

## Supporting information

### VCD Analysis of Axial Chirality in Synthetic Stereoisomeric Biaryl-Type *bis*-Isochroman Heterodimers with Isolated Blocks of Central and Axial Chirality

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## 1. Table of Contents

1. Table of Contents .....	2
1.1. Table of Figures.....	3
1.2. List of Tables.....	12
2. General Information .....	13
2.1. Computational section .....	13
2.2. Syntheses and characterization of the compounds .....	14
2.2.1. General procedure for synthesis of chiral non-racemic 1-arylpropan-2-ols .....	14
2.2.2. General procedure for acetylation of chiral non-racemic 1-arylpropan-2-ols .....	16
2.2.3. General procedure for the halogenation of 1-arylpropan-2-yl acetates or isochroman derivatives with <i>N</i> -halosuccinimides (NXS, X = I or Br) .....	18
2.2.4. General procedure for Miyaura borylation of chiral non-racemic 1-(2-haloaryl)propan-2-yl acetates .....	23
2.2.5. General procedure for oxa-Pictet-Spengler reactions of chiral non-racemic 1-arylpropan-2-ol derivatives .....	25
2.2.6. General procedure for the Suzuki coupling reaction of chiral non-racemic 1-[(2-pinacolatoboryl)aryl]propan-2-yl acetate and 5-iodoisochroman derivatives .....	49
2.2.7. General procedure for deacetylation of chiral non-racemic 1-[2-(6,7,8-trimethoxy-3-methylisochroman-5-yl)-4,5-dimethoxyphenyl]propan-2-yl acetate derivatives .....	55
3. Spectra of the compounds .....	62
3.1. NMR spectra.....	62
3.2. ECD and VCD spectra .....	144
3.3. MS spectra.....	170
3.4. IR spectra.....	180
4. X-ray analysis.....	197
4.1. Data of the X-ray analysis .....	198
5. Structures, populations and Cartesian coordinates of the low-energy DFT conformers .....	229
6. References .....	429

## 1.1. Table of Figures

Figure S1. $^1\text{H}$ NMR (400 MHz) spectrum of ( <i>S</i> )- <b>11</b> in $\text{CDCl}_3$ .....	62
Figure S2. $^{13}\text{C}$ NMR (100 MHz) spectrum of ( <i>S</i> )- <b>11</b> in $\text{CDCl}_3$ .....	62
Figure S3. $^1\text{H}$ NMR (400 MHz) spectrum of ( <i>S</i> )- <b>12</b> in $\text{CDCl}_3$ .....	63
Figure S4. $^{13}\text{C}$ NMR (100 MHz) spectrum of ( <i>S</i> )- <b>12</b> in $\text{CDCl}_3$ .....	63
Figure S5. $^1\text{H}$ NMR (400 MHz) spectrum of ( <i>S</i> )- <b>13</b> in $\text{CDCl}_3$ .....	64
Figure S6. $^{13}\text{C}$ NMR (100 MHz) spectrum of ( <i>S</i> )- <b>13</b> in $\text{CDCl}_3$ .....	64
Figure S7. $^1\text{H}$ NMR (400 MHz) spectrum of ( <i>S</i> )- <b>14</b> in $\text{CDCl}_3$ .....	65
Figure S8. $^{13}\text{C}$ NMR (100 MHz) spectrum of ( <i>S</i> )- <b>14</b> in $\text{CDCl}_3$ .....	65
Figure S9. $^1\text{H}$ NMR (400 MHz) spectrum of ( <i>S</i> )- <b>8</b> in $\text{CDCl}_3$ .....	66
Figure S10. $^{13}\text{C}$ NMR (100 MHz) spectrum of ( <i>S</i> )- <b>8</b> in $\text{CDCl}_3$ .....	66
Figure S11. $^1\text{H}$ NMR (400 MHz) spectrum of ( <i>S</i> )- <b>16</b> in $\text{CDCl}_3$ .....	67
Figure S12. $^{13}\text{C}$ NMR (100 MHz) spectrum of ( <i>S</i> )- <b>16</b> in $\text{CDCl}_3$ .....	67
Figure S13. $^1\text{H}$ NMR (400 MHz) spectrum of <i>cis</i> -(1 <i>R</i> ,3 <i>S</i> )- <b>17</b> in $\text{CDCl}_3$ . ....	68
Figure S14. $^{13}\text{C}$ NMR (100 MHz) spectrum of <i>cis</i> -(1 <i>R</i> ,3 <i>S</i> )- <b>17</b> in $\text{CDCl}_3$ . ....	68
Figure S15. $^1\text{H}$ - $^1\text{H}$ COSY NMR (400 MHz) spectrum of <i>cis</i> -(1 <i>R</i> ,3 <i>S</i> )- <b>17</b> in $\text{CDCl}_3$ . ....	69
Figure S16. $^1\text{H}$ - $^{13}\text{C}$ HSQC NMR (400 MHz) spectrum of <i>cis</i> -(1 <i>R</i> ,3 <i>S</i> )- <b>17</b> in $\text{CDCl}_3$ . ....	69
Figure S17. $^1\text{H}$ - $^{13}\text{C}$ HMBC NMR (400 MHz) spectrum of <i>cis</i> -(1 <i>R</i> ,3 <i>S</i> )- <b>17</b> in $\text{CDCl}_3$ . ....	70
Figure S18. Characteristic NOE correlation shown on the structure of <i>cis</i> -(1 <i>R</i> ,3 <i>S</i> )- <b>17</b> suggesting (1 <i>R</i> ,3 <i>S</i> ) configuration of isochroman unit. ....	71
Figure S19. $^1\text{H}$ - $^1\text{H}$ NOESY NMR (400 MHz) spectrum of <i>cis</i> -(1 <i>R</i> ,3 <i>S</i> )- <b>17</b> in $\text{CDCl}_3$ .....	71
Figure S20. $^1\text{H}$ NMR (400 MHz) spectrum of <i>trans</i> -(1 <i>S</i> ,3 <i>S</i> )- <b>17</b> in $\text{CDCl}_3$ . ....	72
Figure S21. $^{13}\text{C}$ NMR (100 MHz) spectrum of <i>trans</i> -(1 <i>S</i> ,3 <i>S</i> )- <b>17</b> in $\text{CDCl}_3$ . ....	72
Figure S22. $^1\text{H}$ - $^1\text{H}$ COSY NMR (400 MHz) spectrum of <i>trans</i> -(1 <i>S</i> ,3 <i>S</i> )- <b>17</b> in $\text{CDCl}_3$ . ....	73
Figure S23. $^1\text{H}$ - $^{13}\text{C}$ HSQC NMR (400 MHz) spectrum of <i>trans</i> -(1 <i>S</i> ,3 <i>S</i> )- <b>17</b> in $\text{CDCl}_3$ . ....	73
Figure S24. $^1\text{H}$ - $^{13}\text{C}$ HMBC NMR (400 MHz) spectrum of <i>trans</i> -(1 <i>S</i> ,3 <i>S</i> )- <b>17</b> in $\text{CDCl}_3$ . ....	74
Figure S25. Characteristic NOE correlation shown on the structure of <i>trans</i> -(1 <i>S</i> ,3 <i>S</i> )- <b>17</b> suggesting (1 <i>S</i> ,3 <i>S</i> ) configuration of isochroman unit.....	75
Figure S26. $^1\text{H}$ - $^1\text{H}$ NOESY NMR (400 MHz) spectrum of <i>trans</i> -(1 <i>S</i> ,3 <i>S</i> )- <b>17</b> in $\text{CDCl}_3$ . ....	75
Figure S27. $^1\text{H}$ NMR (400 MHz) spectrum of <i>cis</i> -(1 <i>R</i> ,3 <i>S</i> )- <b>18</b> in $\text{CDCl}_3$ . ....	76
Figure S28. $^{13}\text{C}$ NMR (100 MHz) spectrum of <i>cis</i> -(1 <i>R</i> ,3 <i>S</i> )- <b>18</b> in $\text{CDCl}_3$ . ....	76
Figure S29. $^1\text{H}$ NMR (400 MHz) spectrum of <i>trans</i> -(1 <i>S</i> ,3 <i>S</i> )- <b>18</b> in $\text{CDCl}_3$ . ....	77
Figure S30. $^{13}\text{C}$ NMR (100 MHz) spectrum of <i>trans</i> -(1 <i>S</i> ,3 <i>S</i> )- <b>18</b> in $\text{CDCl}_3$ . ....	77
Figure S31. $^1\text{H}$ NMR (400 MHz) spectrum of the mixture of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>19</b> and (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>19</b> in $\text{CDCl}_3$ . ....	78
Figure S32. $^{13}\text{C}$ NMR (100 MHz) spectrum of the mixture of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>19</b> and (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>19</b> in $\text{CDCl}_3$ . ....	78
Figure S33. $^1\text{H}$ NMR (400 MHz) spectrum of (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>19</b> in $\text{CDCl}_3$ . ....	79
Figure S34. $^{13}\text{C}$ NMR (100 MHz) spectrum of (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>19</b> in $\text{CDCl}_3$ . ....	79
Figure S35. $^1\text{H}$ - $^1\text{H}$ COSY NMR (400 MHz) spectrum of (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>19</b> in $\text{CDCl}_3$ . ....	80
Figure S36. $^1\text{H}$ - $^{13}\text{C}$ HSQC NMR (400 MHz) spectrum of (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>19</b> in $\text{CDCl}_3$ . ....	80
Figure S37. $^1\text{H}$ - $^{13}\text{C}$ HMBC NMR (400 MHz) spectrum of (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>19</b> in $\text{CDCl}_3$ . ....	81
Figure S38. $^1\text{H}$ - $^1\text{H}$ NOESY NMR (400 MHz) spectrum of (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>19</b> in $\text{CDCl}_3$ . ....	81
Figure S39. $^1\text{H}$ NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>19</b> in $\text{CDCl}_3$ .....	82
Figure S40. $^{13}\text{C}$ NMR (100 MHz) spectrum of (a <i>R</i> ,1 <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>19</b> in $\text{CDCl}_3$ .....	82
Figure S41. $^1\text{H}$ NMR (400 MHz) spectrum of (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>20</b> in $\text{CDCl}_3$ .....	83
Figure S42. $^{13}\text{C}$ NMR (100 MHz) spectrum of (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>20</b> in $\text{CDCl}_3$ .....	83

Figure S43. $^1\text{H}$ - $^1\text{H}$ COSY NMR (400 MHz) spectrum of (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>20</b> in $\text{CDCl}_3$ .	84
Figure S44. $^1\text{H}$ - $^{13}\text{C}$ HSQC NMR (400 MHz) spectrum of (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>20</b> in $\text{CDCl}_3$ .	84
Figure S45. $^1\text{H}$ - $^{13}\text{C}$ HMBC NMR (400 MHz) spectrum of (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>20</b> in $\text{CDCl}_3$ .	85
Figure S46. $^1\text{H}$ - $^1\text{H}$ NOESY NMR (400 MHz) spectrum of (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>20</b> in $\text{CDCl}_3$ .	85
Figure S47. $^1\text{H}$ NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>20</b> in $\text{CDCl}_3$ .	86
Figure S48. $^{13}\text{C}$ NMR (100 MHz) spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>20</b> in $\text{CDCl}_3$ .	86
Figure S49. $^1\text{H}$ - $^1\text{H}$ COSY NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>20</b> in $\text{CDCl}_3$ .	87
Figure S50. $^1\text{H}$ - $^{13}\text{C}$ HSQC NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>20</b> in $\text{CDCl}_3$ .	87
Figure S51. $^1\text{H}$ - $^{13}\text{C}$ HMBC NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>20</b> in $\text{CDCl}_3$ .	88
Figure S52. $^1\text{H}$ - $^1\text{H}$ NOESY NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>20</b> in $\text{CDCl}_3$ .	88
Figure S53. $^1\text{H}$ NMR (400 MHz) spectrum of (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>20</b> in $\text{CDCl}_3$ .	89
Figure S54. $^{13}\text{C}$ NMR (100 MHz) spectrum of (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>20</b> in $\text{CDCl}_3$ .	89
Figure S55. $^1\text{H}$ - $^1\text{H}$ COSY NMR (400 MHz) spectrum of (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>20</b> in $\text{CDCl}_3$ .	90
Figure S56. $^1\text{H}$ NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>20</b> in $\text{CDCl}_3$ .	90
Figure S57. $^{13}\text{C}$ NMR (100 MHz) spectrum of (a <i>R</i> ,1 <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>20</b> in $\text{CDCl}_3$ .	91
Figure S58. $^1\text{H}$ NMR (400 MHz) spectrum of (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> in $\text{CDCl}_3$ .	91
Figure S59. $^{13}\text{C}$ NMR (100 MHz) spectrum of (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> in $\text{CDCl}_3$ .	92
Figure S60. $^1\text{H}$ - $^1\text{H}$ COSY NMR (400 MHz) spectrum of (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> in $\text{CDCl}_3$ .	92
Figure S61. $^1\text{H}$ - $^{13}\text{C}$ HSQC NMR (400 MHz) spectrum of (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> in $\text{CDCl}_3$ .	93
Figure S62. $^1\text{H}$ - $^{13}\text{C}$ HMBC NMR (400 MHz) spectrum of (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> in $\text{CDCl}_3$ .	93
Figure S63. Characteristic NOE correlations shown on the lowest-energy computed conformer of (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> suggesting (1 <i>S</i> ,3 <i>S</i> ) configuration of isochroman subunit and (a <i>S</i> ) axial chirality.	94
Figure S64. $^1\text{H}$ - $^1\text{H}$ NOESY NMR (400 MHz) spectrum of (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> in $\text{CDCl}_3$ .	94
Figure S65. $^1\text{H}$ NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> in $\text{CDCl}_3$ .	95
Figure S66. $^{13}\text{C}$ NMR (100 MHz) spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> in $\text{CDCl}_3$ .	95
Figure S67. $^1\text{H}$ - $^1\text{H}$ COSY NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> in $\text{CDCl}_3$ .	96
Figure S68. $^1\text{H}$ - $^{13}\text{C}$ HSQC NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> in $\text{CDCl}_3$ .	96
Figure S69. $^1\text{H}$ - $^{13}\text{C}$ HMBC NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> in $\text{CDCl}_3$ .	97
Figure S70. Characteristic NOE correlations shown on the the lowest-energy computed conformer of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> suggesting (1 <i>S</i> ,3 <i>S</i> ) configuration of isochroman subunit and (a <i>R</i> ) axial chirality.	98
Figure S71. $^1\text{H}$ - $^1\text{H}$ NOESY NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> in $\text{CDCl}_3$ .	98
Figure S72. $^1\text{H}$ NMR (400 MHz) spectrum of (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> in $\text{CDCl}_3$ .	99
Figure S73. $^{13}\text{C}$ NMR (100 MHz) spectrum of (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> in $\text{CDCl}_3$ .	99
Figure S74. $^1\text{H}$ - $^1\text{H}$ COSY NMR (400 MHz) spectrum of (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> in $\text{CDCl}_3$ .	100
Figure S75. $^1\text{H}$ - $^{13}\text{C}$ HSQC NMR (400 MHz) spectrum of (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> in $\text{CDCl}_3$ .	100
Figure S76. $^1\text{H}$ - $^{13}\text{C}$ HMBC NMR (400 MHz) spectrum of (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> in $\text{CDCl}_3$ .	101
Figure S77. Characteristic NOE correlations shown on the lowest-energy computed conformer of (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> suggesting (1 <i>R</i> ,3 <i>S</i> ) configuration of isochroman subunit and (a <i>S</i> ) axial chirality.	102
Figure S78. $^1\text{H}$ - $^1\text{H}$ NOESY NMR (400 MHz) spectrum of (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> in $\text{CDCl}_3$ .	102
Figure S79. $^1\text{H}$ NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> in $\text{CDCl}_3$ .	103
Figure S80. $^{13}\text{C}$ NMR (100 MHz) spectrum of (a <i>R</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> in $\text{CDCl}_3$ .	103
Figure S81. $^1\text{H}$ - $^1\text{H}$ COSY NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> in $\text{CDCl}_3$ .	104
Figure S82. $^1\text{H}$ - $^{13}\text{C}$ HSQC NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> in $\text{CDCl}_3$ .	104
Figure S83. $^1\text{H}$ - $^{13}\text{C}$ HMBC NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> in $\text{CDCl}_3$ .	105
Figure S84. Characteristic NOE correlations shown on the lowest-energy computed conformer of (a <i>R</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> suggesting (1 <i>R</i> ,3 <i>S</i> ) configuration of isochroman subunit and (a <i>R</i> ) axial chirality.	106
Figure S85. $^1\text{H}$ - $^1\text{H}$ NOESY NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> in $\text{CDCl}_3$ .	106
Figure S86. $^1\text{H}$ NMR (400 MHz) spectrum of (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> in $\text{CDCl}_3$ .	107



Figure S87. $^{13}\text{C}$ NMR (100 MHz) spectrum of (aS,1 <i>R</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> in $\text{CDCl}_3$ .....	107
Figure S88. $^1\text{H}$ - $^1\text{H}$ COSY NMR (400 MHz) spectrum of (aS,1 <i>R</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> in $\text{CDCl}_3$ .....	108
Figure S89. $^1\text{H}$ - $^{13}\text{C}$ HSQC NMR (400 MHz) spectrum of (aS,1 <i>R</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> in $\text{CDCl}_3$ .....	108
Figure S90. $^1\text{H}$ - $^{13}\text{C}$ HMBC NMR (400 MHz) spectrum of (aS,1 <i>R</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> in $\text{CDCl}_3$ .....	109
Figure S91. Characteristic NOE correlations shown on the structure of (aS,1 <i>R</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> suggesting (1 <i>R</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> ) configurations of isochroman subunits and (aS) axial chirality.....	110
Figure S92. $^1\text{H}$ - $^1\text{H}$ NOESY NMR (400 MHz) spectrum of (aS,1 <i>R</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> in $\text{CDCl}_3$ .....	110
Figure S93. $^1\text{H}$ NMR (400 MHz) spectrum of (aS,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> in $\text{CDCl}_3$ .....	111
Figure S94. $^{13}\text{C}$ NMR (100 MHz) spectrum of (aS,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> in $\text{CDCl}_3$ .....	111
Figure S95. $^1\text{H}$ - $^1\text{H}$ COSY NMR (400 MHz) spectrum of (aS,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> in $\text{CDCl}_3$ .....	112
Figure S96. $^1\text{H}$ - $^{13}\text{C}$ HSQC NMR (400 MHz) spectrum of (aS,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> in $\text{CDCl}_3$ .....	112
Figure S97. $^1\text{H}$ - $^{13}\text{C}$ HMBC NMR (400 MHz) spectrum of (aS,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> in $\text{CDCl}_3$ .....	113
Figure S98. Characteristic NOE correlations shown on the lowest-energy computed conformer of (aS,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> suggesting (1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> ) configurations of isochroman subunits and (aS) axial chirality.....	114
Figure S99. $^1\text{H}$ - $^1\text{H}$ NOESY NMR (400 MHz) spectrum of (aS,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> in $\text{CDCl}_3$ .....	114
Figure S100. $^1\text{H}$ NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> in $\text{CDCl}_3$ .....	115
Figure S101. $^{13}\text{C}$ NMR (100 MHz) spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> in $\text{CDCl}_3$ .....	115
Figure S102. $^1\text{H}$ - $^1\text{H}$ COSY NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> in $\text{CDCl}_3$ .....	116
Figure S103. $^1\text{H}$ - $^{13}\text{C}$ HSQC NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> in $\text{CDCl}_3$ .....	116
Figure S104. $^1\text{H}$ - $^{13}\text{C}$ HMBC NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> in $\text{CDCl}_3$ .....	117
Figure S105. Characteristic NOE correlations shown on the lowest-energy computed conformer of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> suggesting (1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> ) configurations of isochroman subunits and (a <i>R</i> ) axial chirality.....	118
Figure S106. $^1\text{H}$ - $^1\text{H}$ NOESY NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> in $\text{CDCl}_3$ .....	118
Figure S107. $^1\text{H}$ NMR (400 MHz) spectrum of (aS,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> in $\text{CDCl}_3$ .....	119
Figure S108. $^{13}\text{C}$ NMR (100 MHz) spectrum of (aS,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> in $\text{CDCl}_3$ .....	119
Figure S109. $^1\text{H}$ - $^1\text{H}$ COSY NMR (400 MHz) spectrum of (aS,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> in $\text{CDCl}_3$ .....	120
Figure S110. $^1\text{H}$ - $^{13}\text{C}$ HSQC NMR (400 MHz) spectrum of (aS,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> in $\text{CDCl}_3$ .....	120
Figure S111. $^1\text{H}$ - $^{13}\text{C}$ HMBC NMR (400 MHz) spectrum of (aS,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> in $\text{CDCl}_3$ .....	121
Figure S112. Characteristic NOE correlations shown on the structure of (aS,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> suggesting (1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> ) configurations of isochroman subunits and (aS) axial chirality.....	122
Figure S113. $^1\text{H}$ - $^1\text{H}$ NOESY NMR (400 MHz) spectrum of (aS,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> in $\text{CDCl}_3$ .....	122
Figure S114. $^1\text{H}$ NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> in $\text{CDCl}_3$ .....	123
Figure S115. $^{13}\text{C}$ NMR (100 MHz) spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> in $\text{CDCl}_3$ .....	123
Figure S116. $^1\text{H}$ - $^1\text{H}$ COSY NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> in $\text{CDCl}_3$ .....	124
Figure S117. $^1\text{H}$ - $^{13}\text{C}$ HSQC NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> in $\text{CDCl}_3$ .....	124
Figure S118. $^1\text{H}$ - $^{13}\text{C}$ HMBC NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> in $\text{CDCl}_3$ .....	125
Figure S119. Characteristic NOE correlations shown on the structure of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> suggesting (1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> ) configurations of isochroman subunits and (a <i>R</i> ) axial chirality.....	126
Figure S120. $^1\text{H}$ - $^1\text{H}$ NOESY NMR (400 MHz) spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> in $\text{CDCl}_3$ .....	126
Figure S121. $^1\text{H}$ NMR (400 MHz) spectrum of (aS,1 <i>R</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> in $\text{CDCl}_3$ .....	127
Figure S122. $^{13}\text{C}$ NMR (100 MHz) spectrum of (aS,1 <i>R</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> in $\text{CDCl}_3$ .....	127
Figure S123. $^1\text{H}$ - $^1\text{H}$ COSY NMR (400 MHz) spectrum of (aS,1 <i>R</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> in $\text{CDCl}_3$ .....	128
Figure S124. $^1\text{H}$ - $^{13}\text{C}$ HSQC NMR (400 MHz) spectrum of (aS,1 <i>R</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> in $\text{CDCl}_3$ .....	128
Figure S125. $^1\text{H}$ - $^{13}\text{C}$ HMBC NMR (400 MHz) spectrum of (aS,1 <i>R</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> in $\text{CDCl}_3$ .....	129
Figure S126. Characteristic NOE correlations shown on the structure of (aS,1 <i>R</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> suggesting (1 <i>R</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> ) configurations of isochroman subunits and (aS) axial chirality.....	130

Figure S127. $^1\text{H}$ - $^1\text{H}$ NOESY NMR (400 MHz) spectrum of (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> in $\text{CDCl}_3$ .....	130
Figure S128. $^1\text{H}$ NMR (400 MHz) spectrum of ( <i>S</i> )- <b>24</b> in $\text{CDCl}_3$ .....	131
Figure S129. $^{13}\text{C}$ NMR (100 MHz) spectrum of ( <i>S</i> )- <b>24</b> in $\text{CDCl}_3$ .....	131
Figure S130. $^1\text{H}$ NMR (400 MHz) spectrum of ( <i>S</i> )- <b>25</b> in $\text{CDCl}_3$ .....	132
Figure S131. $^{13}\text{C}$ NMR (100 MHz) spectrum of ( <i>S</i> )- <b>25</b> in $\text{CDCl}_3$ .....	132
Figure S132. $^1\text{H}$ NMR (400 MHz) spectrum of the mixture of (a <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>26</b> and (a <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>26</b> in $\text{CDCl}_3$ . ....	133
Figure S133. $^{13}\text{C}$ NMR (100 MHz) spectrum of the mixture of (a <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>26</b> and (a <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>26</b> in $\text{CDCl}_3$ . ....	133
Figure S134. $^1\text{H}$ - $^1\text{H}$ COSY NMR (400 MHz) spectrum of the mixture of (a <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>26</b> and (a <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>26</b> in $\text{CDCl}_3$ . ....	134
Figure S135. $^1\text{H}$ - $^{13}\text{C}$ HSQC NMR (400 MHz) spectrum of the mixture of (a <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>26</b> and (a <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>26</b> in $\text{CDCl}_3$ . ....	134
Figure S136. $^1\text{H}$ - $^{13}\text{C}$ HMBC NMR (400 MHz) spectrum of the mixture of (a <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>26</b> and (a <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>26</b> in $\text{CDCl}_3$ . ....	135
Figure S137. $^1\text{H}$ NMR (400 MHz) spectrum of the mixture of (a <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>27</b> and (a <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>27</b> in $\text{CDCl}_3$ . ....	135
Figure S138. $^{13}\text{C}$ NMR (100 MHz) spectrum of the mixture of (a <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>27</b> and (a <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>27</b> in $\text{CDCl}_3$ . ....	136
Figure S139. $^1\text{H}$ NMR (400 MHz) spectrum of (a <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>28</b> in $\text{CDCl}_3$ . ....	136
Figure S140. $^{13}\text{C}$ NMR (100 MHz) spectrum of (a <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>28</b> in $\text{CDCl}_3$ . ....	137
Figure S141. $^1\text{H}$ - $^1\text{H}$ COSY NMR (400 MHz) spectrum of (a <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>28</b> in $\text{CDCl}_3$ . ....	137
Figure S142. $^1\text{H}$ - $^{13}\text{C}$ HSQC NMR (400 MHz) spectrum of (a <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>28</b> in $\text{CDCl}_3$ . ....	138
Figure S143. $^1\text{H}$ - $^{13}\text{C}$ HMBC NMR (400 MHz) spectrum of (a <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>28</b> in $\text{CDCl}_3$ . ....	138
Figure S144. Characteristic NOE correlations shown on the structure of (a <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>28</b> suggesting (a <i>R</i> ) axial chirality. ....	139
Figure S145. $^1\text{H}$ - $^1\text{H}$ NOESY NMR (400 MHz) spectrum of (a <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>28</b> in $\text{CDCl}_3$ . ....	139
Figure S146. $^1\text{H}$ NMR (400 MHz) spectrum of (a <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>28</b> in $\text{CDCl}_3$ .....	140
Figure S147. $^{13}\text{C}$ NMR (100 MHz) spectrum of (a <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>28</b> in $\text{CDCl}_3$ .....	140
Figure S148. $^1\text{H}$ - $^1\text{H}$ COSY NMR (400 MHz) spectrum of (a <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>28</b> in $\text{CDCl}_3$ . ....	141
Figure S149. $^1\text{H}$ - $^{13}\text{C}$ HSQC NMR (400 MHz) spectrum of (a <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>28</b> in $\text{CDCl}_3$ . ....	141
Figure S150. $^1\text{H}$ - $^{13}\text{C}$ HMBC NMR (400 MHz) spectrum of (a <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>28</b> in $\text{CDCl}_3$ . ....	142
Figure S151. Characteristic NOE correlation shown on the structure of (a <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>28</b> suggesting (a <i>S</i> ) axial chirality.....	143
Figure S152. $^1\text{H}$ - $^1\text{H}$ NOESY NMR (400 MHz) spectrum of (a <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>28</b> in $\text{CDCl}_3$ .....	143
Figure S153. Experimental ECD spectra of enantiomeric (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (black) and (a <i>R</i> ,1 <i>R</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (blue) in MeCN.....	144
Figure S154. Experimental VCD spectra of enantiomeric (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (red) and (a <i>R</i> ,1 <i>R</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (black) in $\text{CDCl}_3$ .....	144
Figure S155. Experimental ECD spectra of enantiomeric (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (black) and (a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (blue) in MeCN. ....	145
Figure S156. Experimental VCD spectra of enantiomeric (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (red) and (a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (black) in $\text{CDCl}_3$ .....	145
Figure S157. Experimental ECD spectra of enantiomeric (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (black) and (a <i>R</i> ,1 <i>S</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (blue) in MeCN. ....	146
Figure S158. Experimental VCD spectra of enantiomeric (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (red) and (a <i>R</i> ,1 <i>S</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (black) in $\text{CDCl}_3$ .....	146
Figure S159. Experimental ECD spectrum of (a <i>R</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> in MeCN. ....	147

Figure S160. Experimental VCD spectrum of (a <i>R</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> in CDCl <sub>3</sub> .	147
Figure S161. Overlapped experimental ECD spectra of stereoisomeric (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (red), (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (blue), (a <i>R</i> ,1 <i>R</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (wine) and (a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (black) in MeCN.	148
Figure S162. Overlapped experimental VCD spectra of stereoisomeric (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (red), (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (blue), (a <i>R</i> ,1 <i>R</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (wine) and (a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (black) in CDCl <sub>3</sub> .	148
Figure S163. Overlapped experimental ECD spectra of stereoisomeric (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (red), (a <i>R</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (blue) and (a <i>R</i> ,1 <i>S</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (wine) in MeCN.	149
Figure S164. Overlapped experimental VCD spectra of stereoisomeric (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (red), (a <i>R</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (blue) and (a <i>R</i> ,1 <i>S</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (wine) in CDCl <sub>3</sub> .	149
Figure S165. Overlapped experimental ECD spectra of stereoisomeric (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (blue), (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (red), (a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (black) and (a <i>R</i> ,1 <i>S</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (wine) in MeCN.	150
Figure S166. Overlapped experimental VCD spectra of stereoisomeric (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (blue), (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (red), (a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (black) and (a <i>R</i> ,1 <i>S</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (wine) in CDCl <sub>3</sub> .	150
Figure S167. Overlapped experimental ECD spectra of stereoisomeric (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (blue), (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (red), (a <i>R</i> ,1 <i>R</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (black) and (a <i>R</i> ,1 <i>S</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (wine) in MeCN.	151
Figure S168. Overlapped experimental VCD spectra of stereoisomeric (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (blue), (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (red), (a <i>R</i> ,1 <i>R</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (black) and (a <i>R</i> ,1 <i>S</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (wine) in CDCl <sub>3</sub> .	151
Figure S169. Overlapped experimental ECD spectra of stereoisomeric (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (blue), (a <i>R</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (red) and (a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (black) in MeCN.	152
Figure S170. Overlapped experimental VCD spectra of stereoisomeric (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (blue), (a <i>R</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (red) and (a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (black) in CDCl <sub>3</sub> .	152
Figure S171. Overlapped experimental ECD spectra of stereoisomeric (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (blue), (a <i>R</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (red) and (a <i>R</i> ,1 <i>R</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (black) in MeCN.	153
Figure S172. Overlapped experimental VCD spectra of stereoisomeric (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (blue), (a <i>R</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (red) and (a <i>R</i> ,1 <i>R</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (black) in CDCl <sub>3</sub> .	153
Figure S173. Experimental ECD spectra of enantiomeric (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> (black) and (a <i>R</i> ,1 <i>S</i> ,3 <i>R</i> ,1' <i>R</i> ,3' <i>R</i> )- <b>22</b> (blue) in MeCN.	154
Figure S174. Experimental VCD spectra of enantiomeric (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> (red) and (a <i>R</i> ,1 <i>S</i> ,3 <i>R</i> ,1' <i>R</i> ,3' <i>R</i> )- <b>22</b> (black) in CDCl <sub>3</sub> .	154
Figure S175. Experimental ECD spectra of enantiomeric (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> (black) and (a <i>R</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>R</i> ,3' <i>R</i> )- <b>22</b> (blue) in MeCN.	155
Figure S176. Experimental VCD spectra of enantiomeric (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> (red) and (a <i>R</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>R</i> ,3' <i>R</i> )- <b>22</b> (black) in CDCl <sub>3</sub> .	155
Figure S177. Experimental ECD spectra of enantiomeric (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> (black) and (a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>R</i> ,3' <i>R</i> )- <b>22</b> (blue) in MeCN.	156
Figure S178. Experimental VCD spectra of enantiomeric (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> (red) and (a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>R</i> ,3' <i>R</i> )- <b>22</b> (black) in CDCl <sub>3</sub> .	156
Figure S179. Overlapped experimental ECD spectra of stereoisomeric (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> (blue), (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> (red), (a <i>R</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>R</i> ,3' <i>R</i> )- <b>22</b> (black) and (a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>R</i> ,3' <i>R</i> )- <b>22</b> (wine) in MeCN.	157
Figure S180. Overlapped experimental VCD spectra of stereoisomeric (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> (blue), (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> (red), (a <i>R</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>R</i> ,3' <i>R</i> )- <b>22</b> (black) and (a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>R</i> ,3' <i>R</i> )- <b>22</b> (wine) in CDCl <sub>3</sub> .	157
Figure S181. Overlapped experimental ECD spectra of stereoisomeric (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> (blue), (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> (red), (a <i>R</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>R</i> ,3' <i>R</i> )- <b>22</b> (black) and (a <i>R</i> ,1 <i>S</i> ,3 <i>R</i> ,1' <i>R</i> ,3' <i>R</i> )- <b>22</b> (wine) in MeCN.	158

Figure S182. Overlapped experimental VCD spectra of stereoisomeric (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> (blue), (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> (red), (a <i>R</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>R</i> ,3' <i>R</i> )- <b>22</b> (black) and (a <i>R</i> ,1 <i>S</i> ,3 <i>R</i> ,1' <i>R</i> ,3' <i>R</i> )- <b>22</b> (wine) in CDCl <sub>3</sub> .	158
Figure S183. Overlapped experimental ECD spectra of stereoisomeric (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> (blue), (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> (red), (a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>R</i> ,3' <i>R</i> )- <b>22</b> (black) and (a <i>R</i> ,1 <i>S</i> ,3 <i>R</i> ,1' <i>R</i> ,3' <i>R</i> )- <b>22</b> (wine) in MeCN.	159
Figure S184. Overlapped experimental VCD spectra of stereoisomeric (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> (blue), (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> (red), (a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>R</i> ,3' <i>R</i> )- <b>22</b> (black) and (a <i>R</i> ,1 <i>S</i> ,3 <i>R</i> ,1' <i>R</i> ,3' <i>R</i> )- <b>22</b> (wine) in CDCl <sub>3</sub> .	159
Figure S185. Experimental ECD spectra of enantiomeric (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> (black) and (a <i>R</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>S</i> ,3' <i>R</i> )- <b>23</b> (blue) in MeCN.	160
Figure S186. Experimental VCD spectra of enantiomeric (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> (red) and (a <i>R</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>S</i> ,3' <i>R</i> )- <b>23</b> (black) in CDCl <sub>3</sub> .	160
Figure S187. Experimental ECD spectra of enantiomeric (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> (black) and (a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>S</i> ,3' <i>R</i> )- <b>23</b> (blue) in MeCN.	161
Figure S188. Experimental VCD spectra of enantiomeric (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> (red) and (a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>S</i> ,3' <i>R</i> )- <b>23</b> (black) in CDCl <sub>3</sub> .	161
Figure S189. Experimental ECD spectra of enantiomeric (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> (black) and (a <i>R</i> ,1 <i>S</i> ,3 <i>R</i> ,1' <i>S</i> ,3' <i>R</i> )- <b>23</b> (blue) in MeCN.	162
Figure S190. Experimental VCD spectra of enantiomeric (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> (red) and (a <i>R</i> ,1 <i>S</i> ,3 <i>R</i> ,1' <i>S</i> ,3' <i>R</i> )- <b>23</b> (black) in CDCl <sub>3</sub> .	162
Figure S191. Overlapped experimental ECD spectra of stereoisomeric (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> (blue), (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> (red), (a <i>R</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>S</i> ,3' <i>R</i> )- <b>23</b> (black) and (a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>S</i> ,3' <i>R</i> )- <b>23</b> (wine) in MeCN.	163
Figure S192. Overlapped experimental VCD spectra of stereoisomeric (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> (blue), (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> (red), (a <i>R</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>S</i> ,3' <i>R</i> )- <b>23</b> (black) and (a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>S</i> ,3' <i>R</i> )- <b>23</b> (wine) in CDCl <sub>3</sub> .	163
Figure S193. Overlapped experimental ECD spectra of stereoisomeric (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> (blue), (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> (red), (a <i>R</i> ,1 <i>S</i> ,3 <i>R</i> ,1' <i>S</i> ,3' <i>R</i> )- <b>23</b> (black) and (a <i>R</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>S</i> ,3' <i>R</i> )- <b>23</b> (wine) in MeCN.	164
Figure S194. Overlapped experimental VCD spectra of stereoisomeric (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> (blue), (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> (red), (a <i>R</i> ,1 <i>S</i> ,3 <i>R</i> ,1' <i>S</i> ,3' <i>R</i> )- <b>23</b> (black) and (a <i>R</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>S</i> ,3' <i>R</i> )- <b>23</b> (wine) in CDCl <sub>3</sub> .	164
Figure S195. Overlapped experimental ECD spectra of stereoisomeric (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> (blue), (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> (red), (a <i>R</i> ,1 <i>S</i> ,3 <i>R</i> ,1' <i>S</i> ,3' <i>R</i> )- <b>23</b> (black) and (a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>S</i> ,3' <i>R</i> )- <b>23</b> (wine) in MeCN.	165
Figure S196. Overlapped experimental VCD spectra of stereoisomeric (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> (blue), (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> (red), (a <i>R</i> ,1 <i>S</i> ,3 <i>R</i> ,1' <i>S</i> ,3' <i>R</i> )- <b>23</b> (black) and (a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>S</i> ,3' <i>R</i> )- <b>23</b> (wine) in CDCl <sub>3</sub> .	165
Figure S197. Overlapped experimental VCD spectra of stereoisomeric (a <i>R</i> ,1 <i>R</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (black), (a <i>R</i> ,1 <i>S</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (orange), (a <i>R</i> ,1 <i>S</i> ,3 <i>R</i> ,1' <i>R</i> ,3' <i>R</i> )- <b>22</b> (violet), (a <i>R</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>R</i> ,3' <i>R</i> )- <b>22</b> (red), (a <i>R</i> ,1 <i>S</i> ,3 <i>R</i> ,1' <i>S</i> ,3' <i>R</i> )- <b>23</b> (blue) and (a <i>R</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>S</i> ,3' <i>R</i> )- <b>23</b> (magenta) in CDCl <sub>3</sub> .	166
Figure S198. Overlapped experimental VCD spectra of stereoisomeric (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (blue), (a <i>R</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (black), (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> (red) and (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> (magenta) in CDCl <sub>3</sub> .	166
Figure S199. Overlapped experimental VCD spectra of stereoisomeric (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (black), (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> (orange), (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> (violet), (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> (red), (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> (blue) and (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> (magenta) in CDCl <sub>3</sub> .	167

Figure S200. Overlapped experimental VCD spectra of stereoisomeric (a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> (blue), (a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>R</i> ,3' <i>R</i> )- <b>22</b> (red) and (a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>S</i> ,3' <i>R</i> )- <b>23</b> (black) in CDCl <sub>3</sub> .....	167
Figure S201. Experimental ECD spectrum of (a <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>28</b> in MeCN. ....	168
Figure S202. Experimental VCD spectrum of (a <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>28</b> in CDCl <sub>3</sub> . ....	168
Figure S203. Experimental ECD spectrum of (a <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>28</b> in MeCN. ....	169
Figure S204. Experimental VCD spectrum of (a <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>28</b> in CDCl <sub>3</sub> .....	169
Figure S205. Experimental ESI-HRMS spectrum of ( <i>S</i> )- <b>11</b> . ....	170
Figure S206. Experimental ESI-HRMS spectrum of ( <i>S</i> )- <b>12</b> . ....	170
Figure S207. Experimental ESI-HRMS spectrum of ( <i>S</i> )- <b>13</b> . ....	170
Figure S208. Experimental ESI-HRMS spectrum of ( <i>S</i> )- <b>14</b> . ....	171
Figure S209. Experimental ESI-HRMS spectrum of ( <i>S</i> )- <b>8</b> . ....	171
Figure S210. Experimental ESI-HRMS spectrum of ( <i>S</i> )- <b>16</b> . ....	171
Figure S211. Experimental ESI-HRMS spectrum of <i>cis</i> -(1 <i>R</i> ,3 <i>S</i> )- <b>17</b> . ....	172
Figure S212. Experimental ESI-HRMS spectrum of <i>trans</i> -(1 <i>S</i> ,3 <i>S</i> )- <b>17</b> . ....	172
Figure S213. Experimental ESI-HRMS spectrum of <i>cis</i> -(1 <i>R</i> ,3 <i>S</i> )- <b>18</b> . ....	172
Figure S214. Experimental ESI-HRMS spectrum of <i>trans</i> -(1 <i>S</i> ,3 <i>S</i> )- <b>18</b> . ....	173
Figure S215. Experimental ESI-HRMS spectrum of the mixture of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>19</b> and (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>19</b> .....	173
Figure S216. Experimental ESI-HRMS spectrum of the mixture of (a <i>R</i> ,1 <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>19</b> and (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>19</b> . ....	173
Figure S217. Experimental ESI-HRMS spectrum of (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>20</b> . ....	174
Figure S218. Experimental ESI-HRMS spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>20</b> . ....	174
Figure S219. Experimental ESI-HRMS spectrum of (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>20</b> . ....	174
Figure S220. Experimental ESI-HRMS spectrum of (a <i>R</i> ,1 <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>20</b> . ....	174
Figure S221. Experimental ESI-HRMS spectrum of (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> . ....	175
Figure S222. Experimental ESI-HRMS spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> . ....	175
Figure S223. Experimental ESI-HRMS spectrum of (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> . ....	175
Figure S224. Experimental ESI-HRMS spectrum of (a <i>R</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> . ....	175
Figure S225. Experimental ESI-HRMS spectrum of (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> . ....	176
Figure S226. Experimental ESI-HRMS spectrum of (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> . ....	176
Figure S227. Experimental ESI-HRMS spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> . ....	176
Figure S228. Experimental ESI-HRMS spectrum of (a <i>S</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> . ....	176
Figure S229. Experimental ESI-HRMS spectrum of (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> . ....	177
Figure S230. Experimental ESI-HRMS spectrum of (a <i>S</i> ,1 <i>R</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> . ....	177
Figure S231. Experimental ESI-HRMS spectrum of ( <i>S</i> )- <b>24</b> . ....	177
Figure S232. Experimental ESI-HRMS spectrum of ( <i>S</i> )- <b>25</b> . ....	178
Figure S233. Experimental ESI-HRMS spectrum of the mixture of (a <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>26</b> and (a <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>26</b> . ....	178
Figure S234. Experimental ESI-HRMS spectrum of the mixture of (a <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>27</b> and (a <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>27</b> . ....	178
Figure S235. Experimental ESI-HRMS spectrum of the mixture of (a <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>28</b> and (a <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>28</b> . ....	179
Figure S236. Experimental IR spectrum of ( <i>S</i> )- <b>11</b> recorded as KBr disc. ....	180
Figure S237. Experimental IR spectrum of ( <i>S</i> )- <b>12</b> recorded as KBr disc. ....	180
Figure S238. Experimental IR spectrum of ( <i>S</i> )- <b>13</b> recorded as KBr disc. ....	181
Figure S239. Experimental IR spectrum of ( <i>S</i> )- <b>14</b> recorded as KBr disc. ....	181
Figure S240. Experimental IR spectrum of ( <i>S</i> )- <b>8</b> recorded as KBr disc. ....	182
Figure S241. Experimental IR spectrum of ( <i>S</i> )- <b>16</b> recorded as KBr disc. ....	182

Figure S242. Experimental IR spectrum of <i>cis</i> -(1 <i>R</i> ,3 <i>S</i> )- <b>17</b> recorded as KBr disc. ....	183
Figure S243. Experimental IR spectrum of <i>trans</i> -(1 <i>S</i> ,3 <i>S</i> )- <b>17</b> recorded as KBr disc. ....	183
Figure S244. Experimental IR spectrum of <i>cis</i> -(1 <i>R</i> ,3 <i>S</i> )- <b>18</b> recorded as KBr disc. ....	184
Figure S245. Experimental IR spectrum of <i>trans</i> -(1 <i>S</i> ,3 <i>S</i> )- <b>18</b> recorded as KBr disc. ....	184
Figure S246. Experimental IR spectrum of the mixture of ( <i>aR</i> ,1 <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>19</b> and ( <i>aS</i> ,1 <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>19</b> recorded as KBr disc. ....	185
Figure S247. Experimental IR spectrum of ( <i>aS</i> ,1 <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>19</b> recorded as KBr disc. ....	185
Figure S248. Experimental IR spectrum of ( <i>aR</i> ,1 <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>19</b> recorded as KBr disc. ....	186
Figure S249. Experimental IR spectrum of ( <i>aS</i> ,1 <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>20</b> recorded as KBr disc. ....	186
Figure S250. Experimental IR spectrum of ( <i>aR</i> ,1 <i>S</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>20</b> recorded as KBr disc. ....	187
Figure S251. Experimental IR spectrum of ( <i>aS</i> ,1 <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>20</b> recorded as KBr disc. ....	187
Figure S252. Experimental IR spectrum of ( <i>aR</i> ,1 <i>R</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>20</b> recorded as KBr disc. ....	188
Figure S253. Experimental IR spectrum of ( <i>aS</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> recorded as KBr disc. ....	188
Figure S254. Experimental IR spectrum of ( <i>aR</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> recorded as KBr disc. ....	189
Figure S255. Experimental IR spectrum of ( <i>aS</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> recorded as KBr disc. ....	189
Figure S256. Experimental IR spectrum of ( <i>aR</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> recorded as KBr disc. ....	190
Figure S257. Experimental IR spectrum of ( <i>aS</i> ,1 <i>R</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> recorded as KBr disc. ....	190
Figure S258. Experimental IR spectrum of ( <i>aS</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> recorded as KBr disc. ....	191
Figure S259. Experimental IR spectrum of ( <i>aR</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> recorded as KBr disc. ....	191
Figure S260. Experimental IR spectrum of ( <i>aS</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> recorded as KBr disc. ....	192
Figure S261. Experimental IR spectrum of ( <i>aR</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> recorded as KBr disc. ....	192
Figure S262. Experimental IR spectrum of ( <i>aS</i> ,1 <i>R</i> ,3 <i>S</i> ,1' <i>R</i> ,3' <i>S</i> )- <b>23</b> recorded as KBr disc. ....	193
Figure S263. Experimental IR spectrum of ( <i>S</i> )- <b>24</b> recorded as KBr disc. ....	193
Figure S264. Experimental IR spectrum of ( <i>S</i> )- <b>25</b> recorded as KBr disc. ....	194
Figure S265. Experimental IR spectrum of the mixture of ( <i>aR</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>26</b> and ( <i>aS</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>26</b> recorded as KBr disc. ....	194
Figure S266. Experimental IR spectrum of the mixture of ( <i>aR</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>27</b> and ( <i>aS</i> ,3 <i>S</i> ,2' <i>S</i> )- <b>27</b> recorded as KBr disc. ....	195
Figure S267. Experimental IR spectrum of ( <i>aR</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>28</b> recorded as KBr disc. ....	195
Figure S268. Experimental IR spectrum of ( <i>aS</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>28</b> recorded as KBr disc. ....	196
Figure S269. ORTEP view of ( <i>aR</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> at 50% probability level with numbering scheme. ....	199
Figure S270. ORTEP view of ( <i>aS</i> ,1 <i>R</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> at 50% probability level with numbering scheme. ....	204
Figure S271. ORTEP view of ( <i>aS</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>R</i> ,3' <i>R</i> )- <b>22</b> at 50% probability level with numbering scheme. Only one molecule from the asymmetric unit is shown and solvent molecules are omitted for clarity. The numbering of the other molecules were systematically changed; <i>e.g.</i> C1 corresponds to C21 and C31. ....	210
Figure S272. Overlay of the three isomers of in the asymmetric unit of structure ( <i>aS</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>R</i> ,3' <i>R</i> )- <b>22</b> . ....	211
Figure S273. Structures and populations of the low-energy $\omega$ B97X/TZVP PCM/MeCN conformers ( $\geq 1\%$ ) of ( <i>aS</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> . ....	229
Figure S274. Overlapped structures of the 12 low-energy $\omega$ B97X/TZVP PCM/MeCN conformers ( $\geq 1\%$ ) of ( <i>aS</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> . ....	229
Figure S275. Structures and populations of the low-energy $\omega$ B97X/TZVP PCM/MeCN conformers ( $\geq 1\%$ ) of ( <i>aR</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> . ....	230
Figure S276. Structures and populations of the low-energy $\omega$ B97X/TZVP PCM/MeCN conformers ( $\geq 1\%$ ) of ( <i>aS</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> . ....	231
Figure S277. Structures and populations of the low-energy $\omega$ B97X/TZVP PCM/MeCN conformers ( $\geq 1\%$ ) of ( <i>aR</i> ,1 <i>R</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> . ....	232

Figure S278. Structures and populations of the low-energy $\omega$ B97X/TZVP PCM/MeCN conformers ( $\geq 1\%$ ) of ( <i>aS</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> . .....	233
Figure S279. Structures and populations of the low-energy $\omega$ B97X/TZVP PCM/MeCN conformers ( $\geq 1\%$ ) of ( <i>aR</i> ,1 <i>S</i> ,3 <i>S</i> ,1' <i>S</i> ,3' <i>S</i> )- <b>22</b> . .....	234
Figure S280. Structures and populations of the low-energy $\omega$ B97X/TZVP PCM/MeCN conformers ( $\geq 1\%$ ) of ( <i>aS</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>28</b> . .....	235
Figure S281. Structures and populations of the low-energy $\omega$ B97X/TZVP PCM/MeCN conformers ( $\geq 1\%$ ) of ( <i>aR</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>28</b> . .....	236

## 1.2. List of Tables

<b>Table S1.</b> Experimental details of the structural elucidation by single crystal X-ray diffraction. ....	198
<b>Table S2.</b> Geometric parameters (Å, °) for (a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b> . ....	199
<b>Table S3.</b> Geometric parameters (Å, °) for (a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b> . ....	205
<b>Table S4.</b> Geometric parameters (Å, °) for (a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>R</i> ,3' <i>R</i> )- <b>22</b> . ....	211
<b>Table S5.</b> Cartesian coordinates and energies of the low-energy conformers calculated at the ωB97X/TZVP PCM/MeCN level. ....	237
<b>Table S6.</b> Cartesian coordinates and energies of the low-energy conformers calculated at the B3LYP/TZVP PCM/CHCl <sub>3</sub> level. ....	354



## 2. General Information

Chemicals were purchased puriss p.a. from commercial suppliers. Thin-layer chromatography (TLC) was performed on Silica gel 60 F<sub>254</sub> (Merck) with visualization by UV light (254 nm) and immersing into aqueous solution of sulfuric acidic ammonium molybdate or 5 % ethanolic phosphomolybdic acid solution followed by heating. Flash column chromatography was performed on Silica gel 60 (Merck 0.040-0.063 mm). Melting points were determined on a Kofler hot-stage apparatus and are uncorrected. Anhydrous solvents were used for all the reactions and distilled solvents were used as eluent for flash chromatography. HPLC-grade solvents were used for chiral HPLC separations. Preparative chiral HPLC was performed by Agilent 1260 Infinity II apparatus using Chiralpak IC column. The <sup>1</sup>H NMR (400 MHz) and <sup>13</sup>C NMR (100 MHz) spectra were recorded with Bruker Avance I 400 MHz spectrometer at 298 K. Chemical shifts are referenced to Me<sub>4</sub>Si (0.00 ppm for <sup>1</sup>H) and to the residual solvent signals (CDCl<sub>3</sub>: 77.16 ppm for <sup>13</sup>C). Chemical shifts were reported as  $\delta$  in ppm, and <sup>1</sup>J<sub>C,F</sub>, <sup>2</sup>J<sub>H,H</sub> and <sup>3</sup>J<sub>H,H</sub> coupling constants in Hz. IR spectra were recorded on a JASCO FT/IR-4100 spectrometer and absorption bands are presented as wavenumber in cm<sup>-1</sup>. Optical rotations were measured at room temperature with a Perkin-Elmer 241 automatic polarimeter (*c* [g/100ml]). ECD spectra were recorded on a J-810 spectropolarimeter. VCD measurements were performed on a BioTools ChiralIR-2X spectrometer at a resolution of 4 cm<sup>-1</sup> under ambient temperature for 18 × 3000 scans, respectively. Sample were dissolved in CDCl<sub>3</sub> and the solutions were placed in a 100  $\mu$ m BaF<sub>2</sub> cell. For spectroscopic measurements spectroscopic grade solvents were used. Diffraction intensity data were collected at room temperature and in case of (a*S*,1*R*,3*R*,1'*R*,3'*R*)-**22** at low temperature (120 K) using a Bruker-D8 Venture diffractometer (Bruker AXS GmbH, Karlsruhe, Germany) equipped with INCOATEC I $\mu$ S 3.0 (Incoatec GmbH, Geesthacht, Germany) dual (Cu and Mo) sealed tube micro sources and a Photon II Charge-Integrating Pixel Array detector (Bruker AXS GmbH, Karlsruhe, Germany) using Mo K $\alpha$  ( $\lambda$  = 0.71073 Å) radiation. Electrospray quadrupole time-of-flight HRMS measurements were performed with a MicroTOF-Q type QqTOF MS instrument equipped with an ESI source from Bruker (Bruker Daltoniks, Bremen, Germany).

### 2.1. Computational section

Mixed torsional/low-frequency mode conformational searches were carried out by means of the MacroModel 10.8.011 software, using the Merck Molecular Force Field (MMFF) with an implicit solvent model for CHCl<sub>3</sub> [1]. All quantum chemical calculations were carried out with the Gaussian 09 software package [2-3]. The B3LYP (VCD) and  $\omega$ B97X [4] (ECD) functionals

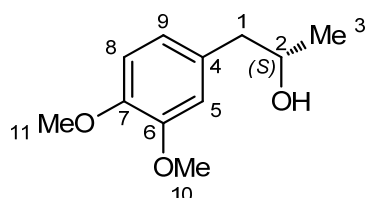
with the TZVP basis set and PCM solvent model for CHCl<sub>3</sub> (VCD) and MeCN (ECD) were used to re-optimize the initial MMFF geometries. TDDFT-ECD and -OR calculations were performed at the B3LYP/TZVP, BH&HLYP/TZVP, CAM-B3LYP/TZVP and the PBE0/TZVP levels of theory with the PCM solvent model for MeCN. ECD spectra were generated as sums of Gaussians with 2100-3000 cm<sup>-1</sup> widths at half-height, using dipole-velocity-computed rotational strength values [5]. VCD calculations were performed at the B3LYP/TZVP PCM/CHCl<sub>3</sub> level, while the spectra were gained by applying a 8 cm<sup>-1</sup> half-height width and scaled by a factor of 0.985. Boltzmann distributions were estimated from the B3LYP and  $\omega$ B97X energies. The MOLEKEL 5.4 software package was used for visualization of the results [6].

## 2.2. Syntheses and characterization of the compounds

### 2.2.1. General procedure for synthesis of chiral non-racemic 1-arylpropan-2-ols

The corresponding aryl bromide (1.3 or 1.5 equiv) was dissolved in anhydrous THF (~1 g aryl bromide/10 ml anhydrous THF) under Ar or N<sub>2</sub> atmosphere and the solution was cooled to -80 °C. Then 2.5 M *n*-BuLi in hexane (1.3 or 1.5 equiv.) was added and after stirring for 20 minutes, (*S*)- or (*R*)-propylene oxide (1.0 equiv.) was added and the reaction mixture was stirred for 20 minutes at -80 °C. Next BF<sub>3</sub>·Et<sub>2</sub>O (1.1 equiv.) was added to the solution, which was stirred further for 30 minutes at -80 °C. Then the cooling was stopped and a saturated solution of NH<sub>4</sub>Cl was added to the reaction mixture. The mixture was stirred for 10 minutes and concentrated in *vacuo*. The suspension was diluted with EtOAc and the organic phase was washed twice with brine. The organic phase was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, filtered, and the solvent was evaporated in *vacuo*. The residue was purified by flash chromatography to yield the optically active 1-arylpropan-2-ol derivative.

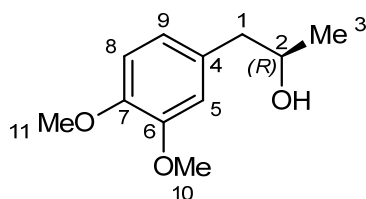
#### (*S*)-1-(3,4-dimethoxyphenyl)propan-2-ol [(*S*)-11] [7]



Starting from 4-bromoveratrole **9** (2.00 ml, 3.02 g, 13.90 mmol, 1.3 equiv.): anhydrous THF (30 ml), 2.5 M *n*-BuLi in hexane (5.56 ml, 13.90 mmol, 1.3 equiv.), (*S*)-propylene oxide (749  $\mu$ l, 621 mg, 10.70 mmol, 1.0 equiv.,  $\geq 98.0$  ee%), BF<sub>3</sub>·Et<sub>2</sub>O (1.45 ml, 1.67 g, 11.77 mmol, 1.1

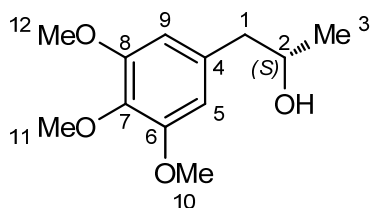
equiv.). (*S*)-**11**: 1.38 g (yield: 66%) yellow syrup;  $[\alpha]_{\text{D}}^{20} +28$  ( $c = 0.50$ ;  $\text{CHCl}_3$ ). Flash chromatography (hexane/EtOAc 7:3  $\rightarrow$  6:4  $\rightarrow$  4:6  $\rightarrow$  3:7);  $R_f = 0.24$  (hexane/EtOAc 6:4);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta = 6.85 - 6.79$  (m, 1H, *H*-5 or *H*-8 or *H*-9), 6.78 – 6.72 (m, 2H, *H*-5, *H*-8, or *H*-5, *H*-9, or *H*-8, *H*-9), 4.02 – 3.93 (m, 1H, *H*-2), 3.87, 3.85 (2s, 2 x 3H, *H*-10, *H*-11), 2.72 (dd,  $J = 13.6, 4.8$  Hz, 1H, *H*-1-*a*), 2.62 (dd,  $J = 13.6, 8.0$  Hz, 1H, *H*-1-*b*), 1.89 (bs, 1H, OH), 1.23 (d,  $J = 6.2$  Hz, 3H, *H*-3);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta = 148.9, 147.7, 131.1$  (3C, *C*-4, *C*-6, *C*-7), 121.3, 112.6, 111.4 (3C, *C*-5, *C*-8, *C*-9) 68.9 (1C, *C*-2), 55.9, 55.8 (2C, *C*-10, *C*-11), 45.3 (1C, *C*-1), 22.7 (1C, *C*-3); IR (KBr)  $\nu = 3398$  ( $\nu$  OH), 3061, 3000 ( $\nu$  Ar =CH), 2963, 2933 ( $\nu_{\text{as}}$  Me,  $\nu_{\text{as}}$  CH<sub>2</sub>), 2858, 2841 ( $\nu_{\text{s}}$  Me,  $\nu_{\text{s}}$  CH<sub>2</sub>), 2007, 1905, 1830, 1789, 1716, 1682 ( $\gamma$  Ar =CH,  $\gamma$  Ar C=C overtone and combination bands), 1604, 1588, 1519, 1464 ( $\nu$  Ar C=C,  $\delta_{\text{as}}$  Me,  $\beta_{\text{s}}$  CH<sub>2</sub>), 1371, 1334 ( $\delta_{\text{s}}$  Me,  $\delta$  CH), 1261 ( $\nu_{\text{as}}$  Ar-O-Me), 1119, 1071 ( $\nu$  C-OH), 1038, 1021 ( $\nu_{\text{s}}$  Ar-O-Me), 889, 829 (1,2,4-trisubstituted  $\gamma_{\text{s}}$  Ar =CH)  $\text{cm}^{-1}$ ; ESI-TOF-HRMS:  $m/z$  calculated for  $\text{C}_{11}\text{H}_{16}\text{NaO}_3$   $[\text{M}+\text{Na}]^+$  219.0992, found 219.0990.

#### (*R*)-1-(3,4-dimethoxyphenyl)-propan-2-ol [(*R*)-11] [8]



Starting from 4-bromoveratrole **9** (4.31 ml, 6.51 g, 29.98 mmol, 1.5 equiv.): anhydrous THF (65 ml), 2.5 M *n*-BuLi in hexane (11.99 ml, 29.98 mmol, 1.5 equiv.), (*R*)-propylene oxide (1.40 ml, 1.16 g, 19.98 mmol, 1.0 equiv.,  $\geq 99.0$  *ee*%),  $\text{BF}_3\cdot\text{Et}_2\text{O}$  (2.71 ml, 3.12 g, 21.98 mmol, 1.1 equiv.). (*R*)-**11**: 2.90 g (yield: 74%) yellow syrup;  $[\alpha]_{\text{D}}^{20} -36$  ( $c = 0.51$ ;  $\text{CHCl}_3$ ). Chromatographic and spectral data except for the chiroptical ones were identical with those of (*S*)-**11**.

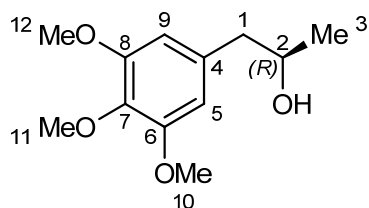
#### (*S*)-1-(3,4,5-trimethoxyphenyl)propan-2-ol [(*S*)-16] [9]



Starting from 5-bromo-1,2,3-trimethoxybenzene **15** (9.52 g, 38.54 mmol, 1.5 equiv.): anhydrous THF (95 ml), 2.5 M *n*-BuLi in hexane (15.42 ml, 38.54 mmol, 1.5 equiv.), (*S*)-propylene oxide (1.80 ml, 1.49 g, 25.69 mmol, 1.0 equiv.,  $\geq 98.0$  *ee*%),  $\text{BF}_3\cdot\text{Et}_2\text{O}$  (3.49 ml, 4.01

g, 28.26 mmol, 1.1 equiv.). (*S*)-**16**: 5.21 g (yield: 90%) yellow syrup;  $[\alpha]_D^{20} +25$  ( $c = 0.52$ ; CHCl<sub>3</sub>). Flash chromatography (hexane/EtOAc 7:3  $\rightarrow$  6:4  $\rightarrow$  4:6  $\rightarrow$  3:7);  $R_f = 0.33$  (hexane/EtOAc 1:1); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta = 6.43$  (s, 2H, *H*-5, *H*-9), 4.06 – 3.97 (m, 1H, *H*-2), 3.85 (s, 6H, *H*-10, *H*-12), 3.83 (s, 3H, *H*-11), 2.73 (dd,  $J = 13.5, 4.6$  Hz, 1H, *H*-1-*a*), 2.61 (dd,  $J = 13.5, 8.2$  Hz, 1H, *H*-1-*b*), 1.96 (bs, 1H, OH), 1.26 (d,  $J = 6.2$  Hz, 3H, *H*-3); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta = 153.2, 136.6, 134.4$  (4C, *C*-4, *C*-6, *C*-7, *C*-8), 106.3 (2C, *C*-5, *C*-9), 68.8 (1C, *C*-2), 60.9 (1C, *C*-11), 56.1 (2C, *C*-10, *C*-12), 46.2 (1C, *C*-1), 22.9 (1C, *C*-3); IR (KBr)  $\nu = 3444$  ( $\nu$  OH), 2936 ( $\nu_{as}$  CH<sub>2</sub>), 2837 ( $\nu_s$  CH<sub>2</sub>), 2012, 1965 ( $\gamma$  Ar =CH,  $\gamma$  Ar C=C overtone and combination bands), 1589, 1507, 1454 ( $\nu$  Ar C=C,  $\delta_{as}$  Me,  $\beta_s$  CH<sub>2</sub>), 1371, 1333 ( $\delta_s$  Me,  $\delta$  CH), 1237 ( $\nu_{as}$  Ar-O-Me), 1126 ( $\nu$  C-OH), 1054 ( $\nu_s$  Ar-O-Me), 852 (1,2,3,5-tetrasubstituted  $\gamma_s$  Ar =CH) cm<sup>-1</sup>; ESI-TOF-HRMS:  $m/z$  calculated for C<sub>12</sub>H<sub>18</sub>NaO<sub>4</sub> [M+Na]<sup>+</sup> 249.1097, found 249.1096.

### (*R*)-1-(3,4,5-trimethoxy-phenyl)propan-2-ol [(*R*)-**16**] [9]



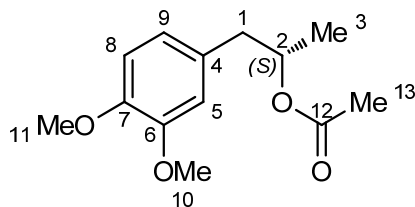
Starting from 5-bromo-1,2,3-trimethoxybenzene **15** (6.35 g, 25.69 mmol, 1.5 equiv.): anhydrous THF (65 ml), 2.5 M *n*-BuLi in hexane (10.28 ml, 25.69 mmol, 1.5 equiv.), (*R*)-propylene oxide (1.20 ml, 1.00 g, 17.13 mmol, 1.0 equiv.,  $\geq 99.0$  ee%), BF<sub>3</sub>·Et<sub>2</sub>O (2.33 ml, 2.67 g, 18.84 mmol, 1.1 equiv.). (*R*)-**16**: 3.41 g (yield: 88%) yellow syrup;  $[\alpha]_D^{20} -31$  ( $c = 0.52$ ; CHCl<sub>3</sub>). Chromatographic and spectral data except for the chiroptical ones were identical with those of (*S*)-**16**.

### 2.2.2. General procedure for acetylation of chiral non-racemic 1-arylpropan-2-ols

The corresponding 1-arylpropan-2-ol (1.0 equiv.) was dissolved in anhydrous CH<sub>2</sub>Cl<sub>2</sub> (20-70 ml) and anhydrous C<sub>5</sub>H<sub>5</sub>N (3.0 equiv.) and AcCl (2.0 equiv.) were added and the reaction mixture was stirred at room temperature. When the starting material was consumed (2.5-3 hours) on the basis of TLC monitoring, a saturated solution of NaHCO<sub>3</sub> was added to the reaction mixture and stirred for 10 minutes. The mixture was diluted with CH<sub>2</sub>Cl<sub>2</sub> and the phases were separated in a separatory funnel. The organic phase was washed twice with a 10% solution of NaHSO<sub>4</sub>, twice with a saturated solution of NaHCO<sub>3</sub> and twice with brine. The

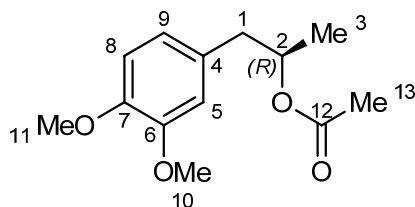
organic phase was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, filtered, and the solvent was evaporated in *vacuo*. The residue was purified by flash chromatography to yield the 1-arylpropan-2-yl acetate target derivative.

**(*S*)-1-(3,4-dimethoxyphenyl)propan-2-yl acetate [(*S*)-12] [10]**



Starting from (*S*)-**11** (1.30 g, 6.63 mmol, 1.0 equiv.): anhydrous CH<sub>2</sub>Cl<sub>2</sub> (20 ml), anhydrous C<sub>5</sub>H<sub>5</sub>N (1.60 ml, 1.57 g, 19.89 mmol, 3.0 equiv.), AcCl (943 ml, 1.04 g, 13.26 mmol, 2.0 equiv.), reaction time: 2.5 hours. (*S*)-**12**: 1.32 g (yield: 84%) yellow syrup; [ $\alpha$ ]<sub>D</sub><sup>20</sup> +6 (*c* = 0.52; CHCl<sub>3</sub>). Flash chromatography (hexane/EtOAc 8:2 → 7:3); R<sub>f</sub> = 0.60 (hexane/EtOAc 6:4); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  = 6.81 – 6.77 (m, 1H, *H*-5 or *H*-8 or *H*-9), 6.76 – 6.71 (m, 2H, *H*-5, *H*-8, or *H*-5, *H*-9, or *H*-8, *H*-9), 5.14 – 5.03 (m, 1H, *H*-2), 3.87, 3.86 (2s, 2 x 3H, *H*-10, *H*-11), 2.88 (dd, *J* = 13.7, 6.6 Hz, 1H, *H*-1-*a*), 2.68 (dd, *J* = 13.7, 6.6 Hz, 1H, *H*-1-*b*), 2.01 (s, 3H, *H*-13), 1.21 (d, *J* = 6.3 Hz, 3H, *H*-3); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  = 170.6 (1C, C-12), 148.8, 147.7, 130.3 (3C, C-4, C-6, C-7), 121.5, 112.6, 111.1 (3C, C-5, C-8, C-9), 71.7 (1C, C-2), 55.9 (2C, C-10, C-11), 41.9 (1C, C-1), 21.5 (1C, C-13), 19.5 (1C, C-3); IR (KBr)  $\nu$  = 2935 ( $\nu_{\text{as}}$  CH<sub>2</sub>), 2835 ( $\nu_{\text{s}}$  CH<sub>2</sub>), 2061 ( $\gamma$  Ar =CH,  $\gamma$  Ar C=C overtone and combination bands), 1731 ( $\nu$  C=O), 1607, 1590, 1517, 1455 ( $\nu$  Ar C=C,  $\delta_{\text{as}}$  Me,  $\beta_{\text{s}}$  CH<sub>2</sub>), 1372, 1331 ( $\delta_{\text{s}}$  Me,  $\delta$  CH), 1240 ( $\nu_{\text{as}}$  C-O-C=O,  $\nu_{\text{as}}$  Ar-O-Me), 1029 ( $\nu_{\text{s}}$  C-O-C=O,  $\nu_{\text{s}}$  Ar-O-Me), 856, 806 (1,2,4-trisubstituted  $\gamma_{\text{s}}$  Ar =CH) cm<sup>-1</sup>; ESI-TOF-HRMS: *m/z* calculated for C<sub>13</sub>H<sub>18</sub>NaO<sub>4</sub> [M+Na]<sup>+</sup> 261.1097, found 261.1096.

**(*R*)-1-(3,4-dimethoxyphenyl)propan-2-yl acetate [(*R*)-12]**



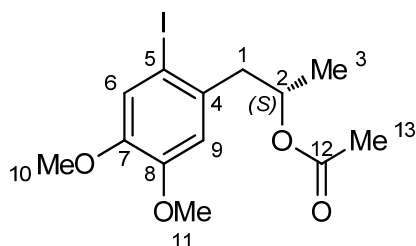
Starting from (*R*)-**11** (3.74 g, 19.07 mmol, 1.0 equiv.): anhydrous CH<sub>2</sub>Cl<sub>2</sub> (70 ml), anhydrous C<sub>5</sub>H<sub>5</sub>N (4.61 ml, 4.53 g, 57.22 mmol, 3.0 equiv.), AcCl (2.71 ml, 2.99 g, 38.15 mmol, 2.0 equiv.), reaction time: 3 hours. (*R*)-**12**: 4.12 g (yield: 91%) yellow syrup; [ $\alpha$ ]<sub>D</sub><sup>20</sup> -16 (*c* = 0.54;

CHCl<sub>3</sub>). Chromatographic and spectral data except for the chiroptical ones were identical with those of (*S*)-**12**.

### 2.2.3. General procedure for the halogenation of 1-arylpropan-2-yl acetates or isochroman derivatives with *N*-halosuccinimides (NXS, X = I or Br)

The corresponding 1-arylpropan-2-yl acetate (1.0 equiv.) was dissolved in anhydrous MeCN (5-30 ml), then NIS (1.1 or 1.3 equiv.) and F<sub>3</sub>CCOOH (0.3 equiv.) or NBS (1.2 equiv.) were added, and the solution was stirred at room temperature. When the starting material was consumed (1.5-16 hours) on the basis of TLC monitoring, the solvent was evaporated in *vacuo* and the residual solid was dissolved in EtOAc. The organic phase was washed with water, twice with a 10% aqueous solution of Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> and once with brine. The organic phase was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, filtered, and the solvent was evaporated in *vacuo*. The residue was purified by flash chromatography to yield the 1-(2-halo)arylpropan-2-yl acetate or isochroman target derivatives.

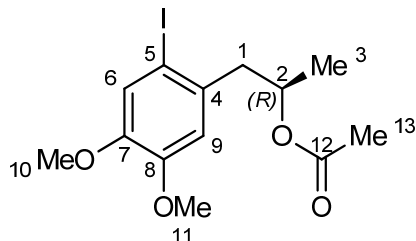
#### (*S*)-1-(2-iodo-4,5-dimethoxyphenyl)propan-2-yl acetate [(*S*)-**13**]



Starting from (*S*)-**12** (1.28 g, 5.39 mmol, 1.0 equiv.): anhydrous MeCN (20 ml), NIS (1.58 g, 7.01 mmol, 1.3 equiv.) and F<sub>3</sub>CCOOH (124  $\mu$ l, 184 mg, 1.62 mmol, 0.3 equiv.), reaction time: 16 hours. (*S*)-**13**: 1.88 g (yield: 96%) yellow syrup;  $[\alpha]_D^{20} +6$  ( $c = 0.55$ ; CHCl<sub>3</sub>). Flash chromatography (CH<sub>2</sub>Cl<sub>2</sub>/EtOAc 10:0  $\rightarrow$  10:0.05  $\rightarrow$  10:0.1);  $R_f = 0.35$  (CH<sub>2</sub>Cl<sub>2</sub>/EtOAc 10:0.05); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta = 7.21, 6.74$  (2s, 2 x 1H, *H*-6, *H*-9), 5.20 – 5.11 (m, 1H, *H*-2), 3.85 (s, 6H, *H*-10, *H*-11), 2.96 (dd,  $J = 14.0, 7.7$  Hz, 1H, *H*-1-*a*), 2.89 (dd,  $J = 14.0, 5.7$  Hz, 1H, *H*-1-*b*), 1.99 (s, 3H, *H*-13), 1.29 (d,  $J = 6.2$  Hz, 3H, *H*-3); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta = 170.4$  (1C, C-12), 149.2, 148.3, 133.1 (3C, C-4, C-7, C-8), 121.7, 113.2 (2C, C-6, C-9), 89.0 (1C, C-5), 71.0 (1C, C-2), 56.2, 56.0 (2C, C-10, C-11), 46.0 (1C, C-1), 21.4 (1C, C-13), 19.8 (1C, C-3); IR (KBr)  $\nu = 3078$  ( $\nu$  Ar =CH), 2976, 2933 ( $\nu_{as}$  Me,  $\nu_{as}$  CH<sub>2</sub>), 2840 ( $\nu_s$  CH<sub>2</sub>), 2048, 1997 ( $\gamma$  Ar =CH,  $\gamma$  Ar C=C overtone and combination bands), 1737 ( $\nu$  C=O), 1596, 1567, 1507, 1441 ( $\nu$  Ar C=C,  $\delta_{as}$  Me,  $\beta_s$  CH<sub>2</sub>), 1373, 1334 ( $\delta_s$  Me,  $\delta$  CH), 1257 ( $\nu_{as}$  C-O-C=O,  $\nu_{as}$  Ar-O-Me), 1051 ( $\nu$  Ar C-I), 1028 ( $\nu_s$  C-O-C=O,  $\nu_s$  Ar-O-Me), 858 (1,2,4,5-tetrasubstituted

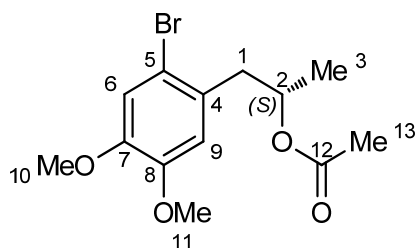
$\gamma_s$  Ar =CH)  $\text{cm}^{-1}$ ; ESI-TOF-HRMS:  $m/z$  calculated for  $\text{C}_{13}\text{H}_{17}\text{INaO}_4$   $[\text{M}+\text{Na}]^+$  387.0064, found 387.0064.

**(*R*)-1-(2-iodo-4,5-dimethoxyphenyl)propan-2-yl acetate [(*R*)-13]**



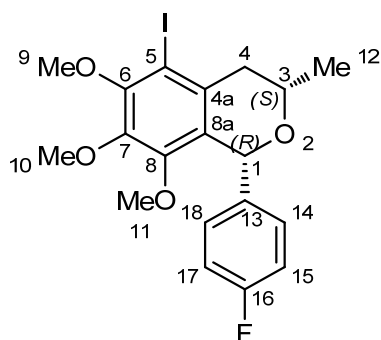
Starting from (*R*)-**12** (1.75 g, 7.35 mmol, 1.0 equiv.): anhydrous MeCN (30 ml), NIS (2.15 g, 9.55 mmol, 1.3 equiv.),  $\text{F}_3\text{CCOOH}$  (169  $\mu\text{l}$ , 251 mg, 2.21 mmol, 0.3 equiv.), reaction time: 16 hours. (*R*)-**13**: 2.47 g (yield: 93%) yellow syrup;  $[\alpha]_D^{20}$   $-17$  ( $c = 0.53$ ;  $\text{CHCl}_3$ ). Chromatographic and spectral data except for the chiroptical ones were identical with those of (*S*)-**13**.

**(*S*)-1-(2-bromo-4,5-dimethoxyphenyl)propan-2-yl acetate [(*S*)-14]**



Starting from (*S*)-**12** (1.36 g, 5.71 mmol, 1.0 equiv.): anhydrous MeCN (15 ml), NBS (1.22 g, 6.85 mmol, 1.2 equiv.), reaction time: 16 hours. (*S*)-**14**: 1.76 g (yield: 97%) pale yellow syrup;  $[\alpha]_D^{20}$   $+8$  ( $c = 0.52$ ;  $\text{CHCl}_3$ ). Flash chromatography ( $\text{CH}_2\text{Cl}_2/\text{EtOAc}$  10:0.05  $\rightarrow$  10:0.1);  $R_f = 0.40$  ( $\text{CH}_2\text{Cl}_2/\text{EtOAc}$  10:0.05);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta = 7.00, 6.74$  (2s, 2 x 1H, *H*-6, *H*-9), 5.22 – 5.13 (m, 1H, *H*-2), 3.85 (s, 6H, *H*-10, *H*-11), 2.93 (d,  $J = 6.6$  Hz, 2H, *H*-1), 1.99 (s, 3H, *H*-13), 1.27 (d,  $J = 6.3$  Hz, 3H, *H*-3);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta = 170.5$  (1C, *C*-12), 149.2, 148.3, 133.1 (3C, *C*-4, *C*-7, *C*-8), 115.5, 113.9 (2C, *C*-6, *C*-9), 114.9 (1C, *C*-5), 70.8 (1C, *C*-2), 56.2, 56.1 (2C, *C*-10, *C*-11), 41.6 (1C, *C*-1), 21.4 (1C, *C*-13), 19.8 (1C, *C*-3); IR (KBr)  $\nu = 3081$  ( $\nu$  Ar =CH), 2978, 2934 ( $\nu_{\text{as}}$  Me,  $\nu_{\text{as}}$   $\text{CH}_2$ ), 2842 ( $\nu_s$   $\text{CH}_2$ ), 2057 ( $\gamma$  Ar =CH,  $\gamma$  Ar C=C overtone and combination bands), 1736 ( $\nu$  C=O), 1604, 1573, 1509, 1461 ( $\nu$  Ar C=C,  $\delta_{\text{as}}$  Me,  $\beta_s$   $\text{CH}_2$ ), 1373, 1337 ( $\delta_s$  Me,  $\delta$  CH), 1244, 1207 ( $\nu_{\text{as}}$  C-O-C=O,  $\nu_{\text{as}}$  Ar-O-Me), 1051, 1031 ( $\nu$  Ar C-Br,  $\nu_s$  C-O-C=O,  $\nu_s$  Ar-O-Me), 859 (1,2,4,5-tetrasubstituted  $\gamma_s$  Ar =CH)  $\text{cm}^{-1}$ ; ESI-TOF-HRMS:  $m/z$  calculated for  $\text{C}_{13}\text{H}_{17}\text{BrNaO}_4$   $[\text{M}+\text{Na}]^+$  339.0202, found 339.0201.

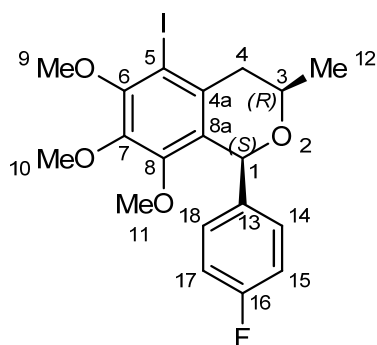
**(1*R*,3*S*)-1-(4-fluorophenyl)-5-iodo-6,7,8-trimethoxy-3-methylisochroman [*cis*-(1*R*,3*S*)-18]**



Starting from *cis*-(1*R*,3*S*)-17 (1.02 g, 3.06 mmol, 1.0 equiv.): anhydrous MeCN (30 ml), NIS (757 mg, 3.36 mmol, 1.1 equiv.), F<sub>3</sub>CCOOH (70  $\mu$ l, 105 mg, 0.92 mmol, 0.3 equiv.), reaction time: 16 hours. *cis*-(1*R*,3*S*)-18: 968 mg (yield 69%) white powder; mp 168-172 °C;  $[\alpha]_D^{20}$  -5 ( $c$  = 0.53; CHCl<sub>3</sub>). Flash chromatography (hexane/CH<sub>2</sub>Cl<sub>2</sub> 7:3  $\rightarrow$  6:4  $\rightarrow$  1:1  $\rightarrow$  4:6  $\rightarrow$  3:7  $\rightarrow$  0:10); R<sub>f</sub> = 0.22 (hexane/CH<sub>2</sub>Cl<sub>2</sub> 1:1); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  = 7.28 – 7.20 (m, 2H, *H*-14, *H*-18), 7.04 – 6.96 (m, 2H, *H*-15, *H*-17), 5.72 (s, 1H, *H*-1), 3.87 (s, 3H, *H*-9), 3.77 (s, 3H, *H*-10), 3.82 – 3.69 (m, 1H, *H*-3), 3.08 (s, 3H, *H*-11), 2.73 (dd,  $J$  = 16.4, 1.3 Hz, 1H, *H*-4<sub>eq</sub>), 2.60 (ddd,  $J$  = 16.4, 10.6, 1.4 Hz, 1H, *H*-4<sub>ax</sub>), 1.38 (d,  $J$  = 6.2 Hz, 3H, *H*-12); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  = 162.3 (1C, d,  $J_{C-F}$  = 245.5 Hz, C-16), 152.8 (1C, C-6), 150.9 (1C, C-8), 144.7 (1C, C-7), 139.7 (1C, d,  $J_{C-F}$  = 3.0 Hz, C-13), 133.9 (1C, C-4a), 130.1 (2C, d,  $J_{C-F}$  = 8.1 Hz, C-14, C-18), 129.2 (1C, C-8a), 115.2 (2C, d,  $J_{C-F}$  = 21.4 Hz, C-15, C-17), 92.5 (1C, C-5), 77.5 (1C, C-1), 71.0 (1C, C-3), 60.8, 60.7, 59.3 (3C, C-9, C-10, C-11), 42.8 (1C, C-4), 21.6 (1C, C-12); IR (KBr)  $\nu$  = 3042 ( $\nu$  Ar=CH), 2974, 2937 ( $\nu_{as}$  Me,  $\nu_{as}$  CH<sub>2</sub>), 2898, 2858 ( $\nu_s$  Me,  $\nu_s$  CH<sub>2</sub>,  $\nu$  CH), 1902 ( $\gamma$  Ar C=C overtone and combination bands), 1604, 1579, 1552, 1513, 1505, 1462 ( $\nu$  Ar C=C,  $\beta_s$  CH<sub>2</sub>,  $\delta_{as}$  Me), 1385, 1354, 1335, 1304 ( $\delta_s$  Me,  $\delta$  CH,  $\gamma_s$  CH<sub>2</sub>), 1290, 1274, 1262, 1225, 1153, 1120, 1100 ( $\nu_{as}$  Ar-O-Me,  $\nu$  Ar C-F), 1085, 1073, 1051, 1024 ( $\nu_{as}$  C-O-C,  $\nu$  Ar C-I,  $\nu_s$  Ar-O-Me) cm<sup>-1</sup>; ESI-TOF-HRMS:  $m/z$  calculated for C<sub>19</sub>H<sub>20</sub>FINaO<sub>4</sub> [M+Na]<sup>+</sup> 481.0283, found 481.0282.

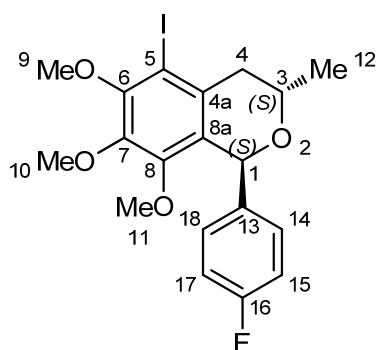
**(1*S*,3*R*)-1-(4-fluorophenyl)-5-iodo-6,7,8-trimethoxy-3-methylisochroman [*cis*-(1*S*,3*R*)-18]**





Starting from *cis*-(1*S*,3*R*)-**17** (1.45 g, 4.36 mmol, 1.0 equiv.): anhydrous MeCN (30 ml), NIS (1.08 g, 4.80 mmol, 1.1 equiv.), F<sub>3</sub>CCOOH (100  $\mu$ l, 149 mg, 1.31 mmol, 0.3 equiv.), reaction time: 16 hours. *cis*-(1*S*,3*R*)-**18**: 1.40 g (yield 70%) white powder; mp 168-171 °C; [ $\alpha$ ]<sub>D</sub><sup>20</sup> +48 (*c* = 0.52; CHCl<sub>3</sub>). Chromatographic and spectral data except for the chiroptical ones were identical with those of *cis*-(1*R*,3*S*)-**18**.

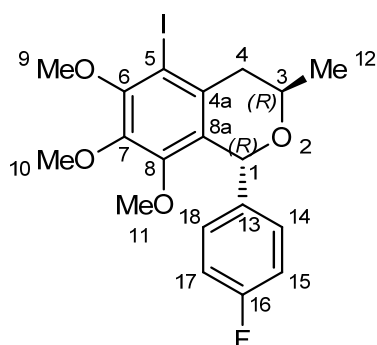
**(1*S*,3*S*)-1-(4-fluorophenyl)-5-iodo-6,7,8-trimethoxy-3-methylisochroman** [*trans*-(1*S*,3*S*)-**18**]



Starting from *trans*-(1*S*,3*S*)-**17** (1.21 g, 3.65 mmol, 1.0 equiv.): anhydrous MeCN (30 ml), NIS (902 mg, 4.01 mmol, 1.1 equiv.), F<sub>3</sub>CCOOH (84  $\mu$ l, 125 mg, 1.09 mmol, 0.3 equiv.), reaction time: 16 hours. *trans*-(1*S*,3*S*)-**18**: 1.54 g (yield: 92%) white solid; mp 55-59 °C; [ $\alpha$ ]<sub>D</sub><sup>20</sup> +5 (*c* = 0.53; CHCl<sub>3</sub>). Flash chromatography (hexane/EtOAc 97:3  $\rightarrow$  95:5  $\rightarrow$  93:7); R<sub>f</sub> = 0.45 (hexane/EtOAc 9:1); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  = 7.21 – 7.14 (m, 2H, *H*-14, *H*-18), 7.03 – 6.95 (m, 2H, *H*-15, *H*-17), 5.94 (s, 1H, *H*-1), 3.91 (s, 3H, *H*-9), 3.86 (s, 3H, *H*-10), 3.75 – 3.63 (m, 1H, *H*-3), 3.55 (s, 3H, *H*-11), 2.69 (dd, *J* = 17.0, 3.7 Hz, 1H, *H*-4<sub>eq</sub>), 2.41 (dd, *J* = 17.0, 10.9 Hz, 1H, *H*-4<sub>ax</sub>), 1.23 (d, *J* = 6.1 Hz, 3H, *H*-12); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  = 162.3 (1C, d, *J*<sub>C-F</sub> = 246.4 Hz, *C*-16), 153.0 (1C, *C*-6), 150.4 (1C, *C*-8), 144.1 (1C, *C*-7), 137.6 (1C, d, *J*<sub>C-F</sub> = 3.0 Hz, *C*-13), 132.9 (1C, *C*-4a), 130.3 (2C, d, *J*<sub>C-F</sub> = 8.0 Hz, *C*-14, *C*-18), 126.7 (1C, *C*-8a), 114.8 (2C, d, *J*<sub>C-F</sub> = 21.2 Hz, *C*-15, *C*-17), 92.8 (1C, *C*-5), 73.3 (1C, *C*-1), 63.8 (1C, *C*-3), 60.8, 60.7, 60.2 (3C, *C*-9, *C*-10, *C*-11), 41.7 (1C, *C*-4), 21.6 (1C, *C*-12); IR (KBr)  $\nu$  = 3044 ( $\nu$  Ar

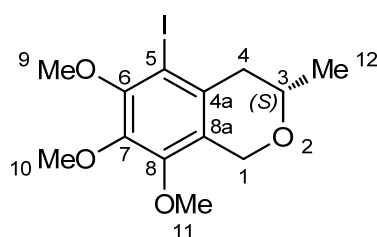
=CH), 2968, 2936 ( $\nu_{\text{as}}$  Me,  $\nu_{\text{as}}$  CH<sub>2</sub>), 2890, 2833 ( $\nu_{\text{s}}$  Me,  $\nu_{\text{s}}$  CH<sub>2</sub>,  $\nu$  CH), 2021, 1914 ( $\gamma$  Ar C=C overtone and combination bands), 1603, 1557, 1507, 1462 ( $\nu$  Ar C=C,  $\beta_{\text{s}}$  CH<sub>2</sub>,  $\delta_{\text{as}}$  Me), 1383, 1362, 1334 ( $\delta_{\text{s}}$  Me,  $\delta$  CH,  $\gamma_{\text{s}}$  CH<sub>2</sub>), 1283, 1263, 1225, 1197, 1160, 1141, 1122, 1110 ( $\nu_{\text{as}}$  Ar-O-Me,  $\nu$  Ar C-F), 1089, 1068, 1047, 1022 ( $\nu_{\text{as}}$  C-O-C,  $\nu$  Ar C-I,  $\nu_{\text{s}}$  Ar-O-Me) cm<sup>-1</sup>; ESI-TOF-HRMS:  $m/z$  calculated for C<sub>19</sub>H<sub>20</sub>FINaO<sub>4</sub> [M+Na]<sup>+</sup> 481.0283, found 481.0282.

**(1*R*,3*R*)-1-(4-fluorophenyl)-5-iodo-6,7,8-trimethoxy-3-methylisochroman** [*trans*-(1*R*,3*R*)-**18**]



Starting from *trans*-(1*R*,3*R*)-**17** (1.27 g, 3.82 mmol, 1.0 equiv.): anhydrous MeCN (30 ml), NIS (946 mg, 4.20 mmol, 1.1 equiv.), F<sub>3</sub>CCOOH (88  $\mu$ l, 131 mg, 1.15 mmol, 0.3 equiv.), reaction time: 16 hours. *trans*-(1*R*,3*R*)-**18**: 1.63 g (yield: 93%) white solid; mp 57-59 °C; [ $\alpha$ ]<sub>D</sub><sup>20</sup> -11 ( $c$  = 0.53; CHCl<sub>3</sub>). Chromatographic and spectral data except for the chiroptical ones were identical with those of *trans*-(1*S*,3*S*)-**18**.

**(*S*)-5-iodo-6,7,8-trimethoxy-3-methylisochroman** [(*S*)-**25**]



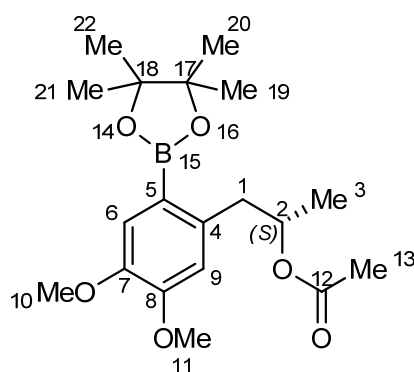
Starting from (*S*)-**24** (556 mg, 2.33 mmol, 1.0 equiv.): anhydrous MeCN (10 ml), NIS (683 mg, 3.03 mmol, 1.3 equiv.), F<sub>3</sub>CCOOH (54  $\mu$ l, 80 mg, 0.70 mmol, 0.3 equiv.) reaction time: 1.5 hours. (*S*)-**25**: 787 mg (yield: 93%) white solid; mp 33-36 °C; [ $\alpha$ ]<sub>D</sub><sup>20</sup> : +72 ( $c$  = 0.53; CHCl<sub>3</sub>). Flash chromatography (hexane/Et<sub>2</sub>O 95:5  $\rightarrow$  9:1); R<sub>f</sub> = 0.47 (hexane/Et<sub>2</sub>O 8:2); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  = 4.87 (d,  $J$  = 15.6 Hz, 1H, *H*-1-*a*), 4.57 (d,  $J$  = 15.6 Hz, 1H, *H*-1-*b*), 3.88, 3.86 (2s, 3 x 3H, *H*-9, *H*-10, *H*-11), 3.74 – 3.61 (m, 1H, *H*-3), 2.64 (dd,  $J$  = 16.7, 2.1 Hz, 1H, *H*-4-*a*), 2.39 (dd,  $J$  = 16.8, 10.7 Hz, 1H, *H*-4-*b*), 1.38 (d,  $J$  = 6.1 Hz, 3H, *H*-12); <sup>13</sup>C NMR (100

MHz, CDCl<sub>3</sub>)  $\delta$  = 152.2, 149.7, 143.9, 132.4, 126.3 (5C, C-4a, C-8a, C-6, C-7, C-8), 92.8 (1C, C-5), 71.4 (1C, C-3), 64.6 (1C, C-1), 61.0, 60.7, 60.5 (3C, C-9, C-10, C-11), 41.6 (1C, C-4), 21.5 (1C, C-12); IR (KBr)  $\nu$  = 2963, 2928 ( $\nu_{\text{as}}$  Me,  $\nu_{\text{as}}$  CH<sub>2</sub>), 2881, 2837 ( $\nu_{\text{s}}$  Me,  $\nu_{\text{s}}$  CH<sub>2</sub>), 2018, 1952, 1915, 1893, 1732 ( $\gamma$  Ar C=C overtone and combination bands), 1648, 1588, 1558, 1466, 1416 ( $\nu$  Ar C=C,  $\beta_{\text{s}}$  CH<sub>2</sub>,  $\delta_{\text{as}}$  Me), 1387, 1367, 1350, 1334 ( $\delta_{\text{s}}$  Me,  $\delta$  CH,  $\gamma_{\text{s}}$  CH<sub>2</sub>), 1261, 1240, 1211 ( $\nu_{\text{as}}$  Ar-O-Me), 1082, 1051, 1025 ( $\nu_{\text{as}}$  C-O-C,  $\nu$  Ar C-I,  $\nu_{\text{s}}$  Ar-O-Me) cm<sup>-1</sup>; ESI-TOF-HRMS:  $m/z$  calculated for C<sub>13</sub>H<sub>17</sub>INaO<sub>4</sub> [M+Na]<sup>+</sup> 387.0064, found 387.0063.

#### 2.2.4. General procedure for Miyaura borylation of chiral non-racemic 1-(2-haloaryl)propan-2-yl acetates

To the solution of 1-(2-haloaryl)propan-2-yl acetate (1.0 equiv.) in anhydrous DMF (18-37 ml), Ph<sub>3</sub>P (0.2 equiv.), (Ph<sub>3</sub>P)<sub>2</sub>PdCl<sub>2</sub> (0.1 equiv.) and anhydrous NaOAc (4.0 equiv.) or annealed KOAc (4.0 equiv.) were added under Ar or N<sub>2</sub> atmosphere, and the solution was stirred for 15 minutes with inert gas bubbling at room temperature. Then B<sub>2</sub>Pin<sub>2</sub> (3.0 equiv.) was added to the reaction mixture and the temperature was raised to 150 °C. When the starting material was consumed (1 hour-3 hours) on the basis of TLC monitoring, the reaction mixture was poured on ice and diluted with Et<sub>2</sub>O and the mixture was filtered on a short pad of Celite. The Celite was washed with Et<sub>2</sub>O and the two layers were separated in a separatory funnel. The aqueous phase was extracted twice with Et<sub>2</sub>O and the combined organic layers were washed twice with brine and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated in *vacuo*. The residue was purified by flash chromatography to yield the 1-[2-(pinacolatoboryl)aryl]propan-2-yl acetate target derivative.

#### (S)-1-[4,5-dimethoxy-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]propan-2-yl acetate [(S)-8]



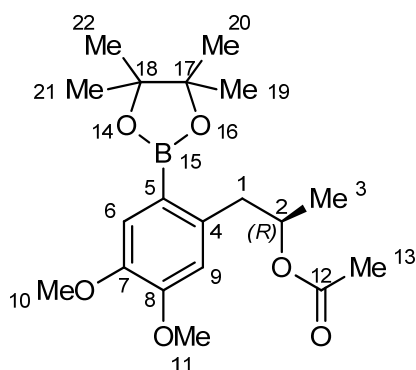
Starting from (S)-**13** (939 mg, 2.58 mmol, 1.0 equiv.): anhydrous DMF (20 ml), Ph<sub>3</sub>P (135 mg, 0.52 mmol, 0.2 equiv.), (Ph<sub>3</sub>P)<sub>2</sub>PdCl<sub>2</sub> (181 mg, 0.26 mmol, 0.1 equiv.), anhydrous NaOAc (846

mg, 10.31 mmol, 4.0 equiv.), B<sub>2</sub>Pin<sub>2</sub> (1.96 g, 7.73 mmol, 3.0 equiv.), reaction time: 1 hour. (*S*)-**8**: 524 mg (yield: 56%) pale yellow syrup.

Starting from (*S*)-**14** (1.76 g, 5.54 mmol, 1.0 equiv.): anhydrous DMF (18 ml), Ph<sub>3</sub>P (291 mg, 1.11 mmol, 0.2 equiv.), (Ph<sub>3</sub>P)<sub>2</sub>PdCl<sub>2</sub> (389 mg, 0.55 mmol, 0.1 equiv.), annealed KOAc (2.18 g, 22.16 mmol, 4.0 equiv.), B<sub>2</sub>Pin<sub>2</sub> (4.22 g, 16.62 mmol, 3.0 equiv.), reaction time: 3 hours. (*S*)-**8**: 1.92 g (yield: 95%) colorless syrup; [ $\alpha$ ]<sub>D</sub><sup>20</sup> +14 (*c* = 0.43; CHCl<sub>3</sub>).

Flash chromatography (hexane/EtOAc 9:1 → 85:15 → 8:2 → 7:3); R<sub>f</sub> = 0.43 (hexane/EtOAc 8:2); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  = 7.27, 6.72 (2s, 2 x 1H, *H*-6, *H*-9), 5.13 – 5.00 (m, 1H, *H*-2), 3.90, 3.88 (2s, 2 x 3H, *H*-10, *H*-11), 3.21 (dd, *J* = 13.2, 5.7 Hz, 1H, *H*-1-*a*), 3.02 (dd, *J* = 13.2, 7.6 Hz, 1H, *H*-1-*b*), 1.96 (s, 3H, *H*-13), 1.33 (s, 12H, *H*-19, *H*-20, *H*-21, *H*-22), 1.22 (d, *J* = 6.2 Hz, 3H, *H*-3); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  = 170.5 (1C, *C*-12), 150.8, 146.8, 138.9 (3C, *C*-4, *C*-7, *C*-8), 118.2, 113.6 (2C, *C*-6, *C*-9), 83.5 (2C, *C*-17, *C*-18), 73.3 (1C, *C*-2), 56.0, 55.8 (2C, *C*-10, *C*-11), 41.2 (1C, *C*-1), 25.0 (4C, *C*-19, *C*-20, *C*-21, *C*-22), 21.4 (1C, *C*-13), 19.7 (1C, *C*-3); IR (KBr)  $\nu$  = 2978, 2934 ( $\nu_{\text{as}}$  Me,  $\nu_{\text{as}}$  CH<sub>2</sub>), 1736 ( $\nu$  C=O), 1600, 1571, 1519 ( $\nu$  Ar C=C), 1371, 1349, 1320 ( $\delta_{\text{s}}$  Me,  $\delta$  CH,  $\nu_{\text{as}}$  O-B-O), 1251, 1221, 1204 ( $\nu_{\text{as}}$  C-O-C=O,  $\nu_{\text{as}}$  Ar-O-Me), 1160, 1144 ( $\nu_{\text{s}}$  O-B-O), 1054 ( $\nu$  C-O-B,  $\nu_{\text{s}}$  C-O-C=O,  $\nu_{\text{s}}$  Ar-O-Me), 860 (1,2,4,5-tetrasubstituted  $\gamma_{\text{s}}$  Ar=CH) cm<sup>-1</sup>; ESI-TOF-HRMS: *m/z* calculated for C<sub>19</sub>H<sub>29</sub>BNaO<sub>6</sub> [M+Na]<sup>+</sup> 387.1953, found 387.1957.

**(*R*)-1-[4,5-dimethoxy-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]propan-2-yl acetate [(*R*)-**8**]**



Starting from (*R*)-**13** (2.50 g, 6.85 mmol, 1.0 equiv.): anhydrous DMF (37 ml), Ph<sub>3</sub>P (360 mg, 1.37 mmol, 0.2 equiv.), (Ph<sub>3</sub>P)<sub>2</sub>PdCl<sub>2</sub> (481 mg, 0.69 mmol, 0.1 equiv.), anhydrous NaOAc (2.25 g, 27.42 mmol, 4.0 equiv.), B<sub>2</sub>Pin<sub>2</sub> (5.22 g, 20.56 mmol, 3.0 equiv.), reaction time: 3 hours. (*R*)-**8**: 1.50 g (yield: 60%) pale yellow syrup; [ $\alpha$ ]<sub>D</sub><sup>20</sup> -23 (*c* = 0.44; CHCl<sub>3</sub>). Chromatographic and spectral data except for the chiroptical ones were identical with those of (*S*)-**8**.

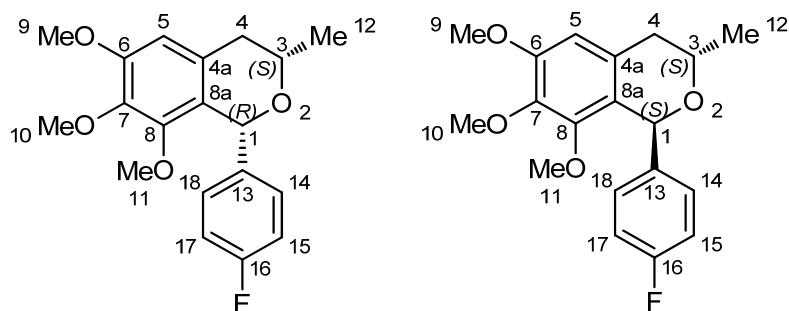
### 2.2.5. General procedure for oxa-Pictet-Spengler reactions of chiral non-racemic 1-arylpropan-2-ol derivatives

**Method A:** The 1-arylpropan-2-ol derivative (1.0 equiv.) was dissolved in anhydrous Et<sub>2</sub>O (5-20 ml), and the solution was cooled to 0 °C. The reagent MOMCl (5.0-10.0 equiv.) and annealed ZnCl<sub>2</sub> (0.3 equiv.) were added to the solution. When the starting material was consumed (2-4 hours) on the basis of TLC monitoring, the reaction was quenched with water and stirred for 15 minutes. Et<sub>2</sub>O was added to the mixture and the layers were separated. The organic layer was extracted twice with a saturated solution of NaHCO<sub>3</sub> and once with brine. The organic phase was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, filtered, and the solvent was evaporated in *vacuo*. The residue was purified by flash chromatography to yield the chiral non-racemic isochroman target derivative.

**Method B:** The 1-arylpropan-2-ol derivative (1.0 equiv.) was dissolved in anhydrous CH<sub>2</sub>Cl<sub>2</sub> (30-55 ml), and 4-fluorobenzaldehyde (1.2 equiv.) was added to the solution. The solution was cooled to 0 °C and BF<sub>3</sub>·Et<sub>2</sub>O (0.3 equiv.) was added. The reaction mixture was allowed to warm up to room temperature. When the starting material was consumed (4 hours) on the basis of TLC monitoring, the reaction was quenched with water and stirred for 20 minutes. CH<sub>2</sub>Cl<sub>2</sub> was added to the mixture and the layers were separated. The organic layer was extracted twice with a saturated solution of NaHCO<sub>3</sub> and once with brine. The organic phase was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, filtered, and the solvent was evaporated in *vacuo*. The residue was purified by flash chromatography to yield the chiral non-racemic isochroman target derivatives.

**Method C:** The 1-arylpropan-2-ol derivative (1.0 equiv.) was dissolved in anhydrous toluene (3 ml) and the solution was cooled to 0 °C. Then ethyl-3,3-diethoxypropionate (90%, technical grade, 2.0 equiv.) and BF<sub>3</sub>·Et<sub>2</sub>O (0.3 equiv.) were added to the solution and the reaction was allowed to warm up to room temperature. When the starting material was consumed (3-16 hours) on the basis of TLC monitoring, the reaction was quenched with a saturated solution of NaHCO<sub>3</sub> and stirred for 10 minutes. EtOAc was added to the mixture, and the layers were separated. The organic layer was extracted twice with a saturated solution of NaHCO<sub>3</sub> and once with brine. The organic phase was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, filtered, and the solvent was evaporated in *vacuo*. The residue was purified by flash chromatography to yield the chiral non-racemic isochroman target derivatives.

**(1*R*,3*S*)-1-(4-fluorophenyl)-6,7,8-trimethoxy-3-methylisochroman [cis-(1*R*,3*S*)-17] and (1*S*,3*S*)-1-(4-fluorophenyl)-6,7,8-trimethoxy-3-methylisochroman [trans-(1*S*,3*S*)-17]**

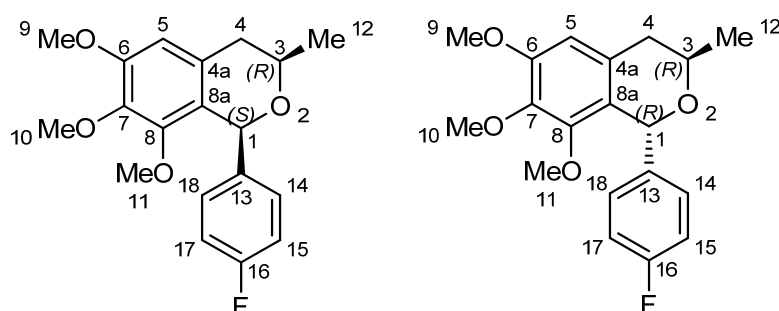


Starting from (*S*)-**16** (2.13 g, 9.39 mmol, 1.0 equiv.) using **method B**: anhydrous CH<sub>2</sub>Cl<sub>2</sub> (30 ml), 4-fluorobenzaldehyde (1.21 ml, 1.40 g, 11.27 mmol, 2.0 equiv.), BF<sub>3</sub>·Et<sub>2</sub>O (348  $\mu$ l, 400 mg, 2.82 mmol, 0.3 equiv.), reaction time: 4 hours. *cis*-(1*R*,3*S*)-**17**: 1.12 g (yield: 36%) colorless syrup;  $[\alpha]_D^{20} +16$  ( $c = 0.47$ ; CHCl<sub>3</sub>); *trans*-(1*S*,3*S*)-**17**: 1.90g (yield: 61%) white solid; mp 49-51 °C;  $[\alpha]_D^{20} -18$  ( $c = 0.50$ ; CHCl<sub>3</sub>); *dr cis:trans* = 1.0:1.7. Flash chromatography (hexane/CH<sub>2</sub>Cl<sub>2</sub> 7:3  $\rightarrow$  65:35  $\rightarrow$  6:4  $\rightarrow$  55:45  $\rightarrow$  1:1  $\rightarrow$  4:6  $\rightarrow$  3:7, then CH<sub>2</sub>Cl<sub>2</sub>/EtOAc 1:1). *cis*-(1*R*,3*S*)-**17**:  $R_f = 0.38$  (CH<sub>2</sub>Cl<sub>2</sub>); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta = 7.30 - 7.23$  (m, 2H, *H*-14, *H*-18), 7.02 – 6.94 (m, 2H, *H*-15, *H*-17), 6.44 (s, 1H, *H*-5), 5.76 (s, 1H, *H*-1), 3.84 (s, 3H, *H*-9), 3.83 – 3.77 (m, 1H, *H*-3), 3.74 (s, 3H, *H*-10), 3.10 (s, 3H, *H*-11), 2.80 (dd,  $J = 15.8, 10.7$  Hz, 1H, *H*-4<sub>ax</sub>), 2.61 (d,  $J = 15.6$  Hz, 1H, *H*-4<sub>eq</sub>), 1.33 (d,  $J = 6.2$  Hz, 3H, *H*-12); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta = 162.2$  (1C, d,  $J_{C-F} = 245.1$  Hz, *C*-16), 152.7 (1C, *C*-6), 150.3 (1C, *C*-8), 140.6 (1C, *C*-7), 140.2 (1C, d,  $J_{C-F} = 2.8$  Hz, *C*-13), 130.6 (1C, *C*-4a), 130.0 (2C, d,  $J_{C-F} = 8.1$  Hz, *C*-14, *C*-18), 123.4 (1C, *C*-8a), 115.0 (2C, d,  $J_{C-F} = 21.3$  Hz, *C*-15, *C*-17), 106.7 (1C, *C*-5), 77.2 (1C, *C*-1), 70.4 (1C, *C*-3), 60.5 (1C, *C*-10), 59.2 (1C, *C*-11), 55.9 (1C, *C*-9), 36.9 (1C, *C*-4), 21.7 (1C, *C*-12); IR (KBr)  $\nu = 3045$  ( $\nu$  Ar =CH), 2970, 2937 ( $\nu_{as}$  Me,  $\nu_{as}$  CH<sub>2</sub>), 2895, 2840 ( $\nu_s$  Me,  $\nu_s$  CH<sub>2</sub>), 1894, 1747 ( $\gamma$  Ar C=C overtone and combination bands), 1602, 1583, 1509, 1492, 1457 ( $\nu$  Ar C=C,  $\beta_s$  CH<sub>2</sub>,  $\delta_{as}$  Me), 1383, 1342, 1305 ( $\delta_s$  Me,  $\delta$  CH,  $\gamma_s$  CH<sub>2</sub>), 1258, 1240, 1221, 1148, 1114 ( $\nu_{as}$  Ar-O-Me,  $\nu$  Ar C-F), 1083, 1055, 1024 ( $\nu_{as}$  C-O-C,  $\nu_s$  Ar-O-Me), 859 (1,2,3,4,5-pentasubstituted  $\gamma_s$  Ar =CH) cm<sup>-1</sup>; ESI-TOF-HRMS:  $m/z$  calculated for C<sub>19</sub>H<sub>21</sub>FN<sub>4</sub>O<sub>4</sub> [M+Na]<sup>+</sup> 355.1316, found 355.1315.

*trans*-(1*S*,3*S*)-**17**:  $R_f = 0.24$  (CH<sub>2</sub>Cl<sub>2</sub>); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta = 7.24 - 7.15$  (m, 2H, *H*-14, *H*-18), 7.01 – 6.94 (m, 2H, *H*-15, *H*-17), 6.48 (s, 1H, *H*-5), 5.95 (s, 1H, *H*-1), 3.87 (s, 3H, *H*-9), 3.82 (s, 3H, *H*-10), 3.79 – 3.68 (m, 1H, *H*-3), 3.53 (s, 3H, *H*-11), 2.71 – 2.58 (m, 2H, *H*-4), 1.18 (d,  $J = 6.1$  Hz, 3H, *H*-12); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta = 162.1$  (1C, d,  $J_{C-F} = 245.7$  Hz, *C*-16), 152.9 (1C, *C*-6), 149.8 (1C, *C*-8), 140.0 (1C, *C*-7), 138.3 (1C, d,  $J_{C-F} = 2.9$  Hz, *C*-13), 130.2 (2C, d,  $J_{C-F} = 8.0$  Hz, *C*-14, *C*-18), 129.8 (1C, *C*-4a), 121.0 (1C, *C*-8a), 114.7 (2C, d,  $J_{C-F} = 21.3$  Hz, *C*-15, *C*-17), 106.9 (1C, *C*-5), 73.2 (1C, *C*-1), 63.0 (1C, *C*-3), 60.7 (1C, *C*-10), 60.0 (1C, *C*-11), 55.9 (1C, *C*-9), 35.4 (1C, *C*-4), 21.5 (1C, *C*-12); IR (KBr)  $\nu = 3047, 3011$

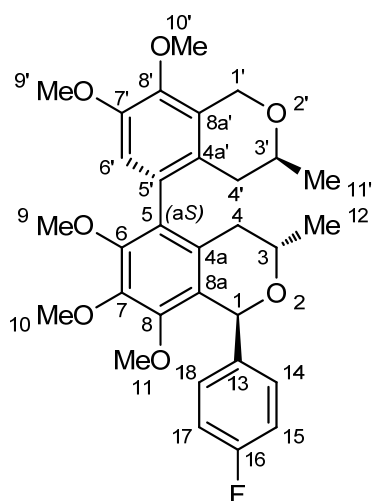
( $\nu$  Ar =CH), 2969, 2943 ( $\nu_{\text{as}}$  Me,  $\nu_{\text{as}}$  CH<sub>2</sub>), 2882, 2846 ( $\nu_{\text{s}}$  Me,  $\nu_{\text{s}}$  CH<sub>2</sub>), 1904 ( $\gamma$  Ar C=C overtone and combination bands), 1602, 1584, 1505, 1492, 1460 ( $\nu$  Ar C=C,  $\beta_{\text{s}}$  CH<sub>2</sub>,  $\delta_{\text{as}}$  Me), 1385, 1365, 1344, 1329 ( $\delta_{\text{s}}$  Me,  $\delta$  CH,  $\gamma_{\text{s}}$  CH<sub>2</sub>), 1265, 1241, 1223, 1201, 1172, 1161, 1145, 1120 ( $\nu_{\text{as}}$  Ar-O-Me,  $\nu$  Ar C-F), 1097, 1069, 1051, 1023 ( $\nu_{\text{as}}$  C-O-C,  $\nu_{\text{s}}$  Ar-O-Me), 882 (1,2,3,4,5-pentasubstituted  $\gamma_{\text{s}}$  Ar =CH) cm<sup>-1</sup>; ESI-TOF-HRMS:  $m/z$  calculated for C<sub>19</sub>H<sub>21</sub>FN<sub>4</sub>O<sub>4</sub> [M+Na]<sup>+</sup> 355.1316, found 355.1315.

**(1*S*,3*R*)-1-(4-fluorophenyl)-6,7,8-trimethoxy-3-methylisochroman** [*cis*-(1*S*,3*R*)-17] and **(1*R*,3*R*)-1-(4-fluorophenyl)-6,7,8-trimethoxy-3-methylisochroman** [*trans*-(1*R*,3*R*)-17]



Starting from (*R*)-**16** (3.95 g, 17.48 mmol, 1.0 equiv.) using **method B**: anhydrous CH<sub>2</sub>Cl<sub>2</sub> (55 ml), 4-fluorobenzaldehyde (2.25 ml, 2.60 g, 20.97 mmol, 1.2 equiv.), BF<sub>3</sub>·Et<sub>2</sub>O (647  $\mu$ l, 744 mg, 5.24 mmol, 0.3 equiv.), reaction time: 4 hours. *cis*-(1*S*,3*R*)-**17**: 2.03 g (yield: 35%) colorless syrup; [ $\alpha$ ]<sub>D</sub><sup>20</sup> -16 ( $c$  = 0.50; CHCl<sub>3</sub>); *trans*-(1*R*,3*R*)-**17**: 3.45 g (yield: 59%) white solid; mp 47-50 °C; [ $\alpha$ ]<sub>D</sub><sup>20</sup> +14 ( $c$  = 0.49; CHCl<sub>3</sub>); *dr cis:trans* = 1.0:1.7. Chromatographic and spectral data except for the chiroptical ones were identical with those of *cis*-(1*R*,3*S*)-**17** and *trans*-(1*S*,3*S*)-**17**.

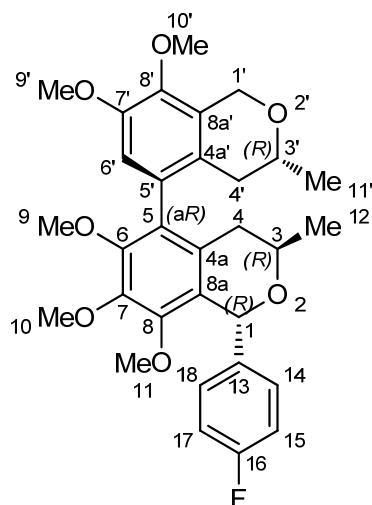
**(a*S*,1*S*,3*S*,3'*S*)-1-(4-fluorophenyl)-6,7,7',8,8'-pentamethoxy-3,3'-dimethyl-5,5'-bis-isochroman** [(a*S*,1*S*,3*S*,3'*S*)-21]



Starting from (aS,1S,3S,2'S)-**20** (70 mg, 0.13 mmol, 1.0 equiv.) using **method A**: anhydrous Et<sub>2</sub>O (5 ml), MOMCl (100  $\mu$ l, 106 mg, 1.32 mmol, 10.0 equiv.), annealed ZnCl<sub>2</sub> (5 mg, 0.04 mmol, 0.3 equiv.), reaction time: 4 hours. (aS,1S,3S,3'S)-**21**: 68 mg (yield: 96%) white amorphous solid foam;  $[\alpha]_{\text{D}}^{20} +66$ ;  $[\alpha]_{578}^{20} +69$ ;  $[\alpha]_{546}^{20} +78$ ;  $[\alpha]_{436}^{20} +130$ ;  $[\alpha]_{365}^{20} +203$  ( $c = 0.51$ ; MeCN); ECD: ( $c = 1.94 \times 10^{-4}$  M; MeCN)  $\lambda$  [nm], ( $\Delta\epsilon$ ) = 287sh (−0.35), 271 (−0.96), 263sh (−1.57), 243 (−5.99), 221 (1.12), 215 (−1.23), 198sh (34.62). Flash chromatography (hexane/EtOAc 9:1  $\rightarrow$  85:15  $\rightarrow$  8:2  $\rightarrow$  7:3);  $R_f = 0.29$  (hexane/EtOAc 8:2); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  = 7.22 – 7.17 (m, 2H, *H*-14, *H*-18), 7.06 – 6.99 (m, 2H, *H*-15, *H*-17), 6.61 (s, 1H, *H*-6'), 6.04 (s, 1H, *H*-1), 5.07 (d,  $J = 15.8$  Hz, 1H, *H*-1'<sub>eq</sub>), 4.77 (d,  $J = 15.8$  Hz, 1H, *H*-1'<sub>ax</sub>), 3.89 (s, 3H, *H*-10), 3.89 (s, 3H, *H*-10'), 3.83 (s, 3H, *H*-9'), 3.71 – 3.66 (m, 1H, *H*-3'), 3.66 (s, 3H, *H*-9), 3.64 – 3.58 (m, 1H, *H*-3), 3.57 (s, 3H, *H*-11), 2.41 (dd,  $J = 16.4, 10.6$  Hz, 1H, *H*-4'<sub>ax</sub>), 2.25 (dd,  $J = 17.1, 11.0$  Hz, 1H, *H*-4<sub>ax</sub>), 2.08 (dd,  $J = 16.4, 2.5$  Hz, 1H, *H*-4'<sub>eq</sub>), 1.97 (dd,  $J = 17.1, 3.5$  Hz, 1H, *H*-4<sub>eq</sub>), 1.30 (d,  $J = 6.1$  Hz, 1H, *H*-11'), 1.08 (d,  $J = 6.1$  Hz, 1H, *H*-12); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  = 162.3 (d,  $J_{\text{C-F}} = 246.1$  Hz, 1C, *C*-16), 151.2 (1C, *C*-6), 150.0 (1C, *C*-7'), 149.4 (1C, *C*-8), 144.1 (1C, *C*-7), 143.7 (1C, *C*-8'), 138.3 (d,  $J_{\text{C-F}} = 2.9$  Hz, 1C, *C*-13), 131.3 (1C, *C*-5'), 130.3 (d,  $J_{\text{C-F}} = 8.0$  Hz, 2C, *C*-14, *C*-18), 128.8 (2C, *C*-5, *C*-8a'), 128.3 (1C, *C*-4a), 125.1 (1C, *C*-4a'), 124.3 (1C, *C*-8a), 114.9 (d,  $J_{\text{C-F}} = 21.1$  Hz, 2C, *C*-15, *C*-17), 112.6 (1C, *C*-6'), 73.4 (1C, *C*-1), 70.8 (1C, *C*-3'), 64.9 (1C, *C*-1'), 63.3 (1C, *C*-3), 61.2 (1C, *C*-9), 60.8 (1C, *C*-10), 60.3 (1C, *C*-10'), 60.1 (1C, *C*-11), 55.9 (1C, *C*-9'), 34.4 (1C, *C*-4), 33.7 (1C, *C*-4'), 21.8 (2C, *C*-11', *C*-12); IR (KBr)  $\nu$  = 2967, 2935 ( $\nu_{\text{as}}$  Me,  $\nu_{\text{as}}$  CH<sub>2</sub>), 2838 ( $\nu_{\text{s}}$  CH<sub>2</sub>), 1603, 1578, 1507, 1491, 1464, 1420, 1408 ( $\nu$  Ar C=C,  $\beta_{\text{s}}$  CH<sub>2</sub>,  $\delta_{\text{as}}$  Me), 1383, 1363, 1316, ( $\delta_{\text{s}}$  Me,  $\delta$  CH,  $\gamma_{\text{s}}$  CH<sub>2</sub>), 1254, 1223, 1199, 1157, 1114 ( $\nu_{\text{as}}$  Ar-O-Me,  $\nu$  Ar C-F), 1085, 1064, 1028 ( $\nu_{\text{as}}$  C-O-C,  $\nu_{\text{s}}$  Ar-O-Me), 864 (1,2,3,4,5-pentasubstituted  $\gamma_{\text{s}}$  Ar =CH) cm<sup>−1</sup>; ESI-TOF-HRMS:  $m/z$  calculated for C<sub>31</sub>H<sub>35</sub>FN<sub>3</sub>O<sub>7</sub> [M+Na]<sup>+</sup> 561.2259, found 561.2257.

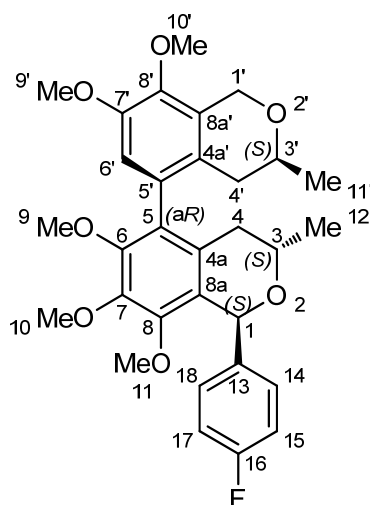


**(a*R*,1*R*,3*R*,3'*R*)-1-(4-fluorophenyl)-6,7,7',8,8'-pentamethoxy-3,3'-dimethyl-5,5'-bis-isochroman [(a*R*,1*R*,3*R*,3'*R*)-21]**



Starting from (a*R*,1*R*,3*R*,2'*R*)-**20** (310 mg, 0.59 mmol, 1.0 equiv.) using **method A**: anhydrous Et<sub>2</sub>O (20 ml), MOMCl (447  $\mu$ l, 474 mg, 5.89 mmol, 10.0 equiv.), annealed ZnCl<sub>2</sub> (24 mg, 0.18 mmol, 0.3 equiv.), reaction time: 4 hours. (a*R*,1*R*,3*R*,3'*R*)-**21**: 272 mg (yield: 86%) white amorphous solid foam;  $[\alpha]_D^{20}$  -57;  $[\alpha]_{578}^{20}$  -59;  $[\alpha]_{546}^{20}$  -67;  $[\alpha]_{436}^{20}$  -103;  $[\alpha]_{365}^{20}$  -158 ( $c = 0.52$ ; MeCN); ECD: ( $c = 1.71 \times 10^{-4}$  M; MeCN)  $\lambda$  [nm], ( $\Delta\epsilon$ ) = 287sh (0.45), 271 (0.98), 263sh (1.56), 242 (5.56), 220 (-0.67), 214 (0.77), 198 (-31.91). Chromatographic and spectral data except for the chiroptical ones were identical with those of (a*S*,1*S*,3*S*,3'*S*)-**21**.

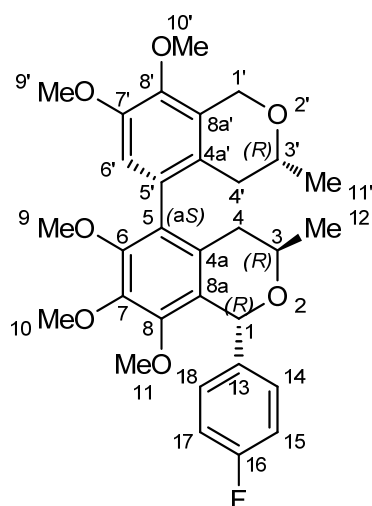
**(a*R*,1*S*,3*S*,3'*S*)-1-(4-fluorophenyl)-6,7,7',8,8'-pentamethoxy-3,3'-dimethyl-5,5'-bis-isochroman [(a*R*,1*S*,3*S*,3'*S*)-21]**



Starting from (a*R*,1*S*,3*S*,2'*S*)-**20** (93 mg, 0.18 mmol, 1.0 equiv.) using **method A**: anhydrous Et<sub>2</sub>O (5 ml), MOMCl (100  $\mu$ l, 106 mg, 1.32 mmol, 7.5 equiv.), annealed ZnCl<sub>2</sub> (7 mg, 0.05 mmol, 0.3 equiv.), reaction time: 4 hours. (a*R*,1*S*,3*S*,3'*S*)-**21**: 94 mg (yield: 99%) off-white

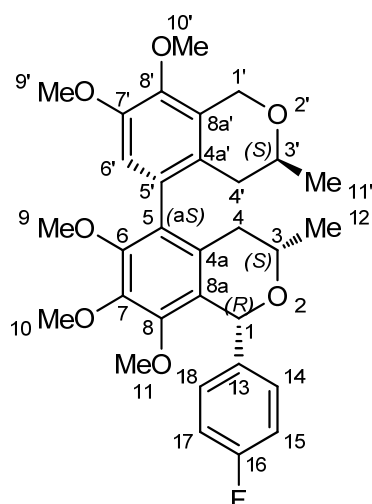
solid; mp 147-150 °C;  $[\alpha]_{\text{D}}^{20} +80$ ;  $[\alpha]_{578}^{20} +83$ ;  $[\alpha]_{546}^{20} +96$ ;  $[\alpha]_{436}^{20} +173$ ;  $[\alpha]_{365}^{20} +301$  ( $c = 0.49$ ; MeCN); ECD: ( $c = 2.24 \times 10^{-4}$  M; MeCN)  $\lambda$  [nm], ( $\Delta\epsilon$ ) = 286 (0.09), 271 (−0.43), 264 (−0.51), 259sh (−0.20), 255 (0.12), 243 (−0.73), 234sh (1.68), 219sh (5.73), 206 (20.54). Purification was not required for the crude product.  $R_f = 0.27$  (hexane/EtOAc 8:2);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta = 7.29 - 7.22$  (m, 2H, *H*-14, *H*-18), 7.08 – 6.97 (m, 2H, *H*-15, *H*-17), 6.61 (s, 1H, *H*-6'), 6.01 (s, 1H, *H*-1), 5.06 (d,  $J = 15.8$  Hz, 1H, *H*-1'<sub>eq</sub>), 4.78 (d,  $J = 15.8$  Hz, 1H, *H*-1'<sub>ax</sub>), 3.89 (s, 3H, *H*-10), 3.88 (s, 3H, *H*-10'), 3.86 (s, 3H, *H*-9'), 3.76 – 3.67 (m, 1H, *H*-3'), 3.67 (s, 3H, *H*-9), 3.66 – 3.62 (m, 1H, *H*-3), 3.57 (s, 3H, *H*-11), 2.27 (dd,  $J = 16.3, 3.3$  Hz, 1H, *H*-4'<sub>eq</sub>), 2.26 (dd,  $J = 17.0, 3.7$  Hz, 1H, *H*-4'<sub>eq</sub>), 2.14 (dd,  $J = 16.3, 10.4$  Hz, 1H, *H*-4'<sub>ax</sub>), 2.05 (dd,  $J = 17.0, 10.7$  Hz, 1H, *H*-4<sub>ax</sub>), 1.26 (d,  $J = 6.1$  Hz, 3H, *H*-11'), 1.08 (d,  $J = 6.1$  Hz, 3H, *H*-12);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta = 162.3$  (d,  $J_{\text{C-F}} = 245.8$  Hz, 1C, *C*-16), 150.3 (1C, *C*-6), 149.9 (1C, *C*-7'), 149.4 (1C, *C*-8), 143.9 (1C, *C*-7), 143.8 (1C, *C*-8'), 138.3 (d,  $J_{\text{C-F}} = 2.9$  Hz, 1C, *C*-13), 131.5 (1C, *C*-5'), 130.4 (d,  $J_{\text{C-F}} = 8.0$  Hz, 2C, *C*-14, *C*-18), 129.3 (1C, *C*-5), 129.0 (1C, *C*-4a), 128.9 (1C, *C*-8a'), 125.8 (1C, *C*-4a'), 124.5 (1C, *C*-8a), 114.8 (d,  $J_{\text{C-F}} = 21.2$  Hz, 2C, *C*-15, *C*-17), 112.4 (1C, *C*-6'), 73.4 (1C, *C*-1), 70.8 (1C, *C*-3'), 65.0 (1C, *C*-1'), 63.4 (1C, *C*-3), 61.0 (1C, *C*-9), 60.8 (1C, *C*-10), 60.2 (1C, *C*-10'), 60.1 (1C, *C*-11), 56.1 (1C, *C*-9'), 33.5 (1C, *C*-4'), 33.3 (1C, *C*-4), 21.7 (1C, *C*-11'), 21.6 (1C, *C*-12); IR (KBr)  $\nu = 2963, 2934$  ( $\nu_{\text{as}}$  Me,  $\nu_{\text{as}}$   $\text{CH}_2$ ), 2837 ( $\nu_{\text{s}}$   $\text{CH}_2$ ), 1907, 1729 ( $\gamma$  Ar=CH,  $\gamma$  Ar C=C overtone and combination bands), 1602, 1579, 1506, 1489, 1465, 1421, 1408 ( $\nu$  Ar C=C,  $\beta_{\text{s}}$   $\text{CH}_2$ ,  $\delta_{\text{as}}$  Me), 1383, 1361, 1315, ( $\delta_{\text{s}}$  Me,  $\delta$  CH,  $\gamma_{\text{s}}$   $\text{CH}_2$ ), 1267, 1253, 1233, 1218, 1198, 1159, 1129, 1117 ( $\nu_{\text{as}}$  Ar-O-Me,  $\nu$  Ar C-F), 1096, 1086, 1066, 1052, 1027 ( $\nu_{\text{as}}$  C-O-C,  $\nu_{\text{s}}$  Ar-O-Me)  $\text{cm}^{-1}$ ; ESI-TOF-HRMS:  $m/z$  calculated for  $\text{C}_{31}\text{H}_{35}\text{FNaO}_7$   $[\text{M}+\text{Na}]^+$  561.2259, found 561.2257.

**(a*S*,1*R*,3*R*,3'*R*)-1-(4-fluorophenyl)-6,7,7',8,8'-pentamethoxy-3,3'-dimethyl-5,5'-bis-isochroman [(a*S*,1*R*,3*R*,3'*R*)-21]**



Starting from (aS,1*R*,3*R*,2'*R*)-**20** (300 mg, 0.57 mmol, 1.0 equiv.) using **method A**: anhydrous Et<sub>2</sub>O (20 ml), MOMCl (325  $\mu$ l, 344 mg, 4.27 mmol, 7.5 equiv.), annealed ZnCl<sub>2</sub> (23 mg, 0.17 mmol, 0.3 equiv.), reaction time: 4 hours. (aS,1*R*,3*R*,3'*R*)-**21**: 304 mg (yield: 99%) off-white solid; mp 150-151 °C;  $[\alpha]_{\text{D}}^{20}$  -84;  $[\alpha]_{578}^{20}$  -88;  $[\alpha]_{546}^{20}$  -101;  $[\alpha]_{436}^{20}$  -155;  $[\alpha]_{365}^{20}$  -298 ( $c = 0.50$ ; MeCN); ECD ( $c = 1.44 \times 10^{-4}$  M; MeCN)  $\lambda$  [nm], ( $\Delta\epsilon$ ) = 286 (-0.15), 271 (0.40), 264 (0.48), 259sh (0.16), 253 (-0.06), 243 (0.70), 232sh (-1.62), 219sh (-6.00), 206 (-20.88). Purification was not required for the crude product. Chromatographic and spectral data except for the chiroptical ones were identical with those of (a*R*,1*S*,3*S*,3'*S*)-**21**.

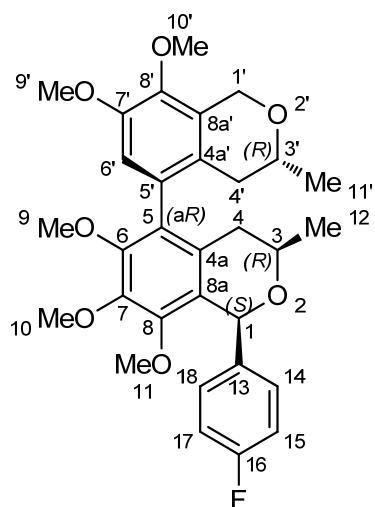
**(aS,1*R*,3*S*,3'*S*)-1-(4-fluorophenyl)-6,7,7',8,8'-pentamethoxy-3,3'-dimethyl-5,5'-bis-isochroman [(aS,1*R*,3*S*,3'*S*)-**21**]**



Starting from (aS,1*R*,3*S*,2'*S*)-**20** (63 mg, 0.12 mmol, 1.0 equiv.) using **method A**: anhydrous Et<sub>2</sub>O (5 ml), MOMCl (91  $\mu$ l, 97 mg, 1.20 mmol, 10.0 equiv.), annealed ZnCl<sub>2</sub> (5 mg, 0.04 mmol, 0.3 equiv.), reaction time: 4 hours. (aS,1*R*,3*S*,3'*S*)-**21**: 63 mg (yield: 97%) off-white amorphous solid foam;  $[\alpha]_{\text{D}}^{20}$  -55;  $[\alpha]_{578}^{20}$  -57;  $[\alpha]_{546}^{20}$  -68;  $[\alpha]_{436}^{20}$  -141;  $[\alpha]_{365}^{20}$  -279 ( $c = 0.49$ ;

MeCN); ECD ( $c = 1.65 \times 10^{-4}$  M; MeCN)  $\lambda$  [nm], ( $\Delta\epsilon$ ) = 287 (−1.45), 270sh (−1.14), 249sh (−5.90), 224 (−28.53), 201 (31.60). Flash chromatography (hexane/EtOAc 9:1  $\rightarrow$  85:15);  $R_f$  = 0.28 (hexane/EtOAc 85:15);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  = 7.39 – 7.31 (m, 2H, *H*-14, *H*-18), 7.08 – 6.99 (m, 2H, *H*-15, *H*-17), 6.65 (s, 1H, *H*-6'), 5.82 (s, 1H, *H*-1), 5.07 (d,  $J$  = 15.8 Hz, 1H, *H*-1' *ax*), 4.77 (d,  $J$  = 15.8 Hz, 1H, *H*-1' *eq*), 3.90 (s, 3H, *H*-10'), 3.87 (s, 3H, *H*-9'), 3.80 (s, 3H, *H*-10), 3.76 – 3.59 (m, 2H, *H*-3, *H*-3'), 3.57 (s, 3H, *H*-9), 3.15 (s, 3H, *H*-11), 2.41 (dd,  $J$  = 16.4, 10.9 Hz, 1H, *H*-4' *ax*), 2.41 (dd,  $J$  = 16.4, 10.9 Hz, 1H, *H*-4 *ax*), 1.99 (ddd,  $J$  = 16.4, 2.3, 1.2 Hz, 1H, *H*-4' *eq*), 1.97 (ddd,  $J$  = 16.4, 3.2, 1.0 Hz, 1H, *H*-4 *eq*), 1.26 (d,  $J$  = 6.1 Hz, 3H, *H*-11'), 1.23 (d,  $J$  = 6.1 Hz, 3H, *H*-12);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  = 162.3 (d,  $J_{\text{C-F}}$  = 245.0 Hz, 1C, *C*-16), 150.9 (1C, *C*-6), 149.8 (1C, *C*-7'), 149.8 (1C, *C*-8), 144.6 (1C, *C*-7), 143.8 (1C, *C*-8'), 140.2 (d,  $J_{\text{C-F}}$  = 2.7 Hz, 1C, *C*-13), 131.3 (1C, *C*-5'), 130.2 (d,  $J_{\text{C-F}}$  = 8.1 Hz, 2C, *C*-14, *C*-18), 129.2 (1C, *C*-4a), 128.7 (1C, *C*-8a'), 128.4 (1C, *C*-5), 126.7 (1C, *C*-8a), 125.8 (1C, *C*-4a'), 115.1 (d,  $J_{\text{C-F}}$  = 21.3 Hz, 2C, *C*-15, *C*-17), 113.0 (1C, *C*-6'), 77.6 (1C, *C*-1), 70.8, 70.6 (2C, *C*-3, *C*-3'), 65.0 (1C, *C*-1'), 61.0 (1C, *C*-9), 60.7 (1C, *C*-10), 60.3 (1C, *C*-10'), 59.4 (1C, *C*-11), 56.1 (1C, *C*-9'), 35.6 (1C, *C*-4), 33.5 (1C, *C*-4'), 21.8 (1C, *C*-12), 21.7 (1C, *C*-11'); IR (KBr)  $\nu$  = 2970, 2936 ( $\nu_{\text{as}}$  Me,  $\nu_{\text{as}}$  CH<sub>2</sub>), 2843 ( $\nu_{\text{s}}$  CH<sub>2</sub>), 1604, 1575, 1510, 1490, 1463, 1420 ( $\nu$  Ar C=C,  $\beta_{\text{s}}$  CH<sub>2</sub>,  $\delta_{\text{as}}$  Me), 1383, 1361, 1317, ( $\delta_{\text{s}}$  Me,  $\delta$  CH,  $\gamma_{\text{s}}$  CH<sub>2</sub>), 1279, 1255, 1232, 1200, 1148, 1118 ( $\nu_{\text{as}}$  Ar-O-Me,  $\nu$  Ar C-F), 1102, 1085, 1029 ( $\nu_{\text{as}}$  C-O-C,  $\nu_{\text{s}}$  Ar-O-Me)  $\text{cm}^{-1}$ ; ESI-TOF-HRMS:  $m/z$  calculated for  $\text{C}_{31}\text{H}_{35}\text{FNaO}_7$   $[\text{M}+\text{Na}]^+$  561.2259, found 561.2256.

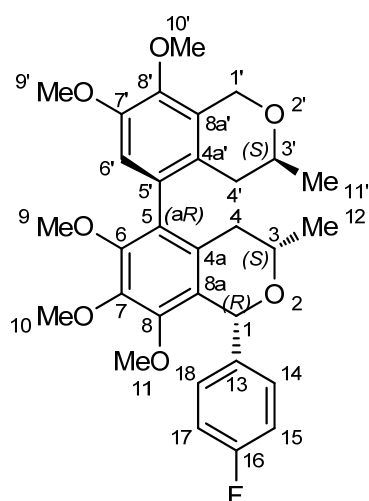
**(a*R*,1*S*,3*R*,3'*R*)-1-(4-fluorophenyl)-6,7,7',8,8'-pentamethoxy-3,3'-dimethyl-5,5'-bis-  
isochroman [(a*R*,1*S*,3*R*,3'*R*)-21]**



Starting from (a*R*,1*S*,3*R*,2'*R*)-**20** (100 mg, 0.19 mmol, 1.0 equiv.) using **method A**: anhydrous Et<sub>2</sub>O (5 ml), MOMCl (144  $\mu\text{l}$ , 153 mg, 1.90 mmol, 10.0 equiv.), annealed ZnCl<sub>2</sub> (8 mg, 0.06

mmol, 0.3 equiv.), reaction time: 4 hours. (*aR,1S,3R,3'R*)-**21**: 90 mg (yield: 88%) off-white amorphous solid foam;  $[\alpha]_{\text{D}}^{20} +49$ ;  $[\alpha]_{578}^{20} +51$ ;  $[\alpha]_{546}^{20} +61$ ;  $[\alpha]_{436}^{20} +116$ ;  $[\alpha]_{365}^{20} +269$  ( $c = 0.49$ ; MeCN); ECD ( $c = 1.94 \times 10^{-4}$  M; MeCN)  $\lambda$  [nm], ( $\Delta\epsilon$ ) = 287 (1.13), 270sh (1.00), 248sh (5.02), 223 (24.51), 201 (−28.82). Chromatographic and spectral data except for the chiroptical ones were identical with those of (*aS,1R,3S,3'S*)-**21**.

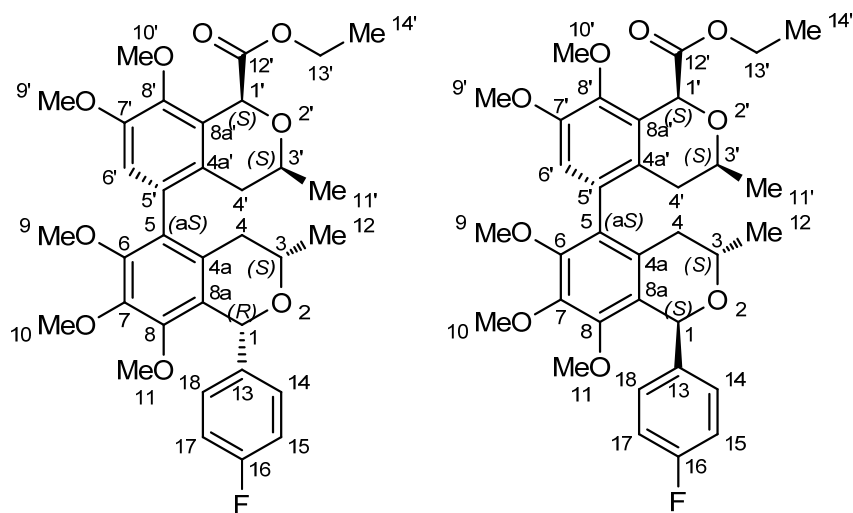
**(*aR,1R,3S,3'S*)-1-(4-fluorophenyl)-6,7,7',8,8'-pentamethoxy-3,3'-dimethyl-5,5'-bis-  
isochroman [(*aR,1R,3S,3'S*)-**21**]**



Starting from (*aR,1R,3S,2'S*)-**20** (41 mg, 0.08 mmol, 1.0 equiv.) using **method A**: anhydrous Et<sub>2</sub>O (7 ml), MOMCl (30  $\mu$ l, 31 mg, 0.39 mmol, 5.0 equiv.), annealed ZnCl<sub>2</sub> (3 mg, 0.02 mmol, 0.3 equiv.), reaction time: 3 hours. (*aR,1R,3S,3'S*)-**21**: 37 mg (yield: 89%) off-white amorphous solid foam;  $[\alpha]_{\text{D}}^{20} -35$ ;  $[\alpha]_{578}^{20} -37$ ;  $[\alpha]_{546}^{20} -43$ ;  $[\alpha]_{436}^{20} -87$ ;  $[\alpha]_{365}^{20} -147$  ( $c = 0.46$ ; MeCN); ECD ( $c = 1.98 \times 10^{-4}$  M; MeCN)  $\lambda$  [nm], ( $\Delta\epsilon$ ) = 287 (−0.49), 271sh (−0.66), 226 (−14.37), 205 (13.86), 202sh (12.76). Flash chromatography (hexane/EtOAc 9:1  $\rightarrow$  85:15);  $R_f = 0.42$  (hexane/EtOAc 8:2); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  = 7.31 – 7.22 (m, 2H, *H*-14, *H*-18), 7.07 – 6.99 (m, 2H, *H*-15, *H*-17), 6.61 (s, 1H, *H*-6'), 5.83 (s, 1H, *H*-1), 5.08 (d,  $J = 15.8$  Hz, 1H, *H*-1'<sub>ax</sub>), 4.79 (d,  $J = 15.8$  Hz, 1H, *H*-1'<sub>eq</sub>), 3.89 (s, 3H, *H*-10'), 3.84 (s, 3H, *H*-9'), 3.82 (s, 3H, *H*-10), 3.78 – 3.68 (m, 2H, *H*-3, *H*-3'), 3.61 (s, 3H, *H*-9), 3.17 (s, 3H, *H*-11), 2.35 – 2.18 (m, 4H, *H*-4', *H*-4), 1.32 (d,  $J = 6.1$  Hz, 3H, *H*-11'), 1.22 (d,  $J = 6.1$  Hz, 3H, *H*-12); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  = 162.3 (d,  $J_{\text{C-F}} = 245.3$  Hz, 1C, *C*-16), 150.3 (1C, *C*-6), 150.0 (1C, *C*-7'), 149.7 (1C, *C*-8), 144.6 (1C, *C*-7), 143.8 (1C, *C*-8'), 140.2 (d,  $J_{\text{C-F}} = 3.0$  Hz, 1C, *C*-13), 131.3 (1C, *C*-5'), 130.1, (1C, *C*-4a), 130.0 (d,  $J_{\text{C-F}} = 8.0$  Hz, 2C, *C*-14, *C*-18), 128.9 (1C, *C*-8a'), 128.7 (1C, *C*-5), 126.9 (1C, *C*-8a), 125.6 (1C, *C*-4a'), 115.2 (d,  $J_{\text{C-F}} = 21.4$  Hz, 2C, *C*-15, *C*-17), 112.6 (1C, *C*-6'), 77.3 (1C, *C*-1), 70.7 (1C, *C*-3'), 70.5 (1C, *C*-3), 65.1 (1C, *C*-1'), 60.9 (1C, *C*-9), 60.7 (1C, *C*-10),

60.3 (1C, C-10'), 59.3 (1C, C-11), 56.0 (1C, C-9'), 34.4 (1C, C-4), 33.6 (1C, C-4'), 21.8 (2C, C-11', C-12); IR (KBr)  $\nu$  = 2970, 2935 ( $\nu_{\text{as}}$  Me,  $\nu_{\text{as}}$  CH<sub>2</sub>), 2847 ( $\nu_{\text{s}}$  CH<sub>2</sub>), 1730 ( $\gamma$  Ar=CH,  $\gamma$  Ar C=C overtone and combination bands), 1604, 1577, 1509, 1490, 1463, 1421, 1407 ( $\nu$  Ar C=C,  $\beta_{\text{s}}$  CH<sub>2</sub>,  $\delta_{\text{as}}$  Me), 1384, 1359, 1317, ( $\delta_{\text{s}}$  Me,  $\delta$  CH,  $\gamma_{\text{s}}$  CH<sub>2</sub>), 1279, 1255, 1223, 1201, 1152, 1116 ( $\nu_{\text{as}}$  Ar-O-Me,  $\nu$  Ar C-F), 1074, 1054, 1029 ( $\nu_{\text{as}}$  C-O-C,  $\nu_{\text{s}}$  Ar-O-Me) cm<sup>-1</sup>; ESI-TOF-HRMS:  $m/z$  calculated for C<sub>31</sub>H<sub>35</sub>FNaO<sub>7</sub> [M+Na]<sup>+</sup> 561.2259, found 561.2251.

**(a*S*,1*R*,3*S*,1'*S*,3'*S*)-ethyl 1-(4-fluorophenyl)-6,7,7',8,8'-pentamethoxy-3,3'-dimethyl-[5,5'-bis-isochroman]-1'-carboxylate [(a*S*,1*R*,3*S*,1'*S*,3'*S*)-22]** and **(a*S*,1*S*,3*S*,1'*S*,3'*S*)-ethyl 1-(4-fluorophenyl)-6,7,7',8,8'-pentamethoxy-3,3'-dimethyl-[5,5'-bis-isochroman]-1'-carboxylate [(a*S*,1*S*,3*S*,1'*S*,3'*S*)-22]**



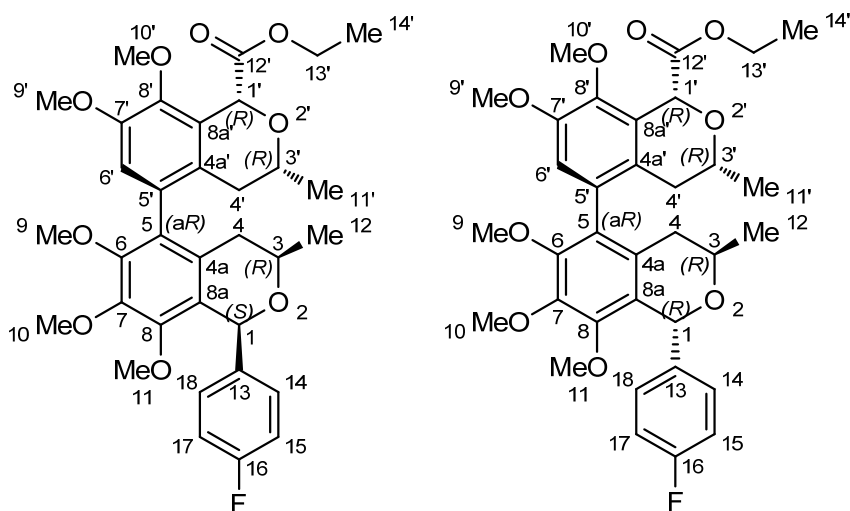
(a*S*,1*R*,3*S*,2'*S*)-**20** (141 mg, 0.27 mmol, 1 equiv.) was dissolved in anhydrous toluene (3 ml), and the solution was cooled to 0 °C. Then ethyl-diethoxyacetate (96  $\mu$ l, 94 mg, 0.54 mmol, 2 equiv.) and BF<sub>3</sub>·Et<sub>2</sub>O (10  $\mu$ l, 11 mg, 0.08 mmol, 0.3 equiv.) were added to the solution, and the reaction was allowed to warm up to room temperature. After stirring overnight, another portion of BF<sub>3</sub>·Et<sub>2</sub>O (10  $\mu$ l, 11 mg, 0.08 mmol, 0.3 equiv.) was added to the solution and stirred for overnight. The reaction was stirred for 4 hours at 60 °C and allowed to cool down to room temperature. After another day, the reaction was quenched with a saturated solution of NaHCO<sub>3</sub> and stirred for 10 minutes. EtOAc was added to the mixture and the layers were separated. The organic layer was extracted twice with a saturated solution of NaHCO<sub>3</sub> and once with brine. The organic phase was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, filtered, and the solvent was evaporated in *vacuo*. The residue was purified by flash chromatography (hexane/EtOAc 85:15  $\rightarrow$  6:4). (a*S*,1*R*,3*S*,1'*S*,3'*S*)-**22**: 37 mg (yield: 23%) white amorphous solid foam;  $[\alpha]_{\text{D}}^{20}$  -49;  $[\alpha]_{578}^{20}$  -52;

$[\alpha]_{546}^{20} -62$ ;  $[\alpha]_{436}^{20} -71$ ;  $[\alpha]_{365}^{20} -261$  ( $c = 0.49$ ; MeCN); ECD ( $c = 1.93 \times 10^{-4}$  M; MeCN)  $\lambda$  [nm], ( $\Delta\epsilon$ ) = 288 (−1.69), 271sh (−1.44), 252sh (−6.17), 225 (−27.82), 201 (33.46).

(a*S*,1*R*,3*S*,1'*S*,3'*S*)-**22**:  $R_f = 0.21$  (hexane/EtOAc 8:2);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta = 7.40 - 7.29$  (m, 2H, *H*-14, *H*-18), 7.09 – 6.98 (m, 2H, *H*-15, *H*-17), 6.72 (s, 1H, *H*-6'), 5.82 (s, 1H, *H*-1), 5.47 (s, 1H, *H*-1'), 4.36 – 4.18 (m, 2H, *H*-13'), 3.88 (s, 3H, *H*-10'), 3.87 (s, 3H, *H*-9'), 3.80 (s, 3H, *H*-10), 3.73 – 3.61 (m, 2H, *H*-3, *H*-3'), 3.54 (s, 3H, *H*-9), 3.15 (s, 3H, *H*-11), 2.56 (ddd,  $J = 16.2, 11.3, 0.9$  Hz, 1H, *H*-4'<sub>ax</sub>), 2.43 (ddd,  $J = 16.3, 10.9, 1.4$  Hz, 1H, *H*-4<sub>ax</sub>), 1.99 (dd,  $J = 16.0, 2.5$  Hz, 1H, *H*-4'<sub>eq</sub>), 1.97 (d,  $J = 16.2$  Hz, 1H, *H*-4<sub>eq</sub>), 1.32 (t,  $J = 7.2$  Hz, 3H, *H*-14'), 1.29 (d,  $J = 6.1$  Hz, 3H, *H*-11'), 1.23 (d,  $J = 6.1$  Hz, 3H, *H*-12');  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta = 171.0$  (1C, *C*-12'), 162.3 (d,  $J_{\text{C-F}} = 245.3$  Hz, 1C, *C*-16), 151.2 (1C, *C*-6), 149.9 (2C, *C*-7', *C*-8), 144.6 (1C, *C*-7), 144.5 (1C, *C*-8'), 140.2 (d,  $J_{\text{C-F}} = 2.9$  Hz, 1C, *C*-13), 130.5 (1C, *C*-5'), 130.2 (d,  $J_{\text{C-F}} = 8.1$  Hz, 2C, *C*-14, *C*-18), 129.2 (1C, *C*-4a), 128.0 (1C, *C*-5), 127.0 (1C, *C*-4a'), 126.7 (1C, *C*-8a), 126.6 (1C, *C*-8a'), 115.1 (d,  $J_{\text{C-F}} = 21.4$  Hz, 2C, *C*-15, *C*-17), 114.3 (1C, *C*-6'), 77.6 (1C, *C*-1), 75.6 (1C, *C*-1'), 71.2 (1C, *C*-3'), 70.6 (1C, *C*-3), 61.4 (1C, *C*-13'), 60.9 (1C, *C*-9), 60.8 (1C, *C*-10), 60.1 (1C, *C*-10'), 59.4 (1C, *C*-11), 56.2 (1C, *C*-9'), 35.8 (1C, *C*-4), 33.4 (1C, *C*-4'), 21.9 (1C, *C*-12), 21.7 (1C, *C*-11'), 14.3 (1C, *C*-14'); IR (KBr)  $\nu = 2973, 2936$  ( $\nu_{\text{as}}$  Me,  $\nu_{\text{as}}$  CH<sub>2</sub>), 2849 ( $\nu_{\text{s}}$  CH<sub>2</sub>), 1746 ( $\nu$  C=O), 1604, 1576, 1509, 1492, 1463, 1420 ( $\nu$  Ar C=C,  $\beta_{\text{s}}$  CH<sub>2</sub>,  $\delta_{\text{as}}$  Me), 1384, 1361, 1318 ( $\delta_{\text{s}}$  Me,  $\delta$  CH,  $\gamma_{\text{s}}$  CH<sub>2</sub>), 1257, 1232, 1183, 1150, 1116 ( $\nu_{\text{as}}$  Ar-O-Me,  $\nu$  Ar C-F,  $\nu_{\text{as}}$  C-O-C=O), 1068, 1029 ( $\nu_{\text{as}}$  C-O-C,  $\nu_{\text{s}}$  Ar-O-Me,  $\nu_{\text{s}}$  C-O-C=O)  $\text{cm}^{-1}$ ; ESI-TOF-HRMS:  $m/z$  calculated for  $\text{C}_{34}\text{H}_{39}\text{FNaO}_9$   $[\text{M}+\text{Na}]^+$  633.2470, found 633.2470.

Epimerization of **C-1** caused by  $\text{BF}_3 \cdot \text{Et}_2\text{O}$  also resulted in (a*S*,1*S*,3*S*,1'*S*,3'*S*)-**22** (52 mg, yield 32%) as pale yellow amorphous solid foam. Characterization is disclosed elsewhere.

**(a*R*,1*S*,3*R*,1'*R*,3'*R*)-ethyl 1-(4-fluorophenyl)-6,7,7',8,8'-pentamethoxy-3,3'-dimethyl-[5,5'-bis-isochroman]-1'-carboxylate [(a*R*,1*S*,3*R*,1'*R*,3'*R*)-22]** and **(a*R*,1*R*,3*R*,1'*R*,3'*R*)-ethyl 1-(4-fluorophenyl)-6,7,7',8,8'-pentamethoxy-3,3'-dimethyl-[5,5'-bis-isochroman]-1'-carboxylate [(a*R*,1*R*,3*R*,1'*R*,3'*R*)-22]**

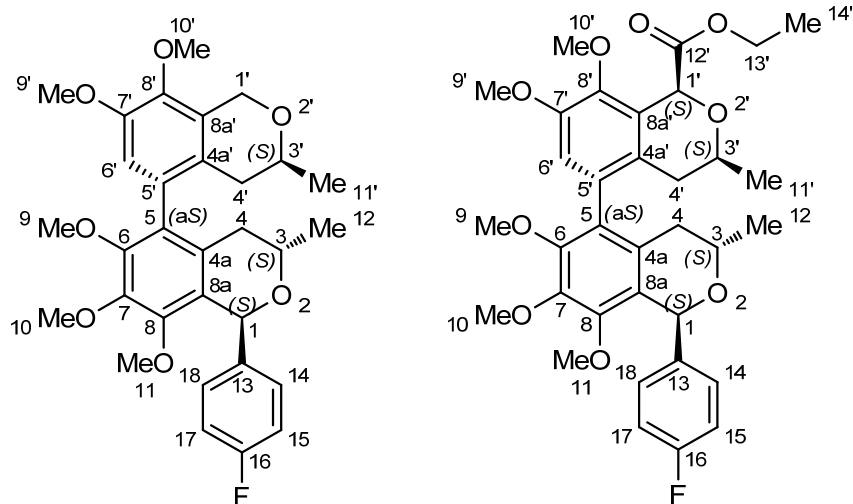


(*aR,1S,3R,2'R*)-**20** (323 mg, 0.61 mmol, 1 equiv.) was dissolved in anhydrous toluene (7 ml), and the solution was cooled to 0 °C. Then ethyl-diethoxyacetate (220  $\mu$ l, 216 mg, 1.22 mmol, 2 equiv.) and  $\text{BF}_3 \cdot \text{Et}_2\text{O}$  (23  $\mu$ l, 26 mg, 0.18 mmol, 0.3 equiv.) were added to the solution, and the reaction were allowed to warm up to room temperature. After stirring overnight, another portion of  $\text{BF}_3 \cdot \text{Et}_2\text{O}$  (11  $\mu$ l, 13 mg, 0.09 mmol, 0.15 equiv.) was added to the solution and the reaction was stirred for 8 hours at 60 °C. Then it was allowed to cool down to room temperature. After stirring overnight, the mixture was quenched with a saturated solution of  $\text{NaHCO}_3$  and stirred for 10 minutes. EtOAc was added to the mixture and the layers were separated. The organic layer was extracted twice with a saturated solution of  $\text{NaHCO}_3$  and once with brine. The organic phase was dried over anhydrous  $\text{Na}_2\text{SO}_4$ , filtered, and the solvent was evaporated in *vacuo*. The residue was purified by flash chromatography. (*aR,1S,3R,1'R,3'R*)-**22**: 62 mg (yield: 17%) white amorphous solid foam;  $[\alpha]_{\text{D}}^{20} +46$ ;  $[\alpha]_{578}^{20} +49$ ;  $[\alpha]_{546}^{20} +58$ ;  $[\alpha]_{436}^{20} +70$ ;  $[\alpha]_{365}^{20} +276$  ( $c = 0.48$ ; MeCN); ECD ( $c = 1.59 \times 10^{-4}$  M; MeCN)  $\lambda$  [nm], ( $\Delta\epsilon$ ) = 288 (1.55), 271sh (1.41), 251sh (6.08), 224 (26.63), 201 (−35.87).

Epimerization of C-1 caused by  $\text{BF}_3 \cdot \text{Et}_2\text{O}$  also resulted in (*aR,1R,3R,1'R,3'R*)-**22** (126 mg, yield 34%) as pale yellow amorphous solid foam. Chromatographic and spectral data except for the chiroptical ones were identical with those of the corresponding enantiomers (*aS,1R,3S,1'S,3'S*)-**22** and (*aS,1S,3S,1'S,3'S*)-**22**.

(*aS,1S,3S,3'S*)-1-(4-fluorophenyl)-6,7,7',8,8'-pentamethoxy-3,3'-dimethyl-5,5'-bis-isochroman [(*aS,1S,3S,3'S*)-**21**] and (*aS,1S,3S,1'S,3'S*)-ethyl 1-(4-fluorophenyl)-6,7,7',8,8'-pentamethoxy-3,3'-dimethyl-[5,5'-bis-isochroman]-1'-carboxylate [(*aS,1S,3S,1'S,3'S*)-**22**]





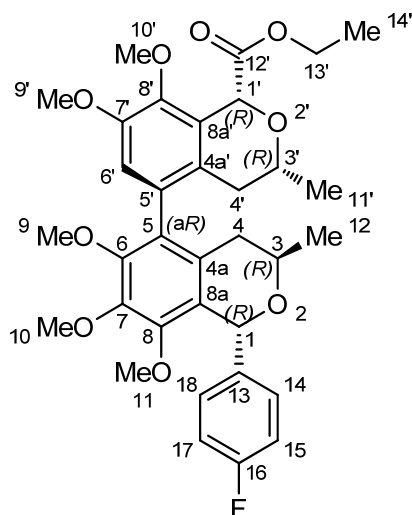
(aS,1S,3S,2'S)-**20** (141 mg, 0.27 mmol, 1.0 equiv.) was dissolved in anhydrous toluene (3 ml), and the solution was cooled to 0 °C. Then ethyl-diethoxyacetate (96  $\mu$ l, 94 mg, 0.53 mmol, 2.0 equiv.) and  $\text{BF}_3 \cdot \text{Et}_2\text{O}$  (10  $\mu$ l, 11 mg, 0.08 mmol, 0.3 equiv.) were added to the solution, and the reaction was allowed to warm up to room temperature. After four days, another portion of ethyl-diethoxyacetate (96  $\mu$ l, 94 mg, 0.53 mmol, 2.0 equiv.) was added to the reaction mixture. The temperature was raised to 60 °C. After stirring overnight, the reaction was allowed to cool down to room temperature and stirred for another day. The reaction was quenched with a saturated solution of  $\text{NaHCO}_3$  and stirred for 10 minutes.  $\text{EtOAc}$  was added to the mixture and the layers were separated. The organic layer was extracted twice with a saturated solution of  $\text{NaHCO}_3$  and once with brine. The organic phase was dried over anhydrous  $\text{Na}_2\text{SO}_4$ , filtered, and the solvent was evaporated in *vacuo*. The residue was purified by flash chromatography (hexane/ $\text{EtOAc}$  95:5  $\rightarrow$  9:1  $\rightarrow$  85:15  $\rightarrow$  75:25  $\rightarrow$  7:3) to yield (aS,1S,3S,1'S,3'S)-**22** (62 mg, 38%) as white amorphous solid foam;  $[\alpha]_{\text{D}}^{20} +42$ ;  $[\alpha]_{578}^{20} +43$ ;  $[\alpha]_{546}^{20} +49$ ;  $[\alpha]_{436}^{20} +55$ ;  $[\alpha]_{365}^{20} +119$  ( $c = 0.50$ ; MeCN); ECD ( $c = 1.3977 \cdot 10^{-4}$  M; MeCN)  $\lambda$  [nm], ( $\Delta\epsilon$ ) = 291 (−0.44), 270 (−1.19), 264sh (−2.05), 239sh (−7.35), 231 (−7.84), 217 (−4.58), 197 (36.15).

(aS,1S,3S,1'S,3'S)-**22**:  $R_f = 0.35$  (hexane/ $\text{EtOAc}$  75:25);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  = 7.22 – 7.16 (m, 2H, *H*-14, *H*-18), 7.06 – 6.99 (m, 2H, *H*-15, *H*-17), 6.67 (s, 1H, *H*-6'), 6.03 (s, 1H, *H*-1), 5.46 (s, 1H, *H*-1'), 4.36 – 4.19 (m, 2H, *H*-13'), 3.89 (s, 3H, *H*-10), 3.87 (s, 3H, *H*-10'), 3.82 (s, 3H, *H*-9'), 3.73 – 3.65 (m, 1H, *H*-3'), 3.63 (s, 3H, *H*-9), 3.62 – 3.58 (m, 1H, *H*-3), 3.57 (s, 3H, *H*-11), 2.54 (ddd,  $J = 16.1, 11.1$  Hz, 1.3 Hz, 1H, *H*-4'<sub>ax</sub>), 2.26 (dd,  $J = 17.0, 11.0$  Hz, 1H, *H*-4<sub>ax</sub>), 2.08 (dd,  $J = 16.1, 2.1$  Hz, 1H, *H*-4'<sub>eq</sub>), 1.93 (dd,  $J = 17.1, 3.5$  Hz, 1H, *H*-4<sub>eq</sub>), 1.33 (t,  $J = 7.1$  Hz, 3H, *H*-14'), 1.33 (d,  $J = 6.1$  Hz, 3H, *H*-11'), 1.08 (d,  $J = 6.1$  Hz, 3H, *H*-12);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  = 170.9 (1C, *C*-12'), 162.3 (d,  $J_{\text{C-F}} = 246.1$  Hz, 1C, *C*-16), 151.5 (1C, *C*-6), 150.1 (1C, *C*-7'), 149.5 (1C, *C*-8), 144.4 (1C, *C*-8'), 144.2 (1C, *C*-7), 138.3 (d,  $J_{\text{C-F}}$

= 3.0 Hz, 1C, C-13), 130.5 (1C, C-5'), 130.3 (d,  $J_{C-F}$  = 8.0 Hz, 2C, C-14, C-18), 128.4 (1C, C-5), 128.3 (1C, C-4a), 126.6 (1C, C-8a'), 126.2 (1C, C-4a'), 124.2 (1C, C-8a), 114.9 (d,  $J_{C-F}$  = 21.3 Hz, 2C, C-15, C-17), 113.9 (1C, C-6'), 75.6 (1C, C-1'), 73.4 (1C, C-1), 71.2 (1C, C-3'), 63.2 (1C, C-3), 61.4 (1C, C-13'), 61.1 (1C, C-9), 60.9 (1C, C-10), 60.2 (1C, C-11), 60.1 (1C, C-10'), 56.0 (1C, C-9'), 34.5 (1C, C-4), 33.6 (1C, C-4'), 21.8 (2C, C-11', C-12), 14.2 (1C, C-14'); IR (KBr)  $\nu$  = 2974, 2935 ( $\nu_{\text{as}}$  Me,  $\nu_{\text{as}}$  CH<sub>2</sub>), 2867 ( $\nu_{\text{s}}$  Me), 1746 ( $\nu$  C=O), 1603, 1579, 1507, 1492, 1464, 1420, 1407 ( $\nu$  Ar C=C,  $\beta_{\text{s}}$  CH<sub>2</sub>,  $\delta_{\text{as}}$  Me), 1384, 1363, 1317 ( $\delta_{\text{s}}$  Me,  $\delta$  CH,  $\gamma_{\text{s}}$  CH<sub>2</sub>), 1282, 1255, 1223, 1182, 1158, 1112 ( $\nu_{\text{as}}$  Ar-O-Me,  $\nu$  Ar C-F,  $\nu_{\text{as}}$  C-O-C=O), 1066, 1028 ( $\nu_{\text{as}}$  C-O-C,  $\nu_{\text{s}}$  Ar-O-Me,  $\nu_{\text{s}}$  C-O-C=O) cm<sup>-1</sup>; ESI-TOF-HRMS:  $m/z$  calculated for C<sub>34</sub>H<sub>39</sub>FNaO<sub>9</sub> [M+Na]<sup>+</sup> 633.2470, found 633.2472.

Hydrolysis of ethyl ester and subsequent decarboxylation of C-1' caused by BF<sub>3</sub>·Et<sub>2</sub>O also resulted in (a*S*,1*S*,3*S*,3'*S*)-**21** (42 mg, 29%) as white amorphous solid foam. Characterization is disclosed elsewhere.

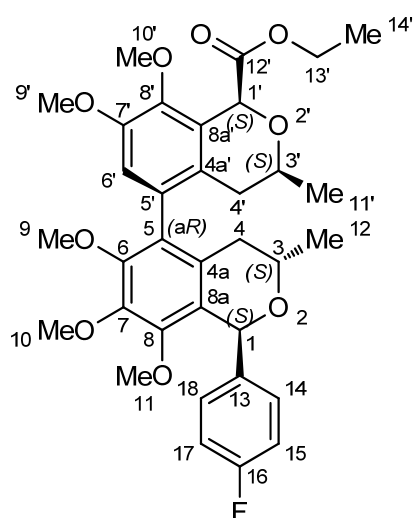
**(a*R*,1*R*,3*R*,1'*R*,3'*R*)-ethyl 1-(4-fluorophenyl)-6,7,7',8,8'-pentamethoxy-3,3'-dimethyl-[5,5'-bis-isochroman]-1'-carboxylate [(a*R*,1*R*,3*R*,1'*R*,3'*R*)-**22**]**



(a*R*,1*R*,3*R*,2'*R*)-**20** (100 mg, 0.19 mmol, 1 equiv.) was dissolved in anhydrous toluene (2 ml), and the solution was cooled to 0 °C. Then ethyl-diethoxyacetate (68  $\mu$ l, 67 mg, 0.38 mmol, 2 equiv.) and BF<sub>3</sub>·Et<sub>2</sub>O (7  $\mu$ l, 8 mg, 0.06 mmol, 0.3 equiv.) were added to the solution, and the reaction were allowed to warm up to room temperature. After stirring overnight, another portion of BF<sub>3</sub>·Et<sub>2</sub>O (4  $\mu$ l, 4 mg, 0.03 mmol, 0.15 equiv.) was added to the solution and the reaction was stirred for 8 hours at 60 °C. Then it was allowed to cool down to room temperature. After stirring overnight, the reaction was quenched with a saturated solution of NaHCO<sub>3</sub> and stirred for 10 minutes. EtOAc was added to the mixture and the layers were separated. The organic

layers were extracted twice with a saturated solution of  $\text{NaHCO}_3$  and once with brine. The organic phase was dried over anhydrous  $\text{Na}_2\text{SO}_4$ , filtered, and the solvent was evaporated in *vacuo*. The residue was purified by flash chromatography to yield (a*R*,1*R*,3*R*,1'*R*,3'*R*)-**22** (45 mg, 39%) as a white amorphous solid foam;  $[\alpha]_{\text{D}}^{20}$  -36;  $[\alpha]_{578}^{20}$  -38;  $[\alpha]_{546}^{20}$  -42;  $[\alpha]_{436}^{20}$  -57;  $[\alpha]_{365}^{20}$  -72 ( $c = 0.44$ ; MeCN); ECD ( $c = 1.7170 \cdot 10^{-4}$  M; MeCN)  $\lambda$  [nm], ( $\Delta\epsilon$ ) = 288 (0.50), 270 (1.04), 263sh (1.85), 239sh (6.54), 230 (7.19), 215 (3.56), 195 (-29.62). Chromatographic and spectral data except for the chiroptical ones were identical with those of (a*S*,1*S*,3*S*,1'*S*,3'*S*)-**22**.

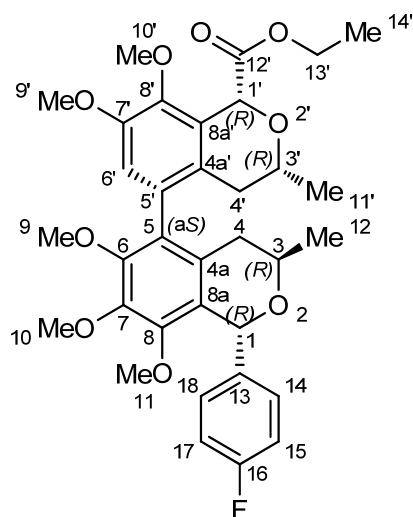
**(a*R*,1*S*,3*S*,1'*S*,3'*S*)-ethyl 1-(4-fluorophenyl)-6,7,7',8,8'-pentamethoxy-3,3'-dimethyl-[5,5'-bis-isochroman]-1'-carboxylate [(a*R*,1*S*,3*S*,1'*S*,3'*S*)-**22**]**



(a*R*,1*S*,3*S*,2'*S*)-**20** (143 mg, 0.27 mmol, 1 equiv.) was dissolved in anhydrous toluene (3 ml), and the solution was cooled to 0 °C. Then ethyl-diethoxyacetate (97  $\mu\text{l}$ , 95 mg, 0.54 mmol, 2 equiv.) and  $\text{BF}_3 \cdot \text{Et}_2\text{O}$  (10  $\mu\text{l}$ , 12 mg, 0.08 mmol, 0.3 equiv.) were added to the solution. After stirring for three days at room temperature, the reaction was quenched with a saturated solution of  $\text{NaHCO}_3$  and stirred for 10 minutes. EtOAc was added to the mixture and the layers were separated. The organic layers were extracted twice with a saturated solution of  $\text{NaHCO}_3$  and once with brine. The organic phase was dried over anhydrous  $\text{Na}_2\text{SO}_4$ , filtered, and the solvent was evaporated in *vacuo*. The residue was purified by flash chromatography to yield (a*R*,1*S*,3*S*,1'*S*,3'*S*)-**22** (118 mg, 71%) as white amorphous solid foam;  $[\alpha]_{\text{D}}^{20}$  +52;  $[\alpha]_{578}^{20}$  +54;  $[\alpha]_{546}^{20}$  +62;  $[\alpha]_{436}^{20}$  +91;  $[\alpha]_{365}^{20}$  +174 ( $c = 0.48$ ; MeCN); ECD ( $c = 1.67 \times 10^{-4}$  M; MeCN)  $\lambda$  [nm], ( $\Delta\epsilon$ ) = 287 (0.44), 279sh (0.18), 270 (-0.48), 264 (-0.69), 257sh (-0.65), 242sh (-3.31), 231 (-4.71), 205 (25.83). Flash chromatography (hexane/EtOAc 9:1  $\rightarrow$  85:15);  $R_f$  = 0.32 (hexane/EtOAc 75:25);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  = 7.28 – 7.22 (m, 2H, *H*-14, *H*-18), 7.06 – 6.99 (m, 2H, *H*-15, *H*-17), 6.68 (s, 1H, *H*-6'), 6.02 (s, 1H, *H*-1), 5.45 (s, 1H, *H*-1'), 4.34 –

4.20 (m, 2H, *H*-13'), 3.89 (s, 3H, *H*-10), 3.87 (s, 3H, *H*-10'), 3.85 (s, 3H, *H*-9'), 3.78 – 3.72 (m, 1H, *H*-3'), 3.71 – 3.60 (m, 1H, *H*-3), 3.64 (s, 3H, *H*-9), 3.57 (s, 3H, *H*-11), 2.32 (dd, *J* = 15.9, 11.3 Hz, 1H, *H*-4'<sub>ax</sub>), 2.29 (dd, *J* = 17.1, 3.3 Hz, 1H, *H*-4<sub>eq</sub>), 2.23 (dd, *J* = 16.0, 2.7 Hz, 1H, *H*-4'<sub>eq</sub>), 2.11 (dd, *J* = 17.0, 10.8 Hz, 1H, *H*-4<sub>ax</sub>), 1.33 (t, *J* = 7.1 Hz, 3H, *H*-14'), 1.30 (d, *J* = 6.0 Hz, 3H, *H*-11'), 1.09 (d, *J* = 6.1 Hz, 3H, *H*-12); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ = 171.0 (1C, *C*-12'), 162.3 (d, *J*<sub>C-F</sub> = 245.9 Hz, 1C, *C*-16), 150.4 (1C, *C*-6), 150.0 (1C, *C*-7'), 149.5 (1C, *C*-8), 144.4 (1C, *C*-8'), 143.8 (1C, *C*-7), 138.3 (d, *J*<sub>C-F</sub> = 2.9 Hz, 1C, *C*-13), 130.8 (1C, *C*-5'), 130.3 (d, *J*<sub>C-F</sub> = 8.0 Hz, 2C, *C*-14, *C*-18), 129.3 (1C, *C*-4a), 128.9 (1C, *C*-5), 126.7 (2C, *C*-8a', *C*-4a'), 124.5 (1C, *C*-8a), 114.8 (d, *J*<sub>C-F</sub> = 21.2 Hz, 2C, *C*-15, *C*-17), 113.7 (1C, *C*-6'), 75.6 (1C, *C*-1'), 73.4 (1C, *C*-1), 71.3 (1C, *C*-3'), 63.4 (1C, *C*-3), 61.3 (1C, *C*-13'), 60.9 (1C, *C*-9), 60.8 (1C, *C*-10), 60.1 (1C, *C*-10'); 60.0 (1C, *C*-11), 56.1 (1C, *C*-9'), 33.3 (2C, *C*-4', *C*-4), 21.6 (2C, *C*-11', *C*-12), 14.2 (1C, *C*-14'); IR (KBr) ν = 2974, 2936 (ν<sub>as</sub> Me, ν<sub>as</sub> CH<sub>2</sub>), 2898 (ν<sub>s</sub> Me), 1747 (ν C=O), 1602, 1579, 1507, 1492, 1464, 1421, 1407 (ν Ar C=C, β<sub>s</sub> CH<sub>2</sub>, δ<sub>as</sub> Me), 1385, 1362, 1315 (δ<sub>s</sub> Me, δ CH, γ<sub>s</sub> CH<sub>2</sub>), 1282, 1266, 1233, 1183, 1159, 1127, 1113 (ν<sub>as</sub> Ar-O-Me, ν Ar C-F, ν<sub>as</sub> C-O-C=O), 1095, 1066, 1053, 1029 (ν<sub>as</sub> C-O-C, ν<sub>s</sub> Ar-O-Me, ν<sub>s</sub> C-O-C=O), 872 (1,2,3,4,5-pentasubstituted γ<sub>s</sub> Ar =CH) cm<sup>-1</sup>; ESI-TOF-HRMS: *m/z* calculated for C<sub>34</sub>H<sub>39</sub>FN<sub>9</sub>O<sub>9</sub> [M+Na]<sup>+</sup> 633.2470, found 633.2461.

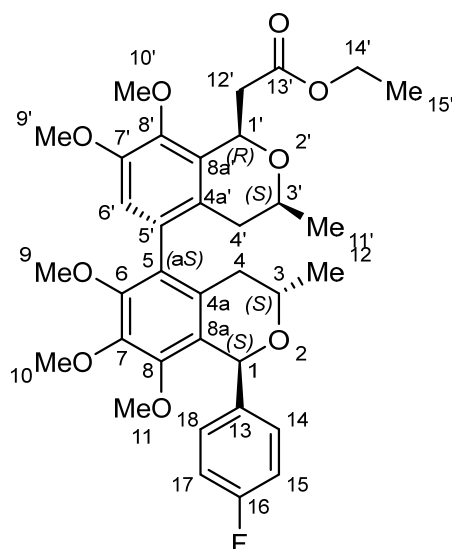
**(a*S*,1*R*,3*R*,1'*R*,3'*R*)-ethyl 1-(4-fluorophenyl)-6,7,7',8,8'-pentamethoxy-3,3'-dimethyl-[5,5'-bis-isochroman]-1'-carboxylate [(a*S*,1*R*,3*R*,1'*R*,3'*R*)-22]**



(a*S*,1*R*,3*R*,2'*R*)-**20** (100 mg, 0.19 mmol, 1 equiv.) was dissolved in anhydrous toluene (2 ml), and the solution was cooled to 0 °C. Then ethyl-diethoxyacetate (68 μl, 67 mg, 0.38 mmol, 2 equiv.) and BF<sub>3</sub>·Et<sub>2</sub>O (7 μl, 8 mg, 0.06 mmol, 0.3 equiv.) were added to the solution. After stirring for 24 hours at room temperature, the reaction was quenched with a saturated solution

of NaHCO<sub>3</sub> and stirred for 10 minutes. EtOAc was added to the mixture and the layers were separated. The organic layers were extracted twice with a saturated solution of NaHCO<sub>3</sub> and once with brine. The organic phase was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, filtered, and the solvent was evaporated in *vacuo*. The residue was purified by flash to yield (a*S*,1*R*,3*R*,1'*R*,3'*R*)-**22** (40 mg, 34%) as white amorphous solid foam;  $[\alpha]_{\text{D}}^{20}$  -45;  $[\alpha]_{578}^{20}$  -48;  $[\alpha]_{546}^{20}$  -54;  $[\alpha]_{436}^{20}$  -90;  $[\alpha]_{365}^{20}$  -147 (*c* = 0.32; MeCN); ECD (*c* = 1.59×10<sup>-4</sup> M; MeCN)  $\lambda$  [nm], ( $\Delta\epsilon$ ) = 287 (-0.34), 279sh (-0.14), 271 (0.45), 264 (0.66), 257sh (0.69), 239sh (3.48), 227 (4.95), 204 (-25.22). Chromatographic and spectral data except for the chiroptical ones were identical with those of (a*R*,1*S*,3*S*,1'*S*,3'*S*)-**22**.

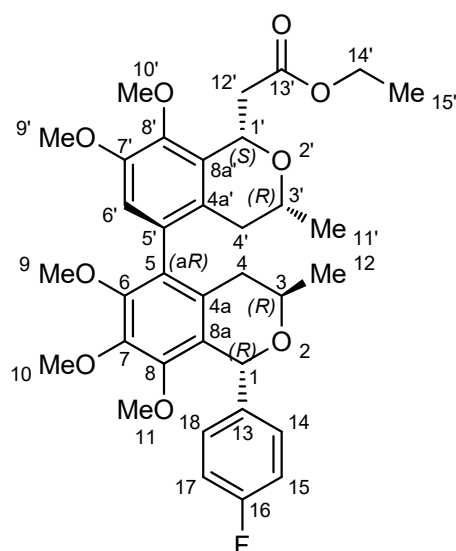
**Ethyl 2'-{(a*S*,1*S*,3*S*,1'*R*,3'*S*)-1-(4-fluorophenyl)-6,7,7',8,8'-pentamethoxy-3,3'-dimethyl-[5,5'-bis-isochroman]-1'-yl}acetate [(a*S*,1*S*,3*S*,1'*R*,3'*S*)-**23**]**



Starting from (a*S*,1*S*,3*S*,2'*S*)-**20** (132 mg, 0.25 mmol, 1.0 equiv.) using **method C**: anhydrous toluene (3 ml), ethyl-3,3-diethoxypropionate (90%, technical grade, 108  $\mu$ l = 98  $\mu$ l, 95 mg, 0.50 mmol, 2.0 equiv.), BF<sub>3</sub>·Et<sub>2</sub>O (9  $\mu$ l, 11 mg, 0.08 mmol, 0.3 equiv.), reaction time: 4 hours. (a*S*,1*S*,3*S*,1'*R*,3'*S*)-**23**: 141 mg (yield: 90%), white amorphous solid foam;  $[\alpha]_{\text{D}}^{20}$  +80;  $[\alpha]_{578}^{20}$  +83;  $[\alpha]_{546}^{20}$  +95;  $[\alpha]_{436}^{20}$  +125;  $[\alpha]_{365}^{20}$  +223 (*c* = 0.51; MeCN); ECD (*c* = 1.82×10<sup>-4</sup> M; MeCN)  $\lambda$  [nm], ( $\Delta\epsilon$ ) = 292 (-0.47), 270 (-1.26), 264sh (-2.30), 242 (-7.40), 220 (3.33), 199 (28.46). Flash chromatography (hexane/EtOAc 9:1 → 85:15 → 8:2 → 75:25 → 7:3); R<sub>f</sub> = 0.40 (hexane/EtOAc 75:25); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  = 7.23 – 7.16 (m, 2H, *H*-14, *H*-18), 7.06 – 6.99 (m, 2H, *H*-15, *H*-17), 6.64 (s, 1H, *H*-6'), 6.04 (s, 1H, *H*-1), 5.44 (dd, *J* = 8.2, 2.9 Hz, 1H, *H*-1'), 4.20 (q, *J* = 7.1 Hz, 2H, *H*-14'), 3.91 (s, 3H, *H*-10'), 3.89 (s, 3H, *H*-10), 3.84 (s, 3H, *H*-9'), 3.66 (s, 3H, *H*-9), 3.64 – 3.58 (m, 2H, *H*-3, *H*-3'), 3.57 (s, 3H, *H*-11), 3.31 (dd, *J* = 15.2,

3.2 Hz, 1H, *H*-12'-*a*), 2.66 (dd, *J* = 15.2, 8.3 Hz, 1H, *H*-12'-*b*), 2.42 (dd, *J* = 15.5, 10.9 Hz, 1H, *H*-4'*ax*), 2.27 (dd, *J* = 17.1, 11.1 Hz, 1H, *H*-4'*ax*), 2.03 (d, *J* = 15.5 Hz, 1H, *H*-4'*eq*), 1.90 (dd, *J* = 17.1, 3.4 Hz, 1H, *H*-4'*eq*), 1.28 (t, *J* = 7.1 Hz, 3H, *H*-15'), 1.24 (d, *J* = 6.1 Hz, 3H, *H*-11'), 1.09 (d, *J* = 6.1 Hz, 3H, *H*-12); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  = 171.9 (1C, C-13'), 162.2 (d, *J*<sub>C-F</sub> = 246.0 Hz, 1C, C-16), 151.3 (1C, C-6), 150.3 (1C, C-7'), 149.3 (1C, C-8), 144.5 (1C, C-8'), 144.1 (1C, C-7), 138.2 (d, *J*<sub>C-F</sub> = 2.8 Hz, 1C, C-13), 130.6 (1C, C-5'), 130.4 (1C, C-8*a*'), 130.2 (d, *J*<sub>C-F</sub> = 8.0 Hz, 2C, C-14, C-18), 128.7 (1C, C-5), 128.2 (1C, C-4*a*), 126.8 (1C, C-4*a*'), 124.1 (1C, C-8*a*), 114.8 (d, *J*<sub>C-F</sub> = 8.0 Hz, 2C, C-15, C-17), 112.8 (1C, C-6'), 73.3 (1C, C-1), 71.6 (1C, C-1'), 69.9 (1C, C-3'), 63.1 (1C, C-3), 61.0 (1C, C-9), 60.7 (1C, C-10), 60.3 (1C, C-10'), 60.2 (1C, C-14'), 60.0 (1C, C-11), 55.9 (1C, C-9'), 41.9 (1C, C-12'), 34.6 (1C, C-4'), 34.4 (1C, C-4), 21.7 (2C, C-11', C-12), 14.3 (1C, C-15'); IR (KBr)  $\nu$  = 2973, 2936 ( $\nu_{\text{as}}$  Me,  $\nu_{\text{as}}$  CH<sub>2</sub>), 2841 ( $\nu_{\text{s}}$  CH<sub>2</sub>), 1737 ( $\nu$  C=O), 1602, 1579, 1507, 1486, 1464, 1420 ( $\nu$  Ar C=C,  $\beta_{\text{s}}$  CH<sub>2</sub>,  $\delta_{\text{as}}$  Me), 1383, 1363, 1314 ( $\delta_{\text{s}}$  Me,  $\delta$  CH,  $\gamma_{\text{s}}$  CH<sub>2</sub>), 1280, 1254, 1223, 1174, 1159, 1112 ( $\nu_{\text{as}}$  Ar-O-Me,  $\nu$  Ar C-F,  $\nu_{\text{as}}$  C-O-C=O), 1093, 1067, 1027 ( $\nu_{\text{as}}$  C-O-C,  $\nu_{\text{s}}$  Ar-O-Me,  $\nu_{\text{s}}$  C-O-C=O) cm<sup>-1</sup>; ESI-TOF-HRMS: *m/z* calculated for C<sub>35</sub>H<sub>41</sub>FNao<sub>9</sub> [M+Na]<sup>+</sup> 647.2627, found 647.2626.

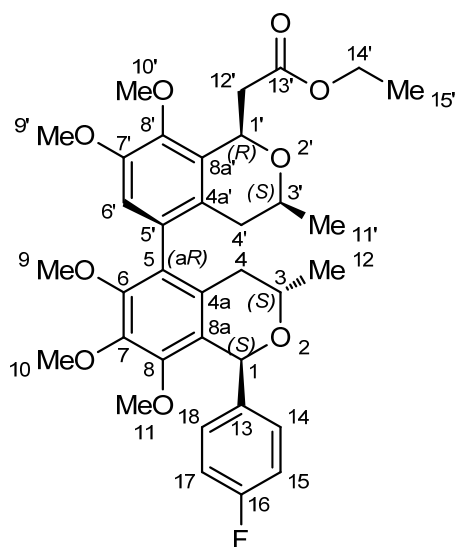
**Ethyl 2'-{(a*R*,1*R*,3*R*,1'*S*,3'*R*)-1-(4-fluorophenyl)-6,7,7',8,8'-pentamethoxy-3,3'-dimethyl-[5,5'-bis-isochroman]-1'-yl}acetate [(a*R*,1*R*,3*R*,1'*S*,3'*R*)-23]**



Starting from (a*R*,1*R*,3*R*,2'*R*)-**20** (170 mg, 0.32 mmol, 1.0 equiv.) using **method C**: anhydrous toluene (4 ml), ethyl-3,3-diethoxypropionate (90%, technical grade, 140  $\mu$ l = 126  $\mu$ l, 123 mg, 0.65 mmol, 2.0 equiv.), BF<sub>3</sub>·Et<sub>2</sub>O (14  $\mu$ l, 12 mg, 0.10 mmol, 0.3 equiv.), reaction time: 4 hours. (a*R*,1*R*,3*R*,1'*S*,3'*R*)-**23**: 140 mg (yield: 69%), white amorphous solid foam; [ $\alpha$ ]<sub>D</sub><sup>20</sup> -75; [ $\alpha$ ]<sub>578</sub><sup>20</sup> -78; [ $\alpha$ ]<sub>546</sub><sup>20</sup> -88; [ $\alpha$ ]<sub>436</sub><sup>20</sup> -121; [ $\alpha$ ]<sub>365</sub><sup>20</sup> -202 (*c* = 0.51; MeCN); ECD (*c* = 1.83×10<sup>-4</sup> M; MeCN)  $\lambda$

[nm], ( $\Delta\epsilon$ ) = 291 (0.45), 270 (1.12), 264sh (2.30), 244 (6.93), 220 (−2.65), 200 (−26.80). Chromatographic and spectral data except for the chiroptical ones were identical with those of (a*S*,1*S*,3*S*,1'*R*,3'*S*)-**23**.

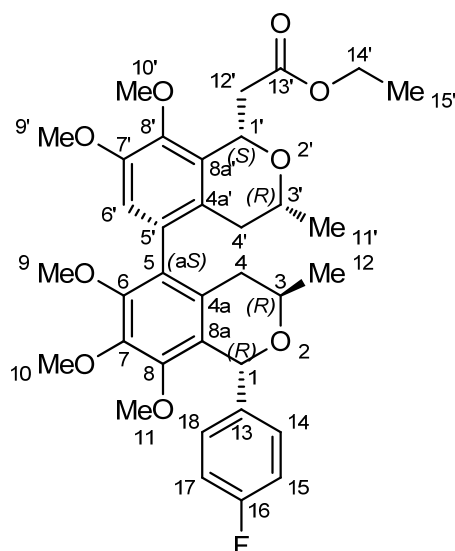
**Ethyl 2'-{(a*R*,1*S*,3*S*,1'*R*,3'*S*)-1-(4-fluorophenyl)-6,7,7',8,8'-pentamethoxy-3,3'-dimethyl-[5,5'-bis-isochroman]-1'-yl}acetate [(a*R*,1*S*,3*S*,1'*R*,3'*S*)-**23**]**



Starting from (a*R*,1*S*,3*S*,2'*S*)-**20** (140 mg, 0.27 mmol, 1.0 equiv.) using **method C**: anhydrous toluene (3 ml), ethyl-3,3-diethoxypropionate (90%, technical grade, 115  $\mu$ l = 103  $\mu$ l, 101 mg, 0.53 mmol, 2.0 equiv.),  $\text{BF}_3 \cdot \text{Et}_2\text{O}$  (10  $\mu$ l, 11 mg, 0.08 mmol, 0.3 equiv.), reaction time: 3 hours. (a*R*,1*S*,3*S*,1'*R*,3'*S*)-**23**: 156 mg (yield: 94%), white amorphous solid foam;  $[\alpha]_{\text{D}}^{20} +72$ ;  $[\alpha]_{578}^{20} +75$ ;  $[\alpha]_{546}^{20} +86$ ;  $[\alpha]_{436}^{20} +122$ ;  $[\alpha]_{365}^{20} +233$  ( $c = 0.50$ ; MeCN); ECD ( $c = 1.66 \times 10^{-4}$  M; MeCN)  $\lambda$  [nm], ( $\Delta\epsilon$ ) = 287 (0.18), 270 (−0.61), 264 (−0.97), 257sh (−1.29), 242sh (−4.07), 233 (−4.18), 206 (27.41). Flash chromatography (hexane/EtOAc 9:1  $\rightarrow$  85:15  $\rightarrow$  8:2  $\rightarrow$  7:3  $\rightarrow$  6:4);  $R_f = 0.49$  (hexane/EtOAc 75:25);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta = 7.28 - 7.22$  (m, 2H, *H*-14, *H*-18), 7.06 – 6.98 (m, 2H, *H*-15, *H*-17), 6.65 (s, 1H, *H*-6'), 6.02 (s, 1H, *H*-1), 5.43 (dd,  $J = 8.0, 3.1$  Hz, 1H, *H*-1'), 4.18 (q,  $J = 7.1$ , 2H, *H*-14'), 3.90 (s, 3H, *H*-10'), 3.89 (s, 3H, *H*-10), 3.87 (s, 3H, *H*-9'), 3.73 – 3.60 (m, 2H, *H*-3', *H*-3), 3.66 (s, 3H, *H*-9), 3.57 (s, 3H, *H*-11), 3.32 (dd,  $J = 15.1, 3.4$  Hz, 1H, *H*-12'-a), 2.66 (dd,  $J = 15.1, 8.1$  Hz, 1H, *H*-12'-b), 2.24 (dd,  $J = 17.0, 3.6$  Hz, 1H, *H*-4<sub>eq</sub>), 2.22 – 2.15 (m, 2H, *H*-4'), 2.11 (dd,  $J = 17.0, 10.7$  Hz, 1H, *H*-4<sub>ax</sub>), 1.27 (t,  $J = 7.1$  Hz, 3H, *H*-15'), 1.21 (d,  $J = 6.1$  Hz, 3H, *H*-11'), 1.09 (d,  $J = 6.1$  Hz, 3H, *H*-12);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta = 171.8$  (1C, *C*-13'), 162.2 (d,  $J_{\text{C-F}} = 245.9$  Hz, 1C, *C*-16), 150.3 (1C, *C*-6), 150.2 (1C, *C*-7'), 149.3 (1C, *C*-8), 144.6 (1C, *C*-8'), 143.8 (1C, *C*-7), 138.2 (d,  $J_{\text{C-F}} = 2.9$  Hz, 1C, *C*-13), 130.9 (1C, *C*-5'), 130.5 (1C, *C*-8a'), 130.3 (d,  $J_{\text{C-F}} = 8.0$  Hz, 2C, *C*-14, *C*-18), 129.2 (2C,

*C-4a*, *C-5*), 127.4 (1C, *C-4a'*), 124.4 (1C, *C-8a*), 114.7 (d,  $J_{C-F}$  = 21.2 Hz, 2C, *C-15*, *C-17*), 112.7 (1C, *C-6'*), 73.4 (1C, *C-1*), 71.7 (1C, *C-1'*), 69.9 (1C, *C-3'*), 63.3 (1C, *C-3*), 60.8 (1C, *C-9*), 60.7 (1C, *C-10*), 60.3 (1C, *C-10'*), 60.2 (1C, *C-14'*), 60.0 (1C, *C-11*), 55.9 (1C, *C-9'*), 41.8 (1C, *C-12'*), 34.4 (1C, *C-4'*), 32.2 (1C, *C-4*), 21.5 (2C, *C-11'*, *C-12*), 14.3 (1C, *C-15'*); IR (KBr)  $\nu$  = 2973, 2935 ( $\nu_{\text{as}}$  Me,  $\nu_{\text{as}}$  CH<sub>2</sub>), 1738 ( $\nu$  C=O), 1602, 1507, 1486, 1464, 1421, 1407 ( $\nu$  Ar C=C,  $\beta_{\text{s}}$  CH<sub>2</sub>,  $\delta_{\text{as}}$  Me), 1384, 1360, 1315 ( $\delta_{\text{s}}$  Me,  $\delta$  CH,  $\gamma_{\text{s}}$  CH<sub>2</sub>), 1267, 1254, 1222, 1174, 1159, 1122 ( $\nu_{\text{as}}$  Ar-O-Me,  $\nu$  Ar C-F,  $\nu_{\text{as}}$  C-O-C=O), 1093, 1066, 1029 ( $\nu_{\text{as}}$  C-O-C,  $\nu_{\text{s}}$  Ar-O-Me,  $\nu_{\text{s}}$  C-O-C=O), 871 (1,2,3,4,5-pentasubstituted  $\gamma_{\text{s}}$  Ar =CH) cm<sup>-1</sup>; ESI-TOF-HRMS:  $m/z$  calculated for C<sub>35</sub>H<sub>41</sub>FNaO<sub>9</sub> [M+Na]<sup>+</sup> 647.2627, found 647.2628.

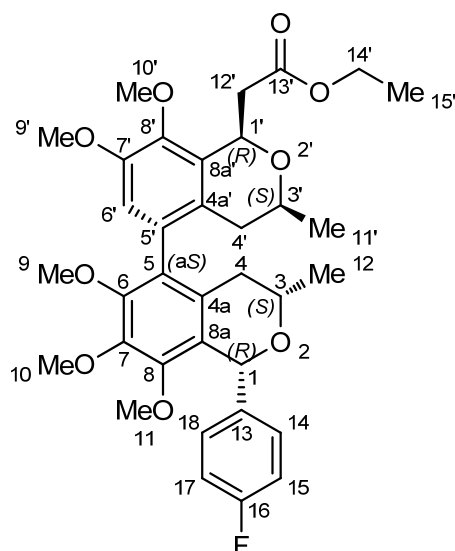
**Ethyl 2'-{(a*S*,1*R*,3*R*,1'*S*,3'*R*)-1-(4-fluorophenyl)-6,7,7',8,8'-pentamethoxy-3,3'-dimethyl-[5,5'-bis-isochroman]-1'-yl}acetate [(a*S*,1*R*,3*R*,1'*S*,3'*R*)-23]**



Starting from (a*S*,1*R*,3*R*,2'*R*)-**20** (100 mg, 0.19 mmol, 1.0 equiv.) using **method C**: anhydrous toluene (2 ml), ethyl-3,3-diethoxypropionate (90%, technical grade, 82  $\mu$ l = 74  $\mu$ l, 72 mg, 0.38 mmol, 2.0 equiv.), BF<sub>3</sub>·Et<sub>2</sub>O (7  $\mu$ l, 8 mg, 0.06 mmol, 0.3 equiv.), reaction time: 3 hours. (a*S*,1*R*,3*R*,1'*S*,3'*R*)-**23**: 98 mg (yield: 83%), white amorphous solid foam;  $[\alpha]_{\text{D}}^{20}$  -70;  $[\alpha]_{578}^{20}$  -74;  $[\alpha]_{546}^{20}$  -84;  $[\alpha]_{436}^{20}$  -131;  $[\alpha]_{365}^{20}$  -230 ( $c$  = 0.50; MeCN); ECD ( $c$  =  $1.87 \times 10^{-4}$  M; MeCN)  $\lambda$  [nm], ( $\Delta\epsilon$ ) = 287 (-0.14), 270 (0.55), 263 (0.89), 257sh (1.28), 241 (4.08), 232sh (3.89), 205 (-24.28). Chromatographic and spectral data except for the chiroptical ones were identical with those of (a*R*,1*S*,3*S*,1'*R*,3'*S*)-**23**.

**Ethyl 2'-{(a*S*,1*R*,3*S*,1'*R*,3'*S*)-1-(4-fluorophenyl)-6,7,7',8,8'-pentamethoxy-3,3'-dimethyl-[5,5'-bis-isochroman]-1'-yl}acetate [(a*S*,1*R*,3*S*,1'*R*,3'*S*)-23]**

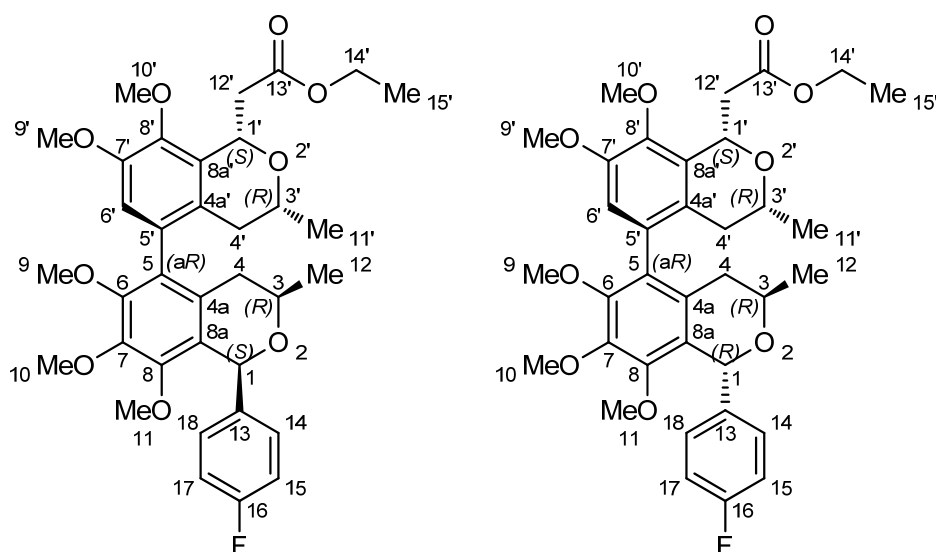




Starting from (aS,1*R*,3*S*,2'*S*)-**20** (140 mg, 0.27 mmol, 1.0 equiv.) using **method C**: anhydrous toluene (3 ml), ethyl-3,3-diethoxypropionate (90%, technical grade, 115  $\mu$ l = 103  $\mu$ l, 101 mg, 0.53 mmol, 2.0 equiv.),  $\text{BF}_3 \cdot \text{Et}_2\text{O}$  (10  $\mu$ l, 11 mg, 0.08 mmol, 0.3 equiv.), reaction time: 16 hours. (aS,1*R*,3*S*,1'*R*,3'*S*)-**23**: 150 mg (yield: 91%), white amorphous solid foam;  $[\alpha]_{\text{D}}^{20} -36$ ;  $[\alpha]_{578}^{20} -38$ ;  $[\alpha]_{546}^{20} -46$ ;  $[\alpha]_{436}^{20} -111$ ;  $[\alpha]_{365}^{20} -253$  ( $c = 0.48$ ; MeCN); ECD ( $c = 1.41 \times 10^{-4}$  M; MeCN)  $\lambda$  [nm], ( $\Delta\epsilon$ ) = 289 (–2.02), 250sh (–7.82), 225 (–30.99), 201 (30.75). Flash chromatography (hexane/EtOAc 95:5  $\rightarrow$  9:1  $\rightarrow$  85:15  $\rightarrow$  8:2);  $R_f = 0.55$  (hexane/EtOAc 75:25);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  = 7.38 – 7.32 (m, 2H, *H*-14, *H*-18), 7.07 – 7.00 (m, 2H, *H*-15, *H*-17), 6.69 (s, 1H, *H*-6'), 5.82 (s, 1H, *H*-1), 5.44 (dd,  $J = 8.4, 3.2$  Hz, 1H, *H*-1'), 4.20 (qd,  $J = 7.1, 1.2$  Hz, 2H, *H*-14'), 3.92 (s, 3H, *H*-10'), 3.88 (s, 3H, *H*-9'), 3.80 (s, 3H, *H*-10), 3.73 – 3.64 (m, 1H, *H*-3), 3.63 – 3.56 (m, 1H, *H*-3'), 3.55 (s, 3H, *H*-9), 3.29 (dd,  $J = 15.1, 3.3$  Hz, 1H, *H*-12'-a), 3.15 (s, 3H, *H*-11), 2.64 (dd,  $J = 15.1, 8.3$  Hz, 1H, *H*-12'-b), 2.49 – 2.38 (m, 2H, *H*-4<sub>ax</sub>, *H*-4'<sub>ax</sub>), 1.99 – 1.91 (m, 1H, *H*-4<sub>eq</sub>), 1.95 – 1.89 (m, 1H, *H*-4'<sub>eq</sub>), 1.28 (t,  $J = 7.1$  Hz, 3H, *H*-15'), 1.23 (d,  $J = 6.1$  Hz, 3H, *H*-12), 1.20 (d,  $J = 6.1$  Hz, 3H, *H*-11');  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  = 172.0 (1C, *C*-13'), 162.2 (d,  $J_{\text{C-F}} = 245.3$  Hz, 1C, *C*-16), 151.1 (1C, *C*-6), 150.1 (1C, *C*-7'), 149.7 (1C, *C*-8), 144.6 (1C, *C*-8'), 144.5 (1C, *C*-7), 140.1 (d,  $J_{\text{C-F}} = 2.8$  Hz, 1C, *C*-13), 130.6 (1C, *C*-5'), 130.3 (1C, *C*-8a'), 130.1 (d,  $J_{\text{C-F}} = 8.0$  Hz, 2C, *C*-14, *C*-18), 129.1 (1C, *C*-4a), 128.4 (1C, *C*-5), 127.6 (1C, *C*-4a'), 126.6 (1C, *C*-8a), 115.0 (d,  $J_{\text{C-F}} = 21.4$  Hz, 2C, *C*-15, *C*-17), 113.3 (1C, *C*-6'), 77.5 (1C, *C*-1), 71.6 (1C, *C*-1'), 70.5 (1C, *C*-3), 69.9 (1C, *C*-3'), 60.9 (1C, *C*-9), 60.6 (1C, *C*-10), 60.4 (1C, *C*-10'), 60.2 (1C, *C*-14'), 59.3 (1C, *C*-11), 56.0 (1C, *C*-9'), 42.0 (1C, *C*-12'), 35.6 (1C, *C*-4), 34.5 (1C, *C*-4'), 21.8 (1C, *C*-12), 21.6 (1C, *C*-11'), 14.3 (1C, *C*-15'); IR (KBr)  $\nu$  = 2974, 2936 ( $\nu_{\text{as}}$  Me,  $\nu_{\text{as}}$   $\text{CH}_2$ ), 2847 ( $\nu_{\text{s}}$   $\text{CH}_2$ ), 1737 ( $\nu$  C=O), 1605, 1576, 1510, 1486, 1462, 1420 ( $\nu$  Ar C=C,  $\beta_{\text{s}}$   $\text{CH}_2$ ,  $\delta_{\text{as}}$  Me), 1383, 1359, 1315 ( $\delta_{\text{s}}$  Me,  $\delta$  CH,  $\gamma_{\text{s}}$   $\text{CH}_2$ ), 1279,

1256, 1224, 1154, 1117 ( $\nu_{\text{as}}$  Ar-O-Me,  $\nu$  Ar C-F,  $\nu_{\text{as}}$  C-O-C=O), 1072, 1029 ( $\nu_{\text{as}}$  C-O-C,  $\nu_{\text{s}}$  Ar-O-Me,  $\nu_{\text{s}}$  C-O-C=O)  $\text{cm}^{-1}$ ; ESI-TOF-HRMS:  $m/z$  calculated for  $\text{C}_{35}\text{H}_{41}\text{FNaO}_9$   $[\text{M}+\text{Na}]^+$  647.2627, found 647.2619.

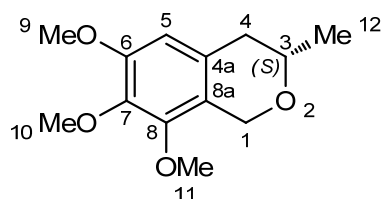
**Ethyl 2'-{(a*R*,1*S*,3*R*,1'*S*,3'*R*)-1-(4-fluorophenyl)-6,7,7',8,8'-pentamethoxy-3,3'-dimethyl-[5,5'-bis-isochroman]-1'-yl}acetate [(a*R*,1*S*,3*R*,1'*S*,3'*R*)-23]** and **ethyl 2'-{(a*R*,1*R*,3*R*,1'*S*,3'*R*)-1-(4-fluorophenyl)-6,7,7',8,8'-pentamethoxy-3,3'-dimethyl-[5,5'-bis-isochroman]-1'-yl}acetate [(a*R*,1*R*,3*R*,1'*S*,3'*R*)-23]**



(a*S*,1*S*,3*S*,2'*S*)-**20** (100 mg, 0.19 mmol, 1.0 equiv.) was dissolved in anhydrous toluene (2 ml), and the solution was cooled to 0 °C. Then ethyl-3,3-diethoxypropionate (90%, technical grade, 82  $\mu\text{l}$  = 74  $\mu\text{l}$ , 72 mg, 0.38 mmol, 2.0 equiv.) and  $\text{BF}_3 \cdot \text{Et}_2\text{O}$  (7  $\mu\text{l}$ , 8 mg, 0.06 mmol, 0.3 equiv.) were added to the solution, and the reaction was allowed to warm up to room temperature. After two days, another portion of  $\text{BF}_3 \cdot \text{Et}_2\text{O}$  (4  $\mu\text{l}$ , 4 mg, 0.03 mmol, 0.15 equiv.) was added to the reaction mixture. The temperature was raised to 60 °C. After stirring 4.5 hours, the reaction was allowed to cool down to room temperature. The reaction was quenched with a saturated solution of  $\text{NaHCO}_3$  and stirred for 10 minutes.  $\text{EtOAc}$  was added to the mixture and the layers were separated. The organic layer was extracted twice with a saturated solution of  $\text{NaHCO}_3$  and once with brine. The organic phase was dried over anhydrous  $\text{Na}_2\text{SO}_4$ , filtered, and the solvent was evaporated in *vacuo*. The residue was purified by flash chromatography to yield the chiral non-racemic isochroman target derivative. (a*R*,1*S*,3*R*,1'*S*,3'*R*)-**23**: 34 mg (yield: 30%), white amorphous solid foam;  $[\alpha]_{\text{D}}^{20} +27$ ;  $[\alpha]_{578}^{20} +28$ ;  $[\alpha]_{546}^{20} +35$ ;  $[\alpha]_{436}^{20} +52$ ;  $[\alpha]_{365}^{20} +205$  ( $c = 0.39$ ; MeCN); ECD ( $c = 1.81 \times 10^{-4}$  M; MeCN)  $\lambda$  [nm], ( $\Delta\epsilon$ ) = 289 (1.57), 250sh (6.47), 225 (25.77), 202 (−28.36).

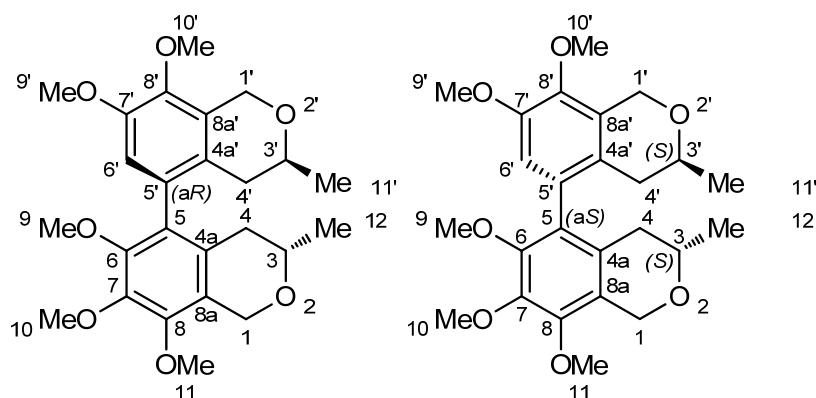
Epimerization of C-1 caused by  $\text{BF}_3 \cdot \text{Et}_2\text{O}$  also resulted in (*aR*,1*R*,3*R*,1'*S*,3'*R*)-**23**: (38 mg, yield: 33%) as white amorphous solid foam. Chromatographic and spectral data except for the chiroptical ones were identical with those of the corresponding enantiomers (*aS*,1*R*,3*S*,1'*R*,3'*S*)-**23** and (*aS*,1*S*,3*S*,1'*R*,3'*S*)-**23**.

**(*S*)-6,7,8-trimethoxy-3-methylisochroman [(*S*)-24]**



Starting from (*S*)-**16** (600 mg, 2.65 mmol, 1.0 equiv.) using **method A**: anhydrous  $\text{Et}_2\text{O}$  (20 ml),  $\text{MOMCl}$  (1.01 ml, 1.07 g, 13.26 mmol, 5.0 equiv.), annealed  $\text{ZnCl}_2$  (109 mg, 0.80 mmol, 0.3 equiv.), reaction time: 2 hours. (*S*)-**24**: 575 mg (yield: 91%), colorless syrup;  $[\alpha]_{\text{D}}^{20} +112$  ( $c = 0.33$ ;  $\text{CHCl}_3$ ). Flash chromatography (hexane/ $\text{EtOAc}$  95:5  $\rightarrow$  93:7  $\rightarrow$  9:1);  $R_f = 0.74$  (hexane/ $\text{EtOAc}$  6:4);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta = 6.39$  (s, 1H, *H*-5), 4.88 (d,  $J = 15.3$  Hz, 1H, *H*-1-*a*), 4.62 (d,  $J = 15.3$  Hz, 1H, *H*-1-*b*), 3.86, 3.83, 3.82 (3s, 3x 3H, *H*-9, *H*-10, *H*-11), 3.78 – 3.65 (m, 1H, *H*-3), 2.59 (d,  $J = 6.8$  Hz, 2H, *H*-4), 1.33 (d,  $J = 6.2$  Hz, 3H, *H*-12);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta = 152.2$ , 149.2, 139.9, 129.1, 120.4 (5C, *C*-4*a*, *C*-8*a*, *C*-6, *C*-7, *C*-8), 107.2 (1C, *C*-5), 70.5 (1C, *C*-3), 64.4 (1C, *C*-1), 60.8, 60.4, 55.9 (3C, *C*-10, *C*-11, *C*-12), 35.5 (1C, *C*-4), 21.5 (1C, *C*-9); IR (KBr)  $\nu = 2969$ , 2936 ( $\nu_{\text{as}}$  Me,  $\nu_{\text{as}}$   $\text{CH}_2$ ), 2837 ( $\nu_{\text{s}}$   $\text{CH}_2$ ), 2017, 1725 ( $\gamma$  Ar =CH,  $\gamma$  Ar C=C overtone and combination bands), 1605, 1589, 1495, 1463 ( $\nu$  Ar C=C,  $\beta_{\text{s}}$   $\text{CH}_2$ ,  $\delta_{\text{as}}$  Me), 1383, 1365, 1336 ( $\delta_{\text{s}}$  Me,  $\delta$  CH), 1263, 1244, 1223 ( $\nu_{\text{as}}$  Ar-O-Me), 1091 ( $\nu_{\text{as}}$  C-O-C), 1050, 1031 ( $\nu_{\text{s}}$  Ar-O-Me), 866 (1,2,3,4,5-pentasubstituted  $\gamma_{\text{s}}$  Ar =CH)  $\text{cm}^{-1}$ ; ESI-TOF-HRMS:  $m/z$  calculated for  $\text{C}_{13}\text{H}_{18}\text{NaO}_4$   $[\text{M}+\text{Na}]^+$  261.1097, found 261.1096.

**(*aR*,3*S*,3'*S*)-6,7,7',8,8'-pentamethoxy-3,3'-dimethyl-5,5'-bis-isochroman [(*aR*,3*S*,3'*S*)-28]**  
**and (*aS*,3*S*,3'*S*)-6,7,7',8,8'-pentamethoxy-3,3'-dimethyl-5,5'-bis-isochroman [(*aS*,3*S*,3'*S*)-28]**



Starting from the mixture of (*aR*,3*S*,2'*S*)-**27** and (*aS*,3*S*,2'*S*)-**27** (136 mg, 0.32 mmol, 1.0 equiv.) using **method A**: anhydrous Et<sub>2</sub>O (5 ml), MOMCl (185  $\mu$ l, 196 mg, 2.44 mmol, 7.7 equiv.), annealed ZnCl<sub>2</sub> (13 mg, 0.10 mmol, 0.3 equiv.), reaction time: 4 hours. The mixture of (*aR*,3*S*,2'*S*)-**28** and (*aS*,3*S*,3'*S*)-**28**: 120 mg, (yield: 86%), yellow syrup. Flash chromatography (hexane/EtOAc 85:15  $\rightarrow$  8:2  $\rightarrow$  7:3); *R<sub>f</sub>* = 0.24 (hexane/EtOAc 8:2); ESI-TOF-HRMS: *m/z* calculated for C<sub>25</sub>H<sub>32</sub>NaO<sub>7</sub> [M+Na]<sup>+</sup> 467.2040, found 467.2040. The atropdiastereomers were separated by preparative chiral HPLC using Chiralpak IC column with isocratic elution (hexane/*i*-PrOH 85:15).

(*aR*,3*S*,3'*S*)-**28**: *t<sub>R</sub>* = 12.29 min [ $\alpha$ ]<sub>D</sub><sup>20</sup> +57; [ $\alpha$ ]<sub>578</sub><sup>20</sup> +60; [ $\alpha$ ]<sub>546</sub><sup>20</sup> +68; [ $\alpha$ ]<sub>436</sub><sup>20</sup> +123; [ $\alpha$ ]<sub>365</sub><sup>20</sup> +197 (*c* = 0.45; MeCN); ECD (*c* = 2.66 $\times$ 10<sup>-4</sup> M; MeCN)  $\lambda$  [nm], ( $\Delta\epsilon$ ) = 289 (−0.07), 268 (0.09), 239 (−1.45), 228sh (−1.36), 204 (34.79); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  = 6.56 (s, 1H, *H*-6'), 5.05 (d, *J* = 15.8 Hz, 1H, *H*-1'*eq*), 4.98 (d, *J* = 15.6 Hz, 1H, *H*-1'*eq*), 4.77 (d, *J* = 15.8 Hz, 1H, *H*-1'*ax*), 4.68 (d, *J* = 15.6 Hz, 1H, *H*-1'*ax*), 3.93 (s, 3H, *H*-11), 3.92 (s, 3H, *H*-10), 3.87 (s, 3H, *H*-10'), 3.82 (s, 3H, *H*-9'), 3.74 – 3.63 (m, 2H, *H*-3, *H*-3'), 3.62 (s, 3H, *H*-9), 2.27 – 2.01 (m, 3H, *H*-4<sub>eq</sub>, *H*-4'), 2.06 (dd, *J* = 17.1, 10.4 Hz, 1H, *H*-4<sub>ax</sub>) 1.25 (d, *J* = 6.2 Hz, 3H, *H*-11'), 1.22 (d, *J* = 6.3 Hz, 3H, *H*-12); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  = 149.9 (1C, *C*-7'), 149.7 (1C, *C*-6), 148.7 (1C, *C*-8), 143.9 (1C, *C*-7), 143.7 (1C, *C*-8'), 131.4 (1C, *C*-5'), 129.4 (1C, *C*-5), 128.8 (1C, *C*-8a'), 128.5 (1C, *C*-4a), 125.7 (1C, *C*-4a'), 124.0 (1C, *C*-8a), 112.4 (1C, *C*-6'), 70.8 (2C, *C*-3, *C*-3'), 65.0 (1C, *C*-1'), 64.7 (1C, *C*-1), 61.1 (1C, *C*-9), 61.0 (1C, *C*-10), 60.6 (1C, *C*-11), 60.3 (1C, *C*-10'), 56.0 (1C, *C*-9'), 33.6 (1C, *C*-4'), 33.4 (1C, *C*-4), 21.7 (2C, *C*-11', *C*-12); IR (KBr)  $\nu$  = 3051 ( $\nu$  Ar =CH), 2967, 2934 ( $\nu_{as}$  Me,  $\nu_{as}$  CH<sub>2</sub>), 2893, 2839 ( $\nu_s$  Me,  $\nu_s$  CH<sub>2</sub>,  $\nu$  CH), 1958, 1733 ( $\gamma$  Ar =CH,  $\gamma$  Ar C=C overtone and combination bands), 1598, 1579, 1489, 1466, 1422, 1408 ( $\nu$  Ar C=C,  $\beta_s$  CH<sub>2</sub>,  $\delta_{as}$  Me), 1384, 1362, 1314 ( $\delta_s$  Me,  $\delta$  CH,  $\gamma_s$  CH<sub>2</sub>), 1280, 1258, 1233, 1215 ( $\nu_{as}$  Ar-O-Me), 1131, 1114, 1083 ( $\nu_{as}$  C-O-C,  $\nu_s$  Ar-O-Me), 869 (1,2,3,4,5-pentasubstituted  $\gamma_s$  Ar =CH) cm<sup>-1</sup>.

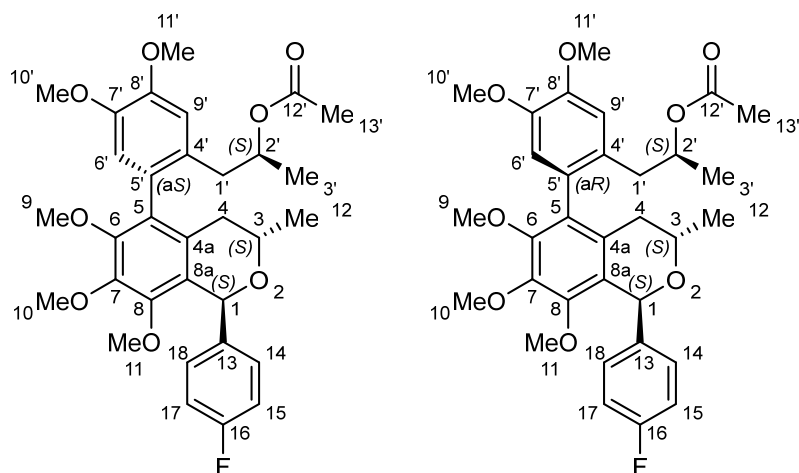
(*aS*,3*S*,3'*S*)-**28**: *t<sub>R</sub>* = 14.33 min; [ $\alpha$ ]<sub>D</sub><sup>20</sup> +69; [ $\alpha$ ]<sub>578</sub><sup>20</sup> +72; [ $\alpha$ ]<sub>546</sub><sup>20</sup> +82; [ $\alpha$ ]<sub>436</sub><sup>20</sup> +135; [ $\alpha$ ]<sub>365</sub><sup>20</sup> +196 (*c* =

0.44; MeCN); ECD ( $c = 2.87 \times 10^{-4}$  M; MeCN)  $\lambda$  [nm], ( $\Delta\epsilon$ ) = 287 (−0.81), 242sh (−4.11), 227 (−6.99), 201 (35.19);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  = 6.57 (s, 1H,  $H-6'$ ), 5.05 (d,  $J = 15.8$  Hz, 1H,  $H-1'_{eq}$ ), 4.97 (d,  $J = 15.5$  Hz, 1H,  $H-1_{eq}$ ), 4.76 (d,  $J = 15.8$  Hz, 1H,  $H-1'_{ax}$ ), 4.69 (d,  $J = 15.5$  Hz, 1H,  $H-1_{ax}$ ), 3.93 (s, 3H,  $H-11$ ), 3.91 (s, 3H,  $H-10$ ), 3.88 (s, 3H,  $H-10'$ ), 3.81 (s, 3H,  $H-9'$ ), 3.72 – 3.57 (m, 2H,  $H-3'$ ,  $H-3$ ), 3.58 (s, 3H,  $H-9$ ), 2.37 (dd,  $J = 16.4, 10.7$  Hz, 1H,  $H-4'_{ax}$ ), 2.25 (dd,  $J = 16.8, 10.6$  Hz, 1H,  $H-4_{ax}$ ), 2.03 (dd,  $J = 16.5, 2.3$  Hz, 1H,  $H-4'_{eq}$ ), 1.94 (dd,  $J = 16.9, 2.0$  Hz, 1H,  $H-4_{eq}$ ), 1.25 (d,  $J = 5.9$  Hz, 3H,  $H-11'$ ), 1.24 (d,  $J = 5.9$  Hz, 3H,  $H-12$ );  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  = 150.4 (1C,  $C-6$ ), 149.9 (1C,  $C-7'$ ), 148.7 (1C,  $C-8$ ), 143.9 (1C,  $C-7$ ), 143.7 (1C,  $C-8'$ ), 131.2 (1C,  $C-5'$ ), 129.1 (1C,  $C-5$ ), 128.6 (1C,  $C-8a'$ ), 127.7 (1C,  $C-4a$ ), 125.5 (1C,  $C-4a'$ ), 123.8 (1C,  $C-8a$ ), 112.7 (1C,  $C-6'$ ), 70.9 (1C,  $C-3$ ), 70.8 (1C,  $C-3'$ ), 64.9 (2C,  $C-1'$ ,  $C-1$ ), 61.1 (1C,  $C-9$ ), 61.0 (1C,  $C-10$ ), 60.6 (1C,  $C-11$ ), 60.3 (1C,  $C-10'$ ), 56.0 (1C,  $C-9'$ ), 34.6 (1C,  $C-4$ ), 33.6 (1C,  $C-4'$ ), 21.8 (1C,  $C-12$ ), 21.7 (1C,  $C-11'$ ); IR (KBr)  $\nu$  = 3051 ( $\nu$  Ar =CH), 2967, 2934 ( $\nu_{as}$  Me,  $\nu_{as}$  CH<sub>2</sub>), 2839 ( $\nu_s$  CH<sub>2</sub>), 1956, 1731 ( $\gamma$  Ar =CH,  $\gamma$  Ar C=C overtone and combination bands), 1598, 1579, 1489, 1465, 1421 ( $\nu$  Ar C=C,  $\beta_s$  CH<sub>2</sub>,  $\delta_{as}$  Me), 1383, 1362, 1314 ( $\delta_s$  Me,  $\delta$  CH,  $\gamma_s$  CH<sub>2</sub>), 1280, 1258, 1233 ( $\nu_{as}$  Ar-O-Me), 1131, 1113, 1084, 1062, 1035 ( $\nu_{as}$  C-O-C,  $\nu_s$  Ar-O-Me), 865 (1,2,3,4,5-pentasubstituted  $\gamma_s$  Ar =CH)  $\text{cm}^{-1}$ .

## 2.2.6. General procedure for the Suzuki coupling reaction of chiral non-racemic 1-[(2-pinacolatoboryl)aryl]propan-2-yl acetate and 5-iodoisochoroman derivatives

To the solution of the 5-iodoisochoroman derivative (1.0 equiv.) in anhydrous DMF (2–22 ml), phosphine ligand (**method D**: SPhos, 0.2 equiv.; **method E**: (*S*)-BINAP, 0.1 equiv.; **method F**: Xantphos, 0.1 equiv.) and  $\text{Pd}(\text{OAc})_2$  (0.1 equiv.) were added under Ar or  $\text{N}_2$  atmosphere, and the solution was stirred for 1 hour with inert gas bubbling at room temperature. To the solution of the 1-[(2-pinacolatoboryl)aryl]propan-2-yl acetate (1.2 equiv.) in anhydrous DMF (2–14 ml), CsF (4.0 equiv.) was added under Ar or  $\text{N}_2$  atmosphere, and the solution was stirred for 0.5 hour with inert gas bubbling at room temperature. The first solution was merged with the second, and the mixture was stirred at 150 °C. When the 5-iodoisochoroman derivative was consumed (1.5–3 hours) on the basis of TLC monitoring, the reaction mixture was poured on ice and diluted with  $\text{Et}_2\text{O}$  and the mixture was filtered on a short pad of Celite. The Celite was washed with  $\text{Et}_2\text{O}$ . The two layers were separated in a separatory funnel. The aqueous phase was extracted twice with  $\text{Et}_2\text{O}$ . The combined organic layers were washed twice with brine. The organic phase was dried over anhydrous  $\text{Na}_2\text{SO}_4$ , filtered, and the solvent was evaporated *in vacuo*. The residue was purified by flash chromatography to yield the 1-[2-(6,7,8-trimethoxy-3-methylisochoroman-5-yl)-4,5-dimethoxyphenyl]propan-2-yl acetate target derivative.

**(2S)-1-{2-[(aS,1S,3S)-1-(4-fluorophenyl)-6,7,8-trimethoxy-3-methylisochroman-5-yl]-4,5-dimethoxyphenyl}propan-2-yl acetate and (2S)-1-{2-[(aR,1S,3S)-1-(4-fluorophenyl)-6,7,8-trimethoxy-3-methylisochroman-5-yl]-4,5-dimethoxyphenyl}propan-2-yl acetate [the mixture of (aR,1S,3S,2'S)-19 and (aS,1S,3S,2'S)-19]**



Starting from *trans*-(1S,3S)-**18** (255 mg, 0.56 mmol, 1.0 equiv.) using **method D**: anhydrous DMF (2.5 ml), SPhos (46 mg, 0.11 mmol, 0.2 equiv.), Pd(OAc)<sub>2</sub> (13 mg, 0.06 mmol, 0.1 equiv.), (*S*)-**8** (243 mg, 0.67 mmol, 1.2 equiv.), anhydrous DMF (2 ml), CsF (338 mg, 2.23 mmol, 4.0 equiv.), reaction time: 2 hours. The mixture of (aR,1S,3S,2'S)-**19** and (aS,1S,3S,2'S)-**19**: 209 mg (yield: 66%, *dr* 1.0:1.2) pale brown amorphous solid foam.

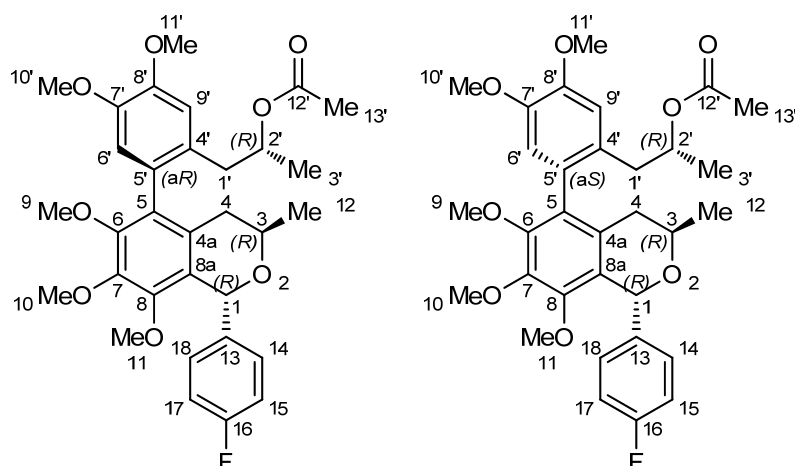
Starting from *trans*-(1S,3S)-**18** (152 mg, 0.33 mmol, 1.0 equiv.) with **method E**: anhydrous DMF (2 ml), (*S*)-BINAP (21 mg, 0.03 mmol, 0.1 equiv.), Pd(OAc)<sub>2</sub> (7 mg, 0.03 mmol, 0.1 equiv.), (*S*)-**8** (145 mg, 0.40 mmol, 1.2 equiv.), anhydrous DMF (2.5 ml), CsF (201 mg, 1.32 mmol, 4.0 equiv.), reaction time: 2 hours. The mixture of (aR,1S,3S,2'S)-**19** and (aS,1S,3S,2'S)-**19**: 102 mg (yield: 54%, *dr* 1.0:1.7) pale brown amorphous solid foam.

Starting from *trans*-(1S,3S)-**18** (815 mg, 1.78 mmol, 1.0 equiv.) with **method F**: anhydrous DMF (5 ml), Xantphos (103 mg, 0.18 mmol, 0.1 equiv.), Pd(OAc)<sub>2</sub> (40 mg, 0.18 mmol, 0.1 equiv.), (*S*)-**8** (778 mg, 2.14 mmol, 1.2 equiv.), anhydrous DMF (3 ml), CsF (1.08 g, 7.12 mmol, 4.0 equiv.), reaction time: 1.5 hours. The mixture of (aR,1S,3S,2'S)-**19** and (aS,1S,3S,2'S)-**19**: 797 mg (yield: 79%, *dr* 1.0:1.4) pale brown amorphous solid foam.

Flash chromatography (hexane/EtOAc 85:15 → 8:2 → 75:25 → 7:3); *R*<sub>f</sub> = 0.27 (hexane/EtOAc 75:25); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ = 7.30 – 7.14 [2m, 2 x 2H, (aR), (aS) *H*-14, *H*-18], 7.08 – 6.96 [2m, 2 x 2H, (aR), (aS) *H*-15, *H*-17], 6.91, 6.85 [2s, 2 x 1H, (aR), (aS) *H*-9'], 6.65, 6.62 [2s, 2 x 1H, (aR), (aS) *H*-6'], 6.04, 6.03 [2s, 2 x 1H, (aR), (aS) *H*-1], 5.21 – 5.08 [m, 1H, (aR) or (aS) *H*-2'], 4.89 – 4.76 [m, 1H, (aR) or (aS) *H*-2'], 3.94, 3.93, 3.89, 3.86, 3.71, 3.65, 3.57,

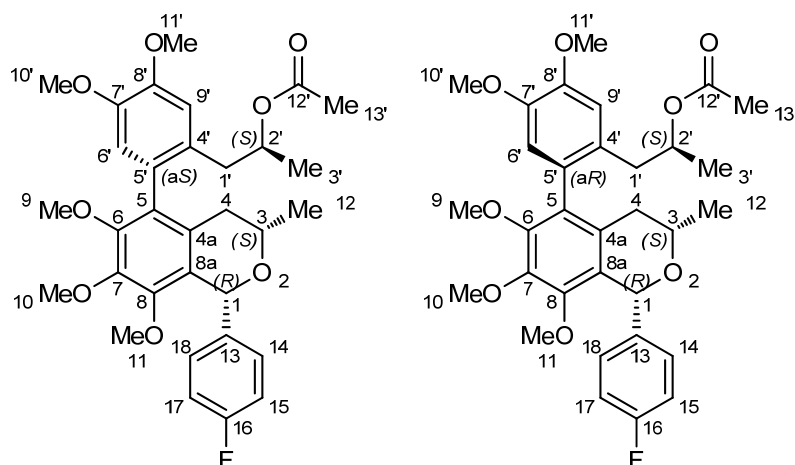
3.55 [10s, 10 x 3H, (aR), (aS) *H-11*, *H-10'*, *H-10*, *H-11'*, *H-9*], 3.69 – 3.62 [2m, 2 x 1H, (aR), (aS) *H-3*], 2.67, 2.55, 2.32, 2.24, 2.21, 2.05, 2.02 [dd,  $J = 14.1$ , 7.4 Hz, 1H, dd,  $J = 13.8$ , 8.0 Hz, 1H, dd,  $J = 13.8$ , 5.8 Hz, 1H, dd,  $J = 14.1$ , 6.4 Hz, 1H, dd,  $J = 17.8$ , 10.2 Hz, 1H, dd,  $J = 17.8$ , 2.5 Hz, 1H, dd,  $J = 17.9$ , 4.3 Hz, 1H, dd,  $J = 17.9$ , 9.8 Hz, 1H, (aR), (aS) *H-1'-a,b*, *H-4-a,b*], 1.99, 1.95 [2s, 2 x 3H, (aR), (aS) *H-13'*], 1.10 [d,  $J = 6.2$  Hz, 3H, (aR) or (aS) *H-12*], 1.08 [d,  $J = 6.1$  Hz, 3H, (aR) or (aS) *H-12*], 1.06 [d,  $J = 5.8$  Hz, 2 x 3H, (aR), (aS) *H-3'*];  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta = 170.5$ , 170.0 [2C, (aR), (aS) *C-12'*], 162.3 [d,  $J_{\text{C-F}} = 245.8$  Hz, 2C, (aR), (aS), *C-16*], 151.1, 150.8 [2C, (aR), (aS) *C-6*], 149.4 [2C, (aR), (aS) *C-8*], 148.2, 147.9 [2C, (aR), (aS) *C-7'*], 147.4, 147.2 [2C, (aR), (aS) *C-8'*], 144.2, 143.9 [2C, (aR), (aS) *C-7*], 138.3 [2C, (aR), (aS) *C-13*], 130.4, 130.3 [2d,  $J_{\text{C-F}} = 7.8$  Hz, 4C, (aR), (aS) *C-14*, *C-18*], 129.6, 129.3, 129.1, 128.6, 128.3, 128.2 [8C, (aR), (aS) *C-5'*, *C-4'*, *C-4a*, *C-5*], 124.5, 124.1 [2C, (aR), (aS) *C-8a*], 114.8 [d,  $J = 21.1$  Hz, 4C, (aR), (aS) *C-15*, *C-17*], 113.5, 113.1, 112.8, 112.1 [4C, (aR), (aS) *C-6'*, *C-9'*], 73.5, 73.3, 71.4, 70.6 [4C, (aR), (aS) *C-2'*, *C-3*], 63.3, 63.1 [2C, (aR), (aS) *C-1*], 61.1, 61.0, 60.8, 60.7, 60.1 [6C, (aR), (aS) *C-9*, *C-10*, *C-11*], 56.1, 56.0, 55.9, 55.8 [4C, (aR), (aS) *C-11'*, *C-10'*], 40.1, 38.7 [2C, (aR), (aS) *C-1'*], 34.4, 33.7 [2C, (aR), (aS) *C-4*], 21.7, 21.6, 21.5, 21.3 [4C, (aR), (aS) *C-12*, *C-13'*], 20.1, 19.8 [2C, (aR), (aS) *C-3*]; IR (KBr)  $\nu = 2930$  ( $\nu_{\text{as}} \text{CH}_2$ ), 2850 ( $\nu_{\text{s}} \text{CH}_2$ ), 1735 ( $\nu \text{C=O}$ ), 1604, 1508, 1463, 1422, 1409 ( $\nu \text{Ar C=C}$ ,  $\beta_{\text{s}} \text{CH}_2$ ,  $\delta_{\text{as}} \text{Me}$ ), 1364, 1329 ( $\delta \text{CH}$ ,  $\gamma_{\text{s}} \text{CH}_2$ ,  $\delta_{\text{s}} \text{Me}$ ), 1249, 1158, 1113 ( $\nu_{\text{as}} \text{C-O-C=O}$ ,  $\nu_{\text{as}} \text{Ar-O-Me}$ ,  $\nu \text{Ar C-F}$ ), 1069, 1025 ( $\nu_{\text{as}} \text{C-O-C}$ ,  $\nu_{\text{s}} \text{C-O-C=O}$ ,  $\nu_{\text{s}} \text{Ar-O-Me}$ )  $\text{cm}^{-1}$ ; ESI-TOF-HRMS:  $m/z$  calculated for  $\text{C}_{32}\text{H}_{37}\text{FNaO}_8$   $[\text{M}+\text{Na}]^+$  591.2365, found 591.2364.

**(2R)-1-{2-[(aR,1R,3R)-1-(4-fluorophenyl)-6,7,8-trimethoxy-3-methylisochroman-5-yl]-4,5-dimethoxyphenyl}propan-2-yl acetate and (2R)-1-{2-[(aS,1R,3R)-1-(4-fluorophenyl)-6,7,8-trimethoxy-3-methylisochroman-5-yl]-4,5-dimethoxyphenyl}propan-2-yl acetate [the mixture of (aR,1R,3R,2'R)-19 and (aS,1R,3R,2'R)-19]**



Starting from *trans*-(1*R*,3*R*)-**18** (1.00 g, 2.18 mmol, 1.0 equiv.) using **method F**: anhydrous DMF (6 ml), Xantphos (126 mg, 0.22 mmol, 0.1 equiv.), Pd(OAc)<sub>2</sub> (49 mg, 0.22 mmol, 0.1 equiv.), (*R*)-**8** (954 mg, 2.62 mmol, 1.2 equiv.), anhydrous DMF (4 ml), CsF (1.33 g, 8.73 mmol, 4.0 equiv.), reaction time: 3 hours. The mixture of (*aR*,1*R*,3*R*,2'*R*)-**19** and (*aS*,1*R*,3*R*,2'*R*)-**19**: 899 mg (yield: 73%, *dr* 1.0:1.4) pale brown amorphous solid foam. Chromatographic and spectral data except for the chiroptical ones were identical with those of the mixture of (*aR*,1*S*,3*S*,2'*S*)-**19** and (*aS*,1*S*,3*S*,2'*S*)-**19**.

**(2*S*)-1-{2-[(*aS*,1*R*,3*S*)-1-(4-fluorophenyl)-6,7,8-trimethoxy-3-methylisochroman-5-yl]-4,5-dimethoxyphenyl}propan-2-yl acetate [(*aS*,1*R*,3*S*,2'*S*)-**19**] and (2*S*)-1-{2-[(*aR*,1*R*,3*S*)-1-(4-fluorophenyl)-6,7,8-trimethoxy-3-methylisochroman-5-yl]-4,5-dimethoxyphenyl}propan-2-yl acetate [(*aR*,1*R*,3*S*,2'*S*)-**19**]**



Starting from *cis*-(1*R*,3*S*)-**18** (500 mg, 1.09 mmol, 1.0 equiv.) using **method F**: anhydrous DMF (8 ml) Xantphos (63 mg, 0.11 mmol, 0.1 equiv.), Pd(OAc)<sub>2</sub> (25 mg, 0.11 mmol, 0.1 equiv.), (*S*)-**8** (477 mg, 1.31 mmol, 1.2 equiv.), anhydrous DMF (5 ml), CsF (663 mg, 4.36 mmol, 4.0 equiv.), reaction time: 1.5 hours. (*aS*,1*R*,3*S*,2'*S*)-**19**: 423 mg (yield: 68%) off-white amorphous solid foam; [ $\alpha$ ]<sub>D</sub><sup>20</sup> -110 (*c* = 0.48; CHCl<sub>3</sub>). (*aR*,1*R*,3*S*,2'*S*)-**19**: 69 mg (yield: 11%) yellow amorphous solid foam; [ $\alpha$ ]<sub>D</sub><sup>20</sup> -45 (*c* = 0.14; CHCl<sub>3</sub>). Flash chromatography (hexane/EtOAc 9:1 → 85:15 → 8:2 → 75:25 → 7:3 → 65:35); ESI-TOF-HRMS: *m/z* calculated for C<sub>32</sub>H<sub>37</sub>FN<sub>2</sub>O<sub>8</sub> [M+Na]<sup>+</sup> 591.2365, found 561.2360.

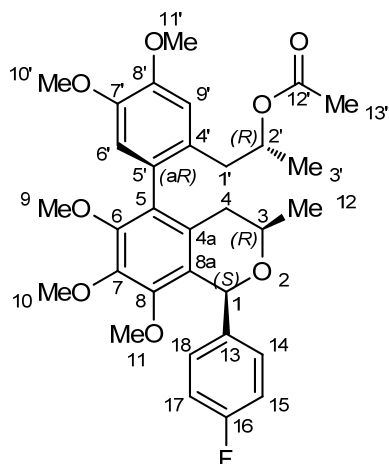
(*aS*,1*R*,3*S*,2'*S*)-**19**: R<sub>f</sub> = 0.31 (hexane/EtOAc 8:2); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  = 7.40 – 7.31 (m, 2H, *H*-14, *H*-18), 7.08 – 6.98 (m, 2H, *H*-15, *H*-17), 6.84 (s, 1H, *H*-9'), 6.67 (s, 1H, *H*-6'), 5.85 (s, 1H, *H*-1), 4.78 – 4.65 (m, 1H, *H*-2'), 3.94 (s, 3H, *H*-11'), 3.90 (s, 3H, *H*-10'), 3.79 (s, 3H, *H*-10), 3.76 – 3.66 (m, 1H, *H*-3), 3.55 (s, 3H, *H*-9), 3.14 (s, 3H, *H*-11), 2.67 – 2.53 (m, 2H, *H*-1'), 2.39 (ddd, *J* = 16.2, 10.7, 1.3 Hz, 1H, *H*-4<sub>ax</sub>), 2.05 (d, *J* = 16.2 Hz, 1H, *H*-4<sub>eq</sub>), 1.93 (s,



3H, *H*-13'), 1.21 (d, *J* = 6.2 Hz, 3H, *H*-12), 1.02 (d, *J* = 6.2 Hz, 3H, *H*-3'); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  = 170.2 (1C, *C*-12'), 162.3 (d, *J*<sub>C-F</sub> = 245.1 Hz, 1C, *C*-16), 150.3 (1C, *C*-6), 149.8 (1C, *C*-8), 148.0 (1C, *C*-8'), 147.4 (1C, *C*-7'), 144.6 (1C, *C*-7), 140.3 (d, *J*<sub>C-F</sub> = 3.0 Hz, 1C, *C*-13), 130.3 (d, *J*<sub>C-F</sub> = 7.9 Hz, 2C, *C*-14, *C*-18), 130.2 (1C, *C*-4a), 129.2 (1C, *C*-4'), 128.8 (1C, *C*-5), 128.2 (1C, *C*-5'), 127.0 (1C, *C*-8a), 115.1 (d, *J*<sub>C-F</sub> = 21.4 Hz, 2C, *C*-15, *C*-17), 113.7 (1C, *C*-6'), 113.4 (1C, *C*-9'), 77.5 (1C, *C*-1), 70.8 (1C, *C*-3), 70.7 (1C, *C*-2'), 61.0 (1C, *C*-9), 60.7 (1C, *C*-10), 59.4 (1C, *C*-11), 56.2 (1C, *C*-10'), 56.0 (1C, *C*-11'), 39.9 (1C, *C*-1'), 35.8 (1C, *C*-4), 21.7 (1C, *C*-12), 21.4 (1C, *C*-13'), 20.3 (1C, *C*-3'); IR (KBr)  $\nu$  = 2974, 2936 ( $\nu_{\text{as}}$  Me,  $\nu_{\text{as}}$  CH<sub>2</sub>), 2845 ( $\nu_{\text{s}}$  CH<sub>2</sub>), 1735 ( $\nu$  C=O), 1606, 1573, 1513, 1462, 1421, 1410 ( $\nu$  Ar C=C,  $\beta_{\text{s}}$  CH<sub>2</sub>,  $\delta_{\text{as}}$  Me), 1371, 1351, 1328 ( $\delta$  CH,  $\gamma_{\text{s}}$  CH<sub>2</sub>,  $\delta_{\text{s}}$  Me), 1251, 1225, 1171, 1154, 1119, 1102 ( $\nu_{\text{as}}$  C-O-C=O,  $\nu_{\text{as}}$  Ar-O-Me,  $\nu$  Ar C-F), 1075, 1051, 1027, 1001 ( $\nu_{\text{as}}$  C-O-C,  $\nu_{\text{s}}$  C-O-C=O,  $\nu_{\text{s}}$  Ar-O-Me), 861 (1,2,4,5-tetrasubstituted  $\gamma_{\text{s}}$  Ar =CH) cm<sup>-1</sup>.

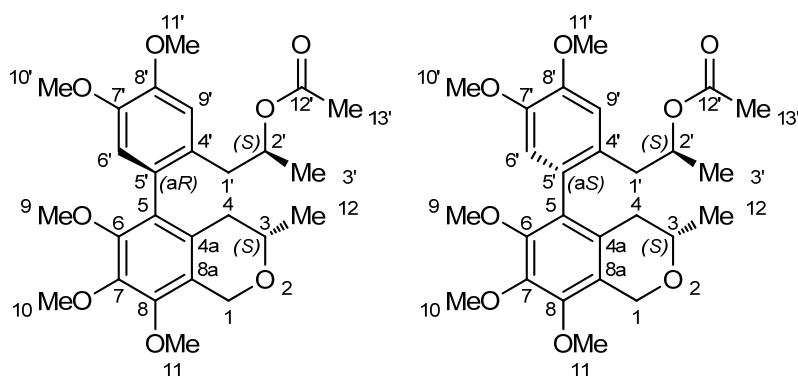
(*aR*,1*R*,3*S*,2'*S*)-**19**: *R*<sub>f</sub> = 0.21 (hexane/EtOAc 8:2); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  = 7.32 – 7.24 (m, 2H, *H*-14, *H*-18), 7.06 – 6.99 (m, 2H, *H*-15, *H*-17), 6.90, 6.62 (2s, 2 x 1H, *H*-6', *H*-9'), 5.84 (s, 1H, *H*-1), 5.18 – 5.08 (m, 1H, *H*-2'), 3.94, 3.86, 3.81, 3.67, 3.20 (5s, 5 x 3H, *H*-9, *H*-10, *H*-11, *H*-10', *H*-11'), 3.78 – 3.71 (m, 1H, *H*-3), 2.39 (dd, *J* = 14.2, 7.7, 1H, *H*-4-a or *H*-1'-a), 2.50 (dd, *J* = 14.2, 6.3 Hz, 1H, *H*-4-b or *H*-1'-b), 2.30 – 2.18 (m, 2H, *H*-4 or *H*-1'), 2.00 (s, 3H, *H*-13'), 1.20, 1.14 (2d, *J* = 6.1 Hz, *J* = 6.2 Hz, 2 x 3H, *H*-12, *H*-3'); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  = 170.5 (1C, *C*-12'), 162.3 (d, *J*<sub>C-F</sub> = 245.4 Hz, 1C, *C*-16), 150.9, 149.7, 148.2, 147.3, 144.6, 130.1, 129.1, 128.9, 128.3, 126.5 (10C, *C*-4a, *C*-5, *C*-6, *C*-7, *C*-8, *C*-8a, *C*-4', *C*-5', *C*-7', *C*-8'), 140.3 (d, *J*<sub>C-F</sub> = 3.0 Hz, 1C, *C*-13), 130.0 (d, *J*<sub>C-F</sub> = 8.1 Hz, 2C, *C*-14, *C*-18), 115.4 (d, *J*<sub>C-F</sub> = 21.4 Hz, 2C, *C*-15, *C*-17), 113.3, 112.3 (2C, *C*-6', *C*-9'), 77.3 (1C, *C*-1), 71.0, 70.4 (2C, *C*-3, *C*-2'), 61.0, 60.5, 59.4, 56.1, 55.9 (5C, *C*-9, *C*-10, *C*-11, *C*-10', *C*-11'), 39.0, 34.8 (3C, *C*-4, *C*-1'), 21.7, 21.5, 20.1 (3C, *C*-12, *C*-3', *C*-13'); IR (KBr)  $\nu$  = 2973, 2936 ( $\nu_{\text{as}}$  Me,  $\nu_{\text{as}}$  CH<sub>2</sub>), 2846 ( $\nu_{\text{s}}$  CH<sub>2</sub>), 1735 ( $\nu$  C=O), 1604, 1575, 1512, 1463, 1421, 1408 ( $\nu$  Ar C=C,  $\beta_{\text{s}}$  CH<sub>2</sub>,  $\delta_{\text{as}}$  Me), 1371, 1352, 1329 ( $\delta$  CH,  $\gamma_{\text{s}}$  CH<sub>2</sub>,  $\delta_{\text{s}}$  Me), 1249, 1172, 1154, 1115 ( $\nu_{\text{as}}$  C-O-C=O,  $\nu_{\text{as}}$  Ar-O-Me,  $\nu$  Ar C-F), 1074, 1050, 1027 ( $\nu_{\text{as}}$  C-O-C,  $\nu_{\text{s}}$  C-O-C=O,  $\nu_{\text{s}}$  Ar-O-Me), 863 (1,2,4,5-tetrasubstituted  $\gamma_{\text{s}}$  Ar =CH) cm<sup>-1</sup>.

**(2*R*)-1-{2-[(*aR*,1*S*,3*R*)-1-(4-fluorophenyl)-6,7,8-trimethoxy-3-methylisochroman-5-yl]-4,5-dimethoxyphenyl}propan-2-yl acetate [(*aR*,1*S*,3*R*,2'*R*)-**19**]**



Starting from *cis*-(1*S*,3*R*)-**18** (1.40 g, 3.06 mmol, 1.0 equiv.) using **method F**: anhydrous DMF (22 ml) Xantphos (177 mg, 0.31 mmol, 0.1 equiv.), Pd(OAc)<sub>2</sub> (69 mg, 0.31 mmol, 0.1 equiv.), (*R*)-**8** (1.34 g, 3.67 mmol, 1.2 equiv.), anhydrous DMF (14 ml), CsF (1.86 g, 12.22 mmol, 4.0 equiv.), reaction time: 3 hours. (*aR*,1*S*,3*R*,2'*R*)-**19**: 983 mg (yield: 57%) off-white amorphous solid foam;  $[\alpha]_D^{20} +90$  ( $c = 0.47$ ; CHCl<sub>3</sub>). Chromatographic and spectral data except for the chiroptical ones were identical with those of (*aS*,1*R*,3*S*,2'*S*)-**19**.

**(2*S*)-1-{2-[(*aR*,3*S*)-6,7,8-trimethoxy-3-methylisochroman-5-yl]-4,5-dimethoxyphenyl}propan-2-yl acetate and (2*S*)-1-{2-[(*aS*,3*S*)-6,7,8-trimethoxy-3-methylisochroman-5-yl]-4,5-dimethoxyphenyl}propan-2-yl acetate [the mixture of (*aR*,3*S*,2'*S*)-**26** and (*aS*,3*S*,2'*S*)-**26**]**



Starting from (*S*)-**25** (415 mg, 1.14 mmol, 1.0 equiv.) using **method D**: anhydrous DMF (4 ml), SPhos (94 mg, 0.23 mmol, 0.2 equiv.), Pd(OAc)<sub>2</sub> (26 mg, 0.11 mmol, 0.1 equiv.), (*S*)-**8** (498 mg, 1.37 mmol, 1.2 equiv.), anhydrous DMF (4 ml), CsF (692 mg, 4.55 mmol, 4.0 equiv.), reaction time: 1.5 hours. The mixture of (*aR*,3*S*,2'*S*)-**26** and (*aS*,3*S*,2'*S*)-**26**: 359 mg (yield: 66%), yellow syrup. Flash chromatography (hexane/acetone 95: 5 → 9:1 → 85:15 → 8:2);  $R_f = 0.46$  (hexane/acetone 7:3); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta = 6.90, 6.84$  [2s, 2 x 1H, (*aR*), (*aS*) *H*-9], 6.60, 6.59 [2s, 2 x 1H, (*aR*), (*aS*) *H*-6], 5.16 – 5.07 [m, 1H, (*aR*) or (*aS*) *H*-2], 5.00, 4.96

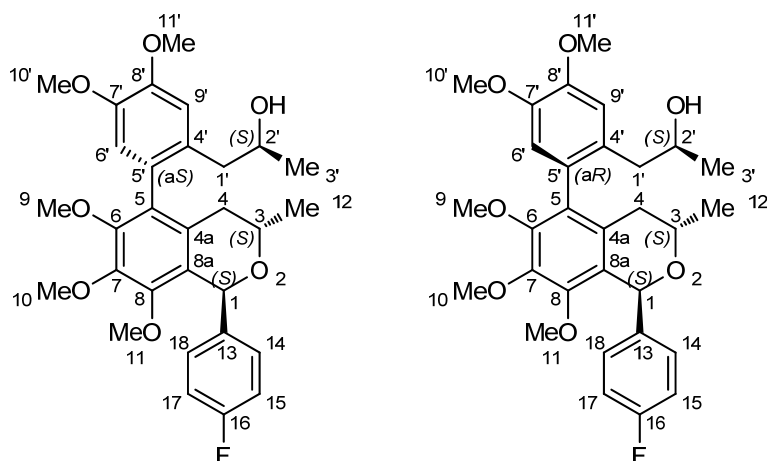
[2d,  $J = 15.4$  Hz, 2 x 1H, (aR), (aS) *H-1-a*], 4.86 – 4.75 [m, 1H, (aR) or (aS) *H-2'*], 4.76 – 4.65 [m, 2 x 1H, (aR), (aS) *H-1-b*], 3.94 [s, 3 x 3H, (aR), (aS) *H-11*, (aR) or (aS) *H-10'*], 3.93 [s, 3H, (aR) or (aS) *H-10'*], 3.91, 3.90 [2s, 2 x 3H, (aR), (aS) *H-10*], 3.85, 3.84 [2s, 2 x 3H, (aR), (aS) *H-11'*], 3.68 [s, 3H, (aR) or (aS) *H-9*], 3.67 – 3.59 [m, 3H, (aR), (aS) *H-3*], 3.56 [s, 3H, (aR), (aS) *H-9*], 2.67 [dd,  $J = 14.1$ , 7.4 Hz, 1H, (aR) or (aS) *H-1'-a*], 2.59 [qd,  $J = 14.1$ , 7.0 Hz, 2H, (aR) or (aS) *H-1'-a,b*], 2.33 [dd,  $J = 14.1$ , 6.4 Hz, 1H, (aR) or (aS) *H-1'-b*], 2.35 – 2.14 [m, 2 x 1H, (aR), (aS) *H-4-a*], 2.08 – 2.01 [m, 2 x 1H, (aR), (aS) *H-4-b*], 1.98, 1.94 [2s, 2 x 3H, (aR), (aS) *H-13'*], 1.22 [2d,  $J = 6.1$  Hz, 2 x 3H, (aR), (aS) *H-12*], 1.08, 1.03 [2d,  $J = 6.2$  Hz, 2 x 3H, (aR), (aS) *H-3'*];  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta = 170.5$ , 170.2 [2C, (aR), (aS) *C-12'*], 150.3, 149.8 [2C, (aR), (aS) *C-6*], 148.6 [2C, (aR), (aS) *C-8*], 148.0, 147.8 [2C, (aR), (aS) *C-7'*], 147.2, 147.1 [2C, (aR), (aS) *C-8'*], 143.8 [2C, (aR), (aS) *C-7*], 129.7, 129.3 [2C, (aR), (aS) *C-5'*], 129.1, 128.8 [2C, (aR), (aS) *C-4'*], 128.5, 128.4 [2C, (aR), (aS) *C-4a*], 128.2, 128.1 [2C, (aR), (aS) *C-5*], 123.9, 123.5 [2C, (aR), (aS) *C-8a*], 113.2, 113.1 [2C, (aR), (aS) *C-6'*], 112.7, 111.9 [2C, (aR), (aS) *C-9'*], 71.3 [1C, (aR) or (aS) *C-2'*], 70.8 [1C, (aR) or (aS) *C-3*], 70.6 [2C, (aR) or (aS) *C-3*, (aR) or (aS) *C-2'*], 64.8, 64.6 [2C, (aR), (aS) *C-1*], 61.0 [2C, (aR), (aS) *C-9*], 60.9, 60.7, 60.5 [4C, (aR), (aS) *C-10*, *C-11*], 55.9 [2C, (aR), (aS) *C-11'*], 55.8 [2C, (aR), (aS) *C-10'*], 39.6, 38.6 [2C, (aR), (aS) *C-1'*], 34.7, 33.7 [2C, (aR), (aS) *C-4*], 21.6, 21.5 [2C, (aR), (aS) *C-12*], 21.4, 21.3 [2C, (aR), (aS) *C-13'*], 20.1, 19.7 [2C, (aR), (aS) *C-3'*]; IR (KBr)  $\nu = 2970$ , 2935 ( $\nu_{\text{as}}$  Me,  $\nu_{\text{as}}$   $\text{CH}_2$ ), 2844 ( $\nu_{\text{s}}$   $\text{CH}_2$ ), 1735 ( $\nu$  C=O), 1606, 1578, 1516, 1465, 1423, 1410 ( $\nu$  Ar C=C,  $\beta_{\text{s}}$   $\text{CH}_2$ ,  $\delta_{\text{as}}$  Me), 1364, 1327 ( $\delta$  CH,  $\gamma_{\text{s}}$   $\text{CH}_2$ ,  $\delta_{\text{s}}$  Me), 1252, 1207, 1174, 1129, 1113 ( $\nu_{\text{as}}$  C-O-C=O,  $\nu_{\text{as}}$  Ar-O-Me), 1072, 1050, 1029 ( $\nu_{\text{as}}$  C-O-C,  $\nu_{\text{s}}$  C-O-C=O,  $\nu_{\text{s}}$  Ar-O-Me), 864 (1,2,4,5-tetrasubstituted  $\gamma_{\text{s}}$  Ar =CH)  $\text{cm}^{-1}$ ; ESI-TOF-HRMS:  $m/z$  calculated for  $\text{C}_{26}\text{H}_{34}\text{NaO}_8$   $[\text{M}+\text{Na}]^+$  497.2146, found 497.2145.

### 2.2.7. General procedure for deacetylation of chiral non-racemic 1-[2-(6,7,8-trimethoxy-3-methylisochroman-5-yl)-4,5-dimethoxyphenyl]propan-2-yl acetate derivatives

The corresponding 1-[2-(6,7,8-trimethoxy-3-methylisochroman-5-yl)-4,5-dimethoxyphenyl]propan-2-yl acetate (1.0 equiv.) was dissolved in a mixture of MeOH:THF:H<sub>2</sub>O. LiOH (2.0 equiv.) was added to the solution and it was stirred at room temperature. When the starting material was consumed (3–4 hours) on the basis of TLC monitoring, the solvent was evaporated in *vacuo*, and the residue was dissolved in  $\text{CH}_2\text{Cl}_2$ . The organic layer was extracted twice with a 10 % aqueous solution of  $\text{NaHSO}_4$ , twice with a saturated aqueous solution of  $\text{NaHCO}_3$  and once with brine. The organic phase was dried over anhydrous  $\text{Na}_2\text{SO}_4$ , filtered, and the solvent was evaporated in *vacuo*. The residue was purified by flash chromatography to yield the 1-[2-

(6,7,8-trimethoxy-3-methylisochroman-5-yl)-4,5-dimethoxyphenyl]propan-2-ol target derivative.

**(2*S*)-1-{2-[(a*S*,1*S*,3*S*)-1-(4-fluorophenyl)-6,7,8-trimethoxy-3-methylisochroman-5-yl]-4,5-dimethoxyphenyl}propan-2-ol [(a*S*,1*S*,3*S*,2'*S*)-20]** and **(2*S*)-1-{2-[(a*R*,1*S*,3*S*)-1-(4-fluorophenyl)-6,7,8-trimethoxy-3-methylisochroman-5-yl]-4,5-dimethoxyphenyl}propan-2-ol [(a*R*,1*S*,3*S*,2'*S*)-20]**



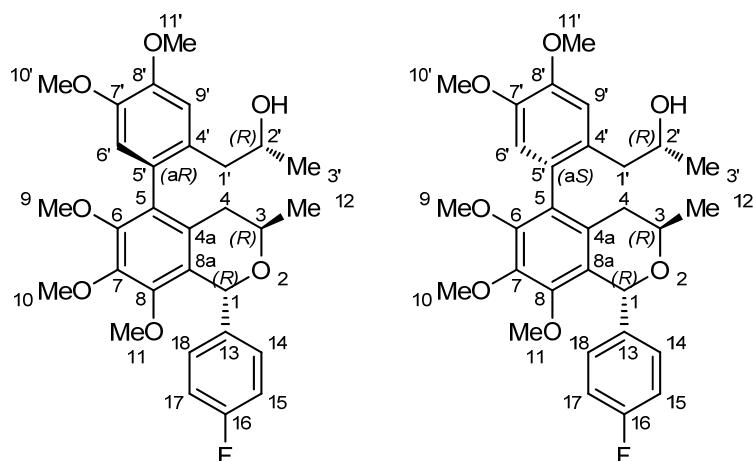
Starting from the mixture of (a*R*,1*S*,3*S*,2'*S*)-**19** and (a*S*,1*S*,3*S*,2'*S*)-**19** (893 mg, 1.57 mmol, 1.0 equiv.), a mixture of MeOH:THF:H<sub>2</sub>O (5:2:3 ml), LiOH (75 mg, 3.14 mmol, 2.0 equiv.), reaction time: 4 hours. (a*S*,1*S*,3*S*,2'*S*)-**20**: 327 mg (yield 40%) off-white amorphous solid foam;  $[\alpha]_D^{20} +36$  ( $c = 0.49$ ; CHCl<sub>3</sub>). (a*R*,1*S*,3*S*,2'*S*)-**20**: 440 mg (yield: 53%) white amorphous solid foam;  $[\alpha]_D^{20} +76$  ( $c = 0.51$ ; CHCl<sub>3</sub>). Flash chromatography (CH<sub>2</sub>Cl<sub>2</sub>/EtOAc 10:0.1 → 10:0.3 → 10:1 → 9:1 → 7:3).

(a*S*,1*S*,3*S*,2'*S*)-**20**:  $R_f = 0.28$  (hexane/EtOAc 6:4); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta = 7.22 - 7.12$  (m, 2H, *H*-14, *H*-18), 7.07 – 6.96 (m, 2H, *H*-15, *H*-17), 6.88 (s, 1H, *H*-9'), 6.63 (s, 1H, *H*-6'), 6.03 (s, 1H, *H*-1), 3.95 (s, 3H, *H*-11'), 3.93 – 3.89 (m, 1H, *H*-2'), 3.88 (s, 3H, *H*-10), 3.86 (s, 3H, *H*-10'), 3.68 (s, 3H, *H*-9), 3.63 (s, 3H, *H*-11), 3.62 – 3.54 (m, 1H, *H*-3), 2.63 (dd,  $J = 13.9$ , 3.2 Hz, 1H, *H*-1'-a), 2.29 (dd,  $J = 13.9$ , 9.4 Hz, 1H, *H*-1'-b), 2.24 (dd,  $J = 17.1$ , 11.0 Hz, 1H, *H*-4<sub>ax</sub>), 2.02 (dd,  $J = 17.1$ , 3.5 Hz, 1H, *H*-4<sub>eq</sub>), 1.16 (d,  $J = 6.1$  Hz, 3H, *H*-3'), 1.06 (d,  $J = 6.1$  Hz, 3H, *H*-12); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta = 162.8$  (d,  $J_{C-F} = 246.1$  Hz, 1C, *C*-16), 150.4 (1C, *C*-6), 149.4 (1C, *C*-8), 148.5 (1C, *C*-8'), 147.5 (1C, *C*-7'), 144.2 (1C, *C*-7), 138.1 (d,  $J_{C-F} = 3.0$  Hz, 1C, *C*-13), 130.2 (d,  $J_{C-F} = 8.0$  Hz, 2C, *C*-14, *C*-18), 129.7 (1C, *C*-4'), 129.6 (1C, *C*-5), 129.0 (1C, *C*-4a), 128.1 (1C, *C*-5'), 124.6 (1C, *C*-8a), 114.9 (d,  $J_{C-F} = 21.3$  Hz, 2C, *C*-15, *C*-17), 113.0 (1C, *C*-6'), 112.7 (1C, *C*-9'), 73.3 (1C, *C*-1), 68.7 (1C, *C*-2'), 63.2 (1C, *C*-3), 61.3 (1C, *C*-9), 61.0 (1C, *C*-10), 60.3 (1C, *C*-11), 56.1 (1C, *C*-10'), 55.9 (1C, *C*-11'), 43.0 (1C, *C*-

1'), 34.4 (1C, C-4), 23.8 (1C, C-3'), 21.7 (1C, C-12); IR (KBr)  $\nu$  = 3461 ( $\nu$  OH), 2967, 2935 ( $\nu_{\text{as}}$  Me,  $\nu_{\text{as}}$  CH<sub>2</sub>), 2843 ( $\nu_{\text{s}}$  CH<sub>2</sub>), 1605, 1577, 1508, 1464, 1421, 1409 ( $\nu$  Ar C=C,  $\beta_{\text{s}}$  CH<sub>2</sub>,  $\delta_{\text{as}}$  Me), 1363, 1330 ( $\delta$  CH,  $\gamma_{\text{s}}$  CH<sub>2</sub>), 1250, 1221, 1199, 1171, 1158, 1110 ( $\nu_{\text{as}}$  Ar-O-Me,  $\nu$  Ar C-F,  $\nu$  C-OH), 1070, 1024 ( $\nu_{\text{as}}$  C-O-C,  $\nu_{\text{s}}$  Ar-O-Me) cm<sup>-1</sup>; ESI-TOF-HRMS:  $m/z$  calculated for C<sub>30</sub>H<sub>35</sub>FN<sub>3</sub>O<sub>7</sub> [M+Na]<sup>+</sup> 549.2259, found 549.2255.

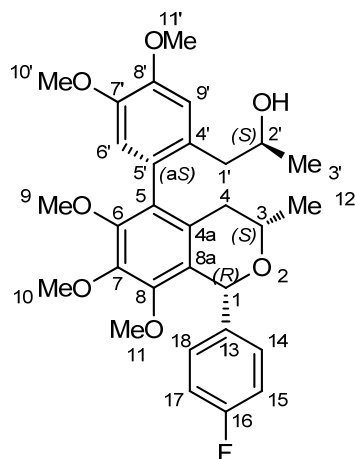
(aR,1S,3S,2'S)-**20**: R<sub>f</sub> = 0.19 (hexane/EtOAc 6:4); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  = 7.30 – 7.20 (m, 2H, H-14, H-18), 7.08 – 6.97 (m, 2H, H-15, H-17), 6.90 (s, 1H, H-9'), 6.64 (s, 1H, H-6'), 6.02 (s, 1H, H-1), 3.94 (s, 3H, H-11'), 3.90 – 3.80 (m, 1H, H-2'), 3.89 (s, 3H, H-10'), 3.84 (s, 3H, H-10), 3.73 (s, 3H, H-9), 3.73 – 3.60 (m, 1H, H-3), 3.53 (s, 3H, H-11), 2.43 (dd,  $J$  = 13.7, 7.7 Hz, 1H, H-1'-a), 2.41 (dd,  $J$  = 13.7, 5.1 Hz, 1H, H-1'-b), 2.23 (dd,  $J$  = 17.0, 3.5 Hz, 1H, H-4<sub>eq</sub>), 2.03 (dd,  $J$  = 17.0, 10.7 Hz, 1H, H-4<sub>ax</sub>), 1.94 (bs, 1H, OH), 1.10 (d,  $J$  = 6.1 Hz, 3H, H-3'), 1.06 (d,  $J$  = 6.1 Hz, 3H, H-12); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  = 162.3 (d,  $J_{\text{C-F}}$  = 245.9 Hz, 1C, C-16), 151.1 (1C, C-6), 149.4 (1C, C-8), 148.1 (1C, C-8'), 147.4 (1C, C-7'), 143.8 (1C, C-7), 138.3 (d,  $J_{\text{C-F}}$  = 2.9 Hz, 1C, C-13), 130.4 (d,  $J_{\text{C-F}}$  = 8.0 Hz, 2C, C-14, C-18), 129.9 (1C, C-4'), 129.8 (1C, C-5), 128.9 (1C, C-4a), 128.3 (1C, C-5'), 124.4 (1C, C-8a), 114.8 (d,  $J_{\text{C-F}}$  = 21.2 Hz, 2C, C-15, C-17), 113.8 (1C, C-9'), 113.2 (1C, C-6'), 73.5 (1C, C-1), 67.5 (1C, C-2'), 63.3 (1C, C-3), 61.2 (1C, C-9), 60.6 (1C, C-10), 60.1 (1C, C-11), 56.2 (1C, C-10'), 55.9 (1C, C-11'), 43.2 (1C, C-1'), 33.7 (1C, C-4), 23.1 (1C, C-3'), 21.6 (1C, C-12); IR (KBr)  $\nu$  = 3430 ( $\nu$  OH), 2966, 2934 ( $\nu_{\text{as}}$  Me,  $\nu_{\text{as}}$  CH<sub>2</sub>), 2843 ( $\nu_{\text{s}}$  CH<sub>2</sub>), 1604, 1578, 1508, 1464, 1421, 1409 ( $\nu$  Ar C=C,  $\beta_{\text{s}}$  CH<sub>2</sub>,  $\delta_{\text{as}}$  Me), 1360, 1330 ( $\delta$  CH,  $\gamma_{\text{s}}$  CH<sub>2</sub>), 1251, 1220, 1158, 1112 ( $\nu_{\text{as}}$  Ar-O-Me,  $\nu$  Ar C-F,  $\nu$  C-OH), 1069, 1026 ( $\nu_{\text{as}}$  C-O-C,  $\nu_{\text{s}}$  Ar-O-Me) cm<sup>-1</sup>; ESI-TOF-HRMS:  $m/z$  calculated for C<sub>30</sub>H<sub>36</sub>FO<sub>7</sub> [M+H]<sup>+</sup> 527.2440, found 527.2431.

**(2R)-1-{2-[(aR,1R,3R)-1-(4-fluorophenyl)-6,7,8-trimethoxy-3-methylisochroman-5-yl]-4,5-dimethoxyphenyl}propan-2-ol [(aR,1R,3R,2'R)-20]** and **(2R)-1-{2-[(aS,1R,3R)-1-(4-fluorophenyl)-6,7,8-trimethoxy-3-methylisochroman-5-yl]-4,5-dimethoxyphenyl}propan-2-ol [(aS,1R,3R,2'R)-20]**



Starting from the mixture of (*aR*,1*R*,3*R*,2'*R*)-**19** and (*aS*,1*R*,3*R*,2'*R*)-**19** (899 mg, 1.58 mmol, 1.0 equiv.), a mixture of MeOH:THF:H<sub>2</sub>O (5:2:3 ml), LiOH (76 mg, 3.16 mmol, 2.0 equiv.), reaction time: 4 hours. (*aR*,1*R*,3*R*,2'*R*)-**20**: 353 mg (yield 42%), off-white amorphous solid foam;  $[\alpha]_D^{20}$   $-48$  ( $c = 0.42$ ; CHCl<sub>3</sub>). (*aS*,1*R*,3*R*,2'*R*)-**20**: 447 mg (yield: 54%), white amorphous solid foam;  $[\alpha]_D^{20}$   $-80$  ( $c = 0.52$ ; CHCl<sub>3</sub>). Chromatographic and spectral data except for the chiroptical ones were identical with those of the mixture of (*aS*,1*S*,3*S*,2'*S*)-**20** and (*aR*,1*S*,3*S*,2'*S*)-**20**.

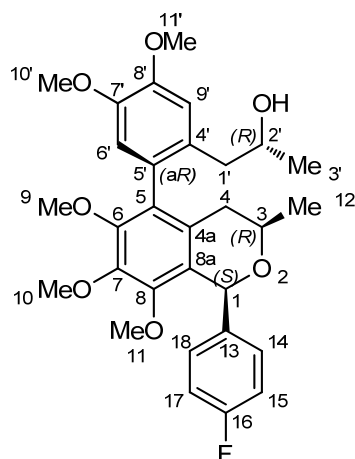
**(2*S*)-1-{2-[(*aS*,1*R*,3*S*)-1-(4-fluorophenyl)-6,7,8-trimethoxy-3-methylisochroman-5-yl]-4,5-dimethoxyphenyl}propan-2-ol [(*aS*,1*R*,3*S*,2'*S*)-**20**]**



Starting from (*aS*,1*R*,3*S*,2'*S*)-**19** (403 mg, 0.71 mmol, 1.0 equiv.), a mixture of MeOH:THF:H<sub>2</sub>O (5:2:3 ml), LiOH (34 mg, 1.42 mmol, 2.0 equiv.), reaction time: 4 hours. (*aS*,1*R*,3*S*,2'*S*)-**20**: 359 mg (yield: 96%), white amorphous solid foam;  $[\alpha]_D^{20}$   $-92$  ( $c = 0.48$ ; CHCl<sub>3</sub>). Flash chromatography (hexane/EtOAc 65:35  $\rightarrow$  6:4  $\rightarrow$  55:45);  $R_f = 0.21$  (hexane/EtOAc 6:4); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta = 7.40 - 7.30$  (m, 2H, *H*-14, *H*-18), 7.09 – 6.98 (m, 2H, *H*-15, *H*-17), 6.88 (s, 1H, *H*-9'), 6.65 (s, 1H, *H*-6'), 5.83 (s, 1H, *H*-1), 4.00 – 3.89

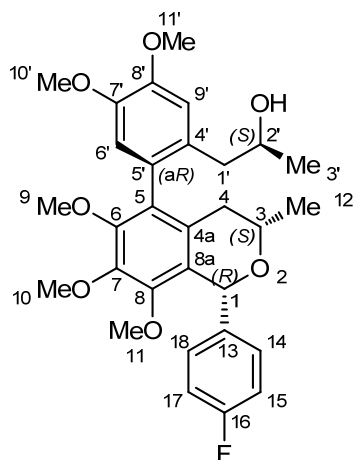
(m), 1H, *H*-2'), 3.95 (s, 3H, *H*-11'), 3.90 (s, 3H, *H*-10'), 3.78 (s, 3H, *H*-10), 3.75 – 3.67 (m, 1H, *H*-3), 3.63 (s, 3H, *H*-9), 3.11 (s, 3H, *H*-11), 2.78 (bs, 1H, OH), 2.58 (dd, *J* = 14.1, 3.1 Hz, 1H, *H*-1'-*a*), 2.36 (ddd, *J* = 16.4, 10.9, 1.4 Hz, 1H, *H*-4<sub>ax</sub>), 2.18 (dd, *J* = 14.1, 9.7 Hz, 1H, *H*-1'-*b*), 2.03 (d, *J* = 16.4 Hz, 1H, *H*-4<sub>eq</sub>), 1.21 (d, *J* = 6.1 Hz, 3H, *H*-12), 1.13 (d, *J* = 6.1 Hz, 3H, *H*-3'); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  = 162.3 (d, *J*<sub>C-F</sub> = 245.2 Hz, 1C, C-16), 149.9, 149.8 (2C, C-6, C-8), 148.6 (1C, C-8'), 147.5 (1C, C-7'), 144.6 (1C, C-7), 140.1 (d, *J*<sub>C-F</sub> = 2.9 Hz, 1C, C-13), 130.2 (d, *J*<sub>C-F</sub> = 8.0 Hz, 2C, C-14, C-18), 130.1, 130.0, 129.1, 128.1, 127.2 (5C, C-4', C-5', C-4a, C-5, C-8a), 115.0 (d, *J*<sub>C-F</sub> = 21.4 Hz, 2C, C-15, C-17), 113.2, 112.3 (2C, C-6', C-9'), 77.5 (1C, C-1), 70.5, 68.6 (2C, C-2', C-3), 61.2 (1C, C-9), 60.8 (1C, C-10), 59.4 (1C, C-11), 56.2 (1C, C-10'), 55.9 (1C, C-11'), 42.7 (1C, C-1'), 35.4 (1C, C-4), 24.0, 21.7 (2C, C-12, C-3'); IR (KBr)  $\nu$  = 3493 ( $\nu$  OH), 2968, 2936 ( $\nu_{\text{as}}$  Me,  $\nu_{\text{as}}$  CH<sub>2</sub>), 2845 ( $\nu_{\text{s}}$  CH<sub>2</sub>), 1606, 1574, 1512, 1462, 1421, 1410 ( $\nu$  Ar C=C,  $\beta_{\text{s}}$  CH<sub>2</sub>,  $\delta_{\text{as}}$  Me), 1352, 1329 ( $\delta$  CH,  $\gamma_{\text{s}}$  CH<sub>2</sub>), 1251, 1222, 1171, 1155, 1118 ( $\nu_{\text{as}}$  Ar-O-Me,  $\nu$  Ar C-F,  $\nu$  C-OH), 1075, 1049, 1026 ( $\nu_{\text{as}}$  C-O-C,  $\nu_{\text{s}}$  Ar-O-Me), 854 (1,2,4,5-tetrasubstituted  $\gamma_{\text{s}}$  Ar =CH) cm<sup>-1</sup>; ESI-TOF-HRMS: *m/z* calculated for C<sub>30</sub>H<sub>35</sub>FNao<sub>7</sub> [M+Na]<sup>+</sup> 549.2259, found 549.2259.

**(2*R*)-1-{2-[(*aR*,1*S*,3*R*)-1-(4-fluorophenyl)-6,7,8-trimethoxy-3-methylisochroman-5-yl]-4,5-dimethoxyphenyl}propan-2-ol [(*aR*,1*S*,3*R*,2'*R*)-20]**



Starting from (*aR*,1*S*,3*R*,2'*R*)-**19** (983 mg, 1.73 mmol, 1.0 equiv.), a mixture of MeOH:THF:H<sub>2</sub>O (12:5:7 ml), LiOH (83 mg, 3.46 mmol, 2.0 equiv.), reaction time: 4 hours. (*aR*,1*S*,3*R*,2'*R*)-**20**: 878 mg (yield: 96%) white amorphous solid foam; [ $\alpha$ ]<sub>D</sub><sup>20</sup> +71 (*c* = 0.31; CHCl<sub>3</sub>). Chromatographic and spectral data except for the chiroptical ones were identical with those of (*aS*,1*R*,3*S*,2'*S*)-**20**.

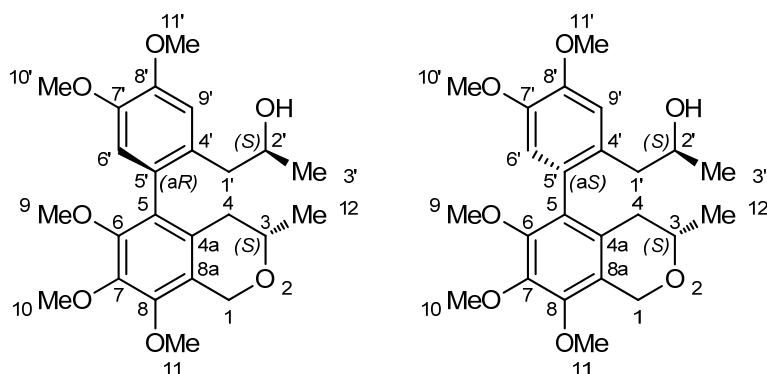
**(2*S*)-1-{2-[(*aR*,1*R*,3*S*)-1-(4-fluorophenyl)-6,7,8-trimethoxy-3-methylisochroman-5-yl]-4,5-dimethoxyphenyl}propan-2-ol [(*aR*,1*R*,3*S*,2'*S*)-20]**



Starting from (*aR*,1*R*,3*S*,2'*S*)-**19** (55 mg, 0.10 mmol, 1.0 equiv.), a mixture of MeOH:THF:H<sub>2</sub>O (1:0.8:0.5 ml), LiOH (5 mg, 0.19 mmol, 2.0 equiv.), reaction time: 4 hours. (*aR*,1*R*,3*S*,2'*S*)-**20**: 48 mg (yield: 94%), off-white amorphous solid foam;  $[\alpha]_{\text{D}}^{20} -36$  ( $c = 0.10$ ; CHCl<sub>3</sub>). Purification was not required for the crude product.  $R_f = 0.29$  (hexane/EtOAc 1:1); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta = 7.28 - 7.21$  (m, 2H, *H*-14, *H*-18), 7.07 – 6.96 (m, 2H, *H*-15, *H*-17), 6.89, 6.65 (2s, 2 x H, *H*-6', *H*-9'), 5.83 (s, 1H, *H*-1), 3.95, 3.87, 3.80, 3.71, 3.21 (5s, 5 x 3H, *H*-9, *H*-10, *H*-11, *H*-10', *H*-11'), 3.86 – 3.81 (m, 1H, *H*-2'), 3.78 – 3.72 (m, 1H, *H*-3), 2.56 (dd,  $J = 13.7, 4.6$  Hz, 1H, *H*-4-*a* or *H*-1'-*a*), 2.49 (dd,  $J = 13.7, 8.3$  Hz, 1H, *H*-4-*b* or *H*-1'-*b*), 2.32 – 2.19 (m, 2H, *H*-4 or *H*-1'), 1.78 (bs, 1H, OH), 1.20, 1.13 (2d,  $J = 6.1$  Hz,  $J = 6.2$  Hz, 2 x 3H, *H*-12, *H*-3'); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta = 162.3$  (d,  $J_{\text{C-F}} = 245.4$  Hz, 1C, C-16), 150.9, 149.7, 148.2, 147.4, 144.5, 129.8, 129.1, 128.4, 126.7 (10C, C-4a, C-5, C-6, C-7, C-8, C-8a, C-4', C-5', C-7', C-8'), 140.2 (d,  $J_{\text{C-F}} = 3.0$  Hz, 1C, C-13), 129.9 (d,  $J_{\text{C-F}} = 8.4$  Hz, 2C, C-14, C-18), 115.2 (d,  $J_{\text{C-F}} = 21.4$  Hz, 2C, C-15, C-17), 113.6, 113.5 (2C, C-6', C-9'), 77.2 (1C, C-1), 70.4, 67.7 (2C, C-3, C-2'), 61.1, 60.5, 59.4, 56.2, 56.0 (5C, C-9, C-10, C-11, C-10', C-11'), 43.3 (1C, C-1'), 34.8 (1C, C-4), 23.2, 21.7 (2C, C-12, C-3'); IR (KBr)  $\nu = 3443$  ( $\nu$  OH), 2967, 2935 ( $\nu_{\text{as}}$  Me,  $\nu_{\text{as}}$  CH<sub>2</sub>), 2847 ( $\nu_{\text{s}}$  CH<sub>2</sub>), 1606, 1577, 1512, 1463, 1422, 1408 ( $\nu$  Ar C=C,  $\beta_{\text{s}}$  CH<sub>2</sub>,  $\delta_{\text{as}}$  Me), 1352, 1330 ( $\delta$  CH,  $\gamma_{\text{s}}$  CH<sub>2</sub>), 1251, 1221, 1171, 1154, 1114 ( $\nu_{\text{as}}$  Ar-O-Me,  $\nu$  Ar C-F,  $\nu$  C-OH), 1074, 1049, 1027 ( $\nu_{\text{as}}$  C-O-C,  $\nu_{\text{s}}$  Ar-O-Me), 867 (1,2,4,5-tetrasubstituted  $\gamma_{\text{s}}$  Ar =CH) cm<sup>-1</sup>; ESI-TOF-HRMS:  $m/z$  calculated for C<sub>30</sub>H<sub>35</sub>FNao<sub>7</sub> [M+Na]<sup>+</sup> 549.2259, found 549.2254.

**(2*S*)-1-{2-[(*aR*,3*S*)-6,7,8-trimethoxy-3-methylisochroman-5-yl]-4,5-dimethoxyphenyl}propan-2-ol and (2*S*)-1-{2-[(*aS*,3*S*)-6,7,8-trimethoxy-3-methylisochroman-5-yl]-4,5-dimethoxyphenyl}propan-2-ol [the mixture of (*aR*,3*S*,2'*S*)-27 and (*aS*,3*S*,2'*S*)-27]**





Starting from the mixture of (aR,3S,2'S)-**26** and (aS,3S,2'S)-**26** (338 mg, 0.71 mmol, 1.0 equiv.), MeOH:THF:H<sub>2</sub>O (7:2:2 ml), LiOH (34 mg, 1.43 mmol, 2.0 equiv.), reaction time: 3 hours. The mixture of (aR,3S,2'S)-**27** and (aS,3S,2'S)-**27**: 281 mg (yield: 91%), light yellow goo. Purification was not required for the crude product. *R*<sub>f</sub> = 0.18 (hexane/EtOAc 6:4); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  = 6.91, 6.88 [2s, 2 x 1H, (aR), (aS) *H*-9'], 6.61, 6.59 [2s, 2 x 1H, (aR), (aS) *H*-6'], 4.98 [d, *J* = 14.8 Hz, 1H, (aR) or (aS) *H*-1-*a*], 4.94 [d, *J* = 14.6 Hz, 1H, (aR) or (aS) *H*-1-*a*], 4.70 [d, *J* = 14.7 Hz, 1H, (aR) or (aS) *H*-1-*b*], 4.66 [d, *J* = 14.7 Hz, 1H, (aR) or (aS) *H*-1-*b*], 3.94, 3.89, 3.88, 3.85, 3.84, 3.69, 3.63 [9s, 10 x 3H, (aR), (aS) *H*-10', *H*-11', *H*-9, *H*-10, *H*-11], 3.87 – 3.78 [m, 2 x 1H, (aR), (aS) *H*-2' or *H*-3], 3.68 – 3.56 [m, 2 x 1H, (aR), (aS) *H*-2' or *H*-3], 2.91 [s, 2H, (aR), (aS) OH], 2.56, 2.44, 2.38, 2.32 – 2.16, 2.10 – 1.96 [dd, *J* = 14.0, 3.4 Hz, 1H, dd, *J* = 13.7, 8.0 Hz, dd, *J* = 13.7, 4.9 Hz, 2m, 3H, (aR), (aS) *H*-1'-*a,b*, *H*-1-*a,b*, *H*-4-*a,b*], 1.21 [2d, *J* = 5.9 Hz, *J* = 5.8 Hz, 2 x 3H, (aR), (aS) *H*-12], 1.12, 1.07 [2d, *J* = 6.0 Hz, *J* = 6.1 Hz, 2 x 3H, (aR), (aS) *H*-3']; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  = 150.1, 149.2 [2C, (aR), (aS) C-6], 148.4, 148.2, 147.7, 147.1, 147.0 [6C, (aR), (aS) C-7', C-8', C-8], 143.6, 143.5 [2C, (aR), (aS) C-7], 129.8, 129.7, 129.6, 128.1, 128.0, 127.9, 127.8 [8C, (aR), (aS) C-4', C-5', C-4a, C-5], 123.9, 123.5 [2C, (aR), (aS) C-8a], 113.4, 112.8, 112.7, 112.1 [4C, (aR), (aS) C-6', C-9], 70.5, 70.4, 68.3, 67.3 [4C, (aR), (aS) C-3, C-2'], 64.5, 64.3 [2C, (aR), (aS) C-1], 60.9, 60.9, 60.8, 60.5, 60.3, 55.8, 55.6 [10C, (aR), (aS) C-9, C-10, C-11, C-10', C-11'], 42.7, 42.4 [2C, (aR), (aS) C-1'], 34.2, 33.4 [2C, (aR), (aS) C-4], 23.6, 22.9 [2C, (aR), (aS) C-12], 21.4, 21.3 [2C, (aR), (aS) C-3']; IR (KBr)  $\nu$  = 3499 ( $\nu$  OH), 2935 ( $\nu_{as}$  CH<sub>2</sub>), 2844 ( $\nu_s$  CH<sub>2</sub>), 2049, 1958, 1715 ( $\gamma$  Ar =CH,  $\gamma$  Ar C=C overtone and combination bands), 1606, 1579, 1515, 1465, 1409 ( $\nu$  Ar C=C,  $\beta_s$  CH<sub>2</sub>,  $\delta_{as}$  Me), 1391, 1363, 1328 ( $\delta_s$  Me,  $\delta$  CH,  $\gamma_s$  CH<sub>2</sub>), 1253, 1219, 1174, 1111 ( $\nu_{as}$  Ar-O-Me,  $\nu$  C-OH), 1073, 1029 ( $\nu_{as}$  C-O-C,  $\nu_s$  Ar-O-Me), 866 (1,2,4,5-tetrasubstituted  $\gamma_s$  Ar =CH) cm<sup>-1</sup>; ESI-TOF-HRMS: *m/z* calculated for C<sub>24</sub>H<sub>32</sub>NaO<sub>7</sub> [M+Na]<sup>+</sup> 455.2040, found 455.2040.

### 3. Spectra of the compounds

#### 3.1. NMR spectra

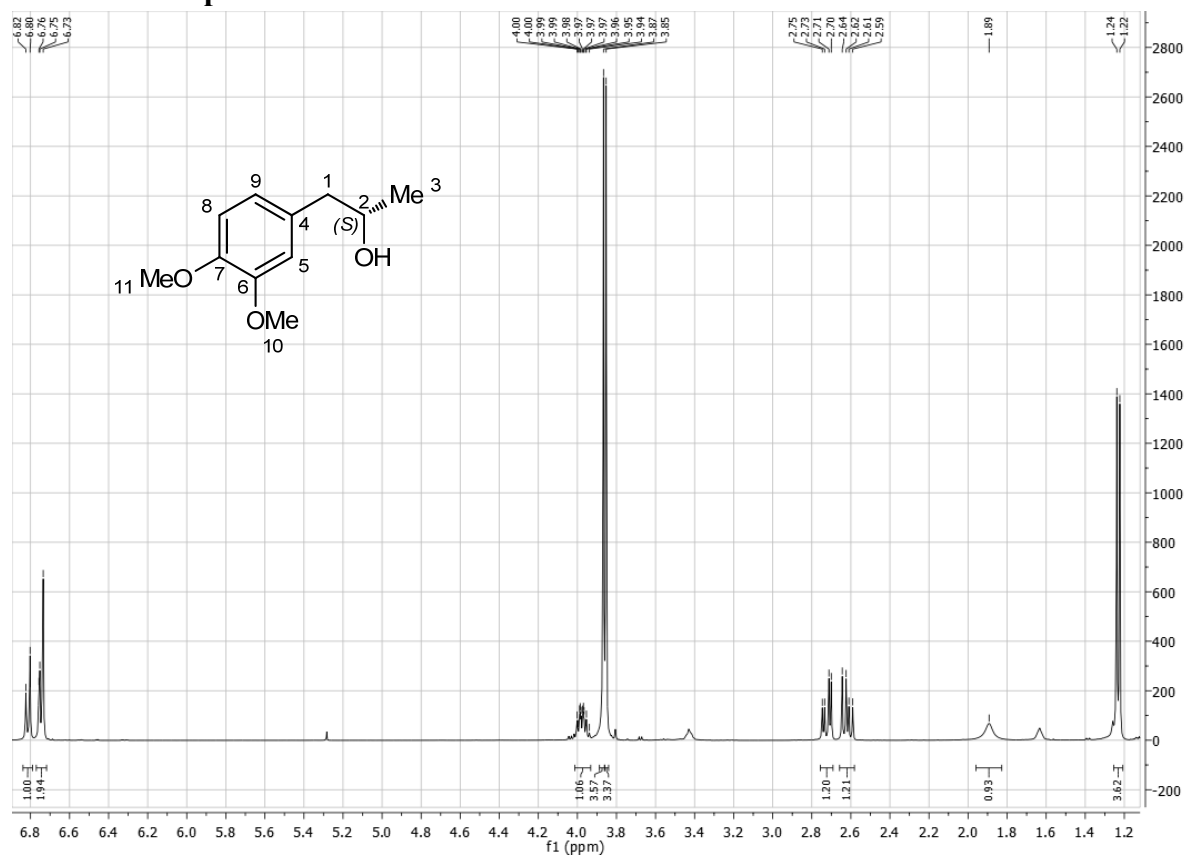


Figure S1. <sup>1</sup>H NMR (400 MHz) spectrum of (S)-11 in CDCl<sub>3</sub>.

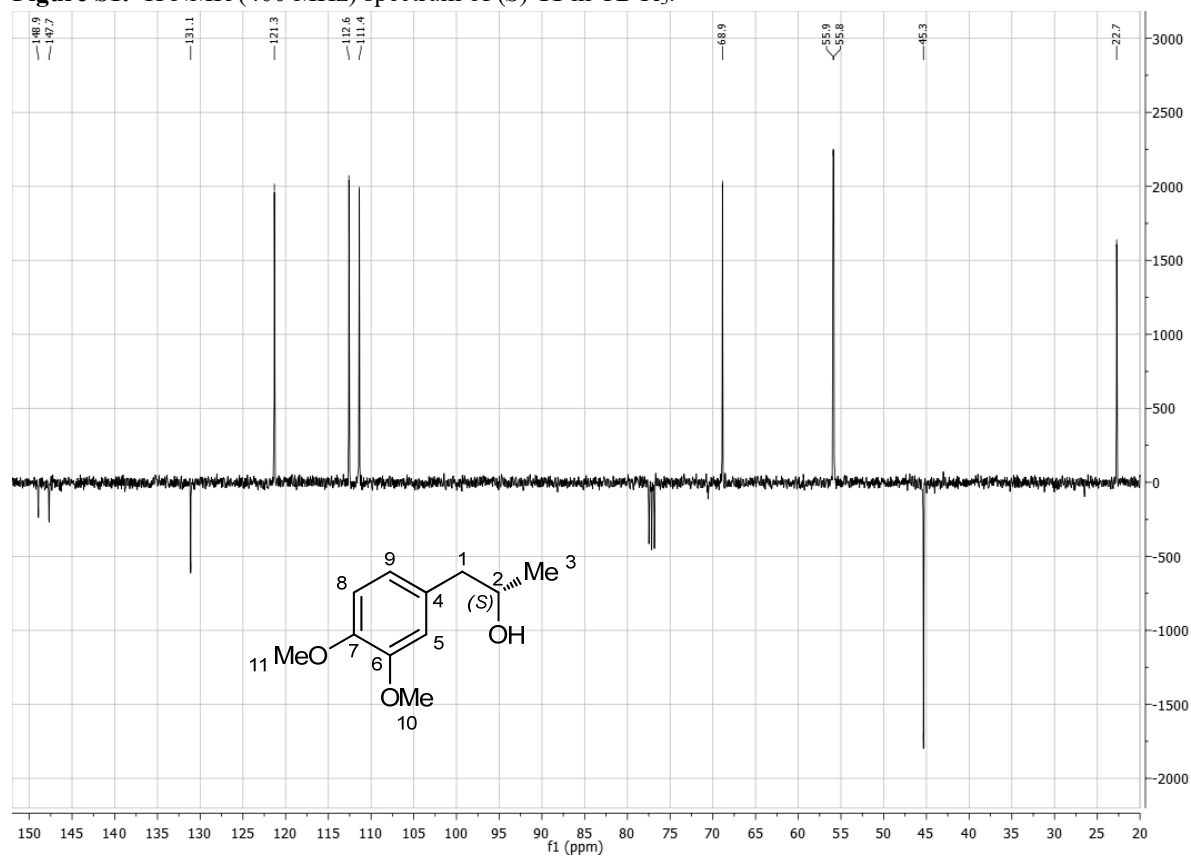
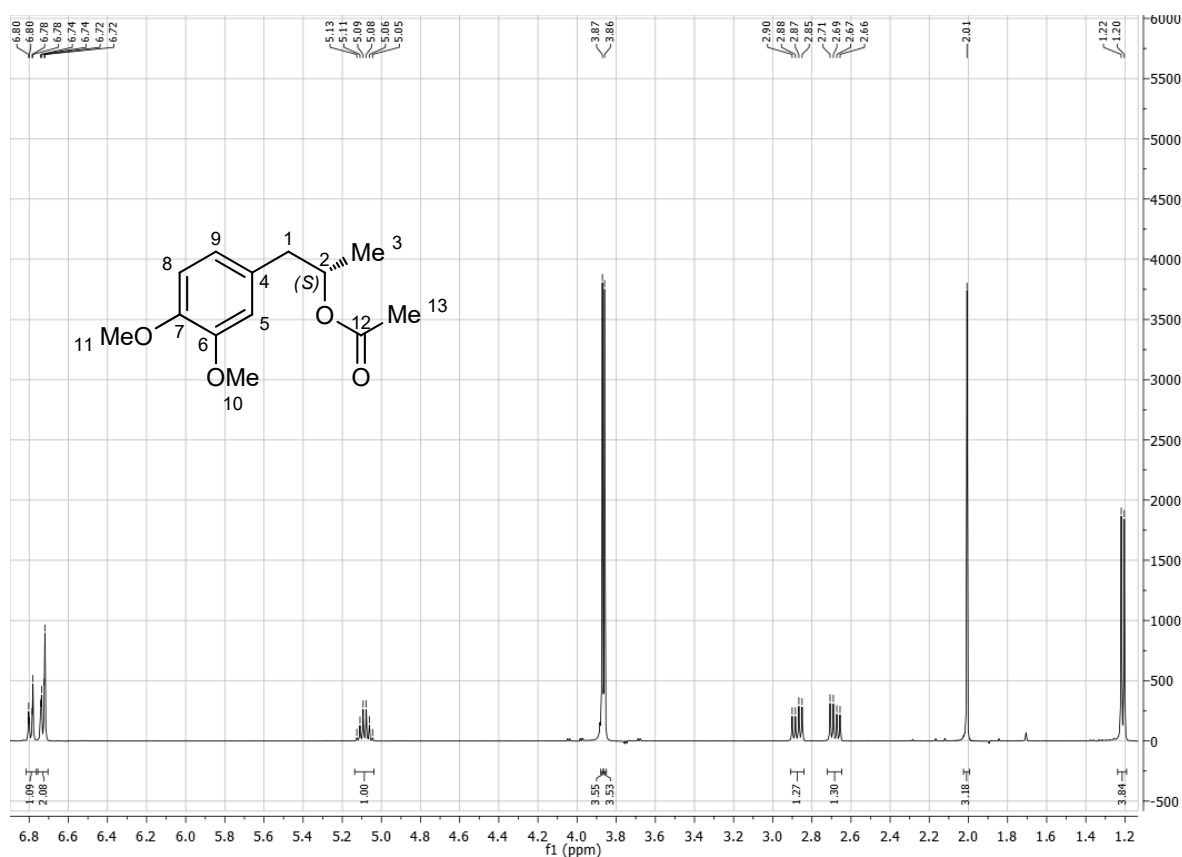
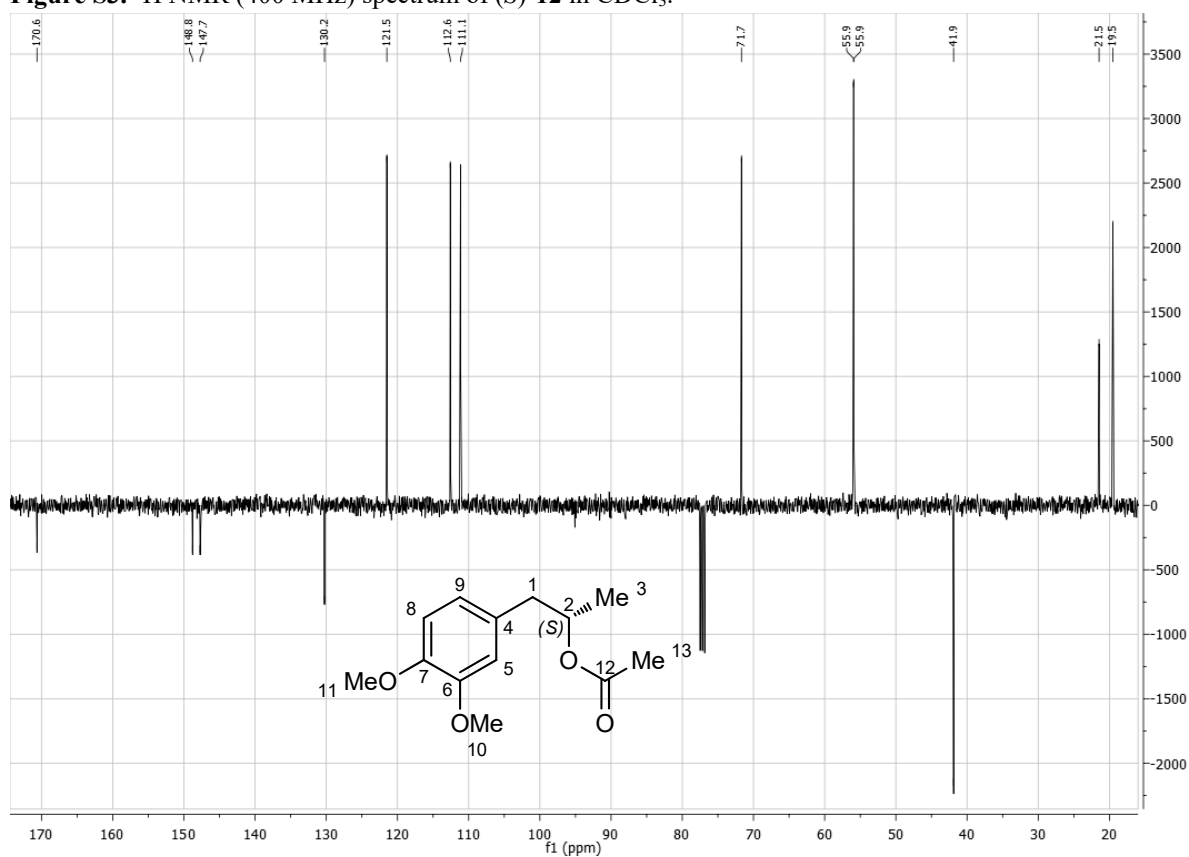


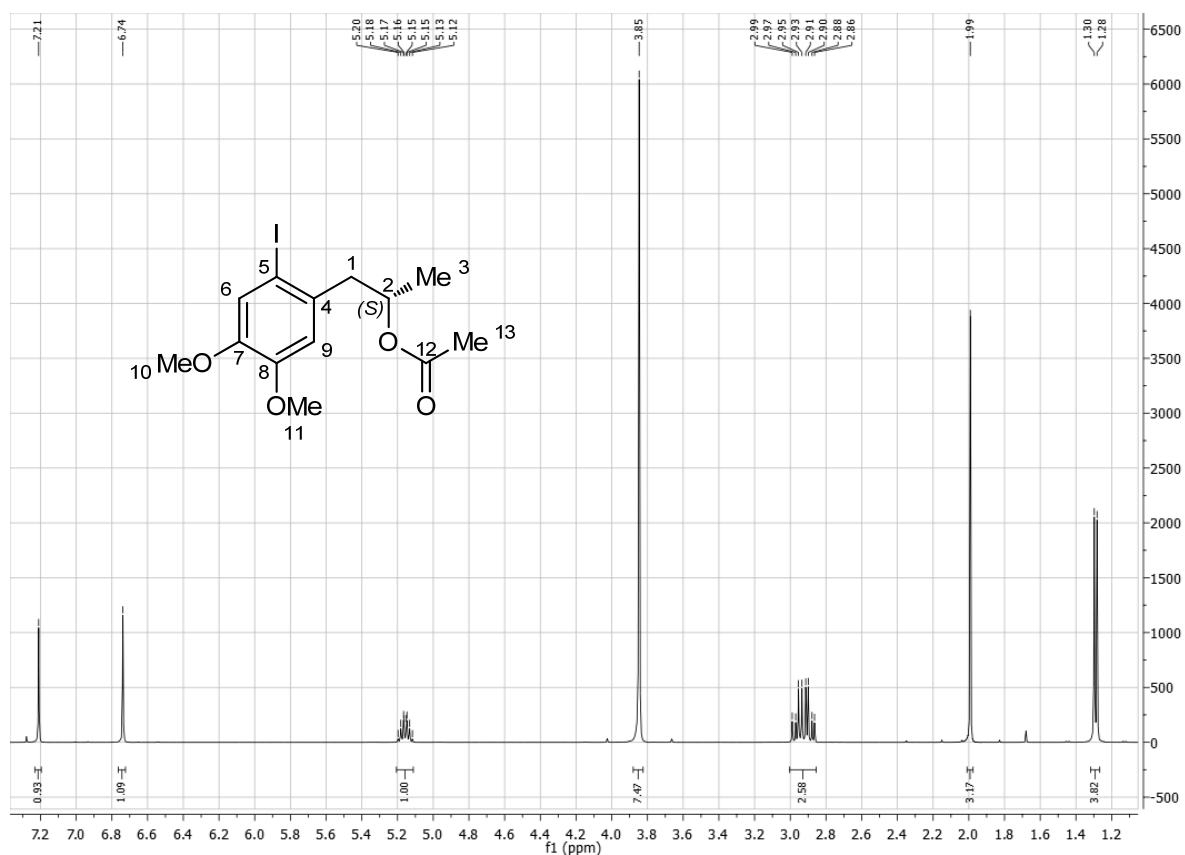
Figure S2. <sup>13</sup>C NMR (100 MHz) spectrum of (S)-11 in CDCl<sub>3</sub>.



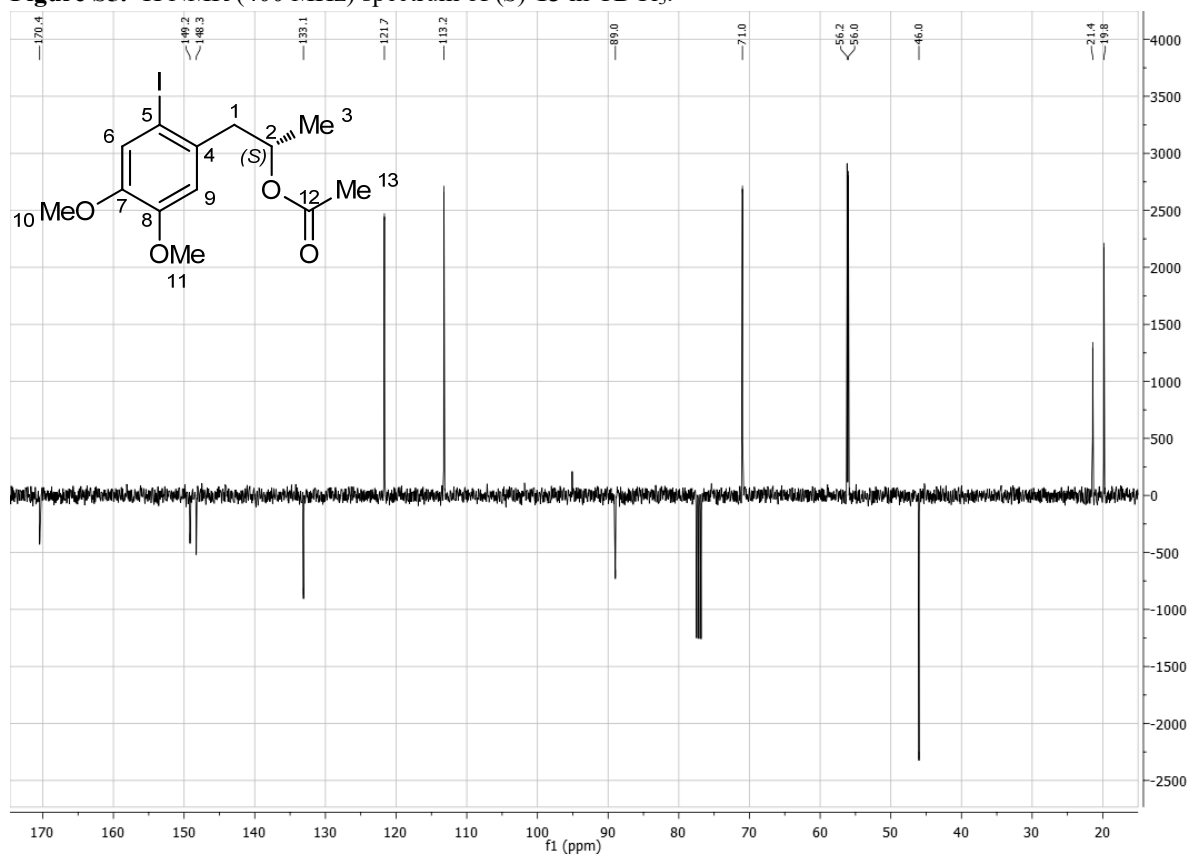
**Figure S3.** <sup>1</sup>H NMR (400 MHz) spectrum of *(S)*-12 in CDCl<sub>3</sub>.



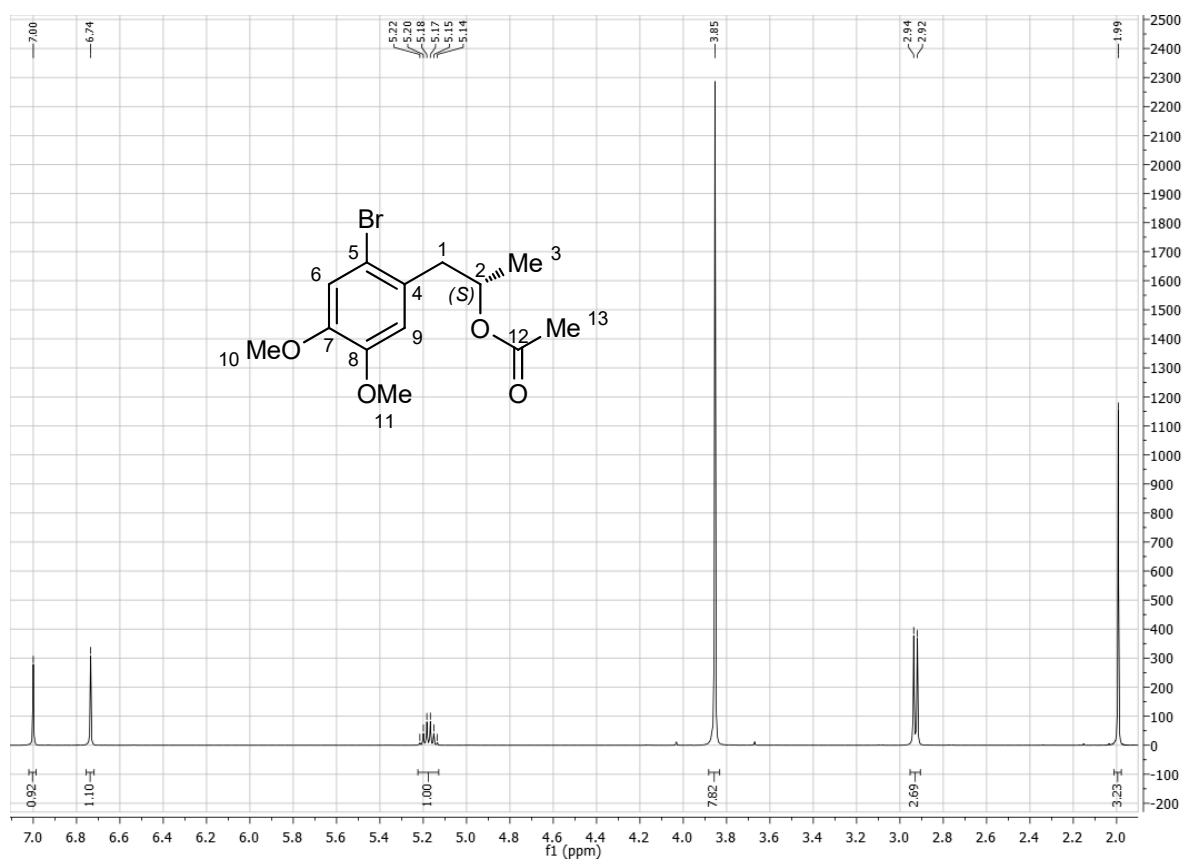
**Figure S4.** <sup>13</sup>C NMR (100 MHz) spectrum of *(S)*-12 in CDCl<sub>3</sub>.



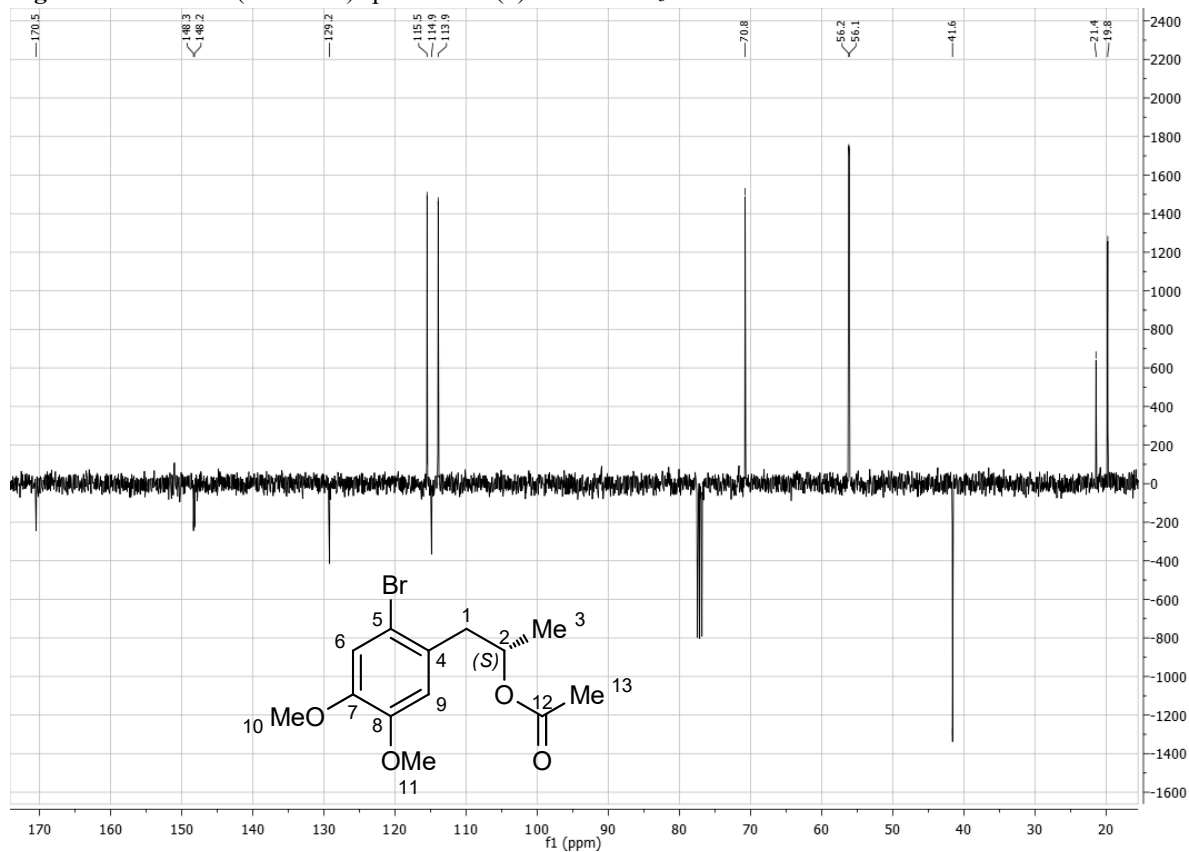
**Figure S5.**  $^1\text{H}$  NMR (400 MHz) spectrum of *(S)*-13 in  $\text{CDCl}_3$ .



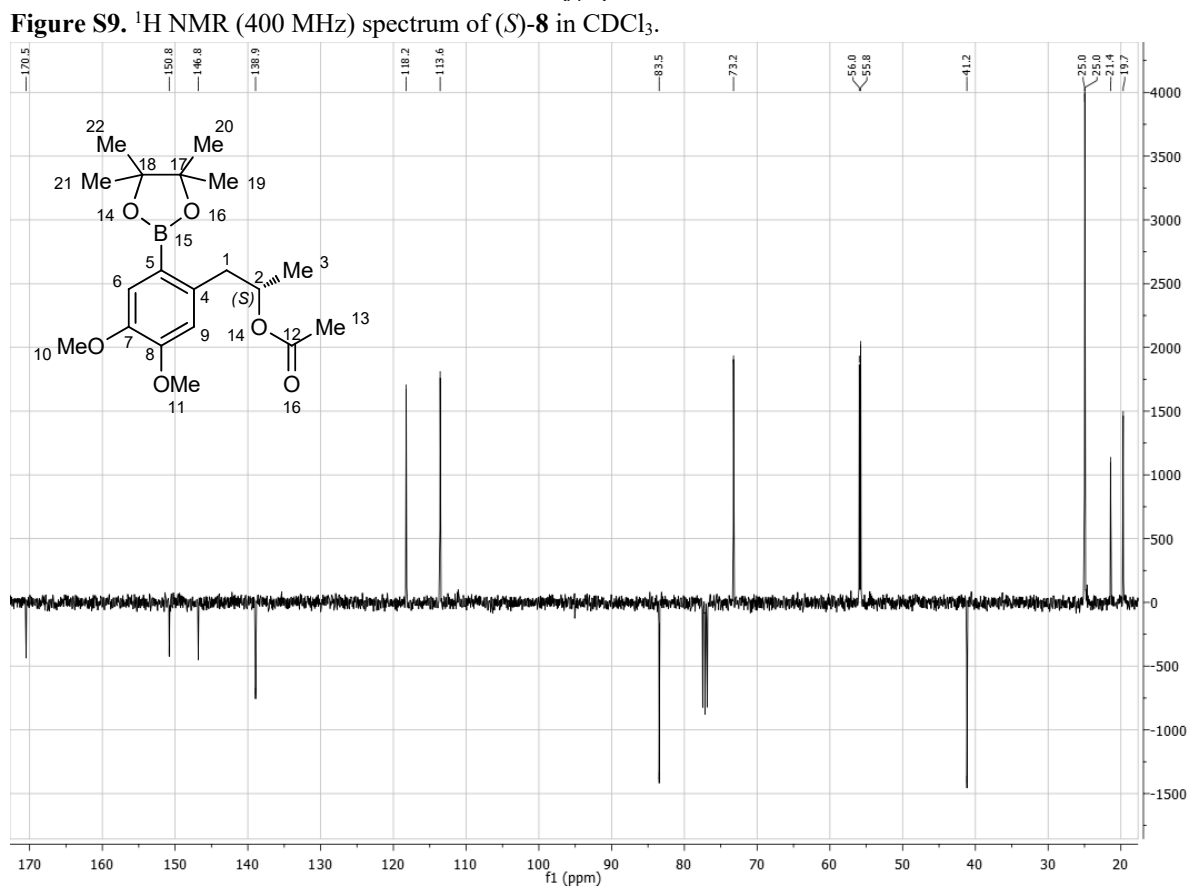
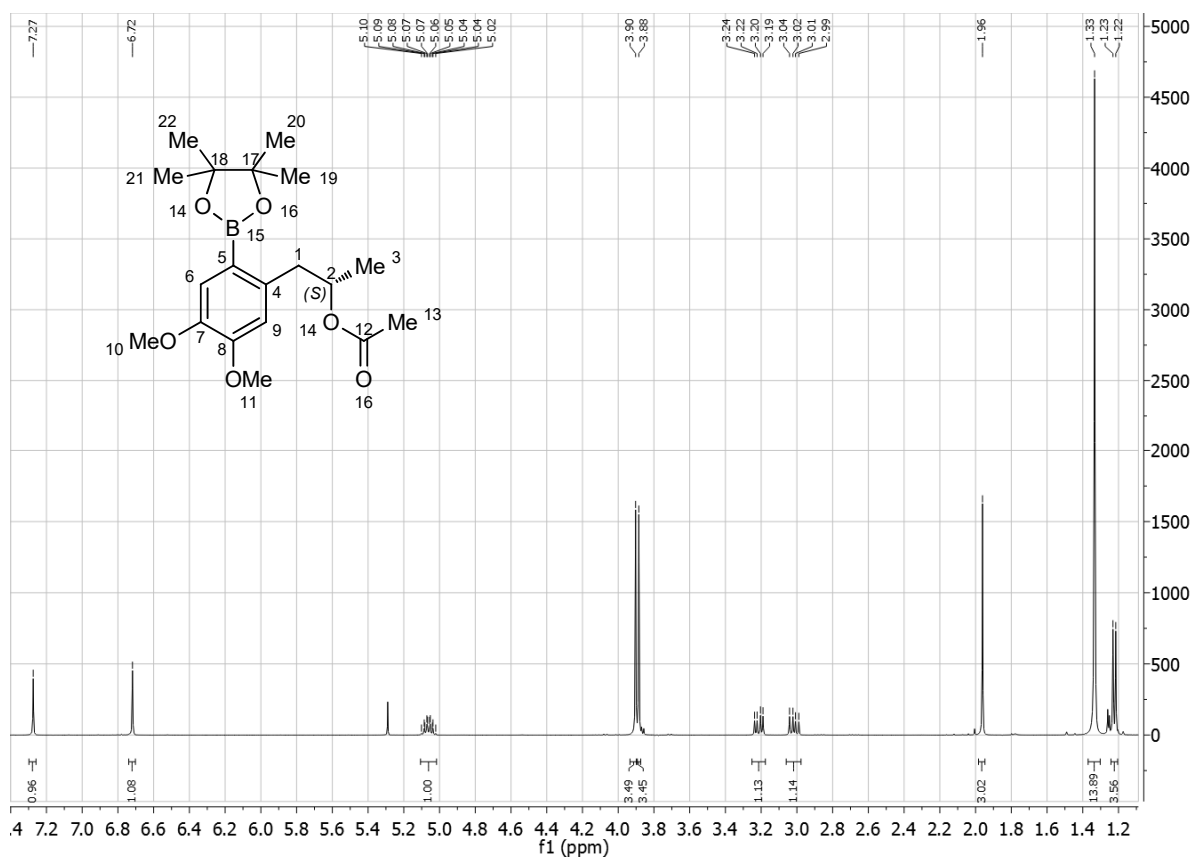
**Figure S6.**  $^{13}\text{C}$  NMR (100 MHz) spectrum of *(S)*-13 in  $\text{CDCl}_3$ .

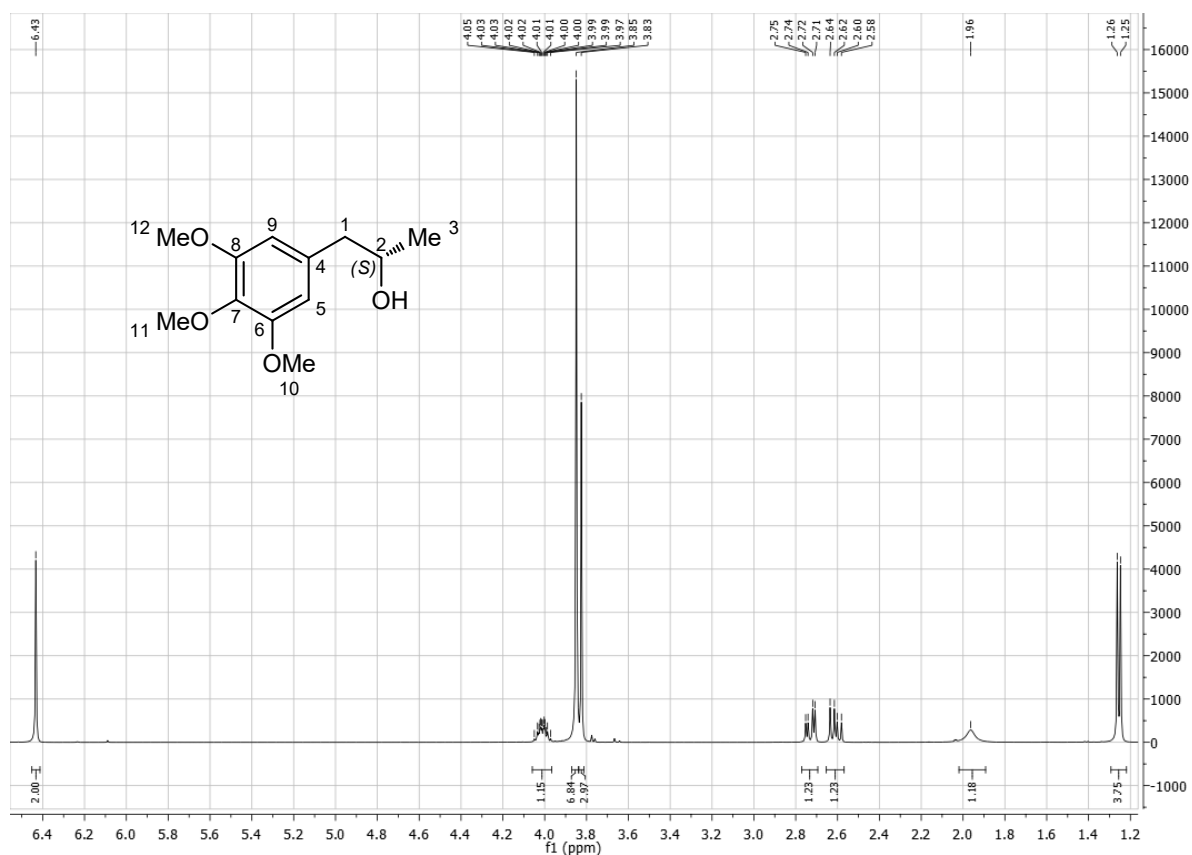


**Figure S7.**  $^1\text{H}$  NMR (400 MHz) spectrum of (*S*)-**14** in  $\text{CDCl}_3$ .

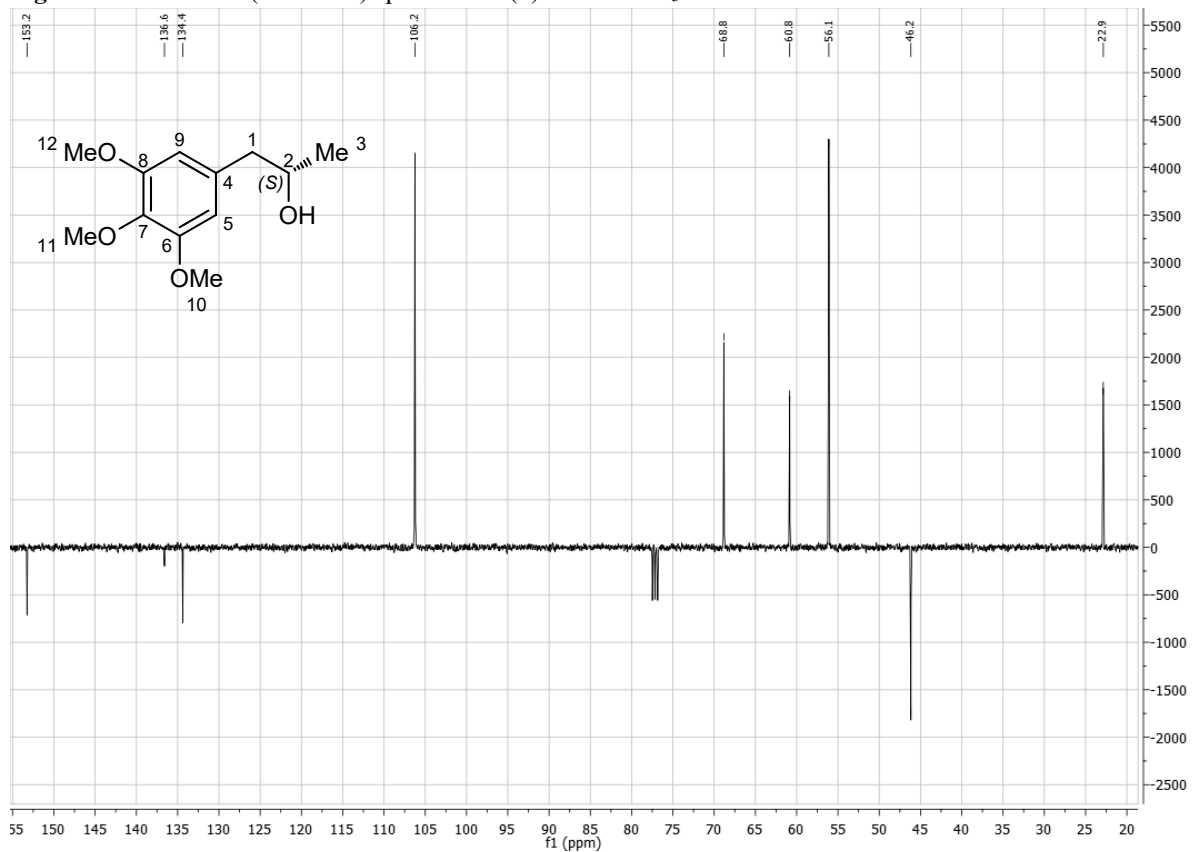


**Figure S8.**  $^{13}\text{C}$  NMR (100 MHz) spectrum of (*S*)-**14** in  $\text{CDCl}_3$ .

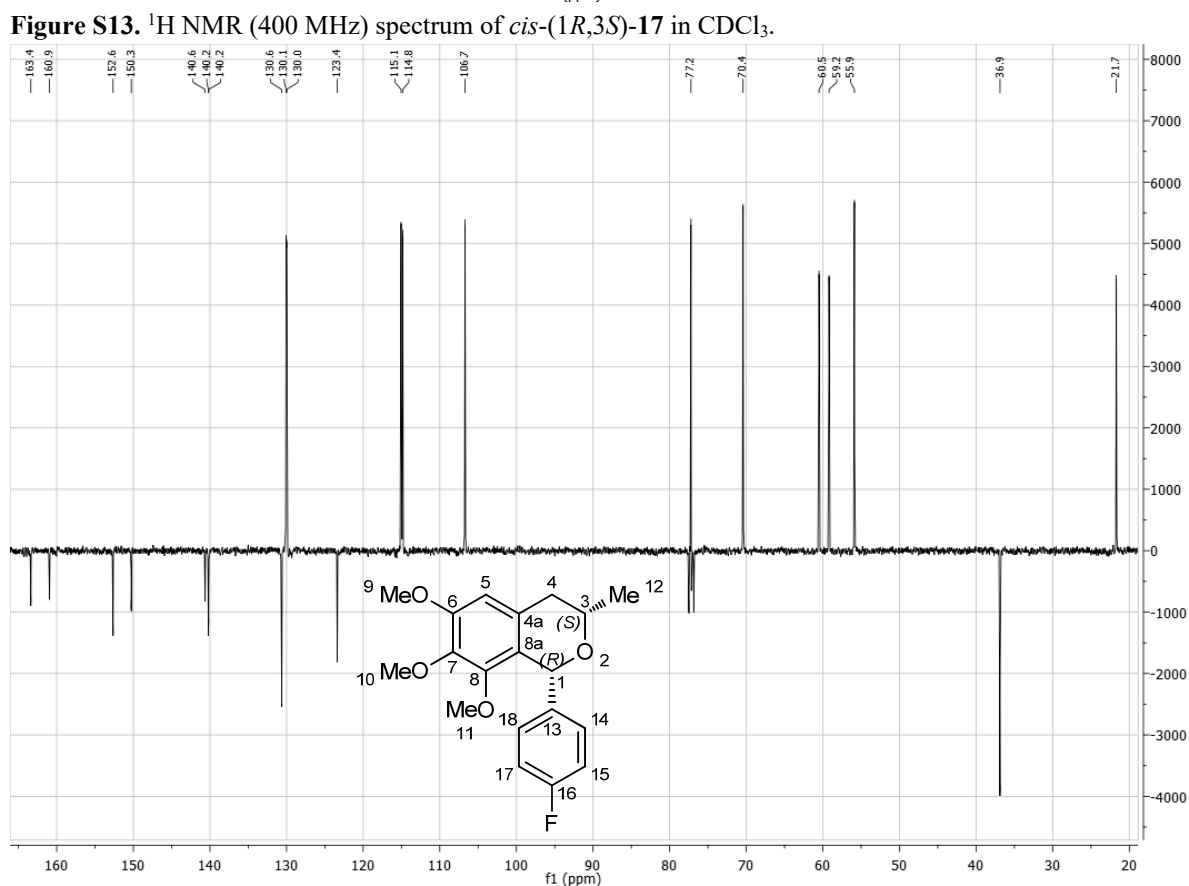
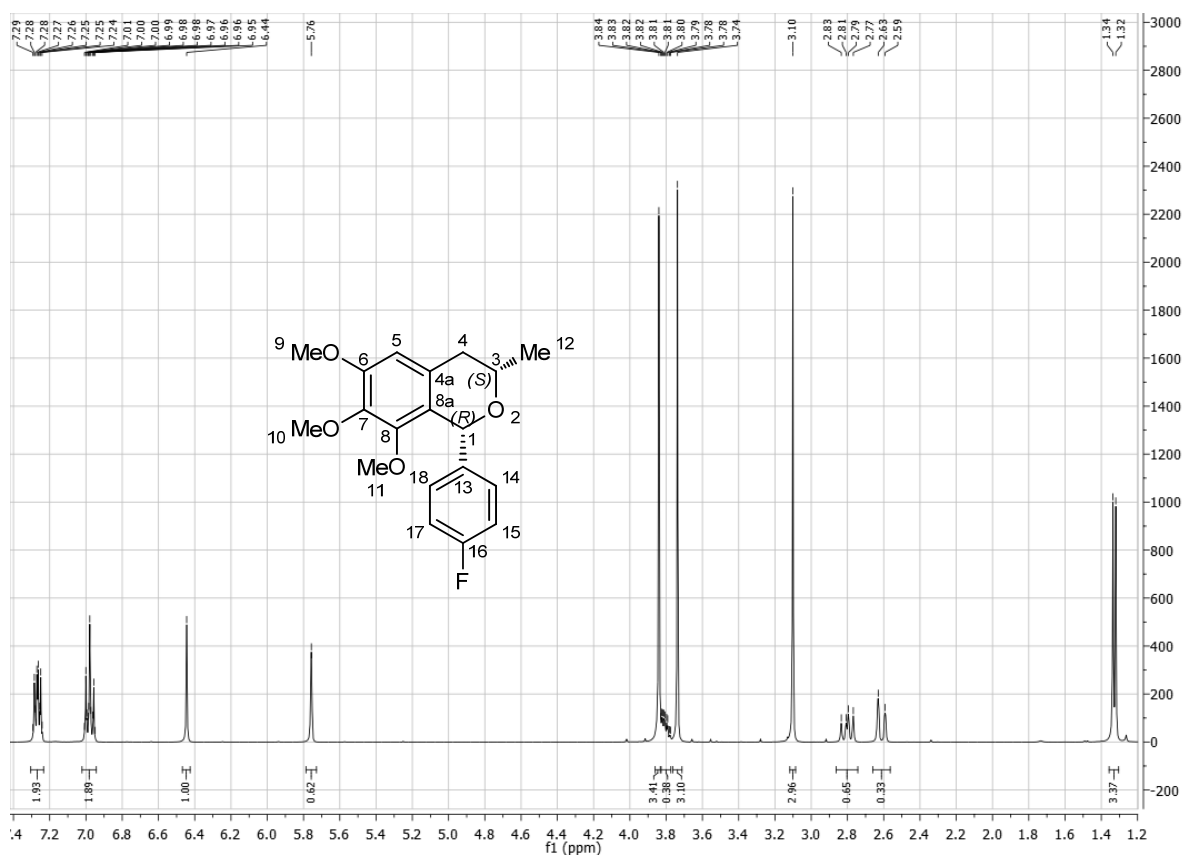




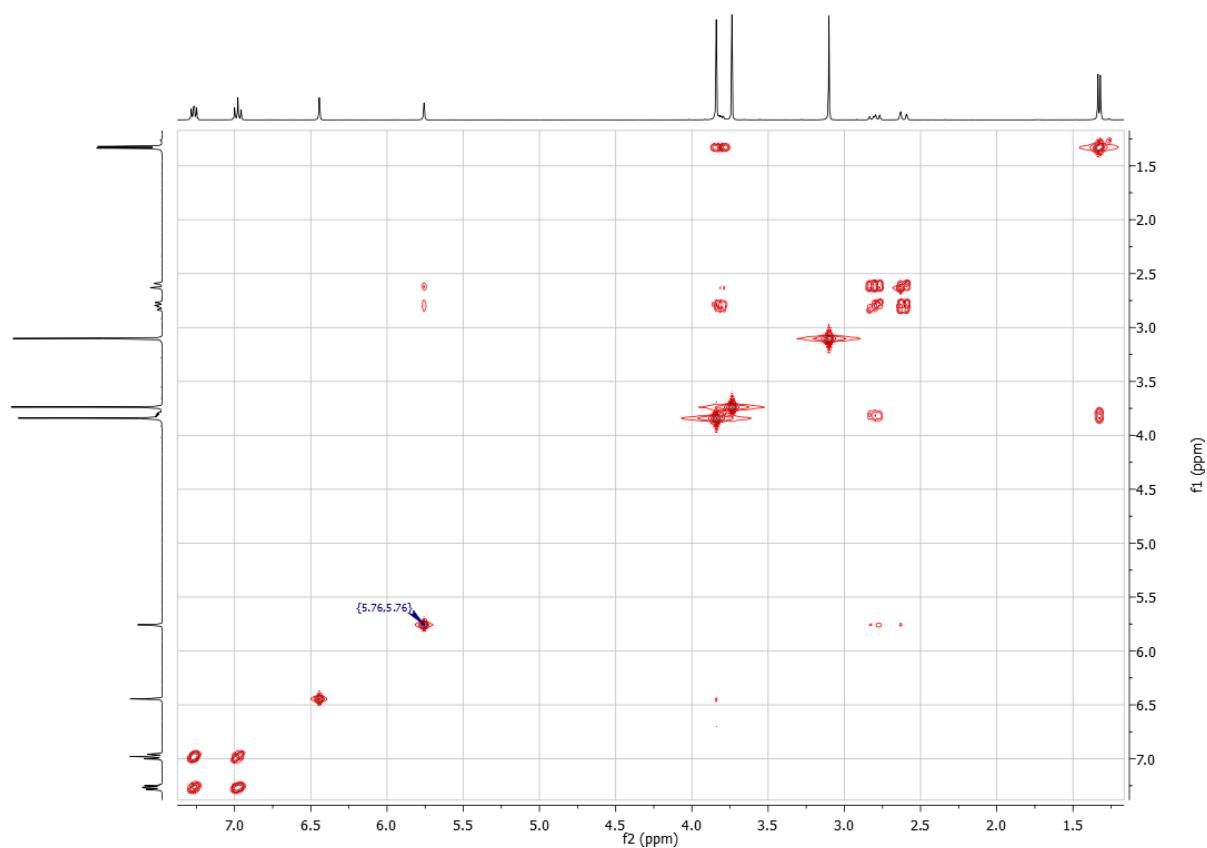
**Figure S11.** <sup>1</sup>H NMR (400 MHz) spectrum of (S)-16 in CDCl<sub>3</sub>.



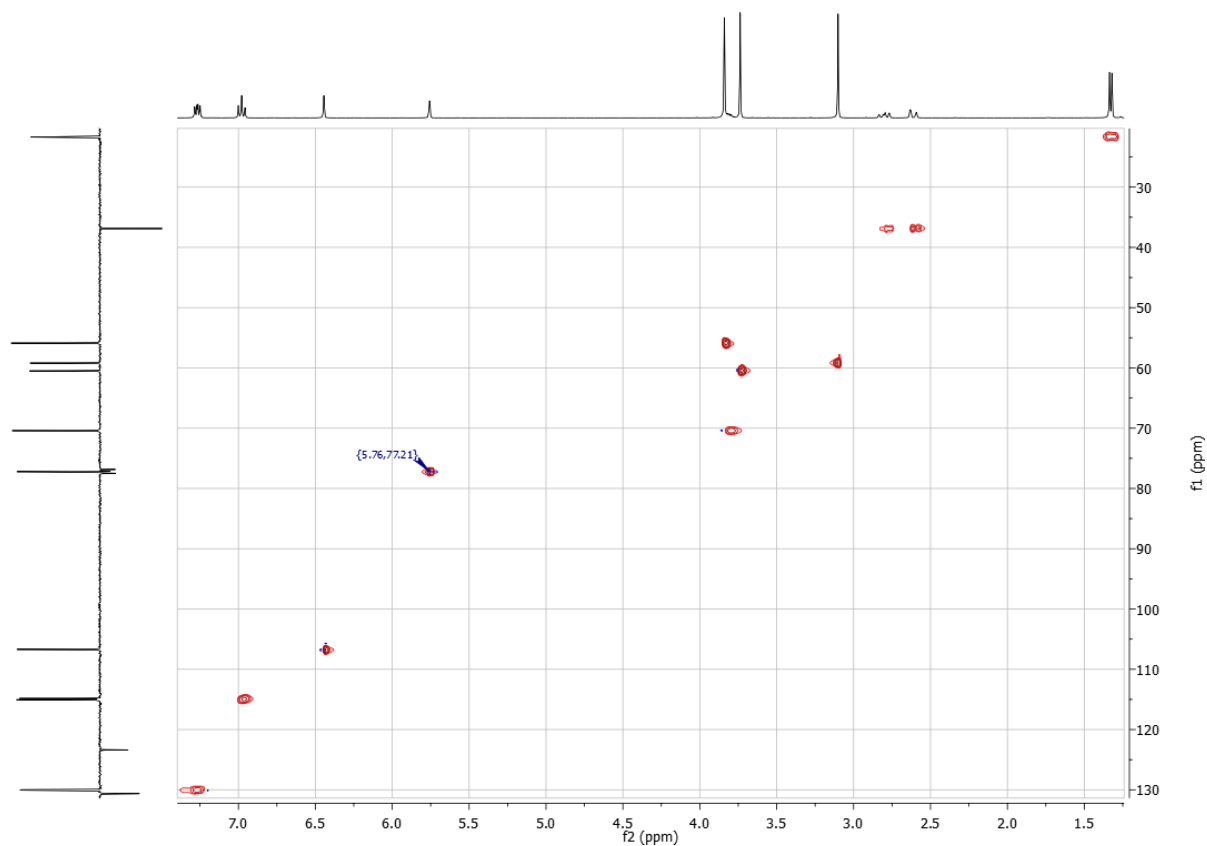
**Figure S12.** <sup>13</sup>C NMR (100 MHz) spectrum of (S)-16 in CDCl<sub>3</sub>.



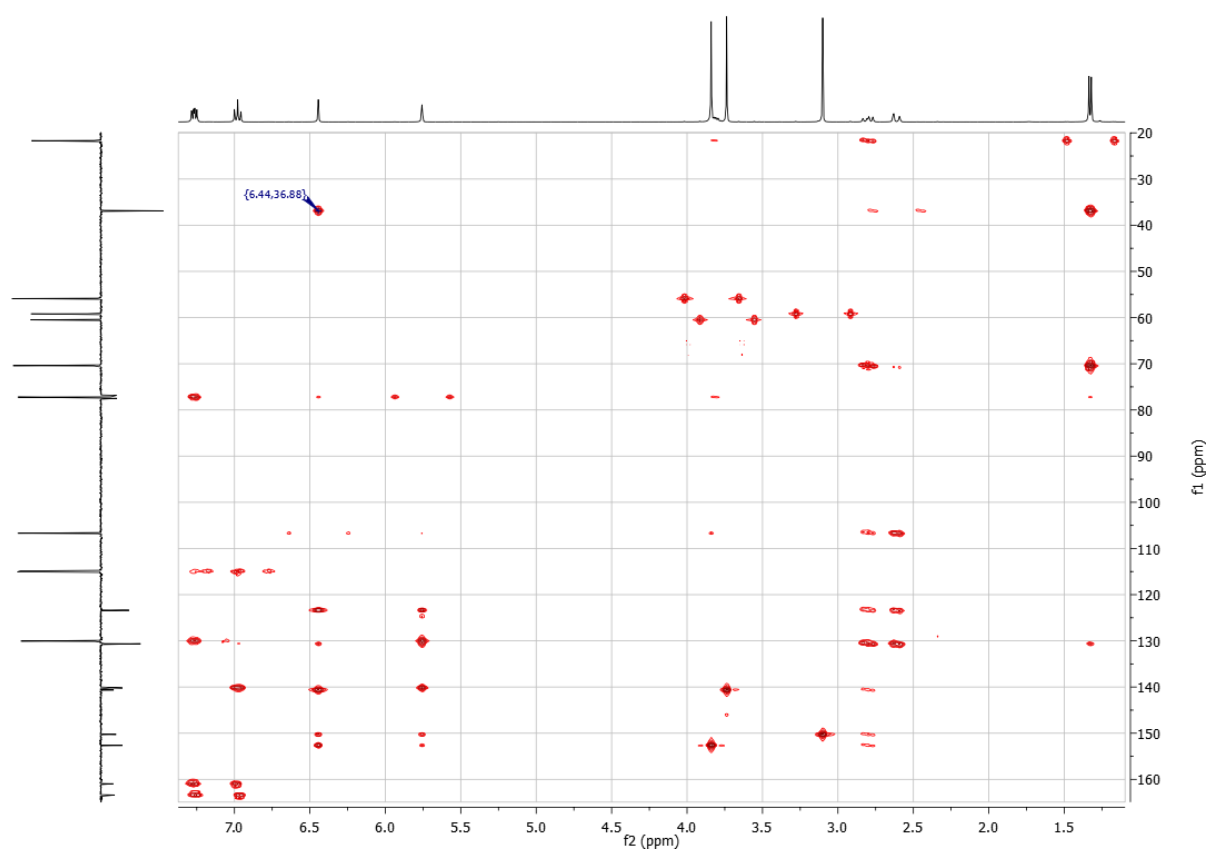




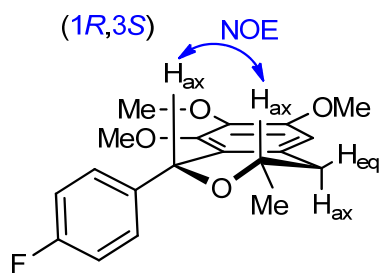
**Figure S15.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR (400 MHz) spectrum of *cis*-(1*R*,3*S*)-**17** in  $\text{CDCl}_3$ .



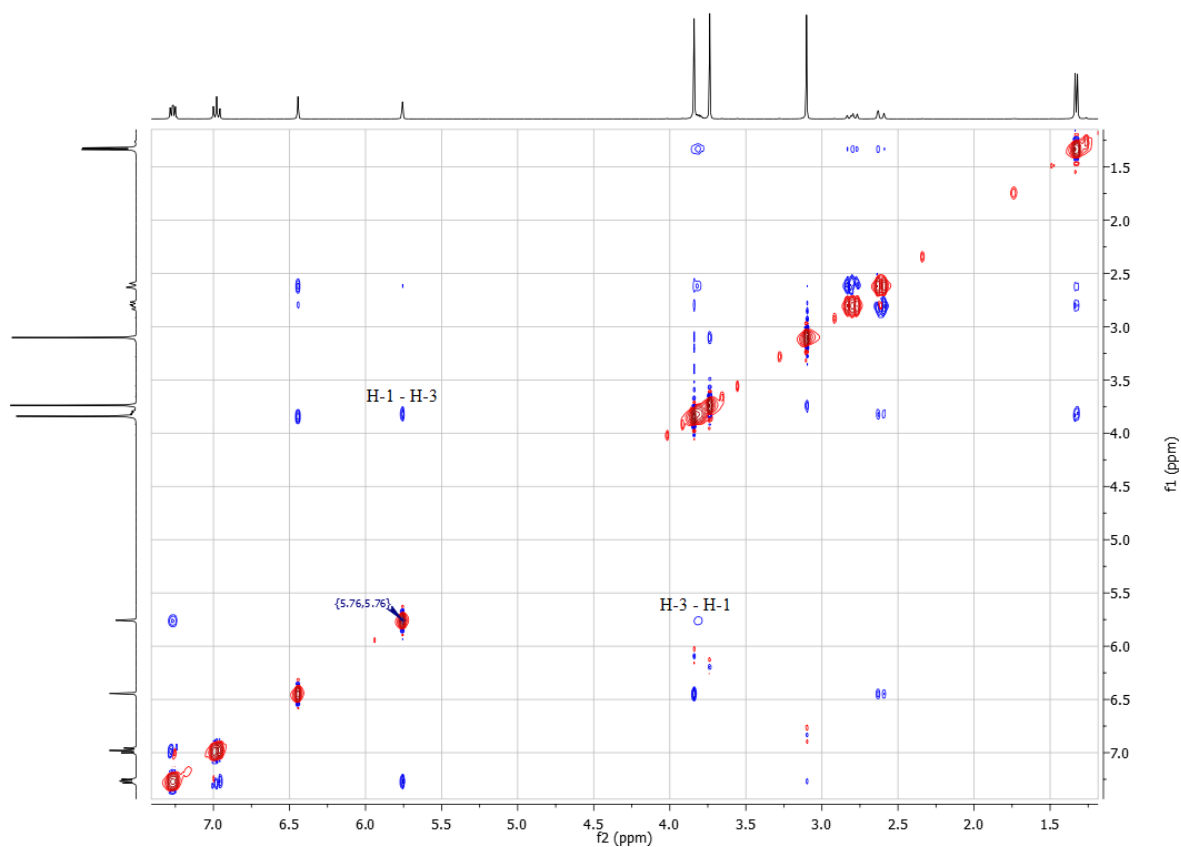
**Figure S16.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR (400 MHz) spectrum of *cis*-(1*R*,3*S*)-**17** in  $\text{CDCl}_3$ .



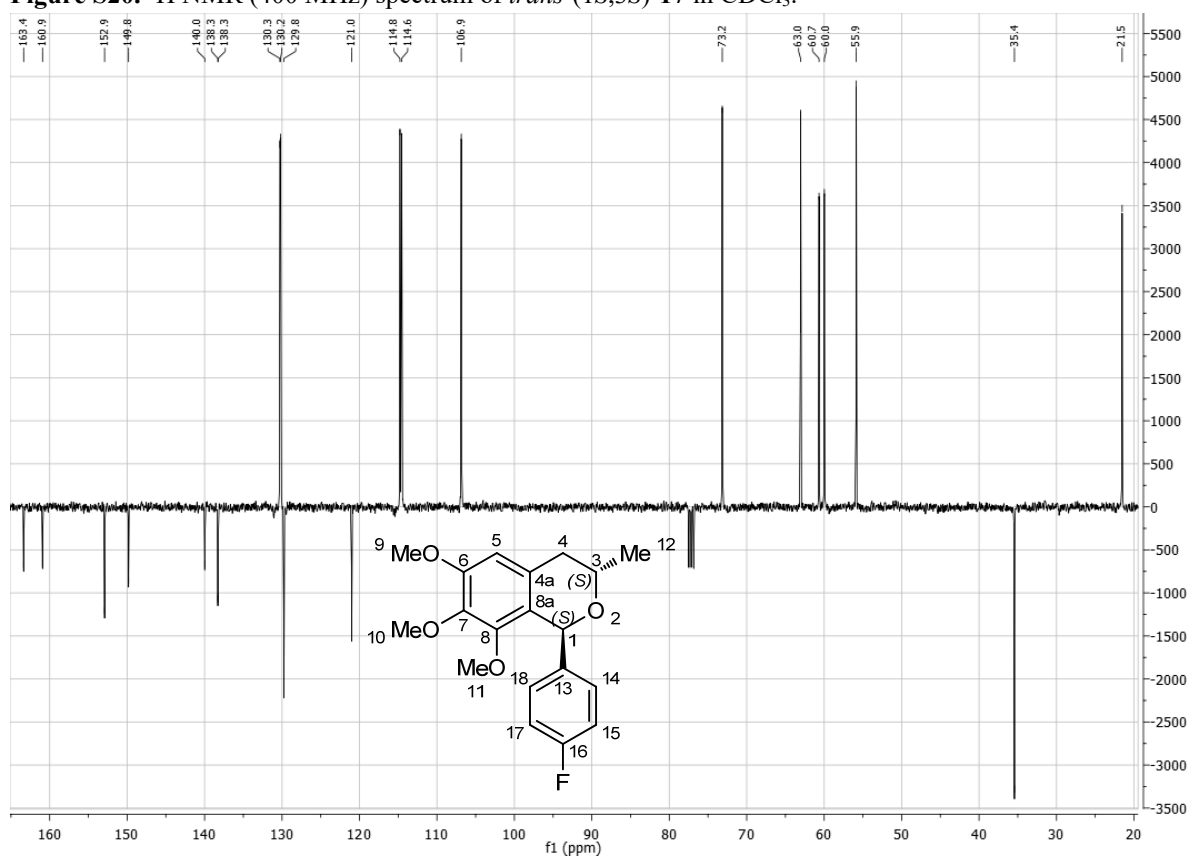
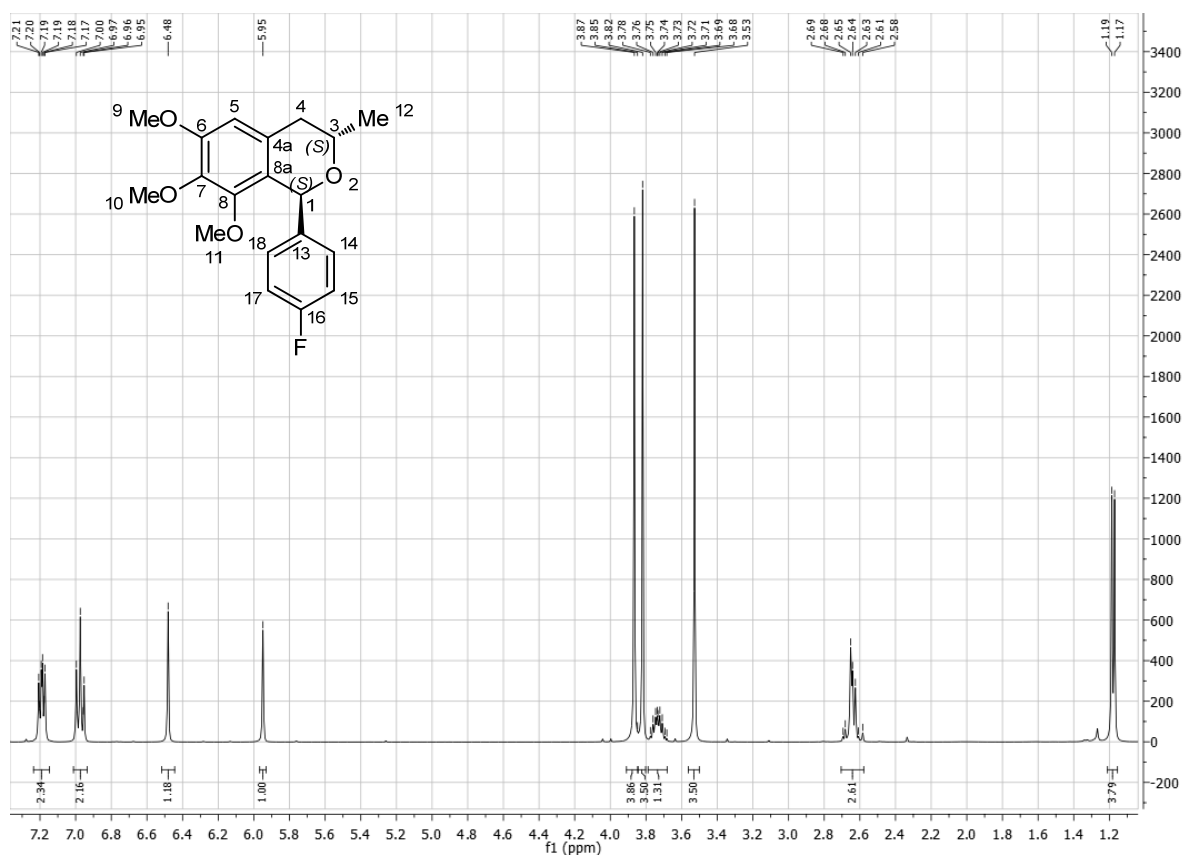
**Figure S17.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC NMR (400 MHz) spectrum of *cis*-(1*R*,3*S*)-**17** in  $\text{CDCl}_3$ .

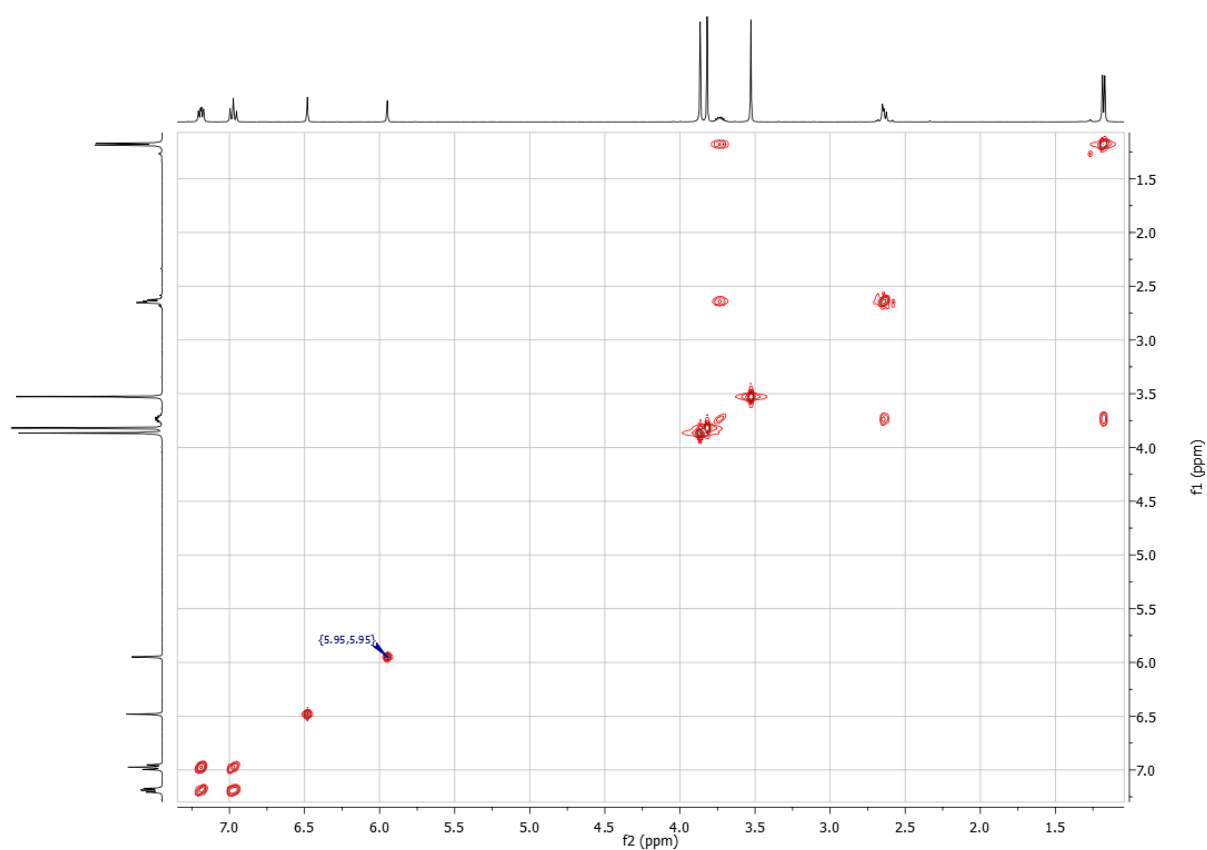


**Figure S18.** Characteristic NOE correlation shown on the structure of *cis*-(1*R*,3*S*)-**17** suggesting (1*R*,3*S*) configuration of isochroman unit.

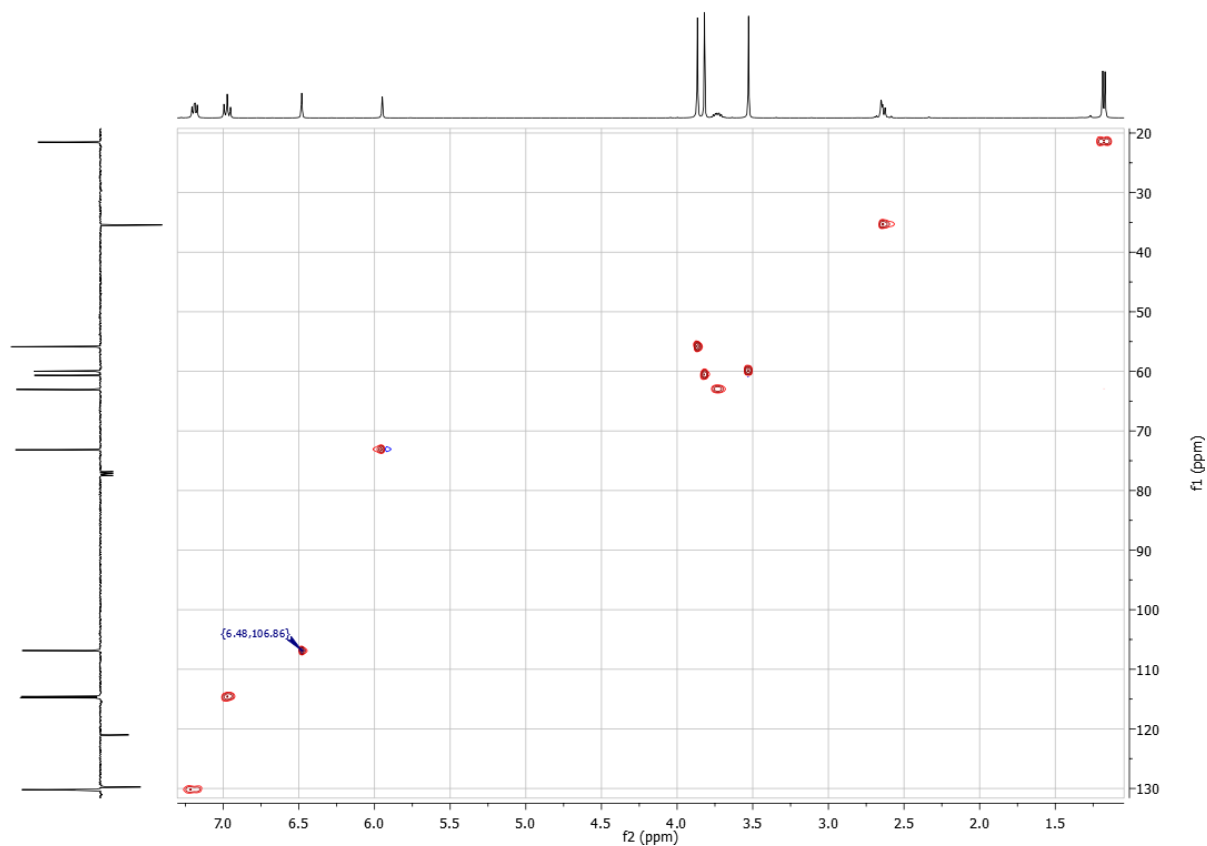


**Figure S19.**  $^1\text{H}$ - $^1\text{H}$  NOESY NMR (400 MHz) spectrum of *cis*-(1*R*,3*S*)-**17** in  $\text{CDCl}_3$ .

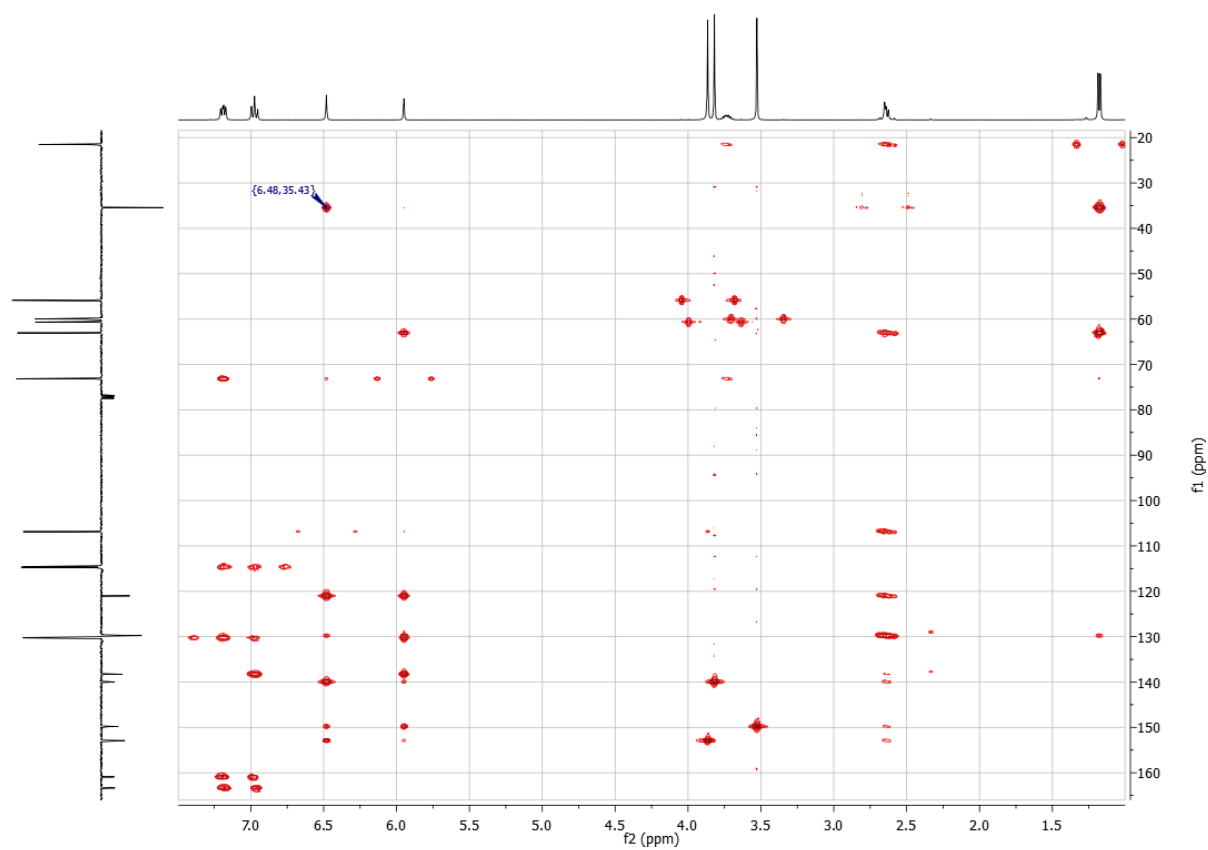




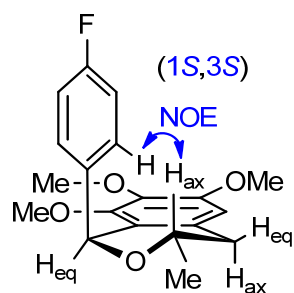
**Figure S22.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR (400 MHz) spectrum of *trans*-(1*S*,3*S*)-**17** in  $\text{CDCl}_3$ .



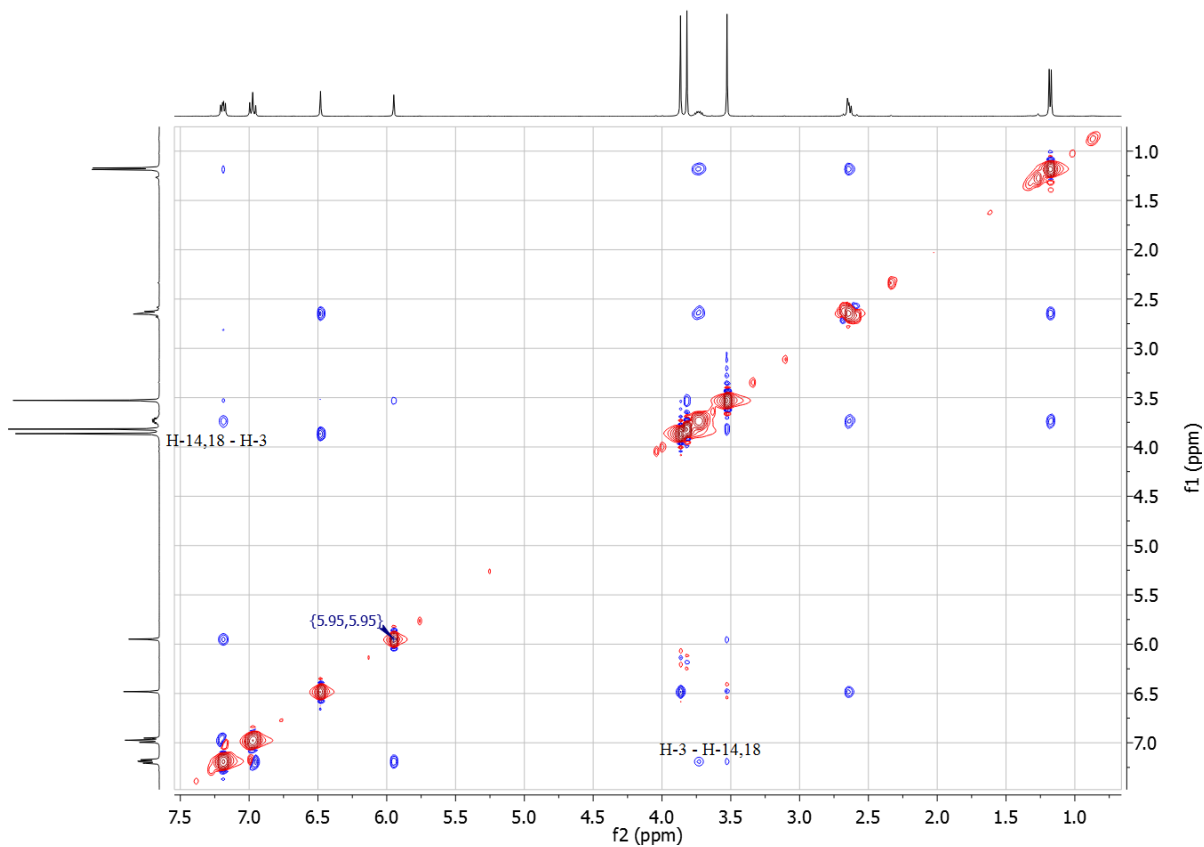
**Figure S23.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR (400 MHz) spectrum of *trans*-(1*S*,3*S*)-**17** in  $\text{CDCl}_3$ .



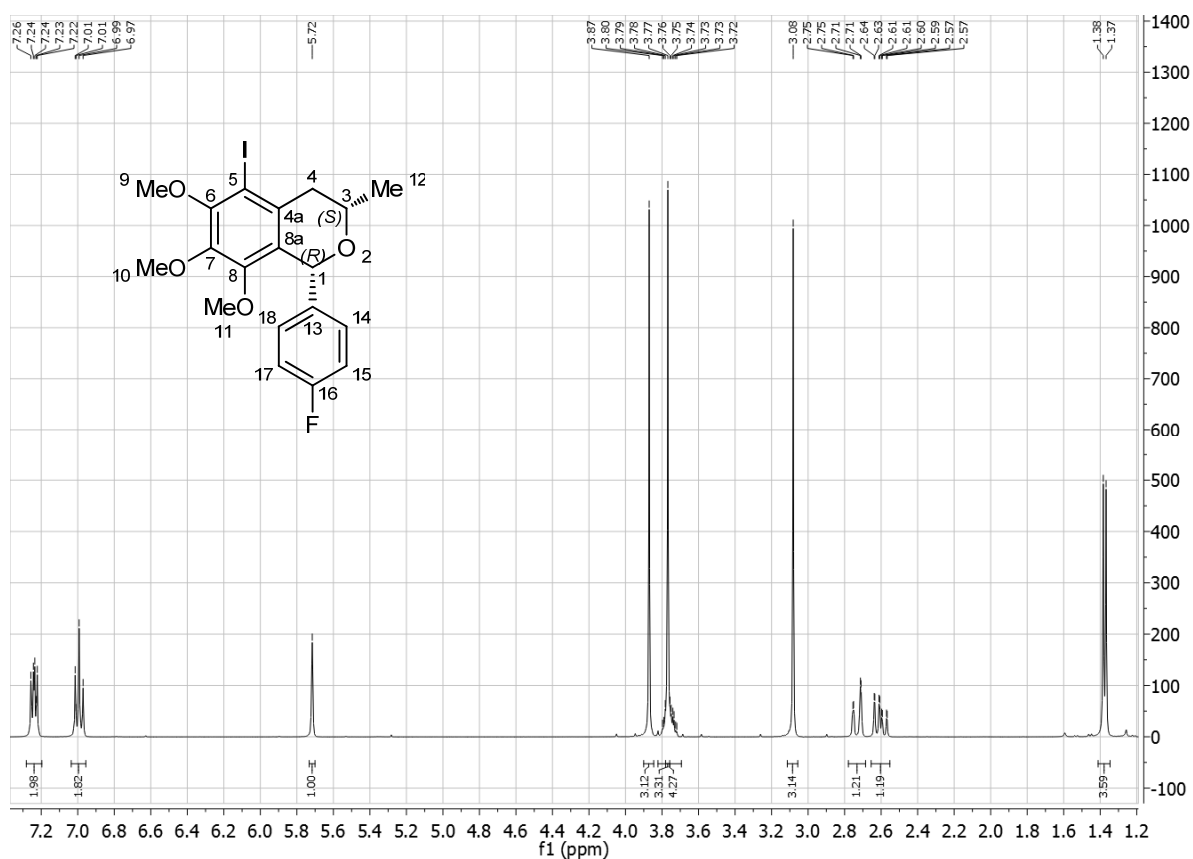
**Figure S24.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC NMR (400 MHz) spectrum of *trans*-(1*S*,3*S*)-**17** in  $\text{CDCl}_3$ .



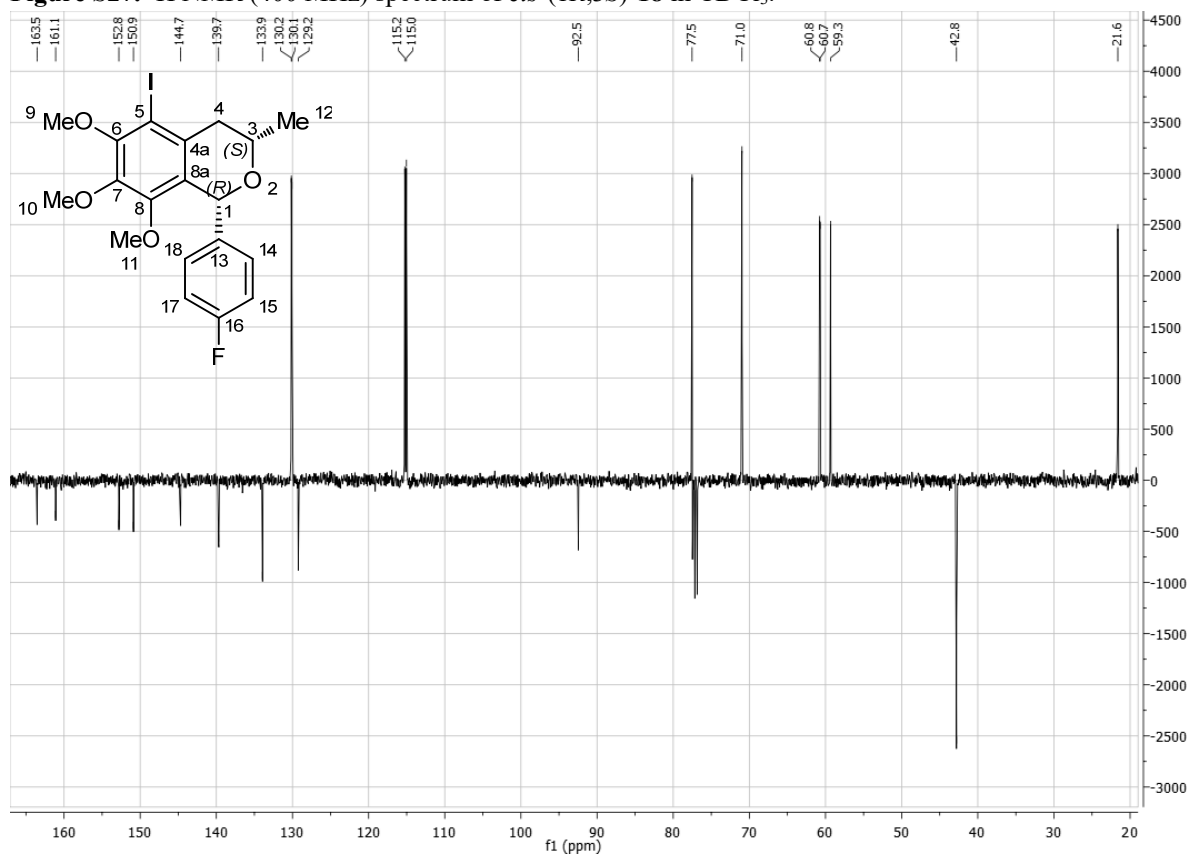
**Figure S25.** Characteristic NOE correlation shown on the structure of *trans*-(1*S*,3*S*)-**17** suggesting (1*S*,3*S*) configuration of isochroman unit.



**Figure S26.** <sup>1</sup>H-<sup>1</sup>H NOESY NMR (400 MHz) spectrum of *trans*-(1*S*,3*S*)-**17** in CDCl<sub>3</sub>.

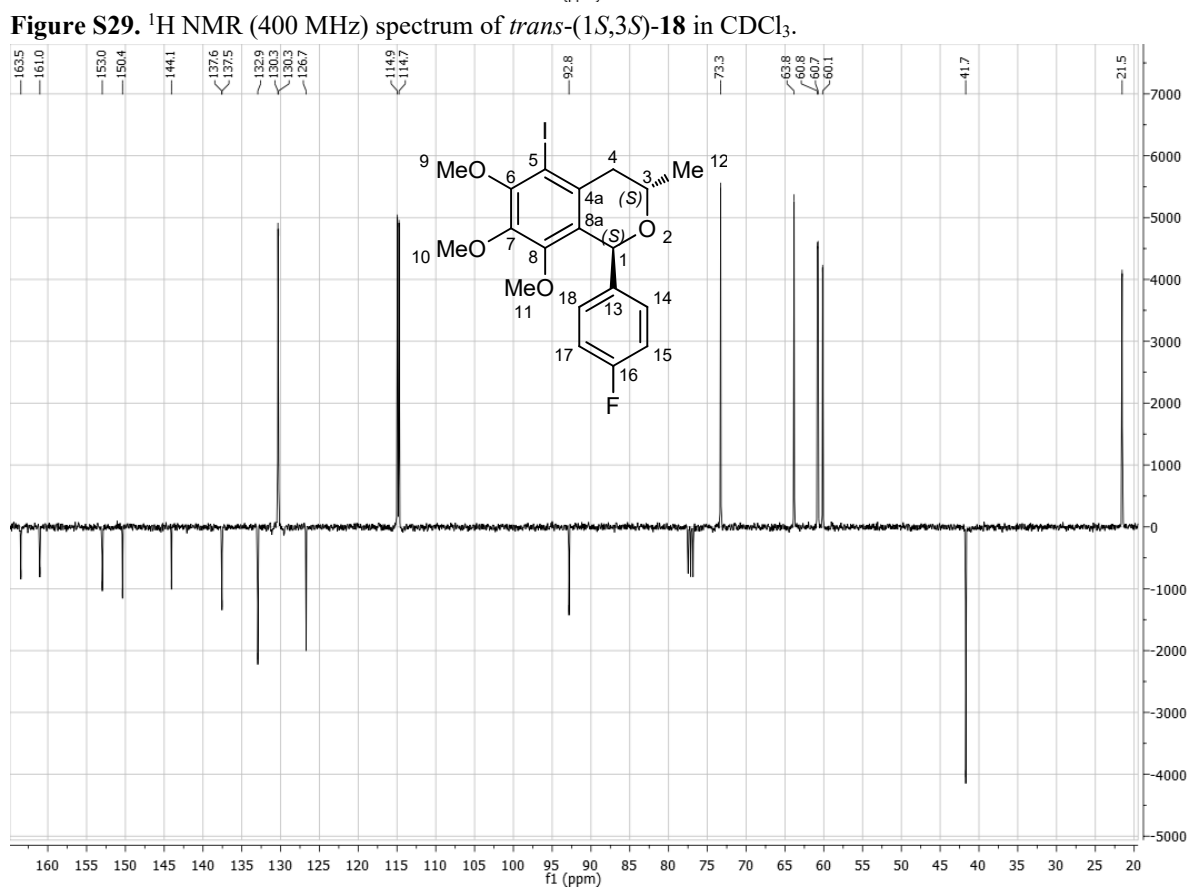
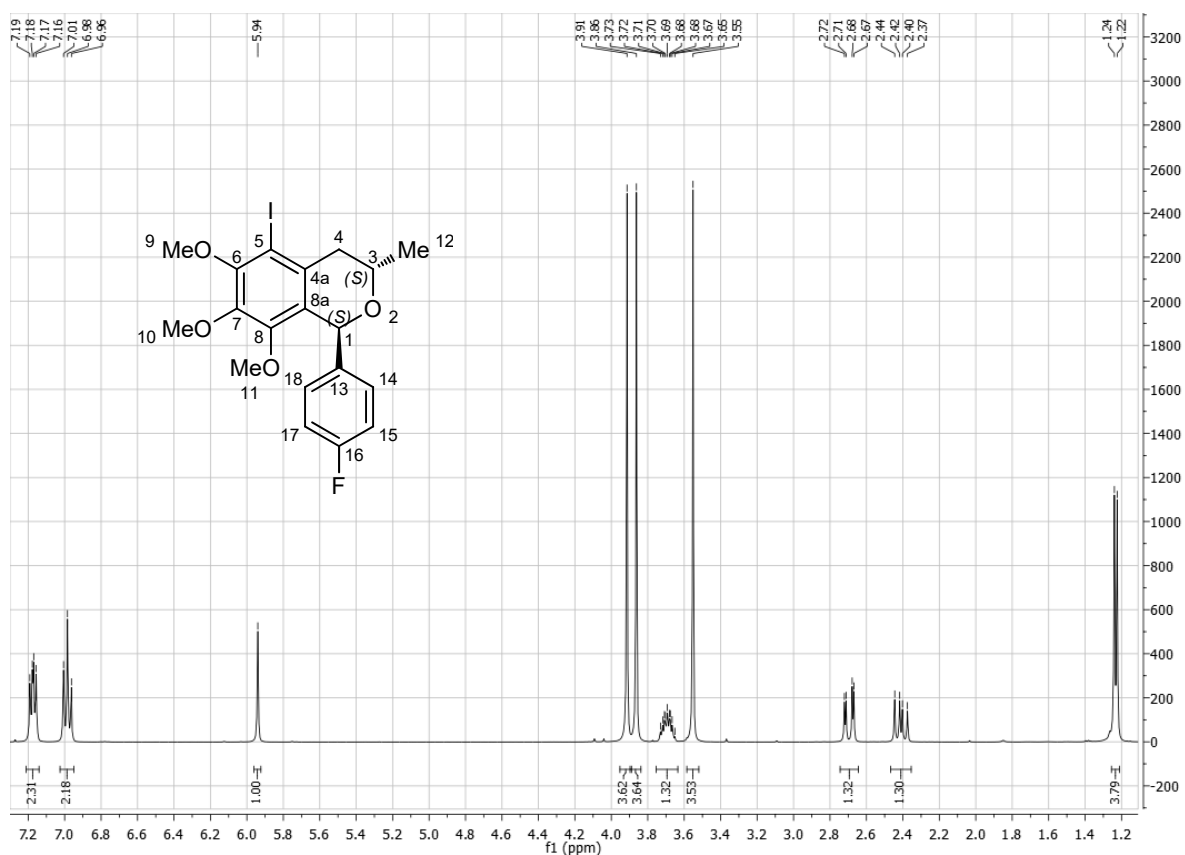


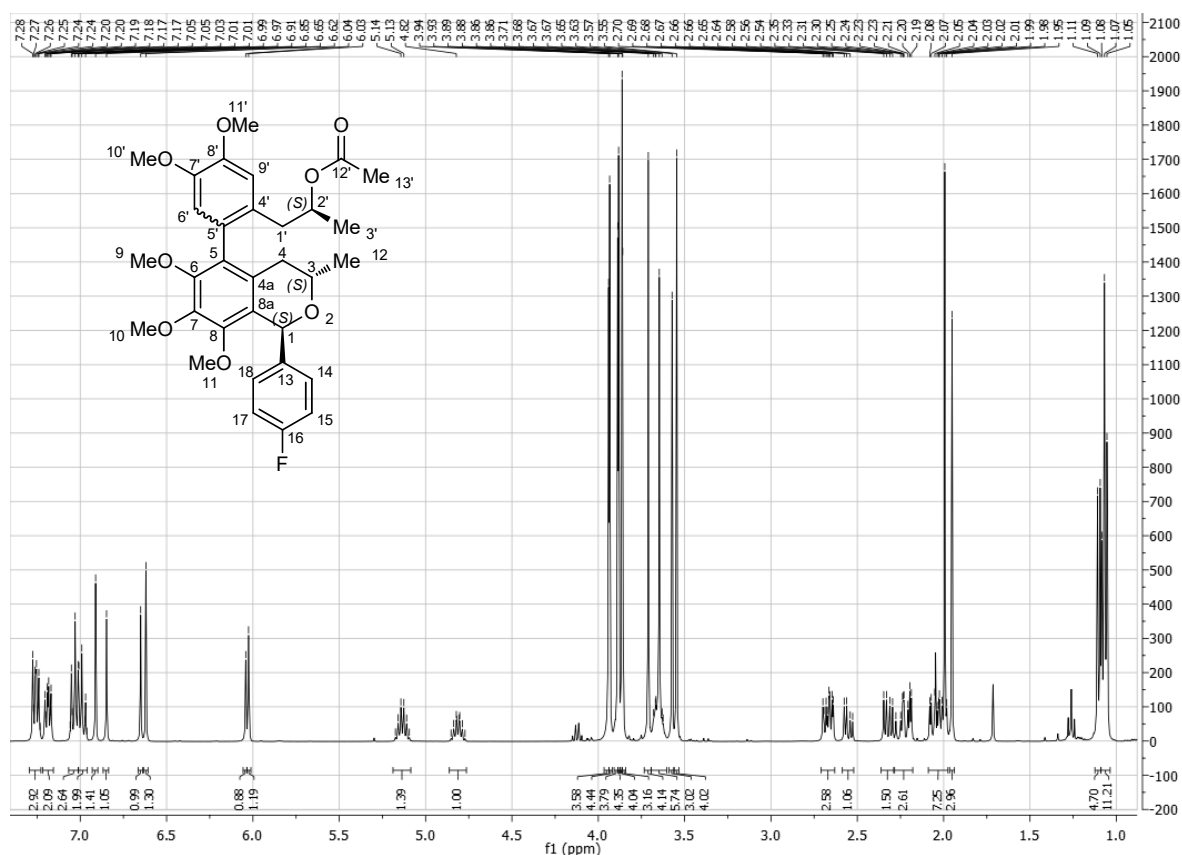
**Figure S27.**  $^1\text{H}$  NMR (400 MHz) spectrum of *cis*-(1*R*,3*S*)-**18** in  $\text{CDCl}_3$ .



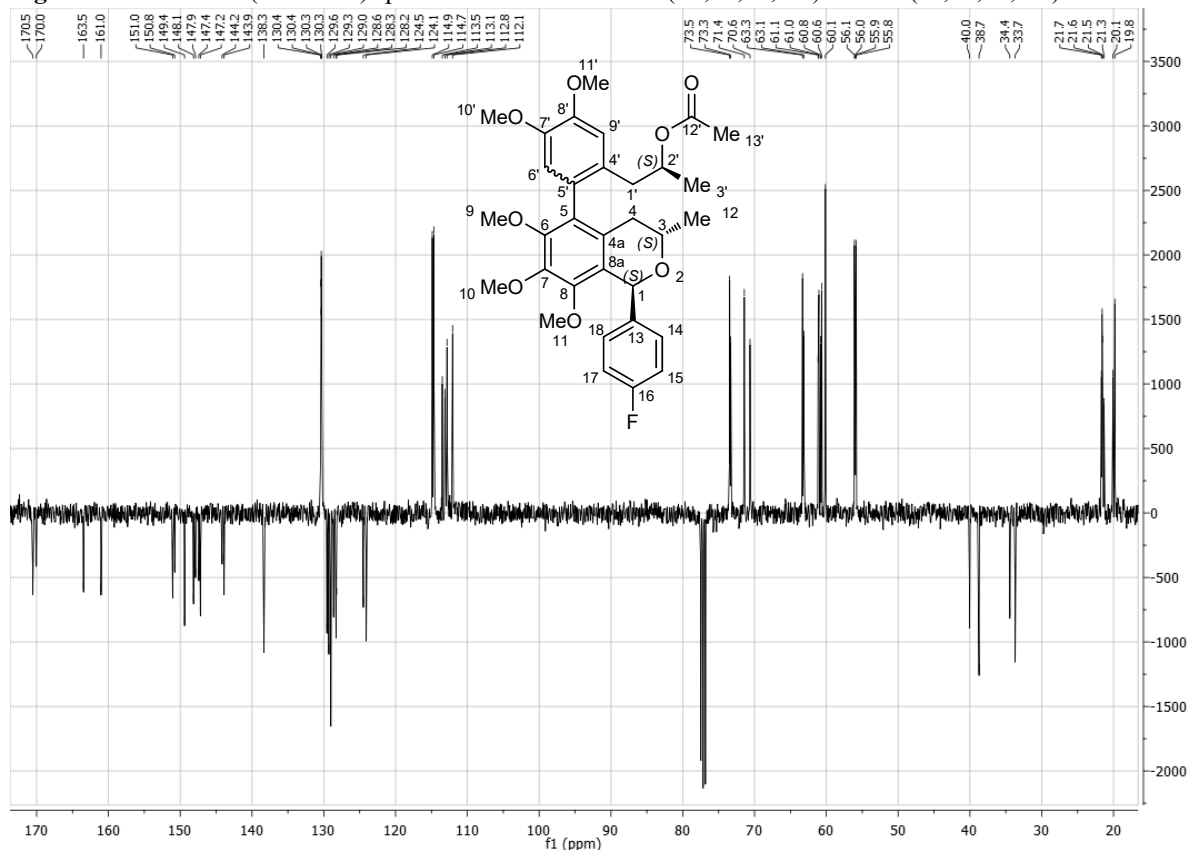
**Figure S28.**  $^{13}\text{C}$  NMR (100 MHz) spectrum of *cis*-(1*R*,3*S*)-**18** in  $\text{CDCl}_3$ .



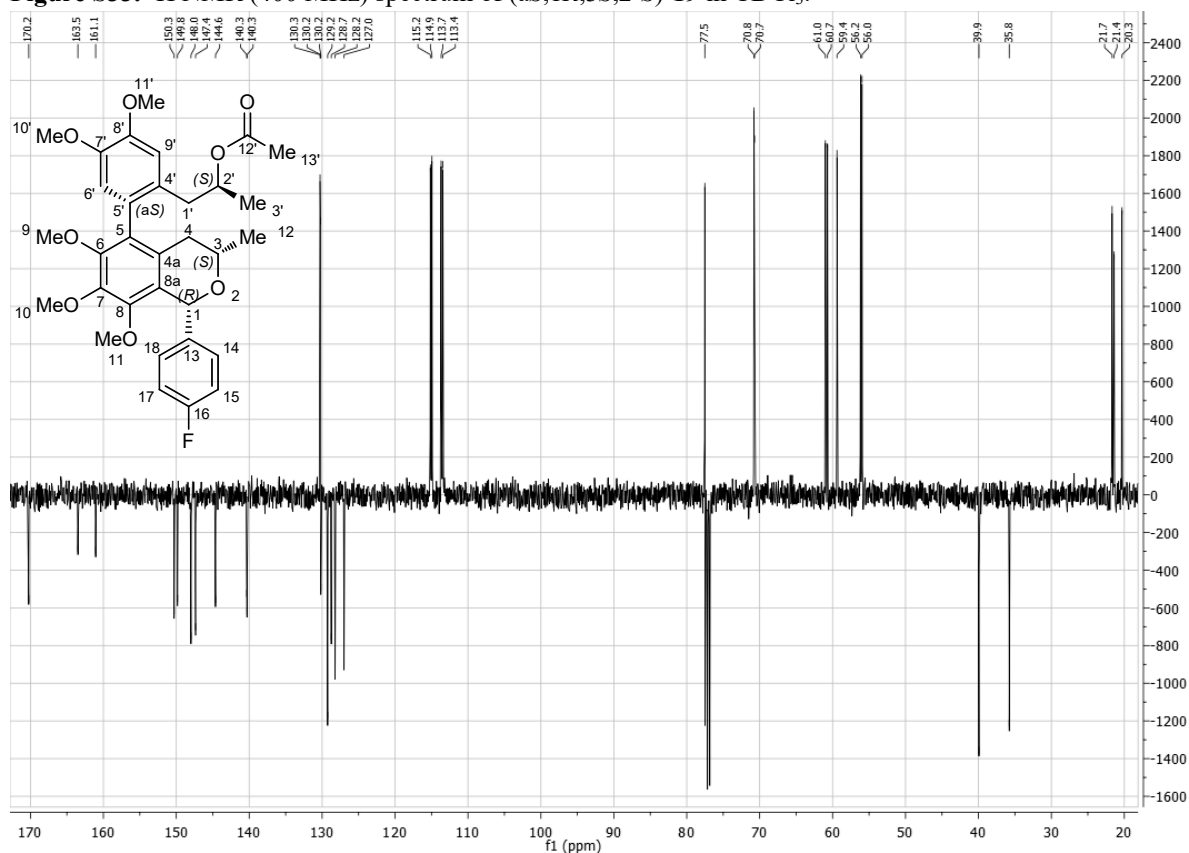
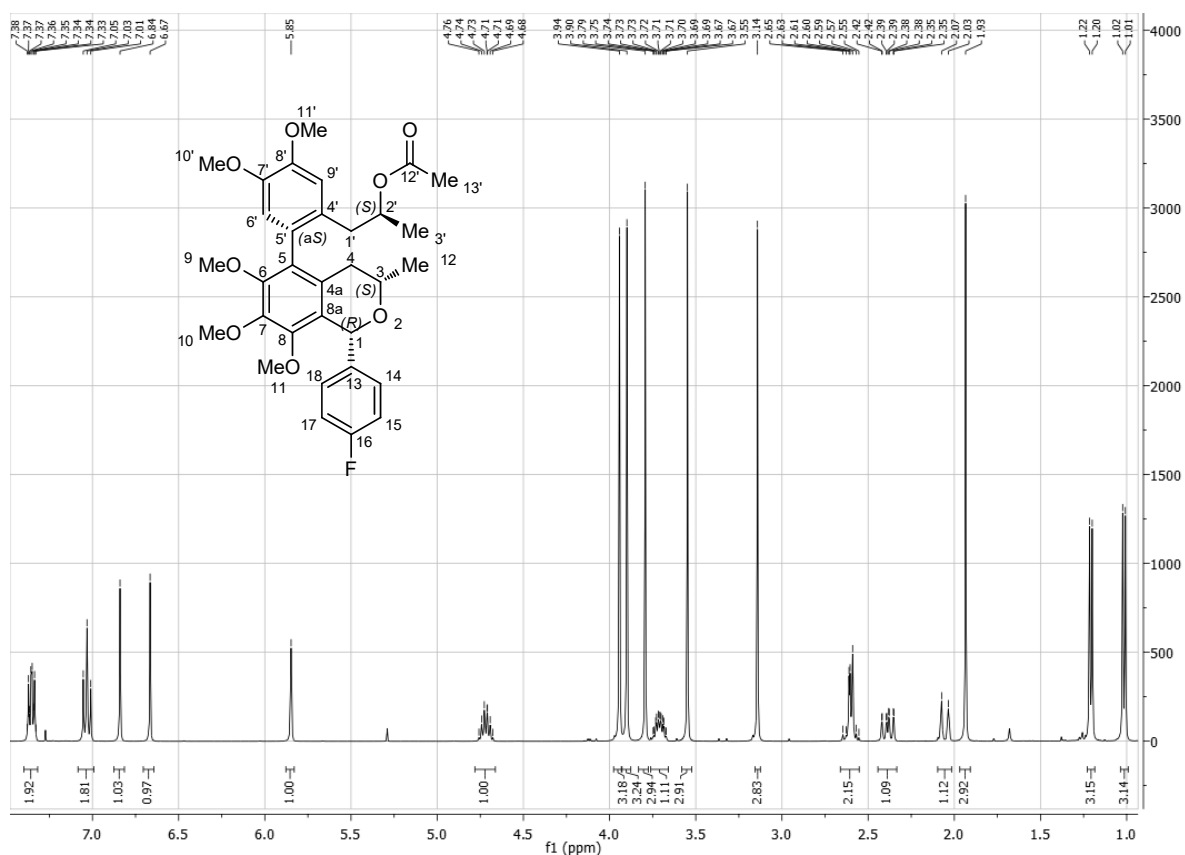




**Figure S31.** <sup>1</sup>H NMR (400 MHz) spectrum of the mixture of (aR,1S,3S,2'S)-19 and (aS,1S,3S,2'S)-19 in CDCl<sub>3</sub>.



**Figure S32.** <sup>13</sup>C NMR (100 MHz) spectrum of the mixture of (aR,1S,3S,2'S)-19 and (aS,1S,3S,2'S)-19 in CDCl<sub>3</sub>.



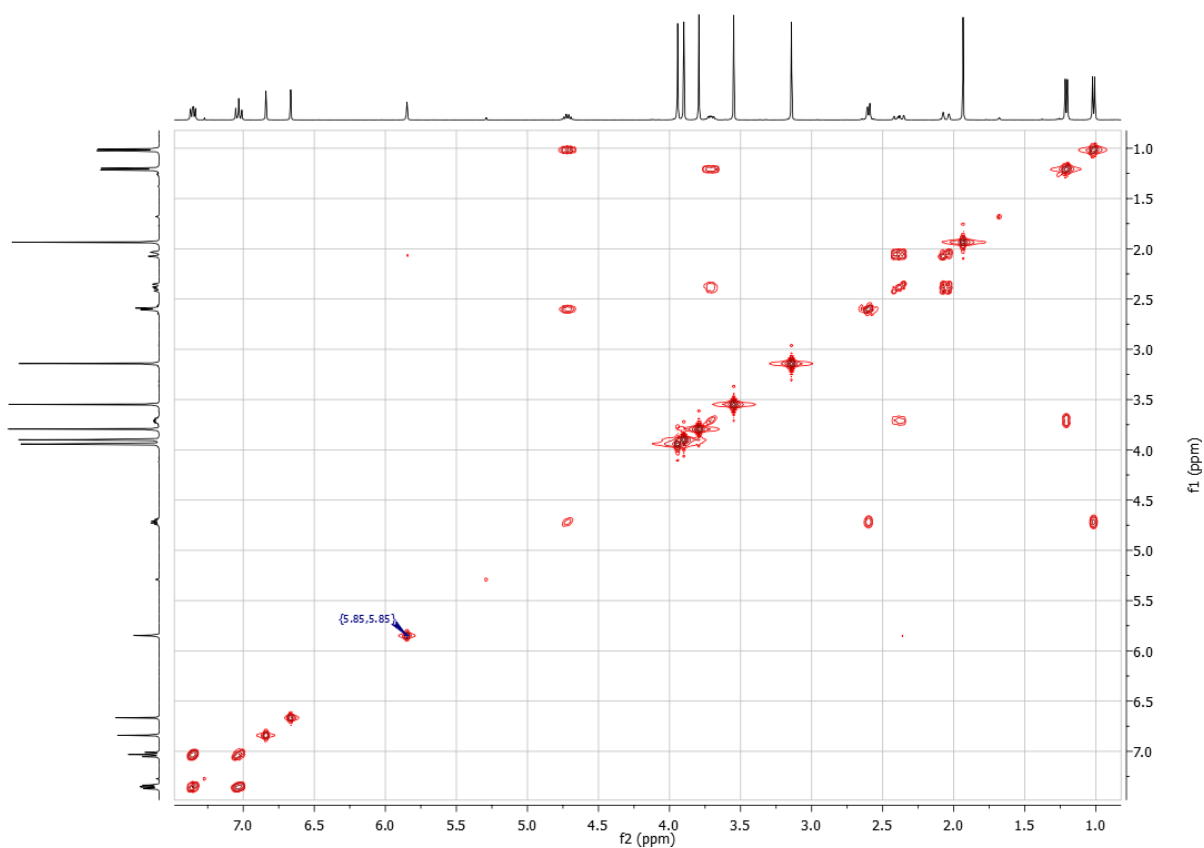


Figure S35.  $^1\text{H}$ - $^1\text{H}$  COSY NMR (400 MHz) spectrum of (aS,1R,3S,2'S)-**19** in  $\text{CDCl}_3$ .

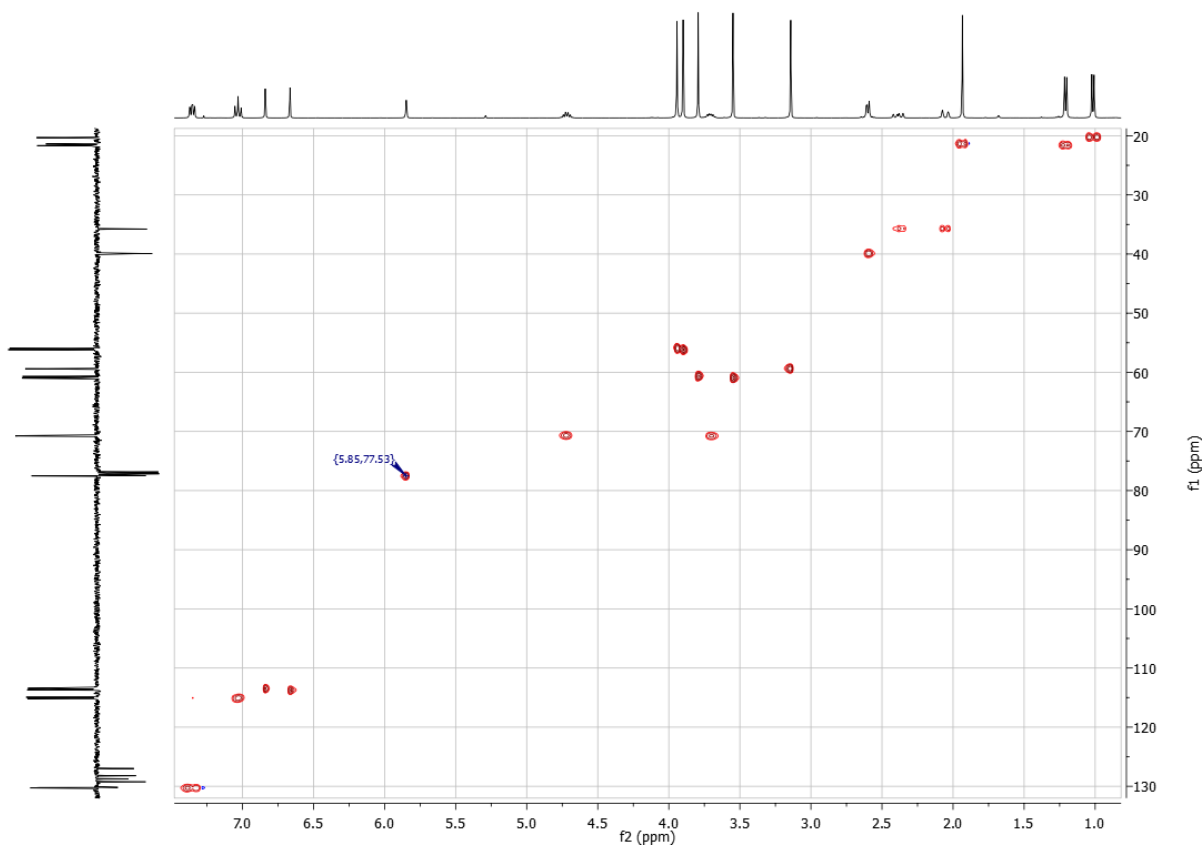
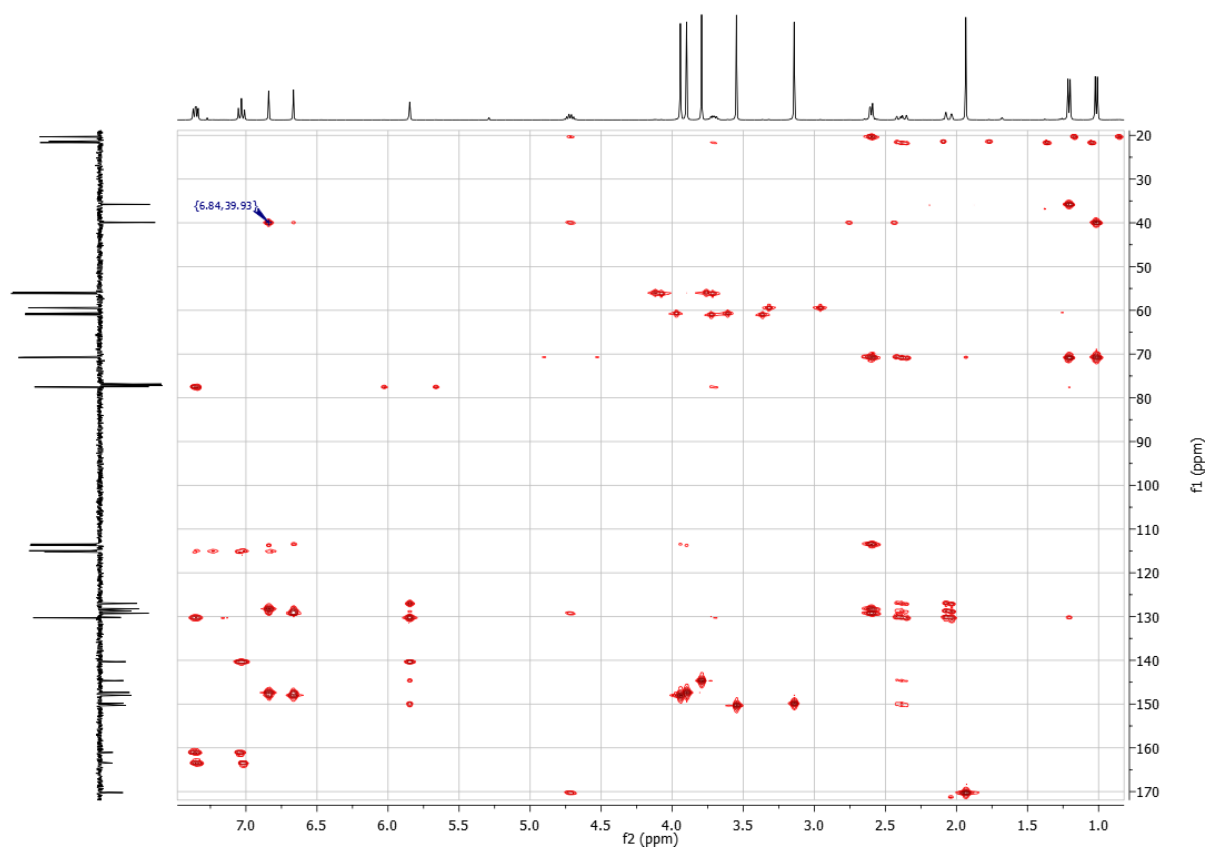
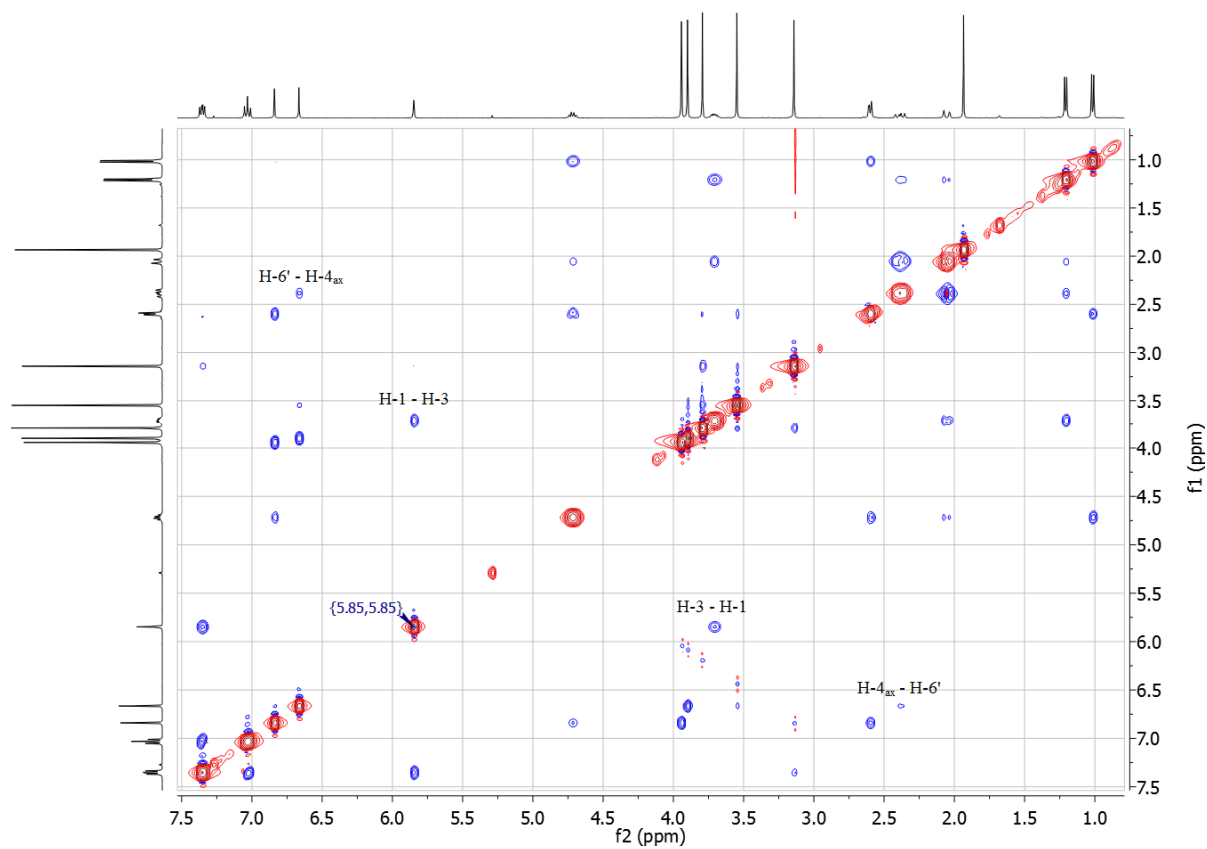


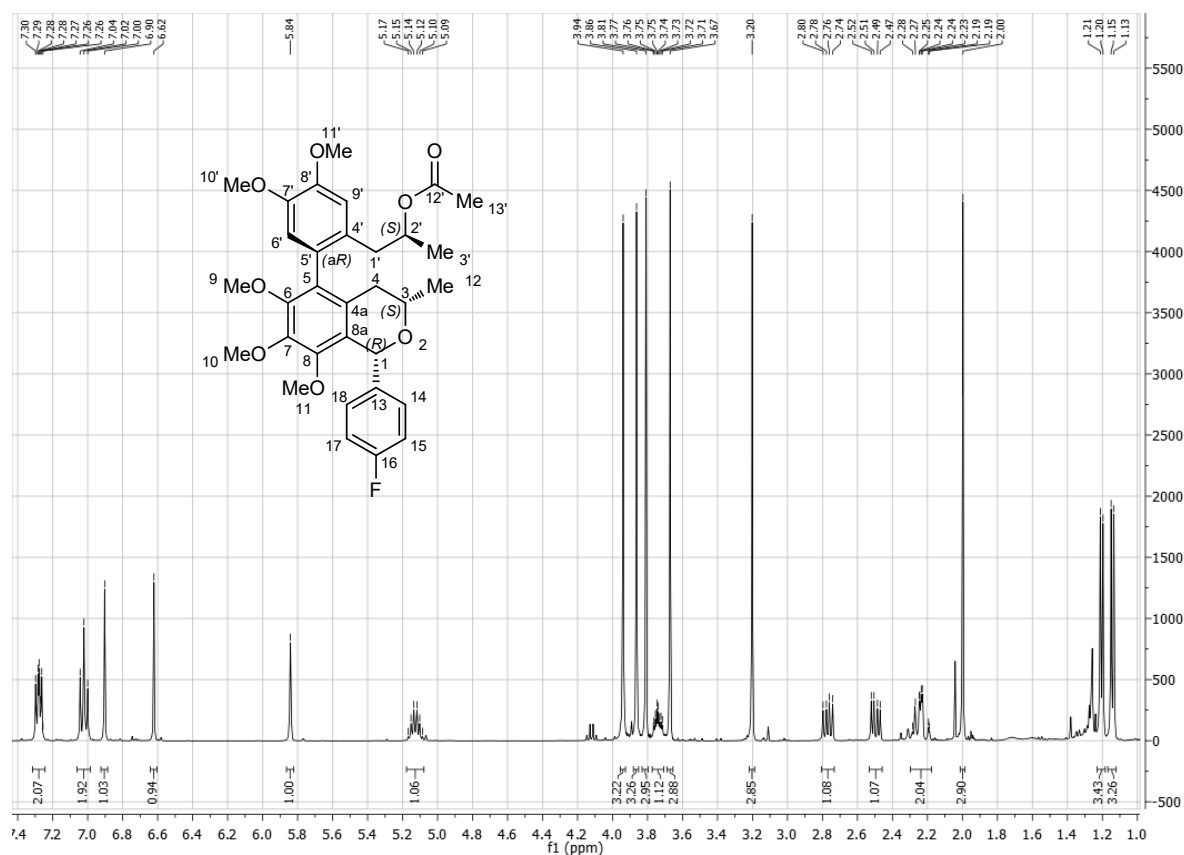
Figure S36.  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR (400 MHz) spectrum of (aS,1R,3S,2'S)-**19** in  $\text{CDCl}_3$ .



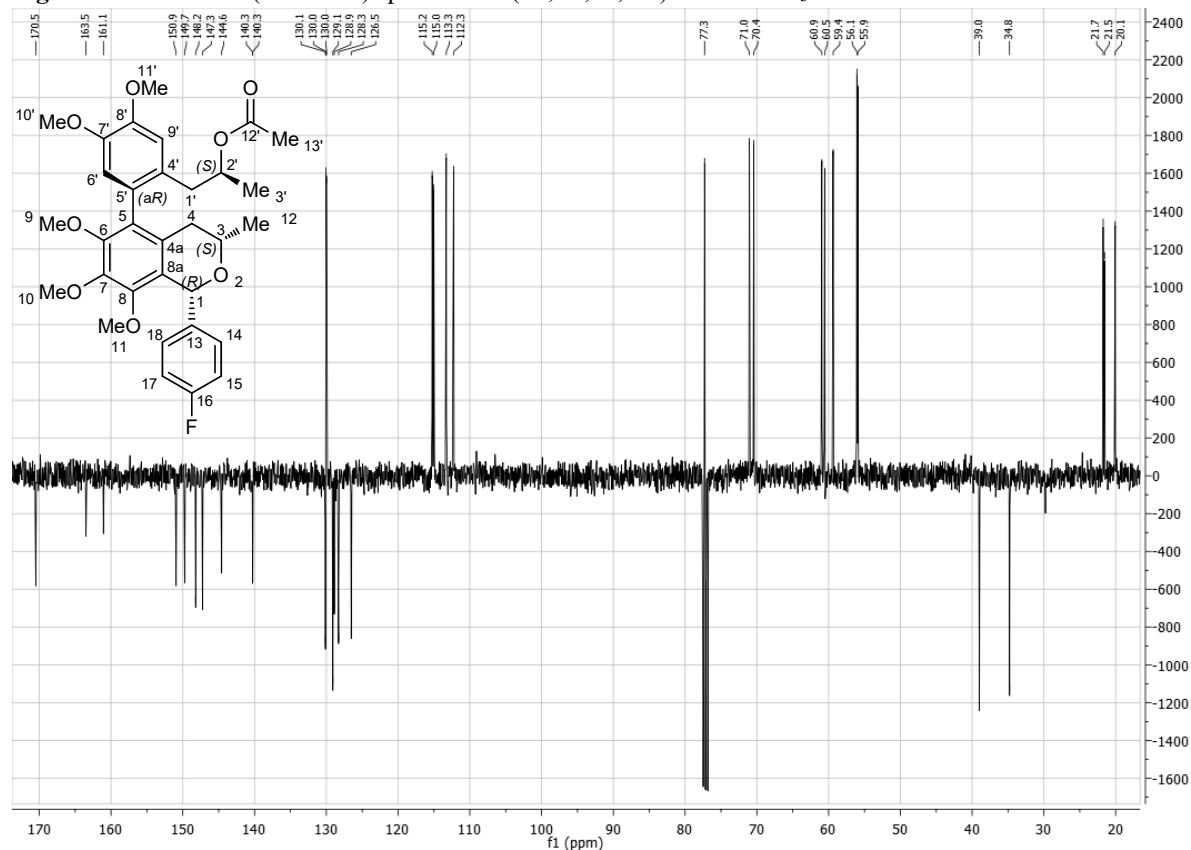
**Figure S37.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC NMR (400 MHz) spectrum of  $(aS,1R,3S,2'S)$ -**19** in  $\text{CDCl}_3$ .



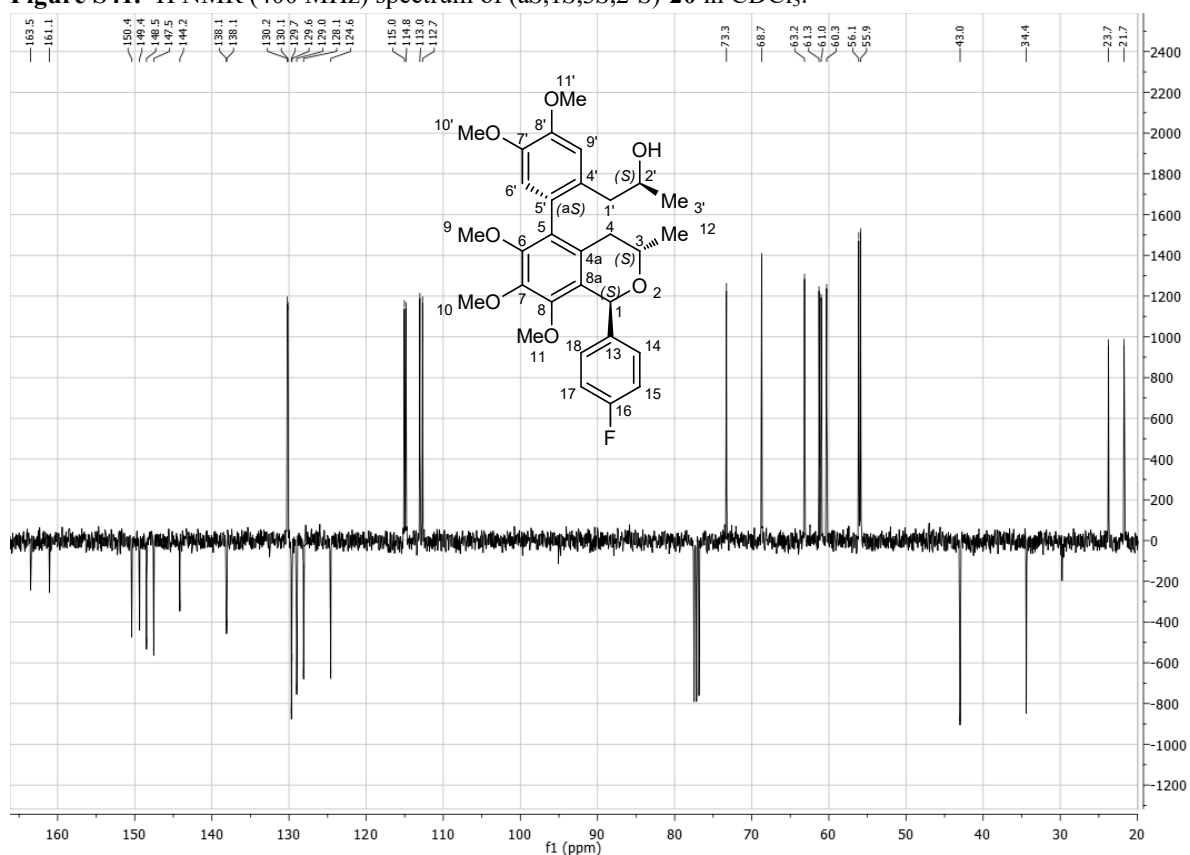
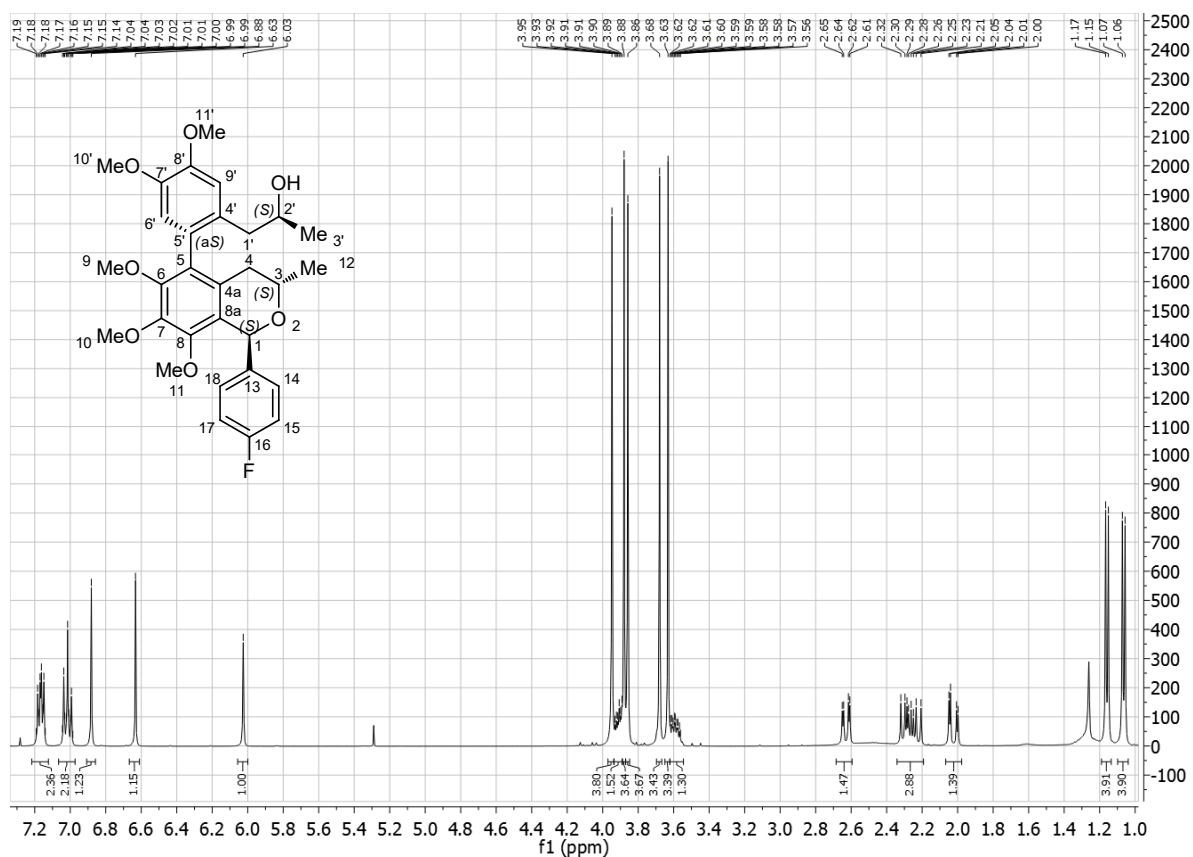
**Figure S38.**  $^1\text{H}$ - $^1\text{H}$  NOESY NMR (400 MHz) spectrum of  $(aS,1R,3S,2'S)$ -**19** in  $\text{CDCl}_3$ .



**Figure S39.**  $^1\text{H}$  NMR (400 MHz) spectrum of (aR,1R,3S,2'S)-19 in  $\text{CDCl}_3$ .



**Figure S40.**  $^{13}\text{C}$  NMR (100 MHz) spectrum of (aR,1R,3S,2'S)-19 in  $\text{CDCl}_3$ .



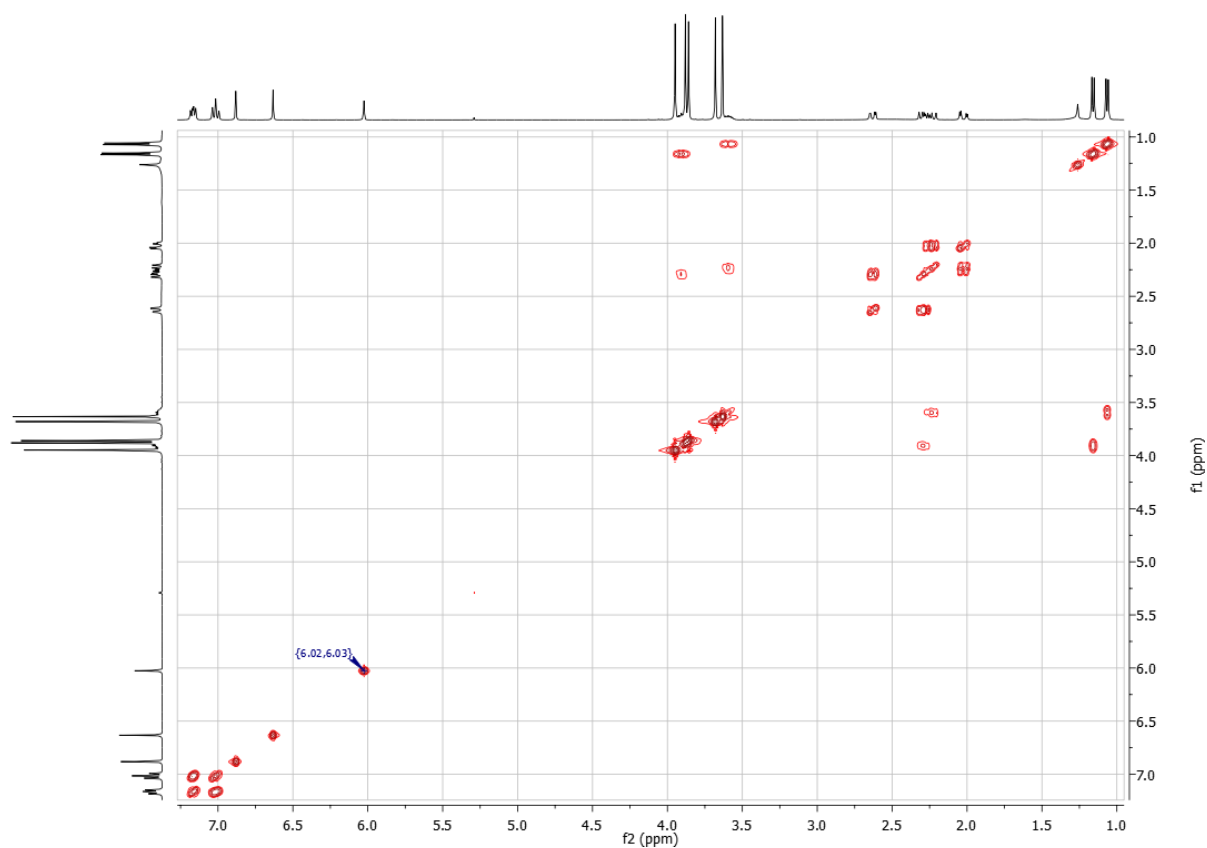


Figure S43.  $^1\text{H}$ - $^1\text{H}$  COSY NMR (400 MHz) spectrum of  $(aS,1S,3S,2'S)$ -**20** in  $\text{CDCl}_3$ .

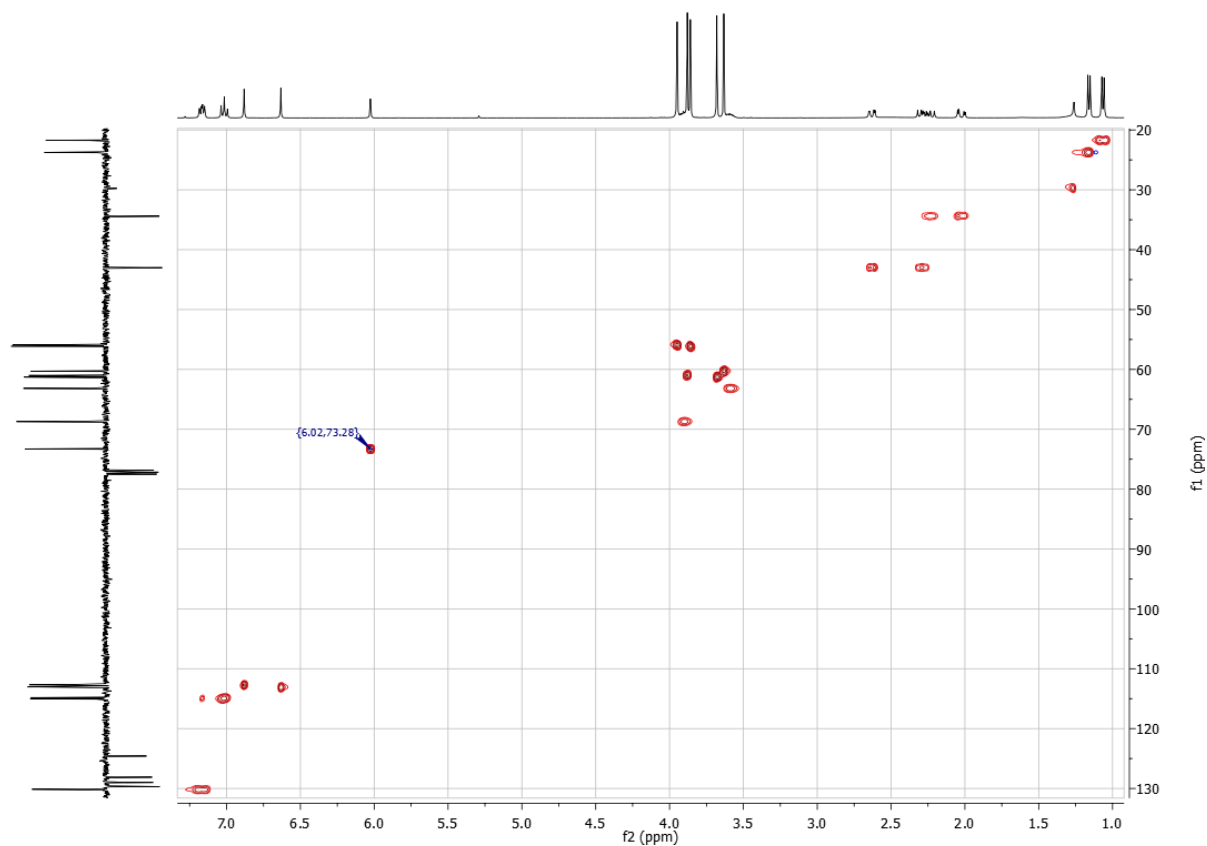


Figure S44.  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR (400 MHz) spectrum of  $(aS,1S,3S,2'S)$ -**20** in  $\text{CDCl}_3$ .



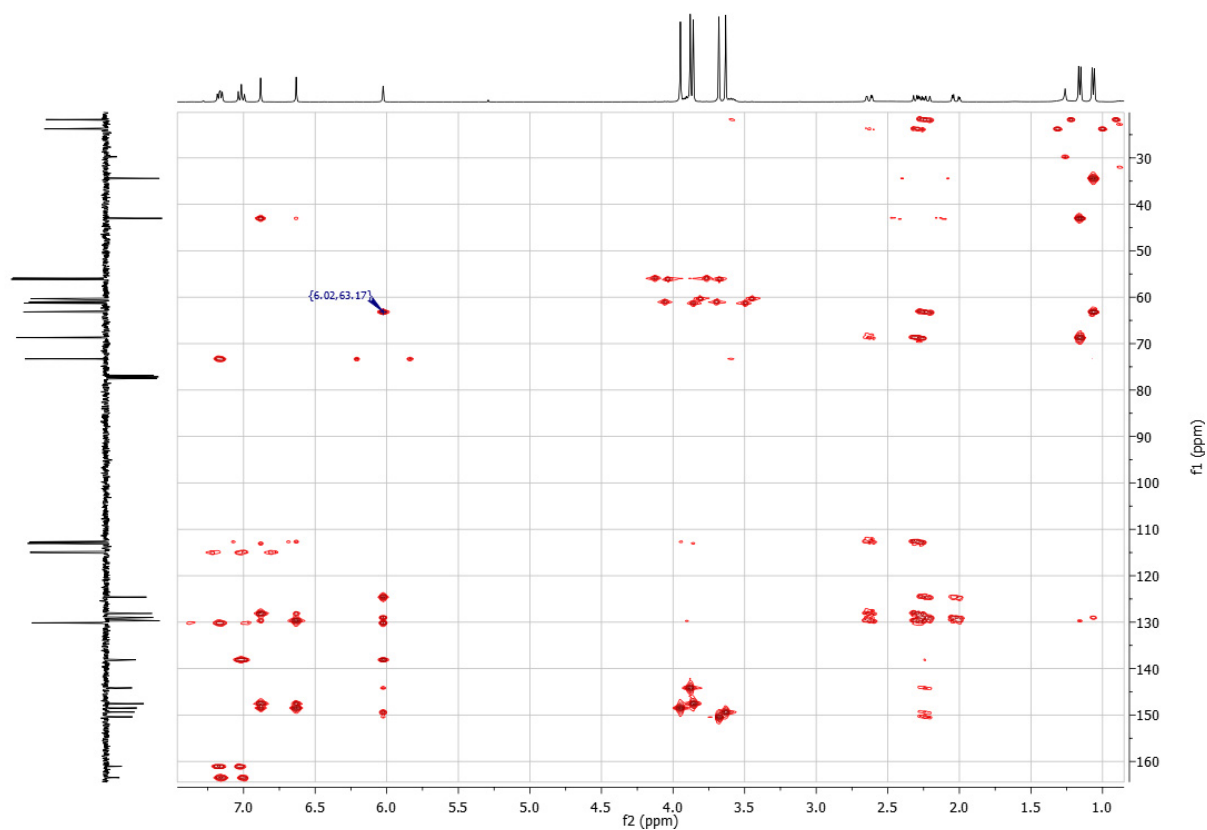


Figure S45.  $^1\text{H}$ - $^{13}\text{C}$  HMBC NMR (400 MHz) spectrum of (aS,1S,3S,2'S)-**20** in  $\text{CDCl}_3$ .

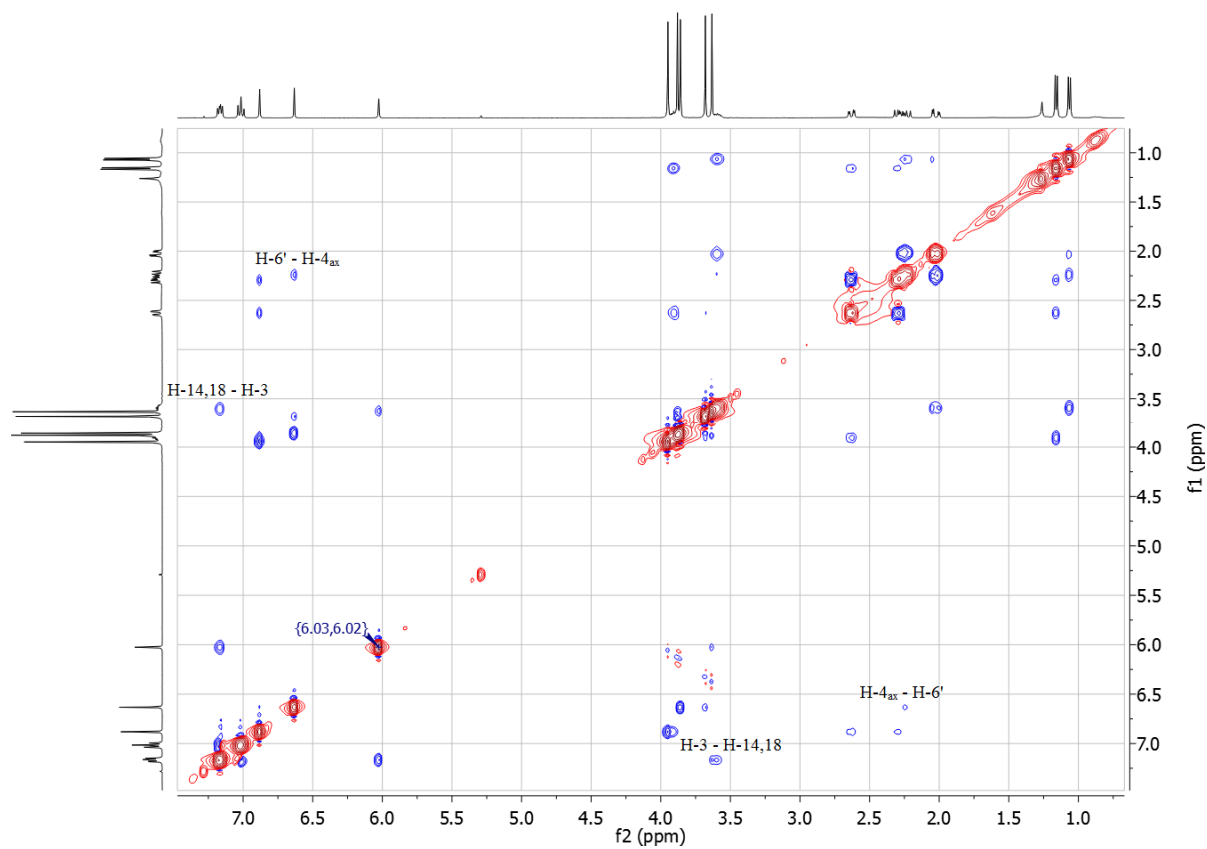
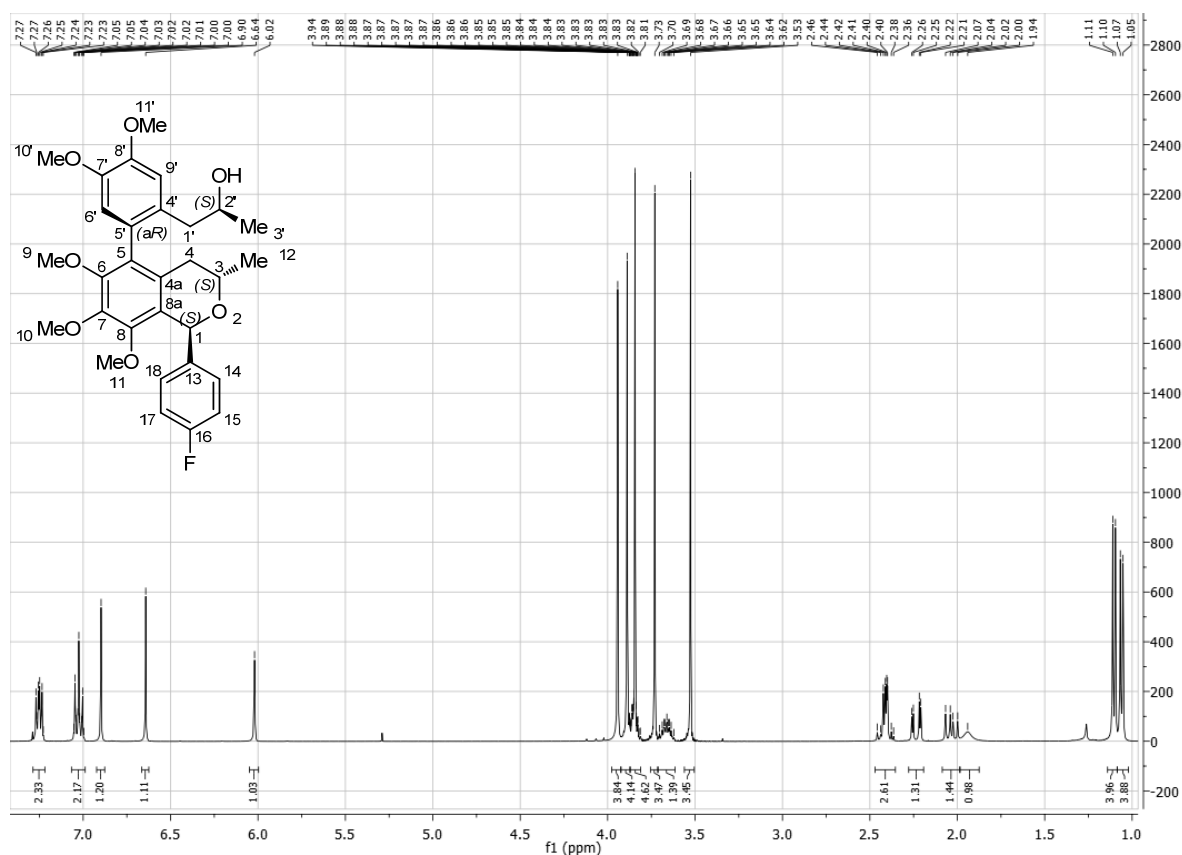
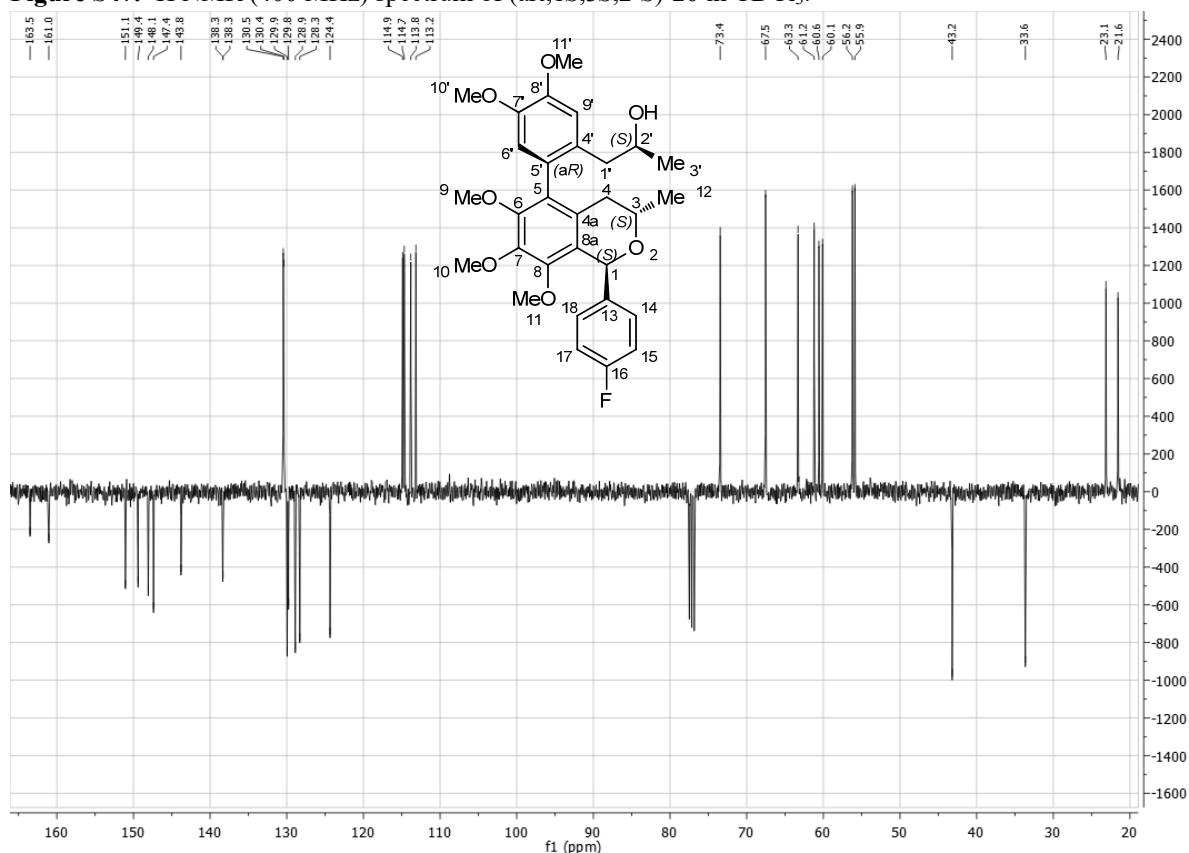


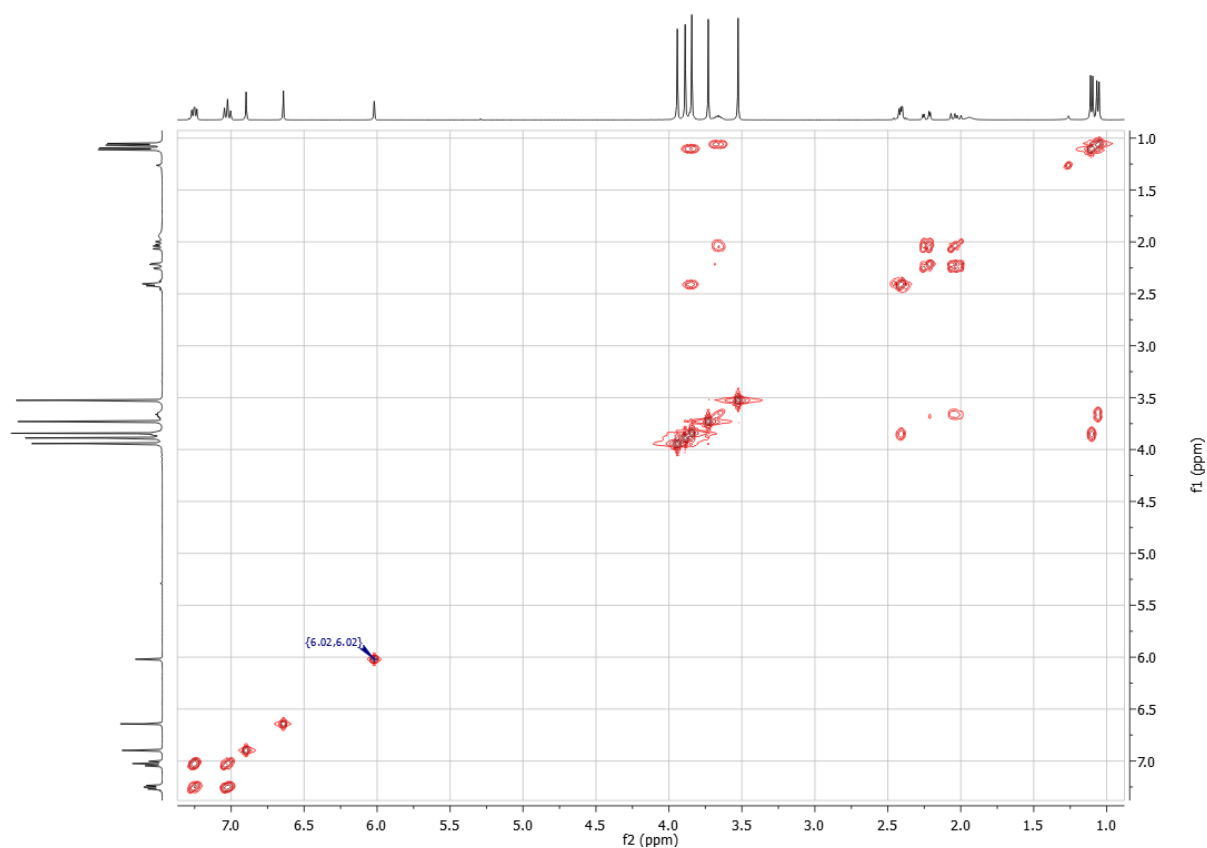
Figure S46.  $^1\text{H}$ - $^1\text{H}$  NOESY NMR (400 MHz) spectrum of (aS,1S,3S,2'S)-**20** in  $\text{CDCl}_3$ .



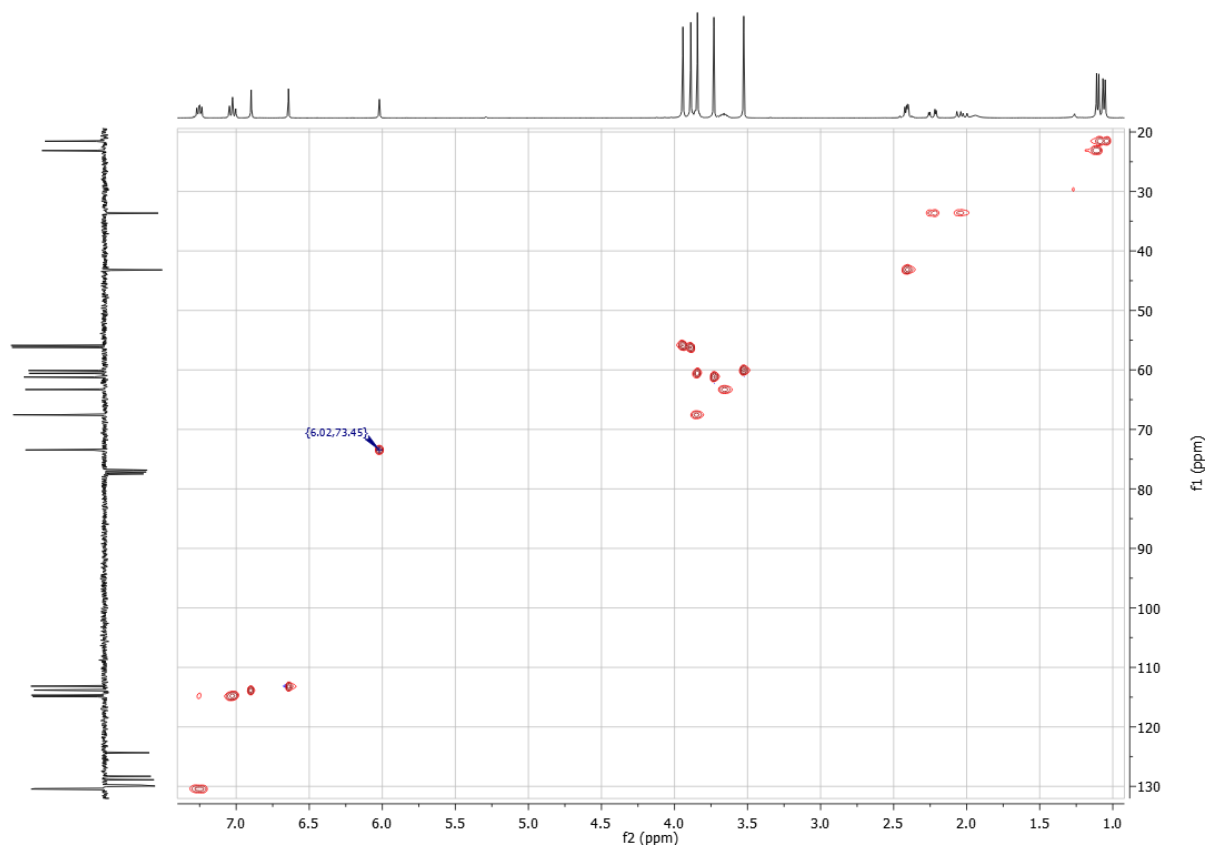
**Figure S47.**  $^1\text{H}$  NMR (400 MHz) spectrum of (aR,1S,3S,2'S)-20 in  $\text{CDCl}_3$ .



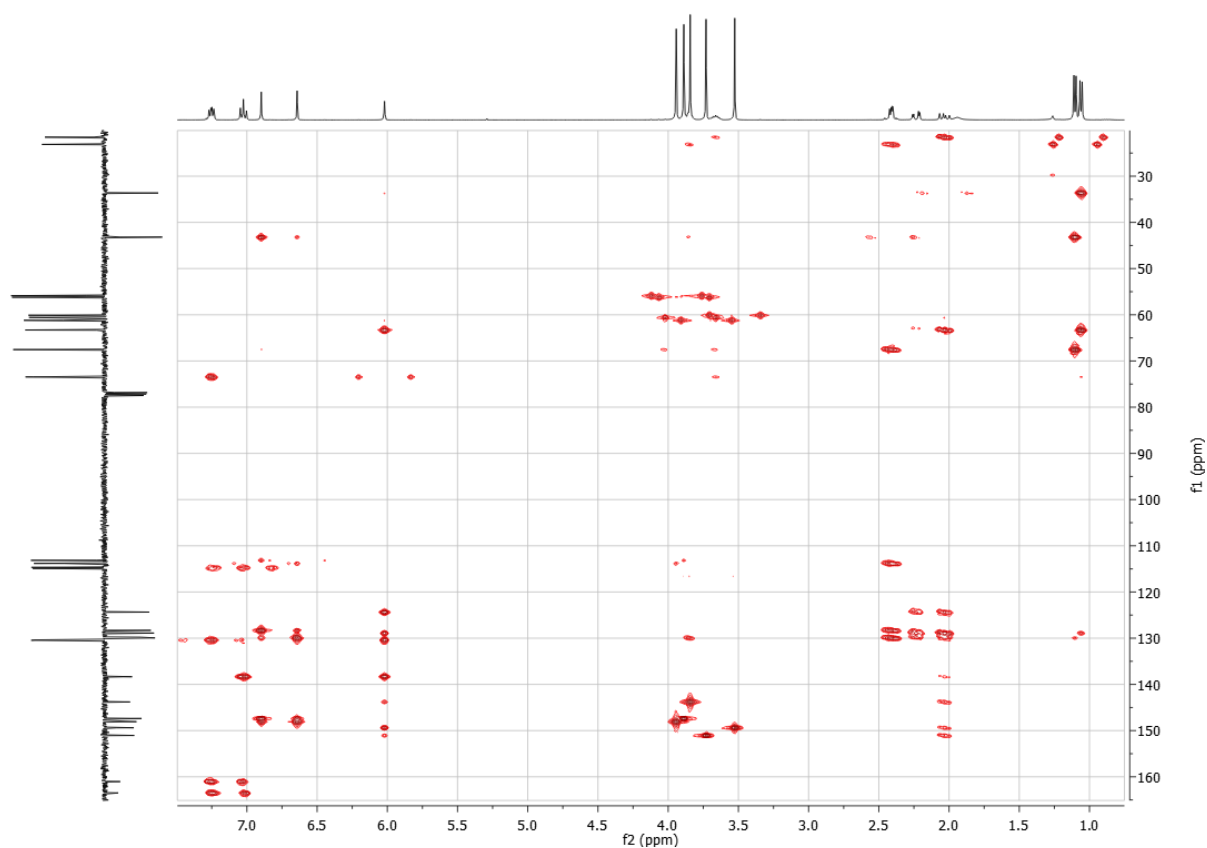
**Figure S48.**  $^{13}\text{C}$  NMR (100 MHz) spectrum of (aR,1S,3S,2'S)-20 in  $\text{CDCl}_3$ .



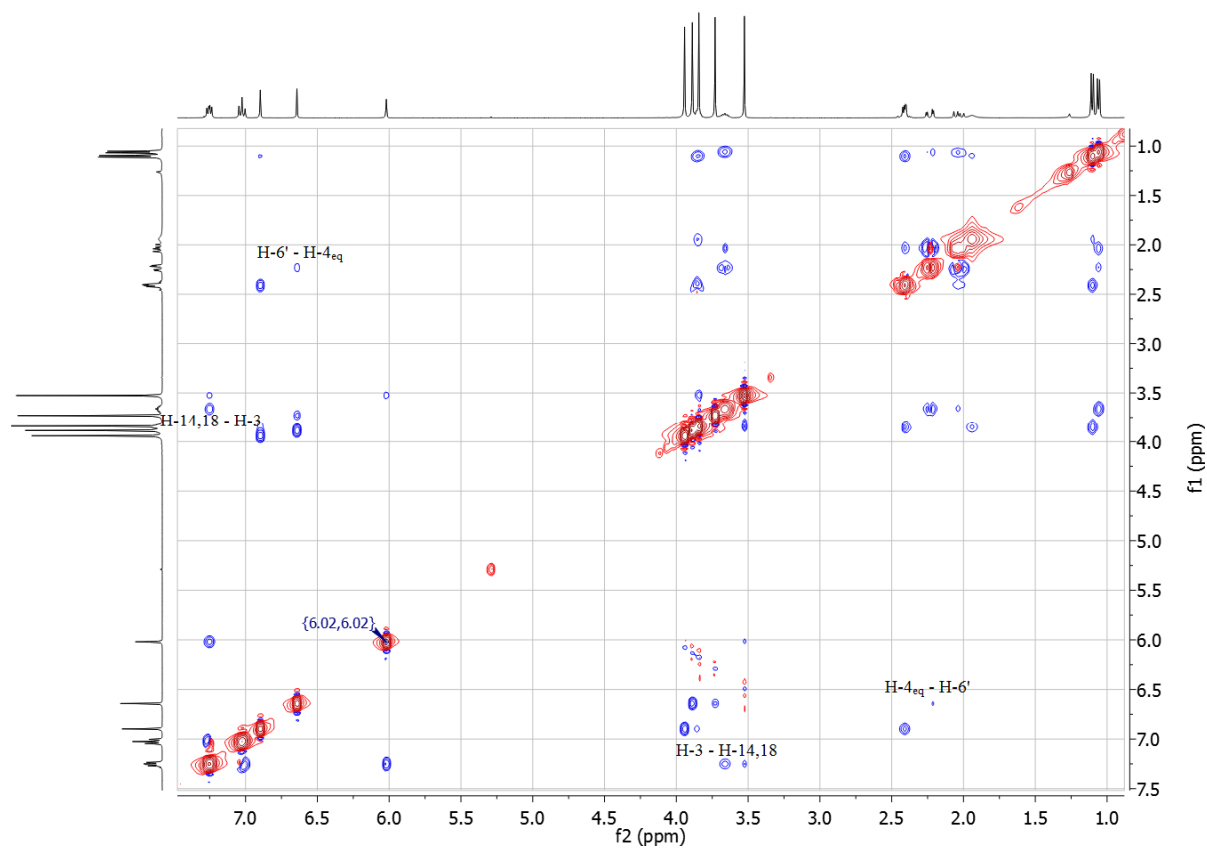
**Figure S49.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR (400 MHz) spectrum of (a*R*,1*S*,3*S*,2'*S*)-**20** in  $\text{CDCl}_3$ .



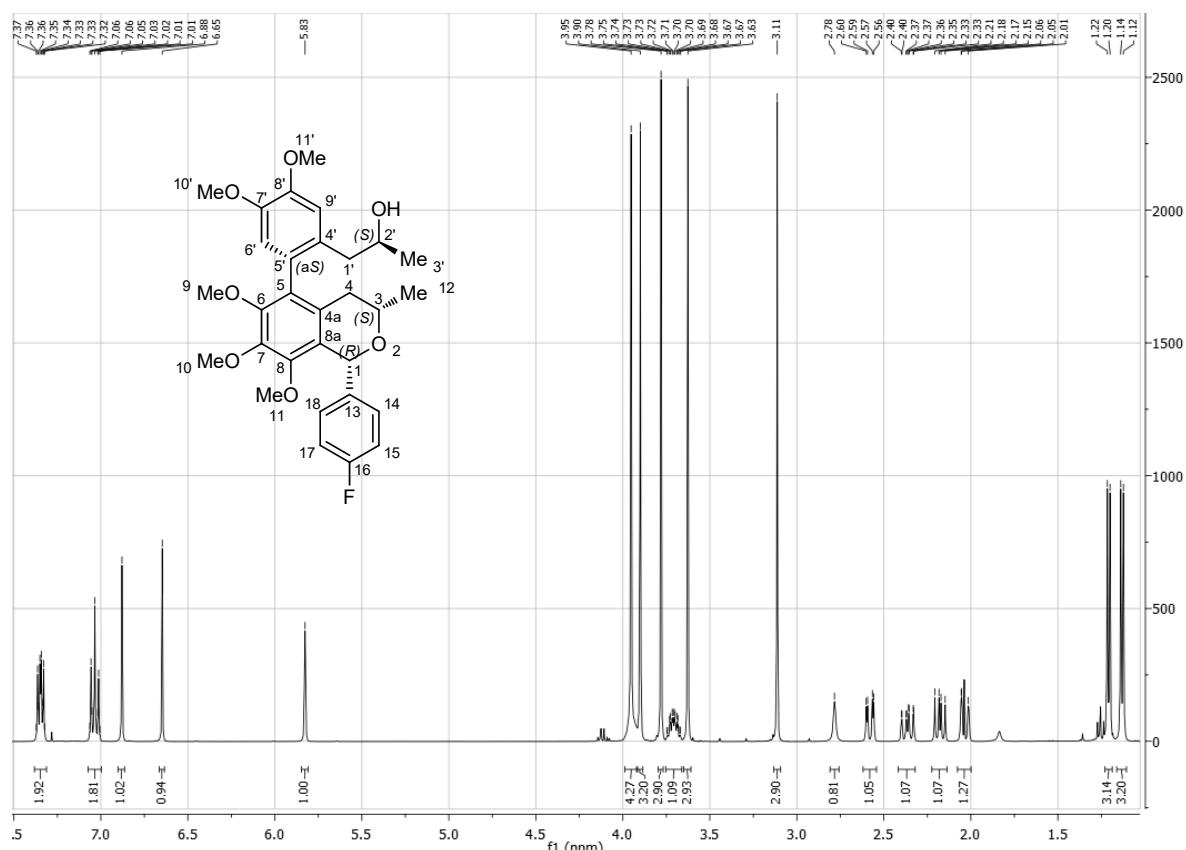
**Figure S50.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR (400 MHz) spectrum of (a*R*,1*S*,3*S*,2'*S*)-**20** in  $\text{CDCl}_3$ .



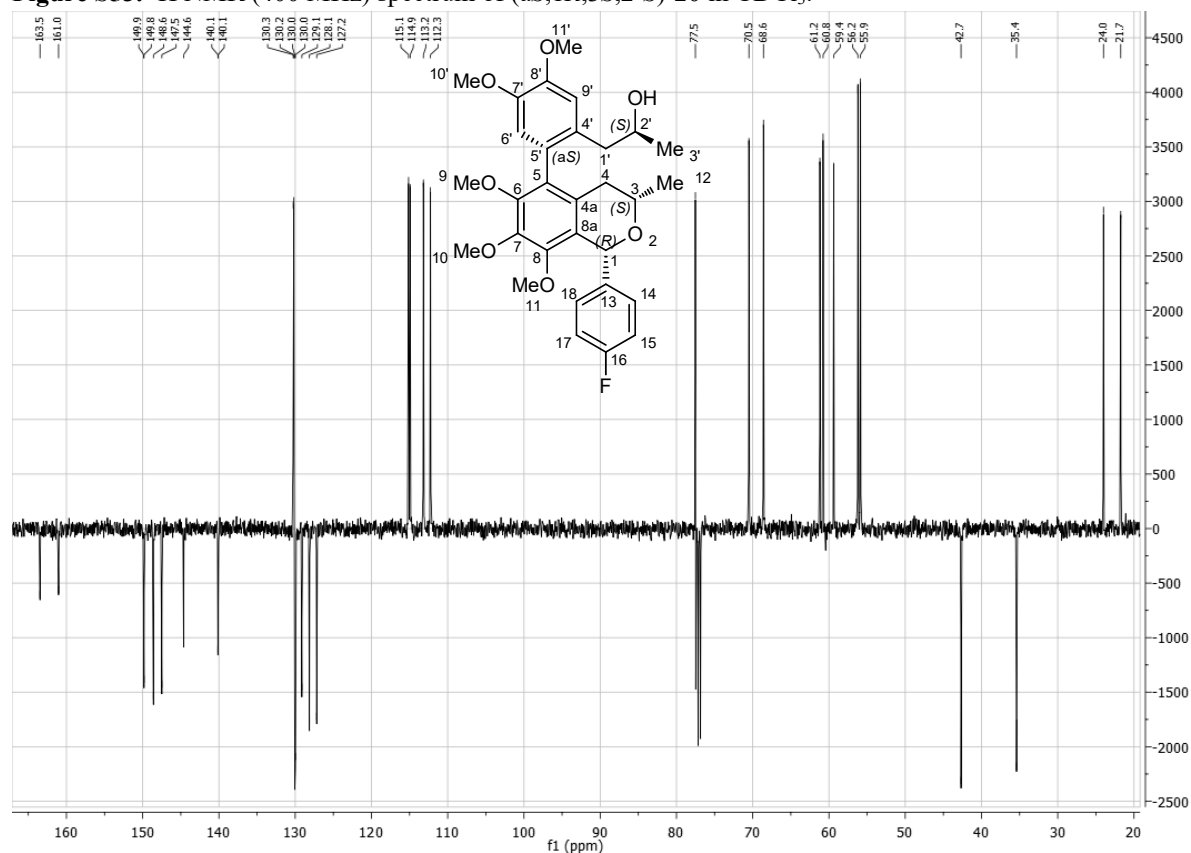
**Figure S51.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC NMR (400 MHz) spectrum of (a*R*,1*S*,3*S*,2'*S*)-**20** in  $\text{CDCl}_3$ .



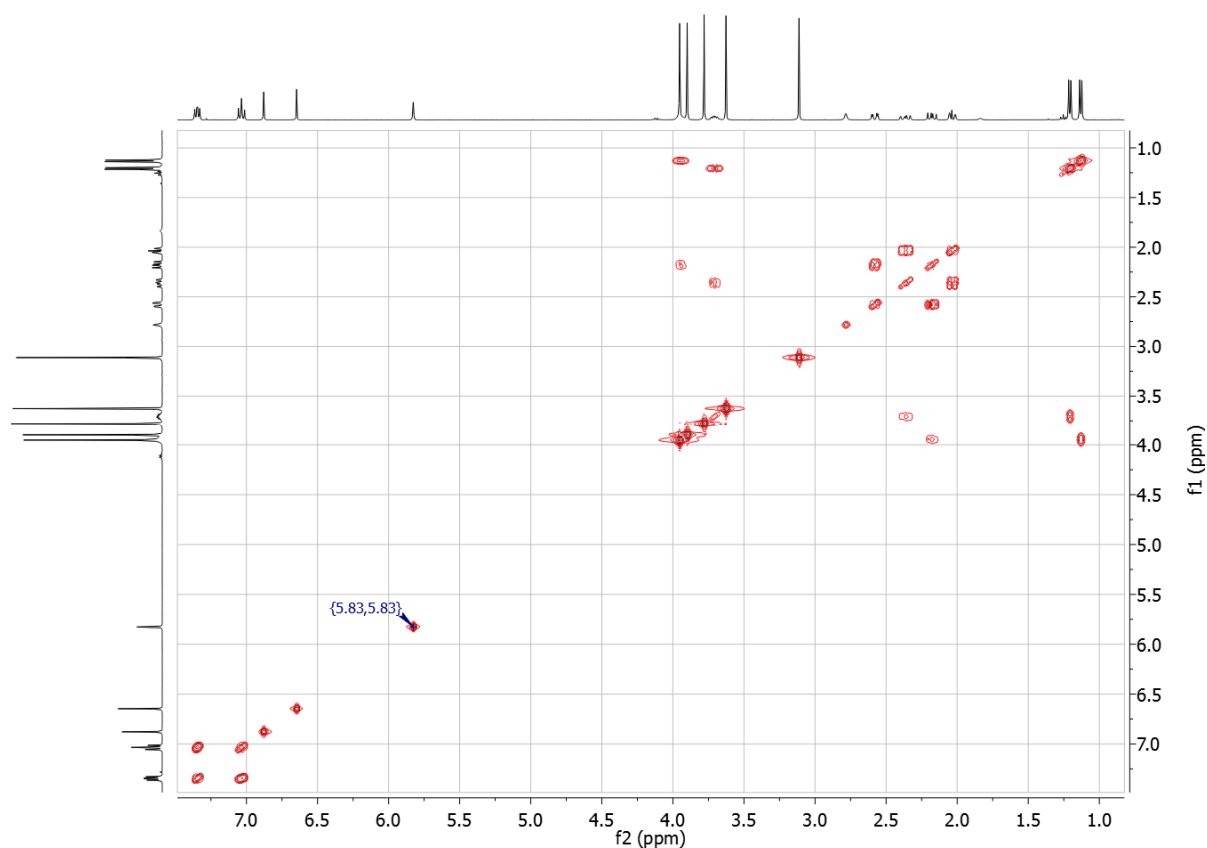
**Figure S52.**  $^1\text{H}$ - $^1\text{H}$  NOESY NMR (400 MHz) spectrum of (a*R*,1*S*,3*S*,2'*S*)-**20** in  $\text{CDCl}_3$ .



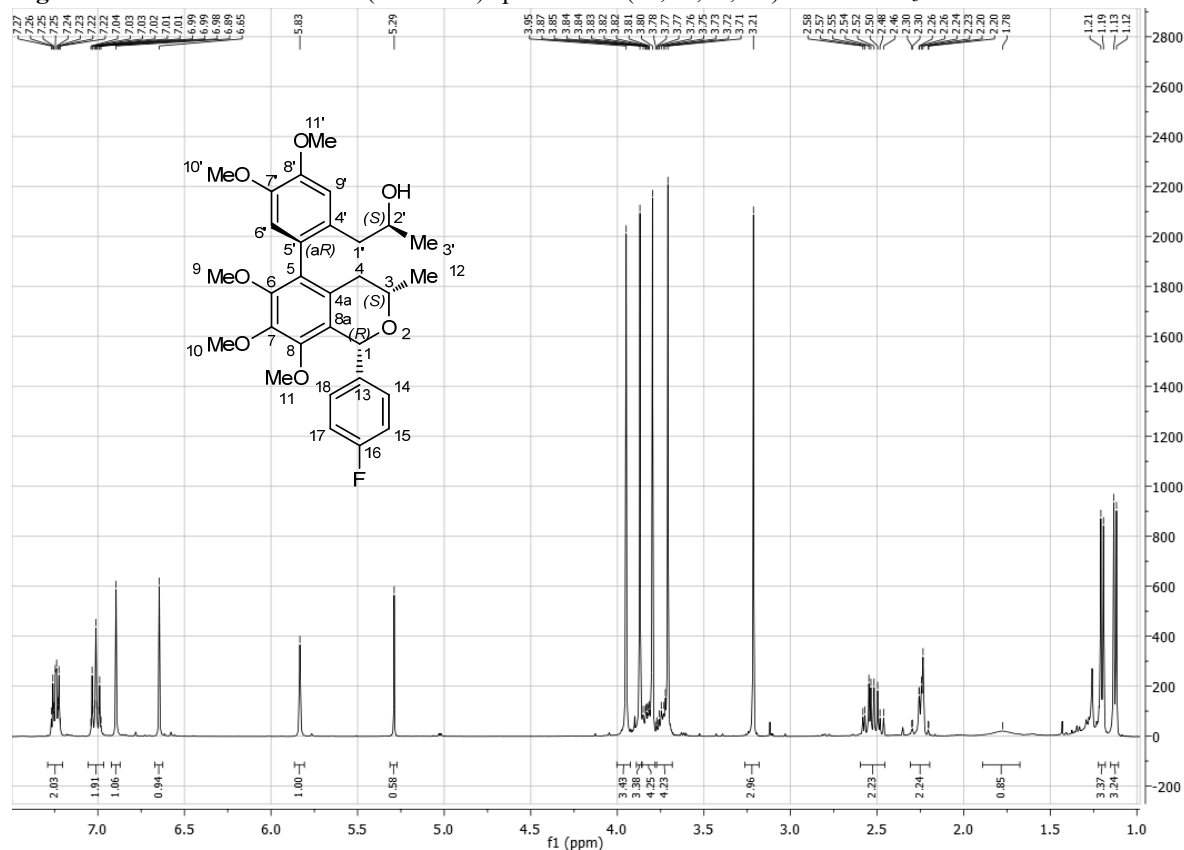
**Figure S53.** <sup>1</sup>H NMR (400 MHz) spectrum of (aS,1R,3S,2'S)-20 in CDCl<sub>3</sub>.



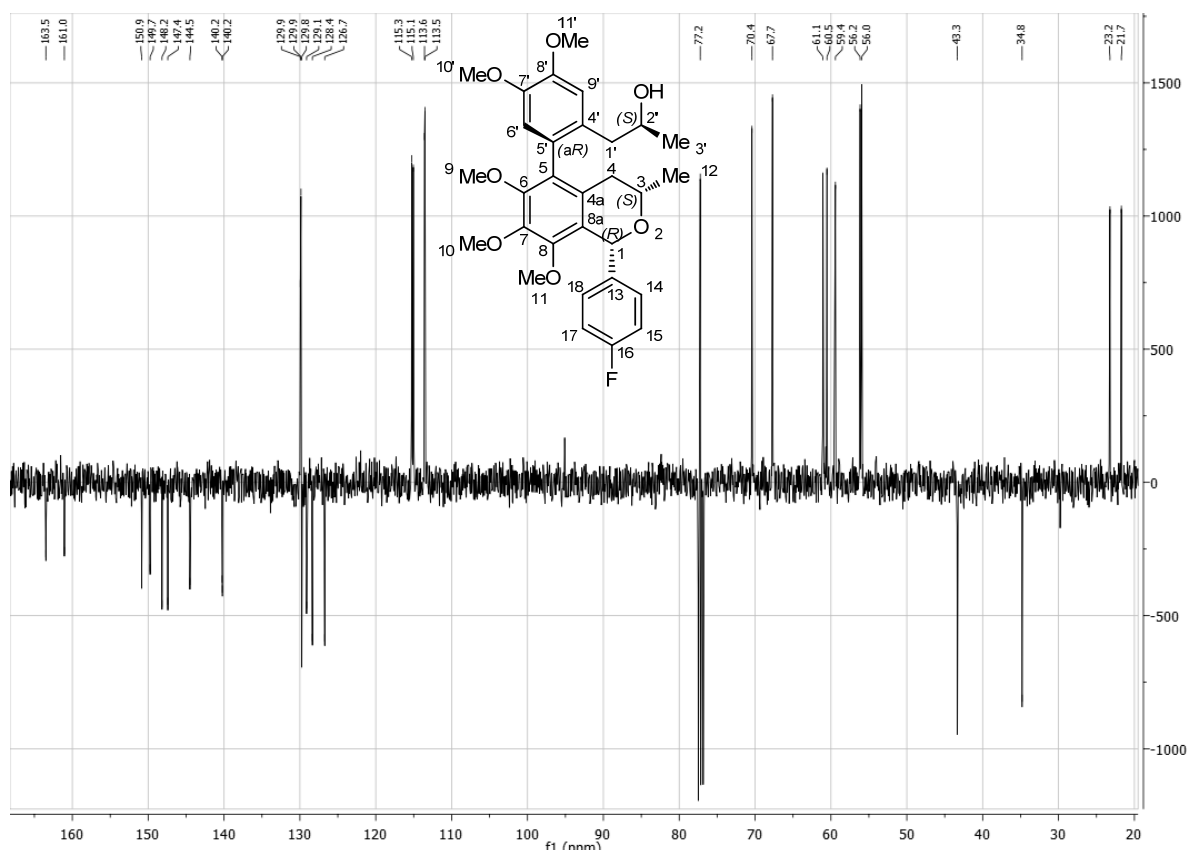
**Figure S54.** <sup>13</sup>C NMR (100 MHz) spectrum of (aS,1R,3S,2'S)-20 in CDCl<sub>3</sub>.



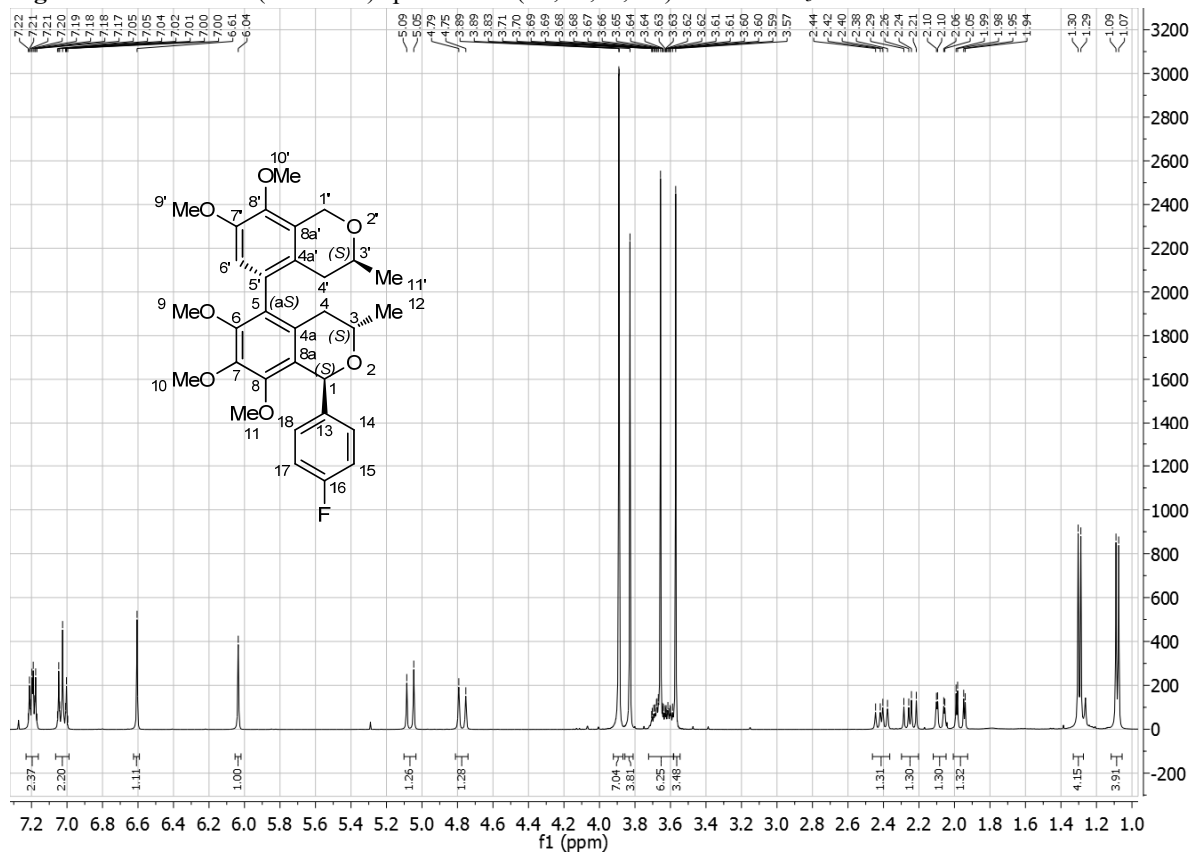
**Figure S55.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR (400 MHz) spectrum of (a*S*,1*R*,3*S*,2'*S*)-**20** in  $\text{CDCl}_3$ .



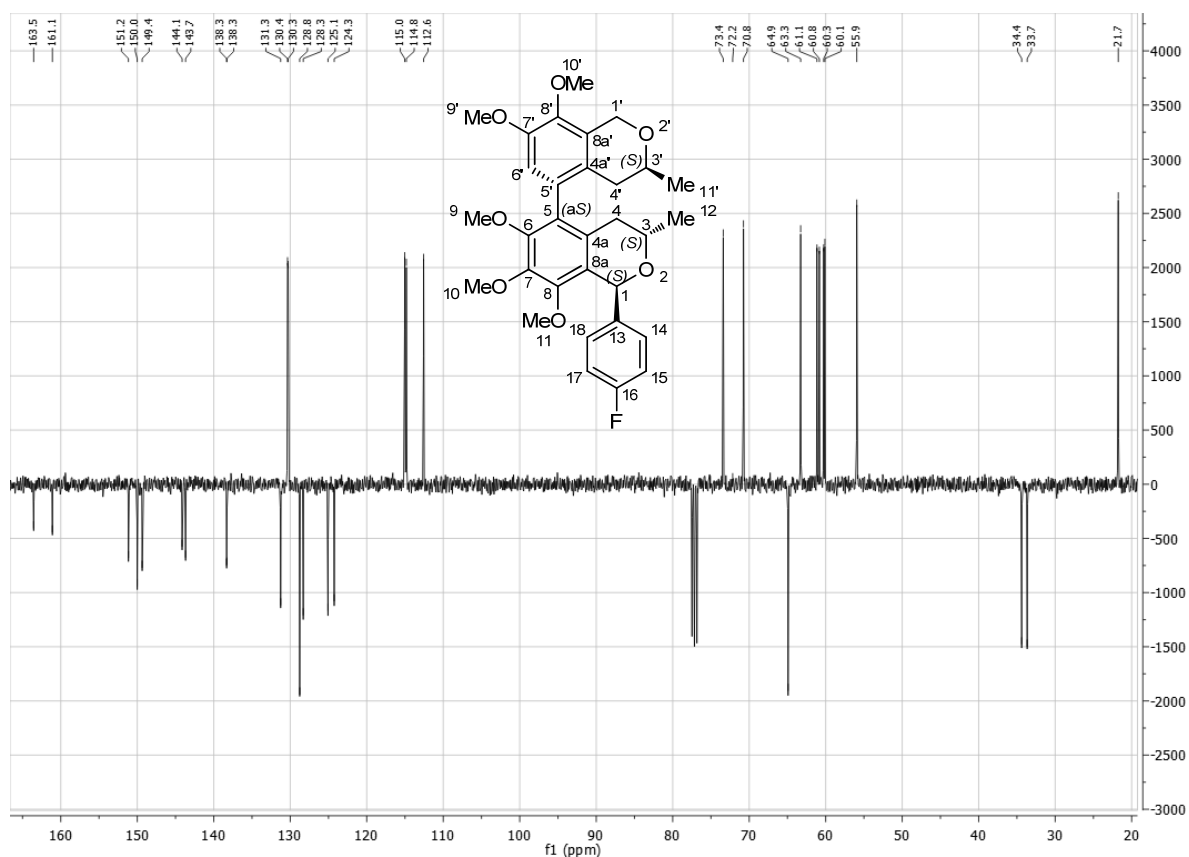
**Figure S56.**  $^1\text{H}$  NMR (400 MHz) spectrum of (a*R*,1*R*,3*S*,2'*S*)-**20** in  $\text{CDCl}_3$ .



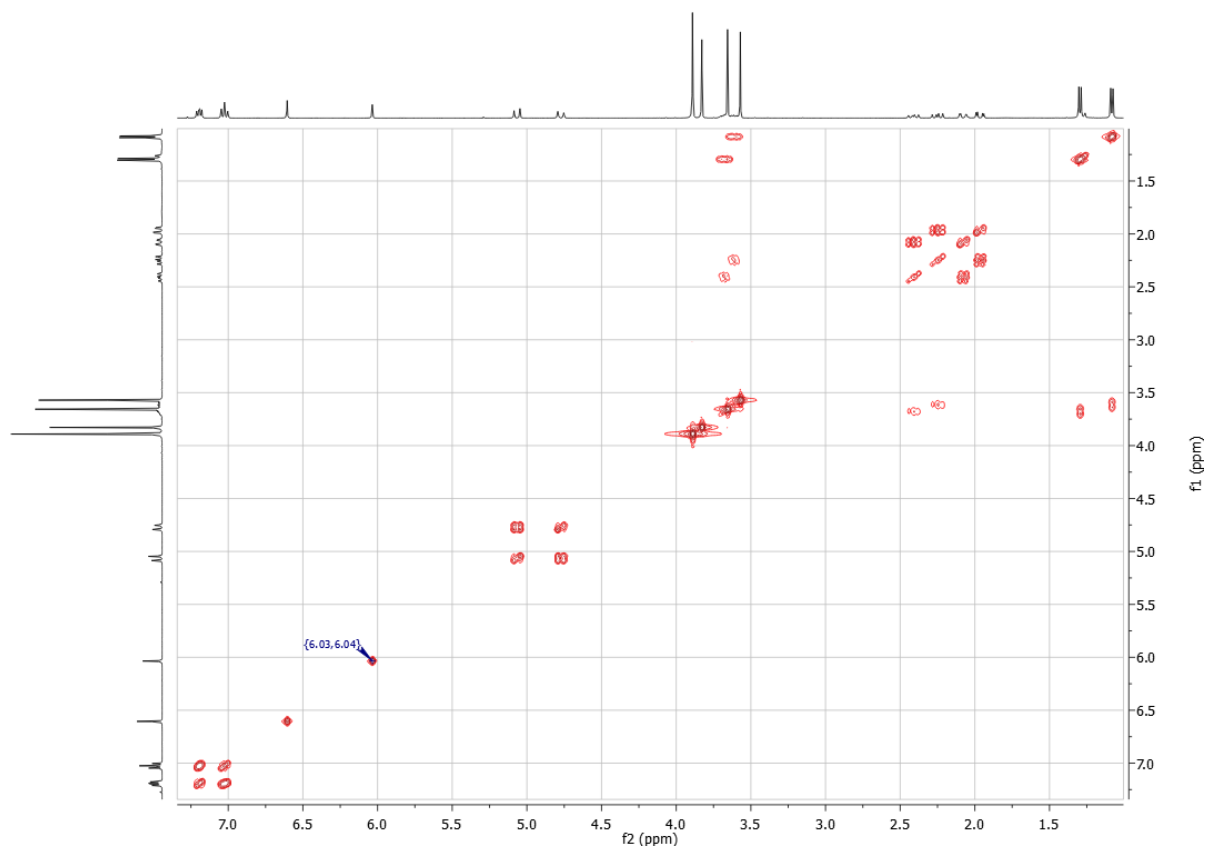
**Figure S57.**  $^{13}\text{C}$  NMR (100 MHz) spectrum of (aR,1R,3S,2'S)-**20** in  $\text{CDCl}_3$ .



**Figure S58.**  $^1\text{H}$  NMR (400 MHz) spectrum of (aS,1S,3S,3'S)-**21** in  $\text{CDCl}_3$ .

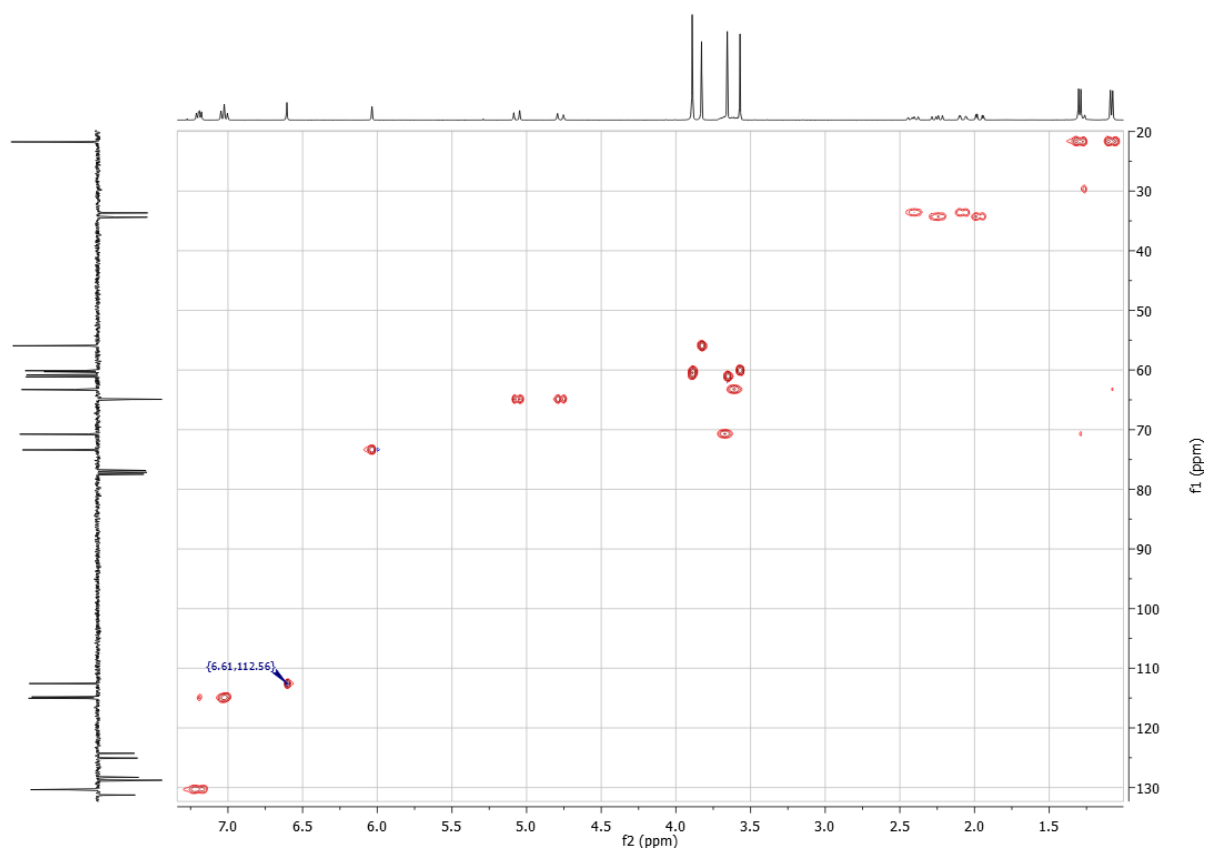


**Figure S59.**  $^{13}\text{C}$  NMR (100 MHz) spectrum of (aS,1S,3S,3'S)-**21** in  $\text{CDCl}_3$ .

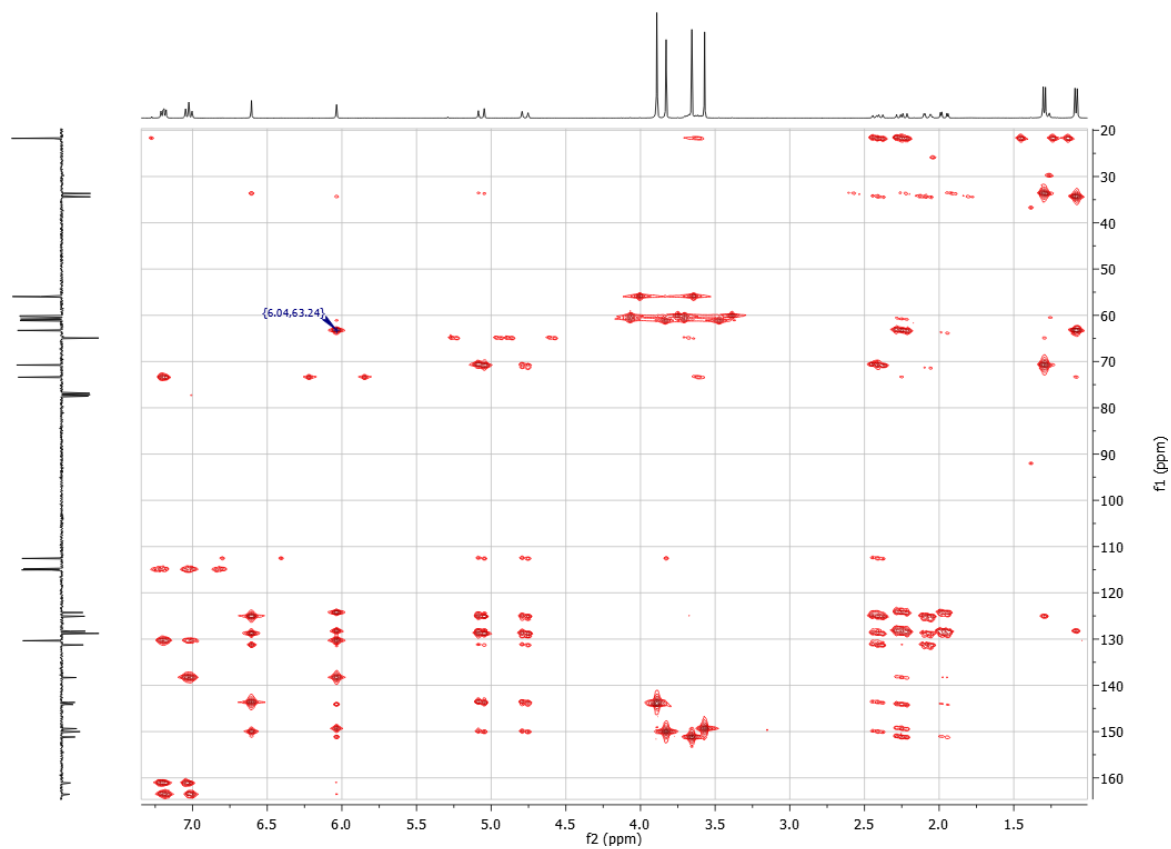


**Figure S60.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR (400 MHz) spectrum of (aS,1S,3S,3'S)-**21** in  $\text{CDCl}_3$ .

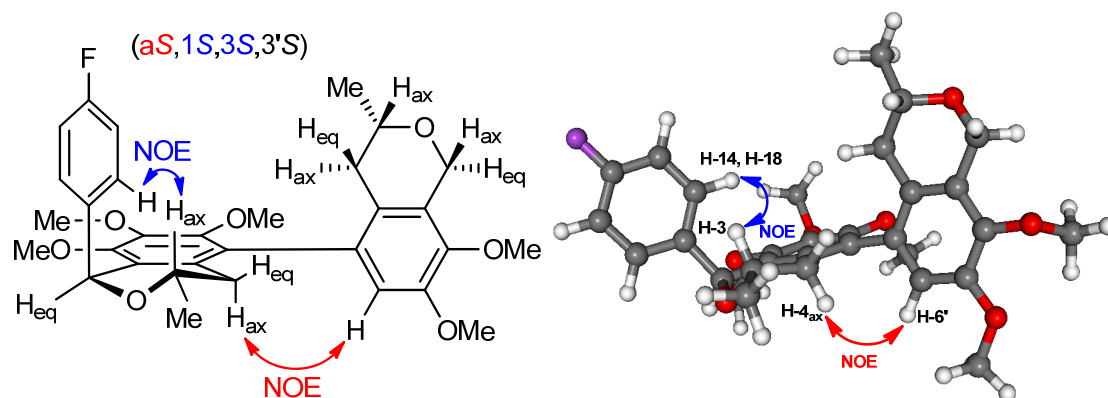




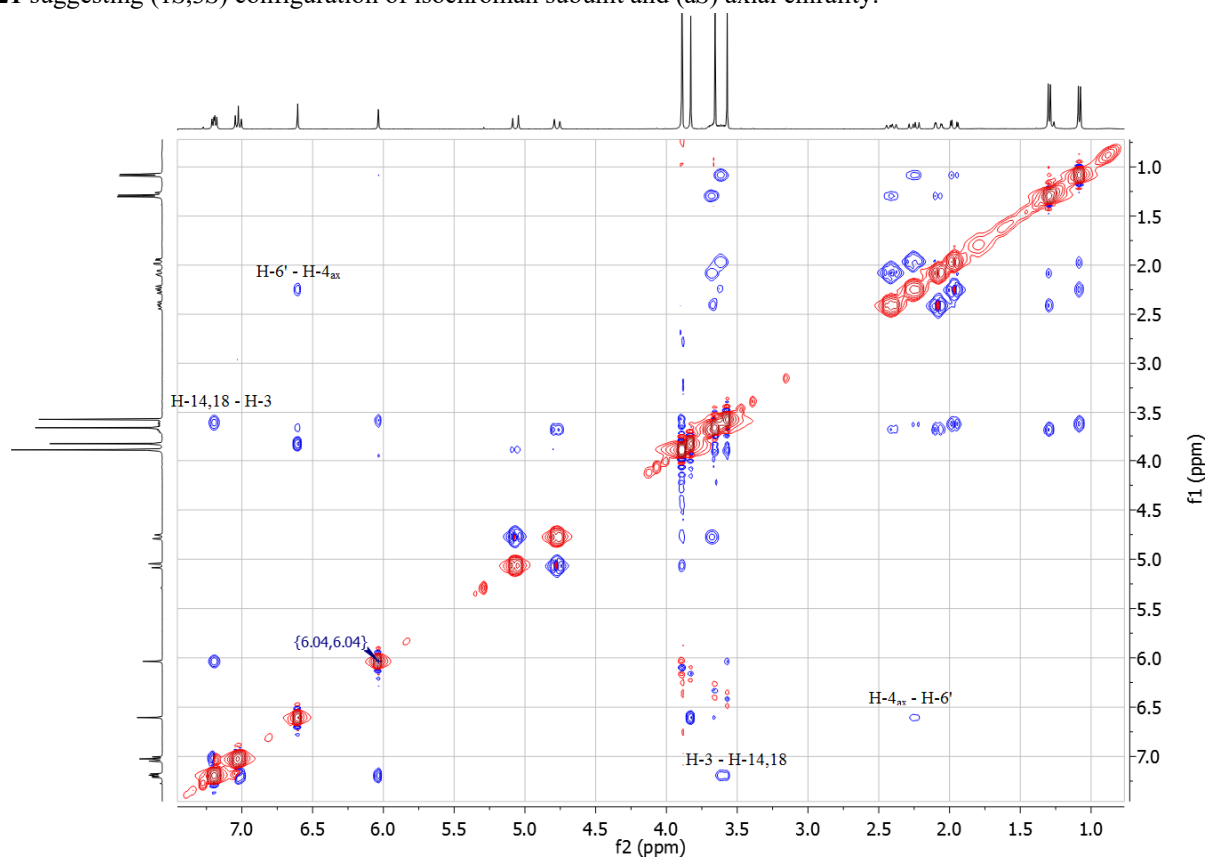
**Figure S61.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR (400 MHz) spectrum of  $(aS,1S,3S,3'S)$ -**21** in  $\text{CDCl}_3$ .



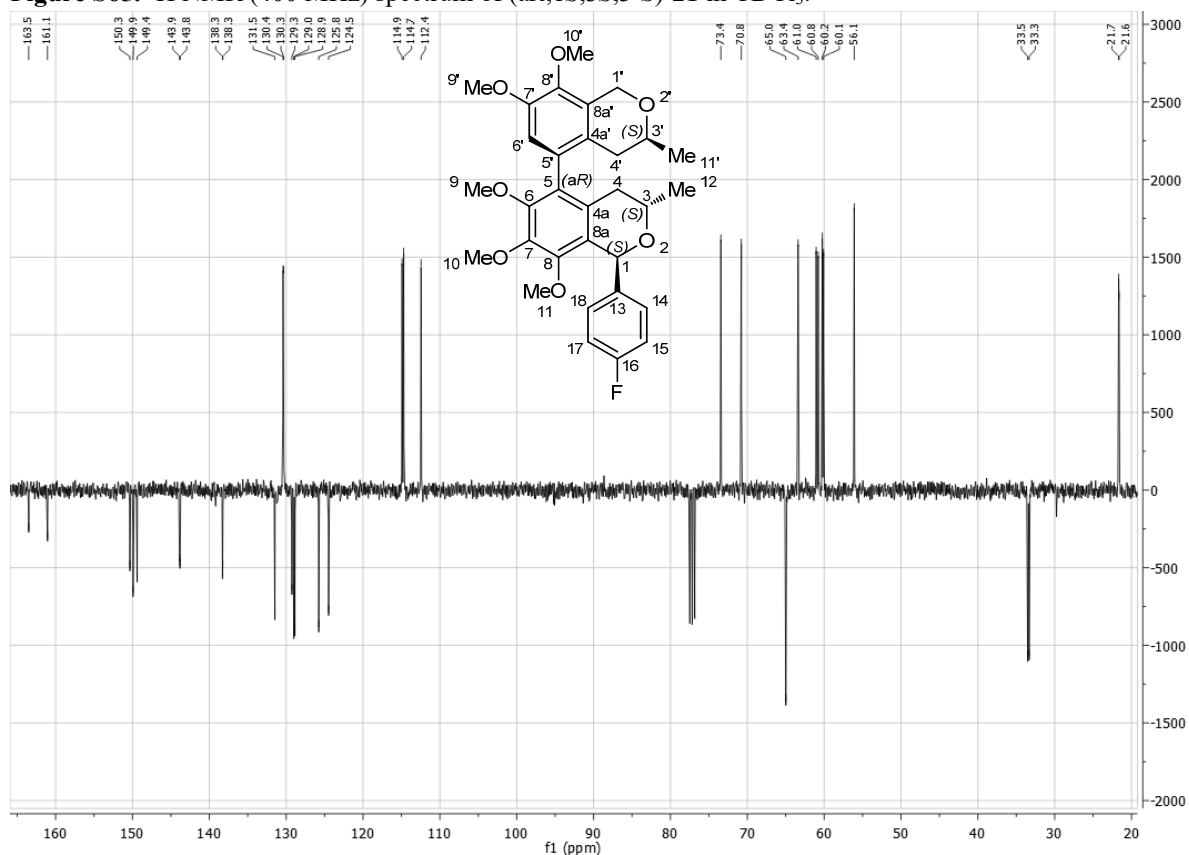
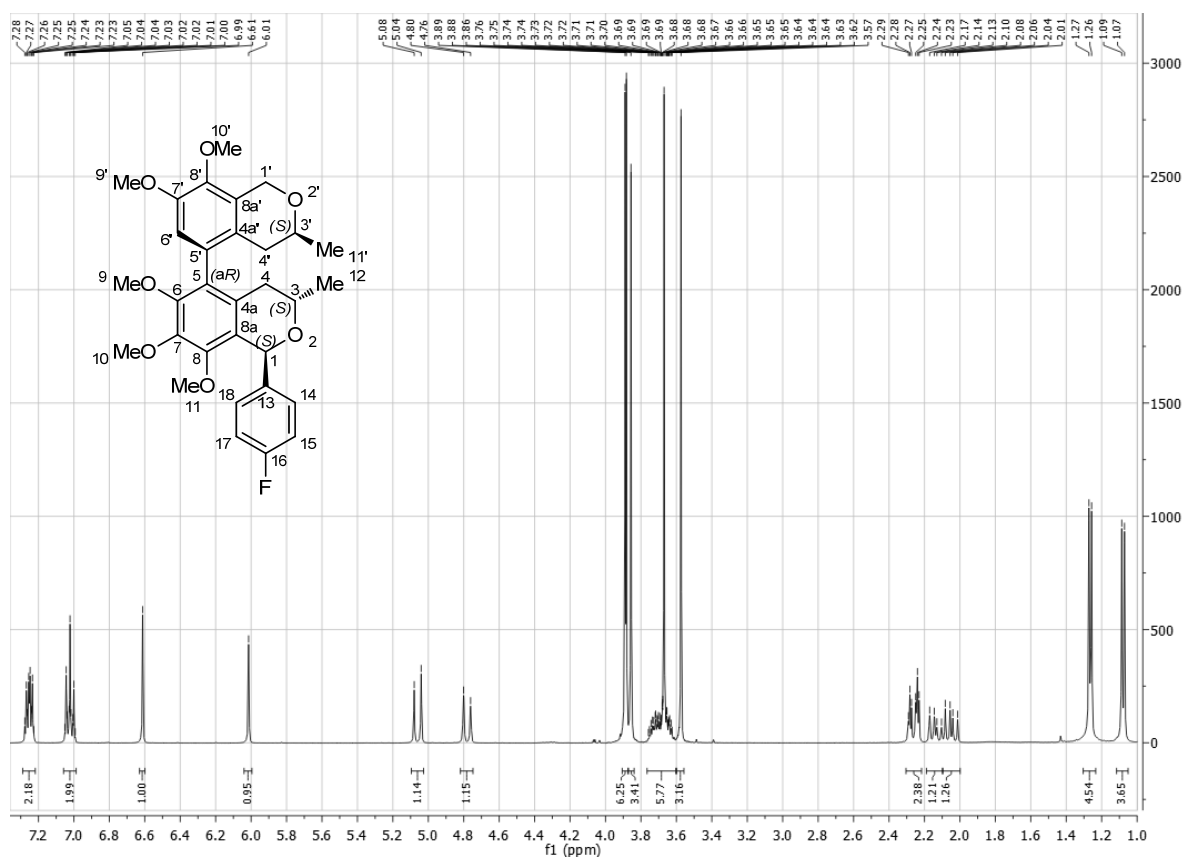
**Figure S62.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC NMR (400 MHz) spectrum of  $(aS,1S,3S,3'S)$ -**21** in  $\text{CDCl}_3$ .

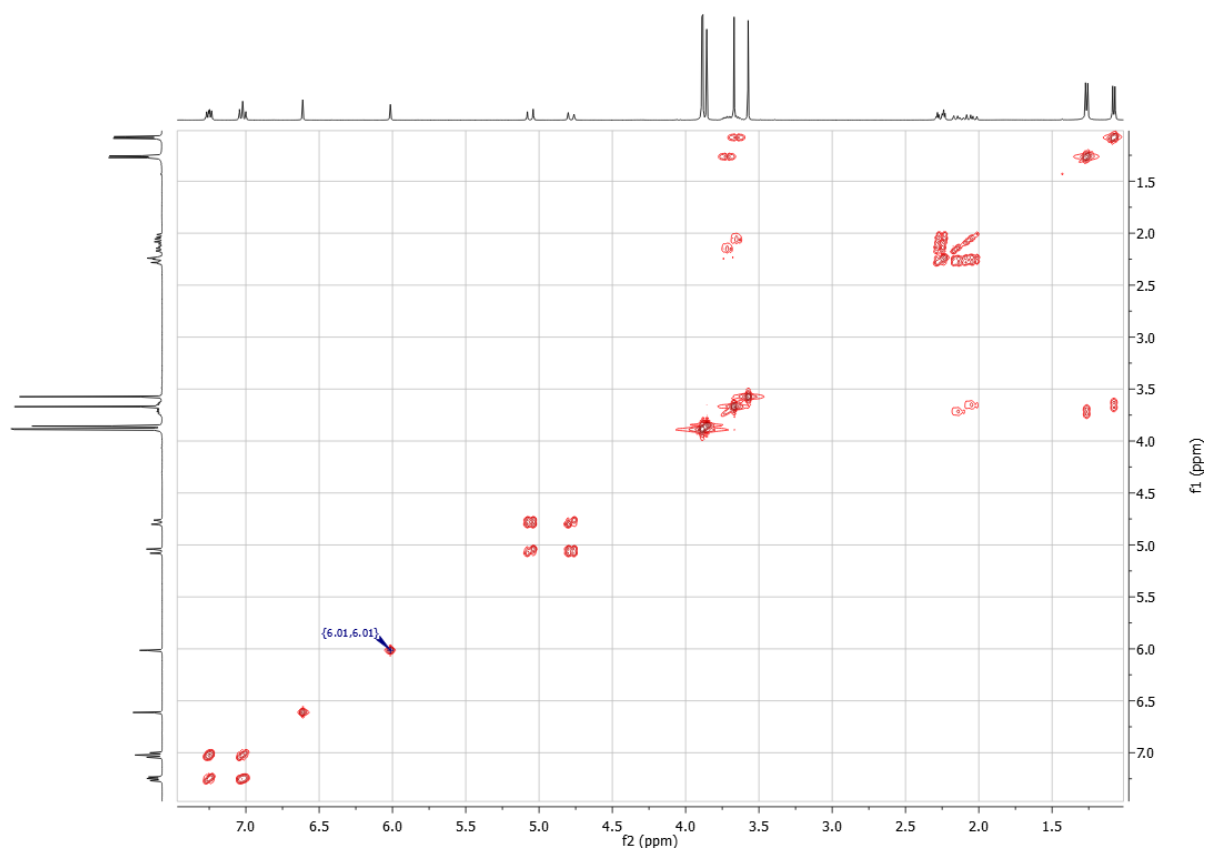


**Figure S63.** Characteristic NOE correlations shown on the lowest-energy computed conformer of (a*S*,1*S*,3*S*,3'*S*)-**21** suggesting (1*S*,3*S*) configuration of isochroman subunit and (a*S*) axial chirality.

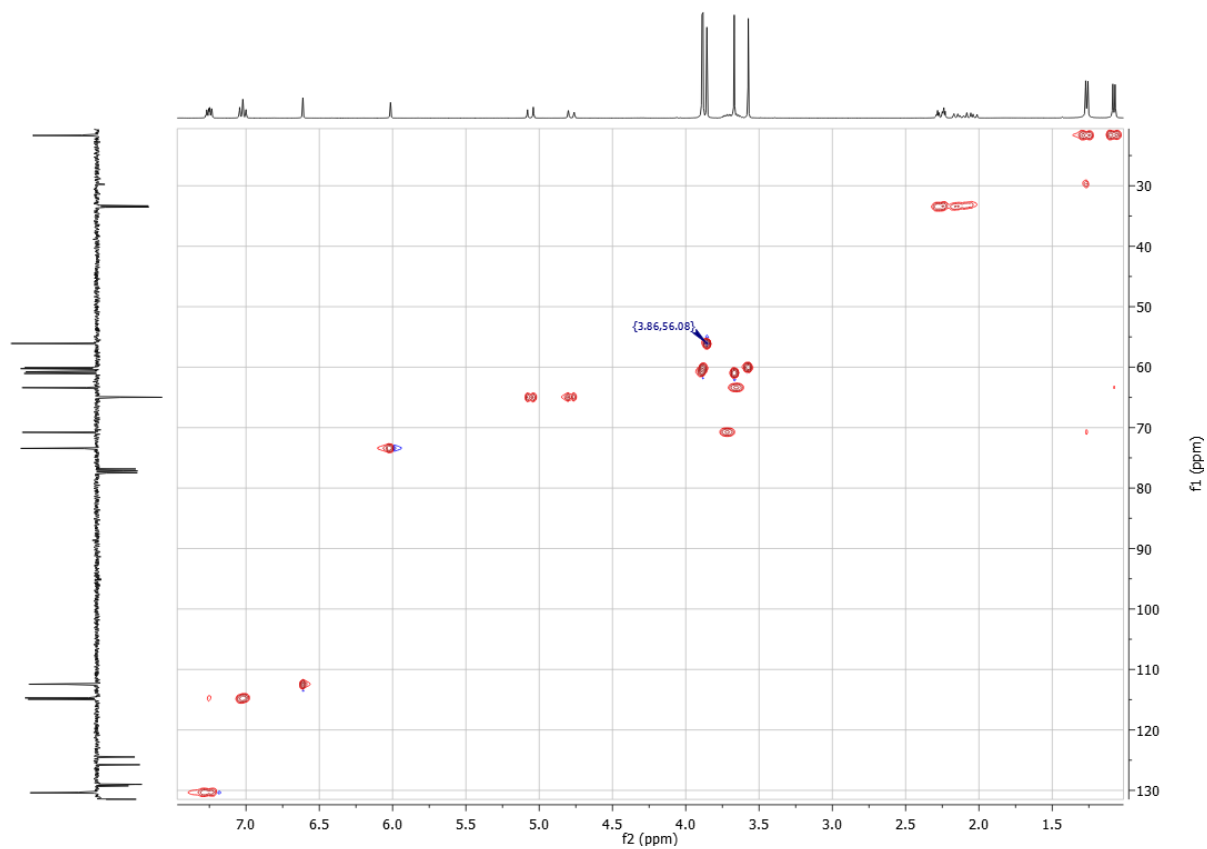


**Figure S64.**  $^1\text{H}$ - $^1\text{H}$  NOESY NMR (400 MHz) spectrum of (a*S*,1*S*,3*S*,3'*S*)-**21** in  $\text{CDCl}_3$ .

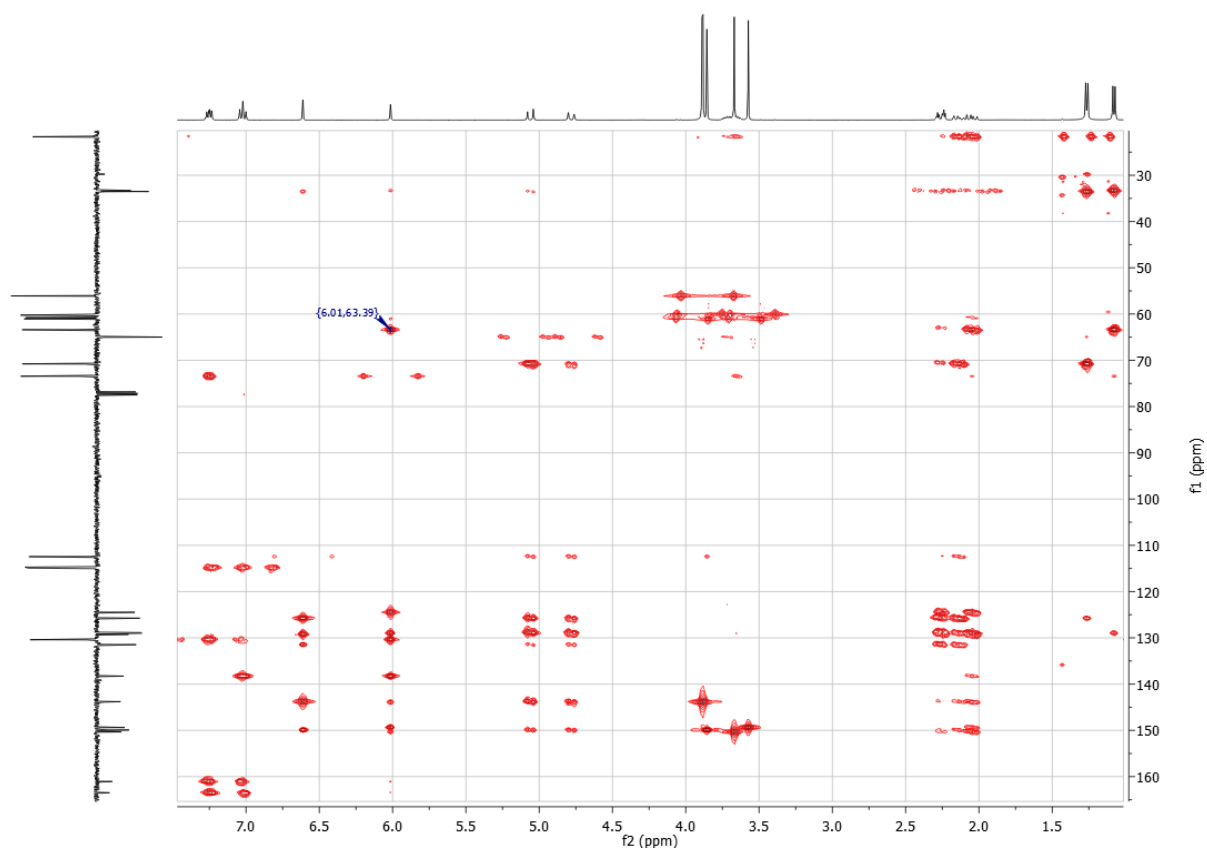




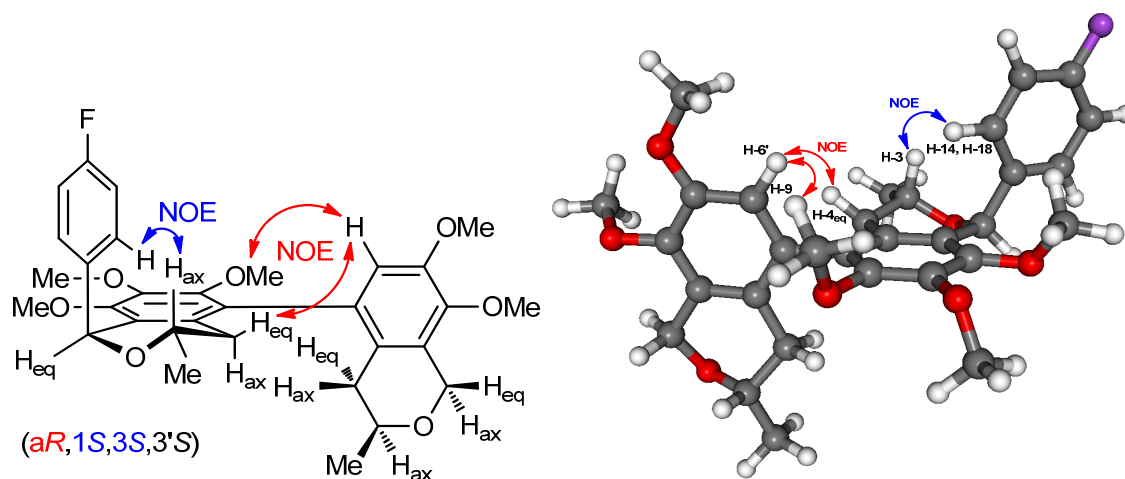
**Figure S67.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR (400 MHz) spectrum of (aR,1S,3S,3'S)-**21** in  $\text{CDCl}_3$ .



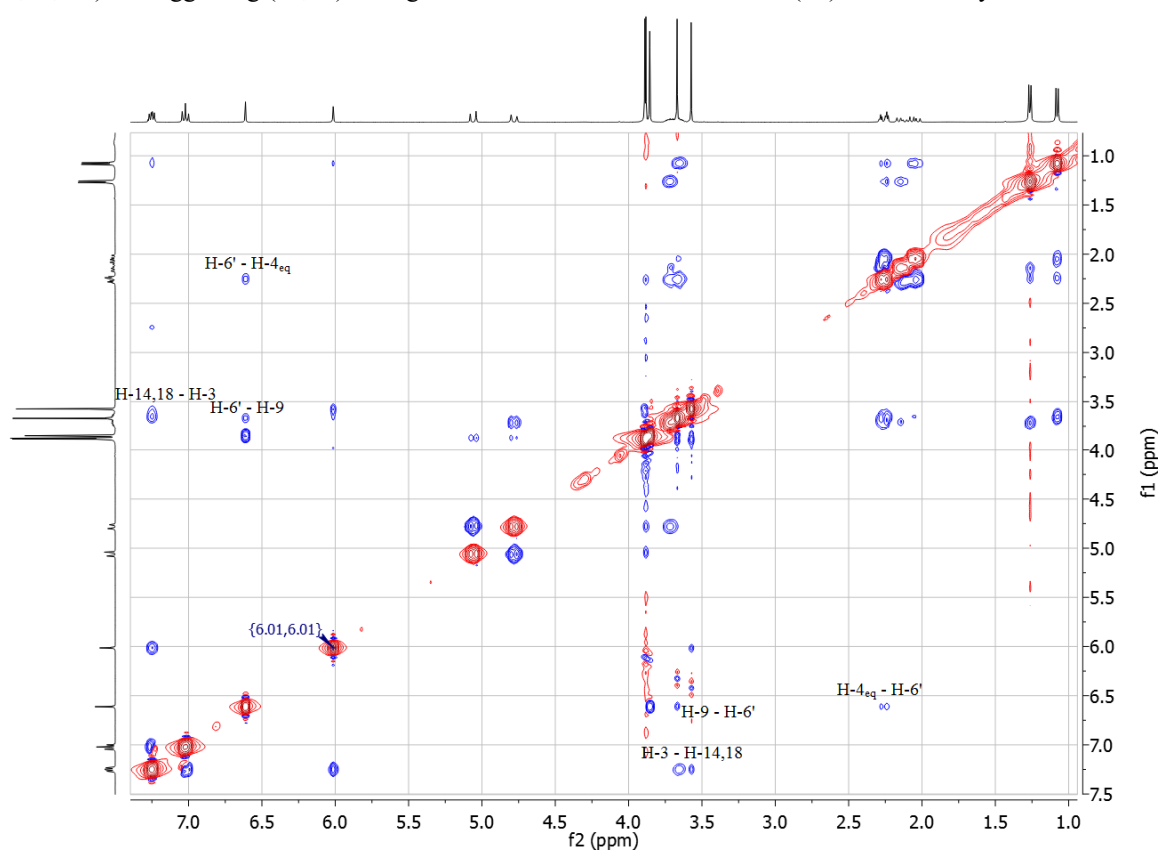
**Figure S68.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR (400 MHz) spectrum of (aR,1S,3S,3'S)-**21** in  $\text{CDCl}_3$ .



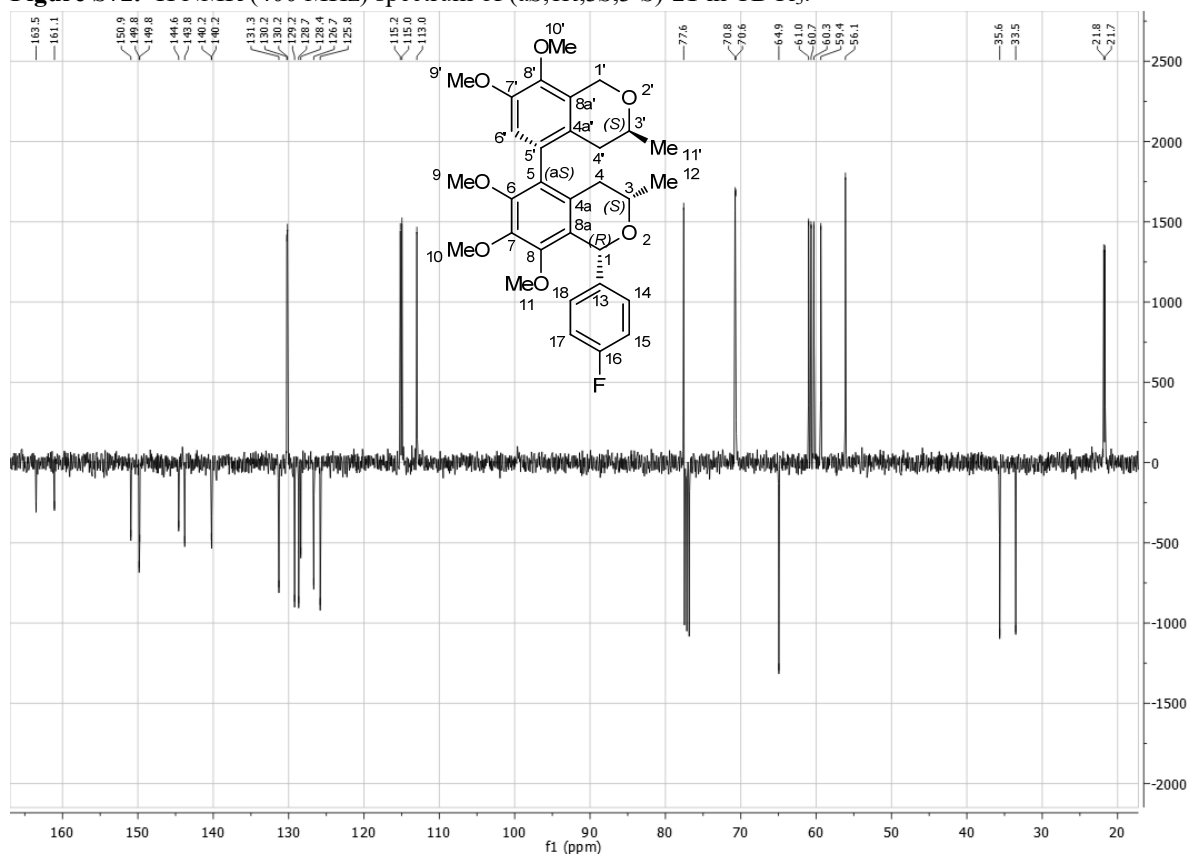
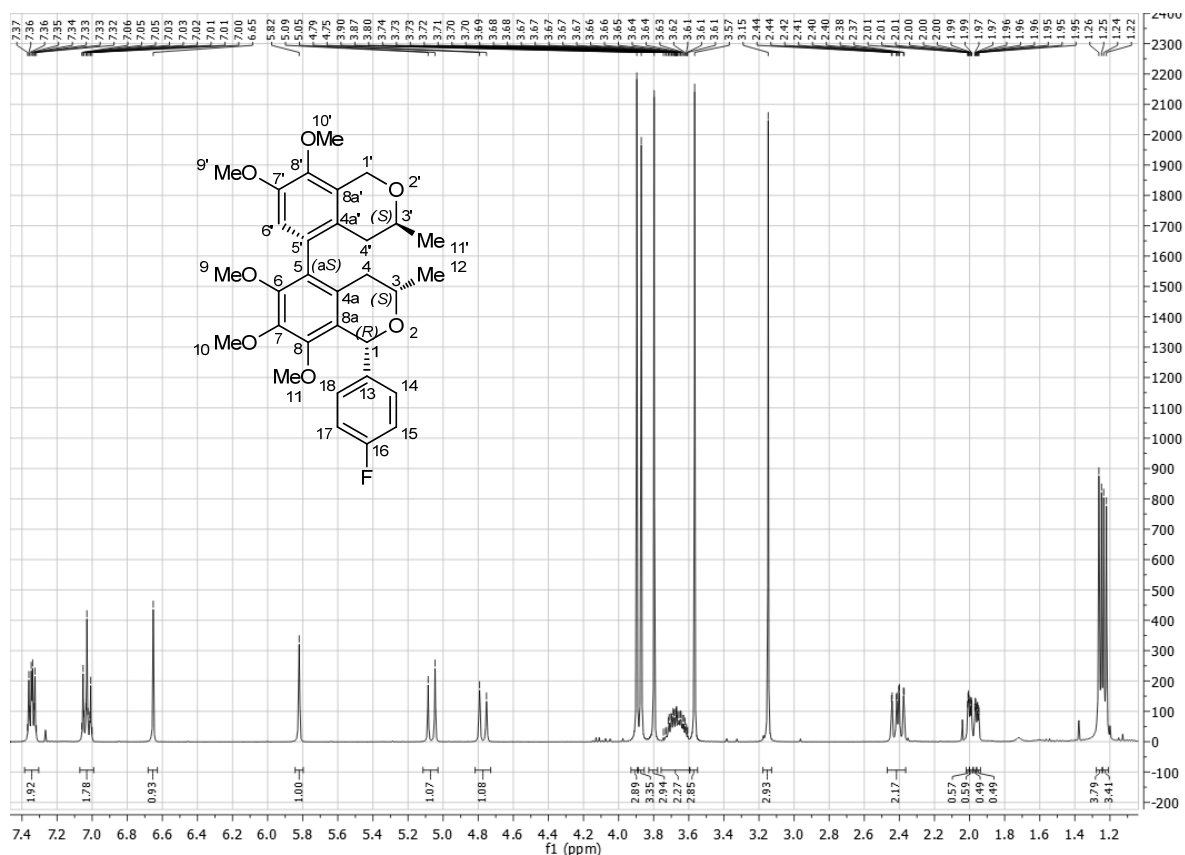
**Figure S69.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC NMR (400 MHz) spectrum of (a*R*,1*S*,3*S*,3'*S*)-**21** in  $\text{CDCl}_3$ .

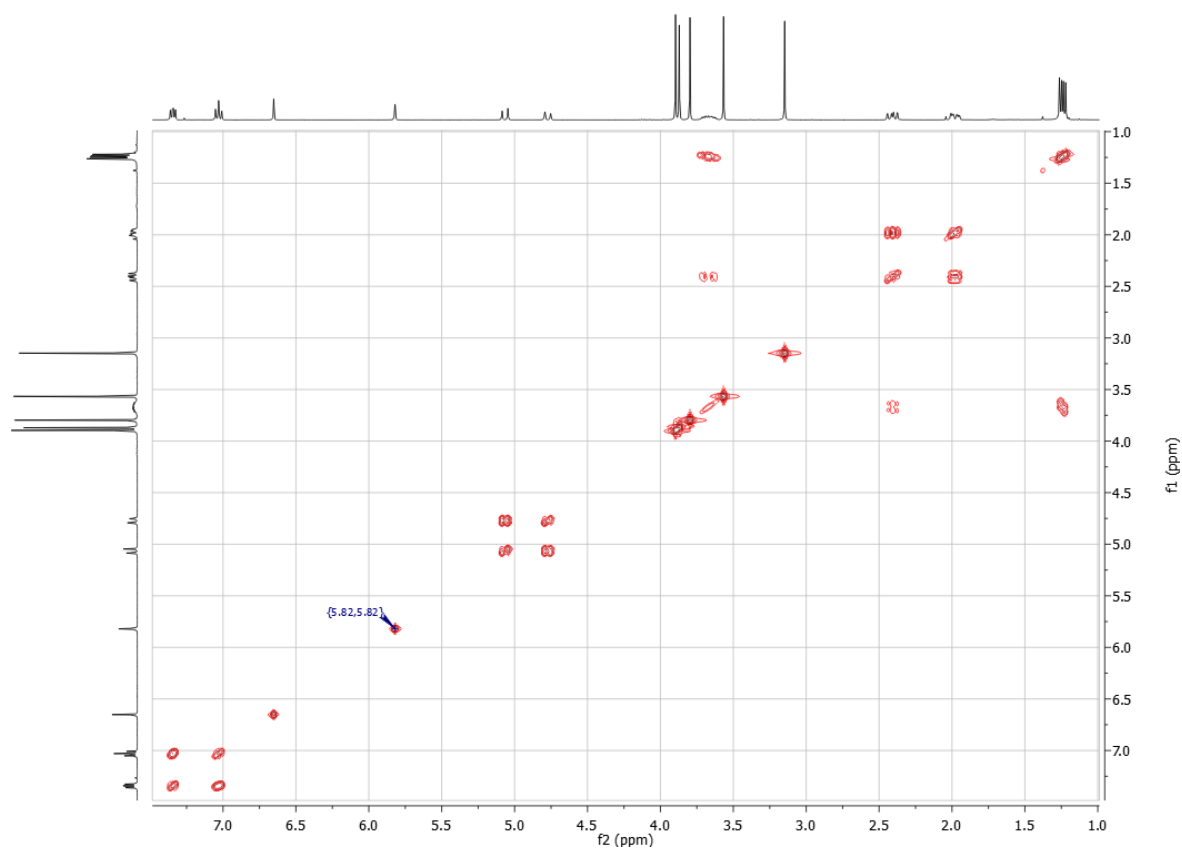


**Figure S70.** Characteristic NOE correlations shown on the the lowest-energy computed conformer of  $(aR,1S,3S,3'S)$ -**21** suggesting  $(1S,3S)$  configuration of isochroman subunit and  $(aR)$  axial chirality.

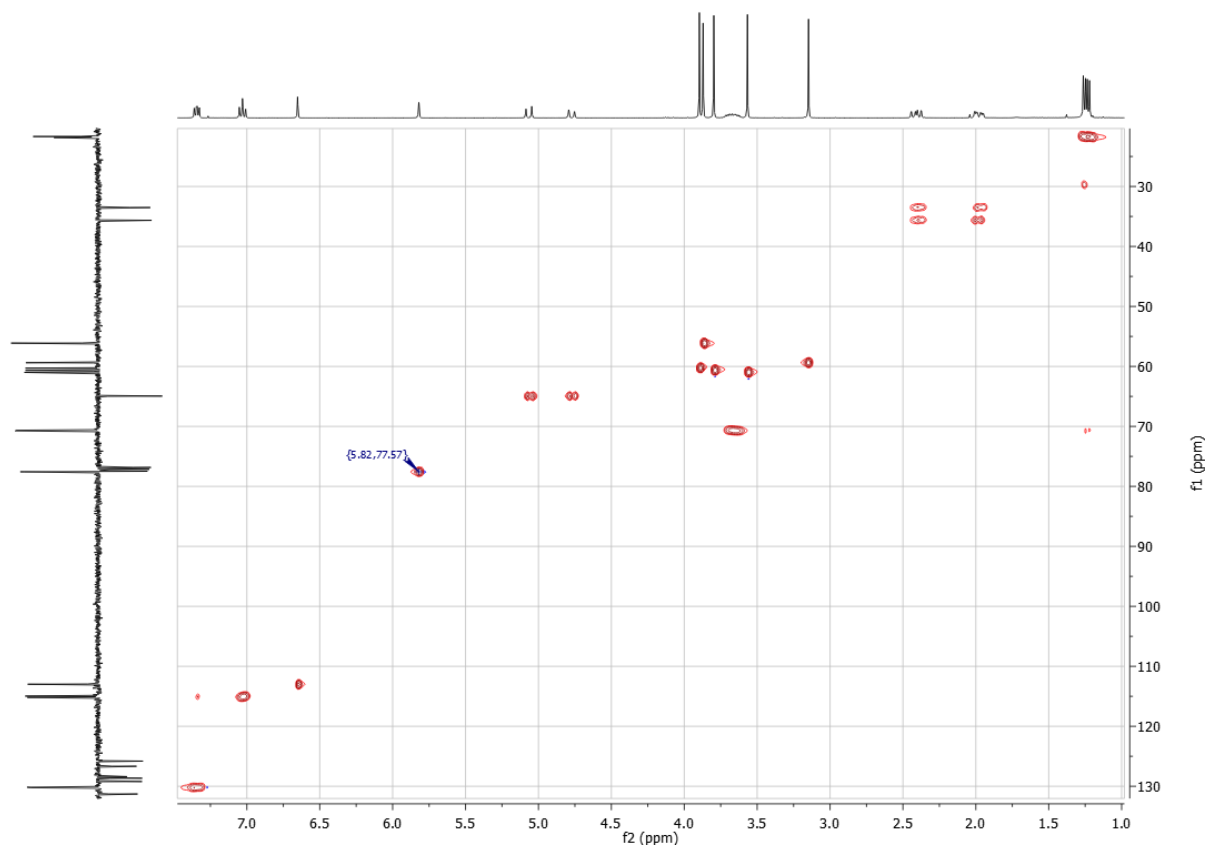


**Figure S71.**  $^1\text{H}$ - $^1\text{H}$  NOESY NMR (400 MHz) spectrum of  $(aR,1S,3S,3'S)$ -**21** in  $\text{CDCl}_3$ .



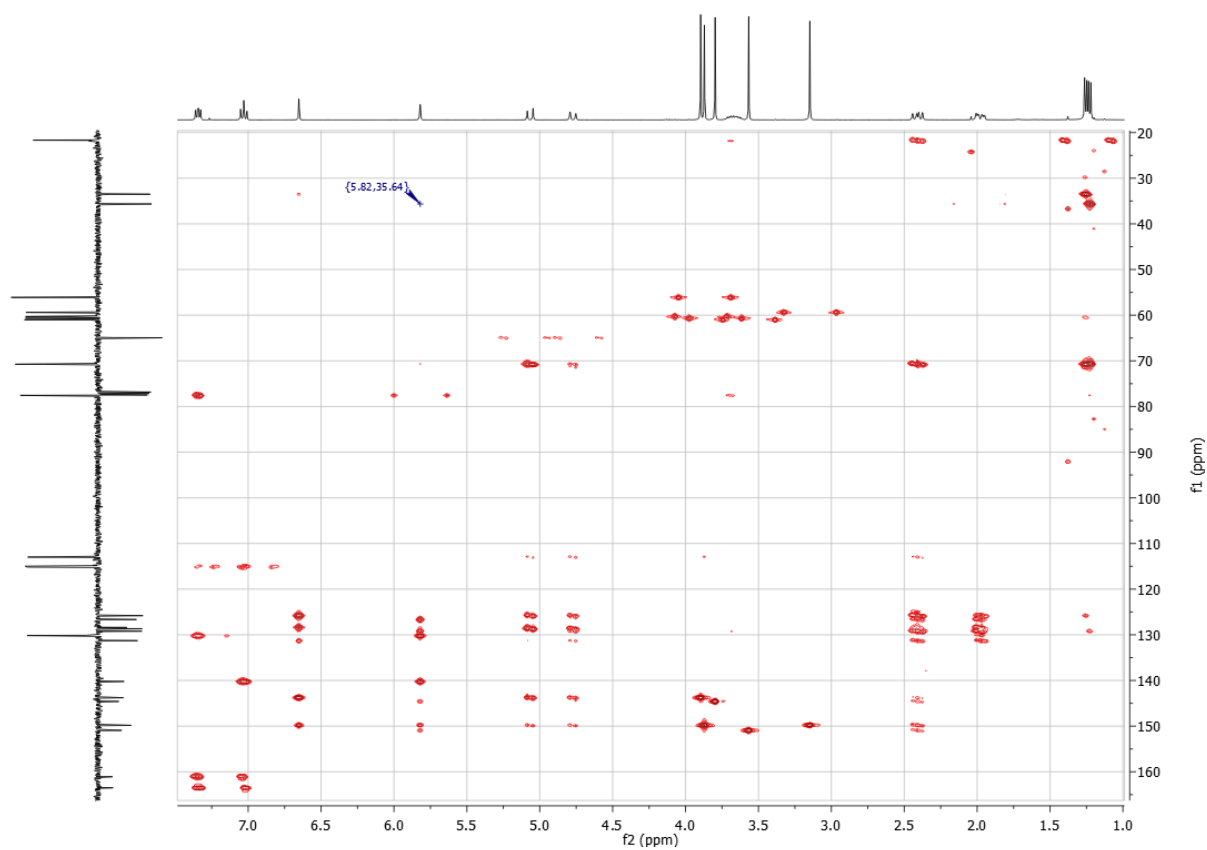


**Figure S74.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR (400 MHz) spectrum of (aS,1R,3S,3'S)-**21** in  $\text{CDCl}_3$ .

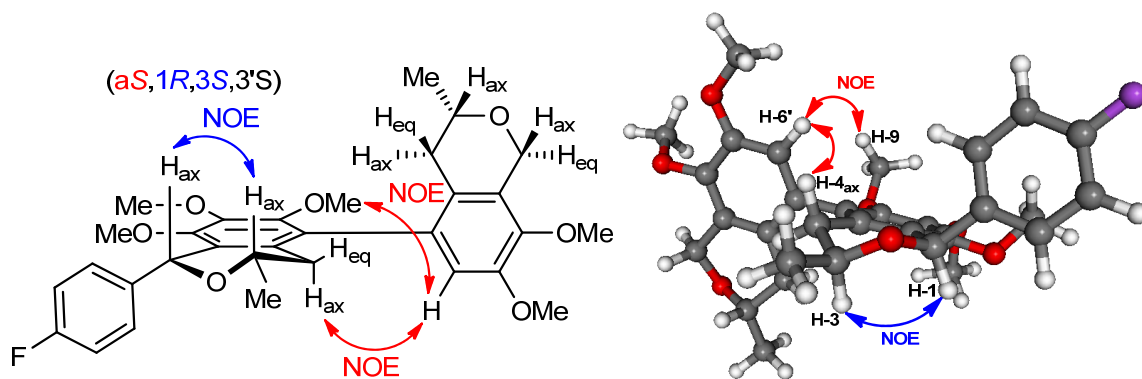


**Figure S75.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR (400 MHz) spectrum of (aS,1R,3S,3'S)-**21** in  $\text{CDCl}_3$ .

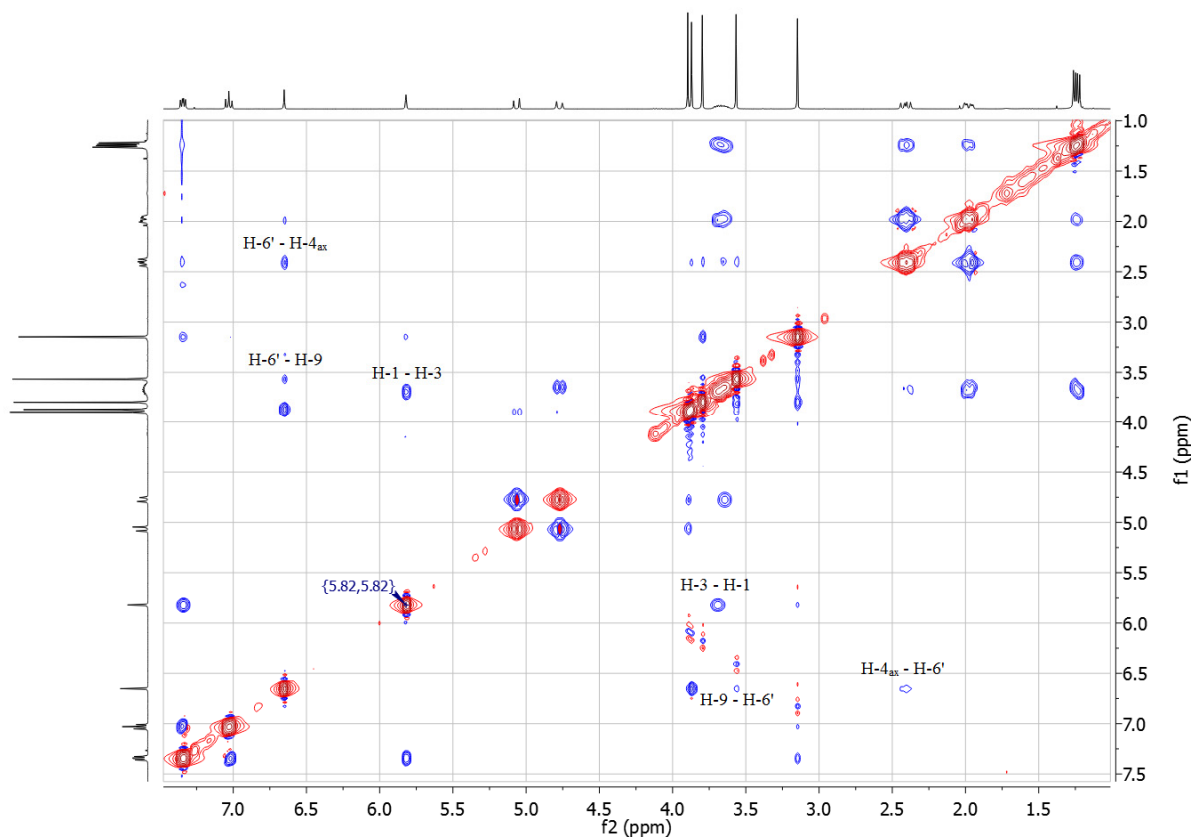




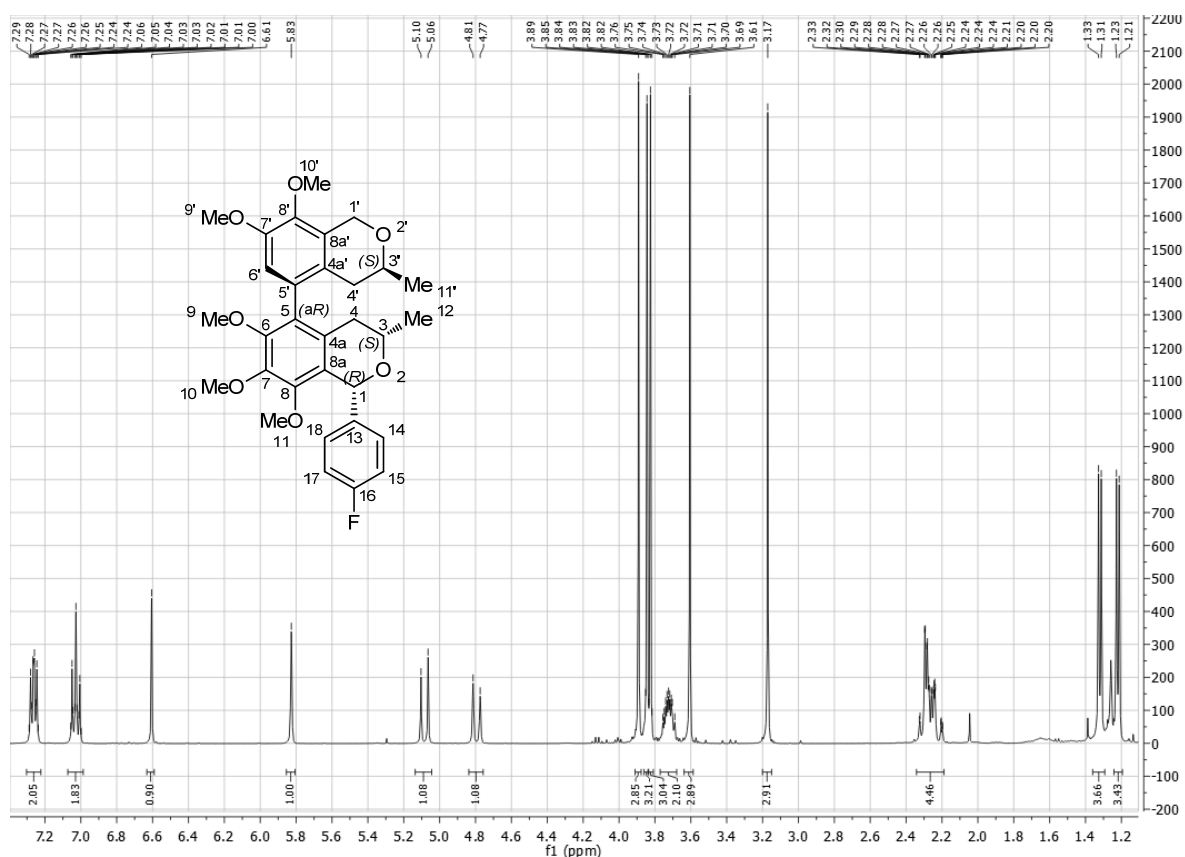
**Figure S76.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC NMR (400 MHz) spectrum of (*aS*,1*R*,3*S*,3'*S*)-**21** in  $\text{CDCl}_3$ .



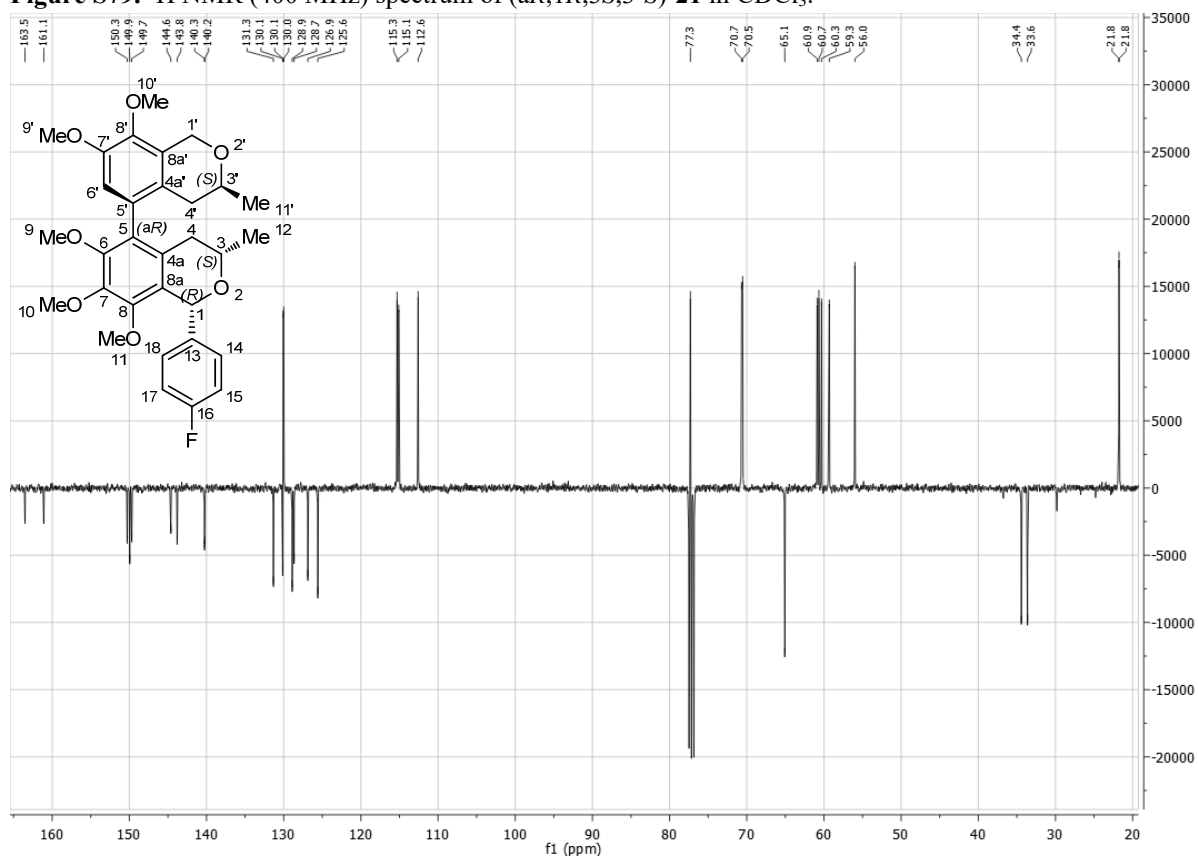
**Figure S77.** Characteristic NOE correlations shown on the lowest-energy computed conformer of (aS,1R,3S,3'S)-**21** suggesting (1R,3S) configuration of isochroman subunit and (aS) axial chirality.



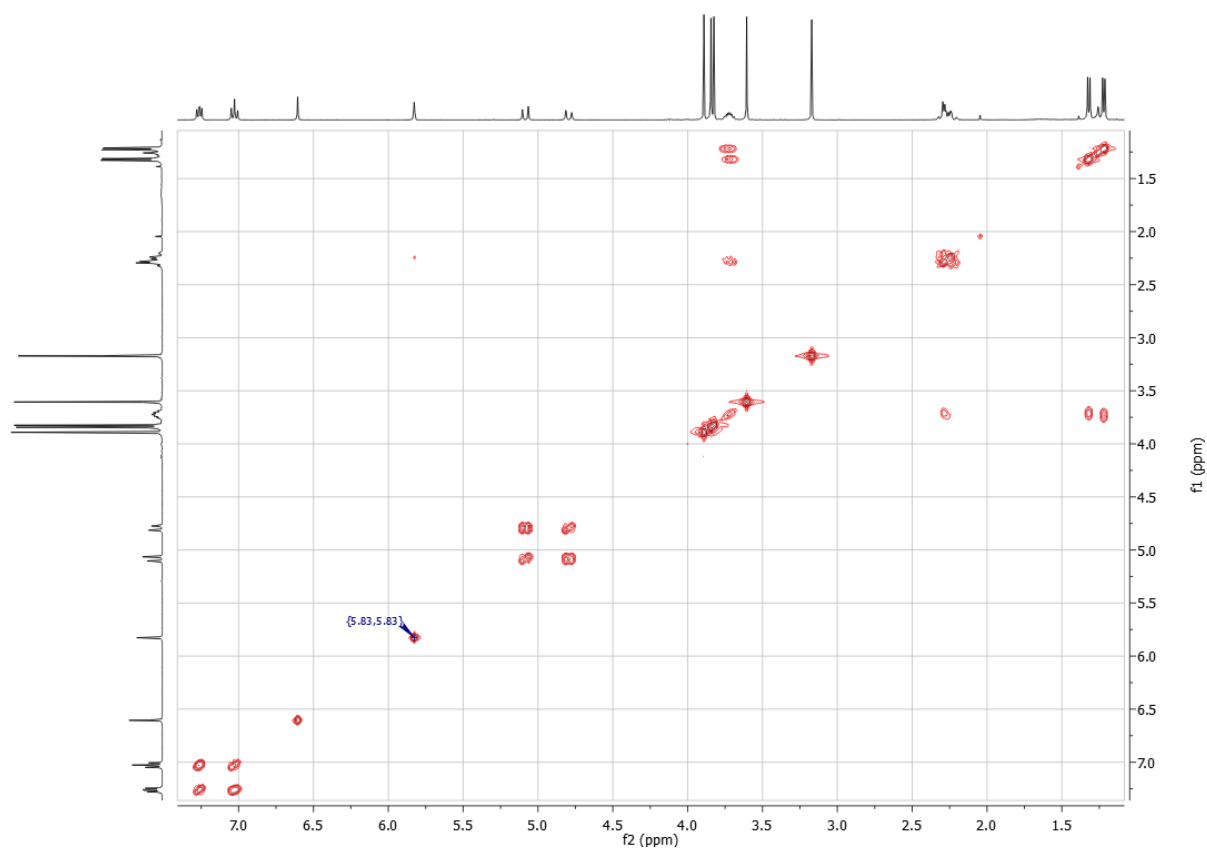
**Figure S78.** <sup>1</sup>H-<sup>1</sup>H NOESY NMR (400 MHz) spectrum of (aS,1R,3S,3'S)-**21** in CDCl<sub>3</sub>.



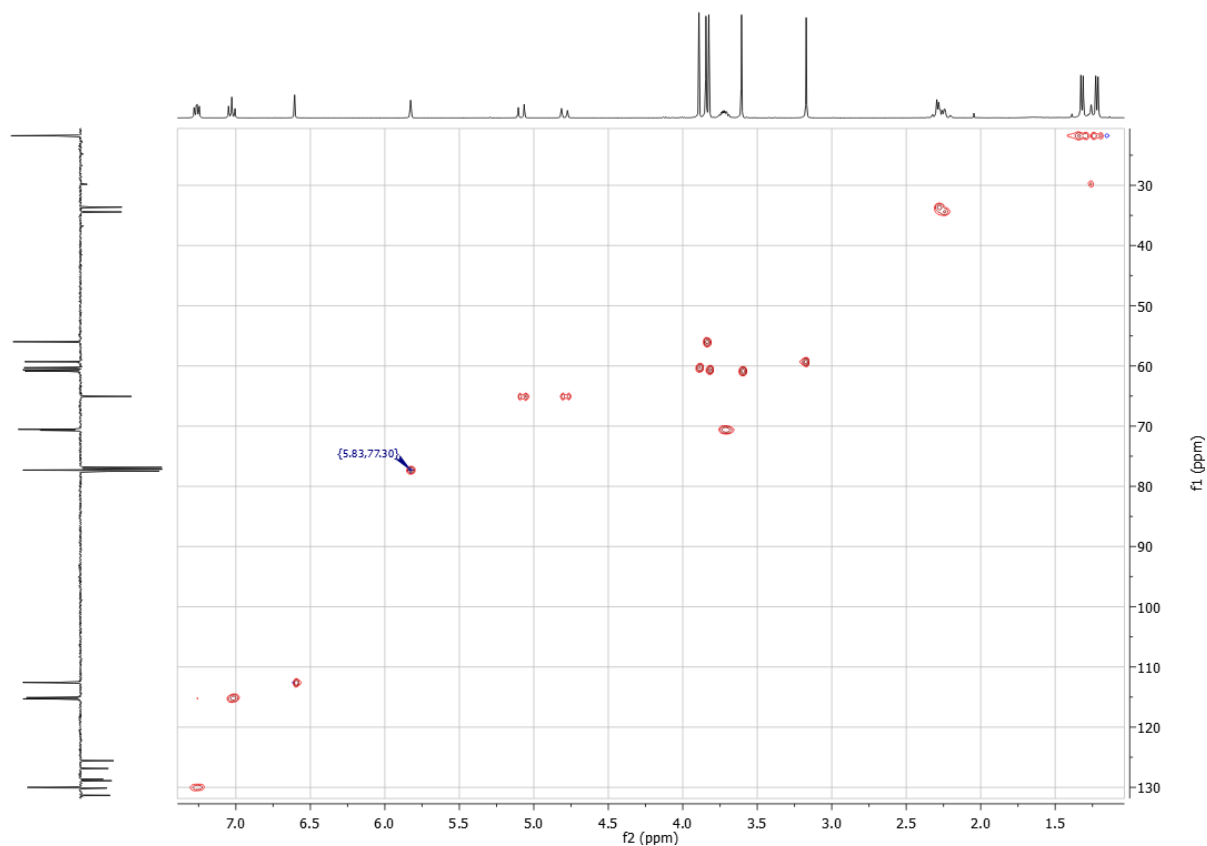
**Figure S79.**  $^1\text{H}$  NMR (400 MHz) spectrum of (aR,1R,3S,3'S)-21 in  $\text{CDCl}_3$ .



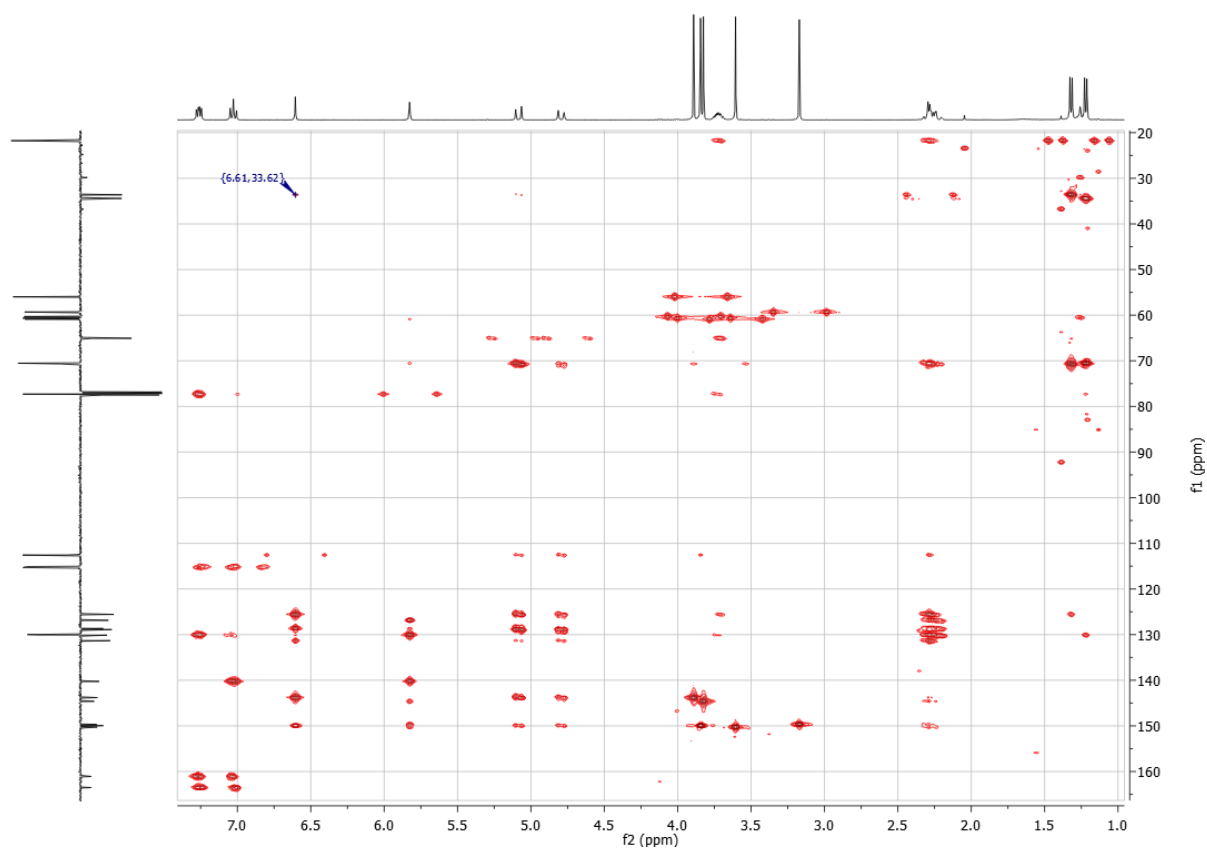
**Figure S80.**  $^{13}\text{C}$  NMR (100 MHz) spectrum of (aR,1R,3S,3'S)-21 in  $\text{CDCl}_3$ .



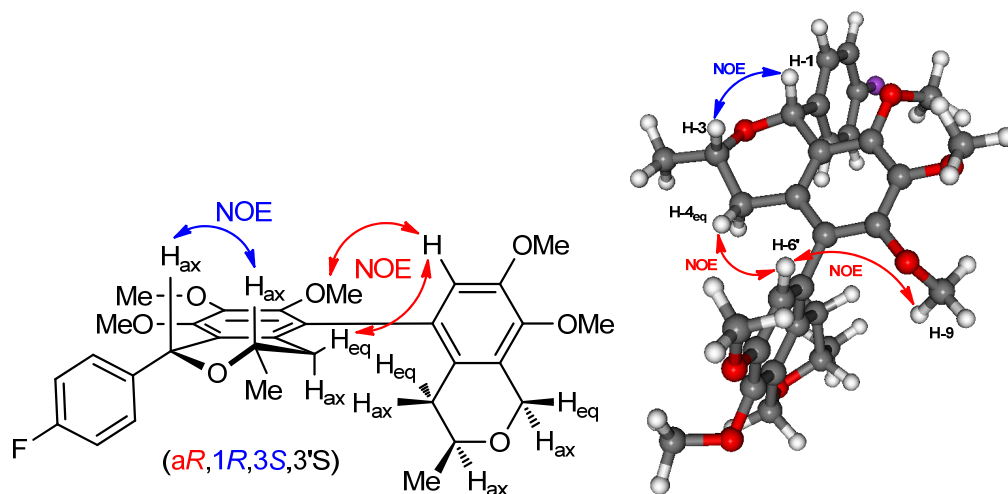
**Figure S81.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR (400 MHz) spectrum of (aR,1R,3S,3'S)-**21** in  $\text{CDCl}_3$ .



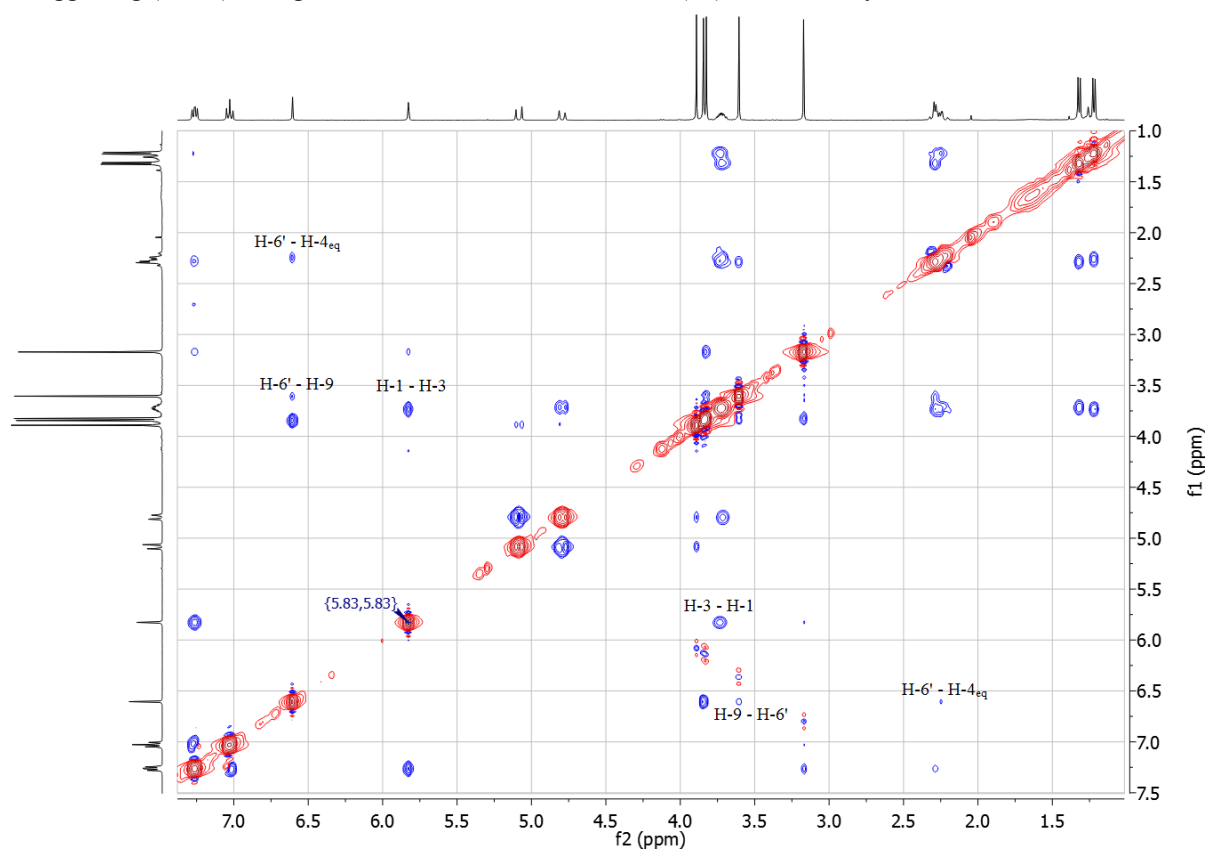
**Figure S82.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR (400 MHz) spectrum of (aR,1R,3S,3'S)-**21** in  $\text{CDCl}_3$ .



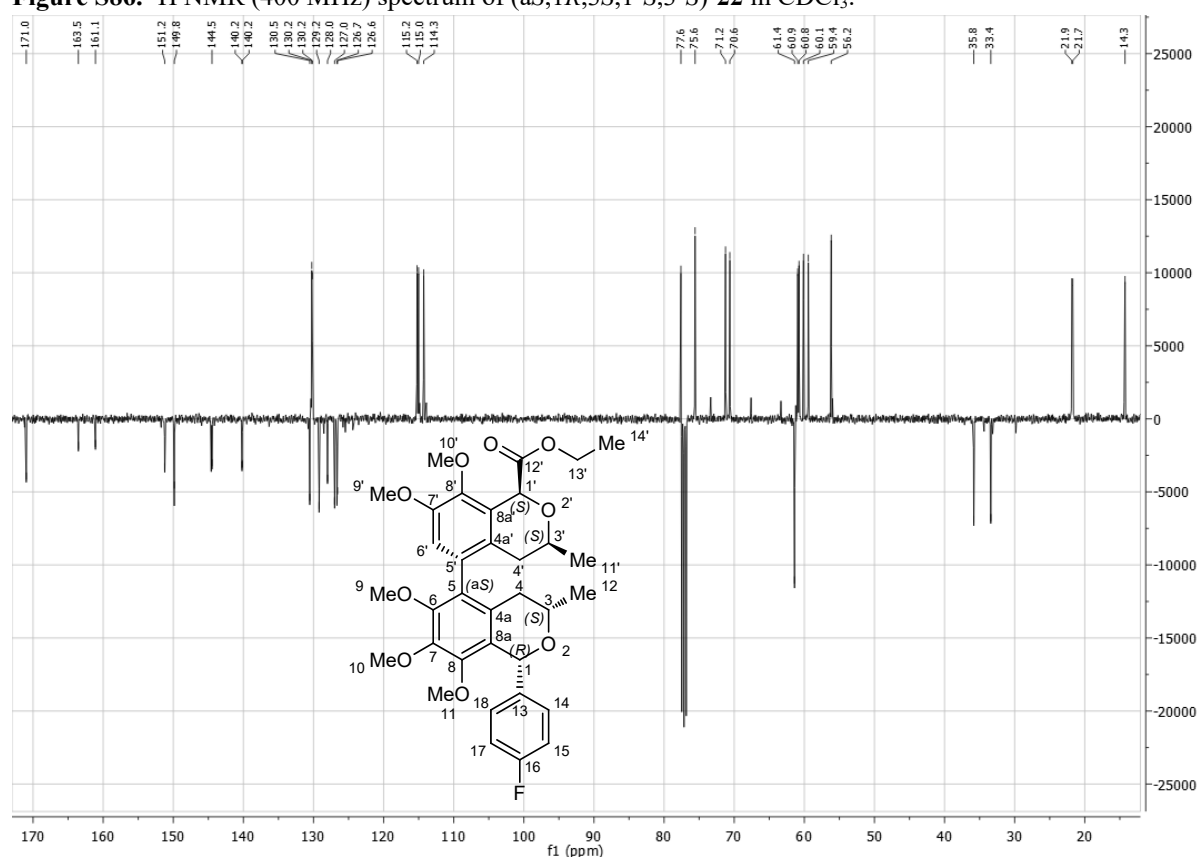
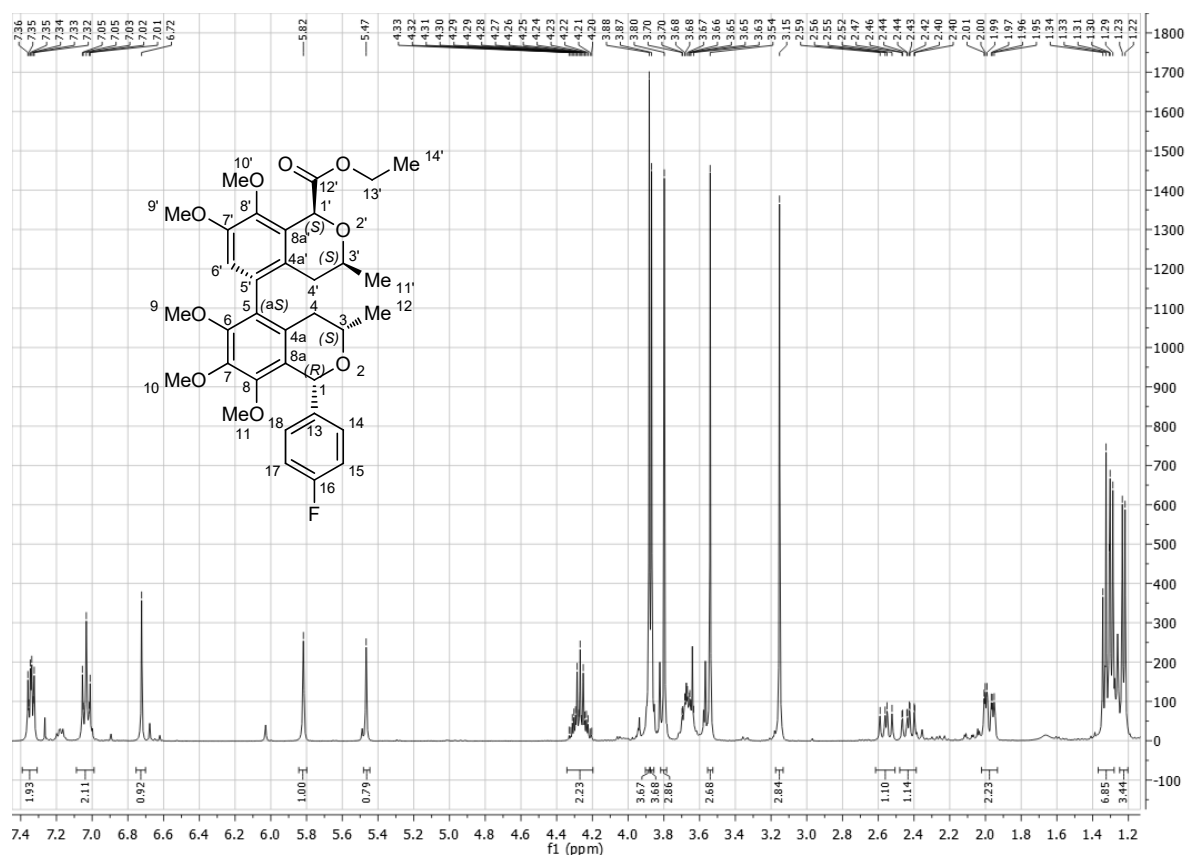
**Figure S83.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC NMR (400 MHz) spectrum of (*aR*,*1R*,*3S*,*3'S*)-**21** in  $\text{CDCl}_3$ .

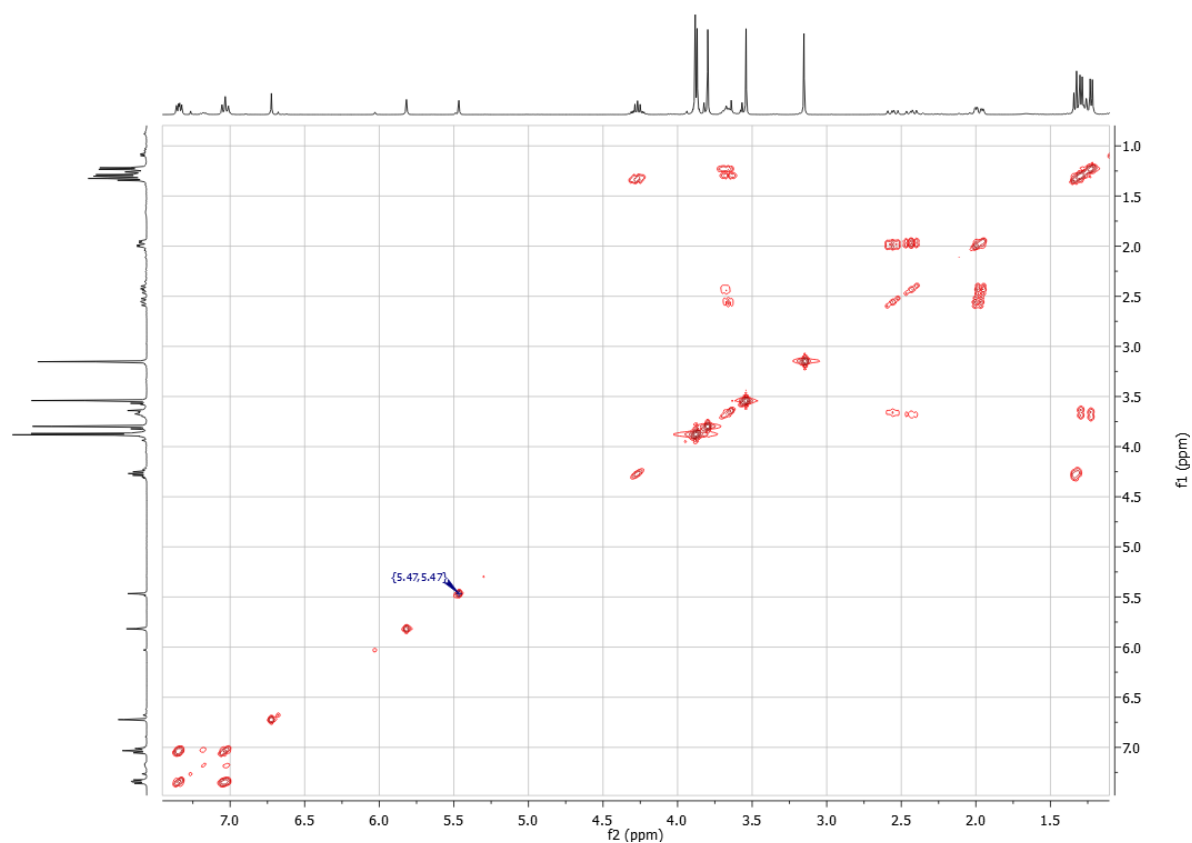


**Figure S84.** Characteristic NOE correlations shown on the lowest-energy computed conformer of (aR,1R,3S,3'S)-**21** suggesting (1R,3S) configuration of isochroman subunit and (aR) axial chirality.

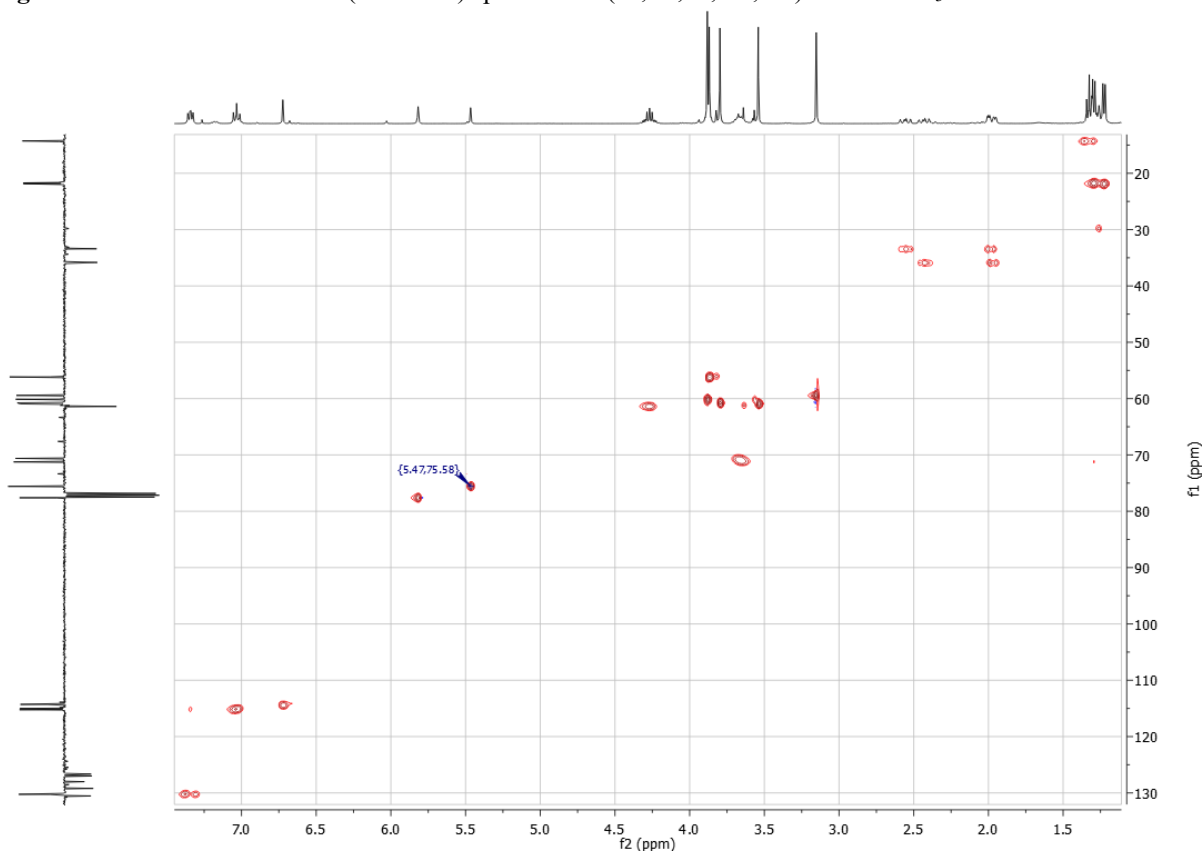


**Figure S85.** <sup>1</sup>H-<sup>1</sup>H NOESY NMR (400 MHz) spectrum of (aR,1R,3S,3'S)-**21** in CDCl<sub>3</sub>.



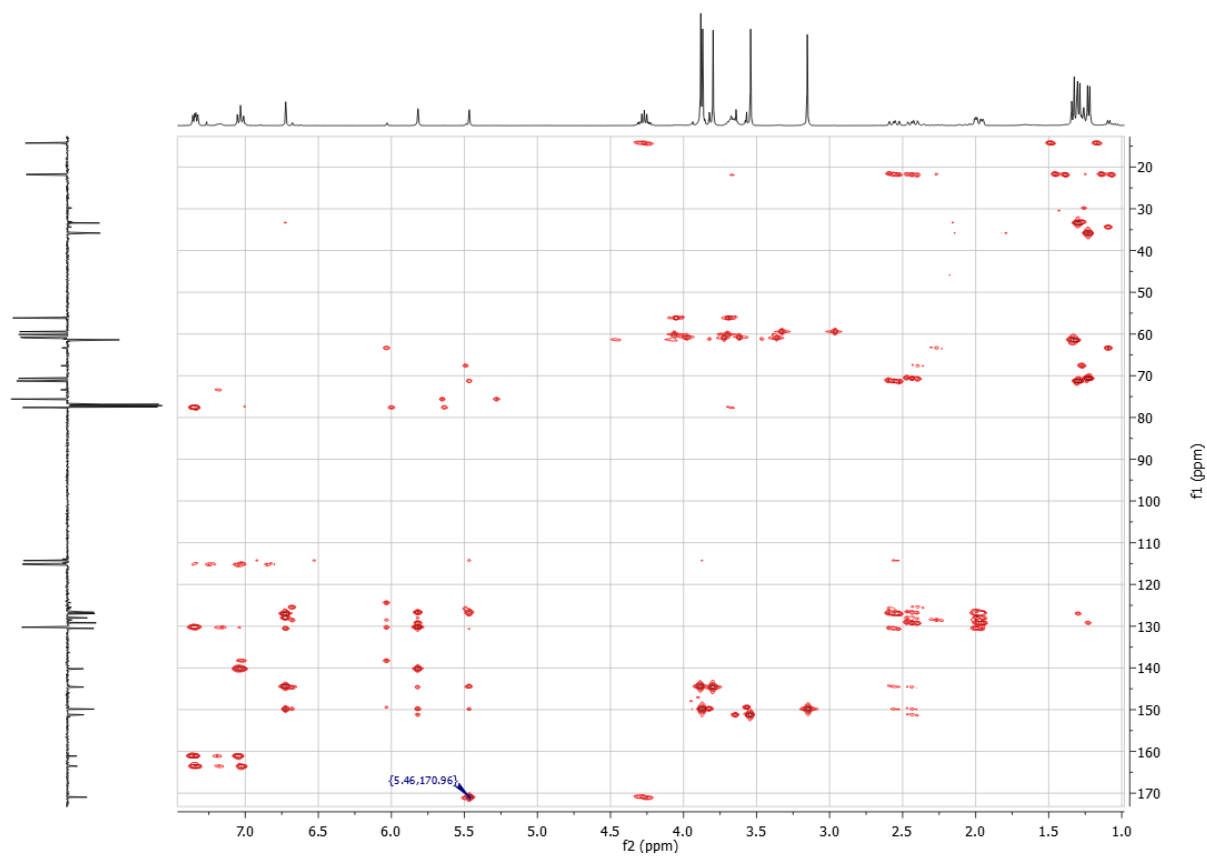


**Figure S88.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR (400 MHz) spectrum of (aS,1R,3S,1'S,3'S)-**22** in  $\text{CDCl}_3$ .

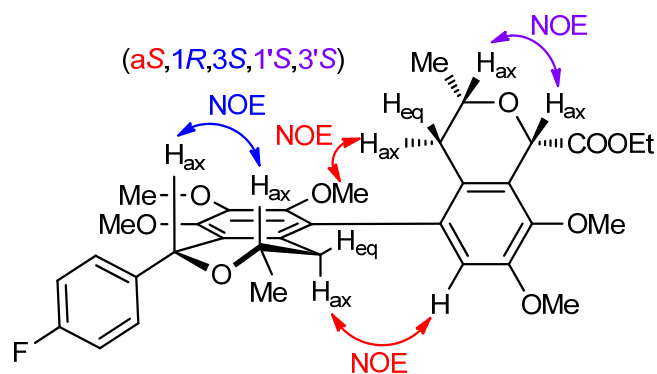


**Figure S89.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR (400 MHz) spectrum of (aS,1R,3S,1'S,3'S)-**22** in  $\text{CDCl}_3$ .

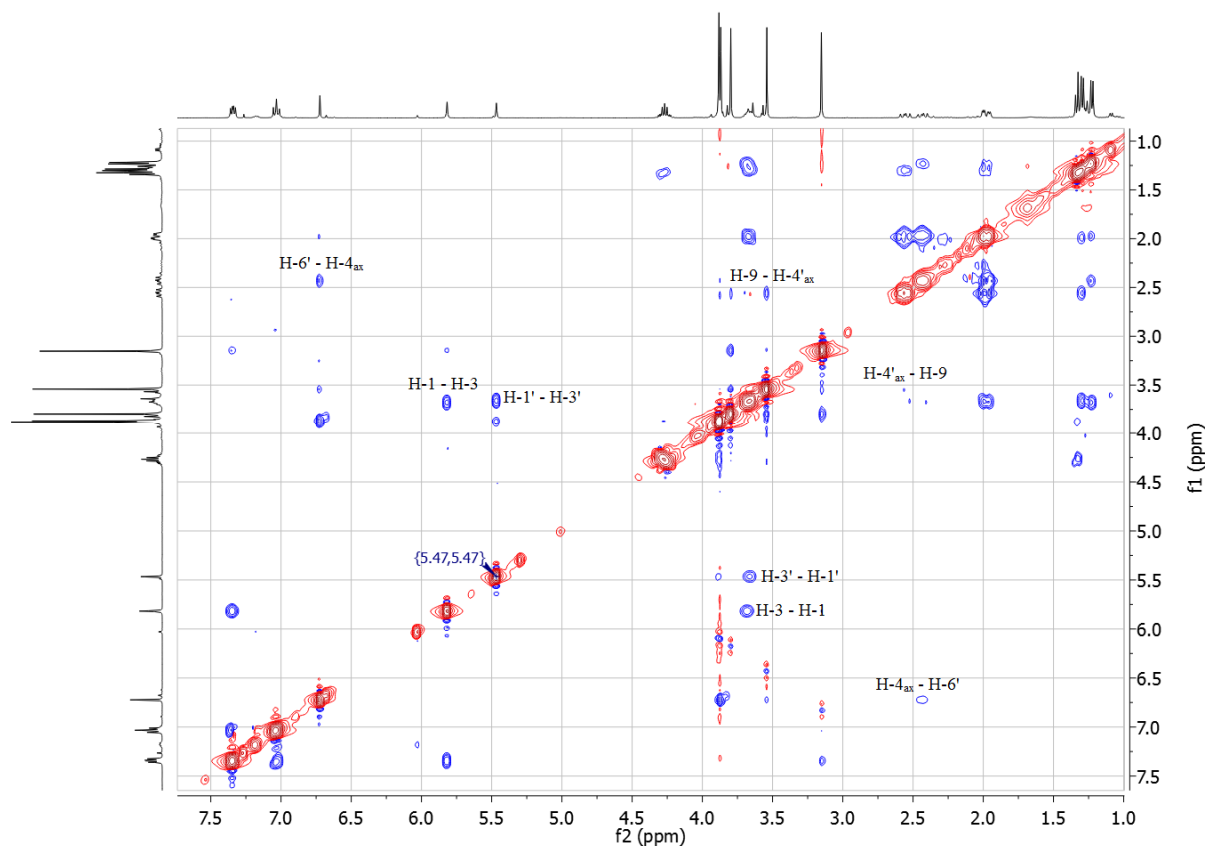




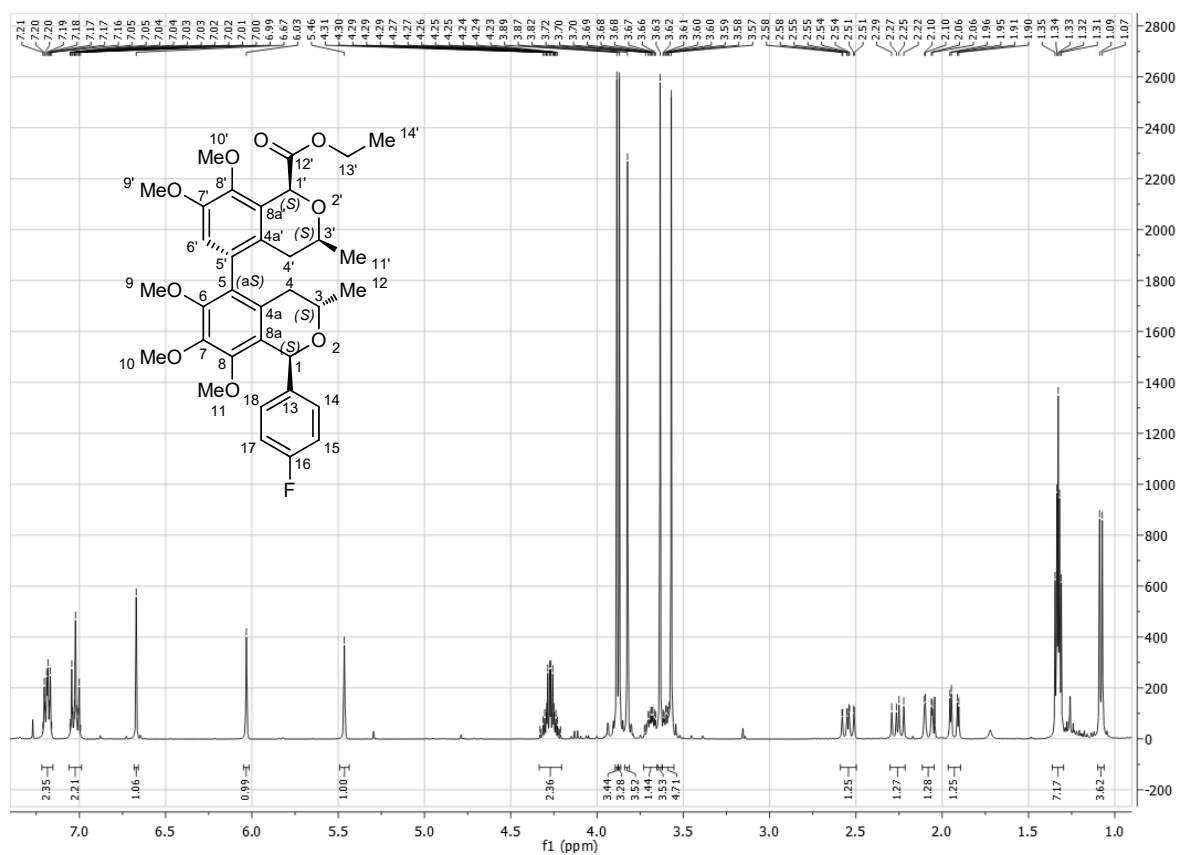
**Figure S90.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC NMR (400 MHz) spectrum of (*aS*,1*R*,3*S*,1'*S*,3'*S*)-**22** in  $\text{CDCl}_3$ .



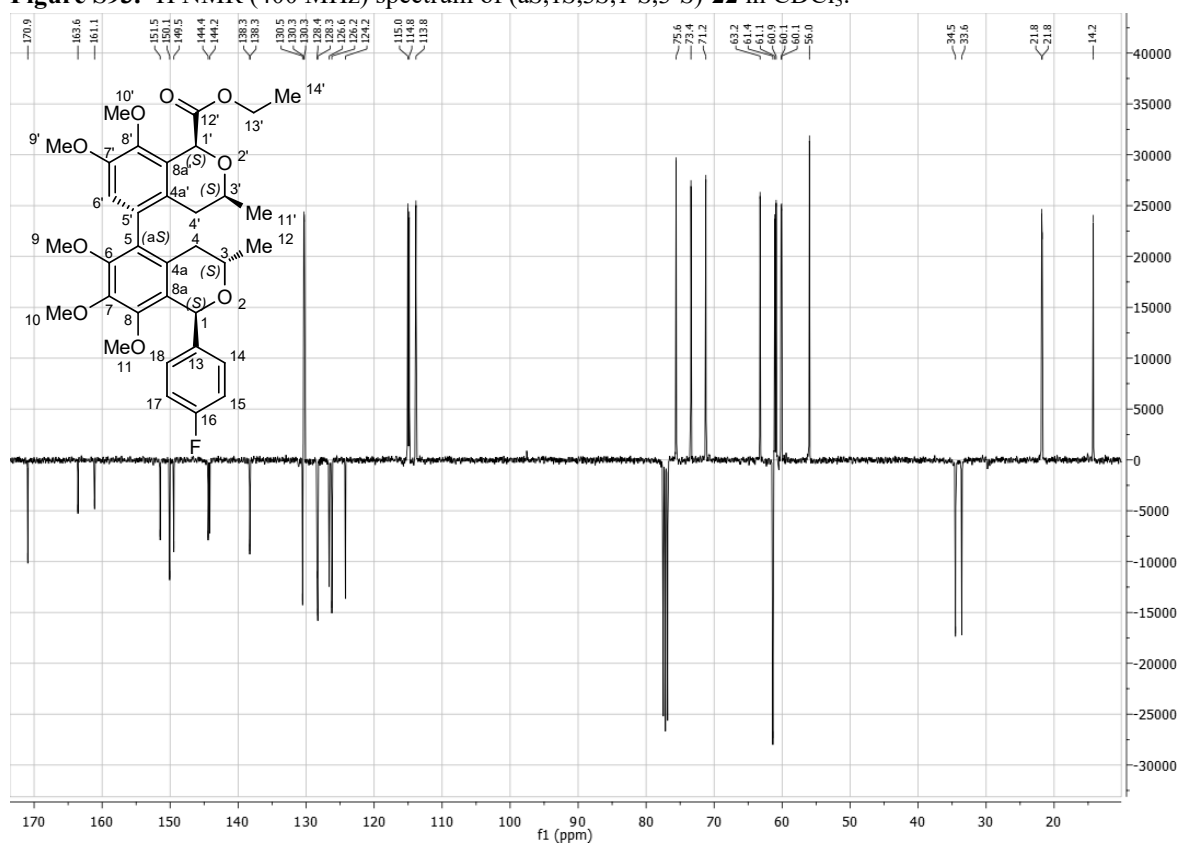
**Figure S91.** Characteristic NOE correlations shown on the structure of (aS,1R,3S,1'S,3'S)-22 suggesting (1R,3S,1'S,3'S) configurations of isochroman subunits and (aS) axial chirality.



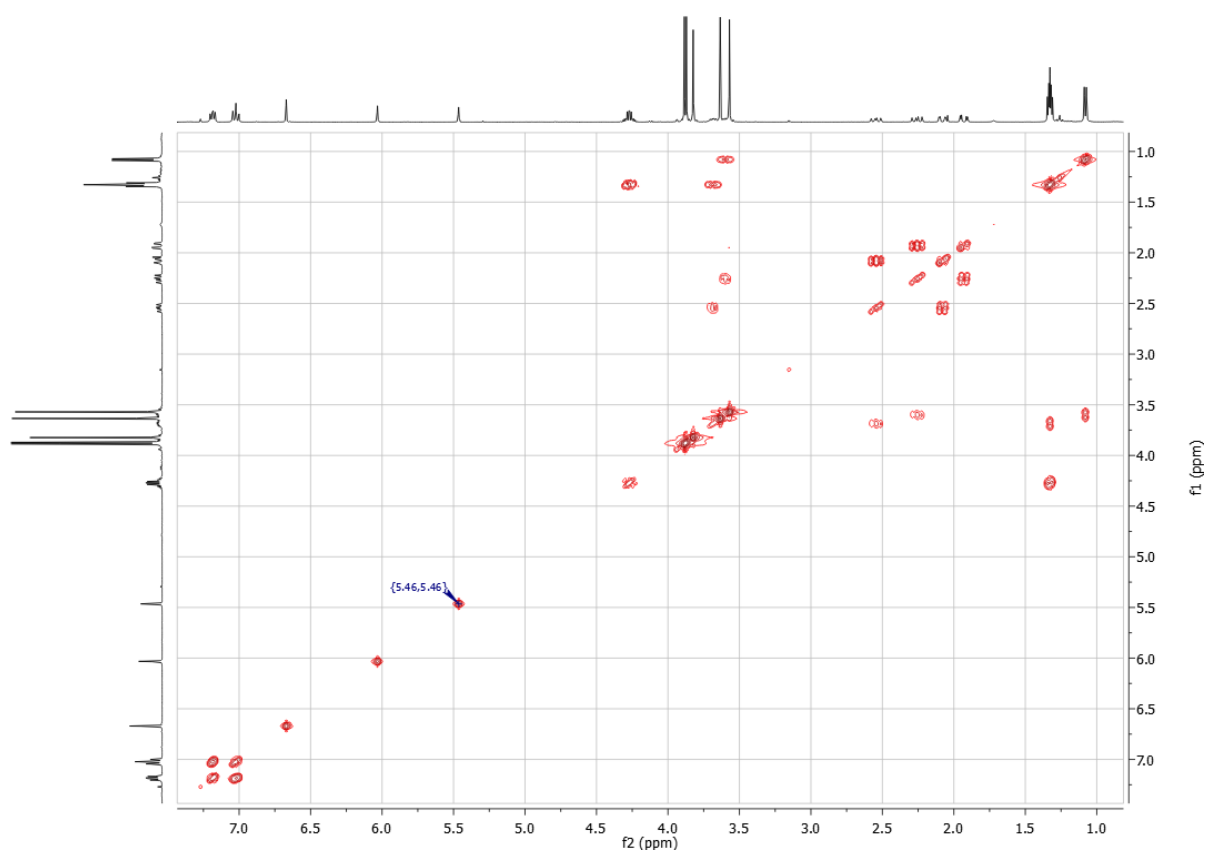
**Figure S92.** <sup>1</sup>H-<sup>1</sup>H NOESY NMR (400 MHz) spectrum of (aS,1R,3S,1'S,3'S)-22 in CDCl<sub>3</sub>.



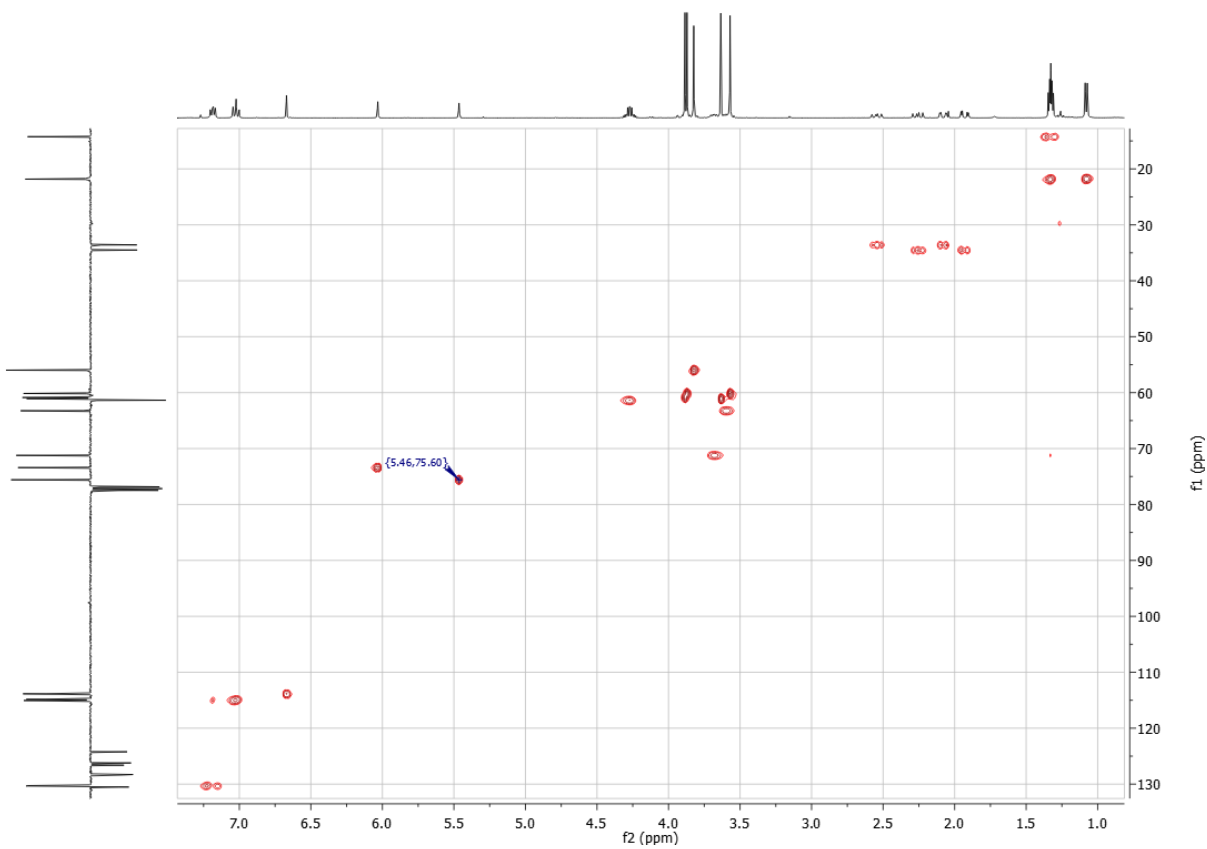
**Figure S93.**  $^1\text{H}$  NMR (400 MHz) spectrum of (aS,1S,3S,1'S,3'S)-**22** in  $\text{CDCl}_3$ .



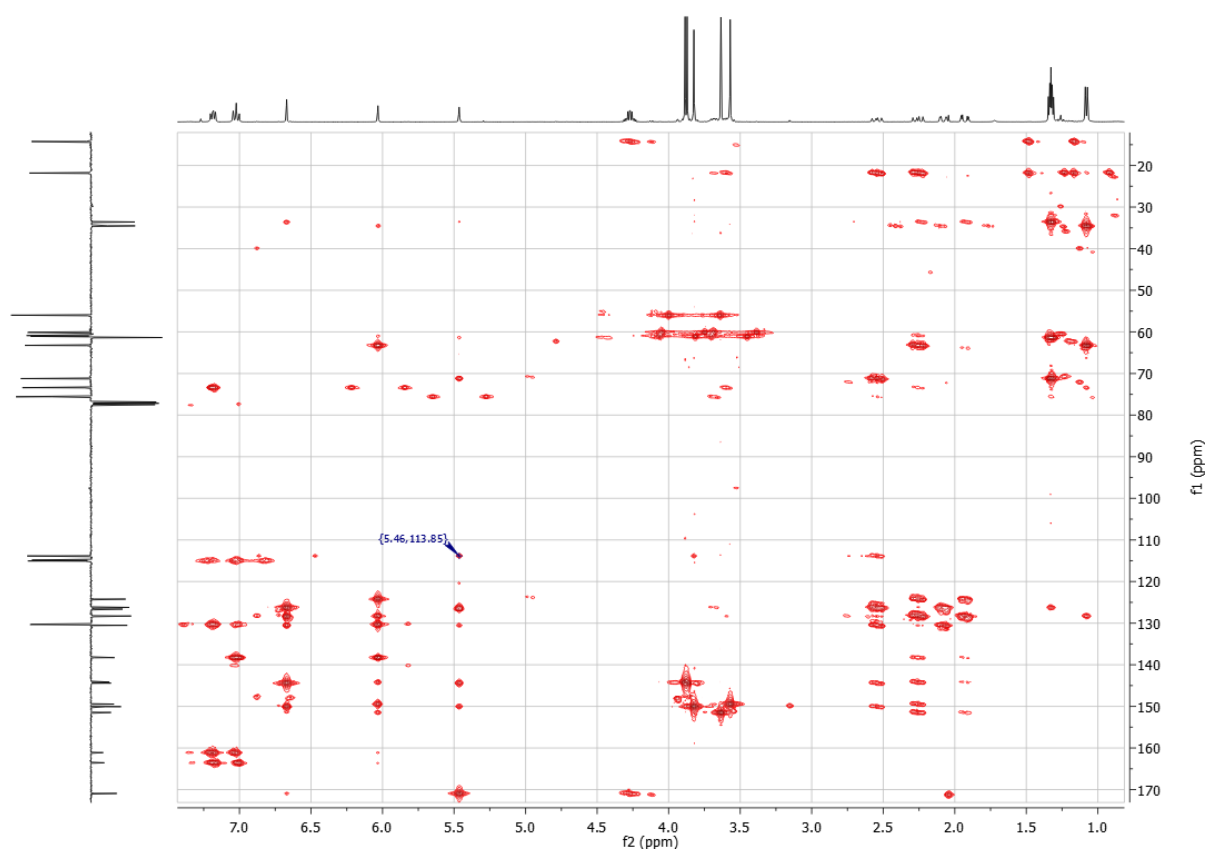
**Figure S94.**  $^{13}\text{C}$  NMR (100 MHz) spectrum of (aS,1S,3S,1'S,3'S)-**22** in  $\text{CDCl}_3$ .



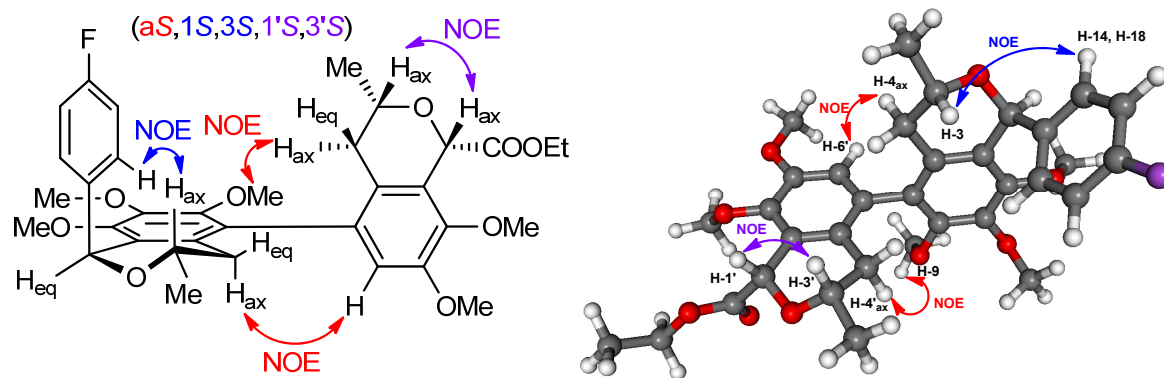
**Figure S95.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR (400 MHz) spectrum of (aS,1S,3S,1'S,3'S)-**22** in  $\text{CDCl}_3$ .



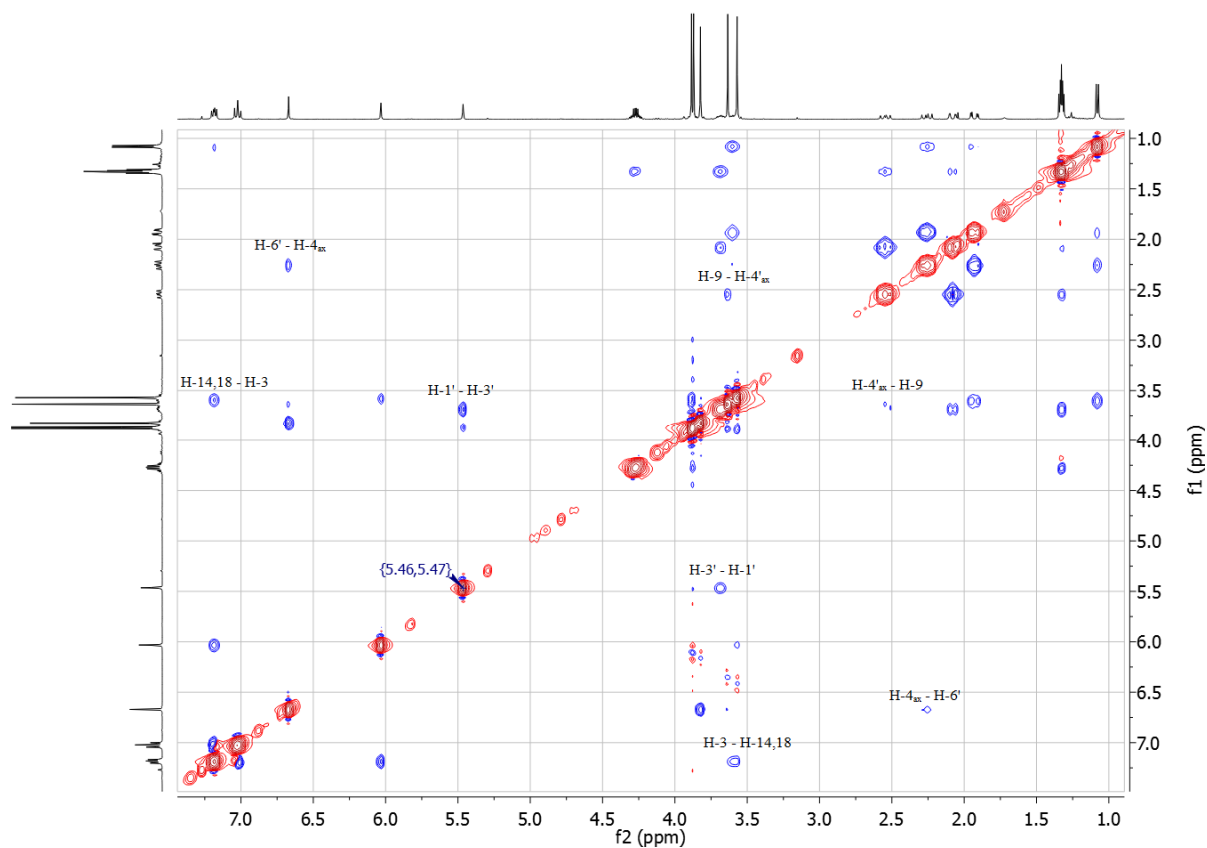
**Figure S96.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR (400 MHz) spectrum of (aS,1S,3S,1'S,3'S)-**22** in  $\text{CDCl}_3$ .



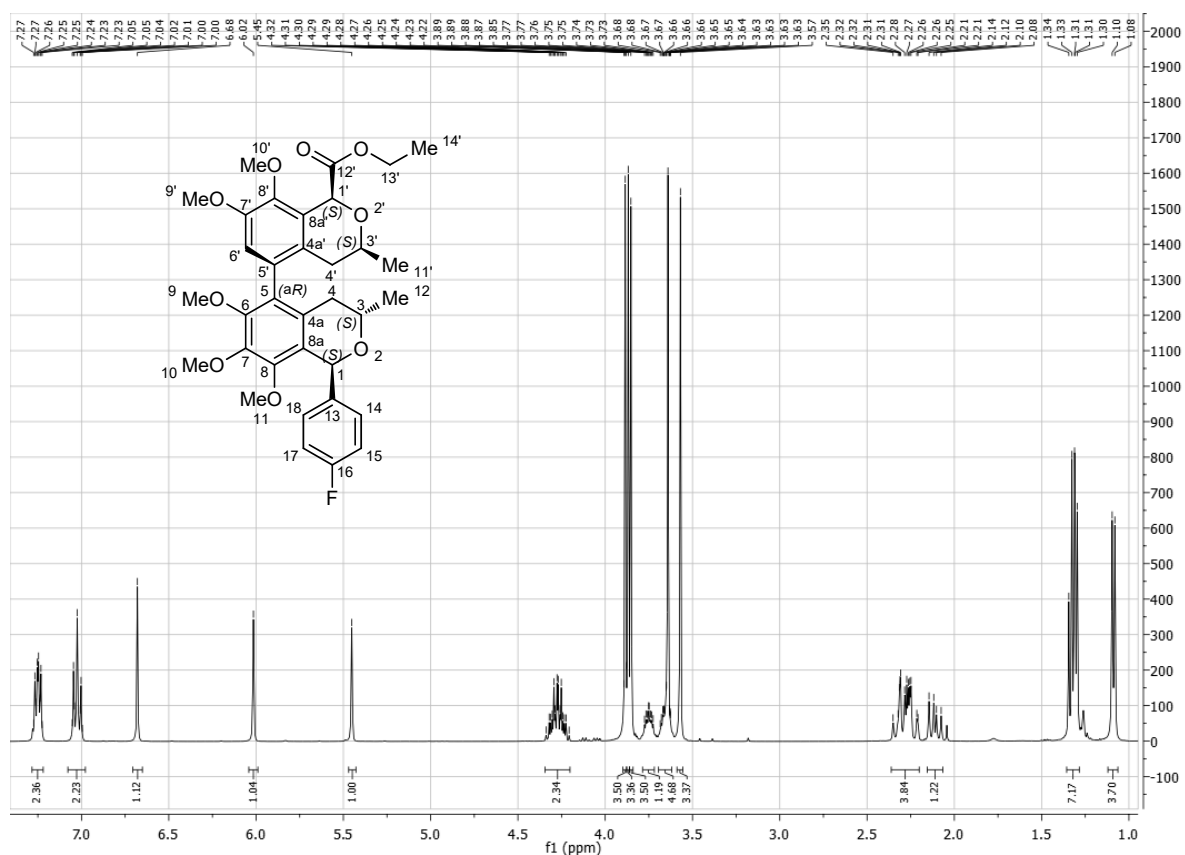
**Figure S97.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC NMR (400 MHz) spectrum of (*aS*,1*S*,3*S*,1'*S*,3'*S*)-**22** in  $\text{CDCl}_3$ .



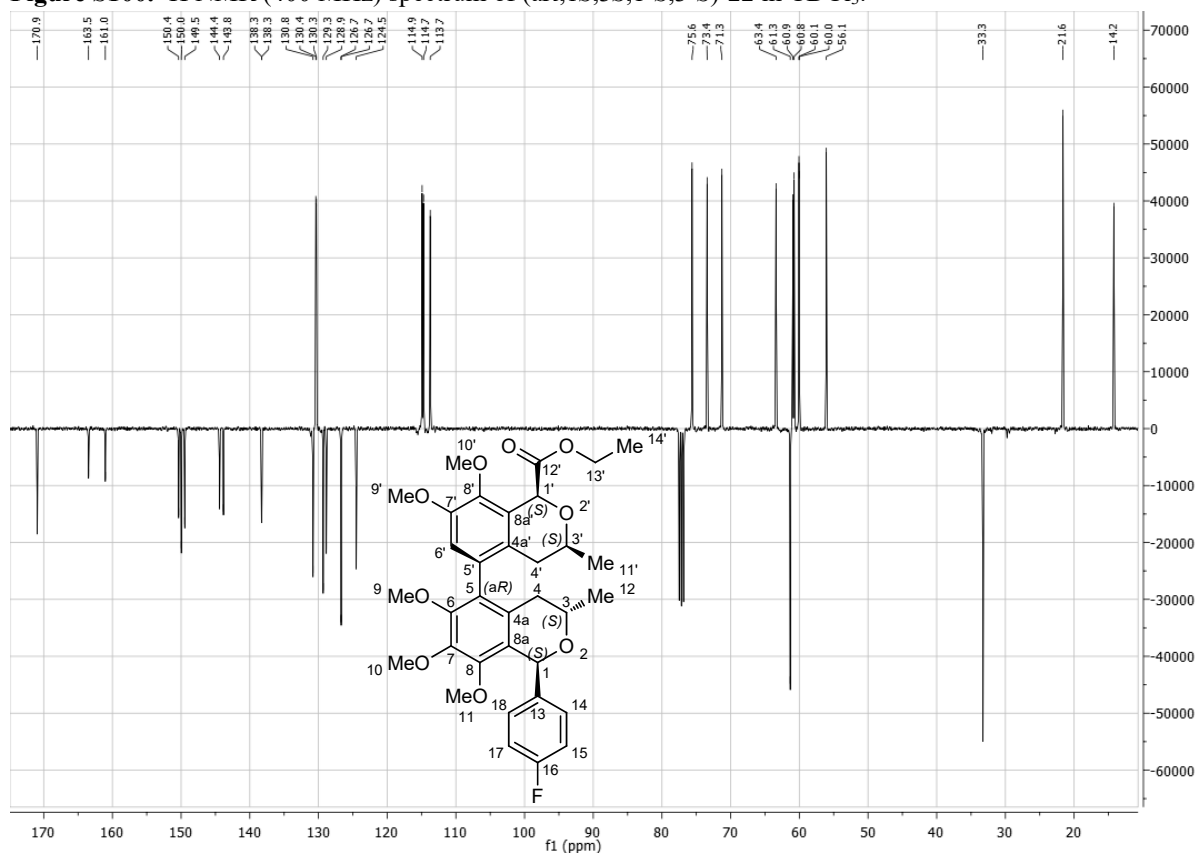
**Figure S98.** Characteristic NOE correlations shown on the lowest-energy computed conformer of (aS,1S,3S,1'S,3'S)-**22** suggesting (1S,3S,1'S,3'S) configurations of isochroman subunits and (aS) axial chirality.



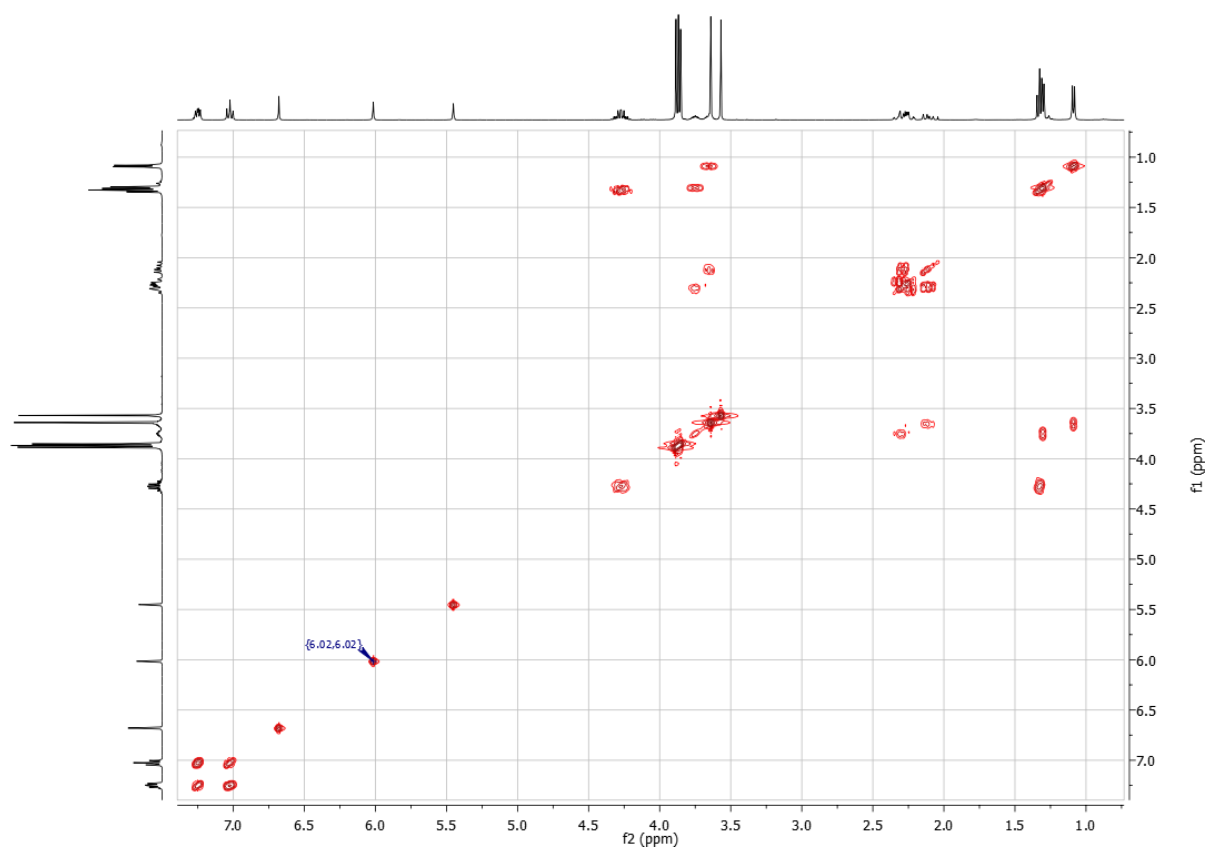
**Figure S99.**  $^1\text{H}$ - $^1\text{H}$  NOESY NMR (400 MHz) spectrum of (aS,1S,3S,1'S,3'S)-**22** in  $\text{CDCl}_3$ .



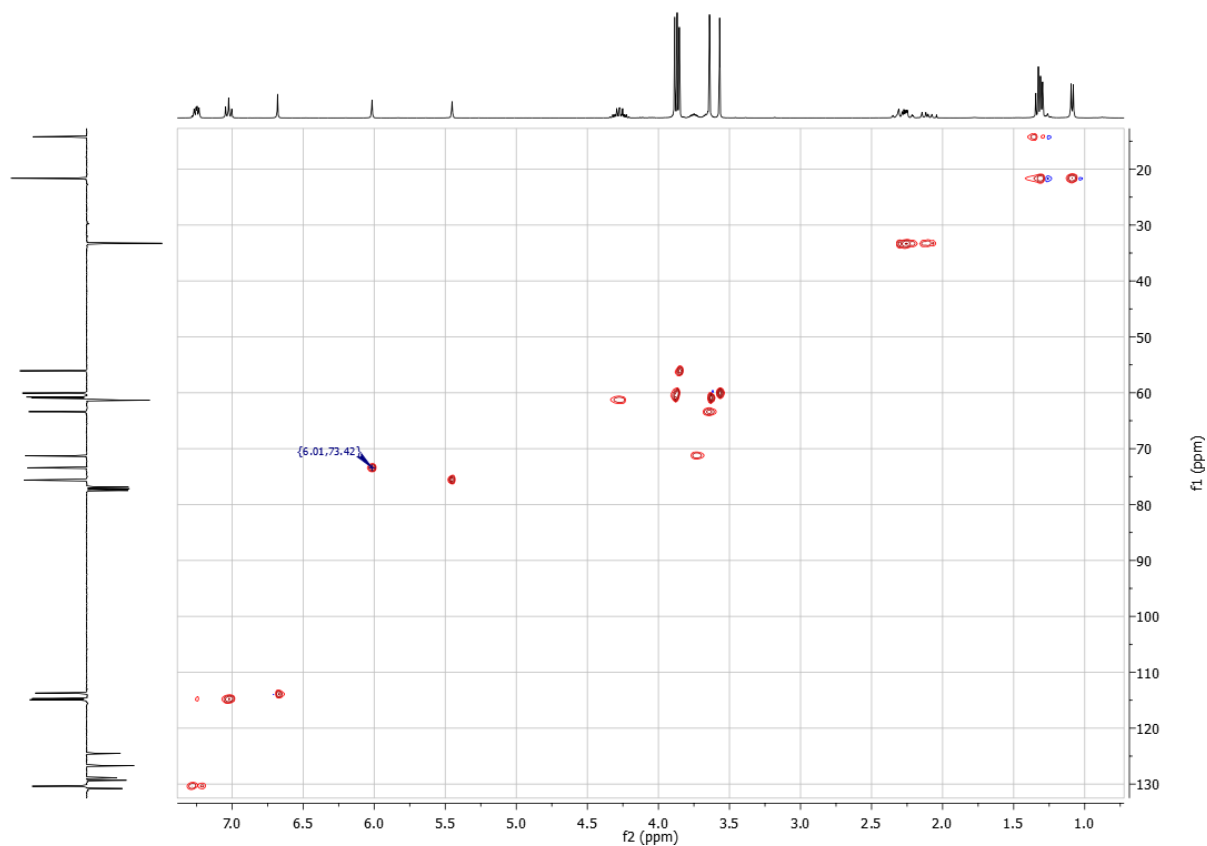
**Figure S100.**  $^1\text{H}$  NMR (400 MHz) spectrum of (aR,1S,3S,1'S,3'S)-**22** in  $\text{CDCl}_3$ .



**Figure S101.**  $^{13}\text{C}$  NMR (100 MHz) spectrum of (aR,1S,3S,1'S,3'S)-**22** in  $\text{CDCl}_3$ .

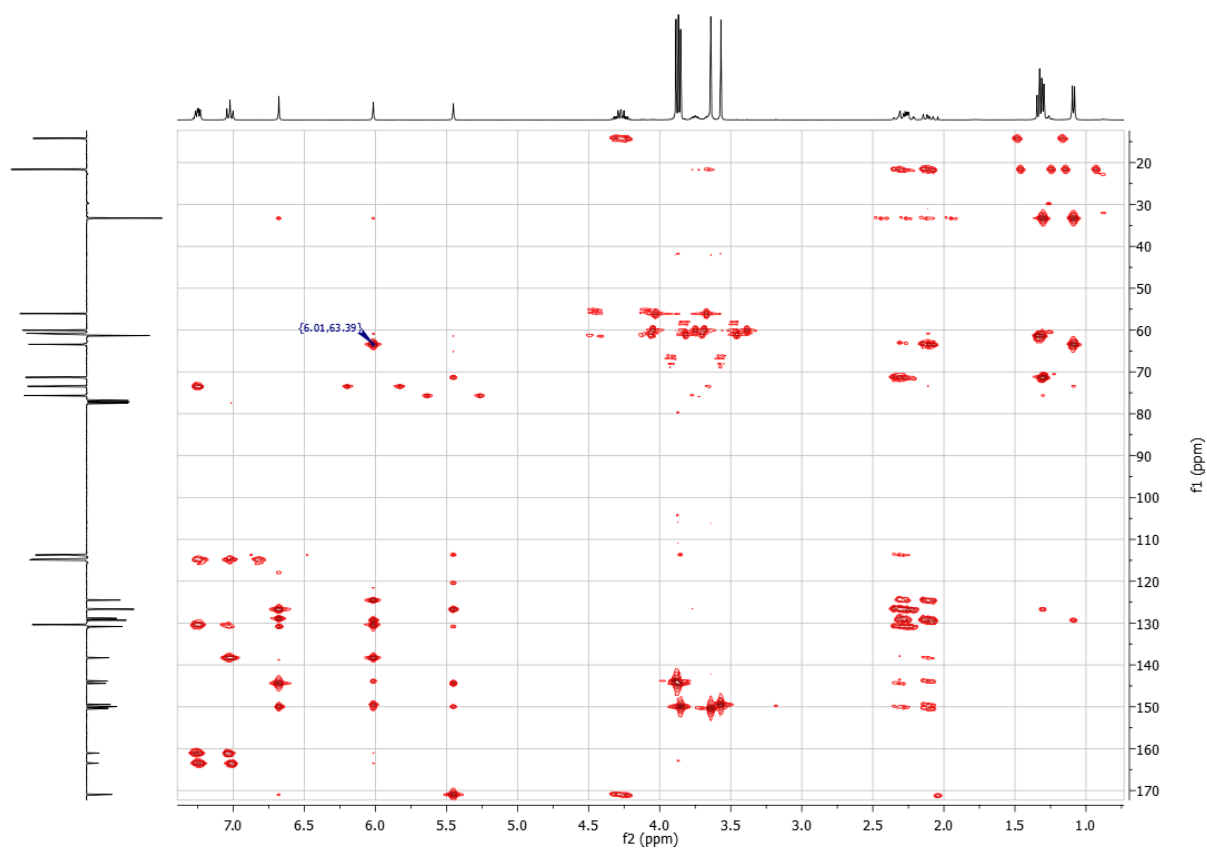


**Figure S102.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR (400 MHz) spectrum of (aR,1S,3S,1'S,3'S)-**22** in  $\text{CDCl}_3$ .

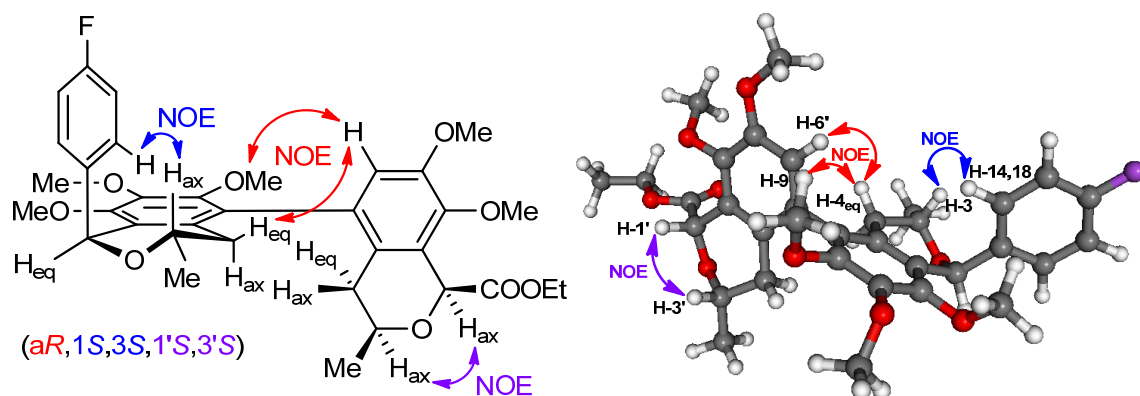


**Figure S103.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR (400 MHz) spectrum of (aR,1S,3S,1'S,3'S)-**22** in  $\text{CDCl}_3$ .

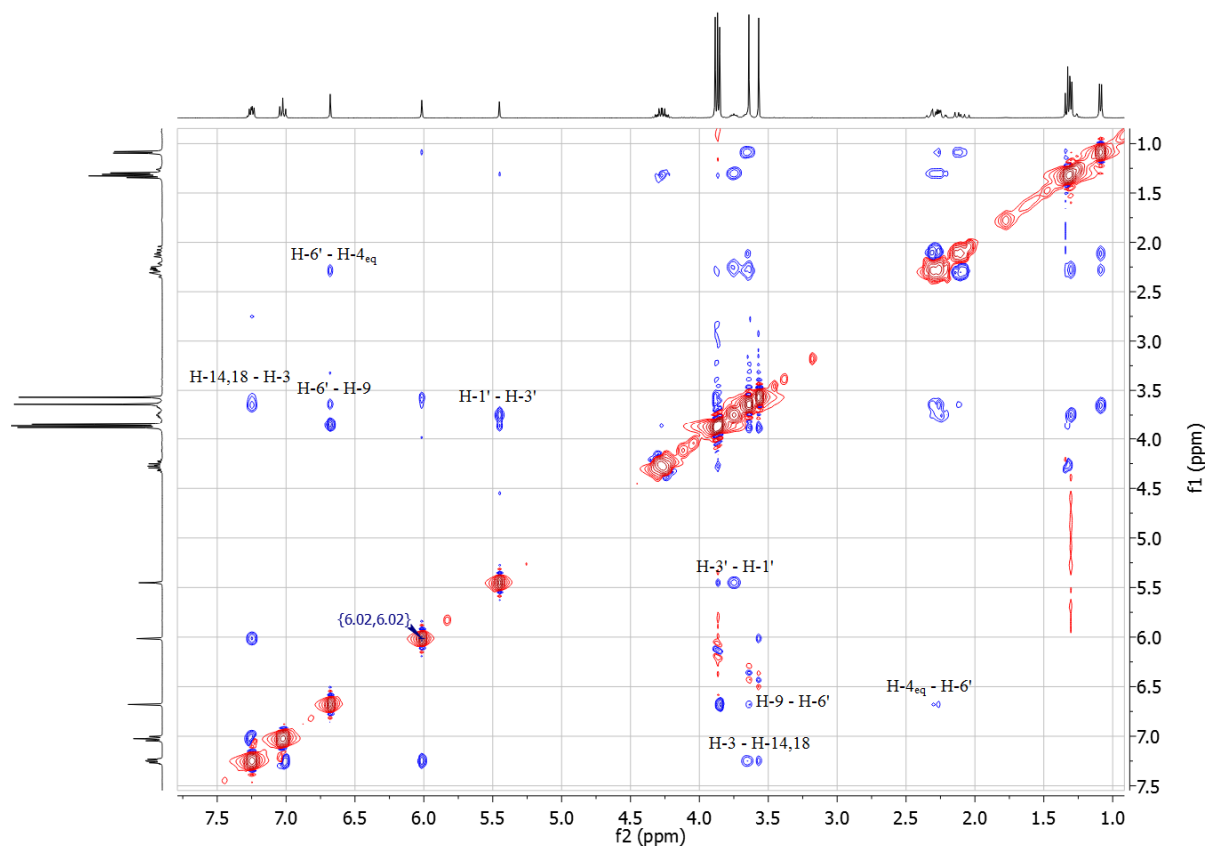




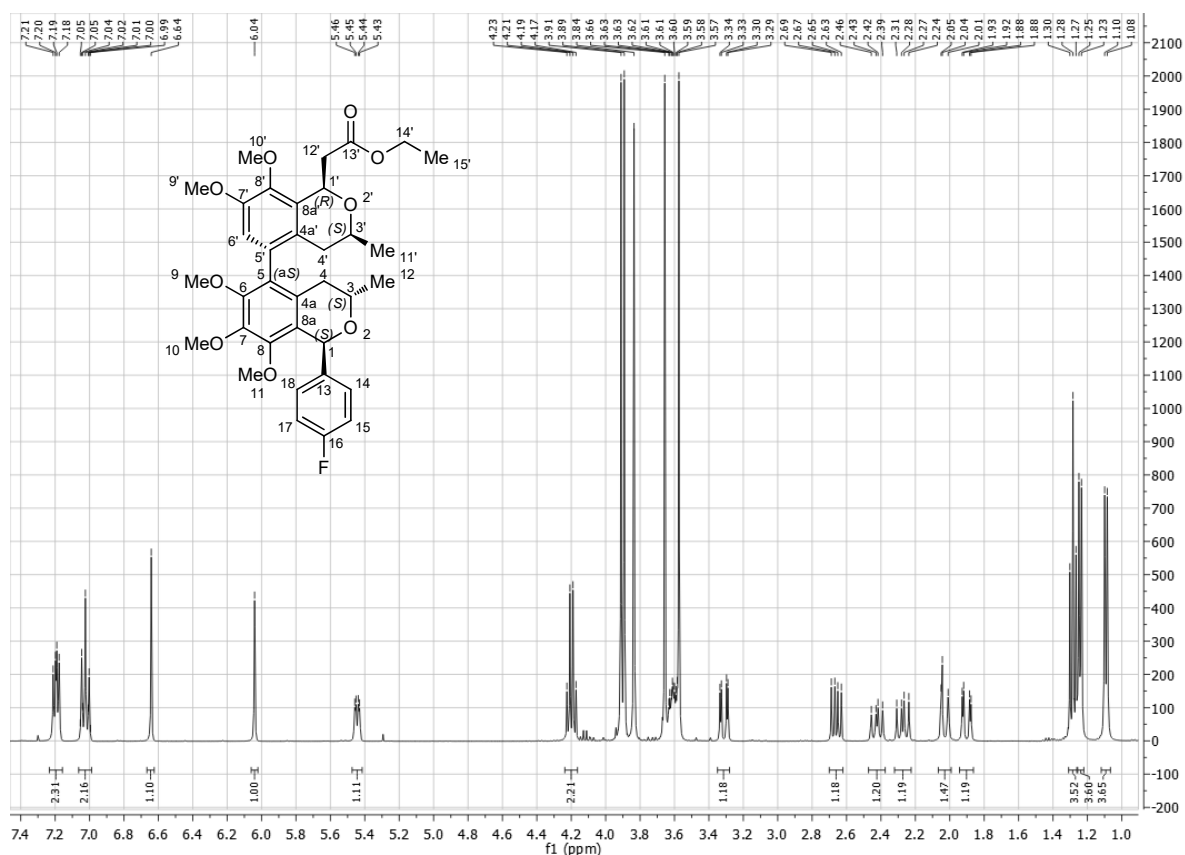
**Figure S104.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC NMR (400 MHz) spectrum of (*aR*,1*S*,3*S*,1'*S*,3'*S*)-**22** in  $\text{CDCl}_3$ .



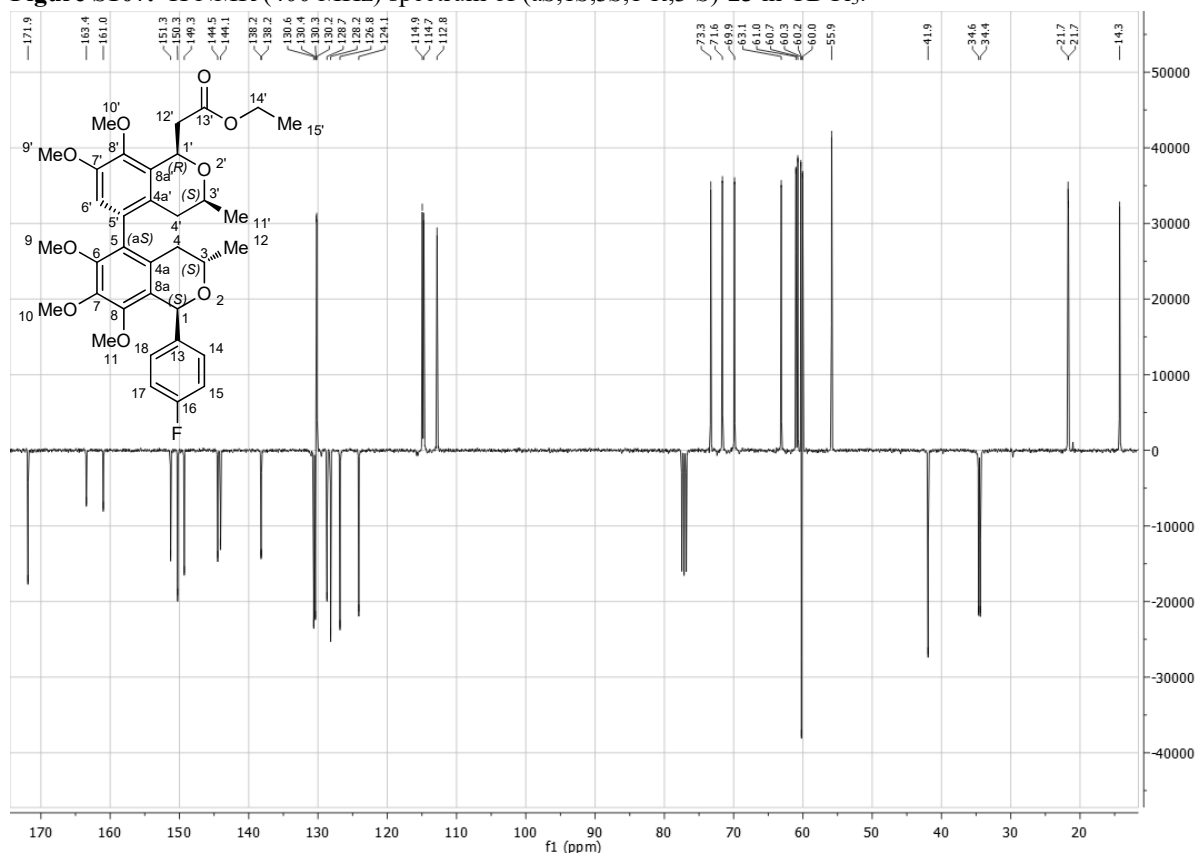
**Figure S105.** Characteristic NOE correlations shown on the lowest-energy computed conformer of (*aR*,1*S*,3*S*,1'*S*,3'*S*)-**22** suggesting (1*S*,3*S*,1'*S*,3'*S*) configurations of isochroman subunits and (*aR*) axial chirality.



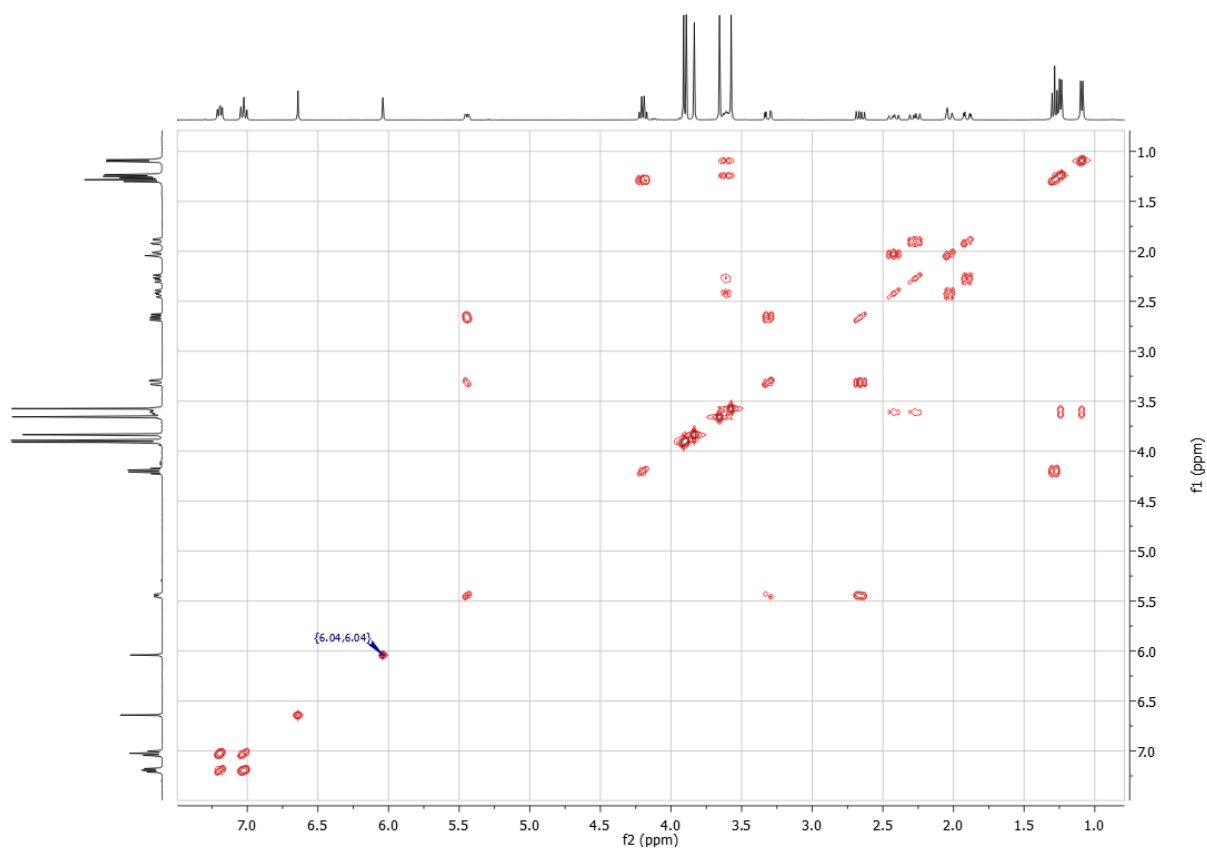
**Figure S106.**  $^1\text{H}$ - $^1\text{H}$  NOESY NMR (400 MHz) spectrum of (*aR*,1*S*,3*S*,1'*S*,3'*S*)-**22** in  $\text{CDCl}_3$ .



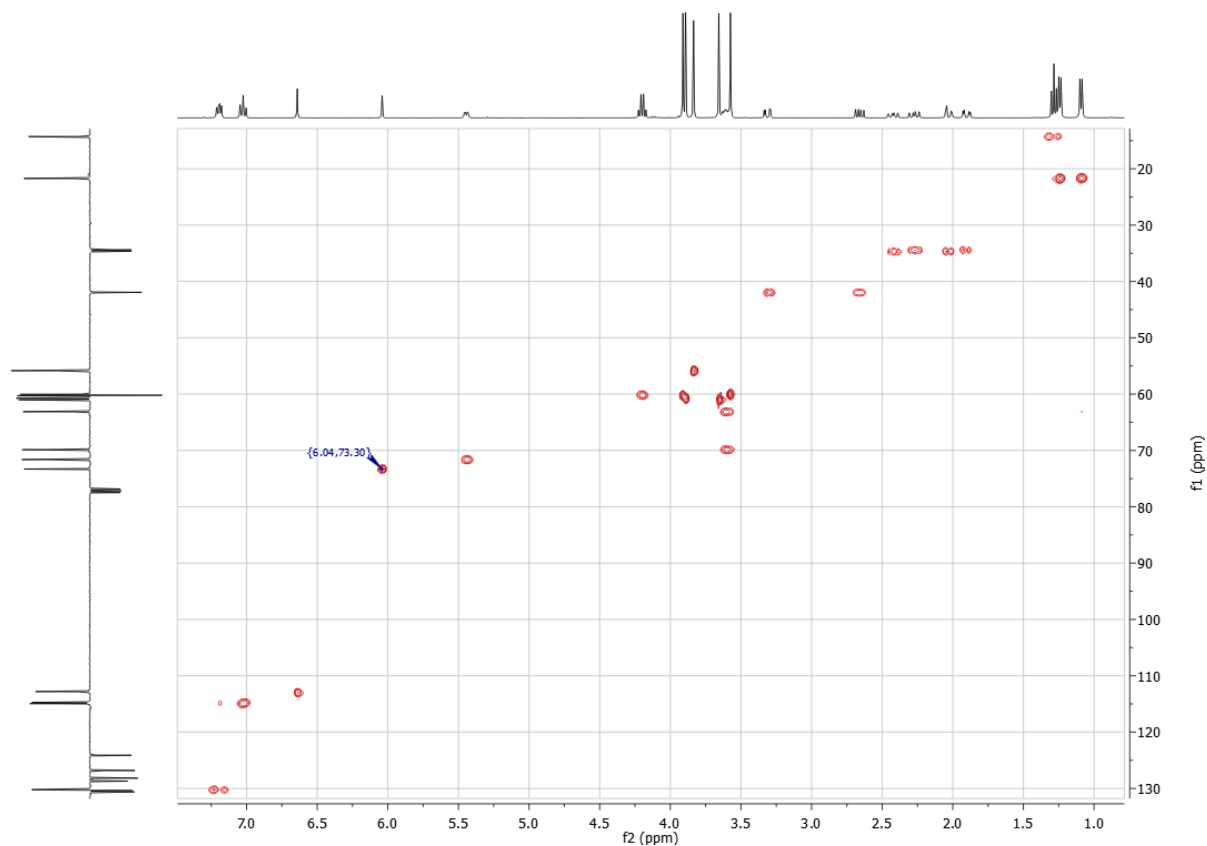
**Figure S107.**  $^1\text{H}$  NMR (400 MHz) spectrum of  $(aS,1S,3S,1'R,3'S)$ -**23** in  $\text{CDCl}_3$ .



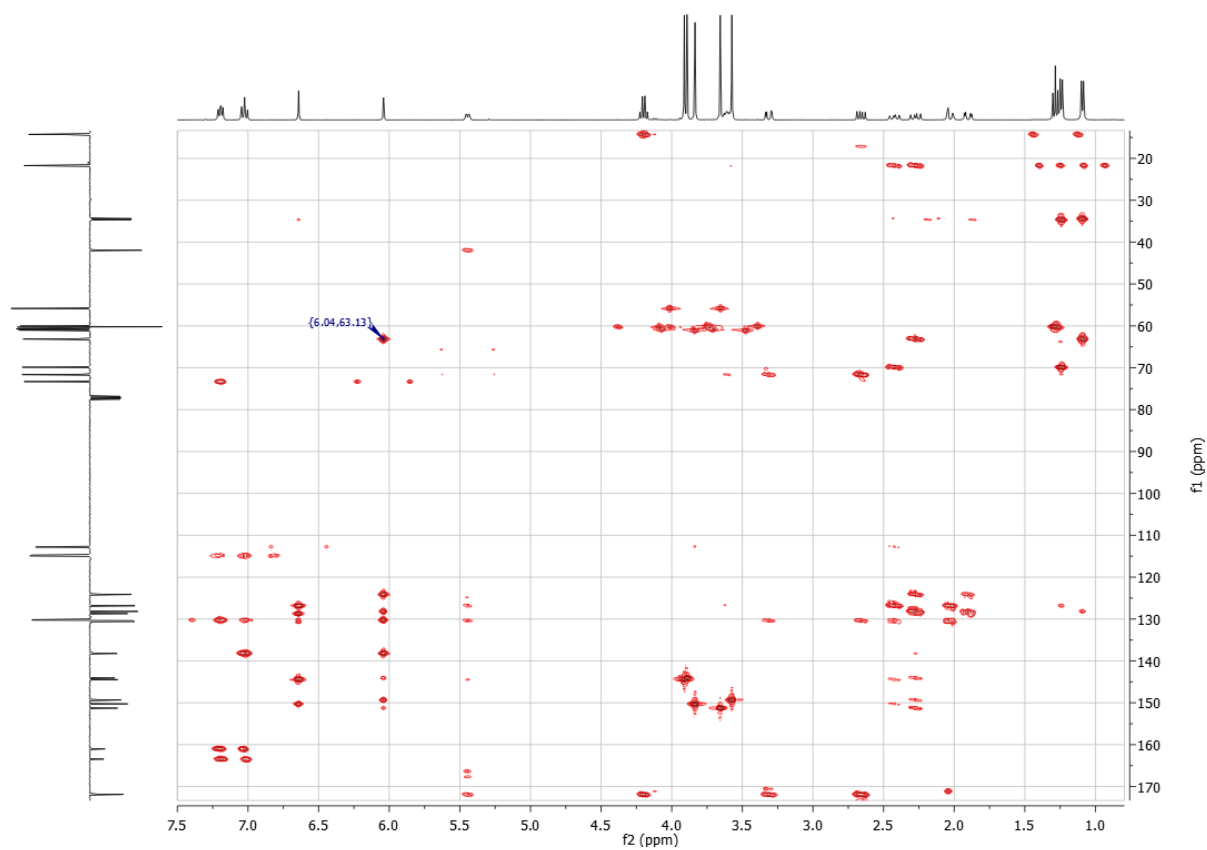
**Figure S108.**  $^{13}\text{C}$  NMR (100 MHz) spectrum of  $(aS,1S,3S,1'R,3'S)$ -**23** in  $\text{CDCl}_3$ .



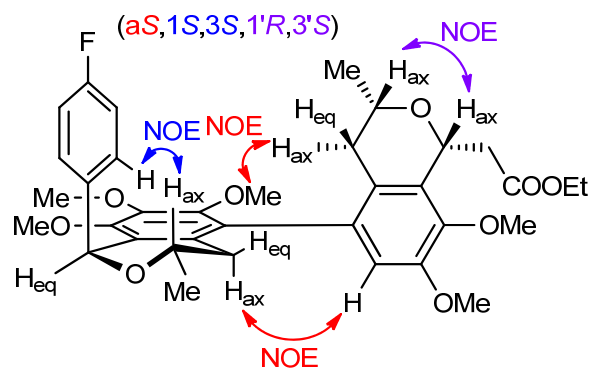
**Figure S109.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR (400 MHz) spectrum of (aS,1S,3S,1'R,3'S)-**23** in  $\text{CDCl}_3$ .



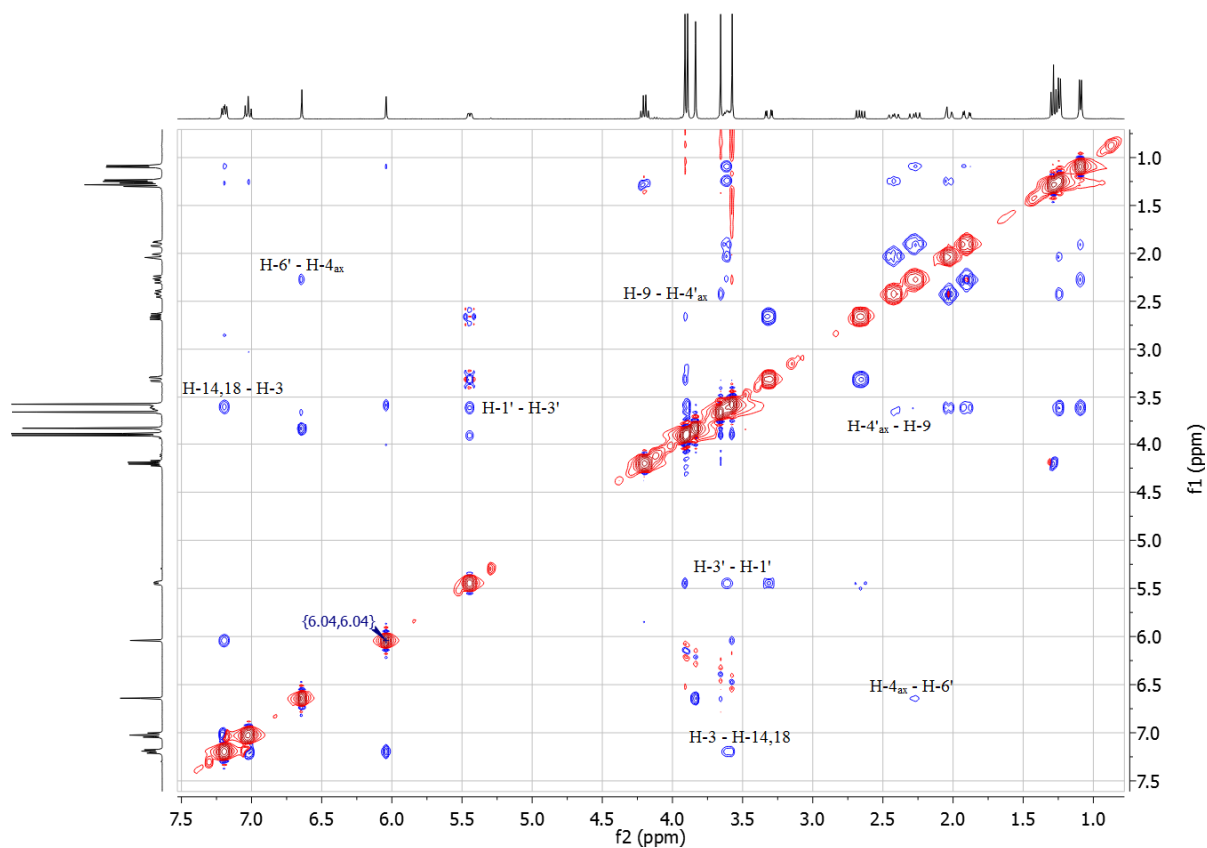
**Figure S110.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR (400 MHz) spectrum of (aS,1S,3S,1'R,3'S)-**23** in  $\text{CDCl}_3$ .



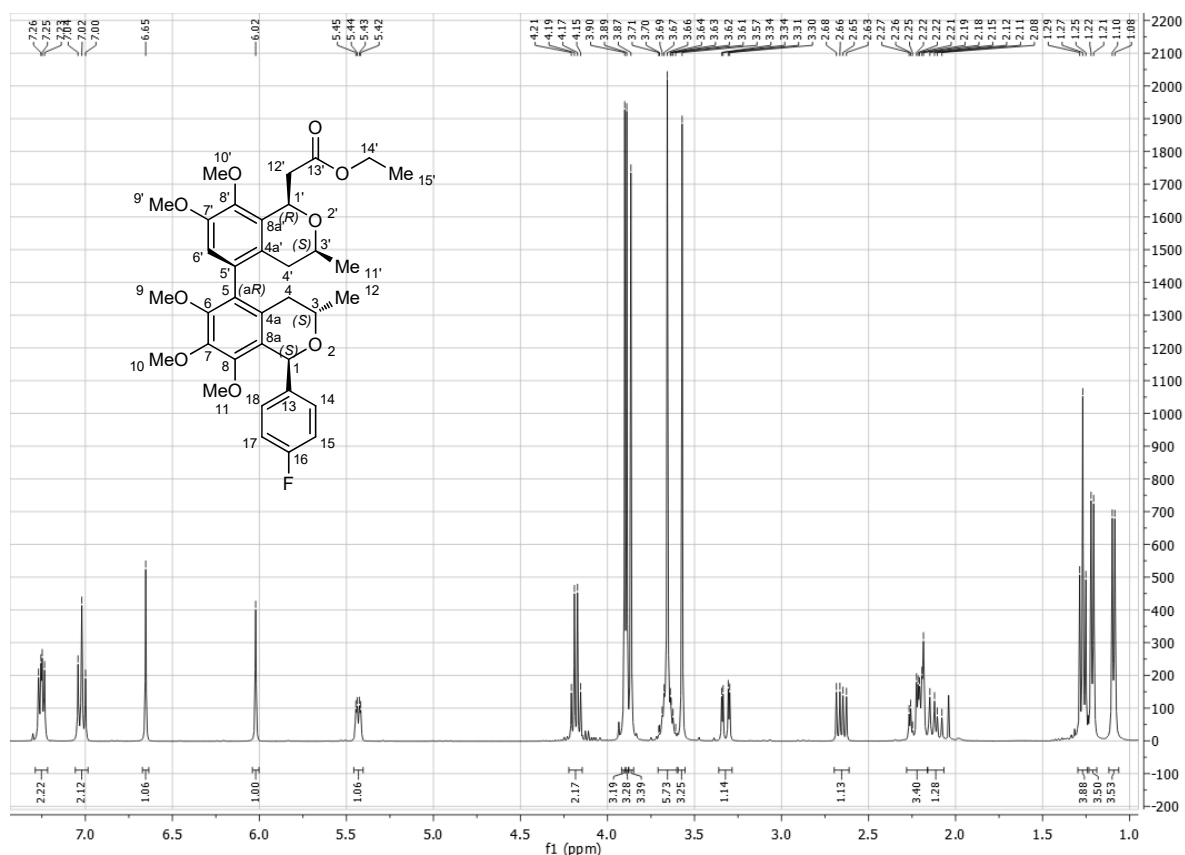
**Figure S111.** <sup>1</sup>H-<sup>13</sup>C HMBC NMR (400 MHz) spectrum of (aS,1S,3S,1'R,3'S)-**23** in CDCl<sub>3</sub>.



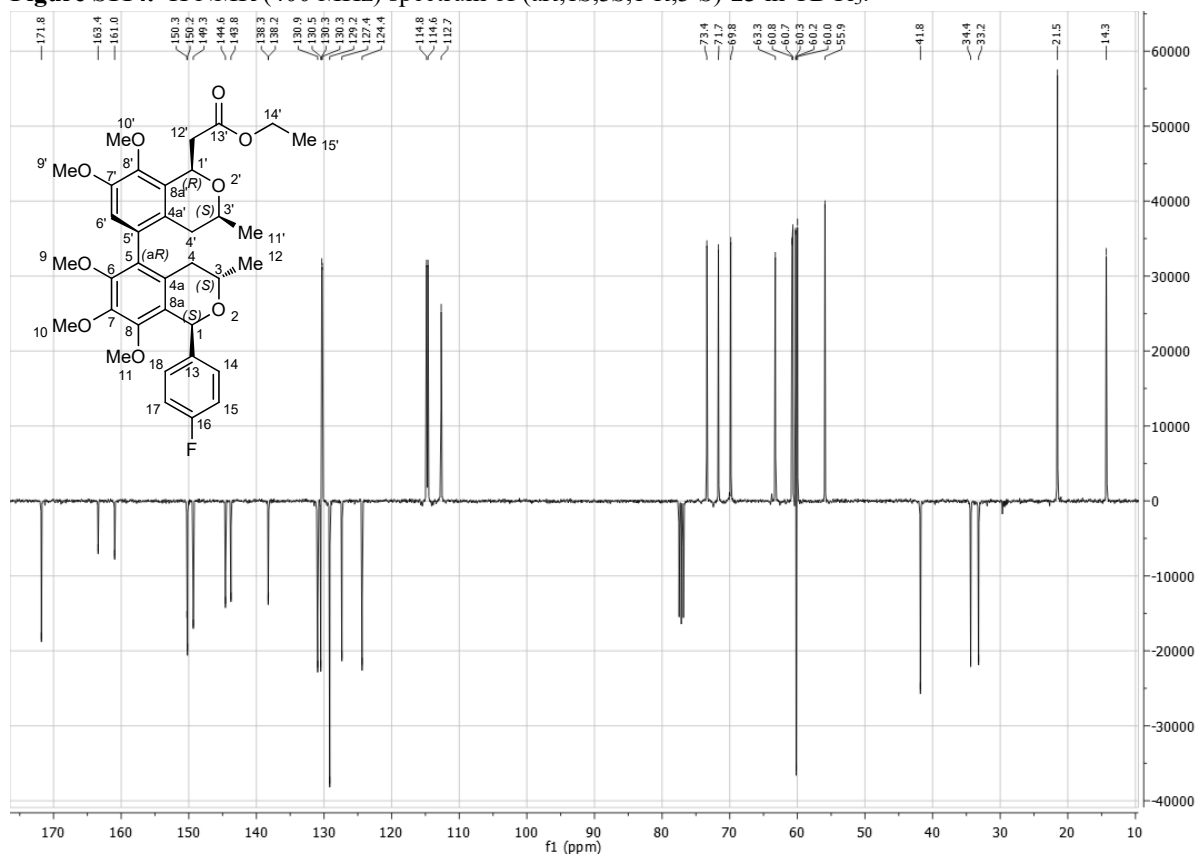
**Figure S112.** Characteristic NOE correlations shown on the structure of (aS,1S,3S,1'R,3'S)-**23** suggesting (1S,3S,1'R,3'S) configurations of isochroman subunits and (aS) axial chirality.



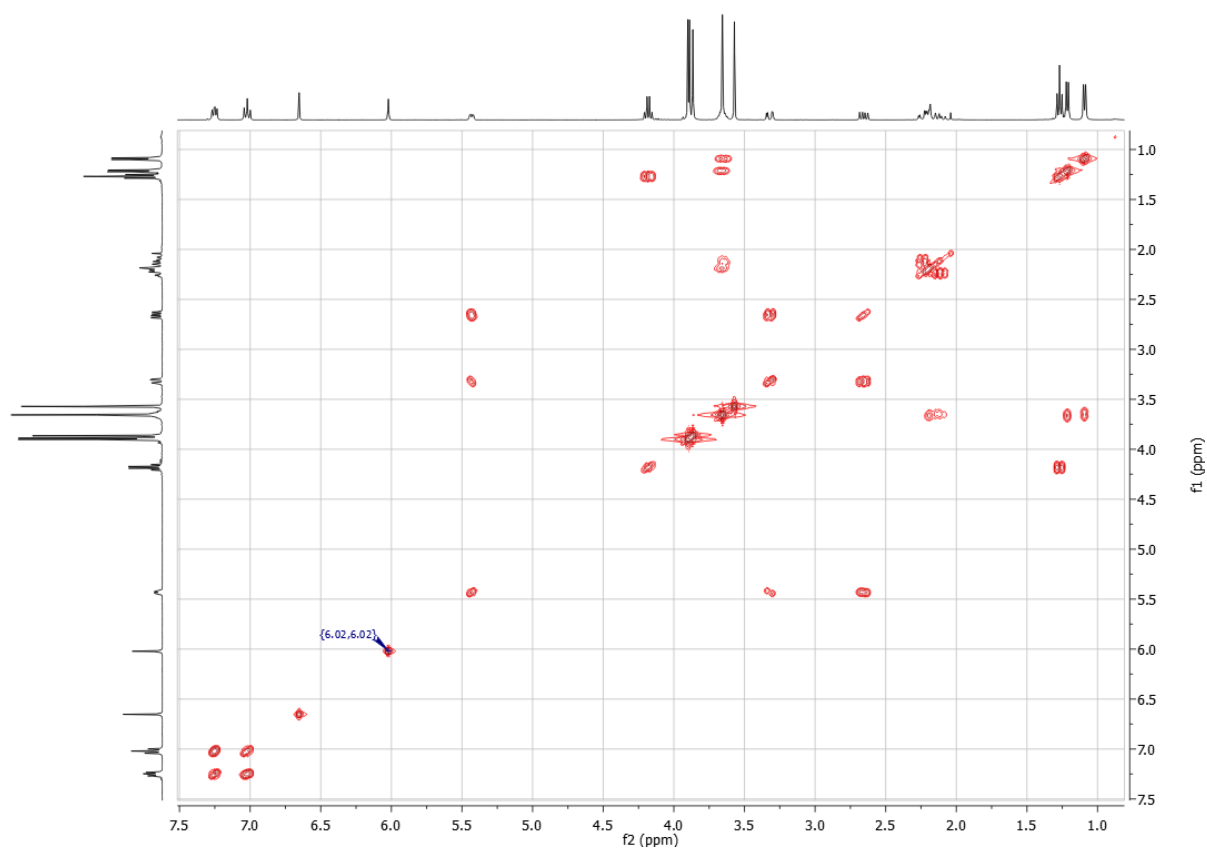
**Figure S113.** <sup>1</sup>H-<sup>1</sup>H NOESY NMR (400 MHz) spectrum of (aS,1S,3S,1'R,3'S)-**23** in CDCl<sub>3</sub>.



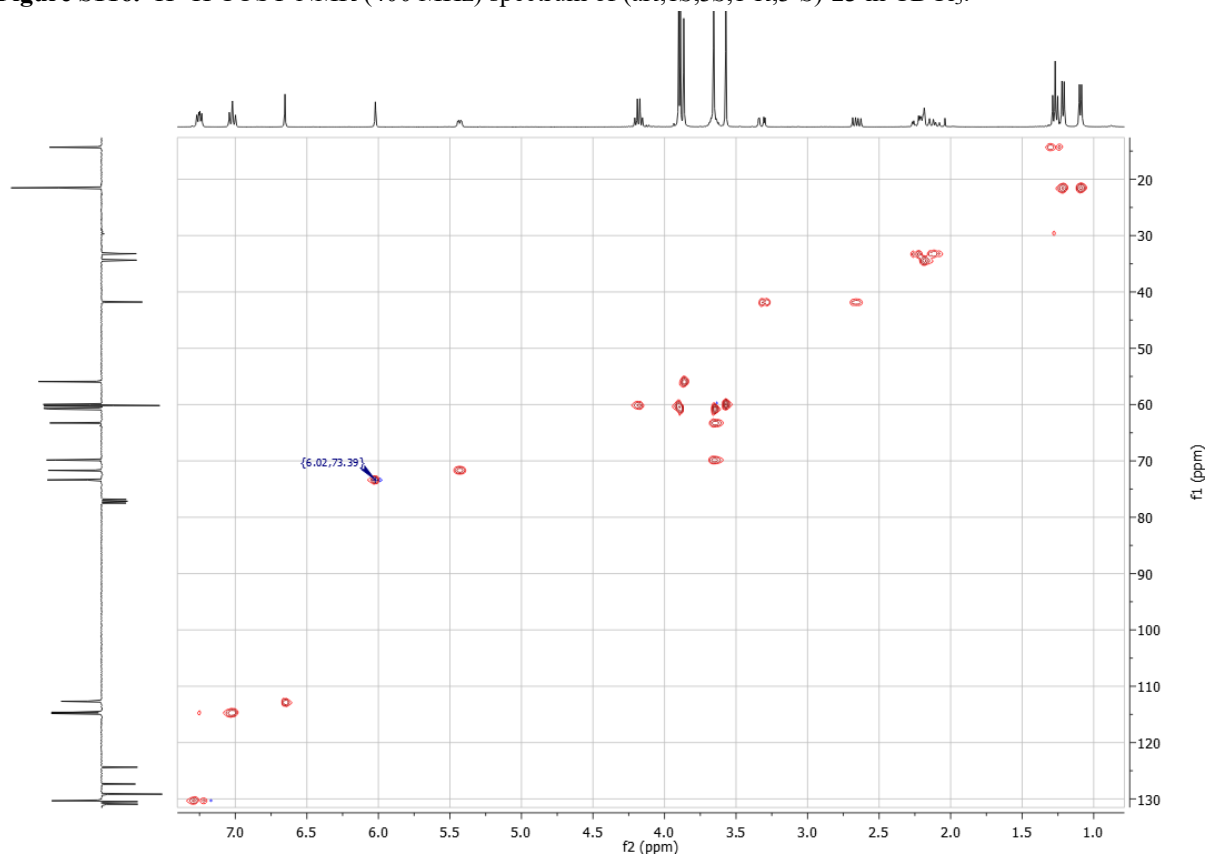
**Figure S114.**  $^1\text{H}$  NMR (400 MHz) spectrum of (aR,1S,3S,1'R,3'S)-23 in  $\text{CDCl}_3$ .



**Figure S115.**  $^{13}\text{C}$  NMR (100 MHz) spectrum of (aR,1S,3S,1'R,3'S)-23 in  $\text{CDCl}_3$ .

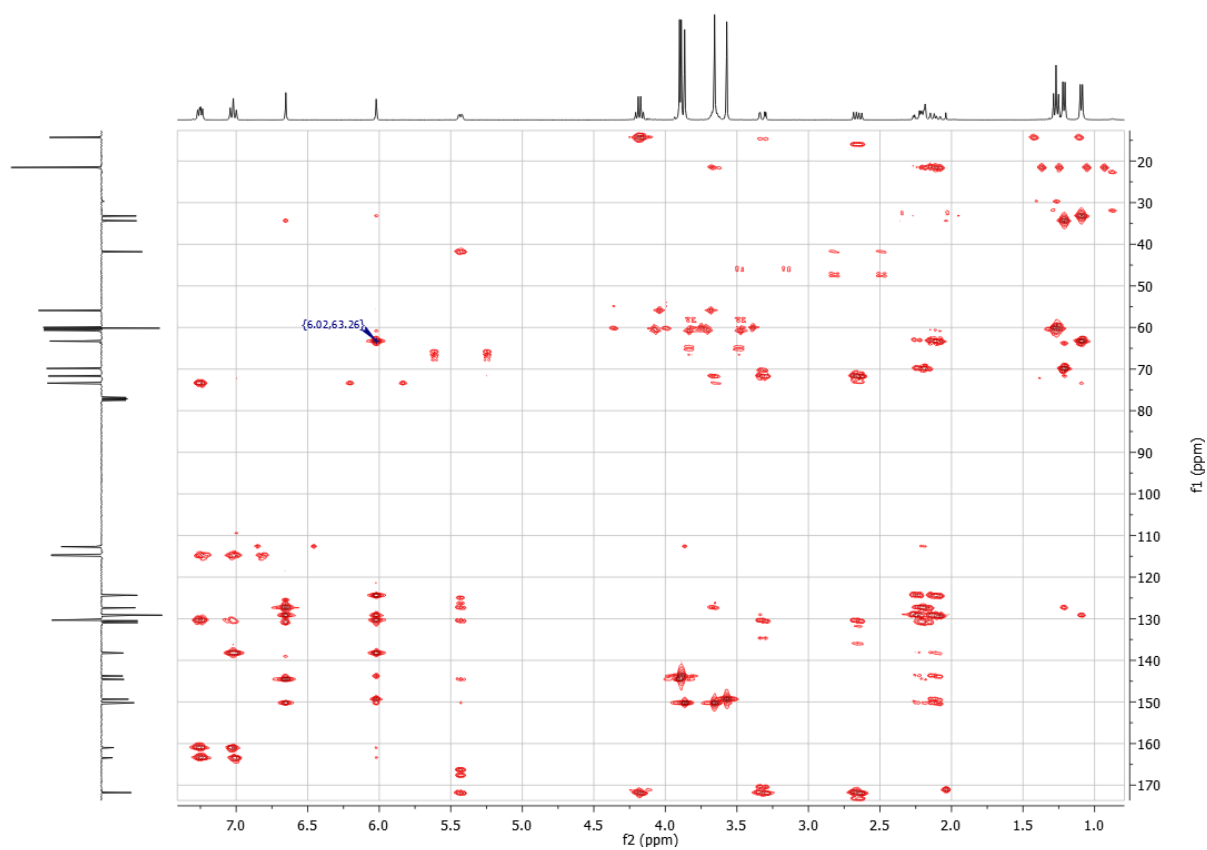


**Figure S116.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR (400 MHz) spectrum of (aR,1S,3S,1'R,3'S)-**23** in  $\text{CDCl}_3$ .

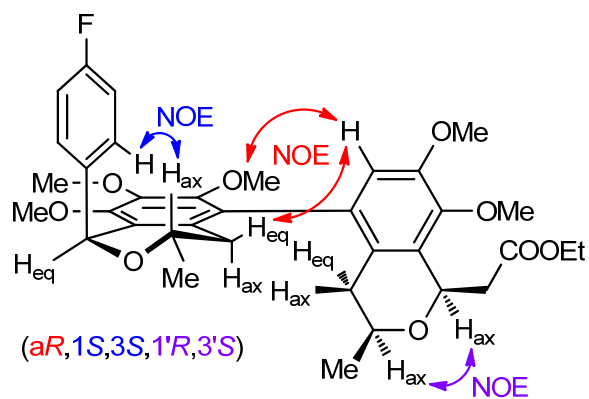


**Figure S117.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR (400 MHz) spectrum of (aR,1S,3S,1'R,3'S)-**23** in  $\text{CDCl}_3$ .

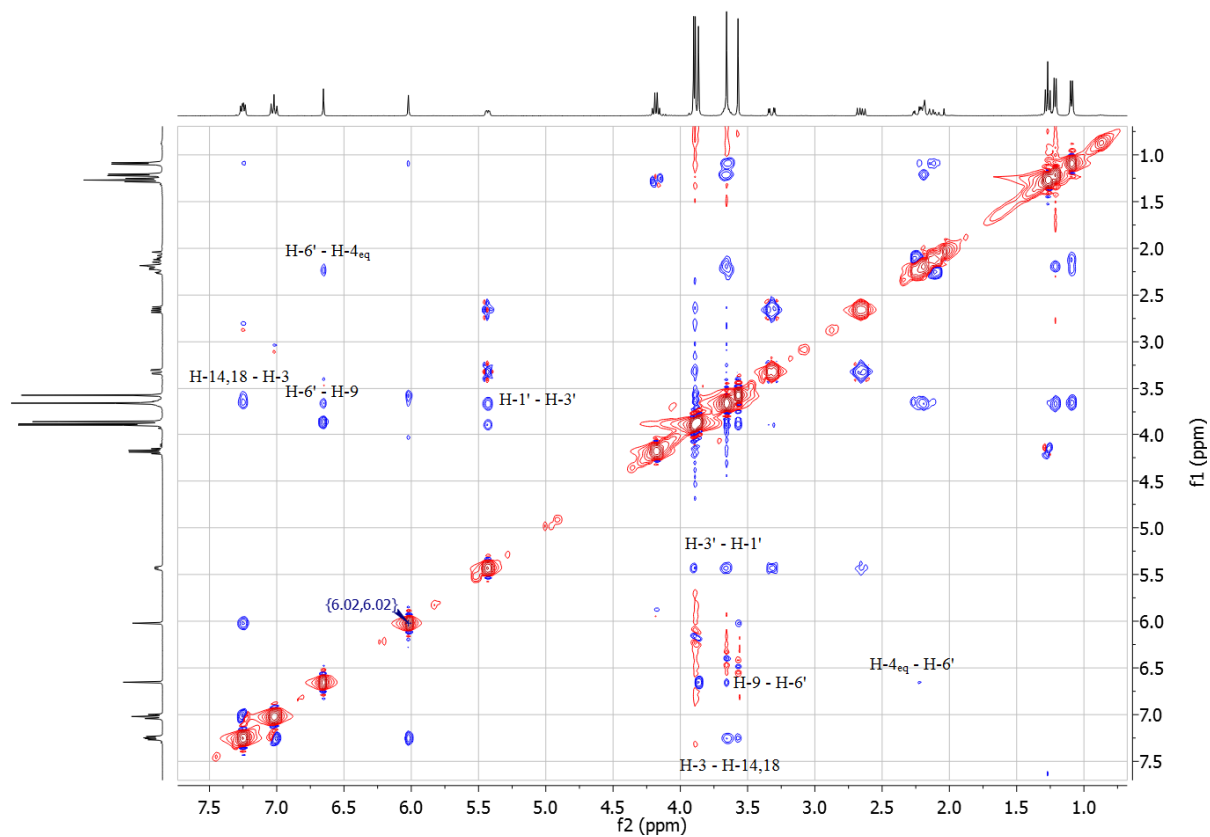




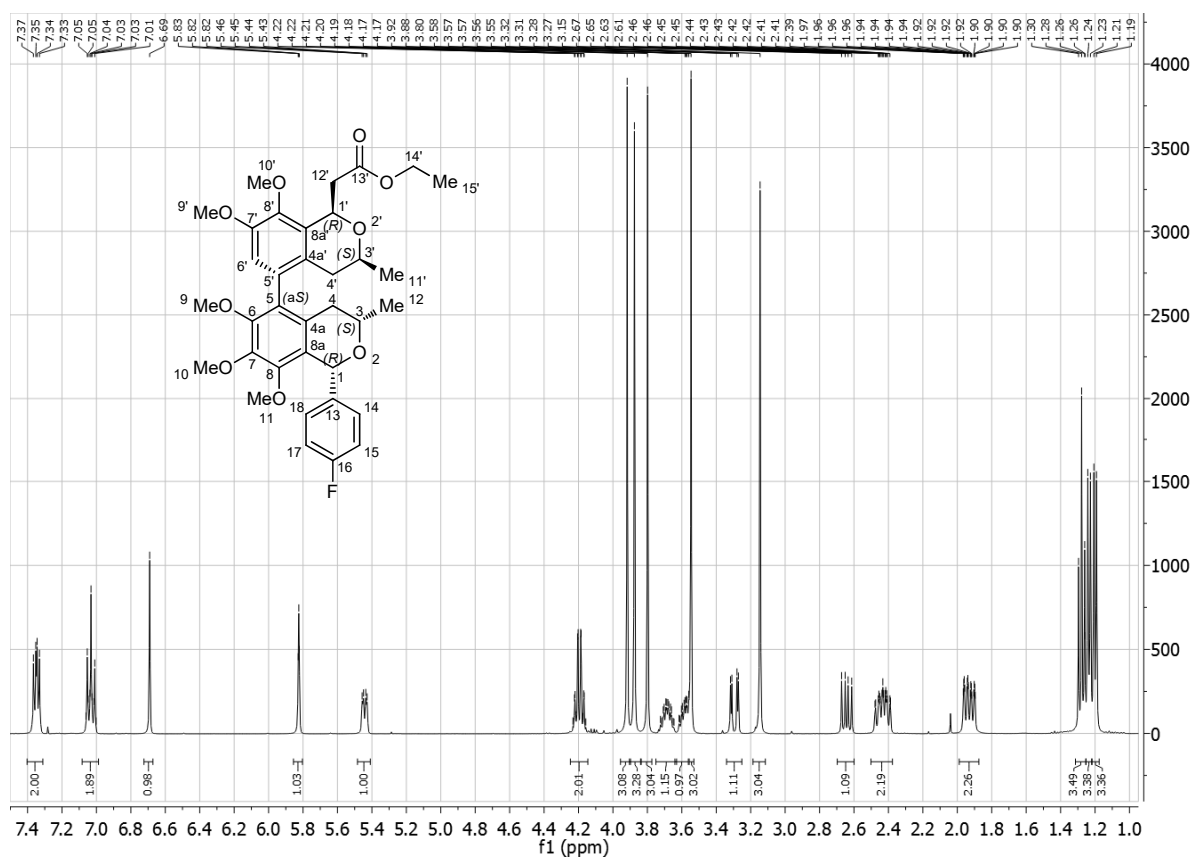
**Figure S118.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC NMR (400 MHz) spectrum of (*aR*,1*S*,3*S*,1'*R*,3'*S*)-**23** in  $\text{CDCl}_3$ .



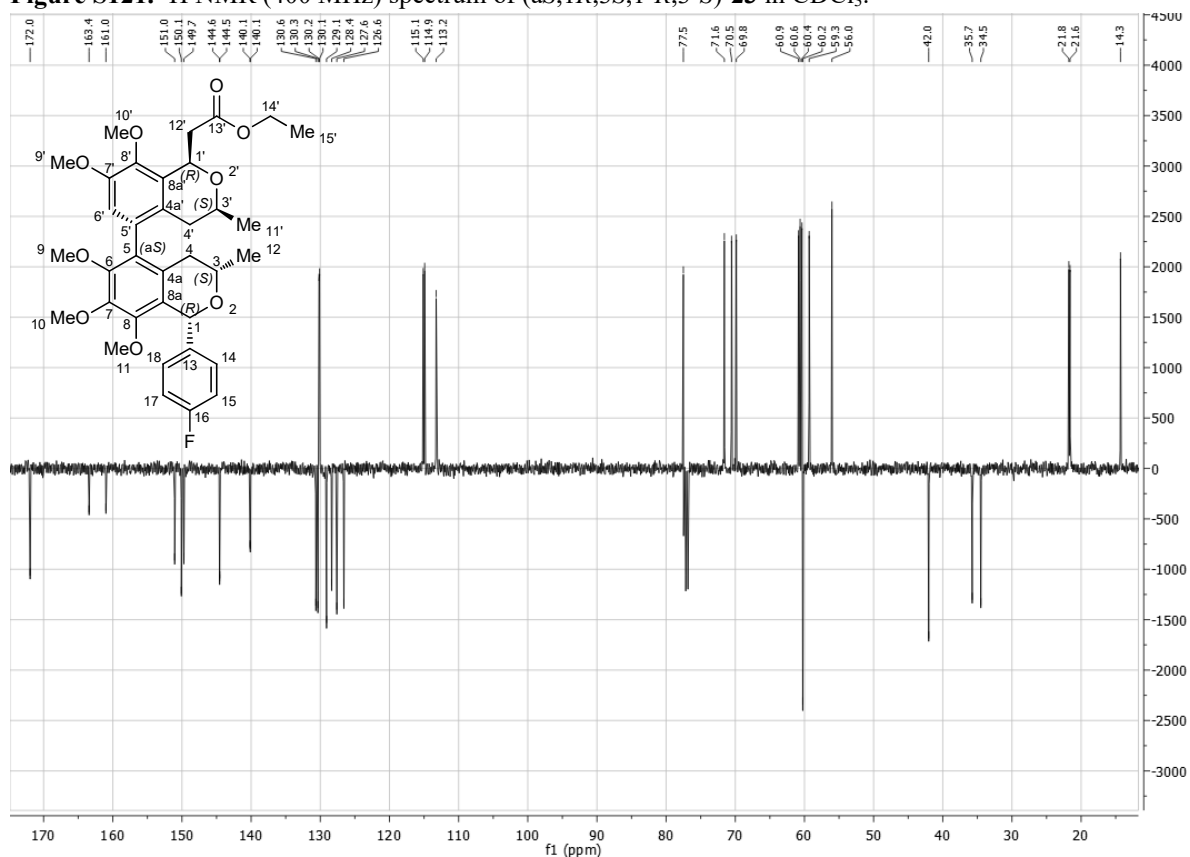
**Figure S119.** Characteristic NOE correlations shown on the structure of  $(aR,1S,3S,1'R,3'S)$ -**23** suggesting  $(1S,3S,1'R,3'S)$  configurations of isochroman subunits and  $(aR)$  axial chirality.



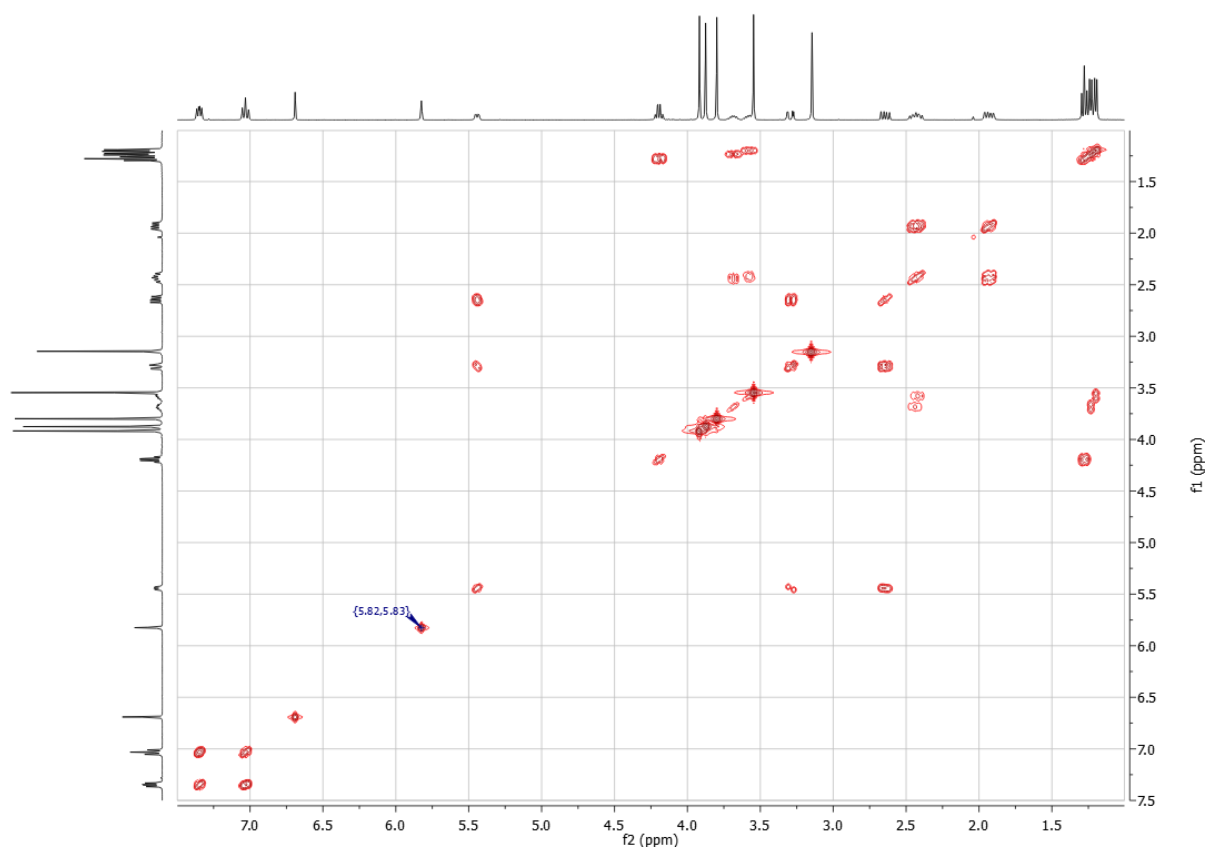
**Figure S120.**  $^1H$ - $^1H$  NOESY NMR (400 MHz) spectrum of  $(aR,1S,3S,1'R,3'S)$ -**23** in  $CDCl_3$ .



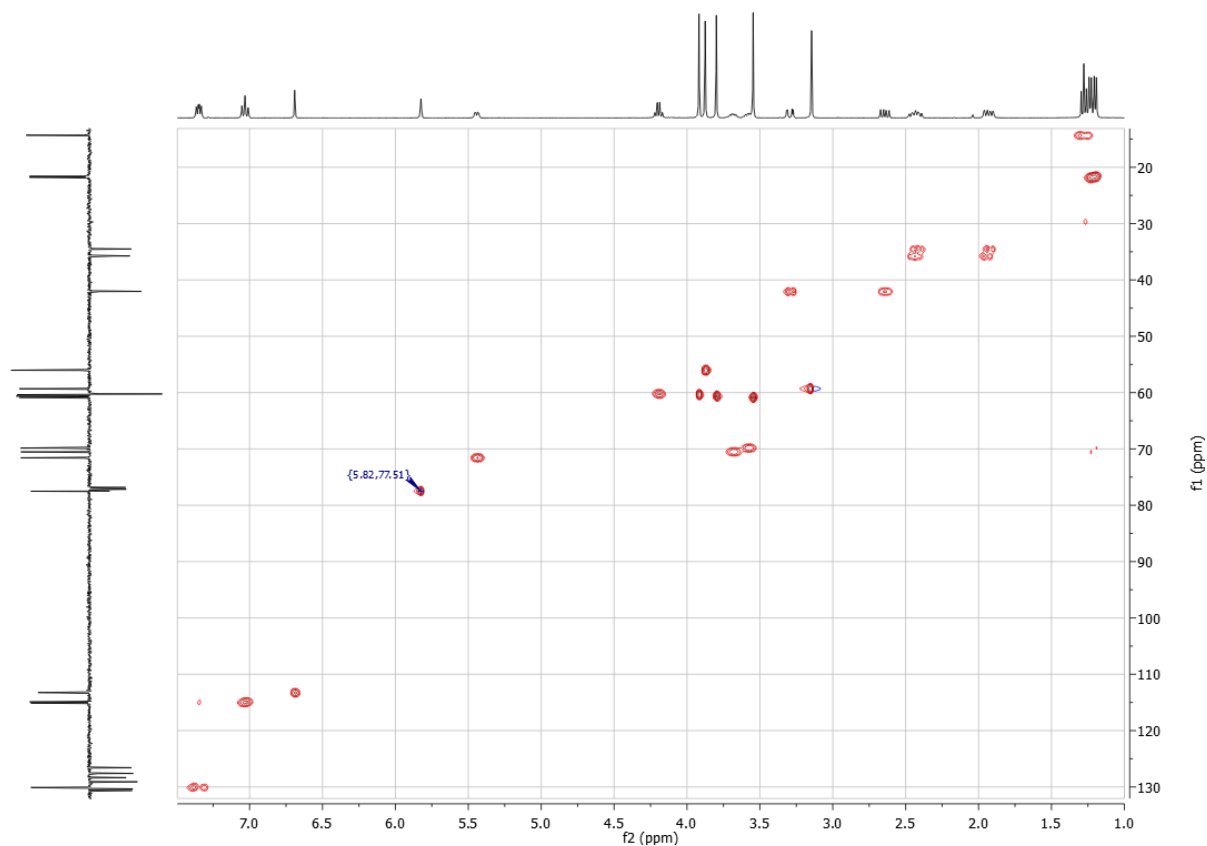
**Figure S121.** <sup>1</sup>H NMR (400 MHz) spectrum of (aS,1R,3S,1'R,3'S)-23 in CDCl<sub>3</sub>.



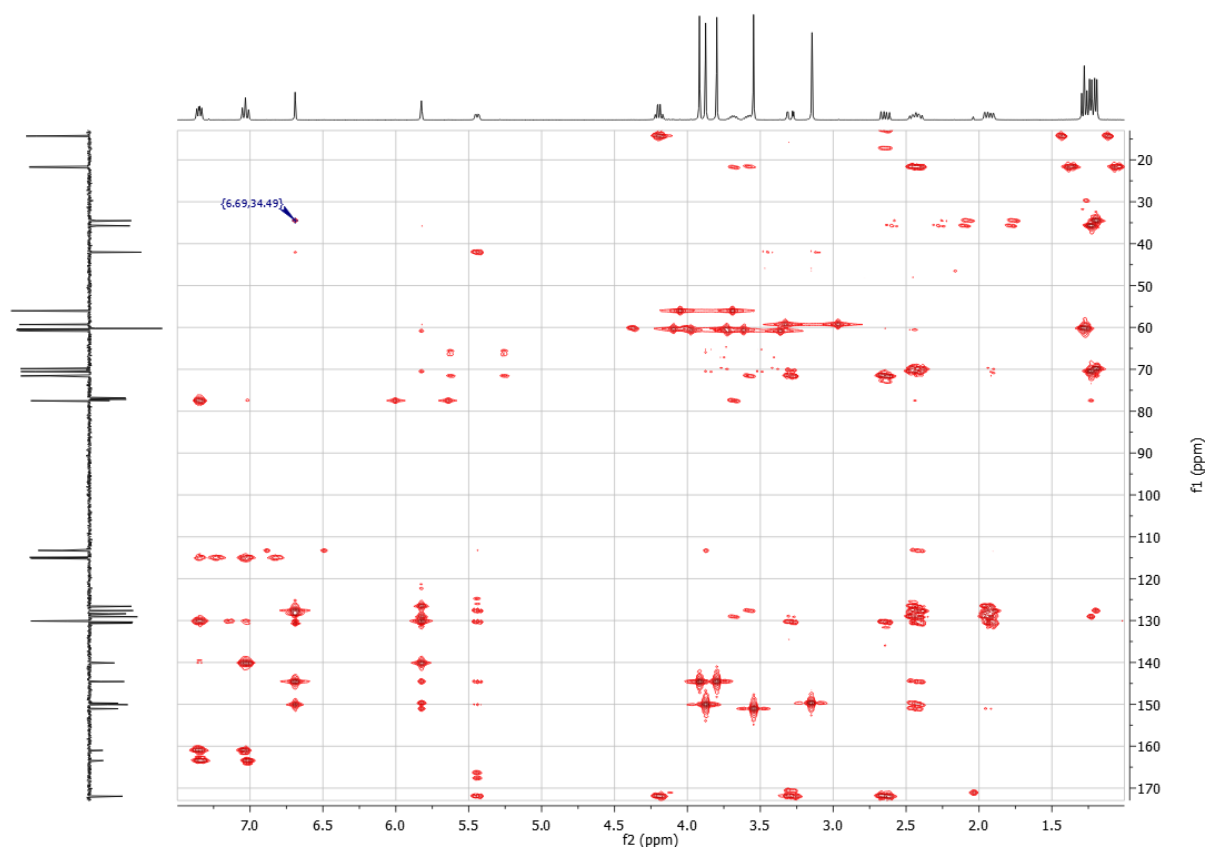
**Figure S122.** <sup>13</sup>C NMR (100 MHz) spectrum of (aS,1R,3S,1'R,3'S)-23 in CDCl<sub>3</sub>.



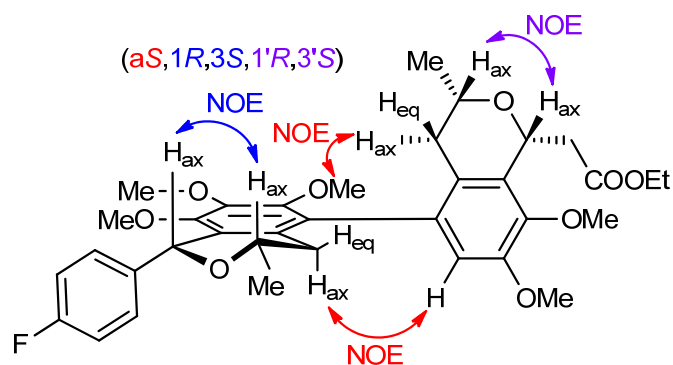
**Figure S123.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR (400 MHz) spectrum of (aS,1*R*,3*S*,1'*R*,3'*S*)-**23** in  $\text{CDCl}_3$ .



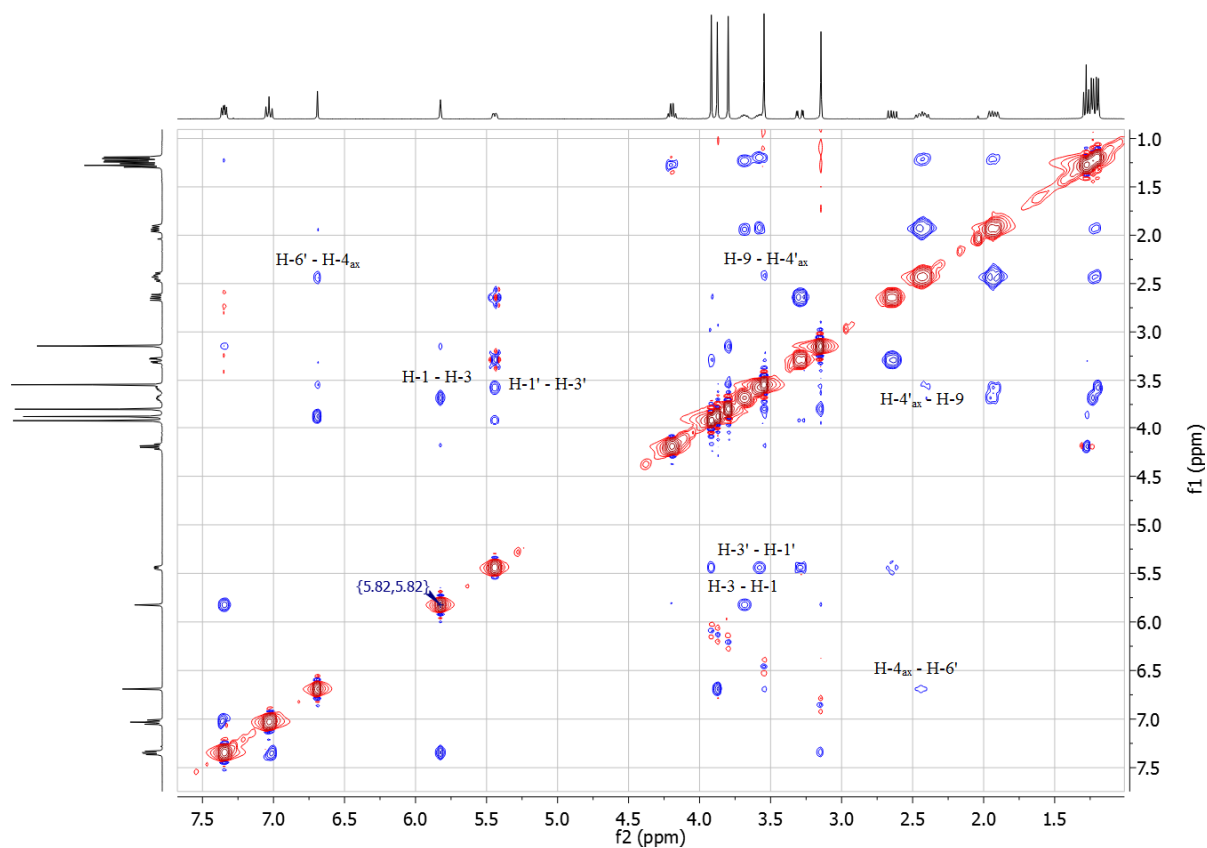
**Figure S124.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR (400 MHz) spectrum of (aS,1*R*,3*S*,1'*R*,3'*S*)-**23** in  $\text{CDCl}_3$ .



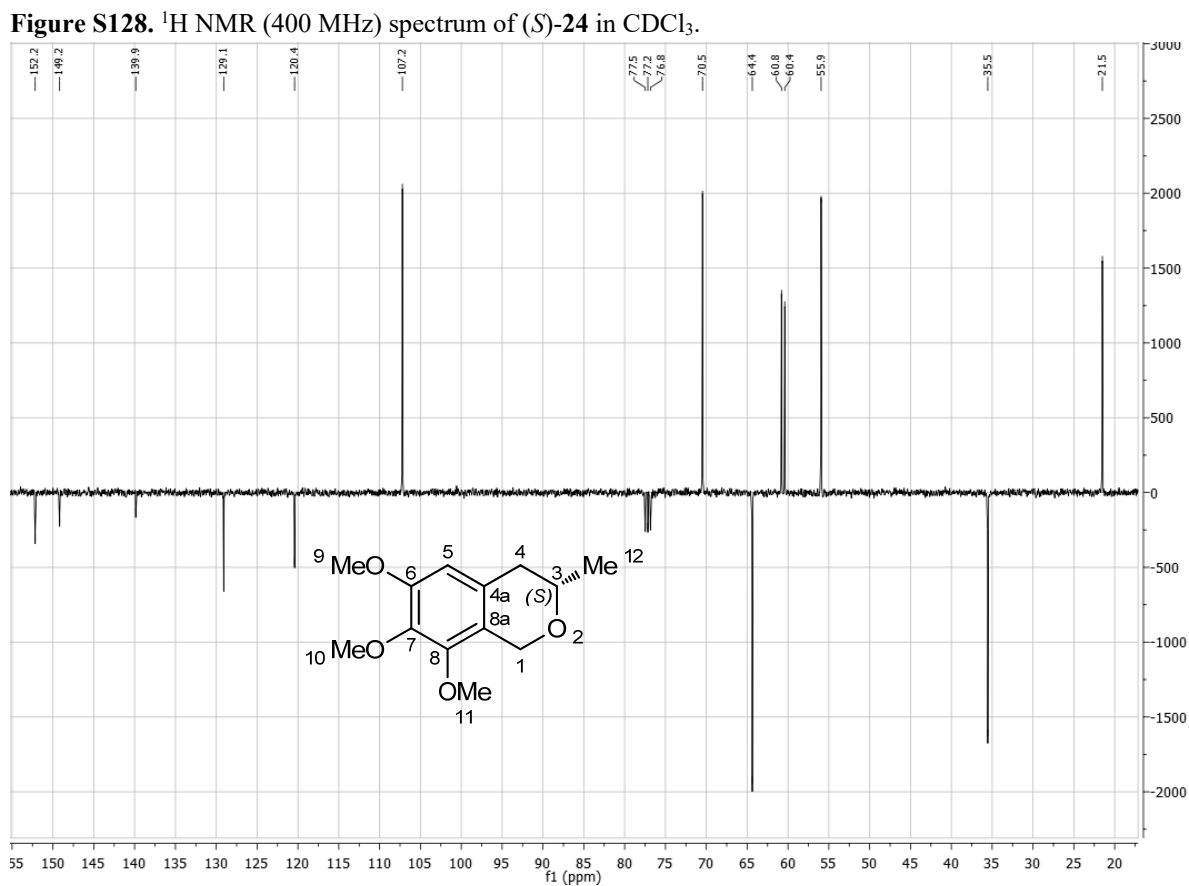
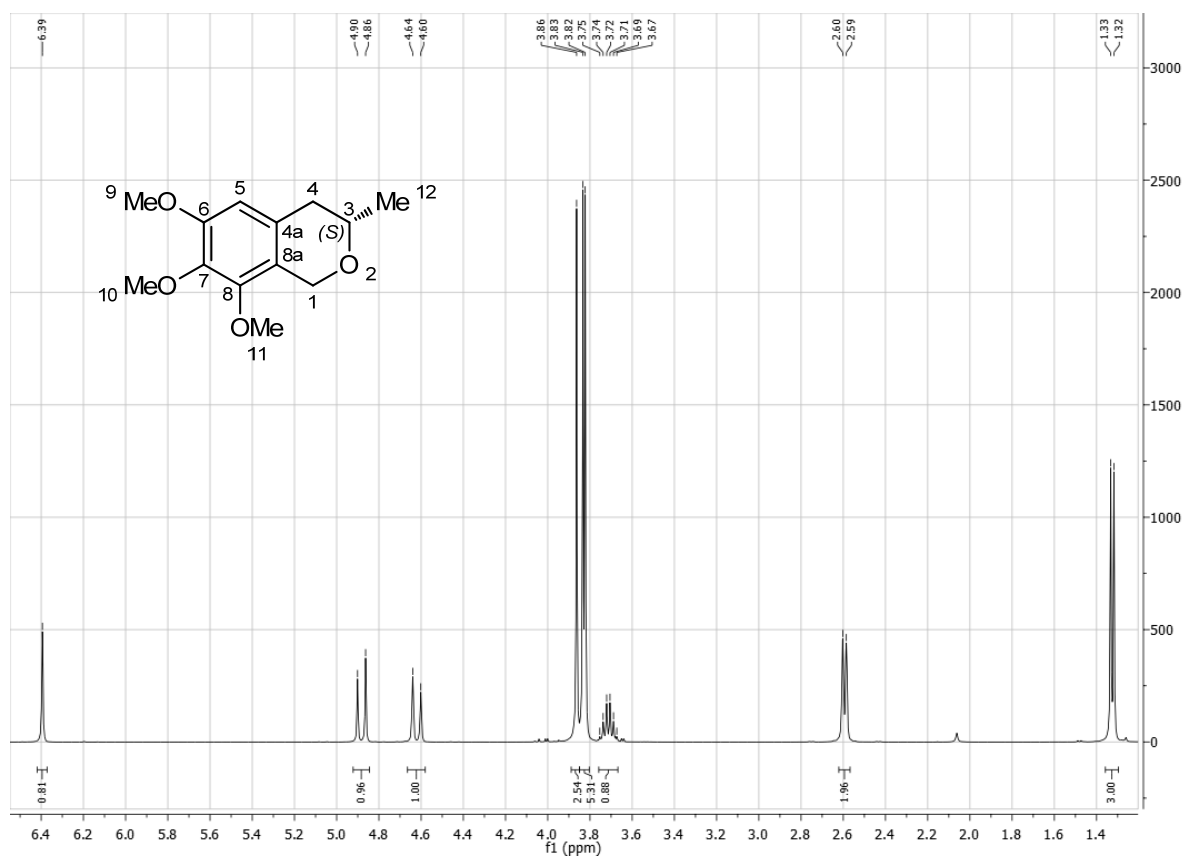
**Figure S125.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC NMR (400 MHz) spectrum of (aS,1R,3S,1'R,3'S)-**23** in  $\text{CDCl}_3$ .

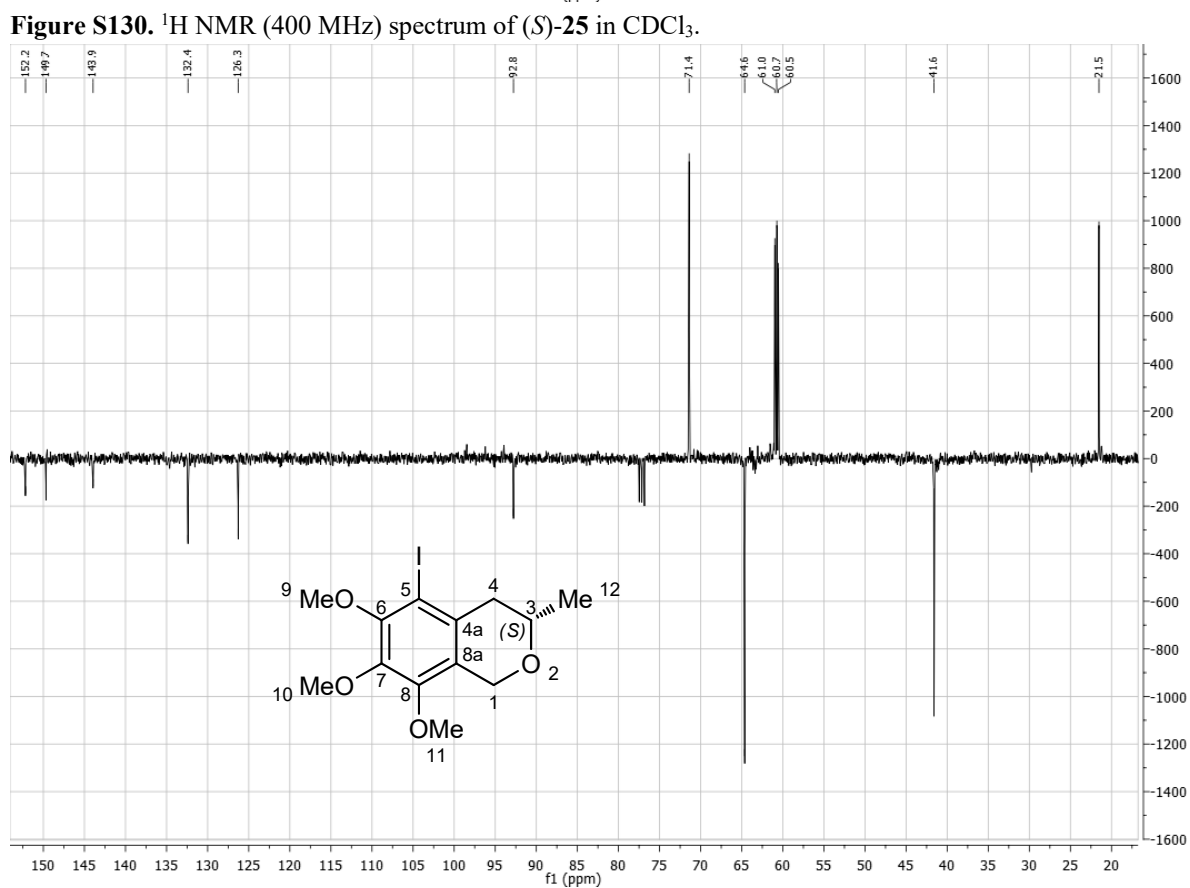
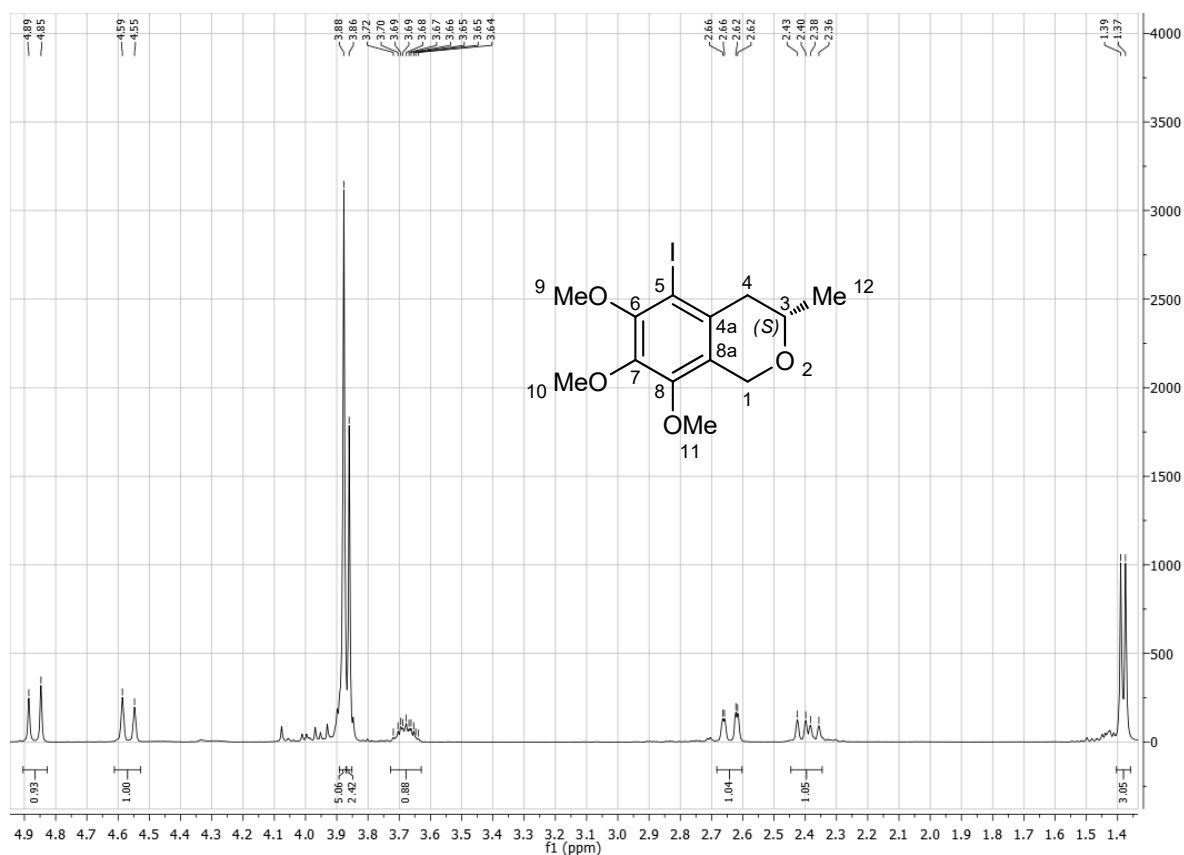


**Figure S126.** Characteristic NOE correlations shown on the structure of (aS,1R,3S,1'R,3'S)-**23** suggesting (1R,3S,1'R,3'S) configurations of isochroman subunits and (aS) axial chirality.

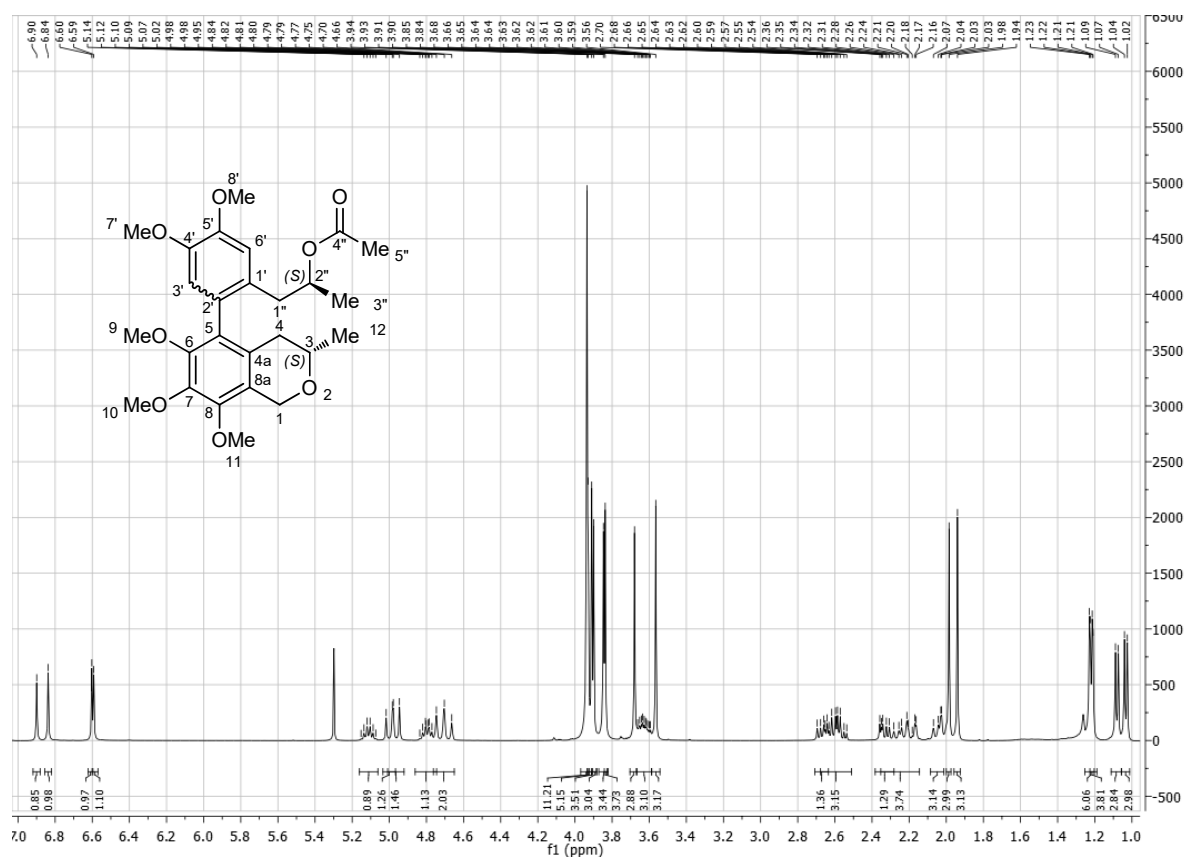


**Figure S127.** <sup>1</sup>H-<sup>1</sup>H NOESY NMR (400 MHz) spectrum of (aS,1R,3S,1'R,3'S)-**23** in CDCl<sub>3</sub>.

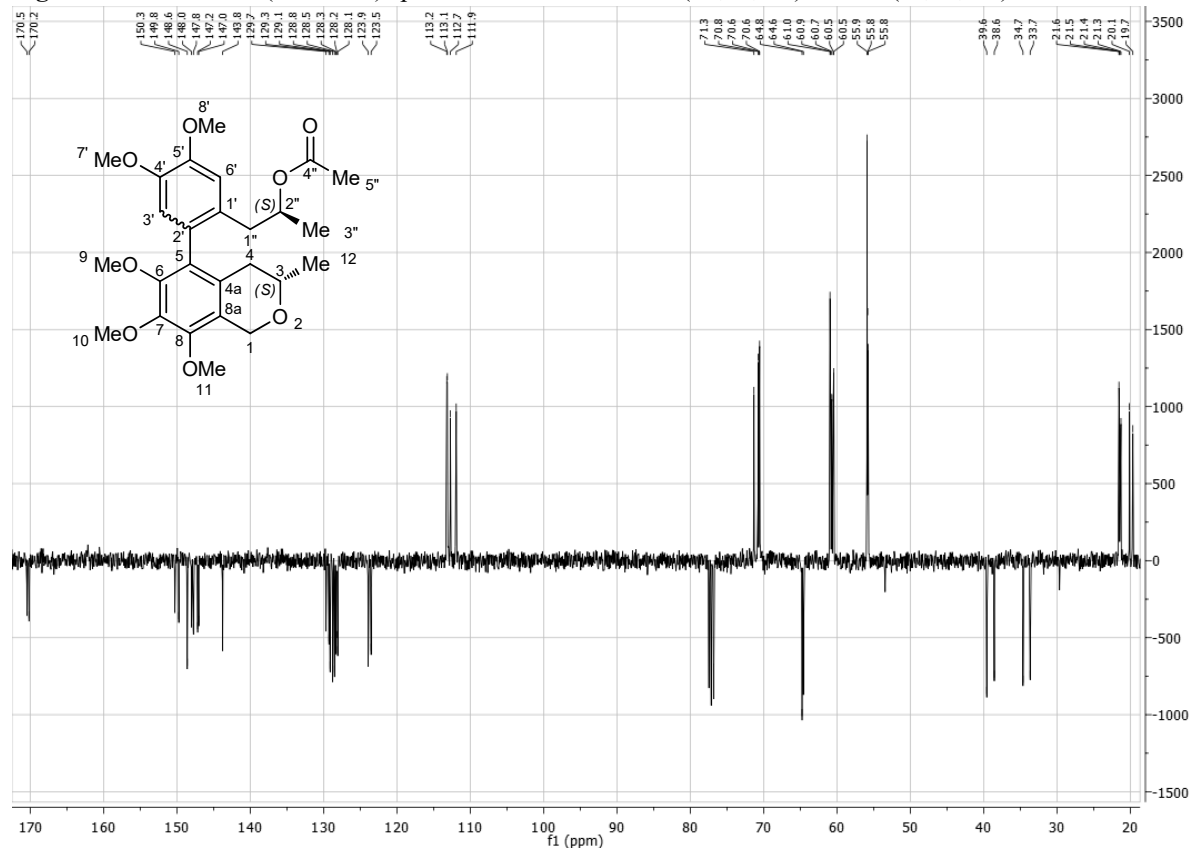




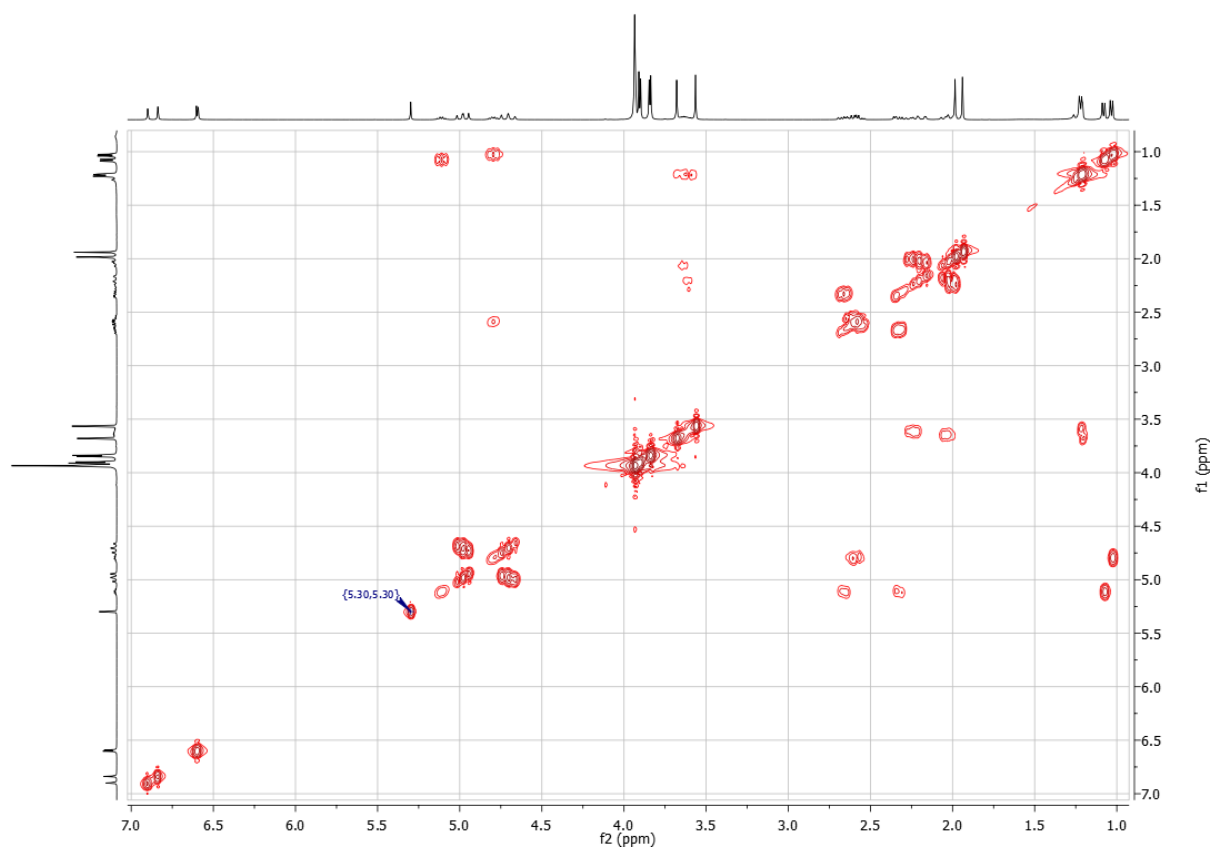




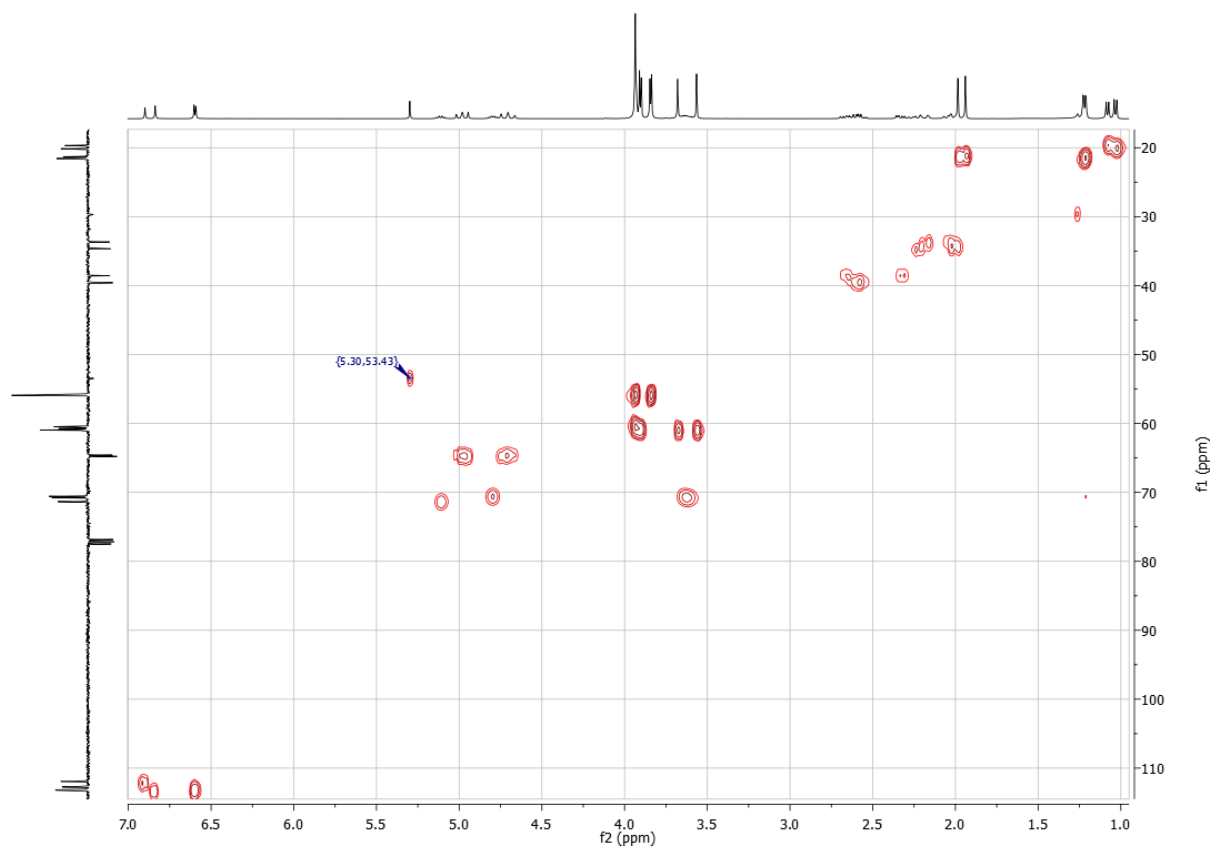
**Figure S132.**  $^1\text{H}$  NMR (400 MHz) spectrum of the mixture of  $(aR,3S,2'S)$ -**26** and  $(aS,3S,2'S)$ -**26** in  $\text{CDCl}_3$ .



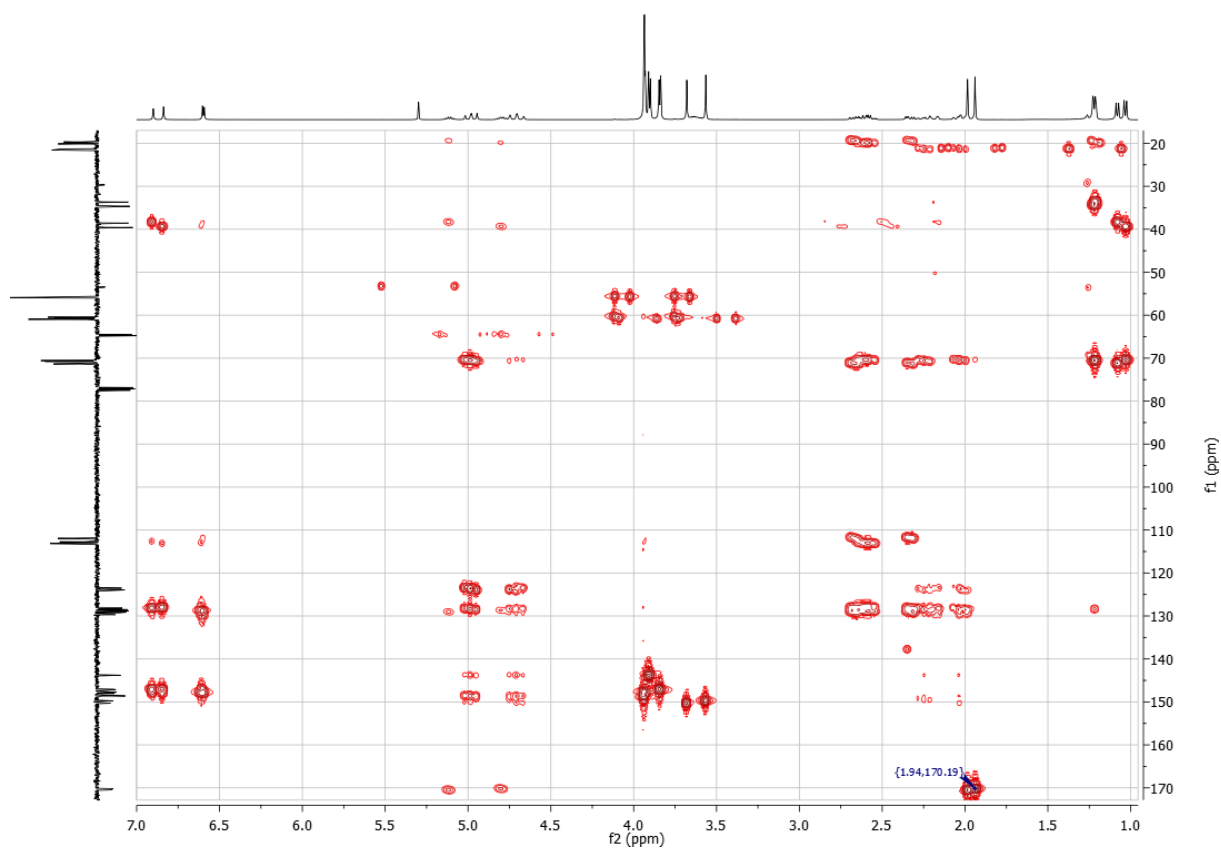
**Figure S133.**  $^{13}\text{C}$  NMR (100 MHz) spectrum of the mixture of  $(aR,3S,2'S)$ -**26** and  $(aS,3S,2'S)$ -**26** in  $\text{CDCl}_3$ .



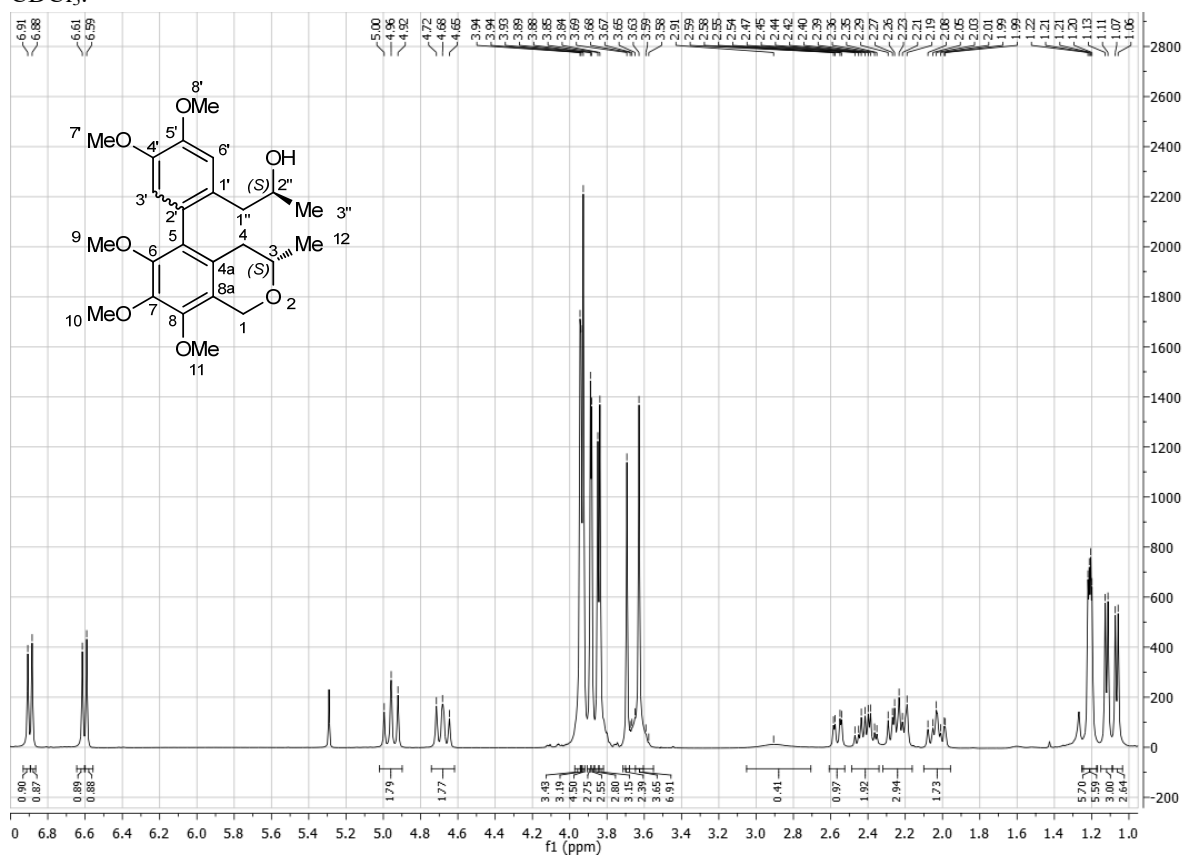
**Figure S134.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR (400 MHz) spectrum of the mixture of (aR,3S,2'S)-**26** and (aS,3S,2'S)-**26** in  $\text{CDCl}_3$ .



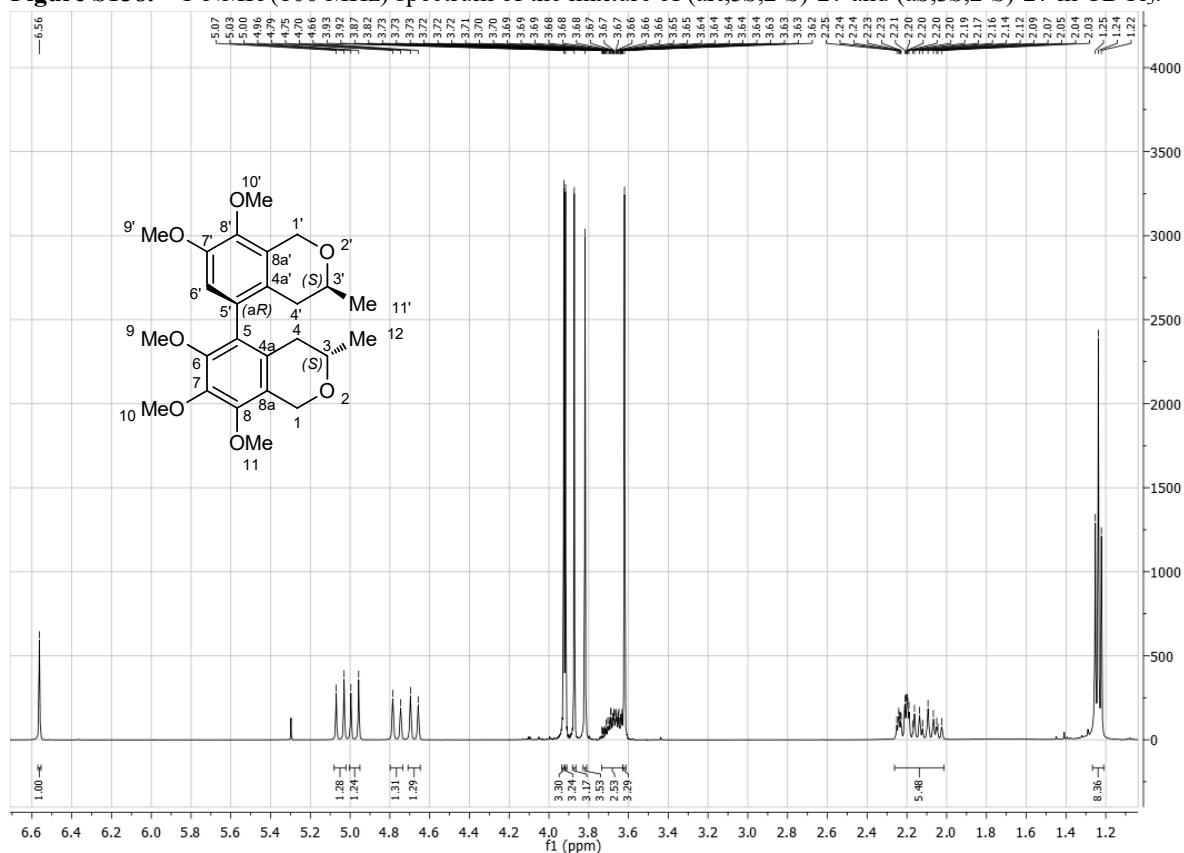
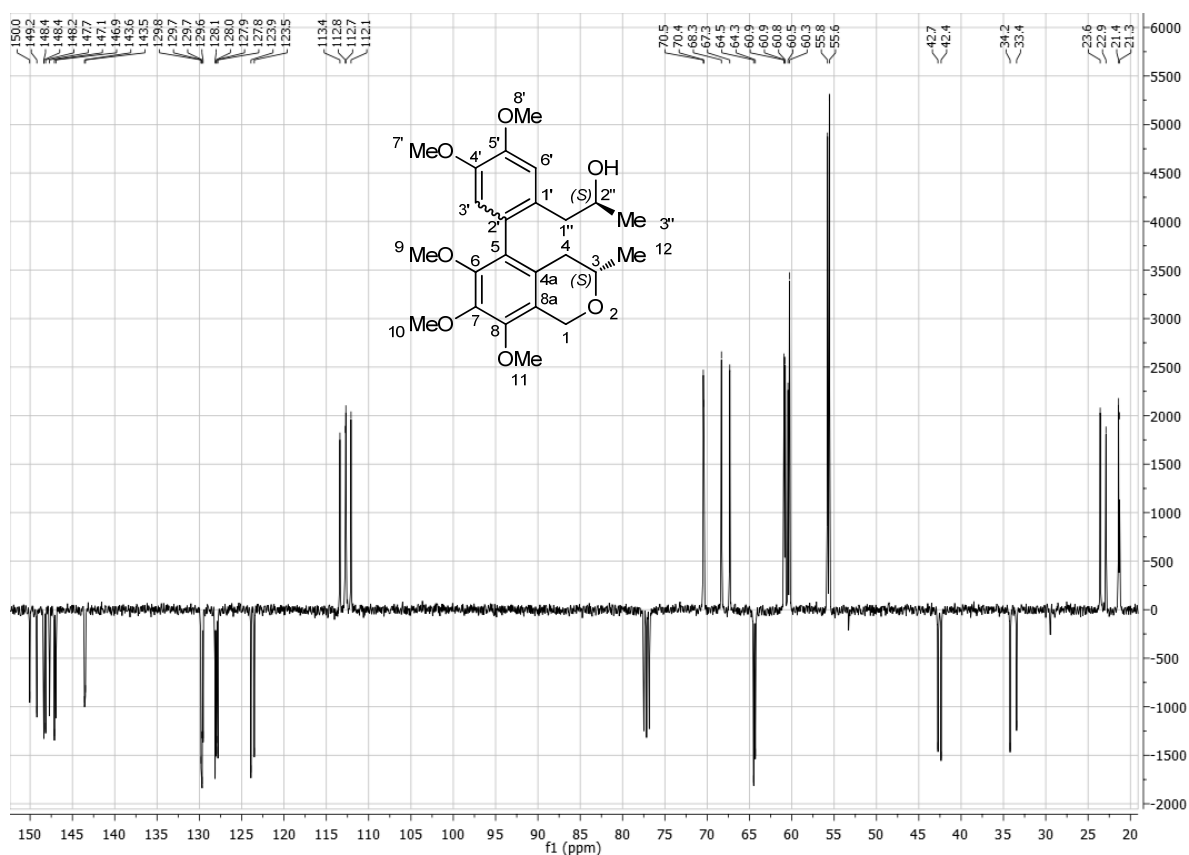
**Figure S135.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR (400 MHz) spectrum of the mixture of (aR,3S,2'S)-**26** and (aS,3S,2'S)-**26** in  $\text{CDCl}_3$ .

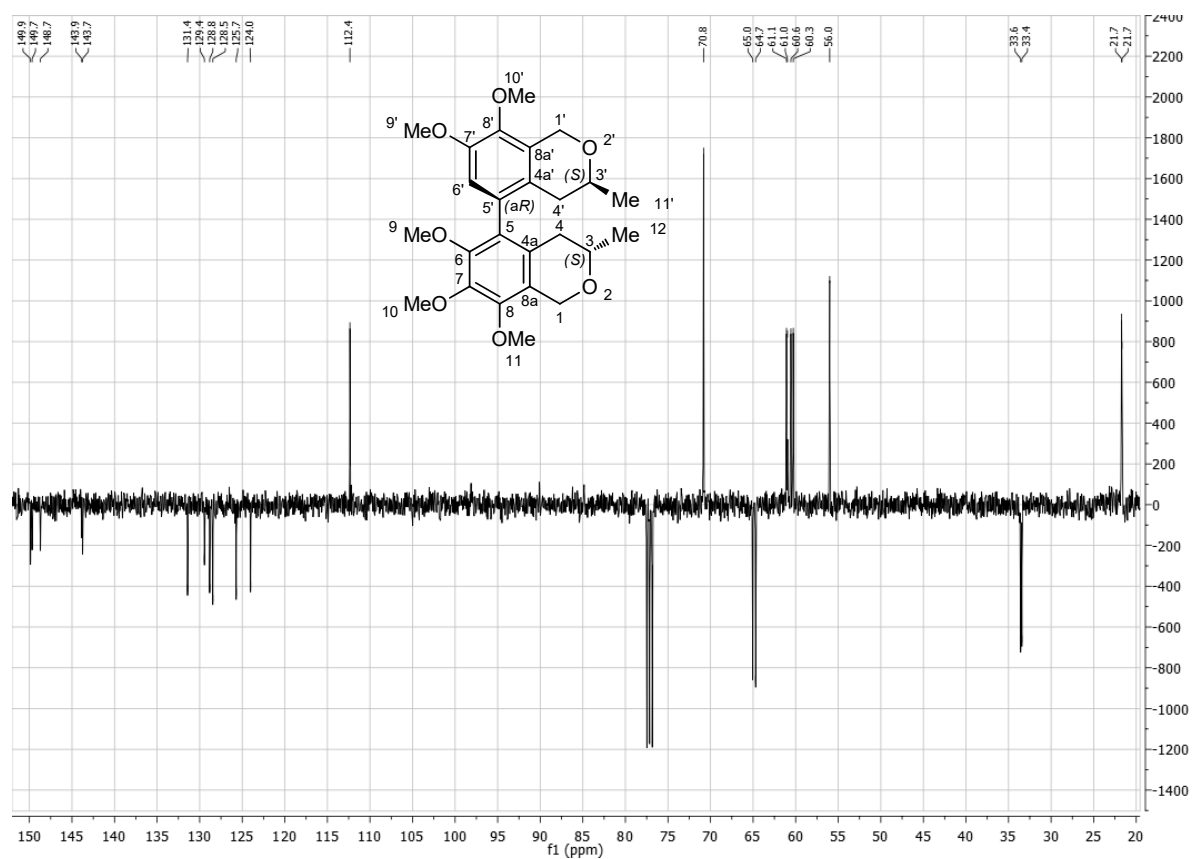


**Figure S136.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC NMR (400 MHz) spectrum of the mixture of (aR,3S,2'S)-**26** and (aS,3S,2'S)-**26** in  $\text{CDCl}_3$ .

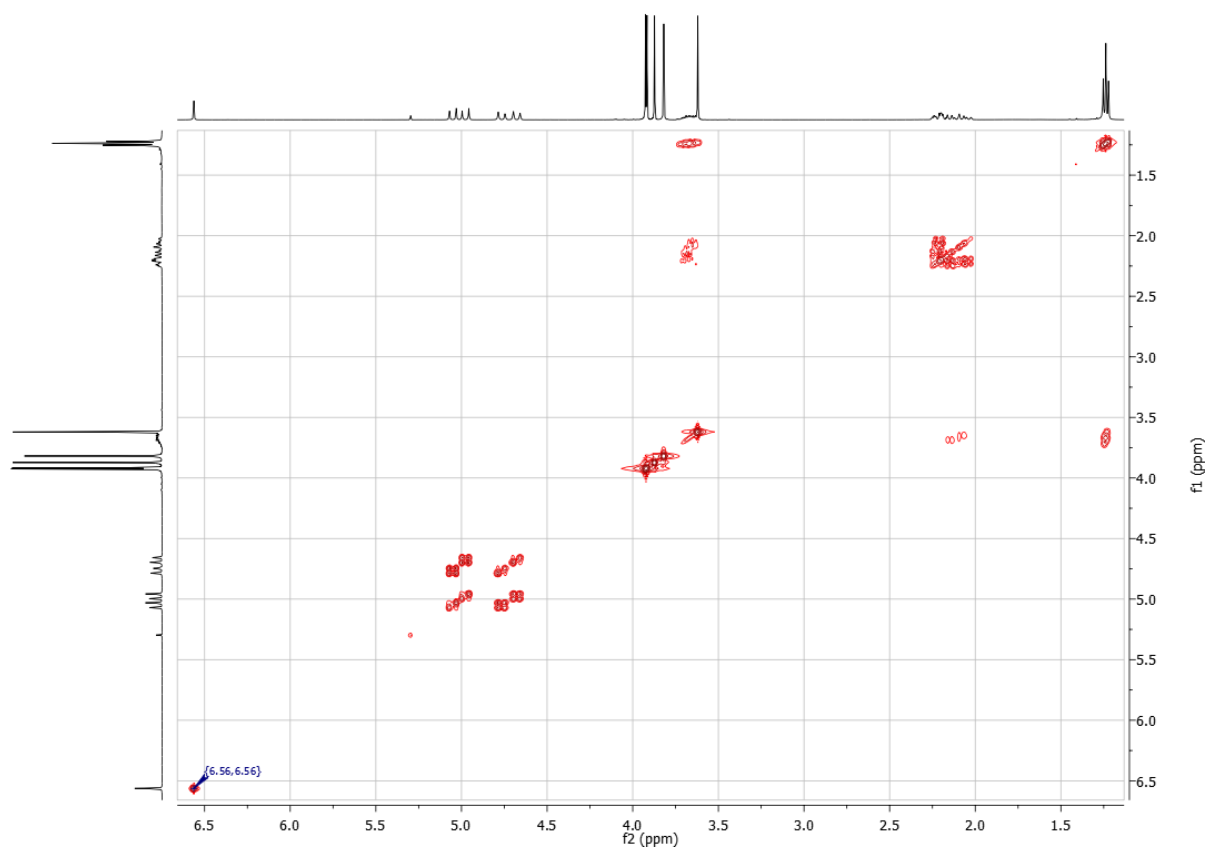


**Figure S137.**  $^1\text{H}$  NMR (400 MHz) spectrum of the mixture of (aR,3S,2'S)-**27** and (aS,3S,2'S)-**27** in  $\text{CDCl}_3$ .





**Figure S140.**  $^{13}\text{C}$  NMR (100 MHz) spectrum of (aR,3S,3'S)-**28** in  $\text{CDCl}_3$ .



**Figure S141.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR (400 MHz) spectrum of (aR,3S,3'S)-**28** in  $\text{CDCl}_3$ .

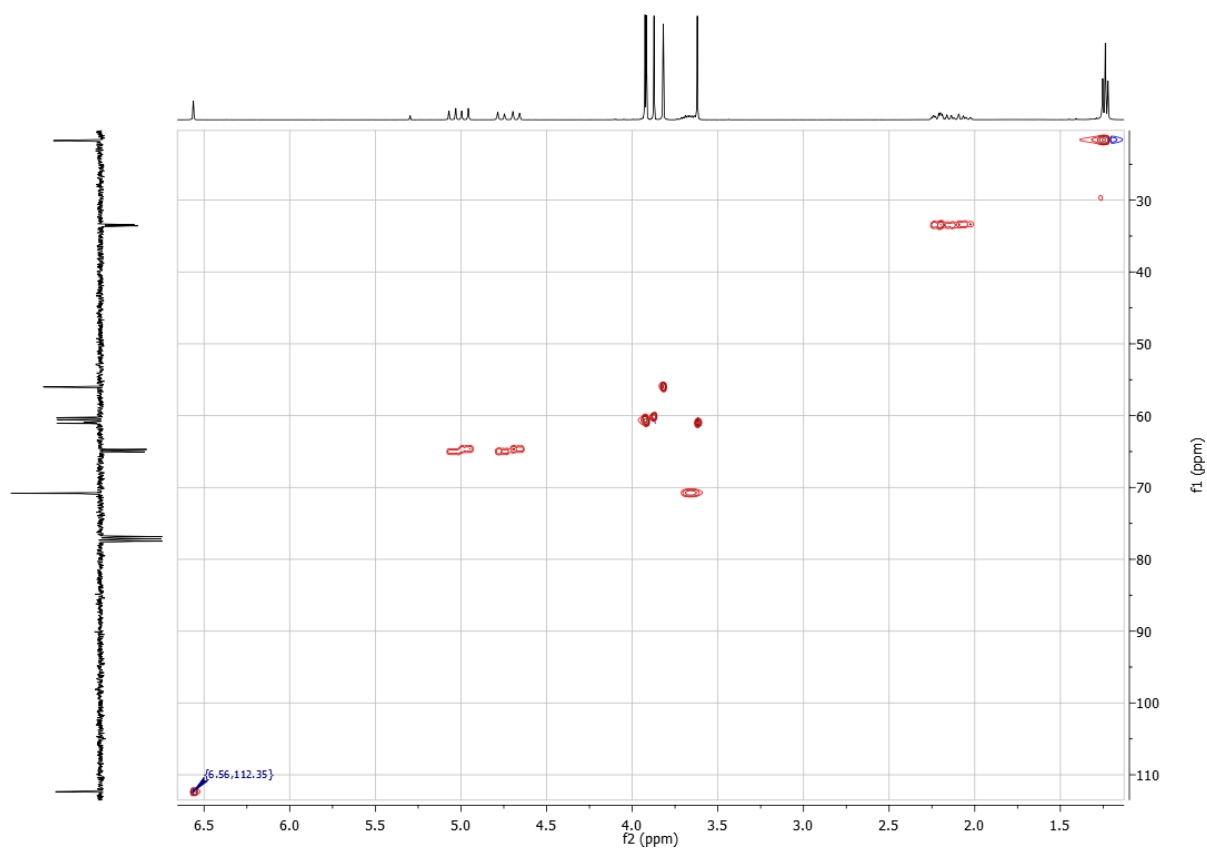


Figure S142.  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR (400 MHz) spectrum of  $(aR,3S,3'S)$ -**28** in  $\text{CDCl}_3$ .

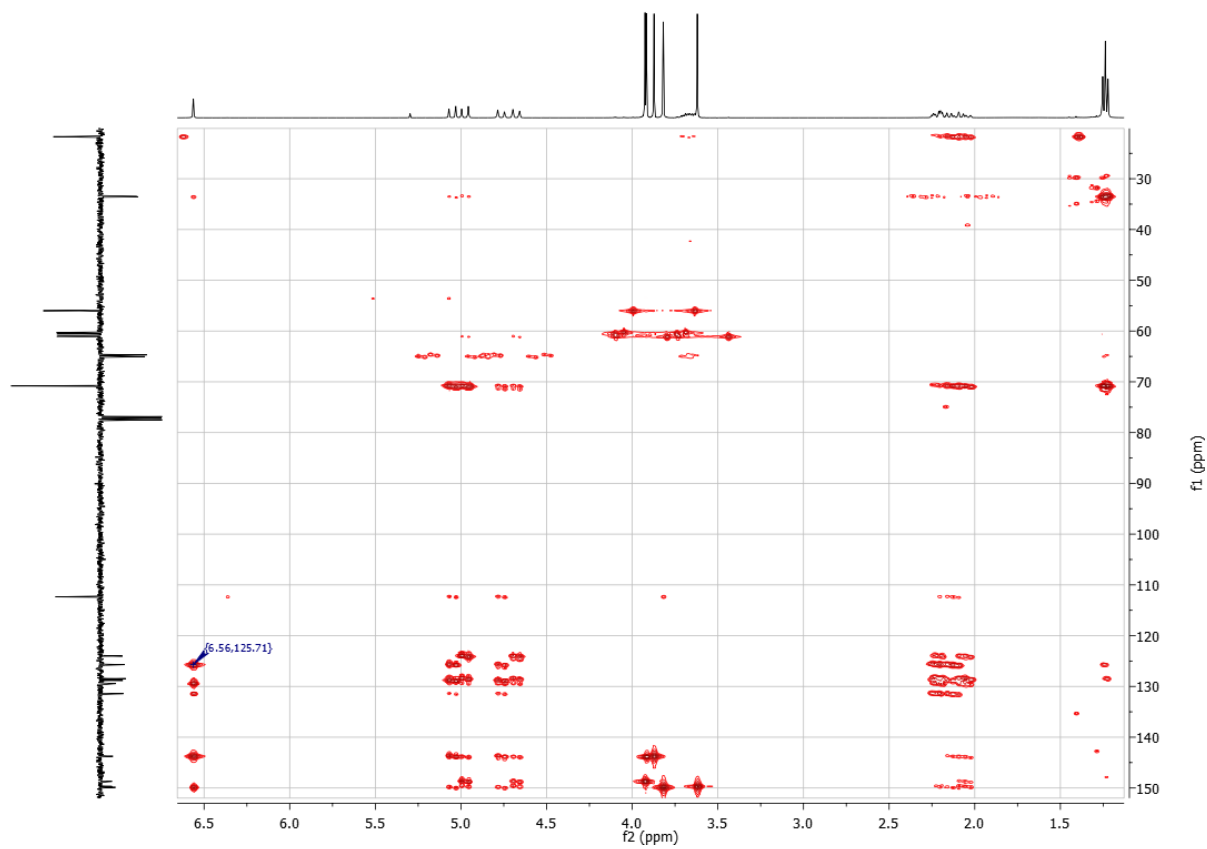
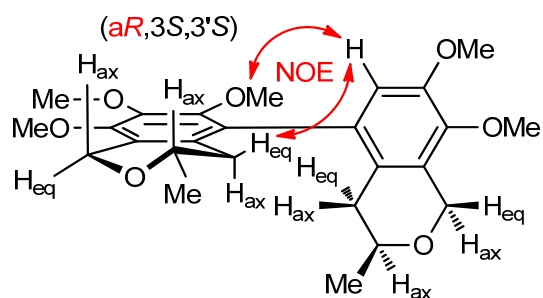
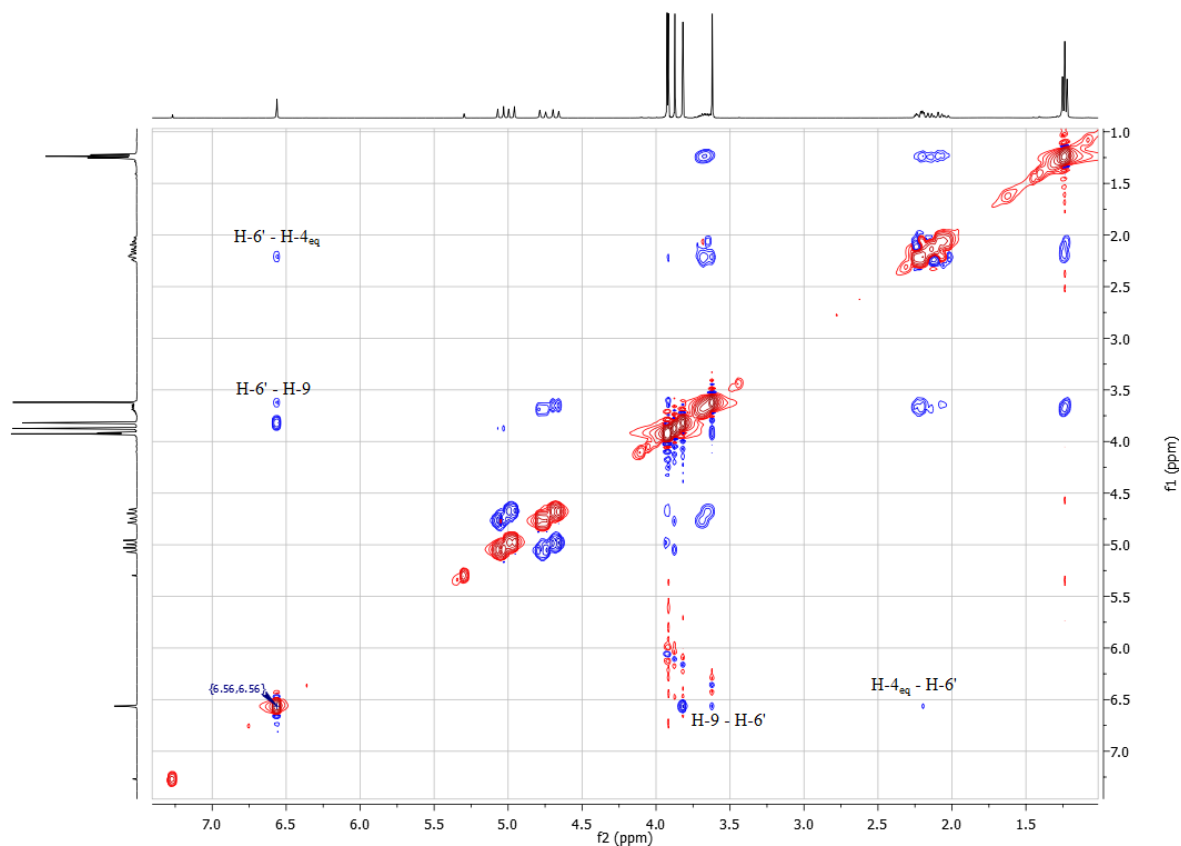


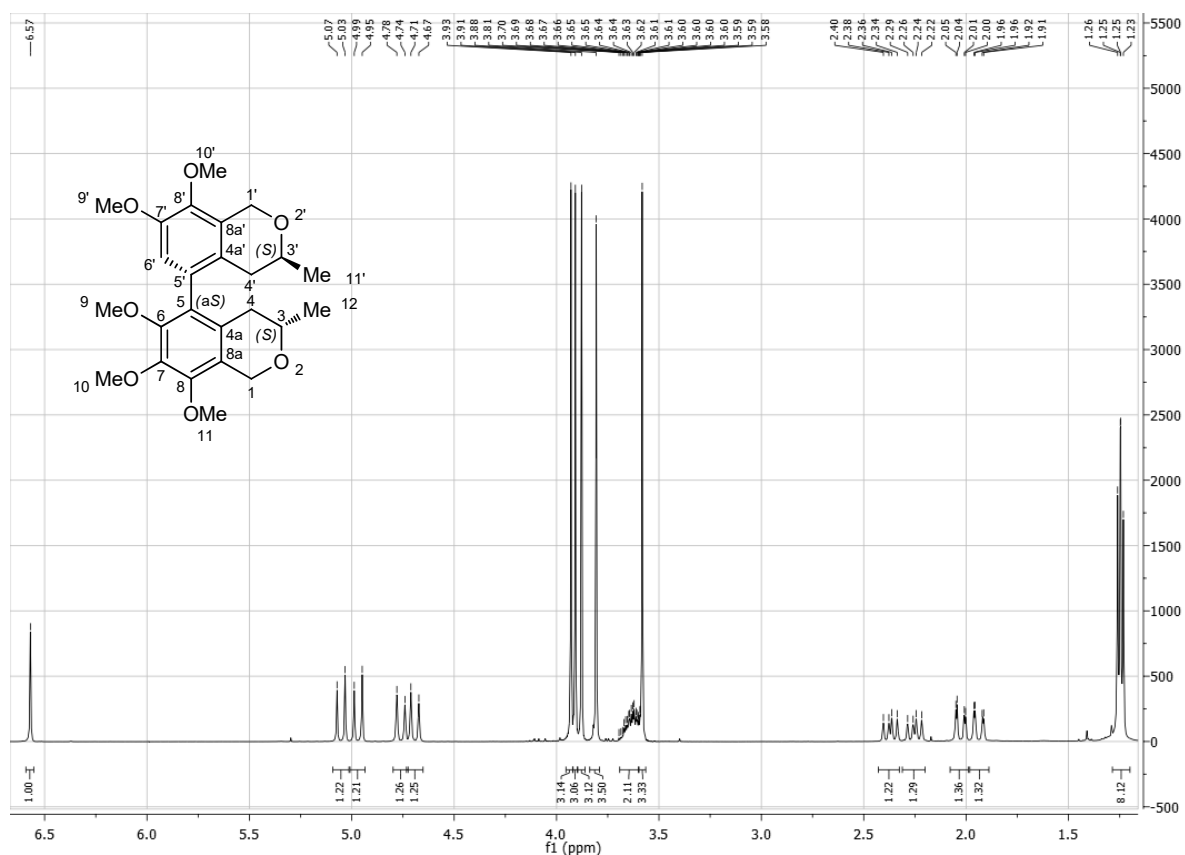
Figure S143.  $^1\text{H}$ - $^{13}\text{C}$  HMBC NMR (400 MHz) spectrum of  $(aR,3S,3'S)$ -**28** in  $\text{CDCl}_3$ .



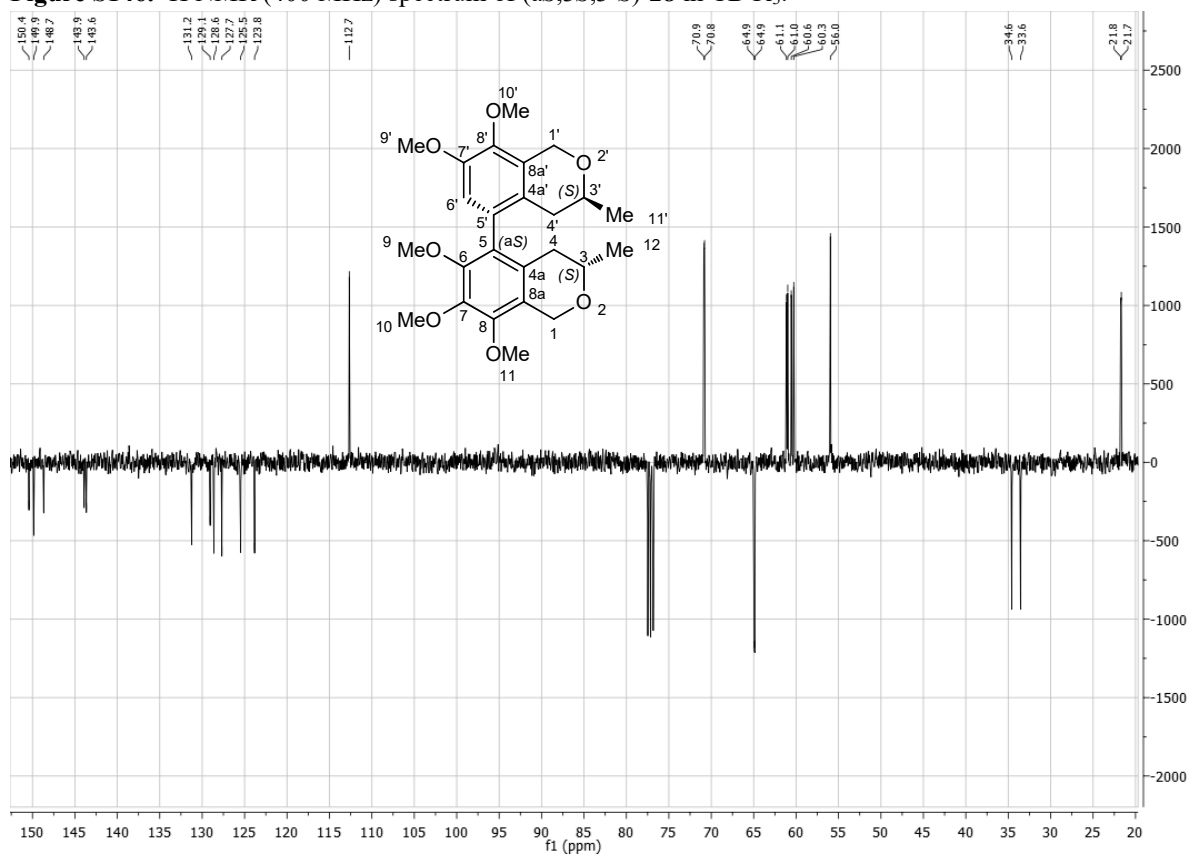
**Figure S144.** Characteristic NOE correlations shown on the structure of (aR,3S,3'S)-28 suggesting (aR) axial chirality.



**Figure S145.** <sup>1</sup>H-<sup>1</sup>H NOESY NMR (400 MHz) spectrum of (aR,3S,3'S)-28 in CDCl<sub>3</sub>.



**Figure S146.**  $^1\text{H}$  NMR (400 MHz) spectrum of (aS,3S,3'S)-28 in  $\text{CDCl}_3$ .



**Figure S147.**  $^{13}\text{C}$  NMR (100 MHz) spectrum of (aS,3S,3'S)-28 in  $\text{CDCl}_3$ .



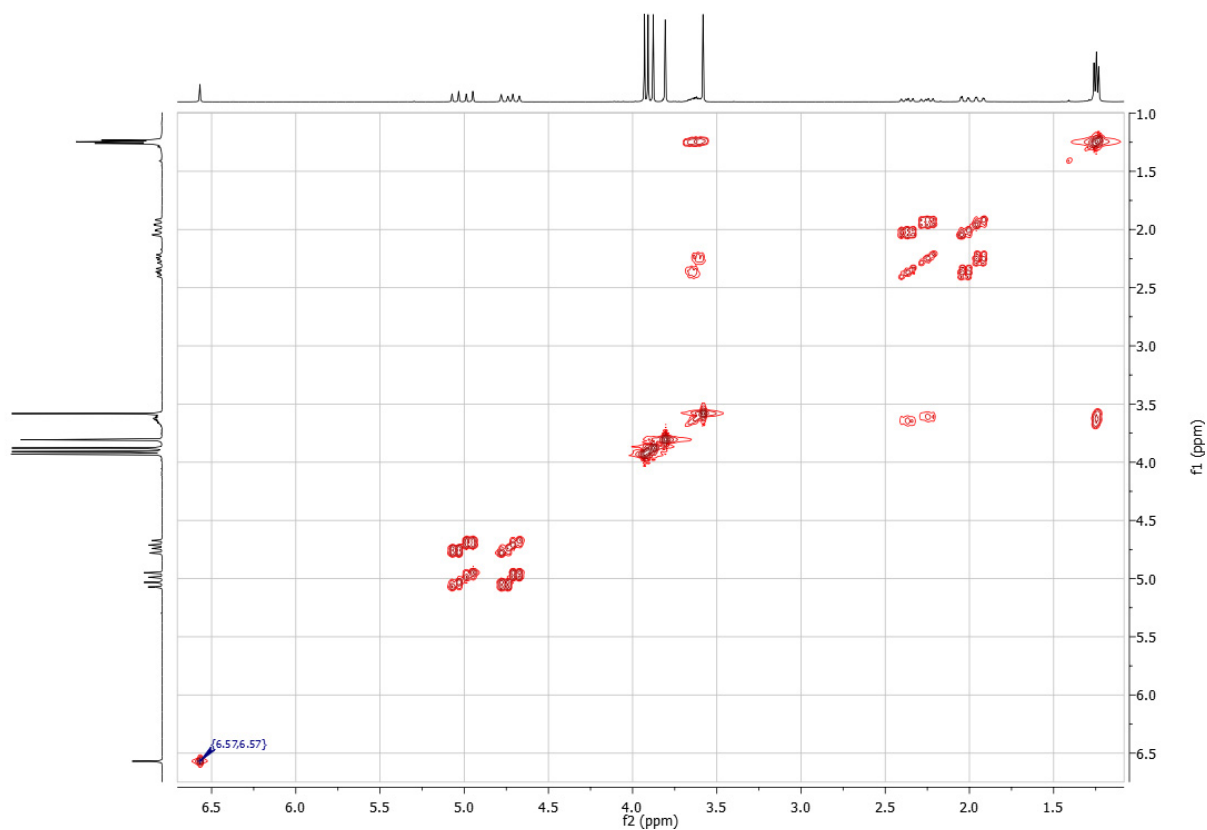


Figure S148.  $^1\text{H}$ - $^1\text{H}$  COSY NMR (400 MHz) spectrum of (aS,3S,3'S)-**28** in  $\text{CDCl}_3$ .

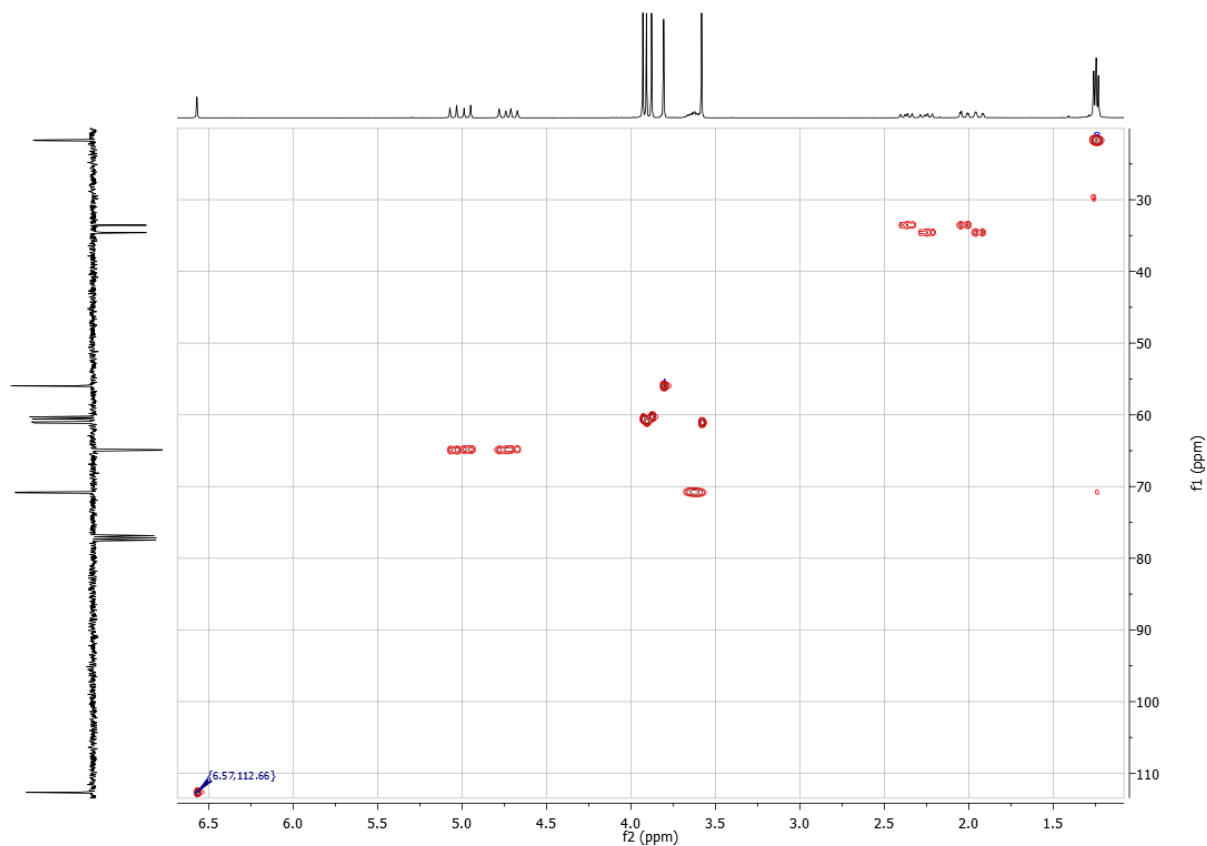


Figure S149.  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR (400 MHz) spectrum of (aS,3S,3'S)-**28** in  $\text{CDCl}_3$ .

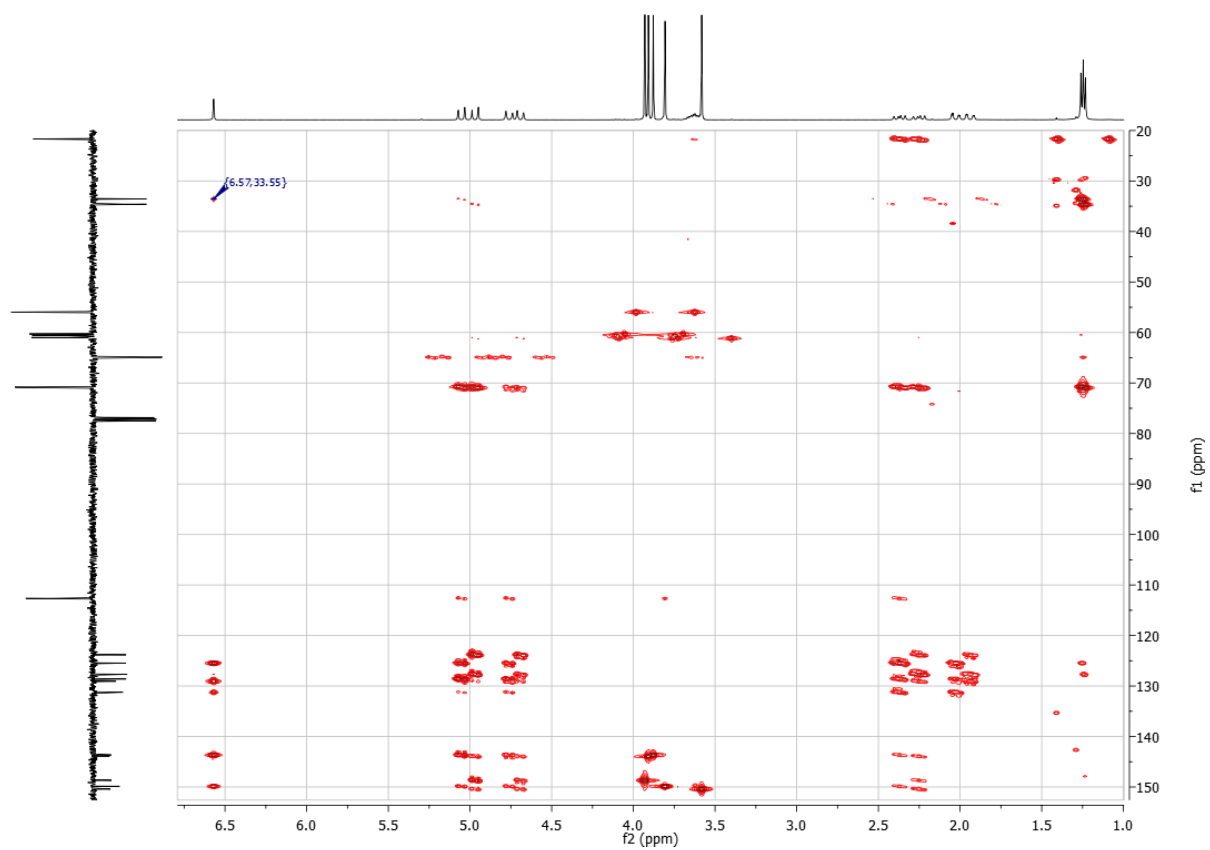
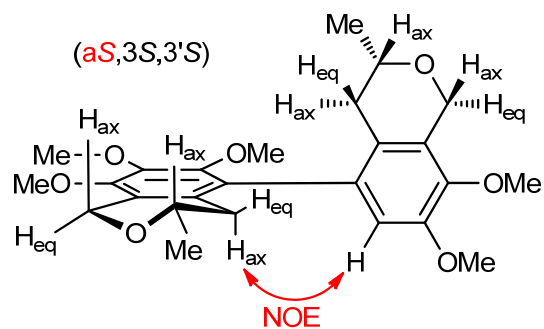
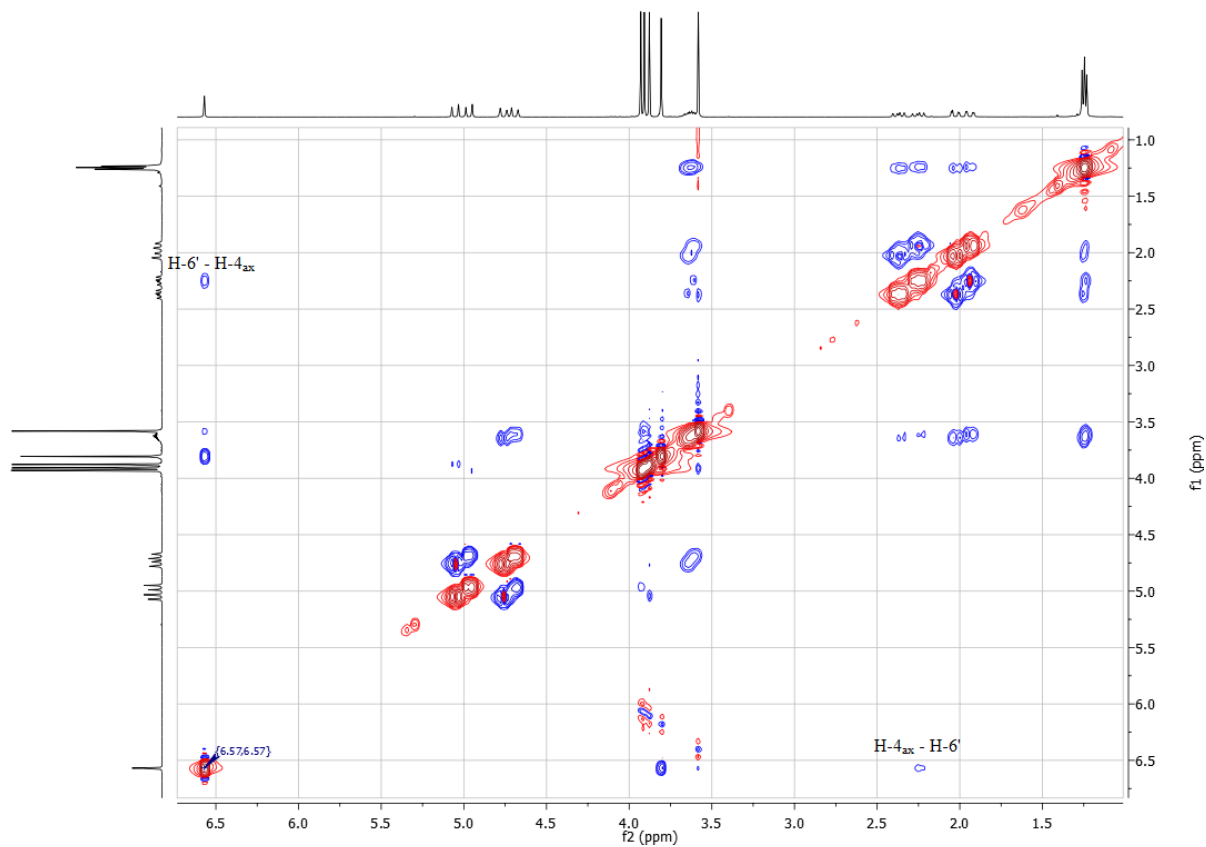


Figure S150.  $^1\text{H}$ - $^{13}\text{C}$  HMBC NMR (400 MHz) spectrum of (*aS*,3*S*,3'*S*)-**28** in  $\text{CDCl}_3$ .

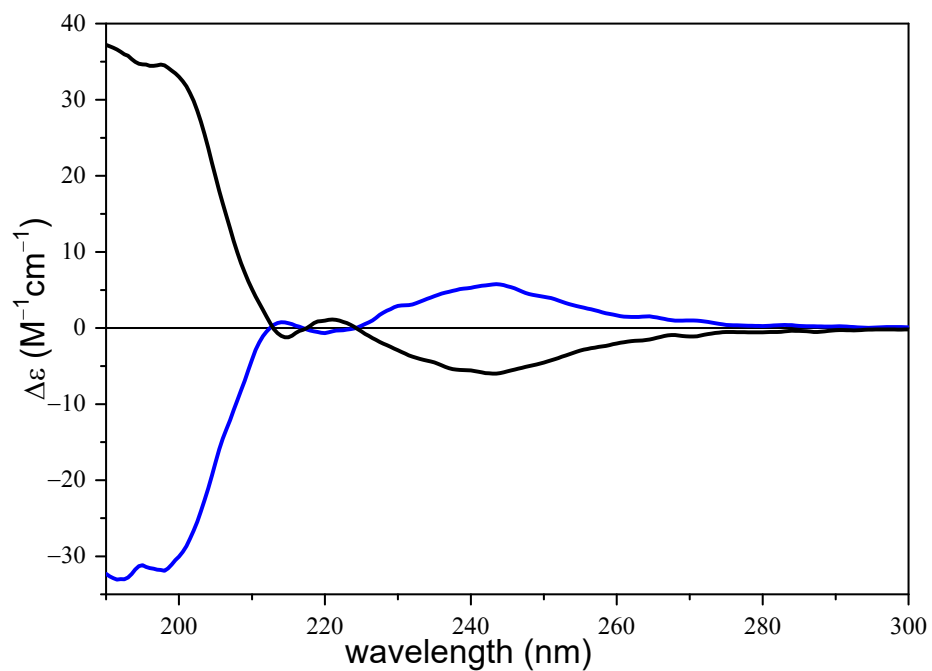


**Figure S151.** Characteristic NOE correlation shown on the structure of (aS,3S,3'S)-28 suggesting (aS) axial chirality.

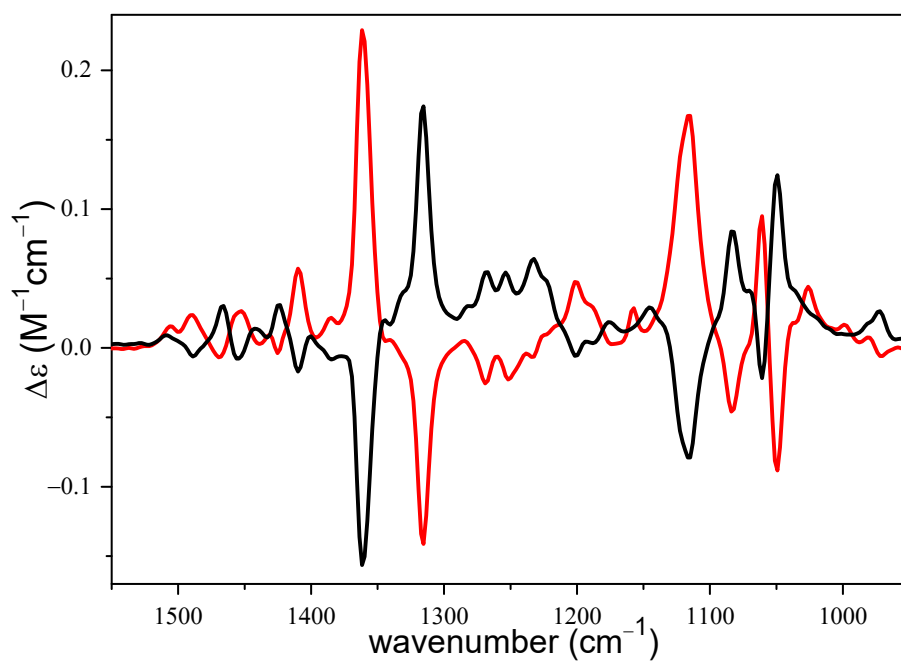


**Figure S152.** <sup>1</sup>H-<sup>1</sup>H NOESY NMR (400 MHz) spectrum of (aS,3S,3'S)-28 in CDCl<sub>3</sub>.

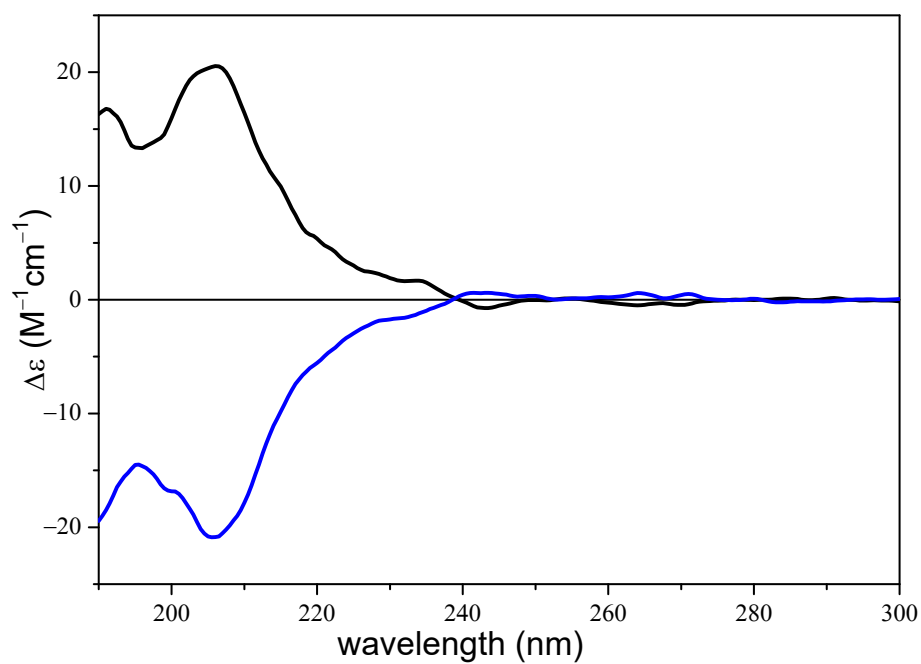
### 3.2. ECD and VCD spectra



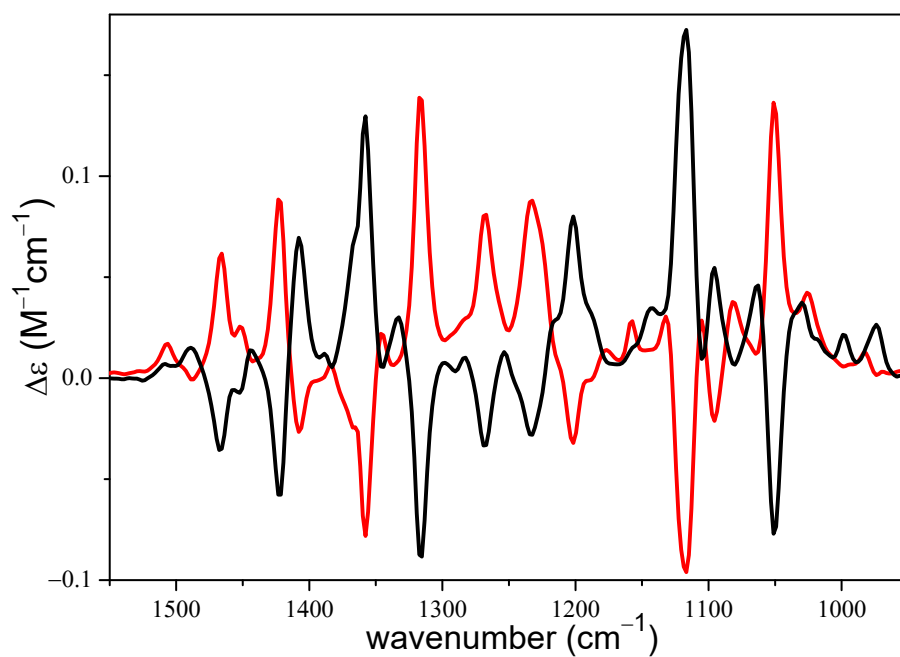
**Figure S153.** Experimental ECD spectra of enantiomeric (aS,1S,3S,3'S)-**21** (black) and (aR,1R,3R,3'R)-**21** (blue) in MeCN.



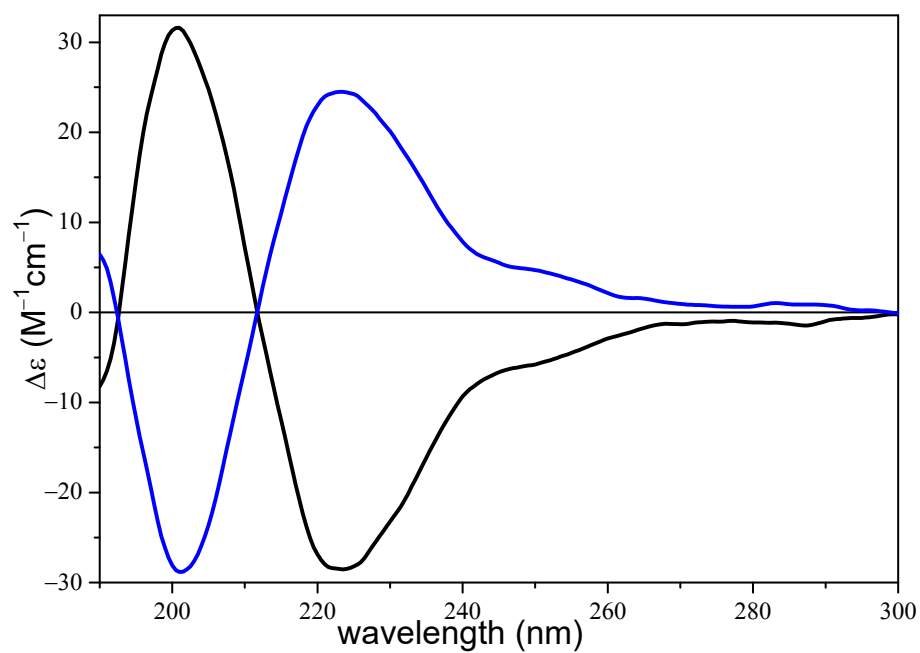
**Figure S154.** Experimental VCD spectra of enantiomeric (aS,1S,3S,3'S)-**21** (red) and (aR,1R,3R,3'R)-**21** (black) in CDCl<sub>3</sub>.



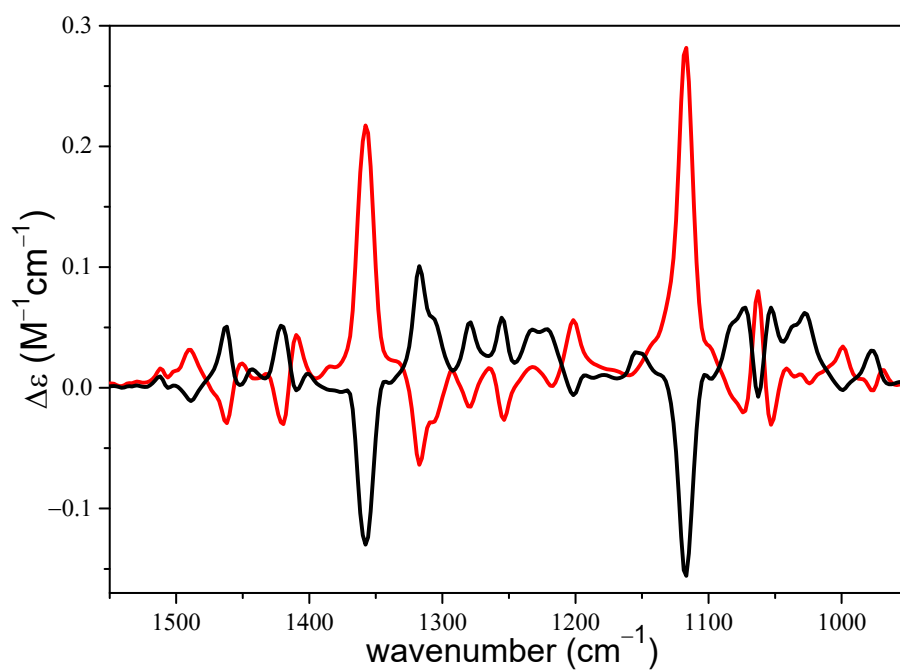
**Figure S155.** Experimental ECD spectra of enantiomeric (*aR*,1*S*,3*S*,3'*S*)-**21** (black) and (*aS*,1*R*,3*R*,3'*R*)-**21** (blue) in MeCN.



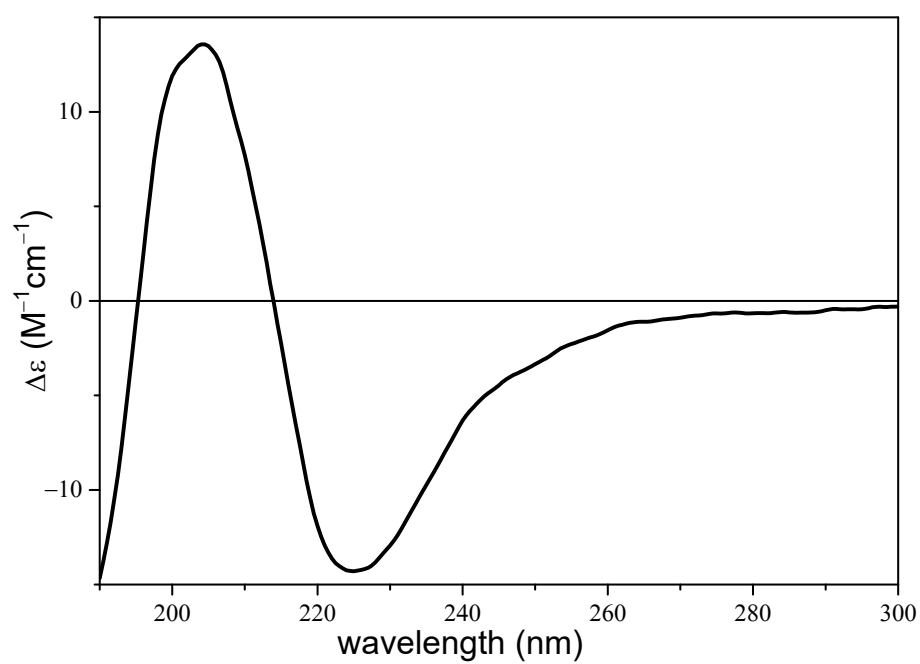
**Figure S156.** Experimental VCD spectra of enantiomeric (*aR*,1*S*,3*S*,3'*S*)-**21** (red) and (*aS*,1*R*,3*R*,3'*R*)-**21** (black) in CDCl<sub>3</sub>.



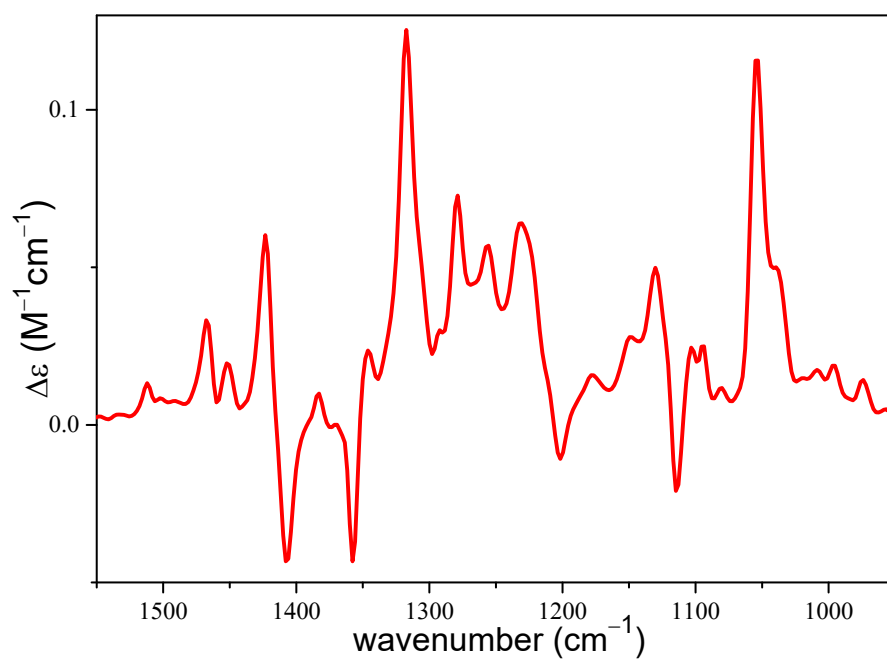
**Figure S157.** Experimental ECD spectra of enantiomeric (*aS*,1*R*,3*S*,3'*S*)-**21** (black) and (*aR*,1*S*,3*R*,3'*R*)-**21** (blue) in MeCN.



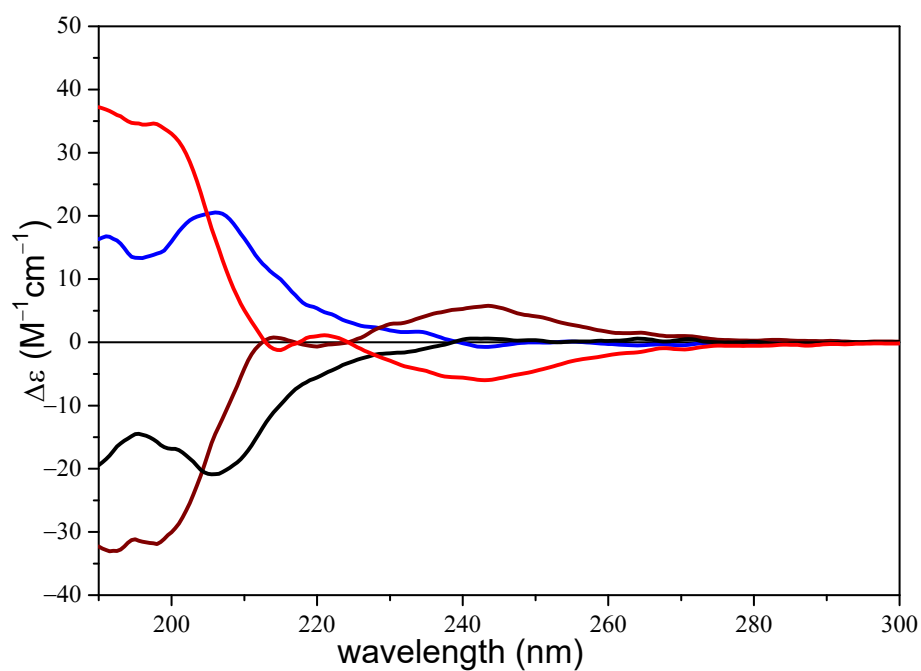
**Figure S158.** Experimental VCD spectra of enantiomeric (*aS*,1*R*,3*S*,3'*S*)-**21** (red) and (*aR*,1*S*,3*R*,3'*R*)-**21** (black) in CDCl<sub>3</sub>.



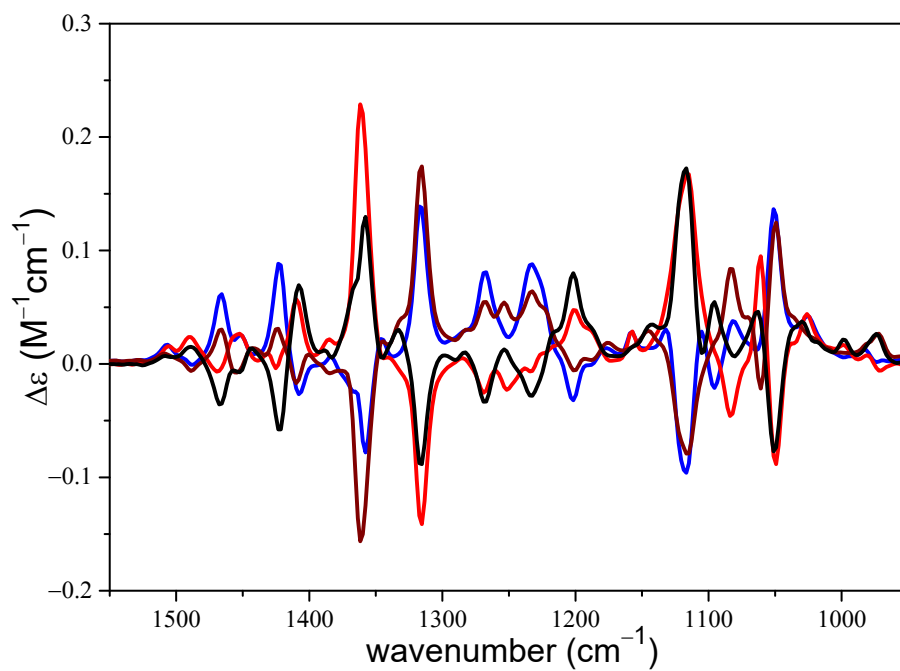
**Figure S159.** Experimental ECD spectrum of (a*R*,1*R*,3*S*,3'*S*)-**21** in MeCN.



**Figure S160.** Experimental VCD spectrum of (a*R*,1*R*,3*S*,3'*S*)-**21** in CDCl<sub>3</sub>.

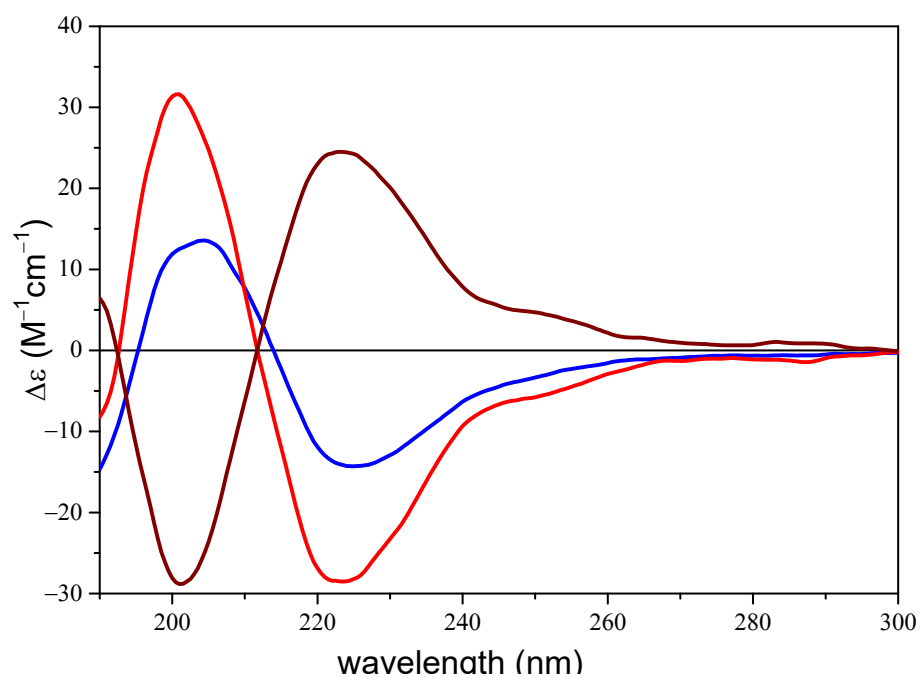


**Figure S161.** Overlapped experimental ECD spectra of stereoisomeric (*aS*,1*S*,3*S*,3'*S*)-**21** (red), (*aR*,1*S*,3*S*,3'*S*)-**21** (blue), (*aR*,1*R*,3*R*,3'*R*)-**21** (wine) and (*aS*,1*R*,3*R*,3'*R*)-**21** (black) in MeCN.

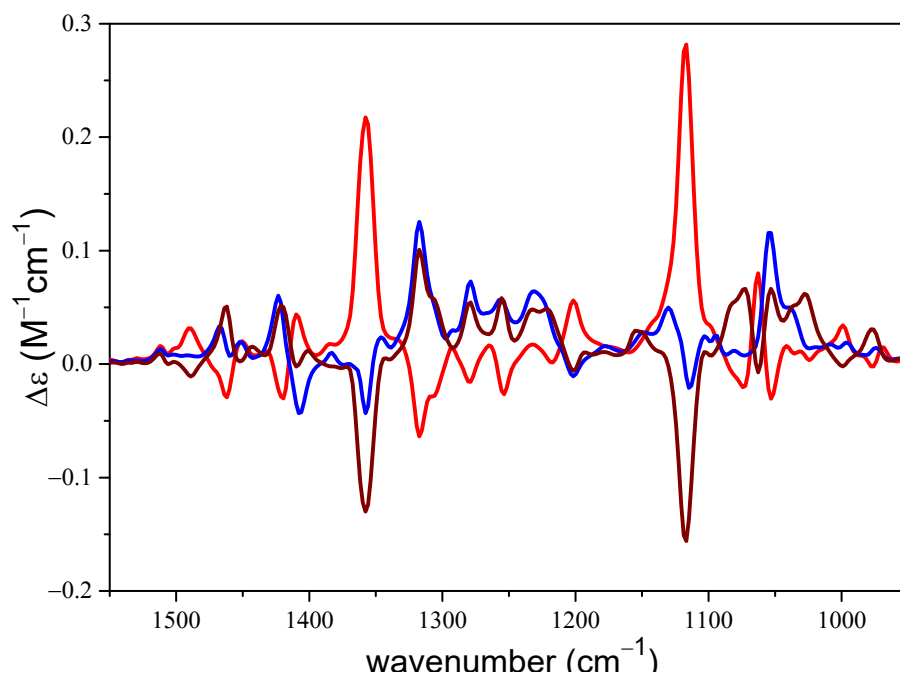


**Figure S162.** Overlapped experimental VCD spectra of stereoisomeric (*aS*,1*S*,3*S*,3'*S*)-**21** (red), (*aR*,1*S*,3*S*,3'*S*)-**21** (blue), (*aR*,1*R*,3*R*,3'*R*)-**21** (wine) and (*aS*,1*R*,3*R*,3'*R*)-**21** (black) in CDCl<sub>3</sub>.

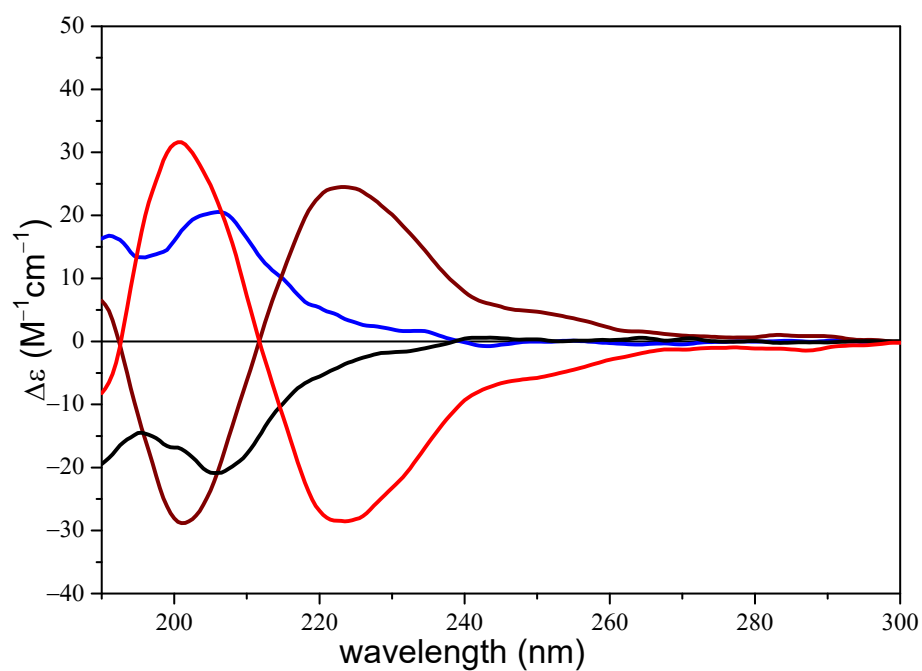




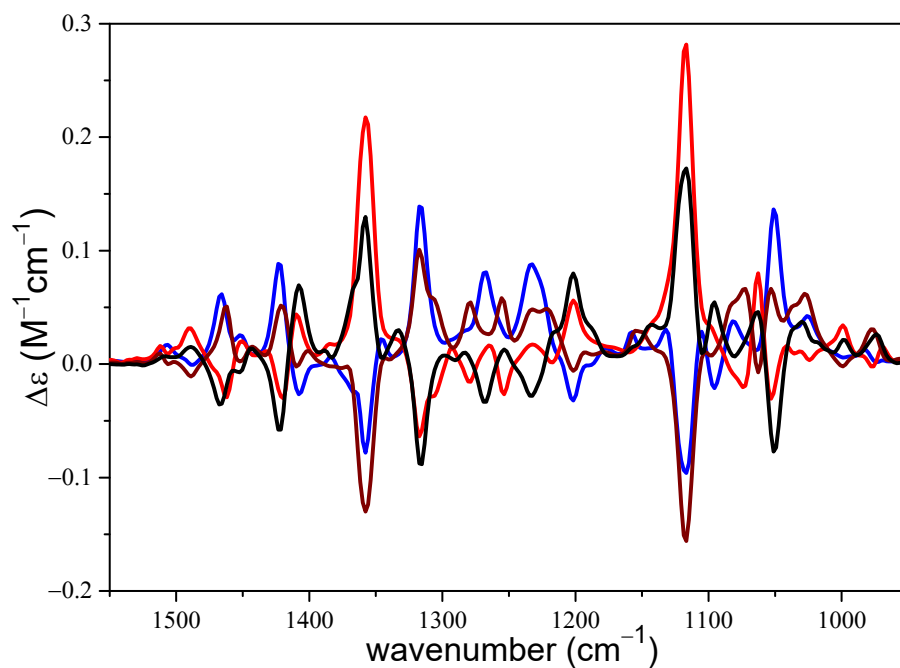
**Figure S163.** Overlapped experimental ECD spectra of stereoisomeric (*aS*,1*R*,3*S*,3'*S*)-**21** (red), (*aR*,1*R*,3*S*,3'*S*)-**21** (blue) and (*aR*,1*S*,3*R*,3'*R*)-**21** (wine) in MeCN.



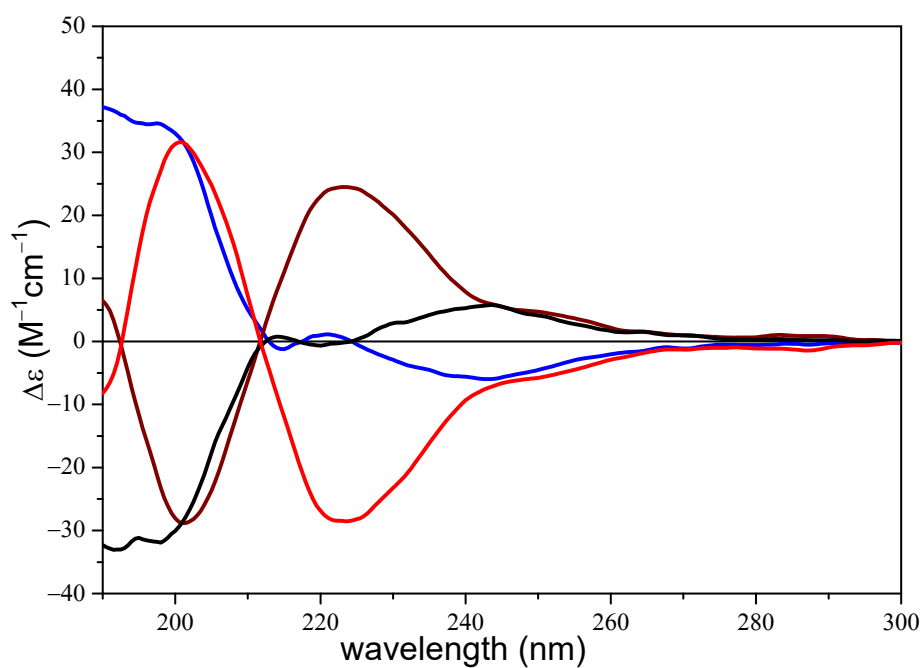
**Figure S164.** Overlapped experimental VCD spectra of stereoisomeric (*aS*,1*R*,3*S*,3'*S*)-**21** (red), (*aR*,1*R*,3*S*,3'*S*)-**21** (blue) and (*aR*,1*S*,3*R*,3'*R*)-**21** (wine) in CDCl<sub>3</sub>.



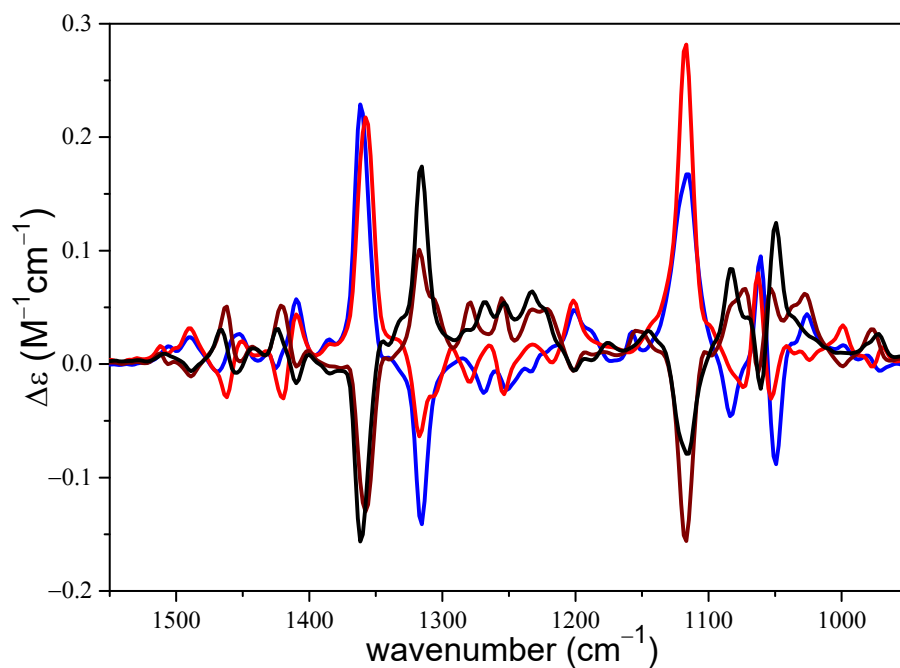
**Figure S165.** Overlapped experimental ECD spectra of stereoisomeric (*aR*,1*S*,3*S*,3'*S*)-**21** (blue), (*aS*,1*R*,3*S*,3'*S*)-**21** (red), (*aS*,1*R*,3*R*,3'*R*)-**21** (black) and (*aR*,1*S*,3*R*,3'*R*)-**21** (wine) in MeCN.



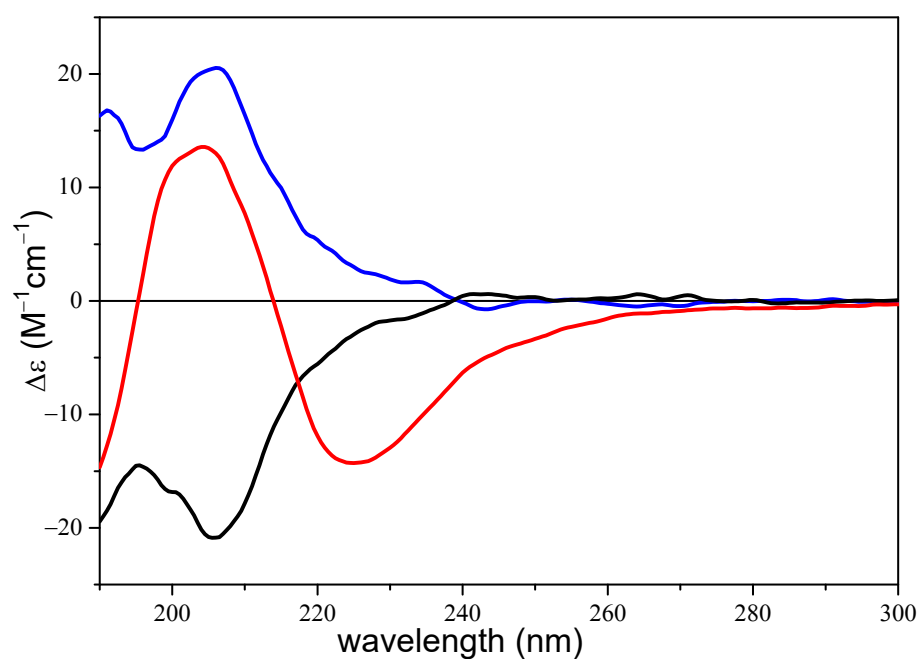
**Figure S166.** Overlapped experimental VCD spectra of stereoisomeric (*aR*,1*S*,3*S*,3'*S*)-**21** (blue), (*aS*,1*R*,3*S*,3'*S*)-**21** (red), (*aS*,1*R*,3*R*,3'*R*)-**21** (black) and (*aR*,1*S*,3*R*,3'*R*)-**21** (wine) in CDCl<sub>3</sub>.



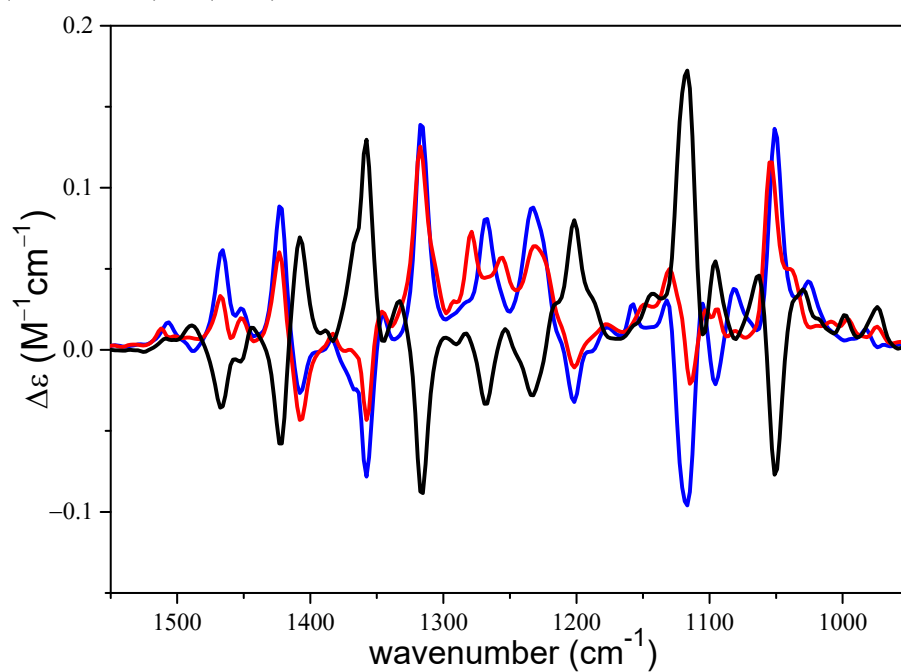
**Figure S167.** Overlapped experimental ECD spectra of stereoisomeric (*aS*,1*S*,3*S*,3'*S*)-**21** (blue), (*aS*,1*R*,3*S*,3'*S*)-**21** (red), (*aR*,1*R*,3*R*,3'*R*)-**21** (black) and (*aR*,1*S*,3*R*,3'*R*)-**21** (wine) in MeCN.



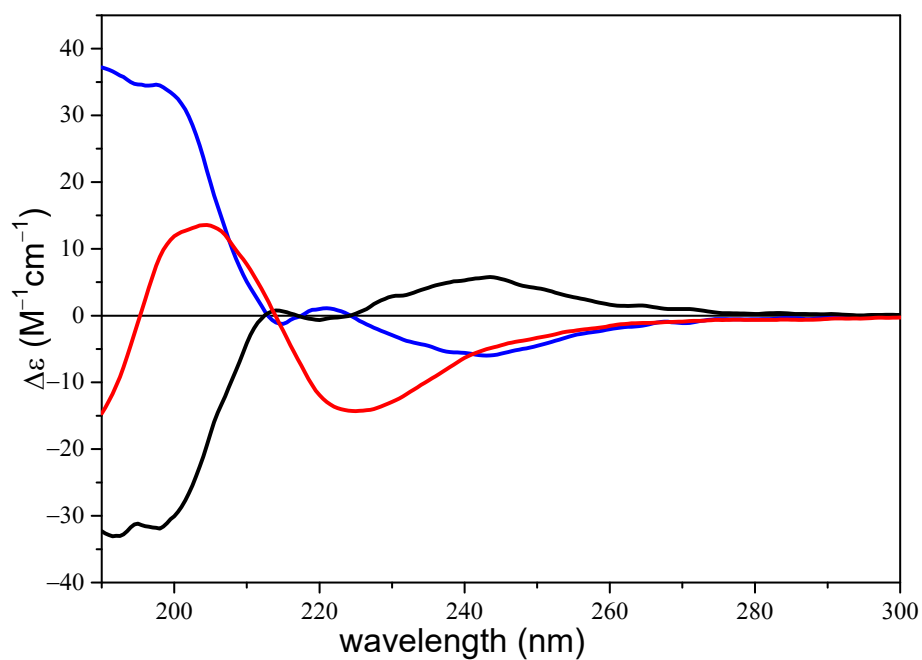
**Figure S168.** Overlapped experimental VCD spectra of stereoisomeric (*aS*,1*S*,3*S*,3'*S*)-**21** (blue), (*aS*,1*R*,3*S*,3'*S*)-**21** (red), (*aR*,1*R*,3*R*,3'*R*)-**21** (black) and (*aR*,1*S*,3*R*,3'*R*)-**21** (wine) in CDCl<sub>3</sub>.



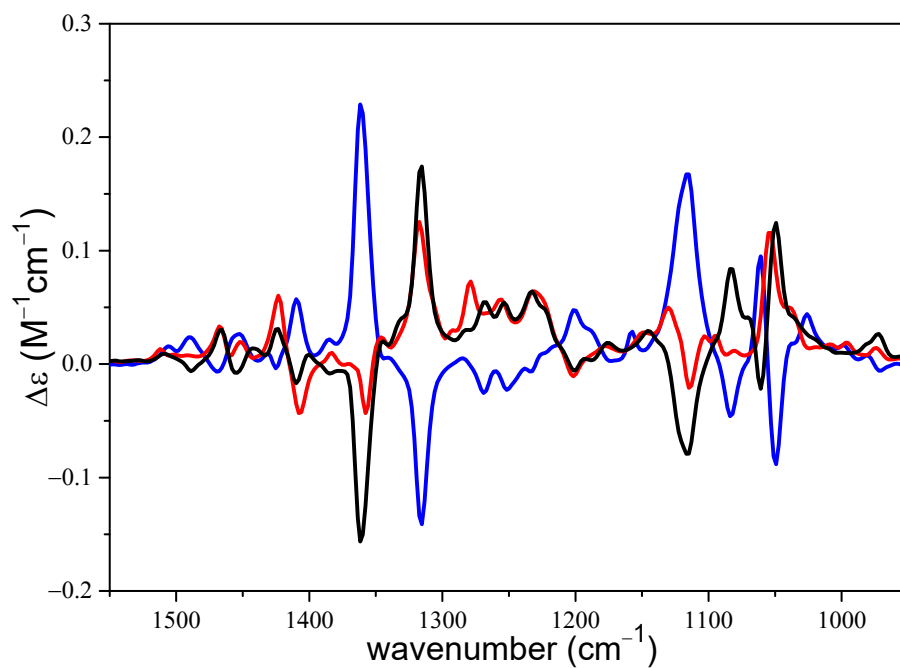
**Figure S169.** Overlapped experimental ECD spectra of stereoisomeric (aR,1S,3S,3'S)-**21** (blue), (aR,1R,3S,3'S)-**21** (red) and (aS,1R,3R,3'R)-**21** (black) in MeCN.



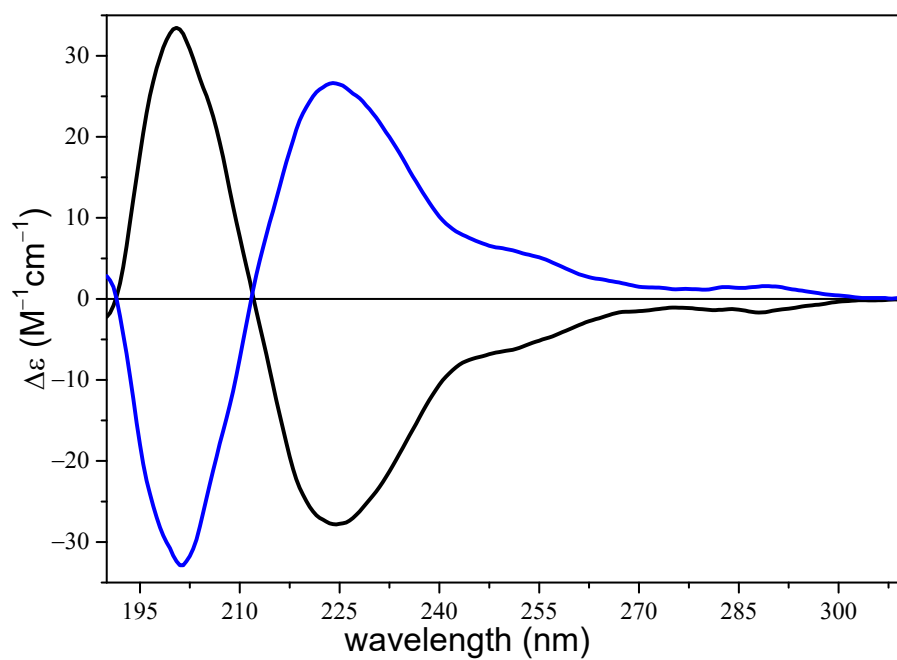
**Figure S170.** Overlapped experimental VCD spectra of stereoisomeric (aR,1S,3S,3'S)-**21** (blue), (aR,1R,3S,3'S)-**21** (red) and (aS,1R,3R,3'R)-**21** (black) in CDCl<sub>3</sub>.



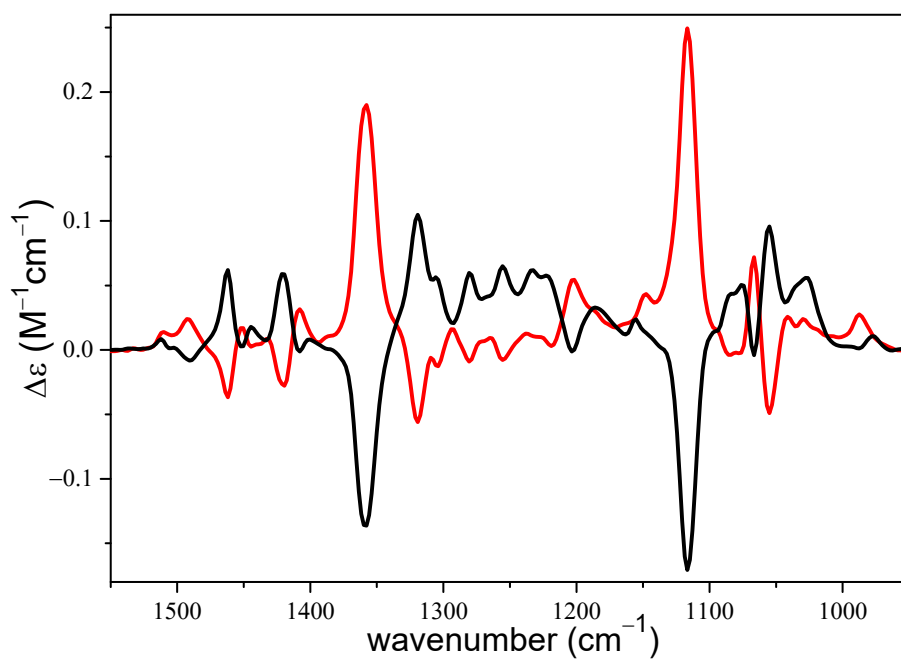
**Figure S171.** Overlapped experimental ECD spectra of stereoisomeric (*aS*,1*S*,3*S*,3'*S*)-**21** (blue), (*aR*,1*R*,3*S*,3'*S*)-**21** (red) and (*aR*,1*R*,3*R*,3'*R*)-**21** (black) in MeCN.



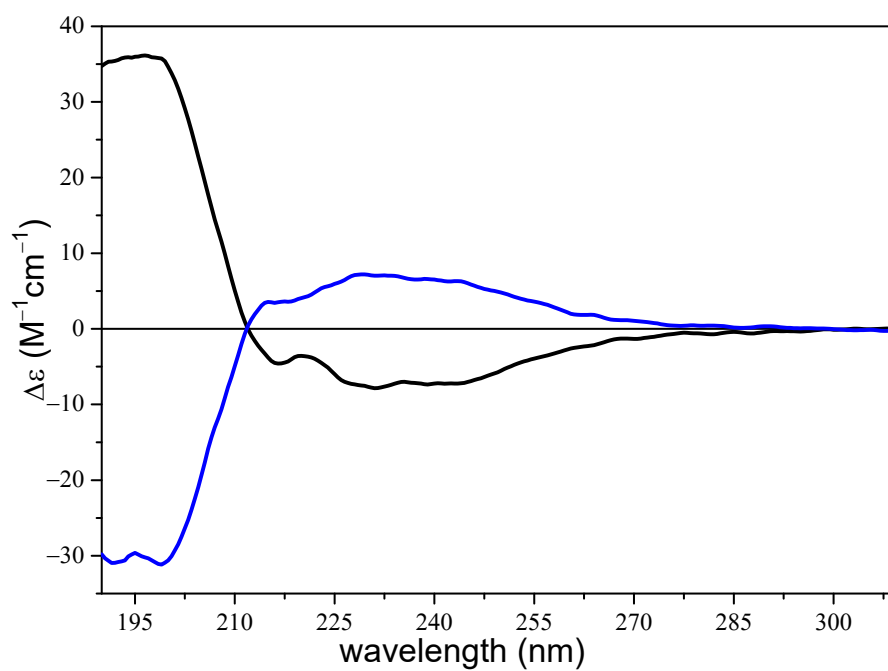
**Figure S172.** Overlapped experimental VCD spectra of stereoisomeric (*aS*,1*S*,3*S*,3'*S*)-**21** (blue), (*aR*,1*R*,3*S*,3'*S*)-**21** (red) and (*aR*,1*R*,3*R*,3'*R*)-**21** (black) in CDCl<sub>3</sub>.



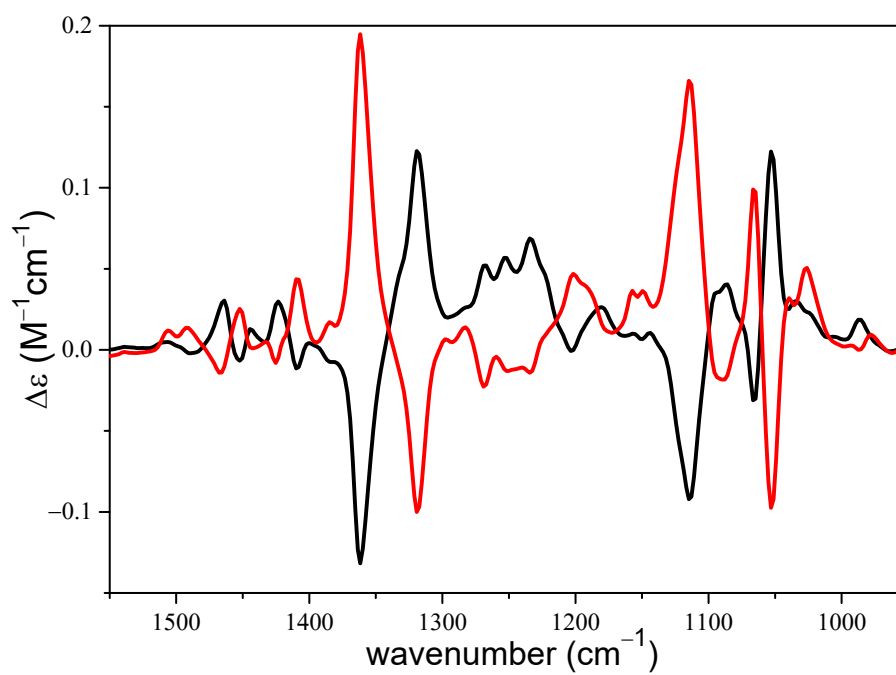
**Figure S173.** Experimental ECD spectra of enantiomeric (*aS*,1*R*,3*S*,1'*S*,3'*S*)-**22** (black) and (*aR*,1*S*,3*R*,1'*R*,3'*R*)-**22** (blue) in MeCN.



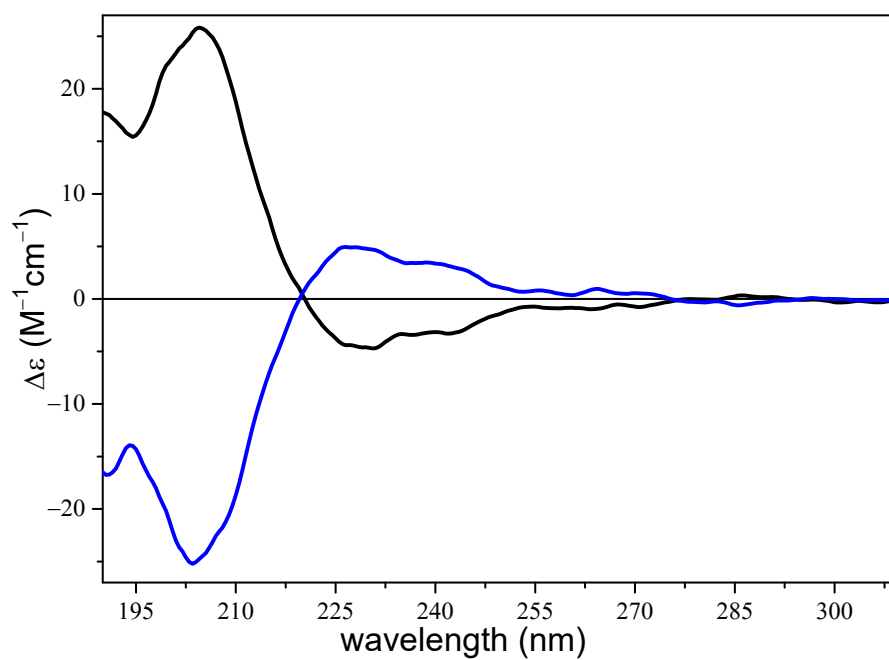
**Figure S174.** Experimental VCD spectra of enantiomeric (*aS*,1*R*,3*S*,1'*S*,3'*S*)-**22** (red) and (*aR*,1*S*,3*R*,1'*R*,3'*R*)-**22** (black) in CDCl<sub>3</sub>.



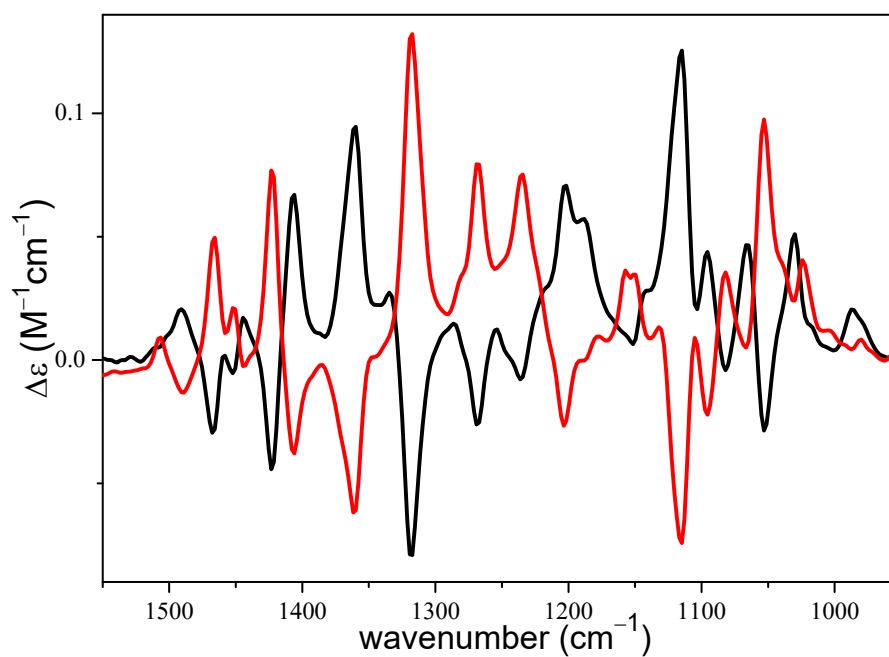
**Figure S175.** Experimental ECD spectra of enantiomeric (*aS*,1*S*,3*S*,1'*S*,3'*S*)-**22** (black) and (*aR*,1*R*,3*R*,1'*R*,3'*R*)-**22** (blue) in MeCN.



**Figure S176.** Experimental VCD spectra of enantiomeric (*aS*,1*S*,3*S*,1'*S*,3'*S*)-**22** (red) and (*aR*,1*R*,3*R*,1'*R*,3'*R*)-**22** (black) in CDCl<sub>3</sub>.

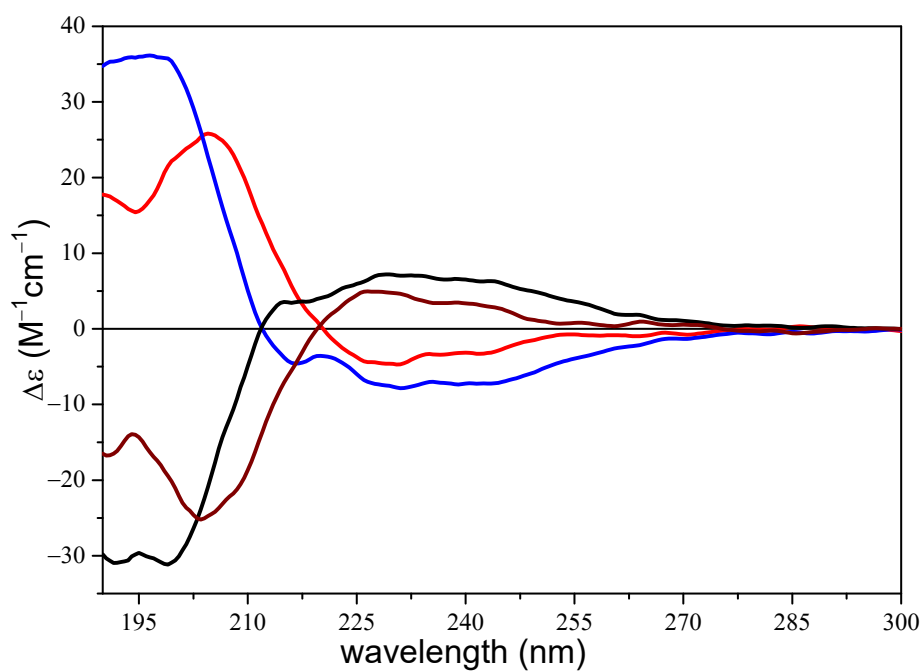


**Figure S177.** Experimental ECD spectra of enantiomeric (*aR,1S,3S,1'S,3'S*)-**22** (black) and (*aS,1R,3R,1'R,3'R*)-**22** (blue) in MeCN.

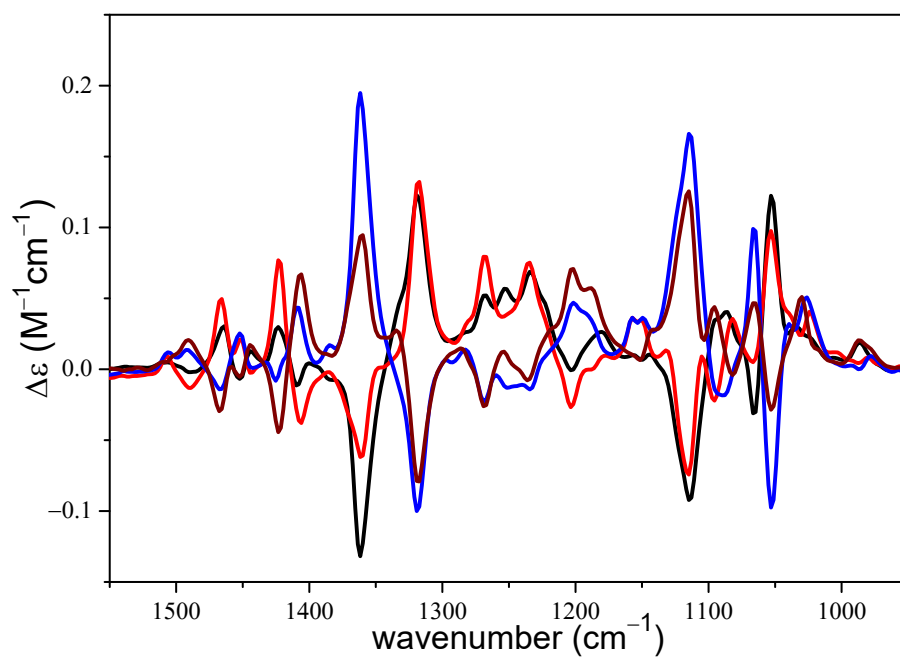


**Figure S178.** Experimental VCD spectra of enantiomeric (*aR,1S,3S,1'S,3'S*)-**22** (red) and (*aS,1R,3R,1'R,3'R*)-**22** (black) in CDCl<sub>3</sub>.

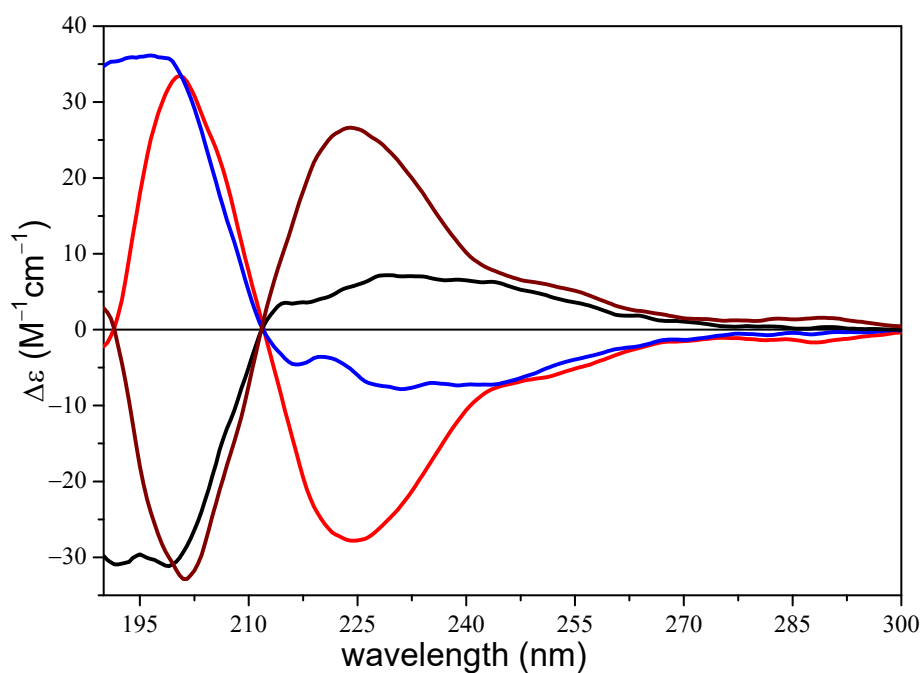




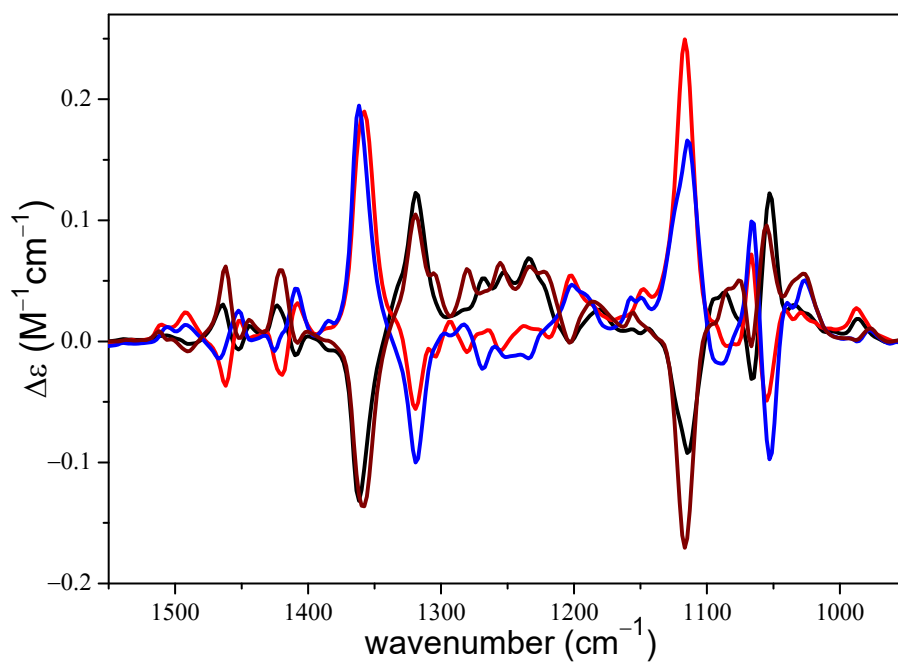
**Figure S179.** Overlapped experimental ECD spectra of stereoisomeric (aS,1S,3S,1'S,3'S)-**22** (blue), (aR,1S,3S,1'S,3'S)-**22** (red), (aR,1R,3R,1'R,3'R)-**22** (black) and (aS,1R,3R,1'R,3'R)-**22** (wine) in MeCN.



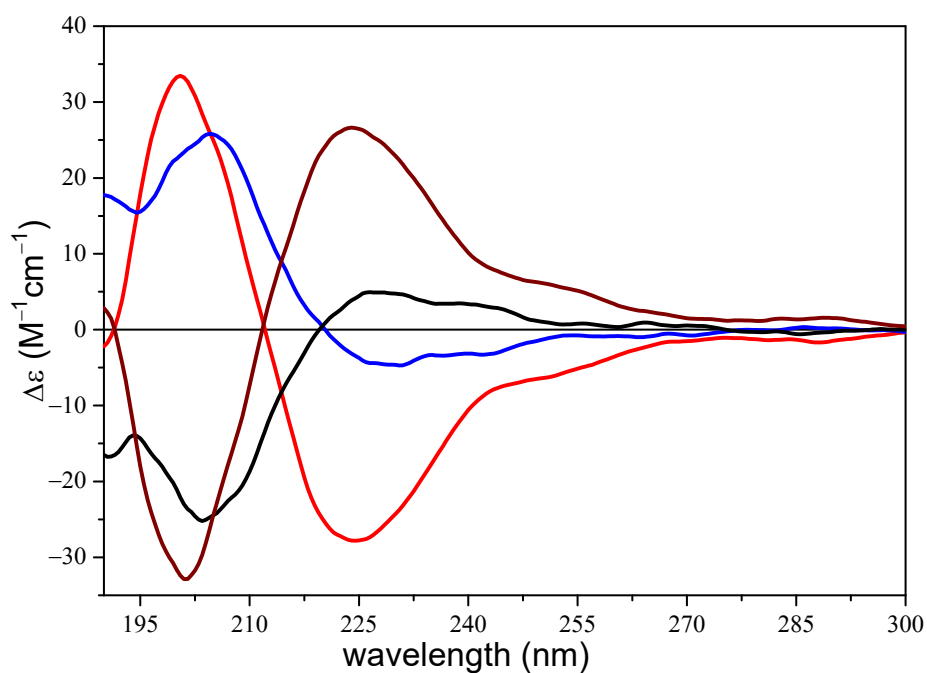
**Figure S180.** Overlapped experimental VCD spectra of stereoisomeric (aS,1S,3S,1'S,3'S)-**22** (blue), (aR,1S,3S,1'S,3'S)-**22** (red), (aR,1R,3R,1'R,3'R)-**22** (black) and (aS,1R,3R,1'R,3'R)-**22** (wine) in CDCl<sub>3</sub>.



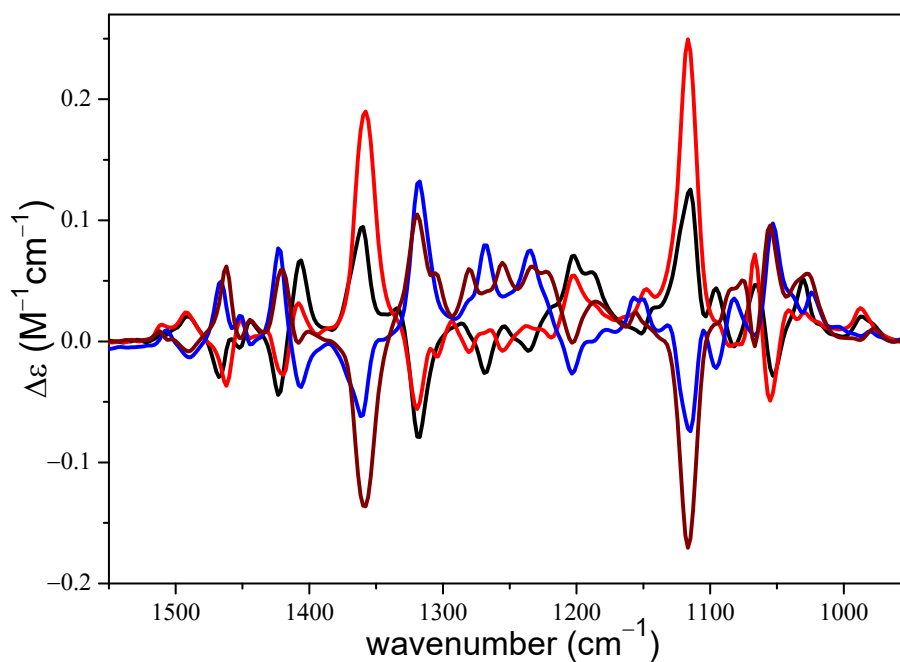
**Figure S181.** Overlapped experimental ECD spectra of stereoisomeric (aS,1S,3S,1'S,3'S)-**22** (blue), (aS,1R,3S,1'S,3'S)-**22** (red), (aR,1R,3R,1'R,3'R)-**22** (black) and (aR,1S,3R,1'R,3'R)-**22** (wine) in MeCN.



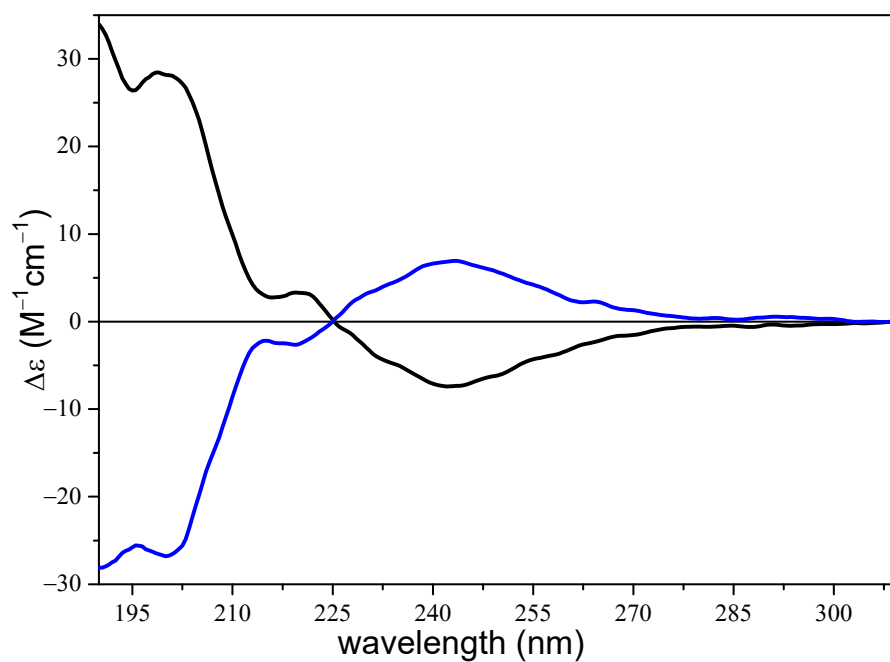
**Figure S182.** Overlapped experimental VCD spectra of stereoisomeric (aS,1S,3S,1'S,3'S)-**22** (blue), (aS,1R,3S,1'S,3'S)-**22** (red), (aR,1R,3R,1'R,3'R)-**22** (black) and (aR,1S,3R,1'R,3'R)-**22** (wine) in CDCl<sub>3</sub>.



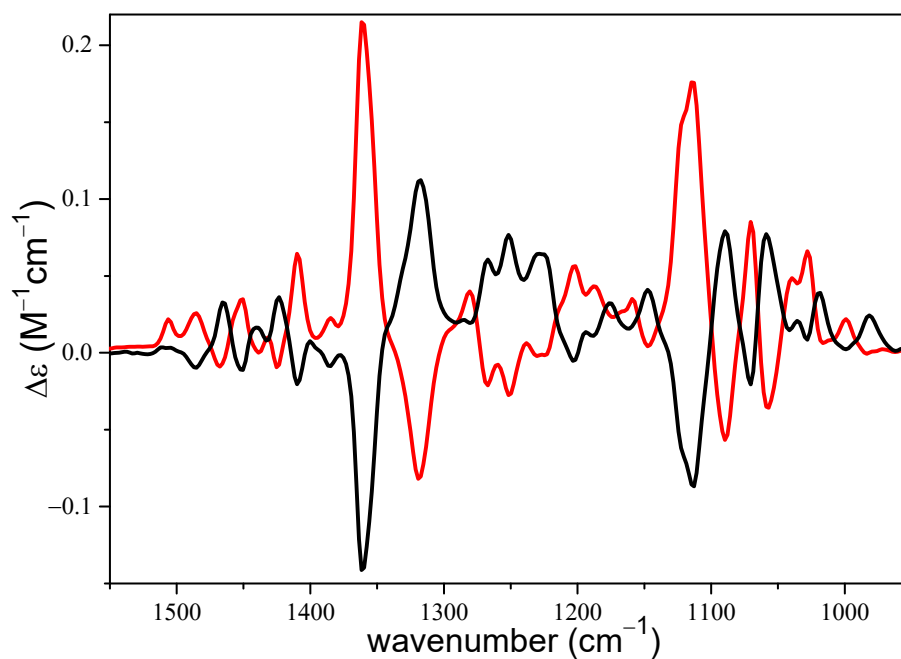
**Figure S183.** Overlapped experimental ECD spectra of stereoisomeric (*aR*,1*S*,3*S*,1'*S*,3'*S*)-**22** (blue), (*aS*,1*R*,3*S*,1'*S*,3'*S*)-**22** (red), (*aS*,1*R*,3*R*,1'*R*,3'*R*)-**22** (black) and (*aR*,1*S*,3*R*,1'*R*,3'*R*)-**22** (wine) in MeCN.



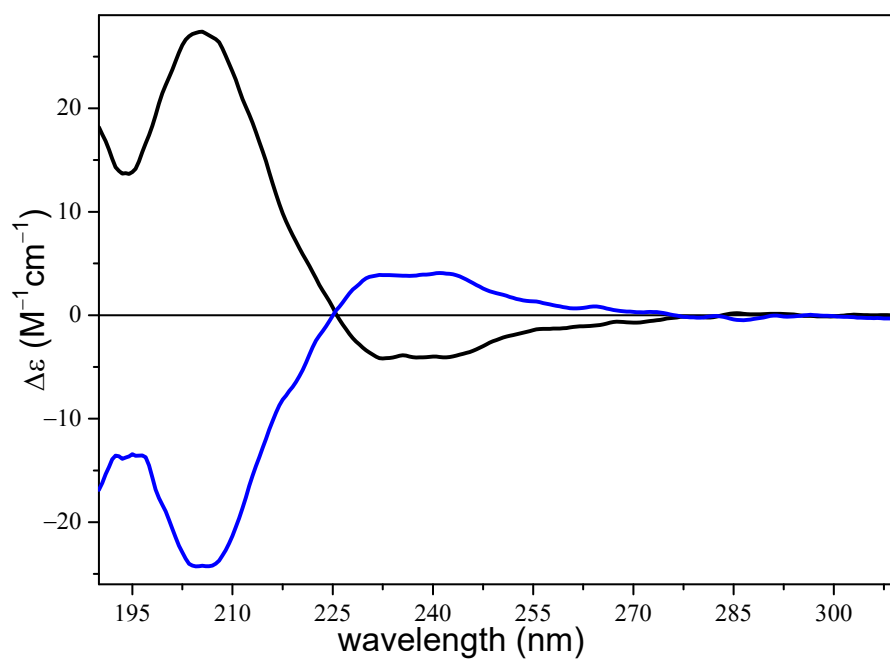
**Figure S184.** Overlapped experimental VCD spectra of stereoisomeric (*aR*,1*S*,3*S*,1'*S*,3'*S*)-**22** (blue), (*aS*,1*R*,3*S*,1'*S*,3'*S*)-**22** (red), (*aS*,1*R*,3*R*,1'*R*,3'*R*)-**22** (black) and (*aR*,1*S*,3*R*,1'*R*,3'*R*)-**22** (wine) in CDCl<sub>3</sub>.



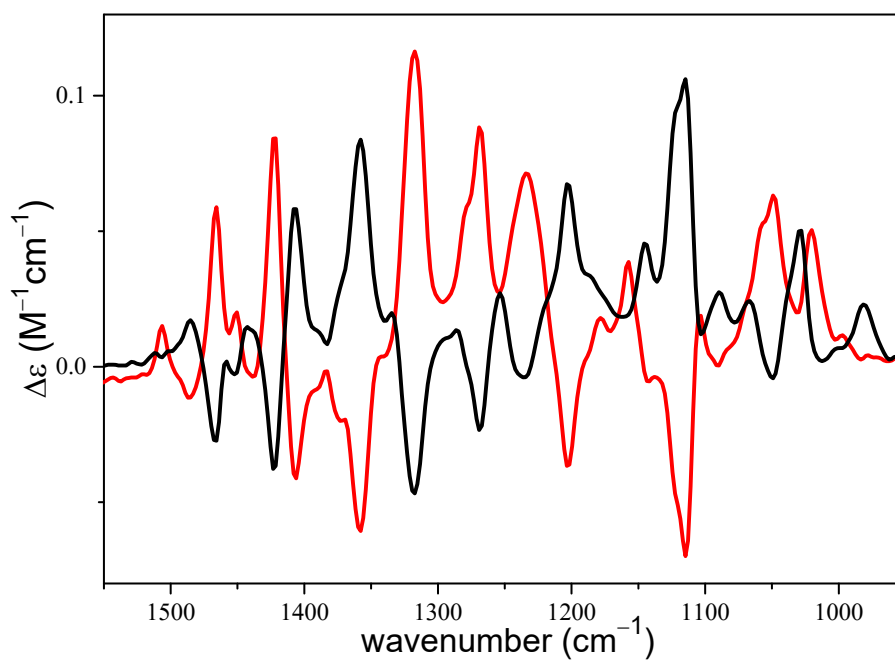
**Figure S185.** Experimental ECD spectra of enantiomeric (*aS*,1*S*,3*S*,1'*R*,3'*S*)-**23** (black) and (*aR*,1*R*,3*R*,1'*S*,3'*R*)-**23** (blue) in MeCN.



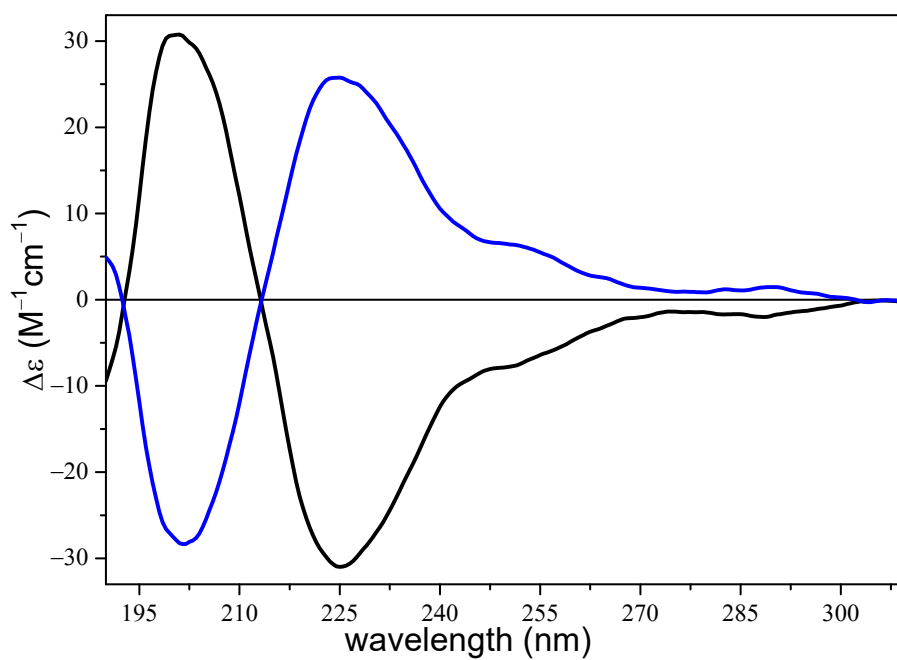
**Figure S186.** Experimental VCD spectra of enantiomeric (*aS*,1*S*,3*S*,1'*R*,3'*S*)-**23** (red) and (*aR*,1*R*,3*R*,1'*S*,3'*R*)-**23** (black) in CDCl<sub>3</sub>.



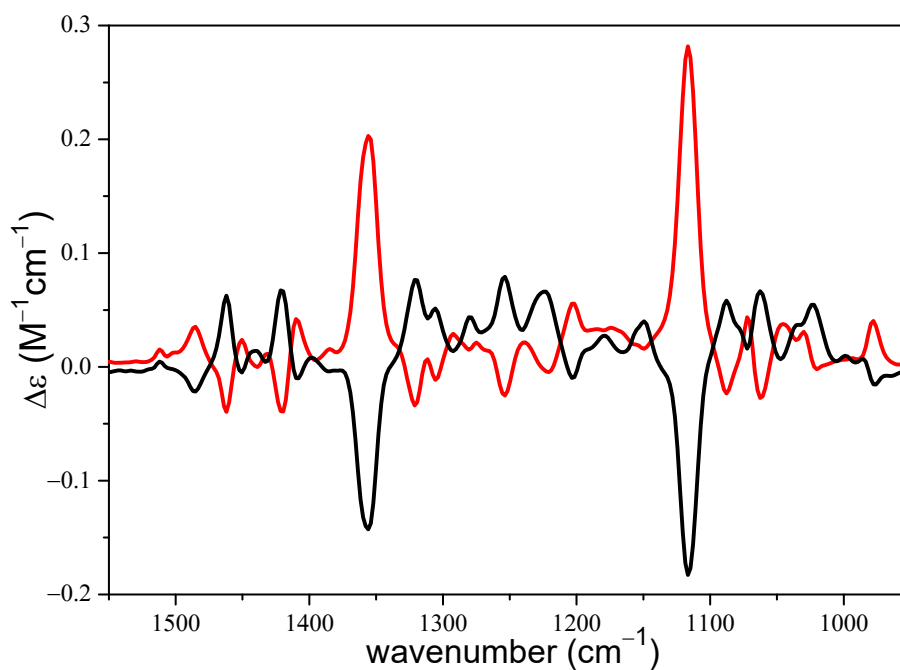
**Figure S187.** Experimental ECD spectra of enantiomeric (*aR*,1*S*,3*S*,1'*R*,3'*S*)-**23** (black) and (*aS*,1*R*,3*R*,1'*S*,3'*R*)-**23** (blue) in MeCN.



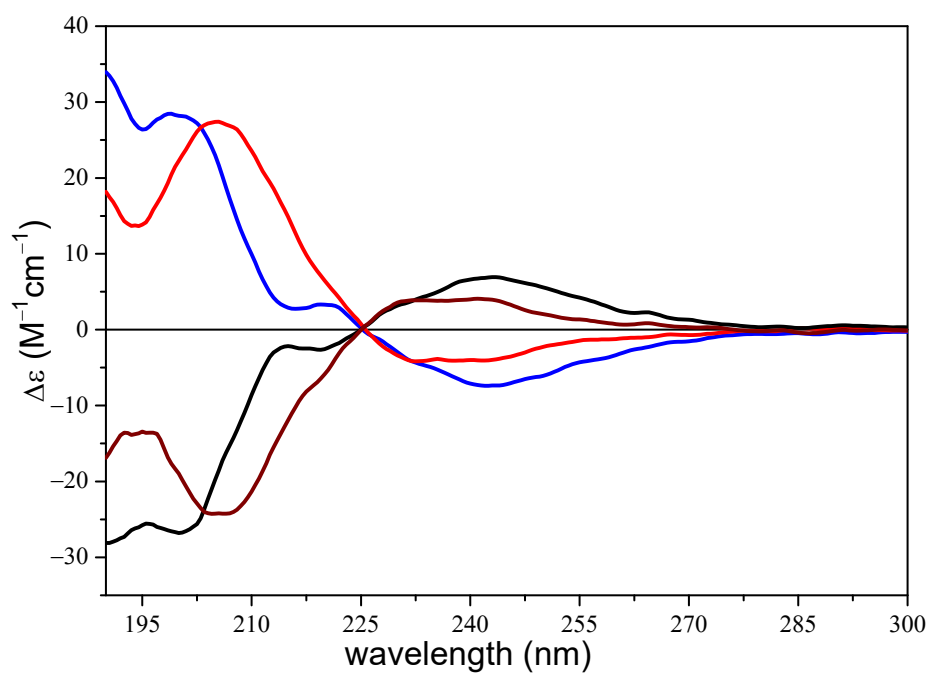
**Figure S188.** Experimental VCD spectra of enantiomeric (*aR*,1*S*,3*S*,1'*R*,3'*S*)-**23** (red) and (*aS*,1*R*,3*R*,1'*S*,3'*R*)-**23** (black) in CDCl<sub>3</sub>.



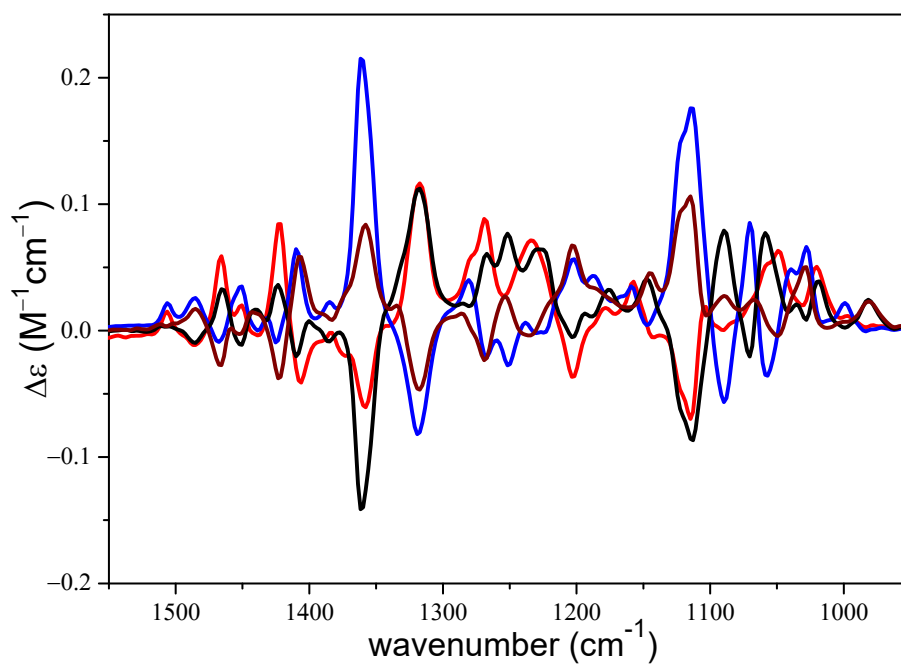
**Figure S189.** Experimental ECD spectra of enantiomeric (*aS*,1*R*,3*S*,1'*R*,3'*S*)-**23** (black) and (*aR*,1*S*,3*R*,1'*S*,3'*R*)-**23** (blue) in MeCN.



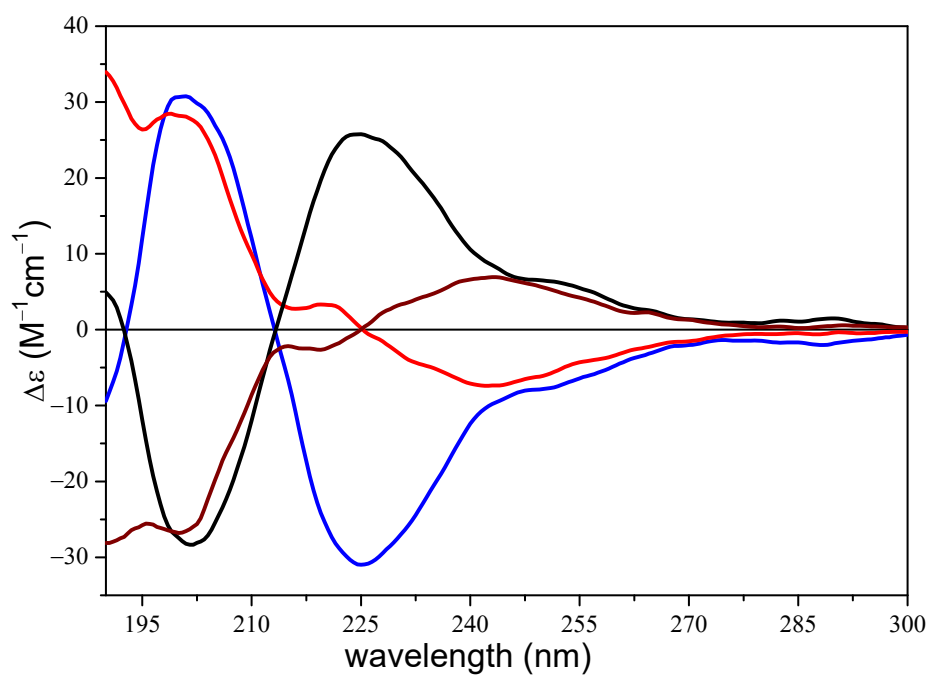
**Figure S190.** Experimental VCD spectra of enantiomeric (*aS*,1*R*,3*S*,1'*R*,3'*S*)-**23** (red) and (*aR*,1*S*,3*R*,1'*S*,3'*R*)-**23** (black) in CDCl<sub>3</sub>.



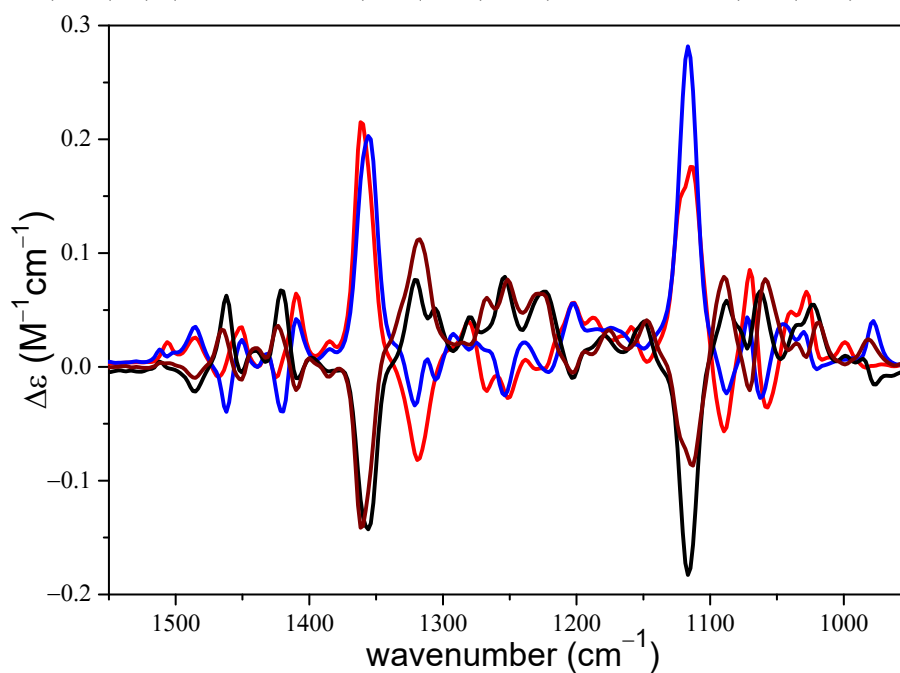
**Figure S191.** Overlapped experimental ECD spectra of stereoisomeric (aS,1S,3S,1'R,3'S)-**23** (blue), (aR,1S,3S,1'R,3'S)-**23** (red), (aR,1R,3R,1'S,3'R)-**23** (black) and (aS,1R,3R,1'S,3'R)-**23** (wine) in MeCN.



**Figure S192.** Overlapped experimental VCD spectra of stereoisomeric (aS,1S,3S,1'R,3'S)-**23** (blue), (aR,1S,3S,1'R,3'S)-**23** (red), (aR,1R,3R,1'S,3'R)-**23** (black) and (aS,1R,3R,1'S,3'R)-**23** (wine) in CDCl<sub>3</sub>.

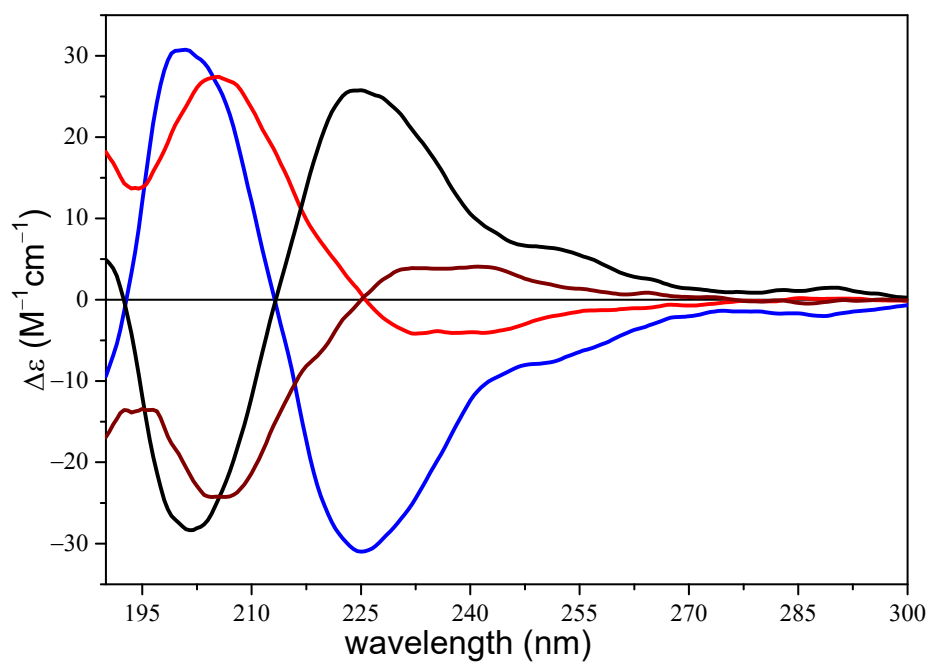


**Figure S193.** Overlapped experimental ECD spectra of stereoisomeric (*aS*,1*R*,3*S*,1'*R*,3'*S*)-**23** (blue), (*aS*,1*S*,3*S*,1'*R*,3'*S*)-**23** (red), (*aR*,1*S*,3*R*,1'*S*,3'*R*)-**23** (black) and (*aR*,1*R*,3*R*,1'*S*,3'*R*)-**23** (wine) in MeCN.

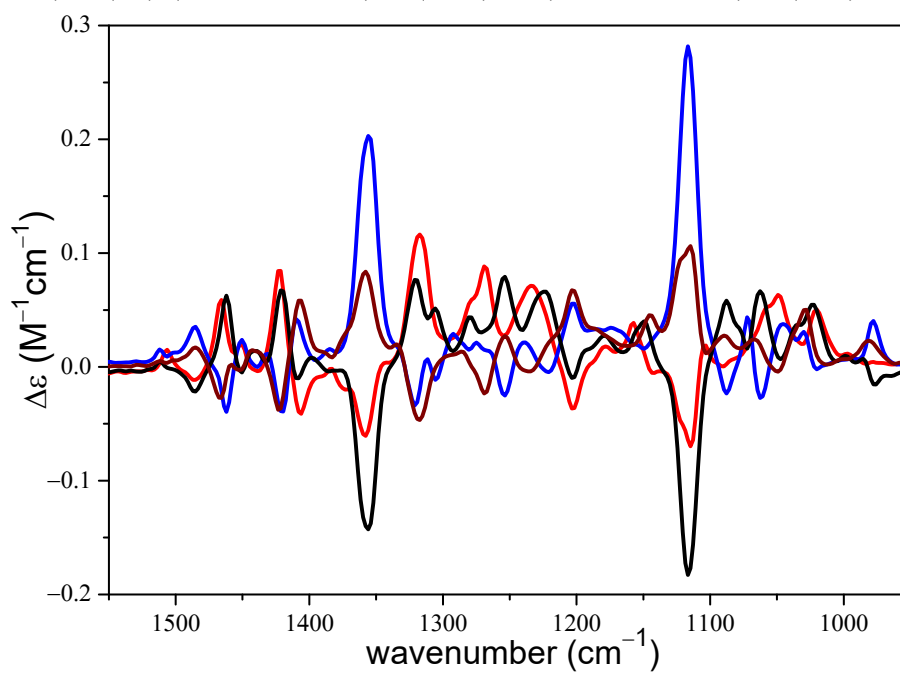


**Figure S194.** Overlapped experimental VCD spectra of stereoisomeric (*aS*,1*R*,3*S*,1'*R*,3'*S*)-**23** (blue), (*aS*,1*S*,3*S*,1'*R*,3'*S*)-**23** (red), (*aR*,1*S*,3*R*,1'*S*,3'*R*)-**23** (black) and (*aR*,1*R*,3*R*,1'*S*,3'*R*)-**23** (wine) in CDCl<sub>3</sub>.

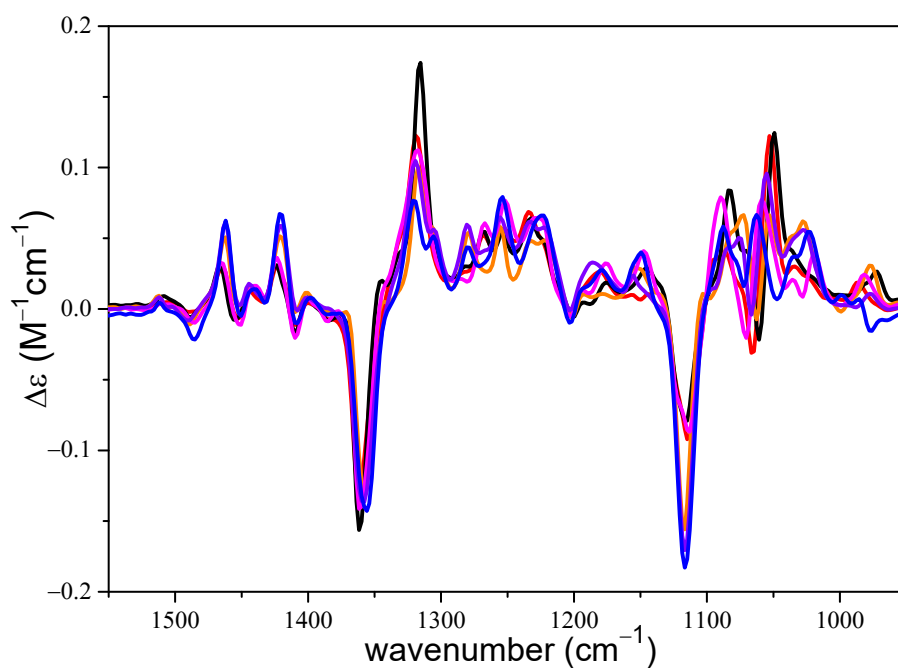




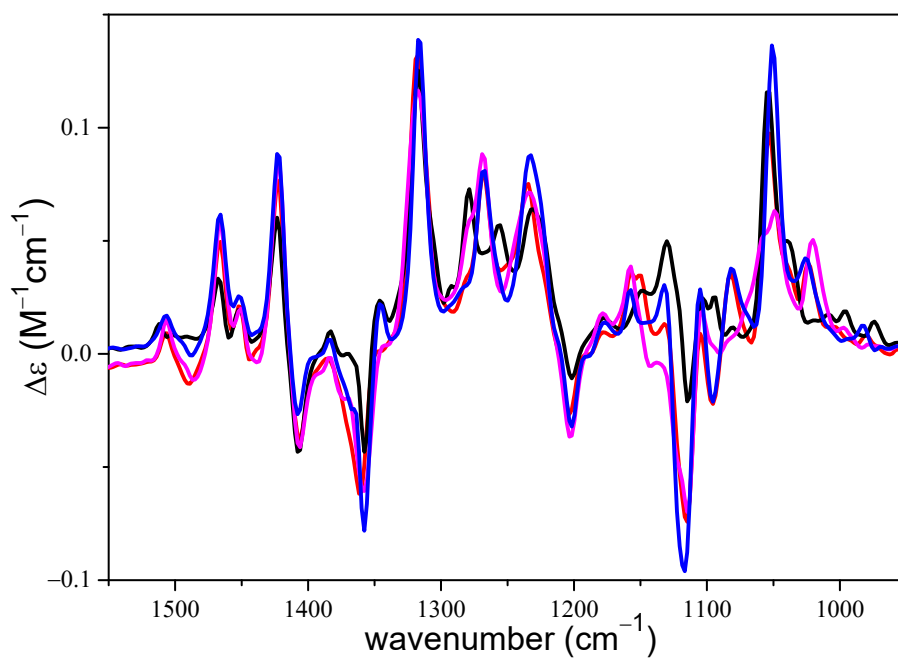
**Figure S195.** Overlapped experimental ECD spectra of stereoisomeric (aS,1R,3S,1'R,3'S)-**23** (blue), (aR,1S,3S,1'R,3'S)-**23** (red), (aR,1S,3R,1'S,3'R)-**23** (black) and (aS,1R,3R,1'S,3'R)-**23** (wine) in MeCN.



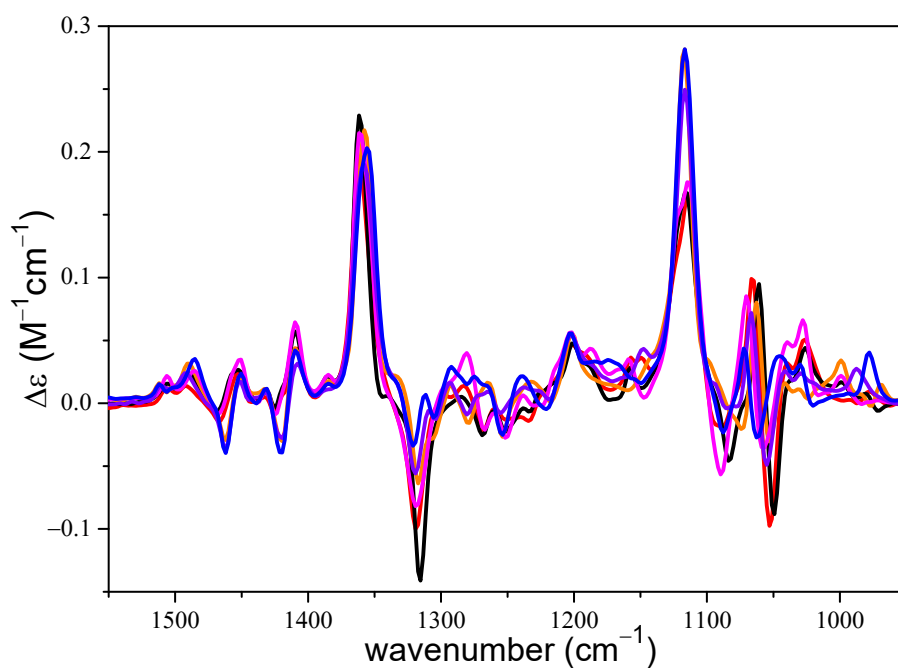
**Figure S196.** Overlapped experimental VCD spectra of stereoisomeric (aS,1R,3S,1'R,3'S)-**23** (blue), (aR,1S,3S,1'R,3'S)-**23** (red), (aR,1S,3R,1'S,3'R)-**23** (black) and (aS,1R,3R,1'S,3'R)-**23** (wine) in CDCl<sub>3</sub>.



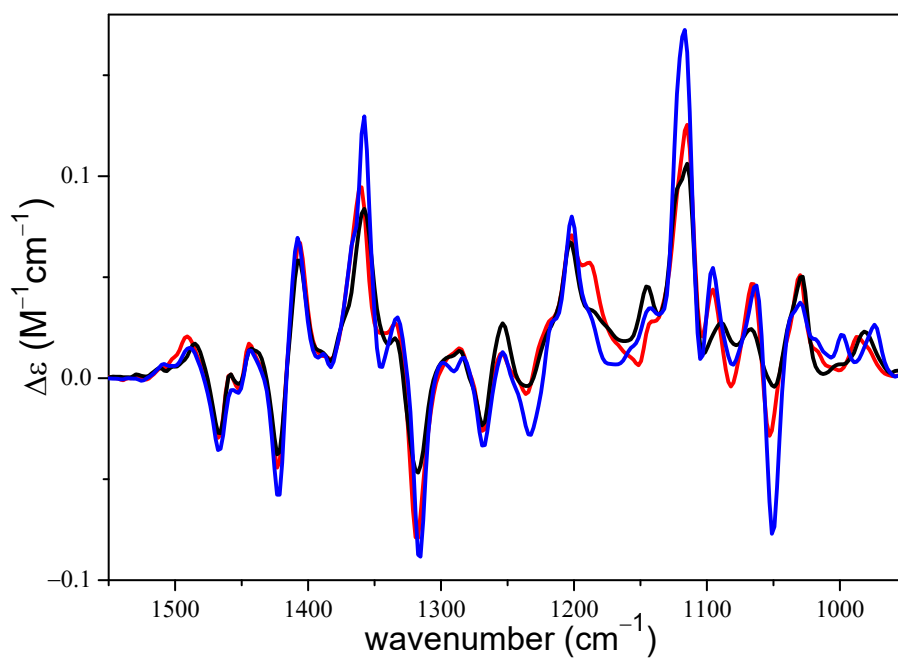
**Figure S197.** Overlapped experimental VCD spectra of stereoisomeric (*aR*,1*R*,3*R*,3'*R*)-**21** (black), (*aR*,1*S*,3*R*,3'*R*)-**21** (orange), (*aR*,1*S*,3*R*,1'*R*,3'*R*)-**22** (violet), (*aR*,1*R*,3*R*,1'*R*,3'*R*)-**22** (red), (*aR*,1*S*,3*R*,1'*S*,3'*R*)-**23** (blue) and (*aR*,1*R*,3*R*,1'*S*,3'*R*)-**23** (magenta) in  $\text{CDCl}_3$ .



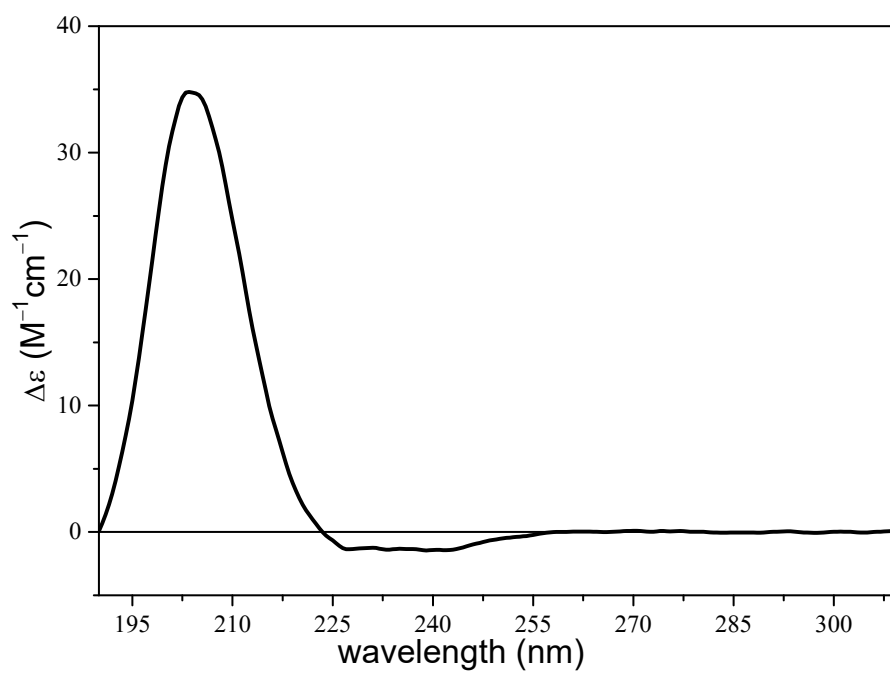
**Figure S198.** Overlapped experimental VCD spectra of stereoisomeric (*aR*,1*S*,3*S*,3'*S*)-**21** (blue), (*aR*,1*R*,3*S*,3'*S*)-**21** (black), (*aR*,1*S*,3*S*,1'*S*,3'*S*)-**22** (red) and (*aR*,1*S*,3*S*,1'*R*,3'*S*)-**23** (magenta) in  $\text{CDCl}_3$ .



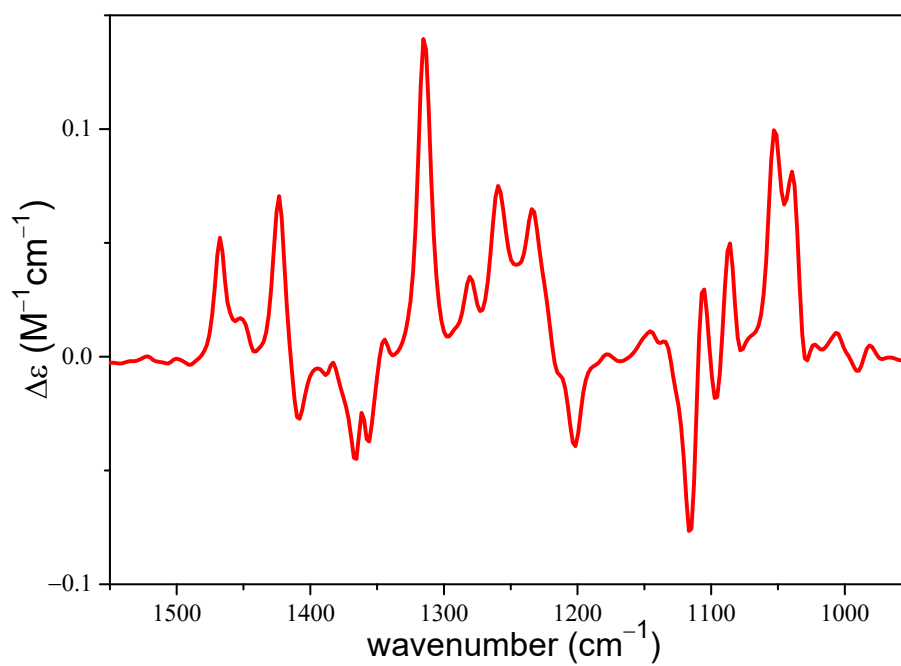
**Figure S199.** Overlapped experimental VCD spectra of stereoisomeric (*aS*,1*S*,3*S*,3'*S*)-**21** (black), (*aS*,1*R*,3*S*,3'*S*)-**21** (orange), (*aS*,1*R*,3*S*,1'*S*,3'*S*)-**22** (violet), (*aS*,1*S*,3*S*,1'*S*,3'*S*)-**22** (red), (*aS*,1*R*,3*S*,1'*R*,3'*S*)-**23** (blue) and (*aS*,1*S*,3*S*,1'*R*,3'*S*)-**23** (magenta) in  $\text{CDCl}_3$ .



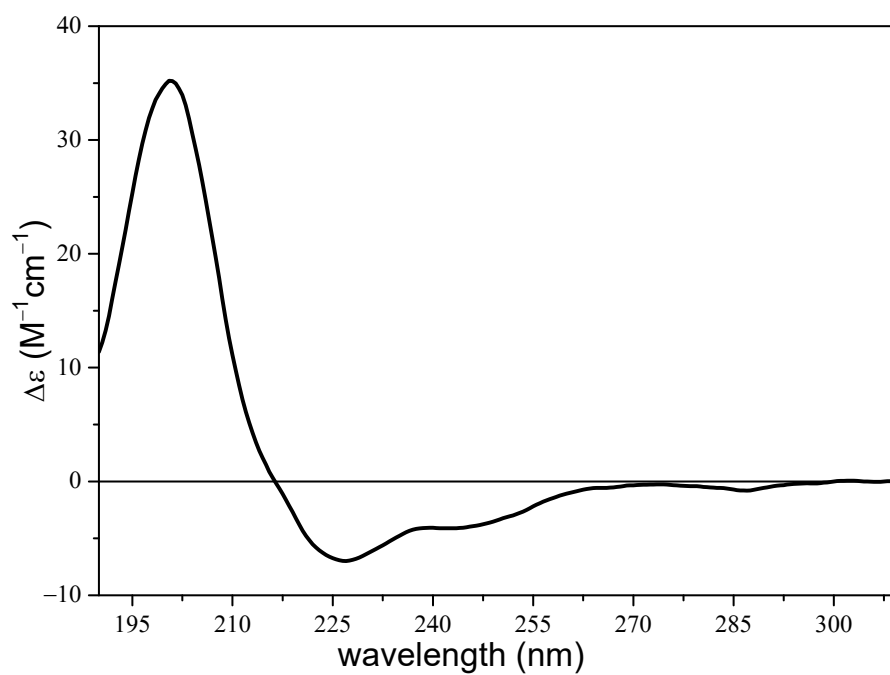
**Figure S200.** Overlapped experimental VCD spectra of stereoisomeric (*aS*,1*R*,3*R*,3'*R*)-**21** (blue), (*aS*,1*R*,3*R*,1'*R*,3'*R*)-**22** (red) and (*aS*,1*R*,3*R*,1'*S*,3'*R*)-**23** (black) in  $\text{CDCl}_3$ .



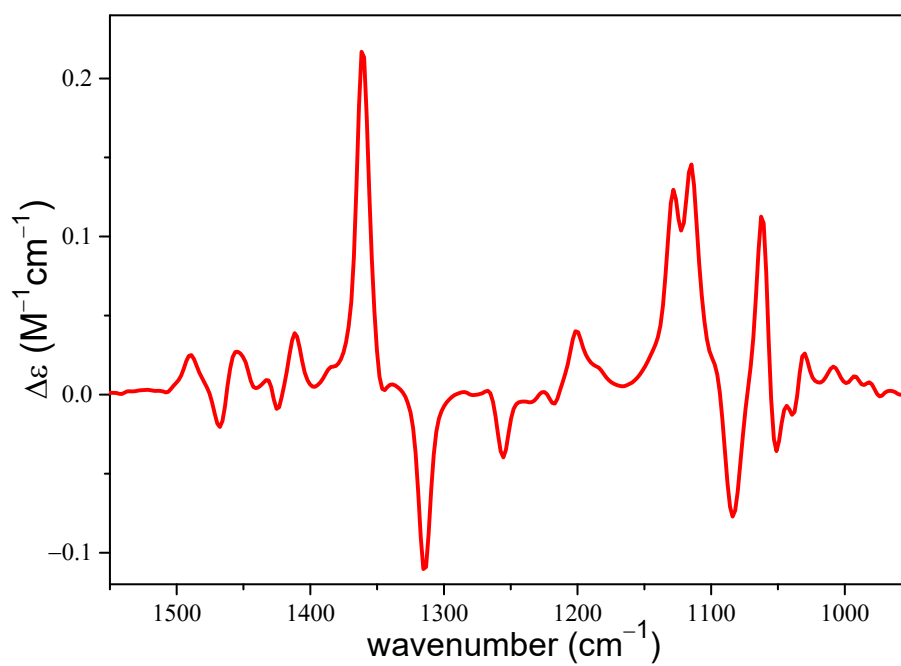
**Figure S201.** Experimental ECD spectrum of (a*R*,3*S*,3'*S*)-**28** in MeCN.



**Figure S202.** Experimental VCD spectrum of (a*R*,3*S*,3'*S*)-**28** in CDCl<sub>3</sub>.

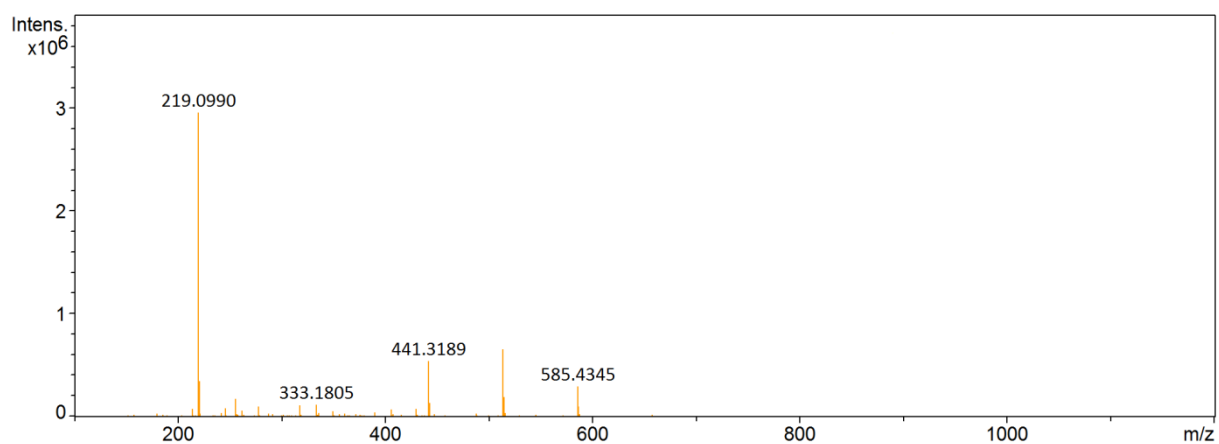


**Figure S203.** Experimental ECD spectrum of (aS,3S,3'S)-**28** in MeCN.

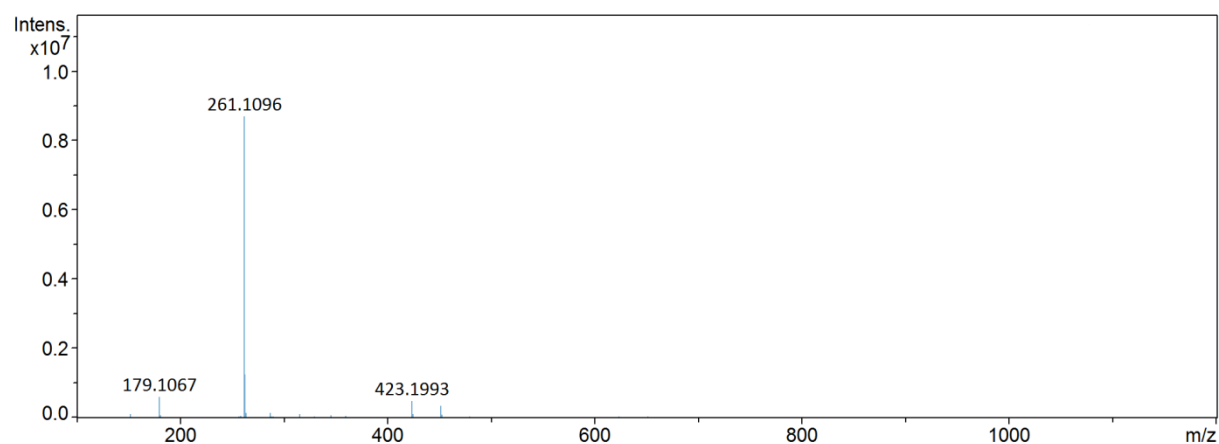


**Figure S204.** Experimental VCD spectrum of (aS,3S,3'S)-**28** in CDCl<sub>3</sub>.

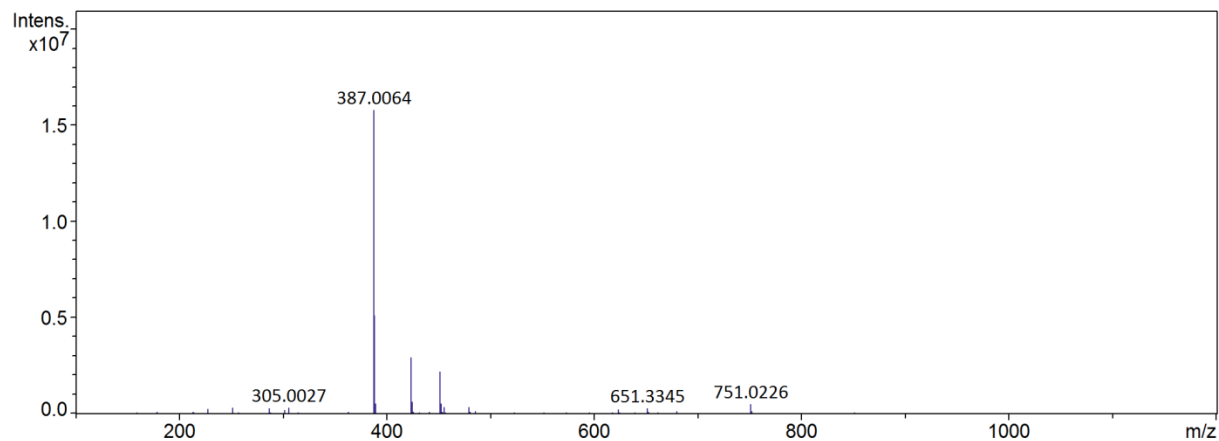
### 3.3. MS spectra



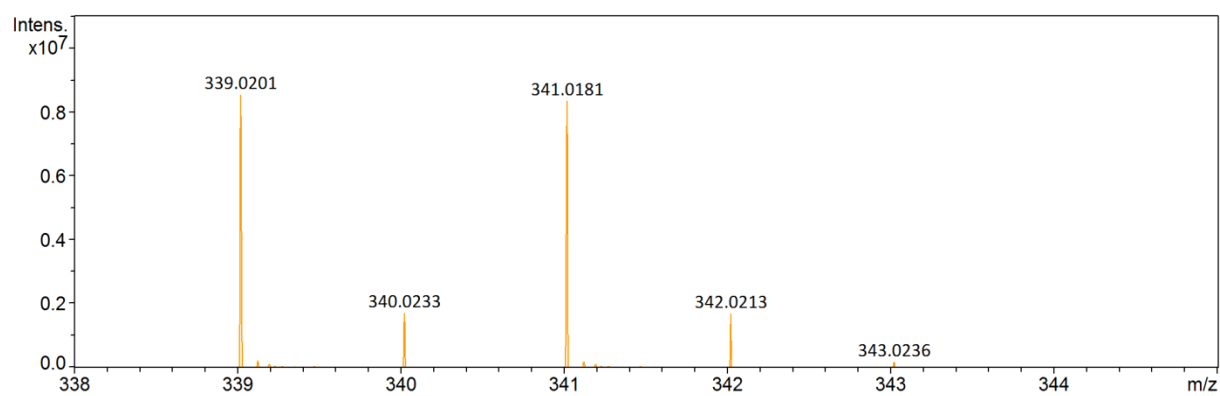
**Figure S205.** Experimental ESI-HRMS spectrum of (S)-11.



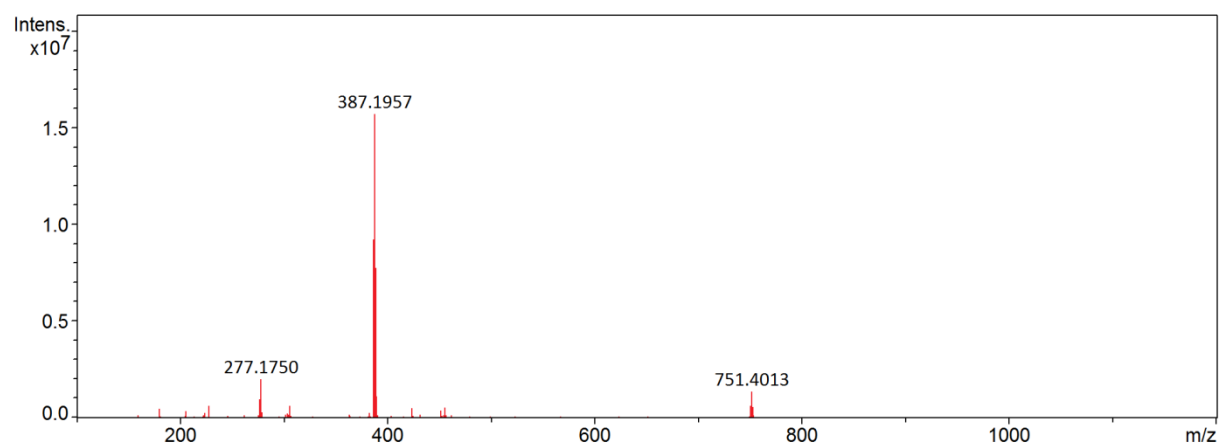
**Figure S206.** Experimental ESI-HRMS spectrum of (S)-12.



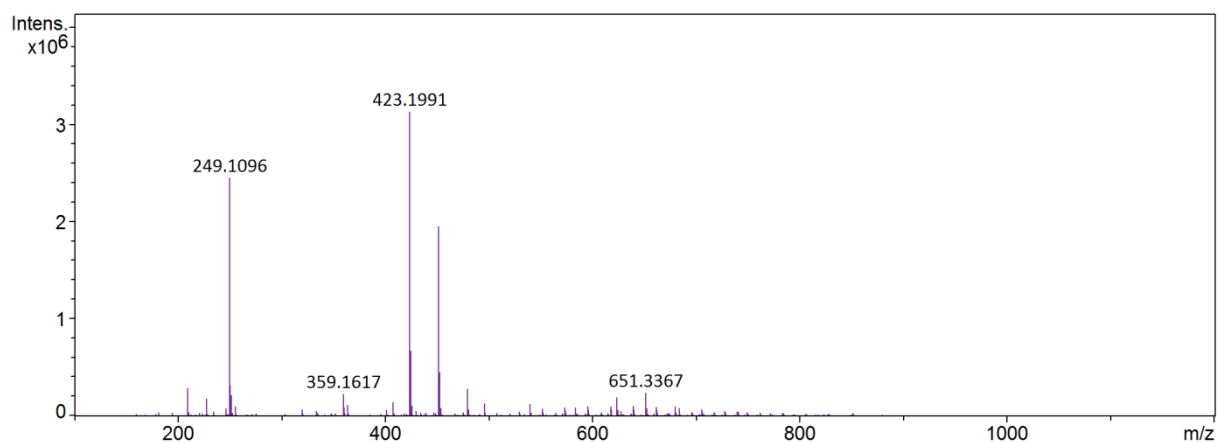
**Figure S207.** Experimental ESI-HRMS spectrum of (S)-13.



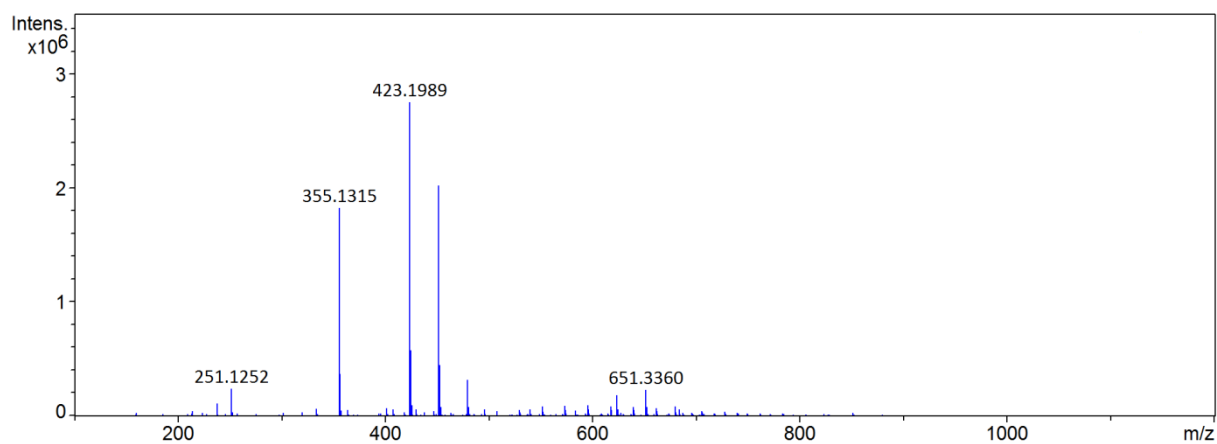
**Figure S208.** Experimental ESI-HRMS spectrum of (S)-14.



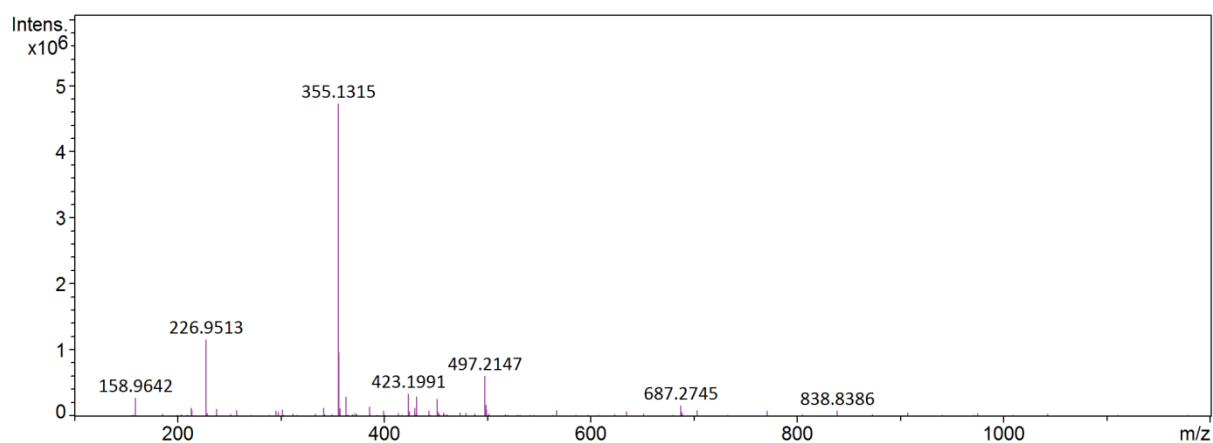
**Figure S209.** Experimental ESI-HRMS spectrum of (S)-8.



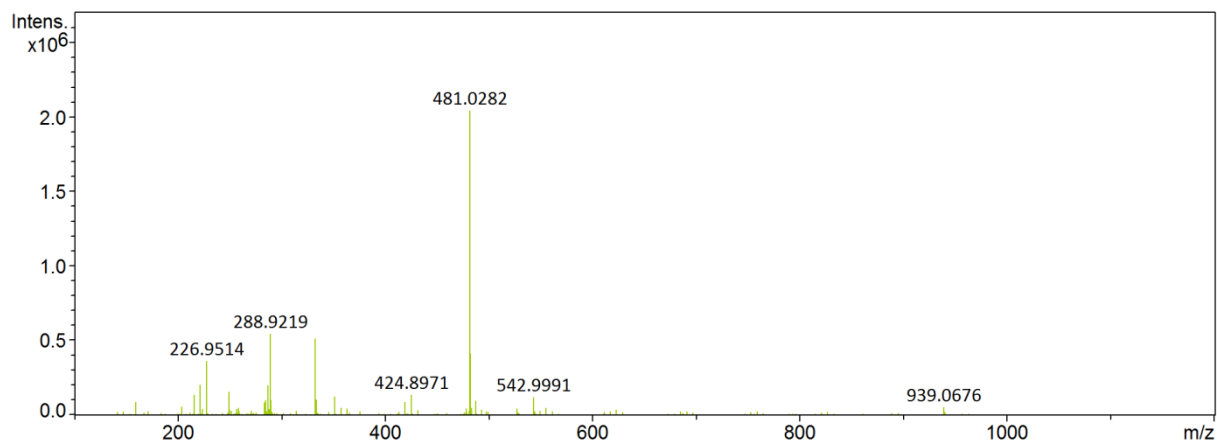
**Figure S210.** Experimental ESI-HRMS spectrum of (S)-16.



**Figure S211.** Experimental ESI-HRMS spectrum of *cis*-(1*R*,3*S*)-17.

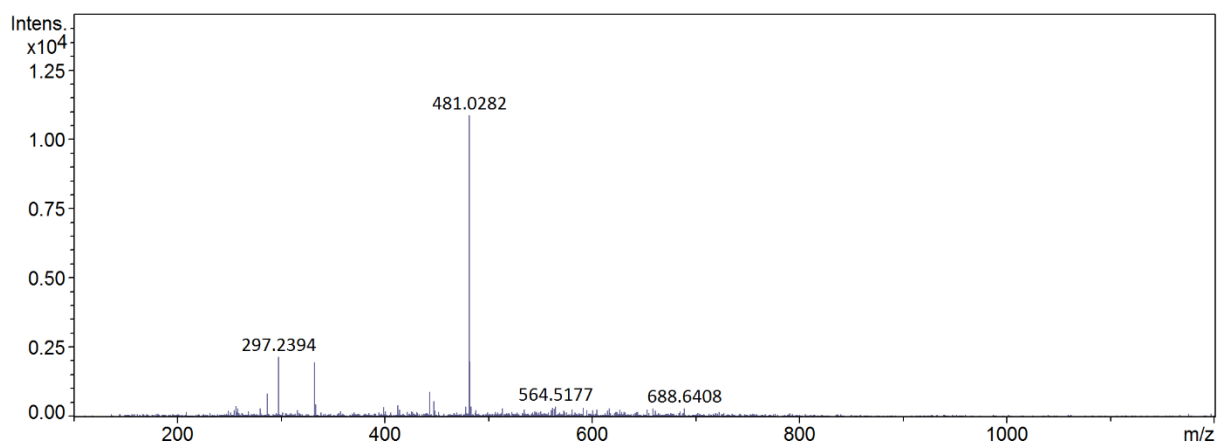


**Figure S212.** Experimental ESI-HRMS spectrum of *trans*-(1*S*,3*S*)-17.

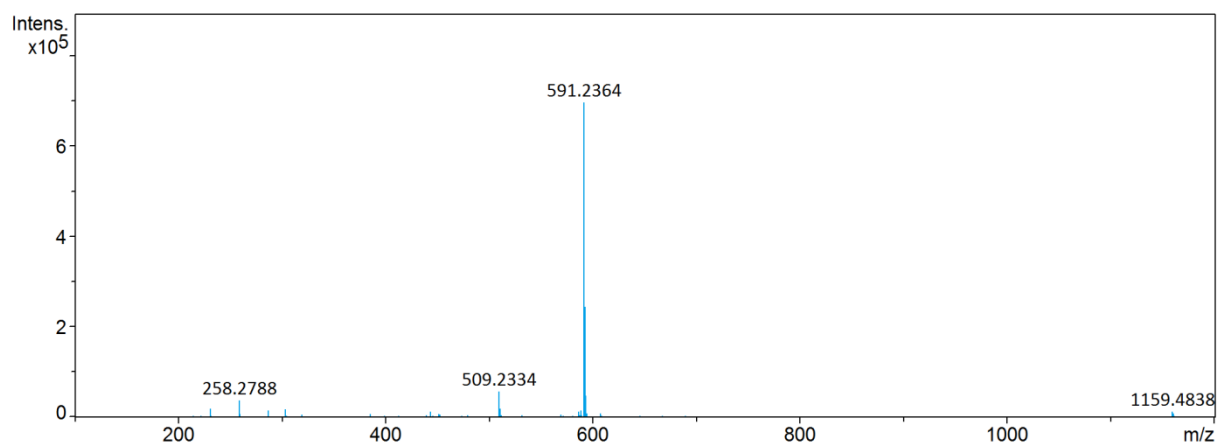


**Figure S213.** Experimental ESI-HRMS spectrum of *cis*-(1*R*,3*S*)-18.

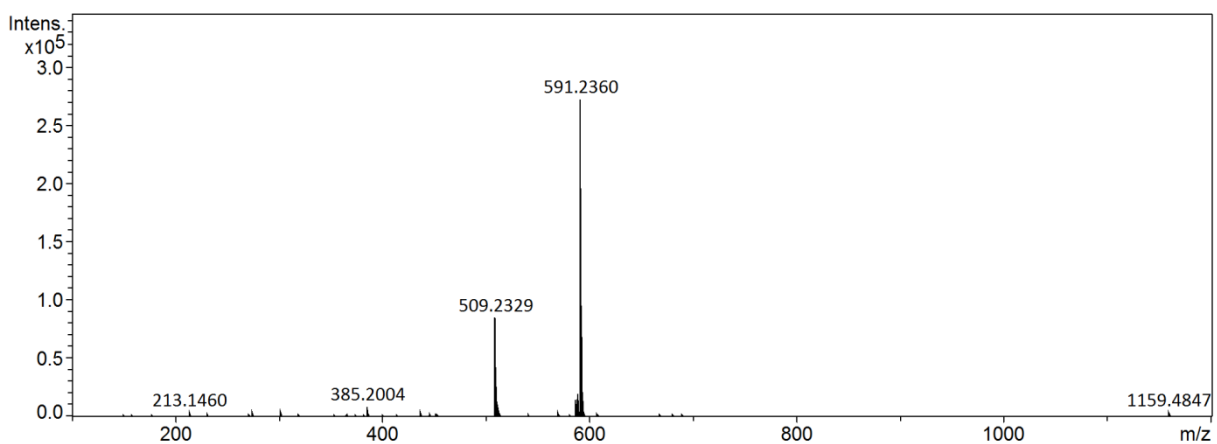




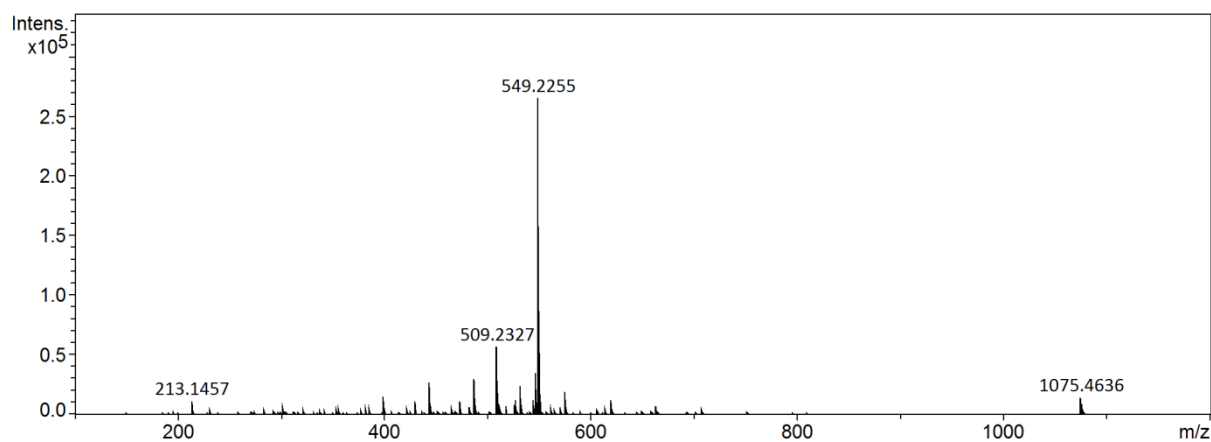
**Figure S214.** Experimental ESI-HRMS spectrum of *trans*-(1*S*,3*S*)-**18**.



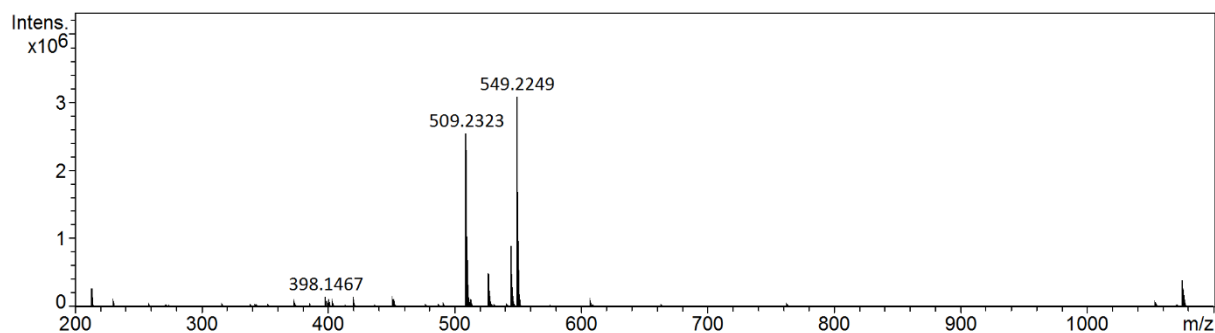
**Figure S215.** Experimental ESI-HRMS spectrum of the mixture of (*aR*,1*S*,3*S*,2'*S*)-**19** and (*aS*,1*S*,3*S*,2'*S*)-**19**.



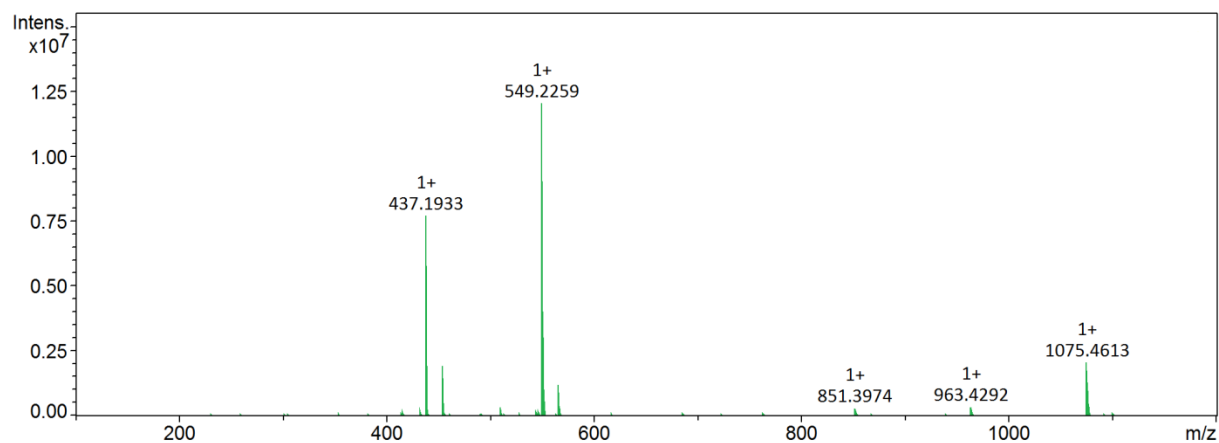
**Figure S216.** Experimental ESI-HRMS spectrum of the mixture of (*aR*,1*R*,3*S*,2'*S*)-**19** and (*aS*,1*R*,3*S*,2'*S*)-**19**.



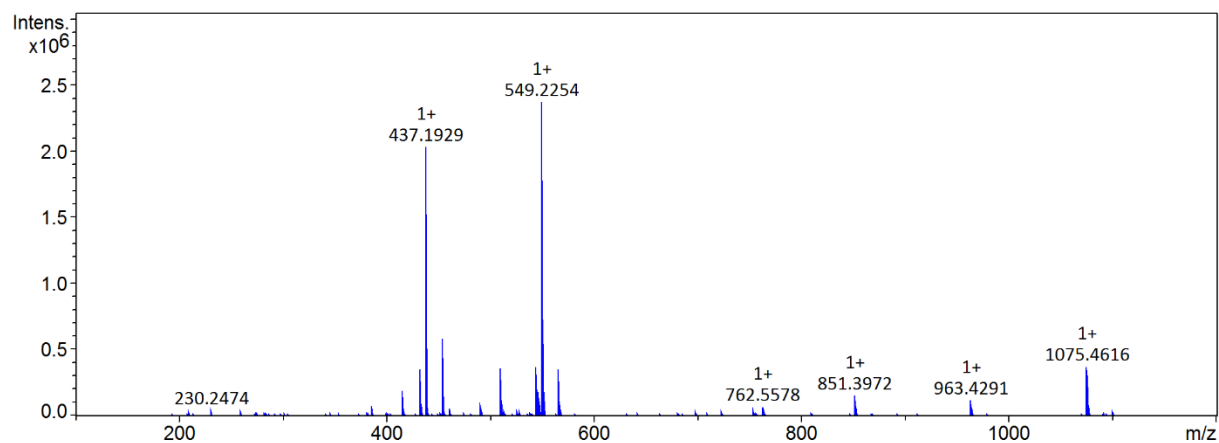
**Figure S217.** Experimental ESI-HRMS spectrum of (aS,1S,3S,2'S)-20.



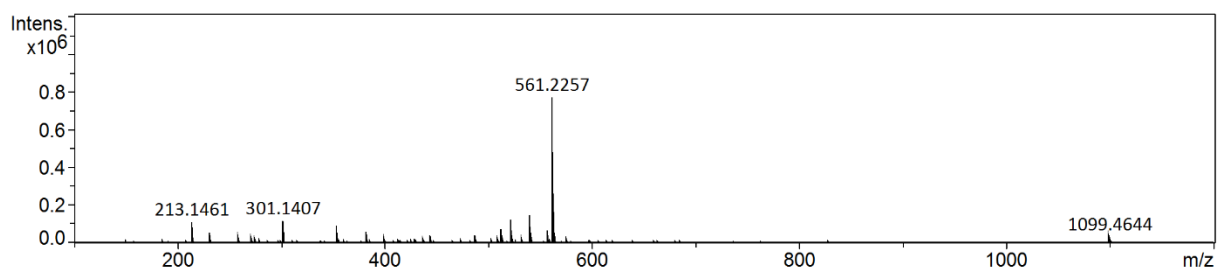
**Figure S218.** Experimental ESI-HRMS spectrum of (aR,1S,3S,2'S)-20.



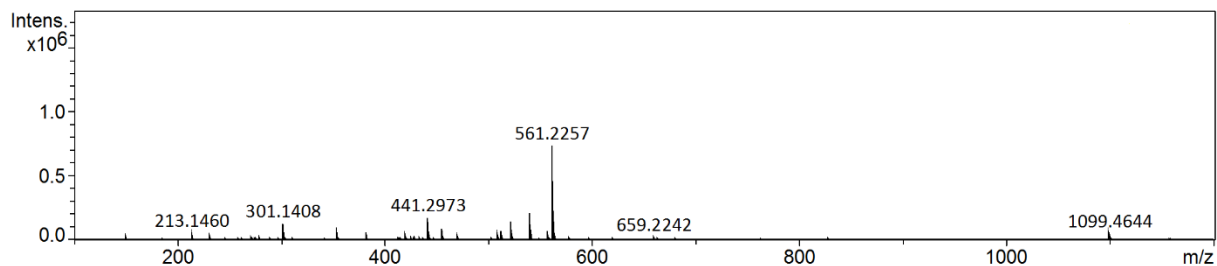
**Figure S219.** Experimental ESI-HRMS spectrum of (aS,1R,3S,2'S)-20.



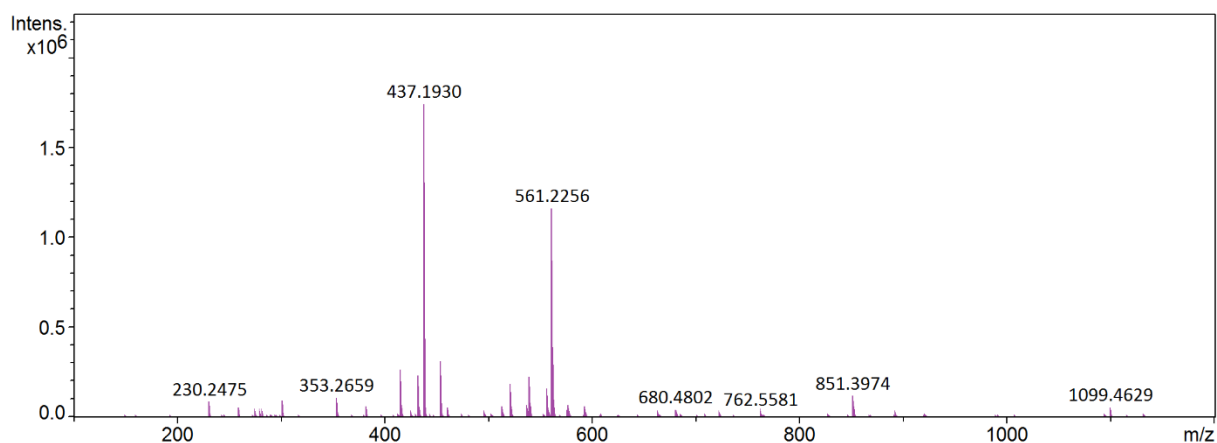
**Figure S220.** Experimental ESI-HRMS spectrum of (aR,1R,3S,2'S)-20.



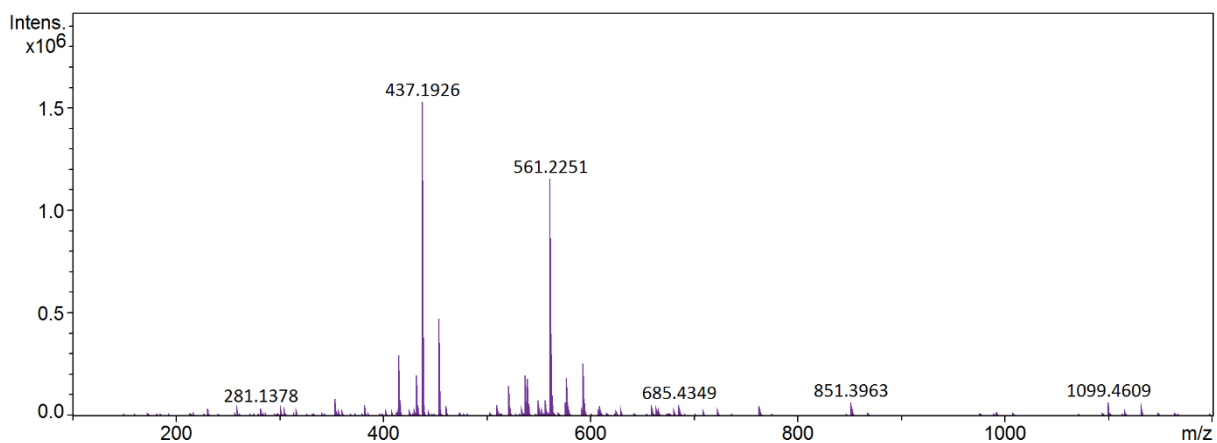
**Figure S221.** Experimental ESI-HRMS spectrum of (aS,1S,3S,3'S)-21.



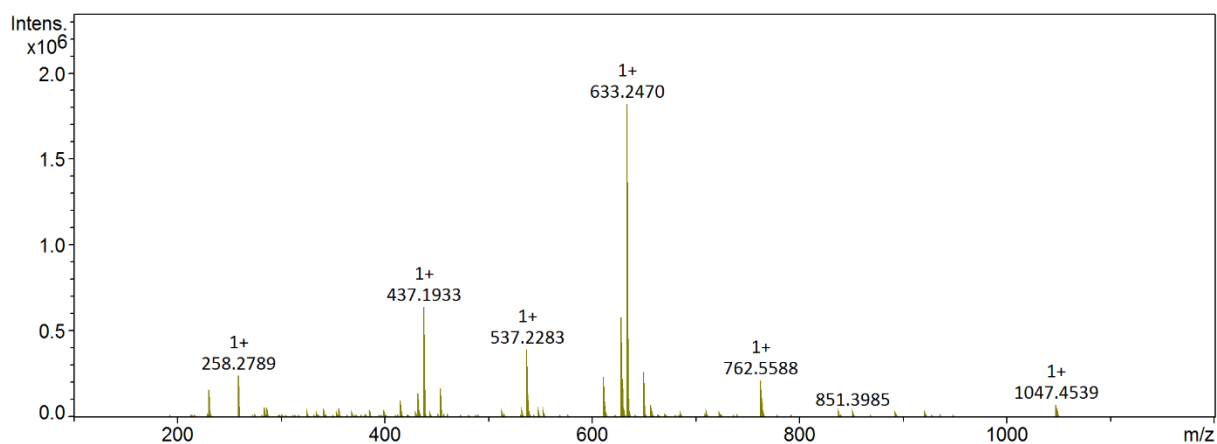
**Figure S222.** Experimental ESI-HRMS spectrum of (aR,1S,3S,3'S)-21.



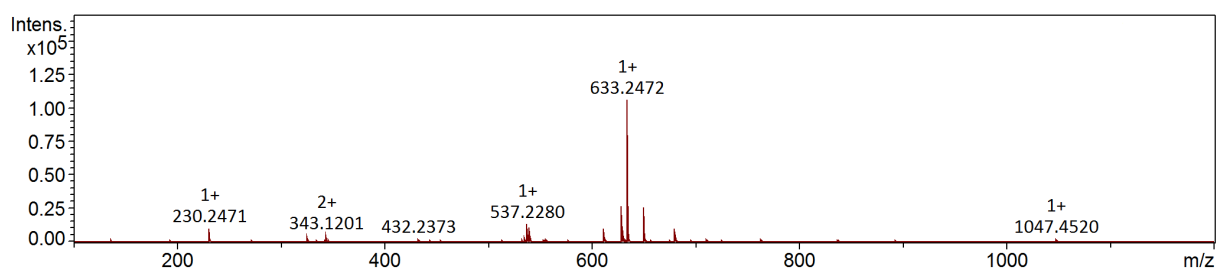
**Figure S223.** Experimental ESI-HRMS spectrum of (aS,1R,3S,3'S)-21.



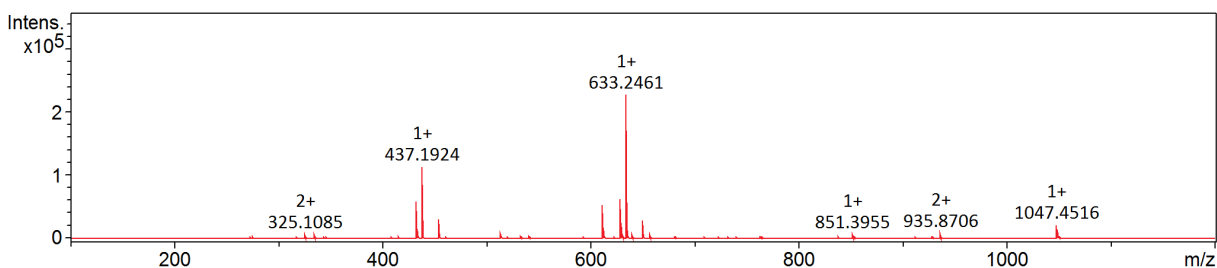
**Figure S224.** Experimental ESI-HRMS spectrum of (aR,1R,3S,3'S)-21.



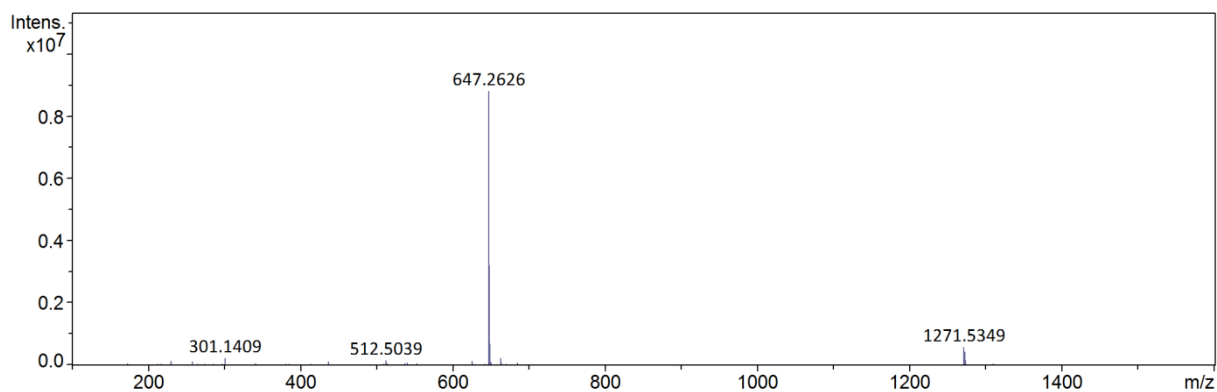
**Figure S225.** Experimental ESI-HRMS spectrum of (aS,1R,3S,1'S,3'S)-22.



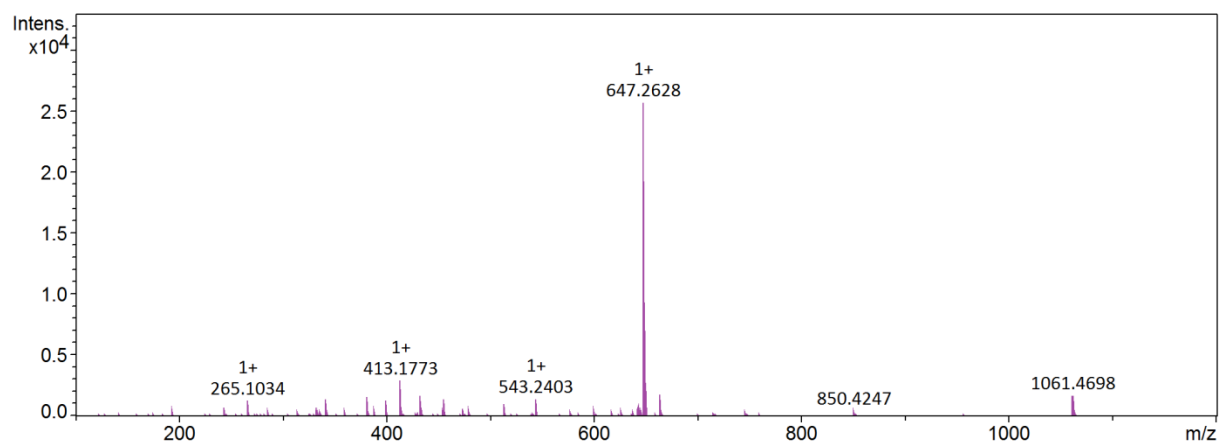
**Figure S226.** Experimental ESI-HRMS spectrum of (aS,1S,3S,1'S,3'S)-22.



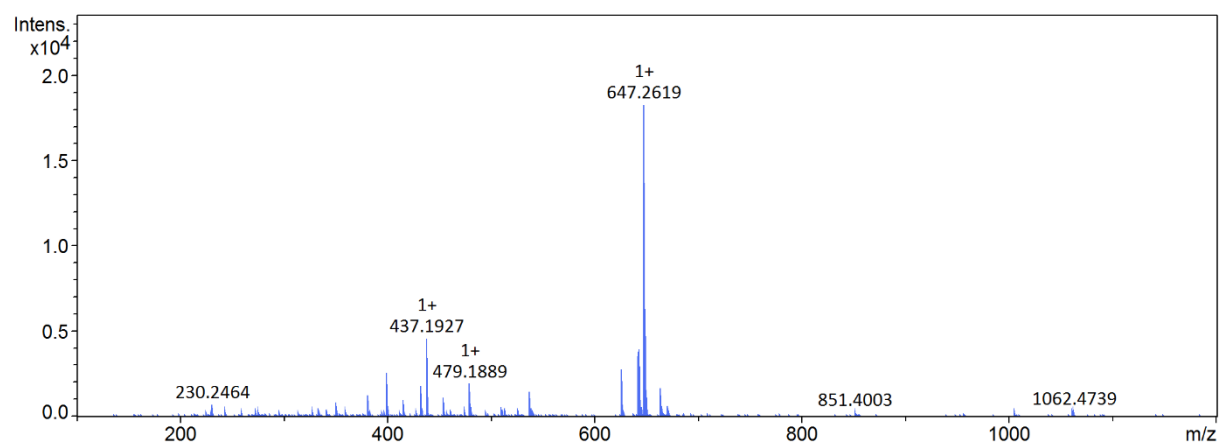
**Figure S227.** Experimental ESI-HRMS spectrum of (aR,1S,3S,1'S,3'S)-22.



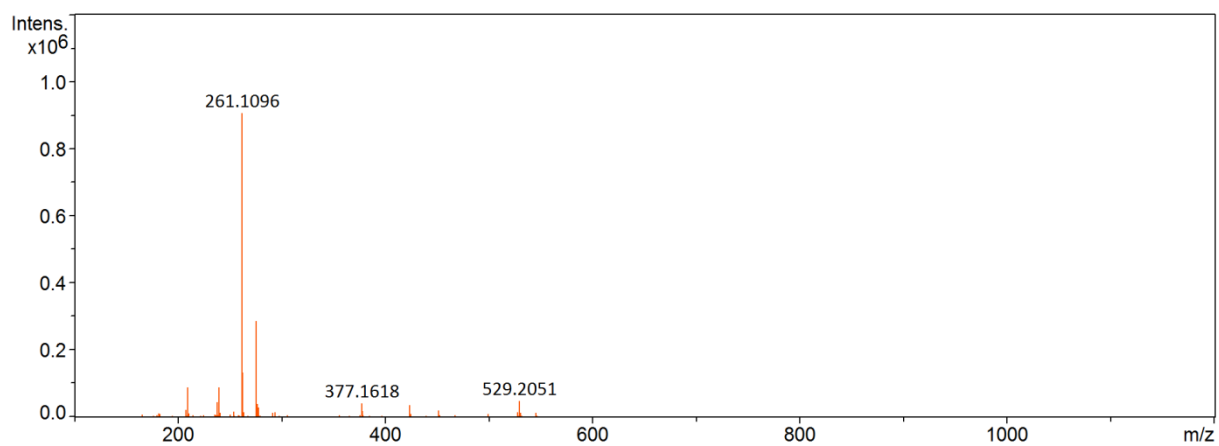
**Figure S228.** Experimental ESI-HRMS spectrum of (aS,1S,3S,1'R,3'S)-23.



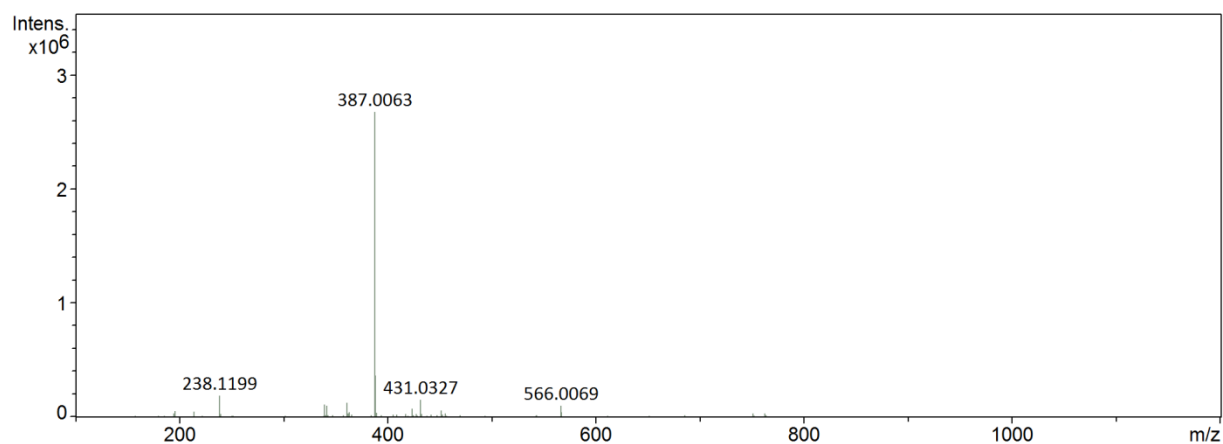
**Figure S229.** Experimental ESI-HRMS spectrum of (aR,1S,3S,1'R,3'S)-23.



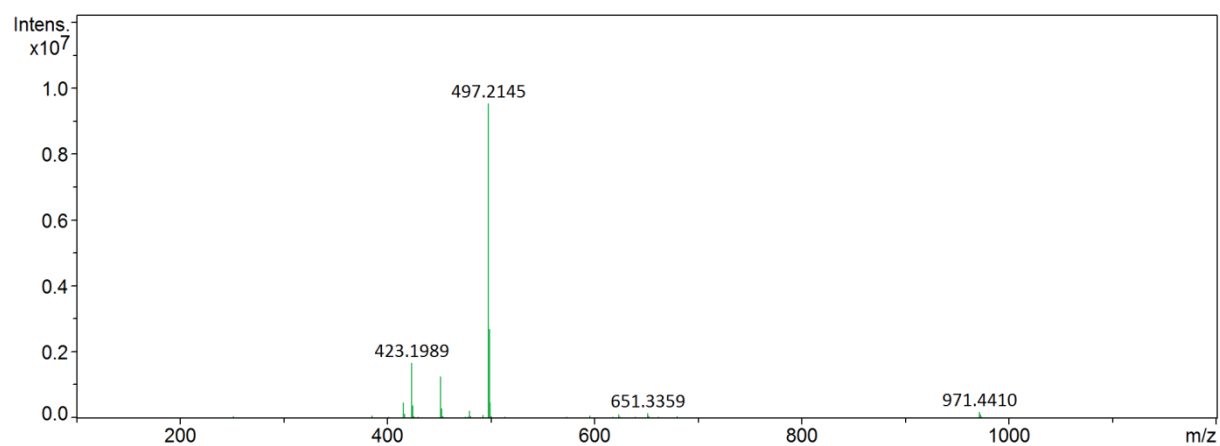
**Figure S230.** Experimental ESI-HRMS spectrum of (aS,1R,3S,1'R,3'S)-23.



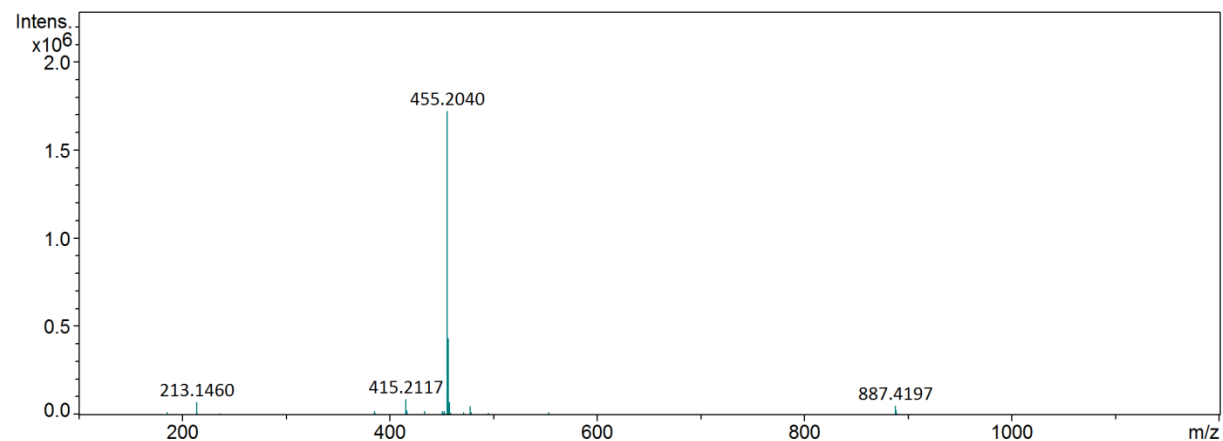
**Figure S231.** Experimental ESI-HRMS spectrum of (S)-24.



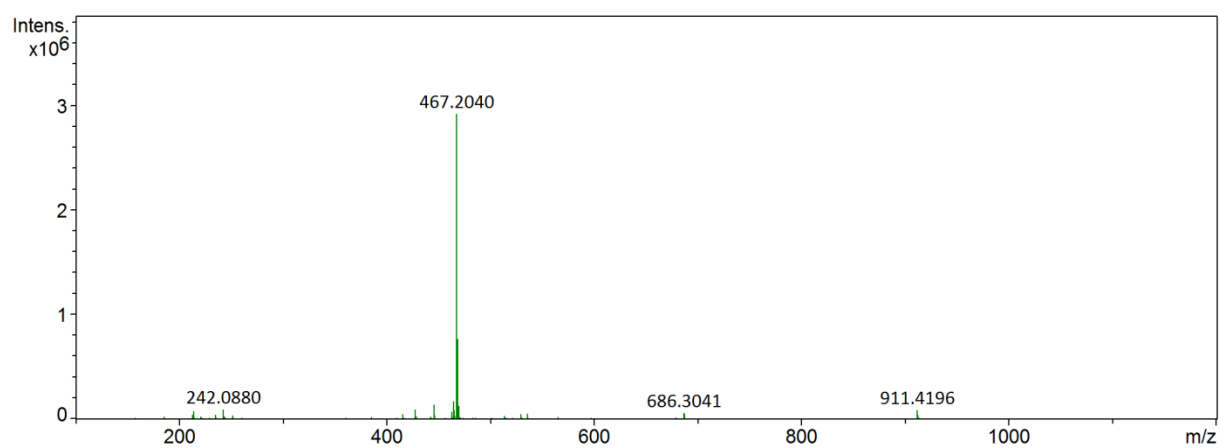
**Figure S232.** Experimental ESI-HRMS spectrum of (S)-25.



**Figure S233.** Experimental ESI-HRMS spectrum of the mixture of (aR,3S,2'S)-26 and (aS,3S,2'S)-26.

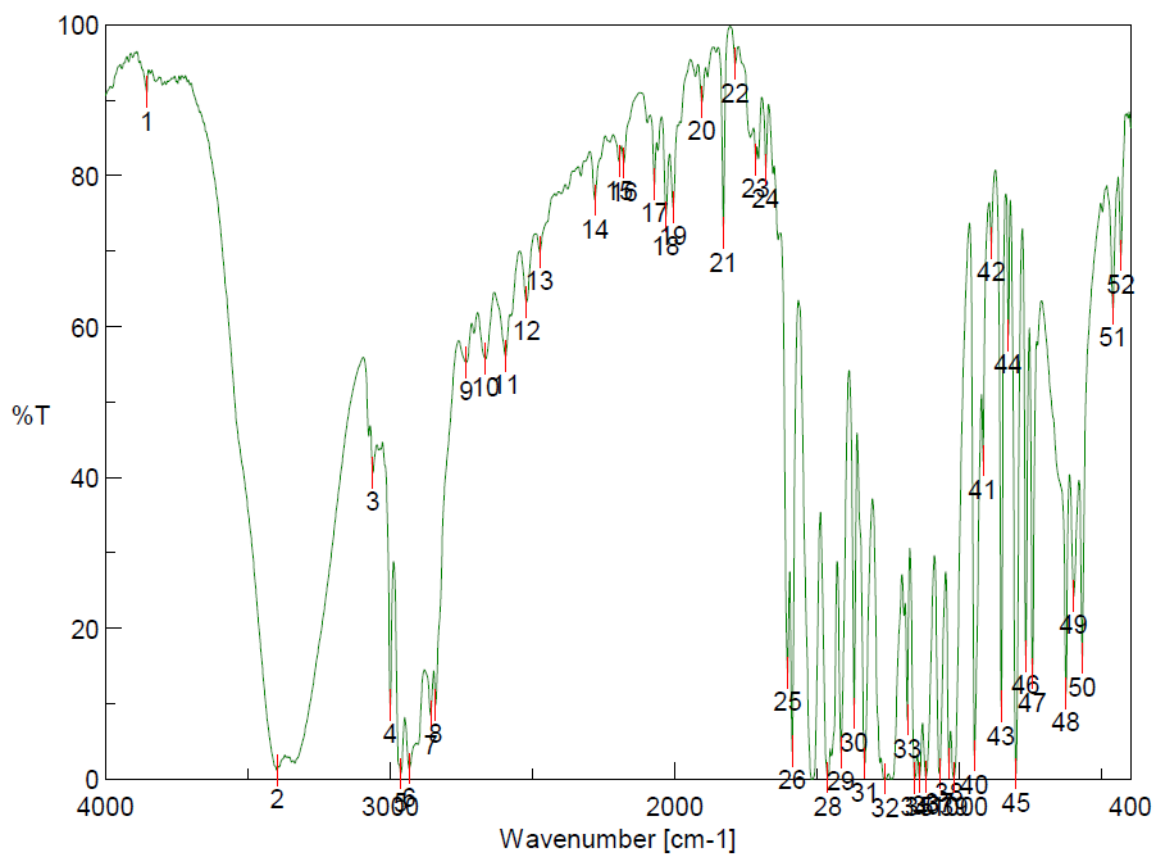


**Figure S234.** Experimental ESI-HRMS spectrum of the mixture of (aR,3S,2'S)-27 and (aS,3S,2'S)-27.

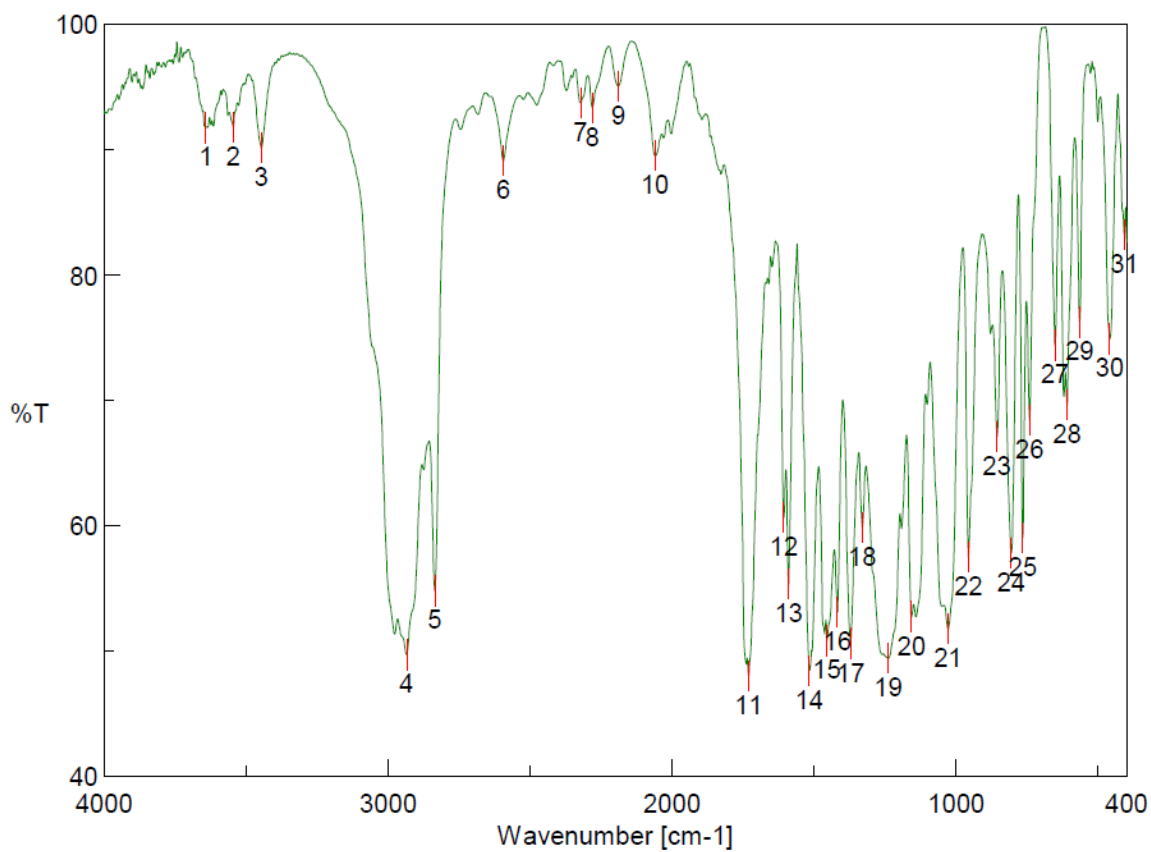


**Figure S235.** Experimental ESI-HRMS spectrum of the mixture of (a*R*,3*S*,3'*S*)-**28** and (a*S*,3*S*,3'*S*)-**28**.

### 3.4. IR spectra

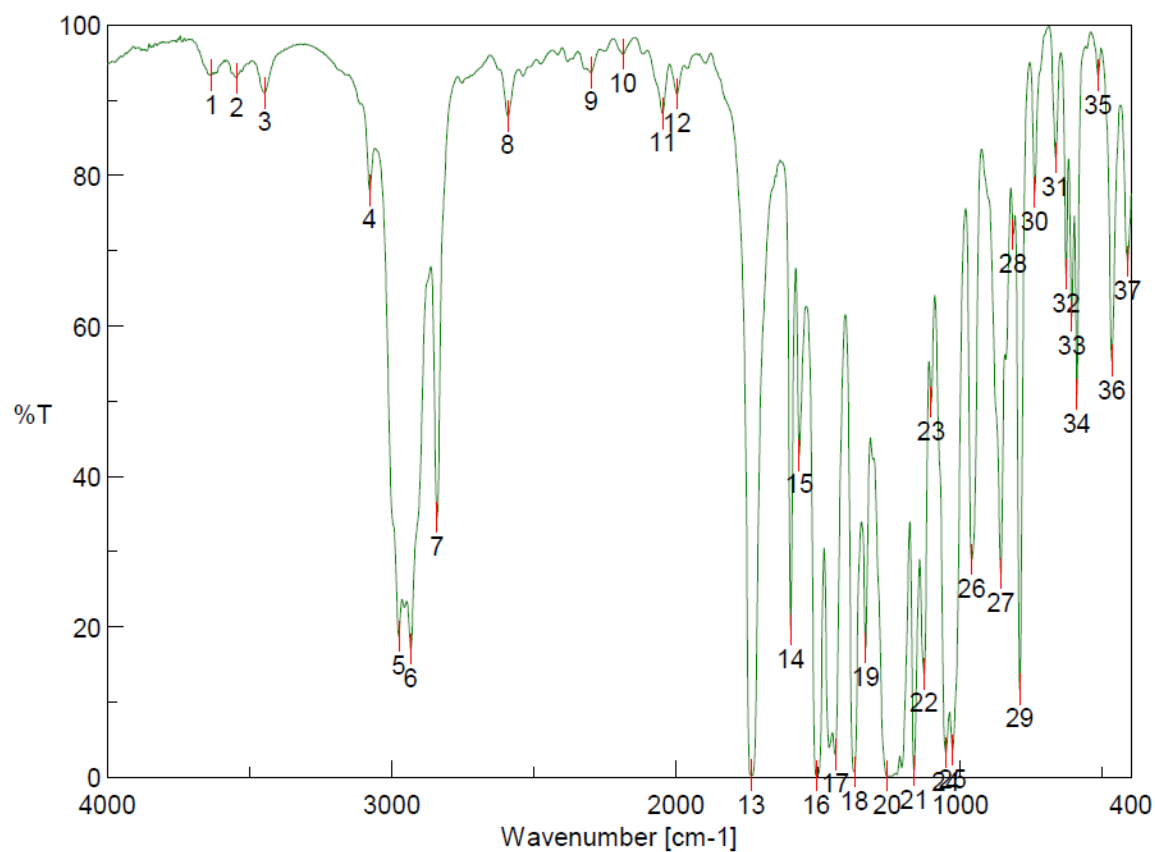


**Figure S236.** Experimental IR spectrum of (S)-11 recorded as KBr disc.

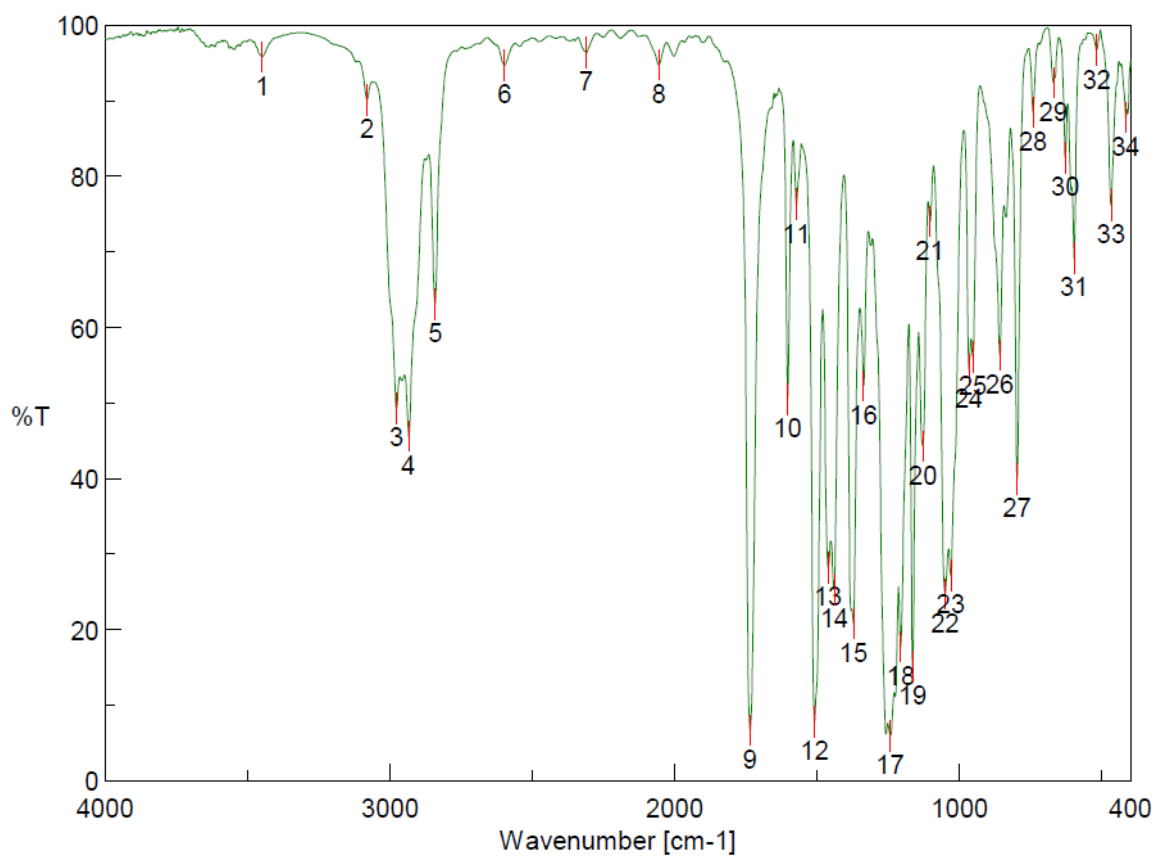


**Figure S237.** Experimental IR spectrum of (S)-12 recorded as KBr disc.

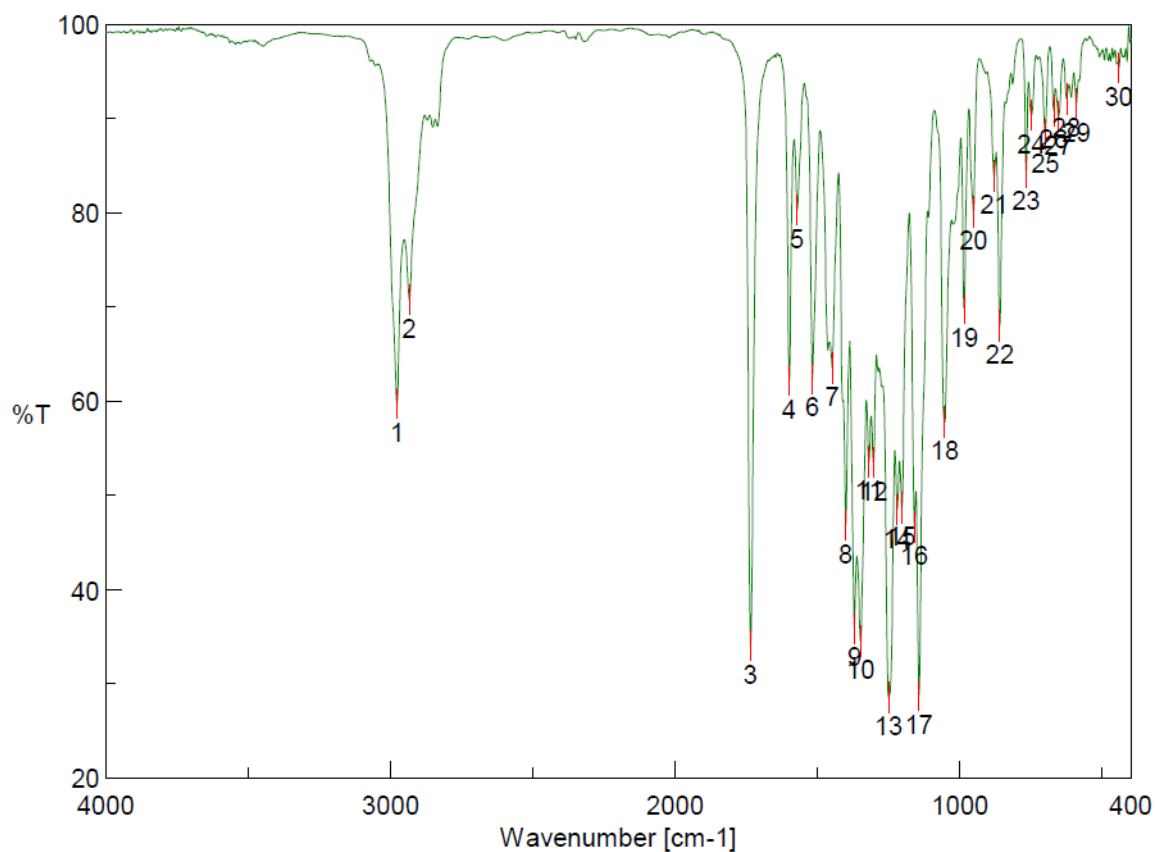




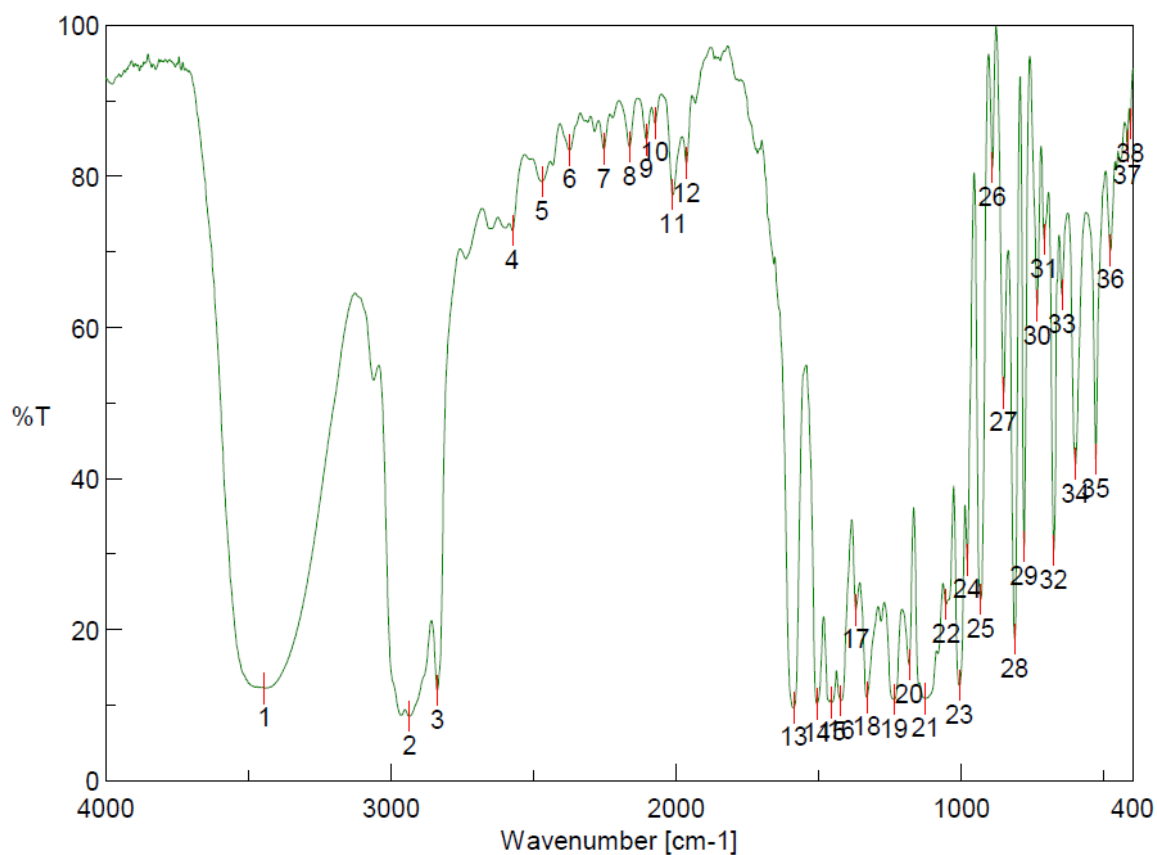
**Figure S238.** Experimental IR spectrum of (S)-13 recorded as KBr disc.



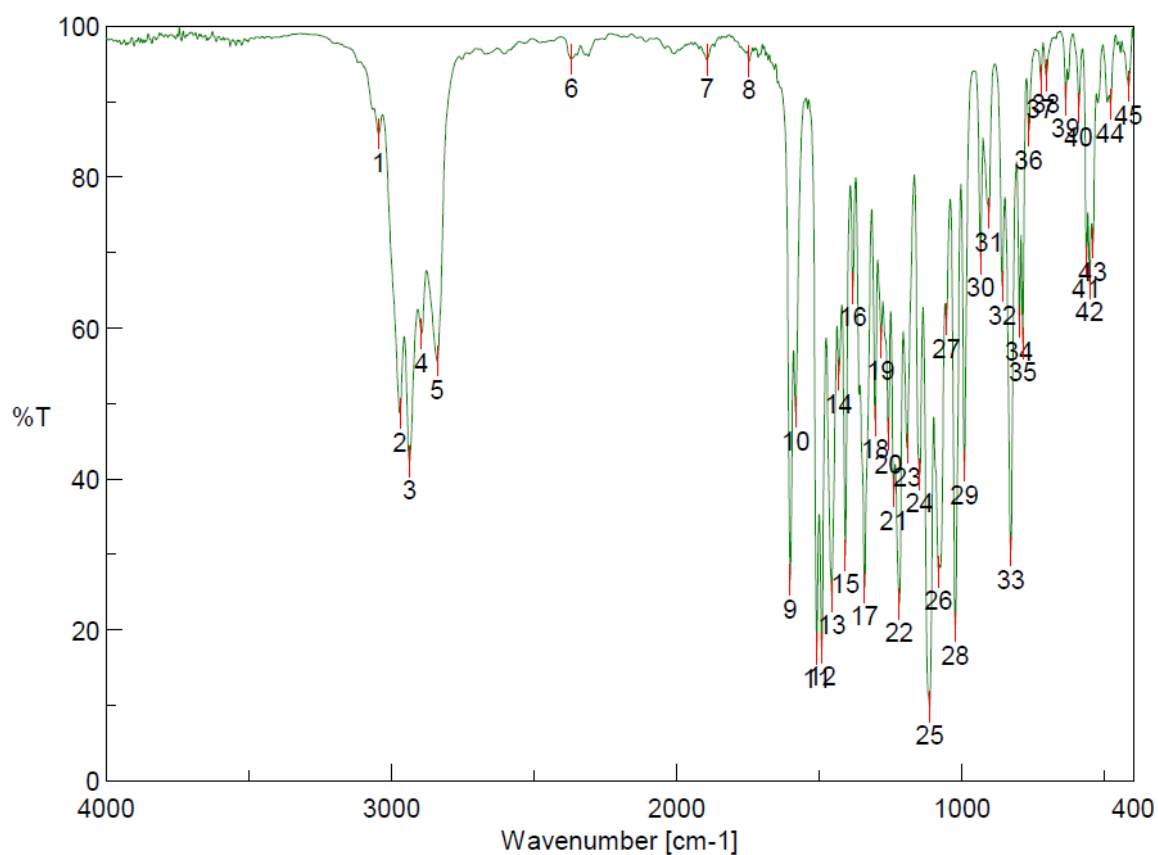
**Figure S239.** Experimental IR spectrum of (S)-14 recorded as KBr disc.



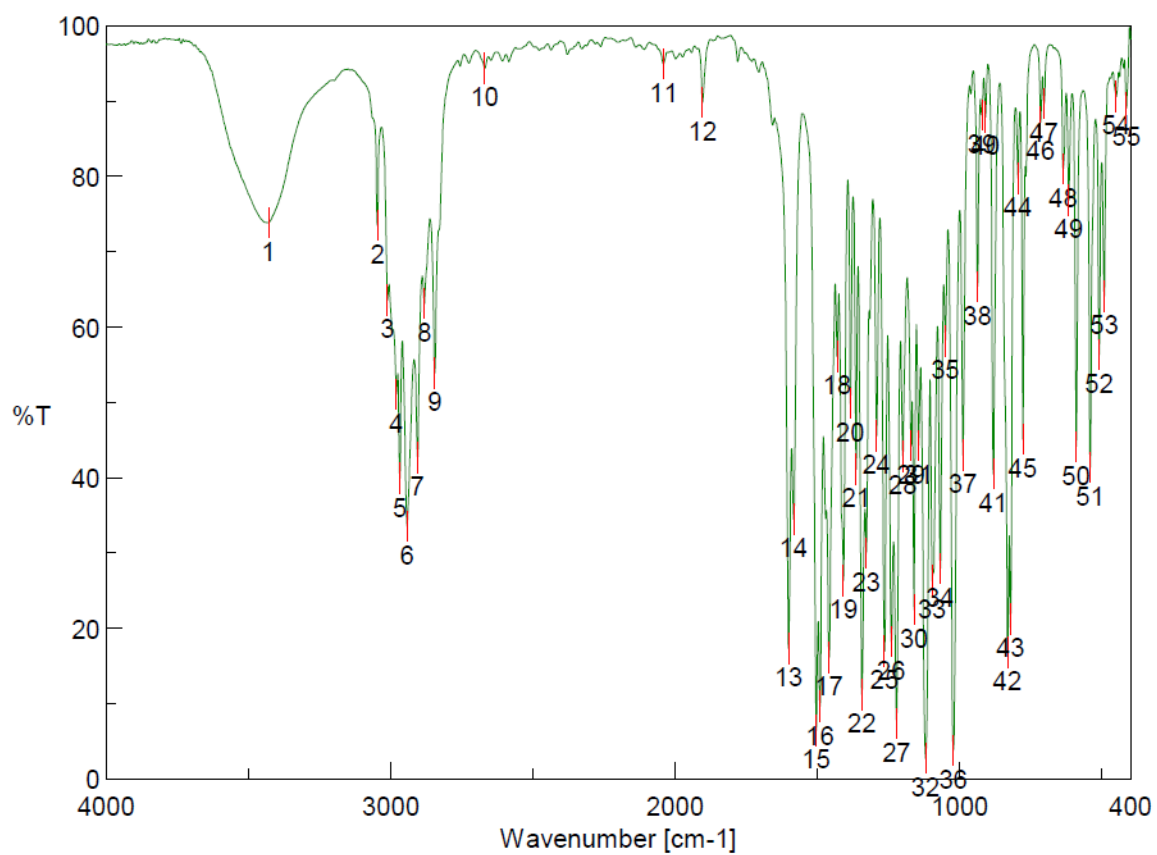
**Figure S240.** Experimental IR spectrum of (*S*)-**8** recorded as KBr disc.



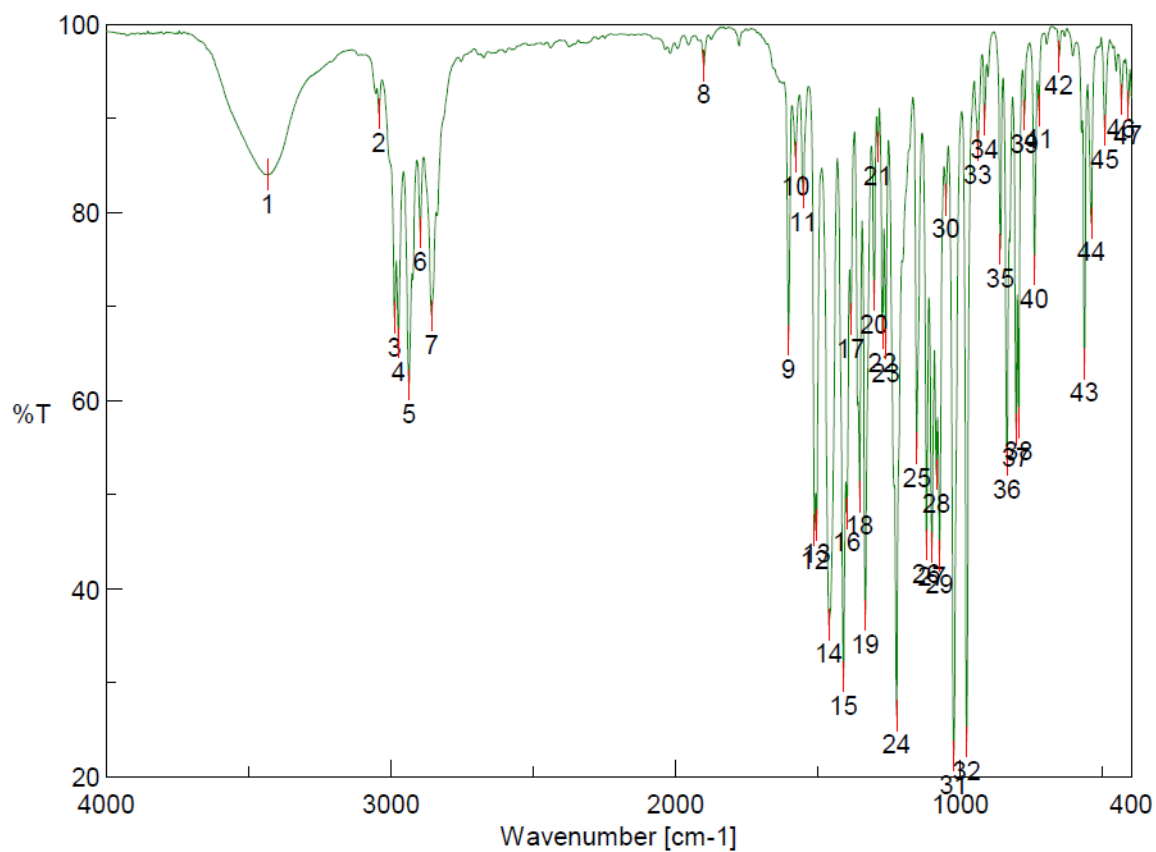
**Figure S241.** Experimental IR spectrum of (*S*)-**16** recorded as KBr disc.



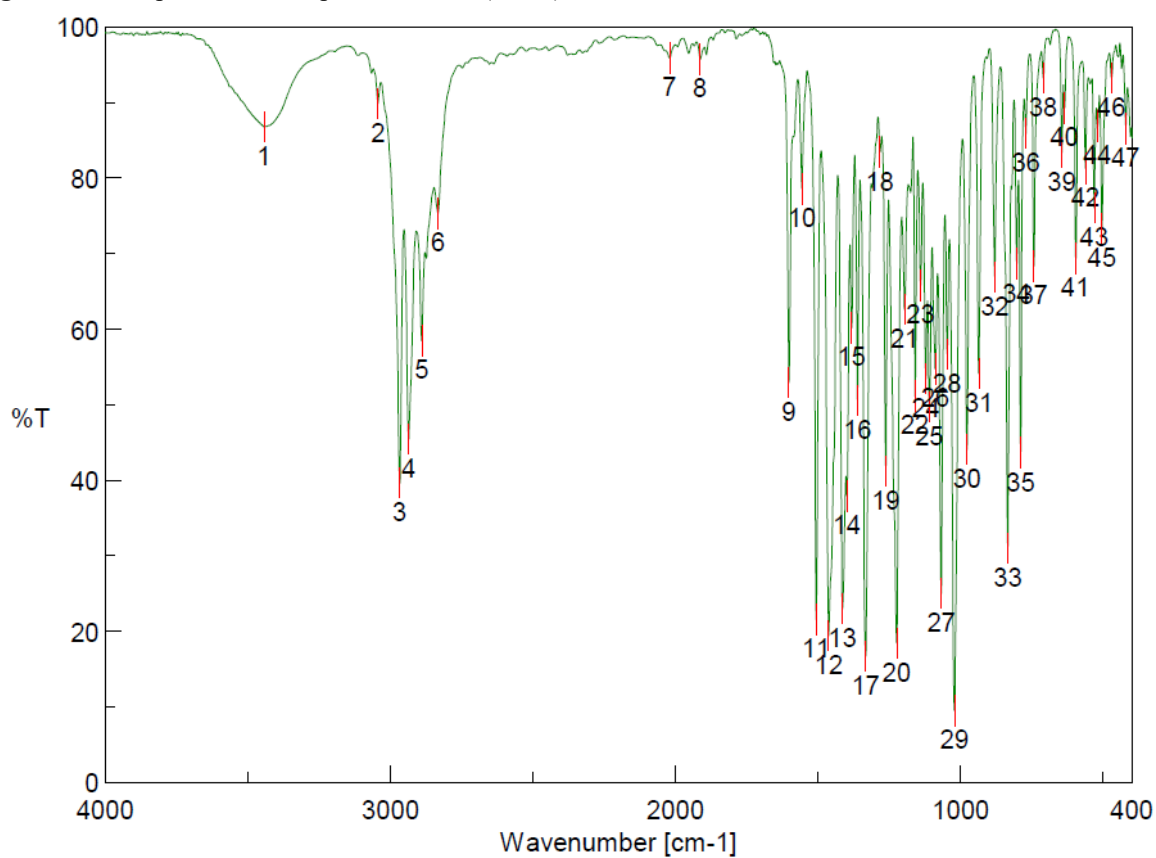
**Figure S242.** Experimental IR spectrum of *cis*-(1*R*,3*S*)-**17** recorded as KBr disc.



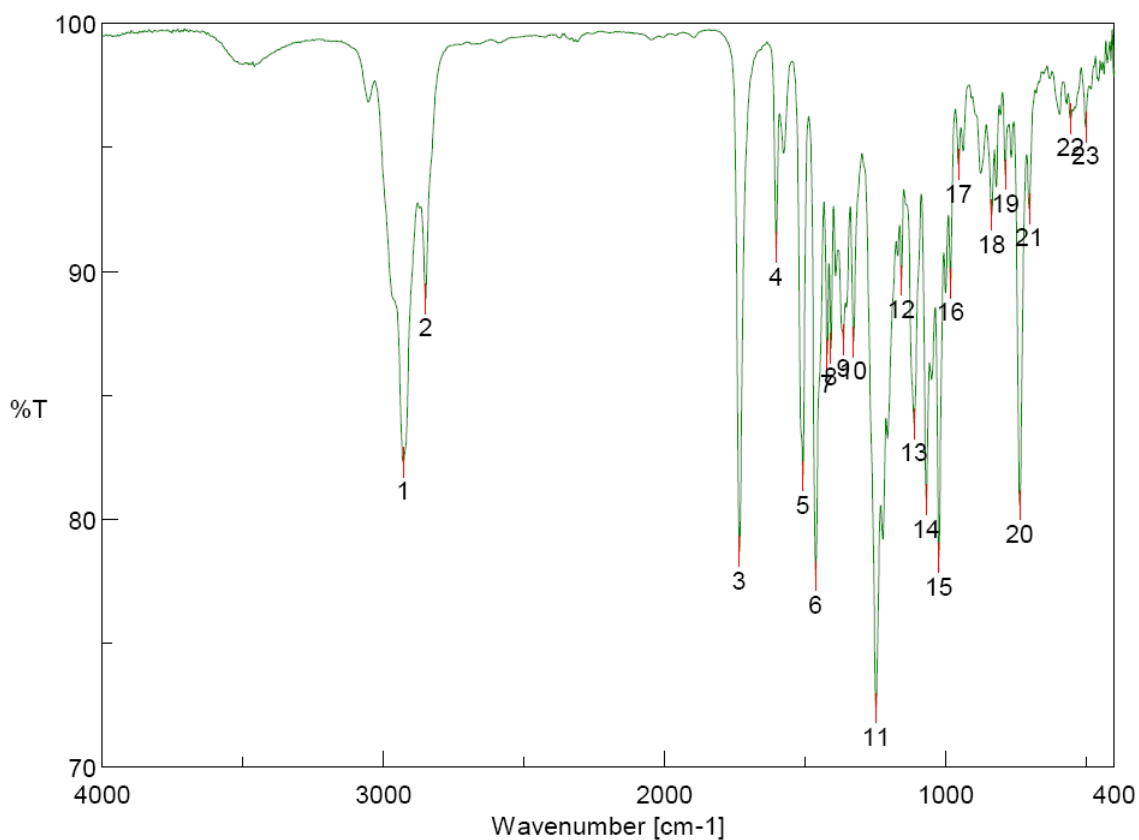
**Figure S243.** Experimental IR spectrum of *trans*-(1*S*,3*S*)-**17** recorded as KBr disc.



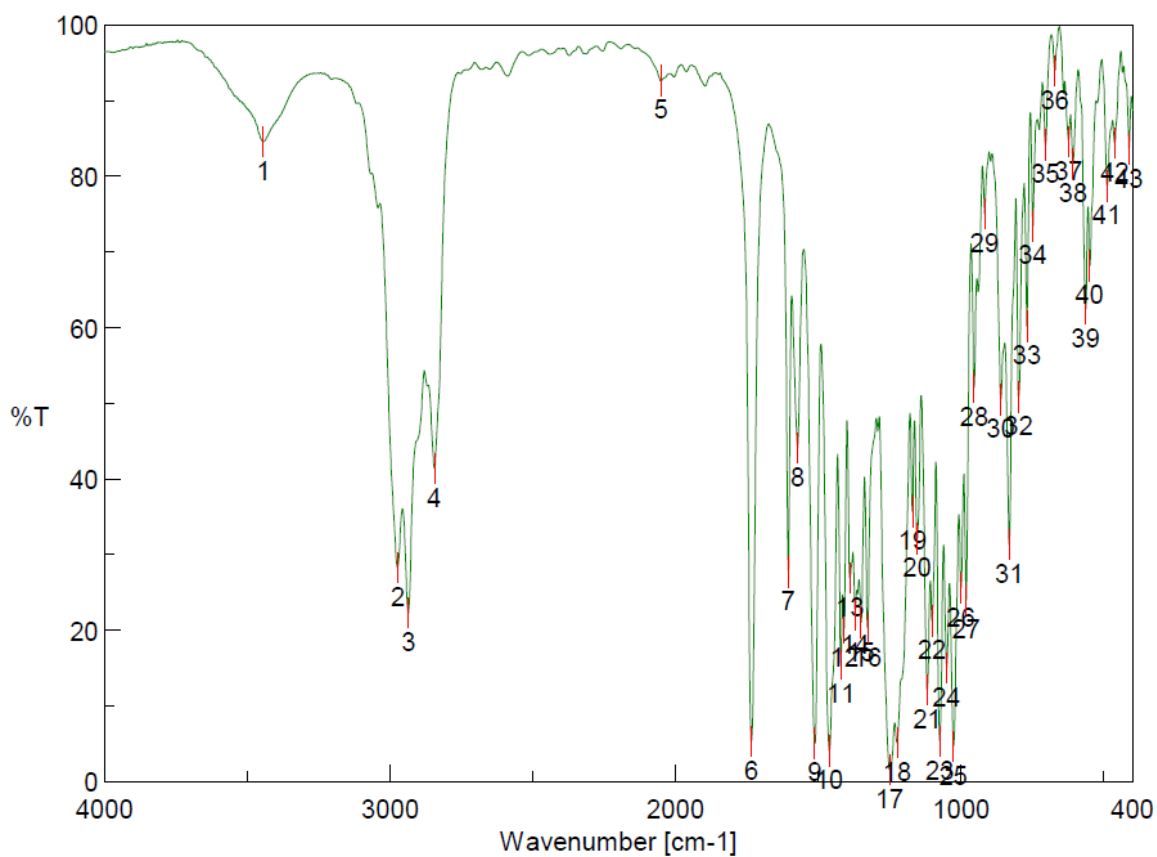
**Figure S244.** Experimental IR spectrum of *cis*-(1*R*,3*S*)-**18** recorded as KBr disc.



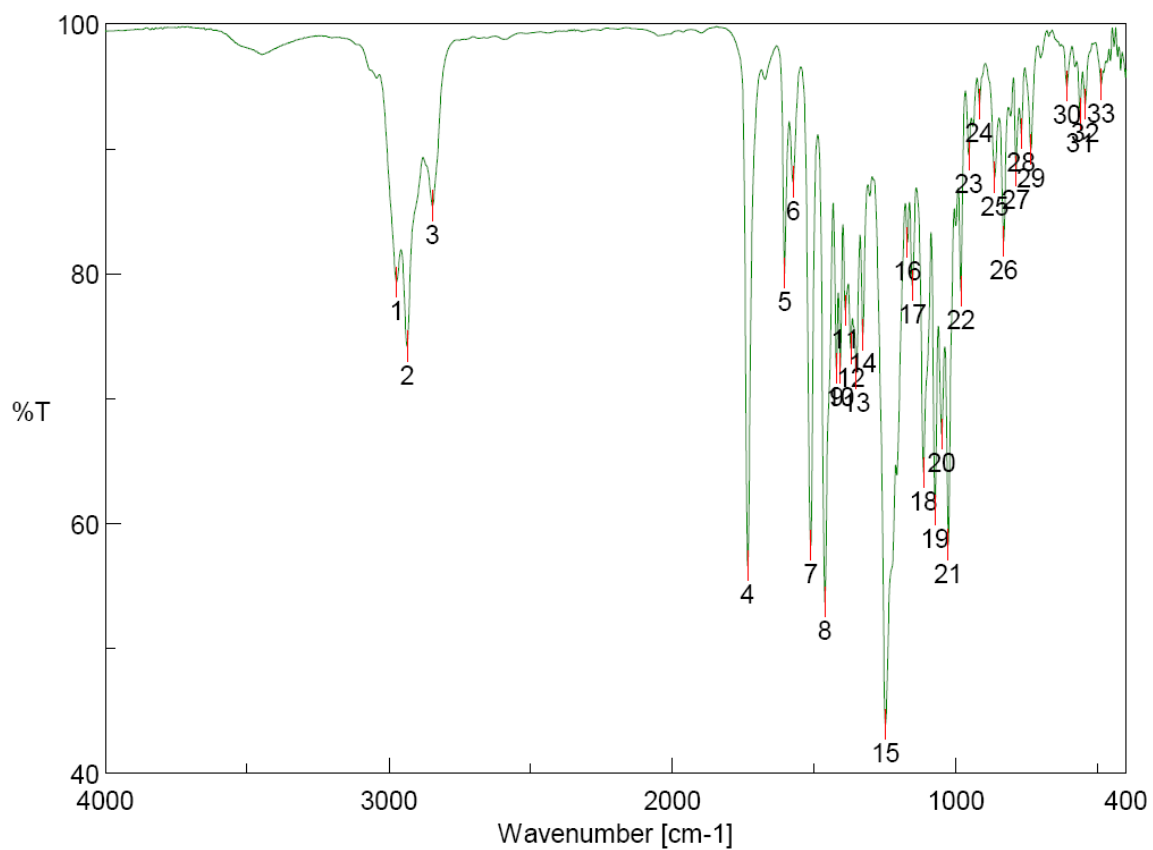
**Figure S245.** Experimental IR spectrum of *trans*-(1*S*,3*S*)-**18** recorded as KBr disc.



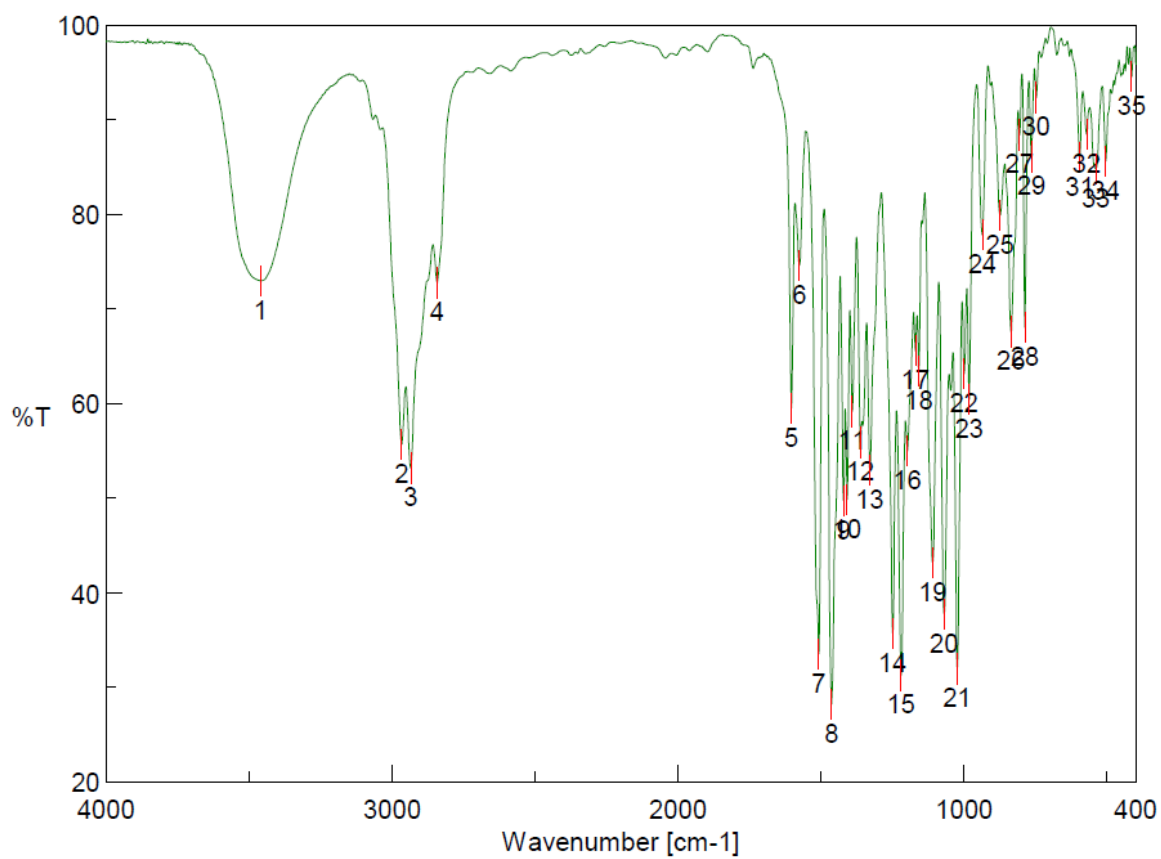
**Figure S246.** Experimental IR spectrum of the mixture of (aR,1S,3S,2'S)-**19** and (aS,1S,3S,2'S)-**19** recorded as KBr disc.



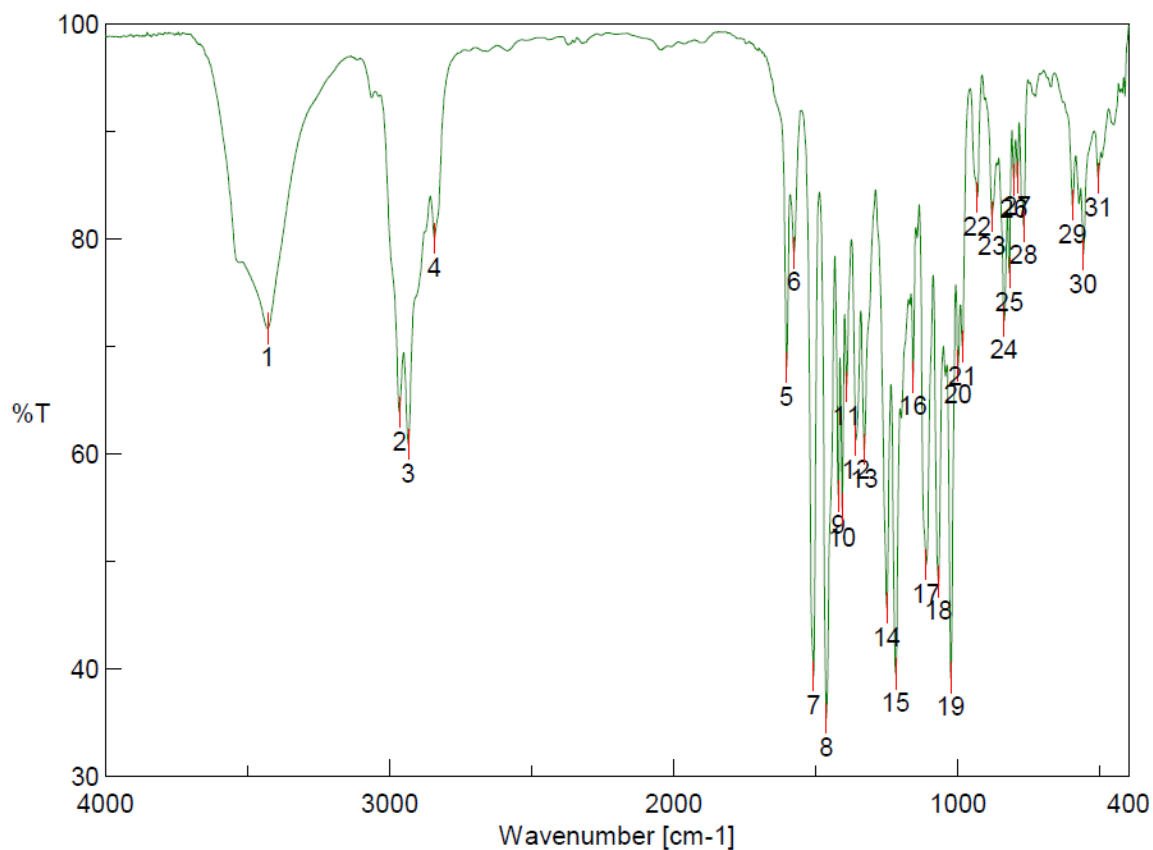
**Figure S247.** Experimental IR spectrum of (aS,1R,3S,2'S)-**19** recorded as KBr disc.



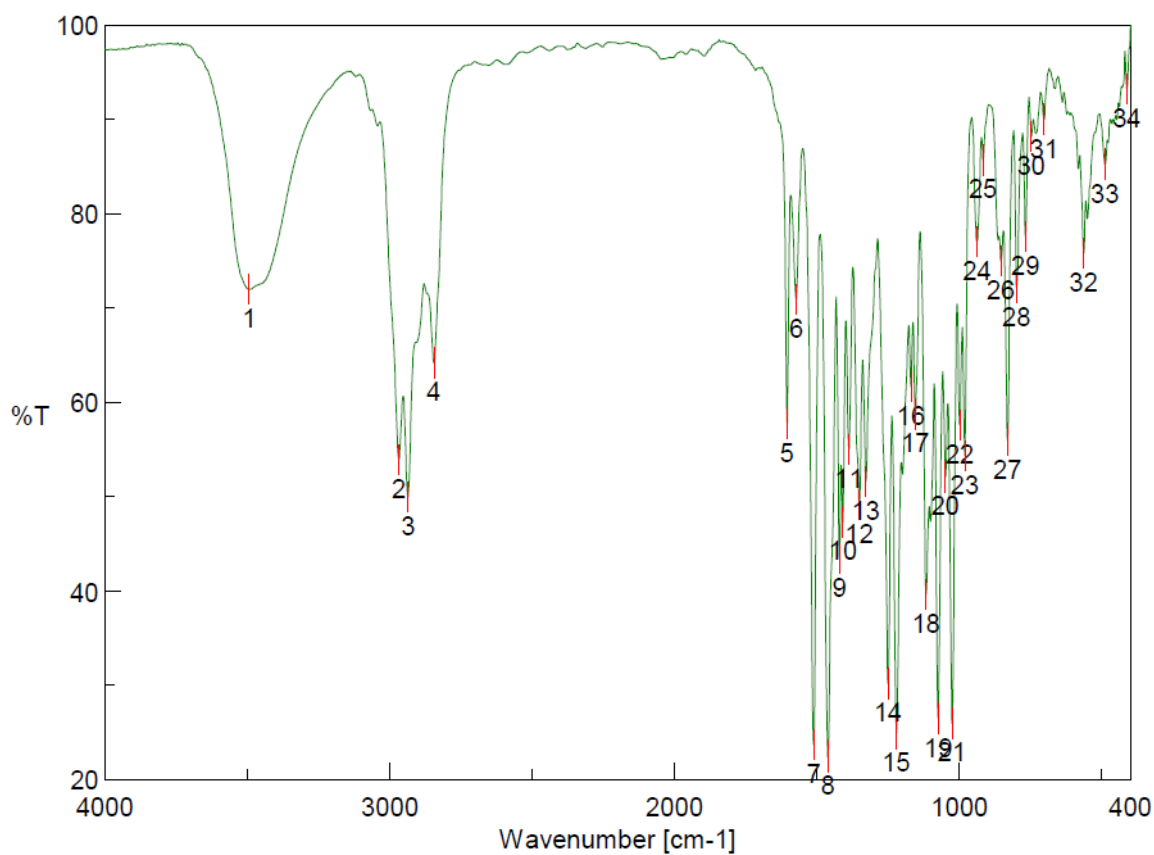
**Figure S248.** Experimental IR spectrum of (aR,1R,3S,2'S)-**19** recorded as KBr disc.



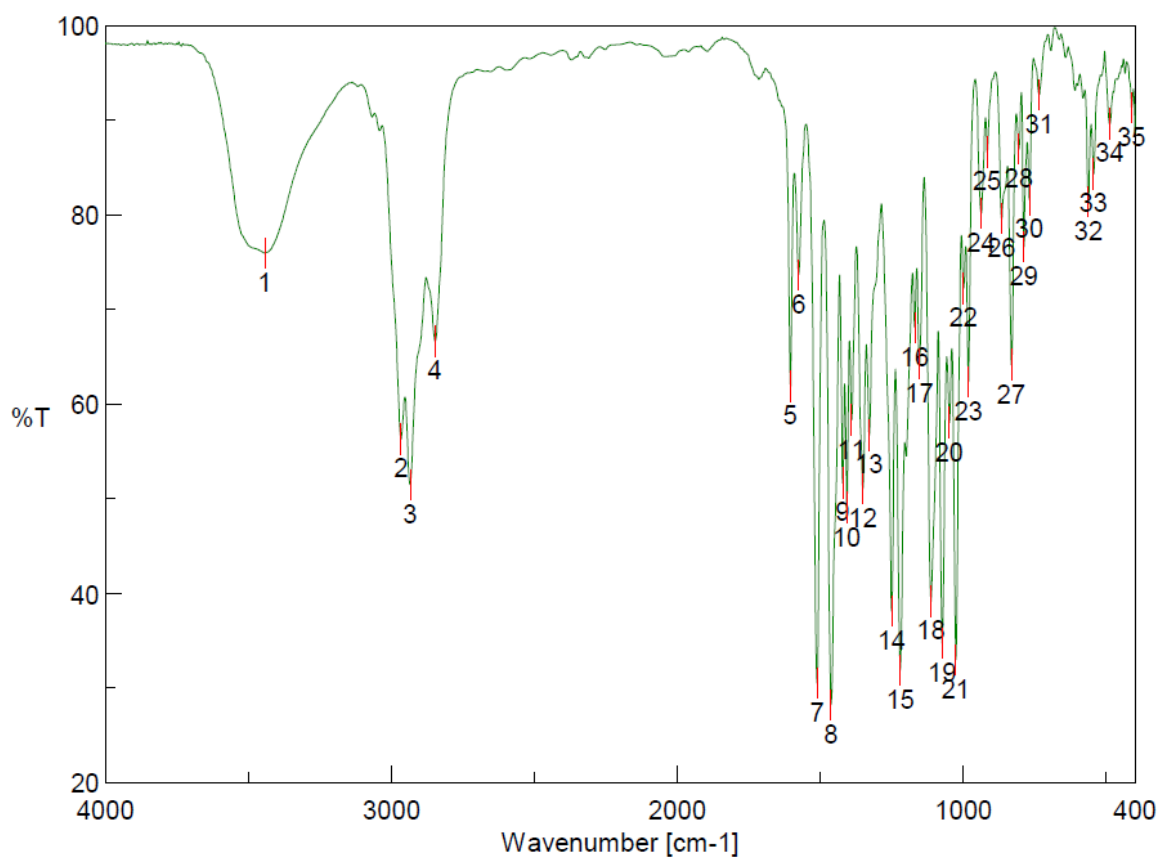
**Figure S249.** Experimental IR spectrum of (aS,1S,3S,2'S)-**20** recorded as KBr disc.



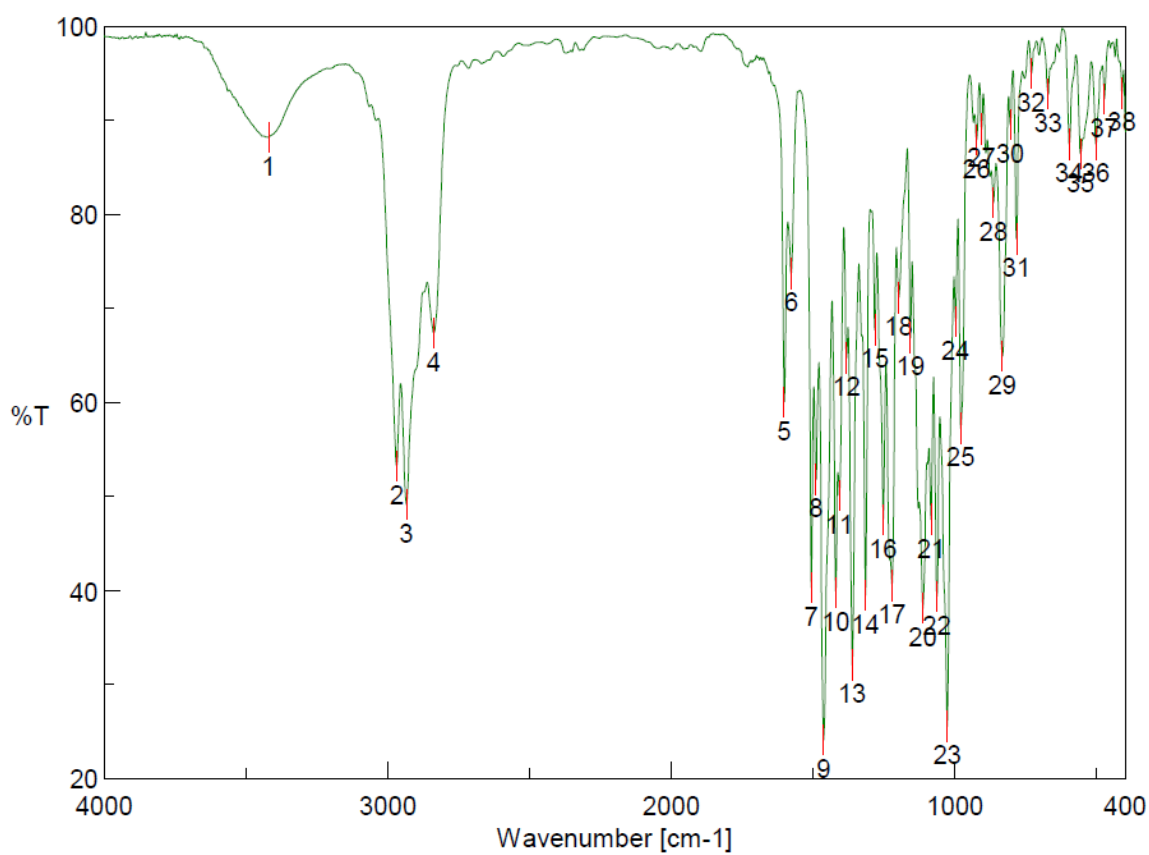
**Figure S250.** Experimental IR spectrum of (aR,1S,3S,2'S)-**20** recorded as KBr disc.



**Figure S251.** Experimental IR spectrum of (aS,1R,3S,2'S)-**20** recorded as KBr disc.

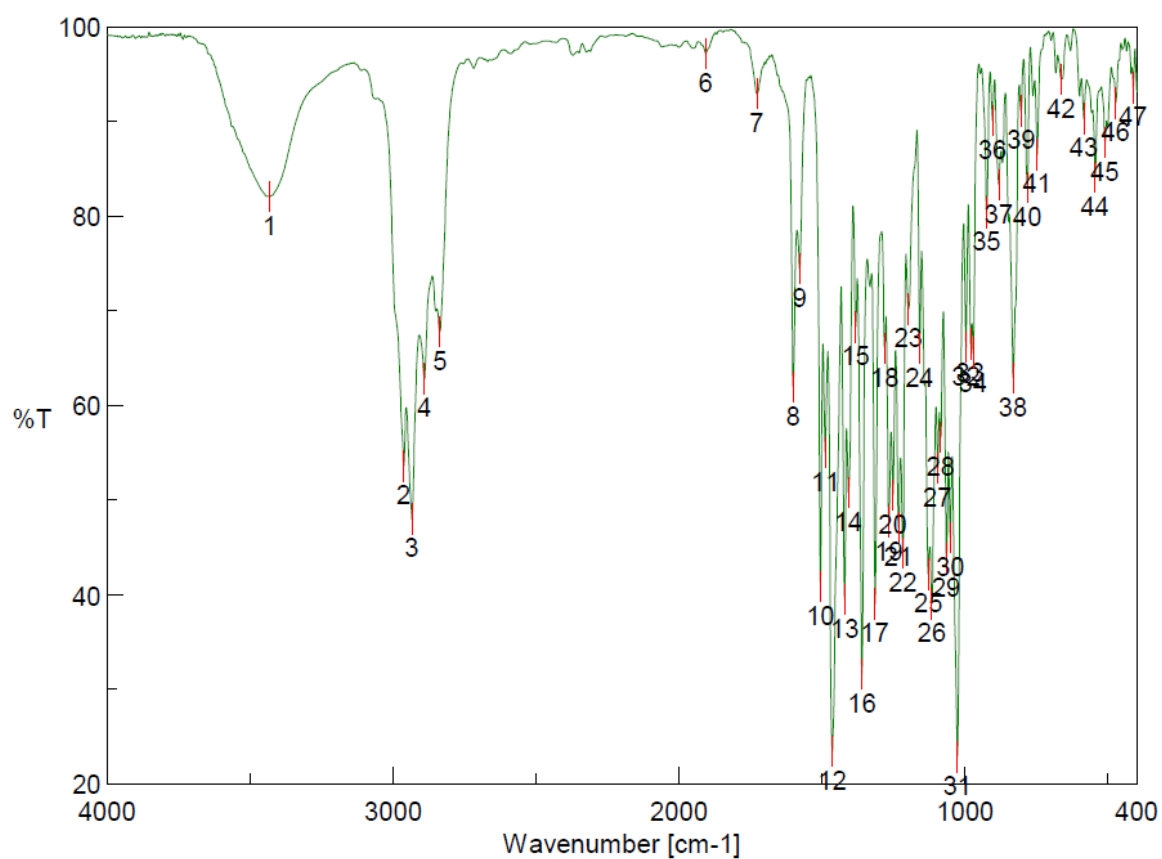


**Figure S252.** Experimental IR spectrum of (aR,1R,3S,2'S)-**20** recorded as KBr disc.

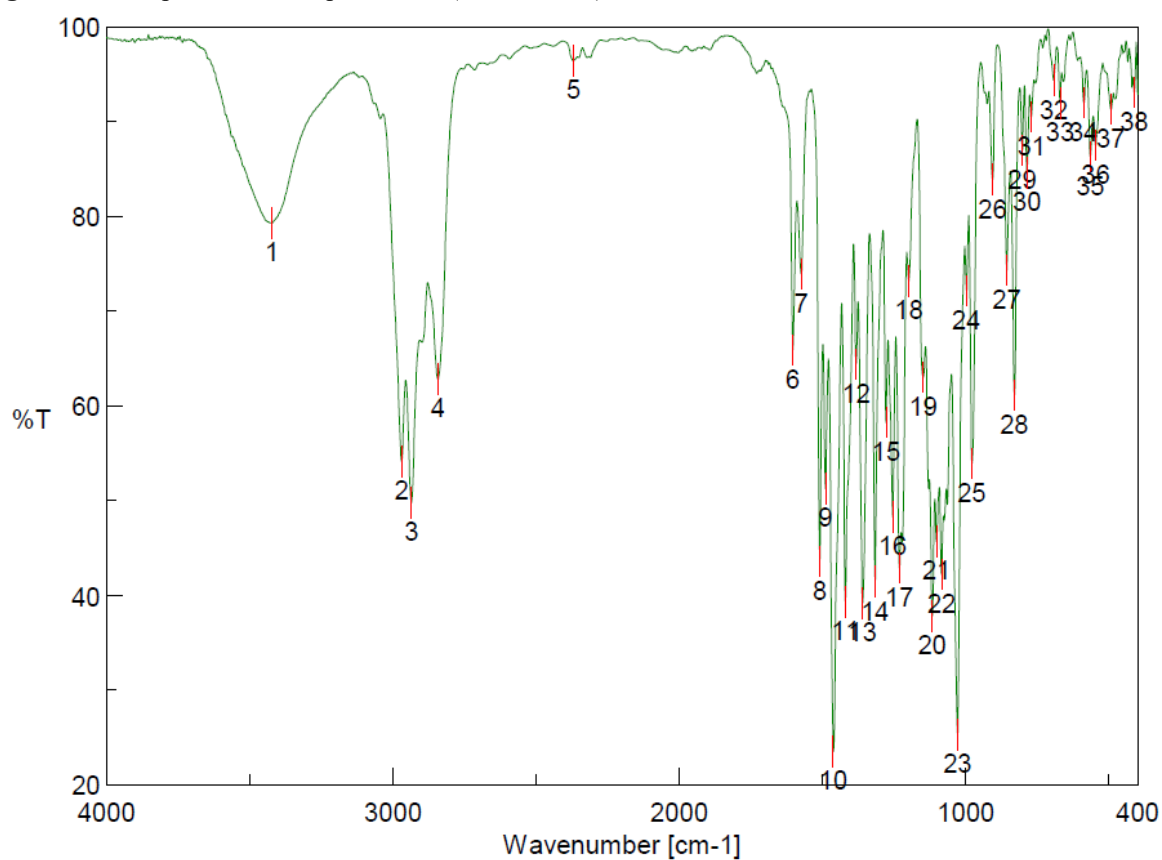


**Figure S253.** Experimental IR spectrum of (aS,1S,3S,3'S)-**21** recorded as KBr disc.

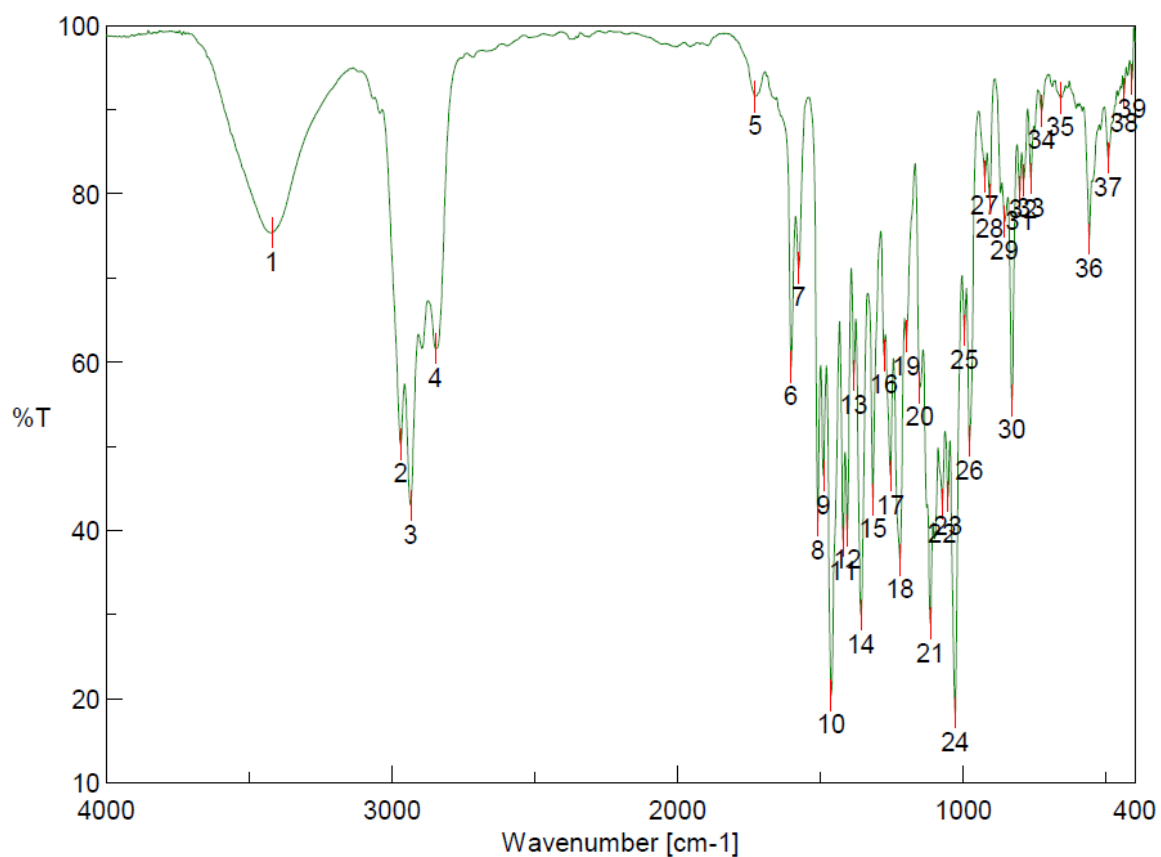




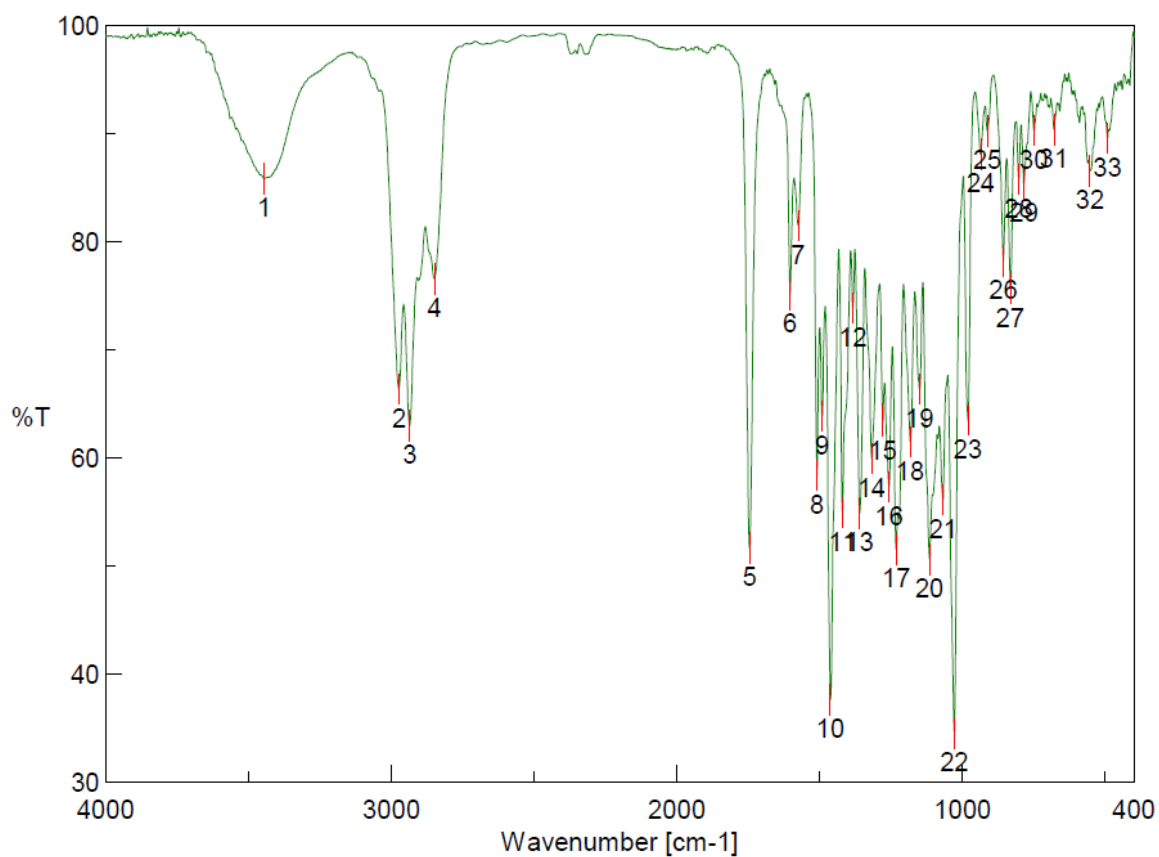
**Figure S254.** Experimental IR spectrum of (aR,1S,3S,3'S)-**21** recorded as KBr disc.



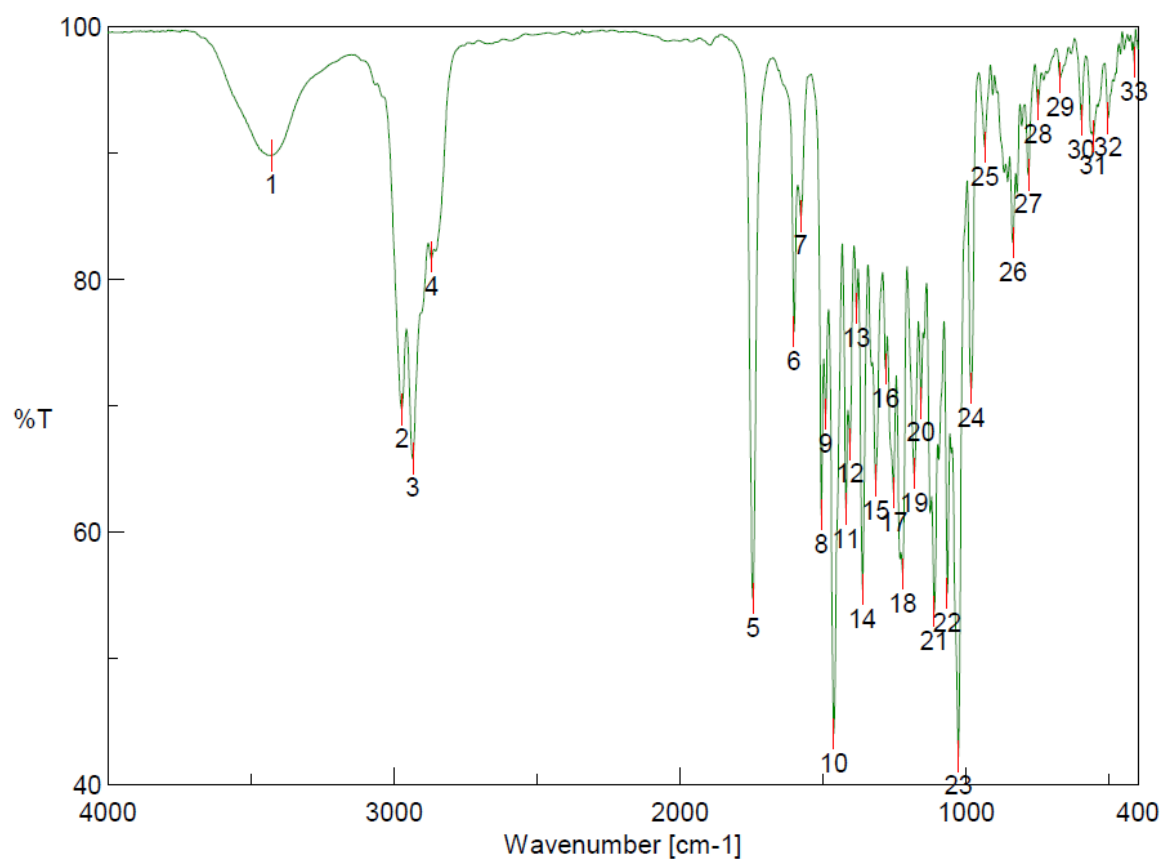
**Figure S255.** Experimental IR spectrum of (aS,1R,3S,3'S)-**21** recorded as KBr disc.



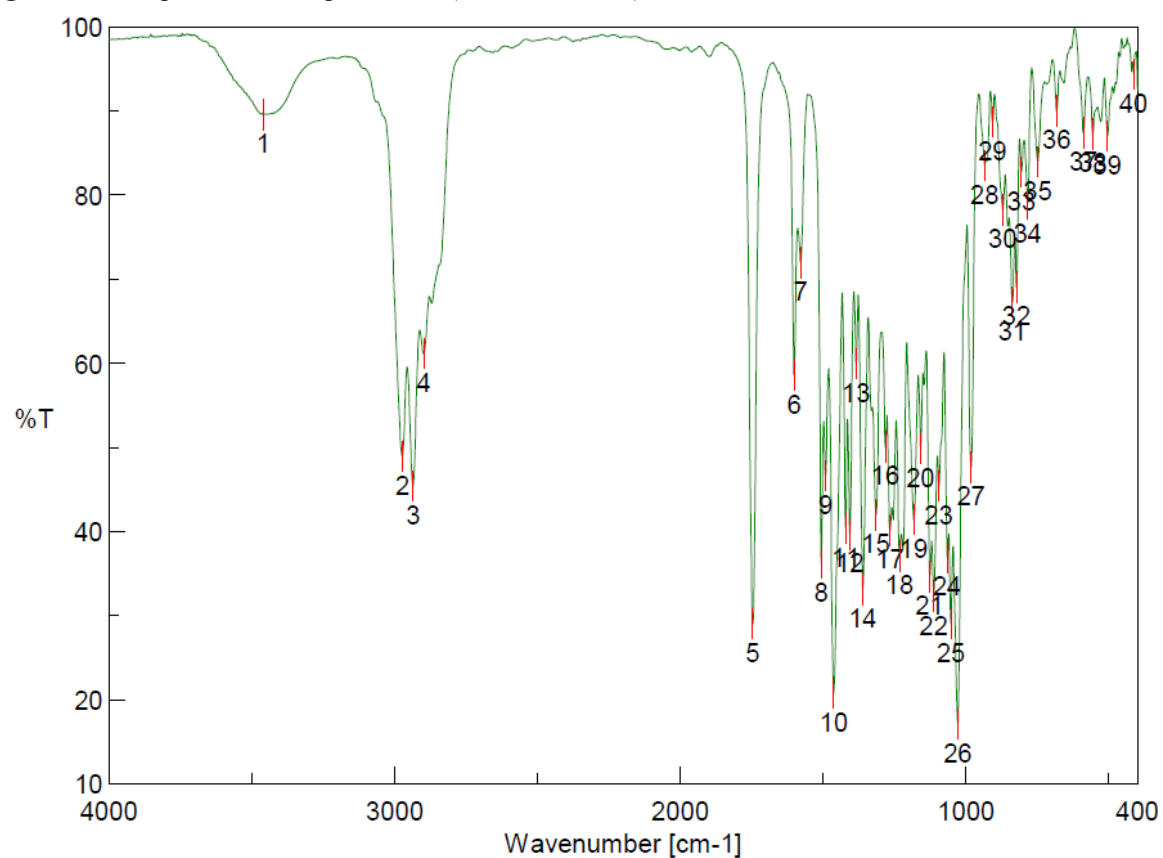
**Figure S256.** Experimental IR spectrum of (aR,1R,3S,3'S)-**21** recorded as KBr disc.



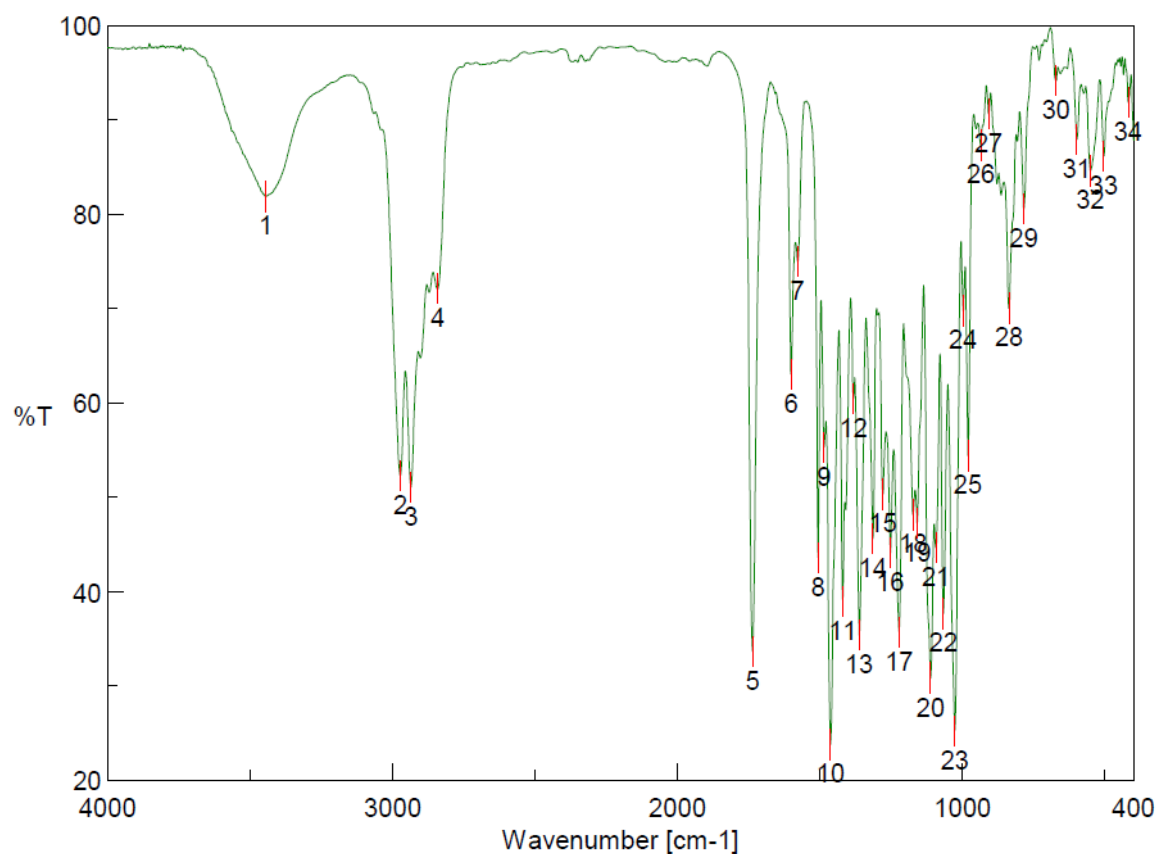
**Figure S257.** Experimental IR spectrum of (aS,1R,3S,1'S,3'S)-**22** recorded as KBr disc.



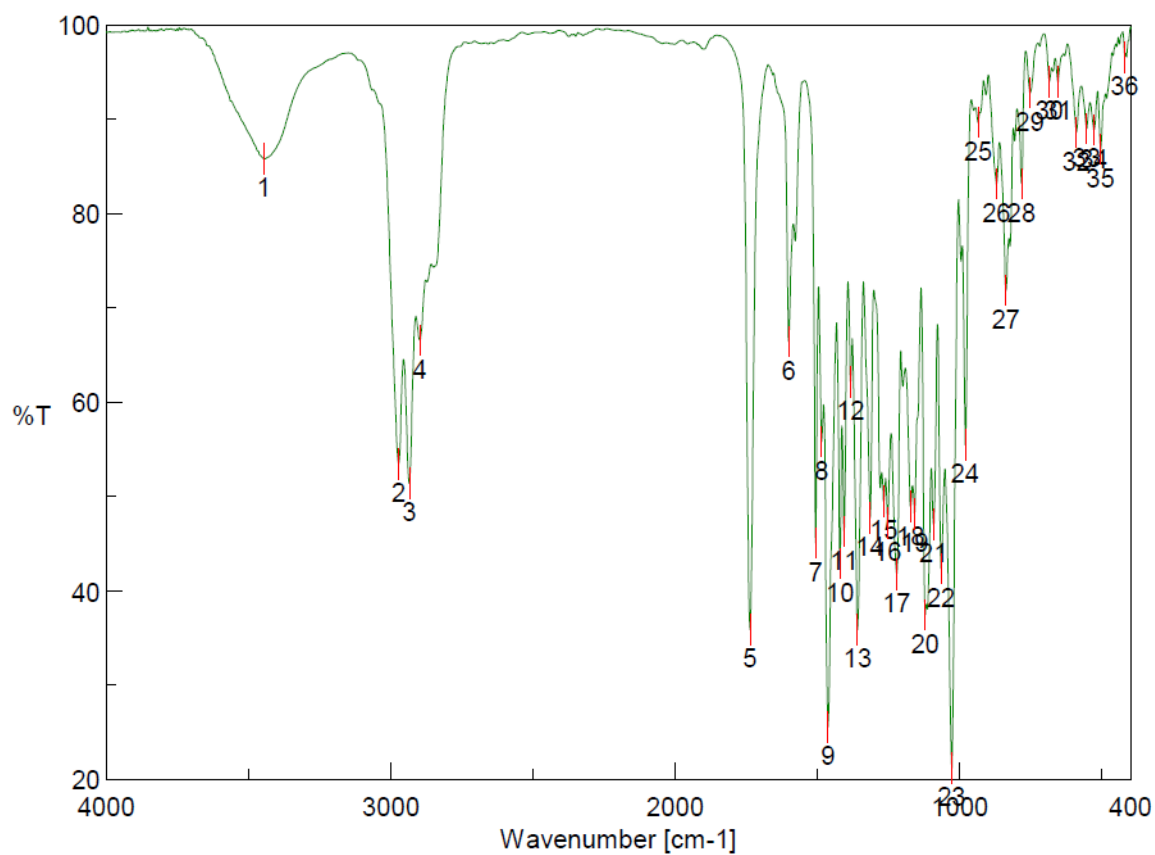
**Figure S258.** Experimental IR spectrum of (aS,1S,3S,1'S,3'S)-**22** recorded as KBr disc.



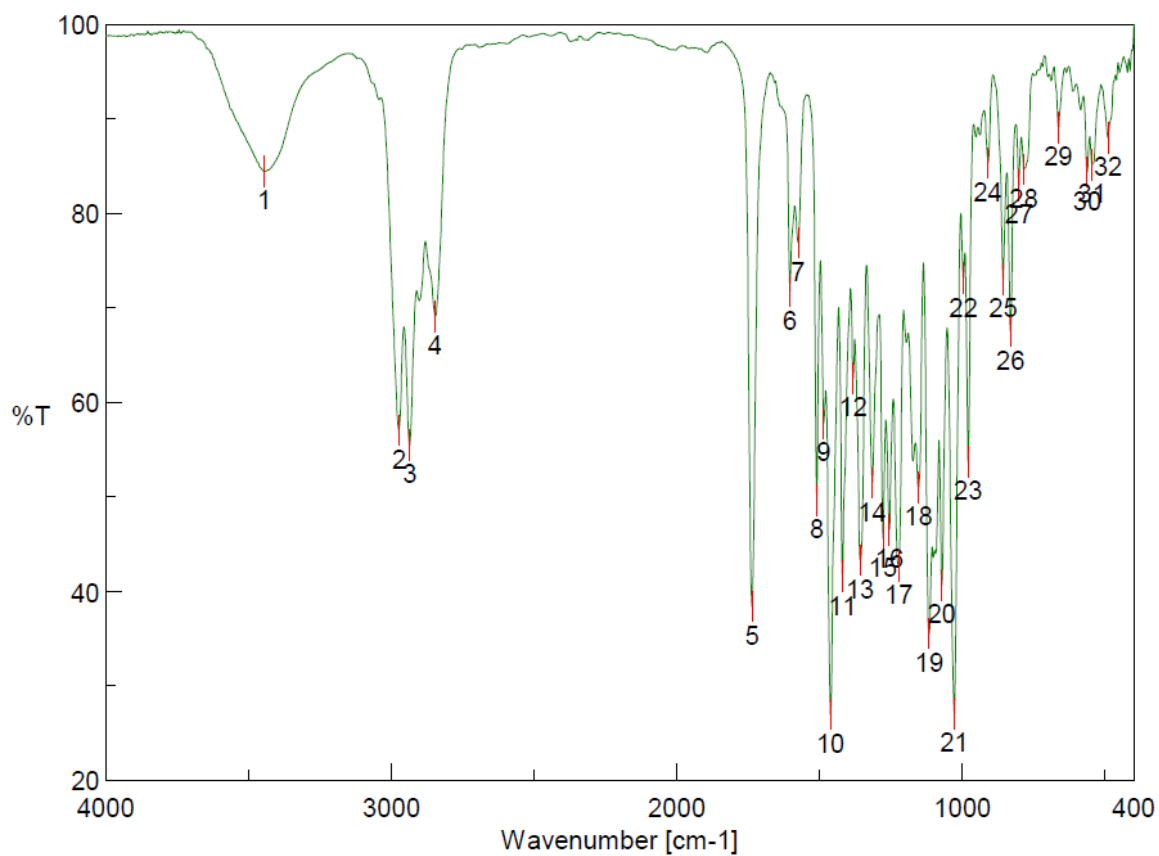
**Figure S259.** Experimental IR spectrum of (aR,1S,3S,1'S,3'S)-**22** recorded as KBr disc.



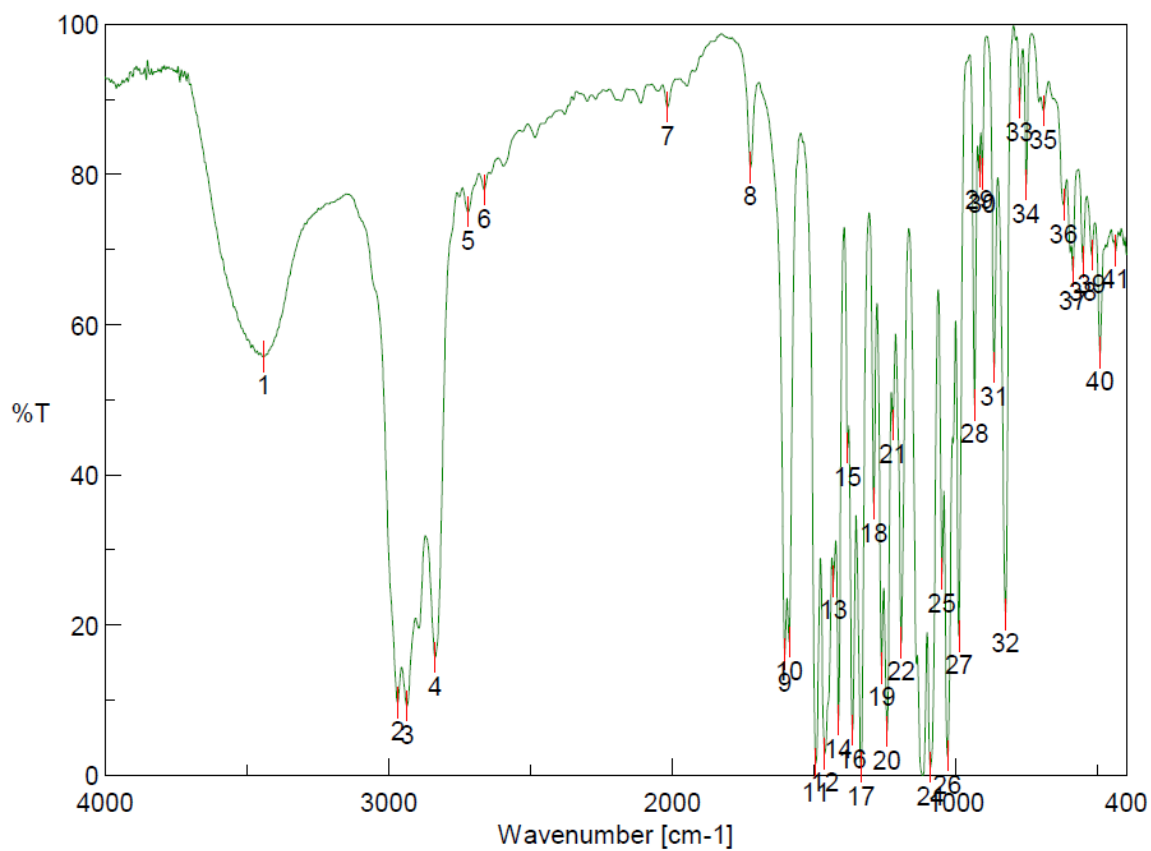
**Figure S260.** Experimental IR spectrum of (aS,1S,3S,1'R,3'S)-**23** recorded as KBr disc.



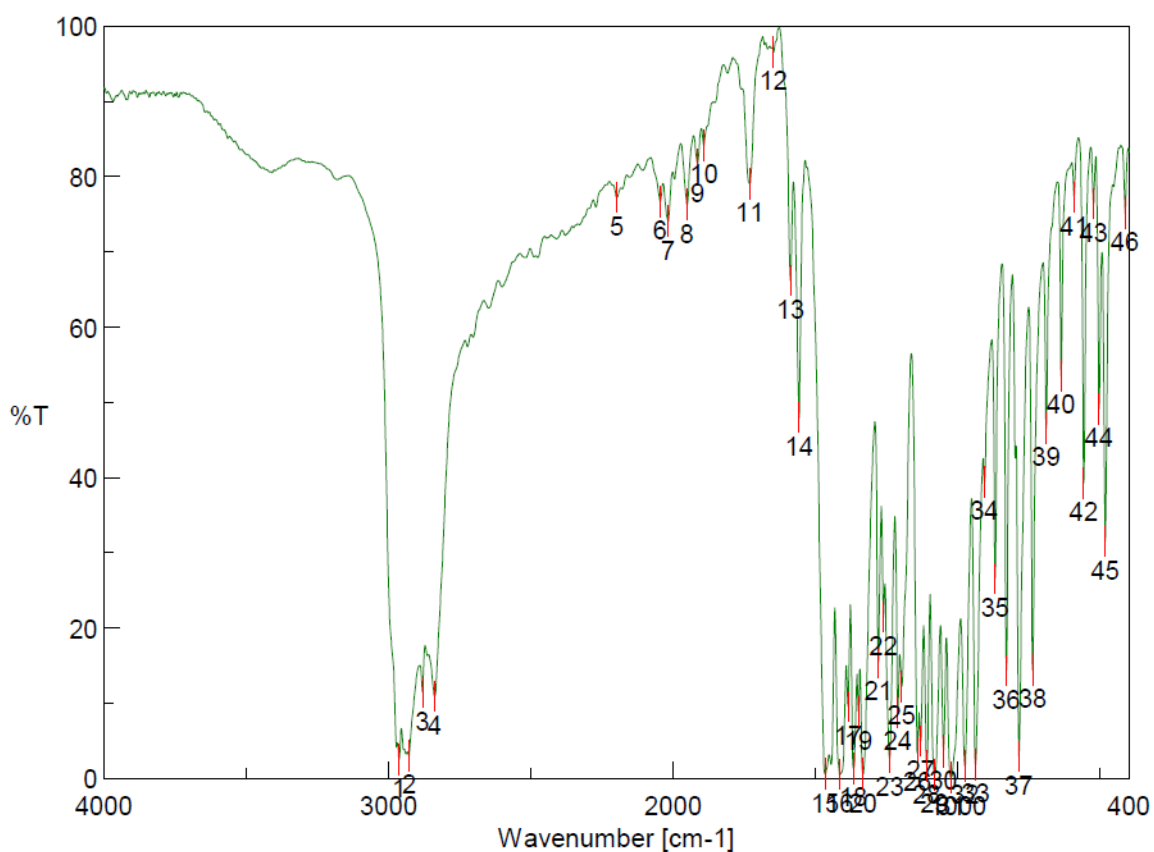
**Figure S261.** Experimental IR spectrum of (aR,1S,3S,1'R,3'S)-**23** recorded as KBr disc.



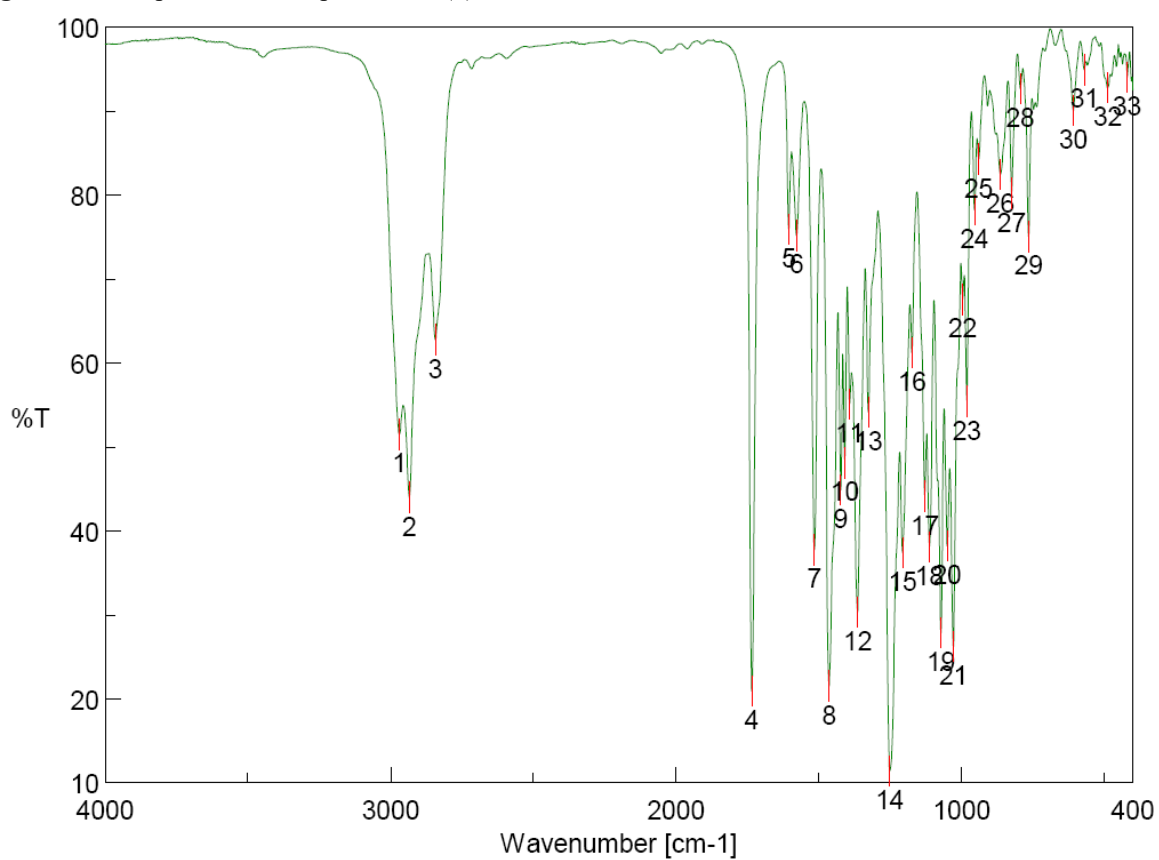
**Figure S262.** Experimental IR spectrum of (aS,1R,3S,1'R,3'S)-**23** recorded as KBr disc.



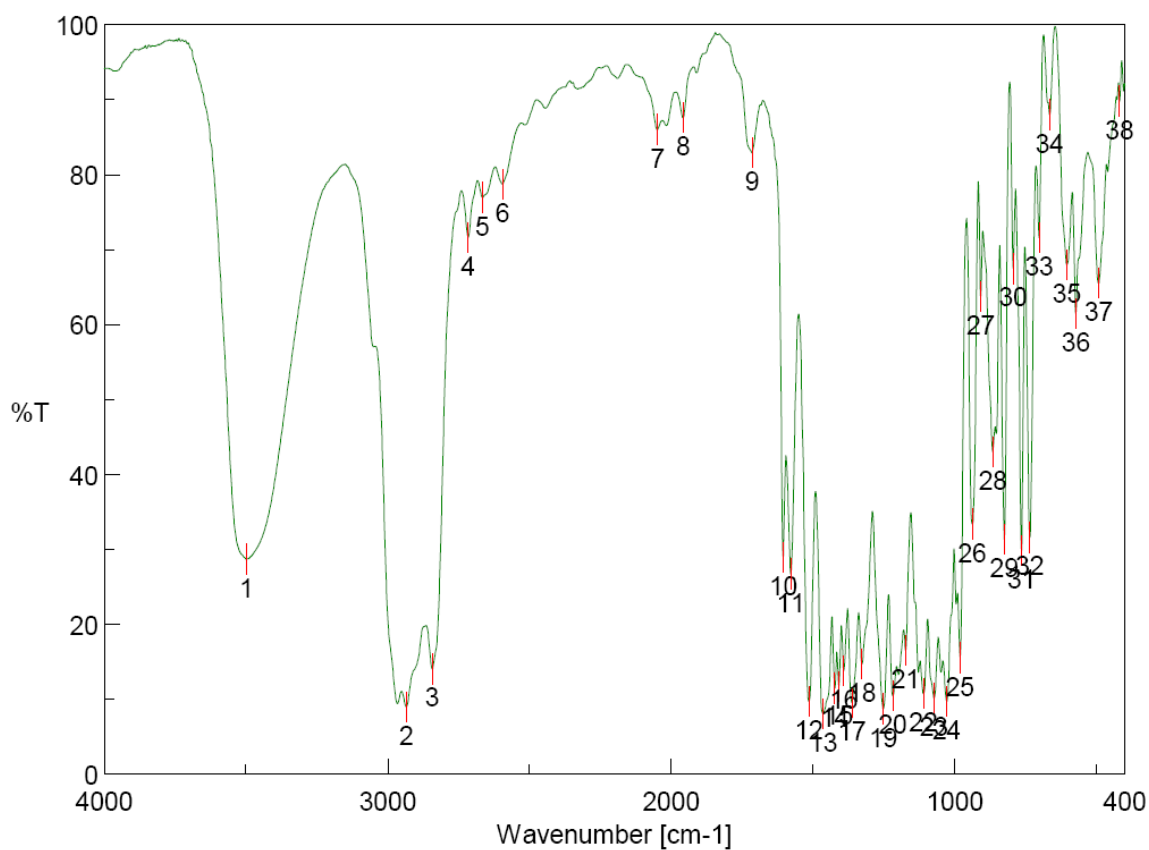
**Figure S263.** Experimental IR spectrum of (S)-**24** recorded as KBr disc.



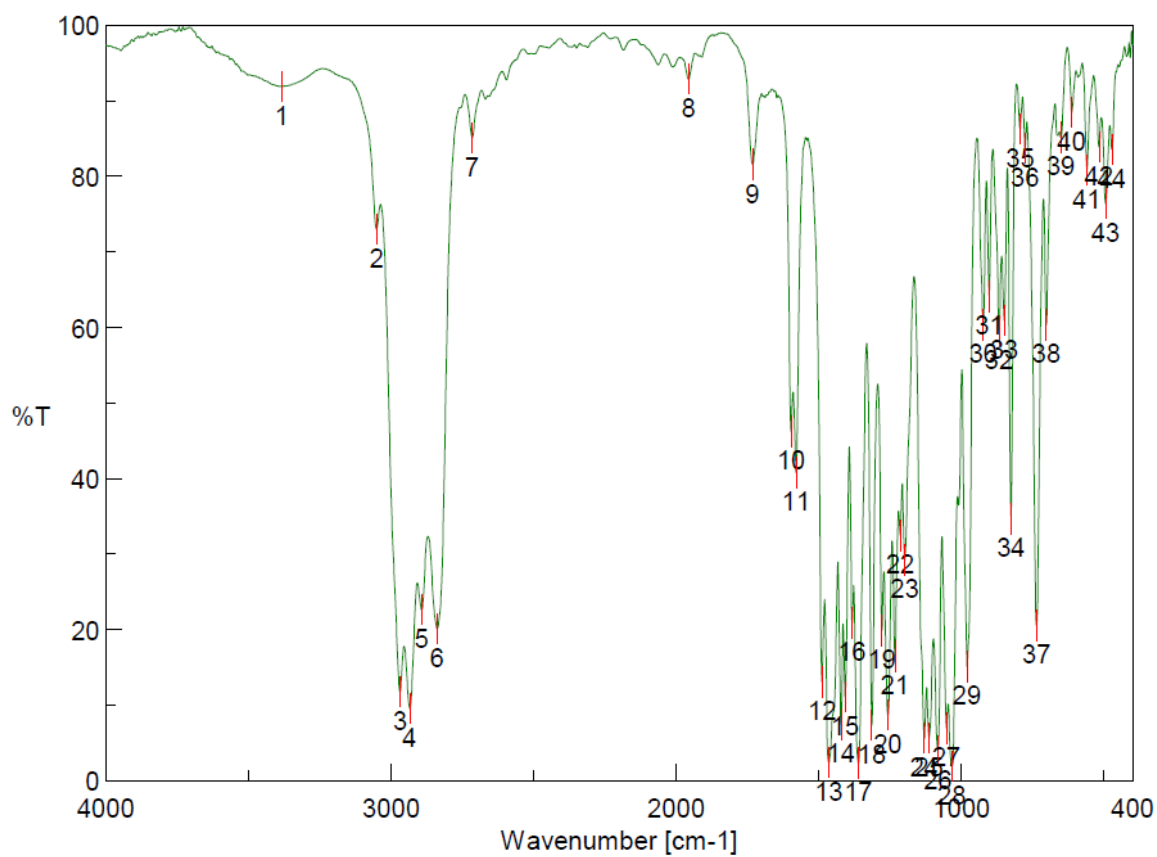
**Figure S264.** Experimental IR spectrum of (*S*)-**25** recorded as KBr disc.



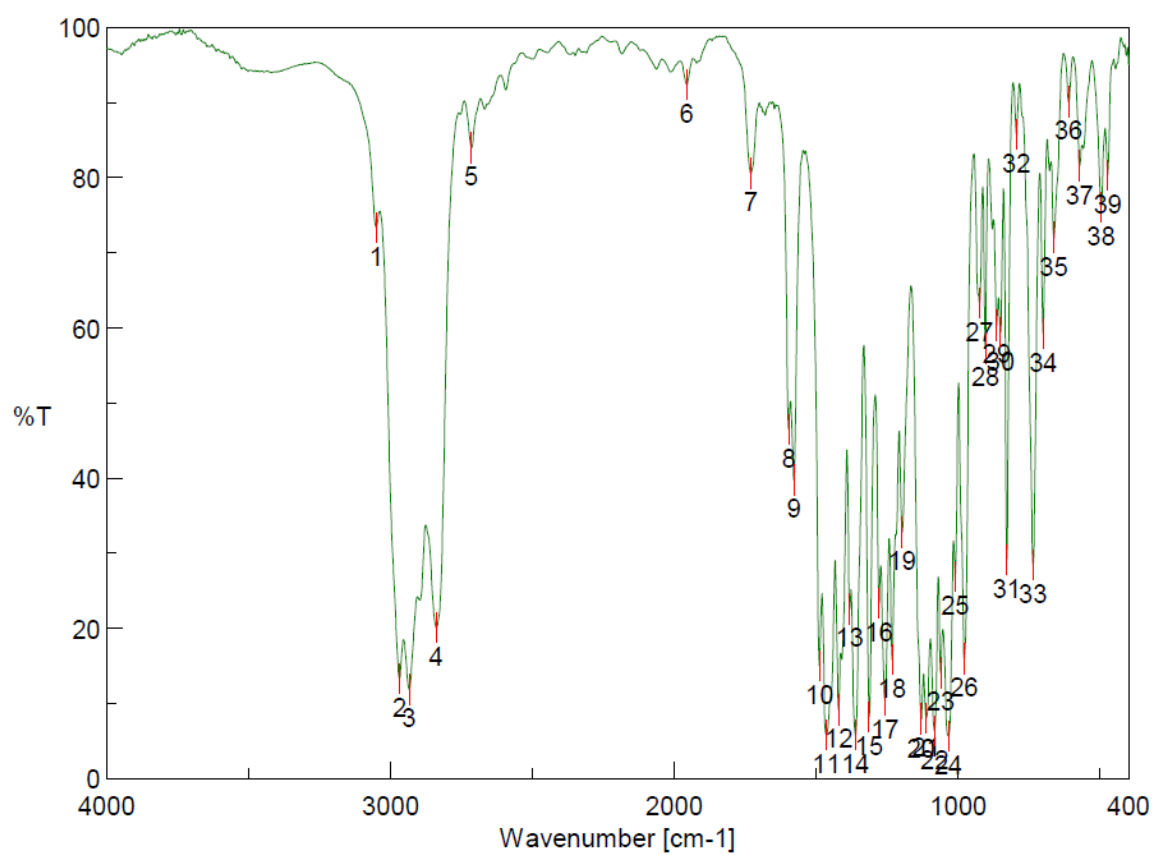
**Figure S265.** Experimental IR spectrum of the mixture of (*aR*,3*S*,2'*S*)-**26** and (*aS*,3*S*,2'*S*)-**26** recorded as KBr disc.



**Figure S266.** Experimental IR spectrum of the mixture of (aR,3S,2'S)-27 and (aS,3S,2'S)-27 recorded as KBr disc.



**Figure S267.** Experimental IR spectrum of (aR,3S,3'S)-28 recorded as KBr disc.



**Figure S268.** Experimental IR spectrum of (a*S*,3*S*,3'*S*)-**28** recorded as KBr disc.



#### 4. X-ray analysis

X-ray-quality crystals were grown by slow evaporation of the sample dissolved in a mixture of hexane and EtOH. A crystal well-looking in polarized light microscope was fixed under a microscope onto a Mitegen loop using high-density oil. Diffraction intensity data were collected at room temperature and in case of (a*S*,1*R*,3*R*,1'*R*,3'*R*)-**22** at low temperature (120 K) using a Bruker-D8 Venture diffractometer (Bruker AXS GmbH, Karlsruhe, Germany) equipped with INCOATEC I $\mu$ S 3.0 (Incoatec GmbH, Geesthacht, Germany) dual (Cu and Mo) sealed tube micro sources and a Photon II Charge-Integrating Pixel Array detector (Bruker AXS GmbH, Karlsruhe, Germany) using Mo K $\alpha$  ( $\lambda = 0.71073$  Å) radiation. The absolute configurations were assigned relative of the known configuration of C-3 and hence the applied radiation the Flack parameter is meaningless [11], but the assignment is unambiguous. Other spectroscopic methods (VCD, ECD) support the 100% enantiopurity of the samples. High multiplicity data collection and integration were performed using APEX4 (version 2021-4.0, Bruker AXS Inc., 2021, Madison, USA) software. Data reduction and multi-scan absorption correction were performed using SAINT (version 8.40B, Bruker AXS Inc., 2019, Madison, USA). The structures were routinely solved using direct methods and refined on F<sup>2</sup> using the SHELXL program [12] incorporated into the APEX4 suite. Refinement was performed anisotropically for all non-hydrogen atoms. Hydrogen atoms were placed into geometric positions except for the hydrogen atoms of solvent ethanol molecules in the structure of (a*S*,1*R*,3*R*,1'*R*,3'*R*)-**22**. These atoms could be found on the difference electron density map and the respective O-H distances should be restrained. Multi-scan absorption correction had to be applied because of the irregular shape of the crystals especially in the case of (a*S*,1*R*,3*R*,3'*R*)-**21** (large crystals) and (a*S*,1*R*,3*R*,1'*R*,3'*R*)-**22** (very small needle crystals). In latter case, RIGU command was used to regulate the refinement resulting in significant number of restrains. Further experimental details are shown in Table S1. The CIF file was manually edited using PubCIF software [13], while graphics were prepared by using the Mercury program [14]. The results for the X-ray diffraction structure determinations were good enough and acceptable according to the CheckCIF functionality of the PLATON software (Utrecht University, Utrecht, The Netherlands) [15]. Structural parameters such as bond length and angle data were in the expected range (Figure S269 and Table S2, Figure S270 and Table S3 as well as Figure S271 and Table S4 for (a*R*,1*S*,3*S*,3'*S*)-**21**, (a*S*,1*R*,3*R*,3'*R*)-**21** and (a*S*,1*R*,3*R*,1'*R*,3'*R*)-**22**, respectively. The solid-state structures are stabilized by van der Waals interactions as well as by weak C-H $\cdots$ O and in case of (a*S*,1*R*,3*R*,1'*R*,3'*R*)-**22** by strong O-H $\cdots$ O hydrogen bonds. As expected, (a*R*,1*S*,3*S*,3'*S*)-**21** and (a*S*,1*R*,3*R*,3'*R*)-**21** crystallized in unit cells of identical

geometric parameters. The most interesting structure is (a*S*,1*R*,3*R*,1'*R*,3'*R*)-**22** in which there were three molecules in the asymmetric unit together with two (slightly disordered) solvent ethanol molecules. There were only minor conformational differences among the molecules (Figure S272) and they have the same axial chirality.

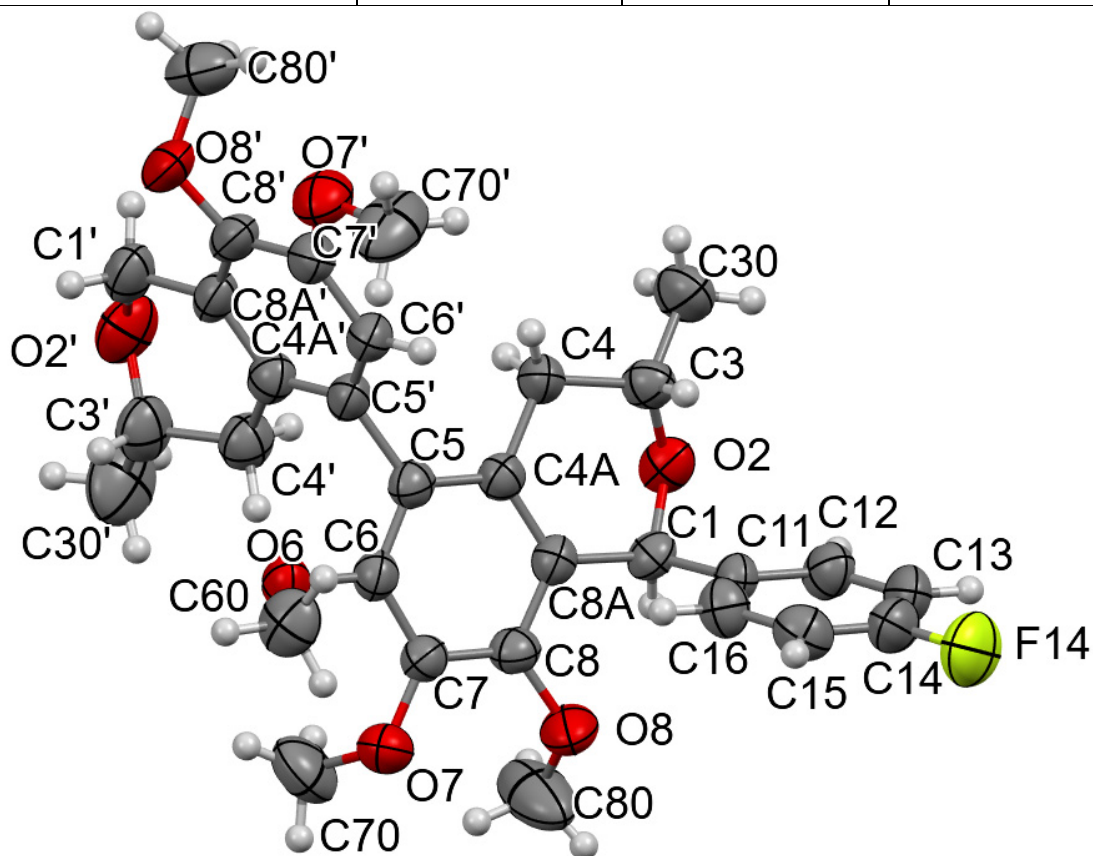
The supplementary crystallographic data can be obtained free of charge from the Cambridge Crystallographic Data Centre via [http://www.ccdc.cam.ac.uk/data\\_request/cif](http://www.ccdc.cam.ac.uk/data_request/cif), using reference deposition number 2249290 for (a*R*,1*S*,3*S*,3'*S*)-**21**, 2249291 for (a*S*,1*R*,3*R*,3'*R*)-**21**, and 2249292 for (a*S*,1*R*,3*R*,1'*R*,3'*R*)-**22**.

#### 4.1. Data of the X-ray analysis

**Table S1.** Experimental details of the structural elucidation by single crystal X-ray diffraction.

Compound	(a <i>R</i> ,1 <i>S</i> ,3 <i>S</i> ,3' <i>S</i> )- <b>21</b>	(a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,3' <i>R</i> )- <b>21</b>	(a <i>S</i> ,1 <i>R</i> ,3 <i>R</i> ,1' <i>R</i> ,3' <i>R</i> )- <b>22</b>
Crystal data			
Chemical formula	C <sub>31</sub> H <sub>35</sub> FO <sub>7</sub>	C <sub>31</sub> H <sub>35</sub> FO <sub>7</sub>	3(C <sub>34</sub> H <sub>39</sub> FO <sub>9</sub> )·2(C <sub>2</sub> H <sub>6</sub> O)
<i>M</i> <sub>r</sub>	538.59	538.59	1924.08
Crystal system, space group	Monoclinic, <i>P</i> 2 <sub>1</sub>	Monoclinic, <i>P</i> 2 <sub>1</sub>	Triclinic, <i>P</i> 1
Temperature (K)	295	302	120
<i>a</i> , <i>b</i> , <i>c</i> (Å)	8.2171 (10), 15.7142 (16), 11.5070 (14)	8.1885 (7), 15.6600 (14), 11.4825 (10)	9.8692 (15), 11.5507 (18), 22.357 (3)
α,β,γ (°)	90, 108.055 (4), 90	90, 108.025 (3), 90	85.927 (8), 82.008 (8), 87.066 (8)
<i>V</i> (Å <sup>3</sup> )	1412.7 (3)	1400.2 (2)	2515.3 (7)
<i>Z</i>	2	2	1
Radiation type	Mo <i>K</i>		
μ (mm <sup>-1</sup> )	0.09	0.09	0.10
Crystal size (mm)	0.32 × 0.21 × 0.07	0.55 × 0.47 × 0.31	0.29 × 0.07 × 0.04
Data collection			
Diffractometer	Bruker D8 VENTURE		
Absorption correction	Multi-scan <i>SADABS2016/2</i> - Bruker AXS area detector scaling and absorption correction		
<i>T</i> <sub>min</sub> , <i>T</i> <sub>max</sub>	0.97, 0.99	0.95, 0.97	0.97, 1.00
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )]	13016, 5165, 2976	17212, 5645, 3805	80197, 17554, 10225

reflections			
$R_{\text{int}}$	0.084	0.112	0.191
$(\sin \Theta / \lambda)_{\text{max}} (\text{\AA}^{-1})$	0.604	0.627	0.604
Refinement			
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.070, 0.194, 1.06	0.077, 0.203, 0.99	0.104, 0.231, 1.08
No. of reflections	5165	5645	17554
No. of parameters	360	360	1272
No. of restraints	1	1	1086
H-atom treatment	H-atom parameters constrained		H atoms treated by a mixture of independent and constrained refinement
$\Delta_{\text{max}}, \Delta_{\text{min}} (\text{e \AA}^{-3})$	0.57, -0.60	0.40, -0.50	0.54, -0.53



**Figure S269.** ORTEP view of (aR,1S,3S,3'S)-**21** at 50% probability level with numbering scheme.

**Table S2.** Geometric parameters ( $\text{\AA}$ ,  $^\circ$ ) for (aR,1S,3S,3'S)-**21**.

Bond distances ( $\text{\AA}$ )
---------------------------------

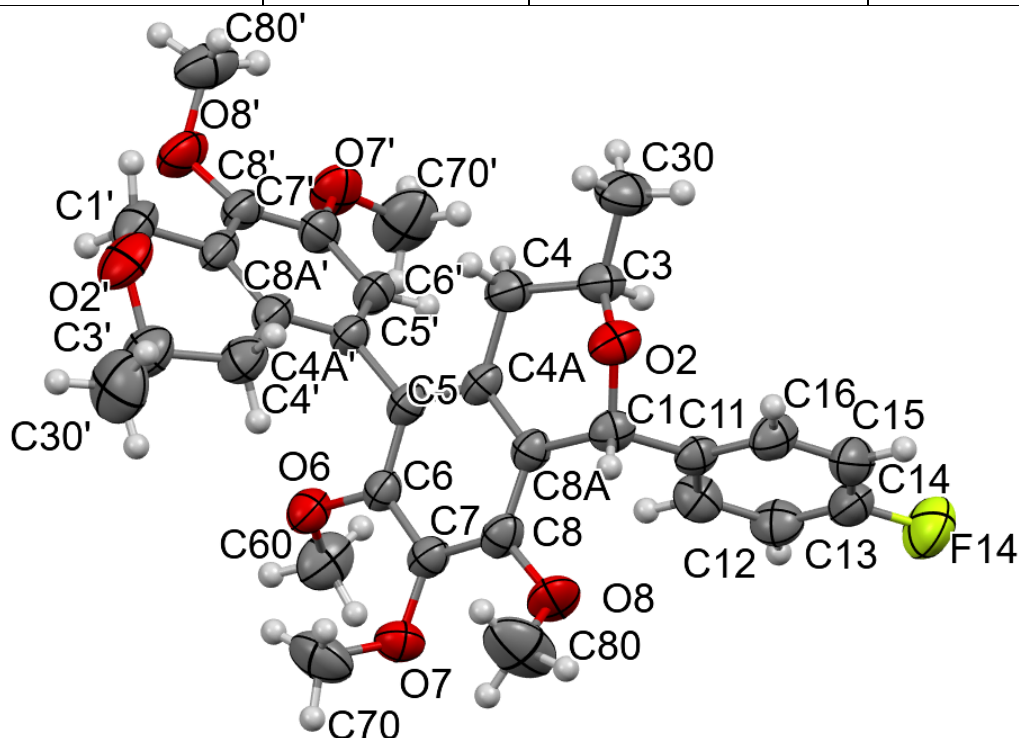
C1—O2	1.433 (8)	C8'—C8A'	1.392 (11)
C1—C8A	1.502 (9)	C11—C12	1.379 (10)
C1—C11	1.529 (9)	C11—C16	1.381 (10)
C1—H1	0.9800	C12—C13	1.380 (11)
C1'—O2'	1.430 (11)	C12—H12	0.9300
C1'—C8A'	1.520 (10)	C13—C14	1.358 (12)
C1'—H1'A	0.9700	C13—H13	0.9300
C1'—H1'B	0.9700	C14—F14	1.354 (9)
C3—O2	1.428 (9)	C14—C15	1.362 (11)
C3—C30	1.518 (10)	C15—C16	1.384 (11)
C3—C4	1.532 (10)	C15—H5'	0.9300
C3—H3	0.9800	C16—H6'	0.9300
C3'—O2'	1.427 (10)	C30—H30A	0.9600
C3'—C30'	1.490 (13)	C30—H30B	0.9600
C3'—C4'	1.496 (10)	C30—H30C	0.9600
C3'—H3'	0.9800	C30'—H30D	0.9600
C4—C4A	1.521 (9)	C30'—H30E	0.9600
C4—H4A	0.9700	C30'—H30F	0.9600
C4—H4B	0.9700	C60—O6	1.432 (9)
C4'—C4A'	1.493 (11)	C60—H60A	0.9600
C4'—H4'A	0.9700	C60—H60B	0.9600
C4'—H4'B	0.9700	C60—H60C	0.9600
C5—C4A	1.393 (9)	C70—O7	1.427 (9)
C5—C6	1.397 (9)	C70—H70A	0.9600
C5—C5'	1.509 (10)	C70—H70B	0.9600
C4A—C8A	1.401 (9)	C70—H70C	0.9600
C5'—C4A'	1.392 (9)	C70'—O7'	1.413 (11)
C5'—C6'	1.400 (10)	C70'—H70D	0.9600
C6—C7	1.378 (10)	C70'—H70E	0.9600
C6—O6	1.389 (8)	C70'—H7'E	0.9600
C6'—C7'	1.386 (10)	C80—O8	1.368 (12)
C6'—H6''	0.9300	C80—H80A	0.9600
C7—O7	1.381 (8)	C80—H80B	0.9600
C7—C8	1.389 (10)	C80—H80C	0.9600
C7'—O7'	1.386 (10)	C80'—O8'	1.422 (10)

C7'—C8'	1.392 (10)	C80'—H80D	0.9600
C8—O8	1.369 (9)	C80'—H80E	0.9600
C8—C8A	1.393 (9)	C80'—H80F	0.9600
C8'—O8'	1.385 (9)	C4A'—C8A'	1.384 (10)
Angles (°)			
O2—C1—C8A	111.6 (5)	C11—C12—H12	119.6000
O2—C1—C11	110.2 (5)	C13—C12—H12	119.6000
C8A—C1—C11	114.4 (5)	C14—C13—C12	119.3 (8)
O2—C1—H1	106.7000	C14—C13—H13	120.4000
C8A—C1—H1	106.7000	C12—C13—H13	120.4000
C11—C1—H1	106.7000	F14—C14—C13	119.1 (8)
O2'—C1'—C8A'	112.9 (7)	F14—C14—C15	119.5 (8)
O2'—C1'—H1'A	109.0000	C13—C14—C15	121.5 (8)
C8A'—C1'—H1'A	109.0000	C14—C15—C16	119.4 (8)
O2'—C1'—H1'B	109.0000	C14—C15—H5'	120.3000
C8A'—C1'—H1'B	109.0000	C16—C15—H5'	120.3000
H1'A—C1'—H1'B	107.8000	C11—C16—C15	120.3 (7)
O2—C3—C30	109.1 (6)	C11—C16—H6'	119.8000
O2—C3—C4	109.8 (5)	C15—C16—H6'	119.8000
C30—C3—C4	112.1 (7)	C3—C30—H30A	109.5000
O2—C3—H3	108.6000	C3—C30—H30B	109.5000
C30—C3—H3	108.6000	H30A—C30—H30B	109.5000
C4—C3—H3	108.6000	C3—C30—H30C	109.5000
O2'—C3'—C30'	107.8 (8)	H30A—C30—H30C	109.5000
O2'—C3'—C4'	108.8 (7)	H30B—C30—H30C	109.5000
C30'—C3'—C4'	113.4 (8)	C3'—C30'—H30D	109.5000
O2'—C3'—H3'	108.9000	C3'—C30'—H30E	109.5000
C30'—C3'—H3'	108.9000	H30D—C30'—H30E	109.5000
C4'—C3'—H3'	108.9000	C3'—C30'—H30F	109.5000
C4A—C4—C3	111.7 (6)	H30D—C30'—H30F	109.5000
C4A—C4—H4A	109.3000	H30E—C30'—H30F	109.5000
C3—C4—H4A	109.3000	O6—C60—H60A	109.5000
C4A—C4—H4B	109.3000	O6—C60—H60B	109.5000
C3—C4—H4B	109.3000	H60A—C60—H60B	109.5000
H4A—C4—H4B	107.9000	O6—C60—H60C	109.5000

C4A'—C4'—C3'	112.5 (7)	H60A—C60—H60C	109.5000
C4A'—C4'—H4'A	109.1000	H60B—C60—H60C	109.5000
C3'—C4'—H4'A	109.1000	O7—C70—H70A	109.5000
C4A'—C4'—H4'B	109.1000	O7—C70—H70B	109.5000
C3'—C4'—H4'B	109.1000	H70A—C70—H70B	109.5000
H4'A—C4'—H4'B	107.8000	O7—C70—H70C	109.5000
C4A—C5—C6	119.1 (6)	H70A—C70—H70C	109.5000
C4A—C5—C5'	122.2 (6)	H70B—C70—H70C	109.5000
C6—C5—C5'	118.7 (6)	O7'—C70'—H70D	109.5000
C5—C4A—C8A	120.0 (6)	O7'—C70'—H70E	109.5000
C5—C4A—C4	120.9 (6)	H70D—C70'—H70E	109.5000
C8A—C4A—C4	119.0 (6)	O7'—C70'—H7'E	109.5000
C4A'—C5'—C6'	120.8 (7)	H70D—C70'—H7'E	109.5000
C4A'—C5'—C5	119.4 (6)	H70E—C70'—H7'E	109.5000
C6'—C5'—C5	119.7 (6)	O8—C80—H80A	109.5000
C7—C6—O6	119.6 (6)	O8—C80—H80B	109.5000
C7—C6—C5	121.4 (6)	H80A—C80—H80B	109.5000
O6—C6—C5	118.9 (6)	O8—C80—H80C	109.5000
C7'—C6'—C5'	119.8 (6)	H80A—C80—H80C	109.5000
C7'—C6'—H6"	120.1000	H80B—C80—H80C	109.5000
C5'—C6'—H6"	120.1000	O8'—C80'—H80D	109.5000
C6—C7—O7	121.3 (6)	O8'—C80'—H80E	109.5000
C6—C7—C8	119.1 (6)	H80D—C80'—H80E	109.5000
O7—C7—C8	119.5 (6)	O8'—C80'—H80F	109.5000
C6'—C7'—O7'	123.7 (7)	H80D—C80'—H80F	109.5000
C6'—C7'—C8'	119.5 (7)	H80E—C80'—H80F	109.5000
O7'—C7'—C8'	116.7 (7)	C8A'—C4A'—C5'	118.8 (7)
O8—C8—C7	121.9 (6)	C8A'—C4A'—C4'	119.0 (7)
O8—C8—C8A	117.4 (6)	C5'—C4A'—C4'	122.2 (7)
C7—C8—C8A	120.7 (6)	C4A'—C8A'—C8'	120.7 (7)
O8'—C8'—C7'	121.7 (8)	C4A'—C8A'—C1'	120.9 (8)
O8'—C8'—C8A'	117.8 (7)	C8'—C8A'—C1'	118.3 (7)
C7'—C8'—C8A'	120.3 (7)	C3—O2—C1	112.7 (5)
C8—C8A—C4A	119.5 (6)	C3'—O2'—C1'	112.3 (6)
C8—C8A—C1	118.6 (6)	C6—O6—C60	113.7 (6)

C4A—C8A—C1	121.9 (6)	C7—O7—C70	113.4 (6)
C12—C11—C16	118.8 (7)	C7'—O7'—C70'	117.4 (6)
C12—C11—C1	118.2 (6)	C80—O8—C8	119.8 (8)
C16—C11—C1	123.0 (6)	C8'—O8'—C80'	117.3 (6)
C11—C12—C13	120.8 (7)		
Torsion angles (°)			
O2—C3—C4—C4A	47.5 (8)	C8A—C1—C11—C12	−177.3 (7)
C30—C3—C4—C4A	169.0 (7)	O2—C1—C11—C16	132.3 (7)
O2'—C3'—C4'—C4A'	52.7 (9)	C8A—C1—C11—C16	5.5 (9)
C30'—C3'—C4'—C4A'	172.7 (8)	C16—C11—C12—C13	0.4 (12)
C6—C5—C4A—C8A	0.1 (9)	C1—C11—C12—C13	−176.9 (7)
C5'—C5—C4A—C8A	−176.3 (6)	C11—C12—C13—C14	0.3 (12)
C6—C5—C4A—C4	176.6 (6)	C12—C13—C14—F14	179.4 (7)
C5'—C5—C4A—C4	0.2 (9)	C12—C13—C14—C15	−0.3 (13)
C3—C4—C4A—C5	166.1 (6)	F14—C14—C15—C16	179.8 (7)
C3—C4—C4A—C8A	−17.4 (9)	C13—C14—C15—C16	−0.5 (13)
C4A—C5—C5'—C4A'	101.6 (7)	C12—C11—C16—C15	−1.2 (11)
C6—C5—C5'—C4A'	−74.8 (8)	C1—C11—C16—C15	175.9 (7)
C4A—C5—C5'—C6'	−78.8 (8)	C14—C15—C16—C11	1.3 (12)
C6—C5—C5'—C6'	104.8 (7)	C6'—C5'—C4A'—C8A'	1.1 (10)
C4A—C5—C6—C7	−4.4 (9)	C5—C5'—C4A'—C8A'	−179.3 (6)
C5'—C5—C6—C7	172.1 (6)	C6'—C5'—C4A'—C4'	−178.4 (7)
C4A—C5—C6—O6	−179.8 (6)	C5—C5'—C4A'—C4'	1.3 (10)
C5'—C5—C6—O6	−3.3 (9)	C3'—C4'—C4A'—C8A'	−20.3 (10)
C4A'—C5'—C6'—C7'	0.5 (10)	C3'—C4'—C4A'—C5'	159.2 (7)
C5—C5'—C6'—C7'	−179.2 (6)	C5'—C4A'—C8A'—C8'	−2.2 (10)
O6—C6—C7—O7	0.1 (10)	C4'—C4A'—C8A'—C8'	177.3 (6)
C5—C6—C7—O7	−175.2 (6)	C5'—C4A'—C8A'—C1'	−179.3 (6)
O6—C6—C7—C8	−179.1 (6)	C4'—C4A'—C8A'—C1'	0.2 (10)
C5—C6—C7—C8	5.6 (10)	O8'—C8'—C8A'—C4A'	−171.8 (6)
C5'—C6'—C7'—O7'	176.2 (6)	C7'—C8'—C8A'—C4A'	1.8 (10)
C5'—C6'—C7'—C8'	−0.9 (10)	O8'—C8'—C8A'—C1'	5.3 (10)
C6—C7—C8—O8	175.1 (6)	C7'—C8'—C8A'—C1'	178.9 (7)
O7—C7—C8—O8	−4.1 (10)	O2'—C1'—C8A'—C4A'	−12.4 (10)
C6—C7—C8—C8A	−2.4 (10)	O2'—C1'—C8A'—C8'	170.5 (6)

O7—C7—C8—C8A	178.4 (6)	C30—C3—O2—C1	169.2 (6)
C6'—C7'—C8'—O8'	173.1 (7)	C4—C3—O2—C1	−67.6 (7)
O7'—C7'—C8'—O8'	−4.2 (10)	C8A—C1—O2—C3	52.0 (7)
C6'—C7'—C8'—C8A'	−0.2 (10)	C11—C1—O2—C3	−76.3 (7)
O7'—C7'—C8'—C8A'	−177.5 (6)	C30'—C3'—O2'—C1'	169.0 (8)
O8—C8—C8A—C4A	−179.4 (6)	C4'—C3'—O2'—C1'	−67.6 (9)
C7—C8—C8A—C4A	−1.8 (10)	C8A'—C1'—O2'—C3'	46.4 (9)
O8—C8—C8A—C1	3.0 (9)	C7—C6—O6—C60	68.8 (9)
C7—C8—C8A—C1	−179.4 (6)	C5—C6—O6—C60	−115.8 (7)
C5—C4A—C8A—C8	2.9 (9)	C6—C7—O7—C70	70.3 (9)
C4—C4A—C8A—C8	−173.6 (6)	C8—C7—O7—C70	−110.5 (8)
C5—C4A—C8A—C1	−179.5 (6)	C6'—C7'—O7'—C70'	−7.5 (11)
C4—C4A—C8A—C1	3.9 (9)	C8'—C7'—O7'—C70'	169.8 (8)
O2—C1—C8A—C8	157.9 (6)	C7—C8—O8—C80	64.6 (11)
C11—C1—C8A—C8	−76.1 (8)	C8A—C8—O8—C80	−117.8 (9)
O2—C1—C8A—C4A	−19.7 (8)	C7'—C8'—O8'—C80'	67.2 (9)
C11—C1—C8A—C4A	106.3 (7)	C8A'—C8'—O8'—C80'	−119.2 (8)
O2—C1—C11—C12	−50.5 (8)		



**Figure S270.** ORTEP view of (aS,1R,3R,3'R)-**21** at 50% probability level with numbering scheme.



**Table S3.** Geometric parameters (Å, °) for (a*S*,1*R*,3*R*,3'*R*)-**21**.

Distances (Å)			
C1—O2	1.425 (6)	C8'—C8A'	1.389 (8)
C1—C8A	1.508 (7)	C11—C16	1.367 (7)
C1—C11	1.533 (7)	C11—C12	1.384 (8)
C1—H1	0.9800	C12—C13	1.384 (8)
C1'—O2'	1.429 (8)	C12—H12	0.9300
C1'—C8A'	1.504 (8)	C13—C14	1.341 (9)
C1'—H1'A	0.9700	C13—H13	0.9300
C1'—H1'B	0.9700	C14—F14	1.361 (7)
C3—O2	1.433 (5)	C14—C15	1.371 (9)
C3—C30	1.505 (8)	C15—C16	1.367 (9)
C3—C4	1.518 (7)	C15—H15	0.9300
C3—H3	0.9800	C16—H16	0.9300
C3'—O2'	1.440 (8)	C30—H30A	0.9600
C3'—C4'	1.484 (8)	C30—H30B	0.9600
C3'—C30'	1.502 (10)	C30—H30C	0.9600
C3'—H3'	0.9800	C30'—H30D	0.9600
C4—C4A	1.507 (7)	C30'—H30E	0.9600
C4—H4A	0.9700	C30'—H30F	0.9600
C4—H4B	0.9700	C60—O6	1.436 (7)
C4'—C4A'	1.502 (8)	C60—H60A	0.9600
C4'—H4'A	0.9700	C60—H60B	0.9600
C4'—H4'B	0.9700	C60—H60C	0.9600
C5—C6	1.385 (7)	C70—O7	1.411 (8)
C5—C4A	1.396 (7)	C70—H70A	0.9600
C5—C5'	1.495 (6)	C70—H70B	0.9600
C4A—C8A	1.402 (6)	C70—H70C	0.9600
C5'—C6'	1.386 (7)	C70'—O7'	1.396 (9)
C5'—C4A'	1.394 (7)	C70'—H70D	0.9600
C6—O6	1.378 (6)	C70'—H70E	0.9600
C6—C7	1.409 (6)	C70'—H70F	0.9600
C6'—C7'	1.382 (6)	C80—O8	1.379 (9)
C6'—H6'	0.9300	C80—H80D	0.9600

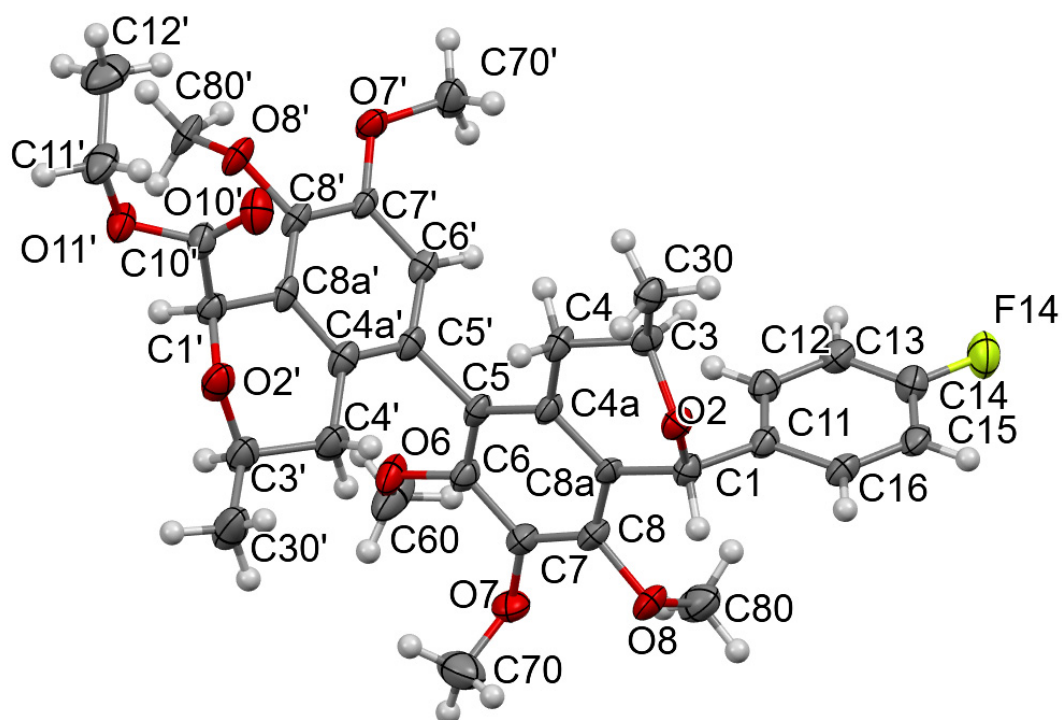
C7—C8	1.368 (7)	C80—H80E	0.9600
C7—O7	1.370 (6)	C80—H80F	0.9600
C7'—C8'	1.387 (8)	C80'—O8'	1.413 (8)
C7'—O7'	1.387 (7)	C80'—H80A	0.9600
C8—O8	1.376 (5)	C80'—H80B	0.9600
C8—C8A	1.387 (7)	C80'—H80C	0.9600
C8'—O8'	1.380 (6)	C4A'—C8A'	1.394 (6)
Angles (°)			
O2—C1—C8A	111.6 (4)	C13—C12—H12	120.3000
O2—C1—C11	110.7 (4)	C11—C12—H12	120.3000
C8A—C1—C11	113.8 (4)	C14—C13—C12	119.6 (6)
O2—C1—H1	106.8000	C14—C13—H13	120.2000
C8A—C1—H1	106.8000	C12—C13—H13	120.2000
C11—C1—H1	106.8000	C13—C14—F14	120.3 (6)
O2'—C1'—C8A'	113.4 (4)	C13—C14—C15	122.3 (5)
O2'—C1'—H1'A	108.9000	F14—C14—C15	117.4 (6)
C8A'—C1'—H1'A	108.9000	C16—C15—C14	117.7 (5)
O2'—C1'—H1'B	108.9000	C16—C15—H15	121.1000
C8A'—C1'—H1'B	108.9000	C14—C15—H15	121.1000
H1'A—C1'—H1'B	107.7000	C15—C16—C11	122.0 (5)
O2—C3—C30	107.6 (5)	C15—C16—H16	119.0000
O2—C3—C4	109.1 (4)	C11—C16—H16	119.0000
C30—C3—C4	113.3 (5)	C3—C30—H30A	109.5000
O2—C3—H3	108.9000	C3—C30—H30B	109.5000
C30—C3—H3	108.9000	H30A—C30—H30B	109.5000
C4—C3—H3	108.9000	C3—C30—H30C	109.5000
O2'—C3'—C4'	108.3 (5)	H30A—C30—H30C	109.5000
O2'—C3'—C30'	107.6 (6)	H30B—C30—H30C	109.5000
C4'—C3'—C30'	113.3 (6)	C3'—C30'—H30D	109.5000
O2'—C3'—H3'	109.2000	C3'—C30'—H30E	109.5000
C4'—C3'—H3'	109.2000	H30D—C30'—H30E	109.5000
C30'—C3'—H3'	109.2000	C3'—C30'—H30F	109.5000
C4A—C4—C3	112.7 (4)	H30D—C30'—H30F	109.5000
C4A—C4—H4A	109.1000	H30E—C30'—H30F	109.5000
C3—C4—H4A	109.1000	O6—C60—H60A	109.5000

C4A—C4—H4B	109.1000	O6—C60—H60B	109.5000
C3—C4—H4B	109.1000	H60A—C60—H60B	109.5000
H4A—C4—H4B	107.8000	O6—C60—H60C	109.5000
C3'—C4'—C4A'	112.7 (5)	H60A—C60—H60C	109.5000
C3'—C4'—H4'A	109.0000	H60B—C60—H60C	109.5000
C4A'—C4'—H4'A	109.0000	O7—C70—H70A	109.5000
C3'—C4'—H4'B	109.0000	O7—C70—H70B	109.5000
C4A'—C4'—H4'B	109.0000	H70A—C70—H70B	109.5000
H4'A—C4'—H4'B	107.8000	O7—C70—H70C	109.5000
C6—C5—C4A	119.0 (4)	H70A—C70—H70C	109.5000
C6—C5—C5'	118.9 (4)	H70B—C70—H70C	109.5000
C4A—C5—C5'	122.0 (4)	O7'—C70'—H70D	109.5000
C5—C4A—C8A	120.0 (4)	O7'—C70'—H70E	109.5000
C5—C4A—C4	121.2 (4)	H70D—C70'—H70E	109.5000
C8A—C4A—C4	118.6 (4)	O7'—C70'—H70F	109.5000
C6'—C5'—C4A'	120.5 (4)	H70D—C70'—H70F	109.5000
C6'—C5'—C5	120.7 (4)	H70E—C70'—H70F	109.5000
C4A'—C5'—C5	118.7 (4)	O8—C80—H80D	109.5000
O6—C6—C5	119.3 (4)	O8—C80—H80E	109.5000
O6—C6—C7	119.4 (4)	H80D—C80—H80E	109.5000
C5—C6—C7	121.2 (4)	O8—C80—H80F	109.5000
C7'—C6'—C5'	120.2 (5)	H80D—C80—H80F	109.5000
C7'—C6'—H6'	119.9000	H80E—C80—H80F	109.5000
C5'—C6'—H6'	119.9000	O8'—C80'—H80A	109.5000
C8—C7—O7	121.0 (4)	O8'—C80'—H80B	109.5000
C8—C7—C6	118.5 (4)	H80A—C80'—H80B	109.5000
O7—C7—C6	120.5 (4)	O8'—C80'—H80C	109.5000
C6'—C7'—C8'	119.7 (5)	H80A—C80'—H80C	109.5000
C6'—C7'—O7'	123.9 (5)	H80B—C80'—H80C	109.5000
C8'—C7'—O7'	116.4 (4)	C8A'—C4A'—C5'	119.0 (5)
C7—C8—O8	121.5 (5)	C8A'—C4A'—C4'	118.6 (5)
C7—C8—C8A	121.7 (4)	C5'—C4A'—C4'	122.4 (4)
O8—C8—C8A	116.8 (4)	C8'—C8A'—C4A'	120.1 (5)
O8'—C8'—C7'	122.1 (5)	C8'—C8A'—C1'	119.1 (4)
O8'—C8'—C8A'	117.0 (5)	C4A'—C8A'—C1'	120.8 (5)

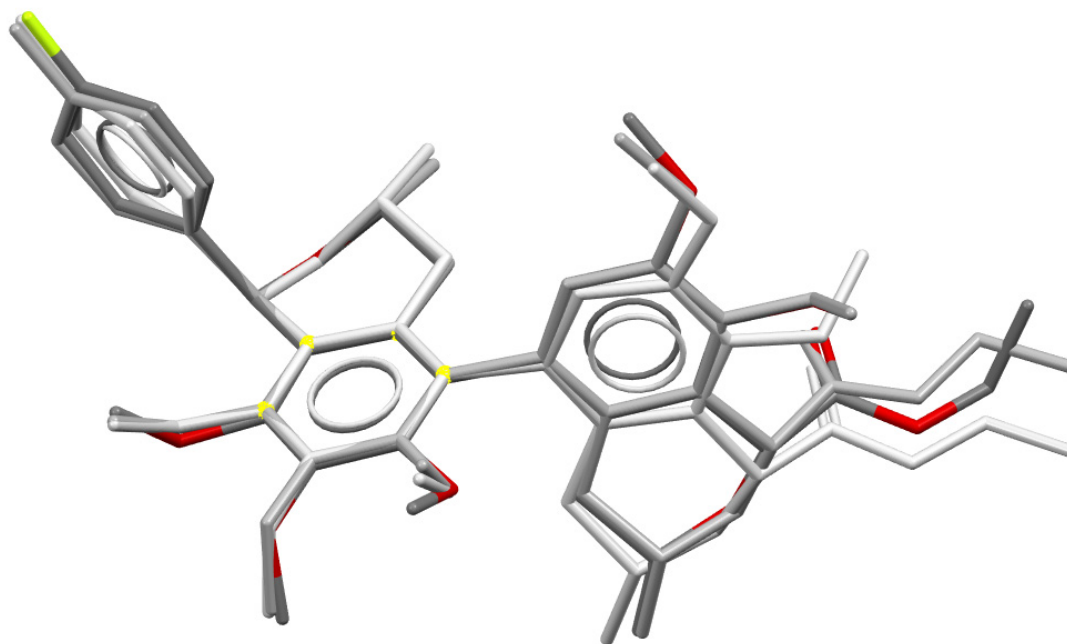
C7'—C8'—C8A'	120.5 (4)	C1—O2—C3	112.4 (4)
C8—C8A—C4A	119.3 (4)	C1'—O2'—C3'	111.9 (5)
C8—C8A—C1	119.0 (4)	C6—O6—C60	114.2 (4)
C4A—C8A—C1	121.6 (4)	C7—O7—C70	114.7 (5)
C16—C11—C12	118.8 (5)	C7'—O7'—C70'	117.4 (4)
C16—C11—C1	118.0 (4)	C8—O8—C80	118.7 (6)
C12—C11—C1	123.1 (4)	C8'—O8'—C80'	117.5 (5)
C13—C12—C11	119.5 (5)		
Torsion angles (°)			
O2—C3—C4—C4A	−48.3 (6)	C8A—C1—C11—C16	177.2 (4)
C30—C3—C4—C4A	−168.2 (5)	O2—C1—C11—C12	−132.0 (5)
O2'—C3'—C4'—C4A'	−52.7 (7)	C8A—C1—C11—C12	−5.4 (6)
C30'—C3'—C4'—C4A'	−172.0 (6)	C16—C11—C12—C13	1.5 (7)
C6—C5—C4A—C8A	−0.5 (7)	C1—C11—C12—C13	−175.9 (5)
C5'—C5—C4A—C8A	176.9 (4)	C11—C12—C13—C14	−0.8 (8)
C6—C5—C4A—C4	−176.4 (5)	C12—C13—C14—F14	−179.6 (5)
C5'—C5—C4A—C4	0.9 (7)	C12—C13—C14—C15	0.1 (9)
C3—C4—C4A—C5	−166.1 (5)	C13—C14—C15—C16	−0.2 (9)
C3—C4—C4A—C8A	17.9 (7)	F14—C14—C15—C16	179.5 (5)
C6—C5—C5'—C6'	−105.2 (6)	C14—C15—C16—C11	1.1 (9)
C4A—C5—C5'—C6'	77.5 (7)	C12—C11—C16—C15	−1.7 (8)
C6—C5—C5'—C4A'	75.1 (6)	C1—C11—C16—C15	175.8 (5)
C4A—C5—C5'—C4A'	−102.2 (5)	C6'—C5'—C4A'—C8A'	0.7 (8)
C4A—C5—C6—O6	−179.5 (4)	C5—C5'—C4A'—C8A'	−179.6 (5)
C5'—C5—C6—O6	3.1 (7)	C6'—C5'—C4A'—C4'	178.3 (5)

C4A—C5—C6—C7	4.1 (7)	C5—C5'—C4A'—C4'	−2.0 (7)
C5'—C5—C6—C7	−173.3 (4)	C3'—C4'—C4A'—C8A'	19.2 (7)
C4A'—C5'—C6'—C7'	−2.3 (8)	C3'—C4'—C4A'—C5'	−158.4 (5)
C5—C5'—C6'—C7'	178.1 (5)	O8'—C8'—C8A'—C4A'	172.9 (5)
O6—C6—C7—C8	179.0 (4)	C7'—C8'—C8A'—C4A'	−0.4 (8)
C5—C6—C7—C8	−4.6 (7)	O8'—C8'—C8A'—C1'	−6.2 (7)
O6—C6—C7—O7	−1.5 (7)	C7'—C8'—C8A'—C1'	−179.5 (5)
C5—C6—C7—O7	174.9 (4)	C5'—C4A'—C8A'—C8'	0.6 (7)
C5'—C6'—C7'—C8'	2.5 (8)	C4'—C4A'—C8A'—C8'	−177.1 (5)
C5'—C6'—C7'—O7'	−175.8 (5)	C5'—C4A'—C8A'—C1'	179.7 (5)
O7—C7—C8—O8	5.1 (7)	C4'—C4A'—C8A'—C1'	2.0 (8)
C6—C7—C8—O8	−175.4 (5)	O2'—C1'—C8A'—C8'	−169.9 (5)
O7—C7—C8—C8A	−178.0 (5)	O2'—C1'—C8A'—C4A'	11.0 (8)
C6—C7—C8—C8A	1.5 (7)	C8A—C1—O2—C3	−52.3 (5)
C6'—C7'—C8'—O8'	−174.1 (5)	C11—C1—O2—C3	75.6 (5)
O7'—C7'—C8'—O8'	4.3 (8)	C30—C3—O2—C1	−168.7 (5)
C6'—C7'—C8'—C8A'	−1.2 (8)	C4—C3—O2—C1	68.0 (6)
O7'—C7'—C8'—C8A'	177.3 (5)	C8A'—C1'—O2'—C3'	−46.4 (7)
C7—C8—C8A—C4A	2.0 (7)	C4'—C3'—O2'—C1'	68.2 (6)
O8—C8—C8A—C4A	179.0 (4)	C30'—C3'—O2'—C1'	−169.1 (6)
C7—C8—C8A—C1	179.2 (5)	C5—C6—O6—C60	115.4 (5)
O8—C8—C8A—C1	−3.7 (7)	C7—C6—O6—C60	−68.1 (6)
C5—C4A—C8A—C8	−2.5 (7)	C8—C7—O7—C70	111.2 (6)
C4—C4A—C8A—C8	173.5 (5)	C6—C7—O7—C70	−68.3 (7)
C5—C4A—C8A—C1	−179.7 (4)	C6'—C7'—O7'—C70'	8.3 (9)
C4—C4A—C8A—C1	−3.6 (7)	C8'—C7'—O7'—C70'	−170.0 (6)

O2—C1—C8A—C8	−157.6 (4)	C7—C8—O8—C80	−65.1 (9)
C11—C1—C8A—C8	76.2 (5)	C8A—C8—O8—C80	117.9 (7)
O2—C1—C8A—C4A	19.6 (6)	C7'—C8'—O8'—C80'	−66.9 (7)
C11—C1—C8A—C4A	−106.6 (5)	C8A'—C8'—O8'—C80'	119.9 (6)
O2—C1—C11—C16	50.5 (5)		



**Figure S271.** ORTEP view of (*aS,1R,3R,1'R,3'R*)-**22** at 50% probability level with numbering scheme. Only one molecule from the asymmetric unit is shown and solvent molecules are omitted for clarity. The numbering of the other molecules were systematically changed; *e.g.* C1 corresponds to C21 and C31.



**Figure S272.** Overlay of the three isomers of in the asymmetric unit of structure (aS,1*R*,3*R*,1'*R*,3'*R*)-**22**.

**Table S4.** Geometric parameters (Å, °) for (aS,1*R*,3*R*,1'*R*,3'*R*)-**22**.

Distances (Å)			
C1—O2	1.424 (15)	C35—H35	0.9500
C1—C11	1.522 (17)	C36—H36	0.9500
C1—C8A	1.533 (17)	C41—O42	1.431 (14)
C1—H1	1.0000	C41—C51	1.500 (17)
C1'—O2'	1.428 (14)	C41—C48E	1.514 (17)
C1'—C10'	1.510 (18)	C41—H41	1.0000
C1'—C8A'	1.512 (17)	C41'—O42'	1.422 (15)
C1'—H1'	1.0000	C41'—C48F	1.525 (16)
C3—O2	1.447 (14)	C41'—C50D	1.530 (18)
C3—C30	1.504 (18)	C41'—H41'	1.0000
C3—C4	1.530 (17)	C43—O42	1.456 (14)
C3—H3	1.0000	C43—C44	1.527 (17)
C3'—O2'	1.457 (17)	C43—H43	1.0000
C3'—C30'	1.503 (19)	C43'—O42'	1.433 (15)
C3'—C4'	1.523 (18)	C43'—C44'	1.526 (16)
C3'—H3'	1.0000	C43'—H43'	1.0000

C4—C4A	1.502 (17)	C44—C44E	1.519 (17)
C4—H4A	0.9900	C44—H44A	0.9900
C4—H4B	0.9900	C44—H44B	0.9900
C4'—C4A'	1.508 (18)	C44'—C44F	1.481 (17)
C4'—H4'A	0.9900	C44'—H44C	0.9900
C4'—H4'B	0.9900	C44'—H44D	0.9900
C5—C6	1.396 (17)	C45—C46	1.390 (17)
C5—C4A	1.401 (17)	C45—C44E	1.405 (17)
C5—C5'	1.533 (17)	C45—C45'	1.506 (16)
C4A—C8A	1.399 (16)	C44E—C48E	1.389 (16)
C5'—C4A'	1.365 (18)	C44F—C45'	1.401 (16)
C5'—C6'	1.398 (18)	C44F—C48F	1.421 (16)
C6—O6	1.380 (15)	C45'—C46'	1.391 (17)
C6—C7	1.389 (17)	C46—C47	1.376 (17)
C6'—C7'	1.400 (16)	C46—O46	1.385 (14)
C6'—H6'	0.9500	C46'—C47'	1.367 (17)
C7—O7	1.379 (15)	C46'—H46'	0.9500
C7—C8	1.386 (18)	C47—O47	1.368 (15)
C7'—O7'	1.375 (15)	C47—C48	1.418 (17)
C7'—C8'	1.385 (17)	C47'—O47'	1.387 (15)
C8—C8A	1.368 (17)	C47'—C48'	1.402 (17)
C8—O8	1.418 (15)	C48—C48E	1.383 (17)
C8'—C8A'	1.368 (18)	C48—O48	1.386 (14)
C8'—O8'	1.404 (14)	C48'—C48F	1.387 (16)
C10'—O10'	1.198 (15)	C48'—O48'	1.405 (14)
C10'—O11'	1.336 (15)	C51—C56	1.387 (18)
C11—C12	1.372 (18)	C51—C52	1.394 (17)
C11—C16	1.416 (17)	C50D—O50D	1.201 (15)
C11'—O11'	1.463 (16)	C50D—O51D	1.334 (15)
C11'—C12'	1.53 (2)	C52—C53	1.413 (18)
C11'—H11A	0.9900	C52—H52	0.9500
C11'—H11B	0.9900	C51D—C52D	1.47 (2)
C12—C13	1.384 (18)	C51D—O51D	1.466 (16)
C12—H12	0.9500	C51D—H51A	0.9900
C12'—H12A	0.9800	C51D—H51B	0.9900



C12'—H12B	0.9800	C53—C54	1.347 (19)
C12'—H12C	0.9800	C53—H53	0.9500
C13—C14	1.380 (19)	C52D—H52A	0.9800
C13—H13	0.9500	C52D—H52B	0.9800
C14—C15	1.355 (19)	C52D—H52C	0.9800
C14—F14	1.366 (15)	C54—F54	1.370 (16)
C15—C16	1.375 (18)	C54—C55	1.386 (19)
C15—H15	0.9500	C55—C56	1.396 (19)
C16—H16	0.9500	C55—H55	0.9500
C21—O22	1.443 (15)	C56—H56	0.9500
C21—C28B	1.512 (17)	C60—O6	1.441 (17)
C21—C31	1.517 (17)	C60—H60A	0.9800
C21—H21	1.0000	C60—H60B	0.9800
C21'—O22'	1.420 (14)	C60—H60C	0.9800
C21'—C28C	1.492 (16)	C60B—O26	1.433 (15)
C21'—C30D	1.517 (18)	C60B—H60D	0.9800
C21'—H21'	1.0000	C60B—H60E	0.9800
C23—O22	1.445 (14)	C60B—H60F	0.9800
C23—C30B	1.508 (18)	C60C—O46	1.430 (14)
C23—C24	1.523 (16)	C60C—H60G	0.9800
C23—H23	1.0000	C60C—H60H	0.9800
C23'—O22'	1.436 (14)	C60C—H60I	0.9800
C23'—C24'	1.483 (17)	C70—O7	1.433 (17)
C23'—C30C	1.509 (17)	C70—H70A	0.9800
C23'—H23'	1.0000	C70—H70B	0.9800
C24—C24B	1.496 (17)	C70—H70C	0.9800
C24—H24A	0.9900	C70'—O7'	1.432 (15)
C24—H24B	0.9900	C70'—H70D	0.9800
C24'—C24C	1.505 (16)	C70'—H70E	0.9800
C24'—H24C	0.9900	C70'—H70F	0.9800
C24'—H24D	0.9900	C70B—O27	1.424 (16)
C25—C26	1.394 (17)	C70B—H70G	0.9800
C25—C24B	1.409 (16)	C70B—H70H	0.9800
C25—C25'	1.525 (16)	C70B—H70I	0.9800
C24B—C28B	1.387 (16)	C70C—O27'	1.437 (15)

C24C—C25'	1.400 (16)	C70C—H70J	0.9800
C24C—C28C	1.412 (16)	C70C—H70K	0.9800
C25'—C26'	1.391 (17)	C70C—H70L	0.9800
C26—O26	1.383 (14)	C70E—O47	1.425 (15)
C26—C27	1.397 (17)	C70E—H70M	0.9800
C26'—C27'	1.396 (17)	C70E—H70N	0.9800
C26'—H26'	0.9500	C70E—H70O	0.9800
C27—C28	1.380 (17)	C70F—O47'	1.439 (15)
C27—O27	1.383 (15)	C70F—H70P	0.9800
C27'—C28'	1.383 (17)	C70F—H70Q	0.9800
C27'—O27'	1.384 (14)	C70F—H70R	0.9800
C28—O28	1.385 (14)	C80—O8	1.422 (16)
C28—C28B	1.402 (17)	C80—H80A	0.9800
C28'—C28C	1.396 (17)	C80—H80B	0.9800
C28'—O28'	1.399 (14)	C80—H80C	0.9800
C30—H30A	0.9800	C80'—O8'	1.440 (15)
C30—H30B	0.9800	C80'—H80D	0.9800
C30—H30C	0.9800	C80'—H80E	0.9800
C30'—H30D	0.9800	C80'—H80F	0.9800
C30'—H30E	0.9800	C81—O81	1.422 (18)
C30'—H30F	0.9800	C81—C82	1.53 (2)
C31—C36	1.374 (17)	C81—H81A	0.9900
C31—C32	1.418 (17)	C81—H81B	0.9900
C30B—H30G	0.9800	C80B—O28	1.442 (16)
C30B—H30H	0.9800	C80B—H80G	0.9800
C30B—H30I	0.9800	C80B—H80H	0.9800
C30C—H30J	0.9800	C80B—H80I	0.9800
C30C—H30K	0.9800	C80C—O28'	1.425 (15)
C30C—H30L	0.9800	C80C—H80J	0.9800
C30D—O30D	1.222 (16)	C80C—H80K	0.9800
C30D—O31D	1.340 (15)	C80C—H80L	0.9800
C30E—C43	1.483 (18)	C80E—O48	1.442 (15)
C30E—H30M	0.9800	C80E—H80M	0.9800
C30E—H30N	0.9800	C80E—H80N	0.9800
C30E—H30O	0.9800	C80E—H80O	0.9800

C30F—C43'	1.513 (17)	C80F—O48'	1.425 (15)
C30F—H30P	0.9800	C80F—H80P	0.9800
C30F—H30Q	0.9800	C80F—H80Q	0.9800
C30F—H30R	0.9800	C80F—H80R	0.9800
C32—C33	1.385 (18)	C82—H82A	0.9800
C32—H32	0.9500	C82—H82B	0.9800
C31D—O31D	1.471 (16)	C82—H82C	0.9800
C31D—C32D	1.51 (2)	C91—C92	1.32 (3)
C31D—H31A	0.9900	C91—O91	1.34 (2)
C31D—H31B	0.9900	C91—H91A	0.9900
C33—C34	1.368 (18)	C91—H91B	0.9900
C33—H33	0.9500	C92—H92A	0.9800
C32D—H32A	0.9800	C92—H92B	0.9800
C32D—H32B	0.9800	C92—H92C	0.9800
C32D—H32C	0.9800	C4A'—C8A'	1.416 (17)
C34—F34	1.372 (15)	O81—H81	0.8500 (15)
C34—C35	1.395 (18)	O91—H91	0.8400
C35—C36	1.369 (17)		
Angles (°)			
O2—C1—C11	111.3 (10)	O42'—C41'—C48F	112.9 (10)
O2—C1—C8A	112.7 (10)	O42'—C41'—C50D	104.4 (10)
C11—C1—C8A	113.1 (11)	C48F—C41'—C50D	110.0 (10)
O2—C1—H1	106.4000	O42'—C41'—H41'	109.8000
C11—C1—H1	106.4000	C48F—C41'—H41'	109.8000
C8A—C1—H1	106.4000	C50D—C41'—H41'	109.8000
O2'—C1'—C10'	102.8 (10)	O42—C43—C30E	106.5 (10)
O2'—C1'—C8A'	113.6 (10)	O42—C43—C44	108.8 (10)
C10'—C1'—C8A'	112.3 (11)	C30E—C43—C44	112.5 (11)
O2'—C1'—H1'	109.3000	O42—C43—H43	109.7000
C10'—C1'—H1'	109.3000	C30E—C43—H43	109.7000
C8A'—C1'—H1'	109.3000	C44—C43—H43	109.7000
O2—C3—C30	105.7 (10)	O42'—C43'—C30F	106.0 (10)
O2—C3—C4	110.0 (10)	O42'—C43'—C44'	109.1 (10)
C30—C3—C4	112.4 (11)	C30F—C43'—C44'	111.5 (10)
O2—C3—H3	109.6000	O42'—C43'—H43'	110.0000

C30—C3—H3	109.6000	C30F—C43'—H43'	110.0000
C4—C3—H3	109.6000	C44'—C43'—H43'	110.0000
O2'—C3'—C30'	105.7 (12)	C44E—C44—C43	113.6 (10)
O2'—C3'—C4'	108.7 (11)	C44E—C44—H44A	108.8000
C30'—C3'—C4'	114.2 (12)	C43—C44—H44A	108.8000
O2'—C3'—H3'	109.4000	C44E—C44—H44B	108.8000
C30'—C3'—H3'	109.4000	C43—C44—H44B	108.8000
C4'—C3'—H3'	109.4000	H44A—C44—H44B	107.7000
C4A—C4—C3	113.1 (10)	C44F—C44'—C43'	110.8 (10)
C4A—C4—H4A	109.0000	C44F—C44'—H44C	109.5000
C3—C4—H4A	109.0000	C43'—C44'—H44C	109.5000
C4A—C4—H4B	109.0000	C44F—C44'—H44D	109.5000
C3—C4—H4B	109.0000	C43'—C44'—H44D	109.5000
H4A—C4—H4B	107.8000	H44C—C44'—H44D	108.1000
C4A'—C4'—C3'	111.7 (11)	C46—C45—C44E	119.4 (11)
C4A'—C4'—H4'A	109.3000	C46—C45—C45'	120.5 (11)
C3'—C4'—H4'A	109.3000	C44E—C45—C45'	120.1 (11)
C4A'—C4'—H4'B	109.3000	C48E—C44E—C45	119.6 (11)
C3'—C4'—H4'B	109.3000	C48E—C44E—C44	119.8 (11)
H4'A—C4'—H4'B	107.9000	C45—C44E—C44	120.6 (11)
C6—C5—C4A	120.3 (11)	C45'—C44F—C48F	118.2 (11)
C6—C5—C5'	120.0 (11)	C45'—C44F—C44'	122.2 (11)
C4A—C5—C5'	119.5 (11)	C48F—C44F—C44'	119.7 (10)
C8A—C4A—C5	119.1 (11)	C46'—C45'—C44F	120.8 (11)
C8A—C4A—C4	120.4 (11)	C46'—C45'—C45	120.1 (10)
C5—C4A—C4	120.5 (11)	C44F—C45'—C45	119.1 (11)
C4A'—C5'—C6'	122.0 (12)	C47—C46—O46	118.6 (11)
C4A'—C5'—C5	120.2 (12)	C47—C46—C45	122.0 (11)
C6'—C5'—C5	117.7 (11)	O46—C46—C45	119.3 (10)
O6—C6—C7	122.7 (11)	C47'—C46'—C45'	120.6 (12)
O6—C6—C5	116.9 (11)	C47'—C46'—H46'	119.7000
C7—C6—C5	120.3 (12)	C45'—C46'—H46'	119.7000
C5'—C6'—C7'	118.8 (12)	O47—C47—C46	122.1 (11)
C5'—C6'—H6'	120.6000	O47—C47—C48	119.9 (11)
C7'—C6'—H6'	120.6000	C46—C47—C48	118.0 (11)

O7—C7—C8	119.8 (11)	C46'—C47'—O47'	125.1 (11)
O7—C7—C6	122.2 (12)	C46'—C47'—C48'	120.2 (12)
C8—C7—C6	118.0 (12)	O47'—C47'—C48'	114.7 (10)
O7'—C7'—C8'	116.7 (10)	C48E—C48—O48	117.4 (11)
O7'—C7'—C6'	124.1 (11)	C48E—C48—C47	120.8 (11)
C8'—C7'—C6'	119.2 (12)	O48—C48—C47	121.6 (11)
C8A—C8—C7	123.1 (12)	C48F—C48'—C47'	120.1 (11)
C8A—C8—O8	117.6 (11)	C48F—C48'—O48'	117.3 (10)
C7—C8—O8	119.0 (11)	C47'—C48'—O48'	122.5 (11)
C8A'—C8'—C7'	121.5 (11)	C48—C48E—C44E	120.2 (11)
C8A'—C8'—O8'	117.6 (11)	C48—C48E—C41	118.4 (11)
C7'—C8'—O8'	120.7 (11)	C44E—C48E—C41	121.3 (11)
C8—C8A—C4A	118.9 (11)	C48'—C48F—C44F	120.1 (11)
C8—C8A—C1	121.2 (11)	C48'—C48F—C41'	119.2 (10)
C4A—C8A—C1	119.7 (11)	C44F—C48F—C41'	120.6 (10)
O10'—C10'—O11'	124.0 (13)	C56—C51—C52	117.2 (12)
O10'—C10'—C1'	125.1 (12)	C56—C51—C41	123.7 (11)
O11'—C10'—C1'	110.8 (11)	C52—C51—C41	119.1 (11)
C12—C11—C16	116.9 (13)	O50D—C50D—O51D	124.5 (12)
C12—C11—C1	124.9 (12)	O50D—C50D—C41'	123.5 (12)
C16—C11—C1	118.0 (12)	O51D—C50D—C41'	111.9 (11)
O11'—C11'—C12'	110.1 (12)	C51—C52—C53	122.4 (13)
O11'—C11'—H11A	109.6000	C51—C52—H52	118.8000
C12'—C11'—H11A	109.6000	C53—C52—H52	118.8000
O11'—C11'—H11B	109.6000	C52D—C51D—O51D	107.4 (13)
C12'—C11'—H11B	109.6000	C52D—C51D—H51A	110.2000
H11A—C11'—H11B	108.2000	O51D—C51D—H51A	110.2000
C11—C12—C13	122.5 (13)	C52D—C51D—H51B	110.2000
C11—C12—H12	118.8000	O51D—C51D—H51B	110.2000
C13—C12—H12	118.8000	H51A—C51D—H51B	108.5000
C11'—C12'—H12A	109.5000	C54—C53—C52	116.9 (13)
C11'—C12'—H12B	109.5000	C54—C53—H53	121.6000
H12A—C12'—H12B	109.5000	C52—C53—H53	121.6000
C11'—C12'—H12C	109.5000	C51D—C52D—H52A	109.5000
H12A—C12'—H12C	109.5000	C51D—C52D—H52B	109.5000

H12B—C12'—H12C	109.5000	H52A—C52D—H52B	109.5000
C14—C13—C12	118.0 (13)	C51D—C52D—H52C	109.5000
C14—C13—H13	121.0000	H52A—C52D—H52C	109.5000
C12—C13—H13	121.0000	H52B—C52D—H52C	109.5000
C15—C14—F14	119.6 (12)	C53—C54—F54	118.1 (13)
C15—C14—C13	122.3 (14)	C53—C54—C55	124.1 (13)
F14—C14—C13	118.2 (13)	F54—C54—C55	117.8 (13)
C14—C15—C16	118.9 (13)	C54—C55—C56	117.3 (13)
C14—C15—H15	120.6000	C54—C55—H55	121.3000
C16—C15—H15	120.6000	C56—C55—H55	121.3000
C15—C16—C11	121.5 (13)	C51—C56—C55	122.1 (13)
C15—C16—H16	119.3000	C51—C56—H56	119.0000
C11—C16—H16	119.3000	C55—C56—H56	119.0000
O22—C21—C28B	110.5 (9)	O6—C60—H60A	109.5000
O22—C21—C31	110.7 (10)	O6—C60—H60B	109.5000
C28B—C21—C31	114.0 (10)	H60A—C60—H60B	109.5000
O22—C21—H21	107.1000	O6—C60—H60C	109.5000
C28B—C21—H21	107.1000	H60A—C60—H60C	109.5000
C31—C21—H21	107.1000	H60B—C60—H60C	109.5000
O22'—C21'—C28C	113.7 (10)	O26—C60B—H60D	109.5000
O22'—C21'—C30D	102.7 (10)	O26—C60B—H60E	109.5000
C28C—C21'—C30D	112.7 (10)	H60D—C60B—H60E	109.5000
O22'—C21'—H21'	109.2000	O26—C60B—H60F	109.5000
C28C—C21'—H21'	109.2000	H60D—C60B—H60F	109.5000
C30D—C21'—H21'	109.2000	H60E—C60B—H60F	109.5000
O22—C23—C30B	106.5 (10)	O46—C60C—H60G	109.5000
O22—C23—C24	108.3 (10)	O46—C60C—H60H	109.5000
C30B—C23—C24	113.0 (11)	H60G—C60C—H60H	109.5000
O22—C23—H23	109.7000	O46—C60C—H60I	109.5000
C30B—C23—H23	109.7000	H60G—C60C—H60I	109.5000
C24—C23—H23	109.7000	H60H—C60C—H60I	109.5000
O22'—C23'—C24'	109.6 (10)	O7—C70—H70A	109.5000
O22'—C23'—C30C	107.3 (10)	O7—C70—H70B	109.5000
C24'—C23'—C30C	113.2 (11)	H70A—C70—H70B	109.5000
O22'—C23'—H23'	108.9000	O7—C70—H70C	109.5000

C24'—C23'—H23'	108.9000	H70A—C70—H70C	109.5000
C30C—C23'—H23'	108.9000	H70B—C70—H70C	109.5000
C24B—C24—C23	112.5 (10)	O7'—C70'—H70D	109.5000
C24B—C24—H24A	109.1000	O7'—C70'—H70E	109.5000
C23—C24—H24A	109.1000	H70D—C70'—H70E	109.5000
C24B—C24—H24B	109.1000	O7'—C70'—H70F	109.5000
C23—C24—H24B	109.1000	H70D—C70'—H70F	109.5000
H24A—C24—H24B	107.8000	H70E—C70'—H70F	109.5000
C23'—C24'—C24C	113.6 (11)	O27—C70B—H70G	109.5000
C23'—C24'—H24C	108.8000	O27—C70B—H70H	109.5000
C24C—C24'—H24C	108.8000	H70G—C70B—H70H	109.5000
C23'—C24'—H24D	108.8000	O27—C70B—H70I	109.5000
C24C—C24'—H24D	108.8000	H70G—C70B—H70I	109.5000
H24C—C24'—H24D	107.7000	H70H—C70B—H70I	109.5000
C26—C25—C24B	119.6 (11)	O27'—C70C—H70J	109.5000
C26—C25—C25'	118.8 (10)	O27'—C70C—H70K	109.5000
C24B—C25—C25'	121.2 (11)	H70J—C70C—H70K	109.5000
C28B—C24B—C25	119.5 (11)	O27'—C70C—H70L	109.5000
C28B—C24B—C24	120.1 (11)	H70J—C70C—H70L	109.5000
C25—C24B—C24	120.4 (11)	H70K—C70C—H70L	109.5000
C25'—C24C—C28C	118.7 (11)	O47—C70E—H70M	109.5000
C25'—C24C—C24'	122.6 (11)	O47—C70E—H70N	109.5000
C28C—C24C—C24'	118.6 (11)	H70M—C70E—H70N	109.5000
C26'—C25'—C24C	121.6 (11)	O47—C70E—H70O	109.5000
C26'—C25'—C25	120.5 (11)	H70M—C70E—H70O	109.5000
C24C—C25'—C25	117.8 (11)	H70N—C70E—H70O	109.5000
O26—C26—C25	119.0 (10)	O47'—C70F—H70P	109.5000
O26—C26—C27	120.2 (11)	O47'—C70F—H70Q	109.5000
C25—C26—C27	120.7 (11)	H70P—C70F—H70Q	109.5000
C25'—C26'—C27'	119.0 (12)	O47'—C70F—H70R	109.5000
C25'—C26'—H26'	120.5000	H70P—C70F—H70R	109.5000
C27'—C26'—H26'	120.5000	H70Q—C70F—H70R	109.5000
C28—C27—O27	120.9 (11)	O8—C80—H80A	109.5000
C28—C27—C26	119.2 (11)	O8—C80—H80B	109.5000
O27—C27—C26	119.7 (11)	H80A—C80—H80B	109.5000

C28'—C27'—O27'	116.8 (11)	O8—C80—H80C	109.5000
C28'—C27'—C26'	120.0 (11)	H80A—C80—H80C	109.5000
O27'—C27'—C26'	123.2 (11)	H80B—C80—H80C	109.5000
C27—C28—O28	122.6 (11)	O8'—C80'—H80D	109.5000
C27—C28—C28B	120.9 (11)	O8'—C80'—H80E	109.5000
O28—C28—C28B	116.5 (11)	H80D—C80'—H80E	109.5000
C27'—C28'—C28C	121.3 (11)	O8'—C80'—H80F	109.5000
C27'—C28'—O28'	121.8 (11)	H80D—C80'—H80F	109.5000
C28C—C28'—O28'	116.5 (11)	H80E—C80'—H80F	109.5000
C24B—C28B—C28	120.0 (11)	O81—C81—C82	107.7 (15)
C24B—C28B—C21	121.4 (11)	O81—C81—H81A	110.2000
C28—C28B—C21	118.4 (11)	C82—C81—H81A	110.2000
C28'—C28C—C24C	119.1 (11)	O81—C81—H81B	110.2000
C28'—C28C—C21'	120.7 (11)	C82—C81—H81B	110.2000
C24C—C28C—C21'	120.2 (11)	H81A—C81—H81B	108.5000
C3—C30—H30A	109.5000	O28—C80B—H80G	109.5000
C3—C30—H30B	109.5000	O28—C80B—H80H	109.5000
H30A—C30—H30B	109.5000	H80G—C80B—H80H	109.5000
C3—C30—H30C	109.5000	O28—C80B—H80I	109.5000
H30A—C30—H30C	109.5000	H80G—C80B—H80I	109.5000
H30B—C30—H30C	109.5000	H80H—C80B—H80I	109.5000
C3'—C30'—H30D	109.5000	O28'—C80C—H80J	109.5000
C3'—C30'—H30E	109.5000	O28'—C80C—H80K	109.5000
H30D—C30'—H30E	109.5000	H80J—C80C—H80K	109.5000
C3'—C30'—H30F	109.5000	O28'—C80C—H80L	109.5000
H30D—C30'—H30F	109.5000	H80J—C80C—H80L	109.5000
H30E—C30'—H30F	109.5000	H80K—C80C—H80L	109.5000
C36—C31—C32	118.4 (12)	O48—C80E—H80M	109.5000
C36—C31—C21	125.2 (11)	O48—C80E—H80N	109.5000
C32—C31—C21	116.0 (11)	H80M—C80E—H80N	109.5000
C23—C30B—H30G	109.5000	O48—C80E—H80O	109.5000
C23—C30B—H30H	109.5000	H80M—C80E—H80O	109.5000
H30G—C30B—H30H	109.5000	H80N—C80E—H80O	109.5000
C23—C30B—H30I	109.5000	O48'—C80F—H80P	109.5000
H30G—C30B—H30I	109.5000	O48'—C80F—H80Q	109.5000



H30H—C30B—H30I	109.5000	H80P—C80F—H80Q	109.5000
C23'—C30C—H30J	109.5000	O48'—C80F—H80R	109.5000
C23'—C30C—H30K	109.5000	H80P—C80F—H80R	109.5000
H30J—C30C—H30K	109.5000	H80Q—C80F—H80R	109.5000
C23'—C30C—H30L	109.5000	C81—C82—H82A	109.5000
H30J—C30C—H30L	109.5000	C81—C82—H82B	109.5000
H30K—C30C—H30L	109.5000	H82A—C82—H82B	109.5000
O30D—C30D—O31D	123.5 (12)	C81—C82—H82C	109.5000
O30D—C30D—C21'	123.8 (12)	H82A—C82—H82C	109.5000
O31D—C30D—C21'	112.7 (11)	H82B—C82—H82C	109.5000
C43—C30E—H30M	109.5000	C92—C91—O91	127 (3)
C43—C30E—H30N	109.5000	C92—C91—H91A	105.5000
H30M—C30E—H30N	109.5000	O91—C91—H91A	105.5000
C43—C30E—H30O	109.5000	C92—C91—H91B	105.5000
H30M—C30E—H30O	109.5000	O91—C91—H91B	105.5000
H30N—C30E—H30O	109.5000	H91A—C91—H91B	106.1000
C43'—C30F—H30P	109.5000	C91—C92—H92A	109.5000
C43'—C30F—H30Q	109.5000	C91—C92—H92B	109.5000
H30P—C30F—H30Q	109.5000	H92A—C92—H92B	109.5000
C43'—C30F—H30R	109.5000	C91—C92—H92C	109.4000
H30P—C30F—H30R	109.5000	H92A—C92—H92C	109.5000
H30Q—C30F—H30R	109.5000	H92B—C92—H92C	109.5000
C33—C32—C31	120.6 (12)	C5'—C4A'—C8A'	118.5 (12)
C33—C32—H32	119.7000	C5'—C4A'—C4'	121.1 (12)
C31—C32—H32	119.7000	C8A'—C4A'—C4'	120.3 (12)
O31D—C31D—C32D	107.4 (12)	C8'—C8A'—C4A'	119.9 (11)
O31D—C31D—H31A	110.2000	C8'—C8A'—C1'	120.3 (11)
C32D—C31D—H31A	110.2000	C4A'—C8A'—C1'	119.9 (11)
O31D—C31D—H31B	110.2000	C1—O2—C3	111.8 (9)
C32D—C31D—H31B	110.2000	C1'—O2'—C3'	112.6 (10)
H31A—C31D—H31B	108.5000	C6—O6—C60	118.3 (11)
C34—C33—C32	117.8 (12)	C7—O7—C70	112.7 (11)
C34—C33—H33	121.1000	C7'—O7'—C70'	118.2 (10)
C32—C33—H33	121.1000	C8—O8—C80	111.3 (11)
C31D—C32D—H32A	109.5000	C8'—O8'—C80'	114.1 (9)

C31D—C32D—H32B	109.5000	C10'—O11'—C11'	117.5 (10)
H32A—C32D—H32B	109.5000	C21—O22—C23	111.1 (9)
C31D—C32D—H32C	109.5000	C21'—O22'—C23'	112.1 (9)
H32A—C32D—H32C	109.5000	C26—O26—C60B	112.9 (9)
H32B—C32D—H32C	109.5000	C27—O27—C70B	115.1 (10)
C33—C34—F34	119.2 (11)	C27'—O27'—C70C	117.7 (10)
C33—C34—C35	123.4 (13)	C28—O28—C80B	116.1 (10)
F34—C34—C35	117.5 (12)	C28'—O28'—C80C	115.7 (10)
C36—C35—C34	117.3 (13)	C30D—O31D—C31D	115.5 (11)
C36—C35—H35	121.3000	C41—O42—C43	113.6 (9)
C34—C35—H35	121.3000	C41'—O42'—C43'	113.1 (9)
C35—C36—C31	122.4 (12)	C46—O46—C60C	112.2 (9)
C35—C36—H36	118.8000	C47—O47—C70E	111.4 (10)
C31—C36—H36	118.8000	C47'—O47'—C70F	115.2 (9)
O42—C41—C51	111.2 (10)	C48—O48—C80E	115.7 (10)
O42—C41—C48E	111.7 (10)	C48'—O48'—C80F	113.8 (10)
C51—C41—C48E	113.8 (10)	C50D—O51D—C51D	114.3 (10)
O42—C41—H41	106.5000	C81—O81—H81	130 (6)
C51—C41—H41	106.5000	C91—O91—H91	109.5000
C48E—C41—H41	106.5000		
Torsion angles (°)			
O2—C3—C4—C4A	−44.9 (14)	C43—C44—C44E—C45	−169.2 (11)
C30—C3—C4—C4A	−162.3 (11)	C43'—C44'—C44F—C45'	−159.9 (11)
O2'—C3'—C4'—C4A'	−50.2 (15)	C43'—C44'—C44F—C48F	19.4 (15)
C30'—C3'—C4'—C4A'	−167.9 (14)	C48F—C44F—C45'—C46'	−2.4 (17)
C6—C5—C4A—C8A	2.9 (19)	C44'—C44F—C45'—C46'	176.9 (11)
C5'—C5—C4A—C8A	178.7 (12)	C48F—C44F—C45'—C45	176.8 (10)
C6—C5—C4A—C4	−174.2 (12)	C44'—C44F—C45'—C45	−4.0 (17)
C5'—C5—C4A—C4	1.6 (19)	C46—C45—C45'—C46'	−98.3 (14)
C3—C4—C4A—C8A	15.0 (18)	C44E—C45—C45'—C46'	82.5 (15)
C3—C4—C4A—C5	−167.9 (12)	C46—C45—C45'—C44F	82.5 (15)
C6—C5—C5'—C4A'	80.7 (16)	C44E—C45—C45'—	−96.6 (14)

		C44F	
C4A—C5—C5'—C4A'	−95.1 (15)	C44E—C45—C46—C47	1.0 (18)
C6—C5—C5'—C6'	−102.9 (14)	C45'—C45—C46—C47	−178.2 (11)
C4A—C5—C5'—C6'	81.3 (15)	C44E—C45—C46—O46	176.3 (11)
C4A—C5—C6—O6	176.5 (12)	C45'—C45—C46—O46	−2.8 (17)
C5'—C5—C6—O6	0.8 (18)	C44F—C45'—C46'— C47'	0.4 (18)
C4A—C5—C6—C7	1 (2)	C45—C45'—C46'—C47'	−178.8 (11)
C5'—C5—C6—C7	−175.0 (12)	O46—C46—C47—O47	4.4 (18)
C4A'—C5'—C6'—C7'	−1.2 (19)	C45—C46—C47—O47	179.8 (11)
C5—C5'—C6'—C7'	−177.5 (11)	O46—C46—C47—C48	−178.9 (10)
O6—C6—C7—O7	2 (2)	C45—C46—C47—C48	−3.5 (18)
C5—C6—C7—O7	177.4 (13)	C45'—C46'—C47'—O47'	−179.7 (11)
O6—C6—C7—C8	−178.3 (13)	C45'—C46'—C47'—C48'	1.1 (18)
C5—C6—C7—C8	−3 (2)	O47—C47—C48—C48E	−179.6 (11)
C5'—C6'—C7'—O7'	178.2 (11)	C46—C47—C48—C48E	3.6 (18)
C5'—C6'—C7'—C8'	0.4 (17)	O47—C47—C48—O48	−5.2 (18)
O7—C7—C8—C8A	−179.0 (13)	C46—C47—C48—O48	178.1 (11)
C6—C7—C8—C8A	1 (2)	C46'—C47'—C48'— C48F	−0.5 (18)
O7—C7—C8—O8	−5 (2)	O47'—C47'—C48'— C48F	−179.7 (11)
C6—C7—C8—O8	174.7 (12)	C46'—C47'—C48'—O48'	174.8 (11)
O7'—C7'—C8'—C8A'	−175.9 (11)	O47'—C47'—C48'—O48'	−4.4 (17)
C6'—C7'—C8'—C8A'	2.0 (18)	O48—C48—C48E— C44E	−175.9 (11)
O7'—C7'—C8'—O8'	−0.4 (17)	C47—C48—C48E— C44E	−1.3 (19)
C6'—C7'—C8'—O8'	177.5 (11)	O48—C48—C48E—C41	0.9 (17)
C7—C8—C8A—C4A	3 (2)	C47—C48—C48E—C41	175.6 (11)
O8—C8—C8A—C4A	−171.2 (11)	C45—C44E—C48E— C48	−1.3 (18)
C7—C8—C8A—C1	178.3 (12)	C44—C44E—C48E— C48	175.7 (12)
O8—C8—C8A—C1	4.7 (19)	C45—C44E—C48E— C41	−178.0 (11)
C5—C4A—C8A—C8	−4.5 (19)	C44—C44E—C48E— C41	−1.1 (18)

C4—C4A—C8A—C8	172.6 (12)	O42—C41—C48E—C48	−157.7 (11)
C5—C4A—C8A—C1	179.6 (12)	C51—C41—C48E—C48	75.3 (15)
C4—C4A—C8A—C1	−3.3 (18)	O42—C41—C48E— C44E	19.1 (16)
O2—C1—C8A—C8	−154.2 (12)	C51—C41—C48E— C44E	−107.9 (13)
C11—C1—C8A—C8	78.5 (15)	C47'—C48'—C48F— C44F	−1.6 (17)
O2—C1—C8A—C4A	21.6 (16)	O48'—C48'—C48F— C44F	−177.1 (10)
C11—C1—C8A—C4A	−105.7 (13)	C47'—C48'—C48F— C41'	178.6 (11)
O2'—C1'—C10'—O10'	79.2 (16)	O48'—C48'—C48F— C41'	3.1 (16)
C8A'—C1'—C10'—O10'	−43.3 (19)	C45'—C44F—C48F— C48'	3.0 (17)
O2'—C1'—C10'—O11'	−96.3 (12)	C44'—C44F—C48F— C48'	−176.3 (11)
C8A'—C1'—C10'—O11'	141.2 (11)	C45'—C44F—C48F— C41'	−177.2 (11)
O2—C1—C11—C12	−96.6 (14)	C44'—C44F—C48F— C41'	3.5 (16)
C8A—C1—C11—C12	31.5 (17)	O42'—C41'—C48F— C48'	−172.9 (11)
O2—C1—C11—C16	77.5 (14)	C50D—C41'—C48F— C48'	−56.8 (14)
C8A—C1—C11—C16	−154.4 (11)	O42'—C41'—C48F— C44F	7.4 (16)
C16—C11—C12—C13	−1.5 (19)	C50D—C41'—C48F— C44F	123.5 (12)
C1—C11—C12—C13	172.8 (12)	O42—C41—C51—C56	−99.7 (14)
C11—C12—C13—C14	0 (2)	C48E—C41—C51—C56	27.6 (18)
C12—C13—C14—C15	1 (2)	O42—C41—C51—C52	78.4 (14)
C12—C13—C14—F14	179.5 (11)	C48E—C41—C51—C52	−154.3 (12)
F14—C14—C15—C16	−179.2 (12)	O42'—C41'—C50D— O50D	68.3 (15)
C13—C14—C15—C16	−1 (2)	C48F—C41'—C50D— O50D	−53.1 (16)
C14—C15—C16—C11	−0.5 (19)	O42'—C41'—C50D— O51D	−109.6 (11)

C12—C11—C16—C15	1.7 (19)	C48F—C41'—C50D— O51D	129.1 (11)
C1—C11—C16—C15	−172.9 (12)	C56—C51—C52—C53	2 (2)
O22—C23—C24—C24B	−46.4 (14)	C41—C51—C52—C53	−175.9 (12)
C30B—C23—C24—C24B	−164.2 (11)	C51—C52—C53—C54	−2 (2)
O22'—C23'—C24'—C24C	−47.8 (14)	C52—C53—C54—F54	178.6 (12)
C30C—C23'—C24'—C24C	−167.5 (11)	C52—C53—C54—C55	0 (2)
C26—C25—C24B—C28B	2.0 (18)	C53—C54—C55—C56	1 (2)
C25'—C25—C24B—C28B	174.9 (11)	F54—C54—C55—C56	−177.2 (13)
C26—C25—C24B—C24	−178.9 (12)	C52—C51—C56—C55	−1 (2)
C25'—C25—C24B—C24	−6.0 (18)	C41—C51—C56—C55	177.3 (13)
C23—C24—C24B—C28B	11.0 (17)	C54—C55—C56—C51	−1 (2)
C23—C24—C24B—C25	−168.1 (11)	C6'—C5'—C4A'—C8A'	−0.4 (19)
C23'—C24'—C24C—C25'	−161.9 (11)	C5—C5'—C4A'—C8A'	175.8 (11)
C23'—C24'—C24C—C28C	15.8 (16)	C6'—C5'—C4A'—C4'	−179.0 (12)
C28C—C24C—C25'—C26'	−0.2 (18)	C5—C5'—C4A'—C4'	−2.8 (19)
C24'—C24C—C25'—C26'	177.5 (12)	C3'—C4'—C4A'—C5'	−162.6 (13)
C28C—C24C—C25'—C25	176.8 (11)	C3'—C4'—C4A'—C8A'	18.8 (18)
C24'—C24C—C25'—C25	−5.5 (17)	C7'—C8'—C8A'—C4A'	−3.6 (19)
C26—C25—C25'—C26'	−102.5 (15)	O8'—C8'—C8A'—C4A'	−179.3 (11)
C24B—C25—C25'—C26'	84.5 (16)	C7'—C8'—C8A'—C1'	178.4 (11)
C26—C25—C25'—C24C	80.4 (15)	O8'—C8'—C8A'—C1'	2.7 (18)
C24B—C25—C25'—C24C	−92.5 (15)	C5'—C4A'—C8A'—C8'	2.8 (18)
C24B—C25—C26—O26	174.4 (11)	C4'—C4A'—C8A'—C8'	−178.6 (13)
C25'—C25—C26—O26	1.3 (17)	C5'—C4A'—C8A'—C1'	−179.2 (12)
C24B—C25—C26—C27	−1.0 (18)	C4'—C4A'—C8A'—C1'	−0.6 (18)
C25'—C25—C26—C27	−174.1 (11)	O2'—C1'—C8A'—C8'	−167.5 (11)
C24C—C25'—C26'—C27'	−2.2 (19)	C10'—C1'—C8A'—C8'	−51.4 (16)
C25—C25'—C26'—C27'	−179.1 (11)	O2'—C1'—C8A'—C4A'	14.4 (16)
O26—C26—C27—C28	−175.5 (11)	C10'—C1'—C8A'—C4A'	130.6 (12)
C25—C26—C27—C28	−0.1 (19)	C11—C1—O2—C3	75.0 (12)
O26—C26—C27—O27	−0.2 (18)	C8A—C1—O2—C3	−53.4 (13)
C25—C26—C27—O27	175.1 (11)	C30—C3—O2—C1	−172.4 (10)
C25'—C26'—C27'—C28'	4.6 (19)	C4—C3—O2—C1	66.0 (12)
C25'—C26'—C27'—O27'	−176.8 (12)	C10'—C1'—O2'—C3'	−170.1 (10)
O27—C27—C28—O28	2.4 (19)	C8A'—C1'—O2'—C3'	−48.5 (14)

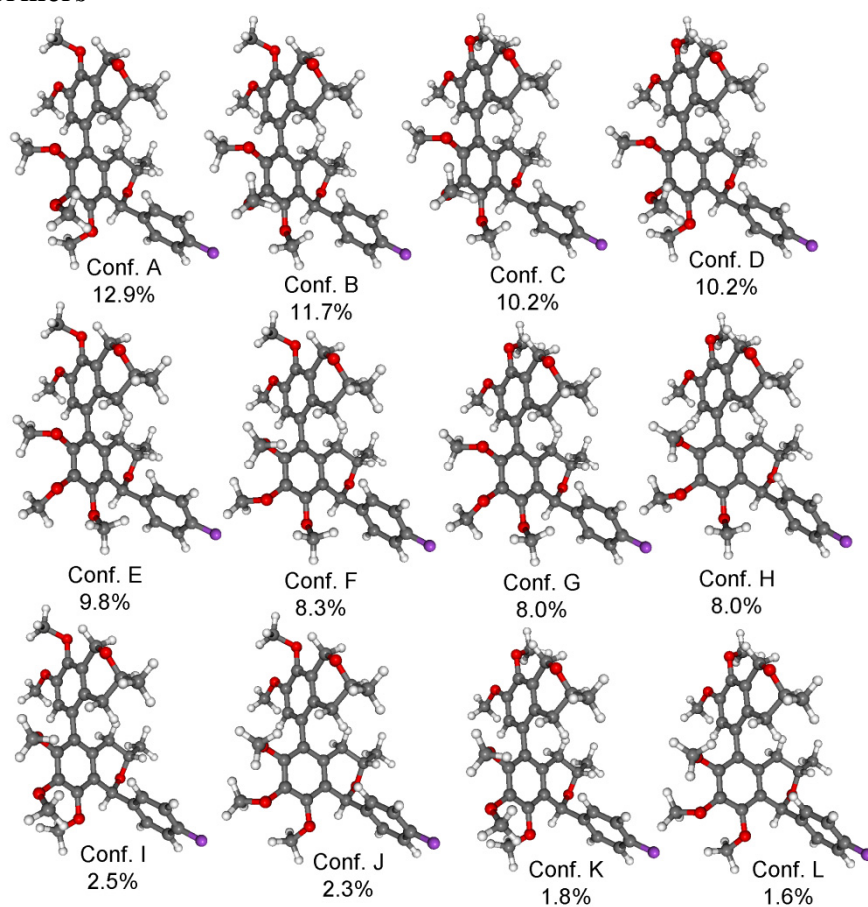
C26—C27—C28—O28	177.6 (11)	C30'—C3'—O2'—C1'	−169.5 (11)
O27—C27—C28—C28B	−174.9 (11)	C4'—C3'—O2'—C1'	67.5 (13)
C26—C27—C28—C28B	0.3 (19)	C7—C6—O6—C60	−45.4 (19)
O27'—C27'—C28'—C28C	176.6 (12)	C5—C6—O6—C60	138.9 (13)
C26'—C27'—C28'—C28C	−4.8 (19)	C8—C7—O7—C70	95.5 (16)
O27'—C27'—C28'—O28'	3.5 (18)	C6—C7—O7—C70	−84.6 (17)
C26'—C27'—C28'—O28'	−177.9 (12)	C8'—C7'—O7'—C70'	161.9 (11)
C25—C24B—C28B—C28	−1.9 (18)	C6'—C7'—O7'—C70'	−15.9 (17)
C24—C24B—C28B—C28	179.0 (12)	C8A—C8—O8—C80	−108.8 (14)
C25—C24B—C28B—C21	−176.6 (11)	C7—C8—O8—C80	77.3 (16)
C24—C24B—C28B—C21	4.3 (18)	C8A'—C8'—O8'—C80'	−112.8 (13)
C27—C28—C28B—C24B	1 (2)	C7'—C8'—O8'—C80'	71.5 (15)
O28—C28—C28B—C24B	−176.7 (10)	O10'—C10'—O11'—C11'	−1 (2)
C27—C28—C28B—C21	175.6 (11)	C1'—C10'—O11'—C11'	174.4 (11)
O28—C28—C28B—C21	−1.9 (17)	C12'—C11'—O11'—C10'	86.7 (15)
O22—C21—C28B—C24B	16.2 (16)	C28B—C21—O22—C23	−54.0 (12)
C31—C21—C28B—C24B	−109.3 (13)	C31—C21—O22—C23	73.3 (11)
O22—C21—C28B—C28	−158.5 (11)	C30B—C23—O22—C21	−167.7 (10)
C31—C21—C28B—C28	76.0 (15)	C24—C23—O22—C21	70.5 (12)
C27'—C28'—C28C—C24C	2.3 (19)	C28C—C21'—O22'—C23'	−49.7 (14)
O28'—C28'—C28C—C24C	175.8 (10)	C30D—C21'—O22'—C23'	−171.8 (10)
C27'—C28'—C28C—C21'	−175.7 (12)	C24'—C23'—O22'—C21'	66.5 (13)
O28'—C28'—C28C—C21'	−2.2 (18)	C30C—C23'—O22'—C21'	−170.2 (10)
C25'—C24C—C28C—C28'	0.2 (17)	C25—C26—O26—C60B	117.1 (13)
C24'—C24C—C28C—C28'	−177.6 (12)	C27—C26—O26—C60B	−67.4 (15)
C25'—C24C—C28C—C21'	178.2 (11)	C28—C27—O27—C70B	82.2 (15)
C24'—C24C—C28C—C21'	0.4 (17)	C26—C27—O27—C70B	−92.9 (14)
O22'—C21'—C28C—C28'	−166.1 (11)	C28'—C27'—O27'—C70C	−171.4 (12)
C30D—C21'—C28C—C28'	−49.7 (16)	C26'—C27'—O27'—C70C	10.1 (18)
O22'—C21'—C28C—C24C	15.9 (16)	C27—C28—O28—C80B	54.1 (17)
C30D—C21'—C28C—C24C	132.3 (12)	C28B—C28—O28—C80B	−128.4 (13)

O22—C21—C31—C36	−110.2 (14)	C27'—C28'—O28'— C80C	−66.2 (15)
C28B—C21—C31—C36	15.2 (18)	C28C—C28'—O28'— C80C	120.4 (12)
O22—C21—C31—C32	62.4 (14)	O30D—C30D—O31D— C31D	0.2 (19)
C28B—C21—C31—C32	−172.2 (11)	C21'—C30D—O31D— C31D	178.3 (11)
O22'—C21'—C30D—O30D	74.4 (15)	C32D—C31D—O31D— C30D	165.1 (12)
C28C—C21'—C30D— O30D	−48.3 (17)	C51—C41—O42—C43	76.1 (12)
O22'—C21'—C30D—O31D	−103.7 (12)	C48E—C41—O42—C43	−52.3 (13)
C28C—C21'—C30D— O31D	133.5 (11)	C30E—C43—O42—C41	−173.1 (10)
C36—C31—C32—C33	−1 (2)	C44—C43—O42—C41	65.4 (12)
C21—C31—C32—C33	−174.1 (12)	C48F—C41'—O42'— C43'	−43.6 (14)
C31—C32—C33—C34	1.4 (19)	C50D—C41'—O42'— C43'	−163.1 (10)
C32—C33—C34—F34	177.2 (11)	C30F—C43'—O42'— C41'	−171.3 (10)
C32—C33—C34—C35	−3 (2)	C44'—C43'—O42'—C41'	68.5 (12)
C33—C34—C35—C36	3 (2)	C47—C46—O46—C60C	−74.9 (14)
F34—C34—C35—C36	−176.6 (12)	C45—C46—O46—C60C	109.6 (12)
C34—C35—C36—C31	−3 (2)	C46—C47—O47—C70E	−91.5 (14)
C32—C31—C36—C35	2 (2)	C48—C47—O47—C70E	91.9 (13)
C21—C31—C36—C35	174.0 (13)	C46'—C47'—O47'— C70F	−1.0 (17)
O42—C43—C44—C44E	−43.6 (14)	C48'—C47'—O47'— C70F	178.2 (11)
C30E—C43—C44—C44E	−161.3 (11)	C48E—C48—O48— C80E	−126.8 (13)
O42'—C43'—C44'—C44F	−53.8 (13)	C47—C48—O48—C80E	58.5 (16)
C30F—C43'—C44'—C44F	−170.6 (10)	C48F—C48'—O48'— C80F	−113.2 (12)
C46—C45—C44E—C48E	1.5 (18)	C47'—C48'—O48'— C80F	71.4 (15)
C45'—C45—C44E—C48E	−179.4 (11)	O50D—C50D—O51D— C51D	4.5 (19)

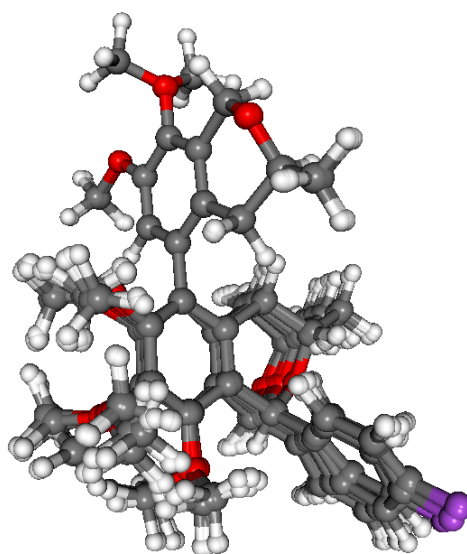
C46—C45—C44E—C44	−175.5 (11)	C41'—C50D—O51D— C51D	−177.7 (11)
C45'—C45—C44E—C44	3.7 (18)	C52D—C51D—O51D— C50D	−174.2 (13)
C43—C44—C44E—C48E	13.8 (17)		



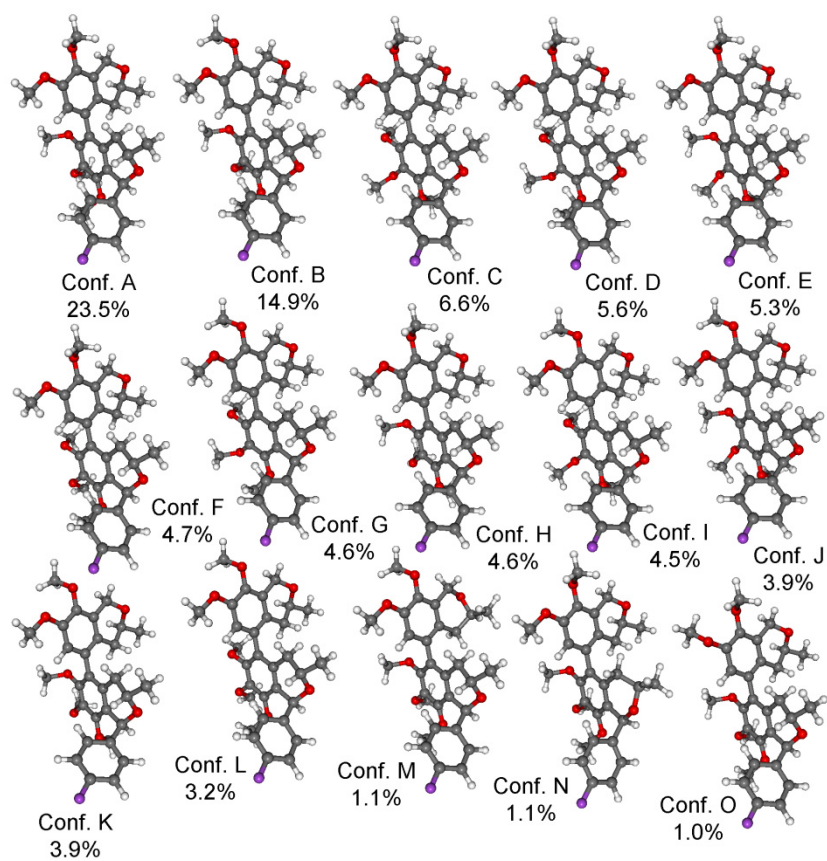
5. Structures, populations and Cartesian coordinates of the low-energy DFT conformers



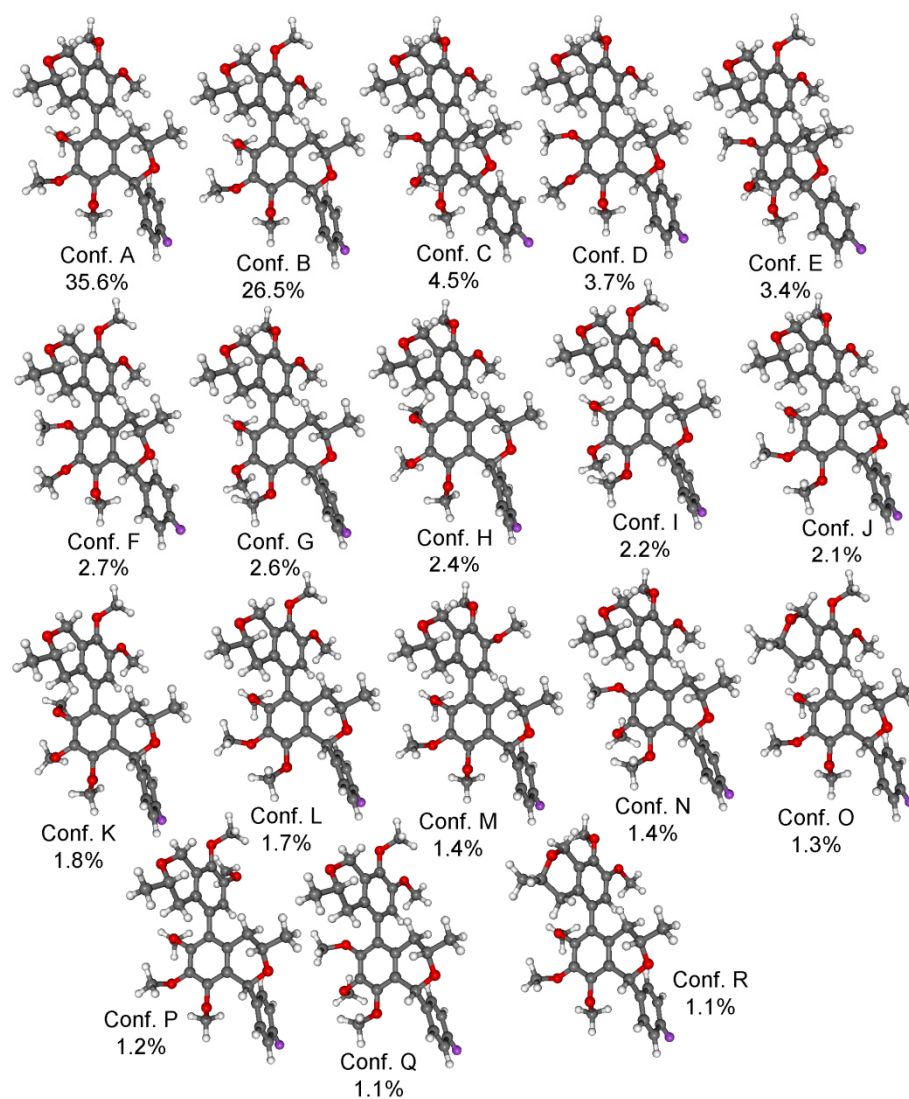
**Figure S273.** Structures and populations of the low-energy  $\omega$ B97X/TZVP PCM/MeCN conformers ( $\geq 1\%$ ) of (*aS*,1*S*,3*S*,3'*S*)-**21**.



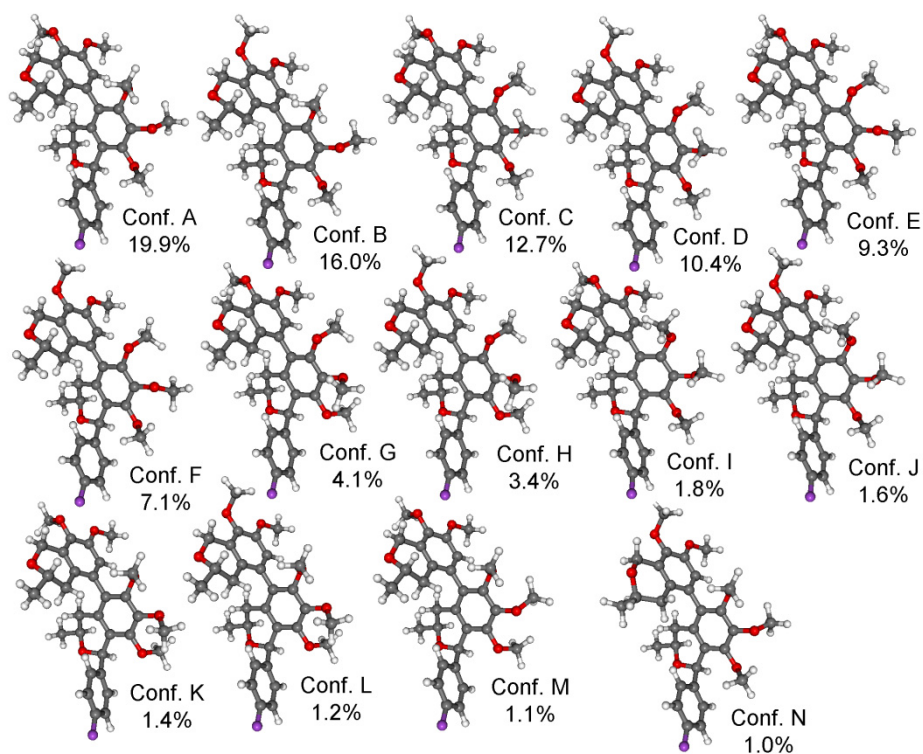
**Figure S274.** Overlapped structures of the 12 low-energy  $\omega$ B97X/TZVP PCM/MeCN conformers ( $\geq 1\%$ ) of (*aS*,1*S*,3*S*,3'*S*)-**21**.



**Figure S275.** Structures and populations of the low-energy  $\omega$ B97X/TZVP PCM/MeCN conformers ( $\geq 1\%$ ) of *(aR,1S,3S,3'S)*-**21**.

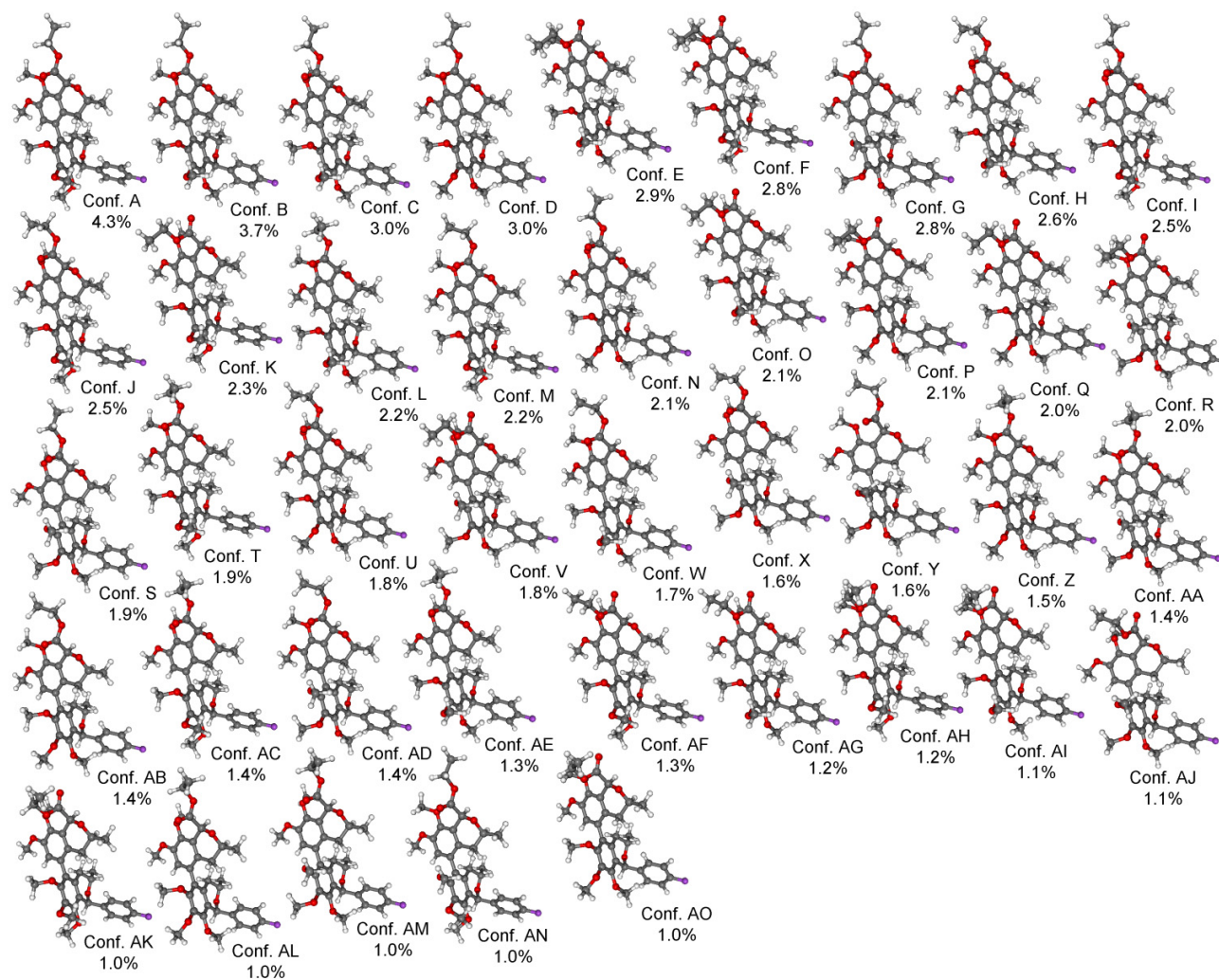


**Figure S276.** Structures and populations of the low-energy  $\omega$ B97X/TZVP PCM/MeCN conformers ( $\geq 1\%$ ) of (*aS*,1*R*,3*S*,3'*S*)-**21**.

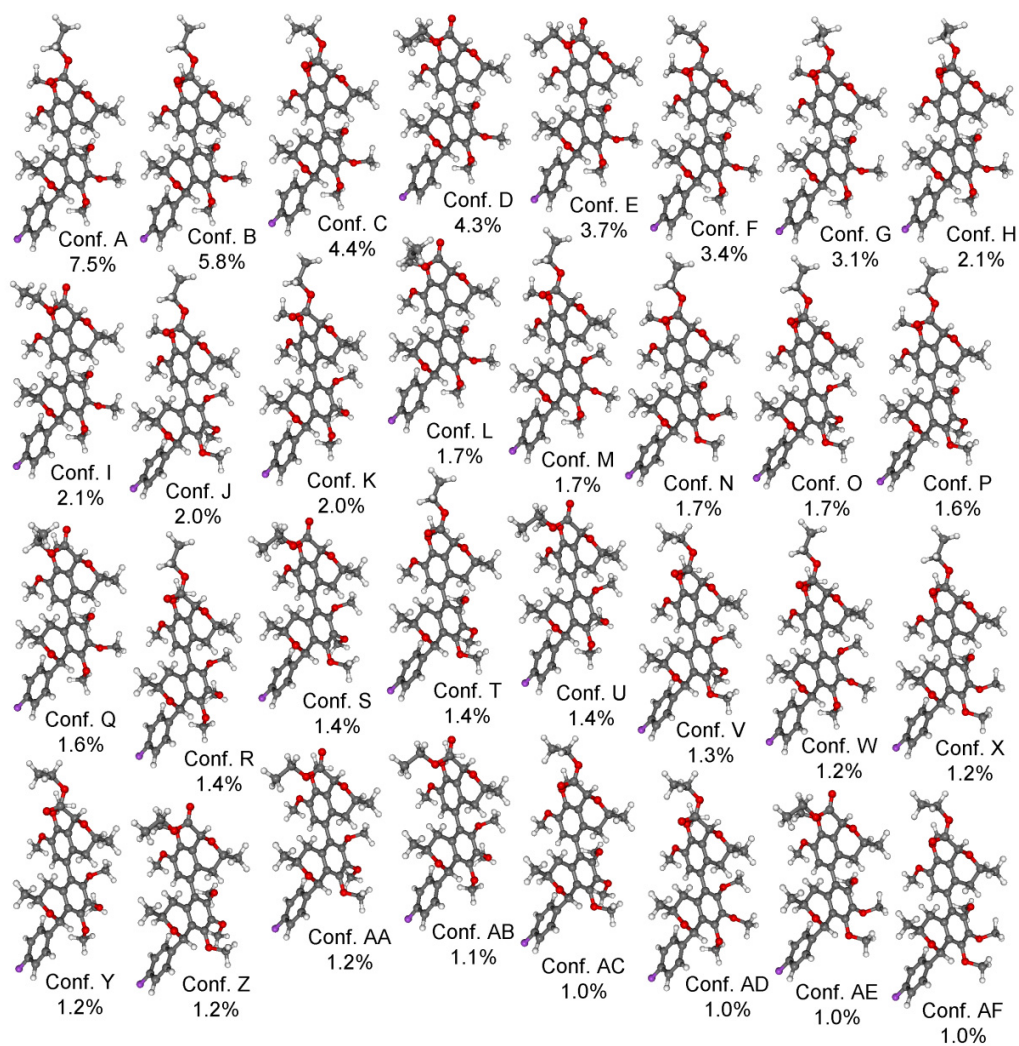


**Figure S277.** Structures and populations of the low-energy  $\omega$ B97X/TZVP PCM/MeCN conformers ( $\geq 1\%$ ) of (*aR,1R,3S,3'S*)-**21**.

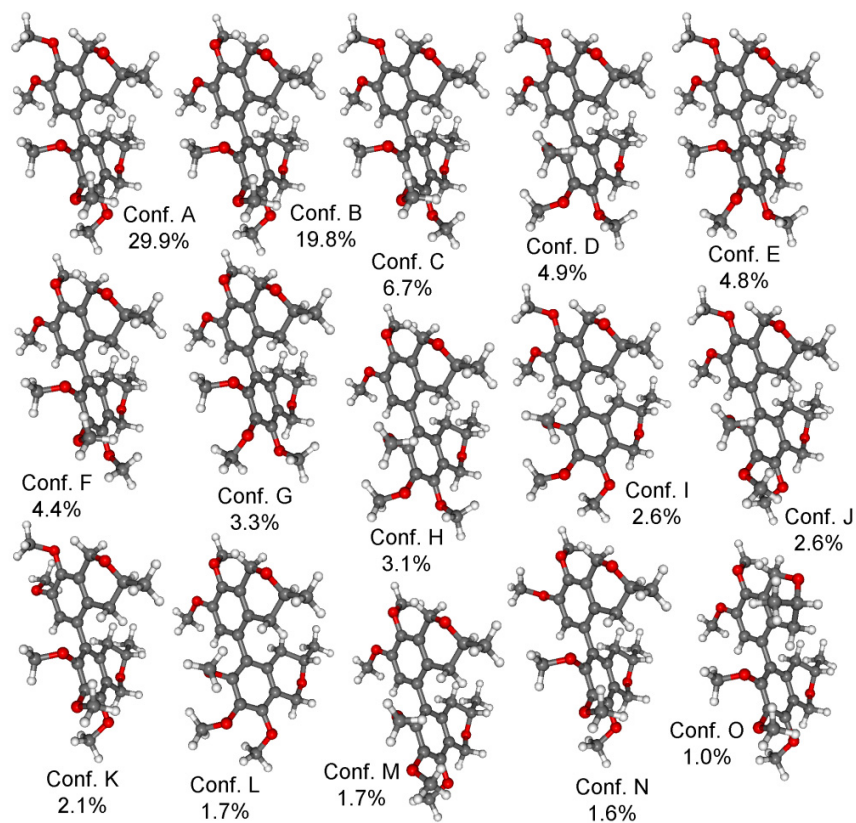




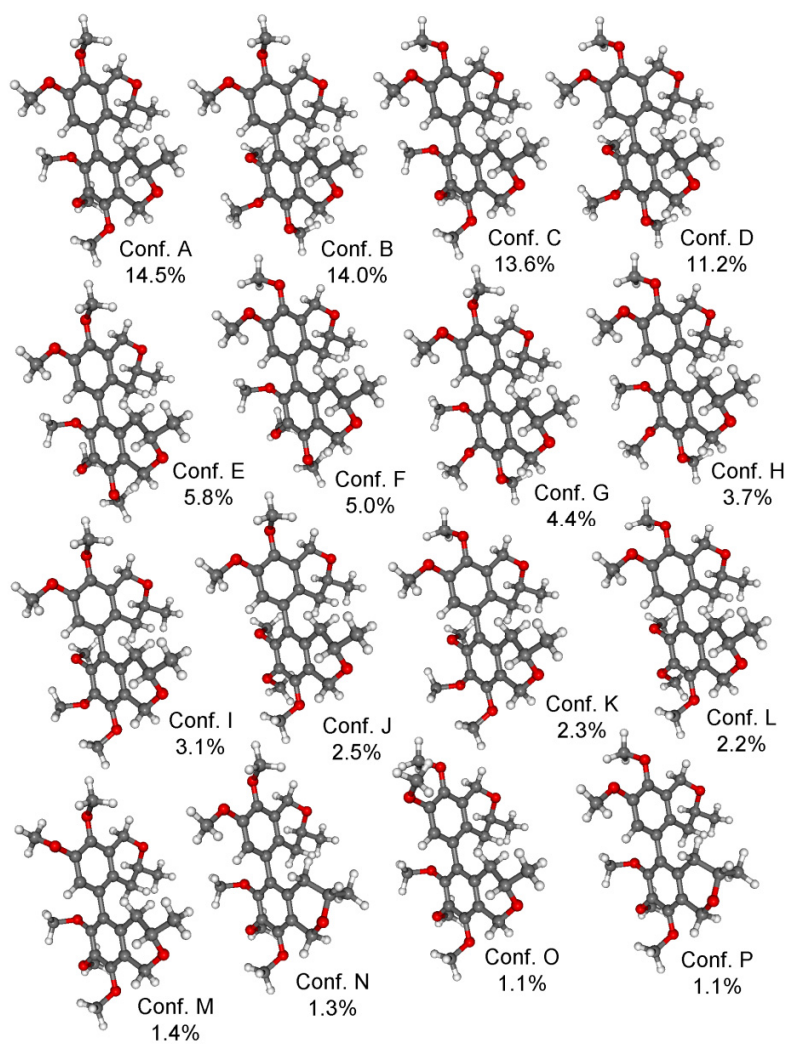
**Figure S278.** Structures and populations of the low-energy  $\omega$ B97X/TZVP PCM/MeCN conformers ( $\geq 1\%$ ) of (*aS,1S,3S,1'S,3'S*)-**22**.



**Figure S279.** Structures and populations of the low-energy  $\omega$ B97X/TZVP PCM/MeCN conformers ( $\geq 1\%$ ) of *(aR,1S,3S,1'S,3'S)*-**22**.



**Figure S280.** Structures and populations of the low-energy  $\omega$ B97X/TZVP PCM/MeCN conformers ( $\geq 1\%$ ) of (*aS,3S,3'S*)-**28**.



**Figure S281.** Structures and populations of the low-energy  $\omega$ B97X/TZVP PCM/MeCN conformers ( $\geq 1\%$ ) of (*aR,3S,3'S*)-**28**.



**Table S5.** Cartesian coordinates and energies of the low-energy conformers calculated at the  $\omega$ B97X/TZVP PCM/MeCN level.

(*aS*,1*S*,3*S*,3'*S*)-**21**, Conf A

C	2.709496	0.616496	-1.323124
C	3.996849	0.120643	-1.476552
C	4.506569	-0.749861	-0.506340
C	3.731917	-1.118796	0.582816
C	2.429042	-0.636030	0.725436
C	1.928692	0.242920	-0.230984
C	1.603617	-1.059134	1.916361
C	2.198233	-2.271810	2.617817
C	1.568317	-2.528798	3.967681
O	3.594920	-2.066322	2.820453
C	0.284853	1.857611	0.721096
C	-0.996360	2.403266	0.815426
C	-2.023835	1.862257	0.049566
C	-1.788030	0.767209	-0.779222
C	-0.508521	0.225554	-0.866826
C	0.540449	0.784790	-0.126126
C	-0.255294	-0.946865	-1.785209
C	-1.544966	-1.611583	-2.237224
C	-1.337564	-2.560059	-3.395935
O	-2.469290	-0.609108	-2.660138
C	-2.937073	0.201471	-1.587969
C	4.309241	-2.073058	1.602418
C	-3.975203	-0.550690	-0.764098
C	-3.723222	-1.051681	0.507370
C	-4.691391	-1.771567	1.197085
C	-5.911739	-1.976405	0.590150
C	-6.203721	-1.493729	-0.670903
C	-5.222951	-0.780479	-1.340333
F	-6.863270	-2.672802	1.256340
O	4.816573	0.413153	-2.519694
C	4.327044	1.298931	-3.515507
O	5.760894	-1.295485	-0.641155
C	6.828609	-0.377322	-0.400792
O	-1.220674	3.476885	1.636116
C	-1.806052	3.122587	2.890907
O	-3.297829	2.361402	0.140683
C	-3.470433	3.663966	-0.426043
O	1.285412	2.355613	1.514542
C	1.857585	3.571422	1.031877
H	2.290285	1.292465	-2.057821
H	1.538634	-0.228600	2.629117
H	0.580135	-1.286846	1.603918
H	2.072355	-3.157093	1.976209
H	1.737550	-1.676387	4.629703
H	0.491799	-2.674231	3.860197
H	1.994540	-3.420175	4.429951
H	0.380241	-1.682900	-1.285152
H	0.298654	-0.604877	-2.666792
H	-1.984432	-2.160701	-1.393656
H	-0.958330	-2.017666	-4.265137

H	-2.275696	-3.045348	-3.668632
H	-0.613116	-3.330952	-3.126670
H	-3.450126	1.031994	-2.077665
H	4.326230	-3.089695	1.183524
H	5.338272	-1.801715	1.838167
H	-2.761566	-0.877801	0.978085
H	-4.505830	-2.166523	2.188317
H	-7.177877	-1.671970	-1.109244
H	-5.432182	-0.392679	-2.331897
H	3.434798	0.893510	-4.000353
H	5.123458	1.396247	-4.249178
H	4.099438	2.281348	-3.092799
H	6.756843	0.036972	0.609585
H	7.754079	-0.942180	-0.495196
H	6.816763	0.432708	-1.132004
H	-1.138882	2.460845	3.449856
H	-2.772692	2.635462	2.740728
H	-1.945636	4.049922	3.442862
H	-4.522552	3.913770	-0.306181
H	-3.218132	3.651296	-1.490383
H	-2.852870	4.398622	0.092771
H	2.325457	3.411003	0.055571
H	1.098019	4.352851	0.956857
H	2.616794	3.867899	1.752919

$\omega$ B97X Energy = -1828.88132787 a.u.

(*aS*,1*S*,3*S*,3'*S*)-**21**, Conf B

C	2.736424	-0.540025	-1.366386
C	4.025015	-0.977484	-1.093517
C	4.511307	-0.875450	0.214938
C	3.711298	-0.360773	1.223573
C	2.406298	0.056790	0.952986
C	1.930936	-0.023827	-0.353101
C	1.548194	0.595725	2.072068
C	2.127659	0.265909	3.439975
C	1.461484	1.036781	4.556693
O	3.517028	0.586431	3.456960
C	0.288172	1.776647	-0.858588
C	-0.991351	2.235252	-1.190830
C	-2.013979	1.307240	-1.364813
C	-1.764863	-0.056818	-1.199764
C	-0.493328	-0.502100	-0.858749
C	0.546297	0.422049	-0.692839
C	-0.241705	-1.980406	-0.677607
C	-1.533130	-2.769570	-0.537971
C	-1.323872	-4.259701	-0.684597
O	-2.447141	-2.363692	-1.555908
C	-2.910628	-1.027857	-1.397077
C	4.265761	-0.276494	2.626941
C	-3.975873	-0.950790	-0.309696
C	-3.725532	-0.452319	0.963905

C	-4.716291	-0.443428	1.938123
C	-5.959729	-0.940235	1.611332
C	-6.251154	-1.443610	0.358275
C	-5.247188	-1.443973	-0.596479
F	-6.934316	-0.930962	2.551255
O	4.869328	-1.513229	-2.012841
C	4.402088	-1.635330	-3.347929
O	5.767198	-1.333949	0.533870
C	6.831221	-0.503863	0.065388
O	-1.228119	3.562381	-1.431568
C	-1.144084	4.415117	-0.285116
O	-3.270195	1.666775	-1.766273
C	-3.978844	2.608226	-0.959460
O	1.298263	2.689439	-0.680743
C	1.897587	3.132070	-1.899653
H	2.335183	-0.604815	-2.370021
H	1.455723	1.683689	1.972839
H	0.536492	0.185534	1.998650
H	2.023044	-0.814237	3.623481
H	1.607224	2.109646	4.410836
H	0.389154	0.832883	4.570128
H	1.880803	0.755734	5.523668
H	0.386042	-2.146981	0.202042
H	0.318608	-2.363592	-1.537973
H	-1.982260	-2.561518	0.442622
H	-0.929725	-4.488903	-1.677390
H	-2.264783	-4.794819	-0.549518
H	-0.610768	-4.615969	0.061195
H	-3.397058	-0.794406	-2.345745
H	4.302710	-1.282503	3.069294
H	5.285091	0.109457	2.610274
H	-2.746062	-0.054907	1.207877
H	-4.530820	-0.054856	2.931906
H	-7.243278	-1.820418	0.142032
H	-5.456979	-1.835341	-1.586580
H	5.215897	-2.086670	-3.910114
H	4.163874	-0.657475	-3.775447
H	3.521890	-2.281991	-3.400767
H	6.822817	-0.437850	-1.024026
H	6.751765	0.498837	0.496604
H	7.758085	-0.967631	0.397444
H	-0.141783	4.393710	0.143690
H	-1.875549	4.111724	0.469636
H	-1.377657	5.419569	-0.632612
H	-3.669574	3.629517	-1.182085
H	-3.826116	2.396482	0.102570
H	-5.033455	2.482518	-1.198874
H	1.153413	3.596317	-2.551350
H	2.654092	3.865278	-1.627173
H	2.372796	2.292895	-2.416515

$\omega$ B97X Energy = -1828.88124038 a.u.

(aS,1S,3S,3'S)-**21**, Conf C

C	2.745246	-0.364807	-1.414406
C	4.056856	-0.748114	-1.171643

C	4.564747	-0.637127	0.127556
C	3.776381	-0.131054	1.149928
C	2.453918	0.246497	0.906626
C	1.947209	0.131345	-0.385210
C	1.607944	0.769365	2.042137
C	2.231191	0.468028	3.397150
C	1.566130	1.222338	4.525775
O	3.608043	0.838064	3.377593
C	0.222650	1.867167	-0.846738
C	-1.079187	2.273838	-1.158895
C	-2.064303	1.305318	-1.328844
C	-1.756023	-0.048577	-1.180658
C	-0.462558	-0.442354	-0.858562
C	0.539561	0.523123	-0.696362
C	-0.146293	-1.910467	-0.695080
C	-1.401499	-2.755691	-0.556005
C	-1.130696	-4.234004	-0.720141
O	-2.338269	-2.377773	-1.563881
C	-2.859757	-1.066157	-1.382944
C	4.369141	-0.000338	2.534246
C	-3.920193	-1.054857	-0.288345
C	-3.688889	-0.554918	0.988170
C	-4.672391	-0.608894	1.968414
C	-5.888878	-1.170027	1.644525
C	-6.160751	-1.677189	0.388537
C	-5.164744	-1.613627	-0.572305
F	-6.856089	-1.223430	2.590622
O	4.909347	-1.226023	-2.114903
C	4.420297	-1.358973	-3.441046
O	5.870176	-0.972754	0.396601
C	6.111785	-2.378859	0.450532
O	-1.373828	3.591420	-1.387906
C	-1.310759	4.440563	-0.237610
O	-3.338879	1.615458	-1.712859
C	-4.076488	2.519616	-0.889656
O	1.195865	2.820492	-0.676784
C	1.760745	3.292067	-1.901356
H	2.324720	-0.443091	-2.409077
H	1.481387	1.853273	1.937595
H	0.607664	0.328460	1.996887
H	2.169152	-0.614039	3.588863
H	1.672374	2.298577	4.371018
H	0.501899	0.982832	4.566459
H	2.017813	0.961531	5.483825
H	0.494560	-2.058477	0.178471
H	0.423957	-2.260099	-1.563148
H	-1.852807	-2.577280	0.429458
H	-0.731610	-4.435866	-1.716881
H	-2.048045	-4.809136	-0.587439
H	-0.400472	-4.568664	0.019057
H	-3.362503	-0.840995	-2.325119
H	4.469473	-0.996793	2.989806
H	5.366917	0.433427	2.473812
H	-2.730436	-0.108127	1.230013
H	-4.501678	-0.220006	2.964714
H	-7.132064	-2.106094	0.175033

H	-5.359221	-2.007171	-1.564660
H	3.579025	-2.056276	-3.484170
H	5.246624	-1.753242	-4.027389
H	4.114784	-0.391744	-3.849529
H	7.163483	-2.506697	0.699793
H	5.495778	-2.844924	1.225649
H	5.905762	-2.846612	-0.514261
H	-0.301961	4.462968	0.175648
H	-2.015900	4.099939	0.526260
H	-1.595572	5.435178	-0.575136
H	-3.811433	3.554704	-1.105463
H	-3.904060	2.304383	0.168654
H	-5.127644	2.353568	-1.119441
H	0.990302	3.732926	-2.538663
H	2.494497	4.050231	-1.635105
H	2.258027	2.473745	-2.430775

$\omega$ B97X Energy = -1828.88111088 a.u.

(*a*S,1S,3S,3'S)-**21**, Conf D

C	2.789626	0.839377	-1.141741
C	4.104072	0.400958	-1.227623
C	4.574600	-0.516992	-0.282148
C	3.748072	-0.959376	0.739841
C	2.424901	-0.520303	0.823691
C	1.954249	0.385021	-0.123404
C	1.538798	-1.033169	1.933095
C	2.127406	-2.268307	2.599083
C	1.415980	-2.634898	3.881351
O	3.497124	-2.027866	2.913822
C	0.219257	1.961904	0.722954
C	-1.083730	2.461598	0.755563
C	-2.062817	1.861017	-0.028918
C	-1.757277	0.752589	-0.816261
C	-0.456605	0.257535	-0.842832
C	0.543779	0.876039	-0.082823
C	-0.126326	-0.929353	-1.716451
C	-1.373294	-1.659807	-2.186430
C	-1.092168	-2.635167	-3.306688
O	-2.322571	-0.709670	-2.670891
C	-2.856122	0.117743	-1.643024
C	4.298375	-1.934418	1.755091
C	-3.892418	-0.644497	-0.826119
C	-5.117561	-0.928717	-1.425924
C	-6.093374	-1.652295	-0.760107
C	-5.819320	-2.089520	0.521344
C	-4.621231	-1.830837	1.151704
C	-3.657976	-1.101443	0.465286
F	-6.766556	-2.794781	1.184330
O	4.991767	0.803961	-2.173338
C	4.544636	1.742216	-3.140534
O	5.879556	-0.946292	-0.315324
C	6.161820	-1.887836	-1.351010
O	-1.376794	3.547184	1.538103
C	-1.979066	3.202015	2.787403
O	-3.357268	2.311750	0.004938

C	-3.559485	3.592847	-0.599602
O	1.171059	2.516232	1.538449
C	1.710328	3.745319	1.051404
H	2.396843	1.542970	-1.864977
H	1.400655	-0.250345	2.688286
H	0.545352	-1.270692	1.540974
H	2.080176	-3.113019	1.894948
H	1.504720	-1.822374	4.606280
H	0.356019	-2.811277	3.689006
H	1.844757	-3.538723	4.316296
H	0.521936	-1.623495	-1.174455
H	0.441858	-0.589936	-2.590085
H	-1.817540	-2.199143	-1.339052
H	-0.704307	-2.106011	-4.180231
H	-2.002240	-3.163601	-3.593878
H	-0.349502	-3.369593	-2.989499
H	-3.382947	0.911283	-2.177485
H	4.404262	-2.927027	1.292402
H	5.289244	-1.618343	2.080140
H	-5.313446	-0.575740	-2.433136
H	-7.050674	-1.871955	-1.216435
H	-4.449167	-2.191094	2.158479
H	-2.714414	-0.884584	0.954406
H	5.394961	1.932370	-3.790776
H	4.232198	2.677567	-2.668037
H	3.718445	1.337954	-3.731816
H	5.535836	-2.778642	-1.241585
H	6.001802	-1.443123	-2.335151
H	7.208222	-2.166504	-1.241962
H	-1.305116	2.572647	3.374828
H	-2.927324	2.682899	2.627064
H	-2.158376	4.136089	3.316040
H	-3.273064	3.563630	-1.654924
H	-2.986267	4.362498	-0.080608
H	-4.623337	3.805940	-0.518797
H	2.439241	4.079968	1.786876
H	2.209524	3.587695	0.090299
H	0.924924	4.496880	0.944489

$\omega$ B97X Energy = -1828.88110805 a.u.

(*a*S,1S,3S,3'S)-**21**, Conf E

C	-2.733379	0.612778	1.273555
C	-4.017655	0.105372	1.413940
C	-4.503835	-0.781938	0.446941
C	-3.708102	-1.157795	-0.624576
C	-2.407465	-0.664985	-0.752434
C	-1.931348	0.232560	0.199198
C	-1.557555	-1.099149	-1.921827
C	-2.129919	-2.327257	-2.614928
C	-1.473951	-2.600274	-3.949096
O	-3.524308	-2.135524	-2.845786
C	-0.287218	1.838974	-0.762476
C	0.988365	2.406599	-0.844876
C	2.021222	1.851880	-0.092342
C	1.770229	0.797712	0.786094

C	0.489721	0.266327	0.892892
C	-0.546798	0.786372	0.107570
C	0.225434	-0.859853	1.864490
C	1.506391	-1.520183	2.347176
C	1.286035	-2.402759	3.554829
O	2.448141	-0.514062	2.718055
C	2.916356	0.257027	1.616853
C	-4.260545	-2.130139	-1.640846
C	3.949138	-0.522427	0.813811
C	5.249319	-0.601052	1.307766
C	6.224861	-1.334979	0.652020
C	5.873868	-1.994841	-0.509540
C	4.599646	-1.944352	-1.033585
C	3.639136	-1.199245	-0.361107
F	6.818912	-2.712881	-1.160563
O	-4.856001	0.401982	2.441075
C	-4.387974	1.299530	3.436605
O	-5.754855	-1.338075	0.568286
C	-6.827692	-0.432351	0.304538
O	1.186091	3.456027	-1.701183
C	1.586095	4.682404	-1.083007
O	3.292967	2.363899	-0.137562
C	3.966189	2.248157	-1.394968
O	-1.286014	2.307897	-1.576458
C	-1.945304	3.474265	-1.089385
H	-2.333063	1.302847	2.005709
H	-1.486049	-0.279334	-2.646013
H	-0.538364	-1.313547	-1.586601
H	-2.009267	-3.201548	-1.957405
H	-1.636370	-1.759179	-4.627097
H	-0.398657	-2.737065	-3.820190
H	-1.886170	-3.501278	-4.405382
H	-0.421005	-1.610211	1.401473
H	-0.321454	-0.469365	2.730248
H	1.933422	-2.121947	1.534033
H	0.915732	-1.809037	4.393812
H	2.217146	-2.886547	3.853019
H	0.550147	-3.176255	3.327087
H	3.431305	1.102460	2.076122
H	-4.278606	-3.140997	-1.208276
H	-5.286897	-1.868823	-1.898752
H	5.506073	-0.075988	2.222029
H	7.239241	-1.396614	1.026492
H	4.368239	-2.472754	-1.950204
H	2.637080	-1.140939	-0.772793
H	-4.163595	2.280893	3.009740
H	-3.498661	0.905747	3.936245
H	-5.194954	1.394973	4.158892
H	-6.835360	0.382847	1.030074
H	-6.743900	-0.024579	-0.707551
H	-7.748832	-1.005914	0.388282
H	0.872589	4.968886	-0.305125
H	1.586840	5.434686	-1.868885
H	2.582451	4.600566	-0.645528
H	4.054629	1.197184	-1.681798
H	4.959095	2.667892	-1.247257

H	3.442401	2.801721	-2.176152
H	-2.718184	3.723142	-1.813914
H	-2.406972	3.277034	-0.116957
H	-1.248000	4.311533	-1.003436

ωB97X Energy = -1828.88106565 a.u.

(αS,1S,3S,3'S)-**21**, Conf F

C	-2.796359	0.764722	1.226860
C	-4.082849	0.262185	1.362013
C	-4.522928	-0.720894	0.468243
C	-3.680332	-1.193889	-0.525625
C	-2.377512	-0.703797	-0.646718
C	-1.947252	0.288046	0.230556
C	-1.472866	-1.255834	-1.722993
C	-2.007998	-2.559028	-2.298809
C	-1.286611	-2.978617	-3.559185
O	-3.388590	-2.402716	-2.618235
C	-0.298732	1.923348	-0.685586
C	0.980051	2.488636	-0.731052
C	2.007201	1.911480	0.009481
C	1.757609	0.815395	0.833833
C	0.472773	0.288387	0.914187
C	-0.561311	0.840370	0.148983
C	0.199837	-0.872726	1.840811
C	1.477246	-1.557095	2.298184
C	1.250610	-2.496486	3.461005
O	2.418237	-0.571027	2.720362
C	2.895154	0.248341	1.657906
C	-4.184750	-2.269253	-1.459588
C	3.944744	-0.489137	0.837485
C	5.240409	-0.573338	1.342202
C	6.231364	-1.269134	0.668189
C	5.900318	-1.885044	-0.522938
C	4.631214	-1.827435	-1.058746
C	3.655115	-1.120758	-0.367527
F	6.860410	-2.565549	-1.192086
O	-4.966712	0.650887	2.317405
C	-4.545645	1.641966	3.242837
O	-5.775034	-1.273992	0.594946
C	-6.838913	-0.412780	0.186115
O	1.236563	3.602961	-1.487806
C	0.744675	4.813743	-0.908058
O	3.258320	2.468956	0.026066
C	3.980293	2.414070	-1.207692
O	-1.338944	2.468175	-1.387335
C	-1.177752	2.572777	-2.804003
H	-2.430426	1.526971	1.902969
H	-1.372493	-0.526993	-2.536155
H	-0.467480	-1.419694	-1.323674
H	-1.918655	-3.351096	-1.539799
H	-1.407801	-2.216909	-4.333050
H	-0.220307	-3.103684	-3.361820
H	-1.683074	-3.923026	-3.934449
H	-0.448719	-1.602719	1.348990
H	-0.347760	-0.511990	2.719134

H	1.907230	-2.119624	1.458713
H	0.877068	-1.943510	4.325965
H	2.180096	-2.994820	3.739696
H	0.515237	-3.257404	3.193090
H	3.397768	1.077855	2.158245
H	-4.229754	-3.228564	-0.924044
H	-5.195160	-2.037757	-1.796874
H	5.481308	-0.082176	2.279314
H	7.242388	-1.334446	1.051007
H	4.416165	-2.320865	-1.998543
H	2.657065	-1.055509	-0.787868
H	-3.677345	1.304394	3.815281
H	-5.383719	1.798725	3.917468
H	-4.306458	2.580681	2.735845
H	-6.864434	0.490982	0.797718
H	-6.727502	-0.141988	-0.868337
H	-7.763214	-0.971524	0.320126
H	1.205035	4.981754	0.069048
H	-0.342805	4.780306	-0.802831
H	1.022979	5.618165	-1.585940
H	4.136613	1.374580	-1.508969
H	4.943807	2.883152	-1.018324
H	3.452567	2.957426	-1.991850
H	-0.730428	1.660511	-3.207882
H	-2.177433	2.696645	-3.215975
H	-0.555576	3.426810	-3.072893

$\omega$ B97X Energy = -1828.88090967 a.u.

(aS,1S,3S,3'S)-**21**, Conf G

C	2.817741	0.839715	-1.083757
C	4.128143	0.387416	-1.158641
C	4.574368	-0.552459	-0.223055
C	3.727775	-1.003859	0.778331
C	2.408535	-0.551246	0.850684
C	1.962240	0.376986	-0.086029
C	1.498876	-1.076769	1.934664
C	2.064090	-2.330485	2.586134
C	1.328689	-2.713546	3.849960
O	3.430931	-2.110271	2.927215
C	0.226096	1.950435	0.763309
C	-1.072929	2.469916	0.780725
C	-2.056103	1.849967	0.013244
C	-1.734501	0.775834	-0.816895
C	-0.432473	0.290850	-0.858179
C	0.555223	0.879076	-0.058596
C	-0.090658	-0.862028	-1.771851
C	-1.328844	-1.589315	-2.269083
C	-1.034402	-2.515682	-3.427176
O	-2.290955	-0.635248	-2.717423
C	-2.828206	0.163200	-1.668208
C	4.251988	-2.003194	1.783622
C	-3.867908	-0.616808	-0.874746
C	-5.144823	-0.753939	-1.414494
C	-6.124207	-1.490273	-0.767292
C	-5.800717	-2.092806	0.432737

C	-4.549992	-1.983677	1.002479
C	-3.585278	-1.237143	0.337610
F	-6.749981	-2.812266	1.076129
O	5.034104	0.796270	-2.084325
C	4.613205	1.758259	-3.039754
O	5.874596	-0.996862	-0.245758
C	6.157858	-1.926968	-1.291456
O	-1.342468	3.538020	1.593512
C	-1.767089	4.726413	0.920144
O	-3.349667	2.305307	-0.000087
C	-4.054077	2.217564	1.242172
O	1.177558	2.479178	1.596711
C	1.779217	3.682359	1.124532
H	2.443676	1.559918	-1.800613
H	1.355125	-0.307529	2.702525
H	0.510225	-1.296472	1.520485
H	2.019671	-3.161334	1.865546
H	1.411954	-1.914445	4.590273
H	0.270634	-2.878046	3.637620
H	1.743408	-3.628176	4.275892
H	0.564270	-1.568150	-1.254112
H	0.474187	-0.486709	-2.632881
H	-1.764242	-2.169264	-1.444571
H	-0.652957	-1.946768	-4.278243
H	-1.937291	-3.043950	-3.736459
H	-0.282547	-3.252506	-3.138508
H	-3.351056	0.971803	-2.181968
H	4.355986	-2.988081	1.304305
H	5.240310	-1.703093	2.130763
H	-5.380194	-0.272459	-2.358001
H	-7.120907	-1.596644	-1.177452
H	-4.340210	-2.468654	1.947845
H	-2.602060	-1.132923	0.784365
H	3.792912	1.375139	-3.652964
H	5.476444	1.951856	-3.671726
H	4.303085	2.687614	-2.554050
H	5.519567	-2.811325	-1.202430
H	6.014954	-1.466385	-2.270971
H	7.199355	-2.220342	-1.174289
H	-2.740948	4.589027	0.447137
H	-1.035328	5.018584	0.161573
H	-1.830455	5.501818	1.680663
H	-3.643465	2.908407	1.980562
H	-4.012601	1.197302	1.631786
H	-5.087611	2.479392	1.024942
H	2.530102	3.965853	1.859360
H	2.261788	3.516642	0.156484
H	1.040245	4.482379	1.036389

$\omega$ B97X Energy = -1828.88087275 a.u.

(aS,1S,3S,3'S)-**21**, Conf H

C	2.894938	1.012528	-0.951530
C	4.205645	0.561263	-1.009389
C	4.589704	-0.508044	-0.191897
C	3.682265	-1.085210	0.682533

C	2.361204	-0.631628	0.739898
C	1.976884	0.424299	-0.083849
C	1.389376	-1.307415	1.679524
C	1.908157	-2.658576	2.149176
C	1.090123	-3.237010	3.281065
O	3.248534	-2.511584	2.610654
C	0.246359	2.049817	0.685795
C	-1.053303	2.565948	0.677443
C	-2.035265	1.930947	-0.073781
C	-1.718278	0.813607	-0.847742
C	-0.417646	0.321892	-0.858990
C	0.572737	0.935824	-0.079468
C	-0.074669	-0.856990	-1.738997
C	-1.312302	-1.596205	-2.219092
C	-1.014610	-2.566235	-3.339959
O	-2.265700	-0.654537	-2.709209
C	-2.806126	0.185221	-1.694513
C	4.143057	-2.229841	1.555503
C	-3.865997	-0.554795	-0.889780
C	-5.138203	-0.692347	-1.440428
C	-6.135292	-1.393856	-0.781666
C	-5.834371	-1.961082	0.441250
C	-4.589210	-1.849802	1.022752
C	-3.606594	-1.138166	0.345972
F	-6.800836	-2.646701	1.095741
O	5.169024	1.086253	-1.809563
C	4.809308	2.170067	-2.653514
O	5.886014	-0.963977	-0.200712
C	6.229669	-1.731835	-1.354598
O	-1.359967	3.686749	1.404855
C	-0.987147	4.905273	0.756771
O	-3.303467	2.442020	-0.153767
C	-4.064968	2.412583	1.057309
O	1.224938	2.702258	1.389952
C	1.137711	2.561460	2.808711
H	2.567697	1.833467	-1.576686
H	1.212666	-0.677877	2.559391
H	0.418752	-1.440533	1.193151
H	1.910514	-3.358612	1.299648
H	1.118368	-2.569154	4.145209
H	0.050097	-3.359439	2.972838
H	1.480555	-4.210806	3.579522
H	0.578931	-1.552014	-1.205733
H	0.491879	-0.502675	-2.608021
H	-1.756460	-2.143192	-1.376560
H	-0.622884	-2.031522	-4.208343
H	-1.918642	-3.099616	-3.636824
H	-0.269964	-3.296872	-3.018697
H	-3.312025	0.982541	-2.241622
H	4.285108	-3.128491	0.936930
H	5.104081	-1.992011	2.010588
H	-5.355606	-0.238512	-2.401754
H	-7.128434	-1.500275	-1.200322
H	-4.397510	-2.306563	1.985830
H	-2.627983	-1.030601	0.801681
H	4.029745	1.877322	-3.362041

H	5.711140	2.437938	-3.198518
H	4.468945	3.029676	-2.069912
H	7.259898	-2.055301	-1.218712
H	5.581666	-2.609680	-1.437856
H	6.151263	-1.128715	-2.261236
H	-1.509029	5.004336	-0.198792
H	0.092972	4.940117	0.596247
H	-1.284952	5.714754	1.420245
H	-5.036614	2.839374	0.816636
H	-3.582581	3.005639	1.834597
H	-4.196259	1.381624	1.397388
H	1.252614	1.512085	3.095058
H	1.958584	3.139531	3.228200
H	0.187054	2.946747	3.182065

$\omega$ B97X Energy = -1828.88087212 a.u.

(aS,1S,3S,3'S)-**21**, Conf I

C	-2.778045	0.778028	1.289762
C	-4.073602	0.300123	1.429049
C	-4.555452	-0.629566	0.500350
C	-3.744644	-1.075079	-0.532047
C	-2.433086	-0.610581	-0.658058
C	-1.961201	0.328760	0.254732
C	-1.564160	-1.133776	-1.777084
C	-2.139654	-2.400675	-2.393047
C	-1.450792	-2.788324	-3.681445
O	-3.521743	-2.199922	-2.680012
C	-0.285218	1.949774	-0.637024
C	1.010763	2.474222	-0.697294
C	2.016568	1.880350	0.062886
C	1.755847	0.756463	0.841577
C	0.464567	0.241835	0.900383
C	-0.562906	0.849028	0.171292
C	0.177516	-0.956512	1.773613
C	1.449182	-1.670573	2.200044
C	1.215842	-2.663726	3.315682
O	2.394503	-0.709407	2.669652
C	2.886593	0.137537	1.637030
C	-4.293744	-2.095297	-1.502196
C	3.918263	-0.597300	0.789387
C	5.154702	-0.881273	1.365983
C	6.128339	-1.580106	0.671366
C	5.840851	-1.992347	-0.615518
C	4.631456	-1.733147	-1.223467
C	3.670282	-1.029085	-0.508006
F	6.786008	-2.673242	-1.306433
O	-4.927295	0.663649	2.421233
C	-4.462601	1.600053	3.382178
O	-5.817197	-1.160265	0.626959
C	-6.870230	-0.256355	0.288496
O	1.242594	3.607473	-1.430818
C	2.126951	3.447972	-2.544426
O	3.295442	2.379155	0.041375
C	3.453732	3.637075	0.704733
O	-1.328080	2.529228	-1.302282

C	-1.199498	2.702064	-2.713780
H	-2.380070	1.499397	1.992081
H	-1.466561	-0.373280	-2.561261
H	-0.554039	-1.334574	-1.407930
H	-2.055600	-3.223140	-1.666446
H	-1.570957	-1.997315	-4.425482
H	-0.383764	-2.940938	-3.508937
H	-1.872665	-3.710939	-4.082332
H	-0.476316	-1.657112	1.247083
H	-0.368724	-0.632088	2.666749
H	1.879291	-2.191922	1.334130
H	0.843163	-2.151395	4.205719
H	2.142451	-3.179410	3.571495
H	0.477319	-3.407206	3.010195
H	3.410452	0.936068	2.166778
H	-4.355741	-3.075117	-1.007010
H	-5.303325	-1.822855	-1.810358
H	5.360587	-0.548709	2.378129
H	7.093972	-1.799714	1.109811
H	4.449007	-2.073464	-2.235338
H	2.717312	-0.812751	-0.978650
H	-3.590207	1.215836	3.917691
H	-5.281601	1.743598	4.082676
H	-4.212434	2.555875	2.914041
H	-7.802485	-0.807312	0.397370
H	-6.873224	0.605718	0.957902
H	-6.766305	0.081359	-0.747220
H	3.123221	3.150288	-2.214808
H	2.174381	4.416173	-3.038745
H	1.732641	2.702473	-3.241065
H	2.869429	4.416373	0.211870
H	4.512864	3.880456	0.653204
H	3.148703	3.554740	1.751773
H	-2.212262	2.770526	-3.107478
H	-0.649874	3.612272	-2.952675
H	-0.698241	1.840620	-3.164835

$\omega$ B97X Energy = -1828.87979073 a.u.

(aS,1S,3S,3'S)-**21**, Conf J

C	-2.822352	0.938287	1.031057
C	-4.104902	0.439523	1.209311
C	-4.487864	-0.708251	0.505539
C	-3.593850	-1.343731	-0.341675
C	-2.295000	-0.853726	-0.504871
C	-1.922109	0.300722	0.179870
C	-1.336901	-1.589661	-1.412991
C	-1.818417	-3.000888	-1.715720
C	-1.029777	-3.663031	-2.822289
O	-3.183734	-2.954623	-2.122903
C	-0.312438	1.890401	-0.870657
C	0.959236	2.462998	-0.995706
C	2.006173	1.953484	-0.232763
C	1.785792	0.913640	0.669912
C	0.511321	0.378949	0.820681
C	-0.545707	0.866702	0.042329

C	0.268228	-0.694482	1.855465
C	1.559424	-1.313331	2.366516
C	1.358292	-2.113210	3.633519
O	2.500927	-0.280960	2.656825
C	2.949683	0.406902	1.494905
C	-4.039354	-2.597630	-1.058201
C	3.942925	-0.447953	0.716503
C	3.648667	-1.036898	-0.507154
C	4.576205	-1.845431	-1.153390
C	5.799114	-2.049319	-0.551584
C	6.132681	-1.480558	0.662552
C	5.192303	-0.679419	1.288885
F	6.711105	-2.832617	-1.175187
O	-5.036102	0.982386	2.035549
C	-4.673873	2.143912	2.767739
O	-5.733231	-1.260990	0.686137
C	-6.797988	-0.521019	0.086714
O	1.215492	3.464832	-1.893216
C	0.547067	4.704272	-1.636705
O	3.286271	2.420675	-0.369333
C	3.508984	3.772626	0.034766
O	-1.359043	2.369092	-1.616796
C	-1.277530	2.103456	-3.018643
H	-2.499509	1.826660	1.558696
H	-1.222655	-1.050421	-2.360441
H	-0.342386	-1.635411	-0.959973
H	-1.752478	-3.607412	-0.799517
H	-1.136225	-3.097022	-3.750679
H	0.029566	-3.703511	-2.561831
H	-1.384471	-4.680480	-2.991943
H	-0.373396	-1.480077	1.447914
H	-0.278142	-0.256098	2.698774
H	1.980323	-1.964810	1.588609
H	0.997700	-1.464250	4.434998
H	2.294852	-2.573593	3.951049
H	0.621463	-2.901859	3.469453
H	3.495251	1.269580	1.882278
H	-4.104812	-3.424818	-0.336745
H	-5.032396	-2.459363	-1.486083
H	2.684631	-0.864949	-0.973670
H	4.357409	-2.308763	-2.107555
H	7.107414	-1.661991	1.098324
H	5.433995	-0.224278	2.243680
H	-5.548739	2.414138	3.353981
H	-4.415595	2.968945	2.098472
H	-3.835039	1.941241	3.439150
H	-6.637134	-0.423466	-0.991309
H	-7.710716	-1.085959	0.266367
H	-6.885398	0.469466	0.536539
H	0.772532	5.056821	-0.626093
H	-0.532380	4.600735	-1.753783
H	0.933056	5.415783	-2.363919
H	4.587713	3.898815	0.104091
H	3.058934	3.958639	1.014170
H	3.107257	4.474986	-0.696239
H	-2.181162	2.515789	-3.462589

H        -0.398422   2.577195   -3.459958  
H        -1.243800   1.025987   -3.201136  
ωB97X Energy = -1828.87968944 a.u.

(aS,1S,3S,3'S)-**21**, Conf K

C	2.776833	0.545621	-1.408630
C	4.093510	0.106688	-1.391091
C	4.588303	-0.503644	-0.233170
C	3.781837	-0.646335	0.885540
C	2.455019	-0.210117	0.864780
C	1.961181	0.391118	-0.289882
C	1.591724	-0.404639	2.088012
C	2.201400	-1.408012	3.055645
C	1.508412	-1.417274	4.398945
O	3.571182	-1.079001	3.274185
C	0.210727	2.118047	0.137965
C	-1.103055	2.591027	0.044073
C	-2.070461	1.784046	-0.552242
C	-1.753967	0.511781	-1.018306
C	-0.443909	0.050806	-0.931804
C	0.544610	0.861058	-0.364986
C	-0.094905	-1.313755	-1.477760
C	-1.327817	-2.160053	-1.752582
C	-1.023614	-3.366481	-2.611431
O	-2.300051	-1.375074	-2.442397
C	-2.845046	-0.335385	-1.638087
C	4.358670	-1.295950	2.122415
C	-3.840243	-0.902092	-0.631371
C	-5.039141	-1.420366	-1.117490
C	-5.972812	-1.989602	-0.267205
C	-5.684617	-2.032036	1.083432
C	-4.512593	-1.530041	1.606153
C	-3.590686	-0.963102	0.734260
F	-6.591355	-2.583717	1.924626
O	4.962243	0.227927	-2.428144
C	4.491937	0.849440	-3.614765
O	5.897621	-0.916819	-0.166479
C	6.172407	-2.113995	-0.894338
O	-1.390401	3.865520	0.455567
C	-2.295343	3.967907	1.559283
O	-3.366497	2.221143	-0.673164
C	-3.554119	3.259212	-1.639972
O	1.218886	2.881437	0.652349
C	1.037457	3.445000	1.951697
H	2.366447	1.018889	-2.291714
H	1.460888	0.551569	2.608692
H	0.593097	-0.741836	1.794771
H	2.155292	-2.412287	2.607679
H	1.603883	-0.439305	4.876591
H	0.446724	-1.638748	4.274945
H	1.946154	-2.170273	5.055601
H	0.561350	-1.841886	-0.780550
H	0.471564	-1.194878	-2.408419
H	-1.758722	-2.493083	-0.798724
H	-0.641918	-3.049746	-3.584917

H	-1.922587	-3.964771	-2.765910
H	-0.268519	-3.991266	-2.130641
H	-3.407989	0.284769	-2.338548
H	4.477971	-2.375858	1.949350
H	5.346952	-0.887874	2.332525
H	-5.246031	-1.378044	-2.181785
H	-6.908478	-2.391568	-0.635941
H	-4.327464	-1.582492	2.671963
H	-2.666996	-0.560118	1.135213
H	3.656279	0.293800	-4.049045
H	5.328512	0.843898	-4.309181
H	4.184527	1.881357	-3.424820
H	7.223601	-2.343915	-0.731071
H	5.557914	-2.939342	-0.521966
H	5.990040	-1.970879	-1.961181
H	-3.263215	3.528142	1.315194
H	-2.411827	5.030660	1.761659
H	-1.878577	3.472957	2.441002
H	-3.014700	4.163773	-1.352656
H	-4.622859	3.460119	-1.673115
H	-3.214959	2.926097	-2.625008
H	2.034726	3.595259	2.362294
H	0.512240	4.398316	1.899328
H	0.484838	2.757719	2.598886

ωB97X Energy = -1828.87947933 a.u.

(aS,1S,3S,3'S)-**21**, Conf L

C	-2.854912	1.051484	0.895040
C	-4.161993	0.597616	0.999078
C	-4.549813	-0.522746	0.255393
C	-3.651344	-1.146689	-0.595766
C	-2.334932	-0.688593	-0.702124
C	-1.945306	0.416482	0.051795
C	-1.374379	-1.416093	-1.614202
C	-1.883914	-2.804079	-1.972515
C	-1.077080	-3.459389	-3.070019
O	-3.232063	-2.704835	-2.424375
C	-0.226203	2.000529	-0.824054
C	1.071600	2.525374	-0.855009
C	2.060550	1.926595	-0.079220
C	1.757483	0.837936	0.738516
C	0.458299	0.346151	0.792878
C	-0.542137	0.929119	0.004838
C	0.128310	-0.788694	1.733693
C	1.372279	-1.501283	2.237393
C	1.088474	-2.403907	3.416620
O	2.334886	-0.535098	2.656956
C	2.861557	0.231499	1.579536
C	-4.116285	-2.350671	-1.382742
C	3.874198	-0.585363	0.786245
C	5.102670	-0.861314	1.383295
C	6.056852	-1.633525	0.741360
C	5.757948	-2.128043	-0.513492
C	4.556306	-1.878590	-1.140710
C	3.615000	-1.099613	-0.478594



F	6.683576	-2.882181	-1.152773
O	-5.117328	1.165467	1.779473
C	-4.753271	2.303307	2.547123
O	-5.840913	-0.989758	0.314133
C	-6.161946	-1.674652	1.525615
O	1.408871	3.566542	-1.677882
C	0.778695	4.816532	-1.378478
O	3.362659	2.347099	-0.123438
C	3.616261	3.671214	0.349079
O	-1.215428	2.571182	-1.584061
C	-1.091701	2.359861	-2.991870
H	-2.523796	1.910301	1.464838
H	-1.229801	-0.850461	-2.542011
H	-0.390515	-1.499909	-1.144037
H	-1.866855	-3.437331	-1.072085
H	-1.129754	-2.862919	-3.983810
H	-0.030241	-3.544358	-2.772439
H	-1.459274	-4.458506	-3.283352
H	-0.529921	-1.511314	1.244624
H	-0.429655	-0.391404	2.589644
H	1.803560	-2.096137	1.420772
H	0.711758	-1.818165	4.258353
H	1.994927	-2.923437	3.730280
H	0.336434	-3.148496	3.149045
H	3.406330	1.044343	2.063860
H	-4.249622	-3.202654	-0.699491
H	-5.082679	-2.148765	-1.843862
H	5.317882	-0.463169	2.369451
H	7.016244	-1.847951	1.195794
H	4.364778	-2.284311	-2.126450
H	2.668664	-0.890124	-0.965611
H	-5.649060	2.600348	3.086901
H	-4.426930	3.125164	1.904190
H	-3.961702	2.061203	3.261450
H	-5.486879	-2.522449	1.676926
H	-6.102764	-0.999108	2.381100
H	-7.181365	-2.039956	1.416830
H	-0.298610	4.762005	-1.538891
H	1.218388	5.549099	-2.052320
H	0.979858	5.105533	-0.342862
H	4.694065	3.749796	0.477532
H	3.123879	3.835072	1.311920
H	3.280301	4.418163	-0.370502
H	-0.173890	2.807122	-3.379004
H	-1.103067	1.290296	-3.218766
H	-1.955931	2.834593	-3.451711

$\omega$ B97X Energy = -1828.87934419 a.u.

(aR,1S,3S,3'S)-**21**, Conf A

C	-2.030320	-1.044059	-1.384732
C	-3.270012	-1.656111	-1.507664
C	-4.301582	-1.274423	-0.642228
C	-4.091787	-0.287051	0.308009
C	-2.851668	0.347724	0.413265

C	-1.819629	-0.048798	-0.432374
C	-2.658711	1.440285	1.437994
C	-3.987520	1.952209	1.975505
C	-3.824457	2.828311	3.196334
O	-4.809663	0.845139	2.339467
C	-0.152637	1.684136	-1.091465
C	1.107355	2.281509	-1.008766
C	2.068171	1.730229	-0.167046
C	1.763529	0.617763	0.617366
C	0.500789	0.038765	0.544525
C	-0.462069	0.565975	-0.325715
C	0.168601	-1.142079	1.425828
C	1.407740	-1.785426	2.026819
C	1.079289	-2.727860	3.162668
O	2.268596	-0.773246	2.547375
C	2.827793	0.067793	1.544474
C	-5.236295	0.113350	1.209692
C	3.966074	-0.635920	0.816735
C	5.212117	-0.701488	1.435905
C	6.276098	-1.361828	0.841979
C	6.069139	-1.961099	-0.385163
C	4.852481	-1.922475	-1.032303
C	3.801866	-1.251126	-0.420085
F	7.102414	-2.605566	-0.976479
O	-3.570426	-2.612522	-2.423854
C	-2.546738	-3.009571	-3.323725
O	-5.555103	-1.826110	-0.756546
C	-5.649676	-3.175751	-0.298185
O	1.378051	3.391748	-1.764929
C	1.308120	4.615272	-1.029066
O	3.298307	2.316076	-0.018814
C	4.139976	2.306462	-1.176566
O	-1.118407	2.258319	-1.876089
C	-0.965322	2.007205	-3.273067
H	-1.210708	-1.330343	-2.031784
H	-2.058464	1.067540	2.277055
H	-2.102466	2.271998	0.997216
H	-4.502375	2.515138	1.182292
H	-3.364689	2.260426	4.008548
H	-3.183237	3.681242	2.965952
H	-4.791166	3.202720	3.535762
H	-0.389633	-1.889839	0.857588
H	-0.490316	-0.809648	2.237192
H	1.944364	-2.336987	1.243473
H	0.596742	-2.182728	3.977312
H	1.985023	-3.199318	3.546396
H	0.398973	-3.509509	2.819432
H	3.261721	0.901925	2.098219
H	-5.965680	0.702331	0.635105
H	-5.753171	-0.770648	1.583472
H	5.356004	-0.222777	2.399003
H	7.250056	-1.411506	1.312971
H	4.733856	-2.402832	-1.995654
H	2.844624	-1.201169	-0.927536
H	-2.989770	-3.763759	-3.969423
H	-1.696036	-3.442388	-2.790330

H	-2.206391	-2.166018	-3.930839
H	-6.690232	-3.472115	-0.416161
H	-5.011052	-3.833593	-0.890263
H	-5.370673	-3.242441	0.757931
H	0.307788	4.750479	-0.609073
H	1.518173	5.415922	-1.735376
H	2.051408	4.626263	-0.228121
H	3.688075	2.869800	-1.993651
H	4.334808	1.278451	-1.493842
H	5.074938	2.774863	-0.875930
H	-1.777833	2.529348	-3.774673
H	-0.006905	2.387654	-3.632948
H	-1.042634	0.934844	-3.477555

$\omega$ B97X Energy = -1828.88182768 a.u.

(aR,1S,3S,3'S)-21, Conf B

C	-2.022228	-1.257989	-1.176186
C	-3.249086	-1.906272	-1.211477
C	-4.270349	-1.467722	-0.361356
C	-4.050794	-0.419564	0.519108
C	-2.818059	0.237118	0.549551
C	-1.805840	-0.193006	-0.303898
C	-2.618279	1.399324	1.493078
C	-3.943043	1.927966	2.023782
C	-3.767404	2.897141	3.170265
O	-4.734051	0.837360	2.490224
C	-0.220015	1.529105	-1.154719
C	1.021588	2.168898	-1.167337
C	2.029693	1.714092	-0.323873
C	1.791074	0.656693	0.554190
C	0.546537	0.035364	0.574928
C	-0.464404	0.464773	-0.294517
C	0.286782	-1.083090	1.556356
C	1.567789	-1.636401	2.159850
C	1.310113	-2.495997	3.376696
O	2.408100	-0.557847	2.568218
C	2.904399	0.216978	1.482629
C	-5.174766	0.013432	1.432037
C	4.043414	-0.505226	0.774461
C	5.306099	-0.490394	1.362699
C	6.374680	-1.159984	0.787893
C	6.155429	-1.849799	-0.388576
C	4.922144	-1.893488	-1.003033
C	3.866695	-1.211728	-0.410591
F	7.193173	-2.503504	-0.961776
O	-3.543839	-2.958725	-2.017252
C	-2.529911	-3.422467	-2.896046
O	-5.487702	-2.105425	-0.344466
C	-6.314805	-1.818098	-1.472492
O	1.228368	3.227596	-2.012711
C	1.105785	4.498841	-1.370791
O	3.243130	2.348557	-0.266657
C	4.043077	2.276587	-1.451373
O	-1.232088	2.012347	-1.942493
C	-1.116584	1.669395	-3.323494

H	-1.213451	-1.577675	-1.821311
H	-1.995070	1.093257	2.342340
H	-2.084169	2.206264	0.984130
H	-4.486407	2.420787	1.203247
H	-3.279343	2.400180	4.011966
H	-3.146921	3.740164	2.860497
H	-4.732584	3.280771	3.503735
H	-0.263197	-1.891335	1.068415
H	-0.355586	-0.710246	2.363349
H	2.097724	-2.230138	1.403263
H	0.834549	-1.904258	4.162325
H	2.243897	-2.905391	3.764463
H	0.647777	-3.324785	3.119443
H	3.326188	1.106450	1.953473
H	-5.943653	0.537687	0.845121
H	-5.647056	-0.858088	1.884516
H	5.458845	0.057628	2.286689
H	7.361112	-1.147614	1.234768
H	4.794640	-2.443186	-1.927415
H	2.895439	-1.227000	-0.893051
H	-2.228473	-2.641402	-3.599654
H	-2.965299	-4.254507	-3.443884
H	-1.654864	-3.771677	-2.341154
H	-5.854798	-2.179871	-2.394083
H	-7.258639	-2.334427	-1.307871
H	-6.498582	-0.742195	-1.549758
H	1.856048	4.606264	-0.583447
H	0.104605	4.617257	-0.947736
H	1.268878	5.253606	-2.137494
H	4.253967	1.233357	-1.701683
H	4.975522	2.787452	-1.219974
H	3.547252	2.768815	-2.288681
H	-0.182096	2.050210	-3.741003
H	-1.168687	0.583740	-3.451884
H	-1.959870	2.133637	-3.831150

$\omega$ B97X Energy = -1828.88139827 a.u.

(aR,1S,3S,3'S)-21, Conf C

C	2.075062	-0.960628	1.494490
C	3.326142	-1.546787	1.615111
C	4.316905	-1.226180	0.678860
C	4.053295	-0.329723	-0.343965
C	2.795642	0.271433	-0.458229
C	1.807897	-0.057273	0.467105
C	2.546681	1.249260	-1.583160
C	3.847803	1.762592	-2.181530
C	3.633806	2.537882	-3.461326
O	4.694258	0.654664	-2.479907
C	0.122129	1.643428	1.164210
C	-1.138779	2.237199	1.080447
C	-2.081427	1.715287	0.201835
C	-1.785098	0.591732	-0.567234
C	-0.526157	0.004148	-0.482030
C	0.442103	0.541909	0.376255
C	-0.205708	-1.197379	-1.339970

C	-1.452333	-1.837341	-1.929330
C	-1.135352	-2.809854	-3.042617
O	-2.297236	-0.823378	-2.473533
C	-2.854410	0.031219	-1.481391
C	5.162686	0.016870	-1.310466
C	-3.989887	-0.669348	-0.744335
C	-5.197284	-0.853251	-1.414705
C	-6.255217	-1.521412	-0.819577
C	-6.081931	-2.007202	0.461970
C	-4.905232	-1.846467	1.161232
C	-3.859075	-1.170627	0.545654
F	-7.109933	-2.659800	1.054611
O	3.680282	-2.417671	2.594849
C	2.699835	-2.755714	3.564641
O	5.583744	-1.746312	0.794324
C	5.689505	-3.122811	0.428090
O	-1.431525	3.333033	1.849192
C	-2.086535	3.004599	3.076164
O	-3.338398	2.256641	0.125584
C	-3.392899	3.552618	-0.478559
O	1.024108	2.120051	2.080154
C	1.685361	3.323632	1.690476
H	1.291058	-1.187065	2.205711
H	1.967401	0.767659	-2.379978
H	1.948245	2.093353	-1.230956
H	4.359207	2.399041	-1.443211
H	3.175920	1.895701	-4.217288
H	2.971554	3.387060	-3.282638
H	4.581760	2.912730	-3.849518
H	0.343225	-1.939366	-0.754896
H	0.456023	-0.892666	-2.159032
H	-1.999083	-2.362183	-1.134599
H	-0.643972	-2.290588	-3.868852
H	-2.047067	-3.277337	-3.416950
H	-0.466572	-3.592903	-2.680406
H	-3.292107	0.857299	-2.045650
H	5.897731	0.658346	-0.803252
H	5.684656	-0.884621	-1.631635
H	-5.314777	-0.463417	-2.420570
H	-7.199622	-1.663061	-1.330473
H	-4.811848	-2.241352	2.165387
H	-2.931527	-1.031096	1.090076
H	2.371268	-1.871907	4.118099
H	3.180469	-3.451868	4.247552
H	1.835330	-3.239212	3.101646
H	6.735796	-3.397334	0.547937
H	5.069989	-3.746928	1.074523
H	5.393803	-3.265446	-0.615912
H	-1.446924	2.366154	3.691334
H	-3.037195	2.501269	2.881605
H	-2.269967	3.943938	3.593960
H	-2.994804	3.512798	-1.496642
H	-2.831821	4.279187	0.110874
H	-4.443616	3.833155	-0.510963
H	2.320814	3.147095	0.817100
H	0.961149	4.110987	1.470999

H 2.307862 3.623677 2.531111  
 ωB97X Energy = -1828.88062572 a.u.

(aR,1S,3S,3'S)-**21**, Conf D

C	2.100263	-0.506641	1.679175
C	3.358747	-1.016478	1.961603
C	4.350841	-0.954527	0.975399
C	4.080190	-0.386278	-0.258696
C	2.815313	0.140606	-0.539208
C	1.826858	0.070276	0.440034
C	2.560585	0.758609	-1.894925
C	3.857154	1.093621	-2.617021
C	3.636587	1.465170	-4.065604
O	4.718490	-0.041694	-2.585260
C	0.123771	1.878380	0.639916
C	-1.143266	2.423282	0.398342
C	-2.072349	1.676738	-0.319758
C	-1.751440	0.394566	-0.770531
C	-0.496668	-0.144715	-0.515226
C	0.455825	0.607386	0.185727
C	-0.169326	-1.535951	-1.003532
C	-1.414836	-2.315929	-1.390992
C	-1.095752	-3.572768	-2.168531
O	-2.244472	-1.500199	-2.217182
C	-2.803757	-0.383443	-1.534562
C	5.189923	-0.310740	-1.282099
C	-3.988823	-0.809712	-0.677565
C	-3.885535	-1.035015	0.691096
C	-4.977758	-1.471232	1.430263
C	-6.173582	-1.671691	0.774346
C	-6.320708	-1.456693	-0.582098
C	-5.216047	-1.026206	-1.300071
F	-7.246456	-2.089404	1.486913
O	3.718923	-1.571582	3.147466
C	2.733453	-1.649530	4.166652
O	5.625120	-1.399807	1.233417
C	5.753600	-2.821605	1.282099
O	-1.452356	3.701393	0.781213
C	-1.555132	3.908325	2.193756
O	-3.295137	2.177511	-0.672743
C	-4.172708	2.574270	0.381893
O	1.039004	2.605413	1.360384
C	1.676636	3.652834	0.628235
H	1.315581	-0.535646	2.424279
H	1.985647	0.066884	-2.521899
H	1.954345	1.662619	-1.796192
H	4.358940	1.922551	-2.094314
H	3.183382	0.628758	-4.602758
H	2.968325	2.325236	-4.138391
H	4.582138	1.717888	-4.547124
H	0.379152	-2.082335	-0.232202
H	0.492276	-1.474155	-1.875166
H	-1.972291	-2.584011	-0.483548
H	-0.586045	-3.320799	-3.101415
H	-2.009219	-4.119707	-2.406094

H	-0.443768	-4.223184	-1.582446
H	-3.190353	0.256022	-2.329822
H	5.912068	0.460684	-0.978090
H	5.727335	-1.257854	-1.331400
H	-2.943489	-0.860070	1.199432
H	-4.906183	-1.648470	2.496275
H	-7.280280	-1.619869	-1.056995
H	-5.313284	-0.850572	-2.366439
H	1.884051	-2.260467	3.849096
H	2.381250	-0.654670	4.452355
H	3.218593	-2.119441	5.018595
H	6.806304	-3.033067	1.459681
H	5.153237	-3.239581	2.091987
H	5.449141	-3.266411	0.329712
H	-0.594600	3.744911	2.683213
H	-2.306357	3.238964	2.623177
H	-1.870019	4.941048	2.329986
H	-4.185334	1.820887	1.174534
H	-5.165272	2.644812	-0.059570
H	-3.884208	3.542277	0.791481
H	0.939598	4.343096	0.211729
H	2.314644	4.181356	1.333747
H	2.293867	3.239197	-0.174715

$\omega$ B97X Energy = -1828.88046454 a.u.

(aR,1S,3S,3'S)-21, Conf E

C	2.069998	-1.015994	1.368115
C	3.320990	-1.607519	1.475772
C	4.336908	-1.204682	0.601458
C	4.100271	-0.217822	-0.342925
C	2.848797	0.396670	-0.432458
C	1.833008	-0.019514	0.423203
C	2.625252	1.487268	-1.453058
C	3.938001	2.019553	-2.010141
C	3.742442	2.889142	-3.230848
O	4.773645	0.925596	-2.382743
C	0.147433	1.684680	1.108388
C	-1.127785	2.256763	1.053474
C	-2.066588	1.724282	0.173161
C	-1.763658	0.601582	-0.595222
C	-0.500692	0.024758	-0.518824
C	0.464652	0.574264	0.333631
C	-0.165826	-1.161864	-1.391279
C	-1.404108	-1.803582	-1.995951
C	-1.073909	-2.751453	-3.126589
O	-2.259588	-0.789740	-2.523395
C	-2.826221	0.044506	-1.519475
C	5.227037	0.203660	-1.257179
C	-3.956198	-0.675455	-0.793168
C	-5.163252	-0.857287	-1.464829
C	-6.215776	-1.541712	-0.878748
C	-6.037515	-2.045867	0.395039
C	-4.861099	-1.887816	1.095338
C	-3.820369	-1.195471	0.488916
F	-7.060278	-2.714420	0.978811

O	3.646948	-2.562372	2.384805
C	2.639728	-2.980226	3.293797
O	5.600763	-1.735360	0.700524
C	5.713557	-3.081738	0.236663
O	-1.385239	3.363259	1.816004
C	-2.426676	3.215427	2.785770
O	-3.320597	2.270161	0.060511
C	-3.352614	3.572566	-0.531546
O	1.117994	2.261396	1.885601
C	1.025884	1.967894	3.277600
H	1.261923	-1.319779	2.021699
H	2.018053	1.105810	-2.283180
H	2.063234	2.310321	-1.003612
H	4.454332	2.593380	-1.225802
H	3.281559	2.310626	-4.034905
H	3.089319	3.731118	-2.993781
H	4.697419	3.279653	-3.584970
H	0.385721	-1.908741	-0.815259
H	0.499999	-0.836756	-2.199962
H	-1.946826	-2.349010	-1.212295
H	-0.587087	-2.210942	-3.941789
H	-1.979352	-3.222451	-3.511591
H	-0.396613	-3.533222	-2.777687
H	-3.270285	0.874525	-2.072439
H	5.951164	0.807335	-0.691252
H	5.756677	-0.670703	-1.635656
H	-5.284663	-0.452773	-2.464401
H	-7.159878	-1.681996	-1.390573
H	-4.763823	-2.297460	2.093182
H	-2.892998	-1.057977	1.034123
H	3.102406	-3.729478	3.931410
H	1.790721	-3.425203	2.767742
H	2.291930	-2.144994	3.908165
H	6.759539	-3.361709	0.346307
H	5.089707	-3.751638	0.830897
H	5.428107	-3.149202	-0.817675
H	-3.399267	3.089794	2.307870
H	-2.420229	4.126286	3.380845
H	-2.226883	2.356096	3.432466
H	-4.402369	3.844021	-0.619939
H	-2.896404	3.548194	-1.524996
H	-2.831231	4.300755	0.092901
H	1.092038	0.889030	3.448031
H	1.869734	2.460810	3.756417
H	0.095364	2.352461	3.701468

$\omega$ B97X Energy = -1828.88042503 a.u.

(aR,1S,3S,3'S)-21, Conf F

C	-2.056906	-0.988761	-1.511921
C	-3.302334	-1.585048	-1.640540
C	-4.305601	-1.262915	-0.718197
C	-4.059412	-0.355689	0.299344
C	-2.806584	0.253921	0.423208
C	-1.806776	-0.075052	-0.489346
C	-2.578282	1.240466	1.545068

C	-3.890760	1.759099	2.113125
C	-3.701483	2.554218	3.384635
O	-4.738325	0.652598	2.413599
C	-0.122120	1.627258	-1.181870
C	1.128916	2.245666	-1.077512
C	2.082702	1.698311	-0.222881
C	1.770683	0.594592	0.571227
C	0.509745	0.013844	0.497047
C	-0.445034	0.532097	-0.387736
C	0.179056	-1.169168	1.376378
C	1.419106	-1.811699	1.976312
C	1.091676	-2.757685	3.109480
O	2.275520	-0.797491	2.500504
C	2.835085	0.044995	1.499158
C	-5.184233	-0.005683	1.246727
C	3.974241	-0.659067	0.773123
C	5.221401	-0.717514	1.390612
C	6.286089	-1.378917	0.799087
C	6.078521	-1.986761	-0.423712
C	4.860584	-1.955648	-1.068872
C	3.809355	-1.282917	-0.459247
F	7.112461	-2.632392	-1.012614
O	-3.639477	-2.467635	-2.615728
C	-2.644847	-2.810063	-3.569422
O	-5.567575	-1.792485	-0.843015
C	-5.668386	-3.166224	-0.465152
O	1.386995	3.335184	-1.864623
C	1.666411	4.548899	-1.161376
O	3.328785	2.255800	-0.090048
C	4.155370	2.223293	-1.257847
O	-1.019692	2.085056	-2.112214
C	-1.774597	3.226157	-1.714716
H	-1.263879	-1.215568	-2.212926
H	-2.017581	0.763899	2.357854
H	-1.970526	2.080751	1.199983
H	-4.391578	2.382851	1.356790
H	-3.253181	1.925758	4.157676
H	-3.040506	3.404027	3.204241
H	-4.657545	2.930010	3.751463
H	-0.378234	-1.915733	0.805293
H	-0.477401	-0.843773	2.191564
H	1.958513	-2.360045	1.192877
H	0.606415	-2.215964	3.924815
H	1.998209	-3.227525	3.493310
H	0.414110	-3.540450	2.763352
H	3.268157	0.878992	2.053800
H	-5.917707	0.621750	0.720078
H	-5.702786	-0.907207	1.573338
H	5.365719	-0.232414	2.350446
H	7.260958	-1.423008	1.268752
H	4.741457	-2.442363	-2.028958
H	2.851252	-1.238416	-0.965689
H	-2.314943	-1.930379	-4.128584
H	-3.112302	-3.516930	-4.250483
H	-1.783164	-3.282690	-3.090201
H	-5.040188	-3.792482	-1.101061

H	-5.380293	-3.297845	0.582420
H	-6.712103	-3.447890	-0.590782
H	2.621619	4.493747	-0.636655
H	0.871937	4.766168	-0.441700
H	1.700959	5.335112	-1.912564
H	5.111376	2.652155	-0.964670
H	3.719174	2.809856	-2.068177
H	4.305102	1.192314	-1.588108
H	-1.119610	4.060804	-1.453146
H	-2.390225	3.506037	-2.567332
H	-2.422707	2.985731	-0.866385

$\omega_{B97X}$  Energy = -1828.88029870 a.u.

(*aR*,1*S*,3*S*,3'*S*)-**21**, Conf G

C	-2.092928	-0.319613	-1.712051
C	-3.334316	-0.825407	-2.067725
C	-4.310564	-0.982377	-1.076523
C	-4.028404	-0.669453	0.243417
C	-2.774738	-0.164649	0.603751
C	-1.811232	0.010669	-0.387539
C	-2.511058	0.179147	2.051833
C	-3.805725	0.328388	2.836428
C	-3.577198	0.437150	4.326679
O	-4.625443	-0.814287	2.603973
C	-0.181323	1.890441	-0.265054
C	1.066810	2.433703	0.062555
C	2.038267	1.604114	0.613655
C	1.775822	0.247818	0.817751
C	0.538361	-0.286306	0.480316
C	-0.456121	0.544581	-0.054137
C	0.275282	-1.757491	0.700990
C	1.556340	-2.543067	0.929633
C	1.299948	-3.931602	1.470303
O	2.368039	-1.858336	1.882589
C	2.871774	-0.614096	1.410188
C	-5.112476	-0.859067	1.279889
C	4.053942	-0.827500	0.473385
C	5.301198	-1.100870	1.030064
C	6.406844	-1.347684	0.231523
C	6.240326	-1.319582	-1.139266
C	5.024354	-1.054192	-1.732255
C	3.931261	-0.804933	-0.911903
F	7.313642	-1.556667	-1.929906
O	-3.688139	-1.191199	-3.326621
C	-2.720774	-1.041150	-4.355073
O	-5.544312	-1.502770	-1.384637
C	-6.397985	-0.608125	-2.099170
O	1.312892	3.774552	-0.066825
C	1.384373	4.257835	-1.412158
O	3.247762	2.078186	1.040937
C	4.085575	2.711459	0.073354
O	-1.134414	2.706071	-0.823704
C	-1.842796	3.517741	0.113227
H	-1.323076	-0.175914	-2.459356
H	-1.911344	-0.607256	2.524950

H	-1.929224	1.101335	2.126948
H	-4.344134	1.219538	2.478632
H	-3.089118	-0.466311	4.699597
H	-2.937592	1.292922	4.550580
H	-4.524272	0.564487	4.852607
H	-0.259381	-2.173916	-0.156301
H	-0.377240	-1.888190	1.571752
H	2.108827	-2.620203	-0.016308
H	0.800609	-3.871982	2.440130
H	2.238097	-4.474463	1.593287
H	0.660780	-4.492510	0.785899
H	3.251413	-0.117033	2.304368
H	-5.887496	-0.090521	1.140795
H	-5.589632	-1.830122	1.150707
H	5.413077	-1.117328	2.109301
H	7.381574	-1.552992	0.656572
H	4.938113	-1.038526	-2.811743
H	2.972660	-0.582102	-1.367966
H	-2.432159	0.006433	-4.476500
H	-3.195706	-1.393395	-5.267405
H	-1.831620	-1.644309	-4.152465
H	-7.348667	-1.121405	-2.230269
H	-6.557574	0.310152	-1.525907
H	-5.974986	-0.363932	-3.075326
H	2.176727	3.740874	-1.961451
H	1.622941	5.317366	-1.343583
H	0.432062	4.123681	-1.925598
H	4.097711	2.138816	-0.858446
H	5.087434	2.721915	0.499140
H	3.759510	3.733273	-0.121079
H	-1.151951	4.112685	0.715222
H	-2.482083	4.178546	-0.468933
H	-2.465166	2.897375	0.765084

ωB97X Energy = -1828.88028885 a.u.

(aR,1S,3S,3'S)-**21**, Conf H

C	2.004527	-1.118132	1.338348
C	3.242179	-1.740689	1.422558
C	4.261681	-1.339062	0.551858
C	4.042058	-0.323743	-0.366014
C	2.804272	0.320844	-0.431996
C	1.784448	-0.093093	0.420232
C	2.599604	1.440248	-1.425151
C	3.921363	1.958461	-1.973954
C	3.740828	2.865541	-3.169417
O	4.730872	0.856837	-2.379774
C	0.139351	1.626641	1.161586
C	-1.115302	2.244905	1.118035
C	-2.090348	1.732216	0.265614
C	-1.812886	0.623126	-0.536491
C	-0.556574	0.029455	-0.502123
C	0.430094	0.534556	0.353666
C	-0.251710	-1.133935	-1.416192
C	-1.506647	-1.743764	-2.019547
C	-1.204844	-2.653586	-3.188777

O	-2.362377	-0.705022	-2.493830
C	-2.901116	0.096603	-1.448302
C	5.173111	0.094834	-1.276351
C	-4.013926	-0.647240	-0.719186
C	-3.856814	-1.188682	0.551309
C	-4.883966	-1.899801	1.159352
C	-6.068547	-2.054943	0.472362
C	-6.267824	-1.529980	-0.789892
C	-5.228676	-0.826760	-1.377549
F	-7.078124	-2.742060	1.057836
O	3.551960	-2.726022	2.304270
C	2.540730	-3.147133	3.207319
O	5.513335	-1.901554	0.628790
C	5.591385	-3.236361	0.125869
O	-1.425698	3.283188	1.955445
C	-0.720230	4.504440	1.711536
O	-3.358612	2.237847	0.213121
C	-3.504721	3.630573	-0.070931
O	1.110707	2.129977	1.990687
C	0.946277	1.784184	3.367015
H	1.193576	-1.419848	1.989345
H	1.981737	1.091536	-2.261846
H	2.056025	2.263726	-0.954168
H	4.453175	2.499156	-1.176403
H	3.264262	2.320034	-3.987300
H	3.107738	3.715144	-2.906537
H	4.703093	3.244267	-3.516576
H	0.301252	-1.904227	-0.873338
H	0.404108	-0.790578	-2.225590
H	-2.039533	-2.312350	-1.245690
H	-0.728488	-2.088274	-3.993258
H	-2.120905	-3.103995	-3.573392
H	-0.527734	-3.452285	-2.880106
H	-3.357139	0.945866	-1.960416
H	5.914856	0.666026	-0.699615
H	5.679548	-0.781436	-1.681212
H	-2.923035	-1.053486	1.086073
H	-4.770138	-2.325778	2.148572
H	-7.217454	-1.669077	-1.291731
H	-5.366375	-0.406048	-2.368264
H	2.215505	-2.322750	3.848155
H	2.990077	-3.924938	3.819784
H	1.678829	-3.557444	2.674166
H	5.295833	-3.266949	-0.927416
H	6.631355	-3.543620	0.218386
H	4.956833	-3.908440	0.706172
H	-1.108978	5.229565	2.423780
H	-0.908984	4.857108	0.693457
H	0.351489	4.372600	1.862503
H	-3.347171	4.233914	0.822563
H	-4.524440	3.762712	-0.427885
H	-2.806425	3.938026	-0.854293
H	1.019674	0.700599	3.498778
H	1.756856	2.268896	3.907673
H	-0.014057	2.140529	3.746715

ωB97X Energy = -1828.88028143 a.u.

(aR,1S,3S,3'S)-**21**, Conf I

C	-2.028372	-1.234497	-1.252411
C	-3.255978	-1.878282	-1.290363
C	-4.258536	-1.475833	-0.399759
C	-4.014663	-0.475626	0.527547
C	-2.774582	0.169950	0.569944
C	-1.786413	-0.215516	-0.332480
C	-2.550668	1.263376	1.588418
C	-3.866169	1.799336	2.133303
C	-3.676889	2.720467	3.316561
O	-4.675332	0.705075	2.557329
C	-0.195447	1.470637	-1.244583
C	1.044754	2.111649	-1.271478
C	2.035260	1.714175	-0.379753
C	1.808591	0.665510	0.508873
C	0.570066	0.030448	0.533235
C	-0.445523	0.444026	-0.338288
C	0.323609	-1.083165	1.523968
C	1.611182	-1.614692	2.133677
C	1.363658	-2.465530	3.358522
O	2.437555	-0.520292	2.530958
C	2.930410	0.232539	1.429226
C	-5.125821	-0.076740	1.471779
C	4.052435	-0.520580	0.722355
C	5.266685	-0.668882	1.389788
C	6.315339	-1.376285	0.824887
C	6.126581	-1.936865	-0.423727
C	4.942934	-1.813936	-1.118394
C	3.905356	-1.098921	-0.532830
F	7.145932	-2.628238	-0.986769
O	-3.572882	-2.889916	-2.138704
C	-2.576314	-3.323925	-3.052157
O	-5.480678	-2.104191	-0.391946
C	-6.320058	-1.767533	-1.497320
O	1.264734	3.129461	-2.161646
C	2.012725	2.729246	-3.312384
O	3.274240	2.300966	-0.406634
C	3.305175	3.652547	0.061808
O	-1.148717	1.816892	-2.166691
C	-1.816149	3.049511	-1.896819
H	-1.239320	-1.514819	-1.938538
H	-1.959210	0.880732	2.428742
H	-1.975197	2.082816	1.150231
H	-4.398201	2.332708	1.330367
H	-3.194569	2.184964	4.137654
H	-3.046587	3.567511	3.039236
H	-4.637111	3.102358	3.665867
H	-0.215608	-1.902037	1.041357
H	-0.322577	-0.714478	2.329122
H	2.150343	-2.207158	1.382501
H	0.879924	-1.872557	4.138257
H	2.302350	-2.859321	3.750632
H	0.712172	-3.305218	3.108933
H	3.369566	1.124136	1.881402

H	-5.899491	0.470458	0.912705
H	-5.595896	-0.964034	1.894851
H	5.395459	-0.221334	2.369851
H	7.264297	-1.492243	1.333820
H	4.837011	-2.268093	-2.095850
H	2.971427	-0.991767	-1.073443
H	-3.024794	-4.133462	-3.622721
H	-1.693337	-3.696536	-2.525875
H	-2.283981	-2.518694	-3.731564
H	-6.500231	-0.688642	-1.527504
H	-5.872450	-2.092585	-2.438429
H	-7.263975	-2.286627	-1.342333
H	1.475613	1.952921	-3.863860
H	3.000270	2.362709	-3.021525
H	2.119533	3.612978	-3.938181
H	2.950971	3.704189	1.095441
H	2.694364	4.297947	-0.571159
H	4.345144	3.969336	0.018720
H	-2.499986	3.221548	-2.725673
H	-2.388487	2.980393	-0.966513
H	-1.101253	3.872404	-1.833787

ωB97X Energy = -1828.88027260 a.u.

(aR,1S,3S,3'S)-**21**, Conf J

C	2.056698	-1.288579	1.103236
C	3.294469	-1.916831	1.096871
C	4.301710	-1.418553	0.262972
C	4.057462	-0.331321	-0.561871
C	2.814338	0.305649	-0.549027
C	1.816384	-0.183428	0.289351
C	2.586182	1.510088	-1.431303
C	3.896158	2.083173	-1.952393
C	3.691722	3.100797	-3.051231
O	4.698511	1.028451	-2.477576
C	0.219099	1.482571	1.224634
C	-1.031476	2.106955	1.278610
C	-2.019298	1.709376	0.381286
C	-1.789176	0.666331	-0.514108
C	-0.548621	0.038861	-0.550127
C	0.465917	0.455577	0.320084
C	-0.291801	-1.054303	-1.560366
C	-1.574102	-1.576702	-2.188544
C	-1.317502	-2.398500	-3.431244
O	-2.403728	-0.477427	-2.564765
C	-2.904853	0.249821	-1.449751
C	5.164829	0.164540	-1.463136
C	-4.029544	-0.518968	-0.764773
C	-5.238186	-0.660078	-1.444051
C	-6.289367	-1.378242	-0.897951
C	-6.109103	-1.956441	0.343985
C	-4.931260	-1.841428	1.049666
C	-3.890789	-1.115594	0.482696
F	-7.131386	-2.657964	0.888729
O	3.612795	-3.003300	1.846918
C	2.615969	-3.522196	2.714495

O	5.529576	-2.033315	0.206340
C	6.357832	-1.789725	1.343910
O	-1.214256	3.132464	2.165154
C	-2.244268	2.935122	3.138324
O	-3.252408	2.312325	0.375258
C	-3.249173	3.664146	-0.093403
O	1.235666	1.929422	2.028103
C	1.163303	1.493516	3.383507
H	1.258095	-1.655087	1.736005
H	1.955153	1.236670	-2.285974
H	2.048302	2.283235	-0.876256
H	4.441579	2.546692	-1.116357
H	3.202257	2.634298	-3.909357
H	3.061126	3.918215	-2.696694
H	4.646710	3.515166	-3.377091
H	0.245407	-1.882139	-1.091350
H	0.361612	-0.666321	-2.351246
H	-2.114313	-2.188133	-1.453330
H	-0.832851	-1.785705	-4.194873
H	-2.252684	-2.787273	-3.836539
H	-0.663406	-3.240804	-3.197851
H	-3.343160	1.149803	-1.885549
H	5.929682	0.675310	-0.859312
H	5.648341	-0.676271	-1.959743
H	-5.360221	-0.198443	-2.418417
H	-7.234114	-1.488853	-1.415843
H	-4.832042	-2.309445	2.021256
H	-2.961057	-1.014542	1.031561
H	3.070955	-4.369209	3.221977
H	1.741390	-3.862542	2.153412
H	2.308369	-2.777205	3.453670
H	7.306010	-2.288834	1.153261
H	6.531292	-0.716709	1.469612
H	5.904422	-2.197917	2.249270
H	-2.142467	3.744257	3.858621
H	-2.109921	1.975752	3.646325
H	-3.234024	2.965859	2.680830
H	-2.844913	3.713232	-1.108326
H	-2.661496	4.307255	0.564919
H	-4.286906	3.990804	-0.098953
H	0.256150	1.861290	3.868302
H	1.194658	0.400950	3.438098
H	2.033999	1.905563	3.889830

$\omega$ B97X Energy = -1828.88013279 a.u.

(aR,1S,3S,3'S)-**21**, Conf K

C	-1.978027	-1.365643	-1.083536
C	-3.199159	-2.025256	-1.064350
C	-4.213871	-1.545913	-0.228286
C	-3.992825	-0.445740	0.585723
C	-2.766677	0.223196	0.559411
C	-1.761589	-0.247231	-0.281018
C	-2.564700	1.440424	1.430544
C	-3.885565	1.983192	1.956718
C	-3.699448	3.013477	3.047005

O	-4.656352	0.911786	2.495229
C	-0.214211	1.449423	-1.242829
C	1.013133	2.117672	-1.303551
C	2.039905	1.717414	-0.452150
C	1.840205	0.679931	0.458934
C	0.607385	0.040303	0.532272
C	-0.428619	0.426558	-0.326259
C	0.383988	-1.041432	1.562369
C	1.684451	-1.544874	2.168081
C	1.463968	-2.348454	3.429442
O	2.514770	-0.433908	2.506427
C	2.983568	0.277430	1.366673
C	-5.106952	0.028696	1.490205
C	4.090630	-0.501743	0.665000
C	5.308468	-0.651031	1.325902
C	6.345871	-1.377871	0.765203
C	6.142572	-1.956346	-0.473015
C	4.955037	-1.833142	-1.160774
C	3.928608	-1.098784	-0.579206
F	7.151087	-2.666713	-1.032123
O	-3.494344	-3.125677	-1.803182
C	-2.490465	-3.626419	-2.673361
O	-5.425057	-2.191657	-0.158675
C	-6.267750	-1.976862	-1.291377
O	1.251501	3.097195	-2.229777
C	0.489189	4.297777	-2.067650
O	3.287329	2.277366	-0.513187
C	3.378325	3.666510	-0.192913
O	-1.236214	1.834137	-2.074270
C	-1.095884	1.382837	-3.422616
H	-1.173774	-1.717169	-1.717641
H	-1.920761	1.190584	2.282797
H	-2.050840	2.223281	0.866196
H	-4.448842	2.426354	1.121522
H	-3.191964	2.565602	3.904551
H	-3.092868	3.844496	2.682285
H	-4.662378	3.405449	3.377215
H	-0.157293	-1.879631	1.117205
H	-0.254226	-0.647185	2.362634
H	2.211327	-2.164061	1.429705
H	0.994040	-1.726760	4.195113
H	2.411387	-2.724887	3.817678
H	0.809995	-3.198449	3.225468
H	3.431810	1.185009	1.775783
H	-5.888335	0.515358	0.887619
H	-5.566016	-0.820330	1.995908
H	5.448275	-0.189581	2.297942
H	7.297229	-1.495228	1.269334
H	4.837706	-2.301430	-2.130231
H	2.991393	-0.991654	-1.113953
H	-2.206180	-2.879784	-3.420156
H	-2.927676	-4.488290	-3.171342
H	-1.604100	-3.940673	-2.115558
H	-5.812963	-2.383292	-2.196841
H	-7.203215	-2.494648	-1.088158
H	-6.465576	-0.909062	-1.425374



H	0.644427	4.716646	-1.069023
H	-0.573481	4.112034	-2.225239
H	0.858969	4.997439	-2.814626
H	2.826958	3.884869	0.726118
H	3.001348	4.285759	-1.007157
H	4.434989	3.875004	-0.036927
H	-0.172407	1.761912	-3.866318
H	-1.104864	0.289447	-3.460972
H	-1.952308	1.770762	-3.970519

$\omega$ B97X Energy = -1828.88013235 a.u.

(aR,1S,3S,3'S)-**21**, Conf L

C	-2.028591	-1.183981	-1.340523
C	-3.253812	-1.829625	-1.410886
C	-4.256799	-1.478665	-0.499267
C	-4.016922	-0.525366	0.477139
C	-2.779589	0.122827	0.551421
C	-1.789882	-0.212485	-0.369728
C	-2.562675	1.166653	1.622198
C	-3.882100	1.673921	2.184445
C	-3.700536	2.542988	3.407719
O	-4.686681	0.558157	2.558687
C	-0.191667	1.509510	-1.198460
C	1.042048	2.169249	-1.175621
C	2.042819	1.697299	-0.329876
C	1.795046	0.630447	0.534059
C	0.551930	0.007644	0.537768
C	-0.449228	0.447225	-0.338009
C	0.290767	-1.133436	1.492834
C	1.570499	-1.699901	2.086593
C	1.310222	-2.586752	3.283131
O	2.408151	-0.629444	2.521209
C	2.907356	0.167783	1.453306
C	-5.130178	-0.179709	1.439885
C	4.043576	-0.544567	0.730833
C	3.860385	-1.240306	-0.459711
C	4.912585	-1.916259	-1.064285
C	6.149431	-1.877616	-0.456530
C	6.375133	-1.198259	0.724703
C	5.309468	-0.534611	1.311894
F	7.184066	-2.525783	-1.041504
O	-3.568045	-2.796343	-2.311010
C	-2.571565	-3.175385	-3.248667
O	-5.475818	-2.112821	-0.523525
C	-6.323044	-1.710448	-1.600511
O	1.238634	3.220557	-2.029882
C	1.502331	4.478651	-1.402333
O	3.274116	2.299593	-0.275583
C	4.060900	2.216897	-1.468250
O	-1.140296	1.887655	-2.113727
C	-1.891459	3.046887	-1.764182
H	-1.238825	-1.425596	-2.040312
H	-1.977600	0.745402	2.448113
H	-1.984456	2.006144	1.227972
H	-4.414658	2.239173	1.404043

H	-3.215044	1.974956	4.204694
H	-3.076252	3.406134	3.169082
H	-4.663812	2.902012	3.772537
H	-0.258098	-1.929735	0.984080
H	-0.350427	-0.783070	2.309796
H	2.103197	-2.276395	1.319017
H	0.832447	-2.013338	4.080969
H	2.243285	-3.004413	3.663749
H	0.648983	-3.409804	3.005508
H	3.332224	1.045314	1.943341
H	-5.910458	0.383428	0.906471
H	-5.590673	-1.089465	1.824202
H	2.886716	-1.250973	-0.937523
H	4.779924	-2.457441	-1.992950
H	7.364074	-1.189494	1.166086
H	5.467332	0.004955	2.239989
H	-2.282619	-2.332186	-3.881916
H	-3.018241	-3.952755	-3.863655
H	-1.686778	-3.574217	-2.745162
H	-7.260410	-2.250024	-1.479408
H	-6.515748	-0.634244	-1.554901
H	-5.874932	-1.963888	-2.563156
H	2.472513	4.478541	-0.902931
H	0.721535	4.713326	-0.673185
H	1.493877	5.223424	-2.195372
H	4.242014	1.171553	-1.730594
H	5.007919	2.702446	-1.241904
H	3.572703	2.726824	-2.300539
H	-1.243455	3.919549	-1.654165
H	-2.593355	3.220745	-2.577417
H	-2.448669	2.882683	-0.836900

$\omega$ B97X Energy = -1828.87993546 a.u.

(aR,1S,3S,3'S)-**21**, Conf M

C	-2.119321	-0.332403	-1.601854
C	-3.372122	-0.846973	-1.905518
C	-4.352530	-0.873676	-0.907321
C	-4.076405	-0.391707	0.362988
C	-2.813313	0.121190	0.669516
C	-1.838832	0.148031	-0.324284
C	-2.553241	0.662875	2.055280
C	-3.537938	0.098692	3.072516
C	-3.241498	-1.345714	3.451865
O	-4.868676	0.275243	2.579100
C	-0.175969	2.003547	-0.281234
C	1.093969	2.519455	-0.009231
C	2.076986	1.675061	0.495513
C	1.789603	0.336103	0.761738
C	0.521518	-0.169840	0.497051
C	-0.467720	0.666873	-0.036770
C	0.209550	-1.612182	0.819702
C	1.462768	-2.434083	1.073585
C	1.164289	-3.763717	1.728594
O	2.335589	-1.716493	1.944801
C	2.873763	-0.533442	1.364111

C	-5.155315	-0.477023	1.417199
C	4.004802	-0.865031	0.400466
C	3.819325	-0.959979	-0.974949
C	4.865953	-1.315667	-1.816213
C	6.100093	-1.566468	-1.254675
C	6.328806	-1.477954	0.104450
C	5.268319	-1.127141	0.924898
F	7.128704	-1.906692	-2.066302
O	-3.726617	-1.348974	-3.116634
C	-2.761735	-1.306098	-4.157189
O	-5.587292	-1.426301	-1.150958
C	-6.439313	-0.619566	-1.965764
O	1.351058	3.844381	-0.246883
C	1.303548	4.653311	0.930931
O	3.315850	2.154326	0.832900
C	4.123482	2.619514	-0.252949
O	-1.164645	2.846016	-0.718338
C	-1.058430	3.213206	-2.093888
H	-1.337829	-0.312505	-2.350877
H	-1.530304	0.441208	2.369646
H	-2.644591	1.753650	2.039188
H	-3.507018	0.709795	3.976214
H	-3.165534	-1.995435	2.576453
H	-2.289890	-1.393831	3.985048
H	-4.021217	-1.735812	4.108731
H	-0.364035	-2.063734	0.006670
H	-0.428694	-1.652091	1.711642
H	1.979617	-2.609570	0.120861
H	0.691338	-3.607647	2.701088
H	2.082835	-4.333831	1.874032
H	0.486991	-4.349309	1.104099
H	3.312166	0.005843	2.205361
H	-6.096408	-0.087683	1.027030
H	-5.327503	-1.531221	1.672005
H	2.848208	-0.744808	-1.407552
H	4.730927	-1.393401	-2.887929
H	7.316074	-1.675386	0.503452
H	5.429096	-1.049984	1.995214
H	-3.245060	-1.731700	-5.033097
H	-1.880211	-1.901524	-3.904341
H	-2.458723	-0.277415	-4.372002
H	-7.385727	-1.150240	-2.050273
H	-6.609304	0.353603	-1.494960
H	-6.007437	-0.477714	-2.958012
H	2.062969	4.333616	1.648786
H	0.312921	4.598669	1.390106
H	1.503603	5.675682	0.616637
H	4.267126	1.822146	-0.987349
H	5.085067	2.889877	0.178610
H	3.672452	3.489802	-0.730836
H	-1.871799	3.907605	-2.295360
H	-0.102055	3.701514	-2.291899
H	-1.167073	2.331329	-2.732956

ωB97X Energy = -1828.87896180 a.u.

(aR,1S,3S,3'S)-**21**, Conf N

C	2.118721	1.586656	-0.861372
C	3.400408	2.116069	-0.790389
C	4.413872	1.356784	-0.194850
C	4.144798	0.089078	0.297778
C	2.863271	-0.456621	0.195192
C	1.849944	0.309124	-0.375338
C	2.601206	-1.848972	0.717852
C	3.893797	-2.610904	0.972514
C	3.675629	-3.879276	1.765252
O	4.795241	-1.784752	1.706186
C	0.065447	-0.934317	-1.589675
C	-1.225227	-1.454231	-1.690517
C	-2.140791	-1.220206	-0.669244
C	-1.771058	-0.479924	0.456511
C	-0.465073	-0.007680	0.569820
C	0.453622	-0.214680	-0.466033
C	-0.049703	0.701256	1.835637
C	-0.928971	0.279137	3.003079
C	-0.677982	-1.146000	3.474117
O	-2.292668	0.509237	2.646480
C	-2.794141	-0.267261	1.564719
C	5.265734	-0.704556	0.927720
C	-4.036787	0.458006	1.090478
C	-5.298415	-0.077077	1.308412
C	-6.441018	0.594883	0.892621
C	-6.288876	1.813833	0.266389
C	-5.050762	2.384719	0.040965
C	-3.924745	1.693942	0.460133
F	-7.395133	2.479600	-0.142950
O	3.759273	3.335742	-1.267647
C	2.752949	4.128877	-1.879197
O	5.703388	1.828422	-0.137093
C	5.906952	2.872401	0.816352
O	-1.580189	-2.193970	-2.788844
C	-1.323241	-3.590892	-2.631474
O	-3.384730	-1.791594	-0.709458
C	-4.259853	-1.307690	-1.733495
O	0.980869	-1.218460	-2.569579
C	0.827490	-0.438120	-3.755433
H	1.311655	2.157352	-1.303144
H	2.030443	-1.796986	1.654173
H	1.985921	-2.406404	0.006303
H	4.362334	-2.854512	0.007130
H	3.251839	-3.643759	2.744387
H	2.982592	-4.538464	1.239158
H	4.617344	-4.410223	1.910477
H	-0.132777	1.784363	1.703319
H	0.998562	0.491960	2.059247
H	-0.760238	0.958809	3.840126
H	-0.763337	-1.870193	2.660398
H	-1.390035	-1.416329	4.255856
H	0.329433	-1.224251	3.888338
H	-3.097823	-1.254403	1.936911
H	5.940721	-1.074749	0.142587
H	5.854743	-0.070379	1.590392

H	-5.396730	-1.039903	1.798104
H	-7.430773	0.184823	1.051023
H	-4.978211	3.346198	-0.452227
H	-2.942655	2.122899	0.290395
H	2.331104	3.626562	-2.754154
H	3.243474	5.047315	-2.191965
H	1.953031	4.366552	-1.172756
H	5.311384	3.751580	0.564140
H	5.649107	2.527487	1.822443
H	6.965236	3.124018	0.781048
H	-1.894607	-3.992668	-1.790495
H	-0.256100	-3.767789	-2.473758
H	-1.641008	-4.074376	-3.553131
H	-5.202345	-1.836040	-1.603386
H	-3.850387	-1.513288	-2.722707
H	-4.428095	-0.233993	-1.611029
H	-0.166018	-0.579641	-4.186595
H	0.992591	0.621684	-3.537981
H	1.583165	-0.784799	-4.457589

ωB97X Energy = -1828.87894652 a.u.

(aR,1S,3S,3'S)-**21**, Conf O

C	-2.033272	-0.979986	-1.390879
C	-3.283206	-1.566941	-1.513988
C	-4.286592	-1.233510	-0.606057
C	-4.039399	-0.294894	0.392232
C	-2.790740	0.314829	0.495127
C	-1.776208	-0.046473	-0.395728
C	-2.554748	1.350533	1.568376
C	-3.857191	1.835602	2.188622
C	-3.635885	2.629507	3.455666
O	-4.674622	0.713296	2.513436
C	-0.117574	1.718402	-0.980216
C	1.146693	2.305417	-0.890295
C	2.125824	1.696143	-0.112336
C	1.836307	0.534589	0.603904
C	0.570421	-0.036442	0.522934
C	-0.411680	0.551175	-0.285005
C	0.255487	-1.272670	1.331630
C	1.507328	-1.953667	1.860349
C	1.205646	-2.972930	2.935525
O	2.378412	-0.977048	2.429675
C	2.918535	-0.071393	1.473298
C	-5.148215	0.057336	1.356439
C	4.046513	-0.724683	0.685750
C	5.300324	-0.828655	1.283954
C	6.355147	-1.454439	0.638735
C	6.131346	-1.980135	-0.618879
C	4.907189	-1.899345	-1.247749
C	3.865697	-1.263657	-0.583747
F	7.154941	-2.592119	-1.259446
O	-3.490079	-2.495777	-2.504179
C	-4.362087	-2.056526	-3.547721
O	-5.546407	-1.774101	-0.697388
C	-5.623099	-3.163871	-0.369637

O	1.402885	3.463824	-1.575997
C	1.351775	4.634999	-0.757957
O	3.362311	2.265352	0.044802
C	4.171554	2.341843	-1.133165
O	-1.101825	2.347987	-1.696347
C	-0.987390	2.193926	-3.111117
H	-1.258748	-1.263787	-2.095627
H	-1.919517	0.931759	2.358234
H	-2.013995	2.203115	1.148848
H	-4.397382	2.452265	1.454691
H	-3.150543	2.005537	4.209756
H	-2.994459	3.489705	3.254997
H	-4.583826	2.989718	3.857472
H	-0.316408	-1.981501	0.728338
H	-0.384058	-0.994454	2.178270
H	2.026637	-2.449058	1.029178
H	0.741314	-2.486759	3.796694
H	2.120488	-3.467410	3.264781
H	0.518532	-3.730943	2.554799
H	3.359763	0.726372	2.072995
H	-5.892982	0.685856	0.847132
H	-5.658687	-0.845447	1.692166
H	5.457267	-0.408305	2.271940
H	7.334475	-1.534369	1.094193
H	4.775257	-2.322388	-2.235944
H	2.902205	-1.182233	-1.075176
H	-4.407340	-2.864120	-4.275564
H	-3.959184	-1.158644	-4.025121
H	-5.362502	-1.851047	-3.161256
H	-5.018323	-3.760948	-1.054683
H	-5.288494	-3.331340	0.658301
H	-6.670198	-3.445460	-0.460304
H	0.359937	4.744706	-0.311203
H	1.552386	5.481204	-1.412017
H	2.109704	4.589946	0.028007
H	4.316346	1.345169	-1.558879
H	5.132346	2.741628	-0.815236
H	3.721390	3.001881	-1.875434
H	-0.038982	2.599516	-3.469983
H	-1.070186	1.138065	-3.386571
H	-1.813101	2.748079	-3.553210

ωB97X Energy = -1828.87887908 a.u.

(aS,1R,3S,3'S)-**21**, Conf A

C	2.009453	-1.497712	-0.892200
C	3.260136	-2.098059	-0.932495
C	4.343686	-1.445375	-0.333424
C	4.164819	-0.226426	0.302787
C	2.901475	0.366092	0.363094
C	1.828163	-0.272828	-0.252631
C	2.730451	1.684914	1.077327
C	3.923814	2.009366	1.963763
C	3.914077	3.439789	2.452568
O	5.129364	1.807497	1.229192

C	0.161911	1.399209	-1.051943
C	-1.100317	1.993296	-1.025041
C	-2.084914	1.473634	-0.190756
C	-1.810489	0.373289	0.626000
C	-0.526976	-0.170166	0.640123
C	0.459548	0.324527	-0.222862
C	-0.195961	-1.249519	1.642598
C	-1.185991	-1.228904	2.792473
C	-1.004911	-2.383370	3.751306
O	-2.502149	-1.320380	2.254573
C	-2.912953	-0.170979	1.527835
C	5.354419	0.440999	0.953509
C	-4.151629	-0.588405	0.763214
C	-5.398762	-0.079434	1.097259
C	-6.539272	-0.475336	0.410420
C	-6.401265	-1.397670	-0.605426
C	-5.179159	-1.936082	-0.959982
C	-4.053989	-1.522000	-0.264340
F	-7.506021	-1.792594	-1.282189
O	3.521744	-3.297918	-1.513505
C	2.441004	-3.984963	-2.126372
O	5.589689	-2.024793	-0.314921
C	6.256107	-2.028739	-1.578578
O	-1.366687	3.079177	-1.817904
C	-0.918942	4.313498	-1.253300
O	-3.303619	2.088585	-0.086353
C	-4.126614	2.053047	-1.256647
O	1.135058	1.941160	-1.852032
C	1.038254	1.551171	-3.221981
H	1.154447	-1.978563	-1.350767
H	2.601769	2.485253	0.339335
H	1.821304	1.667102	1.685629
H	3.929577	1.324569	2.825463
H	3.969000	4.127131	1.605161
H	2.993706	3.644392	3.002822
H	4.762105	3.629629	3.111947
H	0.818600	-1.100812	2.021085
H	-0.218275	-2.239152	1.173079
H	-1.090638	-0.277358	3.335974
H	-1.133250	-3.333322	3.227395
H	-1.735638	-2.329592	4.559304
H	-0.003993	-2.359856	4.185926
H	-3.194866	0.618041	2.238514
H	5.611600	-0.090615	1.881117
H	6.223822	0.391349	0.297843
H	-5.484995	0.649943	1.895378
H	-7.517020	-0.079638	0.656075
H	-5.118226	-2.661258	-1.762079
H	-3.084005	-1.929909	-0.528633
H	2.858638	-4.906105	-2.525270
H	2.010437	-3.398243	-2.942451
H	1.661853	-4.224682	-1.397640
H	7.230312	-2.485797	-1.415829
H	5.694958	-2.610537	-2.311821
H	6.390963	-1.005886	-1.943497
H	0.164097	4.298237	-1.108351

H	-1.419544	4.500067	-0.299310
H	-1.182232	5.095664	-1.962565
H	-5.057071	2.550152	-0.989024
H	-4.338231	1.017924	-1.539179
H	-3.648223	2.577700	-2.083661
H	1.847773	2.053475	-3.747983
H	1.158162	0.467784	-3.319339
H	0.079027	1.858446	-3.645138

ωB97X Energy = -1828.88139278 a.u.

(aS,1R,3S,3'S)-**21**, Conf B

C	2.022732	-1.339811	-1.141174
C	3.285777	-1.899878	-1.275242
C	4.370355	-1.282616	-0.641955
C	4.188689	-0.116283	0.085762
C	2.917017	0.444280	0.224065
C	1.836520	-0.174423	-0.400094
C	2.743633	1.701000	1.041994
C	3.955784	1.977388	1.918844
C	3.932116	3.361604	2.525779
O	5.141565	1.864813	1.134868
C	0.108880	1.514422	-1.009628
C	-1.162274	2.077740	-0.890662
C	-2.104615	1.475331	-0.063730
C	-1.780178	0.319574	0.651995
C	-0.487504	-0.195975	0.577513
C	0.457481	0.385920	-0.277592
C	-0.100091	-1.344001	1.478384
C	-1.050844	-1.439219	2.657518
C	-0.814390	-2.664420	3.510886
O	-2.382715	-1.515365	2.157018
C	-2.839821	-0.318938	1.542270
C	5.387871	0.532369	0.738666
C	-4.097767	-0.698321	0.789386
C	-4.020194	-1.511882	-0.337145
C	-5.164079	-1.892347	-1.021544
C	-6.384445	-1.442898	-0.554745
C	-6.502558	-0.641355	0.561086
C	-5.343311	-0.277004	1.233743
F	-7.507581	-1.805126	-1.219394
O	3.562374	-3.019886	-1.992388
C	2.482372	-3.670032	-2.645396
O	5.640836	-1.787462	-0.782672
C	5.889145	-2.973117	-0.026825
O	-1.476107	3.216187	-1.586805
C	-1.048399	4.412363	-0.932155
O	-3.328423	2.054394	0.138551
C	-4.198456	2.107193	-0.996403
O	1.040965	2.137767	-1.798717
C	0.892858	1.861171	-3.191667
H	1.164602	-1.797835	-1.616919
H	2.582293	2.554100	0.372743
H	1.852027	1.619294	1.670559
H	4.001427	1.223267	2.719204
H	3.946938	4.117644	1.737338

H	3.025251	3.498883	3.117704
H	4.796340	3.515323	3.173425
H	0.923532	-1.201912	1.834463
H	-0.117542	-2.293399	0.931858
H	-0.956001	-0.533635	3.274628
H	-0.941234	-3.570864	2.914541
H	-1.518343	-2.693952	4.343587
H	0.199912	-2.653952	3.913983
H	-3.110534	0.403886	2.324191
H	5.701197	-0.064244	1.608518
H	6.224964	0.558661	0.041654
H	-3.051369	-1.849542	-0.690206
H	-5.118699	-2.522856	-1.900982
H	-7.479744	-0.313744	0.893907
H	-5.414586	0.356850	2.111084
H	1.731949	-4.009352	-1.926087
H	2.912293	-4.530573	-3.151996
H	2.012088	-3.012276	-3.381454
H	6.930905	-3.238427	-0.196675
H	5.731019	-2.788248	1.040035
H	5.243802	-3.788566	-0.359123
H	0.036764	4.411036	-0.802364
H	-1.539361	4.512361	0.039699
H	-1.338724	5.241733	-1.574170
H	-3.776395	2.735916	-1.780302
H	-5.134421	2.533505	-0.640377
H	-4.383074	1.100078	-1.380608
H	-0.086068	2.189224	-3.549288
H	1.675116	2.416000	-3.705978
H	1.020098	0.791157	-3.382491

ωB97X Energy = -1828.88111681 a.u.

(aS,1R,3S,3'S)-**21**, Conf C

C	2.098650	0.728659	-1.593888
C	3.358034	0.588163	-2.158717
C	4.374683	-0.008259	-1.403859
C	4.122136	-0.459339	-0.118101
C	2.849265	-0.331473	0.445771
C	1.842246	0.276301	-0.301093
C	2.604289	-0.860098	1.840216
C	3.697827	-1.821881	2.281371
C	3.623346	-2.150523	3.755041
O	4.971528	-1.233262	2.030277
C	0.093847	1.635155	0.846105
C	-1.196742	1.814319	1.356932
C	-2.114294	0.771023	1.266650
C	-1.770471	-0.423402	0.627901
C	-0.478837	-0.598957	0.140182
C	0.458596	0.436944	0.241769
C	-0.096624	-1.931120	-0.457421
C	-1.027805	-3.021799	0.038890
C	-0.790495	-4.354669	-0.633887
O	-2.368427	-2.633906	-0.245529
C	-2.827307	-1.513770	0.499391
C	5.239746	-1.128632	0.648197

C	-4.081572	-1.042406	-0.207907
C	-5.333941	-1.247736	0.353922
C	-6.487935	-0.844582	-0.305832
C	-6.357057	-0.243659	-1.540071
C	-5.129336	-0.031057	-2.136901
C	-3.991254	-0.437743	-1.458119
F	-7.474947	0.153435	-2.194164
O	3.689529	0.982225	-3.415065
C	2.675873	1.577681	-4.211364
O	5.622131	-0.212454	-1.943606
C	6.407831	0.973517	-2.072170
O	-1.551999	2.964851	2.010676
C	-1.630258	4.132798	1.187274
O	-3.346962	0.847536	1.852309
C	-4.234332	1.868340	1.392888
O	1.005925	2.657946	0.911420
C	1.493361	2.959252	2.220355
H	1.292797	1.186235	-2.153411
H	2.562492	-0.032128	2.557078
H	1.634958	-1.363686	1.893575
H	3.623640	-2.747906	1.690917
H	3.747209	-1.241785	4.348710
H	2.654232	-2.591448	3.995808
H	4.405228	-2.858527	4.032646
H	0.936140	-2.178088	-0.201659
H	-0.149906	-1.890486	-1.551287
H	-0.911262	-3.130131	1.127584
H	-0.937974	-4.263276	-1.712411
H	-1.480765	-5.106941	-0.250023
H	0.230629	-4.694134	-0.450989
H	-3.102827	-1.845739	1.509800
H	5.422174	-2.127193	0.225423
H	6.164381	-0.559922	0.548680
H	-5.415651	-1.718078	1.327923
H	-7.470309	-0.993453	0.125039
H	-5.073366	0.442463	-3.109333
H	-3.017143	-0.277952	-1.908518
H	1.845641	0.885227	-4.374817
H	3.143100	1.812642	-5.164493
H	2.300854	2.496882	-3.753392
H	7.370415	0.667438	-2.477475
H	5.932751	1.683598	-2.751330
H	6.557323	1.441717	-1.094362
H	-0.658930	4.371058	0.751782
H	-1.955041	4.943482	1.836454
H	-2.364832	3.988124	0.389672
H	-3.983634	2.833361	1.833000
H	-5.232628	1.569148	1.708289
H	-4.210429	1.936019	0.301350
H	2.220660	3.759645	2.101008
H	0.685311	3.287575	2.876812
H	1.986662	2.085562	2.654402

ωB97X Energy = -1828.87943253 a.u.

(aS,1R,3S,3'S)-**21**, Conf D

C	2.022104	-1.453226	-1.080391
C	3.269297	-2.060481	-1.129718
C	4.337688	-1.467549	-0.447423
C	4.148060	-0.300319	0.275737
C	2.888621	0.300582	0.339167
C	1.830000	-0.279062	-0.355474
C	2.707975	1.557981	1.155270
C	3.862035	1.773670	2.122828
C	3.845605	3.148087	2.751905
O	5.095856	1.628392	1.423110
C	0.147641	1.376908	-1.166210
C	-1.124839	1.955095	-1.130789
C	-2.088630	1.432415	-0.267644
C	-1.787587	0.367646	0.581492
C	-0.498727	-0.163235	0.579969
C	0.461338	0.319714	-0.313849
C	-0.135912	-1.214480	1.600723
C	-1.095940	-1.164298	2.774869
C	-0.880926	-2.285375	3.765976
O	-2.424290	-1.284737	2.274730
C	-2.867842	-0.169512	1.513995
C	5.320469	0.293073	1.022567
C	-4.106407	-0.643439	0.782275
C	-5.360206	-0.147139	1.109821
C	-6.499633	-0.594788	0.453608
C	-6.353317	-1.555466	-0.524826
C	-5.124035	-2.082980	-0.871007
C	-4.000330	-1.617209	-0.206462
F	-7.456876	-2.001309	-1.171321
O	3.541733	-3.213230	-1.794506
C	2.475292	-3.845207	-2.486893
O	5.577540	-2.061192	-0.434424
C	6.295031	-1.943763	-1.663907
O	-1.418986	2.977196	-1.995637
C	-1.678036	4.243338	-1.382217
O	-3.335696	1.998014	-0.195975
C	-4.150695	1.869318	-1.365807
O	1.105695	1.781689	-2.050713
C	1.442104	3.168366	-2.099926
H	1.177075	-1.889294	-1.598036
H	2.641371	2.427593	0.490871
H	1.767486	1.514842	1.712195
H	3.820127	1.005413	2.909711
H	3.946538	3.915323	1.980616
H	2.903470	3.310728	3.278727
H	4.664800	3.257940	3.463709
H	0.887767	-1.054705	1.948721
H	-0.168394	-2.216013	1.157570
H	-0.994457	-0.194755	3.284628
H	-1.010873	-3.252756	3.275495
H	-1.594347	-2.212765	4.587892
H	0.128964	-2.237821	4.177285
H	-3.159375	0.636969	2.200889
H	5.546044	-0.328105	1.901469
H	6.209851	0.298713	0.392095
H	-5.453048	0.612401	1.878517

H	-7.482849	-0.209805	0.694488
H	-5.056539	-2.838963	-1.643573
H	-3.024864	-2.015513	-0.465219
H	1.675722	-4.134651	-1.799549
H	2.899951	-4.736114	-2.942907
H	2.069833	-3.195172	-3.266868
H	5.758801	-2.437043	-2.476642
H	6.455820	-0.890453	-1.913682
H	7.256957	-2.429714	-1.511947
H	-2.569663	4.201446	-0.754629
H	-1.829240	4.952507	-2.193640
H	-0.822075	4.558427	-0.778766
H	-5.106188	2.329495	-1.122041
H	-4.307252	0.813982	-1.604179
H	-3.698518	2.378528	-2.218022
H	2.467313	3.221471	-2.463382
H	0.782468	3.712423	-2.775225
H	1.393225	3.616199	-1.103318

$\omega$ B97X Energy = -1828.87926012 a.u.

(*a*S,1R,3S,3'S)-**21**, Conf E

C	2.141305	0.125268	-1.778429
C	3.424490	-0.186414	-2.204577
C	4.427242	-0.378298	-1.247410
C	4.148929	-0.227035	0.101967
C	2.857025	0.090698	0.531522
C	1.855800	0.265559	-0.422038
C	2.583762	0.215259	2.012965
C	3.683899	-0.429308	2.842756
C	3.571285	-0.106048	4.315118
O	4.949285	0.043784	2.389124
C	0.029517	1.914578	-0.024591
C	-1.271637	2.251049	0.365092
C	-2.142977	1.242806	0.768036
C	-1.742466	-0.096042	0.734415
C	-0.439118	-0.418167	0.367302
C	0.453093	0.590300	-0.019748
C	0.005774	-1.858650	0.434273
C	-0.883607	-2.646340	1.378284
C	-0.580735	-4.127397	1.377926
O	-2.236401	-2.486075	0.962798
C	-2.749652	-1.170700	1.127264
C	5.264334	-0.438039	1.100353
C	-4.018435	-1.123593	0.300573
C	-5.264490	-1.104365	0.911479
C	-6.430572	-1.089757	0.156612
C	-6.317626	-1.105474	-1.217636
C	-5.096359	-1.135464	-1.862688
C	-3.946188	-1.145377	-1.089034
F	-7.447201	-1.091521	-1.965320
O	3.795525	-0.319618	-3.503933
C	2.799895	-0.129026	-4.498224
O	5.715974	-0.662833	-1.630511
C	5.907200	-1.996307	-2.104307
O	-1.678492	3.557538	0.434172

C	-1.803716	4.222766	-0.826764
O	-3.381330	1.524006	1.273854
C	-4.308993	2.191234	0.416753
O	0.890491	2.898402	-0.440732
C	1.387901	3.746076	0.596434
H	1.344506	0.272540	-2.496193
H	2.507002	1.270685	2.298226
H	1.623396	-0.243355	2.263667
H	3.650361	-1.520301	2.699425
H	3.657382	0.971831	4.470827
H	2.605894	-0.435907	4.703408
H	4.360809	-0.603890	4.879650
H	1.044562	-1.919375	0.766237
H	-0.035697	-2.320059	-0.558881
H	-0.774099	-2.245454	2.397099
H	-0.724819	-4.541692	0.377468
H	-1.236909	-4.654961	2.071311
H	0.454080	-4.301091	1.678705
H	-3.016686	-1.021231	2.182408
H	5.509564	-1.509310	1.152189
H	6.162714	0.087046	0.777092
H	-5.332173	-1.086394	1.993990
H	-7.408410	-1.067941	0.621640
H	-5.054509	-1.150103	-2.944864
H	-2.977059	-1.165814	-1.576523
H	3.299556	-0.266061	-5.454004
H	2.379993	0.879206	-4.448794
H	1.996964	-0.864675	-4.399393
H	6.970437	-2.105410	-2.309578
H	5.609475	-2.721243	-1.340694
H	5.337370	-2.170135	-3.019070
H	-2.493924	3.677991	-1.477485
H	-0.834211	4.316575	-1.317589
H	-2.209407	5.209891	-0.614095
H	-5.291641	2.048081	0.863083
H	-4.300682	1.742754	-0.580820
H	-4.086653	3.256115	0.349780
H	1.996366	3.170917	1.299504
H	2.011481	4.494199	0.111211
H	0.570092	4.235892	1.128737

ωB97X Energy = -1828.87916240 a.u.

(aS,1R,3S,3'S)-**21**, Conf F

C	2.076642	-1.205328	-1.388187
C	3.347425	-1.748803	-1.517757
C	4.390259	-1.223227	-0.746894
C	4.161485	-0.162429	0.115871
C	2.881897	0.382056	0.247980
C	1.843067	-0.145347	-0.515280
C	2.655534	1.513083	1.222515
C	3.801534	1.638706	2.215391
C	3.735690	2.912940	3.025955
O	5.038573	1.636966	1.506789
C	0.078338	1.480942	-1.192189
C	-1.208166	2.017770	-1.084212

C	-2.122789	1.428634	-0.211099
C	-1.758344	0.335743	0.576195
C	-0.456709	-0.156142	0.501809
C	0.455569	0.398115	-0.401123
C	-0.028088	-1.245874	1.453794
C	-0.935542	-1.269645	2.669871
C	-0.650337	-2.426865	3.599894
O	-2.281843	-1.402163	2.223651
C	-2.785584	-0.271299	1.525144
C	5.316294	0.380317	0.926210
C	-4.037779	-0.754063	0.822954
C	-5.292337	-0.324003	1.231576
C	-6.443938	-0.783998	0.605883
C	-6.308296	-1.689982	-0.424817
C	-5.077919	-2.150596	-0.853033
C	-3.942261	-1.673483	-0.217492
F	-7.423802	-2.147960	-1.041590
O	3.669956	-2.770419	-2.352330
C	2.635055	-3.322333	-3.152408
O	5.667918	-1.714056	-0.875113
C	5.874777	-2.979360	-0.246869
O	-1.560830	3.070815	-1.887532
C	-1.831153	4.298207	-1.203711
O	-3.381247	1.952657	-0.063821
C	-4.240909	1.851858	-1.203870
O	0.986572	1.961717	-2.092706
C	1.327878	3.346206	-2.020940
H	1.250004	-1.593734	-1.969513
H	2.554440	2.461743	0.682028
H	1.718000	1.361454	1.765384
H	3.789337	0.769497	2.890679
H	3.808163	3.781175	2.366756
H	2.789238	2.968573	3.567055
H	4.551664	2.953864	3.748618
H	1.007199	-1.082950	1.763507
H	-0.063131	-2.226083	0.965349
H	-0.833174	-0.320415	3.216395
H	-0.781373	-3.375295	3.073947
H	-1.326111	-2.407109	4.455909
H	0.376234	-2.372631	3.966805
H	-3.073337	0.498577	2.254125
H	5.585314	-0.342384	1.710866
H	6.191555	0.512445	0.290734
H	-5.377074	0.393287	2.040806
H	-7.428470	-0.451314	0.910866
H	-5.018966	-2.865510	-1.664452
H	-2.965851	-2.019457	-0.540368
H	1.837858	-3.742787	-2.533372
H	3.096844	-4.116052	-3.734511
H	2.216108	-2.572333	-3.828750
H	6.920763	-3.237191	-0.401756
H	5.672811	-2.912519	0.826598
H	5.238299	-3.745100	-0.694726
H	-2.023534	5.042297	-1.974085
H	-0.964856	4.603927	-0.610263
H	-2.702095	4.203260	-0.553582

H	-3.841236	2.413630	-2.049254
H	-5.198150	2.270241	-0.899154
H	-4.376406	0.804146	-1.484897
H	0.600111	3.961458	-2.549669
H	1.399241	3.674731	-0.979992
H	2.304255	3.445269	-2.492238

ωB97X Energy = -1828.87895828 a.u.

(a*S*,1*R*,3*S*,3'*S*)-**21**, Conf G

C	-2.082404	1.457090	-0.877802
C	-3.343402	2.036639	-0.886101
C	-4.403650	1.358928	-0.273176
C	-4.191651	0.135475	0.343895
C	-2.917679	-0.436460	0.371634
C	-1.867593	0.228546	-0.255948
C	-2.710137	-1.760164	1.066730
C	-3.878921	-2.114388	1.974349
C	-3.835712	-3.550118	2.445443
O	-5.103000	-1.923945	1.267868
C	-0.169640	-1.385446	-1.108858
C	1.112935	-1.940456	-1.118954
C	2.069481	-1.446374	-0.235082
C	1.784378	-0.356216	0.587565
C	0.496527	0.173857	0.606712
C	-0.485291	-0.337971	-0.251008
C	0.155770	1.242815	1.616975
C	1.155797	1.235453	2.758860
C	0.967796	2.387786	3.718846
O	2.466718	1.342433	2.210164
C	2.884282	0.192621	1.486191
C	-5.355760	-0.558312	1.012940
C	4.128531	0.617506	0.734093
C	4.034777	1.345653	-0.447266
C	5.173454	1.787741	-1.103198
C	6.403883	1.490842	-0.550584
C	6.537836	0.778541	0.622599
C	5.383820	0.346519	1.262437
F	7.522062	1.915068	-1.187502
O	-3.635862	3.239185	-1.446452
C	-2.576532	3.956231	-2.062249
O	-5.657870	1.918288	-0.220097
C	-6.352884	1.925269	-1.468128
O	1.362487	-2.996179	-1.952058
C	2.392016	-2.789033	-2.923431
O	3.319716	-2.007984	-0.175407
C	3.348596	-3.324537	0.382401
O	-1.142255	-1.920381	-1.913118
C	-1.095207	-1.472470	-3.265544
H	-1.244432	1.958799	-1.345362
H	-2.584552	-2.550259	0.317548
H	-1.788350	-1.734183	1.655371
H	-3.877535	-1.439844	2.844143
H	-3.898013	-4.228090	1.591055
H	-2.900431	-3.746194	2.973161
H	-4.666035	-3.761546	3.120608

H	-0.852510	1.075087	2.004089
H	0.156659	2.234428	1.151198
H	1.077107	0.282898	3.303388
H	1.081732	3.339088	3.194098
H	1.704267	2.342503	4.522135
H	-0.029960	2.352579	4.159917
H	3.167096	-0.592358	2.202410
H	-5.599950	-0.041261	1.952221
H	-6.240693	-0.515150	0.377894
H	3.059543	1.566363	-0.868476
H	5.115676	2.349947	-2.027135
H	7.522385	0.569165	1.022233
H	5.467628	-0.216811	2.185884
H	-1.790859	4.196126	-1.340569
H	-3.015875	4.877113	-2.437736
H	-2.147971	3.392654	-2.895527
H	-5.815780	2.520304	-2.208696
H	-6.483756	0.904168	-1.839383
H	-7.328547	2.369065	-1.279476
H	3.374690	-2.728999	-2.453668
H	2.203985	-1.871283	-3.488214
H	2.352864	-3.643049	-3.596449
H	2.915940	-3.321178	1.386719
H	4.396582	-3.611529	0.439248
H	2.804176	-4.030318	-0.248592
H	-0.156060	-1.763765	-3.742917
H	-1.925544	-1.949469	-3.782584
H	-1.212011	-0.385344	-3.314253

ωB97X Energy = -1828.87892287 a.u.

(a*S*,1*R*,3*S*,3'*S*)-**21**, Conf H

C	2.039600	-1.381974	-0.975278
C	3.300675	-1.951053	-1.067698
C	4.375017	-1.320189	-0.428198
C	4.174907	-0.158248	0.299555
C	2.899209	0.402797	0.411821
C	1.836080	-0.209566	-0.247556
C	2.708151	1.648756	1.243316
C	3.896996	1.909417	2.155920
C	3.859063	3.285826	2.779730
O	5.103133	1.804754	1.401695
C	0.143529	1.549614	-0.810307
C	-1.113202	2.142246	-0.648389
C	-2.073417	1.496355	0.128278
C	-1.792995	0.271290	0.734215
C	-0.516565	-0.274790	0.626740
C	0.455391	0.356223	-0.160651
C	-0.174160	-1.505651	1.432749
C	-1.165530	-1.702010	2.565263
C	-0.983750	-3.019552	3.284018
O	-2.482672	-1.689029	2.022110
C	-2.889624	-0.417563	1.536132
C	5.355386	0.475476	0.999398
C	-4.146866	-0.668754	0.729605
C	-4.075072	-1.331602	-0.491847



C	-5.220453	-1.599366	-1.225668
C	-6.436199	-1.192078	-0.711292
C	-6.548938	-0.538753	0.497878
C	-5.388426	-0.284793	1.217366
F	-7.560707	-1.446065	-1.422723
O	3.584440	-3.097404	-1.738169
C	2.511850	-3.767962	-2.383020
O	5.631871	-1.874400	-0.459920
C	6.301198	-1.740427	-1.714827
O	-1.402306	3.387242	-1.133553
C	-1.408953	3.543978	-2.552499
O	-3.284021	2.073762	0.392624
C	-4.139155	2.336207	-0.720817
O	1.082889	2.246828	-1.528058
C	1.458102	1.676986	-2.783358
H	1.192339	-1.842778	-1.467557
H	2.566461	2.511602	0.583556
H	1.799763	1.559353	1.846024
H	3.921104	1.145032	2.947246
H	3.899420	4.051565	2.001610
H	2.934872	3.418377	3.345321
H	4.703455	3.428787	3.455397
H	0.836958	-1.410609	1.836659
H	-0.179948	-2.400288	0.800282
H	-1.070788	-0.872459	3.281339
H	-1.117425	-3.849635	2.586526
H	-1.711045	-3.120990	4.090594
H	0.018976	-3.083484	3.710497
H	-3.149316	0.224278	2.389462
H	5.633370	-0.133647	1.871830
H	6.219318	0.505063	0.335151
H	-3.109992	-1.639671	-0.880415
H	-5.179095	-2.111957	-2.178847
H	-7.522691	-0.239221	0.865403
H	-5.455726	0.231607	2.168884
H	1.747266	-4.071924	-1.662830
H	2.944848	-4.651660	-2.845100
H	2.058571	-3.139334	-3.154281
H	5.749661	-2.249697	-2.507131
H	6.425230	-0.683762	-1.971089
H	7.280214	-2.200793	-1.596398
H	-1.931939	2.710553	-3.030964
H	-0.395235	3.618902	-2.946066
H	-1.944442	4.469799	-2.756725
H	-3.819642	3.227727	-1.260503
H	-5.134833	2.492315	-0.308846
H	-4.162479	1.477289	-1.397731
H	2.100021	2.407500	-3.272251
H	2.005848	0.742895	-2.648189
H	0.575507	1.494781	-3.403630

$\omega$ B97X Energy = -1828.87885177 a.u.

(a*S*,1*R*,3*S*,3'*S*)-**21**, Conf I

C	2.068686	-1.310079	-1.114725
C	3.339001	-1.856984	-1.232365

C	4.411467	-1.219042	-0.598921
C	4.210481	-0.045812	0.112512
C	2.931337	0.501553	0.234276
C	1.863105	-0.137620	-0.390009
C	2.736582	1.766466	1.034229
C	3.938804	2.069296	1.916023
C	3.894175	3.461437	2.503362
O	5.131819	1.959822	1.142671
C	0.116322	1.516975	-1.037726
C	-1.171731	2.052322	-0.953912
C	-2.090515	1.468624	-0.084851
C	-1.762671	0.317569	0.631851
C	-0.468453	-0.192280	0.560974
C	0.475027	0.404325	-0.284609
C	-0.078658	-1.334035	1.468496
C	-1.034183	-1.426874	2.644576
C	-0.794616	-2.644823	3.507336
O	-2.363778	-1.513952	2.138883
C	-2.825554	-0.324206	1.513051
C	5.396592	0.624946	0.767001
C	-4.075128	-0.722887	0.755163
C	-5.328267	-0.489323	1.305463
C	-6.483562	-0.899293	0.653229
C	-6.352648	-1.551608	-0.554633
C	-5.124060	-1.809781	-1.130530
C	-3.984333	-1.390497	-0.461820
F	-7.472056	-1.953982	-1.203394
O	3.633623	-2.982758	-1.933215
C	2.565497	-3.653802	-2.584595
O	5.688787	-1.710521	-0.723720
C	5.944338	-2.885663	0.046023
O	-1.464051	3.175574	-1.677653
C	-2.520171	3.039185	-2.632876
O	-3.345464	2.002971	0.063930
C	-3.373712	3.256260	0.752073
O	1.053355	2.134318	-1.824774
C	0.971723	1.796513	-3.207163
H	1.219580	-1.784498	-1.590702
H	2.569274	2.607946	0.352204
H	1.841411	1.681790	1.657308
H	3.987249	1.326935	2.727180
H	3.907197	4.206650	1.704666
H	2.980617	3.596502	3.085415
H	4.750830	3.634135	3.156280
H	0.942672	-1.185294	1.828188
H	-0.090195	-2.286653	0.927512
H	-0.946917	-0.516519	3.255796
H	-0.913315	-3.556131	2.916790
H	-1.502210	-2.672728	4.337004
H	0.217709	-2.625402	3.915038
H	-3.110674	0.398628	2.290858
H	5.708523	0.043814	1.647760
H	6.239665	0.651100	0.077219
H	-5.409854	0.027488	2.255882
H	-7.466678	-0.718568	1.069969
H	-5.068467	-2.325708	-2.081188

H	-3.010300	-1.581756	-0.899944
H	3.008611	-4.515313	-3.078004
H	2.091840	-3.010854	-3.331477
H	1.814748	-3.993158	-1.865619
H	5.310020	-3.711290	-0.282337
H	6.990001	-3.141541	-0.113994
H	5.776813	-2.691638	1.109808
H	-3.480859	2.879544	-2.141419
H	-2.315779	2.205705	-3.311291
H	-2.541331	3.968883	-3.197654
H	-2.911812	3.158494	1.738577
H	-4.422933	3.520405	0.867181
H	-2.856926	4.030170	0.180434
H	0.018226	2.118056	-3.634203
H	1.784816	2.319920	-3.706425
H	1.093375	0.717913	-3.346674

$\omega$ B97X Energy = -1828.87875646 a.u.

(*aS*,1*R*,3*S*,3'*S*)-**21**, Conf J

C	1.989705	-1.563748	-0.808194
C	3.238653	-2.169002	-0.796335
C	4.314006	-1.490984	-0.210736
C	4.128853	-0.241122	0.360359
C	2.867569	0.358461	0.366404
C	1.802560	-0.307619	-0.234485
C	2.689975	1.713359	1.008122
C	3.868714	2.079665	1.898265
C	3.857652	3.534601	2.308536
O	5.086731	1.833361	1.198801
C	0.156540	1.315029	-1.161693
C	-1.101271	1.923521	-1.189347
C	-2.096437	1.455788	-0.334250
C	-1.845570	0.394503	0.537295
C	-0.567124	-0.153765	0.607096
C	0.436423	0.295762	-0.259143
C	-0.264968	-1.178152	1.673344
C	-1.278806	-1.083953	2.799258
C	-1.123291	-2.180354	3.828290
O	-2.584110	-1.203186	2.240558
C	-2.976488	-0.105270	1.427133
C	5.308652	0.453016	1.000544
C	-4.185216	-0.588515	0.652449
C	-4.034762	-1.502035	-0.385816
C	-5.137632	-1.997364	-1.063958
C	-6.391012	-1.562663	-0.679160
C	-6.581354	-0.661964	0.347452
C	-5.462077	-0.181462	1.014302
F	-7.475048	-2.039796	-1.337644
O	3.505618	-3.396728	-1.312873
C	2.432714	-4.110963	-1.908144
O	5.557069	-2.072886	-0.139926
C	6.247227	-2.140229	-1.388997
O	-1.403689	2.912508	-2.085527
C	-0.674368	4.134037	-1.928881
O	-3.356996	1.988897	-0.361187

C	-3.473817	3.332329	0.105147
O	1.138395	1.754933	-2.014250
C	1.007654	1.255630	-3.346359
H	1.140804	-2.064596	-1.256621
H	2.579263	2.476141	0.228483
H	1.769820	1.731040	1.599562
H	3.854743	1.442346	2.795619
H	3.931421	4.174033	1.425762
H	2.928903	3.772962	2.830381
H	4.694943	3.756508	2.971605
H	0.743235	-1.016773	2.063517
H	-0.288347	-2.192562	1.260040
H	-1.188928	-0.102091	3.286972
H	-1.247106	-3.158641	3.358266
H	-1.869200	-2.075910	4.617292
H	-0.130814	-2.135740	4.280244
H	-3.292038	0.723706	2.076610
H	5.541381	-0.030266	1.960461
H	6.191835	0.363161	0.368057
H	-3.041320	-1.830777	-0.673104
H	-5.035682	-2.707981	-1.874953
H	-7.582518	-0.348023	0.616030
H	-5.589999	0.530499	1.822903
H	1.641698	-4.313018	-1.180748
H	2.854081	-5.051433	-2.254568
H	2.016388	-3.564619	-2.758891
H	7.216655	-2.591335	-1.186113
H	5.697941	-2.755663	-2.103473
H	6.392345	-1.136794	-1.800993
H	-1.094537	4.834400	-2.648034
H	0.386893	3.985793	-2.128660
H	-0.805083	4.529862	-0.917316
H	-3.072564	4.040070	-0.621812
H	-2.959485	3.453607	1.062940
H	-4.537612	3.518745	0.241346
H	0.053869	1.561064	-3.783660
H	1.827589	1.681718	-3.921104
H	1.086468	0.164324	-3.352989

$\omega$ B97X Energy = -1828.87871108 a.u.

(*aS*,1*R*,3*S*,3'*S*)-**21**, Conf K

C	2.032330	-1.220272	-1.186332
C	3.299521	-1.753504	-1.367427
C	4.384033	-1.155377	-0.714345
C	4.194435	-0.039257	0.084787
C	2.915661	0.492963	0.274554
C	1.837395	-0.100958	-0.377210
C	2.736713	1.678117	1.192701
C	3.954490	1.896386	2.078074
C	3.917928	3.224070	2.799917
O	5.131846	1.870088	1.273578
C	0.091803	1.653978	-0.767950
C	-1.172985	2.203947	-0.532284
C	-2.092331	1.489037	0.233060
C	-1.763845	0.236962	0.754005

C	-0.480106	-0.270663	0.572301
C	0.451045	0.430225	-0.205425
C	-0.084536	-1.539223	1.290524
C	-1.027742	-1.819841	2.446220
C	-0.791451	-3.168841	3.086284
O	-2.363890	-1.809265	1.951739
C	-2.817254	-0.524496	1.548353
C	5.394247	0.580388	0.764327
C	-4.090922	-0.765580	0.764739
C	-4.037130	-1.363309	-0.490906
C	-5.195724	-1.622809	-1.206511
C	-6.406217	-1.274103	-0.639396
C	-6.501042	-0.685706	0.604141
C	-5.327219	-0.438977	1.304507
F	-7.543631	-1.521069	-1.332530
O	3.582846	-2.826903	-2.149391
C	2.502182	-3.461453	-2.816655
O	5.659376	-1.631840	-0.898590
C	5.932487	-2.856233	-0.215730
O	-1.505160	3.467765	-0.934876
C	-1.572687	3.697774	-2.342291
O	-3.306301	2.019935	0.570352
C	-4.205349	2.321881	-0.497446
O	0.989744	2.419327	-1.468714
C	1.352464	1.934214	-2.762877
H	1.176001	-1.659412	-1.682714
H	2.559204	2.581508	0.599417
H	1.852321	1.532715	1.819671
H	4.021567	1.078667	2.811734
H	3.910731	4.043272	2.077205
H	3.017224	3.296535	3.412319
H	4.788587	3.336587	3.447420
H	0.939639	-1.447783	1.660977
H	-0.099658	-2.395549	0.607297
H	-0.924272	-1.027281	3.201962
H	-0.929308	-3.964012	2.349988
H	-1.488817	-3.330741	3.909212
H	0.226276	-3.230306	3.476038
H	-3.067317	0.061927	2.443334
H	5.738482	-0.079368	1.574767
H	6.214894	0.680074	0.054223
H	-3.076033	-1.625826	-0.920564
H	-5.168673	-2.085941	-2.185169
H	-7.471104	-0.431032	1.012818
H	-5.380335	0.027578	2.282290
H	1.767575	-3.844762	-2.103046
H	2.936181	-4.290995	-3.369338
H	2.011657	-2.776962	-3.514126
H	6.975179	-3.097353	-0.413353
H	5.786109	-2.734456	0.861802
H	5.292727	-3.659316	-0.586624
H	-2.121871	2.892477	-2.839345
H	-0.576772	3.787943	-2.775945
H	-2.109819	4.635527	-2.474857
H	-3.917605	3.242390	-1.005459
H	-5.186951	2.444695	-0.042785

H	-4.242872	1.495380	-1.212979
H	1.929969	2.726327	-3.236045
H	1.960778	1.030955	-2.693297
H	0.460133	1.727267	-3.361082

$\omega$ B97X Energy = -1828.87859887 a.u.

(*aS*,1*R*,3*S*,3'*S*)-**21**, Conf L

C	1.986789	-1.423071	-1.058542
C	3.242980	-2.006118	-1.150784
C	4.330579	-1.369723	-0.541937
C	4.159144	-0.161887	0.117467
C	2.894206	0.422438	0.213113
C	1.810197	-0.216142	-0.384456
C	2.731980	1.726339	0.956036
C	3.940462	2.036225	1.826810
C	3.932011	3.453635	2.352203
O	5.131320	1.861796	1.062320
C	0.108813	1.464536	-1.084268
C	-1.156995	2.051667	-1.004385
C	-2.114071	1.484028	-0.166052
C	-1.816545	0.342346	0.580710
C	-0.529015	-0.187893	0.549653
C	0.436547	0.364242	-0.300790
C	-0.172815	-1.308229	1.496849
C	-1.153621	-1.353567	2.654398
C	-0.946723	-2.545282	3.561076
O	-2.472257	-1.443518	2.121899
C	-2.908369	-0.270528	1.446613
C	5.361715	0.505608	0.744622
C	-4.138290	-0.688311	0.667059
C	-5.403179	-0.461447	1.193001
C	-6.542849	-0.890990	0.526167
C	-6.384534	-1.555742	-0.671593
C	-5.143700	-1.807376	-1.223412
C	-4.019849	-1.368693	-0.540237
F	-7.488619	-1.977293	-1.334575
O	3.509873	-3.167134	-1.803562
C	2.425691	-3.838330	-2.427848
O	5.594789	-1.899336	-0.641117
C	5.815689	-3.049356	0.175928
O	-1.503735	3.119809	-1.786649
C	-0.784621	4.331295	-1.532559
O	-3.383107	1.991692	-0.092504
C	-3.503702	3.296750	0.472741
O	1.050925	2.005193	-1.923433
C	0.884983	1.629189	-3.291430
H	1.126489	-1.895368	-1.516035
H	2.589045	2.541458	0.237101
H	1.834058	1.693450	1.579989
H	3.967826	1.329516	2.670197
H	3.963965	4.162714	1.521709
H	3.022719	3.637853	2.927482
H	4.793249	3.632544	2.997346
H	0.843019	-1.161662	1.872836
H	-0.186327	-2.276183	0.984057

H	-1.069335	-0.424953	3.237949
H	-1.063322	-3.474016	2.997879
H	-1.672240	-2.538461	4.375531
H	0.056770	-2.523669	3.989931
H	-3.212823	0.476200	2.193898
H	5.658326	-0.045082	1.649783
H	6.205498	0.481351	0.055699
H	-5.506194	0.064983	2.136070
H	-7.534778	-0.715685	0.923964
H	-5.066495	-2.332624	-2.167442
H	-3.036686	-1.554166	-0.960071
H	1.667158	-4.129814	-1.696185
H	2.847953	-4.729576	-2.885422
H	1.967553	-3.215262	-3.200766
H	6.854423	-3.339931	0.030730
H	5.649998	-2.808934	1.230499
H	5.160004	-3.869704	-0.122235
H	-1.236513	5.092454	-2.165469
H	0.271263	4.218857	-1.778928
H	-0.887870	4.622075	-0.482958
H	-3.156140	4.062259	-0.222092
H	-2.943035	3.363546	1.409554
H	-4.562744	3.446495	0.674718
H	1.676919	2.124921	-3.849387
H	0.984416	0.545339	-3.403186
H	-0.088495	1.953007	-3.668146

ωB97X Energy = -1828.87851537 a.u.

(aS,1R,3S,3'S)-**21**, Conf M

C	1.983269	-1.364857	-1.038586
C	3.242065	-1.935073	-1.147568
C	4.328018	-1.313479	-0.533180
C	4.137135	-0.148722	0.205933
C	2.866337	0.407511	0.334503
C	1.784259	-0.199169	-0.310769
C	2.683805	1.660809	1.155428
C	3.891776	1.946896	2.034959
C	3.859538	3.334826	2.632834
O	5.081255	1.833530	1.256818
C	0.087465	1.515410	-0.932721
C	-1.183747	2.084055	-0.841755
C	-2.155408	1.468226	-0.059758
C	-1.858315	0.297555	0.643574
C	-0.565458	-0.220955	0.603304
C	0.408189	0.371891	-0.211319
C	-0.211467	-1.385456	1.496983
C	-1.205816	-1.502446	2.637441
C	-1.002709	-2.744961	3.474287
O	-2.517969	-1.567206	2.086193
C	-2.951787	-0.358860	1.477971
C	5.330029	0.498548	0.870871
C	-4.176699	-0.724822	0.666090
C	-5.441266	-0.317296	1.067425
C	-6.570148	-0.670587	0.339265
C	-6.402386	-1.446333	-0.788386

C	-5.161827	-1.881153	-1.213946
C	-4.049049	-1.512487	-0.474205
F	-7.495461	-1.797191	-1.507116
O	3.392881	-3.077560	-1.894791
C	3.710588	-4.244365	-1.133682
O	5.592901	-1.845872	-0.594686
C	6.194627	-1.808891	-1.891545
O	-1.471310	3.237434	-1.524307
C	-1.030071	4.417475	-0.849405
O	-3.385115	2.044626	0.110863
C	-4.212906	2.124981	-1.053742
O	1.046158	2.145050	-1.684381
C	0.935638	1.892356	-3.085557
H	1.150195	-1.856228	-1.530273
H	2.515053	2.511156	0.484827
H	1.790977	1.570229	1.781008
H	3.937021	1.198213	2.840262
H	3.876436	4.085846	1.839651
H	2.948564	3.472563	3.218288
H	4.719174	3.495661	3.284791
H	0.797754	-1.249849	1.894337
H	-0.207453	-2.324923	0.933366
H	-1.133772	-0.609652	3.275945
H	-1.109366	-3.638762	2.855356
H	-1.736616	-2.789386	4.279988
H	-0.003791	-2.745379	3.914218
H	-3.255886	0.347510	2.262642
H	5.630616	-0.094824	1.746690
H	6.177737	0.520240	0.185881
H	-5.551634	0.296137	1.955179
H	-7.561791	-0.353878	0.638161
H	-5.077135	-2.490932	-2.104997
H	-3.064856	-1.838682	-0.793959
H	2.925456	-4.443989	-0.398805
H	4.670379	-4.131746	-0.625101
H	3.763510	-5.069844	-1.840689
H	5.620928	-2.403112	-2.605119
H	6.269121	-0.777181	-2.247191
H	7.192899	-2.227279	-1.780504
H	0.053763	4.397317	-0.711302
H	-1.527225	4.511409	0.119902
H	-1.302687	5.260126	-1.481812
H	-5.161809	2.542269	-0.722093
H	-4.382163	1.127560	-1.469057
H	-3.763295	2.772798	-1.806154
H	-0.027975	2.238966	-3.466410
H	1.739913	2.444660	-3.567565
H	1.054624	0.823921	-3.289548

ωB97X Energy = -1828.87836779 a.u.

(aS,1R,3S,3'S)-**21**, Conf N

C	-2.036329	1.460252	-1.020492
C	-3.286875	2.061696	-1.048396
C	-4.346773	1.450337	-0.369058
C	-4.145500	0.270151	0.329655

C	-2.882302	-0.324644	0.372550
C	-1.831906	0.274399	-0.318160
C	-2.688306	-1.596915	1.161956
C	-3.834719	-1.839609	2.132227
C	-3.806056	-3.226591	2.732591
O	-5.073975	-1.687122	1.443635
C	-0.157754	-1.390548	-1.129768
C	1.122040	-1.949032	-1.119023
C	2.083564	-1.444171	-0.247529
C	1.806151	-0.348675	0.566893
C	0.522349	0.196348	0.559691
C	-0.459355	-0.315624	-0.295147
C	0.185007	1.286141	1.548710
C	1.169865	1.279572	2.703785
C	0.981906	2.443573	3.649693
O	2.488750	1.367382	2.171767
C	2.905238	0.208370	1.461033
C	-5.308918	-0.344873	1.073132
C	4.152758	0.623850	0.708774
C	5.406117	0.346480	1.237967
C	6.563066	0.769740	0.597161
C	6.433662	1.480524	-0.577284
C	5.204995	1.784112	-1.130545
C	4.063646	1.350448	-0.473942
F	7.554536	1.896545	-1.215148
O	-3.570122	3.225286	-1.689394
C	-2.510860	3.877675	-2.373786
O	-5.589183	2.037627	-0.334470
C	-6.315779	1.942121	-1.560523
O	1.448994	-2.991202	-1.948236
C	1.736982	-2.579882	-3.285794
O	3.340309	-1.989418	-0.233688
C	3.411362	-3.288373	0.357826
O	-1.127235	-1.829920	-1.984666
C	-1.400980	-3.232729	-2.026328
H	-1.197920	1.910972	-1.536396
H	-2.620515	-2.452077	0.479129
H	-1.744438	-1.558053	1.713355
H	-3.792456	-1.087671	2.934701
H	-3.906139	-3.978680	1.946422
H	-2.860142	-3.393783	3.251152
H	-4.620702	-3.356385	3.446288
H	-0.830917	1.142050	1.925117
H	0.209302	2.269893	1.067163
H	1.073202	0.333546	3.256808
H	1.110883	3.388405	3.116808
H	1.708893	2.399502	4.461659
H	-0.020993	2.422501	4.079887
H	3.185608	-0.568642	2.187026
H	-5.530613	0.256322	1.966781
H	-6.203359	-0.342111	0.449865
H	5.486400	-0.215420	2.162638
H	7.546241	0.555036	0.997384
H	5.150868	2.344816	-2.055631
H	3.089673	1.575600	-0.895754
H	-2.106266	3.246896	-3.169877

H	-1.708985	4.156418	-1.684676
H	-2.942562	4.775898	-2.808326
H	-7.277348	2.423370	-1.392280
H	-5.786530	2.451696	-2.367759
H	-6.476595	0.893429	-1.828988
H	0.860005	-2.115925	-3.746356
H	2.007630	-3.477914	-3.837660
H	2.573075	-1.875684	-3.296997
H	4.460371	-3.577653	0.342784
H	2.821547	-4.007350	-0.213310
H	3.057840	-3.255240	1.392743
H	-1.212880	-3.695155	-1.054706
H	-2.456409	-3.331400	-2.276788
H	-0.794688	-3.731927	-2.782676

ωB97X Energy = -1828.87834418 a.u.

(a*S*,1*R*,3*S*,3'*S*)-**21**, Conf O

C	2.037189	-1.100359	-1.256921
C	3.299120	-1.648482	-1.442352
C	4.353264	-1.204373	-0.637120
C	4.142471	-0.223016	0.320221
C	2.877835	0.344463	0.490736
C	1.825734	-0.108998	-0.301101
C	2.676114	1.409510	1.541944
C	3.994847	2.056080	1.950600
C	4.516257	3.044879	0.917015
O	4.943944	1.030814	2.257898
C	0.106956	1.636600	-0.759955
C	-1.170561	2.179010	-0.613592
C	-2.128139	1.488319	0.122410
C	-1.811544	0.266803	0.723541
C	-0.513286	-0.230671	0.627892
C	0.445675	0.440517	-0.140571
C	-0.137385	-1.469675	1.403477
C	-1.116449	-1.707178	2.538524
C	-0.894815	-3.026260	3.242938
O	-2.435253	-1.727675	1.999728
C	-2.886568	-0.471234	1.512390
C	5.318760	0.246607	1.143153
C	-4.124708	-0.774383	0.695036
C	-4.014304	-1.450696	-0.516297
C	-5.139878	-1.766773	-1.261161
C	-6.375402	-1.393216	-0.768141
C	-6.525946	-0.728188	0.430456
C	-5.384416	-0.426065	1.161856
F	-7.481021	-1.694280	-1.490230
O	3.600597	-2.594976	-2.368893
C	2.551577	-3.055208	-3.207501
O	5.627418	-1.686680	-0.816759
C	5.821924	-3.026229	-0.360669
O	-1.475693	3.382584	-1.194380
C	-1.066227	4.505446	-0.410769
O	-3.361662	2.036086	0.351731
C	-4.203608	2.200194	-0.793713
O	1.056682	2.345194	-1.450593

C	0.949635	2.222943	-2.869499
H	1.201064	-1.429963	-1.860788
H	1.991440	2.177195	1.173983
H	2.206956	0.965670	2.426573
H	3.856369	2.580992	2.897268
H	4.578627	2.603241	-0.080353
H	3.839757	3.899626	0.859795
H	5.505574	3.408707	1.200975
H	0.875403	-1.362335	1.800388
H	-0.131189	-2.349335	0.750094
H	-1.041983	-0.882372	3.262451
H	-1.002911	-3.852458	2.536488
H	-1.618924	-3.158281	4.047939
H	0.109271	-3.063756	3.669314
H	-3.179917	0.157652	2.364430
H	5.865665	-0.608572	1.541648
H	6.015443	0.799286	0.499133
H	-3.034097	-1.730453	-0.888014
H	-5.068489	-2.289789	-2.206835
H	-7.514209	-0.457369	0.781125
H	-5.481784	0.099235	2.105835
H	2.997651	-3.792906	-3.869957
H	2.134712	-2.237860	-3.802357
H	1.755282	-3.525284	-2.623911
H	5.194728	-3.722467	-0.919975
H	6.871150	-3.262066	-0.527971
H	5.598437	-3.103837	0.707805
H	-1.350329	5.396722	-0.966844
H	0.016565	4.494525	-0.262917
H	-1.574317	4.500529	0.557357
H	-5.146481	2.596594	-0.421687
H	-4.381795	1.234459	-1.274714
H	-3.761289	2.897669	-1.504994
H	1.734477	2.843719	-3.297117
H	1.100957	1.182791	-3.174092
H	-0.025618	2.574036	-3.214824

$\omega$ B97X Energy = -1828.87825231 a.u.

(aS,1R,3S,3'S)-**21**, Conf P

C	1.997646	-1.354768	-1.057329
C	3.265328	-1.902508	-1.175872
C	4.339846	-1.282409	-0.541455
C	4.142283	-0.103695	0.172885
C	2.866267	0.442487	0.293857
C	1.786783	-0.189799	-0.331216
C	2.673297	1.702826	1.101318
C	3.873719	1.999778	1.987435
C	3.828612	3.389240	2.580925
O	5.068226	1.892451	1.216516
C	0.063848	1.494647	-0.961548
C	-1.212438	2.050650	-0.865465
C	-2.168590	1.437047	-0.062978
C	-1.851856	0.279467	0.653309
C	-0.554303	-0.226725	0.605431
C	0.404389	0.364951	-0.227425

C	-0.178702	-1.375703	1.510163
C	-1.158978	-1.487296	2.663450
C	-0.933686	-2.716166	3.514592
O	-2.476611	-1.571754	2.128174
C	-2.928523	-0.374631	1.511162
C	5.329860	0.559654	0.832218
C	-4.162247	-0.759460	0.721729
C	-5.423468	-0.352855	1.134446
C	-6.560225	-0.722710	0.427184
C	-6.403668	-1.514448	-0.690927
C	-5.166707	-1.949052	-1.127018
C	-4.045884	-1.563520	-0.408247
F	-7.504555	-1.881756	-1.389232
O	3.432326	-3.066399	-1.886158
C	4.101513	-2.893463	-3.136683
O	5.615853	-1.779818	-0.648799
C	5.839019	-3.001758	0.058860
O	-1.518797	3.191111	-1.561486
C	-1.097817	4.385617	-0.899398
O	-3.401176	2.004916	0.114952
C	-4.243826	2.063451	-1.040273
O	1.008042	2.125104	-1.730575
C	0.887695	1.852937	-3.127183
H	1.170217	-1.853495	-1.551248
H	2.507537	2.546789	0.421957
H	1.776112	1.614884	1.720824
H	3.918839	1.253711	2.795222
H	3.844826	4.138016	1.785611
H	2.913489	3.522447	3.160919
H	4.683465	3.557978	3.237173
H	0.833539	-1.225127	1.894237
H	-0.171634	-2.322262	0.958642
H	-1.088457	-0.585255	3.289020
H	-1.037152	-3.619550	2.909197
H	-1.658446	-2.757325	4.328723
H	0.069809	-2.699637	3.943657
H	-3.226602	0.339342	2.291258
H	5.640976	-0.028800	1.708249
H	6.172799	0.588783	0.142311
H	-5.524973	0.273396	2.014282
H	-7.549369	-0.406780	0.735040
H	-5.091005	-2.572109	-2.009658
H	-3.064426	-1.889485	-0.736505
H	3.522496	-2.232410	-3.788094
H	4.172422	-3.879265	-3.592043
H	5.102909	-2.482761	-2.990293
H	6.886503	-3.257089	-0.087980
H	5.644335	-2.864469	1.126441
H	5.205140	-3.799769	-0.332317
H	-0.013829	4.385079	-0.760388
H	-1.597102	4.481991	0.068567
H	-1.383672	5.216666	-1.541239
H	-3.808978	2.705649	-1.806054
H	-5.192247	2.476533	-0.702043
H	-4.409341	1.059470	-1.441066
H	-0.084789	2.179981	-3.502735

H 1.678631 2.411205 -3.624179  
H 1.020928 0.783848 -3.319069  
ωB97X Energy = -1828.87820610 a.u.

(aS,1R,3S,3'S)-**21**, Conf Q

C	2.031629	-1.289687	-1.257082
C	3.293922	-1.853614	-1.382031
C	4.362044	-1.283955	-0.680205
C	4.165584	-0.160409	0.107984
C	2.894470	0.403974	0.236395
C	1.830062	-0.167433	-0.456564
C	2.705085	1.605877	1.129882
C	3.881023	1.794849	2.076499
C	3.846093	3.126788	2.790490
O	5.096105	1.730280	1.333373
C	0.098537	1.512325	-1.094181
C	-1.189090	2.044688	-0.999900
C	-2.108699	1.465572	-0.129697
C	-1.781826	0.326088	0.602029
C	-0.490417	-0.192246	0.512706
C	0.449341	0.391922	-0.342789
C	-0.098274	-1.334402	1.418478
C	-1.033877	-1.408376	2.611841
C	-0.787121	-2.618789	3.483256
O	-2.372313	-1.492678	2.130291
C	-2.839411	-0.310393	1.492800
C	5.348088	0.431460	0.840407
C	-4.091299	-0.723010	0.745754
C	-4.004321	-1.402095	-0.465182
C	-5.145639	-1.835022	-1.122116
C	-6.372191	-1.579031	-0.540688
C	-6.499313	-0.915763	0.661463
C	-5.342198	-0.492354	1.302109
F	-7.493246	-1.995028	-1.178195
O	3.584744	-2.935023	-2.150555
C	2.520579	-3.540985	-2.869010
O	5.632211	-1.794005	-0.806463
C	5.844535	-3.018740	-0.103801
O	-1.563659	3.133010	-1.745434
C	-1.888006	2.805999	-3.097987
O	-3.373739	1.982806	-0.034396
C	-3.446510	3.233533	0.652678
O	1.027146	2.026122	-1.953083
C	1.281378	3.432320	-1.902888
H	1.185654	-1.712133	-1.784456
H	2.596282	2.511987	0.522154
H	1.782665	1.502260	1.708542
H	3.884320	0.978704	2.814758
H	3.904940	3.941997	2.065496
H	2.915278	3.230626	3.351199
H	4.682127	3.215772	3.485432
H	0.931340	-1.198781	1.759188
H	-0.133170	-2.288801	0.881585
H	-0.929485	-0.492188	3.211594
H	-0.921522	-3.535452	2.904476

H	-1.480720	-2.633627	4.324999
H	0.232064	-2.601642	3.873613
H	-3.124584	0.419138	2.264498
H	5.637358	-0.232947	1.668322
H	6.203477	0.507431	0.169471
H	-3.031926	-1.590954	-0.907976
H	-5.093063	-2.359676	-2.068181
H	-7.480785	-0.737281	1.083033
H	-5.420849	0.032809	2.248228
H	2.959731	-4.377962	-3.406266
H	2.078099	-2.841912	-3.583833
H	1.746193	-3.910521	-2.191208
H	6.885507	-3.293389	-0.263377
H	5.665259	-2.882468	0.967094
H	5.194074	-3.806328	-0.489188
H	-2.716414	2.093408	-3.129957
H	-1.020418	2.384078	-3.613376
H	-2.185213	3.734268	-3.581898
H	-3.046285	3.134819	1.666247
H	-4.501154	3.496915	0.704435
H	-2.898375	4.006765	0.111469
H	2.326146	3.565016	-2.180787
H	0.642938	3.975250	-2.600424
H	1.120702	3.821443	-0.894928

ωB97X Energy = -1828.87811651 a.u.

(aS,1R,3S,3'S)-**21**, Conf R

C	2.003043	-1.277529	-1.072733
C	3.248734	-1.878317	-1.193798
C	4.307478	-1.400156	-0.414802
C	4.107210	-0.365416	0.486839
C	2.854321	0.239639	0.607600
C	1.805170	-0.224079	-0.182437
C	2.665584	1.362461	1.599394
C	3.994851	1.998977	1.989145
C	4.555633	2.912746	0.908375
O	4.912282	0.969863	2.369635
C	0.154208	1.547101	-0.773638
C	-1.108727	2.135062	-0.688437
C	-2.106884	1.509419	0.051864
C	-1.843579	0.311479	0.722018
C	-0.558765	-0.226982	0.690044
C	0.439989	0.375170	-0.084926
C	-0.241772	-1.432131	1.541996
C	-1.258640	-1.575493	2.659251
C	-1.095098	-2.854827	3.447893
O	-2.561827	-1.592964	2.083369
C	-2.963678	-0.356141	1.510773
C	5.280809	0.109308	1.311032
C	-4.177830	-0.674503	0.663344
C	-5.443985	-0.262158	1.054422
C	-6.563433	-0.573844	0.293361
C	-6.384890	-1.312778	-0.857107
C	-5.142542	-1.751056	-1.273913
C	-4.039299	-1.424302	-0.500966

F	-7.468741	-1.623291	-1.607650
O	3.528236	-2.918337	-2.021481
C	2.471260	-3.431205	-2.818487
O	5.547858	-1.987773	-0.481811
C	6.279341	-1.683412	-1.669801
O	-1.363012	3.316411	-1.335466
C	-0.898896	4.463641	-0.620329
O	-3.331232	2.099992	0.214310
C	-4.131514	2.226473	-0.965251
O	1.142534	2.187589	-1.476978
C	1.062421	1.994992	-2.889784
H	1.165342	-1.624803	-1.664517
H	2.002777	2.125385	1.184600
H	2.177895	0.975972	2.500736
H	3.857156	2.581260	2.901776
H	4.618643	2.413272	-0.061347
H	3.903649	3.780545	0.792891
H	5.550812	3.265970	1.185174
H	0.762541	-1.332015	1.961565
H	-0.244808	-2.347459	0.939589
H	-1.181192	-0.710824	3.334736
H	-1.210807	-3.719726	2.790706
H	-1.842556	-2.916094	4.239921
H	-0.103540	-2.895264	3.902367
H	-3.272447	0.326721	2.314256
H	5.783024	-0.742775	1.769149
H	6.013633	0.598128	0.654155
H	-5.563030	0.321425	1.960941
H	-7.556166	-0.253169	0.584316
H	-5.049032	-2.330890	-2.183870
H	-3.053853	-1.754455	-0.812737
H	2.897817	-4.251187	-3.390948
H	2.087231	-2.670582	-3.503854
H	1.655127	-3.808864	-2.196522
H	6.422067	-0.602797	-1.766681
H	7.248927	-2.167906	-1.571341
H	5.765031	-2.067645	-2.552644
H	0.183052	4.412989	-0.476018
H	-1.400749	4.538409	0.348200
H	-1.147124	5.332394	-1.226943
H	-5.078056	2.657336	-0.644413
H	-4.313427	1.242992	-1.407562
H	-3.651442	2.881597	-1.692135
H	0.112447	2.369817	-3.278030
H	1.884530	2.556329	-3.329379
H	1.173378	0.934447	-3.135544

$\omega$ B97X Energy = -1828.87810776 a.u.

(aR,1R,3S,3'S)-**21**, Conf A

C	2.951226	1.171189	0.723162
C	4.280921	0.776586	0.731216
C	4.644790	-0.391132	0.048981
C	3.692725	-1.133791	-0.630266
C	2.354483	-0.728787	-0.650177

C	1.992114	0.426255	0.039426
C	1.343834	-1.556804	-1.410187
C	2.013455	-2.510033	-2.389320
C	1.052760	-3.529968	-2.956613
O	3.054769	-3.217027	-1.720234
C	0.161401	1.905850	-0.783713
C	-1.164709	2.343678	-0.783902
C	-2.095606	1.713839	0.035168
C	-1.704160	0.665200	0.872485
C	-0.365466	0.283135	0.917005
C	0.569204	0.880036	0.060266
C	0.075135	-0.736587	1.939121
C	-0.934606	-0.827582	3.068448
C	-0.633814	-1.943116	4.043408
O	-2.217467	-1.086821	2.505679
C	-2.752341	-0.009476	1.748969
C	4.132294	-2.370710	-1.379385
C	-3.894752	-0.601543	0.950256
C	-5.212903	-0.296107	1.258279
C	-6.262219	-0.857976	0.541999
C	-5.959811	-1.736165	-0.477230
C	-4.661061	-2.074064	-0.806695
C	-3.630260	-1.497267	-0.081858
F	-6.974102	-2.291263	-1.182358
O	5.283046	1.450628	1.352143
C	4.946752	2.643976	2.044120
O	5.959353	-0.787408	-0.009944
C	6.463591	-1.336710	1.208498
O	-1.545713	3.382497	-1.592861
C	-1.264211	4.667394	-1.034091
O	-3.383586	2.172172	0.107847
C	-4.171010	2.025088	-1.078192
O	1.074907	2.558560	-1.571629
C	1.043205	2.173730	-2.945535
H	2.640896	2.071329	1.238094
H	0.737515	-2.146002	-0.711662
H	0.650278	-0.908446	-1.952344
H	2.462823	-1.928434	-3.208802
H	0.644676	-4.148379	-2.153714
H	0.224536	-3.030206	-3.462523
H	1.557569	-4.178253	-3.674014
H	1.054744	-0.460125	2.335868
H	0.182981	-1.727788	1.483911
H	-0.969328	0.133061	3.602876
H	-0.637028	-2.905936	3.527297
H	-1.380897	-1.970750	4.837618
H	0.348597	-1.795618	4.495574
H	-3.161712	0.742203	2.437802
H	4.675736	-2.072591	-2.287626
H	4.815886	-2.962307	-0.770368
H	-5.430074	0.401406	2.060042
H	-7.295188	-0.623607	0.767671
H	-4.469777	-2.771759	-1.612679
H	-2.602365	-1.744708	-0.326765
H	4.528506	3.389891	1.362896
H	5.876208	3.019865	2.464649



H	4.236188	2.446614	2.851355
H	6.431441	-0.597920	2.011069
H	5.887332	-2.221273	1.497019
H	7.495699	-1.624168	1.017298
H	-1.616692	5.404963	-1.752388
H	-0.189800	4.790889	-0.878617
H	-1.794599	4.796318	-0.086706
H	-4.269849	0.967524	-1.338315
H	-3.730193	2.577027	-1.908151
H	-5.153079	2.431013	-0.843195
H	1.337439	1.125472	-3.057996
H	0.048279	2.327233	-3.369779
H	1.761932	2.805207	-3.464046

ωB97X Energy = -1828.88072464 a.u.

(aR,1R,3S,3'S)-21, Conf B

C	2.932838	1.097209	0.845630
C	4.248217	0.667329	0.940300
C	4.614733	-0.533200	0.319638
C	3.671871	-1.293204	-0.353647
C	2.344977	-0.862015	-0.446255
C	1.985078	0.340003	0.159394
C	1.346792	-1.708223	-1.202338
C	2.035505	-2.718149	-2.108288
C	1.077056	-3.741231	-2.673789
O	3.027617	-3.417537	-1.361268
C	0.227994	1.811367	-0.823889
C	-1.084238	2.282969	-0.901603
C	-2.062916	1.726014	-0.085447
C	-1.733390	0.717995	0.825069
C	-0.408491	0.305546	0.945363
C	0.574858	0.828135	0.094513
C	-0.037221	-0.665677	2.039482
C	-1.090965	-0.665858	3.131584
C	-0.858651	-1.732588	4.177313
O	-2.358419	-0.922788	2.533777
C	-2.832831	0.122303	1.695970
C	4.110390	-2.584230	-1.006484
C	-3.960734	-0.484555	0.887603
C	-3.683988	-1.436592	-0.089456
C	-4.704045	-2.026039	-0.819404
C	-6.004522	-1.643731	-0.550989
C	-6.319205	-0.709340	0.413018
C	-5.280785	-0.135482	1.135607
F	-7.008048	-2.210727	-1.262076
O	5.231986	1.328691	1.602861
C	4.893351	2.552207	2.238590
O	5.901350	-1.005640	0.418358
C	6.847592	-0.304831	-0.389413
O	-1.405010	3.283289	-1.782190
C	-1.110846	4.590277	-1.284460
O	-3.339322	2.220830	-0.089926
C	-4.083834	2.030665	-1.297361
O	1.189637	2.388814	-1.613220
C	1.180505	1.940725	-2.968460

H	2.621731	2.025174	1.308041
H	0.705121	-2.254043	-0.500170
H	0.686047	-1.074560	-1.799941
H	2.534925	-2.183614	-2.931004
H	0.614650	-4.310043	-1.863721
H	0.287689	-3.246932	-3.243212
H	1.599218	-4.435042	-3.333923
H	0.934412	-0.394192	2.458547
H	0.058670	-1.683404	1.644036
H	-1.118652	0.323809	3.610443
H	-0.872146	-2.722120	3.714787
H	-1.633601	-1.694993	4.943895
H	0.111356	-1.587367	4.656189
H	-3.247122	0.923083	2.323785
H	4.713127	-2.355882	-1.898236
H	4.739415	-3.156052	-0.324924
H	-2.654835	-1.718097	-0.287926
H	-4.503088	-2.766379	-1.583891
H	-7.353144	-0.441746	0.592602
H	-5.507429	0.605324	1.894765
H	4.537153	3.288971	1.513530
H	5.808345	2.913676	2.701340
H	4.132356	2.400068	3.008887
H	7.808911	-0.792051	-0.237845
H	6.571767	-0.368592	-1.446414
H	6.916207	0.742386	-0.088675
H	-1.667088	4.781941	-0.362875
H	-1.423594	5.295638	-2.051807
H	-0.039174	4.698718	-1.101145
H	-5.064233	2.469264	-1.121600
H	-4.197656	0.963663	-1.508061
H	-3.598510	2.529981	-2.135859
H	1.944537	2.512175	-3.491799
H	1.426617	0.875475	-3.022411
H	0.207176	2.120251	-3.430602

ωB97X Energy = -1828.88052036 a.u.

(aR,1R,3S,3'S)-21, Conf C

C	-2.909739	0.952748	-0.979392
C	-4.246973	0.582365	-0.951859
C	-4.660718	-0.393223	-0.037136
C	-3.750249	-0.967146	0.836457
C	-2.408874	-0.576066	0.824500
C	-1.995025	0.382087	-0.096525
C	-1.442126	-1.200006	1.802997
C	-2.164963	-1.919609	2.932448
C	-1.241540	-2.791266	3.752538
O	-3.183694	-2.755461	2.387126
C	-0.143784	1.919860	0.546170
C	1.185416	2.351300	0.486768
C	2.093297	1.642876	-0.296027
C	1.693020	0.491791	-0.980843
C	0.360266	0.092457	-0.942587
C	-0.562830	0.802617	-0.165476
C	-0.083632	-1.079719	-1.782847

C	0.910926	-1.345432	-2.898312
C	0.610978	-2.611981	-3.667206
O	2.206892	-1.488409	-2.323963
C	2.733605	-0.288039	-1.774977
C	-4.237070	-2.001558	1.824643
C	3.924668	-0.709928	-0.939235
C	5.218664	-0.471030	-1.381055
C	6.315974	-0.883924	-0.636445
C	6.085845	-1.547137	0.550527
C	4.813702	-1.813114	1.018928
C	3.733554	-1.388408	0.260649
F	7.147790	-1.954144	1.286591
O	-5.208796	1.106688	-1.754391
C	-4.821902	2.110983	-2.680235
O	-5.983586	-0.755332	0.051196
C	-6.444506	-1.564624	-1.031778
O	1.588275	3.499793	1.115675
C	1.598954	3.438084	2.545439
O	3.373798	2.080573	-0.486745
C	4.213034	2.198999	0.662919
O	-1.042114	2.595121	1.333777
C	-1.489266	3.839671	0.792592
H	-2.560547	1.693619	-1.687427
H	-0.794896	-1.917828	1.284010
H	-0.786500	-0.432451	2.222929
H	-2.645363	-1.174038	3.583863
H	-0.805621	-3.571227	3.123832
H	-0.430612	-2.192748	4.171817
H	-1.782811	-3.265280	4.572378
H	-1.071301	-0.881048	-2.204886
H	-0.174710	-1.983087	-1.168096
H	0.921730	-0.487743	-3.586910
H	0.631000	-3.474015	-2.996484
H	1.348213	-2.766231	-4.456181
H	-0.378678	-2.550701	-4.123461
H	3.094136	0.350862	-2.593098
H	-4.809260	-1.505402	2.621934
H	-4.906028	-2.710221	1.336288
H	5.378335	0.055338	-2.315989
H	7.330355	-0.698514	-0.967502
H	4.679663	-2.338517	1.956480
H	2.725927	-1.583984	0.612999
H	-5.728965	2.401388	-3.204538
H	-4.093154	1.727513	-3.399611
H	-4.404418	2.981742	-2.166888
H	-6.353620	-1.033711	-1.981009
H	-5.879908	-2.501060	-1.077048
H	-7.492113	-1.783412	-0.833997
H	1.981251	4.396540	2.891167
H	2.262135	2.637923	2.886997
H	0.594211	3.275023	2.937341
H	4.004062	3.119395	1.208061
H	5.236496	2.215597	0.291437
H	4.086782	1.335700	1.322492
H	-0.651551	4.524580	0.644139
H	-2.008610	3.677656	-0.156442

H -2.184182 4.260090 1.516843  
 ωB97X Energy = -1828.88029948 a.u.

(*aR*,1*R*,3*S*,3'*S*)-**21**, Conf D

C	2.911741	0.947250	0.981735
C	4.229389	0.514543	1.039420
C	4.615168	-0.585683	0.265118
C	3.690233	-1.243441	-0.530811
C	2.366784	-0.800371	-0.597352
C	1.985097	0.298132	0.168447
C	1.387889	-1.516165	-1.498421
C	2.095777	-2.420265	-2.497228
C	1.147477	-3.356310	-3.210878
O	3.060980	-3.215638	-1.812721
C	0.209692	1.819791	-0.694661
C	-1.105671	2.294835	-0.726067
C	-2.058939	1.707188	0.101817
C	-1.716337	0.631022	0.925667
C	-0.396822	0.191448	0.976131
C	0.570351	0.777864	0.150500
C	-0.013537	-0.882708	1.964515
C	-1.049520	-0.986299	3.068536
C	-0.811366	-2.156699	3.995262
O	-2.330536	-1.164946	2.471332
C	-2.805317	-0.027151	1.764513
C	4.140233	-2.440421	-1.336302
C	-3.970784	-0.521494	0.932307
C	-5.275430	-0.180695	1.260831
C	-6.347330	-0.656381	0.516356
C	-6.081498	-1.486193	-0.552444
C	-4.798057	-1.857437	-0.904275
C	-3.743880	-1.366899	-0.149830
F	-7.118230	-1.956942	-1.286340
O	5.194209	1.080366	1.809305
C	4.835965	2.208782	2.593038
O	5.900635	-1.067638	0.327736
C	6.861881	-0.265354	-0.358735
O	-1.453815	3.376175	-1.491729
C	-1.420224	3.160300	-2.906025
O	-3.329289	2.202812	0.198509
C	-4.132020	2.196913	-0.982952
O	1.152847	2.374169	-1.523785
C	1.621586	3.659684	-1.111941
H	2.583786	1.788271	1.579416
H	0.700364	-2.125081	-0.898378
H	0.775144	-0.789563	-2.038802
H	2.624973	-1.797091	-3.233867
H	0.659612	-4.017844	-2.491126
H	0.376764	-2.787667	-3.734552
H	1.683122	-3.967188	-3.938719
H	0.965616	-0.658834	2.393734
H	0.071868	-1.855840	1.466679
H	-1.056442	-0.051084	3.647566
H	-0.843889	-3.094256	3.435524
H	-1.572236	-2.189975	4.776043

H	0.168348	-2.069478	4.468446
H	-3.181380	0.710420	2.486908
H	4.760600	-2.103972	-2.180360
H	4.754964	-3.096128	-0.720321
H	-5.463486	0.477646	2.102196
H	-7.369692	-0.393220	0.758143
H	-4.636000	-2.514925	-1.749567
H	-2.727348	-1.642887	-0.410954
H	4.483786	3.030914	1.963558
H	5.741002	2.513145	3.112888
H	4.065206	1.952658	3.324907
H	6.932885	0.726983	0.090831
H	7.818287	-0.776466	-0.266232
H	6.600385	-0.173416	-1.417302
H	-1.790907	4.075282	-3.363954
H	-2.072879	2.326264	-3.180240
H	-0.404391	2.958639	-3.247629
H	-4.048808	1.235686	-1.498282
H	-3.848951	3.007213	-1.654529
H	-5.160042	2.335994	-0.652717
H	2.115436	3.590920	-0.138262
H	2.343153	3.981067	-1.860392
H	0.799783	4.377169	-1.060388

$\omega$ B97X Energy = -1828.88011080 a.u.

(*aR*,1*R*,3*S*,3'*S*)-**21**, Conf E

C	2.937562	1.110676	0.688356
C	4.264770	0.704975	0.718525
C	4.633841	-0.454807	0.026972
C	3.690644	-1.175845	-0.688489
C	2.359895	-0.753385	-0.738565
C	1.989873	0.389719	-0.035181
C	1.356270	-1.544910	-1.543715
C	2.032821	-2.520378	-2.496552
C	1.066855	-3.526048	-3.080121
O	3.044096	-3.242819	-1.797712
C	0.149277	1.806700	-0.942456
C	-1.173688	2.259945	-0.944131
C	-2.094006	1.670658	-0.079322
C	-1.691628	0.681923	0.821986
C	-0.353329	0.302245	0.874916
C	0.566672	0.844533	-0.030211
C	0.097207	-0.663263	1.943531
C	-0.897271	-0.685448	3.089515
C	-0.587872	-1.744567	4.123023
O	-2.188466	-0.973041	2.560681
C	-2.733130	0.049926	1.737888
C	4.128288	-2.413377	-1.437022
C	-3.866741	-0.606728	0.976899
C	-5.189249	-0.298245	1.262209
C	-6.229910	-0.918604	0.582452
C	-5.914435	-1.858042	-0.376363
C	-4.610848	-2.200699	-0.680753
C	-3.588859	-1.565457	0.006779
F	-6.920258	-2.470444	-1.045444

O	5.256598	1.360428	1.375073
C	4.914484	2.550493	2.069531
O	5.944496	-0.867124	-0.003208
C	6.412275	-1.434605	1.221401
O	-1.533425	3.230031	-1.841262
C	-1.975417	4.462805	-1.265659
O	-3.399049	2.089161	-0.050414
C	-4.160365	1.844318	-1.237348
O	1.034745	2.275850	-1.877666
C	1.557552	3.577705	-1.624204
H	2.621674	1.995029	1.227186
H	0.697691	-2.108793	-0.871470
H	0.716087	-0.867351	-2.115012
H	2.514461	-1.955030	-3.308620
H	0.628425	-4.130932	-2.282894
H	0.260175	-3.014077	-3.608177
H	1.575730	-4.188584	-3.781483
H	1.083699	-0.373208	2.312010
H	0.193114	-1.677299	1.537529
H	-0.921446	0.304484	3.568073
H	-0.597914	-2.734720	3.661783
H	-1.326946	-1.725874	4.924949
H	0.399304	-1.574063	4.556369
H	-3.153540	0.837604	2.377891
H	4.689998	-2.119199	-2.335422
H	4.793848	-3.016346	-0.819222
H	-5.416709	0.447218	2.016549
H	-7.266190	-0.682952	0.790999
H	-4.409064	-2.946534	-1.439662
H	-2.557427	-1.815799	-0.219711
H	4.511815	3.303270	1.385987
H	5.838323	2.918784	2.508673
H	4.188952	2.351680	2.862995
H	7.442770	-1.739664	1.049762
H	6.376349	-0.701343	2.028886
H	5.814130	-2.310632	1.490844
H	-2.940951	4.346363	-0.771006
H	-2.063042	5.170490	-2.087571
H	-1.241853	4.832246	-0.543282
H	-4.171022	0.775699	-1.467313
H	-3.758128	2.400256	-2.085652
H	-5.173810	2.177148	-1.022201
H	2.276873	3.782654	-2.414728
H	0.769425	4.333029	-1.649275
H	2.066333	3.607272	-0.656069

$\omega$ B97X Energy = -1828.88000819 a.u.

(*aR*,1*R*,3*S*,3'*S*)-**21**, Conf F

C	2.923214	1.031550	0.810463
C	4.235272	0.591287	0.918393
C	4.602487	-0.603344	0.288539
C	3.665064	-1.344929	-0.413634
C	2.346532	-0.897522	-0.528331
C	1.983645	0.295203	0.091816
C	1.352166	-1.710749	-1.323203

C	2.040376	-2.742575	-2.205292
C	1.073964	-3.752119	-2.781445
O	3.005797	-3.454673	-1.435094
C	0.222948	1.713382	-0.959113
C	-1.085436	2.200683	-1.039970
C	-2.056628	1.680121	-0.186706
C	-1.719886	0.728034	0.778669
C	-0.396556	0.315147	0.906284
C	0.574783	0.787058	0.015585
C	-0.018164	-0.607579	2.038686
C	-1.057907	-0.546681	3.142341
C	-0.820727	-1.564503	4.234792
O	-2.334764	-0.823357	2.574383
C	-2.815129	0.172524	1.681444
C	4.096525	-2.636796	-1.068790
C	-3.938516	-0.488308	0.909072
C	-3.653547	-1.494603	-0.009333
C	-4.668492	-2.133258	-0.704287
C	-5.972052	-1.745545	-0.459740
C	-6.294698	-0.758164	0.447122
C	-5.261274	-0.135115	1.135347
F	-6.970665	-2.360853	-1.136876
O	5.211992	1.236988	1.606410
C	4.874548	2.462776	2.238029
O	5.882645	-1.089186	0.407026
C	6.847678	-0.394976	-0.383819
O	-1.380045	3.132105	-1.999609
C	-1.812634	4.403806	-1.507295
O	-3.348924	2.135187	-0.231685
C	-4.071669	1.853645	-1.434460
O	1.159401	2.111348	-1.877443
C	1.704195	3.412325	-1.669969
H	2.609499	1.947005	1.295959
H	0.664722	-2.231365	-0.645067
H	0.741115	-1.051554	-1.945514
H	2.565855	-2.224848	-3.022061
H	0.587474	-4.307423	-1.976078
H	0.303493	-3.247109	-3.367111
H	1.594637	-4.459197	-3.428602
H	0.960814	-0.326948	2.433500
H	0.063967	-1.642867	1.686937
H	-1.071545	0.464991	3.573455
H	-0.846105	-2.574509	3.819444
H	-1.586970	-1.485567	5.007032
H	0.155400	-1.403920	4.696052
H	-3.235855	1.003499	2.263990
H	4.709136	-2.412528	-1.954856
H	4.712732	-3.218467	-0.383875
H	-2.622162	-1.779849	-0.190127
H	-4.461106	-2.915048	-1.424526
H	-7.330795	-0.488534	0.610532
H	-5.494134	0.646971	1.849931
H	4.530153	3.201182	1.508483
H	5.786903	2.819150	2.709823
H	4.104879	2.316383	3.000791
H	7.802545	-0.890166	-0.217825

H	6.588575	-0.454129	-1.445294
H	6.920157	0.651126	-0.079743
H	-2.796554	4.335204	-1.040652
H	-1.856154	5.066601	-2.369181
H	-1.095076	4.796422	-0.781048
H	-5.077678	2.238800	-1.280423
H	-4.118249	0.775056	-1.605786
H	-3.613552	2.344419	-2.294533
H	2.461147	3.557594	-2.438316
H	0.937375	4.183337	-1.769139
H	2.172033	3.482014	-0.683373

$\omega$ B97X Energy = -1828.87974789 a.u.

(aR,1R,3S,3'S)-**21**, Conf G

C	2.901418	1.162355	0.699907
C	4.238034	0.793921	0.765555
C	4.650469	-0.374753	0.114691
C	3.740620	-1.140874	-0.596910
C	2.400085	-0.756318	-0.683143
C	1.986835	0.395363	-0.019160
C	1.435404	-1.594651	-1.488685
C	2.159636	-2.568486	-2.406969
C	1.235132	-3.610710	-2.993673
O	3.172958	-3.249788	-1.670812
C	0.141292	1.753664	-0.999580
C	-1.186437	2.181474	-1.038144
C	-2.101342	1.654646	-0.132455
C	-1.715258	0.670454	0.777276
C	-0.378550	0.281806	0.839280
C	0.555085	0.820744	-0.054798
C	0.055751	-0.674517	1.922781
C	-0.946725	-0.676736	3.062878
C	-0.652241	-1.728515	4.108152
O	-2.238149	-0.957827	2.530094
C	-2.767507	0.063640	1.695264
C	4.226885	-2.384942	-1.303729
C	-3.912118	-0.584049	0.942648
C	-5.227587	-0.330048	1.305059
C	-6.281995	-0.958172	0.654856
C	-5.986565	-1.847641	-0.356423
C	-4.690652	-2.132511	-0.741000
C	-3.654557	-1.491902	-0.079787
F	-7.006218	-2.466585	-0.999441
O	5.200036	1.494200	1.420027
C	4.815490	2.696099	2.070542
O	5.972104	-0.751328	0.119133
C	6.432949	-1.271102	1.367271
O	-1.571210	3.127857	-1.951231
C	-2.238257	2.580486	-3.090885
O	-3.409411	2.062806	-0.166055
C	-3.624197	3.390842	0.318280
O	1.028441	2.213716	-1.937133
C	1.476768	3.552104	-1.720782
H	2.552277	2.054095	1.204986
H	0.781616	-2.164755	-0.817216

H	0.786397	-0.948363	-2.085813
H	2.645004	-2.005303	-3.218318
H	0.792476	-4.211369	-2.195584
H	0.429120	-3.130712	-3.551879
H	1.778971	-4.272993	-3.668550
H	1.042046	-0.388944	2.295231
H	0.145209	-1.693665	1.528454
H	-0.964733	0.317975	3.531712
H	-0.668820	-2.722908	3.656344
H	-1.395212	-1.695490	4.905987
H	0.334200	-1.562611	4.544942
H	-3.177813	0.863717	2.327849
H	4.803635	-2.098018	-2.194934
H	4.891358	-2.956342	-0.655486
H	-5.439065	0.376378	2.100830
H	-7.313120	-0.764162	0.923291
H	-4.505185	-2.840372	-1.539497
H	-2.629045	-1.700659	-0.367338
H	4.408720	3.417858	1.356596
H	5.721418	3.100010	2.515632
H	4.079311	2.503976	2.855810
H	5.857239	-2.158342	1.648598
H	7.475701	-1.547456	1.223326
H	6.357946	-0.518195	2.153748
H	-2.495450	3.418654	-3.735503
H	-3.148353	2.056553	-2.788952
H	-1.575377	1.896585	-3.627767
H	-3.096995	4.119624	-0.299970
H	-3.292311	3.476151	1.357226
H	-4.696371	3.568800	0.264807
H	2.152664	3.790417	-2.539756
H	0.635527	4.248058	-1.723790
H	2.017635	3.623975	-0.772128

ωB97X Energy = -1828.87924378 a.u.

(aR,1R,3S,3'S)-**21**, Conf H

C	-2.883363	-1.096566	0.813497
C	-4.204166	-0.696847	0.962540
C	-4.613730	0.513600	0.391839
C	-3.709130	1.309187	-0.293989
C	-2.381960	0.901920	-0.451956
C	-1.976843	-0.305673	0.110326
C	-1.426510	1.771198	-1.235124
C	-2.161065	2.815913	-2.062520
C	-1.233938	3.869703	-2.623837
O	-3.125248	3.474297	-1.244260
C	-0.218707	-1.646862	-1.037176
C	1.092683	-2.106075	-1.165606
C	2.063044	-1.663048	-0.273342
C	1.747112	-0.734479	0.718568
C	0.426588	-0.314777	0.867292
C	-0.561400	-0.766767	-0.016435
C	0.068927	0.578124	2.029870
C	1.118152	0.475898	3.122343
C	0.899483	1.465866	4.243867

O	2.393708	0.755578	2.552121
C	2.855633	-0.219724	1.626811
C	-4.186813	2.616051	-0.884375
C	3.986254	0.448731	0.871264
C	5.307732	0.161402	1.184070
C	6.352342	0.808299	0.536492
C	6.041516	1.750314	-0.421144
C	4.739519	2.069959	-0.754299
C	3.713261	1.410212	-0.096596
F	7.051442	2.387363	-1.061757
O	-5.151614	-1.397580	1.636971
C	-4.770362	-2.636698	2.215296
O	-5.904452	0.958057	0.552110
C	-6.860748	0.280869	-0.263673
O	1.411440	-2.998940	-2.155037
C	1.970468	-2.379512	-3.315404
O	3.356455	-2.098505	-0.401731
C	3.562798	-3.454689	0.000585
O	-1.159754	-2.020894	-1.960527
C	-1.637674	-3.358350	-1.811057
H	-2.537221	-2.023824	1.252347
H	-0.738420	2.284777	-0.552522
H	-0.812098	1.152127	-1.894421
H	-2.692754	2.314511	-2.885441
H	-0.743142	4.409227	-1.810403
H	-0.464771	3.405373	-3.243855
H	-1.786866	4.584936	-3.234229
H	-0.909257	0.296899	2.426163
H	-0.004206	1.623909	1.708884
H	1.124750	-0.547404	3.525360
H	0.933512	2.486553	3.856118
H	1.669603	1.357577	5.008699
H	-0.075469	1.303431	4.706967
H	3.269077	-1.072656	2.183889
H	-4.817458	2.413631	-1.762975
H	-4.797837	3.154066	-0.160165
H	5.531360	-0.585152	1.938825
H	7.387710	0.589252	0.766592
H	4.541823	2.818079	-1.512085
H	2.683236	1.645859	-0.344544
H	-4.419873	-3.337975	1.452771
H	-5.664472	-3.035152	2.688361
H	-3.991403	-2.498307	2.970073
H	-6.614487	0.399495	-1.323258
H	-6.904952	-0.780780	-0.012583
H	-7.825429	0.743674	-0.064363
H	2.175439	-3.175474	-4.028547
H	2.900265	-1.862814	-3.064642
H	1.258075	-1.673092	-3.750075
H	2.975496	-4.136232	-0.617301
H	3.297011	-3.585236	1.053787
H	4.623489	-3.657872	-0.132676
H	-2.354587	-3.523928	-2.612909
H	-0.818397	-4.075000	-1.895956
H	-2.139611	-3.477925	-0.846017

ωB97X Energy = -1828.87906502 a.u.

(aR,1R,3S,3'S)-**21**, Conf I

C	2.895365	1.132362	0.884175
C	4.239256	0.787231	0.880162
C	4.658611	-0.287665	0.087461
C	3.748489	-0.981985	-0.694071
C	2.398092	-0.622306	-0.704910
C	1.978139	0.434512	0.100926
C	1.443532	-1.367245	-1.608759
C	2.182616	-2.161544	-2.675847
C	1.279506	-3.117872	-3.420603
O	3.214768	-2.927610	-2.059452
C	0.119995	2.015807	-0.467985
C	-1.202047	2.457382	-0.338908
C	-2.105640	1.691825	0.394767
C	-1.704994	0.495438	0.991395
C	-0.374022	0.096138	0.910566
C	0.541592	0.844251	0.158464
C	0.080385	-1.098880	1.714248
C	-0.902981	-1.399161	2.831247
C	-0.588613	-2.683863	3.563400
O	-2.202063	-1.535771	2.262175
C	-2.738420	-0.321263	1.756335
C	4.253222	-2.109539	-1.564440
C	-3.925522	-0.717255	0.902715
C	-5.221673	-0.488286	1.343307
C	-6.315213	-0.873574	0.578525
C	-6.079133	-1.498881	-0.627612
C	-4.804596	-1.753383	-1.096251
C	-3.728392	-1.356451	-0.317733
F	-7.137202	-1.878732	-1.383405
O	5.202730	1.426022	1.591890
C	4.807208	2.519067	2.407895
O	5.986209	-0.633761	0.019321
C	6.487812	-1.280332	1.190518
O	-1.612988	3.671420	-0.815492
C	-1.607370	3.836736	-2.233601
O	-3.380707	2.125431	0.631251
C	-4.231966	2.298028	-0.502262
O	0.993335	2.842807	-1.128751
C	1.514692	2.356865	-2.366132
H	2.540794	1.957823	1.487828
H	0.827129	-2.060373	-1.025035
H	0.755554	-0.665782	-2.089386
H	2.649129	-1.462821	-3.387115
H	0.859631	-3.852237	-2.729160
H	0.456715	-2.575255	-3.889746
H	1.833713	-3.646912	-4.196984
H	1.071056	-0.907239	2.133046
H	0.167540	-1.988825	1.081249
H	-0.914416	-0.560490	3.542649
H	-0.607208	-3.527453	2.869588
H	-1.319544	-2.864749	4.352548
H	0.403588	-2.627983	4.014755
H	-3.103940	0.284624	2.596781

H	4.832518	-1.692387	-2.400656
H	4.921730	-2.756934	-0.996559
H	-5.385851	0.009555	2.292916
H	-7.331223	-0.695246	0.908458
H	-4.666002	-2.248936	-2.049246
H	-2.718949	-1.542776	-0.669945
H	5.714509	2.881222	2.884929
H	4.094400	2.202357	3.173949
H	4.367499	3.320443	1.808130
H	6.411364	-0.624807	2.059724
H	5.941530	-2.209751	1.378411
H	7.533839	-1.509089	0.995874
H	-0.594838	3.980004	-2.610958
H	-2.199051	4.726702	-2.441661
H	-2.066743	2.973326	-2.724148
H	-5.246075	2.367343	-0.112262
H	-4.163275	1.434358	-1.170020
H	-3.984718	3.210260	-1.045332
H	0.708084	1.994637	-3.010714
H	2.006482	3.202058	-2.844497
H	2.241987	1.558680	-2.206243

$\omega$ B97X Energy = -1828.87847184 a.u.

(aR,1R,3S,3'S)-**21**, Conf J

C	2.888463	1.059422	0.967081
C	4.216056	0.660810	1.033214
C	4.618566	-0.471046	0.314777
C	3.700500	-1.194656	-0.430492
C	2.364234	-0.791776	-0.499681
C	1.966247	0.340172	0.209912
C	1.404944	-1.566599	-1.373010
C	2.140898	-2.463920	-2.357243
C	1.221985	-3.437312	-3.059380
O	3.123356	-3.221007	-1.655170
C	0.190493	1.939749	-0.538337
C	-1.119237	2.431241	-0.496536
C	-2.077179	1.751733	0.253646
C	-1.740613	0.595436	0.958846
C	-0.421789	0.149270	0.961778
C	0.545933	0.805606	0.189934
C	-0.038071	-0.989685	1.876244
C	-1.068053	-1.157687	2.978368
C	-0.822435	-2.379774	3.833802
O	-2.350722	-1.305315	2.376132
C	-2.829506	-0.127656	1.741619
C	4.180617	-2.410802	-1.188966
C	-3.983444	-0.570709	0.866198
C	-3.740729	-1.333861	-0.272286
C	-4.784442	-1.772141	-1.071979
C	-6.073395	-1.432298	-0.708242
C	-6.354734	-0.684212	0.415473
C	-5.293010	-0.259672	1.204241
F	-7.099753	-1.851546	-1.486425
O	5.176052	1.289719	1.758199
C	4.798940	2.445386	2.492576

O	5.916049	-0.917406	0.380205
C	6.851011	-0.119967	-0.347818
O	-1.473010	3.616920	-1.077736
C	-1.368351	3.694440	-2.499850
O	-3.345995	2.243719	0.395953
C	-4.143652	2.316495	-0.786538
O	1.118119	2.685451	-1.221879
C	1.664051	2.093273	-2.401002
H	2.548202	1.934005	1.506390
H	0.747918	-2.192101	-0.758016
H	0.757625	-0.877812	-1.923362
H	2.655268	-1.837196	-3.101756
H	0.748343	-4.099418	-2.330744
H	0.439219	-2.899388	-3.597475
H	1.778643	-4.046066	-3.773063
H	0.945173	-0.797974	2.311975
H	0.035387	-1.933243	1.324186
H	-1.074687	-0.258002	3.611105
H	-0.853660	-3.283090	3.220231
H	-1.580521	-2.461670	4.613792
H	0.158492	-2.316910	4.308318
H	-3.217386	0.558521	2.506808
H	4.807303	-2.090215	-2.034514
H	4.798291	-3.035639	-0.544291
H	-2.720062	-1.585105	-0.542247
H	-4.610291	-2.363527	-1.962449
H	-7.380859	-0.443376	0.664405
H	-5.492804	0.333968	2.089825
H	4.424335	3.229527	1.829186
H	5.701161	2.792634	2.989890
H	4.039572	2.206134	3.241772
H	6.903884	0.890044	0.062812
H	7.819452	-0.606163	-0.247251
H	6.575601	-0.075275	-1.405884
H	-1.950189	4.563305	-2.803313
H	-1.786996	2.797727	-2.966617
H	-0.332467	3.824396	-2.812499
H	-4.137416	1.357048	-1.311841
H	-3.794537	3.108233	-1.449529
H	-5.157406	2.536620	-0.456831
H	0.867539	1.715893	-3.049409
H	2.205749	2.883339	-2.918233
H	2.353315	1.282499	-2.157265

$\omega$ B97X Energy = -1828.87832878 a.u.

(aR,1R,3S,3'S)-**21**, Conf K

C	2.912194	1.242996	0.752016
C	4.256579	0.907908	0.807619
C	4.694193	-0.246064	0.145681
C	3.799439	-1.032376	-0.561503
C	2.445698	-0.686794	-0.629710
C	2.010205	0.454215	0.039716
C	1.501077	-1.562153	-1.421107
C	2.249397	-2.476133	-2.379787
C	1.359293	-3.534331	-2.990605

O	3.294821	-3.140729	-1.674560
C	0.155359	1.865610	-0.842112
C	-1.182801	2.271158	-0.874242
C	-2.093994	1.662564	-0.015297
C	-1.701865	0.607232	0.809346
C	-0.362604	0.229700	0.854582
C	0.570834	0.854285	0.017118
C	0.078380	-0.797152	1.869314
C	-0.938771	-0.910587	2.990486
C	-0.639355	-2.040456	3.949102
O	-2.217754	-1.164081	2.415445
C	-2.750143	-0.068938	1.682090
C	4.320554	-2.250602	-1.288901
C	-3.916756	-0.636484	0.900397
C	-5.211306	-0.493819	1.381683
C	-6.289195	-1.058618	0.712984
C	-6.038443	-1.771251	-0.440622
C	-4.764800	-1.942315	-0.946861
C	-3.703848	-1.368578	-0.263045
F	-7.081622	-2.325189	-1.104669
O	5.206475	1.628636	1.457425
C	4.795218	2.809721	2.129868
O	6.025846	-0.584941	0.133560
C	6.514577	-1.098207	1.373821
O	-1.530613	3.304880	-1.699318
C	-2.522876	3.009241	-2.686260
O	-3.401086	2.077575	0.023738
C	-3.590759	3.371032	0.603226
O	1.075337	2.520115	-1.619452
C	1.091331	2.120676	-2.987007
H	2.545507	2.131380	1.250025
H	0.905558	-2.184530	-0.742680
H	0.791792	-0.947816	-1.982154
H	2.703079	-1.868191	-3.177496
H	0.947603	-4.176391	-2.208364
H	0.530510	-3.068924	-3.527361
H	1.921893	-4.154269	-3.689890
H	1.052465	-0.517627	2.277235
H	0.197044	-1.782110	1.403569
H	-0.980714	0.041217	3.540175
H	-0.637005	-2.995130	3.418087
H	-1.389914	-2.082819	4.739391
H	0.340526	-1.896899	4.408009
H	-3.139876	0.675722	2.391290
H	4.889803	-1.929811	-2.173308
H	5.001313	-2.813693	-0.650337
H	-5.387117	0.071902	2.290601
H	-7.303900	-0.949593	1.075521
H	-4.614865	-2.509942	-1.857006
H	-2.696048	-1.490867	-0.646648
H	4.368367	3.533439	1.430264
H	5.692903	3.227585	2.578781
H	4.066948	2.585459	2.913925
H	5.968285	-2.003877	1.654910
H	7.563637	-1.342305	1.217908
H	6.424894	-0.352456	2.165540

H	-2.541387	3.860367	-3.363877
H	-3.505495	2.871851	-2.233305
H	-2.251685	2.107095	-3.242364
H	-4.665597	3.534784	0.646077
H	-3.121823	4.147434	-0.005336
H	-3.176702	3.399150	1.615019
H	0.121233	2.292789	-3.459865
H	1.845739	2.729013	-3.481933
H	1.362538	1.064224	-3.079037

$\omega$ B97X Energy = -1828.87821641 a.u.

(aR,1R,3S,3'S)-21, Conf L

C	-2.904649	-1.205999	0.803105
C	-4.232282	-0.829025	0.938018
C	-4.649747	0.389073	0.387861
C	-3.744024	1.216803	-0.255669
C	-2.404314	0.838246	-0.389522
C	-1.994144	-0.381215	0.144718
C	-1.449050	1.758644	-1.113750
C	-2.188748	2.784564	-1.958970
C	-1.276987	3.866225	-2.491758
O	-3.190689	3.411817	-1.162292
C	-0.217196	-1.760954	-0.926975
C	1.105717	-2.199035	-1.046759
C	2.064741	-1.697395	-0.170907
C	1.733220	-0.716416	0.764299
C	0.408863	-0.309157	0.895963
C	-0.571282	-0.823751	0.037370
C	0.038271	0.622543	2.023780
C	1.090692	0.578390	3.117221
C	0.858440	1.605867	4.201606
O	2.360335	0.856720	2.532810
C	2.835220	-0.149890	1.648980
C	-4.237749	2.524688	-0.831080
C	3.954925	0.499193	0.860937
C	5.281261	0.227535	1.167167
C	6.315414	0.856923	0.486515
C	5.989207	1.765224	-0.498209
C	4.682054	2.067791	-0.827126
C	3.666384	1.425648	-0.136294
F	6.988729	2.385353	-1.170874
O	-5.182527	-1.559186	1.576385
C	-4.791420	-2.799239	2.146512
O	-5.951065	0.808145	0.527841
C	-6.880278	0.124399	-0.313559
O	1.393353	-3.159894	-1.976665
C	2.356808	-2.797519	-2.970048
O	3.360652	-2.144520	-0.223111
C	3.537197	-3.492523	0.220358
O	-1.183664	-2.310369	-1.729136
C	-1.228330	-1.783286	-3.052390
H	-2.555132	-2.146035	1.210408
H	-0.819656	2.294301	-0.393103
H	-0.772436	1.181309	-1.749407
H	-2.684431	2.271873	-2.797635

H	-0.818452	4.412366	-1.664102
H	-0.482582	3.426871	-3.098008
H	-1.835134	4.571242	-3.109179
H	-0.934809	0.339397	2.431528
H	-0.051720	1.655051	1.667449
H	1.115370	-0.428735	3.558237
H	0.873999	2.611767	3.775932
H	1.632410	1.539003	4.967228
H	-0.112332	1.444510	4.673757
H	3.260535	-0.972819	2.240748
H	-4.851237	2.322849	-1.721845
H	-4.870848	3.038076	-0.107952
H	5.516800	-0.493237	1.943036
H	7.354325	0.649720	0.711521
H	4.472308	2.789816	-1.606677
H	2.632435	1.648244	-0.379993
H	-4.421926	-3.487844	1.381799
H	-5.685952	-3.214471	2.604143
H	-4.023990	-2.657692	2.912429
H	-7.855886	0.569544	-0.127724
H	-6.615776	0.259108	-1.366808
H	-6.911589	-0.940446	-0.074820
H	2.336630	-3.588755	-3.716549
H	3.356492	-2.713853	-2.542085
H	2.083498	-1.847584	-3.438518
H	4.606744	-3.689667	0.187102
H	3.010940	-4.192604	-0.432187
H	3.176429	-3.606246	1.246494
H	-1.454784	-0.712486	-3.034762
H	-0.283378	-1.950160	-3.575294
H	-2.025848	-2.310408	-3.572329

$\omega$ B97X Energy = -1828.87807643 a.u.

(aR,1R,3S,3'S)-21, Conf M

C	2.904133	1.202469	0.661424
C	4.235411	0.817913	0.716026
C	4.615357	-0.392584	0.123147
C	3.676846	-1.188237	-0.513484
C	2.336241	-0.795296	-0.578913
C	1.958500	0.404677	0.019501
C	1.342139	-1.684896	-1.289417
C	2.032979	-2.690129	-2.198747
C	1.088982	-3.751312	-2.716151
O	3.069703	-3.345186	-1.471777
C	0.142618	1.823041	-0.930014
C	-1.180855	2.273846	-0.973506
C	-2.119972	1.696909	-0.122730
C	-1.748485	0.688302	0.768078
C	-0.413719	0.304716	0.858915
C	0.534940	0.855944	-0.011432
C	0.000272	-0.653147	1.948986
C	-1.031889	-0.663830	3.062316
C	-0.755050	-1.711864	4.116116
O	-2.304661	-0.959529	2.493735
C	-2.822285	0.053035	1.640422



C	4.135952	-2.470289	-1.169508
C	-3.918338	-0.617586	0.836919
C	-3.594800	-1.522444	-0.169302
C	-4.585666	-2.184935	-0.876670
C	-5.903632	-1.924158	-0.555295
C	-6.264262	-1.038020	0.437590
C	-5.254283	-0.387844	1.134987
F	-6.879329	-2.564662	-1.243936
O	5.224922	1.540110	1.301829
C	4.873129	2.777270	1.903032
O	5.933004	-0.782644	0.109785
C	6.423618	-1.240854	1.370643
O	-1.595466	3.210048	-1.881045
C	-1.018704	4.512356	-1.740172
O	-3.436795	2.068783	-0.170595
C	-3.723005	3.386205	0.297423
O	1.070917	2.372986	-1.778856
C	0.999059	1.888389	-3.120245
H	2.581939	2.135100	1.106558
H	0.739766	-2.236908	-0.557964
H	0.643161	-1.083254	-1.876375
H	2.490118	-2.156350	-3.046030
H	0.668706	-4.318909	-1.882629
H	0.267983	-3.290739	-3.268856
H	1.611252	-4.441091	-3.380394
H	0.975021	-0.359967	2.345824
H	0.105935	-1.672295	1.559945
H	-1.073075	0.330889	3.529506
H	-0.750531	-2.706790	3.665194
H	-1.518448	-1.685063	4.894634
H	0.218314	-1.536403	4.577807
H	-3.277713	0.840634	2.257078
H	4.693334	-2.229630	-2.086320
H	4.812675	-3.014695	-0.510798
H	-2.552762	-1.712328	-0.406551
H	-4.348692	-2.890822	-1.663172
H	-7.310520	-0.863219	0.655959
H	-5.516754	0.316252	1.917542
H	4.463686	3.472359	1.164980
H	5.794287	3.185659	2.311335
H	4.149944	2.633897	2.710507
H	7.460265	-1.532898	1.214185
H	6.374526	-0.447810	2.118882
H	5.849392	-2.107465	1.712665
H	-1.548294	5.156480	-2.439318
H	0.045390	4.499128	-1.976378
H	-1.162550	4.885575	-0.721920
H	-3.384962	4.141050	-0.414223
H	-3.254123	3.558757	1.270566
H	-4.804704	3.448165	0.402106
H	0.006047	2.055571	-3.544318
H	1.739096	2.444604	-3.692175
H	1.241868	0.822044	-3.156676

ωB97X Energy = -1828.87801889 a.u.

(aR,1R,3S,3'S)-**21**, Conf N

C	2.893729	0.993651	0.912188
C	4.217102	0.579399	0.934750
C	4.609976	-0.475663	0.102593
C	3.689431	-1.097903	-0.725547
C	2.352356	-0.688035	-0.739788
C	1.964376	0.366202	0.084364
C	1.382481	-1.383422	-1.667466
C	1.879661	-2.767610	-2.067832
C	1.742203	-3.797403	-0.954693
O	3.219936	-2.656482	-2.552816
C	0.162301	1.964000	-0.572348
C	-1.157056	2.421373	-0.522905
C	-2.108221	1.698629	0.188482
C	-1.746014	0.532686	0.869872
C	-0.413918	0.127361	0.876581
C	0.542939	0.824752	0.125911
C	-0.005892	-1.042453	1.738351
C	-1.034732	-1.287560	2.826713
C	-0.763234	-2.544703	3.621327
O	-2.312396	-1.435105	2.214398
C	-2.817917	-0.245304	1.624256
C	4.153991	-2.263065	-1.567824
C	-3.960856	-0.684853	0.733151
C	-5.276493	-0.396722	1.067281
C	-6.326624	-0.817438	0.261082
C	-6.027592	-1.538797	-0.875520
C	-4.731753	-1.855907	-1.235672
C	-3.699971	-1.421552	-0.418704
F	-7.042626	-1.954455	-1.669985
O	5.181861	1.117014	1.724909
C	4.813505	2.185766	2.584059
O	5.898262	-0.952340	0.134911
C	6.859839	-0.093318	-0.479919
O	-1.510629	3.573772	-1.175905
C	-1.220484	4.758437	-0.430925
O	-3.388904	2.164933	0.316137
C	-4.164983	2.216107	-0.885082
O	1.099234	2.702201	-1.248378
C	1.039304	2.567719	-2.668596
H	2.560524	1.804501	1.547222
H	0.395958	-1.465455	-1.205480
H	1.250907	-0.785572	-2.575087
H	1.311936	-3.112523	-2.933676
H	2.202304	-3.461167	-0.022159
H	0.683932	-3.980144	-0.757503
H	2.202789	-4.742032	-1.249751
H	0.971672	-0.847643	2.185463
H	0.094985	-1.955047	1.138182
H	-1.062493	-0.420226	3.502466
H	-0.770108	-3.415937	2.962141
H	-1.522129	-2.684254	4.392302
H	0.214165	-2.482404	4.103138
H	-3.221860	0.402608	2.414191
H	5.068827	-2.003279	-2.101545
H	4.398718	-3.107313	-0.909541

H	-5.490440	0.175691	1.963420
H	-7.357541	-0.594273	0.506599
H	-4.543375	-2.426454	-2.136758
H	-2.674203	-1.654883	-0.685285
H	4.444517	3.042889	2.014335
H	5.718404	2.468077	3.116514
H	4.052658	1.869709	3.302806
H	6.907720	0.867994	0.034515
H	7.821409	-0.597353	-0.404136
H	6.614421	0.064013	-1.534732
H	-1.553862	5.598592	-1.036974
H	-0.146815	4.842493	-0.246402
H	-1.762414	4.754514	0.518680
H	-3.727638	2.911723	-1.601122
H	-5.155526	2.558589	-0.591603
H	-4.244577	1.219607	-1.328650
H	1.251040	1.535476	-2.963153
H	0.059942	2.867994	-3.047251
H	1.806139	3.223409	-3.076182

ωB97X Energy = -1828.87792563 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf A

C	0.778024	-1.552833	1.452622
C	2.098748	-1.742981	1.862198
C	3.132619	-1.450503	0.978673
C	2.858641	-0.943213	-0.289590
C	1.539263	-0.760866	-0.694711
C	0.490414	-1.083176	0.175306
O	3.593132	-0.511031	-2.561383
C	2.479866	0.364736	-2.740562
C	1.250157	-0.240972	-2.083382
C	4.014546	-0.600144	-1.205518
C	2.300945	0.574858	-4.226846
C	4.779676	0.655393	-0.799187
C	-0.935087	-0.918958	-0.239751
C	-1.658956	0.214360	0.121740
C	-2.991862	0.315737	-0.276546
C	-3.580498	-0.670897	-1.057196
C	-2.838134	-1.788888	-1.454001
C	-1.524883	-1.909436	-1.019336
C	6.015653	0.889541	-1.399147
C	6.751239	2.026656	-1.108374
C	6.226625	2.929491	-0.203483
C	5.009259	2.736490	0.412549
C	4.288674	1.588387	0.105900
C	-1.028378	1.328015	0.919442
C	-1.821800	2.616738	0.795115
O	-3.197878	2.343394	1.071369
C	-3.809739	1.540038	0.082558
C	-1.369578	3.683619	1.764723
F	6.938590	4.043253	0.090973
O	-4.868093	-0.460134	-1.479849
C	-5.836606	-1.450481	-1.113321
O	-3.460980	-2.680954	-2.266853

C	-2.726996	-3.822924	-2.684189
C	-5.162190	1.175371	0.691684
O	-5.315191	0.334197	1.542437
O	-6.134967	1.946000	0.219875
C	-8.397005	2.686903	0.084736
C	-7.454803	1.730038	0.769506
O	-0.238943	-1.778343	2.342672
C	-0.577948	-3.155877	2.503359
O	2.357606	-2.230552	3.115794
C	2.743328	-1.220015	4.050623
C	4.869424	-2.950962	1.524831
O	4.440798	-1.595316	1.362555
H	2.708779	1.326267	-2.261661
H	0.451827	0.505370	-2.046312
H	0.879477	-1.062280	-2.707276
H	4.722389	-1.431587	-1.192618
H	1.441380	1.220536	-4.416412
H	3.187310	1.041159	-4.659123
H	2.131064	-0.382593	-4.724813
H	-0.932663	-2.770000	-1.304078
H	6.409633	0.169114	-2.108420
H	7.714404	2.214191	-1.566754
H	4.635583	3.468622	1.117749
H	3.331358	1.425336	0.588801
H	-0.966973	1.043240	1.975990
H	-0.003961	1.498701	0.576866
H	-1.746051	2.993258	-0.235179
H	-3.990215	2.135636	-0.821330
H	-1.944315	4.600337	1.627927
H	-0.313382	3.908893	1.606805
H	-1.499905	3.337132	2.792333
H	-6.806880	-1.029989	-1.373215
H	-5.673864	-2.377971	-1.659805
H	-5.796485	-1.636259	-0.037233
H	-3.399484	-4.397180	-3.316481
H	-1.843360	-3.535169	-3.260328
H	-2.423844	-4.432251	-1.828469
H	-9.403371	2.549192	0.482768
H	-8.097423	3.721080	0.259345
H	-8.424657	2.504625	-0.990379
H	-7.733039	0.688714	0.596451
H	-7.411633	1.898926	1.846701
H	0.283372	-3.727148	2.856714
H	-1.373172	-3.197318	3.244995
H	-0.939666	-3.572347	1.558134
H	3.662637	-0.726388	3.725957
H	1.944967	-0.481560	4.163712
H	2.912530	-1.721410	5.001389
H	4.314907	-3.441655	2.326111
H	4.738678	-3.503490	0.590019
H	5.927032	-2.910562	1.776894

ωB97X Energy = -2096.10614559 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf B

C	0.767966	-0.951342	1.862917
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C	2.088855	-0.989149	2.322341
C	3.122161	-1.057365	1.392375
C	2.842049	-1.078545	0.024680
C	1.527207	-1.033508	-0.423112
C	0.478751	-0.974427	0.504210
O	3.580786	-1.498953	-2.256803
C	2.478087	-0.726564	-2.729931
C	1.243511	-1.054843	-1.906676
C	4.004388	-1.144468	-0.945054
C	2.300519	-1.042569	-4.197700
C	4.847464	0.123916	-0.970633
C	-0.946361	-0.944810	0.058054
C	-1.666743	0.247225	0.047839
C	-2.999218	0.223663	-0.364705
C	-3.589891	-0.954598	-0.802705
C	-2.850512	-2.142546	-0.832419
C	-1.538894	-2.126439	-0.377789
C	6.189473	0.023541	-1.329745
C	6.997528	1.146654	-1.413014
C	6.435039	2.376851	-1.134543
C	5.111660	2.522191	-0.776088
C	4.322560	1.381966	-0.693058
C	-1.033179	1.551549	0.462718
C	-1.827475	2.742090	-0.045087
O	-3.203836	2.564894	0.299490
C	-3.812509	1.502320	-0.405807
C	-1.376463	4.052511	0.556785
F	7.215342	3.480826	-1.209898
O	-4.875246	-0.881435	-1.275214
C	-5.849543	-1.708172	-0.626915
O	-3.474741	-3.239943	-1.332896
C	-2.743253	-4.456435	-1.380952
C	-5.175400	1.346000	0.265567
O	-5.342942	0.821148	1.338603
O	-6.139609	1.920105	-0.443870
C	-8.402786	2.539729	-0.862847
C	-7.470131	1.879069	0.120075
O	-0.255020	-0.877242	2.775340
C	-0.610373	-2.137942	3.345825
O	2.375781	-1.048401	3.659656
C	2.064440	0.133116	4.405377
C	4.985348	-0.136096	2.567466
O	4.431837	-1.180573	1.765738
H	2.716359	0.339371	-2.616031
H	0.446265	-0.345534	-2.144769
H	0.876589	-2.046316	-2.195416
H	4.658580	-1.962688	-0.639343
H	1.448777	-0.492609	-4.602247
H	3.192477	-0.765162	-4.761128
H	2.119085	-2.111156	-4.334363
H	-0.950243	-3.035197	-0.379052
H	6.614582	-0.951952	-1.542136
H	8.044177	1.076222	-1.682333
H	4.711305	3.505524	-0.562358
H	3.284023	1.483167	-0.396292
H	-0.964890	1.602663	1.555351

H	-0.011188	1.608009	0.077483
H	-1.751351	2.789946	-1.140954
H	-3.977221	1.795646	-1.450424
H	-1.952857	4.883985	0.149556
H	-0.320460	4.221807	0.338986
H	-1.507164	4.032447	1.641037
H	-6.815822	-1.392557	-1.017435
H	-5.682502	-2.760106	-0.852535
H	-5.822117	-1.546493	0.453492
H	-3.418180	-5.194182	-1.807630
H	-1.859332	-4.360522	-2.017314
H	-2.441419	-4.776037	-0.379935
H	-9.418332	2.522419	-0.464682
H	-8.118372	3.578952	-1.032832
H	-8.398633	2.012625	-1.817823
H	-7.736878	0.835370	0.296746
H	-7.454160	2.396269	1.080812
H	-1.405069	-1.943451	4.063274
H	-0.977085	-2.817178	2.570382
H	0.245189	-2.586216	3.856875
H	2.593721	0.995914	3.990320
H	0.990921	0.323645	4.402693
H	2.407703	-0.047355	5.422149
H	4.673819	-0.231403	3.607720
H	6.066700	-0.240245	2.497562
H	4.693201	0.842712	2.176637

ωB97X Energy = -2096.10599611 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf C

C	-0.792309	1.091981	-1.825221
C	-2.122684	1.428965	-2.096670
C	-3.136081	0.595020	-1.632761
C	-2.826298	-0.551609	-0.898285
C	-1.502360	-0.871248	-0.621347
C	-0.473838	-0.046698	-1.095831
O	-3.501803	-2.714765	-0.014392
C	-2.408851	-2.653288	0.901036
C	-1.184940	-2.110414	0.182362
C	-3.964396	-1.433307	-0.426812
C	-2.195251	-4.045756	1.449508
C	-4.831747	-0.801989	0.654945
C	0.960184	-0.381196	-0.845409
C	1.694760	0.301081	0.121856
C	3.028836	-0.054862	0.325621
C	3.606064	-1.085004	-0.400494
C	2.871505	-1.763533	-1.377685
C	1.547679	-1.403596	-1.587636
C	-6.135043	-1.269813	0.809202
C	-6.963383	-0.777434	1.804688
C	-6.461315	0.193908	2.648913
C	-5.179066	0.686095	2.531401
C	-4.367393	0.179623	1.523646
C	1.078067	1.397544	0.954010
C	1.898366	1.680700	2.200651
O	3.269195	1.850929	1.828740

C	3.861478	0.651516	1.379442
C	1.465636	2.937632	2.918774
F	-7.261707	0.684622	3.624547
O	4.930036	-1.381063	-0.187836
C	5.159483	-2.595455	0.529984
O	3.527281	-2.736386	-2.058851
C	2.807891	-3.439661	-3.061721
C	5.229983	1.068195	0.840945
O	5.389767	1.712256	-0.165234
O	6.210330	0.682830	1.649856
C	8.500098	0.421604	2.252764
C	7.555880	0.984653	1.220979
O	0.210857	1.910001	-2.281758
C	0.546270	1.697171	-3.654352
O	-2.435958	2.505609	-2.882269
C	-2.149850	3.785559	-2.309106
C	-5.030109	2.045847	-1.513283
O	-4.452895	0.808478	-1.932594
H	-2.675752	-1.977670	1.724860
H	-0.398702	-1.891604	0.910026
H	-0.789476	-2.886901	-0.482038
H	-4.610549	-1.639344	-1.281949
H	-1.355982	-4.051856	2.147561
H	-3.086016	-4.391911	1.975503
H	-1.975611	-4.742922	0.637583
H	0.952982	-1.912717	-2.335790
H	-6.511445	-2.032535	0.135387
H	-7.979326	-1.131961	1.927900
H	-4.826730	1.450465	3.213019
H	-3.360384	0.568468	1.415456
H	1.000184	2.314381	0.358660
H	0.061004	1.119536	1.244061
H	1.833681	0.821380	2.883612
H	4.021019	-0.023835	2.230230
H	2.060900	3.093399	3.819191
H	0.415190	2.861868	3.205387
H	1.584212	3.804282	2.264687
H	4.796412	-3.453986	-0.037958
H	6.235933	-2.675167	0.669385
H	4.667316	-2.561965	1.506410
H	3.504700	-4.161933	-3.479503
H	1.949480	-3.966142	-2.635841
H	2.468066	-2.762837	-3.850245
H	9.529207	0.622404	1.951586
H	8.331816	0.881421	3.227511
H	8.373647	-0.657984	2.346616
H	7.708679	0.532725	0.238909
H	7.656904	2.066492	1.121154
H	0.926364	0.681577	-3.800124
H	-0.323051	1.864362	-4.294980
H	1.326271	2.414843	-3.900453
H	-2.681148	3.906094	-1.360403
H	-1.078627	3.910908	-2.149140
H	-2.507791	4.526364	-3.021371
H	-6.109007	1.906828	-1.554105
H	-4.737247	2.276820	-0.485195

H -4.739839 2.860553 -2.176532  
 ωB97X Energy = -2096.10580625 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf D

C	-0.769287	-1.585124	-1.385650
C	-2.089653	-1.811475	-1.786838
C	-3.124645	-1.447925	-0.928642
C	-2.847124	-0.941166	0.340965
C	-1.530417	-0.763840	0.751067
C	-0.482379	-1.081104	-0.122181
O	-3.594477	-0.464169	2.604914
C	-2.467239	0.392709	2.784179
C	-1.243367	-0.235410	2.136988
C	-4.007197	-0.585057	1.247920
C	-2.292332	0.604446	4.270995
C	-4.774900	0.652227	0.801662
C	0.943181	-0.888526	0.280435
C	1.661688	0.224865	-0.147746
C	2.995403	0.353881	0.239607
C	3.589651	-0.582544	1.075785
C	2.852186	-1.677452	1.540292
C	1.538928	-1.829016	1.115714
C	-4.177688	1.694638	0.099760
C	-4.897021	2.831934	-0.244056
C	-6.224717	2.901141	0.121718
C	-6.857774	1.886993	0.813362
C	-6.118592	0.764132	1.150834
C	1.024433	1.287377	-1.007315
C	1.815906	2.582558	-0.966086
O	3.191552	2.295413	-1.229899
C	3.808435	1.556858	-0.194588
C	1.357577	3.586127	-1.998455
F	-6.937238	4.001842	-0.214817
O	4.877146	-0.341133	1.482226
C	5.849465	-1.348118	1.176265
O	3.479387	-2.516849	2.404430
C	2.745866	-3.626343	2.902137
C	5.160474	1.159972	-0.784285
O	5.313677	0.270208	-1.584036
O	6.131954	1.960929	-0.362928
C	8.393710	2.710180	-0.273561
C	7.448985	1.722898	-0.910042
O	0.251831	-1.830628	-2.266375
C	0.670253	-3.192325	-2.321195
O	-2.316387	-2.332292	-3.031892
C	-2.971133	-3.603949	-3.053060
C	-4.901907	-0.855475	-2.384910
O	-4.438805	-1.631705	-1.275415
H	-2.676065	1.357865	2.304454
H	-0.434791	0.499515	2.097919
H	-0.887955	-1.056037	2.770596
H	-4.708842	-1.420693	1.249640
H	-1.424001	1.237671	4.462640
H	-3.173546	1.085208	4.697833
H	-2.139171	-0.354055	4.772320

H	0.951966	-2.674597	1.451846
H	-3.136698	1.621906	-0.197184
H	-4.440614	3.648474	-0.789797
H	-7.905023	1.979522	1.073503
H	-6.599257	-0.043952	1.692533
H	0.956961	0.937280	-2.043548
H	0.001783	1.476098	-0.668685
H	1.743277	3.022309	0.039086
H	3.988710	2.207971	0.670191
H	1.931386	4.510447	-1.922096
H	0.301638	3.819016	-1.850199
H	1.483888	3.175744	-3.002775
H	6.817767	-0.910622	1.414403
H	5.687584	-2.242952	1.774890
H	5.813270	-1.595588	0.112471
H	3.419845	-4.155196	3.571381
H	1.863833	-3.298254	3.458849
H	2.440408	-4.294418	2.092429
H	9.396743	2.560728	-0.675726
H	8.087883	3.735383	-0.486190
H	8.432664	2.570993	0.807635
H	7.730616	0.690583	-0.694363
H	7.398774	1.845359	-1.993268
H	-0.143487	-3.839240	-2.658866
H	1.488338	-3.239722	-3.037199
H	1.024151	-3.525583	-1.340695
H	-2.973175	-3.928872	-4.091373
H	-2.419990	-4.327429	-2.445523
H	-3.995666	-3.529702	-2.684607
H	-4.387820	-1.136360	-3.305766
H	-5.966119	-1.061909	-2.477936
H	-4.753750	0.209815	-2.190124

ωB97X Energy = -2096.10579153 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf E

C	0.456983	-1.060351	-1.632686
C	1.720766	-1.503214	-2.036863
C	2.833030	-0.718476	-1.745490
C	2.685801	0.486436	-1.055331
C	1.426804	0.915356	-0.651632
C	0.299339	0.137827	-0.947292
O	3.606555	2.634754	-0.378402
C	2.615989	2.711525	0.645887
C	1.287130	2.220560	0.096092
C	3.927903	1.300926	-0.756451
C	2.558009	4.147950	1.113988
C	4.851590	0.655850	0.269544
C	-1.070566	0.573614	-0.542201
C	-1.708185	-0.007170	0.551997
C	-2.994822	0.418037	0.883518
C	-3.616138	1.433525	0.168853
C	-2.957775	2.044055	-0.903756
C	-1.695531	1.589003	-1.260535
C	6.197885	1.014412	0.265489
C	7.082817	0.497355	1.198126

C	6.594231	-0.386880	2.140231
C	5.270164	-0.767977	2.181397
C	4.401980	-0.239368	1.234162
C	-1.036588	-1.074525	1.379613
C	-1.698377	-1.220293	2.738540
O	-3.110044	-1.358791	2.554861
C	-3.718222	-0.176403	2.075626
C	-1.221951	-2.433346	3.502756
F	7.450322	-0.901600	3.054347
O	-4.849339	1.843885	0.603049
C	-5.919597	1.811179	-0.347066
O	-3.607011	3.066958	-1.517487
C	-2.961761	3.700316	-2.612746
C	-5.164074	-0.587913	1.801811
O	-6.060897	-0.417396	2.590378
O	-5.299449	-1.221285	0.643051
C	-6.533643	-2.374140	-1.034150
C	-6.611576	-1.741050	0.331887
O	-0.640691	-1.836281	-1.911564
C	-1.152074	-1.657489	-3.233272
O	1.868862	-2.640889	-2.783903
C	1.575473	-3.864344	-2.101149
C	4.628035	-2.296175	-1.757036
O	4.089580	-1.041609	-2.176437
H	2.922433	2.069848	1.482992
H	0.570171	2.108274	0.913851
H	0.878192	2.983964	-0.575495
H	4.495517	1.410277	-1.682044
H	1.793354	4.263002	1.884583
H	3.518329	4.456360	1.529478
H	2.309804	4.807322	0.279026
H	-1.171246	2.035615	-2.096012
H	6.562817	1.709687	-0.483432
H	8.132313	0.764818	1.197442
H	4.929400	-1.466831	2.935340
H	3.360317	-0.541799	1.250848
H	-1.079132	-2.035253	0.854080
H	0.021053	-0.832045	1.514981
H	-1.517801	-0.311814	3.331004
H	-3.765947	0.568727	2.880253
H	-1.712014	-2.493909	4.475166
H	-0.143392	-2.377003	3.660311
H	-1.442984	-3.343699	2.941082
H	-5.867937	0.898848	-0.947584
H	-6.840506	1.812976	0.234588
H	-5.888617	2.680310	-1.002025
H	-3.645008	4.472991	-2.956200
H	-2.018966	4.159538	-2.303278
H	-2.775637	2.992171	-3.424635
H	-7.507592	-2.788402	-1.298354
H	-6.257002	-1.637151	-1.789985
H	-5.800543	-3.181572	-1.047033
H	-6.888361	-2.462292	1.102516
H	-7.328053	-0.917821	0.360253
H	-0.389611	-1.896522	-3.978715
H	-1.992763	-2.340543	-3.337823

H	-1.498377	-0.628971	-3.372280
H	2.212845	-3.970506	-1.218362
H	0.526780	-3.903451	-1.805446
H	1.793712	-4.666025	-2.803950
H	4.221842	-3.116751	-2.348390
H	5.703877	-2.231086	-1.910159
H	4.427004	-2.464529	-0.695258

$\omega$ B97X Energy = -2096.10575917 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf F

C	0.474441	1.768937	-0.860718
C	1.741590	2.230035	-1.220456
C	2.850642	1.804690	-0.496104
C	2.705339	0.900847	0.554295
C	1.438790	0.444173	0.908186
C	0.312054	0.895307	0.209386
O	3.606793	-0.118767	2.563956
C	2.612904	-1.139669	2.473494
C	1.288006	-0.518053	2.062872
C	3.941033	0.441347	1.299732
C	2.540427	-1.825986	3.818530
C	4.827399	-0.513869	0.507716
C	-1.061685	0.452883	0.594581
C	-1.720691	-0.548020	-0.114869
C	-3.006890	-0.917052	0.280500
C	-3.608042	-0.330470	1.386382
C	-2.929657	0.648946	2.119640
C	-1.666672	1.043948	1.700186
C	4.401534	-1.179675	-0.635048
C	5.237488	-2.069565	-1.298917
C	6.503375	-2.277374	-0.795794
C	6.966409	-1.635842	0.336911
C	6.115574	-0.753800	0.982432
C	-1.070744	-1.233444	-1.290694
C	-1.756508	-2.548118	-1.617923
O	-3.167179	-2.328642	-1.704060
C	-3.748060	-2.017045	-0.453613
C	-1.309038	-3.134895	-2.936376
F	7.327678	-3.139513	-1.437249
O	-4.840657	-0.801979	1.754566
C	-5.900286	0.153788	1.867480
O	-3.561036	1.136766	3.218701
C	-2.886366	2.120264	3.989542
C	-5.202221	-1.691756	-0.790131
O	-6.098301	-2.494065	-0.697293
O	-5.347756	-0.462493	-1.269534
C	-6.604171	1.344828	-2.177263
C	-6.672065	-0.086585	-1.709111
O	-0.611013	2.143928	-1.608549
C	-1.110167	3.444051	-1.294703
O	1.874141	3.108945	-2.262720
C	2.299862	2.487690	-3.477752
C	4.376521	3.601957	-0.592221
O	4.111780	2.217482	-0.840290
H	2.924798	-1.866005	1.710985

H	0.578925	-1.308003	1.800463
H	0.860027	0.010196	2.922396
H	4.542152	1.320814	1.540632
H	1.769603	-2.598762	3.806603
H	3.495398	-2.292131	4.064783
H	2.292299	-1.101891	4.598018
H	-1.124272	1.806011	2.245644
H	3.405118	-1.004178	-1.025648
H	4.915082	-2.591923	-2.191186
H	7.970693	-1.824312	0.695913
H	6.459980	-0.241096	1.874466
H	-1.108287	-0.578147	-2.168449
H	-0.014140	-1.418525	-1.077815
H	-1.571718	-3.268067	-0.807699
H	-3.779965	-2.916664	0.174823
H	-1.805817	-4.087448	-3.124161
H	-0.230441	-3.301622	-2.925462
H	-1.545170	-2.448444	-3.752470
H	-5.853658	0.678277	2.820291
H	-5.850684	0.877113	1.048927
H	-6.827766	-0.413031	1.797084
H	-2.682370	3.016601	3.397684
H	-3.557699	2.372440	4.806604
H	-1.949981	1.728095	4.395801
H	-7.588536	1.659704	-2.526513
H	-6.300055	2.007013	-1.364765
H	-5.895924	1.451579	-2.999833
H	-6.975677	-0.765391	-2.507688
H	-7.364089	-0.210316	-0.873799
H	-1.456850	3.479343	-0.257197
H	-0.340749	4.202705	-1.455486
H	-1.949071	3.627091	-1.963285
H	3.277456	2.016882	-3.346999
H	1.568256	1.741924	-3.800193
H	2.369513	3.275693	-4.224884
H	5.419339	3.767431	-0.854476
H	3.733595	4.236720	-1.203694
H	4.226646	3.831703	0.466582

$\omega$ B97X Energy = -2096.10573808 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf G

C	-0.786131	-1.708715	-1.312505
C	-2.114078	-1.951027	-1.678334
C	-3.139300	-1.543175	-0.830160
C	-2.850839	-0.953149	0.399013
C	-1.526819	-0.765245	0.783034
C	-0.487975	-1.140261	-0.076371
O	-3.565320	-0.357971	2.645173
C	-2.436440	0.507340	2.758633
C	-1.221395	-0.157915	2.132080
C	-3.997882	-0.552277	1.302672
C	-2.240035	0.805099	4.228008
C	-4.777874	0.657611	0.804868
C	0.940111	-0.941126	0.314053
C	1.650454	0.178223	-0.112685

C	2.984852	0.314204	0.270934
C	3.588217	-0.622638	1.099480
C	2.858869	-1.723504	1.562811
C	1.544950	-1.880971	1.143100
C	-6.104563	0.801955	1.204302
C	-6.854503	1.903279	0.823117
C	-6.249859	2.862678	0.034525
C	-4.940156	2.759879	-0.383944
C	-4.209223	1.645112	0.006809
C	1.004950	1.246009	-0.960299
C	1.782556	2.548754	-0.896194
O	3.159537	2.279875	-1.170736
C	3.788620	1.526859	-0.153224
C	1.310660	3.567230	-1.907656
F	-6.973379	3.941640	-0.346250
O	4.876274	-0.375772	1.501724
C	5.852616	-1.374090	1.180966
O	3.494927	-2.561797	2.421403
C	2.767545	-3.672212	2.926326
C	5.136474	1.143644	-0.761232
O	5.285457	0.264186	-1.573163
O	6.108850	1.942907	-0.339052
C	8.367867	2.702025	-0.264002
C	7.422152	1.715053	-0.899480
O	0.254444	-2.092845	-2.109779
C	0.248999	-1.641383	-3.466364
O	-2.421170	-2.585769	-2.854301
C	-2.191411	-3.996159	-2.817339
C	-4.967304	-1.104659	-2.275981
O	-4.448971	-1.799916	-1.138193
H	-2.653013	1.443062	2.226286
H	-0.413479	0.573317	2.041099
H	-0.856770	-0.941452	2.806234
H	-4.696523	-1.388450	1.360219
H	-1.370835	1.450116	4.369798
H	-3.116320	1.307738	4.639532
H	-2.076709	-0.122731	4.781172
H	0.963987	-2.731276	1.477194
H	-6.562423	0.037266	1.823242
H	-7.888549	2.020418	1.123140
H	-4.506647	3.533030	-1.006248
H	-3.182369	1.545983	-0.329078
H	0.949938	0.918476	-2.005154
H	-0.022464	1.417362	-0.627356
H	1.708286	2.967660	0.117670
H	3.974815	2.164741	0.720047
H	1.875671	4.495449	-1.815288
H	0.253063	3.787088	-1.751643
H	1.437939	3.177695	-2.920188
H	5.815539	-1.608007	0.114095
H	6.819426	-0.935572	1.423238
H	5.695746	-2.277547	1.767990
H	3.447017	-4.197031	3.593208
H	1.887819	-3.345016	3.487153
H	2.459397	-4.343500	2.120477
H	9.368095	2.559758	-0.675645

H	8.055740	3.727286	-0.466953
H	8.416608	2.555544	0.815824
H	7.710263	0.682499	-0.693588
H	7.361970	1.845085	-1.981282
H	-0.190197	-0.643400	-3.540411
H	1.291183	-1.602670	-3.779151
H	-0.305931	-2.324315	-4.110276
H	-2.502969	-4.388420	-3.783346
H	-1.132060	-4.213447	-2.656216
H	-2.785901	-4.458348	-2.024995
H	-4.893594	-0.024086	-2.124903
H	-4.436814	-1.394053	-3.183453
H	-6.015378	-1.386865	-2.354574

ωB97X Energy = -2096.10572014 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf H

C	-0.744933	-1.198162	1.763632
C	-2.070939	-1.538449	2.052330
C	-3.088119	-0.672074	1.661864
C	-2.786387	0.512201	0.986255
C	-1.467031	0.838094	0.696197
C	-0.434748	-0.021764	1.093193
O	-3.468072	2.726259	0.245880
C	-2.392269	2.720687	-0.691627
C	-1.158218	2.122391	-0.036580
C	-3.928187	1.422173	0.583021
C	-2.177249	4.146775	-1.145237
C	-4.804372	0.856709	-0.528248
C	0.994869	0.311359	0.816973
C	1.677814	-0.296841	-0.233910
C	3.008038	0.057135	-0.462949
C	3.631810	1.014994	0.320876
C	2.950943	1.614946	1.384549
C	1.630046	1.257856	1.617936
C	-6.100338	1.350846	-0.661605
C	-6.934814	0.916151	-1.678697
C	-6.446969	-0.024309	-2.565290
C	-5.172271	-0.540016	-2.470103
C	-4.353959	-0.090889	-1.440773
C	1.009723	-1.307829	-1.131949
C	1.770334	-1.482096	-2.435266
O	3.152557	-1.706466	-2.142207
C	3.786357	-0.564506	-1.606348
C	1.284795	-2.657882	-3.250381
F	-7.254142	-0.458778	-3.561777
O	4.949960	1.308382	0.072203
C	5.177205	2.595279	-0.506461
O	3.651968	2.513361	2.121047
C	2.986067	3.139154	3.208555
C	5.163326	-1.059278	-1.161884
O	5.347734	-1.752503	-0.193722
O	6.107552	-0.687429	-2.021078
C	8.095000	-0.047615	-0.772495
C	7.470300	-1.057212	-1.708981
O	0.261630	-2.051419	2.141451

C	0.641722	-1.921962	3.512765
O	-2.373948	-2.654534	2.785154
C	-2.116270	-3.903789	2.135801
C	-4.995439	-2.103664	1.510490
O	-4.399689	-0.892972	1.978806
H	-2.679585	2.105675	-1.555219
H	-0.390649	1.944945	-0.794869
H	-0.740559	2.851974	0.666504
H	-4.566548	1.575377	1.454745
H	-1.349426	4.196206	-1.855148
H	-3.073662	4.535226	-1.630523
H	-1.938858	4.783308	-0.289927
H	1.075768	1.709812	2.431014
H	-6.465560	2.088838	0.045098
H	-7.944908	1.291766	-1.786587
H	-4.830495	-1.278162	-3.185144
H	-3.352210	-0.497571	-1.351599
H	0.945140	-2.274930	-0.620487
H	-0.015177	-0.994539	-1.349452
H	1.691877	-0.559529	-3.028293
H	3.931356	0.183661	-2.396693
H	1.838249	-2.734104	-4.187020
H	0.224685	-2.540206	-3.481966
H	1.415511	-3.585571	-2.688893
H	4.647044	2.686225	-1.459052
H	4.856982	3.386067	0.173943
H	6.249249	2.670997	-0.679517
H	3.711855	3.813021	3.656765
H	2.121062	3.712699	2.864569
H	2.665589	2.403039	3.950635
H	9.128486	-0.331691	-0.566669
H	8.096488	0.945969	-1.224069
H	7.550673	-0.002711	0.171526
H	7.473640	-2.059688	-1.281818
H	7.973940	-1.076767	-2.673571
H	1.040287	-0.921118	3.704007
H	-0.209538	-2.115372	4.170117
H	1.419075	-2.661927	3.692475
H	-2.669634	-3.965372	1.194107
H	-1.050414	-4.032263	1.945633
H	-2.468231	-4.678561	2.814126
H	-6.071998	-1.959775	1.583081
H	-4.727787	-2.284517	0.465575
H	-4.696996	-2.953344	2.124397

ωB97X Energy = -2096.10566943 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf I

C	0.829158	-1.799752	1.195215
C	2.166136	-2.047952	1.509953
C	3.162926	-1.573859	0.663447
C	2.835731	-0.832165	-0.469915
C	1.500615	-0.586765	-0.778204
C	0.488683	-1.089848	0.048819
O	3.467741	0.029849	-2.648915
C	2.356320	0.924448	-2.598714

C	1.152506	0.198131	-2.021075
C	3.952007	-0.325667	-1.358945
C	2.114590	1.430865	-4.002323
C	4.764386	0.816255	-0.759888
C	-0.951998	-0.876546	-0.283960
C	-1.690400	0.128183	0.336090
C	-3.028976	0.295596	-0.023579
C	-3.607199	-0.509110	-0.992990
C	-2.868296	-1.524488	-1.607822
C	-1.539073	-1.694491	-1.247113
C	6.001456	1.103465	-1.333358
C	6.779876	2.153695	-0.875801
C	6.295832	2.915530	0.170165
C	5.079233	2.665164	0.767319
C	4.315716	1.605330	0.292368
C	-1.072777	1.036735	1.369669
C	-1.900292	2.293734	1.576209
O	-3.268546	1.925533	1.773379
C	-3.859400	1.399775	0.605094
C	-1.468743	3.092728	2.783698
F	7.048588	3.943768	0.628537
O	-4.935126	-0.330646	-1.293553
C	-5.180280	0.306823	-2.548883
O	-3.524903	-2.277910	-2.525001
C	-2.796972	-3.311374	-3.172976
C	-5.236135	0.906072	1.048414
O	-5.409718	-0.031130	1.785965
O	-6.206777	1.674843	0.568327
C	-8.486678	2.191415	0.119419
C	-7.559711	1.285590	0.889911
O	-0.150562	-2.218964	2.056547
C	-0.483364	-3.601536	1.926302
O	2.477006	-2.775934	2.627568
C	2.872394	-1.971246	3.740731
C	4.922611	-3.135754	0.828047
O	4.486035	-1.779163	0.958722
H	2.615853	1.770518	-1.948109
H	0.361696	0.919823	-1.798240
H	0.748963	-0.483007	-2.778907
H	4.641814	-1.151718	-1.544883
H	1.258815	2.108491	-4.016800
H	2.988706	1.968359	-4.372396
H	1.906540	0.595828	-4.675330
H	-0.939733	-2.468362	-1.710272
H	6.363276	0.493355	-2.154427
H	7.744433	2.380593	-1.312916
H	4.739174	3.286209	1.586875
H	3.359139	1.395708	0.758766
H	-0.982438	0.503793	2.323005
H	-0.060060	1.315692	1.065276
H	-1.841979	2.920560	0.674655
H	-4.006741	2.203448	-0.128369
H	-2.068029	3.998543	2.882296
H	-0.419795	3.378722	2.687697
H	-1.582852	2.495465	3.691006
H	-4.822415	-0.313646	-3.372615



H	-6.258312	0.435593	-2.626534
H	-4.693615	1.285982	-2.583982
H	-3.493815	-3.782868	-3.861337
H	-1.950092	-2.905852	-3.733153
H	-2.438964	-4.052240	-2.453046
H	-9.521712	1.931059	0.345362
H	-8.327680	3.235707	0.391491
H	-8.330914	2.080263	-0.954770
H	-7.690531	0.237934	0.613119
H	-7.700366	1.376862	1.968321
H	-0.882451	-3.804320	0.927629
H	0.391613	-4.228463	2.112719
H	-1.248617	-3.810751	2.671114
H	3.765991	-1.390876	3.497847
H	2.060678	-1.299532	4.032785
H	3.091453	-2.655276	4.558145
H	5.986203	-3.140270	1.057072
H	4.389507	-3.784492	1.524528
H	4.769497	-3.486468	-0.196727

$\omega$ B97X Energy = -2096.10564467 a.u.

(*aS*,1*S*,3*S*,1'*S*,3'*S*)-22, Conf J

C	-0.751180	-1.651125	-1.346719
C	-2.074372	-1.908390	-1.708231
C	-3.098201	-1.562610	-0.832837
C	-2.811402	-0.942374	0.381335
C	-1.489587	-0.690664	0.738544
C	-0.449643	-1.059946	-0.124142
O	-3.509682	-0.344023	2.626649
C	-2.421438	0.576624	2.706353
C	-1.187811	-0.043621	2.070188
C	-3.957295	-0.557724	1.293065
C	-2.215194	0.912182	4.165948
C	-4.769851	0.636323	0.804694
C	0.978028	-0.818632	0.243131
C	1.684157	0.252270	-0.300094
C	3.011959	0.443432	0.084374
C	3.609322	-0.396178	1.011382
C	2.905274	-1.479548	1.545596
C	1.587811	-1.676794	1.155664
C	-6.013863	0.862827	1.390584
C	-6.790434	1.951610	1.029738
C	-6.298264	2.813937	0.068921
C	-5.074756	2.626096	-0.536711
C	-4.313053	1.526496	-0.159689
C	1.044366	1.210374	-1.273445
C	1.826458	2.508802	-1.370600
O	3.207034	2.205615	-1.591285
C	3.817452	1.602481	-0.470206
C	1.369530	3.389085	-2.510353
F	-7.049682	3.880652	-0.293661
O	4.925192	-0.179669	1.338938
C	5.135542	0.339769	2.653575
O	3.581960	-2.269622	2.416794
C	2.888682	-3.371351	2.984981

C	5.191862	1.158766	-0.973320
O	5.367941	0.219613	-1.707415
O	6.145045	1.987223	-0.557345
C	8.116007	0.687239	0.030780
C	7.505953	1.677220	-0.935733
O	0.252086	-1.937005	-2.234932
C	0.622065	-3.315762	-2.268815
O	-2.347153	-2.513008	-2.906777
C	-2.712973	-1.590722	-3.935459
C	-4.809300	-3.142393	-1.208472
O	-4.409552	-1.768808	-1.175545
H	-2.692337	1.489127	2.158491
H	-0.415532	0.721044	1.948943
H	-0.776479	-0.795843	2.752822
H	-4.638721	-1.407847	1.365834
H	-1.376344	1.601440	4.279958
H	-3.107795	1.380561	4.582895
H	-1.997938	0.004759	4.734311
H	1.016364	-2.504949	1.555928
H	-6.382294	0.174244	2.143872
H	-7.760072	2.132578	1.476940
H	-4.727663	3.325560	-1.287189
H	-3.350644	1.367137	-0.633774
H	0.987372	0.748685	-2.265548
H	0.018048	1.427273	-0.964223
H	1.743602	3.055786	-0.420419
H	3.967863	2.352646	0.317187
H	1.938228	4.319442	-2.532560
H	0.311503	3.631055	-2.395001
H	1.504494	2.872137	-3.462978
H	4.794471	-0.370421	3.408703
H	6.207740	0.497686	2.755542
H	4.613807	1.293354	2.777115
H	3.596180	-3.860303	3.649929
H	2.020294	-3.037553	3.559506
H	2.568064	-4.076449	2.213427
H	9.151676	0.491881	-0.252784
H	8.108589	1.087338	1.046165
H	7.568419	-0.255838	0.021095
H	7.509712	1.298742	-1.957623
H	8.020012	2.636077	-0.906663
H	-0.231299	-3.937720	-2.548495
H	1.405359	-3.410643	-3.018182
H	1.010012	-3.630252	-1.294983
H	-2.896731	-2.178023	-4.832901
H	-3.620587	-1.047592	-3.660112
H	-1.899426	-0.884212	-4.121059
H	-4.251393	-3.691860	-1.968090
H	-4.657589	-3.605140	-0.228940
H	-5.869913	-3.148498	-1.451012

$\omega$ B97X Energy = -2096.10562824 a.u.

(*aS*,1*S*,3*S*,1'*S*,3'*S*)-22, Conf K

C	-0.482002	1.944849	-0.553237
C	-1.754146	2.518032	-0.570580

C	-2.859813	1.712321	-0.819099
C	-2.703184	0.343797	-1.030797
C	-1.431380	-0.222092	-1.016265
C	-0.309729	0.584891	-0.786698
O	-3.597203	-1.743333	-1.884364
C	-2.583292	-2.457964	-1.177443
C	-1.267927	-1.701610	-1.274506
C	-3.933807	-0.505893	-1.267859
C	-2.501462	-3.843600	-1.776610
C	-4.775415	-0.742945	-0.018167
C	1.068306	0.008922	-0.773909
C	1.716182	-0.255876	0.430677
C	3.003375	-0.792902	0.395215
C	3.613984	-1.089582	-0.813253
C	2.966807	-0.817599	-2.021981
C	1.691624	-0.269547	-1.988066
C	-6.061283	-1.254644	-0.182635
C	-6.866719	-1.538029	0.908250
C	-6.360629	-1.300258	2.171785
C	-5.096482	-0.792695	2.379063
C	-4.306467	-0.515312	1.269966
C	1.053900	0.012281	1.758938
C	1.743510	-0.736848	2.886296
O	3.152152	-0.498476	2.812325
C	3.747764	-1.097872	1.680357
C	1.282455	-0.296538	4.255998
F	-7.139360	-1.572556	3.245754
O	4.893303	-1.587777	-0.795815
C	5.000321	-2.970160	-1.144435
O	3.654966	-1.111306	-3.153863
C	3.025093	-0.846074	-4.398921
C	5.193076	-0.600118	1.697144
O	6.107878	-1.244038	2.149649
O	5.304921	0.635409	1.230503
C	6.516103	2.596894	0.638920
C	6.629662	1.209828	1.218917
O	0.598292	2.732137	-0.248776
C	1.084005	3.497963	-1.352065
O	-1.908546	3.863074	-0.360602
C	-2.008802	4.208952	1.022458
C	-4.431326	3.103855	-1.893711
O	-4.125483	2.237086	-0.797392
H	-2.879129	-2.535285	-0.122685
H	-0.549253	-2.126901	-0.568390
H	-0.844446	-1.848215	-2.274684
H	-4.567335	0.001222	-1.998523
H	-1.715100	-4.420832	-1.286565
H	-3.447942	-4.371939	-1.654132
H	-2.271469	-3.779904	-2.842731
H	1.165213	-0.047870	-2.908079
H	-6.439931	-1.436313	-1.183088
H	-7.867973	-1.933513	0.789521
H	-4.739467	-0.618806	3.386670
H	-3.311576	-0.111051	1.421957
H	1.075565	1.086775	1.973774
H	0.001514	-0.282579	1.717581

H	1.573028	-1.816191	2.764387
H	3.803691	-2.185228	1.823664
H	1.790050	-0.865426	5.035862
H	0.206856	-0.451550	4.357501
H	1.494127	0.765049	4.401646
H	4.698460	-3.130891	-2.180794
H	6.046975	-3.240004	-1.019190
H	4.383761	-3.581789	-0.479259
H	3.731429	-1.158202	-5.164041
H	2.098984	-1.417717	-4.503697
H	2.812502	0.220175	-4.514226
H	7.503935	3.058525	0.603759
H	6.116440	2.561194	-0.375476
H	5.865800	3.222774	1.251483
H	7.012903	1.223233	2.240584
H	7.275616	0.567733	0.617180
H	1.425952	2.835940	-2.153501
H	0.307675	4.168428	-1.728073
H	1.924246	4.081918	-0.981715
H	-2.873486	3.717963	1.477277
H	-1.097101	3.925724	1.554563
H	-2.137656	5.288546	1.067827
H	-5.466562	3.411932	-1.762779
H	-3.780210	3.979076	-1.889230
H	-4.327899	2.568232	-2.841951

$\omega$ B97X Energy = -2096.10556265 a.u.

(*a*S,1S,3S,1'S,3'S)-22, Conf L

C	-0.667219	0.267990	2.026279
C	-1.962860	0.113886	2.530525
C	-3.042122	0.485183	1.733785
C	-2.830448	0.995719	0.451444
C	-1.539900	1.141421	-0.043211
C	-0.445826	0.778266	0.753021
O	-3.686780	2.180776	-1.494756
C	-2.604016	1.657007	-2.262926
C	-1.331562	1.696761	-1.432543
C	-4.040112	1.368108	-0.381285
C	-2.504406	2.483750	-3.524759
C	-4.862499	0.164703	-0.825427
C	0.957482	0.932281	0.265956
C	1.684367	-0.172478	-0.171697
C	3.003171	0.012750	-0.585970
C	3.572658	1.279078	-0.612656
C	2.823963	2.393949	-0.219254
C	1.528032	2.201579	0.240810
C	-6.215563	0.348342	-1.100490
C	-7.006702	-0.697924	-1.548201
C	-6.416554	-1.934849	-1.719912
C	-5.081510	-2.160735	-1.460766
C	-4.309240	-1.098469	-1.008178
C	1.072855	-1.550676	-0.216236
C	1.857304	-2.474359	-1.131336
O	3.241583	-2.411151	-0.778767
C	3.828612	-1.159640	-1.073976

C	1.430568	-3.919552	-1.021018
F	-7.180447	-2.965190	-2.153662
O	4.845628	1.390174	-1.110447
C	5.829334	1.964490	-0.241111
O	3.424066	3.606886	-0.335068
C	2.686380	4.753470	0.062799
C	5.195103	-1.230657	-0.394482
O	5.370312	-1.061895	0.786722
O	6.147194	-1.567303	-1.258235
C	7.644655	-3.143505	-0.146893
C	7.481998	-1.759368	-0.733022
O	0.400145	-0.105217	2.804572
C	0.784842	0.879644	3.765248
O	-2.178424	-0.309794	3.814631
C	-1.838769	-1.676319	4.071952
C	-4.840879	-0.828255	2.599550
O	-4.332783	0.439585	2.182416
H	-2.830087	0.615878	-2.529684
H	-0.542611	1.138499	-1.943821
H	-0.984720	2.734085	-1.362597
H	-4.690679	2.002080	0.223362
H	-1.676372	2.131937	-4.143076
H	-3.425772	2.411026	-4.104210
H	-2.329448	3.533068	-3.276210
H	0.934875	3.046044	0.568447
H	-6.662122	1.326912	-0.957617
H	-8.061237	-0.565425	-1.756388
H	-4.659007	-3.147341	-1.605668
H	-3.260725	-1.268637	-0.787991
H	1.044400	-1.980623	0.791342
H	0.038297	-1.487395	-0.565033
H	1.751743	-2.132672	-2.171029
H	3.987532	-1.069641	-2.155991
H	2.006419	-4.545224	-1.703931
H	0.371839	-4.018690	-1.266897
H	1.584022	-4.280388	-0.001557
H	5.818695	1.457564	0.726789
H	6.790065	1.799910	-0.726255
H	5.657285	3.031139	-0.106977
H	3.339557	5.604749	-0.111968
H	1.776695	4.864472	-0.533464
H	2.425618	4.706451	1.123530
H	8.676835	-3.279302	0.180539
H	6.990147	-3.284120	0.713908
H	7.418478	-3.906639	-0.893018
H	8.131555	-1.610088	-1.593281
H	7.681019	-0.982852	0.006090
H	-0.037076	1.090201	4.454071
H	1.627970	0.466398	4.315172
H	1.094068	1.801059	3.262789
H	-2.424248	-2.341274	3.430253
H	-0.774664	-1.849985	3.910262
H	-2.091041	-1.863530	5.113824
H	-5.925686	-0.736585	2.597425
H	-4.545680	-1.610573	1.894610
H	-4.496258	-1.079819	3.602569

$\omega$ B97X Energy = -2096.10550950 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf M

C	0.725114	-1.600576	1.417427
C	2.040999	-1.827822	1.824521
C	3.083143	-1.527151	0.953614
C	2.822603	-0.977584	-0.299844
C	1.508447	-0.756580	-0.701933
C	0.450892	-1.084110	0.155516
O	3.570593	-0.500241	-2.557712
C	2.476715	0.403311	-2.716614
C	1.232938	-0.190794	-2.075329
C	3.987012	-0.632081	-1.203723
C	2.304038	0.652983	-4.197540
C	4.773198	0.598461	-0.763392
C	-0.969126	-0.875168	-0.258328
C	-1.654780	0.283926	0.095301
C	-2.983431	0.428418	-0.305283
C	-3.603488	-0.540191	-1.084163
C	-2.896082	-1.682369	-1.477996
C	-1.590097	-1.847274	-1.036550
C	4.295262	1.517766	0.162512
C	5.035046	2.645010	0.499487
C	6.258074	2.831113	-0.107422
C	6.770335	1.941027	-1.031818
C	6.015745	0.824674	-1.352732
C	-0.985441	1.386793	0.876153
C	-1.717103	2.705117	0.699391
O	-3.103945	2.504740	0.982576
C	-3.756680	1.685408	0.031756
C	-1.219657	3.787223	1.629108
F	6.988465	3.924595	0.216344
O	-4.880583	-0.284917	-1.514606
C	-5.879721	-1.250522	-1.165415
O	-3.540324	-2.551837	-2.298766
C	-2.837260	-3.710949	-2.722000
C	-5.106546	1.398870	0.688881
O	-5.296051	0.530419	1.503535
O	-6.013414	2.296071	0.316252
C	-8.223731	1.237688	0.357503
C	-7.301019	2.262479	0.976229
O	-0.298973	-1.836648	2.296636
C	-0.659436	-3.213038	2.415018
O	2.286677	-2.358040	3.063379
C	2.685743	-1.382938	4.029653
C	4.791572	-3.073215	1.461642
O	4.387457	-1.706149	1.336552
H	2.725943	1.347944	-2.214828
H	0.452790	0.573359	-2.017709
H	0.842120	-0.985428	-2.721197
H	4.679626	-1.476274	-1.211147
H	1.460242	1.323337	-4.371716
H	3.201491	1.108547	-4.618260
H	2.111987	-0.288053	-4.718230
H	-1.026288	-2.727279	-1.319429

H	3.333170	1.360327	0.637837
H	4.671577	3.366621	1.220677
H	7.738532	2.122310	-1.482026
H	6.399856	0.114421	-2.077509
H	-0.956566	1.133116	1.941964
H	0.051616	1.500122	0.548406
H	-1.622500	3.036931	-0.344631
H	-3.938117	2.256322	-0.887769
H	-1.755977	4.721269	1.457776
H	-0.155218	3.962890	1.463724
H	-1.363660	3.485735	2.668975
H	-5.702514	-2.197993	-1.671128
H	-5.895872	-1.398582	-0.082452
H	-6.829041	-0.827844	-1.489248
H	-2.557716	-4.337072	-1.870425
H	-3.522274	-4.259243	-3.363829
H	-1.941867	-3.443876	-3.289850
H	-9.210310	1.320310	0.816855
H	-8.330519	1.410347	-0.714877
H	-7.853330	0.225570	0.520519
H	-7.141900	2.069979	2.037478
H	-7.688167	3.271800	0.850274
H	-1.025454	-3.595153	1.456938
H	0.191998	-3.808268	2.752404
H	-1.456908	-3.264494	3.153617
H	2.845376	-1.915596	4.964960
H	3.613132	-0.893449	3.722097
H	1.898355	-0.636306	4.164040
H	5.848784	-3.058960	1.718211
H	4.225498	-3.576662	2.246754
H	4.654738	-3.596709	0.511104

ωB97X Energy = -2096.10549169 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf N

C	-0.824233	-1.818030	-1.156068
C	-2.161456	-2.084972	-1.467392
C	-3.159754	-1.561671	-0.648910
C	-2.829550	-0.849992	0.504435
C	-1.496942	-0.625781	0.830617
C	-0.485588	-1.108541	-0.009404
O	-3.482757	0.009254	2.682280
C	-2.346871	0.873286	2.668584
C	-1.151804	0.131656	2.091261
C	-3.950451	-0.332342	1.382067
C	-2.112413	1.335954	4.088741
C	-4.731499	0.821117	0.766128
C	0.954610	-0.876606	0.313087
C	1.677522	0.126198	-0.328750
C	3.015898	0.314863	0.019285
C	3.608757	-0.462295	1.002123
C	2.885993	-1.475668	1.638790
C	1.557385	-1.669653	1.287175
C	-6.050545	1.017152	1.168819
C	-6.801326	2.075737	0.683013
C	-6.205108	2.940310	-0.214067

C	-4.903139	2.783862	-0.639915
C	-4.171364	1.712735	-0.143049
C	1.043521	1.012154	-1.371833
C	1.859425	2.271913	-1.605895
O	3.228466	1.910663	-1.811660
C	3.835461	1.407571	-0.641486
C	1.409624	3.049518	-2.820669
F	-6.929247	3.976762	-0.697666
O	4.935843	-0.259525	1.291550
C	5.178623	0.394383	2.539051
O	3.556581	-2.204667	2.565761
C	2.847634	-3.241441	3.229299
C	5.203931	0.899844	-1.094877
O	5.365328	-0.073112	-1.787521
O	6.181817	1.697248	-0.680026
C	8.468744	2.313245	-0.424286
C	7.527685	1.292625	-1.012435
O	0.162352	-2.230532	-2.013463
C	0.561986	-3.588933	-1.847064
O	-2.442377	-2.807044	-2.595596
C	-3.106717	-4.053923	-2.371472
C	-4.988457	-1.213511	-2.124328
O	-4.488300	-1.779792	-0.909092
H	-2.573294	1.743935	2.039029
H	-0.343937	0.841009	1.892169
H	-0.772319	-0.570597	2.842269
H	-4.654885	-1.148412	1.551361
H	-1.237266	1.986996	4.133693
H	-2.975958	1.889208	4.460328
H	-1.939464	0.477454	4.741854
H	0.970867	-2.443548	1.766430
H	-6.501895	0.326849	1.873958
H	-7.829709	2.231229	0.985005
H	-4.476306	3.482676	-1.348724
H	-3.150811	1.571401	-0.483070
H	0.948792	0.463111	-2.315377
H	0.031431	1.288229	-1.062435
H	1.805943	2.912154	-0.713503
H	3.995111	2.225145	0.073773
H	2.000509	3.958518	-2.938732
H	0.359411	3.328616	-2.718283
H	1.519262	2.439719	-3.720131
H	4.832447	-0.221715	3.370948
H	6.255207	0.537448	2.610209
H	4.679467	1.367494	2.565562
H	3.554508	-3.693099	3.920735
H	1.996434	-2.842663	3.787771
H	2.498868	-3.996624	2.519775
H	9.498356	2.028345	-0.645290
H	8.287329	3.301291	-0.849401
H	8.352601	2.369609	0.659082
H	7.694624	0.296824	-0.596940
H	7.617019	1.231735	-2.098172
H	-0.267467	-4.270188	-2.053013
H	1.361641	-3.769534	-2.562695
H	0.935979	-3.758210	-0.832713

H	-2.521493	-4.682293	-1.693942
H	-4.103436	-3.903147	-1.953323
H	-3.181552	-4.539000	-3.342364
H	-4.531259	-1.682397	-2.997184
H	-6.061007	-1.396498	-2.125211
H	-4.803649	-0.136471	-2.145765

ωB97X Energy = -2096.10547817 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf O

C	-0.478533	1.446999	-1.358135
C	-1.758209	1.941054	-1.633120
C	-2.848691	1.083513	-1.519145
C	-2.665497	-0.243220	-1.123719
C	-1.391820	-0.722735	-0.842998
C	-0.285923	0.127945	-0.967436
O	-3.532977	-2.510532	-0.935575
C	-2.521778	-2.790026	0.031965
C	-1.212697	-2.159512	-0.413338
C	-3.886264	-1.133570	-1.009227
C	-2.427767	-4.292801	0.168370
C	-4.814023	-0.748515	0.135833
C	1.100457	-0.360700	-0.702782
C	1.742908	-0.069537	0.498415
C	3.039583	-0.544598	0.698041
C	3.666407	-1.318482	-0.266265
C	3.024138	-1.605384	-1.474381
C	1.738645	-1.122800	-1.678480
C	-6.166387	-1.064992	0.030721
C	-7.054277	-0.777831	1.055453
C	-6.561722	-0.170218	2.193718
C	-5.231064	0.159317	2.340489
C	-4.360754	-0.132746	1.297913
C	1.063997	0.728856	1.582587
C	1.749999	0.538168	2.924266
O	3.155322	0.751150	2.763290
C	3.777436	-0.254905	1.990578
C	1.263899	1.505883	3.977740
F	-7.420005	0.118030	3.200402
O	4.955482	-1.732304	-0.037835
C	5.094165	-3.129999	0.229575
O	3.726709	-2.341600	-2.371880
C	3.105537	-2.635188	-3.615045
C	5.208189	0.245760	1.793182
O	6.135673	-0.118893	2.473485
O	5.289663	1.173667	0.850061
C	6.440954	2.779876	-0.477022
C	6.593159	1.747141	0.610961
O	0.599911	2.289632	-1.464842
C	1.071919	2.456685	-2.802869
O	-1.942489	3.217057	-2.093992
C	-1.663891	4.254095	-1.147502
C	-4.682996	2.563166	-1.133112
O	-4.117677	1.467393	-1.853954
H	-2.823780	-2.357610	0.995217
H	-0.482758	-2.218237	0.398604

H	-0.802116	-2.742081	-1.245866
H	-4.458353	-1.048633	-1.934626
H	-1.646173	-4.558939	0.882444
H	-3.373608	-4.707369	0.519723
H	-2.184711	-4.744860	-0.795973
H	1.215976	-1.329227	-2.604046
H	-6.535606	-1.540090	-0.872272
H	-8.108812	-1.011985	0.977493
H	-4.887249	0.639115	3.248525
H	-3.314535	0.136613	1.396715
H	1.072381	1.793604	1.322617
H	0.015221	0.430281	1.665743
H	1.597686	-0.494881	3.268461
H	3.859430	-1.177622	2.580212
H	1.767975	1.327992	4.928358
H	0.189253	1.387528	4.127161
H	1.458857	2.533827	3.664125
H	4.782269	-3.720054	-0.633907
H	6.149075	-3.303199	0.432313
H	4.503112	-3.412402	1.105816
H	3.825540	-3.222227	-4.179599
H	2.192166	-3.218981	-3.472527
H	2.872207	-1.718951	-4.164156
H	7.410226	3.236511	-0.682279
H	6.072777	2.324085	-1.397137
H	5.748355	3.565453	-0.172065
H	6.956368	2.185600	1.541903
H	7.273478	0.944587	0.320062
H	1.434251	1.504069	-3.200938
H	0.281457	2.851066	-3.446103
H	1.895121	3.166927	-2.757374
H	-2.292546	4.138565	-0.259652
H	-0.612667	4.245357	-0.858044
H	-1.904827	5.192937	-1.642207
H	-4.290948	3.514589	-1.492488
H	-5.756717	2.520133	-1.307427
H	-4.489259	2.457465	-0.061902

ωB97X Energy = -2096.10547627 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf P

C	0.470727	1.777679	-0.832587
C	1.740353	2.253510	-1.175705
C	2.848083	1.776929	-0.478498
C	2.686375	0.896048	0.591324
C	1.416892	0.457915	0.950777
C	0.299718	0.898305	0.230203
O	3.583012	-0.125655	2.608695
C	2.566176	-1.124615	2.538225
C	1.252808	-0.483306	2.120659
C	3.918439	0.436863	1.344677
C	2.483041	-1.783076	3.896801
C	4.807471	-0.507065	0.546799
C	-1.078256	0.450990	0.594199
C	-1.714420	-0.563773	-0.116352
C	-3.007495	-0.934993	0.253312

C	-3.637831	-0.337149	1.336742
C	-2.982223	0.655643	2.072625
C	-1.711789	1.052549	1.677756
C	6.172153	-0.529238	0.824230
C	7.026359	-1.397339	0.162714
C	6.487433	-2.249817	-0.780820
C	5.142773	-2.261942	-1.086298
C	4.306965	-1.378602	-0.415446
C	-1.032542	-1.260678	-1.267015
C	-1.704301	-2.582500	-1.594941
O	-3.113561	-2.371110	-1.717049
C	-3.725181	-2.048287	-0.484234
C	-1.222730	-3.182123	-2.895466
F	7.312125	-3.100945	-1.434877
O	-4.876470	-0.810440	1.681466
C	-5.943084	0.140983	1.758769
O	-3.642490	1.154278	3.149630
C	-2.995034	2.156812	3.919240
C	-5.173182	-1.736140	-0.857768
O	-6.066680	-2.542299	-0.773540
O	-5.314675	-0.515003	-1.358532
C	-6.559467	1.269454	-2.325415
C	-6.630169	-0.154647	-1.835906
O	-0.615776	2.160369	-1.575782
C	-1.151243	3.433773	-1.222748
O	1.849185	3.131885	-2.219413
C	2.379858	4.418600	-1.890027
C	4.610689	1.834655	-2.066528
O	4.116956	2.204745	-0.775407
H	2.858199	-1.874663	1.791722
H	0.528145	-1.263793	1.873381
H	0.838144	0.066811	2.973057
H	4.515213	1.317226	1.589109
H	1.699072	-2.542615	3.900100
H	3.429998	-2.260824	4.151532
H	2.248287	-1.039807	4.662212
H	-1.186715	1.825094	2.225492
H	6.577251	0.149564	1.567612
H	8.089994	-1.415624	0.366038
H	4.762781	-2.943958	-1.836859
H	3.250303	-1.365930	-0.661232
H	-1.050616	-0.617026	-2.153931
H	0.019255	-1.438513	-1.025525
H	-1.535490	-3.292142	-0.772220
H	-3.766215	-2.940492	0.154139
H	-1.711972	-4.138257	-3.084823
H	-0.144267	-3.345272	-2.855872
H	-1.440492	-2.505427	-3.724708
H	-5.875523	0.858413	0.936315
H	-6.865856	-0.430713	1.668563
H	-5.923872	0.673124	2.708308
H	-3.687703	2.416388	4.715891
H	-2.064979	1.780386	4.353826
H	-2.785233	3.044842	3.316911
H	-7.536985	1.572570	-2.703110
H	-6.278582	1.946381	-1.516721

H	-5.832499	1.367340	-3.132623
H	-6.910164	-0.848167	-2.630478
H	-7.341481	-0.269589	-1.015675
H	-1.470228	3.439469	-0.175895
H	-0.417446	4.226562	-1.388750
H	-2.013533	3.600444	-1.865324
H	2.258084	5.034555	-2.778557
H	1.822653	4.861655	-1.059700
H	3.435976	4.356955	-1.622843
H	5.626514	2.220036	-2.125577
H	4.627691	0.746514	-2.168638
H	4.002971	2.270323	-2.861580

$\omega_{B97X}$  Energy = -2096.10545556 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf Q

C	0.485793	2.007983	-0.139248
C	1.765745	2.551343	-0.287813
C	2.859869	1.836176	0.193735
C	2.674600	0.634662	0.877979
C	1.395056	0.120949	1.056844
C	0.291441	0.809875	0.538258
O	3.538462	-1.053592	2.399605
C	2.504296	-1.943974	1.982839
C	1.205351	-1.172380	1.814444
C	3.892663	-0.091403	1.411832
C	2.398593	-3.034557	3.024990
C	4.755200	-0.719824	0.325523
C	-1.095076	0.279515	0.705490
C	-1.735440	-0.383446	-0.338931
C	-3.028424	-0.866953	-0.134238
C	-3.654346	-0.715927	1.093264
C	-3.015423	-0.042538	2.138417
C	-1.732998	0.447218	1.932494
C	6.114936	-0.893453	0.571975
C	6.942826	-1.501302	-0.358776
C	6.382426	-1.938573	-1.542902
C	5.041812	-1.787306	-1.827927
C	4.232702	-1.169954	-0.882898
C	-1.059615	-0.596046	-1.670307
C	-1.739871	-1.693554	-2.470311
O	-3.148058	-1.442478	-2.502243
C	-3.760031	-1.603495	-1.239433
C	-1.262399	-1.763996	-3.902001
F	7.181178	-2.532293	-2.460338
O	-4.939327	-1.178041	1.236413
C	-5.064033	-2.350239	2.045306
O	-3.718077	0.086261	3.292055
C	-3.094107	0.762375	4.374137
C	-5.201877	-1.142187	-1.450526
O	-6.116607	-1.903860	-1.649007
O	-5.309516	0.178774	-1.466611
C	-6.506545	2.224459	-1.691568
C	-6.628031	0.721711	-1.694229
O	-0.587067	2.650891	-0.700283
C	-1.109964	3.718946	0.086320

O	1.897547	3.742299	-0.948553
C	2.447651	4.815576	-0.179678
C	4.635485	2.418773	-1.269500
O	4.138127	2.317291	0.068551
H	2.788652	-2.391054	1.021415
H	0.472247	-1.801555	1.302392
H	0.789788	-0.953898	2.804701
H	4.513840	0.629620	1.945532
H	1.602557	-3.733154	2.760640
H	3.335731	-3.587965	3.098956
H	2.170209	-2.601388	4.001582
H	-1.212060	0.969643	2.725148
H	6.537793	-0.542149	1.507489
H	8.002379	-1.633980	-0.178115
H	4.643573	-2.141124	-2.770857
H	3.179789	-1.030287	-1.103848
H	-1.077962	0.335253	-2.247546
H	-0.008002	-0.854941	-1.518092
H	-1.576671	-2.661510	-1.974822
H	-3.820037	-2.671559	-0.991233
H	-1.760872	-2.574087	-4.435642
H	-0.185615	-1.940124	-3.930237
H	-1.472349	-0.823056	-4.415370
H	-6.117391	-2.622903	2.034551
H	-4.471144	-3.168908	1.627104
H	-4.745801	-2.147738	3.069407
H	-3.814047	0.751825	5.188590
H	-2.181681	0.248162	4.687985
H	-2.859483	1.797290	4.110627
H	-7.489015	2.668879	-1.857165
H	-6.124290	2.582121	-0.734489
H	-5.838155	2.561754	-2.484882
H	-7.000344	0.342894	-2.647563
H	-7.287600	0.364342	-0.901145
H	-0.364335	4.506394	0.222976
H	-1.962975	4.120527	-0.457096
H	-1.440903	3.350327	1.062165
H	1.898000	4.935542	0.758255
H	3.503010	4.647161	0.040469
H	2.334285	5.713352	-0.783752
H	4.630571	1.437493	-1.750932
H	4.044535	3.122023	-1.859002
H	5.659708	2.776317	-1.185948

ωB97X Energy = -2096.10540626 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf R

C	0.487770	1.889589	-0.725761
C	1.767285	2.365832	-1.028746
C	2.865216	1.850124	-0.346462
C	2.692180	0.909845	0.667878
C	1.412098	0.481112	1.003567
C	0.303325	0.970003	0.303513
O	3.567009	-0.231974	2.629993
C	2.528523	-1.202936	2.506690
C	1.228980	-0.511032	2.127566

C	3.913877	0.392429	1.398400
C	2.433117	-1.932904	3.827436
C	4.786610	-0.521956	0.549076
C	-1.080028	0.525671	0.650087
C	-1.690404	-0.523501	-0.032737
C	-2.987587	-0.893783	0.324210
C	-3.648077	-0.258297	1.366847
C	-3.018702	0.770236	2.076044
C	-1.743507	1.163815	1.693743
C	4.271160	-1.317768	-0.469286
C	5.089724	-2.173157	-1.195153
C	6.433175	-2.210336	-0.886356
C	6.986628	-1.434756	0.113365
C	6.149203	-0.593124	0.828677
C	-0.978330	-1.266989	-1.135727
C	-1.619221	-2.619122	-1.395349
O	-3.027423	-2.439127	-1.566483
C	-3.678427	-2.048280	-0.374067
C	-1.094905	-3.292305	-2.642206
F	7.242033	-3.033673	-1.593722
O	-4.890271	-0.729807	1.701863
C	-5.967085	0.213081	1.709630
O	-3.708610	1.304382	3.116731
C	-3.090462	2.345924	3.858382
C	-5.114221	-1.761625	-0.810525
O	-6.007168	-2.567393	-0.717498
O	-5.243198	-0.566220	-1.372922
C	-6.455113	1.159971	-2.476552
C	-6.543218	-0.234202	-1.909707
O	-0.620222	2.368293	-1.366635
C	-0.637073	2.290174	-2.794180
O	1.957183	3.332102	-1.982678
C	1.579168	4.641964	-1.552923
C	4.665514	2.045151	-1.880305
O	4.126744	2.326766	-0.585321
H	2.803246	-1.917096	1.719219
H	0.485016	-1.261924	1.848179
H	0.830938	0.008467	3.006781
H	4.525955	1.247399	1.690405
H	1.635952	-2.677711	3.790589
H	3.371761	-2.440036	4.054690
H	2.211931	-1.228063	4.632270
H	-1.238353	1.964446	2.219063
H	3.215990	-1.264791	-0.715717
H	4.697752	-2.795482	-1.990137
H	8.048709	-1.490582	0.317932
H	6.566366	0.025989	1.616171
H	-1.001283	-0.681893	-2.062727
H	0.074664	-1.406878	-0.875993
H	-1.459601	-3.270922	-0.524348
H	-3.739027	-2.902822	0.312242
H	-1.568655	-4.264291	-2.784240
H	-0.016395	-3.439827	-2.562782
H	-1.296676	-2.672381	-3.518614
H	-6.882073	-0.371026	1.619351
H	-5.978117	0.785302	2.635770

H	-5.883665	0.895783	0.859527
H	-3.803797	2.628889	4.628362
H	-2.165947	1.999709	4.328239
H	-2.877884	3.210857	3.224470
H	-7.421004	1.442363	-2.897662
H	-6.194467	1.881096	-1.700053
H	-5.706181	1.210932	-3.267845
H	-6.800114	-0.971166	-2.672255
H	-7.278937	-0.302886	-1.105987
H	-0.138124	1.380244	-3.137113
H	-1.685731	2.259353	-3.085308
H	-0.152561	3.156350	-3.245971
H	0.507793	4.687904	-1.339958
H	2.143929	4.928092	-0.661824
H	1.819516	5.319296	-2.369951
H	5.658403	2.490121	-1.900230
H	4.749350	0.964946	-2.029020
H	4.047539	2.486021	-2.662835

$\omega$ B97X Energy = -2096.10540617 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf S

C	0.841286	1.924546	-1.080549
C	2.186367	2.185637	-1.361674
C	3.171543	1.630613	-0.550343
C	2.826797	0.871089	0.566463
C	1.486444	0.659159	0.872468
C	0.487765	1.183453	0.044132
O	3.445636	-0.083036	2.716334
C	2.295999	-0.925753	2.652368
C	1.118913	-0.136345	2.102811
C	3.932492	0.313555	1.438529
C	2.043286	-1.453621	4.046420
C	4.719282	-0.813748	0.783154
C	-0.956578	0.955081	0.349972
C	-1.652537	-0.097583	-0.240008
C	-2.996721	-0.280372	0.088490
C	-3.622496	0.553747	1.001276
C	-2.926318	1.616103	1.585888
C	-1.591513	1.802902	1.254165
C	6.039965	-1.018053	1.176051
C	6.795053	-2.054301	0.649969
C	6.201269	-2.888422	-0.276914
C	4.897576	-2.723040	-0.694333
C	4.162068	-1.674146	-0.157587
C	-0.985194	-1.051362	-1.199877
C	-1.771265	-2.344250	-1.333278
O	-3.139252	-2.029752	-1.607490
C	-3.790365	-1.426138	-0.510024
C	-1.276032	-3.223848	-2.457409
F	6.929526	-3.902695	-0.799792
O	-4.954291	0.352360	1.269576
C	-5.224076	-0.199732	2.560194
O	-3.628185	2.396657	2.445273
C	-2.946911	3.480448	3.060980
C	-5.135781	-0.960722	-1.066642

O	-5.265442	-0.036685	-1.829593
O	-6.129381	-1.740506	-0.656471
C	-8.424506	-2.354334	-0.479281
C	-7.453764	-1.393004	-1.116852
O	-0.161551	2.450332	-1.845575
C	-0.125268	2.181400	-3.249538
O	2.549212	2.978774	-2.419456
C	2.342299	4.373875	-2.185413
C	5.043670	1.375929	-1.985715
O	4.496660	1.896682	-0.770658
H	2.511887	-1.768249	1.981867
H	0.296031	-0.819844	1.876348
H	0.752651	0.546824	2.877750
H	4.636628	1.118815	1.654200
H	1.155836	-2.089346	4.054344
H	2.893925	-2.040858	4.394908
H	1.882170	-0.625515	4.740524
H	-1.025415	2.614983	1.692660
H	6.489768	-0.351423	1.904593
H	7.824971	-2.215348	0.943703
H	4.472785	-3.397584	-1.427461
H	3.141052	-1.523821	-0.492016
H	-0.894371	-0.589145	-2.189820
H	0.030005	-1.275934	-0.861110
H	-1.728816	-2.894716	-0.382407
H	-3.983411	-2.179119	0.265207
H	-1.848343	-4.151046	-2.503479
H	-0.224333	-3.471703	-2.303372
H	-1.373033	-2.703805	-3.413006
H	-4.904979	0.486575	3.346525
H	-6.300869	-0.347841	2.615359
H	-4.717796	-1.162203	2.679118
H	-3.675301	3.964267	3.706869
H	-2.105224	3.127015	3.662671
H	-2.589519	4.196063	2.315864
H	-9.437467	-2.119906	-0.809576
H	-8.199736	-3.383004	-0.764190
H	-8.390895	-2.275016	0.608317
H	-7.655255	-0.359004	-0.830979
H	-7.470258	-1.457497	-2.206138
H	0.243272	1.169936	-3.438622
H	-1.151730	2.264627	-3.602409
H	0.507150	2.896769	-3.776047
H	2.688860	4.893188	-3.076615
H	1.282570	4.587792	-2.023257
H	2.921511	4.704550	-1.319394
H	6.104063	1.620269	-1.971128
H	4.923256	0.289533	-2.020879
H	4.568861	1.833799	-2.853677

$\omega$ B97X Energy = -2096.10539029 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf T

C	0.685330	-0.970280	1.838831
C	1.982070	-1.009844	2.352656
C	3.060741	-1.024607	1.475647



C	2.853494	-0.980305	0.098531
C	1.557370	-0.946198	-0.409007
C	0.463347	-0.954607	0.465884
O	3.697054	-1.351613	-2.145537
C	2.611131	-0.585407	-2.667299
C	1.341295	-0.925691	-1.904041
C	4.055530	-0.971040	-0.822605
C	2.503471	-0.894337	-4.143134
C	4.823460	0.346797	-0.836454
C	-0.939125	-0.939408	-0.048117
C	-1.685186	0.236690	-0.057682
C	-2.997526	0.195563	-0.528522
C	-3.541267	-0.981564	-1.026088
C	-2.774430	-2.151881	-1.055983
C	-1.485272	-2.120768	-0.541555
C	6.076367	0.363960	-1.446699
C	6.817161	1.531083	-1.533290
C	6.280324	2.685892	-0.997252
C	5.046644	2.712929	-0.384346
C	4.320980	1.529836	-0.309018
C	-1.101278	1.542094	0.421290
C	-1.899695	2.728903	-0.088684
O	-3.285209	2.512433	0.190832
C	-3.840660	1.453961	-0.563640
C	-1.505495	4.031056	0.568620
F	6.997097	3.832448	-1.073979
O	-4.806355	-0.921389	-1.551844
C	-5.788800	-1.787887	-0.971189
O	-3.350457	-3.247416	-1.615160
C	-2.593170	-4.448207	-1.656588
C	-5.218950	1.247238	0.061625
O	-5.405756	0.664742	1.101003
O	-6.168206	1.847169	-0.648814
C	-7.737200	2.891815	0.902186
C	-7.516675	1.804685	-0.125061
O	-0.372832	-0.892123	2.706488
C	-0.742803	-2.144598	3.284361
O	2.185509	-1.049110	3.706846
C	2.299029	0.248530	4.294981
C	4.761403	-2.250413	2.551799
O	4.345459	-1.019188	1.953798
H	2.838062	0.480929	-2.534231
H	0.557910	-0.206790	-2.159254
H	0.980867	-1.907578	-2.231218
H	4.747938	-1.748118	-0.491795
H	1.664999	-0.350721	-4.582548
H	3.416826	-0.604847	-4.664620
H	2.338619	-1.963831	-4.293395
H	-0.877650	-3.016915	-0.539422
H	6.479633	-0.552718	-1.864074
H	7.792902	1.553133	-2.002773
H	4.663058	3.639376	0.024908
H	3.350256	1.539519	0.174437
H	-1.083861	1.562576	1.516838
H	-0.064507	1.632266	0.085007
H	-1.777718	2.809731	-1.178406

H	-3.979742	1.772270	-1.604533
H	-2.086519	4.860315	0.163512
H	-0.446538	4.231749	0.396643
H	-1.676585	3.974979	1.645927
H	-6.744910	-1.478055	-1.389967
H	-5.591034	-2.828443	-1.223383
H	-5.808417	-1.661416	0.114020
H	-3.229248	-5.186154	-2.138965
H	-1.678514	-4.318511	-2.241381
H	-2.338910	-4.789855	-0.649627
H	-8.777195	2.871925	1.232568
H	-7.098060	2.744402	1.773299
H	-7.532615	3.873880	0.473377
H	-8.147828	1.946761	-1.000126
H	-7.697523	0.813583	0.291742
H	-1.070054	-2.841371	2.506565
H	0.093089	-2.574331	3.841071
H	-1.569777	-1.943873	3.962532
H	2.465352	0.097245	5.359642
H	3.145636	0.790051	3.864521
H	1.377505	0.816946	4.144563
H	4.146310	-2.487776	3.421083
H	4.705225	-3.064305	1.822948
H	5.795808	-2.110025	2.858502

ωB97X Energy = -2096.10537681 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf U

C	0.754385	1.822740	-1.107165
C	2.083193	2.139942	-1.407379
C	3.095639	1.629593	-0.598145
C	2.785512	0.878882	0.535997
C	1.459901	0.603282	0.851446
C	0.435628	1.074427	0.020424
O	3.460182	-0.022834	2.690606
C	2.353396	-0.922613	2.643674
C	1.136434	-0.199409	2.089778
C	3.920780	0.376580	1.404284
C	2.133005	-1.444309	4.045448
C	4.748475	-0.726838	0.758625
C	-0.996865	0.785103	0.330464
C	-1.682658	-0.223324	-0.342736
C	-3.014511	-0.468145	-0.006380
C	-3.636873	0.255582	0.998810
C	-2.952659	1.276632	1.665242
C	-1.630646	1.527712	1.324214
C	6.074959	-0.877832	1.156036
C	6.868629	-1.891498	0.643336
C	6.307707	-2.757299	-0.275115
C	4.999840	-2.644327	-0.696828
C	4.224748	-1.617495	-0.172979
C	-1.014754	-1.059429	-1.405394
C	-1.781615	-2.344619	-1.665495
O	-3.161897	-2.031013	-1.873776
C	-3.796782	-1.564966	-0.702110
C	-1.296775	-3.083573	-2.890918

F	7.073714	-3.750227	-0.784862
O	-4.956441	-0.005748	1.274562
C	-5.186559	-0.671147	2.518147
O	-3.651359	1.957125	2.608619
C	-2.982965	3.003398	3.298765
C	-5.168617	-1.080844	-1.173565
O	-5.344121	-0.068700	-1.803474
O	-6.119401	-1.956729	-0.862642
C	-8.109314	-0.745004	-0.160458
C	-7.477827	-1.616213	-1.222786
O	-0.242186	2.223857	-1.958531
C	-0.691185	3.561682	-1.756328
O	2.344299	2.895778	-2.518062
C	2.966940	4.158400	-2.265058
C	4.940206	1.377346	-2.074224
O	4.417241	1.896827	-0.847811
H	2.608490	-1.762142	1.983544
H	0.349058	-0.925378	1.869751
H	0.738189	0.469339	2.861315
H	4.592782	1.212987	1.603442
H	1.283114	-2.129199	4.063729
H	3.015927	-1.977997	4.399766
H	1.926402	-0.617415	4.728865
H	-1.073913	2.308755	1.826832
H	6.498032	-0.187060	1.878085
H	7.902919	-2.011900	0.941190
H	4.601639	-3.342186	-1.423032
H	3.199012	-1.509490	-0.509698
H	-0.942343	-0.487352	-2.337190
H	0.007495	-1.302115	-1.101647
H	-1.708802	-2.997665	-0.783831
H	-3.950140	-2.400189	-0.006280
H	-1.852134	-4.012079	-3.028290
H	-0.237281	-3.324592	-2.787444
H	-1.424944	-2.462589	-3.780219
H	-4.865676	-0.048222	3.354809
H	-6.259084	-0.846564	2.580661
H	-4.658383	-1.628852	2.543584
H	-3.707981	3.412493	3.997878
H	-2.119307	2.623272	3.851073
H	-2.660106	3.787069	2.608157
H	-9.141773	-0.523872	-0.436713
H	-8.115033	-1.256523	0.803672
H	-7.567592	0.195665	-0.054707
H	-7.470634	-1.124931	-2.195465
H	-7.983977	-2.575811	-1.309380
H	0.115535	4.277688	-1.932923
H	-1.489785	3.735479	-2.474819
H	-1.080676	3.687817	-0.741501
H	2.357181	4.755540	-1.580974
H	3.964799	4.031321	-1.841752
H	3.033771	4.663597	-3.226225
H	4.483383	1.863882	-2.937561
H	6.009118	1.579969	-2.057797
H	4.776123	0.298265	-2.130844

ωB97X Energy = -2096.10531262 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf V

C	0.499114	2.060756	0.081266
C	1.787740	2.596716	-0.006858
C	2.872754	1.833806	0.415294
C	2.678171	0.573338	0.976931
C	1.389011	0.068833	1.116679
C	0.293518	0.812037	0.663124
O	3.522136	-1.263338	2.330110
C	2.467770	-2.089435	1.838433
C	1.182494	-1.281299	1.762380
C	3.886652	-0.213310	1.440332
C	2.354343	-3.276740	2.767945
C	4.742859	-0.741378	0.297125
C	-1.097827	0.283819	0.793364
C	-1.715149	-0.372194	-0.269205
C	-3.013775	-0.854108	-0.097591
C	-3.668325	-0.707044	1.115094
C	-3.051552	-0.042107	2.178966
C	-1.763564	0.445800	2.005700
C	4.214806	-1.063730	-0.949168
C	5.017362	-1.589455	-1.953259
C	6.357231	-1.778738	-1.687985
C	6.922950	-1.468147	-0.466981
C	6.101329	-0.950097	0.522024
C	-1.008720	-0.589228	-1.584397
C	-1.666068	-1.696221	-2.390465
O	-3.071621	-1.442744	-2.466225
C	-3.721432	-1.587626	-1.220100
C	-1.146279	-1.785230	-3.806311
F	7.149962	-2.282476	-2.662728
O	-4.958149	-1.165657	1.223986
C	-5.107525	-2.342603	2.021590
O	-3.780356	0.080543	3.316786
C	-3.179254	0.744813	4.419084
C	-5.150362	-1.109521	-1.476416
O	-6.066711	-1.860336	-1.706097
O	-5.242621	0.212637	-1.492985
C	-6.409191	2.272173	-1.750603
C	-6.546224	0.770815	-1.765526
O	-0.597151	2.770440	-0.320292
C	-0.596705	3.285324	-1.654231
O	2.000346	3.858192	-0.499579
C	1.635079	4.896529	0.412524
C	4.687111	2.573274	-0.922514
O	4.143042	2.344756	0.380701
H	2.733653	-2.443067	0.833467
H	0.427493	-1.849472	1.212139
H	0.788144	-1.140105	2.775275
H	4.515291	0.445607	2.041425
H	1.543532	-3.933029	2.446148
H	3.282687	-3.849531	2.774045
H	2.144561	-2.940301	3.785934
H	-1.259832	0.963438	2.812281
H	3.162855	-0.893286	-1.152290

H	4.615196	-1.841975	-2.926592	C	6.184929	-0.285744	-1.259782
H	7.981667	-1.626486	-0.302864	C	-1.012602	1.650289	0.112121
H	6.528342	-0.699000	1.487426	C	-1.754745	2.726311	-0.659822
H	-1.022029	0.333254	-2.176717	O	-3.143232	2.660859	-0.325645
H	0.041626	-0.838421	-1.409790	C	-3.775369	1.485573	-0.795286
H	-1.517903	-2.657629	-1.877912	C	-1.280412	4.123375	-0.333940
H	-3.802201	-2.653232	-0.967540	F	7.255762	3.126017	-1.742559
H	-1.630956	-2.600566	-4.344530	O	-4.872695	-0.995759	-1.228053
H	-0.069645	-1.964452	-3.799672	C	-5.868951	-1.692068	-0.469665
H	-1.338366	-0.850212	-4.337309	O	-3.509346	-3.348984	-0.836901
H	-6.158431	-2.619995	1.969612	C	-2.795661	-4.563723	-0.657937
H	-4.495485	-3.156469	1.621974	C	-5.139197	1.528859	-0.106805
H	-4.828892	-2.144390	3.057944	O	-5.341987	1.162227	1.023813
H	-3.917575	0.728708	5.216813	O	-6.042757	2.116099	-0.884467
H	-2.275678	0.224980	4.748745	C	-8.242096	1.166700	-0.362754
H	-2.935915	1.781337	4.170804	C	-7.346942	2.383631	-0.316610
H	-7.380578	2.727654	-1.948361	O	-0.329216	-0.329825	2.858976
H	-6.057509	2.620947	-0.778658	C	-0.727608	-1.464275	3.630683
H	-5.709762	2.606492	-2.518015	O	2.278029	-0.386587	3.818970
H	-6.887177	0.400612	-2.733873	C	1.988103	0.917470	4.332873
H	-7.238101	0.416719	-0.999027	C	4.928043	0.267598	2.644154
H	-0.091125	2.595501	-2.334537	O	4.368904	-0.889994	2.022076
H	-1.641828	3.380261	-1.944194	H	2.775258	-0.184120	-2.615598
H	-0.108409	4.258929	-1.705038	H	0.484625	-0.694217	-2.061798
H	2.203824	4.805260	1.341463	H	0.849554	-2.388729	-1.790401
H	1.878810	5.838596	-0.074412	H	4.629302	-2.090568	-0.190286
H	0.564554	4.862123	0.632037	H	1.516498	-1.361422	-4.426009
H	5.683676	2.982605	-0.769091	H	3.254851	-1.700539	-4.491121
H	4.762741	1.630698	-1.471753	H	2.138574	-2.910457	-3.829814
H	4.077720	3.285320	-1.479519	H	-1.007258	-3.012275	0.131665
$\omega$ B97X Energy = -2096.10529428 a.u.				H	3.308812	1.354062	-0.564953
(aS,1S,3S,1'S,3'S)-22, Conf W				H	4.760360	3.297103	-1.083210
C	0.708633	-0.585026	1.997427	H	8.047986	0.664074	-1.806433
C	2.019553	-0.562404	2.486026	H	6.594879	-1.289257	-1.308932
C	3.068475	-0.815175	1.606682	H	-0.985001	1.921988	1.173533
C	2.813231	-1.078758	0.259506	H	0.024345	1.605125	-0.232081
C	1.508665	-1.091902	-0.218650	H	-1.650739	2.538496	-1.738168
C	0.444308	-0.848848	0.659552	H	-3.936506	1.559443	-1.878304
O	3.582094	-1.935288	-1.884087	H	-1.826936	4.863074	-0.920132
C	2.508778	-1.245453	-2.522907	H	-0.216312	4.220751	-0.556326
C	1.250508	-1.374806	-1.679851	H	-1.433040	4.333619	0.726956
C	3.990339	-1.339607	-0.657593	H	-5.905669	-1.300014	0.550109
C	2.346598	-1.840497	-3.903433	H	-6.815987	-1.496396	-0.969009
C	4.848512	-0.106138	-0.910315	H	-5.672138	-2.762432	-0.453551
C	-0.971488	-0.878098	0.184797	H	-3.470217	-5.355194	-0.974802
C	-1.667796	0.302927	-0.059300	H	-1.893352	-4.585958	-1.275091
C	-2.993068	0.226004	-0.489161	H	-2.526842	-4.713815	0.391060
C	-3.598842	-1.002547	-0.719394	H	-9.244965	1.446341	-0.035068
C	-2.879869	-2.187652	-0.520732	H	-8.311774	0.776061	-1.379554
C	-1.578466	-2.109345	-0.043853	H	-7.873145	0.381060	0.296412
C	4.343125	1.188250	-0.846954	H	-7.213843	2.745591	0.703231
C	5.145643	2.286027	-1.130742	H	-7.740698	3.189644	-0.932820
C	6.462581	2.062657	-1.471619	H	-1.099551	-2.258028	2.975907
C	7.005807	0.794743	-1.542330	H	0.107247	-1.837124	4.229149
				H	-1.528637	-1.130539	4.287246
				H	2.566068	1.675952	3.796641

H	0.923884	1.139753	4.252367
H	2.287055	0.907324	5.379199
H	6.008988	0.150827	2.588063
H	4.637015	1.172896	2.103732
H	4.620794	0.341666	3.687437

$\omega$ B97X Energy = -2096.10524763 a.u.

(*aS*,1*S*,3*S*,1'*S*,3'*S*)-**22**, Conf X

C	0.767670	1.926148	-1.008453
C	2.103115	2.244122	-1.276048
C	3.105930	1.695893	-0.482011
C	2.786670	0.885581	0.606198
C	1.453937	0.615533	0.900267
C	0.438474	1.133687	0.088560
O	3.435077	-0.126151	2.721190
C	2.316836	-1.006588	2.619913
C	1.113209	-0.238078	2.099227
C	3.910371	0.338888	1.462108
C	2.081474	-1.598938	3.990929
C	4.744977	-0.729165	0.768418
C	-0.996981	0.842464	0.382078
C	-1.665079	-0.187279	-0.276815
C	-3.000243	-0.434286	0.044920
C	-3.644590	0.310813	1.019803
C	-2.977862	1.352668	1.671758
C	-1.651952	1.604235	1.346487
C	6.076798	-0.881622	1.146548
C	6.876185	-1.864484	0.584596
C	6.315240	-2.698379	-0.362691
C	5.001879	-2.583008	-0.766813
C	4.221696	-1.586647	-0.194426
C	-0.975729	-1.052211	-1.302806
C	-1.721868	-2.357858	-1.517652
O	-3.100860	-2.069329	-1.764851
C	-3.763734	-1.558010	-0.627834
C	-1.206374	-3.146129	-2.698965
F	7.086609	-3.661074	-0.920197
O	-4.967402	0.046937	1.277861
C	-5.218530	-0.578633	2.538041
O	-3.696803	2.051235	2.586269
C	-3.045713	3.115122	3.266184
C	-5.123535	-1.094171	-1.151475
O	-5.285882	-0.098873	-1.811062
O	-6.078052	-1.968521	-0.848107
C	-8.098454	-0.755961	-0.241430
C	-7.426407	-1.647666	-1.260902
O	-0.252244	2.442219	-1.756238
C	-0.193106	2.255880	-3.172849
O	2.438859	3.087378	-2.303681
C	2.190873	4.465329	-2.015330
C	4.987535	1.554407	-1.919231
O	4.420855	2.017269	-0.689870
H	2.563735	-1.813174	1.916912
H	0.314458	-0.940174	1.845097
H	0.723726	0.401477	2.899537

H	4.580642	1.162645	1.712886
H	1.221893	-2.271555	3.969433
H	2.954985	-2.163144	4.320433
H	1.883024	-0.806419	4.716232
H	-1.108608	2.401822	1.837226
H	6.500202	-0.215559	1.891282
H	7.914872	-1.985165	0.866612
H	4.603900	-3.255204	-1.516948
H	3.192260	-1.474421	-0.518047
H	-0.908318	-0.522861	-2.260433
H	0.048893	-1.265824	-0.986062
H	-1.657051	-2.967888	-0.605162
H	-3.934067	-2.365591	0.096061
H	-1.751281	-4.084850	-2.804974
H	-0.147244	-3.372747	-2.564107
H	-1.322337	-2.567504	-3.618091
H	-6.291402	-0.756711	2.585913
H	-4.687261	-1.532624	2.605069
H	-4.916205	0.072981	3.359499
H	-3.784589	3.533820	3.944818
H	-2.189413	2.751105	3.840358
H	-2.715623	3.886644	2.565617
H	-9.123594	-0.551821	-0.555438
H	-8.129698	-1.243111	0.734700
H	-7.569079	0.192514	-0.143423
H	-7.390266	-1.180055	-2.244520
H	-7.922685	-2.613003	-1.340449
H	-1.223544	2.260788	-3.524653
H	0.366804	3.057342	-3.655685
H	0.270307	1.296942	-3.417439
H	2.764573	4.780409	-1.139884
H	2.515882	5.029020	-2.887549
H	1.125980	4.640593	-1.839948
H	4.906298	0.466013	-1.988197
H	4.497303	2.021461	-2.773726
H	6.038405	1.836256	-1.895057

$\omega$ B97X Energy = -2096.10521619 a.u.

(*aS*,1*S*,3*S*,1'*S*,3'*S*)-**22**, Conf Y

C	0.769773	1.956908	-1.081727
C	2.105458	2.241207	-1.384041
C	3.112725	1.702172	-0.592666
C	2.794854	0.924003	0.521569
C	1.464543	0.672988	0.838038
C	0.442132	1.183167	0.025895
O	3.461002	-0.014645	2.664778
C	2.333824	-0.887638	2.610833
C	1.131094	-0.129141	2.073831
C	3.923756	0.396805	1.383011
C	2.108970	-1.424865	4.006033
C	4.738620	-0.705558	0.719901
C	-0.993949	0.927729	0.350049
C	-1.635091	-0.234601	-0.072479
C	-2.978358	-0.420130	0.261401
C	-3.658451	0.513321	1.031500

C	-2.997312	1.658529	1.492711
C	-1.675210	1.862170	1.124556
C	6.066957	-0.870784	1.105536
C	6.849840	-1.883115	0.573981
C	6.276344	-2.733128	-0.351378
C	4.966272	-2.605868	-0.762053
C	4.202302	-1.580402	-0.219606
C	-0.910211	-1.310356	-0.844450
C	-1.606694	-2.651167	-0.696900
O	-2.984361	-2.492137	-1.042647
C	-3.703726	-1.691609	-0.124845
C	-1.037011	-3.717482	-1.603167
F	7.031828	-3.724402	-0.879606
O	-4.949356	0.220405	1.391220
C	-5.949694	1.171200	1.006258
O	-3.702330	2.488793	2.303393
C	-3.045055	3.641829	2.809290
C	-5.024901	-1.429815	-0.847106
O	-5.193374	-0.558091	-1.662927
O	-5.928346	-2.349978	-0.526517
C	-8.154544	-1.334044	-0.661286
C	-7.185280	-2.337033	-1.243668
O	-0.228089	2.514634	-1.837673
C	-0.363759	1.963005	-3.148915
O	2.422604	3.040063	-2.451931
C	2.286632	4.436785	-2.177130
C	4.973331	1.499651	-2.050965
O	4.429505	1.997897	-0.824841
H	2.565277	-1.722909	1.936208
H	0.323119	-0.834713	1.863190
H	0.757179	0.548368	2.850275
H	4.605298	1.222801	1.592667
H	1.242760	-2.089106	4.019810
H	2.980854	-1.984898	4.346702
H	1.926746	-0.603430	4.702809
H	-1.145136	2.744826	1.458662
H	6.500204	-0.192026	1.832928
H	7.885524	-2.014181	0.862324
H	4.558142	-3.291453	-1.494404
H	3.175529	-1.460459	-0.548718
H	-0.864258	-1.057982	-1.909973
H	0.122421	-1.395126	-0.496294
H	-1.547348	-2.979363	0.350980
H	-3.919598	-2.270971	0.781878
H	-1.553762	-4.666312	-1.454735
H	0.023760	-3.863306	-1.391517
H	-1.144433	-3.419949	-2.648605
H	-5.918809	1.329711	-0.074919
H	-6.904927	0.728576	1.282270
H	-5.812862	2.116559	1.528358
H	-3.774163	4.151236	3.434419
H	-2.176619	3.366835	3.413891
H	-2.732670	4.306924	2.000004
H	-9.120982	-1.439285	-1.157356
H	-8.297863	-1.510153	0.406291
H	-7.802152	-0.313369	-0.810141

H	-6.983267	-2.135664	-2.295966
H	-7.557750	-3.354351	-1.139755
H	-0.606867	0.898213	-3.089726
H	-1.185930	2.493506	-3.624727
H	0.551466	2.103257	-3.726831
H	2.567064	4.962246	-3.087809
H	1.253347	4.677811	-1.916940
H	2.954920	4.731638	-1.363671
H	4.871600	0.411788	-2.096586
H	4.481275	1.957808	-2.909145
H	6.029318	1.762589	-2.044282

ωB97X Energy = -2096.10517991 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf Z

C	-0.702177	-1.497448	-1.491782
C	-2.012721	-1.685139	-1.943131
C	-3.068352	-1.392053	-1.082800
C	-2.822076	-0.996205	0.231894
C	-1.515782	-0.859546	0.688005
C	-0.446969	-1.104163	-0.183163
O	-3.624617	-0.700344	2.507904
C	-2.497845	0.130681	2.784538
C	-1.261235	-0.452890	2.120390
C	-4.002998	-0.706092	1.135708
C	-2.361224	0.223147	4.287404
C	-4.749192	0.571395	0.773563
C	0.967660	-0.942351	0.268657
C	1.669794	0.230259	0.001093
C	2.992774	0.333660	0.430096
C	3.592228	-0.691393	1.150230
C	2.870908	-1.851181	1.454498
C	1.568193	-1.971099	0.988251
C	-4.131403	1.653611	0.155103
C	-4.831945	2.822798	-0.111959
C	-6.162043	2.883900	0.246132
C	-6.815110	1.831459	0.857421
C	-6.094603	0.676721	1.118735
C	1.026803	1.385152	-0.725104
C	1.784482	2.678682	-0.483009
O	3.171020	2.461902	-0.757905
C	3.789350	1.595892	0.172587
C	1.320736	3.811387	-1.368725
F	-6.856567	4.015839	-0.016153
O	4.867753	-0.480263	1.607315
C	5.864757	-1.422749	1.194019
O	3.502019	-2.783716	2.213728
C	2.790978	-3.970895	2.532864
C	5.152707	1.303832	-0.452171
O	5.329960	0.509823	-1.342457
O	6.097973	2.082518	0.063863
C	7.552190	2.813640	-1.755181
C	7.425787	1.976877	-0.502428
O	0.341613	-1.664287	-2.364449
C	0.751191	-3.017370	-2.548100
O	-2.210140	-2.094811	-3.233899

C	-2.865122	-3.357874	-3.381436
C	-4.807343	-0.677249	-2.532846
O	-4.374076	-1.539013	-1.475719
H	-2.688603	1.132272	2.377150
H	-0.446674	0.275066	2.164405
H	-0.928903	-1.327818	2.690815
H	-4.711028	-1.532101	1.051738
H	-1.495444	0.833807	4.550653
H	-3.251212	0.674787	4.727680
H	-2.225343	-0.772450	4.716242
H	0.992367	-2.862849	1.201788
H	-3.088367	1.588089	-0.136118
H	-4.359422	3.670094	-0.593301
H	-7.863424	1.919766	1.114767
H	-6.590809	-0.161353	1.597157
H	0.995385	1.182222	-1.801584
H	-0.008644	1.504270	-0.393998
H	1.684176	2.966187	0.573516
H	3.952244	2.124109	1.120541
H	1.872403	4.725903	-1.147790
H	0.257598	4.000087	-1.209257
H	1.473124	3.554918	-2.419393
H	6.822776	-0.985716	1.471130
H	5.730840	-2.378849	1.697401
H	5.827205	-1.560232	0.110651
H	3.467137	-4.573185	3.134417
H	1.890455	-3.748091	3.111569
H	2.518211	-4.522588	1.629167
H	8.575973	2.754002	-2.128647
H	6.881485	2.453944	-2.536143
H	7.324106	3.859695	-1.545641
H	8.083208	2.335883	0.286993
H	7.638670	0.925442	-0.696807
H	1.591536	-2.998795	-3.239256
H	1.071161	-3.454886	-1.597492
H	-0.055778	-3.616820	-2.976727
H	-3.894725	-3.315808	-3.022145
H	-2.852765	-3.585005	-4.445350
H	-2.323409	-4.135855	-2.835777
H	-4.279617	-0.895243	-3.462920
H	-5.871826	-0.863312	-2.659563
H	-4.651404	0.369002	-2.257671

ωB97X Energy = -2096.10516274 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf AA

C	0.722288	-1.499074	1.543704
C	2.039632	-1.667734	1.982551
C	3.087613	-1.406056	1.104919
C	2.832867	-1.039998	-0.215575
C	1.520054	-0.931963	-0.663440
C	0.458123	-1.156400	0.220125
O	3.612949	-0.809990	-2.507795
C	2.477694	0.005123	-2.795282
C	1.251429	-0.570222	-2.105314
C	4.004209	-0.777605	-1.139321

C	2.326962	0.057901	-4.298786
C	4.754349	0.508788	-0.819356
C	-0.958269	-1.017426	-0.233505
C	-1.656024	0.171416	-0.033500
C	-2.978424	0.255945	-0.469773
C	-3.581416	-0.805807	-1.130830
C	-2.864758	-1.984343	-1.366774
C	-1.563323	-2.083144	-0.892589
C	4.141340	1.608683	-0.227680
C	4.844540	2.783823	0.003198
C	6.172928	2.833083	-0.363321
C	6.821422	1.763317	-0.948666
C	6.098065	0.602745	-1.174311
C	-1.009874	1.366638	0.622714
C	-1.759179	2.646829	0.297254
O	-3.146954	2.455328	0.582499
C	-3.767992	1.536549	-0.294080
C	-1.291355	3.830794	1.110954
F	6.870201	3.970868	-0.135795
O	-4.854930	-0.615332	-1.603034
C	-5.857412	-1.526801	-1.137051
O	-3.499196	-2.955427	-2.073108
C	-2.790933	-4.159101	-2.331040
C	-5.135727	1.293897	0.342027
O	-5.322488	0.558810	1.279729
O	-6.073157	2.045039	-0.226231
C	-7.533293	2.891852	1.537324
C	-7.404942	1.981828	0.336966
O	-0.339403	-1.739186	2.369237
C	-0.371557	-1.046991	3.620091
O	2.313434	-2.082013	3.260417
C	2.068252	-3.473844	3.475296
C	4.872289	-0.711298	2.505593
O	4.389102	-1.593392	1.488176
H	2.664328	1.018511	-2.415795
H	0.429712	0.148541	-2.165256
H	0.923187	-1.464943	-2.646660
H	4.712826	-1.601285	-1.039147
H	1.453870	0.654602	-4.569796
H	3.209353	0.505214	-4.758356
H	2.195610	-0.949408	-4.700840
H	-0.991848	-2.988791	-1.051682
H	3.100161	1.552082	0.071727
H	4.375815	3.644694	0.463710
H	7.868525	1.842933	-1.213682
H	6.590777	-0.248926	-1.631873
H	-0.988101	1.236427	1.711089
H	0.028769	1.458715	0.293464
H	-1.654501	2.865755	-0.775143
H	-3.923817	2.006034	-1.273600
H	-1.841247	4.731018	0.834063
H	-0.227900	4.006987	0.939700
H	-1.444089	3.640038	2.175510
H	-5.819156	-1.604833	-0.047800
H	-6.813097	-1.099574	-1.436746
H	-5.730308	-2.509923	-1.587403

H	-3.466682	-4.787027	-2.906284
H	-1.887068	-3.967451	-2.915544
H	-2.524474	-4.667725	-1.400772
H	-8.560993	2.865095	1.903769
H	-6.873560	2.571564	2.344384
H	-7.291909	3.921402	1.269003
H	-8.054810	2.298180	-0.476600
H	-7.626261	0.944908	0.591080
H	-1.422697	-0.937726	3.882222
H	0.147532	-1.608540	4.397577
H	0.084343	-0.058301	3.526693
H	2.327242	-3.678602	4.512169
H	1.015235	-3.713543	3.305155
H	2.694969	-4.077807	2.814048
H	4.782492	0.328703	2.179741
H	4.330004	-0.859121	3.439752
H	5.923617	-0.954814	2.646023

ωB97X Energy = -2096.10510860 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf AB

C	-0.721122	-1.645132	-1.334071
C	-2.037291	-1.915392	-1.722510
C	-3.078800	-1.535155	-0.879643
C	-2.810710	-0.966573	0.365643
C	-1.497639	-0.743175	0.764224
C	-0.444116	-1.078020	-0.095619
O	-3.562972	-0.414882	2.610236
C	-2.455971	0.474801	2.751477
C	-1.219130	-0.148913	2.124859
C	-3.976201	-0.597597	1.260292
C	-2.281456	0.748956	4.228138
C	-4.769912	0.605785	0.768658
C	0.977244	-0.840073	0.297911
C	1.658869	0.294833	-0.133195
C	2.989930	0.466545	0.248845
C	3.616298	-0.449740	1.083975
C	2.912338	-1.564210	1.556139
C	1.604005	-1.758513	1.134641
C	-4.201291	1.623705	0.009635
C	-4.945041	2.732062	-0.374795
C	-6.267682	2.797184	0.009355
C	-6.872735	1.806511	0.757825
C	-6.109783	0.712426	1.134284
C	0.982315	1.342109	-0.981349
C	1.714591	2.669616	-0.904662
O	3.100395	2.449654	-1.177640
C	3.755865	1.703808	-0.169899
C	1.212146	3.680135	-1.909387
F	-7.003701	3.869559	-0.365911
O	4.895803	-0.167730	1.490108
C	5.892800	-1.152470	1.191525
O	3.562582	-2.377731	2.428001
C	2.861767	-3.503552	2.936130
C	5.111829	1.387757	-0.799983
O	5.309623	0.479585	-1.568027

O	6.013539	2.305502	-0.466913
C	8.224053	1.244402	-0.449892
C	7.305825	2.243416	-1.115606
O	0.305215	-1.910192	-2.202919
C	0.738290	-3.268501	-2.210712
O	-2.254125	-2.495528	-2.942945
C	-2.886072	-3.778379	-2.906967
C	-4.868745	-1.044545	-2.357819
O	-4.389261	-1.760920	-1.215525
H	-2.689467	1.415072	2.234998
H	-0.429765	0.604186	2.051217
H	-0.839691	-0.932915	2.790247
H	-4.660968	-1.446279	1.297355
H	-1.429575	1.411918	4.390873
H	-3.173488	1.222929	4.639861
H	-2.101341	-0.184955	4.765623
H	1.043388	-2.618973	1.477689
H	-3.163927	1.554181	-0.300472
H	-4.511232	3.529044	-0.966023
H	-7.917029	1.894504	1.031097
H	-6.568141	-0.076729	1.721331
H	0.942635	1.013079	-2.025929
H	-0.051402	1.477848	-0.651429
H	1.624344	3.077834	0.112317
H	3.926839	2.338551	0.708898
H	1.748255	4.624634	-1.809761
H	0.148204	3.866461	-1.752757
H	1.351789	3.301907	-2.924504
H	5.915793	-1.347762	0.116159
H	6.841885	-0.720541	1.503417
H	5.707091	-2.075772	1.737309
H	2.575317	-4.187472	2.132739
H	3.551446	-4.006164	3.609603
H	1.970971	-3.196224	3.490708
H	9.214888	1.312217	-0.902462
H	8.320150	1.457229	0.616293
H	7.857200	0.226189	-0.578742
H	7.153686	2.008440	-2.169362
H	7.692825	3.256840	-1.028024
H	-0.066861	-3.935578	-2.528788
H	1.559247	-3.330749	-2.922285
H	1.092755	-3.564399	-1.218538
H	-2.331424	-4.459064	-2.254850
H	-3.917144	-3.704045	-2.557319
H	-2.866725	-4.157255	-3.926671
H	-4.352873	-1.359188	-3.266679
H	-5.929674	-1.272545	-2.437011
H	-4.737862	0.030795	-2.212620

ωB97X Energy = -2096.10505961 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf AC

C	0.747948	-1.503285	1.569768
C	2.069312	-1.643665	1.997521
C	3.103585	-1.392226	1.101642
C	2.828792	-0.978378	-0.200068

C	1.509088	-0.848985	-0.623641
C	0.460880	-1.126708	0.262084
O	3.570094	-0.685022	-2.491876
C	2.438400	0.149230	-2.739637
C	1.217938	-0.435369	-2.047141
C	3.982723	-0.669274	-1.130494
C	2.265836	0.248849	-4.238092
C	4.708363	0.632598	-0.805976
C	-0.963639	-0.999739	-0.169341
C	-1.680462	0.166801	0.086932
C	-3.003759	0.248843	-0.346624
C	-3.587189	-0.796021	-1.046075
C	-2.872394	-1.972134	-1.291319
C	-1.558280	-2.059119	-0.850430
C	5.943023	0.861232	-1.410742
C	6.642644	2.036687	-1.192488
C	6.083528	2.983411	-0.355625
C	4.866048	2.797556	0.262396
C	4.182017	1.610609	0.029125
C	-1.054085	1.342836	0.793556
C	-1.835150	2.619834	0.535372
O	-3.217550	2.384584	0.817605
C	-3.824678	1.498065	-0.099072
C	-1.388399	3.772986	1.403253
F	6.760460	4.134885	-0.132461
O	-4.898440	-0.671798	-1.434946
C	-5.084211	-0.486860	-2.840533
O	-3.534366	-2.955635	-1.951076
C	-2.835140	-4.164720	-2.209339
C	-5.180286	1.177373	0.531614
O	-5.328034	0.428780	1.464325
O	-6.154665	1.879435	-0.038257
C	-7.700956	2.586989	1.715774
C	-7.488161	1.716375	0.498148
O	-0.270688	-1.682013	2.468436
C	-0.592288	-3.050497	2.718909
O	2.328320	-2.042180	3.282004
C	2.695074	-0.967152	4.150296
C	4.867736	-2.817878	1.750434
O	4.411408	-1.484377	1.503426
H	2.641708	1.147795	-2.329868
H	0.403644	0.294162	-2.067128
H	0.868839	-1.307491	-2.611753
H	4.713196	-1.477532	-1.056453
H	1.392892	0.858950	-4.477926
H	3.144372	0.704427	-4.696977
H	2.121839	-0.744938	-4.668496
H	-0.977098	-2.954457	-1.032536
H	6.364588	0.106217	-2.066119
H	7.604591	2.220715	-1.654839
H	4.464629	3.564518	0.913253
H	3.225005	1.452787	0.514391
H	-1.015595	1.156357	1.872831
H	-0.022085	1.475827	0.456904
H	-1.742166	2.893663	-0.525457
H	-4.002888	2.013538	-1.051789

H	-1.955197	4.674963	1.169494
H	-0.328670	3.976278	1.239262
H	-1.535392	3.529772	2.457834
H	-4.549645	0.404140	-3.182914
H	-4.738093	-1.361479	-3.393786
H	-6.152434	-0.351121	-2.996890
H	-3.533537	-4.808271	-2.738309
H	-1.957628	-3.987178	-2.836874
H	-2.527796	-4.648742	-1.278398
H	-8.732342	2.484361	2.057682
H	-7.038835	2.290981	2.529992
H	-7.521893	3.636317	1.476686
H	-8.143252	2.008580	-0.320386
H	-7.645334	0.661527	0.723944
H	-0.943558	-3.533201	1.801697
H	0.275058	-3.584902	3.112865
H	-1.390619	-3.053688	3.458315
H	3.608582	-0.482308	3.797430
H	1.885536	-0.234923	4.212327
H	2.867132	-1.404052	5.131852
H	5.920523	-2.738272	2.013079
H	4.313423	-3.273279	2.572393
H	4.762590	-3.427785	0.848563

ωB97X Energy = -2096.10505931 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf AD

C	-0.734916	-1.704010	-1.312756
C	-2.056642	-1.978043	-1.678883
C	-3.091525	-1.593343	-0.831835
C	-2.817408	-0.994038	0.396246
C	-1.498491	-0.775251	0.780985
C	-0.450631	-1.127272	-0.077580
O	-3.548730	-0.405961	2.639275
C	-2.437993	0.482263	2.751942
C	-1.208411	-0.160292	2.130006
C	-3.974358	-0.615087	1.296878
C	-2.250585	0.789031	4.220692
C	-4.779025	0.575499	0.791788
C	0.971979	-0.894596	0.314239
C	1.651228	0.250483	-0.093888
C	2.981531	0.418304	0.293405
C	3.609855	-0.513171	1.109381
C	2.908542	-1.639002	1.557985
C	1.601322	-1.828239	1.131606
C	-6.111741	0.689664	1.180551
C	-6.884249	1.772254	0.790667
C	-6.296358	2.743916	0.004436
C	-4.981049	2.670816	-0.403231
C	-4.227442	1.574397	-0.004276
C	0.973425	1.318248	-0.915803
C	1.697185	2.647224	-0.793789
O	3.083567	2.443501	-1.074736
C	3.744283	1.667763	-0.093093
C	1.188924	3.688207	-1.763881
F	-7.041732	3.804260	-0.384737



O	4.888569	-0.235591	1.522051
C	5.888810	-1.208989	1.199043
O	3.560852	-2.468069	2.413541
C	2.859222	-3.599691	2.907346
C	5.097120	1.370129	-0.738184
O	5.293089	0.479902	-1.527327
O	5.998597	2.282163	-0.388860
C	8.212939	1.230456	-0.400866
C	7.287759	2.237464	-1.044759
O	0.313482	-2.064824	-2.111698
C	0.303480	-1.589406	-3.460014
O	-2.348794	-2.619491	-2.854841
C	-2.075720	-4.022248	-2.823565
C	-4.930898	-1.199660	-2.276890
O	-4.394571	-1.882081	-1.139881
H	-2.671987	1.411706	2.215933
H	-0.414300	0.586096	2.040863
H	-0.831035	-0.936141	2.806078
H	-4.654759	-1.465985	1.356429
H	-1.395922	1.453283	4.361804
H	-3.138286	1.274070	4.628864
H	-2.068443	-0.133211	4.777322
H	1.043208	-2.698026	1.454103
H	-6.556587	-0.084258	1.797520
H	-7.923157	1.865761	1.082122
H	-4.560943	3.452551	-1.024034
H	-3.196156	1.498197	-0.332407
H	0.946703	1.026972	-1.972443
H	-0.064436	1.436230	-0.592724
H	1.604119	3.019525	0.236577
H	3.919383	2.275990	0.803387
H	1.720311	4.631461	-1.632532
H	0.124162	3.863878	-1.600911
H	1.330609	3.345693	-2.791365
H	6.837155	-0.779754	1.517011
H	5.709349	-2.144642	1.725607
H	5.909078	-1.381451	0.119708
H	3.548383	-4.111227	3.574614
H	1.968517	-3.298653	3.465535
H	2.572347	-4.273510	2.095769
H	9.200887	1.308431	-0.858016
H	8.314556	1.426257	0.668045
H	7.848141	0.213357	-0.543905
H	7.131860	2.020325	-2.101752
H	7.671214	3.250718	-0.941079
H	1.343378	-1.558935	-3.780821
H	-0.266579	-2.252827	-4.111142
H	-0.122454	-0.584215	-3.511978
H	-2.649956	-4.504378	-2.028123
H	-2.382746	-4.421230	-3.788238
H	-1.009180	-4.207755	-2.670926
H	-4.888984	-0.117671	-2.123788
H	-4.391142	-1.471806	-3.184294
H	-5.970162	-1.512227	-2.357801

ωB97X Energy = -2096.10504969 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf AE

C	-0.713056	0.213223	2.094939
C	-2.026178	0.052048	2.549983
C	-3.075912	0.446517	1.725649
C	-2.818777	0.986960	0.464066
C	-1.511559	1.138477	0.017759
C	-0.447149	0.751692	0.842237
O	-3.603116	2.221749	-1.480756
C	-2.497012	1.710438	-2.223559
C	-1.253172	1.725048	-1.350114
C	-3.998037	1.384941	-0.399504
C	-2.351196	2.564495	-3.462521
C	-4.810929	0.197165	-0.899556
C	0.971845	0.908641	0.403471
C	1.692831	-0.185227	-0.070307
C	3.018049	0.004585	-0.462400
C	3.598904	1.262294	-0.414155
C	2.877554	2.358754	0.067698
C	1.562506	2.168323	0.470418
C	-4.258702	-1.065046	-1.091801
C	-5.020405	-2.111610	-1.595912
C	-6.344241	-1.871281	-1.896307
C	-6.933157	-0.634869	-1.716739
C	-6.152466	0.395732	-1.217379
C	1.068975	-1.553599	-0.186667
C	1.863113	-2.445874	-1.125277
O	3.242379	-2.408963	-0.748769
C	3.843781	-1.153239	-0.985766
C	1.423369	-3.890668	-1.081058
F	-7.098120	-2.886397	-2.380485
O	4.914267	1.391134	-0.787001
C	5.116310	2.066724	-2.030688
O	3.536667	3.543868	0.110071
C	2.839190	4.671085	0.620261
C	5.202061	-1.251768	-0.290589
O	5.351081	-1.198110	0.903992
O	6.177121	-1.470657	-1.167201
C	7.748143	-3.058595	-0.178912
C	7.514349	-1.638409	-0.641632
O	0.325916	-0.183782	2.899176
C	0.676376	0.770463	3.903116
O	-2.287538	-0.401449	3.815245
C	-1.961078	-1.774934	4.051996
C	-4.905434	-0.879526	2.503840
O	-4.381531	0.394582	2.127220
H	-2.717952	0.676640	-2.521288
H	-0.449779	1.174575	-1.847296
H	-0.904036	2.758485	-1.243682
H	-4.665374	2.008338	0.197814
H	-1.503607	2.222685	-4.059641
H	-3.252115	2.508959	-4.075081
H	-2.180918	3.607324	-3.185092
H	0.978711	2.999162	0.846630
H	-3.219475	-1.246837	-0.839269
H	-4.598616	-3.097334	-1.748648

H	-7.979075	-0.491052	-1.958250
H	-6.598248	1.373629	-1.067696
H	1.015646	-2.025786	0.800878
H	0.042402	-1.465683	-0.553416
H	1.776700	-2.061138	-2.151691
H	4.017582	-1.022271	-2.061764
H	2.003445	-4.492569	-1.781519
H	0.367403	-3.970190	-1.345324
H	1.559620	-4.295093	-0.075613
H	4.601224	1.541100	-2.840185
H	4.760161	3.096595	-1.972136
H	6.188365	2.057937	-2.217011
H	3.540495	5.500680	0.578593
H	1.962793	4.904480	0.009560
H	2.531033	4.507441	1.656425
H	8.783697	-3.167062	0.148265
H	7.096094	-3.311823	0.657592
H	7.570776	-3.763612	-0.992478
H	8.163843	-1.378439	-1.475390
H	7.663245	-0.920837	0.165439
H	-0.172878	0.969454	4.561364
H	1.491374	0.334139	4.477092
H	1.015120	1.702399	3.440729
H	-2.536679	-2.423477	3.385059
H	-0.894734	-1.951672	3.909504
H	-2.236439	-1.981221	5.084366
H	-5.989280	-0.788460	2.456662
H	-4.579706	-1.651332	1.800717
H	-4.603072	-1.145298	3.516786

$\omega$ B97X Energy = -2096.10504262 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf AF

C	0.568305	1.885897	-0.854526
C	1.864634	2.308451	-1.154032
C	2.929588	1.817013	-0.405794
C	2.712162	0.886450	0.608391
C	1.417485	0.469279	0.902933
C	0.335476	0.985384	0.179362
O	3.503090	-0.232490	2.610869
C	2.469070	-1.205767	2.463061
C	1.186369	-0.518734	2.022033
C	3.901633	0.346163	1.373784
C	2.321201	-1.915756	3.789503
C	4.760075	-0.628987	0.575346
C	-1.066143	0.577380	0.496035
C	-1.705059	-0.417512	-0.239875
C	-3.010544	-0.772546	0.103008
C	-3.650089	-0.167474	1.173779
C	-3.014587	0.842810	1.901891
C	-1.718697	1.201412	1.556674
C	4.322628	-1.250265	-0.588144
C	5.128020	-2.161808	-1.260003
C	6.375767	-2.436554	-0.743866
C	6.849609	-1.841047	0.409314
C	6.029100	-0.936110	1.062657

C	-1.013518	-1.119580	-1.381564
C	-1.704393	-2.426204	-1.732133
O	-3.106734	-2.187323	-1.881988
C	-3.738332	-1.861711	-0.660881
C	-1.207493	-3.026329	-3.026664
F	7.170767	-3.320376	-1.392614
O	-4.943472	-0.529693	1.456865
C	-5.095184	-1.316942	2.640104
O	-3.732599	1.405421	2.906400
C	-3.116045	2.439687	3.659776
C	-5.172246	-1.504944	-1.054186
O	-6.090378	-2.282549	-0.962660
O	-5.257720	-0.290713	-1.580878
C	-7.381557	0.691163	-0.884659
C	-6.558422	0.151266	-2.032008
O	-0.475989	2.321727	-1.627063
C	-0.914578	3.645378	-1.320395
O	2.066881	3.212088	-2.163447
C	2.528264	2.614755	-3.377685
C	4.527254	3.553063	-0.389673
O	4.217505	2.189067	-0.693159
H	2.775511	-1.928988	1.695541
H	0.457217	-1.272159	1.711412
H	0.746967	0.003232	2.879723
H	4.539155	1.186059	1.657624
H	1.523768	-2.659112	3.733361
H	3.248894	-2.421856	4.060054
H	2.071333	-1.198558	4.574807
H	-1.197706	1.974472	2.107654
H	3.340696	-1.022874	-0.988546
H	4.795989	-2.649978	-2.167950
H	7.839181	-2.081591	0.777978
H	6.382981	-0.458098	1.970187
H	-1.002730	-0.470236	-2.264577
H	0.030059	-1.319235	-1.122238
H	-1.565719	-3.144178	-0.910940
H	-3.813845	-2.759797	-0.033331
H	-1.709976	-3.972121	-3.232454
H	-0.133191	-3.209286	-2.966123
H	-1.395898	-2.340330	-3.855470
H	-6.155783	-1.544572	2.726918
H	-4.528209	-2.248755	2.555876
H	-4.765195	-0.760602	3.519180
H	-2.219980	2.076127	4.169891
H	-2.855544	3.289590	3.023066
H	-3.850719	2.752404	4.397422
H	-8.329938	1.070914	-1.269252
H	-7.591310	-0.088210	-0.151654
H	-6.859301	1.509503	-0.386674
H	-6.337913	0.925227	-2.764750
H	-7.057222	-0.680792	-2.529278
H	-0.102061	4.363074	-1.453860
H	-1.722273	3.875132	-2.012530
H	-1.290426	3.694184	-0.293660
H	1.796523	1.891353	-3.747378
H	2.640106	3.420545	-4.100328

H	3.491602	2.122614	-3.222994
H	3.922839	4.232217	-0.992590
H	4.360718	3.751434	0.672993
H	5.581315	3.688670	-0.622443

$\omega$ B97X Energy = -2096.10498380 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf AG

C	0.553026	-1.477237	-1.407989
C	1.849427	-1.925464	-1.683980
C	2.912239	-1.037786	-1.542333
C	2.686403	0.273933	-1.120265
C	1.396576	0.707814	-0.838838
C	0.318366	-0.173376	-0.990521
O	3.480177	2.563233	-0.881547
C	2.455036	2.792542	0.084297
C	1.169300	2.128808	-0.380058
C	3.877546	1.199808	-0.978557
C	2.312326	4.288847	0.247012
C	4.809086	0.821888	0.165700
C	-1.082616	0.270869	-0.724536
C	-1.715113	-0.041043	0.476554
C	-3.021033	0.405320	0.683200
C	-3.666546	1.172726	-0.273888
C	-3.036539	1.474262	-1.485071
C	-1.741538	1.021032	-1.695691
C	6.152802	1.176891	0.073589
C	7.042676	0.897864	1.098843
C	6.560801	0.259021	2.224468
C	5.238950	-0.109383	2.358133
C	4.366654	0.175164	1.315147
C	-1.013775	-0.826424	1.556034
C	-1.694915	-0.648861	2.901918
O	-3.096315	-0.890816	2.750183
C	-3.745415	0.099828	1.979457
C	-1.183163	-1.606000	3.952946
F	7.421143	-0.021478	3.231584
O	-4.959653	1.566062	-0.034298
C	-5.118791	2.962082	0.229753
O	-3.758434	2.197585	-2.377764
C	-3.148579	2.507827	-3.622522
C	-5.166512	-0.434573	1.797346
O	-6.089380	-0.091703	2.494977
O	-5.234978	-1.367982	0.857217
C	-7.384010	-1.131180	-0.277469
C	-6.522302	-1.984692	0.625146
O	-0.499282	-2.348800	-1.539846
C	-0.951764	-2.508894	-2.885505
O	2.078275	-3.184277	-2.171174
C	1.819840	-4.252186	-1.253795
C	4.789262	-2.462785	-1.161462
O	4.194570	-1.377690	-1.874887
H	2.765378	2.352887	1.041548
H	0.434748	2.146867	0.429659
H	0.742608	2.714708	-1.202110
H	4.458727	1.151267	-1.900931

H	1.518923	4.517116	0.961200
H	3.242737	4.726604	0.611202
H	2.060119	4.750195	-0.710557
H	-1.226341	1.243995	-2.621618
H	6.513710	1.675968	-0.819774
H	8.090800	1.161998	1.030852
H	4.903692	-0.612887	3.256483
H	3.327921	-0.125179	1.403277
H	-1.002120	-1.891224	1.296308
H	0.029318	-0.506908	1.632627
H	-1.561169	0.387379	3.244346
H	-3.843953	1.021521	2.568149
H	-1.684365	-1.436800	4.906674
H	-0.109995	-1.467272	4.095345
H	-1.360869	-2.637705	3.641470
H	-6.174786	3.118809	0.440566
H	-4.525363	3.256933	1.100289
H	-4.823790	3.554576	-0.638000
H	-3.884218	3.078755	-4.183441
H	-2.248712	3.112690	-3.482003
H	-2.895667	1.598318	-4.174180
H	-8.326376	-1.647286	-0.469945
H	-7.604640	-0.169788	0.186926
H	-6.886577	-0.954720	-1.232232
H	-6.282024	-2.939721	0.161803
H	-7.001963	-2.163798	1.587507
H	-0.143947	-2.872334	-3.525377
H	-1.755882	-3.241549	-2.859471
H	-1.335425	-1.560620	-3.273855
H	2.416430	-4.127182	-0.345367
H	0.761519	-4.296919	-0.995439
H	2.117801	-5.168630	-1.759352
H	5.861770	-2.387406	-1.332118
H	4.589507	-2.371905	-0.090034
H	4.426105	-3.422189	-1.529946

$\omega$ B97X Energy = -2096.10490117 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf AH

C	-0.512989	0.981694	1.780523
C	-1.786349	1.080752	2.342866
C	-2.897391	1.122541	1.507419
C	-2.746330	1.044459	0.124642
C	-1.473383	0.949677	-0.431175
C	-0.346753	0.932233	0.400655
O	-3.658743	1.418356	-2.091253
C	-2.626185	0.601075	-2.643020
C	-1.314721	0.894980	-1.932399
C	-3.981738	1.069472	-0.750460
C	-2.561508	0.888501	-4.125726
C	-4.800327	-0.217004	-0.715925
C	1.031818	0.851004	-0.168865
C	1.700168	-0.367870	-0.252766
C	2.991372	-0.391390	-0.780376
C	3.588157	0.769389	-1.254005
C	2.900653	1.986508	-1.202653

C	1.631833	2.015330	-0.639574
C	-4.323908	-1.412849	-0.193191
C	-5.098431	-2.566711	-0.223473
C	-6.354146	-2.497528	-0.786300
C	-6.866240	-1.328616	-1.315956
C	-6.076818	-0.191216	-1.274789
C	1.057473	-1.651105	0.211172
C	1.753061	-2.864338	-0.380477
O	3.160919	-2.746623	-0.157685
C	3.747547	-1.699534	-0.904209
C	1.303227	-4.165745	0.241211
F	-7.118252	-3.615258	-0.818434
O	4.828359	0.650339	-1.823498
C	5.876782	1.462259	-1.283550
O	3.530516	3.065907	-1.734072
C	2.856459	4.315218	-1.690524
C	5.190637	-1.648001	-0.404045
O	6.106314	-2.187057	-0.974899
O	5.296472	-1.009201	0.756146
C	6.855802	-2.257148	2.160435
C	6.597564	-0.983626	1.387877
O	0.576391	0.876295	2.605488
C	1.010336	2.119710	3.157497
O	-1.931807	1.151427	3.703259
C	-2.174650	-0.119722	4.309763
C	-4.504286	2.433982	2.627224
O	-4.161728	1.177539	2.034859
H	-2.892454	-0.453107	-2.487925
H	-0.574989	0.136759	-2.203800
H	-0.921291	1.853810	-2.288983
H	-4.630553	1.877702	-0.406179
H	-1.763222	0.305494	-4.588880
H	-3.504900	0.631509	-4.609395
H	-2.358656	1.948510	-4.295461
H	1.082390	2.946331	-0.579578
H	-3.335500	-1.456251	0.251081
H	-4.735564	-3.502819	0.182697
H	-7.860213	-1.316814	-1.745920
H	-6.460291	0.735875	-1.687818
H	1.094997	-1.713446	1.304807
H	0.001093	-1.664296	-0.071512
H	1.579522	-2.890885	-1.465878
H	3.807652	-1.986301	-1.962095
H	1.816176	-5.011193	-0.218727
H	0.228332	-4.295082	0.102711
H	1.516626	-4.165825	1.312443
H	5.840165	2.469511	-1.695353
H	5.801010	1.508622	-0.194051
H	6.810467	0.975747	-1.562982
H	2.654916	4.619156	-0.659828
H	3.527283	5.033616	-2.154976
H	1.918627	4.277457	-2.251337
H	7.815306	-2.179233	2.674578
H	6.077855	-2.418886	2.908015
H	6.892602	-3.119348	1.493829
H	7.355705	-0.816639	0.622106

H	6.557471	-0.117928	2.046794
H	1.321467	2.802714	2.360980
H	0.215452	2.577456	3.750611
H	1.862271	1.897105	3.796921
H	-3.092483	-0.563476	3.915193
H	-1.331507	-0.793269	4.134412
H	-2.284527	0.057496	5.377729
H	-5.524858	2.335108	2.991113
H	-3.836384	2.667126	3.457707
H	-4.459682	3.230874	1.879142

$\omega$ B97X Energy = -2096.10489948 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf AI

C	-0.504262	-0.383919	1.964032
C	-1.775333	-0.682214	2.466532
C	-2.886447	-0.075296	1.888023
C	-2.730931	0.810129	0.819605
C	-1.464861	1.096880	0.323313
C	-0.339175	0.498665	0.903863
O	-3.654694	2.563329	-0.589667
C	-2.630073	2.307741	-1.549632
C	-1.314123	2.061279	-0.829961
C	-3.971671	1.432592	0.214051
C	-2.573163	3.499529	-2.478120
C	-4.833432	0.442625	-0.560501
C	1.038637	0.795378	0.409759
C	1.698938	-0.093676	-0.434907
C	2.993453	0.213492	-0.854585
C	3.601664	1.402786	-0.475437
C	2.920348	2.313983	0.338702
C	1.648381	1.987503	0.789586
C	-6.183055	0.737718	-0.740501
C	-7.010223	-0.097725	-1.474142
C	-6.460553	-1.237313	-2.028510
C	-5.131025	-1.567595	-1.875580
C	-4.321580	-0.716953	-1.133164
C	1.042012	-1.368357	-0.902432
C	1.729352	-1.925853	-2.136069
O	3.137082	-1.992499	-1.893109
C	3.738146	-0.717124	-1.791649
C	1.266933	-3.319188	-2.493019
F	-7.259855	-2.062520	-2.744980
O	4.845622	1.664796	-0.987355
C	5.895547	1.912571	-0.045860
O	3.558805	3.479625	0.617726
C	2.891730	4.420270	1.446779
C	5.178174	-1.019425	-1.379791
O	6.091603	-1.074827	-2.165565
O	5.282372	-1.282848	-0.081819
C	6.799367	-3.174566	0.192962
C	6.576674	-1.695967	0.415226
O	0.594987	-0.985522	2.524736
C	1.039897	-0.363151	3.731401
O	-1.934179	-1.486062	3.563476
C	-1.610110	-2.865771	3.363609

C	-4.666872	-1.583751	2.403499
O	-4.152167	-0.251886	2.374290
H	-2.901058	1.412825	-2.125787
H	-0.574270	1.682447	-1.540485
H	-0.927560	3.016425	-0.456503
H	-4.583923	1.835454	1.022378
H	-1.790234	3.359634	-3.225977
H	-3.525718	3.630013	-2.993421
H	-2.353772	4.408638	-1.913372
H	1.103840	2.670070	1.429934
H	-6.597174	1.637050	-0.296420
H	-8.061782	0.120566	-1.613947
H	-4.740656	-2.472345	-2.325002
H	-3.276023	-0.972698	-0.998113
H	1.071695	-2.118638	-0.104005
H	-0.012537	-1.184193	-1.126037
H	1.560105	-1.247726	-2.984818
H	3.801406	-0.256458	-2.785946
H	1.768242	-3.673564	-3.394383
H	0.189930	-3.323006	-2.670042
H	1.485770	-4.009683	-1.675477
H	5.849345	1.190527	0.773623
H	6.828502	1.782349	-0.592260
H	5.831766	2.923568	0.353215
H	3.569641	5.264316	1.546267
H	1.957151	4.756282	0.989570
H	2.686697	3.999598	2.434830
H	7.748238	-3.469370	0.644357
H	6.002696	-3.757330	0.657600
H	6.837604	-3.410199	-0.871052
H	7.346630	-1.094664	-0.069142
H	6.545087	-1.451972	1.475784
H	1.339409	0.671281	3.538006
H	0.254778	-0.386083	4.491017
H	1.901313	-0.931343	4.076718
H	-2.225886	-3.290240	2.565187
H	-0.554557	-2.987053	3.119066
H	-1.833948	-3.371172	4.301012
H	-4.258544	-2.145390	3.243608
H	-5.745494	-1.489540	2.515904
H	-4.447638	-2.100328	1.464737

ωB97X Energy = -2096.10487362 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf AJ

C	0.589446	2.034123	-0.791368
C	1.903092	2.437898	-1.051314
C	2.947185	1.861247	-0.337669
C	2.685732	0.925296	0.663813
C	1.375352	0.555116	0.944764
C	0.318011	1.103314	0.205685
O	3.428128	-0.249445	2.660420
C	2.349258	-1.169518	2.502439
C	1.100939	-0.419012	2.066571
C	3.851421	0.348243	1.440139
C	2.166594	-1.881103	3.823971

C	4.705227	-0.614922	0.625964
C	-1.098001	0.717406	0.487394
C	-1.661668	-0.419039	-0.090073
C	-2.986583	-0.738745	0.215257
C	-3.719637	0.042031	1.094237
C	-3.157655	1.189698	1.662335
C	-1.843314	1.511557	1.355599
C	4.190906	-1.375136	-0.419574
C	4.989308	-2.276119	-1.112087
C	6.312116	-2.395402	-0.741875
C	6.864307	-1.657436	0.286747
C	6.046910	-0.768762	0.967291
C	-0.873089	-1.324297	-1.005563
C	-1.508779	-2.700365	-1.103946
O	-2.894381	-2.548852	-1.421441
C	-3.639192	-1.977715	-0.365286
C	-0.890744	-3.562194	-2.180012
F	7.101855	-3.264114	-1.415525
O	-5.027326	-0.296877	1.337555
C	-5.273742	-0.824381	2.643283
O	-3.961763	1.912952	2.481139
C	-3.419943	3.084193	3.075011
C	-5.025882	-1.739924	-0.964427
O	-5.940731	-2.514214	-0.825006
O	-5.067421	-0.645464	-1.712330
C	-7.271711	0.365586	-1.422820
C	-6.318111	-0.331086	-2.366715
O	-0.447051	2.623286	-1.466951
C	-0.548050	2.266170	-2.846872
O	2.165644	3.387981	-2.003792
C	1.935040	4.725517	-1.554111
C	4.809773	1.956926	-1.804639
O	4.241000	2.267492	-0.528970
H	2.619696	-1.902976	1.731236
H	0.333312	-1.137646	1.767745
H	0.694354	0.129299	2.924295
H	4.496296	1.171912	1.750415
H	1.339329	-2.590542	3.760629
H	3.071560	-2.426866	4.094325
H	1.944427	-1.158866	4.612927
H	-1.379477	2.391425	1.782825
H	3.153685	-1.258279	-0.714863
H	4.597680	-2.870616	-1.928236
H	7.910541	-1.777737	0.539477
H	6.463797	-0.178868	1.777055
H	-0.812866	-0.893389	-2.011405
H	0.154381	-1.425495	-0.646215
H	-1.431680	-3.206370	-0.130550
H	-3.779847	-2.721348	0.430462
H	-1.364678	-4.543983	-2.206595
H	0.175382	-3.695848	-1.988282
H	-1.010718	-3.088451	-3.156822
H	-6.332605	-1.072349	2.682178
H	-4.681333	-1.728979	2.808945
H	-5.040525	-0.082809	3.409062
H	-4.215764	3.507404	3.682743

H	-2.564371	2.844079	3.711899
H	-3.118501	3.809030	2.314285
H	-8.174184	0.649426	-1.967338
H	-7.556738	-0.288709	-0.598640
H	-6.817551	1.269046	-1.013323
H	-6.030397	0.316293	-3.192969
H	-6.745643	-1.251345	-2.765225
H	0.355271	2.548426	-3.390267
H	-0.723467	1.191559	-2.950906
H	-1.402861	2.809137	-3.244646
H	0.883867	4.868062	-1.292939
H	2.567217	4.951680	-0.691287
H	2.199290	5.382173	-2.380604
H	5.833221	2.325908	-1.778883
H	4.818481	0.874774	-1.962167
H	4.258826	2.449005	-2.606510

ωB97X Energy = -2096.10483296 a.u.

(*aS*,1*S*,3*S*,1'*S*,3'*S*)-22, Conf AK

C	-0.534457	-0.565567	1.949114
C	-1.816422	-0.869489	2.408930
C	-2.912999	-0.239096	1.830295
C	-2.738689	0.666886	0.786126
C	-1.457168	0.970589	0.334933
C	-0.345139	0.363112	0.930894
O	-3.620087	2.481096	-0.563911
C	-2.574606	2.266650	-1.512274
C	-1.275816	1.978106	-0.776400
C	-3.961461	1.307336	0.164479
C	-2.491669	3.501003	-2.381104
C	-4.785734	0.359355	-0.698635
C	1.044434	0.694149	0.494033
C	1.745674	-0.147399	-0.365983
C	3.042975	0.205853	-0.740353
C	3.613418	1.385702	-0.288663
C	2.912281	2.226497	0.580800
C	1.625689	1.870734	0.961335
C	-4.275347	-0.817771	-1.233488
C	-5.052017	-1.627522	-2.053029
C	-6.345982	-1.237140	-2.322766
C	-6.892883	-0.077080	-1.809325
C	-6.099429	0.715895	-0.996341
C	1.130793	-1.413551	-0.906686
C	1.869292	-1.905825	-2.139360
O	3.270575	-1.953836	-1.854878
C	3.841043	-0.672677	-1.683622
C	1.448345	-3.292751	-2.565710
F	-7.113029	-2.021944	-3.116222
O	4.904457	1.673758	-0.656369
C	5.029472	2.731313	-1.610215
O	3.562829	3.342197	0.996436
C	2.879873	4.212793	1.886807
C	5.271516	-0.952953	-1.222779
O	6.218648	-0.934852	-1.969986
O	5.325828	-1.284542	0.060511

C	6.955780	-3.086996	0.304924
C	6.617068	-1.643940	0.602799
O	0.540191	-1.232329	2.476954
C	0.992475	-0.708127	3.725620
O	-1.977572	-1.763219	3.434247
C	-2.324361	-3.077570	2.992769
C	-4.520452	-0.075715	3.548682
O	-4.187219	-0.540200	2.236806
H	-2.837667	1.401483	-2.135598
H	-0.525287	1.621031	-1.487127
H	-0.887587	2.913222	-0.356945
H	-4.609460	1.663230	0.968074
H	-1.692314	3.393172	-3.116753
H	-3.431718	3.660260	-2.911046
H	-2.281993	4.381011	-1.768551
H	1.056553	2.503324	1.631072
H	-3.257631	-1.119161	-1.010031
H	-4.662835	-2.546118	-2.474523
H	-7.917147	0.188654	-2.040060
H	-6.511453	1.630700	-0.582974
H	1.151167	-2.194711	-0.138395
H	0.080294	-1.241473	-1.157342
H	1.711849	-1.197416	-2.965408
H	3.931942	-0.174797	-2.658143
H	1.982449	-3.599189	-3.465818
H	0.377032	-3.312000	-2.773466
H	1.659391	-4.011202	-1.770567
H	6.091295	2.830040	-1.826354
H	4.491448	2.483456	-2.529986
H	4.648450	3.667729	-1.199103
H	3.569006	5.026893	2.096936
H	1.971654	4.613848	1.428852
H	2.625573	3.702489	2.819727
H	7.897737	-3.344734	0.792309
H	6.179534	-3.751864	0.686741
H	7.068167	-3.251485	-0.767060
H	7.366318	-0.961475	0.200928
H	6.513372	-1.471543	1.672355
H	1.334202	0.324381	3.604017
H	0.197632	-0.751479	4.473769
H	1.827007	-1.330651	4.042226
H	-3.275110	-3.063678	2.453894
H	-1.538445	-3.482878	2.349791
H	-2.418399	-3.692701	3.885418
H	-5.565444	-0.331872	3.710014
H	-3.898075	-0.560051	4.302486
H	-4.398404	1.009645	3.609311

ωB97X Energy = -2096.10480941 a.u.

(*aS*,1*S*,3*S*,1'*S*,3'*S*)-22, Conf AL

C	-0.739598	-1.561477	-1.464663
C	-2.060660	-1.756706	-1.880351
C	-3.095833	-1.415798	-1.012822
C	-2.819180	-0.964273	0.277663
C	-1.502592	-0.819030	0.700317

C	-0.454118	-1.111980	-0.180653
O	-3.570769	-0.569575	2.555775
C	-2.434211	0.265480	2.774177
C	-1.215203	-0.351814	2.107930
C	-3.978769	-0.629110	1.193251
C	-2.264538	0.416676	4.268908
C	-4.726004	0.637175	0.795997
C	0.970421	-0.946401	0.237739
C	1.692625	0.186260	-0.130580
C	3.016386	0.304533	0.293387
C	3.594475	-0.669434	1.092671
C	2.873811	-1.812241	1.452104
C	1.560095	-1.936369	1.020185
C	-6.063632	0.763267	1.163512
C	-6.783467	1.911434	0.872985
C	-6.137339	2.936296	0.209647
C	-4.815176	2.853713	-0.172692
C	-4.115212	1.691418	0.124428
C	1.070080	1.286475	-0.952375
C	1.864260	2.577112	-0.846093
O	3.244822	2.298074	-1.095380
C	3.840393	1.521667	-0.077036
C	1.426425	3.621107	-1.846734
F	-6.831084	4.061771	-0.081001
O	4.906472	-0.516244	1.468440
C	5.091787	-0.176093	2.844485
O	3.530994	-2.728975	2.206137
C	2.827681	-3.906544	2.575008
C	5.207158	1.138711	-0.645569
O	5.369021	0.311796	-1.506890
O	6.174717	1.880556	-0.115538
C	7.777183	2.428450	-1.875222
C	7.519213	1.658162	-0.600061
O	0.283934	-1.779856	-2.349549
C	0.682887	-3.143278	-2.469189
O	-2.287640	-2.222534	-3.146903
C	-2.957262	-3.484250	-3.224379
C	-4.858906	-0.747812	-2.455130
O	-4.410388	-1.569240	-1.372524
H	-2.628714	1.251124	2.331352
H	-0.397157	0.373584	2.102169
H	-0.873592	-1.202599	2.708449
H	-4.692527	-1.453693	1.158296
H	-1.389376	1.030912	4.489322
H	-3.141938	0.891609	4.709906
H	-2.125917	-0.562349	4.733499
H	0.974997	-2.807287	1.288073
H	-6.554424	-0.053328	1.682907
H	-7.825896	2.015535	1.147733
H	-4.348077	3.679604	-0.694805
H	-3.078639	1.608859	-0.185075
H	1.015905	0.981352	-2.003497
H	0.043409	1.464776	-0.620260
H	1.773745	2.977819	0.173832
H	4.001572	2.140587	0.815234
H	1.999581	4.540743	-1.723559

H	0.368172	3.849928	-1.708918
H	1.570754	3.250209	-2.863888
H	4.730784	-0.976443	3.492804
H	6.161645	-0.040118	2.989299
H	4.570821	0.756301	3.081487
H	3.524318	-4.502188	3.159524
H	1.951875	-3.669187	3.185092
H	2.516698	-4.472119	1.692429
H	8.816062	2.287709	-2.178610
H	7.133228	2.077816	-2.682327
H	7.606035	3.495077	-1.722517
H	8.157116	2.004413	0.210967
H	7.665912	0.587033	-0.739714
H	-0.137531	-3.760326	-2.844131
H	1.505526	-3.167121	-3.181104
H	1.024801	-3.530217	-1.504295
H	-2.408573	-4.243676	-2.659933
H	-3.977022	-3.417007	-2.841634
H	-2.973837	-3.756165	-4.277663
H	-4.346331	-1.003059	-3.384183
H	-5.925618	-0.935834	-2.557904
H	-4.696403	0.307815	-2.222958

ωB97X Energy = -2096.10477165 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf AM

C	-0.748650	-1.629732	-1.463232
C	-2.076095	-1.820238	-1.860851
C	-3.104039	-1.474889	-0.988507
C	-2.819993	-1.003948	0.292113
C	-1.497583	-0.873301	0.704150
C	-0.455617	-1.180515	-0.178069
O	-3.551141	-0.592887	2.574395
C	-2.405893	0.234128	2.775552
C	-1.197314	-0.401405	2.107465
C	-3.970568	-0.661936	1.215503
C	-2.224073	0.400302	4.267310
C	-4.720609	0.602109	0.815987
C	0.970491	-1.022765	0.237791
C	1.676983	0.138045	-0.069445
C	3.001501	0.248319	0.354519
C	3.596863	-0.762051	1.092802
C	2.892380	-1.932445	1.390166
C	1.577711	-2.047966	0.958688
C	-4.118378	1.646421	0.121553
C	-4.820159	2.806970	-0.178264
C	-6.135576	2.897932	0.224842
C	-6.773396	1.882950	0.911060
C	-6.051813	0.736390	1.203631
C	1.038837	1.284348	-0.813748
C	1.806758	2.576951	-0.596449
O	3.189758	2.347845	-0.879945
C	3.811963	1.493207	0.057003
C	1.342514	3.698997	-1.495397
F	-6.831076	4.021803	-0.068052
O	4.909069	-0.610103	1.468885

C	5.100500	-0.370222	2.865363
O	3.565379	-2.882178	2.087412
C	2.873996	-4.080984	2.407781
C	5.161119	1.157831	-0.579649
O	5.301895	0.371695	-1.482066
O	6.137421	1.891807	-0.055099
C	7.644326	2.546892	-1.862252
C	7.462980	1.721026	-0.608877
O	0.294248	-1.950565	-2.285014
C	0.305977	-1.371299	-3.592470
O	-2.378996	-2.338932	-3.093235
C	-2.155239	-3.747384	-3.191637
C	-4.908460	-0.878680	-2.407752
O	-4.414500	-1.679370	-1.330085
H	-2.594506	1.216695	2.322923
H	-0.370682	0.314163	2.095271
H	-0.862660	-1.253593	2.710089
H	-4.685459	-1.485973	1.192518
H	-1.342063	1.009186	4.474858
H	-3.094217	0.887527	4.709268
H	-2.090643	-0.574818	4.741518
H	1.005259	-2.940582	1.177167
H	-3.087492	1.556800	-0.204351
H	-4.359654	3.625200	-0.718022
H	-7.810862	1.993302	1.201719
H	-6.536143	-0.072531	1.740801
H	1.006104	1.069977	-1.888408
H	0.004399	1.415949	-0.484663
H	1.715921	2.880442	0.456425
H	3.999376	2.039370	0.990579
H	1.900625	4.613602	-1.291937
H	0.281593	3.895746	-1.331132
H	1.486257	3.426478	-2.543282
H	6.168355	-0.220252	3.010959
H	4.560387	0.528995	3.176334
H	4.764198	-1.225876	3.453309
H	3.579152	-4.695481	2.961791
H	1.999941	-3.877717	3.032410
H	2.562592	-4.610001	1.503204
H	8.669412	2.439389	-2.221186
H	6.968594	2.215652	-2.651311
H	7.461300	3.603011	-1.658773
H	8.129824	2.050112	0.185764
H	7.626465	0.659968	-0.797953
H	-0.134799	-0.371544	-3.576188
H	1.351988	-1.301805	-3.886570
H	-0.239073	-1.991038	-4.305148
H	-1.101474	-3.986014	-3.024720
H	-2.773418	-4.283255	-2.466748
H	-2.440983	-4.037613	-4.200734
H	-4.802511	0.183511	-2.170346
H	-4.384734	-1.108632	-3.335889
H	-5.964425	-1.121433	-2.509147

ωB97X Energy = -2096.10474404 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf AN

C	0.788124	-1.647219	1.414389
C	2.120930	-1.835477	1.796790
C	3.134560	-1.498803	0.901877
C	2.837906	-0.945819	-0.340484
C	1.510752	-0.769628	-0.719392
C	0.482070	-1.134737	0.154700
O	3.529996	-0.440422	-2.610508
C	2.406357	0.430168	-2.742640
C	1.193159	-0.207730	-2.085094
C	3.976000	-0.570171	-1.265517
C	2.200193	0.686250	-4.218224
C	4.745032	0.674073	-0.834313
C	-0.949280	-0.980901	-0.245230
C	-1.671991	0.158653	0.099230
C	-3.008283	0.250198	-0.291055
C	-3.602099	-0.753064	-1.045172
C	-2.860829	-1.876910	-1.427052
C	-1.544028	-1.986475	-1.001134
C	5.979779	0.918632	-1.432634
C	6.717959	2.048496	-1.121170
C	6.196897	2.933689	-0.197026
C	4.981071	2.729831	0.418650
C	4.257926	1.588966	0.091254
C	-1.038284	1.295595	0.861728
C	-1.830140	2.580774	0.695961
O	-3.203696	2.319570	0.994991
C	-3.826018	1.481554	0.042077
C	-1.368654	3.682943	1.620651
F	6.911064	4.040424	0.117788
O	-4.894588	-0.553192	-1.458691
C	-5.855890	-1.538254	-1.060451
O	-3.489218	-2.784920	-2.217603
C	-2.755171	-3.930601	-2.624918
C	-5.167713	1.128474	0.681256
O	-5.305035	0.307263	1.553951
O	-6.149982	1.885208	0.206667
C	-8.412876	2.628659	0.101213
C	-7.460645	1.678378	0.781250
O	-0.250970	-2.017028	2.219124
C	-0.290944	-1.481848	3.542633
O	2.393570	-2.422009	3.003800
C	3.096389	-1.602187	3.942764
C	4.866174	-3.051042	1.296144
O	4.453140	-1.682210	1.236737
H	2.635135	1.378118	-2.237152
H	0.389504	0.530292	-2.011635
H	0.818456	-1.011902	-2.728666
H	4.686608	-1.398691	-1.292328
H	1.332785	1.330875	-4.372201
H	3.075581	1.172828	-4.650503
H	2.028528	-0.256246	-4.743371
H	-0.952650	-2.851807	-1.272261
H	6.371013	0.211707	-2.156891
H	7.680259	2.243749	-1.578136
H	4.610566	3.448389	1.139324



H	3.301899	1.416907	0.573691	C	-1.774766	2.906485	-0.275267
H	-0.979930	1.052354	1.929104	O	-3.180627	2.772273	-0.049142
H	-0.012773	1.452594	0.516246	C	-3.765957	1.752870	-0.834021
H	-1.762345	2.917259	-0.348640	C	-1.328511	4.183112	0.398427
H	-4.022996	2.046848	-0.877662	F	7.152946	3.528229	-0.821543
H	-1.943093	4.594650	1.452888	O	-4.843886	-0.565297	-1.832217
H	-0.313353	3.900334	1.446561	C	-5.888105	-1.401028	-1.321281
H	-1.492239	3.377130	2.661945	O	-3.540950	-2.980958	-1.828289
H	-6.830632	-1.124799	-1.314903	C	-2.863313	-4.228955	-1.830462
H	-5.698205	-2.475560	-1.591592	C	-5.206936	1.676957	-0.331000
H	-5.800442	-1.703956	0.018282	O	-6.126845	2.233584	-0.877723
H	-3.431819	-4.516613	-3.241824	O	-5.306058	0.994940	0.804869
H	-1.878512	-3.648298	-3.214249	C	-6.867061	2.180812	2.260788
H	-2.441140	-4.525678	-1.763282	C	-6.605117	0.939473	1.438733
H	-9.412710	2.496552	0.517205	O	-0.588993	-0.786250	2.567810
H	-8.109324	3.664284	0.259649	C	-1.105539	-2.012629	3.079132
H	-8.458438	2.434727	-0.971237	O	1.880632	-1.075036	3.686296
H	-7.743389	0.635507	0.625301	C	2.431359	-2.275727	4.234234
H	-7.399175	1.859951	1.855441	C	4.608969	-0.072766	2.775274
H	0.319817	-2.071940	4.225446	O	4.158840	-1.178923	1.987194
H	0.049580	-0.442225	3.550548	H	2.860535	0.354250	-2.573544
H	-1.333339	-1.517667	3.854844	H	0.552292	-0.261282	-2.266115
H	4.099530	-1.366683	3.584921	H	0.928242	-1.974484	-2.284425
H	2.546283	-0.674893	4.126274	H	4.603878	-1.933132	-0.406215
H	3.156745	-2.176059	4.865313	H	1.743937	-0.496097	-4.640669
H	5.932143	-3.041545	1.513587	H	3.489407	-0.801653	-4.650400
H	4.331521	-3.587980	2.082120	H	2.359433	-2.119858	-4.287414
H	4.694657	-3.541203	0.333641	H	-1.093227	-2.896732	-0.670990
$\omega$ B97X Energy = -2096.10473283 a.u.				H	3.183777	1.504708	-0.314956
(aS,1S,3S,1'S,3'S)-22, Conf AO				H	4.603180	3.537488	-0.386717
C	0.503436	-0.926891	1.751604	H	8.038555	1.125897	-1.191226
C	1.774393	-1.046501	2.322357	H	6.619008	-0.913468	-1.145462
C	2.886978	-1.075925	1.485001	H	-1.091812	1.693580	1.356831
C	2.730302	-1.063431	0.098976	H	-0.015820	1.701742	-0.034502
C	1.460132	-0.988526	-0.461822	H	-1.608527	2.980173	-1.359600
C	0.336707	-0.912116	0.371411	H	-3.830717	2.080308	-1.879733
O	3.656210	-1.490834	-2.108658	H	-1.847267	5.044580	-0.023713
C	2.610895	-0.708905	-2.685631	H	-0.254759	4.323300	0.261527
C	1.303719	-0.995830	-1.964399	H	-1.537507	4.136671	1.469487
C	3.970025	-1.122769	-0.769860	H	-6.824214	-0.904919	-1.574646
C	2.549363	-1.051953	-4.156891	H	-5.852410	-2.389897	-1.775364
C	4.801436	0.152719	-0.738078	H	-5.806075	-1.493386	-0.235202
C	-1.041602	-0.814871	-0.196222	H	-3.530142	-4.930724	-2.325127
C	-1.711416	0.405592	-0.240377	H	-1.923573	-4.166965	-2.385920
C	-3.004856	0.443798	-0.761414	H	-2.664620	-4.572551	-0.811700
C	-3.601415	-0.701594	-1.271598	H	-7.824698	2.078262	2.774090
C	-2.911829	-1.918454	-1.262478	H	-6.087786	2.317182	3.012047
C	-1.642273	-1.964052	-0.702264	H	-6.909970	3.068319	1.628623
C	4.244433	1.409166	-0.522167	H	-7.364597	0.799189	0.668932
C	5.028336	2.555504	-0.553419	H	-6.559643	0.048857	2.063199
C	6.378506	2.418169	-0.796963	H	-1.396989	-2.678202	2.260767
C	6.972601	1.189926	-1.010772	H	-0.371188	-2.512172	3.716237
C	6.169715	0.060434	-0.981015	H	-1.983387	-1.760296	3.670791
C	-1.068335	1.674092	0.261461	H	2.318069	-2.197653	5.313479
				H	1.881864	-3.149219	3.871949
				H	3.486954	-2.382891	3.978692

H	4.044851	0.005993	3.706196
H	5.657934	-0.262508	2.993366
H	4.518267	0.858423	2.210227

ωB97X Energy = -2096.10472392 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf A

C	-1.029441	2.050541	0.700135
C	-2.321383	2.448631	0.348339
C	-3.128127	1.580594	-0.378175
C	-2.640893	0.337089	-0.782213
C	-1.347079	-0.047111	-0.444926
C	-0.536692	0.810243	0.311194
O	-2.795356	-1.573754	-2.278539
C	-1.918638	-2.300321	-1.418112
C	-0.816352	-1.379526	-0.919455
C	-3.537699	-0.559947	-1.609998
C	-1.382313	-3.474258	-2.205643
C	-4.695704	-1.160535	-0.824506
C	0.854472	0.421818	0.692849
C	1.922660	0.655886	-0.169347
C	3.198317	0.239648	0.213997
C	3.414440	-0.354278	1.450257
C	2.346233	-0.544688	2.334410
C	1.069787	-0.176952	1.930718
C	-4.618512	-1.432410	0.537864
C	-5.678491	-2.025059	1.211700
C	-6.817258	-2.332666	0.497715
C	-6.937769	-2.075286	-0.853833
C	-5.864847	-1.488628	-1.506670
C	1.732031	1.364537	-1.488155
C	3.045023	1.919207	-2.012299
O	4.026831	0.879615	-1.992974
C	4.392416	0.496943	-0.682743
C	2.948491	2.423932	-3.433032
F	-7.859436	-2.903044	1.146509
O	4.708271	-0.655962	1.791361
C	4.986197	-2.026072	2.105597
O	2.643337	-1.065595	3.552509
C	1.581733	-1.227253	4.482070
C	5.245233	-0.754000	-0.885740
O	4.796014	-1.847225	-1.126905
O	6.541444	-0.473761	-0.830081
C	8.855545	-1.029631	-0.920207
C	7.455083	-1.571583	-1.053614
O	-0.213038	2.931739	1.360284
C	-0.504617	3.078476	2.750770
O	-2.784378	3.684246	0.719223
C	-2.473268	4.709457	-0.226744
C	-5.348128	2.144494	0.239859
O	-4.375955	1.962995	-0.794617
H	-2.494040	-2.673677	-0.560847
H	-0.267444	-1.873287	-0.113807
H	-0.097661	-1.213158	-1.730954
H	-3.966521	0.038924	-2.415076

H	-0.685089	-4.051359	-1.595314
H	-2.194758	-4.131476	-2.518523
H	-0.854745	-3.121968	-3.095007
H	0.223770	-0.336337	2.587239
H	-3.724883	-1.169666	1.093558
H	-5.627403	-2.239003	2.272125
H	-7.853601	-2.325978	-1.374769
H	-5.942303	-1.277527	-2.568217
H	1.317266	0.677135	-2.234852
H	1.013235	2.179516	-1.371718
H	3.387948	2.728056	-1.351396
H	5.024826	1.272530	-0.232382
H	3.904177	2.831916	-3.764152
H	2.193357	3.208991	-3.500797
H	2.662766	1.610486	-4.103629
H	4.657817	-2.673826	1.288878
H	6.067530	-2.095771	2.212478
H	4.501671	-2.319469	3.035493
H	2.033476	-1.630065	5.385067
H	1.107653	-0.268142	4.708295
H	0.831088	-1.928322	4.107734
H	9.573304	-1.836273	-1.076031
H	9.044749	-0.253357	-1.662760
H	9.017717	-0.612250	0.074446
H	7.246066	-2.348734	-0.315991
H	7.267905	-1.982173	-2.047125
H	-0.355981	2.128200	3.272679
H	0.194427	3.816768	3.138633
H	-1.528488	3.428290	2.897596
H	-1.390980	4.805708	-0.345314
H	-2.935378	4.491464	-1.193233
H	-2.880759	5.636642	0.171347
H	-5.039023	2.928805	0.931353
H	-6.271807	2.433006	-0.257810
H	-5.505014	1.206627	0.779746

ωB97X Energy = -2096.10658614 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf B

C	-0.978231	2.038952	0.557678
C	-2.265903	2.451188	0.206763
C	-3.108409	1.564429	-0.453327
C	-2.661846	0.286255	-0.791186
C	-1.372008	-0.112740	-0.455954
C	-0.525090	0.765845	0.232624
O	-2.901807	-1.709091	-2.162005
C	-2.024085	-2.403813	-1.276895
C	-0.886461	-1.484620	-0.861158
C	-3.600025	-0.633132	-1.545586
C	-1.537706	-3.639071	-2.000432
C	-4.760370	-1.143968	-0.702427
C	0.864391	0.367084	0.610527
C	1.921528	0.544952	-0.278885
C	3.200192	0.144876	0.112641
C	3.420896	-0.391338	1.371348
C	2.358377	-0.576623	2.260909

C	1.083642	-0.193049	1.867007
C	-4.656156	-1.353537	0.669240
C	-5.721205	-1.865044	1.399006
C	-6.892698	-2.153904	0.731401
C	-7.040707	-1.955689	-0.627247
C	-5.961846	-1.450707	-1.336326
C	1.720299	1.180438	-1.632907
C	3.033411	1.677452	-2.213345
O	4.001417	0.626675	-2.140506
C	4.385492	0.332945	-0.814666
C	2.919924	2.086775	-3.663244
F	-7.939873	-2.644424	1.435049
O	4.691377	-0.794360	1.702332
C	5.363802	0.062647	2.628023
O	2.664542	-1.131184	3.460072
C	1.607917	-1.314982	4.391410
C	5.229077	-0.936885	-0.926413
O	4.776716	-2.026255	-1.174174
O	6.522886	-0.676420	-0.780154
C	8.820260	-1.287119	-0.637338
C	7.421861	-1.804413	-0.860345
O	-0.128247	2.934247	1.154029
C	-0.379241	3.145760	2.544158
O	-2.691594	3.716773	0.515525
C	-2.337492	4.687905	-0.471562
C	-5.302919	2.217404	0.168549
O	-4.353694	1.954959	-0.869665
H	-2.588243	-2.707664	-0.385291
H	-0.330404	-1.944335	-0.040582
H	-0.184697	-1.386340	-1.698003
H	-4.026407	-0.072469	-2.379001
H	-0.844917	-4.198497	-1.369003
H	-2.375226	-4.289325	-2.256672
H	-1.018722	-3.358575	-2.919895
H	0.240087	-0.330938	2.531794
H	-3.736802	-1.103850	1.187701
H	-5.649010	-2.031081	2.466736
H	-7.981421	-2.188190	-1.110898
H	-6.060789	-1.285942	-2.404243
H	1.277870	0.458994	-2.329994
H	1.019957	2.015592	-1.552520
H	3.399012	2.523558	-1.614213
H	5.026838	1.136112	-0.428800
H	3.874579	2.459886	-4.035907
H	2.172189	2.874277	-3.772619
H	2.614753	1.232950	-4.272316
H	6.357469	-0.357134	2.772252
H	5.451070	1.073937	2.219961
H	4.833925	0.092073	3.581821
H	2.061984	-1.749358	5.278428
H	1.140656	-0.361071	4.651212
H	0.850774	-1.998990	3.998804
H	9.527198	-2.116403	-0.688710
H	9.091767	-0.556696	-1.400591
H	8.910019	-0.819803	0.344372
H	7.127743	-2.529988	-0.099657

H	7.308684	-2.269676	-1.840855
H	0.337573	3.892348	2.880178
H	-1.395054	3.513759	2.703018
H	-0.226219	2.217611	3.103227
H	-2.719090	5.644468	-0.119971
H	-1.251608	4.744205	-0.581928
H	-2.796979	4.441450	-1.432482
H	-4.966945	3.036005	0.805593
H	-6.230209	2.493173	-0.329683
H	-5.467342	1.317374	0.767426

$\omega$ B97X Energy = -2096.10634044 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf C

C	-0.972039	2.051791	0.597888
C	-2.272743	2.447246	0.276394
C	-3.108877	1.559911	-0.390855
C	-2.643804	0.298605	-0.765261
C	-1.341459	-0.083154	-0.459736
C	-0.500083	0.795641	0.235583
O	-2.866123	-1.666581	-2.181061
C	-1.963420	-2.366350	-1.325524
C	-0.837075	-1.436416	-0.903121
C	-3.575758	-0.620141	-1.527963
C	-1.464780	-3.573994	-2.086467
C	-4.713172	-1.175385	-0.681568
C	0.902463	0.414261	0.581648
C	1.938668	0.614895	-0.327443
C	3.229982	0.226713	0.033012
C	3.484402	-0.316680	1.282079
C	2.443029	-0.525293	2.191196
C	1.155415	-0.155000	1.827612
C	-5.914791	-1.497039	-1.307872
C	-6.972961	-2.041952	-0.597284
C	-6.804157	-2.264470	0.755185
C	-5.631726	-1.962215	1.415110
C	-4.587532	-1.410973	0.683979
C	1.703222	1.263575	-1.669679
C	2.998832	1.784441	-2.268469
O	3.980150	0.744357	-2.230020
C	4.393497	0.434668	-0.916185
C	2.851647	2.213068	-3.709741
F	-7.831213	-2.793790	1.460396
O	4.767027	-0.706703	1.579604
C	5.444273	0.133356	2.516781
O	2.780886	-1.089209	3.377581
C	1.746553	-1.295050	4.329056
C	5.241990	-0.828805	-1.066293
O	4.785449	-1.922868	-1.282345
O	6.539266	-0.545910	-1.001932
C	7.668406	-2.307596	0.241048
C	7.466147	-1.651012	-1.105813
O	-0.129309	2.948468	1.202337
C	-0.370777	3.133766	2.597984
O	-2.717931	3.697056	0.620106
C	-2.385177	4.699761	-0.342607

C	-5.305848	2.154705	0.278951
O	-4.367537	1.936148	-0.779111
H	-2.509297	-2.702454	-0.434186
H	-0.261783	-1.904559	-0.100712
H	-0.148571	-1.306681	-1.746642
H	-4.025353	-0.047606	-2.340883
H	-0.751745	-4.134974	-1.479408
H	-2.293397	-4.234100	-2.346398
H	-0.965395	-3.260662	-3.006159
H	0.327840	-0.311450	2.508066
H	-6.030141	-1.312964	-2.370980
H	-7.913672	-2.286587	-1.074916
H	-5.542922	-2.148181	2.478296
H	-3.667919	-1.151133	1.196941
H	1.257164	0.545306	-2.367654
H	0.993742	2.088414	-1.565755
H	3.366285	2.626279	-1.664477
H	5.038879	1.235741	-0.532866
H	3.794490	2.602049	-4.095931
H	2.093479	2.993754	-3.792736
H	2.543569	1.364731	-4.324978
H	4.928794	0.133583	3.478727
H	6.443858	-0.280941	2.635861
H	5.516468	1.155232	2.132837
H	2.224030	-1.734122	5.201366
H	1.274777	-0.349232	4.609519
H	0.988635	-1.983057	3.945073
H	8.400961	-3.111254	0.147804
H	8.042667	-1.585225	0.968513
H	6.734623	-2.729265	0.614666
H	7.090997	-2.356597	-1.846759
H	8.385096	-1.199272	-1.474575
H	0.341282	3.881922	2.940542
H	-1.388934	3.488146	2.771538
H	-0.203554	2.197947	3.139927
H	-2.781400	5.639978	0.035841
H	-1.301009	4.777660	-0.456210
H	-2.845117	4.470758	-1.307625
H	-6.245328	2.425250	-0.198862
H	-5.444537	1.236973	0.857055
H	-4.975757	2.963372	0.931558

$\omega_{B97X}$  Energy = -2096.10609784 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf D

C	-0.926383	2.218321	0.493923
C	-2.233881	2.524078	0.108827
C	-3.005352	1.548991	-0.514421
C	-2.467269	0.290959	-0.786384
C	-1.160077	-0.003162	-0.413207
C	-0.386055	0.962288	0.243881
O	-2.546415	-1.779079	-2.060896
C	-1.642293	-2.369578	-1.128184
C	-0.576516	-1.357165	-0.741125
C	-3.328170	-0.726044	-1.507294
C	-1.060676	-3.604155	-1.779089

C	-4.463459	-1.279238	-0.656732
C	1.017400	0.665958	0.660898
C	2.079921	0.870385	-0.215745
C	3.367427	0.527742	0.198920
C	3.598033	0.036532	1.476708
C	2.534870	-0.125055	2.371294
C	1.248137	0.169957	1.940721
C	-4.378402	-1.394073	0.727206
C	-5.414553	-1.951940	1.464906
C	-6.537416	-2.384785	0.791800
C	-6.665458	-2.284053	-0.579652
C	-5.616157	-1.729694	-1.295763
C	1.867308	1.464469	-1.586669
C	3.163919	2.007039	-2.161760
O	4.175270	1.001543	-2.055376
C	4.554208	0.747081	-0.717794
C	3.052101	2.382292	-3.620948
F	-7.556182	-2.923315	1.502158
O	4.899638	-0.206141	1.829445
C	5.213815	-1.519844	2.303340
O	2.846823	-0.551120	3.622134
C	1.787485	-0.693739	4.557384
C	5.504253	-0.444916	-0.821391
O	6.704234	-0.332055	-0.870133
O	4.857718	-1.599143	-0.931567
C	4.730751	-3.967192	-1.144771
C	5.663114	-2.782553	-1.130337
O	-0.143729	3.197585	1.047760
C	-0.423954	3.468142	2.421410
O	-2.738176	3.774435	0.353722
C	-2.676467	4.642739	-0.780151
C	-5.242510	2.102078	0.056574
O	-4.271741	1.825834	-0.958134
H	-2.202685	-2.665526	-0.231470
H	-0.007012	-1.736904	0.110476
H	0.133689	-1.252518	-1.570312
H	-3.778157	-0.237537	-2.373118
H	-0.341964	-4.080158	-1.109276
H	-1.846894	-4.323525	-2.012047
H	-0.546391	-3.336389	-2.704992
H	0.405484	0.030539	2.606142
H	-3.497460	-1.034250	1.247789
H	-5.356846	-2.046392	2.542221
H	-7.568365	-2.629900	-1.067578
H	-5.699615	-1.640237	-2.373925
H	1.465811	0.708718	-2.272261
H	1.129427	2.268784	-1.532512
H	3.485061	2.879722	-1.575286
H	5.158574	1.581030	-0.338220
H	3.996350	2.784092	-3.990219
H	2.276550	3.138478	-3.754917
H	2.787036	1.505334	-4.215819
H	6.290326	-1.634805	2.184367
H	4.937658	-1.634598	3.350214
H	4.697474	-2.274955	1.704168
H	2.249138	-1.024149	5.484442

H	1.278494	0.259810	4.723311
H	1.063834	-1.442564	4.224736
H	5.305621	-4.880541	-1.303834
H	4.200497	-4.057110	-0.195039
H	3.998142	-3.877077	-1.947824
H	6.204444	-2.675388	-2.071789
H	6.392688	-2.846803	-0.320920
H	-0.208930	2.587365	3.034496
H	0.232425	4.283497	2.719064
H	-1.465618	3.768205	2.553233
H	-3.105437	5.593372	-0.469740
H	-1.638388	4.792656	-1.088744
H	-3.255552	4.232138	-1.611145
H	-4.990401	3.012459	0.601306
H	-6.192712	2.229188	-0.458174
H	-5.315780	1.259720	0.749897

$\omega$ B97X Energy = -2096.10605516 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf E

C	-0.869220	2.216215	0.320760
C	-2.167230	2.534386	-0.085884
C	-2.971714	1.542138	-0.634797
C	-2.475754	0.249385	-0.809348
C	-1.175425	-0.056309	-0.421901
C	-0.367428	0.930680	0.158275
O	-2.632076	-1.912204	-1.915150
C	-1.735428	-2.454816	-0.946809
C	-0.635465	-1.447983	-0.651850
C	-3.374529	-0.793930	-1.441193
C	-1.197658	-3.753279	-1.504557
C	-4.517285	-1.241688	-0.539957
C	1.030477	0.624816	0.587459
C	2.088312	0.728567	-0.312580
C	3.372446	0.397078	0.121969
C	3.598818	0.004969	1.431745
C	2.536425	-0.102861	2.334038
C	1.256010	0.210630	1.898049
C	-4.428745	-1.229465	0.848327
C	-5.474228	-1.691465	1.637404
C	-6.609254	-2.159824	1.010272
C	-6.740287	-2.185910	-0.364444
C	-5.682078	-1.724803	-1.131640
C	1.881305	1.214309	-1.726110
C	3.187899	1.676579	-2.347916
O	4.174751	0.656491	-2.168494
C	4.557418	0.496545	-0.818096
C	3.075212	1.939388	-3.831330
F	-7.637253	-2.605289	1.770013
O	4.875018	-0.343071	1.799692
C	5.525427	0.596253	2.659419
O	2.846498	-0.522515	3.586210
C	1.788379	-0.631041	4.527698
C	5.456889	-0.739476	-0.819641
O	6.660952	-0.678110	-0.870213
O	4.763096	-1.868901	-0.835911

C	4.540672	-4.239922	-0.824432
C	5.522307	-3.096828	-0.873645
O	-0.057337	3.207558	0.807955
C	-0.334093	3.582751	2.157879
O	-2.637700	3.813607	0.058900
C	-2.343146	4.650800	-1.061496
C	-5.188754	2.208843	-0.110709
O	-4.227659	1.828228	-1.100387
H	-2.293409	-2.661765	-0.023988
H	-0.064629	-1.778706	0.219071
H	0.064819	-1.427975	-1.495622
H	-3.818216	-0.361869	-2.339592
H	-0.480956	-4.193833	-0.808843
H	-2.006029	-4.467118	-1.668461
H	-0.691241	-3.573655	-2.455776
H	0.412478	0.127096	2.571837
H	-3.537934	-0.842321	1.331100
H	-5.414384	-1.684594	2.718737
H	-7.652182	-2.556470	-0.816181
H	-5.767487	-1.736542	-2.213333
H	1.458363	0.415673	-2.347015
H	1.163717	2.038510	-1.735373
H	3.534992	2.583708	-1.833092
H	5.197947	1.334634	-0.512633
H	4.025950	2.288957	-4.235400
H	2.316323	2.700673	-4.020309
H	2.786265	1.025106	-4.354452
H	6.528664	0.212515	2.833175
H	5.588162	1.576177	2.177392
H	4.993897	0.683262	3.608524
H	2.245533	-0.966656	5.455089
H	1.303577	0.335710	4.689262
H	1.045146	-1.364055	4.202965
H	5.083112	-5.185909	-0.857240
H	3.956537	-4.210448	0.096449
H	3.858576	-4.205257	-1.675032
H	6.117585	-3.107620	-1.788397
H	6.202934	-3.106443	-0.020476
H	0.357266	4.385580	2.406243
H	-1.361646	3.938312	2.259132
H	-0.163988	2.736766	2.830888
H	-2.771287	5.627456	-0.844803
H	-1.262519	4.745471	-1.195488
H	-2.796222	4.246071	-1.970379
H	-4.893706	3.135126	0.382637
H	-6.128854	2.353614	-0.639251
H	-5.307862	1.411372	0.627960

$\omega$ B97X Energy = -2096.10591385 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf F

C	-1.034924	2.086242	0.675565
C	-2.339996	2.445784	0.329690
C	-3.129195	1.544273	-0.376816
C	-2.609932	0.312546	-0.775267
C	-1.304673	-0.033858	-0.441857

C	-0.514020	0.852684	0.300905
O	-2.722358	-1.616087	-2.251429
C	-1.822690	-2.311084	-1.388815
C	-0.742267	-1.357344	-0.904408
C	-3.488049	-0.616359	-1.587777
C	-1.259140	-3.477994	-2.167697
C	-4.624563	-1.241419	-0.790080
C	0.887129	0.500837	0.681242
C	1.946069	0.737065	-0.191409
C	3.230515	0.344981	0.188634
C	3.465413	-0.220155	1.435187
C	2.406459	-0.404669	2.332335
C	1.121149	-0.068662	1.929159
C	-5.781957	-1.620588	-1.465960
C	-6.833634	-2.233591	-0.803099
C	-6.703842	-2.465029	0.552291
C	-5.576259	-2.106896	1.260350
C	-4.537348	-1.488923	0.576170
C	1.738681	1.432178	-1.514488
C	3.038616	2.022015	-2.031535
O	4.041935	1.003608	-2.022450
C	4.414910	0.601937	-0.718253
C	2.933165	2.539067	-3.447224
F	-7.725416	-3.061038	1.210901
O	4.766683	-0.494908	1.770689
C	5.060889	-1.847602	2.139361
O	2.718454	-0.887773	3.562568
C	1.664843	-1.043139	4.502199
C	5.256310	-0.650043	-0.965850
O	4.801500	-1.756325	-1.118310
O	6.542439	-0.338443	-1.086160
C	7.880527	-2.225685	-0.282938
C	7.456234	-1.392934	-1.470810
O	-0.232768	2.995318	1.313953
C	-0.519471	3.166161	2.702160
O	-2.821169	3.674986	0.697266
C	-2.833694	4.627024	-0.369423
C	-5.353752	2.063855	0.268123
O	-4.396013	1.878030	-0.779155
H	-2.383943	-2.690982	-0.525014
H	-0.178200	-1.828682	-0.095839
H	-0.030880	-1.181513	-1.720335
H	-3.937912	-0.037471	-2.396017
H	-0.544409	-4.030876	-1.555177
H	-2.055315	-4.159170	-2.471023
H	-0.744606	-3.120252	-3.062516
H	0.282470	-0.228148	2.594897
H	-5.866828	-1.429518	-2.530724
H	-7.740148	-2.524630	-1.319322
H	-5.517138	-2.302758	2.323847
H	-3.652302	-1.188339	1.126408
H	1.349014	0.730685	-2.261635
H	0.996107	2.226296	-1.404098
H	3.362797	2.831202	-1.361640
H	5.061122	1.364837	-0.265845
H	3.881754	2.966701	-3.773908

H	2.164859	3.311851	-3.507189
H	2.661615	1.727682	-4.126152
H	4.567723	-2.114854	3.072219
H	4.753119	-2.529036	1.341887
H	6.141124	-1.896183	2.263318
H	1.176600	-0.086410	4.707252
H	0.923473	-1.765282	4.150192
H	2.128221	-1.415860	5.412206
H	8.648078	-2.935217	-0.596895
H	8.299449	-1.593314	0.501842
H	7.039777	-2.787995	0.123246
H	6.980316	-2.002498	-2.239257
H	8.301170	-0.863710	-1.907141
H	-1.548094	3.501943	2.847938
H	-0.352136	2.229697	3.243174
H	0.169198	3.923783	3.070913
H	-3.489464	4.292803	-1.176976
H	-3.211939	5.557809	0.048377
H	-1.821823	4.782172	-0.753239
H	-5.447831	1.149353	0.860090
H	-5.072838	2.898326	0.911795
H	-6.302079	2.275582	-0.221527

$\omega$ B97X Energy = -2096.10585458 a.u.

(aR,lS,3S,l'S,3'S)-22, Conf G

C	-1.022674	2.102280	0.562004
C	-2.311095	2.466244	0.164157
C	-3.101896	1.542917	-0.510212
C	-2.601358	0.277522	-0.817891
C	-1.311787	-0.074538	-0.432675
C	-0.518598	0.839276	0.273549
O	-2.720851	-1.733848	-2.179354
C	-1.856213	-2.393401	-1.255475
C	-0.767226	-1.434340	-0.801506
C	-3.479664	-0.680241	-1.596104
C	-1.299593	-3.616112	-1.949127
C	-4.648809	-1.230498	-0.790708
C	0.865811	0.487209	0.710937
C	1.954678	0.681262	-0.135112
C	3.223799	0.308154	0.308960
C	3.412551	-0.204315	1.585637
C	2.321807	-0.359350	2.448632
C	1.053216	-0.033886	1.987961
C	-5.807245	-1.603954	-1.467694
C	-6.888708	-2.150933	-0.794875
C	-6.787295	-2.322621	0.571710
C	-5.659813	-1.967213	1.281536
C	-4.591163	-1.415166	0.587210
C	1.791329	1.301626	-1.501202
C	3.112592	1.830905	-2.031429
O	4.103537	0.806342	-1.913375
C	4.438984	0.524080	-0.570226
C	3.047608	2.230704	-3.486965
F	-7.837565	-2.854451	1.239929
O	4.700589	-0.461542	1.979390

C	4.993709	-1.801069	2.394133
O	2.590326	-0.804559	3.702873
C	1.504411	-0.930574	4.609576
C	5.317282	-0.722654	-0.659900
O	4.889260	-1.835461	-0.842064
O	6.606741	-0.414009	-0.575207
C	7.837757	-1.794489	-2.169128
C	7.559899	-1.493971	-0.713851
O	-0.220234	3.033971	1.167665
C	-0.523448	3.268338	2.543369
O	-2.784176	3.722627	0.440298
C	-2.521748	4.664544	-0.602132
C	-5.333007	2.136130	0.035828
O	-4.346512	1.884251	-0.969978
H	-2.445276	-2.710394	-0.384769
H	-0.233039	-1.867924	0.047358
H	-0.033033	-1.321894	-1.608356
H	-3.896968	-0.141652	-2.448415
H	-0.611712	-4.145400	-1.287072
H	-2.102956	-4.298111	-2.230946
H	-0.756397	-3.324129	-2.850887
H	0.190727	-0.164414	2.629272
H	-5.869570	-1.459431	-2.541309
H	-7.796321	-2.436524	-1.312199
H	-5.623793	-2.115093	2.353788
H	-3.706098	-1.115669	1.138054
H	1.396991	0.564193	-2.210414
H	1.065695	2.117510	-1.454411
H	3.431653	2.688846	-1.422488
H	5.045124	1.341401	-0.159439
H	4.007556	2.624424	-3.823041
H	2.286890	3.000111	-3.630449
H	2.787004	1.367249	-4.103145
H	6.077893	-1.858790	2.477471
H	4.534269	-2.020963	3.356353
H	4.648334	-2.513505	1.640999
H	0.773538	-1.661215	4.253119
H	1.935201	-1.277739	5.545343
H	1.012121	0.032622	4.770077
H	8.607073	-2.565441	-2.238674
H	6.941441	-2.157860	-2.672867
H	8.198258	-0.902971	-2.684324
H	8.449986	-1.131228	-0.203465
H	7.175066	-2.368212	-0.188036
H	-1.553885	3.609999	2.661152
H	-0.362827	2.357646	3.128501
H	0.160709	4.042316	2.885500
H	-1.445066	4.774604	-0.755829
H	-3.000002	4.348565	-1.533006
H	-2.943299	5.614438	-0.279401
H	-5.047808	2.985585	0.657182
H	-6.257572	2.358287	-0.493265
H	-5.475815	1.247457	0.656770

ωB97X Energy = -2096.10575637 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf H

C	-0.977379	2.089200	0.387047
C	-2.257579	2.457083	-0.032929
C	-3.076603	1.507071	-0.632444
C	-2.611447	0.208804	-0.845065
C	-1.327963	-0.146464	-0.443119
C	-0.506932	0.796441	0.189170
O	-2.805682	-1.907827	-2.030222
C	-1.941892	-2.508011	-1.066096
C	-0.821077	-1.543056	-0.714258
C	-3.525048	-0.784460	-1.533606
C	-1.428446	-3.800019	-1.660450
C	-4.702443	-1.224580	-0.674511
C	0.871446	0.441794	0.643852
C	1.960715	0.570678	-0.214383
C	3.226612	0.213739	0.252364
C	3.404100	-0.231722	1.552712
C	2.309082	-0.370709	2.410859
C	1.047457	-0.029462	1.942894
C	-4.631237	-1.301424	0.712994
C	-5.709639	-1.753992	1.461918
C	-6.860531	-2.119762	0.796235
C	-6.975770	-2.053259	-0.578358
C	-5.884144	-1.605049	-1.305761
C	1.808352	1.115973	-1.612928
C	3.138064	1.603440	-2.162768
O	4.117380	0.574777	-1.991235
C	4.446728	0.352283	-0.636307
C	3.082772	1.932268	-3.636316
F	-7.920529	-2.554105	1.517514
O	4.666571	-0.589164	1.957552
C	5.281538	0.329744	2.863879
O	2.572226	-0.840797	3.655601
C	1.481602	-0.973233	4.555975
C	5.291275	-0.922188	-0.655757
O	4.838250	-2.025595	-0.827772
O	6.584672	-0.645126	-0.525573
C	7.847226	-2.118140	-2.007052
C	7.509399	-1.756162	-0.578469
O	-0.149714	3.040007	0.925707
C	-0.441609	3.370516	2.284094
O	-2.696123	3.742834	0.149178
C	-2.385349	4.602720	-0.949364
C	-5.284803	2.211987	-0.123940
O	-4.315461	1.843485	-1.110135
H	-2.522396	-2.733262	-0.161669
H	-0.276505	-1.921034	0.154153
H	-0.104312	-1.511194	-1.543671
H	-3.934232	-0.308320	-2.426062
H	-0.738872	-4.286001	-0.967701
H	-2.252858	-4.483988	-1.866528
H	-0.897925	-3.600596	-2.594421
H	0.180088	-0.130369	2.583161
H	-3.727619	-0.992579	1.227424
H	-5.663234	-1.817724	2.542042
H	-7.901269	-2.342866	-1.060557

H	-5.957187	-1.543362	-2.386641
H	1.410784	0.344441	-2.282920
H	1.091134	1.940496	-1.615233
H	3.463997	2.486686	-1.595142
H	5.075166	1.173685	-0.268029
H	4.048048	2.299024	-3.987308
H	2.330800	2.701594	-3.820368
H	2.815336	1.042365	-4.210505
H	5.352774	1.323212	2.411500
H	4.719009	0.387100	3.797371
H	6.281493	-0.052003	3.059895
H	1.904184	-1.345740	5.485686
H	0.999024	-0.008497	4.735233
H	0.744210	-1.687597	4.180190
H	8.596478	-2.911647	-2.012040
H	6.965629	-2.475206	-2.540303
H	8.257492	-1.256441	-2.535670
H	8.385383	-1.401044	-0.039000
H	7.073179	-2.598220	-0.040995
H	-0.311056	2.493648	2.925703
H	0.268781	4.141016	2.577033
H	-1.459688	3.753729	2.380220
H	-2.851551	4.234275	-1.867001
H	-2.788216	5.583419	-0.704275
H	-1.303046	4.674256	-1.085226
H	-6.213635	2.390878	-0.661891
H	-5.430583	1.394950	0.588132
H	-4.979868	3.116808	0.402310

ωB97X Energy = -2096.10540689 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf I

C	-0.900928	2.128402	0.514536
C	-2.208163	2.486030	0.175692
C	-3.026453	1.553596	-0.453163
C	-2.534694	0.289760	-0.779821
C	-1.226719	-0.055084	-0.455094
C	-0.405926	0.865757	0.208640
O	-2.720534	-1.740791	-2.106012
C	-1.806569	-2.383708	-1.218425
C	-0.696568	-1.415536	-0.841876
C	-3.449555	-0.678449	-1.501193
C	-1.287161	-3.618586	-1.919256
C	-4.577329	-1.216791	-0.631270
C	1.000342	0.523485	0.579782
C	2.043699	0.724664	-0.320676
C	3.339534	0.379065	0.067270
C	3.589215	-0.124424	1.333870
C	2.540210	-0.337210	2.233190
C	1.249331	-0.007346	1.843407
C	-5.765214	-1.605358	-1.245949
C	-6.811824	-2.142992	-0.513351
C	-6.645397	-2.290223	0.849710
C	-5.486746	-1.919604	1.498850
C	-4.453840	-1.377276	0.745161
C	1.809169	1.332208	-1.682147

C	3.098201	1.872216	-2.277767
O	4.107124	0.861501	-2.197658
C	4.510635	0.598639	-0.869872
C	2.960169	2.257818	-3.732003
F	-7.661189	-2.812524	1.576288
O	4.876606	-0.472121	1.659922
C	5.515349	0.411223	2.584871
O	2.874465	-0.863662	3.437886
C	1.832040	-1.067427	4.380953
C	5.457128	-0.596625	-0.985805
O	6.657656	-0.480580	-1.019780
O	4.802872	-1.741413	-1.130198
C	6.052797	-3.473625	0.052693
C	5.590665	-2.944047	-1.285903
O	-0.073016	3.062723	1.079576
C	-0.323794	3.311038	2.463216
O	-2.663193	3.743079	0.476100
C	-2.666409	4.632876	-0.642840
C	-5.228421	2.159497	0.200507
O	-4.297321	1.878069	-0.849218
H	-2.347059	-2.684864	-0.311323
H	-0.109167	-1.837019	-0.022673
H	-0.014112	-1.308428	-1.693558
H	-3.908543	-0.151805	-2.339531
H	-0.567028	-4.138148	-1.284296
H	-2.104575	-4.303622	-2.148369
H	-0.790329	-3.342878	-2.852319
H	0.416508	-0.164603	2.517271
H	-5.878613	-1.479945	-2.317757
H	-7.741631	-2.440229	-0.982433
H	-5.399156	-2.048960	2.570486
H	-3.544445	-1.066290	1.247881
H	1.391248	0.584394	-2.366545
H	1.077052	2.140237	-1.608433
H	3.434373	2.739530	-1.691754
H	5.123274	1.430989	-0.498618
H	3.898761	2.658590	-4.116479
H	2.185091	3.017716	-3.846158
H	2.680557	1.385869	-4.327558
H	4.989511	0.414931	3.541210
H	6.527063	0.035016	2.723127
H	5.555984	1.426294	2.179035
H	1.337469	-0.124842	4.631411
H	1.093241	-1.780112	4.004711
H	2.306725	-1.474924	5.269951
H	6.591848	-4.410826	-0.097483
H	6.718798	-2.765243	0.545880
H	5.200942	-3.667683	0.706139
H	4.917801	-3.641620	-1.781016
H	6.431326	-2.727789	-1.945362
H	-0.153275	2.402832	3.049541
H	0.381065	4.079353	2.774775
H	-1.345189	3.666102	2.614567
H	-3.025920	5.592398	-0.276544
H	-1.654724	4.748539	-1.040898
H	-3.333475	4.265265	-1.426468



H	-5.296003	1.309378	0.884834
H	-4.940690	3.056901	0.749205
H	-6.191901	2.312000	-0.281581

$\omega$ B97X Energy = -2096.10536729 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf J

C	-1.061353	2.094372	0.639420
C	-2.358605	2.458794	0.273228
C	-3.143695	1.558029	-0.438556
C	-2.658900	0.289558	-0.749923
C	-1.366261	-0.071081	-0.379406
C	-0.553133	0.842887	0.303067
O	-2.806084	-1.717121	-2.104947
C	-1.946437	-2.386961	-1.182775
C	-0.841123	-1.440480	-0.742324
C	-3.557066	-0.672141	-1.499011
C	-1.413534	-3.622973	-1.870794
C	-4.693749	-1.247199	-0.660467
C	0.847364	0.493255	0.688654
C	1.890711	0.595862	-0.229059
C	3.179191	0.241294	0.178335
C	3.427063	-0.178540	1.477365
C	2.381837	-0.246238	2.406781
C	1.097265	0.072813	1.992361
C	-5.724653	-1.909180	-1.324960
C	-6.771879	-2.490250	-0.629036
C	-6.769264	-2.397676	0.749651
C	-5.770680	-1.752106	1.445845
C	-4.730190	-1.176190	0.726673
C	1.671603	1.093641	-1.637775
C	2.964241	1.605752	-2.248337
O	3.967952	0.597113	-2.108944
C	4.355564	0.388298	-0.766715
C	2.839064	1.917096	-3.721450
F	-7.789446	-2.959591	1.440767
O	4.729314	-0.431586	1.825412
C	5.019754	-1.750781	2.303366
O	2.713445	-0.600348	3.674731
C	1.673968	-0.662737	4.640869
C	5.219754	-0.870079	-0.819870
O	4.779220	-1.987300	-0.933291
O	6.513650	-0.575411	-0.794187
C	8.829933	-1.128892	-0.755183
C	7.435291	-1.685148	-0.889874
O	-0.310316	2.959820	1.390987
C	0.244712	4.052714	0.659620
O	-2.832011	3.701660	0.601330
C	-3.697025	3.700507	1.739572
C	-4.544105	2.886133	-1.795499
O	-4.430708	1.876403	-0.787645
H	-2.537228	-2.685760	-0.306367
H	-0.308134	-1.874005	0.107575
H	-0.110973	-1.347354	-1.554519
H	-4.008216	-0.137395	-2.337539
H	-0.728478	-4.157425	-1.209956

H	-2.229263	-4.295005	-2.140971
H	-0.872966	-3.346489	-2.779060
H	0.271071	0.026052	2.690113
H	-5.706927	-1.973214	-2.407987
H	-7.579569	-3.002418	-1.137305
H	-5.808661	-1.700744	2.527018
H	-3.941139	-0.662235	1.264477
H	1.285256	0.288087	-2.272824
H	0.921656	1.888090	-1.647402
H	3.296701	2.501459	-1.703913
H	4.985919	1.220843	-0.429210
H	3.783350	2.291392	-4.118488
H	2.070480	2.675525	-3.880486
H	2.558053	1.017591	-4.273757
H	4.666163	-2.497166	1.587581
H	6.104176	-1.808879	2.383304
H	4.565945	-1.921642	3.278186
H	2.149473	-0.958705	5.572574
H	1.196664	0.312261	4.769846
H	0.921596	-1.405859	4.364134
H	9.553679	-1.941909	-0.828038
H	9.040705	-0.409057	-1.547128
H	8.960623	-0.638181	0.210234
H	7.201143	-2.397864	-0.097019
H	7.281803	-2.178556	-1.851082
H	0.967222	3.692765	-0.079537
H	-0.540470	4.626784	0.163444
H	0.757373	4.683705	1.382907
H	-4.582910	3.089734	1.549353
H	-3.167975	3.324570	2.619297
H	-3.993538	4.733931	1.907187
H	-5.607745	3.012376	-1.986069
H	-4.114419	3.828354	-1.452258
H	-4.045087	2.562696	-2.713533

$\omega$ B97X Energy = -2096.10534483 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf K

C	-1.078716	2.179496	0.006280
C	-2.381655	2.409795	-0.450934
C	-3.140072	1.331494	-0.896344
C	-2.613550	0.038397	-0.869272
C	-1.324146	-0.184212	-0.401862
C	-0.543015	0.897053	0.029287
O	-2.720308	-2.278840	-1.605122
C	-1.866258	-2.638887	-0.520189
C	-0.775489	-1.591283	-0.368143
C	-3.482064	-1.101686	-1.360520
C	-1.312480	-4.014460	-0.815148
C	-4.668677	-1.403100	-0.454310
C	0.858282	0.692706	0.505223
C	1.906356	0.526356	-0.398173
C	3.192322	0.306230	0.100912
C	3.435380	0.285511	1.466896
C	2.386072	0.490641	2.371035
C	1.103190	0.671616	1.875730

C	-5.800355	-1.990168	-1.015327
C	-6.895032	-2.331155	-0.236609
C	-6.834765	-2.076731	1.119594
C	-5.735293	-1.497249	1.716300
C	-4.651913	-1.159426	0.915106
C	1.696116	0.593702	-1.891944
C	2.993360	0.904695	-2.617416
O	3.991267	-0.024566	-2.187562
C	4.372062	0.159402	-0.839170
C	2.875836	0.778293	-4.118419
F	-7.898777	-2.403573	1.890511
O	4.736637	0.145757	1.876640
C	5.026156	-0.966366	2.732490
O	2.711427	0.521320	3.688596
C	1.667647	0.742379	4.626305
C	5.214593	-1.074896	-0.521888
O	4.754901	-2.164915	-0.286171
O	6.513009	-0.813392	-0.607530
C	8.821692	-1.391077	-0.513264
C	7.415879	-1.921213	-0.389132
O	-0.333947	3.241483	0.456655
C	0.262514	4.025063	-0.577225
O	-2.887436	3.678521	-0.547134
C	-3.122419	4.340324	0.700362
C	-5.393292	2.064812	-0.605658
O	-4.385182	1.491637	-1.439564
H	-2.461948	-2.678931	0.401479
H	-0.237084	-1.758942	0.567980
H	-0.047342	-1.722701	-1.176489
H	-3.881807	-0.827890	-2.338360
H	-0.623793	-4.321409	-0.025770
H	-2.116780	-4.748597	-0.878882
H	-0.769990	-4.006436	-1.763403
H	0.273662	0.825665	2.553794
H	-5.829913	-2.180795	-2.083154
H	-7.781507	-2.781276	-0.666121
H	-5.731261	-1.311573	2.783304
H	-3.787361	-0.689990	1.371974
H	1.311580	-0.360746	-2.269164
H	0.947566	1.350961	-2.136815
H	3.327937	1.918434	-2.353043
H	5.015202	1.044338	-0.753420
H	3.825571	1.013178	-4.600270
H	2.115856	1.465498	-4.494286
H	2.587723	-0.239942	-4.389046
H	6.111709	-1.017146	2.801377
H	4.596822	-0.819875	3.722319
H	4.645292	-1.890747	2.291292
H	2.139234	0.732756	5.605716
H	1.189194	1.711505	4.462155
H	0.916765	-0.050514	4.576399
H	9.531510	-2.205358	-0.360910
H	8.991575	-0.967674	-1.504032
H	9.014883	-0.622129	0.235915
H	7.221702	-2.335143	0.602177
H	7.202021	-2.692277	-1.131041

H	1.023490	3.445291	-1.108209
H	-0.492383	4.379611	-1.282890
H	0.735681	4.875573	-0.090488
H	-3.596701	5.289546	0.458986
H	-3.794907	3.746049	1.325941
H	-2.186341	4.515711	1.230975
H	-5.384930	1.596606	0.382642
H	-5.259623	3.142237	-0.509452
H	-6.344835	1.856889	-1.091676

$\omega$ B97X Energy = -2096.10531944 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf L

C	-0.974845	2.224834	0.361127
C	-2.270437	2.504853	-0.079930
C	-3.026110	1.492603	-0.660805
C	-2.483663	0.218394	-0.832990
C	-1.186285	-0.049309	-0.409452
C	-0.427848	0.957052	0.203582
O	-2.537347	-1.935915	-1.962054
C	-1.652009	-2.459450	-0.973040
C	-0.594819	-1.420725	-0.635675
C	-3.329282	-0.847396	-1.499725
C	-1.057850	-3.734383	-1.527776
C	-4.481376	-1.340630	-0.634640
C	0.962790	0.686723	0.677450
C	2.050732	0.835196	-0.179145
C	3.324067	0.512641	0.291181
C	3.515957	0.095743	1.601346
C	2.427346	-0.009128	2.473392
C	1.155023	0.265735	1.990173
C	-5.613463	-1.854589	-1.262731
C	-6.676747	-2.357247	-0.529377
C	-6.583883	-2.341319	0.848622
C	-5.482103	-1.843257	1.511210
C	-4.431084	-1.339720	0.755616
C	1.880952	1.348519	-1.587890
C	3.197003	1.852748	-2.153879
O	4.198817	0.849763	-1.963415
C	4.537994	0.666448	-0.603627
C	3.129227	2.148625	-3.633834
F	-7.617136	-2.827513	1.575552
O	4.805165	-0.133877	2.003663
C	5.098069	-1.421690	2.556197
O	2.702607	-0.364729	3.754429
C	1.616439	-0.461809	4.664311
C	5.472321	-0.542957	-0.610736
O	6.674750	-0.448205	-0.610870
O	4.805886	-1.689699	-0.687860
C	5.988264	-3.156820	-2.238867
C	5.578698	-2.906881	-0.805436
O	-0.209827	3.238234	0.877909
C	-0.531691	3.589947	2.224012
O	-2.785363	3.766888	0.064832
C	-2.514246	4.615864	-1.052489
C	-5.278561	2.079435	-0.194182

O	-4.277219	1.742856	-1.159606
H	-2.229715	-2.694355	-0.069166
H	-0.040055	-1.741562	0.249203
H	0.129591	-1.369315	-1.457493
H	-3.761700	-0.421421	-2.406486
H	-0.347015	-4.159621	-0.816744
H	-1.838751	-4.471130	-1.720916
H	-0.531709	-3.529334	-2.463003
H	0.293043	0.168008	2.638078
H	-5.668982	-1.857522	-2.346436
H	-7.563935	-2.751772	-1.009152
H	-5.452174	-1.845706	2.593822
H	-3.566680	-0.928882	1.265981
H	1.496160	0.555635	-2.240272
H	1.146023	2.157212	-1.602471
H	3.506275	2.754578	-1.606571
H	5.143815	1.512466	-0.254415
H	4.085761	2.526367	-3.996860
H	2.361913	2.899351	-3.830895
H	2.876723	1.241673	-4.187756
H	4.807552	-1.472010	3.604348
H	4.581224	-2.204803	1.995159
H	6.174595	-1.555127	2.457840
H	2.051159	-0.745220	5.619539
H	1.103185	0.498142	4.768652
H	0.902534	-1.227004	4.348266
H	6.501982	-4.117315	-2.306475
H	5.112818	-3.189744	-2.889069
H	6.665529	-2.379838	-2.594808
H	6.443156	-2.838701	-0.144319
H	4.908801	-3.683427	-0.440150
H	0.113322	4.424745	2.491072
H	-1.577593	3.893001	2.306408
H	-0.332845	2.749121	2.895688
H	-2.968934	5.579656	-0.832275
H	-1.436539	4.740724	-1.185753
H	-2.955869	4.202024	-1.962882
H	-6.208990	2.191930	-0.747168
H	-5.387157	1.273082	0.536367
H	-5.033537	3.012891	0.312940

ωB97X Energy = -2096.10520155 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf M

C	-1.070001	2.022663	0.827739
C	-2.362603	2.425593	0.474506
C	-3.156815	1.561795	-0.274895
C	-2.646555	0.345282	-0.728861
C	-1.346424	-0.030548	-0.410056
C	-0.551264	0.813015	0.377164
O	-2.788964	-1.532281	-2.267413
C	-1.896562	-2.268245	-1.431169
C	-0.802446	-1.344424	-0.920494
C	-3.539655	-0.546322	-1.567492
C	-1.350942	-3.415536	-2.250916
C	-4.677926	-1.186507	-0.784132

C	0.847881	0.435425	0.741808
C	1.898296	0.616013	-0.155900
C	3.183380	0.225743	0.229083
C	3.422004	-0.303741	1.489130
C	2.369972	-0.449255	2.401844
C	1.088616	-0.095254	2.006519
C	-4.581565	-1.488712	0.570472
C	-5.622472	-2.118863	1.240206
C	-6.761661	-2.433357	0.530018
C	-6.900692	-2.147092	-0.813931
C	-5.846650	-1.523122	-1.462854
C	1.693403	1.235567	-1.517659
C	2.991412	1.804116	-2.063207
O	3.993699	0.786025	-2.010601
C	4.367474	0.446793	-0.690864
C	2.881767	2.255269	-3.500943
F	-7.785478	-3.040313	1.174963
O	4.721992	-0.587036	1.821934
C	5.007476	-1.939833	2.198296
O	2.691258	-0.911158	3.637298
C	1.644304	-1.050214	4.587279
C	5.214862	-0.813450	-0.857439
O	4.760043	-1.913819	-1.050868
O	6.512214	-0.534712	-0.829382
C	8.823806	-1.101926	-0.912940
C	7.420775	-1.641790	-1.026212
O	-0.326003	2.816222	1.662359
C	0.324735	3.914417	1.029464
O	-2.817286	3.633959	0.928059
C	-3.158065	4.583731	-0.085812
C	-5.370350	2.038681	0.435893
O	-4.434762	1.901602	-0.638455
H	-2.460144	-2.669757	-0.579013
H	-0.239665	-1.848384	-0.130767
H	-0.095391	-1.154068	-1.735968
H	-3.987700	0.063507	-2.353669
H	-0.639971	-3.996496	-1.660424
H	-2.156723	-4.076985	-2.571994
H	-0.836589	-3.034692	-3.136268
H	0.257338	-0.201579	2.691522
H	-3.687938	-1.220903	1.123825
H	-5.556224	-2.356284	2.294774
H	-7.816116	-2.404808	-1.332158
H	-5.938877	-1.289546	-2.518500
H	1.321311	0.488010	-2.227349
H	0.938272	2.023620	-1.467398
H	3.317671	2.643925	-1.432439
H	5.006447	1.234857	-0.272717
H	3.830575	2.663984	-3.850346
H	2.115786	3.027118	-3.594160
H	2.605444	1.413874	-4.140266
H	6.091491	-2.007494	2.275178
H	4.551029	-2.182654	3.156509
H	4.652699	-2.628504	1.427447
H	2.111874	-1.423110	5.495069
H	1.167760	-0.087861	4.791633

H	0.892868	-1.766493	4.244755
H	9.537968	-1.914644	-1.052830
H	9.012059	-0.344143	-1.674593
H	8.992249	-0.661562	0.070707
H	7.211918	-2.398138	-0.267311
H	7.227930	-2.078091	-2.007645
H	-0.397109	4.571959	0.539109
H	0.839050	4.466299	1.813742
H	1.057962	3.561636	0.297502
H	-3.333991	5.527279	0.426529
H	-2.332383	4.701438	-0.793425
H	-4.055634	4.282537	-0.628402
H	-5.085656	2.851173	1.106719
H	-6.331213	2.258146	-0.024910
H	-5.441712	1.103769	0.997530

ωB97X Energy = -2096.10519018 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf N

C	-1.058052	1.984247	0.907562
C	-2.350073	2.415369	0.585731
C	-3.153068	1.603831	-0.212306
C	-2.669051	0.384460	-0.691026
C	-1.376800	-0.025238	-0.384086
C	-0.562433	0.781119	0.420507
O	-2.819837	-1.404567	-2.324488
C	-1.948862	-2.198870	-1.519492
C	-0.846241	-1.321291	-0.950257
C	-3.569199	-0.460606	-1.567718
C	-1.414376	-3.313326	-2.389978
C	-4.702536	-1.152842	-0.819530
C	0.831092	0.363414	0.759963
C	1.892409	0.682817	-0.083351
C	3.168889	0.219689	0.237494
C	3.393420	-0.506143	1.399608
C	2.333436	-0.782484	2.270850
C	1.055268	-0.365683	1.924012
C	-5.761560	-1.667241	-1.565168
C	-6.807528	-2.342041	-0.957264
C	-6.774273	-2.495048	0.415443
C	-5.747397	-2.001502	1.190587
C	-4.709523	-1.326724	0.559084
C	1.691685	1.526963	-1.317924
C	3.002335	2.125276	-1.797625
O	3.977458	1.084505	-1.899922
C	4.354703	0.559032	-0.643308
C	2.891311	2.775420	-3.156971
F	-7.793016	-3.150541	1.021360
O	4.687517	-0.856738	1.688720
C	4.953307	-2.255978	1.844672
O	2.640232	-1.434768	3.421386
C	1.586872	-1.697663	4.337008
C	5.185783	-0.673254	-0.995600
O	4.715506	-1.719556	-1.368704
O	6.487319	-0.428124	-0.907526
C	8.788094	-1.035246	-1.036463

C	7.376732	-1.505824	-1.279224
O	-0.251680	2.781076	1.681157
C	-0.568547	2.765820	3.074289
O	-2.862302	3.574234	1.105974
C	-2.253472	4.781203	0.635427
C	-4.688956	3.177453	-1.151681
O	-4.447115	1.921353	-0.514739
H	-2.530021	-2.629732	-0.693140
H	-0.302759	-1.873550	-0.179761
H	-0.122128	-1.097504	-1.743099
H	-4.023178	0.192473	-2.315593
H	-0.718022	-3.933802	-1.822778
H	-2.227799	-3.944861	-2.749820
H	-0.885879	-2.898105	-3.251236
H	0.214494	-0.592983	2.567160
H	-5.769059	-1.536434	-2.642302
H	-7.637192	-2.740671	-1.528019
H	-5.762245	-2.141585	2.264444
H	-3.899357	-0.927985	1.159676
H	1.261259	0.924523	-2.126743
H	0.981470	2.330426	-1.107633
H	3.358493	2.858932	-1.060435
H	5.003546	1.273452	-0.121066
H	3.845013	3.211700	-3.456115
H	2.139365	3.566027	-3.133769
H	2.593390	2.036452	-3.904041
H	4.594539	-2.807201	0.971815
H	6.035891	-2.349899	1.914486
H	4.488279	-2.644019	2.749486
H	2.046367	-2.197180	5.186209
H	1.115874	-0.769536	4.672500
H	0.831910	-2.353115	3.894841
H	9.486534	-1.823711	-1.320365
H	9.011177	-0.148431	-1.631107
H	8.944212	-0.801167	0.017440
H	7.129052	-2.381979	-0.677126
H	7.201288	-1.749736	-2.328351
H	-1.597728	3.089997	3.243566
H	-0.422448	1.763416	3.487617
H	0.118396	3.458525	3.556373
H	-2.784767	5.599841	1.116848
H	-1.196878	4.816137	0.902381
H	-2.362615	4.865685	-0.449665
H	-4.693458	3.991909	-0.427946
H	-3.936615	3.368111	-1.922046
H	-5.668377	3.096464	-1.619383

ωB97X Energy = -2096.10517428 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf O

C	-1.006846	2.068830	0.529248
C	-2.297083	2.456241	0.161849
C	-3.116853	1.550267	-0.502702
C	-2.674637	0.255152	-0.763857
C	-1.388332	-0.127803	-0.393595
C	-0.540747	0.789344	0.240648

O	-2.908722	-1.810967	-2.015841
C	-2.048300	-2.459562	-1.079504
C	-0.907925	-1.525378	-0.707038
C	-3.614869	-0.712932	-1.450886
C	-1.563722	-3.741174	-1.718104
C	-4.754116	-1.205459	-0.564973
C	0.853995	0.415842	0.625588
C	1.892386	0.481410	-0.301248
C	3.180436	0.130186	0.111253
C	3.423871	-0.265708	1.415985
C	2.376844	-0.351628	2.339798
C	1.098186	-0.001049	1.932640
C	-4.743897	-1.093886	0.820123
C	-5.788925	-1.595072	1.586707
C	-6.839826	-2.208100	0.939629
C	-6.890041	-2.338985	-0.434923
C	-5.836867	-1.832420	-1.178769
C	1.672882	0.937821	-1.723665
C	2.969111	1.414773	-2.355673
O	3.963275	0.400524	-2.187596
C	4.355784	0.232807	-0.842364
C	2.840725	1.679115	-3.837596
F	-7.865289	-2.696628	1.677061
O	4.700672	-0.631244	1.764107
C	5.382289	0.304901	2.602323
O	2.704700	-0.778305	3.584791
C	1.662317	-0.878386	4.544834
C	5.207033	-1.036807	-0.844834
O	4.760218	-2.146877	-0.989157
O	6.500129	-0.755979	-0.734676
C	8.799662	-1.338445	-0.525212
C	7.407455	-1.880170	-0.728426
O	-0.220699	2.939079	1.238042
C	0.341046	4.000004	0.465596
O	-2.730283	3.724718	0.444476
C	-3.592325	3.793581	1.583100
C	-4.490811	2.860513	-1.902165
O	-4.397564	1.893812	-0.851075
H	-2.627667	-2.699723	-0.177829
H	-0.366266	-1.936380	0.148392
H	-0.195666	-1.487107	-1.539342
H	-4.063605	-0.206337	-2.307921
H	-0.879288	-4.262634	-1.046378
H	-2.402877	-4.402049	-1.939677
H	-1.035529	-3.522680	-2.649177
H	0.269673	-0.044604	2.628063
H	-3.914195	-0.604902	1.318595
H	-5.790534	-1.511094	2.666486
H	-7.738054	-2.822793	-0.903743
H	-5.857289	-1.926772	-2.259528
H	1.274902	0.115955	-2.330127
H	0.931902	1.739935	-1.757090
H	3.313438	2.324404	-1.842545
H	4.995326	1.071085	-0.536267
H	3.787005	2.030584	-4.250382
H	2.079132	2.439761	-4.018124

H	2.548302	0.765035	-4.359093
H	4.870138	0.409530	3.560371
H	6.382297	-0.094083	2.760948
H	5.452553	1.279355	2.110165
H	2.130149	-1.234762	5.459067
H	1.199353	0.094889	4.727930
H	0.899479	-1.592862	4.224337
H	9.513835	-2.163102	-0.523184
H	9.071397	-0.650833	-1.327207
H	8.877380	-0.814792	0.428715
H	7.110211	-2.556165	0.075349
H	7.308542	-2.409597	-1.677536
H	1.040620	3.605250	-0.277858
H	-0.442094	4.577384	-0.029572
H	0.882035	4.638709	1.160942
H	-4.502803	3.213992	1.412918
H	-3.076909	3.423634	2.473390
H	-3.845662	4.842965	1.719385
H	-5.552131	3.014459	-2.085152
H	-4.024746	3.801948	-1.607483
H	-4.015955	2.479019	-2.810683

$\omega B97X$  Energy = -2096.10516780 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf P

C	-1.013803	2.098577	0.587576
C	-2.313337	2.475605	0.233352
C	-3.104197	1.575624	-0.477117
C	-2.634732	0.297733	-0.775255
C	-1.349265	-0.078211	-0.399659
C	-0.529767	0.831846	0.278332
O	-2.784325	-1.692240	-2.153935
C	-1.937920	-2.380581	-1.233217
C	-0.830725	-1.448323	-0.767973
C	-3.533503	-0.649079	-1.542649
C	-1.407018	-3.610327	-1.933904
C	-4.682846	-1.224512	-0.722151
C	0.865402	0.466801	0.669094
C	1.926035	0.663184	-0.211545
C	3.206623	0.273313	0.182787
C	3.434273	-0.259723	1.444573
C	2.372501	-0.417011	2.342772
C	1.091650	-0.073960	1.931357
C	-5.707103	-1.879504	-1.403956
C	-6.765838	-2.459823	-0.725324
C	-6.782113	-2.373353	0.653761
C	-5.791038	-1.734665	1.366650
C	-4.738292	-1.159583	0.664628
C	1.720537	1.301783	-1.563450
C	3.026141	1.832273	-2.129517
O	4.014075	0.800548	-2.060831
C	4.392557	0.494193	-0.734521
C	2.914588	2.255130	-3.575681
F	-7.813871	-2.934617	1.327941
O	4.732491	-0.535378	1.790470
C	5.023725	-1.884389	2.175332

O	2.679745	-0.881800	3.580965
C	1.622718	-1.019116	4.519623
C	5.259515	-0.755710	-0.874249
O	4.822713	-1.863710	-1.065556
O	6.552546	-0.459369	-0.827599
C	8.872341	-0.996491	-0.869683
C	7.478475	-1.556049	-0.999363
O	-0.180175	3.007709	1.184522
C	-0.418312	3.221500	2.573996
O	-2.733464	3.743197	0.530803
C	-3.869955	3.831381	1.395443
C	-4.431917	2.913827	-1.895853
O	-4.373673	1.911612	-0.875857
H	-2.539387	-2.687400	-0.366797
H	-0.313321	-1.896228	0.083961
H	-0.086947	-1.349513	-1.567801
H	-3.972358	-0.101821	-2.379366
H	-0.731027	-4.158438	-1.274926
H	-2.224578	-4.273266	-2.220513
H	-0.856870	-3.324420	-2.833441
H	0.250942	-0.206781	2.600511
H	-5.674266	-1.938713	-2.486884
H	-7.568181	-2.966913	-1.246983
H	-5.843990	-1.688094	2.447407
H	-3.954579	-0.651352	1.215453
H	1.299757	0.574810	-2.268370
H	1.000746	2.119981	-1.482458
H	3.370278	2.678933	-1.518514
H	5.018295	1.300694	-0.331592
H	3.864895	2.649012	-3.937936
H	2.153982	3.030707	-3.681369
H	2.628349	1.402872	-4.196064
H	6.108126	-1.946895	2.251863
H	4.569029	-2.123030	3.135356
H	4.671637	-2.579593	1.409214
H	2.081319	-1.383537	5.435384
H	1.139687	-0.057053	4.711692
H	0.878034	-1.741010	4.174110
H	9.599272	-1.800738	-0.991735
H	9.062023	-0.242777	-1.635016
H	9.020200	-0.545527	0.112475
H	7.267737	-2.307857	-0.236446
H	7.306605	-2.004274	-1.979340
H	-1.414833	3.634921	2.744475
H	-0.305452	2.286405	3.130965
H	0.329902	3.935747	2.911875
H	-4.766532	3.438454	0.914313
H	-3.686730	3.283086	2.324121
H	-4.001384	4.888166	1.618158
H	-5.485061	3.051927	-2.130998
H	-4.003658	3.855241	-1.546128
H	-3.898675	2.577102	-2.789230

ωB97X Energy = -2096.10514261 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf Q

C	-0.919794	2.213484	0.107957
C	-2.209626	2.486005	-0.353378
C	-3.003574	1.441425	-0.813538
C	-2.504378	0.138872	-0.848357
C	-1.211323	-0.123408	-0.408061
C	-0.415496	0.918477	0.086178
O	-2.636646	-2.118478	-1.744156
C	-1.754780	-2.565239	-0.715043
C	-0.664766	-1.529052	-0.492385
C	-3.390235	-0.964575	-1.388820
C	-1.200772	-3.904423	-1.146326
C	-4.543537	-1.330363	-0.464032
C	0.970585	0.660298	0.580319
C	2.054346	0.675400	-0.294309
C	3.326067	0.397221	0.209425
C	3.513823	0.141489	1.558565
C	2.425000	0.120976	2.435340
C	1.157928	0.382793	1.932367
C	-4.474692	-1.184674	0.917801
C	-5.529691	-1.573873	1.733102
C	-6.654270	-2.105237	1.138213
C	-6.765776	-2.263569	-0.229324
C	-5.698414	-1.872862	-1.022637
C	1.888229	1.011653	-1.755733
C	3.209512	1.427029	-2.379513
O	4.199471	0.441653	-2.070009
C	4.539710	0.417466	-0.698993
C	3.142498	1.542271	-3.884372
F	-7.691431	-2.480599	1.922957
O	4.779494	-0.158283	1.997790
C	5.397486	0.865186	2.781944
O	2.698957	-0.166263	3.732431
C	1.613187	-0.190825	4.647969
C	5.452344	-0.800629	-0.555341
O	6.656236	-0.722494	-0.545579
O	4.767038	-1.936024	-0.516213
C	5.993801	-3.601895	-1.815792
C	5.520735	-3.168001	-0.446834
O	-0.116233	3.250332	0.505789
C	-0.417193	3.764413	1.803747
O	-2.683205	3.772176	-0.347211
C	-2.385236	4.487404	-1.548185
C	-5.230626	2.146102	-0.396804
O	-4.250330	1.678983	-1.329154
H	-2.327953	-2.692524	0.212798
H	-0.112694	-1.773530	0.418279
H	0.054207	-1.585480	-1.318647
H	-3.823947	-0.621827	-2.329633
H	-0.492241	-4.276530	-0.403888
H	-2.002347	-4.635703	-1.258379
H	-0.680756	-3.805334	-2.101958
H	0.294769	0.365356	2.585879
H	-3.591993	-0.749679	1.373873
H	-5.485220	-1.462407	2.809424
H	-7.670065	-2.679605	-0.656041
H	-5.768578	-1.988750	-2.099199

H	1.495439	0.147403	-2.304379
H	1.161642	1.819660	-1.871948
H	3.531290	2.384558	-1.945603
H	5.161917	1.289088	-0.456029
H	4.103201	1.860660	-4.290654
H	2.384755	2.273545	-4.170898
H	2.877683	0.578498	-4.324801
H	6.408868	0.524200	2.993740
H	5.439230	1.804042	2.222040
H	4.854700	1.015778	3.716577
H	2.044458	-0.427536	5.617323
H	1.117097	0.782339	4.698517
H	0.885121	-0.959550	4.375811
H	6.489951	-4.570726	-1.735915
H	5.150468	-3.704231	-2.500421
H	6.703385	-2.886002	-2.231620
H	6.353294	-3.028660	0.243128
H	4.820474	-3.884732	-0.021997
H	-0.265257	2.991942	2.563897
H	0.274112	4.585927	1.981052
H	-1.444362	4.132486	1.847276
H	-2.810269	5.482570	-1.433424
H	-1.304124	4.564380	-1.689877
H	-2.838987	3.992478	-2.410893
H	-4.933668	3.102864	0.033340
H	-6.154649	2.263981	-0.959262
H	-5.380765	1.407567	0.395509

ωB97X Energy = -2096.10512907 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf R

C	-1.028305	2.136692	-0.156470
C	-2.328165	2.369623	-0.621391
C	-3.120319	1.283581	-0.980940
C	-2.631460	-0.018665	-0.859176
C	-1.346289	-0.243204	-0.381271
C	-0.531710	0.844018	-0.036262
O	-2.807149	-2.378574	-1.426268
C	-1.953801	-2.685470	-0.324541
C	-0.835452	-1.658602	-0.248731
C	-3.534663	-1.166562	-1.261242
C	-1.436846	-4.091445	-0.529177
C	-4.720241	-1.367638	-0.326249
C	0.866253	0.633990	0.447558
C	1.904016	0.387963	-0.449834
C	3.190508	0.185761	0.055941
C	3.435614	0.244165	1.417736
C	2.390815	0.475291	2.318558
C	1.112309	0.673939	1.818610
C	-4.679364	-1.035054	1.023888
C	-5.763514	-1.283091	1.856152
C	-6.888715	-1.862744	1.309605
C	-6.973684	-2.202847	-0.026307
C	-5.877565	-1.951130	-0.836442
C	1.688174	0.356546	-1.943807
C	2.988379	0.596060	-2.691798

O	3.973349	-0.318702	-2.203872
C	4.364653	-0.050457	-0.874242
C	2.863263	0.372000	-4.180704
F	-7.953430	-2.102435	2.110860
O	4.712577	0.007852	1.863651
C	5.400088	1.165873	2.343515
O	2.719555	0.484824	3.634228
C	1.679976	0.717465	4.574046
C	5.183216	-1.274405	-0.462948
O	4.705036	-2.354226	-0.221415
O	6.485386	-1.015211	-0.472494
C	8.775970	-1.579027	-0.141343
C	7.363226	-2.104767	-0.112470
O	-0.245522	3.204502	0.206610
C	0.328321	3.919323	-0.888676
O	-2.799969	3.641307	-0.808615
C	-3.004630	4.401467	0.387041
C	-5.351746	2.093434	-0.730902
O	-4.363675	1.440389	-1.529208
H	-2.543370	-2.648499	0.601128
H	-0.299003	-1.775017	0.696240
H	-0.112971	-1.864879	-1.046571
H	-3.936235	-0.952870	-2.253129
H	-0.748118	-4.361120	0.273648
H	-2.259572	-4.807667	-0.535931
H	-0.904090	-4.162123	-1.480300
H	0.284542	0.862898	2.490171
H	-3.794796	-0.565556	1.440483
H	-5.740398	-1.028793	2.908647
H	-7.879706	-2.649574	-0.416816
H	-5.926315	-2.209367	-1.889251
H	1.287436	-0.615656	-2.252777
H	0.951182	1.107005	-2.239098
H	3.340206	1.619592	-2.496618
H	5.025782	0.825764	-0.852305
H	3.814325	0.561019	-4.679800
H	2.111318	1.043396	-4.598911
H	2.560114	-0.657746	-4.382497
H	4.905624	1.569617	3.228659
H	6.407859	0.843971	2.598787
H	5.448979	1.932073	1.564278
H	2.149715	0.685518	5.553833
H	1.221738	1.698237	4.421487
H	0.912795	-0.058966	4.513153
H	9.467164	-2.380596	0.122907
H	9.035812	-1.214856	-1.136184
H	8.902610	-0.766434	0.575486
H	7.079710	-2.459846	0.879986
H	7.215012	-2.918393	-0.824449
H	-0.445068	4.263580	-1.578942
H	0.846505	4.776228	-0.462946
H	1.048132	3.291555	-1.422376
H	-2.059990	4.585651	0.899361
H	-3.449800	5.344762	0.076887
H	-3.691691	3.877888	1.058200
H	-6.310871	1.880602	-1.199590

H        -5.351226   1.689800   0.285552  
H        -5.189073   3.170934   -0.705438  
ωB97X Energy = -2096.10501745 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf S

C	-0.972853	2.262748	0.451269
C	-2.284594	2.527115	0.052164
C	-3.023986	1.526383	-0.567760
C	-2.476966	0.259390	-0.761651
C	-1.169677	-0.000400	-0.360689
C	-0.404025	1.011534	0.234253
O	-2.531798	-1.885278	-1.898042
C	-1.637957	-2.410632	-0.916742
C	-0.577693	-1.371088	-0.592088
C	-3.329011	-0.814581	-1.406159
C	-1.049841	-3.687074	-1.473800
C	-4.444261	-1.344050	-0.511320
C	1.010240	0.757631	0.643014
C	2.044479	0.817480	-0.288916
C	3.343875	0.525530	0.131612
C	3.611233	0.213514	1.456775
C	2.575863	0.190360	2.398109
C	1.280192	0.445723	1.972751
C	-5.470934	-2.073626	-1.107807
C	-6.497523	-2.618057	-0.353657
C	-6.477559	-2.420410	1.013597
C	-5.481933	-1.705680	1.643663
C	-4.463224	-1.167495	0.866842
C	1.802322	1.194406	-1.730773
C	3.079111	1.685393	-2.389559
O	4.103668	0.709067	-2.186079
C	4.508515	0.605182	-0.835704
C	2.937039	1.886500	-3.880075
F	-7.477594	-2.945255	1.760955
O	4.921212	0.004105	1.799387
C	5.239452	-1.239933	2.432295
O	2.925723	-0.067064	3.684320
C	1.892286	-0.106042	4.657992
C	5.427072	-0.616054	-0.818842
O	6.626850	-0.543486	-0.919921
O	4.749991	-1.756371	-0.760397
C	4.550035	-4.126481	-0.695766
C	5.517932	-2.978553	-0.831576
O	-0.270232	3.231411	1.120127
C	0.238480	4.277250	0.291865
O	-2.832479	3.765815	0.259658
C	-3.481664	3.886165	1.527362
C	-4.481926	2.628293	-2.054016
O	-4.325268	1.751519	-0.934482
H	-2.209420	-2.640635	-0.007448
H	-0.013620	-1.688556	0.288440
H	0.137379	-1.324956	-1.421580
H	-3.798157	-0.392145	-2.297251
H	-0.332063	-4.110506	-0.768611
H	-1.832813	-4.424208	-1.656978

H	-0.532686	-3.485043	-2.414731
H	0.460017	0.426244	2.678873
H	-5.468048	-2.218405	-2.183172
H	-7.302733	-3.180983	-0.809438
H	-5.506420	-1.571987	2.718134
H	-3.678270	-0.597699	1.351774
H	1.430881	0.331629	-2.295838
H	1.033983	1.968146	-1.797743
H	3.397861	2.624454	-1.914425
H	5.141062	1.462142	-0.570818
H	3.871734	2.247052	-4.311023
H	2.154354	2.618498	-4.086802
H	2.667934	0.944864	-4.363684
H	4.700046	-2.061234	1.952221
H	6.311075	-1.381287	2.298863
H	4.993825	-1.212956	3.492599
H	2.380068	-0.330358	5.603259
H	1.383530	0.858738	4.731726
H	1.163652	-0.888307	4.429270
H	5.094461	-5.070106	-0.751829
H	4.030931	-4.085942	0.263408
H	3.809459	-4.107771	-1.496295
H	6.046826	-2.998499	-1.785860
H	6.258237	-2.971329	-0.029393
H	0.989341	3.887210	-0.402280
H	-0.567982	4.759591	-0.264291
H	0.707293	4.999901	0.956735
H	-4.291725	3.156781	1.612026
H	-2.763820	3.741005	2.338747
H	-3.890870	4.893227	1.577164
H	-5.551888	2.714674	-2.231405
H	-4.062363	3.611965	-1.838397
H	-3.999064	2.203701	-2.939068

ωB97X Energy = -2096.10500889 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf T

C	-0.968031	2.079275	0.451436
C	-2.262747	2.470444	0.095387
C	-3.085685	1.555100	-0.556403
C	-2.652462	0.251791	-0.793435
C	-1.370060	-0.135790	-0.419280
C	-0.518839	0.787446	0.199293
O	-2.886398	-1.813827	-2.045950
C	-2.031429	-2.465895	-1.107208
C	-0.891268	-1.535214	-0.725503
C	-3.592434	-0.714126	-1.484215
C	-1.546208	-3.746743	-1.746894
C	-4.737868	-1.202073	-0.604005
C	0.873455	0.409793	0.589240
C	1.926591	0.556277	-0.310323
C	3.207816	0.173979	0.090537
C	3.434271	-0.316620	1.366808
C	2.375386	-0.471473	2.266489
C	1.098573	-0.103854	1.864278
C	-4.736061	-1.086155	0.780743



C	-5.787119	-1.582523	1.542348
C	-6.835271	-2.195179	0.890590
C	-6.877200	-2.330230	-0.483910
C	-5.818358	-1.828356	-1.222691
C	1.716609	1.138213	-1.686778
C	3.025189	1.614050	-2.294415
O	3.997306	0.570453	-2.182909
C	4.388711	0.333724	-0.847936
C	2.902511	1.962161	-3.759448
F	-7.866394	-2.679171	1.623023
O	4.706466	-0.706128	1.706995
C	5.381238	0.182060	2.600909
O	2.686748	-0.982670	3.483534
C	1.632853	-1.138613	4.423017
C	5.244019	-0.931419	-0.911989
O	4.802554	-2.032357	-1.125923
O	6.534727	-0.654618	-0.768007
C	8.835298	-1.241076	-0.582144
C	7.444068	-1.776407	-0.807542
O	-0.106133	2.994978	0.996152
C	-0.321109	3.271024	2.378557
O	-2.647894	3.761020	0.335176
C	-3.772508	3.919513	1.205497
C	-4.400451	2.846470	-2.027986
O	-4.352541	1.902732	-0.953291
H	-2.615844	-2.707251	-0.208991
H	-0.359376	-1.948359	0.134845
H	-0.169148	-1.496585	-1.549979
H	-4.035247	-0.206810	-2.343688
H	-0.865423	-4.270993	-1.073634
H	-2.385403	-4.405748	-1.973844
H	-1.013693	-3.526596	-2.675102
H	0.258106	-0.218505	2.537349
H	-3.908050	-0.597905	1.282690
H	-5.795391	-1.495295	2.621837
H	-7.723399	-2.813582	-0.956464
H	-5.832161	-1.925919	-2.303266
H	1.270165	0.389170	-2.351607
H	1.016178	1.975314	-1.634984
H	3.391168	2.485568	-1.733164
H	5.023946	1.157603	-0.497057
H	3.853973	2.321959	-4.152773
H	2.151895	2.742413	-3.897398
H	2.596496	1.082693	-4.330411
H	5.463793	1.179820	2.159936
H	4.856313	0.241084	3.556088
H	6.376773	-0.230408	2.753276
H	2.090178	-1.542456	5.322699
H	1.163562	-0.177903	4.652228
H	0.876762	-1.837217	4.054834
H	9.550306	-2.064607	-0.607933
H	9.107900	-0.525189	-1.358677
H	8.910691	-0.751372	0.389827
H	7.147341	-2.484558	-0.031626
H	7.346371	-2.267793	-1.776942
H	-1.306689	3.712025	2.543947

H	-0.220675	2.357375	2.972369
H	0.445861	3.982718	2.677508
H	-4.685691	3.536573	0.748089
H	-3.597494	3.402104	2.153268
H	-3.868286	4.987800	1.387804
H	-3.935116	3.791705	-1.741530
H	-3.897298	2.441931	-2.910611
H	-5.453391	3.005620	-2.250464

ωB97X Energy = -2096.10499030 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf U

C	-0.969590	2.266028	0.094925
C	-2.284623	2.477183	-0.336513
C	-3.019305	1.395729	-0.812938
C	-2.457051	0.117708	-0.841858
C	-1.155288	-0.086220	-0.401197
C	-0.398028	0.999563	0.060217
O	-2.512153	-2.172284	-1.663616
C	-1.632235	-2.548269	-0.605180
C	-0.567490	-1.477595	-0.430883
C	-3.301457	-1.026396	-1.364771
C	-1.046641	-3.896355	-0.959856
C	-4.467353	-1.393586	-0.455910
C	1.018641	0.818901	0.498556
C	2.049294	0.726447	-0.435188
C	3.353693	0.527326	0.023430
C	3.628652	0.454304	1.381254
C	2.596229	0.582061	2.317625
C	1.296442	0.744672	1.860917
C	-5.585358	-2.000634	-1.023237
C	-6.660522	-2.398619	-0.244471
C	-6.594606	-2.181272	1.117944
C	-5.507824	-1.584804	1.721023
C	-4.443866	-1.189967	0.919802
C	1.797726	0.846941	-1.919358
C	3.065936	1.218422	-2.667050
O	4.102216	0.307263	-2.293243
C	4.513856	0.465356	-0.950390
C	2.912805	1.136653	-4.167865
F	-7.640117	-2.563334	1.888805
O	4.942337	0.330349	1.750084
C	5.284115	-0.781017	2.585188
O	2.954255	0.557839	3.626904
C	1.929557	0.711206	4.598484
C	5.479278	-0.695964	-0.720176
O	6.675504	-0.593855	-0.836707
O	4.849008	-1.835230	-0.460660
C	4.757080	-4.164868	0.026098
C	5.669606	-3.017207	-0.324556
O	-0.248858	3.331444	0.575497
C	0.320201	4.163611	-0.435666
O	-2.824213	3.734753	-0.380927
C	-3.063127	4.345161	0.891632
C	-5.286316	2.065630	-0.473921
O	-4.275183	1.539793	-1.334924

H	-2.211884	-2.638212	0.323169
H	-0.008529	-1.665796	0.489190
H	0.149531	-1.558469	-1.255708
H	-3.721688	-0.726369	-2.326201
H	-0.338617	-4.214424	-0.192248
H	-1.832218	-4.648826	-1.040823
H	-0.518638	-3.837297	-1.914475
H	0.478923	0.840990	2.563759
H	-5.619772	-2.161828	-2.095751
H	-7.536753	-2.864182	-0.678547
H	-5.498625	-1.429579	2.792843
H	-3.589408	-0.707702	1.382222
H	1.425021	-0.101386	-2.322929
H	1.025037	1.594359	-2.114663
H	3.378353	2.232677	-2.378482
H	5.114667	1.378787	-0.852882
H	3.842239	1.416109	-4.665238
H	2.123152	1.811932	-4.501862
H	2.648322	0.119295	-4.464655
H	6.355567	-0.933423	2.462067
H	5.052980	-0.572269	3.628395
H	4.748155	-1.678323	2.264113
H	2.425113	0.669001	5.565123
H	1.425330	1.675056	4.489365
H	1.195746	-0.096283	4.530968
H	5.344426	-5.078774	0.125172
H	4.245799	-3.981868	0.972749
H	4.008768	-4.319259	-0.752369
H	6.192255	-3.182958	-1.268053
H	6.414555	-2.835241	0.452413
H	1.101582	3.625725	-0.981019
H	-0.446515	4.510704	-1.132225
H	0.763189	5.016633	0.074517
H	-3.552180	5.295764	0.688168
H	-3.724039	3.718167	1.497328
H	-2.127134	4.514513	1.424228
H	-5.247777	1.578370	0.504429
H	-5.182843	3.144393	-0.358042
H	-6.238924	1.838653	-0.949220

$\omega_{B97X}$  Energy = -2096.10497249 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf V

C	-0.999183	2.069466	0.605411
C	-2.302655	2.448224	0.277525
C	-3.118283	1.555967	-0.410152
C	-2.657775	0.281621	-0.734011
C	-1.358617	-0.093202	-0.402582
C	-0.515660	0.812129	0.254699
O	-2.877721	-1.732541	-2.069686
C	-1.991133	-2.405489	-1.175661
C	-0.860453	-1.468171	-0.782152
C	-3.592987	-0.672732	-1.446320
C	-1.496990	-3.650697	-1.875934
C	-4.707262	-1.223847	-0.563163
C	0.891852	0.447672	0.599573

C	1.909853	0.554879	-0.345989
C	3.209879	0.204702	0.027995
C	3.485595	-0.226112	1.315053
C	2.459425	-0.352320	2.257477
C	1.168450	-0.005357	1.887956
C	-5.790340	-1.842267	-1.184967
C	-6.819958	-2.401509	-0.445915
C	-6.745701	-2.332185	0.932034
C	-5.693780	-1.729378	1.587034
C	-4.672737	-1.174380	0.825190
C	1.655320	1.054959	-1.747850
C	2.934259	1.556257	-2.396277
O	3.937324	0.543803	-2.279095
C	4.362299	0.345143	-0.947737
C	2.769966	1.860390	-3.867049
F	-7.747745	-2.873136	1.665067
O	4.773323	-0.588982	1.623539
C	5.462322	0.320383	2.484384
O	2.818065	-0.813120	3.481794
C	1.797068	-0.954039	4.459479
C	5.226918	-0.914843	-1.004003
O	4.784210	-2.027665	-1.137028
O	6.520523	-0.611110	-0.965781
C	7.667125	-2.283646	0.383502
C	7.461332	-1.708740	-0.999618
O	-0.215797	2.924824	1.335162
C	0.317613	4.021787	0.593646
O	-2.751870	3.696193	0.619878
C	-3.596661	3.703858	1.773360
C	-4.541877	2.898791	-1.727317
O	-4.411232	1.888775	-0.721873
H	-2.551566	-2.693406	-0.276056
H	-0.297977	-1.904980	0.046707
H	-0.162715	-1.383436	-1.623251
H	-4.065519	-0.137846	-2.272880
H	-0.796303	-4.190825	-1.236453
H	-2.329691	-4.313634	-2.114968
H	-0.984440	-3.384748	-2.803360
H	0.355310	-0.080964	2.598514
H	-5.829845	-1.887909	-2.268361
H	-7.668015	-2.879413	-0.920669
H	-5.675875	-1.695050	2.669398
H	-3.842357	-0.693339	1.330214
H	1.244629	0.251665	-2.370433
H	0.911829	1.855468	-1.737595
H	3.285978	2.453415	-1.866545
H	5.000048	1.182210	-0.634732
H	3.704618	2.228496	-4.291676
H	2.000489	2.621299	-4.009019
H	2.470198	0.959245	-4.406600
H	4.959051	0.396018	3.449702
H	6.463111	-0.084939	2.622423
H	5.530062	1.309183	2.021312
H	2.287564	-1.331219	5.353265
H	1.326716	0.007779	4.680324
H	1.036148	-1.668129	4.133574

H	8.407304	-3.084367	0.337736
H	8.033592	-1.517146	1.068595
H	6.736797	-2.691953	0.779646
H	7.098100	-2.461005	-1.699534
H	8.376014	-1.267781	-1.391319
H	-0.481941	4.602565	0.129543
H	0.857317	4.645020	1.303891
H	1.013183	3.665209	-0.172445
H	-4.498258	3.113035	1.594755
H	-3.060084	3.310501	2.640835
H	-3.868283	4.741985	1.953574
H	-5.608848	3.032680	-1.892242
H	-4.096946	3.838100	-1.395615
H	-4.067626	2.571140	-2.656893

ωB97X Energy = -2096.10496600 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf W

C	-1.019715	2.039490	0.657437
C	-2.311322	2.444666	0.302288
C	-3.138245	1.547423	-0.368005
C	-2.663508	0.290284	-0.742566
C	-1.366018	-0.091995	-0.421267
C	-0.537312	0.788176	0.287248
O	-2.881908	-1.691872	-2.134354
C	-1.988028	-2.384337	-1.263509
C	-0.862317	-1.452052	-0.844753
C	-3.594053	-0.637618	-1.496806
C	-1.486843	-3.602536	-2.005648
C	-4.732816	-1.185579	-0.647172
C	0.859322	0.405031	0.656474
C	1.898273	0.503258	-0.267348
C	3.184928	0.131742	0.131786
C	3.427781	-0.310917	1.421358
C	2.381295	-0.425097	2.342572
C	1.103347	-0.058504	1.947854
C	-4.610364	-1.407576	0.720875
C	-5.654452	-1.956282	1.454154
C	-6.823448	-2.270130	0.793659
C	-6.989047	-2.061190	-0.561369
C	-5.931048	-1.518603	-1.273959
C	1.683440	1.020004	-1.669847
C	2.984051	1.508480	-2.284170
O	3.968047	0.478660	-2.156285
C	4.360287	0.257939	-0.818738
C	2.856917	1.830314	-3.754870
F	-7.850325	-2.797469	1.500727
O	4.703660	-0.692791	1.755194
C	5.390414	0.214145	2.620998
O	2.708590	-0.894520	3.572149
C	1.667048	-1.019036	4.530274
C	5.197287	-1.020368	-0.867207
O	4.736986	-2.120390	-1.042692
O	6.494149	-0.757675	-0.757008
C	8.788808	-1.372064	-0.587881
C	7.388314	-1.891953	-0.790938

O	-0.239879	2.871477	1.418645
C	0.396605	3.927669	0.704715
O	-2.733126	3.690300	0.680586
C	-3.080832	4.575266	-0.388311
C	-5.328738	2.116410	0.348092
O	-4.416604	1.886907	-0.730427
H	-2.541707	-2.708323	-0.372685
H	-0.294033	-1.910915	-0.031913
H	-0.169459	-1.338708	-1.686295
H	-4.042158	-0.075740	-2.317952
H	-0.780675	-4.158222	-1.385822
H	-2.315373	-4.263293	-2.264242
H	-0.978834	-3.302298	-2.925013
H	0.274750	-0.125417	2.641248
H	-3.693268	-1.139513	1.234228
H	-5.567857	-2.131947	2.519269
H	-7.927085	-2.314771	-1.039608
H	-6.043871	-1.345539	-2.339188
H	1.277194	0.228980	-2.310348
H	0.950713	1.830537	-1.669409
H	3.338593	2.394304	-1.737673
H	5.009302	1.077599	-0.483718
H	3.805833	2.189274	-4.154970
H	2.101480	2.603489	-3.905648
H	2.556457	0.939171	-4.310422
H	4.877545	0.294730	3.580971
H	6.387422	-0.196042	2.769525
H	5.468041	1.201804	2.157022
H	2.134727	-1.403206	5.433254
H	1.207412	-0.049966	4.741742
H	0.901540	-1.721543	4.190196
H	9.492823	-2.205063	-0.612206
H	9.061631	-0.668703	-1.375709
H	8.881616	-0.872389	0.377473
H	7.091238	-2.585976	-0.002602
H	7.273428	-2.394527	-1.752737
H	1.092803	3.529428	-0.039902
H	-0.336516	4.572082	0.214207
H	0.951948	4.509177	1.437927
H	-3.235824	5.552522	0.064079
H	-2.266760	4.634717	-1.116356
H	-3.991778	4.250813	-0.893754
H	-5.034097	2.986397	0.937761
H	-6.300530	2.291338	-0.108903
H	-5.383147	1.235435	0.992632

ωB97X Energy = -2096.10488537 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf X

C	-1.010631	2.003476	0.763356
C	-2.300234	2.442606	0.443095
C	-3.137630	1.601351	-0.285810
C	-2.690294	0.343624	-0.696904
C	-1.400649	-0.075710	-0.391331
C	-0.551763	0.761318	0.343297
O	-2.914040	-1.539719	-2.211894

C	-2.044181	-2.302562	-1.376103
C	-0.910818	-1.417034	-0.884712
C	-3.626731	-0.533151	-1.501649
C	-1.553821	-3.481508	-2.185573
C	-4.758325	-1.151490	-0.689202
C	0.841267	0.338964	0.680019
C	1.886405	0.578552	-0.209089
C	3.166808	0.136091	0.126647
C	3.402438	-0.500181	1.334859
C	2.352684	-0.744054	2.225550
C	1.075397	-0.320093	1.884639
C	-5.852444	-1.672087	-1.377542
C	-6.897342	-2.286663	-0.706979
C	-6.826928	-2.372993	0.670150
C	-5.764960	-1.869989	1.390001
C	-4.729215	-1.256009	0.696241
C	1.670522	1.320260	-1.505509
C	2.979945	1.851997	-2.062574
O	3.936365	0.788828	-2.095141
C	4.338090	0.378445	-0.805521
C	2.849082	2.386671	-3.469506
F	-7.843542	-2.970252	1.336740
O	4.673061	-0.944160	1.608101
C	5.372856	-0.175337	2.589181
O	2.672732	-1.395143	3.371463
C	1.629481	-1.645662	4.302237
C	5.150896	-0.894957	-1.039900
O	4.669186	-1.952167	-1.360841
O	6.453242	-0.672996	-0.906191
C	8.739650	-1.339655	-0.871710
C	7.324244	-1.810820	-1.089563
O	-0.170161	2.829082	1.467250
C	-0.453459	2.905804	2.865686
O	-2.775266	3.642892	0.901032
C	-2.154826	4.803920	0.338907
C	-4.661853	3.152914	-1.281403
O	-4.430550	1.928557	-0.581818
H	-2.617147	-2.667978	-0.513376
H	-0.364351	-1.932557	-0.091180
H	-0.198369	-1.261709	-1.703925
H	-4.081814	0.081757	-2.280407
H	-0.862131	-4.084082	-1.593880
H	-2.389516	-4.112621	-2.491084
H	-1.032254	-3.133935	-3.080356
H	0.240776	-0.506081	2.548858
H	-5.888948	-1.594414	-2.459254
H	-7.753912	-2.689972	-1.232919
H	-5.750994	-1.956961	2.469472
H	-3.891443	-0.849923	1.252385
H	1.212310	0.659649	-2.251018
H	0.978264	2.151298	-1.348907
H	3.363926	2.639588	-1.398566
H	5.004008	1.133289	-0.367329
H	3.802113	2.781088	-3.823901
H	2.109062	3.188338	-3.497780
H	2.524680	1.592719	-4.145824

H	5.467288	0.865282	2.265095
H	4.859606	-0.218550	3.551489
H	6.362895	-0.617811	2.680904
H	2.093814	-2.153445	5.143839
H	1.175070	-0.712453	4.646362
H	0.859962	-2.289891	3.868633
H	9.424964	-2.179670	-0.993535
H	9.009396	-0.569105	-1.595097
H	8.865027	-0.937012	0.134446
H	7.034505	-2.580196	-0.371377
H	7.174721	-2.206030	-2.095556
H	-1.470132	3.265763	3.038054
H	-0.321268	1.926561	3.335323
H	0.261368	3.608941	3.288554
H	-2.655689	5.662875	0.781014
H	-1.090811	4.831860	0.575647
H	-2.291926	4.821908	-0.746176
H	-4.647947	4.004335	-0.601643
H	-3.914871	3.292516	-2.067767
H	-5.646863	3.061264	-1.735258

ωB97X Energy = -2096.10485835 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf Y

C	-1.011403	2.157789	-0.043642
C	-2.322388	2.408669	-0.465388
C	-3.116112	1.339959	-0.870465
C	-2.616942	0.036163	-0.835353
C	-1.319967	-0.206787	-0.400343
C	-0.503387	0.864584	-0.012550
O	-2.790820	-2.288333	-1.533529
C	-1.915163	-2.651768	-0.467101
C	-0.800281	-1.624484	-0.356389
C	-3.521845	-1.092699	-1.285032
C	-1.396477	-4.041580	-0.759059
C	-4.688260	-1.356199	-0.341626
C	0.908036	0.638411	0.422114
C	1.921199	0.438735	-0.514285
C	3.221493	0.216084	-0.054406
C	3.504284	0.213023	1.301310
C	2.484971	0.401414	2.240364
C	1.192357	0.617480	1.786144
C	-4.626053	-1.098335	1.023873
C	-5.692803	-1.403000	1.859880
C	-6.822150	-1.963267	1.301850
C	-6.927945	-2.230175	-0.049123
C	-5.849035	-1.922689	-0.863051
C	1.663991	0.478017	-2.001753
C	2.943911	0.745640	-2.774848
O	3.938100	-0.192463	-2.354182
C	4.368633	0.023031	-1.027136
C	2.776326	0.586113	-4.267867
F	-7.870015	-2.257881	2.107045
O	4.792183	-0.045740	1.700789
C	5.497793	1.084988	2.216685
O	2.850833	0.353979	3.545451

C	1.838038	0.543938	4.523334
C	5.203357	-1.212527	-0.687246
O	4.732811	-2.298023	-0.457850
O	6.504184	-0.947036	-0.753564
C	7.621450	-2.127715	1.058959
C	7.416659	-2.023003	-0.435458
O	-0.229902	3.210744	0.363582
C	0.347726	3.963910	-0.703250
O	-2.803393	3.686561	-0.566989
C	-2.988845	4.369722	0.677397
C	-5.345919	2.120467	-0.528122
O	-4.371929	1.518955	-1.382310
H	-2.486768	-2.669281	0.470311
H	-0.244838	-1.789096	0.570299
H	-0.092710	-1.783271	-1.177898
H	-3.943431	-0.824664	-2.255220
H	-0.693579	-4.352581	0.016068
H	-2.216486	-4.760165	-0.792456
H	-0.878880	-4.056209	-1.721014
H	0.383062	0.772432	2.488144
H	-3.738408	-0.643901	1.450522
H	-5.652954	-1.206772	2.924234
H	-7.836417	-2.664485	-0.447858
H	-5.914218	-2.123457	-1.927420
H	1.249058	-0.476541	-2.344754
H	0.923400	1.245045	-2.240590
H	3.305842	1.758604	-2.546057
H	5.027111	0.900713	-0.990146
H	3.714679	0.791133	-4.784396
H	2.017781	1.278889	-4.636314
H	2.460780	-0.432377	-4.504703
H	5.020781	1.457778	3.124642
H	6.505519	0.741897	2.444307
H	5.544383	1.881006	1.467711
H	2.334800	0.471000	5.487483
H	1.374873	1.529411	4.425523
H	1.070111	-0.230783	4.450845
H	8.334965	-2.925197	1.273619
H	8.020214	-1.194016	1.459474
H	6.682897	-2.353941	1.566014
H	7.025978	-2.949664	-0.855412
H	8.338262	-1.757107	-0.949704
H	-0.422864	4.320569	-1.390645
H	0.852365	4.813459	-0.247440
H	1.079649	3.359607	-1.247694
H	-2.034805	4.527533	1.180981
H	-3.445477	5.327591	0.436224
H	-3.659310	3.800226	1.327696
H	-6.313591	1.929562	-0.988586
H	-5.322588	1.659783	0.463460
H	-5.187101	3.195584	-0.444346

ωB97X Energy = -2096.10485223 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf Z

C	-0.937546	2.264026	0.321899
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C	-2.254049	2.520140	-0.075763
C	-2.990218	1.494299	-0.663608
C	-2.450236	0.216024	-0.796167
C	-1.147454	-0.035922	-0.380651
C	-0.382640	0.997520	0.174092
O	-2.503789	-1.961824	-1.869810
C	-1.613697	-2.459568	-0.870943
C	-0.554204	-1.412078	-0.570139
C	-3.300268	-0.872935	-1.418029
C	-1.024327	-3.750782	-1.391657
C	-4.428052	-1.366323	-0.519249
C	1.027269	0.754563	0.604111
C	2.077924	0.879051	-0.301493
C	3.371893	0.581268	0.126901
C	3.620930	0.214453	1.442394
C	2.569920	0.134736	2.361911
C	1.276408	0.383004	1.921917
C	-4.435882	-1.182992	0.858408
C	-5.465427	-1.689006	1.642376
C	-6.483551	-2.378378	1.019880
C	-6.515564	-2.581152	-0.346353
C	-5.477616	-2.069186	-1.107789
C	1.845939	1.339736	-1.719709
C	3.133738	1.829899	-2.358120
O	4.148935	0.839536	-2.173100
C	4.546113	0.708820	-0.822991
C	3.002647	2.070562	-3.843781
F	-7.494474	-2.871386	1.774084
O	4.927941	0.008487	1.798249
C	5.253260	-1.253757	2.389729
O	2.899565	-0.170624	3.643168
C	1.850850	-0.247393	4.597858
C	5.487927	-0.494433	-0.827500
O	6.687750	-0.395375	-0.902562
O	4.833351	-1.649390	-0.820457
C	4.684972	-4.025003	-0.849584
C	5.629248	-2.851725	-0.917320
O	-0.158919	3.284356	0.802156
C	-0.429683	3.664482	2.149438
O	-2.745330	3.789248	0.062118
C	-3.896992	3.920746	0.900937
C	-4.378162	2.558795	-2.244831
O	-4.274155	1.708509	-1.098545
H	-2.188311	-2.664626	0.042369
H	0.005506	-1.706627	0.320927
H	0.165961	-1.385189	-1.396815
H	-3.757545	-0.475101	-2.326159
H	-0.308352	-4.155151	-0.673561
H	-1.806835	-4.492589	-1.557113
H	-0.504747	-3.573790	-2.336260
H	0.442857	0.302786	2.608213
H	-3.633087	-0.632778	1.336762
H	-5.481256	-1.549959	2.716330
H	-7.338733	-3.122679	-0.795916
H	-5.484831	-2.217808	-2.182625
H	1.439915	0.521361	-2.326124

H	1.105539	2.143271	-1.732852
H	3.459697	2.752620	-1.857426
H	5.160047	1.570659	-0.531082
H	3.941254	2.438449	-4.259838
H	2.223764	2.810486	-4.036211
H	2.732583	1.142759	-4.353013
H	4.725640	-2.062983	1.877099
H	6.327263	-1.380506	2.260243
H	4.999255	-1.266633	3.448343
H	1.329682	0.709713	4.688054
H	1.135137	-1.031562	4.337198
H	2.325650	-0.490898	5.544969
H	5.252142	-4.953460	-0.928775
H	4.142664	-4.034093	0.097563
H	3.963035	-3.991468	-1.666501
H	6.182201	-2.824007	-1.857685
H	6.349238	-2.859102	-0.096768
H	-1.443612	4.057441	2.252877
H	-0.292640	2.813909	2.824126
H	0.286058	4.444037	2.402763
H	-4.054921	4.988726	1.035991
H	-4.777062	3.469112	0.441291
H	-3.716259	3.453161	1.873163
H	-3.983951	3.554666	-2.032572
H	-3.838859	2.123335	-3.090609
H	-5.437440	2.624665	-2.483918

ωB97X Energy = -2096.10483125 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf AA

C	-0.902787	2.255562	0.322269
C	-2.209898	2.535551	-0.081683
C	-2.981629	1.522236	-0.640699
C	-2.474945	0.229743	-0.759914
C	-1.172750	-0.045435	-0.353184
C	-0.373350	0.977037	0.174782
O	-2.603791	-1.974443	-1.771080
C	-1.714508	-2.469320	-0.769935
C	-0.622660	-1.443525	-0.512039
C	-3.363668	-0.852125	-1.337720
C	-1.164986	-3.788715	-1.263015
C	-4.489263	-1.291867	-0.408940
C	1.036129	0.706863	0.590011
C	2.063495	0.683780	-0.350973
C	3.360212	0.394508	0.080439
C	3.626263	0.158474	1.419066
C	2.592753	0.172954	2.361513
C	1.303080	0.452573	1.933532
C	-5.569327	-1.975176	-0.963981
C	-6.607232	-2.441369	-0.173483
C	-6.543738	-2.212852	1.187494
C	-5.494816	-1.541076	1.777354
C	-4.466085	-1.080839	0.964646
C	1.822376	0.980535	-1.811297
C	3.108267	1.394509	-2.505005
O	4.108050	0.404881	-2.247242

C	4.519510	0.371466	-0.895789
C	2.962977	1.508389	-4.004425
F	-7.554066	-2.661374	1.969839
O	4.911107	-0.160833	1.782482
C	5.593860	0.853482	2.524291
O	2.940832	-0.100099	3.643793
C	1.910591	-0.105767	4.621812
C	5.389743	-0.881728	-0.798530
O	6.591759	-0.860314	-0.901137
O	4.667795	-1.985747	-0.667619
C	4.374994	-4.332442	-0.403525
C	5.388627	-3.235907	-0.612575
O	-0.160885	3.237084	0.925879
C	0.356367	4.225012	0.034515
O	-2.707861	3.803936	0.058788
C	-3.570304	3.955567	1.188950
C	-4.409726	2.594373	-2.180282
O	-4.276073	1.763558	-1.022781
H	-2.282042	-2.634670	0.155532
H	-0.058891	-1.728031	0.379914
H	0.084957	-1.464113	-1.348922
H	-3.825049	-0.466160	-2.249068
H	-0.450999	-4.192463	-0.542544
H	-1.967867	-4.514342	-1.399952
H	-0.652119	-3.649488	-2.217567
H	0.483119	0.473624	2.639979
H	-5.601310	-2.144639	-2.035284
H	-7.453905	-2.967439	-0.596984
H	-5.486032	-1.380720	2.848412
H	-3.639133	-0.544628	1.417154
H	1.422243	0.096647	-2.321484
H	1.075829	1.770785	-1.920665
H	3.455499	2.351901	-2.089876
H	5.186031	1.219327	-0.689987
H	3.905066	1.814989	-4.460242
H	2.200119	2.248440	-4.252292
H	2.664555	0.547384	-4.429065
H	5.105985	1.022209	3.485550
H	6.607061	0.490185	2.683456
H	5.626005	1.787333	1.955538
H	2.394524	-0.344894	5.565396
H	1.431682	0.874079	4.697055
H	1.157496	-0.865400	4.396007
H	4.884942	-5.296004	-0.362891
H	3.836784	-4.188640	0.534398
H	3.654846	-4.358312	-1.222439
H	5.938158	-3.359743	-1.547327
H	6.108184	-3.183808	0.206299
H	1.066811	3.775847	-0.666668
H	-0.450850	4.713566	-0.514911
H	0.875715	4.957181	0.649610
H	-4.433342	3.290467	1.106711
H	-3.026216	3.746063	2.113785
H	-3.904673	4.991068	1.189952
H	-5.476860	2.689848	-2.369308
H	-3.975173	3.579541	-2.004360

H        -3.927451   2.124360   -3.042210  
 ωB97X Energy = -2096.10482849 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf AB

C	-0.897886	2.251245	-0.050029
C	-2.208499	2.472296	-0.489546
C	-2.976350	1.384532	-0.893687
C	-2.452784	0.090997	-0.839139
C	-1.156757	-0.122438	-0.386084
C	-0.365279	0.968596	-0.000687
O	-2.573033	-2.243687	-1.515338
C	-1.705138	-2.578666	-0.433514
C	-0.611030	-1.529575	-0.319990
C	-3.329671	-1.059299	-1.290104
C	-1.156445	-3.961611	-0.702556
C	-4.505355	-1.335030	-0.362058
C	1.047100	0.773743	0.445738
C	2.068075	0.580475	-0.483589
C	3.369691	0.383657	-0.015661
C	3.646169	0.402828	1.341290
C	2.619297	0.584801	2.273282
C	1.325094	0.773300	1.811041
C	-5.650520	-1.920491	-0.896695
C	-6.736457	-2.238971	-0.096438
C	-6.653485	-1.963662	1.254432
C	-5.540111	-1.384599	1.825321
C	-4.466075	-1.069092	1.002788
C	1.817233	0.601934	-1.972423
C	3.096527	0.884155	-2.740935
O	4.102336	-0.036532	-2.309689
C	4.523097	0.189730	-0.980269
C	2.939393	0.713313	-4.233812
F	-7.708425	-2.268794	2.046353
O	4.936373	0.171102	1.750026
C	5.614946	1.322546	2.258761
O	2.979351	0.557531	3.580649
C	1.959748	0.746606	4.551583
C	5.412092	-1.010323	-0.653665
O	6.613318	-0.990643	-0.766308
O	4.709202	-2.080598	-0.310765
C	4.467063	-4.334876	0.417021
C	5.454912	-3.282241	-0.017614
O	-0.141426	3.322937	0.355408
C	0.432760	4.077893	-0.712046
O	-2.712976	3.739387	-0.610449
C	-2.928054	4.432168	0.623788
C	-5.225325	2.123097	-0.586647
O	-4.228499	1.534810	-1.423517
H	-2.288767	-2.596436	0.496471
H	-0.064702	-1.673644	0.615540
H	0.109825	-1.684251	-1.130686
H	-3.741213	-0.809285	-2.269388
H	-0.457638	-4.250122	0.084938
H	-1.962089	-4.696168	-0.737767
H	-0.626662	-3.977311	-1.657876

H	0.510096	0.922313	2.507719
H	-5.697909	-2.127331	-1.960846
H	-7.633222	-2.687688	-0.505577
H	-5.518324	-1.182187	2.889049
H	-3.591059	-0.599634	1.439224
H	1.419643	-0.362043	-2.309699
H	1.065594	1.354822	-2.221452
H	3.442401	1.903560	-2.516007
H	5.179666	1.069247	-0.944837
H	3.877293	0.929469	-4.746592
H	2.172453	1.392338	-4.610359
H	2.640687	-0.311267	-4.466218
H	6.630289	1.006988	2.489941
H	5.642219	2.113956	1.504100
H	5.126986	1.689997	3.163006
H	2.453272	0.693267	5.518679
H	1.483913	1.724371	4.438612
H	1.202522	-0.039211	4.486413
H	4.998332	-5.260804	0.641980
H	3.932421	-4.018548	1.313744
H	3.741660	-4.538335	-0.371909
H	6.000376	-3.578296	-0.915398
H	6.179512	-3.054541	0.766053
H	-0.337325	4.414527	-1.409974
H	0.917109	4.940299	-0.258407
H	1.181275	3.482854	-1.243952
H	-3.401591	5.377426	0.365990
H	-3.594427	3.856064	1.272463
H	-1.984182	4.616128	1.137391
H	-5.209806	1.666152	0.406822
H	-5.085294	3.200898	-0.504407
H	-6.182541	1.914910	-1.061232

ωB97X Energy = -2096.10474300 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf AC

C	-0.961305	2.085128	0.516151
C	-2.269604	2.464970	0.199496
C	-3.088385	1.559440	-0.470853
C	-2.636098	0.274673	-0.765960
C	-1.340607	-0.103357	-0.429060
C	-0.494468	0.811649	0.208518
O	-2.854919	-1.744745	-2.093671
C	-1.974110	-2.417369	-1.193897
C	-0.843674	-1.482152	-0.794785
C	-3.570611	-0.680244	-1.478802
C	-1.478898	-3.664783	-1.889513
C	-4.692498	-1.222371	-0.600289
C	0.910305	0.444484	0.561766
C	1.943849	0.628139	-0.353630
C	3.237626	0.254229	0.013161
C	3.496007	-0.261232	1.273288
C	2.456509	-0.456167	2.187655
C	1.166997	-0.098009	1.818795
C	-4.664365	-1.169673	0.788087
C	-5.692614	-1.716331	1.546355

C	-6.745063	-2.314119	0.887684
C	-6.813161	-2.386328	-0.490491
C	-5.776569	-1.835391	-1.225884
C	1.700816	1.241474	-1.710920
C	2.991810	1.751128	-2.328964
O	3.978977	0.717904	-2.263913
C	4.397980	0.449350	-0.942897
C	2.837544	2.137420	-3.781407
F	-7.753999	-2.846977	1.617103
O	4.780673	-0.638555	1.578346
C	5.454177	0.225186	2.496434
O	2.798066	-0.995169	3.384574
C	1.764245	-1.193694	4.338152
C	5.262361	-0.806706	-1.059876
O	4.819936	-1.910404	-1.255305
O	6.555868	-0.507161	-0.994601
C	7.695243	-2.238823	0.282609
C	7.496078	-1.602987	-1.074592
O	-0.104952	2.996385	1.076832
C	-0.297001	3.220303	2.471959
O	-2.673371	3.738369	0.494439
C	-3.782610	3.843172	1.392200
C	-4.455945	2.881907	-1.865020
O	-4.369088	1.896950	-0.830423
H	-2.540006	-2.702563	-0.296733
H	-0.291513	-1.917577	0.041548
H	-0.135318	-1.401099	-1.628021
H	-4.035923	-0.147922	-2.310842
H	-0.781969	-4.204847	-1.245889
H	-2.311537	-4.326825	-2.131245
H	-0.961690	-3.401240	-2.815028
H	0.341083	-0.243583	2.503752
H	-3.833220	-0.692694	1.295675
H	-5.679845	-1.679525	2.628707
H	-7.661947	-2.860054	-0.968115
H	-5.811133	-1.883268	-2.309354
H	1.253306	0.503390	-2.387175
H	0.989565	2.066664	-1.625180
H	3.356844	2.611845	-1.750666
H	5.033556	1.268852	-0.582741
H	3.777179	2.519540	-4.182017
H	2.075417	2.911918	-3.883995
H	2.531364	1.270205	-4.370730
H	4.938116	0.245422	3.457867
H	6.455199	-0.182585	2.625479
H	5.522875	1.238216	2.089172
H	2.243855	-1.616169	5.217460
H	1.285503	-0.247105	4.603757
H	1.011597	-1.892747	3.963823
H	8.436136	-3.036487	0.205277
H	8.057670	-1.503125	1.002669
H	6.763041	-2.664455	0.655568
H	7.135160	-2.323040	-1.808660
H	8.412756	-1.145872	-1.442378
H	-0.168837	2.288383	3.030927
H	0.463593	3.934637	2.780771

H	-1.286366	3.637805	2.671770
H	-4.695933	3.452172	0.941901
H	-3.575260	3.301881	2.319928
H	-3.899618	4.902894	1.608836
H	-5.515585	3.024166	-2.066002
H	-4.008931	3.825808	-1.546799
H	-3.956516	2.525699	-2.770298

$\omega$ B97X Energy = -2096.10473443 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf AD

C	-1.005341	2.017437	0.764370
C	-2.305941	2.423927	0.446408
C	-3.130736	1.552250	-0.259552
C	-2.645508	0.322365	-0.704941
C	-1.338707	-0.058316	-0.421301
C	-0.511408	0.794905	0.321000
O	-2.855559	-1.587770	-2.195286
C	-1.942253	-2.312308	-1.371991
C	-0.822972	-1.387641	-0.921108
C	-3.573347	-0.577627	-1.495648
C	-1.436175	-3.484592	-2.181797
C	-4.694546	-1.185045	-0.663086
C	0.897258	0.414413	0.643930
C	1.915878	0.579125	-0.293208
C	3.215144	0.204134	0.058764
C	3.490232	-0.305434	1.316663
C	2.464084	-0.487361	2.249794
C	1.173558	-0.117138	1.902157
C	-5.890726	-1.514035	-1.296030
C	-6.932730	-2.107674	-0.600826
C	-6.753457	-2.371128	0.742957
C	-5.585921	-2.063470	1.408806
C	-4.557794	-1.463587	0.693108
C	1.666100	1.167615	-1.661315
C	2.947648	1.708799	-2.271556
O	3.947497	0.687646	-2.221685
C	4.368796	0.396437	-0.906156
C	2.787176	2.112302	-3.718677
F	-7.765041	-2.948118	1.433167
O	4.777256	-0.689552	1.601701
C	5.469618	0.166454	2.513227
O	2.822449	-1.023386	3.442973
C	1.801963	-1.221884	4.411105
C	5.217007	-0.868557	-1.044391
O	4.759149	-1.966891	-1.234354
O	6.514580	-0.583019	-1.003252
C	7.656501	-2.329496	0.250258
C	7.441033	-1.689017	-1.102255
O	-0.227053	2.820024	1.558288
C	0.408076	3.902514	0.883906
O	-2.737067	3.644233	0.891149
C	-3.100442	4.578168	-0.129550
C	-5.317495	2.063748	0.510404
O	-4.417040	1.894977	-0.589050
H	-2.480119	-2.687913	-0.491804



H	-0.237015	-1.879432	-0.140715	C	3.330869	0.486610	0.196643
H	-0.143762	-1.221703	-1.765102	C	3.580277	-0.049425	1.452585
H	-4.038442	0.019582	-2.281654	C	2.530443	-0.243397	2.356592
H	-0.712521	-4.059929	-1.601331	C	1.237902	0.069707	1.957608
H	-2.259319	-4.143740	-2.460849	C	-5.532331	-1.951632	-1.244142
H	-0.947041	-3.130590	-3.092209	C	-6.544506	-2.578018	-0.535642
H	0.360100	-0.235747	2.606429	C	-6.505947	-2.520751	0.844396
H	-6.014431	-1.298154	-2.352200	C	-5.505862	-1.866375	1.530210
H	-7.869143	-2.358827	-1.083510	C	-4.501377	-1.244320	0.798478
H	-5.488358	-2.282394	2.464936	C	1.804675	1.486090	-1.531902
H	-3.642046	-1.200488	1.211387	C	3.092740	2.044920	-2.110577
H	1.259265	0.406213	-2.336435	O	4.103890	1.035437	-2.052779
H	0.921711	1.965406	-1.603568	C	4.503375	0.738326	-0.729916
H	3.300436	2.567312	-1.681687	C	2.957414	2.466656	-3.555010
H	5.016935	1.202881	-0.539103	F	-7.491588	-3.127464	1.547852
H	3.723470	2.506136	-4.115656	O	4.886869	-0.303994	1.777682
H	2.019651	2.882824	-3.810156	C	5.207676	-1.634450	2.197440
H	2.486508	1.250581	-4.318759	O	2.860972	-0.716269	3.585658
H	4.967094	0.187257	3.481665	C	1.815530	-0.895353	4.530165
H	6.469378	-0.248938	2.626827	C	5.455765	-0.445772	-0.887669
H	5.539823	1.180243	2.108121	O	6.654289	-0.326065	-0.953377
H	2.292649	-1.652441	5.280339	O	4.812099	-1.598827	-1.023396
H	1.332519	-0.274803	4.689873	C	4.692477	-3.960435	-1.303222
H	1.040158	-1.914502	4.043481	C	5.619065	-2.771582	-1.272917
H	8.388596	-3.133850	0.159476	O	-0.153774	3.106338	1.273794
H	8.037260	-1.598471	0.965628	C	-0.453508	3.280121	2.660101
H	6.726626	-2.747211	0.637660	O	-2.792596	3.736831	0.626244
H	7.059110	-2.403476	-1.831222	C	-2.223777	4.877936	-0.024541
H	8.356131	-1.241306	-1.485202	C	-4.611180	2.948057	-1.562952
H	1.113679	3.531914	0.133833	O	-4.343585	1.829267	-0.715319
H	-0.326015	4.556321	0.407014	H	-2.293375	-2.659339	-0.307158
H	0.952430	4.464893	1.639956	H	-0.097153	-1.773226	0.098194
H	-3.261779	5.530330	0.371522	H	0.070221	-1.211291	-1.555409
H	-2.292027	4.682242	-0.858935	H	-3.887923	-0.121875	-2.262264
H	-4.011700	4.270377	-0.644884	H	-0.446969	-4.042808	-1.271350
H	-5.363186	1.148950	1.106714	H	-1.955689	-4.215087	-2.183777
H	-5.017851	2.901241	1.142959	H	-0.645206	-3.202178	-2.818876
H	-6.294549	2.260468	0.073998	H	0.405492	-0.092613	2.630572
$\omega B97X$ Energy = -2096.10472808 a.u.				H	-5.543591	-1.986564	-2.328608
$(aR,1S,3S,1'S,3'S)-22$ , Conf AE				H	-7.352572	-3.098119	-1.035193
C	-0.944354	2.184569	0.634392	H	-5.515288	-1.843680	2.613006
C	-2.251587	2.529339	0.273246	H	-3.711584	-0.722408	1.327454
C	-3.037591	1.590019	-0.389797	H	1.390605	0.753459	-2.234962
C	-2.522022	0.330050	-0.699373	H	1.069208	2.289240	-1.440354
C	-1.215445	0.003382	-0.354416	H	3.425068	2.898197	-1.502183
C	-0.418552	0.937929	0.317894	H	5.111121	1.561431	-0.332430
O	-2.627180	-1.662637	-2.078737	H	3.896047	2.879010	-3.926879
C	-1.728531	-2.319612	-1.185703	H	2.181042	3.227634	-3.651830
C	-0.651273	-1.343833	-0.740033	H	2.681080	1.609539	-4.173195
C	-3.402208	-0.653426	-1.441564	H	4.682568	-2.366277	1.577441
C	-1.161350	-3.519420	-1.909737	H	6.282437	-1.744461	2.059171
C	-4.500934	-1.279831	-0.590485	H	4.946459	-1.788021	3.243104
C	0.988628	0.614628	0.701405	H	1.309343	0.050876	4.740372
C	2.037624	0.846391	-0.184840	H	1.086834	-1.630908	4.179359
				H	2.290433	-1.261386	5.436930
				H	5.268845	-4.865592	-1.499442

H	4.181421	-4.080304	-0.346311
H	3.943923	-3.851602	-2.089072
H	6.140854	-2.634036	-2.221421
H	6.364934	-2.855498	-0.480331
H	-1.486405	3.607460	2.797865
H	-0.284033	2.347130	3.205698
H	0.226825	4.044052	3.031059
H	-2.786540	5.741283	0.324827
H	-1.170515	4.991122	0.233716
H	-2.329844	4.789221	-1.109604
H	-4.606558	3.880966	-0.999553
H	-3.877541	2.999387	-2.372311
H	-5.600274	2.781208	-1.985377

ωB97X Energy = -2096.10468085 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf AF

C	-1.004712	1.985925	0.850872
C	-2.306222	2.415642	0.567858
C	-3.136577	1.596133	-0.193266
C	-2.671126	0.369317	-0.671582
C	-1.369771	-0.038960	-0.403824
C	-0.527600	0.776178	0.362468
O	-2.881829	-1.441614	-2.274039
C	-1.983358	-2.226308	-1.490325
C	-0.860657	-1.343018	-0.971577
C	-3.602733	-0.486433	-1.503916
C	-1.480913	-3.352612	-2.364700
C	-4.707748	-1.166966	-0.704157
C	0.875804	0.359856	0.661092
C	1.908519	0.670197	-0.220575
C	3.197301	0.221273	0.071260
C	3.453691	-0.491609	1.231739
C	2.416773	-0.803923	2.116239
C	1.131434	-0.372317	1.818080
C	-5.799287	-1.683248	-1.399844
C	-6.820940	-2.349034	-0.742441
C	-6.729779	-2.491469	0.628778
C	-5.669192	-1.995528	1.355526
C	-4.656933	-1.329675	0.675056
C	1.668855	1.493169	-1.462425
C	2.965000	2.079037	-1.995742
O	3.936869	1.035570	-2.107182
C	4.356207	0.542436	-0.852067
C	2.811575	2.701661	-3.363752
F	-7.723913	-3.138620	1.282578
O	4.731242	-0.942212	1.456029
C	5.435936	-0.254185	2.491460
O	2.755794	-1.525865	3.213360
C	1.726620	-1.845028	4.138816
C	5.184486	-0.698363	-1.187824
O	4.709791	-1.738620	-1.568153
O	6.486310	-0.452464	-1.080161
C	7.553303	-2.441365	-0.158539
C	7.392071	-1.543559	-1.364455
O	-0.171881	2.789581	1.588676

C	-0.441138	2.785905	2.991940
O	-2.799167	3.580973	1.092129
C	-2.204868	4.781809	0.588588
C	-4.700017	3.166286	-1.092993
O	-4.438809	1.912898	-0.458142
H	-2.534898	-2.646234	-0.638508
H	-0.291149	-1.886466	-0.213832
H	-0.164420	-1.130445	-1.792035
H	-4.083753	0.156484	-2.243527
H	-0.766015	-3.967057	-1.814273
H	-2.307252	-3.987171	-2.687968
H	-0.982179	-2.949310	-3.249068
H	0.306460	-0.610997	2.477517
H	-5.852706	-1.560881	-2.476673
H	-7.675561	-2.749187	-1.273937
H	-5.638093	-2.127413	2.430069
H	-3.820635	-0.928862	1.237192
H	1.210762	0.877223	-2.245445
H	0.967945	2.302605	-1.243814
H	3.344333	2.827419	-1.285310
H	5.016172	1.274246	-0.368230
H	3.755475	3.130864	-3.701723
H	2.060934	3.493261	-3.332859
H	2.490074	1.948236	-4.086217
H	4.938767	-0.389060	3.453520
H	6.432426	-0.690692	2.528887
H	5.513773	0.812167	2.259808
H	2.205571	-2.403401	4.939193
H	1.270724	-0.939817	4.549391
H	0.955653	-2.465175	3.673861
H	8.273522	-3.228859	-0.387376
H	7.925347	-1.874891	0.696911
H	6.605093	-2.905981	0.113162
H	7.018925	-2.092628	-2.228829
H	8.327930	-1.054371	-1.627700
H	0.262425	3.481783	3.444627
H	-1.463738	3.112803	3.192933
H	-0.282260	1.786485	3.407751
H	-2.721182	5.606507	1.075939
H	-1.140617	4.819388	0.822840
H	-2.346977	4.853096	-0.493625
H	-4.691301	3.982729	-0.371536
H	-3.965768	3.357859	-1.880336
H	-5.689188	3.080011	-1.538748

ωB97X Energy = -2096.10467808 a.u.

(aS,3S,3'S)-28, Conf A

C	-1.365688	1.140715	-1.122244
C	-2.739172	1.334514	-1.160280
C	-3.556858	0.546125	-0.342665
C	-2.999447	-0.401989	0.501089
C	-1.615451	-0.582410	0.554071
C	-0.803482	0.188425	-0.273414
C	-1.036223	-1.616179	1.488846

C	-2.046187	-2.068005	2.533719
C	-1.595356	-3.300626	3.284132
O	-3.282501	-2.376458	1.897563
C	1.256403	-1.079794	-0.876765
C	2.640547	-1.256874	-0.887227
C	3.452049	-0.304536	-0.280635
C	2.890816	0.807936	0.340046
C	1.508429	0.969240	0.365096
C	0.681605	0.027485	-0.260495
C	0.921977	2.163431	1.082201
C	1.933879	2.814668	2.013477
C	1.464656	4.153209	2.536716
O	3.154602	3.025035	1.311176
C	3.803442	1.808623	1.010484
C	-3.911927	-1.223681	1.382028
O	4.812290	-0.471294	-0.223860
C	5.480948	-0.330274	-1.478147
O	0.460008	-2.047738	-1.434869
C	0.343655	-1.950964	-2.852838
O	-3.368282	2.251856	-1.941476
C	-2.563870	3.077418	-2.766115
O	-4.917052	0.734228	-0.315669
C	-5.599772	0.285283	-1.485230
O	3.198056	-2.344764	-1.507079
C	3.166218	-3.529906	-0.710443
H	-0.710165	1.735205	-1.746420
H	-0.707917	-2.485245	0.907163
H	-0.148891	-1.215558	1.987903
H	-2.221764	-1.246466	3.245832
H	-2.327543	-3.580257	4.042563
H	-1.475530	-4.136124	2.590808
H	-0.637140	-3.117694	3.774381
H	0.038630	1.859312	1.650563
H	0.582870	2.908364	0.353809
H	2.133585	2.136862	2.857843
H	1.323932	4.851352	1.708389
H	2.196861	4.575404	3.226081
H	0.513854	4.043290	3.061804
H	4.220293	1.368687	1.928096
H	4.642733	2.052240	0.358490
H	-4.284184	-0.598298	2.206763
H	-4.779601	-1.564457	0.817249
H	5.313012	0.669856	-1.889880
H	6.542441	-0.465994	-1.280253
H	5.137787	-1.084652	-2.187900
H	1.323497	-2.042655	-3.328173
H	-0.296236	-2.771777	-3.171167
H	-0.119986	-0.999925	-3.133345
H	-1.995867	2.484715	-3.489147
H	-3.249960	3.732825	-3.297245
H	-1.874861	3.681574	-2.168759
H	-5.275289	0.843592	-2.365097
H	-6.660218	0.458781	-1.311957
H	-5.427658	-0.784264	-1.642913
H	3.723531	-3.380092	0.218403
H	2.134886	-3.812352	-0.485385

H 3.640787 -4.314159 -1.297215  
 ωB97X Energy = -1498.55731613 a.u.

(aS,3S,3'S)-**28**, Conf B

C	-1.363283	0.969984	-1.274467
C	-2.741564	1.070493	-1.399291
C	-3.554536	0.258422	-0.600624
C	-2.989122	-0.653670	0.277236
C	-1.601611	-0.753229	0.403564
C	-0.793114	0.064599	-0.380853
C	-1.014209	-1.745705	1.376628
C	-2.050808	-2.244951	2.372490
C	-1.569813	-3.439446	3.164730
O	-3.229072	-2.635200	1.674618
C	1.378991	-1.061771	-0.858825
C	2.770897	-1.138785	-0.796998
C	3.478444	-0.132875	-0.147866
C	2.807712	0.935104	0.441339
C	1.418054	0.999219	0.389401
C	0.695904	0.002774	-0.279135
C	0.708839	2.147116	1.070405
C	1.619568	2.873813	2.049531
C	1.030942	4.178988	2.534742
O	2.859327	3.166108	1.413217
C	3.607468	1.996903	1.159836
C	-3.899155	-1.532783	1.104220
O	4.842434	-0.204157	-0.019233
C	5.563730	0.004860	-1.234156
O	0.685805	-2.085863	-1.453143
C	0.590629	-1.969410	-2.871194
O	-3.380485	1.907754	-2.258307
C	-2.581396	2.725798	-3.095607
O	-4.921820	0.300907	-0.721122
C	-5.528363	1.470648	-0.176699
O	3.436671	-2.178763	-1.390710
C	3.460371	-3.365336	-0.596372
H	-0.710641	1.588729	-1.877690
H	-0.607912	-2.599112	0.821803
H	-0.177811	-1.291546	1.916270
H	-2.313891	-1.426566	3.061066
H	-2.323866	-3.752683	3.887834
H	-1.364094	-4.274846	2.491795
H	-0.651526	-3.194131	3.701996
H	-0.177408	1.777670	1.593948
H	0.352749	2.863646	0.321755
H	1.819949	2.216773	2.910050
H	0.881664	4.859257	1.693173
H	1.697276	4.657363	3.253544
H	0.066075	4.005776	3.015269
H	3.996667	1.588297	2.103852
H	4.466626	2.296342	0.558985
H	-4.370851	-0.930980	1.896171
H	-4.697420	-1.934980	0.481386
H	6.620444	-0.067542	-0.984160
H	5.306344	-0.755038	-1.973516

H	5.353115	1.000524	-1.637106
H	0.043144	-2.842270	-3.221509
H	0.040849	-1.062850	-3.143342
H	1.584994	-1.952622	-3.324858
H	-1.957495	3.405826	-2.508034
H	-1.945471	2.121190	-3.748736
H	-3.273812	3.304772	-3.701988
H	-5.191144	2.366295	-0.701921
H	-5.301604	1.560948	0.890500
H	-6.602452	1.353306	-0.307962
H	3.966696	-3.177654	0.354585
H	2.444650	-3.724832	-0.414434
H	4.015817	-4.109935	-1.163494

$\omega$ B97X Energy = -1498.55692462 a.u.

(*aS*,3*S*,3'*S*)-**28**, Conf C

C	-1.451474	1.127274	-1.085600
C	-2.831531	1.267122	-1.062796
C	-3.581815	0.437767	-0.221357
C	-2.951447	-0.498168	0.583614
C	-1.560145	-0.623494	0.576423
C	-0.814911	0.189351	-0.273672
C	-0.902426	-1.643960	1.473615
C	-1.850225	-2.146968	2.552627
C	-1.320755	-3.368648	3.269045
O	-3.098002	-2.498385	1.963239
C	1.272769	-0.988987	-0.956224
C	2.664206	-1.109607	-1.034367
C	3.459001	-0.112517	-0.473724
C	2.868381	0.991080	0.143737
C	1.485683	1.089056	0.237627
C	0.674810	0.094165	-0.324279
C	0.880272	2.263361	0.971142
C	1.907238	2.970707	1.842304
C	1.401366	4.288198	2.384610
O	3.072939	3.236799	1.070622
C	3.766643	2.055897	0.730841
C	-3.793902	-1.365912	1.489689
O	4.823163	-0.107786	-0.554454
C	5.525326	-1.279722	-0.147922
O	0.491662	-1.973704	-1.511403
C	0.270912	-1.805574	-2.910849
O	-3.528573	2.167723	-1.804724
C	-2.792555	3.038480	-2.646843
O	-4.945915	0.572862	-0.132986
C	-5.660698	0.102695	-1.274641
O	3.242894	-2.137349	-1.732094
C	3.087592	-3.434247	-1.151794
H	-0.846569	1.753331	-1.729638
H	-0.564154	-2.492761	0.868276
H	-0.012275	-1.213212	1.941573
H	-2.029089	-1.340826	3.281318
H	-2.012450	-3.687874	4.049678
H	-1.192281	-4.190034	2.560580
H	-0.353615	-3.152022	3.727081

H	0.042142	1.924576	1.586359
H	0.471265	2.984652	0.254990
H	2.187353	2.310004	2.677577
H	1.174769	4.970060	1.561858
H	2.150681	4.754497	3.025474
H	0.490764	4.134696	2.966962
H	4.280736	1.653516	1.616412
H	4.534031	2.338968	0.011001
H	-4.156581	-0.766295	2.337465
H	-4.669680	-1.735316	0.956375
H	5.091233	-1.690592	0.768557
H	5.519269	-2.037949	-0.930418
H	6.548814	-0.966585	0.051074
H	-0.345951	-2.642216	-3.233579
H	-0.259188	-0.867699	-3.103010
H	1.218956	-1.814593	-3.455014
H	-2.101182	3.657620	-2.067831
H	-2.235137	2.481501	-3.405572
H	-3.525723	3.676760	-3.134150
H	-5.386946	0.668453	-2.167026
H	-5.464882	-0.961912	-1.438373
H	-6.718206	0.246749	-1.061040
H	3.560941	-3.471346	-0.165725
H	2.033215	-3.698286	-1.064417
H	3.590515	-4.131257	-1.819649

$\omega$ B97X Energy = -1498.55590620 a.u.

(*aS*,3*S*,3'*S*)-**28**, Conf D

C	-1.423899	0.761770	-1.438851
C	-2.802702	0.908296	-1.491162
C	-3.581089	0.362523	-0.464014
C	-2.979530	-0.302013	0.593302
C	-1.589975	-0.429891	0.655846
C	-0.817556	0.097590	-0.375013
C	-0.962455	-1.142061	1.830065
C	-1.938758	-1.297374	2.987534
C	-1.436542	-2.251055	4.047874
O	-3.175915	-1.804413	2.499042
C	1.289475	-1.167556	-0.817124
C	2.683135	-1.266906	-0.837069
C	3.449149	-0.216698	-0.339450
C	2.844171	0.944090	0.129785
C	1.456248	1.049653	0.123111
C	0.672875	-0.006758	-0.353098
C	0.814540	2.309908	0.653944
C	1.789344	3.138877	1.477602
C	1.258725	4.520919	1.784462
O	3.007268	3.291567	0.756927
C	3.709897	2.073653	0.638466
C	-3.850866	-0.861671	1.693970
O	4.818747	-0.272729	-0.380837
C	5.406098	-1.208549	0.522702
O	0.497030	-2.163269	-1.317168
C	0.679804	-3.476843	-0.788243
O	-3.472443	1.559791	-2.477891

C	-2.709613	2.132789	-3.526371
O	-4.945252	0.524184	-0.450031
C	-5.641907	-0.246616	-1.427785
O	3.309041	-2.380270	-1.337445
C	3.336625	-2.421731	-2.764460
H	-0.797081	1.170150	-2.221481
H	-0.624418	-2.138569	1.521839
H	-0.074426	-0.600552	2.169390
H	-2.123982	-0.309230	3.436927
H	-2.150438	-2.324075	4.869248
H	-1.295974	-3.246149	3.619605
H	-0.480172	-1.906774	4.446486
H	-0.059386	2.057524	1.261152
H	0.448194	2.919264	-0.179903
H	2.007463	2.608901	2.418019
H	1.096338	5.072720	0.855848
H	1.965161	5.078132	2.400901
H	0.308203	4.453012	2.317145
H	4.145430	1.797725	1.610902
H	4.536087	2.251809	-0.049307
H	-4.227598	-0.037791	2.317541
H	-4.717177	-1.370847	1.271925
H	6.484076	-1.115747	0.405460
H	5.131741	-0.967760	1.554552
H	5.095493	-2.227341	0.284925
H	0.913246	-3.435637	0.279027
H	-0.265755	-3.997311	-0.931634
H	1.479702	-4.007936	-1.305607
H	-2.018229	2.889983	-3.145443
H	-2.148396	1.369132	-4.072489
H	-3.425287	2.603056	-4.196524
H	-6.702599	-0.054109	-1.277243
H	-5.354183	0.050879	-2.437667
H	-5.443222	-1.313925	-1.287069
H	2.322229	-2.458567	-3.171860
H	3.860744	-1.548402	-3.161536
H	3.875248	-3.326533	-3.040045

$\omega$ B97X Energy = -1498.55560804 a.u.

(aS,3S,3'S)-28, Conf E

C	-1.433658	1.004859	-1.183702
C	-2.811670	1.165084	-1.210360
C	-3.596472	0.421243	-0.321929
C	-3.002516	-0.449959	0.577950
C	-1.613874	-0.594968	0.618685
C	-0.834573	0.130933	-0.277604
C	-0.995639	-1.545507	1.614538
C	-1.976151	-1.936220	2.710644
C	-1.485280	-3.097698	3.544704
O	-3.216619	-2.318864	2.124441
C	1.248645	-1.121856	-0.830458
C	2.639485	-1.254080	-0.872467
C	3.426827	-0.252947	-0.309159
C	2.845173	0.891737	0.227215
C	1.460615	1.022785	0.254238

C	0.654537	0.010601	-0.280554
C	0.851959	2.249756	0.892217
C	1.855261	2.985059	1.768569
C	1.358656	4.344584	2.205289
O	3.064884	3.176518	1.042264
C	3.741339	1.960618	0.809982
C	-3.881224	-1.223590	1.533560
O	4.797595	-0.350996	-0.300113
C	5.311329	-1.351459	0.580885
O	0.458880	-2.142605	-1.292131
C	0.299781	-2.172029	-2.705651
O	-3.474948	2.008862	-2.044790
C	-2.702441	2.800152	-2.931135
O	-4.960027	0.581780	-0.281295
C	-5.653901	0.034573	-1.401304
O	3.176011	-2.393171	-1.408407
C	4.019572	-2.200864	-2.545075
H	-0.802433	1.566378	-1.861133
H	-0.659748	-2.448109	1.091862
H	-0.107723	-1.092165	2.065165
H	-2.157766	-1.065497	3.360080
H	-2.201062	-3.335986	4.332477
H	-1.353276	-3.980469	2.915203
H	-0.525870	-2.855852	4.006303
H	-0.020058	1.965386	1.487529
H	0.491357	2.936803	0.118551
H	2.077595	2.370845	2.655100
H	1.193183	4.980606	1.332770
H	2.086426	4.830499	2.856243
H	0.415572	4.248007	2.746641
H	4.188971	1.595597	1.746764
H	4.558489	2.180643	0.123401
H	-4.256427	-0.545655	2.314306
H	-4.748644	-1.626538	1.010901
H	6.396013	-1.293193	0.515403
H	4.997514	-1.151888	1.609632
H	4.974707	-2.347233	0.283557
H	-0.145538	-1.237656	-3.062503
H	1.257621	-2.338714	-3.205814
H	-0.370929	-2.999541	-2.928908
H	-2.020874	3.456696	-2.382455
H	-2.128995	2.177262	-3.623856
H	-3.411370	3.404387	-3.492138
H	-6.714645	0.197762	-1.219866
H	-5.358710	0.534432	-2.325506
H	-5.460858	-1.039740	-1.485229
H	3.502004	-1.615766	-3.311430
H	4.947215	-1.694891	-2.272783
H	4.237383	-3.193447	-2.934510

$\omega$ B97X Energy = -1498.55558051 a.u.

(aS,3S,3'S)-28, Conf F

C	-1.456346	0.955859	-1.235563
C	-2.841521	0.996494	-1.300355
C	-3.582967	0.138989	-0.479697

C	-2.939457	-0.756326	0.360820
C	-1.544624	-0.794107	0.428089
C	-0.806996	0.067352	-0.379488
C	-0.874798	-1.767318	1.367103
C	-1.847010	-2.316931	2.400383
C	-1.280266	-3.491324	3.165879
O	-3.032982	-2.757672	1.747499
C	1.392808	-0.964365	-0.935953
C	2.791731	-0.982249	-0.941554
C	3.480936	0.071722	-0.346201
C	2.780519	1.129552	0.235415
C	1.391361	1.126525	0.256101
C	0.686101	0.074981	-0.343772
C	0.664035	2.253740	0.951837
C	1.589011	3.036188	1.871974
C	0.962387	4.314995	2.379188
O	2.771216	3.384964	1.161051
C	3.566147	2.257536	0.864251
C	-3.775297	-1.683616	1.213122
O	4.843311	0.177818	-0.357741
C	5.609283	-0.937518	0.090696
O	0.716107	-2.006572	-1.521650
C	0.547354	-1.859405	-2.930763
O	-3.552573	1.815253	-2.119742
C	-2.827404	2.677215	-2.980192
O	-4.954717	0.118810	-0.541447
C	-5.591355	1.258976	0.030984
O	3.480147	-1.964939	-1.603524
C	3.397649	-3.268356	-1.023318
H	-0.857907	1.609299	-1.858036
H	-0.456501	-2.599327	0.789360
H	-0.036916	-1.280864	1.875390
H	-2.119097	-1.514301	3.103783
H	-1.991723	-3.844393	3.913470
H	-1.059574	-4.312353	2.480079
H	-0.355958	-3.204938	3.671627
H	-0.177888	1.854197	1.524004
H	0.240827	2.942180	0.211951
H	1.871743	2.399676	2.725083
H	0.728889	4.975773	1.541295
H	1.643325	4.836757	3.052677
H	0.037335	4.098353	2.917079
H	4.060642	1.894675	1.777664
H	4.348214	2.594964	0.184633
H	-4.244010	-1.111161	2.028194
H	-4.577296	-2.118232	0.617464
H	6.597453	-0.548932	0.330655
H	5.165678	-1.372228	0.991564
H	5.691788	-1.699425	-0.683814
H	-0.054897	-0.973056	-3.152564
H	1.516917	-1.784077	-3.430092
H	0.023455	-2.747887	-3.278051
H	-3.570977	3.230800	-3.548536
H	-2.209320	3.378174	-2.411477
H	-2.194607	2.108769	-3.667769
H	-5.314958	2.169881	-0.503331

H	-5.327555	1.356518	1.089010
H	-6.663454	1.094171	-0.059219
H	3.806367	-3.261738	-0.008081
H	2.366667	-3.622737	-1.002836
H	4.001567	-3.921474	-1.650683

ωB97X Energy = -1498.55550722 a.u.

(aS,3S,3'S)-28, Conf G

C	-1.427006	0.859920	-1.302422
C	-2.809082	0.924924	-1.405919
C	-3.589438	0.134640	-0.554598
C	-2.987941	-0.719257	0.357133
C	-1.596451	-0.781464	0.463313
C	-0.820342	0.012614	-0.376387
C	-0.971969	-1.709245	1.476004
C	-1.980104	-2.168239	2.518909
C	-1.458984	-3.300321	3.374803
O	-3.160558	-2.625292	1.866706
C	1.368229	-1.090497	-0.832886
C	2.764899	-1.129581	-0.803380
C	3.452858	-0.088796	-0.183614
C	2.768540	1.006061	0.334997
C	1.378608	1.045597	0.288817
C	0.671621	-0.008989	-0.300832
C	0.655362	2.219284	0.907680
C	1.560077	3.015519	1.836896
C	0.952106	4.336889	2.249151
O	2.790318	3.290932	1.175699
C	3.557230	2.123575	0.978535
C	-3.864778	-1.573759	1.243909
O	4.824445	-0.094224	-0.100877
C	5.359911	-1.088560	0.774436
O	0.677606	-2.154757	-1.351045
C	0.519093	-2.121257	-2.764536
O	-3.481780	1.706849	-2.291089
C	-2.717341	2.505925	-3.177462
O	-4.959400	0.140627	-0.652167
C	-5.582704	1.321439	-0.152382
O	3.405805	-2.217952	-1.329704
C	4.270825	-1.943353	-2.432556
H	-0.798922	1.462910	-1.946270
H	-0.562674	-2.585400	0.960887
H	-0.132658	-1.213028	1.972348
H	-2.250303	-1.314634	3.160670
H	-2.197072	-3.588669	4.124304
H	-1.237244	-4.169478	2.751573
H	-0.542344	-2.998744	3.885591
H	-0.221431	1.866756	1.457854
H	0.283590	2.886938	0.122396
H	1.776661	2.413136	2.732885
H	0.784178	4.962226	1.369377
H	1.614684	4.869790	2.932165
H	-0.006016	4.175663	2.747036
H	3.969330	1.778989	1.939121
H	4.399188	2.401899	0.345152

H	-4.342158	-0.939789	2.006884
H	-4.660360	-2.029852	0.655695
H	4.953496	-0.966705	1.782635
H	5.136888	-2.093945	0.410434
H	6.436748	-0.933347	0.796673
H	-0.016139	-1.216773	-3.071101
H	1.488332	-2.165059	-3.269638
H	-0.067224	-2.997114	-3.035657
H	-3.434337	3.039838	-3.796543
H	-2.101606	3.227017	-2.631739
H	-2.077100	1.888970	-3.814650
H	-5.344702	1.463837	0.906682
H	-5.270070	2.199085	-0.721521
H	-6.655796	1.177606	-0.264100
H	5.127198	-1.340054	-2.126295
H	4.610158	-2.908725	-2.802902
H	3.726895	-1.421243	-3.225779

ωB97X Energy = -1498.55524483 a.u.

(aS,3S,3'S)-28, Conf H

C	-1.413390	0.588807	-1.537563
C	-2.795802	0.618306	-1.654147
C	-3.572831	0.021558	-0.655037
C	-2.967268	-0.615314	0.417180
C	-1.575681	-0.642191	0.534583
C	-0.803562	-0.037139	-0.452960
C	-0.946493	-1.320283	1.727656
C	-1.955480	-1.547231	2.844208
C	-1.429666	-2.459731	3.929086
O	-3.127696	-2.147977	2.305499
C	1.414349	-1.118667	-0.830909
C	2.811182	-1.104832	-0.795937
C	3.469099	-0.009168	-0.244548
C	2.753867	1.085750	0.227523
C	1.363091	1.078867	0.167958
C	0.688027	-0.023130	-0.366753
C	0.599439	2.267431	0.704024
C	1.472514	3.152824	1.581657
C	0.820002	4.479708	1.897321
O	2.699285	3.420951	0.912194
C	3.503344	2.267038	0.798623
C	-3.840678	-1.267307	1.464515
O	4.839385	0.046313	-0.234176
C	5.465395	-0.857625	0.675775
O	0.725411	-2.161716	-1.384284
C	0.988609	-3.467326	-0.869748
O	-3.471567	1.188366	-2.685874
C	-2.710931	1.769089	-3.731768
O	-4.942889	-0.003060	-0.750552
C	-5.574540	1.255123	-0.525209
O	3.545621	-2.151283	-1.292840
C	3.628299	-2.159115	-2.718395
H	-0.787489	1.044917	-2.294132
H	-0.531547	-2.290327	1.429102
H	-0.110669	-0.722541	2.103320

H	-2.233279	-0.575044	3.280933
H	-2.167885	-2.579510	4.723040
H	-1.205132	-3.444136	3.512292
H	-0.515259	-2.049060	4.361803
H	-0.269795	1.926893	1.273856
H	0.211618	2.865033	-0.128580
H	1.698794	2.619568	2.518298
H	0.641694	5.036754	0.974771
H	1.458804	5.079204	2.546971
H	-0.137682	4.323050	2.397604
H	3.917957	2.002574	1.783323
H	4.340827	2.528188	0.152278
H	-4.332589	-0.489749	2.068571
H	-4.625315	-1.852868	0.986530
H	6.537334	-0.690783	0.589111
H	5.147502	-0.648207	1.701941
H	5.231612	-1.892196	0.418809
H	1.162017	-3.430000	0.209079
H	0.098032	-4.059769	-1.072795
H	1.855685	-3.919430	-1.352726
H	-2.099662	2.598956	-3.365135
H	-2.066855	1.026833	-4.211512
H	-3.431377	2.143450	-4.455102
H	-6.646839	1.082427	-0.596601
H	-5.334040	1.633110	0.473771
H	-5.270611	1.984927	-1.277868
H	2.635669	-2.267871	-3.164663
H	4.094774	-1.238223	-3.078227
H	4.247930	-3.011584	-2.990611

ωB97X Energy = -1498.55519086 a.u.

(aS,3S,3'S)-28, Conf I

C	-1.334509	-1.077843	-1.297232
C	-2.706442	-1.122987	-1.495261
C	-3.539834	-0.411988	-0.624075
C	-2.999151	0.329154	0.414318
C	-1.615575	0.385959	0.605758
C	-0.787545	-0.330866	-0.256054
C	-1.064307	1.218213	1.740795
C	-2.091528	2.211909	2.263076
C	-1.661742	2.869655	3.554775
O	-3.319501	1.535284	2.508051
C	1.351720	-1.339705	0.537198
C	2.742335	-1.332983	0.700628
C	3.474021	-0.250691	0.219385
C	2.828800	0.795420	-0.441720
C	1.449320	0.778907	-0.604126
C	0.699047	-0.295021	-0.106843
C	0.781255	1.916136	-1.341941
C	1.692435	3.128410	-1.465002
C	1.158501	4.159609	-2.433232
O	2.971131	2.714683	-1.932206
C	3.658189	1.941803	-0.972019
C	-3.933773	1.106923	1.312002
O	4.821388	-0.119054	0.407517

C	5.662721	-1.195606	-0.001928
O	0.631066	-2.414502	0.996968
C	0.417432	-2.425816	2.407519
O	-3.320395	-1.808908	-2.494285
C	-2.502455	-2.534963	-3.396498
O	-4.899972	-0.385798	-0.814278
C	-5.563810	-1.606207	-0.489062
O	3.376722	-2.328955	1.396740
C	3.385312	-3.609033	0.761258
H	-0.666115	-1.619768	-1.953902
H	-0.757098	0.570151	2.569787
H	-0.166822	1.754882	1.421551
H	-2.267790	2.982795	1.496134
H	-2.406205	3.595548	3.883874
H	-1.541615	2.116053	4.336420
H	-0.708194	3.383997	3.420398
H	-0.145007	2.205548	-0.839064
H	0.496178	1.581695	-2.346062
H	1.819380	3.585462	-0.470865
H	1.073964	3.726501	-3.432449
H	1.824945	5.021550	-2.482785
H	0.169948	4.500328	-2.119120
H	3.981968	2.581632	-0.137868
H	4.557399	1.561867	-1.456259
H	-4.328206	1.973705	0.762047
H	-4.786377	0.491189	1.598850
H	5.332343	-1.598004	-0.964215
H	6.660602	-0.775070	-0.114112
H	5.679451	-1.989790	0.743930
H	-0.089903	-3.360892	2.637423
H	1.366447	-2.379265	2.946902
H	-0.220620	-1.588626	2.704888
H	-1.928819	-3.308358	-2.877810
H	-3.180596	-3.002731	-4.106257
H	-1.818557	-1.871187	-3.932954
H	-5.394899	-1.865600	0.561019
H	-6.626242	-1.435800	-0.652998
H	-5.219306	-2.420073	-1.129381
H	2.371496	-3.990852	0.634832
H	3.879341	-3.548498	-0.213356
H	3.952880	-4.270733	1.413027

ωB97X Energy = -1498.55501614 a.u.

(a*S*,3*S*,3'*S*)-**28**, Conf J

C	-1.405459	0.855678	-1.437970
C	-2.781878	1.012455	-1.516104
C	-3.588474	0.412370	-0.542388
C	-3.016829	-0.316233	0.488897
C	-1.629984	-0.457409	0.576963
C	-0.829665	0.125406	-0.401226
C	-1.035920	-1.244991	1.720116
C	-2.040440	-1.455333	2.844102
C	-1.570224	-2.467626	3.863883
O	-3.269357	-1.924233	2.300128
C	1.278520	-1.104858	-0.919330

C	2.671780	-1.225423	-0.896101
C	3.427935	-0.215564	-0.302598
C	2.817360	0.885486	0.284970
C	1.430120	0.995603	0.268246
C	0.658879	0.006753	-0.348001
C	0.778259	2.191633	0.921363
C	1.741486	2.930824	1.838984
C	1.208859	4.275495	2.279231
O	2.971675	3.151831	1.157142
C	3.673303	1.947762	0.935072
C	-3.918517	-0.932176	1.533610
O	4.800017	-0.300054	-0.267792
C	5.432396	-0.080504	-1.530481
O	0.481244	-2.018256	-1.547494
C	0.613470	-3.387678	-1.176779
O	-3.424145	1.723501	-2.479792
C	-2.633571	2.346231	-3.478276
O	-4.951972	0.580141	-0.553398
C	-5.625476	-0.125861	-1.594525
O	3.268573	-2.284280	-1.529749
C	3.976611	-3.187531	-0.678238
H	-0.757195	1.304417	-2.179868
H	-0.700069	-2.225278	1.360618
H	-0.150641	-0.734841	2.111261
H	-2.228811	-0.490717	3.340993
H	-2.303084	-2.576559	4.664361
H	-1.428167	-3.440684	3.388057
H	-0.620379	-2.153410	4.300994
H	-0.101141	1.875435	1.489586
H	0.417952	2.883600	0.151737
H	1.945342	2.307354	2.723601
H	1.059947	4.921656	1.411230
H	1.908192	4.763080	2.959487
H	0.251158	4.155896	2.789473
H	4.074893	1.567027	1.885743
H	4.524391	2.193440	0.299633
H	-4.305984	-0.142882	2.194271
H	-4.776975	-1.409821	1.061505
H	5.192098	0.917309	-1.909595
H	6.504276	-0.154028	-1.357424
H	5.122076	-0.832262	-2.259063
H	0.773399	-3.484515	-0.098292
H	-0.327927	-3.867599	-1.439567
H	1.433779	-3.866460	-1.711679
H	-1.947947	3.078254	-3.041821
H	-2.063090	1.609159	-4.050559
H	-3.330695	2.855932	-4.139096
H	-5.435086	-1.200855	-1.513469
H	-5.308475	0.231390	-2.575849
H	-6.688971	0.063606	-1.460820
H	4.351651	-3.982632	-1.320005
H	4.809003	-2.688332	-0.180079
H	3.302950	-3.612928	0.071772

ωB97X Energy = -1498.55499976 a.u.

(a*S*,3*S*,3'*S*)-**28**, Conf K



C	-1.348116	0.984931	-1.253936	H	-4.684443	2.890999	-1.021135
C	-2.725487	1.123083	-1.317302	H	-3.113625	3.732388	-1.156551
C	-3.527240	0.368132	-0.463335	H	-4.243419	3.727428	-2.533499
C	-2.943644	-0.493085	0.461464	H	-5.302182	-1.107780	-1.751829
C	-1.557500	-0.611642	0.539046	H	-6.597792	0.089459	-1.503841
C	-0.755846	0.123981	-0.338838	H	-5.201485	0.491954	-2.539189
C	-0.950233	-1.547728	1.555024	H	3.854920	-4.282975	-0.973089
C	-1.955528	-1.964747	2.618440	H	3.913709	-3.222472	0.458111
C	-1.463252	-3.116274	3.465244	H	2.337041	-3.767514	-0.193135
O	-3.166940	-2.374050	1.991472	$\omega$ B97X Energy = -1498.55479398 a.u.			
C	1.350940	-1.116105	-0.822294	(aS,3S,3'S)-28, Conf L			
C	2.740545	-1.242344	-0.813524	C	-1.308241	-1.235058	-1.195049
C	3.512800	-0.214923	-0.282868	C	-2.680762	-1.388916	-1.323008
C	2.908195	0.922223	0.245379	C	-3.523125	-0.726886	-0.422722
C	1.520739	1.034231	0.251987	C	-2.990378	0.040526	0.601189
C	0.733248	0.015768	-0.299412	C	-1.607206	0.192946	0.732192
C	0.886448	2.260600	0.866098	C	-0.769880	-0.451557	-0.176811
C	1.868040	3.031162	1.737201	C	-1.067544	1.058544	1.847229
C	1.345648	4.393466	2.133265	C	-2.140011	1.977863	2.412543
O	3.084908	3.222375	1.023364	C	-1.701256	2.676965	3.679234
C	3.778644	2.008281	0.834014	O	-3.299506	1.211788	2.719260
C	-3.836452	-1.291871	1.382873	C	1.468808	-1.311530	0.506792
O	4.877844	-0.328030	-0.210010	C	2.860940	-1.205605	0.611516
C	5.546398	-0.257225	-1.470449	C	3.491686	-0.068476	0.113939
O	0.592164	-2.153790	-1.301878	C	2.745090	0.935145	-0.504980
C	0.484382	-2.180858	-2.724126	C	1.364460	0.820303	-0.608745
O	-3.271717	1.971371	-2.249576	C	0.715401	-0.309433	-0.093668
C	-3.863816	3.145909	-1.695503	C	0.586383	1.913294	-1.304304
O	-4.896501	0.484767	-0.475542	C	1.399761	3.191369	-1.442649
C	-5.526738	-0.042335	-1.644463	C	0.751843	4.194370	-2.370178
O	3.341200	-2.354591	-1.342915	O	2.684280	2.880316	-1.969224
C	3.356429	-3.469081	-0.449951	C	3.466303	2.144356	-1.053419
H	-0.739157	1.571741	-1.933652	C	-3.938804	0.723943	1.559898
H	-0.575464	-2.440194	1.041251	O	4.833284	0.157751	0.247039
H	-0.088346	-1.072623	2.032892	C	5.729849	-0.848255	-0.220394
H	-2.177964	-1.100474	3.263687	O	0.849329	-2.441487	0.980927
H	-2.196301	-3.372480	4.231092	C	0.681240	-2.477282	2.397179
H	-1.292167	-3.994759	2.839103	O	-3.287361	-2.150003	-2.270836
H	-0.523976	-2.852846	3.955559	C	-2.458474	-2.881944	-3.158199
H	0.015011	1.971213	1.460188	O	-4.886307	-0.877070	-0.493302
H	0.519323	2.926235	0.077044	C	-5.498902	-0.213431	-1.596882
H	2.087111	2.442399	2.641537	O	3.593166	-2.160615	1.267513
H	1.182026	5.004373	1.242638	C	3.668567	-3.428799	0.612489
H	2.057598	4.906719	2.780677	H	-0.632971	-1.733047	-1.878873
H	0.397230	4.296149	2.665199	H	-0.683849	0.433600	2.661909
H	4.200828	1.664041	1.789427	H	-0.223040	1.655992	1.493353
H	4.615569	2.224524	0.169588	H	-2.409785	2.726601	1.650919
H	-4.255370	-0.627760	2.153273	H	-2.482077	3.347552	4.040032
H	-4.674777	-1.712168	0.827364	H	-1.487771	1.940924	4.457520
H	5.226684	-1.069453	-2.125227	H	-0.796543	3.260423	3.497519
H	5.351712	0.706284	-1.951778	H	-0.339424	2.126663	-0.763778
H	6.610678	-0.348699	-1.262379	H	0.289807	1.570679	-2.302398
H	-0.005059	-1.271853	-3.087233	H	1.533931	3.641812	-0.446417
H	1.470256	-2.282298	-3.184595	H	0.662320	3.772165	-3.373602
H	-0.127453	-3.045260	-2.975034				

H	1.346962	5.106464	-2.428113
H	-0.247191	4.452044	-2.012840
H	3.782469	2.794004	-0.224016
H	4.367005	1.836455	-1.583941
H	-4.451059	1.548565	1.041013
H	-4.704451	0.023591	1.892050
H	5.388914	-1.253267	-1.177901
H	6.691078	-0.357193	-0.361991
H	5.832780	-1.654236	0.505806
H	-0.009518	-1.693516	2.720940
H	0.253416	-3.449483	2.634399
H	1.640348	-2.361699	2.907599
H	-1.815477	-3.578301	-2.612737
H	-3.130134	-3.441490	-3.804848
H	-1.840479	-2.215484	-3.766835
H	-5.145348	-0.624509	-2.544284
H	-6.570527	-0.379240	-1.503091
H	-5.294056	0.861395	-1.560351
H	2.678562	-3.873608	0.505563
H	4.132776	-3.322767	-0.372867
H	4.293781	-4.061247	1.240107

$\omega$ B97X Energy = -1498.55459787 a.u.

(*a*S,3*S*,3'*S*)-**28**, Conf M

C	-1.391363	0.894494	-1.412447
C	-2.769888	0.970067	-1.552096
C	-3.579329	0.194416	-0.714848
C	-3.009403	-0.657992	0.218143
C	-1.621784	-0.731155	0.359348
C	-0.816989	0.049608	-0.465574
C	-1.032556	-1.652345	1.399693
C	-2.071364	-2.085729	2.423611
C	-1.583403	-3.207825	3.311584
O	-3.236902	-2.543473	1.747143
C	1.392638	-1.002280	-0.962055
C	2.789017	-1.027505	-0.883423
C	3.445983	-0.013525	-0.187437
C	2.735161	0.996192	0.448794
C	1.345222	1.011686	0.375797
C	0.672188	0.021206	-0.344160
C	0.584047	2.108745	1.083352
C	1.454378	2.840592	2.094908
C	0.810973	4.108982	2.607251
O	2.690791	3.196968	1.485782
C	3.486274	2.064694	1.208654
C	-3.916762	-1.496182	1.089437
O	4.818285	-0.001904	-0.100022
C	5.480083	0.345089	-1.318349
O	0.686447	-1.916507	-1.687948
C	0.937307	-3.300977	-1.461150
O	-3.412524	1.750668	-2.460072
C	-2.618175	2.530062	-3.338252
O	-4.946794	0.212344	-0.845359
C	-5.570126	1.406195	-0.377893
O	3.486350	-1.990287	-1.565733

C	4.232319	-2.900133	-0.755131
H	-0.741313	1.484359	-2.046177
H	-0.625284	-2.547523	0.914888
H	-0.197233	-1.161745	1.908081
H	-2.349043	-1.218384	3.043223
H	-2.342666	-3.475549	4.047334
H	-1.357015	-4.090710	2.709313
H	-0.676455	-2.907130	3.839899
H	-0.293057	1.690656	1.585560
H	0.207810	2.831426	0.350554
H	1.667481	2.167262	2.939806
H	0.649044	4.806894	1.782682
H	1.448654	4.590928	3.349315
H	-0.153797	3.887434	3.067670
H	3.878614	1.644372	2.146409
H	4.340415	2.415430	0.629226
H	-4.413532	-0.850549	1.829613
H	-4.696661	-1.956562	0.483855
H	5.162630	1.336188	-1.656109
H	6.545863	0.361453	-1.098854
H	5.273020	-0.390038	-2.098807
H	1.131250	-3.492220	-0.401071
H	0.030363	-3.826559	-1.756331
H	1.780263	-3.653574	-2.055152
H	-2.006862	3.250549	-2.786877
H	-1.971076	1.897905	-3.952712
H	-3.314667	3.064849	-3.979623
H	-5.238528	2.271819	-0.954549
H	-5.352575	1.563967	0.683435
H	-6.641924	1.269151	-0.509219
H	4.685679	-3.616735	-1.437520
H	5.008976	-2.380321	-0.192158
H	3.569716	-3.427800	-0.062574

$\omega$ B97X Energy = -1498.55458641 a.u.

(*a*S,3*S*,3'*S*)-**28**, Conf N

C	-1.348557	0.936778	-1.287060
C	-2.727534	1.039699	-1.377637
C	-3.525551	0.307892	-0.500857
C	-2.939462	-0.548304	0.427119
C	-1.552623	-0.647332	0.517805
C	-0.752646	0.103361	-0.349116
C	-0.943772	-1.564399	1.549716
C	-1.952313	-1.971234	2.613766
C	-1.452825	-3.097890	3.489282
O	-3.152738	-2.409047	1.985397
C	1.386238	-1.099421	-0.782251
C	2.777842	-1.196132	-0.752416
C	3.520832	-0.144727	-0.226850
C	2.885136	0.987803	0.274108
C	1.495623	1.071199	0.258601
C	0.737547	0.027343	-0.286455
C	0.826656	2.294566	0.840967
C	1.778708	3.104307	1.709439
C	1.222203	4.463975	2.066056

O	3.002471	3.305152	1.010170
C	3.723236	2.101875	0.857411
C	-3.831896	-1.351498	1.345710
O	4.886734	-0.228627	-0.132866
C	5.571611	-0.163398	-1.384896
O	0.656429	-2.160521	-1.255664
C	0.565710	-2.210225	-2.678098
O	-3.277122	1.890371	-2.305446
C	-3.942228	1.230452	-3.382452
O	-4.897048	0.367500	-0.563788
C	-5.457194	1.606233	-0.126755
O	3.408345	-2.303440	-1.256981
C	3.442451	-3.400923	-0.343835
H	-0.741620	1.520379	-1.971317
H	-0.560690	-2.462189	1.051723
H	-0.087861	-1.076143	2.024845
H	-2.190548	-1.095967	3.238449
H	-2.189734	-3.347888	4.253510
H	-1.263825	-3.987172	2.883859
H	-0.522037	-2.811114	3.982644
H	-0.045913	1.997189	1.429409
H	0.454752	2.935991	0.034457
H	1.995790	2.540438	2.629964
H	1.057856	5.049823	1.158904
H	1.914095	5.007544	2.710529
H	0.268665	4.358904	2.587230
H	4.133972	1.784677	1.827090
H	4.568263	2.321985	0.204612
H	-4.279653	-0.684104	2.097936
H	-4.648887	-1.796714	0.778768
H	5.364175	0.788513	-1.883620
H	6.634496	-0.229739	-1.160766
H	5.277573	-0.992013	-2.031175
H	1.558879	-2.293914	-3.126325
H	-0.022067	-3.092737	-2.923420
H	0.058769	-1.318397	-3.059768
H	-3.242735	0.587359	-3.924839
H	-4.782068	0.634223	-3.018879
H	-4.305650	2.010770	-4.048463
H	-5.120839	2.431676	-0.757462
H	-6.537690	1.500617	-0.202541
H	-5.183884	1.803234	0.914256
H	3.988794	-3.125964	0.562714
H	2.428389	-3.717279	-0.087343
H	3.961515	-4.213105	-0.849357

ωB97X Energy = -1498.55454131 a.u.

(aS,3S,3'S)-28, Conf O

C	1.336540	0.743974	1.351975
C	2.714340	0.851193	1.478997
C	3.530505	0.254980	0.511823
C	2.968930	-0.441605	-0.547750
C	1.582747	-0.567847	-0.663070
C	0.770781	0.037899	0.292015
C	1.001462	-1.333509	-1.827512

C	2.028988	-2.268859	-2.454460
C	2.273423	-3.521811	-1.624281
O	3.229704	-1.539669	-2.715261
C	-1.378934	-1.180806	0.633074
C	-2.770102	-1.269778	0.577362
C	-3.500847	-0.192945	0.086567
C	-2.852978	0.957763	-0.353196
C	-1.463579	1.034193	-0.309828
C	-0.718776	-0.035298	0.200678
C	-0.778327	2.280611	-0.819168
C	-1.710225	3.134994	-1.666148
C	-1.142292	4.507785	-1.946039
O	-2.946980	3.307345	-0.981553
C	-3.675242	2.101333	-0.900722
C	3.891762	-1.096138	-1.548705
O	-4.865374	-0.267355	-0.034047
C	-5.570890	-0.254990	1.208042
O	-0.659723	-2.270266	1.055857
C	-0.572082	-2.390689	2.474047
O	3.348530	1.494591	2.494375
C	2.548016	2.086616	3.503050
O	4.898727	0.291342	0.622667
C	5.481416	1.569377	0.373248
O	-3.410849	-2.397736	1.019794
C	-3.459790	-3.438589	0.043444
H	0.679936	1.200072	2.082482
H	0.134319	-1.911351	-1.500237
H	0.647755	-0.629319	-2.587933
H	1.681118	-2.568947	-3.444639
H	3.091113	-4.106905	-2.049564
H	2.512377	-3.286281	-0.584739
H	1.372922	-4.138918	-1.623034
H	0.104962	2.007466	-1.403433
H	-0.420364	2.879609	0.025770
H	-1.910510	2.616243	-2.616308
H	-0.994294	5.048933	-1.008711
H	-1.819178	5.084680	-2.577346
H	-0.179123	4.423420	-2.453010
H	-4.066015	1.832273	-1.892865
H	-4.533361	2.294337	-0.256451
H	4.651780	-0.387751	-1.880054
H	4.421403	-1.927106	-1.064234
H	-5.294304	-1.115405	1.819560
H	-5.364276	0.670845	1.753942
H	-6.630381	-0.301426	0.963692
H	-0.003066	-3.295905	2.677185
H	-0.047503	-1.528919	2.898627
H	-1.567888	-2.475873	2.916348
H	1.900595	2.866375	3.091342
H	3.240465	2.530739	4.214145
H	1.935909	1.337330	4.013448
H	5.237862	1.911358	-0.637846
H	5.138119	2.304286	1.103387
H	6.558707	1.441608	0.461399
H	-4.008185	-3.105881	-0.842206
H	-2.449593	-3.747512	-0.237066

H        -3.982659   -4.275219   0.503039  
 $\omega$ B97X Energy = -1498.55411257 a.u.

(*aR*,3*S*,3'*S*)-**28**, Conf A

C	-1.365688	1.140715	-1.122244
C	-2.739172	1.334514	-1.160280
C	-3.556858	0.546125	-0.342665
C	-2.999447	-0.401989	0.501089
C	-1.615451	-0.582410	0.554071
C	-0.803482	0.188425	-0.273414
C	-1.036223	-1.616179	1.488846
C	-2.046187	-2.068005	2.533719
C	-1.595356	-3.300626	3.284132
O	-3.282501	-2.376458	1.897563
C	1.256403	-1.079794	-0.876765
C	2.640547	-1.256874	-0.887227
C	3.452049	-0.304536	-0.280635
C	2.890816	0.807936	0.340046
C	1.508429	0.969240	0.365096
C	0.681605	0.027485	-0.260495
C	0.921977	2.163431	1.082201
C	1.933879	2.814668	2.013477
C	1.464656	4.153209	2.536716
O	3.154602	3.025035	1.311176
C	3.803442	1.808623	1.010484
C	-3.911927	-1.223681	1.382028
O	4.812290	-0.471294	-0.223860
C	5.480948	-0.330274	-1.478147
O	0.460008	-2.047738	-1.434869
C	0.343655	-1.950964	-2.852838
O	-3.368282	2.251856	-1.941476
C	-2.563870	3.077418	-2.766115
O	-4.917052	0.734228	-0.315669
C	-5.599772	0.285283	-1.485230
O	3.198056	-2.344764	-1.507079
C	3.166218	-3.529906	-0.710443
H	-0.710165	1.735205	-1.746420
H	-0.707917	-2.485245	0.907163
H	-0.148891	-1.215558	1.987903
H	-2.221764	-1.246466	3.245832
H	-2.327543	-3.580257	4.042563
H	-1.475530	-4.136124	2.590808
H	-0.637140	-3.117694	3.774381
H	0.038630	1.859312	1.650563
H	0.582870	2.908364	0.353809
H	2.133585	2.136862	2.857843
H	1.323932	4.851352	1.708389
H	2.196861	4.575404	3.226081
H	0.513854	4.043290	3.061804
H	4.220293	1.368687	1.928096
H	4.642733	2.052240	0.358490
H	-4.284184	-0.598298	2.206763
H	-4.779601	-1.564457	0.817249
H	5.313012	0.669856	-1.889880

H	6.542441	-0.465994	-1.280253
H	5.137787	-1.084652	-2.187900
H	1.323497	-2.042655	-3.328173
H	-0.296236	-2.771777	-3.171167
H	-0.119986	-0.999925	-3.133345
H	-1.995867	2.484715	-3.489147
H	-3.249960	3.732825	-3.297245
H	-1.874861	3.681574	-2.168759
H	-5.275289	0.843592	-2.365097
H	-6.660218	0.458781	-1.311957
H	-5.427658	-0.784264	-1.642913
H	3.723531	-3.380092	0.218403
H	2.134886	-3.812352	-0.485385
H	3.640787	-4.314159	-1.297215

$\omega$ B97X Energy = -1498.55731613 a.u.

(*aR*,3*S*,3'*S*)-**28**, Conf B

C	-1.363283	0.969984	-1.274467
C	-2.741564	1.070493	-1.399291
C	-3.554536	0.258422	-0.600624
C	-2.989122	-0.653670	0.277236
C	-1.601611	-0.753229	0.403564
C	-0.793114	0.064599	-0.380853
C	-1.014209	-1.745705	1.376628
C	-2.050808	-2.244951	2.372490
C	-1.569813	-3.439446	3.164730
O	-3.229072	-2.635200	1.674618
C	1.378991	-1.061771	-0.858825
C	2.770897	-1.138785	-0.796998
C	3.478444	-0.132875	-0.147866
C	2.807712	0.935104	0.441339
C	1.418054	0.999219	0.389401
C	0.695904	0.002774	-0.279135
C	0.708839	2.147116	1.070405
C	1.619568	2.873813	2.049531
C	1.030942	4.178988	2.534742
O	2.859327	3.166108	1.413217
C	3.607468	1.996903	1.159836
C	-3.899155	-1.532783	1.104220
O	4.842434	-0.204157	-0.019233
C	5.563730	0.004860	-1.234156
O	0.685805	-2.085863	-1.453143
C	0.590629	-1.969410	-2.871194
O	-3.380485	1.907754	-2.258307
C	-2.581396	2.725798	-3.095607
O	-4.921820	0.300907	-0.721122
C	-5.528363	1.470648	-0.176699
O	3.436671	-2.178763	-1.390710
C	3.460371	-3.365336	-0.596372
H	-0.710641	1.588729	-1.877690
H	-0.607912	-2.599112	0.821803
H	-0.177811	-1.291546	1.916270
H	-2.313891	-1.426566	3.061066
H	-2.323866	-3.752683	3.887834
H	-1.364094	-4.274846	2.491795

H	-0.651526	-3.194131	3.701996
H	-0.177408	1.777670	1.593948
H	0.352749	2.863646	0.321755
H	1.819949	2.216773	2.910050
H	0.881664	4.859257	1.693173
H	1.697276	4.657363	3.253544
H	0.066075	4.005776	3.015269
H	3.996667	1.588297	2.103852
H	4.466626	2.296342	0.558985
H	-4.370851	-0.930980	1.896171
H	-4.697420	-1.934980	0.481386
H	6.620444	-0.067542	-0.984160
H	5.306344	-0.755038	-1.973516
H	5.353115	1.000524	-1.637106
H	0.043144	-2.842270	-3.221509
H	0.040849	-1.062850	-3.143342
H	1.584994	-1.952622	-3.324858
H	-1.957495	3.405826	-2.508034
H	-1.945471	2.121190	-3.748736
H	-3.273812	3.304772	-3.701988
H	-5.191144	2.366295	-0.701921
H	-5.301604	1.560948	0.890500
H	-6.602452	1.353306	-0.307962
H	3.966696	-3.177654	0.354585
H	2.444650	-3.724832	-0.414434
H	4.015817	-4.109935	-1.163494

$\omega$ B97X Energy = -1498.55692462 a.u.

(*aR*,3*S*,3'*S*)-**28**, Conf C

C	-1.451474	1.127274	-1.085600
C	-2.831531	1.267122	-1.062796
C	-3.581815	0.437767	-0.221357
C	-2.951447	-0.498168	0.583614
C	-1.560145	-0.623494	0.576423
C	-0.814911	0.189351	-0.273672
C	-0.902426	-1.643960	1.473615
C	-1.850225	-2.146968	2.552627
C	-1.320755	-3.368648	3.269045
O	-3.098002	-2.498385	1.963239
C	1.272769	-0.988987	-0.956224
C	2.664206	-1.109607	-1.034367
C	3.459001	-0.112517	-0.473724
C	2.868381	0.991080	0.143737
C	1.485683	1.089056	0.237627
C	0.674810	0.094165	-0.324279
C	0.880272	2.263361	0.971142
C	1.907238	2.970707	1.842304
C	1.401366	4.288198	2.384610
O	3.072939	3.236799	1.070622
C	3.766643	2.055897	0.730841
C	-3.793902	-1.365912	1.489689
O	4.823163	-0.107786	-0.554454
C	5.525326	-1.279722	-0.147922
O	0.491662	-1.973704	-1.511403
C	0.270912	-1.805574	-2.910849

O	-3.528573	2.167723	-1.804724
C	-2.792555	3.038480	-2.646843
O	-4.945915	0.572862	-0.132986
C	-5.660698	0.102695	-1.274641
O	3.242894	-2.137349	-1.732094
C	3.087592	-3.434247	-1.151794
H	-0.846569	1.753331	-1.729638
H	-0.564154	-2.492761	0.868276
H	-0.012275	-1.213212	1.941573
H	-2.029089	-1.340826	3.281318
H	-2.012450	-3.687874	4.049678
H	-1.192281	-4.190034	2.560580
H	-0.353615	-3.152022	3.727081
H	0.042142	1.924576	1.586359
H	0.471265	2.984652	0.254990
H	2.187353	2.310004	2.677577
H	1.174769	4.970060	1.561858
H	2.150681	4.754497	3.025474
H	0.490764	4.134696	2.966962
H	4.280736	1.653516	1.616412
H	4.534031	2.338968	0.011001
H	-4.156581	-0.766295	2.337465
H	-4.669680	-1.735316	0.956375
H	5.091233	-1.690592	0.768557
H	5.519269	-2.037949	-0.930418
H	6.548814	-0.966585	0.051074
H	-0.345951	-2.642216	-3.233579
H	-0.259188	-0.867699	-3.103010
H	1.218956	-1.814593	-3.455014
H	-2.101182	3.657620	-2.067831
H	-2.235137	2.481501	-3.405572
H	-3.525723	3.676760	-3.134150
H	-5.386946	0.668453	-2.167026
H	-5.464882	-0.961912	-1.438373
H	-6.718206	0.246749	-1.061040
H	3.560941	-3.471346	-0.165725
H	2.033215	-3.698286	-1.064417
H	3.590515	-4.131257	-1.819649

$\omega$ B97X Energy = -1498.55590620 a.u.

(*aR*,3*S*,3'*S*)-**28**, Conf D

C	-1.423899	0.761770	-1.438851
C	-2.802702	0.908296	-1.491162
C	-3.581089	0.362523	-0.464014
C	-2.979530	-0.302013	0.593302
C	-1.589975	-0.429891	0.655846
C	-0.817556	0.097590	-0.375013
C	-0.962455	-1.142061	1.830065
C	-1.938758	-1.297374	2.987534
C	-1.436542	-2.251055	4.047874
O	-3.175915	-1.804413	2.499042
C	1.289475	-1.167556	-0.817124
C	2.683135	-1.266906	-0.837069
C	3.449149	-0.216698	-0.339450
C	2.844171	0.944090	0.129785

C	1.456248	1.049653	0.123111
C	0.672875	-0.006758	-0.353098
C	0.814540	2.309908	0.653944
C	1.789344	3.138877	1.477602
C	1.258725	4.520919	1.784462
O	3.007268	3.291567	0.756927
C	3.709897	2.073653	0.638466
C	-3.850866	-0.861671	1.693970
O	4.818747	-0.272729	-0.380837
C	5.406098	-1.208549	0.522702
O	0.497030	-2.163269	-1.317168
C	0.679804	-3.476843	-0.788243
O	-3.472443	1.559791	-2.477891
C	-2.709613	2.132789	-3.526371
O	-4.945252	0.524184	-0.450031
C	-5.641907	-0.246616	-1.427785
O	3.309041	-2.380270	-1.337445
C	3.336625	-2.421731	-2.764460
H	-0.797081	1.170150	-2.221481
H	-0.624418	-2.138569	1.521839
H	-0.074426	-0.600552	2.169390
H	-2.123982	-0.309230	3.436927
H	-2.150438	-2.324075	4.869248
H	-1.295974	-3.246149	3.619605
H	-0.480172	-1.906774	4.446486
H	-0.059386	2.057524	1.261152
H	0.448194	2.919264	-0.179903
H	2.007463	2.608901	2.418019
H	1.096338	5.072720	0.855848
H	1.965161	5.078132	2.400901
H	0.308203	4.453012	2.317145
H	4.145430	1.797725	1.610902
H	4.536087	2.251809	-0.049307
H	-4.227598	-0.037791	2.317541
H	-4.717177	-1.370847	1.271925
H	6.484076	-1.115747	0.405460
H	5.131741	-0.967760	1.554552
H	5.095493	-2.227341	0.284925
H	0.913246	-3.435637	0.279027
H	-0.265755	-3.997311	-0.931634
H	1.479702	-4.007936	-1.305607
H	-2.018229	2.889983	-3.145443
H	-2.148396	1.369132	-4.072489
H	-3.425287	2.603056	-4.196524
H	-6.702599	-0.054109	-1.277243
H	-5.354183	0.050879	-2.437667
H	-5.443222	-1.313925	-1.287069
H	2.322229	-2.458567	-3.171860
H	3.860744	-1.548402	-3.161536
H	3.875248	-3.326533	-3.040045

$\omega$ B97X Energy = -1498.55560804 a.u.

(aR,3S,3'S)-28, Conf E

C	-1.433658	1.004859	-1.183702
C	-2.811670	1.165084	-1.210360

C	-3.596472	0.421243	-0.321929
C	-3.002516	-0.449959	0.577950
C	-1.613874	-0.594968	0.618685
C	-0.834573	0.130933	-0.277604
C	-0.995639	-1.545507	1.614538
C	-1.976151	-1.936220	2.710644
C	-1.485280	-3.097698	3.544704
O	-3.216619	-2.318864	2.124441
C	1.248645	-1.121856	-0.830458
C	2.639485	-1.254080	-0.872467
C	3.426827	-0.252947	-0.309159
C	2.845173	0.891737	0.227215
C	1.460615	1.022785	0.254238
C	0.654537	0.010601	-0.280554
C	0.851959	2.249756	0.892217
C	1.855261	2.985059	1.768569
C	1.358656	4.344584	2.205289
O	3.064884	3.176518	1.042264
C	3.741339	1.960618	0.809982
C	-3.881224	-1.223590	1.533560
O	4.797595	-0.350996	-0.300113
C	5.311329	-1.351459	0.580885
O	0.458880	-2.142605	-1.292131
C	0.299781	-2.172029	-2.705651
O	-3.474948	2.008862	-2.044790
C	-2.702441	2.800152	-2.931135
O	-4.960027	0.581780	-0.281295
C	-5.653901	0.034573	-1.401304
O	3.176011	-2.393171	-1.408407
C	4.019572	-2.200864	-2.545075
H	-0.802433	1.566378	-1.861133
H	-0.659748	-2.448109	1.091862
H	-0.107723	-1.092165	2.065165
H	-2.157766	-1.065497	3.360080
H	-2.201062	-3.335986	4.332477
H	-1.353276	-3.980469	2.915203
H	-0.525870	-2.855852	4.006303
H	-0.020058	1.965386	1.487529
H	0.491357	2.936803	0.118551
H	2.077595	2.370845	2.655100
H	1.193183	4.980606	1.332770
H	2.086426	4.830499	2.856243
H	0.415572	4.248007	2.746641
H	4.188971	1.595597	1.746764
H	4.558489	2.180643	0.123401
H	-4.256427	-0.545655	2.314306
H	-4.748644	-1.626538	1.010901
H	6.396013	-1.293193	0.515403
H	4.997514	-1.151888	1.609632
H	4.974707	-2.347233	0.283557
H	-0.145538	-1.237656	-3.062503
H	1.257621	-2.338714	-3.205814
H	-0.370929	-2.999541	-2.928908
H	-2.020874	3.456696	-2.382455
H	-2.128995	2.177262	-3.623856
H	-3.411370	3.404387	-3.492138

H	-6.714645	0.197762	-1.219866
H	-5.358710	0.534432	-2.325506
H	-5.460858	-1.039740	-1.485229
H	3.502004	-1.615766	-3.311430
H	4.947215	-1.694891	-2.272783
H	4.237383	-3.193447	-2.934510

$\omega$ B97X Energy = -1498.55558051 a.u.

(*aR*,3*S*,3'*S*)-**28**, Conf F

C	-1.456346	0.955859	-1.235563
C	-2.841521	0.996494	-1.300355
C	-3.582967	0.138989	-0.479697
C	-2.939457	-0.756326	0.360820
C	-1.544624	-0.794107	0.428089
C	-0.806996	0.067352	-0.379488
C	-0.874798	-1.767318	1.367103
C	-1.847010	-2.316931	2.400383
C	-1.280266	-3.491324	3.165879
O	-3.032982	-2.757672	1.747499
C	1.392808	-0.964365	-0.935953
C	2.791731	-0.982249	-0.941554
C	3.480936	0.071722	-0.346201
C	2.780519	1.129552	0.235415
C	1.391361	1.126525	0.256101
C	0.686101	0.074981	-0.343772
C	0.664035	2.253740	0.951837
C	1.589011	3.036188	1.871974
C	0.962387	4.314995	2.379188
O	2.771216	3.384964	1.161051
C	3.566147	2.257536	0.864251
C	-3.775297	-1.683616	1.213122
O	4.843311	0.177818	-0.357741
C	5.609283	-0.937518	0.090696
O	0.716107	-2.006572	-1.521650
C	0.547354	-1.859405	-2.930763
O	-3.552573	1.815253	-2.119742
C	-2.827404	2.677215	-2.980192
O	-4.954717	0.118810	-0.541447
C	-5.591355	1.258976	0.030984
O	3.480147	-1.964939	-1.603524
C	3.397649	-3.268356	-1.023318
H	-0.857907	1.609299	-1.858036
H	-0.456501	-2.599327	0.789360
H	-0.036916	-1.280864	1.875390
H	-2.119097	-1.514301	3.103783
H	-1.991723	-3.844393	3.913470
H	-1.059574	-4.312353	2.480079
H	-0.355958	-3.204938	3.671627
H	-0.177888	1.854197	1.524004
H	0.240827	2.942180	0.211951
H	1.871743	2.399676	2.725083
H	0.728889	4.975773	1.541295
H	1.643325	4.836757	3.052677
H	0.037335	4.098353	2.917079
H	4.060642	1.894675	1.777664

H	4.348214	2.594964	0.184633
H	-4.244010	-1.111161	2.028194
H	-4.577296	-2.118232	0.617464
H	6.597453	-0.548932	0.330655
H	5.165678	-1.372228	0.991564
H	5.691788	-1.699425	-0.683814
H	-0.054897	-0.973056	-3.152564
H	1.516917	-1.784077	-3.430092
H	0.023455	-2.747887	-3.278051
H	-3.570977	3.230800	-3.548536
H	-2.209320	3.378174	-2.411477
H	-2.194607	2.108769	-3.667769
H	-5.314958	2.169881	-0.503331
H	-5.327555	1.356518	1.089010
H	-6.663454	1.094171	-0.059219
H	3.806367	-3.261738	-0.008081
H	2.366667	-3.622737	-1.002836
H	4.001567	-3.921474	-1.650683

$\omega$ B97X Energy = -1498.55550722 a.u.

(*aR*,3*S*,3'*S*)-**28**, Conf G

C	-1.427006	0.859920	-1.302422
C	-2.809082	0.924924	-1.405919
C	-3.589438	0.134640	-0.554598
C	-2.987941	-0.719257	0.357133
C	-1.596451	-0.781464	0.463313
C	-0.820342	0.012614	-0.376387
C	-0.971969	-1.709245	1.476004
C	-1.980104	-2.168239	2.518909
C	-1.458984	-3.300321	3.374803
O	-3.160558	-2.625292	1.866706
C	1.368229	-1.090497	-0.832886
C	2.764899	-1.129581	-0.803380
C	3.452858	-0.088796	-0.183614
C	2.768540	1.006061	0.334997
C	1.378608	1.045597	0.288817
C	0.671621	-0.008989	-0.300832
C	0.655362	2.219284	0.907680
C	1.560077	3.015519	1.836896
C	0.952106	4.336889	2.249151
O	2.790318	3.290932	1.175699
C	3.557230	2.123575	0.978535
C	-3.864778	-1.573759	1.243909
O	4.824445	-0.094224	-0.100877
C	5.359911	-1.088560	0.774436
O	0.677606	-2.154757	-1.351045
C	0.519093	-2.121257	-2.764536
O	-3.481780	1.706849	-2.291089
C	-2.717341	2.505925	-3.177462
O	-4.959400	0.140627	-0.652167
C	-5.582704	1.321439	-0.152382
O	3.405805	-2.217952	-1.329704
C	4.270825	-1.943353	-2.432556
H	-0.798922	1.462910	-1.946270
H	-0.562674	-2.585400	0.960887

H	-0.132658	-1.213028	1.972348
H	-2.250303	-1.314634	3.160670
H	-2.197072	-3.588669	4.124304
H	-1.237244	-4.169478	2.751573
H	-0.542344	-2.998744	3.885591
H	-0.221431	1.866756	1.457854
H	0.283590	2.886938	0.122396
H	1.776661	2.413136	2.732885
H	0.784178	4.962226	1.369377
H	1.614684	4.869790	2.932165
H	-0.006016	4.175663	2.747036
H	3.969330	1.778989	1.939121
H	4.399188	2.401899	0.345152
H	-4.342158	-0.939789	2.006884
H	-4.660360	-2.029852	0.655695
H	4.953496	-0.966705	1.782635
H	5.136888	-2.093945	0.410434
H	6.436748	-0.933347	0.796673
H	-0.016139	-1.216773	-3.071101
H	1.488332	-2.165059	-3.269638
H	-0.067224	-2.997114	-3.035657
H	-3.434337	3.039838	-3.796543
H	-2.101606	3.227017	-2.631739
H	-2.077100	1.888970	-3.814650
H	-5.344702	1.463837	0.906682
H	-5.270070	2.199085	-0.721521
H	-6.655796	1.177606	-0.264100
H	5.127198	-1.340054	-2.126295
H	4.610158	-2.908725	-2.802902
H	3.726895	-1.421243	-3.225779

ωB97X Energy = -1498.55524483 a.u.

(aR,3S,3'S)-**28**, Conf H

C	-1.413390	0.588807	-1.537563
C	-2.795802	0.618306	-1.654147
C	-3.572831	0.021558	-0.655037
C	-2.967268	-0.615314	0.417180
C	-1.575681	-0.642191	0.534583
C	-0.803562	-0.037139	-0.452960
C	-0.946493	-1.320283	1.727656
C	-1.955480	-1.547231	2.844208
C	-1.429666	-2.459731	3.929086
O	-3.127696	-2.147977	2.305499
C	1.414349	-1.118667	-0.830909
C	2.811182	-1.104832	-0.795937
C	3.469099	-0.009168	-0.244548
C	2.753867	1.085750	0.227523
C	1.363091	1.078867	0.167958
C	0.688027	-0.023130	-0.366753
C	0.599439	2.267431	0.704024
C	1.472514	3.152824	1.581657
C	0.820002	4.479708	1.897321
O	2.699285	3.420951	0.912194
C	3.503344	2.267038	0.798623
C	-3.840678	-1.267307	1.464515

O	4.839385	0.046313	-0.234176
C	5.465395	-0.857625	0.675775
O	0.725411	-2.161716	-1.384284
C	0.988609	-3.467326	-0.869748
O	-3.471567	1.188366	-2.685874
C	-2.710931	1.769089	-3.731768
O	-4.942889	-0.003060	-0.750552
C	-5.574540	1.255123	-0.525209
O	3.545621	-2.151283	-1.292840
C	3.628299	-2.159115	-2.718395
H	-0.787489	1.044917	-2.294132
H	-0.531547	-2.290327	1.429102
H	-0.110669	-0.722541	2.103320
H	-2.233279	-0.575044	3.280933
H	-2.167885	-2.579510	4.723040
H	-1.205132	-3.444136	3.512292
H	-0.515259	-2.049060	4.361803
H	-0.269795	1.926893	1.273856
H	0.211618	2.865033	-0.128580
H	1.698794	2.619568	2.518298
H	0.641694	5.036754	0.974771
H	1.458804	5.079204	2.546971
H	-0.137682	4.323050	2.397604
H	3.917957	2.002574	1.783323
H	4.340827	2.528188	0.152278
H	-4.332589	-0.489749	2.068571
H	-4.625315	-1.852868	0.986530
H	6.537334	-0.690783	0.589111
H	5.147502	-0.648207	1.701941
H	5.231612	-1.892196	0.418809
H	1.162017	-3.430000	0.209079
H	0.098032	-4.059769	-1.072795
H	1.855685	-3.919430	-1.352726
H	-2.099662	2.598956	-3.365135
H	-2.066855	1.026833	-4.211512
H	-3.431377	2.143450	-4.455102
H	-6.646839	1.082427	-0.596601
H	-5.334040	1.633110	0.473771
H	-5.270611	1.984927	-1.277868
H	2.635669	-2.267871	-3.164663
H	4.094774	-1.238223	-3.078227
H	4.247930	-3.011584	-2.990611

ωB97X Energy = -1498.55519086 a.u.

(aR,3S,3'S)-**28**, Conf I

C	-1.334509	-1.077843	-1.297232
C	-2.706442	-1.122987	-1.495261
C	-3.539834	-0.411988	-0.624075
C	-2.999151	0.329154	0.414318
C	-1.615575	0.385959	0.605758
C	-0.787545	-0.330866	-0.256054
C	-1.064307	1.218213	1.740795
C	-2.091528	2.211909	2.263076
C	-1.661742	2.869655	3.554775
O	-3.319501	1.535284	2.508051



C	1.351720	-1.339705	0.537198
C	2.742335	-1.332983	0.700628
C	3.474021	-0.250691	0.219385
C	2.828800	0.795420	-0.441720
C	1.449320	0.778907	-0.604126
C	0.699047	-0.295021	-0.106843
C	0.781255	1.916136	-1.341941
C	1.692435	3.128410	-1.465002
C	1.158501	4.159609	-2.433232
O	2.971131	2.714683	-1.932206
C	3.658189	1.941803	-0.972019
C	-3.933773	1.106923	1.312002
O	4.821388	-0.119054	0.407517
C	5.662721	-1.195606	-0.001928
O	0.631066	-2.414502	0.996968
C	0.417432	-2.425816	2.407519
O	-3.320395	-1.808908	-2.494285
C	-2.502455	-2.534963	-3.396498
O	-4.899972	-0.385798	-0.814278
C	-5.563810	-1.606207	-0.489062
O	3.376722	-2.328955	1.396740
C	3.385312	-3.609033	0.761258
H	-0.666115	-1.619768	-1.953902
H	-0.757098	0.570151	2.569787
H	-0.166822	1.754882	1.421551
H	-2.267790	2.982795	1.496134
H	-2.406205	3.595548	3.883874
H	-1.541615	2.116053	4.336420
H	-0.708194	3.383997	3.420398
H	-0.145007	2.205548	-0.839064
H	0.496178	1.581695	-2.346062
H	1.819380	3.585462	-0.470865
H	1.073964	3.726501	-3.432449
H	1.824945	5.021550	-2.482785
H	0.169948	4.500328	-2.119120
H	3.981968	2.581632	-0.137868
H	4.557399	1.561867	-1.456259
H	-4.328206	1.973705	0.762047
H	-4.786377	0.491189	1.598850
H	5.332343	-1.598004	-0.964215
H	6.660602	-0.775070	-0.114112
H	5.679451	-1.989790	0.743930
H	-0.089903	-3.360892	2.637423
H	1.366447	-2.379265	2.946902
H	-0.220620	-1.588626	2.704888
H	-1.928819	-3.308358	-2.877810
H	-3.180596	-3.002731	-4.106257
H	-1.818557	-1.871187	-3.932954
H	-5.394899	-1.865600	0.561019
H	-6.626242	-1.435800	-0.652998
H	-5.219306	-2.420073	-1.129381
H	2.371496	-3.990852	0.634832
H	3.879341	-3.548498	-0.213356
H	3.952880	-4.270733	1.413027

ωB97X Energy = -1498.55501614 a.u.

(aR,3S,3'S)-28, Conf J

C	-1.405459	0.855678	-1.437970
C	-2.781878	1.012455	-1.516104
C	-3.588474	0.412370	-0.542388
C	-3.016829	-0.316233	0.488897
C	-1.629984	-0.457409	0.576963
C	-0.829665	0.125406	-0.401226
C	-1.035920	-1.244991	1.720116
C	-2.040440	-1.455333	2.844102
C	-1.570224	-2.467626	3.863883
O	-3.269357	-1.924233	2.300128
C	1.278520	-1.104858	-0.919330
C	2.671780	-1.225423	-0.896101
C	3.427935	-0.215564	-0.302598
C	2.817360	0.885486	0.284970
C	1.430120	0.995603	0.268246
C	0.658879	0.006753	-0.348001
C	0.778259	2.191633	0.921363
C	1.741486	2.930824	1.838984
C	1.208859	4.275495	2.279231
O	2.971675	3.151831	1.157142
C	3.673303	1.947762	0.935072
C	-3.918517	-0.932176	1.533610
O	4.800017	-0.300054	-0.267792
C	5.432396	-0.080504	-1.530481
O	0.481244	-2.018256	-1.547494
C	0.613470	-3.387678	-1.176779
O	-3.424145	1.723501	-2.479792
C	-2.633571	2.346231	-3.478276
O	-4.951972	0.580141	-0.553398
C	-5.625476	-0.125861	-1.594525
O	3.268573	-2.284280	-1.529749
C	3.976611	-3.187531	-0.678238
H	-0.757195	1.304417	-2.179868
H	-0.700069	-2.225278	1.360618
H	-0.150641	-0.734841	2.111261
H	-2.228811	-0.490717	3.340993
H	-2.303084	-2.576559	4.664361
H	-1.428167	-3.440684	3.388057
H	-0.620379	-2.153410	4.300994
H	-0.101141	1.875435	1.489586
H	0.417952	2.883600	0.151737
H	1.945342	2.307354	2.723601
H	1.059947	4.921656	1.411230
H	1.908192	4.763080	2.959487
H	0.251158	4.155896	2.789473
H	4.074893	1.567027	1.885743
H	4.524391	2.193440	0.299633
H	-4.305984	-0.142882	2.194271
H	-4.776975	-1.409821	1.061505
H	5.192098	0.917309	-1.909595
H	6.504276	-0.154028	-1.357424
H	5.122076	-0.832262	-2.259063
H	0.773399	-3.484515	-0.098292
H	-0.327927	-3.867599	-1.439567

H	1.433779	-3.866460	-1.711679
H	-1.947947	3.078254	-3.041821
H	-2.063090	1.609159	-4.050559
H	-3.330695	2.855932	-4.139096
H	-5.435086	-1.200855	-1.513469
H	-5.308475	0.231390	-2.575849
H	-6.688971	0.063606	-1.460820
H	4.351651	-3.982632	-1.320005
H	4.809003	-2.688332	-0.180079
H	3.302950	-3.612928	0.071772

$\omega_{B97X}$  Energy = -1498.55499976 a.u.

(*aR*,3*S*,3'*S*)-**28**, Conf K

C	-1.348116	0.984931	-1.253936
C	-2.725487	1.123083	-1.317302
C	-3.527240	0.368132	-0.463335
C	-2.943644	-0.493085	0.461464
C	-1.557500	-0.611642	0.539046
C	-0.755846	0.123981	-0.338838
C	-0.950233	-1.547728	1.555024
C	-1.955528	-1.964747	2.618440
C	-1.463252	-3.116274	3.465244
O	-3.166940	-2.374050	1.991472
C	1.350940	-1.116105	-0.822294
C	2.740545	-1.242344	-0.813524
C	3.512800	-0.214923	-0.282868
C	2.908195	0.922223	0.245379
C	1.520739	1.034231	0.251987
C	0.733248	0.015768	-0.299412
C	0.886448	2.260600	0.866098
C	1.868040	3.031162	1.737201
C	1.345648	4.393466	2.133265
O	3.084908	3.222375	1.023364
C	3.778644	2.008281	0.834014
C	-3.836452	-1.291871	1.382873
O	4.877844	-0.328030	-0.210010
C	5.546398	-0.257225	-1.470449
O	0.592164	-2.153790	-1.301878
C	0.484382	-2.180858	-2.724126
O	-3.271717	1.971371	-2.249576
C	-3.863816	3.145909	-1.695503
O	-4.896501	0.484767	-0.475542
C	-5.526738	-0.042335	-1.644463
O	3.341200	-2.354591	-1.342915
C	3.356429	-3.469081	-0.449951
H	-0.739157	1.571741	-1.933652
H	-0.575464	-2.440194	1.041251
H	-0.088346	-1.072623	2.032892
H	-2.177964	-1.100474	3.263687
H	-2.196301	-3.372480	4.231092
H	-1.292167	-3.994759	2.839103
H	-0.523976	-2.852846	3.955559
H	0.015011	1.971213	1.460188
H	0.519323	2.926235	0.077044
H	2.087111	2.442399	2.641537

H	1.182026	5.004373	1.242638
H	2.057598	4.906719	2.780677
H	0.397230	4.296149	2.665199
H	4.200828	1.664041	1.789427
H	4.615569	2.224524	0.169588
H	-4.255370	-0.627760	2.153273
H	-4.674777	-1.712168	0.827364
H	5.226684	-1.069453	-2.125227
H	5.351712	0.706284	-1.951778
H	6.610678	-0.348699	-1.262379
H	-0.005059	-1.271853	-3.087233
H	1.470256	-2.282298	-3.184595
H	-0.127453	-3.045260	-2.975034
H	-4.684443	2.890999	-1.021135
H	-3.113625	3.732388	-1.156551
H	-4.243419	3.727428	-2.533499
H	-5.302182	-1.107780	-1.751829
H	-6.597792	0.089459	-1.503841
H	-5.201485	0.491954	-2.539189
H	3.854920	-4.282975	-0.973089
H	3.913709	-3.222472	0.458111
H	2.337041	-3.767514	-0.193135

$\omega_{B97X}$  Energy = -1498.55479398 a.u.

(*aR*,3*S*,3'*S*)-**28**, Conf L

C	-1.308241	-1.235058	-1.195049
C	-2.680762	-1.388916	-1.323008
C	-3.523125	-0.726886	-0.422722
C	-2.990378	0.040526	0.601189
C	-1.607206	0.192946	0.732192
C	-0.769880	-0.451557	-0.176811
C	-1.067544	1.058544	1.847229
C	-2.140011	1.977863	2.412543
C	-1.701256	2.676965	3.679234
O	-3.299506	1.211788	2.719260
C	1.468808	-1.311530	0.506792
C	2.860940	-1.205605	0.611516
C	3.491686	-0.068476	0.113939
C	2.745090	0.935145	-0.504980
C	1.364460	0.820303	-0.608745
C	0.715401	-0.309433	-0.093668
C	0.586383	1.913294	-1.304304
C	1.399761	3.191369	-1.442649
C	0.751843	4.194370	-2.370178
O	2.684280	2.880316	-1.969224
C	3.466303	2.144356	-1.053419
C	-3.938804	0.723943	1.559898
O	4.833284	0.157751	0.247039
C	5.729849	-0.848255	-0.220394
O	0.849329	-2.441487	0.980927
C	0.681240	-2.477282	2.397179
O	-3.287361	-2.150003	-2.270836
C	-2.458474	-2.881944	-3.158199
O	-4.886307	-0.877070	-0.493302
C	-5.498902	-0.213431	-1.596882

O	3.593166	-2.160615	1.267513
C	3.668567	-3.428799	0.612489
H	-0.632971	-1.733047	-1.878873
H	-0.683849	0.433600	2.661909
H	-0.223040	1.655992	1.493353
H	-2.409785	2.726601	1.650919
H	-2.482077	3.347552	4.040032
H	-1.487771	1.940924	4.457520
H	-0.796543	3.260423	3.497519
H	-0.339424	2.126663	-0.763778
H	0.289807	1.570679	-2.302398
H	1.533931	3.641812	-0.446417
H	0.662320	3.772165	-3.373602
H	1.346962	5.106464	-2.428113
H	-0.247191	4.452044	-2.012840
H	3.782469	2.794004	-0.224016
H	4.367005	1.836455	-1.583941
H	-4.451059	1.548565	1.041013
H	-4.704451	0.023591	1.892050
H	5.388914	-1.253267	-1.177901
H	6.691078	-0.357193	-0.361991
H	5.832780	-1.654236	0.505806
H	-0.009518	-1.693516	2.720940
H	0.253416	-3.449483	2.634399
H	1.640348	-2.361699	2.907599
H	-1.815477	-3.578301	-2.612737
H	-3.130134	-3.441490	-3.804848
H	-1.840479	-2.215484	-3.766835
H	-5.145348	-0.624509	-2.544284
H	-6.570527	-0.379240	-1.503091
H	-5.294056	0.861395	-1.560351
H	2.678562	-3.873608	0.505563
H	4.132776	-3.322767	-0.372867
H	4.293781	-4.061247	1.240107

$\omega$ B97X Energy = -1498.55459787 a.u.

(aR,3S,3'S)-**28**, Conf M

C	-1.391363	0.894494	-1.412447
C	-2.769888	0.970067	-1.552096
C	-3.579329	0.194416	-0.714848
C	-3.009403	-0.657992	0.218143
C	-1.621784	-0.731155	0.359348
C	-0.816989	0.049608	-0.465574
C	-1.032556	-1.652345	1.399693
C	-2.071364	-2.085729	2.423611
C	-1.583403	-3.207825	3.311584
O	-3.236902	-2.543473	1.747143
C	1.392638	-1.002280	-0.962055
C	2.789017	-1.027505	-0.883423
C	3.445983	-0.013525	-0.187437
C	2.735161	0.996192	0.448794
C	1.345222	1.011686	0.375797
C	0.672188	0.021206	-0.344160
C	0.584047	2.108745	1.083352
C	1.454378	2.840592	2.094908

C	0.810973	4.108982	2.607251
O	2.690791	3.196968	1.485782
C	3.486274	2.064694	1.208654
C	-3.916762	-1.496182	1.089437
O	4.818285	-0.001904	-0.100022
C	5.480083	0.345089	-1.318349
O	0.686447	-1.916507	-1.687948
C	0.937307	-3.300977	-1.461150
O	-3.412524	1.750668	-2.460072
C	-2.618175	2.530062	-3.338252
O	-4.946794	0.212344	-0.845359
C	-5.570126	1.406195	-0.377893
O	3.486350	-1.990287	-1.565733
C	4.232319	-2.900133	-0.755131
H	-0.741313	1.484359	-2.046177
H	-0.625284	-2.547523	0.914888
H	-0.197233	-1.161745	1.908081
H	-2.349043	-1.218384	3.043223
H	-2.342666	-3.475549	4.047334
H	-1.357015	-4.090710	2.709313
H	-0.676455	-2.907130	3.839899
H	-0.293057	1.690656	1.585560
H	0.207810	2.831426	0.350554
H	1.667481	2.167262	2.939806
H	0.649044	4.806894	1.782682
H	1.448654	4.590928	3.349315
H	-0.153797	3.887434	3.067670
H	3.878614	1.644372	2.146409
H	4.340415	2.415430	0.629226
H	-4.413532	-0.850549	1.829613
H	-4.696661	-1.956562	0.483855
H	5.162630	1.336188	-1.656109
H	6.545863	0.361453	-1.098854
H	5.273020	-0.390038	-2.098807
H	1.131250	-3.492220	-0.401071
H	0.030363	-3.826559	-1.756331
H	1.780263	-3.653574	-2.055152
H	-2.006862	3.250549	-2.786877
H	-1.971076	1.897905	-3.952712
H	-3.314667	3.064849	-3.979623
H	-5.238528	2.271819	-0.954549
H	-5.352575	1.563967	0.683435
H	-6.641924	1.269151	-0.509219
H	4.685679	-3.616735	-1.437520
H	5.008976	-2.380321	-0.192158
H	3.569716	-3.427800	-0.062574

$\omega$ B97X Energy = -1498.55458641 a.u.

(aR,3S,3'S)-**28**, Conf N

C	-1.348557	0.936778	-1.287060
C	-2.727534	1.039699	-1.377637
C	-3.525551	0.307892	-0.500857
C	-2.939462	-0.548304	0.427119
C	-1.552623	-0.647332	0.517805
C	-0.752646	0.103361	-0.349116

C	-0.943772	-1.564399	1.549716
C	-1.952313	-1.971234	2.613766
C	-1.452825	-3.097890	3.489282
O	-3.152738	-2.409047	1.985397
C	1.386238	-1.099421	-0.782251
C	2.777842	-1.196132	-0.752416
C	3.520832	-0.144727	-0.226850
C	2.885136	0.987803	0.274108
C	1.495623	1.071199	0.258601
C	0.737547	0.027343	-0.286455
C	0.826656	2.294566	0.840967
C	1.778708	3.104307	1.709439
C	1.222203	4.463975	2.066056
O	3.002471	3.305152	1.010170
C	3.723236	2.101875	0.857411
C	-3.831896	-1.351498	1.345710
O	4.886734	-0.228627	-0.132866
C	5.571611	-0.163398	-1.384896
O	0.656429	-2.160521	-1.255664
C	0.565710	-2.210225	-2.678098
O	-3.277122	1.890371	-2.305446
C	-3.942228	1.230452	-3.382452
O	-4.897048	0.367500	-0.563788
C	-5.457194	1.606233	-0.126755
O	3.408345	-2.303440	-1.256981
C	3.442451	-3.400923	-0.343835
H	-0.741620	1.520379	-1.971317
H	-0.560690	-2.462189	1.051723
H	-0.087861	-1.076143	2.024845
H	-2.190548	-1.095967	3.238449
H	-2.189734	-3.347888	4.253510
H	-1.263825	-3.987172	2.883859
H	-0.522037	-2.811114	3.982644
H	-0.045913	1.997189	1.429409
H	0.454752	2.935991	0.034457
H	1.995790	2.540438	2.629964
H	1.057856	5.049823	1.158904
H	1.914095	5.007544	2.710529
H	0.268665	4.358904	2.587230
H	4.133972	1.784677	1.827090
H	4.568263	2.321985	0.204612
H	-4.279653	-0.684104	2.097936
H	-4.648887	-1.796714	0.778768
H	5.364175	0.788513	-1.883620
H	6.634496	-0.229739	-1.160766
H	5.277573	-0.992013	-2.031175
H	1.558879	-2.293914	-3.126325
H	-0.022067	-3.092737	-2.923420
H	0.058769	-1.318397	-3.059768
H	-3.242735	0.587359	-3.924839
H	-4.782068	0.634223	-3.018879
H	-4.305650	2.010770	-4.048463
H	-5.120839	2.431676	-0.757462
H	-6.537690	1.500617	-0.202541
H	-5.183884	1.803234	0.914256
H	3.988794	-3.125964	0.562714

H	2.428389	-3.717279	-0.087343
H	3.961515	-4.213105	-0.849357

ωB97X Energy = -1498.55454131 a.u.

(aR,3S,3'S)-**28**, Conf O

C	1.336540	0.743974	1.351975
C	2.714340	0.851193	1.478997
C	3.530505	0.254980	0.511823
C	2.968930	-0.441605	-0.547750
C	1.582747	-0.567847	-0.663070
C	0.770781	0.037899	0.292015
C	1.001462	-1.333509	-1.827512
C	2.028988	-2.268859	-2.454460
C	2.273423	-3.521811	-1.624281
O	3.229704	-1.539669	-2.715261
C	-1.378934	-1.180806	0.633074
C	-2.770102	-1.269778	0.577362
C	-3.500847	-0.192945	0.086567
C	-2.852978	0.957763	-0.353196
C	-1.463579	1.034193	-0.309828
C	-0.718776	-0.035298	0.200678
C	-0.778327	2.280611	-0.819168
C	-1.710225	3.134994	-1.666148
C	-1.142292	4.507785	-1.946039
O	-2.946980	3.307345	-0.981553
C	-3.675242	2.101333	-0.900722
C	3.891762	-1.096138	-1.548705
O	-4.865374	-0.267355	-0.034047
C	-5.570890	-0.254990	1.208042
O	-0.659723	-2.270266	1.055857
C	-0.572082	-2.390689	2.474047
O	3.348530	1.494591	2.494375
C	2.548016	2.086616	3.503050
O	4.898727	0.291342	0.622667
C	5.481416	1.569377	0.373248
O	-3.410849	-2.397736	1.019794
C	-3.459790	-3.438589	0.043444
H	0.679936	1.200072	2.082482
H	0.134319	-1.911351	-1.500237
H	0.647755	-0.629319	-2.587933
H	1.681118	-2.568947	-3.444639
H	3.091113	-4.106905	-2.049564
H	2.512377	-3.286281	-0.584739
H	1.372922	-4.138918	-1.623034
H	0.104962	2.007466	-1.403433
H	-0.420364	2.879609	0.025770
H	-1.910510	2.616243	-2.616308
H	-0.994294	5.048933	-1.008711
H	-1.819178	5.084680	-2.577346
H	-0.179123	4.423420	-2.453010
H	-4.066015	1.832273	-1.892865
H	-4.533361	2.294337	-0.256451
H	4.651780	-0.387751	-1.880054
H	4.421403	-1.927106	-1.064234
H	-5.294304	-1.115405	1.819560

H	-5.364276	0.670845	1.753942
H	-6.630381	-0.301426	0.963692
H	-0.003066	-3.295905	2.677185
H	-0.047503	-1.528919	2.898627
H	-1.567888	-2.475873	2.916348
H	1.900595	2.866375	3.091342
H	3.240465	2.530739	4.214145
H	1.935909	1.337330	4.013448
H	5.237862	1.911358	-0.637846
H	5.138119	2.304286	1.103387
H	6.558707	1.441608	0.461399
H	-4.008185	-3.105881	-0.842206
H	-2.449593	-3.747512	-0.237066
H	-3.982659	-4.275219	0.503039

ωB97X Energy = -1498.55411257 a.u.

**Table S6.** Cartesian coordinates and energies of the low-energy conformers calculated at the B3LYP/TZVP PCM/CHCl<sub>3</sub> level.

(*aS*,1*S*,3*S*,3'*S*)-**21**, Conf A

C	2.712249	0.607559	-1.315173
C	4.007708	0.123147	-1.470156
C	4.529491	-0.743683	-0.496919
C	3.750859	-1.120607	0.594666
C	2.440153	-0.645931	0.738946
C	1.926304	0.230966	-0.222560
C	1.624966	-1.067491	1.941408
C	2.211196	-2.293073	2.637603
C	1.588584	-2.560873	3.994542
O	3.617790	-2.099237	2.835934
C	0.282540	1.876874	0.697133
C	-1.000252	2.433236	0.776869
C	-2.032376	1.888415	0.010944
C	-1.805132	0.762863	-0.787839
C	-0.523550	0.207475	-0.859264
C	0.534566	0.775463	-0.125553
C	-0.271861	-0.976818	-1.769332
C	-1.558203	-1.647065	-2.238617
C	-1.343961	-2.588592	-3.408685
O	-2.490355	-0.640451	-2.662194
C	-2.959252	0.181553	-1.584976
C	4.334224	-2.080185	1.610311
C	-4.002121	-0.568290	-0.755665
C	-3.766236	-1.029426	0.538252
C	-4.737401	-1.744047	1.236658
C	-5.948026	-1.986682	0.616959
C	-6.225140	-1.544992	-0.666046
C	-5.242046	-0.835434	-1.343939
F	-6.904540	-2.678823	1.291490
O	4.823968	0.422775	-2.522945
C	4.330999	1.295382	-3.536720
O	5.782212	-1.302435	-0.631557
C	6.893636	-0.401980	-0.492888
O	-1.226039	3.528618	1.579512
C	-1.704351	3.209482	2.897663
O	-3.308752	2.396457	0.083525
C	-3.490635	3.720080	-0.451503
O	1.287252	2.369819	1.496099
C	1.834341	3.637072	1.098292
H	2.291832	1.277287	-2.051910
H	1.579638	-0.239643	2.657582
H	0.594747	-1.278264	1.643160
H	2.073890	-3.173789	1.992284
H	1.762566	-1.716683	4.665280
H	0.510976	-2.707265	3.897044
H	2.018667	-3.456021	4.446113
H	0.359269	-1.711440	-1.263696
H	0.292907	-0.642655	-2.646356
H	-2.001262	-2.206191	-1.405109

H	-0.960666	-2.042188	-4.273242
H	-2.281452	-3.069568	-3.690821
H	-0.623298	-3.365153	-3.144474
H	-3.475369	1.001956	-2.085367
H	4.367607	-3.093206	1.182583
H	5.358048	-1.802587	1.856677
H	-2.818900	-0.824421	1.019604
H	-4.561831	-2.102366	2.242521
H	-7.188346	-1.750930	-1.114140
H	-5.442204	-0.485385	-2.349687
H	3.448752	0.876440	-4.027810
H	5.135477	1.390698	-4.261827
H	4.089199	2.281488	-3.131067
H	6.868554	0.092204	0.482475
H	7.790109	-1.014770	-0.564699
H	6.894810	0.346061	-1.285500
H	-0.973571	2.600152	3.433997
H	-2.661112	2.685478	2.845087
H	-1.835904	4.158357	3.413900
H	-4.551366	3.940685	-0.352440
H	-3.210782	3.745480	-1.508144
H	-2.905047	4.451930	0.104004
H	2.289432	3.561760	0.107194
H	1.066850	4.412013	1.099809
H	2.602389	3.879182	1.830117

B3LYP Energy = -1829.33666153 a.u.

(*aS*,1*S*,3*S*,3'*S*)-**21**, Conf B

C	2.732486	0.475033	-1.361297
C	4.050895	0.029751	-1.386458
C	4.571032	-0.616991	-0.254647
C	3.786388	-0.773196	0.885420
C	2.458281	-0.326771	0.907827
C	1.934594	0.303444	-0.226702
C	1.628346	-0.529860	2.156263
C	2.248558	-1.558263	3.098204
C	1.595209	-1.582366	4.466952
O	3.636063	-1.251910	3.284405
C	0.224141	2.040145	0.325962
C	-1.078413	2.554137	0.288443
C	-2.080553	1.834741	-0.364186
C	-1.801380	0.586859	-0.932024
C	-0.501621	0.073789	-0.883246
C	0.525186	0.807852	-0.260930
C	-0.197008	-1.252749	-1.547764
C	-1.452202	-2.045566	-1.896507
C	-1.184978	-3.177271	-2.870895
O	-2.413200	-1.171795	-2.508138
C	-2.924066	-0.177105	-1.610142
C	4.394376	-1.443494	2.100066

C	-3.949730	-0.792233	-0.658809
C	-5.185586	-1.180417	-1.184536
C	-6.149829	-1.788101	-0.390351
C	-5.857629	-2.004006	0.946008
C	-4.650710	-1.634283	1.507513
C	-3.698967	-1.024835	0.692500
F	-6.795100	-2.595409	1.733528
O	4.900904	0.183645	-2.443689
C	4.425386	0.855532	-3.607537
O	5.884783	-1.031418	-0.208992
C	6.223688	-2.148184	-1.045580
O	-1.360177	3.773156	0.862413
C	-1.688928	3.707522	2.261066
O	-3.376565	2.292937	-0.396943
C	-3.605858	3.493001	-1.157219
O	1.199277	2.719579	1.017723
C	1.712315	3.896748	0.373035
H	2.312093	0.972916	-2.223551
H	1.525876	0.421846	2.688857
H	0.617699	-0.847895	1.887126
H	2.174804	-2.556797	2.641229
H	1.703085	-0.612049	4.956495
H	0.530444	-1.806625	4.376923
H	2.055432	-2.342196	5.100152
H	0.449039	-1.855061	-0.904341
H	0.371713	-1.071354	-2.466036
H	-1.887708	-2.458703	-0.978157
H	-0.803566	-2.784580	-3.816025
H	-2.100353	-3.735460	-3.071473
H	-0.444039	-3.865837	-2.459543
H	-3.462244	0.513055	-2.260984
H	4.516691	-2.520128	1.907823
H	5.385043	-1.036757	2.298496
H	-5.397814	-1.007012	-2.232937
H	-7.110055	-2.086081	-0.790526
H	-4.463152	-1.816094	2.557637
H	-2.755130	-0.721477	1.126480
H	5.260546	0.867696	-4.303577
H	4.128354	1.882902	-3.380846
H	3.584092	0.323950	-4.060584
H	5.607253	-3.016942	-0.797343
H	6.104334	-1.900326	-2.100473
H	7.267533	-2.375998	-0.838532
H	-0.848856	3.312230	2.835612
H	-2.574634	3.087900	2.419237
H	-1.897650	4.728355	2.574910
H	-3.291682	3.352532	-2.195050
H	-3.077273	4.340344	-0.722094
H	-4.679267	3.667417	-1.124530
H	2.455861	4.313582	1.049242
H	2.191013	3.634791	-0.574008
H	0.919198	4.625802	0.201824

B3LYP Energy = -1829.33643339 a.u.

(aS,1S,3S,3'S)-**21**, Conf C

C	-2.846642	0.885597	1.063854
C	-4.143816	0.406915	1.215821
C	-4.555901	-0.693754	0.447497
C	-3.668015	-1.302847	-0.435333
C	-2.354125	-0.831865	-0.571279
C	-1.951055	0.278139	0.180446
C	-1.417697	-1.523299	-1.539779
C	-1.917338	-2.910685	-1.934566
C	-1.151525	-3.510733	-3.098400
O	-3.295135	-2.825554	-2.318689
C	-0.328906	1.922200	-0.778884
C	0.941132	2.513614	-0.846694
C	1.993895	1.966606	-0.111453
C	1.769054	0.883459	0.747273
C	0.488443	0.335890	0.857085
C	-0.567386	0.841472	0.075433
C	0.233083	-0.769967	1.859618
C	1.515642	-1.410405	2.379195
C	1.296651	-2.251493	3.622845
O	2.458337	-0.383666	2.718570
C	2.923033	0.366764	1.588066
C	-4.138197	-2.509002	-1.220569
C	3.973636	-0.425499	0.812420
C	5.262668	-0.518789	1.345351
C	6.251248	-1.267982	0.719553
C	5.929536	-1.928895	-0.454085
C	4.669445	-1.863579	-1.017324
C	3.694569	-1.103538	-0.374229
F	6.889874	-2.662380	-1.076508
O	-5.064034	0.927948	2.078680
C	-4.683806	2.038757	2.887973
O	-5.809179	-1.247040	0.599996
C	-6.911565	-0.447392	0.140933
O	1.151883	3.624966	-1.633253
C	0.798998	4.868534	-1.001523
O	3.240836	2.543006	-0.107142
C	3.951768	2.591060	-1.357541
O	-1.383597	2.472839	-1.467105
C	-1.320347	2.411024	-2.902031
H	-2.510726	1.736963	1.638275
H	-1.309576	-0.921469	-2.449098
H	-0.417882	-1.606799	-1.107094
H	-1.842747	-3.580600	-1.064731
H	-1.254873	-2.882906	-3.986105
H	-0.090306	-3.592695	-2.855122
H	-1.528844	-4.506773	-3.333803
H	-0.406644	-1.540277	1.424062
H	-0.325293	-0.355831	2.706768
H	1.950225	-2.041619	1.593878
H	0.913015	-1.634722	4.438504
H	2.232686	-2.709288	3.945407
H	0.574863	-3.045991	3.422476
H	3.429454	1.223912	2.032157
H	-4.216340	-3.377045	-0.549557
H	-5.130072	-2.334336	-1.635041
H	5.498555	0.002542	2.265569

H	7.252041	-1.339054	1.124935
H	4.459192	-2.391828	-1.938065
H	2.708272	-1.036511	-0.814898
H	-3.850484	1.782884	3.547653
H	-5.557687	2.279542	3.488357
H	-4.413445	2.903947	2.276799
H	-6.997943	0.471919	0.719689
H	-6.796185	-0.207087	-0.919766
H	-7.803989	-1.054660	0.279233
H	1.392542	5.021330	-0.097227
H	-0.264793	4.889249	-0.756523
H	1.023741	5.652620	-1.721889
H	4.075762	1.584376	-1.762877
H	4.929270	3.009178	-1.126677
H	3.435658	3.223170	-2.078272
H	-1.255818	1.373272	-3.238131
H	-2.250288	2.846669	-3.261392
H	-0.471977	2.977516	-3.285421

B3LYP Energy = -1829.33568997 a.u.

(aS,1S,3S,3'S)-**21**, Conf D

C	2.852200	0.958088	-0.992627
C	4.172889	0.532113	-1.089077
C	4.607460	-0.521619	-0.269749
C	3.739078	-1.091378	0.657743
C	2.409618	-0.656443	0.757999
C	1.968845	0.373827	-0.081307
C	1.494981	-1.312967	1.770573
C	2.042102	-2.654239	2.252253
C	1.286146	-3.214799	3.441977
O	3.409539	-2.489480	2.645870
C	0.252262	2.011136	0.716286
C	-1.038258	2.560921	0.693284
C	-2.043406	1.924528	-0.036825
C	-1.751184	0.786950	-0.799936
C	-0.450232	0.277715	-0.820090
C	0.559539	0.880979	-0.046984
C	-0.123636	-0.898550	-1.715365
C	-1.367474	-1.624994	-2.213188
C	-1.080250	-2.576361	-3.359895
O	-2.322065	-0.663421	-2.683689
C	-2.853650	0.174031	-1.646550
C	4.258752	-2.203770	1.544584
C	-3.931099	-0.568985	-0.859709
C	-3.705812	-1.138657	0.393214
C	-4.703190	-1.857901	1.048712
C	-5.931449	-1.992101	0.430165
C	-6.199935	-1.438829	-0.810637
C	-5.189510	-0.729207	-1.447405
F	-6.913680	-2.685763	1.063929
O	5.101559	1.073417	-1.929892
C	4.715188	2.173579	-2.750784
O	5.914170	-0.958633	-0.297319
C	6.324455	-1.647576	-1.488733
O	-1.317588	3.719067	1.384898

C	-0.927355	4.924040	0.701901
O	-3.306277	2.456081	-0.133349
C	-4.067510	2.579019	1.081731
O	1.259783	2.646613	1.401772
C	1.141888	2.677121	2.834128
H	2.493455	1.762678	-1.618370
H	1.368243	-0.659916	2.641347
H	0.498688	-1.456963	1.345978
H	2.004812	-3.376983	1.423117
H	1.355145	-2.532795	4.292219
H	0.231745	-3.352035	3.194079
H	1.698643	-4.179921	3.739208
H	0.525726	-1.604520	-1.193523
H	0.448183	-0.540051	-2.578798
H	-1.814041	-2.189212	-1.384747
H	-0.691734	-2.028975	-4.221421
H	-1.988926	-3.098353	-3.662557
H	-0.338555	-3.319309	-3.059847
H	-3.349650	0.979311	-2.188976
H	4.408240	-3.114803	0.945979
H	5.226452	-1.932001	1.964038
H	-2.745592	-1.015865	0.877174
H	-4.534551	-2.301659	2.021174
H	-7.177403	-1.560721	-1.258606
H	-5.383806	-0.292323	-2.419839
H	3.920558	1.892522	-3.447187
H	5.604613	2.450188	-3.311603
H	4.387752	3.023792	-2.146916
H	7.341990	-1.987824	-1.306505
H	5.680988	-2.512252	-1.674927
H	6.308072	-0.983312	-2.352831
H	-1.446945	5.007049	-0.255508
H	0.152337	4.946091	0.542494
H	-1.219183	5.749607	1.347968
H	-5.049041	2.939443	0.781212
H	-3.602644	3.286774	1.766045
H	-4.172340	1.604673	1.564071
H	1.097426	1.661767	3.235376
H	2.042149	3.167428	3.198337
H	0.260629	3.237156	3.146523

B3LYP Energy = -1829.33532556 a.u.

(aS,1S,3S,3'S)-**21**, Conf E

C	2.714087	-0.473605	-1.387057
C	4.008359	-0.936474	-1.170983
C	4.536681	-0.892812	0.128876
C	3.763687	-0.412223	1.182918
C	2.452609	0.032830	0.966623
C	1.933607	0.009980	-0.332975
C	1.639970	0.544226	2.135714
C	2.231752	0.125045	3.478884
C	1.608887	0.851498	4.655900
O	3.636916	0.409041	3.487379
C	0.281193	1.840426	-0.742460
C	-1.004473	2.317615	-1.043429



C	-2.036018	1.397727	-1.255907
C	-1.787202	0.021391	-1.144322
C	-0.508364	-0.441351	-0.831232
C	0.541617	0.474605	-0.629227
C	-0.253567	-1.931149	-0.734848
C	-1.539428	-2.743678	-0.643045
C	-1.324193	-4.226004	-0.885245
O	-2.464106	-2.276839	-1.635769
C	-2.933710	-0.942208	-1.399180
C	4.354255	-0.411255	2.577352
C	-4.019106	-0.943014	-0.323847
C	-3.782300	-0.570495	0.999113
C	-4.787598	-0.646416	1.960950
C	-6.035117	-1.097167	1.573836
C	-6.315228	-1.472597	0.270813
C	-5.296476	-1.392251	-0.670644
F	-7.024988	-1.169361	2.503246
O	4.818018	-1.451366	-2.142367
C	4.309151	-1.547598	-3.470799
O	5.789139	-1.394074	0.411204
C	6.899422	-0.651453	-0.118866
O	-1.234465	3.659191	-1.243945
C	-1.123830	4.508037	-0.086618
O	-3.293568	1.752857	-1.663377
C	-3.997940	2.804698	-0.987635
O	1.298693	2.746469	-0.532031
C	1.879511	3.298242	-1.725563
H	2.290013	-0.494696	-2.380857
H	1.591138	1.637928	2.096918
H	0.610719	0.182968	2.064006
H	2.099902	-0.959767	3.608278
H	1.776582	1.927363	4.570423
H	0.532381	0.671887	4.687772
H	2.043978	0.507297	5.595239
H	0.379244	-2.147238	0.129260
H	0.308376	-2.260857	-1.615266
H	-1.986791	-2.605711	0.349335
H	-0.936910	-4.396240	-1.892160
H	-2.262132	-4.772586	-0.778368
H	-0.606440	-4.627651	-0.167112
H	-3.410606	-0.661720	-2.338690
H	4.397501	-1.441917	2.959430
H	5.375309	-0.032670	2.561133
H	-2.805399	-0.207014	1.290703
H	-4.610243	-0.359057	2.989073
H	-7.307287	-1.814456	0.006306
H	-5.499389	-1.684945	-1.694089
H	5.105536	-1.994774	-4.060614
H	4.065992	-0.562683	-3.878513
H	3.424354	-2.188276	-3.512061
H	6.885333	-0.647598	-1.208572
H	6.887644	0.376223	0.255219
H	7.796912	-1.154717	0.235459
H	-0.121594	4.464827	0.337450
H	-1.858294	4.220859	0.670457
H	-1.337357	5.517166	-0.432988

H	-3.674780	3.783716	-1.335760
H	-3.861848	2.730210	0.093637
H	-5.049498	2.655771	-1.225479
H	1.128512	3.821478	-2.320133
H	2.642799	4.000570	-1.396548
H	2.344784	2.510911	-2.323433

B3LYP Energy = -1829.33509463 a.u.

(*aS*,1*S*,3*S*,3'*S*)-**21**, Conf F

C	2.740092	-0.258553	-1.428538
C	4.058259	-0.663048	-1.240200
C	4.585619	-0.673148	0.060324
C	3.810078	-0.242792	1.134256
C	2.483689	0.166280	0.942157
C	1.950402	0.155694	-0.352051
C	1.666480	0.614296	2.133394
C	2.287591	0.173385	3.455904
C	1.647511	0.831569	4.663467
O	3.679004	0.517032	3.461448
C	0.222251	1.930996	-0.683826
C	-1.083993	2.365702	-0.959091
C	-2.078717	1.412494	-1.198333
C	-1.773950	0.044404	-1.138733
C	-0.475224	-0.376837	-0.849398
C	0.538109	0.573381	-0.621131
C	-0.160542	-1.857671	-0.807365
C	-1.413146	-2.721908	-0.730473
C	-1.143336	-4.187070	-1.018573
O	-2.362706	-2.262039	-1.702387
C	-2.882703	-0.954739	-1.422234
C	4.425305	-0.237030	2.518572
C	-3.964145	-1.031897	-0.345748
C	-3.739711	-0.688211	0.987074
C	-4.739332	-0.831532	1.947167
C	-5.968736	-1.320261	1.548324
C	-6.236148	-1.669376	0.235298
C	-5.223189	-1.521863	-0.704281
F	-6.953214	-1.457818	2.476039
O	4.900119	-1.051165	-2.242491
C	4.412933	-1.035416	-3.582309
O	5.898040	-1.021375	0.296406
C	6.224772	-2.407850	0.114538
O	-1.371716	3.702067	-1.111561
C	-1.278964	4.518392	0.070562
O	-3.352163	1.733684	-1.585080
C	-4.098575	2.711354	-0.845900
O	1.204625	2.868903	-0.449131
C	1.755735	3.482314	-1.626693
H	2.312229	-0.250218	-2.420916
H	1.581344	1.706391	2.130142
H	0.649224	0.220877	2.059911
H	2.201987	-0.920005	3.548067
H	1.769919	1.915729	4.614352
H	0.579763	0.606175	4.698961
H	2.106574	0.473406	5.586050

H	0.490155	-2.077895	0.042325
H	0.403375	-2.134380	-1.704619
H	-1.857256	-2.630158	0.268727
H	-0.755888	-4.311704	-2.032129
H	-2.059224	-4.771902	-0.923776
H	-0.406634	-4.582765	-0.316427
H	-3.372960	-0.663075	-2.351487
H	4.539825	-1.271061	2.877254
H	5.420089	0.205308	2.487764
H	-2.777935	-0.293315	1.287940
H	-4.571660	-0.566460	2.982888
H	-7.214513	-2.042263	-0.038139
H	-5.416309	-1.793111	-1.735493
H	3.569877	-1.719996	-3.708622
H	5.242330	-1.366337	-4.202507
H	4.113479	-0.028563	-3.884966
H	7.269149	-2.513212	0.401895
H	5.606044	-3.037533	0.760374
H	6.098091	-2.709142	-0.925514
H	-0.269963	4.503368	0.480132
H	-1.990525	4.178182	0.827475
H	-1.538148	5.528033	-0.241352
H	-3.820087	3.722596	-1.136049
H	-3.953668	2.578309	0.228634
H	-5.143844	2.530581	-1.089200
H	0.981706	3.998613	-2.197428
H	2.496430	4.199288	-1.278460
H	2.243840	2.733386	-2.254754

B3LYP Energy = -1829.33476331 a.u.

(aS,1S,3S,3'S)-**21**, Conf G

C	-2.734933	0.560633	1.292526
C	-4.022342	0.048911	1.425626
C	-4.518162	-0.809532	0.431709
C	-3.721572	-1.152850	-0.658049
C	-2.418336	-0.652321	-0.779687
C	-1.930765	0.217896	0.201918
C	-1.582456	-1.038388	-1.979463
C	-2.140980	-2.257810	-2.709003
C	-1.501042	-2.482360	-4.065670
O	-3.549025	-2.084386	-2.916494
C	-0.304244	1.883946	-0.707306
C	0.969641	2.468430	-0.773981
C	2.021598	1.882575	-0.063383
C	1.789834	0.790511	0.780640
C	0.505920	0.249266	0.886535
C	-0.547590	0.787312	0.124315
C	0.252268	-0.896583	1.844212
C	1.535134	-1.560647	2.332182
C	1.320909	-2.442966	3.547720
O	2.484906	-0.549341	2.700047
C	2.948136	0.232531	1.590237
C	-4.276597	-2.103657	-1.697554
C	3.981430	-0.548343	0.781294
C	5.283712	-0.642874	1.280245

C	6.256701	-1.387486	0.624943
C	5.905225	-2.043562	-0.542740
C	4.630777	-1.976975	-1.072867
C	3.672449	-1.220808	-0.401327
F	6.849695	-2.772999	-1.193186
O	-4.855133	0.313737	2.474966
C	-4.386897	1.169075	3.514681
O	-5.762095	-1.392681	0.543416
C	-6.887487	-0.509506	0.406887
O	1.157074	3.557260	-1.591941
C	1.544780	4.778646	-0.937060
O	3.294294	2.407025	-0.109758
C	3.966790	2.354221	-1.382405
O	-1.314208	2.349903	-1.515889
C	-1.973373	3.548598	-1.090276
H	-2.335520	1.225206	2.045460
H	-1.539103	-0.194990	-2.677024
H	-0.553400	-1.241172	-1.671674
H	-1.994360	-3.151033	-2.083124
H	-1.684022	-1.625639	-4.717774
H	-0.421856	-2.610983	-3.961037
H	-1.910405	-3.374375	-4.542050
H	-0.390443	-1.644810	1.374768
H	-0.301009	-0.521714	2.712075
H	1.961789	-2.166578	1.523547
H	0.948617	-1.852550	4.387818
H	2.256324	-2.918196	3.846001
H	0.591891	-3.225026	3.325774
H	3.468953	1.069134	2.056666
H	-4.293813	-3.125419	-1.290032
H	-5.303464	-1.841352	-1.947986
H	5.543165	-0.126105	2.196701
H	7.267781	-1.459130	1.003801
H	4.397083	-2.500656	-1.990530
H	2.675646	-1.151326	-0.817231
H	-5.199435	1.231965	4.234329
H	-4.159193	2.169468	3.136660
H	-3.501864	0.753362	4.003507
H	-6.861076	-0.000075	-0.560571
H	-7.773929	-1.138586	0.460033
H	-6.909590	0.226188	1.210728
H	2.520537	4.683919	-0.460545
H	0.802320	5.064338	-0.187471
H	1.583623	5.536841	-1.716194
H	4.958551	2.767535	-1.212592
H	3.441070	2.943731	-2.133297
H	4.056894	1.320756	-1.721177
H	-2.394245	3.423807	-0.089203
H	-1.293360	4.401754	-1.102830
H	-2.779098	3.721263	-1.801035

B3LYP Energy = -1829.33421666 a.u.

(aS,1S,3S,3'S)-**21**, Conf H

C	-2.761101	0.781580	1.261397
C	-4.068592	0.335058	1.424959

C	-4.581707	-0.607711	0.520337
C	-3.781481	-1.099122	-0.507738
C	-2.457264	-0.663738	-0.657632
C	-1.954356	0.293185	0.230894
C	-1.615851	-1.227221	-1.783119
C	-2.206112	-2.514538	-2.352803
C	-1.541978	-2.955956	-3.643319
O	-3.598503	-2.314990	-2.627038
C	-0.294813	1.917664	-0.696541
C	0.998376	2.461207	-0.765935
C	2.016129	1.893069	0.007315
C	1.780207	0.763068	0.792687
C	0.490608	0.227220	0.860173
C	-0.553039	0.811457	0.124602
C	0.217541	-0.950282	1.772005
C	1.493032	-1.641180	2.240665
C	1.263272	-2.583372	3.407387
O	2.439316	-0.650415	2.669465
C	2.922944	0.171450	1.598509
C	-4.358911	-2.142924	-1.440125
C	3.967613	-0.582491	0.775158
C	5.198399	-0.866731	1.374709
C	6.182378	-1.579390	0.701435
C	5.915628	-2.006837	-0.588596
C	4.714449	-1.747010	-1.219577
C	3.742145	-1.029522	-0.525534
F	6.873155	-2.701805	-1.258779
O	-4.906018	0.742442	2.423263
C	-4.420661	1.691327	3.370507
O	-5.849347	-1.128848	0.668607
C	-6.935788	-0.223025	0.415120
O	1.213610	3.602743	-1.503245
C	2.114836	3.480336	-2.619303
O	3.287082	2.428655	-0.010744
C	3.428711	3.693678	0.661923
O	-1.366688	2.479910	-1.334888
C	-1.278212	2.789829	-2.732669
H	-2.348127	1.514344	1.939931
H	-1.535502	-0.493123	-2.592962
H	-0.597478	-1.416926	-1.435199
H	-2.113717	-3.314967	-1.603340
H	-1.666859	-2.193922	-4.415747
H	-0.473445	-3.117125	-3.486806
H	-1.981403	-3.887295	-4.003260
H	-0.427051	-1.675714	1.270592
H	-0.340482	-0.602471	2.648303
H	1.929075	-2.203949	1.405645
H	0.887711	-2.033820	4.273308
H	2.192894	-3.079785	3.688879
H	0.530742	-3.347580	3.139973
H	3.441507	0.984652	2.107742
H	-4.443769	-3.103267	-0.910399
H	-5.362616	-1.862050	-1.756259
H	5.390538	-0.527487	2.385716
H	7.138533	-1.798355	1.158377
H	4.546953	-2.094828	-2.230503

H	2.802126	-0.810993	-1.015133
H	-3.558798	1.300652	3.917822
H	-5.240407	1.862568	4.063930
H	-4.150022	2.634206	2.888028
H	-7.847840	-0.807769	0.518267
H	-6.940397	0.596268	1.133949
H	-6.873316	0.176946	-0.600912
H	3.109400	3.179211	-2.292130
H	2.157755	4.465004	-3.080018
H	1.731340	2.756553	-3.343014
H	2.824100	4.464507	0.182905
H	4.482751	3.954831	0.595929
H	3.140508	3.602090	1.712268
H	-2.304704	2.825260	-3.093473
H	-0.795408	3.751547	-2.896154
H	-0.737023	2.008589	-3.271954

B3LYP Energy = -1829.33408435 a.u.

(*aS*,1*S*,3*S*,3'*S*)-**21**, Conf I

C	2.663618	-0.185141	-1.486825
C	3.972556	-0.632406	-1.358384
C	4.537248	-0.742602	-0.084315
C	3.772172	-0.443055	1.045936
C	2.445794	-0.017812	0.913202
C	1.892426	0.128712	-0.368991
C	1.643064	0.301346	2.154952
C	2.279555	-0.268605	3.419861
C	1.659621	0.273550	4.693571
O	3.673950	0.063589	3.439880
C	0.211148	1.973951	-0.481370
C	-1.083396	2.459678	-0.702930
C	-2.103191	1.566310	-1.035047
C	-1.849541	0.191580	-1.093220
C	-0.556717	-0.289154	-0.863239
C	0.487951	0.606758	-0.569252
C	-0.281272	-1.774010	-0.979742
C	-1.553806	-2.613638	-0.983631
C	-1.320115	-4.039754	-1.445602
O	-2.508841	-2.023718	-1.878307
C	-2.991943	-0.750388	-1.428898
C	4.397226	-0.601211	2.415833
C	-4.022778	-0.932902	-0.315176
C	-3.767552	-0.634819	1.022326
C	-4.726155	-0.863621	2.007346
C	-5.944947	-1.392549	1.628739
C	-6.241747	-1.699832	0.311423
C	-5.270321	-1.465482	-0.653552
F	-6.889618	-1.614184	2.581363
O	4.701901	-0.910096	-2.496352
C	4.937147	-2.306753	-2.738804
O	5.823964	-1.204780	0.097865
C	6.870617	-0.328305	-0.357582
O	-1.337216	3.810265	-0.623985
C	-1.714823	4.265307	0.686968
O	-3.391852	2.003167	-1.232361

C	-3.610568	2.836087	-2.385573
O	1.204074	2.843779	-0.096076
C	1.730207	3.685829	-1.135403
H	2.250794	-0.090777	-2.483808
H	1.553782	1.388052	2.258210
H	0.626223	-0.086526	2.052981
H	2.187797	-1.365111	3.407277
H	1.789549	1.356519	4.747717
H	0.590745	0.052682	4.721185
H	2.127405	-0.175455	5.570862
H	0.369734	-2.100231	-0.165033
H	0.269948	-1.965541	-1.906457
H	-1.981910	-2.629199	0.026401
H	-0.942919	-4.051307	-2.470582
H	-2.248392	-4.611487	-1.411127
H	-0.587436	-4.531911	-0.802759
H	-3.520908	-0.349546	-2.294370
H	4.489088	-1.670576	2.657886
H	5.402813	-0.182960	2.427643
H	-2.815003	-0.208390	1.308767
H	-4.535237	-0.632198	3.047051
H	-7.211117	-2.106478	0.054640
H	-5.486176	-1.703446	-1.688460
H	5.515588	-2.364333	-3.658737
H	3.989734	-2.836315	-2.871843
H	5.499868	-2.759709	-1.920716
H	6.822565	0.629379	0.167415
H	7.807906	-0.826198	-0.117810
H	6.803361	-0.161143	-1.432811
H	-1.888009	5.336232	0.601689
H	-0.912224	4.080627	1.404125
H	-2.631512	3.771343	1.016933
H	-3.318637	2.308380	-3.297495
H	-3.057101	3.770956	-2.305339
H	-4.679404	3.037680	-2.410450
H	0.948664	4.318587	-1.557881
H	2.491943	4.305567	-0.666782
H	2.188327	3.080427	-1.921635

B3LYP Energy = -1829.33401202 a.u.

(*aS*,1*S*,3*S*,3'*S*)-**21**, Conf J

C	2.761453	0.620096	-1.245560
C	4.073630	0.160890	-1.309361
C	4.569990	-0.624745	-0.257506
C	3.771008	-0.897255	0.850606
C	2.450942	-0.430973	0.914302
C	1.947779	0.330247	-0.146704
C	1.608301	-0.751011	2.128506
C	2.198413	-1.888740	2.957789
C	1.537103	-2.040609	4.314373
O	3.592218	-1.638256	3.179925
C	0.234689	2.000717	0.577186
C	-1.060561	2.539883	0.555430
C	-2.069693	1.852461	-0.126024
C	-1.775185	0.695569	-0.856741

C	-0.470006	0.197274	-0.878765
C	0.541371	0.844433	-0.145489
C	-0.148991	-1.026686	-1.710541
C	-1.394077	-1.789048	-2.149156
C	-1.117268	-2.788961	-3.256278
O	-2.369736	-0.860642	-2.644665
C	-2.890002	0.017829	-1.635679
C	4.352151	-1.717276	1.983957
C	-3.922363	-0.710036	-0.778044
C	-5.208741	-0.889150	-1.294673
C	-6.178066	-1.594523	-0.592274
C	-5.838683	-2.124844	0.640991
C	-4.580126	-1.971152	1.190862
C	-3.625484	-1.255698	0.471224
F	-6.779582	-2.815199	1.337702
O	4.937947	0.427240	-2.332330
C	4.485787	1.246383	-3.407788
O	5.874909	-1.068260	-0.250673
C	6.202531	-2.079763	-1.215883
O	-1.310577	3.692220	1.261955
C	-1.710269	4.834357	0.483198
O	-3.360736	2.330158	-0.163400
C	-4.068024	2.377888	1.090505
O	1.202020	2.574553	1.367812
C	1.846623	3.743259	0.847054
H	2.357326	1.219548	-2.048923
H	1.523133	0.140681	2.758873
H	0.592585	-1.014334	1.822119
H	2.103507	-2.831175	2.397283
H	1.667457	-1.130629	4.903797
H	0.467286	-2.225169	4.197973
H	1.973797	-2.875306	4.864655
H	0.512965	-1.695068	-1.154885
H	0.406927	-0.719179	-2.603004
H	-1.818224	-2.319668	-1.287912
H	-0.753321	-2.277748	-4.150176
H	-2.024487	-3.336155	-3.515796
H	-0.359751	-3.507535	-2.936962
H	-3.421456	0.782894	-2.202301
H	4.444414	-2.768462	1.671410
H	5.352908	-1.365099	2.229907
H	-5.458196	-0.470621	-2.262561
H	-7.177098	-1.731349	-0.984897
H	-4.356275	-2.396659	2.160290
H	-2.642080	-1.115656	0.901139
H	3.643379	0.787861	-3.932816
H	5.329514	1.334087	-4.087870
H	4.199090	2.241162	-3.056518
H	5.558155	-2.954710	-1.091035
H	6.112209	-1.697565	-2.232871
H	7.235377	-2.361698	-1.020649
H	-2.667635	4.666214	-0.010383
H	-0.952550	5.070720	-0.268335
H	-1.794618	5.660887	1.185480
H	-3.596355	3.071870	1.785905
H	-4.115450	1.383492	1.537615

H	-5.073949	2.716112	0.851999
H	2.617982	4.010990	1.566323
H	2.311367	3.530521	-0.118987
H	1.144572	4.572538	0.746725

B3LYP Energy = -1829.33390621 a.u.

(aS,1S,3S,3'S)-21, Conf K

C	-2.822472	0.929067	1.012421
C	-4.117342	0.454260	1.193245
C	-4.523664	-0.692860	0.493033
C	-3.631354	-1.352560	-0.347698
C	-2.318472	-0.886386	-0.510097
C	-1.922134	0.272097	0.169463
C	-1.377524	-1.637569	-1.429223
C	-1.873351	-3.047916	-1.738303
C	-1.102659	-3.716661	-2.860696
O	-3.250225	-2.989321	-2.130691
C	-0.310933	1.893136	-0.848351
C	0.954776	2.493997	-0.947955
C	2.013956	1.976612	-0.195564
C	1.801765	0.896876	0.672933
C	0.527436	0.343071	0.808058
C	-0.540853	0.836148	0.036159
C	0.287875	-0.740198	1.839037
C	1.578227	-1.360194	2.364128
C	1.375478	-2.163751	3.634842
O	2.521402	-0.319966	2.659824
C	2.970198	0.381507	1.492902
C	-4.095757	-2.608029	-1.055882
C	3.981618	-0.462969	0.716124
C	5.210581	-0.738770	1.323442
C	6.167320	-1.524314	0.693502
C	5.875612	-2.032676	-0.561432
C	4.675791	-1.783225	-1.198862
C	3.730665	-0.992226	-0.548238
F	6.806549	-2.800098	-1.189019
O	-5.040630	1.021562	2.023134
C	-4.664068	2.176871	2.769189
O	-5.775284	-1.240033	0.676745
C	-6.878715	-0.474417	0.165150
O	1.192204	3.518735	-1.834674
C	0.527778	4.766596	-1.560150
O	3.300404	2.437201	-0.301288
C	3.558389	3.839380	-0.132446
O	-1.360669	2.390859	-1.588910
C	-1.315973	2.129097	-3.001708
H	-2.491379	1.815649	1.534006
H	-1.265257	-1.096416	-2.375095
H	-0.379378	-1.693123	-0.989056
H	-1.800265	-3.662617	-0.828589
H	-1.204860	-3.145027	-3.785745
H	-0.041968	-3.780729	-2.610004
H	-1.477195	-4.726187	-3.035361
H	-0.350019	-1.525392	1.428614
H	-0.267049	-0.308255	2.679697

H	2.007205	-2.011802	1.592377
H	1.001036	-1.523152	4.436358
H	2.315691	-2.611385	3.959577
H	0.651969	-2.964213	3.467180
H	3.508844	1.241657	1.891937
H	-4.170870	-3.432123	-0.331204
H	-5.088095	-2.464213	-1.480953
H	5.421429	-0.336137	2.306979
H	7.121615	-1.738271	1.156713
H	4.488190	-2.194574	-2.182017
H	2.792131	-0.782213	-1.044438
H	-3.829064	1.960719	3.440798
H	-5.538243	2.447262	3.356395
H	-4.397697	3.007877	2.110659
H	-7.770242	-1.072671	0.342835
H	-6.966971	0.481013	0.681935
H	-6.763018	-0.304551	-0.909097
H	0.843741	5.163071	-0.591882
H	-0.554966	4.647748	-1.571518
H	0.834917	5.449758	-2.349242
H	2.994968	4.236771	0.715606
H	3.315749	4.398080	-1.034164
H	4.623728	3.920997	0.074918
H	-1.345652	1.054372	-3.192840
H	-2.205562	2.592990	-3.422625
H	-0.423172	2.559724	-3.456831

B3LYP Energy = -1829.33385979 a.u.

(aS,1S,3S,3'S)-21, Conf L

C	2.674028	0.240754	-1.462534
C	3.981102	-0.229981	-1.447883
C	4.514652	-0.731086	-0.257135
C	3.755436	-0.699347	0.915727
C	2.440931	-0.221578	0.897515
C	1.893514	0.247887	-0.307944
C	1.637700	-0.217014	2.179096
C	2.254118	-1.108914	3.253663
C	1.637620	-0.900681	4.623888
O	3.654673	-0.823453	3.360237
C	0.196171	2.048532	0.056789
C	-1.103956	2.561890	-0.030854
C	-2.113932	1.778339	-0.591381
C	-1.844547	0.472092	-1.014337
C	-0.546934	-0.039841	-0.913887
C	0.487600	0.755917	-0.386755
C	-0.254577	-1.439024	-1.415982
C	-1.518670	-2.256627	-1.654163
C	-1.270574	-3.509322	-2.473155
O	-2.471919	-1.456936	-2.369949
C	-2.974189	-0.357513	-1.598706
C	4.373324	-1.211633	2.200167
C	-4.007968	-0.847706	-0.584417
C	-3.778541	-0.882985	0.789757
C	-4.738028	-1.382821	1.668061
C	-5.931054	-1.843744	1.145923

C	-6.201854	-1.823798	-0.212081
C	-5.230424	-1.322443	-1.069167
F	-6.875972	-2.329587	1.994594
O	4.704631	-0.237697	-2.622306
C	5.765684	0.729434	-2.689141
O	5.809841	-1.200412	-0.188564
C	6.059997	-2.435907	-0.880750
O	-1.374185	3.840752	0.400758
C	-1.705633	3.937014	1.796910
O	-3.407429	2.237251	-0.669130
C	-3.636373	3.345948	-1.557629
O	1.179752	2.799987	0.656995
C	1.698599	3.882938	-0.132233
H	2.273133	0.610778	-2.398250
H	1.571448	0.807404	2.560737
H	0.613657	-0.543054	1.979653
H	2.138715	-2.162700	2.958138
H	1.791047	0.128072	4.956672
H	0.563995	-1.096702	4.592319
H	2.089520	-1.572025	5.355364
H	0.392255	-1.963503	-0.708524
H	0.307558	-1.376058	-2.353898
H	-1.954332	-2.540091	-0.687966
H	-0.890249	-3.249200	-3.463416
H	-2.193829	-4.077440	-2.594527
H	-0.535341	-4.147183	-1.978272
H	-3.504665	0.255675	-2.328377
H	4.453671	-2.308487	2.162046
H	5.382613	-0.818678	2.316061
H	-2.846033	-0.508081	1.191129
H	-4.566939	-1.410888	2.736203
H	-7.151473	-2.188483	-0.581177
H	-5.425573	-1.303611	-2.134858
H	5.364219	1.742995	-2.604852
H	6.231346	0.604676	-3.664712
H	6.504141	0.560252	-1.903746
H	5.892135	-2.327296	-1.952782
H	7.102892	-2.682917	-0.692880
H	5.421695	-3.231449	-0.487177
H	-0.873851	3.592976	2.415018
H	-2.602837	3.355157	2.020549
H	-1.895671	4.990057	1.994832
H	-4.709156	3.526300	-1.540357
H	-3.327050	3.089336	-2.574370
H	-3.103596	4.234546	-1.221275
H	2.173897	3.500301	-1.039081
H	0.908961	4.588709	-0.393307
H	2.445192	4.378246	0.485225

B3LYP Energy = -1829.33380006 a.u.

(*aS*,1*S*,3*S*,3'*S*)-**21**, Conf M

C	2.799223	0.830332	-1.212291
C	4.127001	0.421334	-1.287862
C	4.622115	-0.461262	-0.315214
C	3.803243	-0.881847	0.730088

C	2.467151	-0.464869	0.806272
C	1.968080	0.396622	-0.177086
C	1.604385	-0.950664	1.950660
C	2.206705	-2.168035	2.647279
C	1.510568	-2.516300	3.949210
O	3.583076	-1.905784	2.947017
C	0.230647	2.044790	0.544953
C	-1.081932	2.544617	0.530494
C	-2.057958	1.868798	-0.209336
C	-1.761897	0.678611	-0.876964
C	-0.453319	0.187216	-0.862233
C	0.548879	0.875366	-0.159748
C	-0.115151	-1.059571	-1.651844
C	-1.352430	-1.840886	-2.080079
C	-1.058449	-2.879134	-3.146596
O	-2.323550	-0.933129	-2.621702
C	-2.862302	-0.030331	-1.645772
C	4.382001	-1.810734	1.777133
C	-3.898661	-0.741396	-0.775537
C	-3.679099	-1.074488	0.559944
C	-4.639566	-1.762997	1.298293
C	-5.823397	-2.109488	0.676186
C	-6.084355	-1.795304	-0.647141
C	-5.112079	-1.109976	-1.364409
F	-6.769322	-2.777391	1.388870
O	5.007504	0.826339	-2.249310
C	4.561029	1.765160	-3.225385
O	5.941058	-0.861674	-0.316171
C	6.332774	-1.741949	-1.380740
O	-1.356552	3.740419	1.152470
C	-2.282704	3.687769	2.253551
O	-3.347269	2.354918	-0.272062
C	-3.517363	3.545148	-1.063928
O	1.263898	2.703707	1.153679
C	1.131779	3.126253	2.518115
H	2.396467	1.508123	-1.951289
H	1.481564	-0.151560	2.690669
H	0.602234	-1.195448	1.590226
H	2.159796	-3.031478	1.966426
H	1.589923	-1.687782	4.656392
H	0.452358	-2.719782	3.773121
H	1.960720	-3.400859	4.401968
H	0.543815	-1.708816	-1.070832
H	0.450167	-0.773658	-2.545806
H	-1.788142	-2.339322	-1.204932
H	-0.683989	-2.399088	-4.053344
H	-1.960809	-3.438020	-3.398007
H	-0.303265	-3.583785	-2.792437
H	-3.397034	0.709283	-2.242630
H	4.526345	-2.812292	1.344735
H	5.359656	-1.455042	2.099321
H	-2.753099	-0.788723	1.041427
H	-4.476367	-2.023090	2.335940
H	-7.027338	-2.078685	-1.095958
H	-5.299967	-0.858738	-2.401633
H	3.747832	1.355585	-3.830717

H	5.420486	1.961060	-3.861857
H	4.234741	2.698016	-2.758543
H	7.368571	-2.012445	-1.184697
H	5.716027	-2.645324	-1.380390
H	6.259771	-1.245940	-2.348740
H	-1.898080	3.040861	3.046105
H	-3.259651	3.329730	1.930647
H	-2.364990	4.706752	2.625771
H	-3.193555	3.369557	-2.093083
H	-2.958911	4.381921	-0.643062
H	-4.582474	3.766359	-1.051215
H	0.621192	2.365704	3.114083
H	2.147660	3.246554	2.890145
H	0.597409	4.071810	2.590939

B3LYP Energy = -1829.33377123 a.u.

(*aS*,1*S*,3*S*,3'*S*)-**21**, Conf N

C	-2.842599	1.007374	0.918144
C	-4.158136	0.569367	1.030595
C	-4.566633	-0.549446	0.287991
C	-3.677723	-1.175036	-0.582316
C	-2.353245	-0.728921	-0.698655
C	-1.938480	0.369638	0.064859
C	-1.416858	-1.447514	-1.647267
C	-1.936756	-2.831002	-2.028368
C	-1.155409	-3.470910	-3.160222
O	-3.300921	-2.718883	-2.451477
C	-0.237605	1.987658	-0.804053
C	1.050420	2.548060	-0.824926
C	2.063605	1.952612	-0.066589
C	1.782903	0.834277	0.731173
C	0.487048	0.318258	0.788175
C	-0.535196	0.891408	0.009374
C	0.174651	-0.814093	1.744378
C	1.424137	-1.509033	2.272835
C	1.149551	-2.384681	3.481127
O	2.386616	-0.521097	2.667624
C	2.902031	0.235238	1.563676
C	-4.169318	-2.360398	-1.387383
C	3.920247	-0.591834	0.777696
C	5.121039	-0.929221	1.409682
C	6.080310	-1.704762	0.771163
C	5.820030	-2.139795	-0.517738
C	4.648992	-1.827404	-1.180506
C	3.700666	-1.048056	-0.520636
F	6.753950	-2.896305	-1.154023
O	-5.105743	1.157477	1.817227
C	-4.745172	2.320410	2.559317
O	-5.867706	-1.001625	0.332048
C	-6.284080	-1.606851	1.566052
O	1.353054	3.612180	-1.642882
C	0.720418	4.864799	-1.319588
O	3.368139	2.369634	-0.097620
C	3.671934	3.756322	0.116964
O	-1.243795	2.560527	-1.549684

C	-1.149134	2.392867	-2.974564
H	-2.504172	1.862511	1.485494
H	-1.291702	-0.863542	-2.565850
H	-0.422561	-1.540134	-1.204787
H	-1.900834	-3.485886	-1.144540
H	-1.218758	-2.857092	-4.061327
H	-0.103594	-3.575134	-2.886661
H	-1.552001	-4.461154	-3.388491
H	-0.474721	-1.550484	1.266923
H	-0.394137	-0.412622	2.590936
H	1.861069	-2.124438	1.476162
H	0.765710	-1.784172	4.308859
H	2.062655	-2.883179	3.809043
H	0.408437	-3.148386	3.236418
H	3.447654	1.053235	2.035208
H	-4.315816	-3.223808	-0.721265
H	-5.134484	-2.135916	-1.839421
H	5.308303	-0.582459	2.419009
H	7.013246	-1.965614	1.253454
H	4.486375	-2.181434	-2.190065
H	2.785396	-0.788207	-1.036320
H	-5.644749	2.623502	3.089415
H	-4.423622	3.129176	1.898056
H	-3.954240	2.102945	3.282167
H	-5.635933	-2.450793	1.819184
H	-6.280807	-0.882227	2.380463
H	-7.297241	-1.967588	1.399620
H	-0.364677	4.782394	-1.368712
H	1.072874	5.579099	-2.060707
H	1.018737	5.197878	-0.322247
H	4.725912	3.788768	0.386574
H	3.077037	4.159925	0.940156
H	3.503705	4.342365	-0.784306
H	-0.248683	2.863879	-3.370701
H	-1.154702	1.332780	-3.236639
H	-2.032206	2.870874	-3.393107

B3LYP Energy = -1829.33345252 a.u.

(*aR*,1*S*,3*S*,3'*S*)-**21**, Conf A

C	-1.992368	-1.120850	-1.331123
C	-3.218995	-1.765859	-1.459860
C	-4.277929	-1.383419	-0.621599
C	-4.103064	-0.357390	0.303755
C	-2.873827	0.307027	0.415422
C	-1.811132	-0.092724	-0.401750
C	-2.722685	1.428708	1.420572
C	-4.071472	1.946947	1.913449
C	-3.954355	2.859235	3.119329
O	-4.899698	0.837030	2.286528
C	-0.186334	1.695174	-1.049580
C	1.058765	2.332915	-0.957591
C	2.056450	1.775480	-0.156158
C	1.795653	0.624059	0.598018
C	0.535633	0.022617	0.541804

C	-0.462303	0.550066	-0.299302
C	0.237862	-1.173488	1.421161
C	1.494331	-1.807217	2.007233
C	1.198929	-2.760397	3.150342
O	2.355333	-0.780123	2.518867
C	2.887780	0.083019	1.504267
C	-5.278194	0.053929	1.164782
C	4.043152	-0.598423	0.773815
C	5.284702	-0.667477	1.412382
C	6.363042	-1.320255	0.827839
C	6.179370	-1.909921	-0.411565
C	4.970478	-1.865489	-1.079390
C	3.904116	-1.201877	-0.476237
F	7.228261	-2.548838	-0.994315
O	-3.482456	-2.754234	-2.364244
C	-2.440531	-3.164164	-3.246147
O	-5.529466	-1.948031	-0.743646
C	-5.643346	-3.322049	-0.339018
O	1.304594	3.489850	-1.662662
C	0.780921	4.682288	-1.051084
O	3.272001	2.393320	0.010549
C	4.101998	2.547362	-1.154942
O	-1.186025	2.262751	-1.805556
C	-1.020187	2.169384	-3.229747
H	-1.161416	-1.404902	-1.961095
H	-2.143713	1.082629	2.284900
H	-2.159348	2.252950	0.978039
H	-4.568833	2.486259	1.093761
H	-3.512495	2.321854	3.961205
H	-3.320121	3.717138	2.887337
H	-4.936221	3.227109	3.420595
H	-0.318546	-1.926307	0.859588
H	-0.416051	-0.856897	2.241837
H	2.025754	-2.351974	1.216897
H	0.719451	-2.229443	3.975562
H	2.119500	-3.214877	3.518924
H	0.529869	-3.556408	2.817295
H	3.308441	0.918440	2.064207
H	-6.006843	0.605999	0.552961
H	-5.790158	-0.822839	1.559064
H	5.411760	-0.202531	2.382920
H	7.327964	-1.371172	1.314951
H	4.869182	-2.335692	-2.048758
H	2.957384	-1.151000	-0.998144
H	-2.871415	-3.942059	-3.871663
H	-1.588613	-3.572411	-2.695540
H	-2.105190	-2.336785	-3.877065
H	-6.696160	-3.579912	-0.435848
H	-5.045340	-3.971251	-0.978523
H	-5.334385	-3.442856	0.703265
H	-0.306730	4.632225	-0.975908
H	1.065380	5.508363	-1.699831
H	1.217752	4.828016	-0.060365
H	3.632995	3.202931	-1.886773
H	4.311687	1.573658	-1.603220
H	5.031382	2.988155	-0.800503

H	-1.882692	2.666668	-3.668715
H	-0.104051	2.666104	-3.551446
H	-1.007565	1.122569	-3.544222

B3LYP Energy = -1829.33650259 a.u.

(aR,1S,3S,3'S)-**21**, Conf B

C	-1.993171	-1.260535	-1.183498
C	-3.207569	-1.938826	-1.233169
C	-4.251522	-1.524528	-0.391779
C	-4.056649	-0.474416	0.502138
C	-2.833896	0.209278	0.548860
C	-1.798826	-0.193473	-0.302135
C	-2.666124	1.367373	1.508953
C	-4.005841	1.876394	2.034503
C	-3.863319	2.838976	3.197843
O	-4.790733	0.763837	2.484108
C	-0.236766	1.585811	-1.107481
C	0.996498	2.252111	-1.095989
C	2.030082	1.767294	-0.293164
C	1.818334	0.661051	0.539666
C	0.571528	0.030437	0.559834
C	-0.462934	0.483070	-0.280983
C	0.326295	-1.114130	1.520672
C	1.611103	-1.676108	2.119379
C	1.365102	-2.547964	3.336542
O	2.459403	-0.595465	2.533626
C	2.946528	0.203140	1.446878
C	-5.197598	-0.074175	1.413924
C	4.093637	-0.507113	0.731154
C	5.352224	-0.514394	1.339410
C	6.426263	-1.187611	0.770517
C	6.220790	-1.860904	-0.421945
C	4.994485	-1.879851	-1.058580
C	3.932557	-1.194391	-0.472165
F	7.265169	-2.520851	-0.989244
O	-3.467882	-3.003418	-2.047069
C	-2.428049	-3.479929	-2.897307
O	-5.456610	-2.193261	-0.368247
C	-6.288324	-2.031837	-1.527906
O	1.193190	3.366986	-1.879978
C	0.698861	4.590345	-1.306517
O	3.234824	2.421810	-0.204278
C	4.029964	2.507807	-1.400770
O	-1.272961	2.088574	-1.860936
C	-1.152280	1.915870	-3.282127
H	-1.176811	-1.561535	-1.824667
H	-2.049408	1.063237	2.362800
H	-2.136074	2.185465	1.016448
H	-4.547496	2.371578	1.214774
H	-3.374296	2.346914	4.041332
H	-3.261318	3.701920	2.906217
H	-4.841371	3.194883	3.524860
H	-0.222009	-1.915362	1.021455
H	-0.318386	-0.762317	2.334067
H	2.137291	-2.265905	1.358527



H	0.893477	-1.967357	4.132259
H	2.304696	-2.953651	3.713905
H	0.706808	-3.380890	3.081241
H	3.366548	1.082847	1.934942
H	-5.982281	0.426594	0.827200
H	-5.647309	-0.957250	1.865987
H	5.495811	0.015769	2.273506
H	7.404111	-1.191475	1.233897
H	4.876495	-2.415319	-1.991511
H	2.971737	-1.192974	-0.970389
H	-2.115506	-2.715115	-3.613493
H	-2.849755	-4.325619	-3.434961
H	-1.562733	-3.814205	-2.318686
H	-5.815969	-2.458475	-2.413074
H	-7.213406	-2.563614	-1.313922
H	-6.509277	-0.974547	-1.699762
H	1.197909	4.797783	-0.357066
H	-0.381082	4.537656	-1.156837
H	0.931253	5.378447	-2.020034
H	4.260504	1.508338	-1.776153
H	4.952910	3.004055	-1.108214
H	3.521478	3.088296	-2.168867
H	-0.255453	2.406258	-3.662449
H	-1.133365	0.852939	-3.536752
H	-2.036398	2.375161	-3.719718

B3LYP Energy = -1829.33624493 a.u.

(aR,1S,3S,3'S)-**21**, Conf C

C	2.107308	-0.888896	1.523434
C	3.359462	-1.477985	1.664118
C	4.345901	-1.215853	0.699565
C	4.075739	-0.357390	-0.362630
C	2.819575	0.253782	-0.490187
C	1.828322	-0.030817	0.456552
C	2.570277	1.192677	-1.651994
C	3.869371	1.673234	-2.293003
C	3.651081	2.396517	-3.608255
O	4.712977	0.543488	-2.551311
C	0.138405	1.703062	1.097097
C	-1.133069	2.284481	1.002629
C	-2.079880	1.728258	0.140628
C	-1.792352	0.559959	-0.571809
C	-0.525592	-0.022720	-0.467927
C	0.457225	0.562317	0.352317
C	-0.205805	-1.261062	-1.278458
C	-1.448943	-1.931373	-1.853120
C	-1.128258	-2.941491	-2.938634
O	-2.304279	-0.934146	-2.432427
C	-2.865650	-0.040472	-1.461764
C	5.181180	-0.059147	-1.353676
C	-4.014272	-0.717621	-0.713694
C	-5.196392	-0.974628	-1.414344
C	-6.267192	-1.622381	-0.811401
C	-6.137129	-2.013173	0.510796
C	-4.988073	-1.778302	1.240885

C	-3.927328	-1.125332	0.616393
F	-7.180384	-2.644870	1.112175
O	3.717312	-2.297414	2.695465
C	2.761380	-2.554151	3.721910
O	5.620764	-1.725502	0.820178
C	5.751188	-3.144959	0.639819
O	-1.425339	3.411028	1.737756
C	-2.173185	3.160260	2.940789
O	-3.341695	2.267468	0.038531
C	-3.420748	3.567609	-0.573968
O	1.052779	2.201110	1.994361
C	1.624434	3.481684	1.683324
H	1.333445	-1.076152	2.253901
H	1.972310	0.691320	-2.421559
H	1.985862	2.054706	-1.323385
H	4.391927	2.340346	-1.591272
H	3.178862	1.731454	-4.334617
H	3.002933	3.262902	-3.462469
H	4.600477	2.741011	-4.020530
H	0.343522	-1.978783	-0.665223
H	0.460645	-0.990176	-2.104435
H	-1.994397	-2.434688	-1.045191
H	-0.635276	-2.452822	-3.781907
H	-2.039473	-3.420336	-3.299463
H	-0.461921	-3.714904	-2.551350
H	-3.299790	0.760561	-2.061461
H	5.932414	0.589739	-0.879981
H	5.690279	-0.975634	-1.648894
H	-5.281386	-0.665440	-2.449389
H	-7.186516	-1.819369	-1.347163
H	-4.927603	-2.095451	2.273715
H	-3.027699	-0.926534	1.184323
H	2.455565	-1.630157	4.219270
H	3.263063	-3.200591	4.437814
H	1.879425	-3.066203	3.327553
H	6.816092	-3.361216	0.698968
H	5.220858	-3.690617	1.420136
H	5.373864	-3.443532	-0.342443
H	-1.612256	2.504476	3.610677
H	-3.142736	2.715262	2.708987
H	-2.318924	4.127695	3.417153
H	-3.020435	3.534404	-1.590731
H	-2.880974	4.311424	0.011619
H	-4.478614	3.819060	-0.609272
H	2.197673	3.430591	0.754175
H	0.853322	4.248086	1.604808
H	2.296883	3.718624	2.505310

B3LYP Energy = -1829.33575129 a.u.

(aR,1S,3S,3'S)-**21**, Conf D

C	-2.061070	-1.140944	-1.319547
C	-3.290234	-1.788284	-1.387168
C	-4.295184	-1.434254	-0.472922
C	-4.042750	-0.483033	0.512011
C	-2.800827	0.165422	0.581819

C	-1.808344	-0.169909	-0.346962
C	-2.572278	1.207077	1.656561
C	-3.881605	1.704964	2.263158
C	-3.679021	2.544888	3.509783
O	-4.689159	0.578043	2.625931
C	-0.196917	1.556875	-1.175089
C	1.057736	2.180769	-1.173126
C	2.045963	1.731550	-0.295676
C	1.815031	0.625813	0.528334
C	0.564290	0.000517	0.518232
C	-0.458354	0.478378	-0.322745
C	0.305815	-1.164950	1.450530
C	1.584951	-1.747280	2.041953
C	1.328286	-2.657791	3.227946
O	2.429409	-0.678740	2.496531
C	2.933530	0.135158	1.429817
C	-5.145871	-0.145980	1.493908
C	4.072928	-0.579821	0.703051
C	3.947431	-1.116994	-0.577094
C	5.003097	-1.798164	-1.179660
C	6.186200	-1.930011	-0.478735
C	6.354904	-1.409786	0.793546
C	5.288601	-0.735830	1.375472
F	7.224677	-2.588044	-1.059768
O	-3.602584	-2.765158	-2.287688
C	-2.607039	-3.167758	-3.225622
O	-5.517136	-2.071699	-0.471797
C	-6.375742	-1.790643	-1.588423
O	1.296253	3.241402	-2.017741
C	2.001403	2.893631	-3.222382
O	3.293717	2.311841	-0.285163
C	3.352502	3.663072	0.206799
O	-1.152151	1.945657	-2.084360
C	-1.750175	3.234240	-1.872326
H	-1.278512	-1.386232	-2.023130
H	-1.958339	0.789528	2.462536
H	-2.012883	2.053119	1.251460
H	-4.427236	2.293630	1.510411
H	-3.183352	1.958725	4.286596
H	-3.058931	3.415384	3.286604
H	-4.636860	2.893489	3.898465
H	-0.242761	-1.950182	0.926267
H	-0.340388	-0.833906	2.270638
H	2.118498	-2.310889	1.266554
H	0.850584	-2.103302	4.038620
H	2.264314	-3.077040	3.599303
H	0.671397	-3.481028	2.939898
H	3.366826	0.997443	1.938173
H	-5.934207	0.425441	0.981195
H	-5.604962	-1.057128	1.875113
H	3.020915	-1.000186	-1.124096
H	4.912654	-2.215306	-2.174043
H	7.299788	-1.528999	1.307324
H	5.404143	-0.325619	2.371768
H	-3.066090	-3.948695	-3.826854
H	-1.725265	-3.570823	-2.720470

H	-2.310165	-2.338358	-3.872973
H	-5.940777	-2.152523	-2.520179
H	-7.309328	-2.314189	-1.391780
H	-6.570721	-0.717108	-1.663716
H	1.427204	2.170902	-3.806645
H	2.987313	2.486114	-2.990305
H	2.110587	3.815620	-3.789941
H	4.402470	3.946770	0.181193
H	2.987973	3.709418	1.236460
H	2.770282	4.335915	-0.422389
H	-2.289752	3.255325	-0.921998
H	-1.000034	4.024834	-1.892903
H	-2.456807	3.375946	-2.687626

B3LYP Energy = -1829.33549686 a.u.

(aR,1S,3S,3'S)-21, Conf E

C	1.965370	-1.200412	1.265300
C	3.190510	-1.854056	1.358967
C	4.248369	-1.433388	0.537858
C	4.074047	-0.362232	-0.334820
C	2.847071	0.311598	-0.408612
C	1.784932	-0.124947	0.390666
C	2.695476	1.480633	-1.358604
C	4.043004	2.011722	-1.841507
C	3.920309	2.974165	-3.007235
O	4.862280	0.914627	-2.267836
C	0.170002	1.643559	1.113729
C	-1.072754	2.294085	1.062969
C	-2.076077	1.775242	0.237375
C	-1.829080	0.634148	-0.539957
C	-0.575388	0.020373	-0.513474
C	0.437633	0.525934	0.321909
C	-0.294703	-1.153447	-1.428654
C	-1.559157	-1.754315	-2.032392
C	-1.277104	-2.662467	-3.214649
O	-2.415993	-0.700608	-2.495520
C	-2.937971	0.109404	-1.433874
C	5.245925	0.084178	-1.182561
C	-4.061310	-0.626372	-0.702485
C	-3.944793	-1.099951	0.603003
C	-4.985689	-1.797419	1.212806
C	-6.145154	-2.010249	0.492752
C	-6.304716	-1.554511	-0.805261
C	-5.253684	-0.862297	-1.393427
F	-7.169235	-2.685741	1.079805
O	3.453808	-2.886571	2.212549
C	2.411903	-3.341418	3.072318
O	5.498177	-2.007867	0.626433
C	5.604696	-3.361712	0.156904
O	-1.353036	3.361910	1.883352
C	-0.617383	4.574714	1.636087
O	-3.346387	2.283486	0.185441
C	-3.541241	3.694274	0.004849
O	1.162390	2.148668	1.926426
C	1.014887	1.860127	3.326545

H	1.134533	-1.515680	1.880453
H	2.103957	1.179775	-2.231348
H	2.143845	2.287579	-0.871635
H	4.550386	2.513983	-1.004521
H	3.467213	2.474796	-3.866421
H	3.293829	3.825586	-2.733802
H	4.901616	3.348394	-3.302393
H	0.252116	-1.929804	-0.890242
H	0.363908	-0.821066	-2.239370
H	-2.091185	-2.325074	-1.260837
H	-0.801417	-2.101018	-4.021737
H	-2.202587	-3.097777	-3.593922
H	-0.609224	-3.474372	-2.919584
H	-3.389603	0.959432	-1.946531
H	5.978501	0.609163	-0.551904
H	5.754555	-0.775684	-1.616351
H	-3.036994	-0.918768	1.163687
H	-4.902286	-2.164487	2.227351
H	-7.231407	-1.736251	-1.333707
H	-5.361874	-0.502154	-2.409633
H	2.076443	-2.547712	3.744959
H	2.843069	-4.150177	3.657179
H	1.560091	-3.721199	2.501599
H	5.286974	-3.432318	-0.887332
H	6.657487	-3.626555	0.232973
H	5.009858	-4.038604	0.770025
H	-0.988557	5.301953	2.355244
H	-0.805880	4.936684	0.622161
H	0.451546	4.422528	1.778667
H	-3.411297	4.234894	0.940123
H	-4.564863	3.806860	-0.347511
H	-2.855860	4.087125	-0.750293
H	1.051584	0.782050	3.499976
H	1.857691	2.334022	3.825662
H	0.079469	2.266615	3.714856

B3LYP Energy = -1829.33484405 a.u.

(aR,1S,3S,3'S)-**21**, Conf F

C	-1.945236	-1.369435	-1.065912
C	-3.154338	-2.058588	-1.072622
C	-4.210347	-1.584426	-0.279231
C	-4.031464	-0.464007	0.528458
C	-2.814747	0.232093	0.529680
C	-1.767727	-0.230625	-0.275260
C	-2.662875	1.463585	1.396843
C	-4.008407	1.994515	1.884594
C	-3.875446	3.037514	2.977951
O	-4.783971	0.909930	2.410482
C	-0.221815	1.520911	-1.169636
C	1.003947	2.203714	-1.201344
C	2.044553	1.767380	-0.374385
C	1.851726	0.677197	0.486408
C	0.613449	0.034434	0.542935
C	-0.436500	0.455713	-0.293618
C	0.389511	-1.076968	1.547085

C	1.685997	-1.606146	2.150270
C	1.462497	-2.432320	3.402837
O	2.531954	-0.503274	2.508991
C	3.000777	0.238979	1.375849
C	-5.181212	-0.004418	1.400616
C	4.114973	-0.525076	0.659366
C	5.329976	-0.698768	1.329123
C	6.375899	-1.410460	0.755432
C	6.188113	-1.949507	-0.506431
C	5.005487	-1.800660	-1.204415
C	3.969993	-1.082327	-0.609660
F	7.206925	-2.644886	-1.079299
O	-3.398160	-3.189125	-1.797857
C	-2.344455	-3.729638	-2.591131
O	-5.410582	-2.258566	-0.211648
C	-6.229201	-2.206883	-1.390495
O	1.231969	3.220460	-2.099091
C	0.472770	4.428894	-1.908051
O	3.301074	2.312156	-0.400558
C	3.455335	3.734542	-0.282325
O	-1.248950	1.943160	-1.987311
C	-1.133459	1.550277	-3.364721
H	-1.119048	-1.718708	-1.668843
H	-2.039771	1.234934	2.269271
H	-2.145671	2.248598	0.840923
H	-4.553562	2.426311	1.031971
H	-3.378085	2.611063	3.851791
H	-3.285196	3.885621	2.625187
H	-4.857096	3.402977	3.282764
H	-0.157199	-1.900538	1.084139
H	-0.249888	-0.701457	2.354328
H	2.207541	-2.219133	1.404427
H	0.996441	-1.825493	4.182241
H	2.409751	-2.817036	3.783108
H	0.807158	-3.278844	3.187844
H	3.451228	1.131621	1.811306
H	-5.964059	0.450153	0.775035
H	-5.630220	-0.854855	1.911931
H	5.459954	-0.273975	2.317421
H	7.319754	-1.544555	1.267477
H	4.899864	-2.233084	-2.190743
H	3.043538	-0.952824	-1.153777
H	-2.024955	-3.025969	-3.364644
H	-2.755114	-4.619621	-3.061638
H	-1.485807	-4.009686	-1.975087
H	-5.742664	-2.705166	-2.229284
H	-7.152536	-2.726234	-1.141287
H	-6.456521	-1.170687	-1.656627
H	0.680096	4.859766	-0.925103
H	-0.595544	4.242638	-2.009409
H	0.805119	5.116976	-2.682596
H	2.783444	4.135068	0.480840
H	3.275787	4.232754	-1.232956
H	4.486142	3.894730	0.028328
H	-0.213065	1.935512	-3.806893
H	-1.161660	0.461690	-3.454168

H        -1.993802   1.976522   -3.876914  
B3LYP Energy = -1829.33467513 a.u.

(*aR*,1*S*,3*S*,3'*S*)-**21**, Conf G

C	2.058543	-1.090432	1.317409
C	3.304114	-1.702429	1.423191
C	4.342035	-1.279613	0.578092
C	4.128048	-0.246510	-0.331069
C	2.879949	0.385233	-0.418799
C	1.838299	-0.055616	0.404257
C	2.683863	1.515760	-1.406284
C	4.010072	2.071516	-1.919762
C	3.847629	2.987092	-3.117772
O	4.861133	0.986096	-2.313616
C	0.174237	1.681509	1.088452
C	-1.096022	2.275520	1.028791
C	-2.051095	1.742888	0.158020
C	-1.780075	0.589897	-0.584398
C	-0.517463	-0.004265	-0.510883
C	0.470879	0.549952	0.322021
C	-0.203589	-1.203884	-1.379899
C	-1.451098	-1.844440	-1.978160
C	-1.138474	-2.801744	-3.112998
O	-2.310087	-0.821762	-2.504182
C	-2.861279	0.031525	-1.492440
C	5.279139	0.208072	-1.202630
C	-4.006656	-0.670986	-0.763216
C	-5.195403	-0.895971	-1.463850
C	-6.264084	-1.562704	-0.878118
C	-6.125563	-2.005090	0.426885
C	-4.969907	-1.803294	1.156399
C	-3.911232	-1.130863	0.549207
F	-7.166706	-2.655413	1.011555
O	3.606006	-2.695165	2.310826
C	2.586550	-3.147461	3.198084
O	5.609810	-1.811815	0.677592
C	5.755450	-3.177022	0.254101
O	-1.329133	3.417124	1.757203
C	-2.374487	3.343753	2.744275
O	-3.295098	2.324879	0.036102
C	-3.313614	3.599634	-0.633042
O	1.180604	2.255408	1.826528
C	1.069984	2.175121	3.253172
H	1.243144	-1.406478	1.952541
H	2.094495	1.167084	-2.262480
H	2.112247	2.321783	-0.941353
H	4.507436	2.619410	-1.105882
H	3.405912	2.442658	-3.955245
H	3.194863	3.826359	-2.869582
H	4.813884	3.382996	-3.433557
H	0.346910	-1.952437	-0.806841
H	0.460685	-0.891010	-2.193597
H	-1.991457	-2.385726	-1.191326
H	-0.652038	-2.272639	-3.935373
H	-2.052338	-3.263012	-3.489693

H	-0.469135	-3.592514	-2.768308
H	-3.297019	0.857425	-2.055604
H	5.997156	0.779260	-0.595771
H	5.813940	-0.649147	-1.609312
H	-5.287247	-0.546609	-2.485430
H	-7.188309	-1.735129	-1.413905
H	-4.902880	-2.160648	2.175615
H	-3.006018	-0.958809	1.116891
H	3.046178	-3.922748	3.806155
H	1.739548	-3.570521	2.651083
H	2.236169	-2.339646	3.846008
H	6.816070	-3.407303	0.334017
H	5.183801	-3.850107	0.892979
H	5.436116	-3.293380	-0.785541
H	-3.346693	3.172370	2.283402
H	-2.369031	4.303495	3.256505
H	-2.166546	2.546527	3.462788
H	-4.357804	3.901360	-0.678766
H	-2.916315	3.504591	-1.646779
H	-2.736048	4.343022	-0.082410
H	0.931221	1.138726	3.572348
H	2.011032	2.550028	3.650626
H	0.250042	2.790477	3.623968

B3LYP Energy = -1829.33464125 a.u.

(*aR*,1*S*,3*S*,3'*S*)-**21**, Conf H

C	2.044609	-1.282113	1.120260
C	3.275315	-1.932194	1.133145
C	4.306947	-1.449517	0.313354
C	4.084521	-0.359627	-0.524869
C	2.845768	0.295943	-0.534057
C	1.822604	-0.176601	0.295156
C	2.646023	1.498660	-1.431283
C	3.970059	2.061212	-1.941646
C	3.796501	3.073890	-3.057392
O	4.776756	0.989531	-2.447770
C	0.231033	1.544542	1.163992
C	-1.021453	2.177738	1.186895
C	-2.017611	1.737490	0.310503
C	-1.803601	0.637215	-0.524513
C	-0.557033	0.005733	-0.536975
C	0.470654	0.467361	0.304347
C	-0.302040	-1.130201	-1.505832
C	-1.581938	-1.684906	-2.122126
C	-1.325409	-2.544921	-3.345330
O	-2.426459	-0.598986	-2.533006
C	-2.926181	0.177345	-1.436958
C	5.211144	0.113154	-1.419803
C	-4.062608	-0.560075	-0.728585
C	-5.277599	-0.704494	-1.405116
C	-6.341499	-1.395994	-0.839818
C	-6.171321	-1.945470	0.420005
C	-4.989103	-1.825721	1.124542
C	-3.935632	-1.126709	0.538604
F	-7.207359	-2.621176	0.984668

O	3.563173	-3.031753	1.889652
C	2.535254	-3.580650	2.709982
O	5.527554	-2.087393	0.253700
C	6.358632	-1.964564	1.418361
O	-1.199911	3.271015	2.000393
C	-2.213022	3.151757	3.016547
O	-3.246313	2.362606	0.272666
C	-3.246979	3.679323	-0.310043
O	1.279577	2.027302	1.908278
C	1.191789	1.900261	3.333299
H	1.237496	-1.635433	1.746374
H	2.025169	1.227184	-2.293132
H	2.107278	2.279911	-0.890849
H	4.506527	2.530128	-1.103320
H	3.308782	2.611938	-3.918540
H	3.180578	3.909724	-2.719670
H	4.763901	3.464624	-3.376164
H	0.238947	-1.937289	-1.008216
H	0.352870	-0.773164	-2.308705
H	-2.116581	-2.280084	-1.371158
H	-0.846129	-1.956916	-4.131015
H	-2.261596	-2.946661	-3.735182
H	-0.669661	-3.380519	-3.092243
H	-3.361823	1.055066	-1.915194
H	5.985002	0.606647	-0.812868
H	5.681731	-0.735522	-1.914507
H	-5.394012	-0.271354	-2.391541
H	-7.285689	-1.506714	-1.356760
H	-4.897601	-2.266494	2.108581
H	-3.009141	-1.019970	1.087594
H	2.978076	-4.443148	3.202046
H	1.679505	-3.905111	2.111816
H	2.201626	-2.864343	3.465818
H	7.294388	-2.465246	1.177351
H	6.557314	-0.912351	1.641008
H	5.898075	-2.443890	2.282598
H	-2.173653	4.076924	3.587578
H	-1.995230	2.307275	3.675549
H	-3.202652	3.025451	2.578899
H	-2.884917	3.641236	-1.340566
H	-2.629870	4.367550	0.268720
H	-4.282365	4.013065	-0.300770
H	0.446861	2.578723	3.748826
H	0.956488	0.870795	3.616435
H	2.174585	2.162774	3.720013

B3LYP Energy = -1829.33434393 a.u.

(aR,1S,3S,3'S)-**21**, Conf I

C	-1.984489	-1.080893	-1.324049
C	-3.217728	-1.710072	-1.442371
C	-4.253046	-1.355420	-0.572638
C	-4.055261	-0.344912	0.372274
C	-2.819844	0.304537	0.470069
C	-1.768174	-0.083558	-0.375179
C	-2.636687	1.401811	1.496199

C	-3.967416	1.911451	2.044359
C	-3.808430	2.786648	3.272644
O	-4.791263	0.795635	2.408874
C	-0.140750	1.716845	-0.979736
C	1.112497	2.337395	-0.887050
C	2.120137	1.737655	-0.129942
C	1.862816	0.559372	0.582572
C	0.596543	-0.028758	0.524737
C	-0.412049	0.542762	-0.273862
C	0.304048	-1.258569	1.358055
C	1.564305	-1.922493	1.901212
C	1.277885	-2.916916	3.010883
O	2.440196	-0.921398	2.439142
C	2.964622	-0.024534	1.449770
C	-5.204083	0.046148	1.276983
C	4.103633	-0.686203	0.677303
C	5.356489	-0.779442	1.290225
C	6.420867	-1.418348	0.666127
C	6.211635	-1.969542	-0.586838
C	4.990732	-1.900171	-1.230261
C	3.938755	-1.250847	-0.587643
F	7.246694	-2.594830	-1.207821
O	-3.373056	-2.707467	-2.382607
C	-4.205908	-2.364224	-3.502670
O	-5.500778	-1.937200	-0.659265
C	-5.568395	-3.321143	-0.271304
O	1.351751	3.521369	-1.548705
C	0.929136	4.694783	-0.831792
O	3.344703	2.338601	0.034682
C	4.154001	2.518442	-1.141977
O	-1.150966	2.324110	-1.689290
C	-1.010585	2.298704	-3.119224
H	-1.189371	-1.382016	-1.995132
H	-2.029378	1.033207	2.330932
H	-2.085571	2.234508	1.054285
H	-4.485397	2.477967	1.256430
H	-3.345636	2.221784	4.084742
H	-3.175451	3.647222	3.047354
H	-4.778415	3.151167	3.613700
H	-0.263274	-1.985455	0.773719
H	-0.337463	-0.972693	2.199694
H	2.080279	-2.439993	1.082964
H	0.815010	-2.414977	3.863337
H	2.199901	-3.392700	3.347588
H	0.597462	-3.693970	2.656925
H	3.399945	0.786126	2.034359
H	-5.947712	0.617399	0.701626
H	-5.708033	-0.840032	1.660480
H	5.503744	-0.345317	2.272144
H	7.394318	-1.488048	1.133559
H	4.868841	-2.340739	-2.211103
H	2.982656	-1.181327	-1.090108
H	-4.225931	-3.240374	-4.147737
H	-3.779599	-1.519229	-4.050138
H	-5.219615	-2.119670	-3.181124
H	-4.952257	-3.942467	-0.921885

H	-5.246542	-3.443387	0.766372
H	-6.613113	-3.610888	-0.363147
H	-0.149974	4.678760	-0.666848
H	1.190465	5.546270	-1.457022
H	1.451296	4.768974	0.124897
H	4.351119	1.555247	-1.617645
H	5.091457	2.947313	-0.794309
H	3.674003	3.193525	-1.848673
H	-0.103343	2.816200	-3.432607
H	-0.997260	1.267888	-3.482668
H	-1.883633	2.810920	-3.518501

B3LYP Energy = -1829.33406422 a.u.

(aR,1S,3S,3'S)-**21**, Conf J

C	-1.975587	-1.146177	-1.274895
C	-3.201423	-1.793187	-1.371522
C	-4.252788	-1.394597	-0.541648
C	-4.049524	-0.391925	0.410383
C	-2.813182	0.256220	0.505479
C	-1.766912	-0.125003	-0.349947
C	-2.632442	1.362005	1.522722
C	-3.965691	1.880419	2.055974
C	-3.813715	2.776158	3.270226
O	-4.788674	0.769169	2.435569
C	-0.175591	1.678241	-1.028844
C	1.068106	2.321885	-0.972727
C	2.093370	1.766050	-0.205797
C	1.862469	0.609986	0.551039
C	0.605574	-0.000350	0.528446
C	-0.420366	0.526014	-0.278919
C	0.342288	-1.205011	1.407445
C	1.619038	-1.827629	1.961022
C	1.361485	-2.785717	3.109110
O	2.482058	-0.792734	2.453116
C	2.982563	0.074383	1.425839
C	-5.197690	-0.001818	1.317307
C	4.122542	-0.599469	0.664964
C	3.957574	-1.194036	-0.586100
C	5.011833	-1.851522	-1.216743
C	6.234754	-1.898930	-0.575312
C	6.444023	-1.318061	0.664243
C	5.377588	-0.671271	1.276433
F	7.271899	-2.532202	-1.184651
O	-3.366798	-2.780986	-2.320163
C	-3.456713	-4.116446	-1.796756
O	-5.483674	-2.015221	-0.591470
C	-6.260173	-1.758066	-1.774523
O	1.281603	3.484589	-1.679011
C	0.823200	4.674200	-1.012623
O	3.309936	2.390600	-0.074998
C	4.101763	2.552177	-1.266080
O	-1.202595	2.245617	-1.747311
C	-1.085997	2.155824	-3.177167
H	-1.176780	-1.459809	-1.935784
H	-2.034058	0.998976	2.366326

H	-2.074484	2.188349	1.077538
H	-4.480479	2.433061	1.256124
H	-3.353491	2.225769	4.093590
H	-3.181577	3.634287	3.033488
H	-4.785976	3.144185	3.600932
H	-0.217734	-1.961288	0.854238
H	-0.296272	-0.901032	2.244846
H	2.136215	-2.365350	1.156632
H	0.898467	-2.260934	3.947573
H	2.295400	-3.232247	3.452996
H	0.691614	-3.587412	2.791680
H	3.412421	0.911996	1.975481
H	-5.954244	0.550924	0.740399
H	-5.683510	-0.891650	1.715819
H	2.999738	-1.141738	-1.087302
H	4.890078	-2.315067	-2.186959
H	7.419112	-1.371344	1.130413
H	5.524615	-0.213823	2.247727
H	-2.537787	-4.381228	-1.266399
H	-3.580832	-4.773322	-2.655397
H	-4.311254	-4.221034	-1.126188
H	-6.455037	-0.687544	-1.879725
H	-5.752446	-2.128360	-2.665766
H	-7.202172	-2.285673	-1.639520
H	-0.256145	4.635817	-0.853780
H	1.066522	5.506438	-1.670200
H	1.336970	4.800601	-0.056750
H	4.304933	1.580526	-1.721596
H	5.038182	3.000318	-0.940628
H	3.604588	3.204220	-1.982331
H	-1.082964	1.109961	-3.494759
H	-1.963558	2.653664	-3.584645
H	-0.182244	2.655203	-3.528260

B3LYP Energy = -1829.33384284 a.u.

(aR,1S,3S,3'S)-**21**, Conf K

C	2.114736	-0.344765	1.699395
C	3.368352	-0.843562	2.035906
C	4.358444	-0.917510	1.042793
C	4.087337	-0.477110	-0.249732
C	2.827914	0.043647	-0.582980
C	1.835269	0.097620	0.403299
C	2.582782	0.526755	-1.997324
C	3.884831	0.784945	-2.750166
C	3.676852	1.025366	-4.233208
O	4.741396	-0.356010	-2.610221
C	0.148919	1.941877	0.473865
C	-1.127839	2.475526	0.232704
C	-2.084667	1.683483	-0.408277
C	-1.781032	0.361558	-0.766163
C	-0.517372	-0.168383	-0.501301
C	0.465087	0.629342	0.115779
C	-0.205342	-1.595661	-0.900145
C	-1.454622	-2.399641	-1.240370
C	-1.145951	-3.698145	-1.962087

O	-2.296656	-1.620490	-2.102008
C	-2.850247	-0.461389	-1.464633
C	5.199434	-0.523132	-1.277046
C	-4.033647	-0.854226	-0.581596
C	-3.947849	-0.963236	0.806234
C	-5.038512	-1.382482	1.565417
C	-6.217158	-1.686517	0.911479
C	-6.347483	-1.588504	-0.463613
C	-5.245933	-1.171845	-1.200820
F	-7.289335	-2.090052	1.643869
O	3.725435	-1.259029	3.286182
C	2.765302	-1.158877	4.335497
O	5.638119	-1.337677	1.334362
C	5.790625	-2.729330	1.657207
O	-1.414737	3.790001	0.522007
C	-1.463548	4.138188	1.918092
O	-3.310437	2.155963	-0.797555
C	-4.157752	2.809512	0.158549
O	1.093131	2.718055	1.111217
C	1.697505	3.750216	0.314316
H	1.340126	-0.272943	2.449143
H	2.007195	-0.218729	-2.557069
H	1.977907	1.435892	-1.988634
H	4.392232	1.654404	-2.306118
H	3.217887	0.151113	-4.699956
H	3.021671	1.884171	-4.391776
H	4.629015	1.221542	-4.727976
H	0.345073	-2.095035	-0.099688
H	0.454885	-1.594024	-1.773738
H	-2.004777	-2.625042	-0.318364
H	-0.646522	-3.496736	-2.912323
H	-2.063435	-4.252765	-2.163354
H	-0.490100	-4.324225	-1.353708
H	-3.246180	0.129422	-2.291070
H	5.946861	0.248395	-1.040591
H	5.711304	-1.484154	-1.246046
H	-3.024449	-0.711568	1.311768
H	-4.978483	-1.469170	2.642434
H	-7.289794	-1.829785	-0.937784
H	-5.331376	-1.092296	-2.278123
H	1.888324	-1.780580	4.135475
H	2.451690	-0.123091	4.488989
H	3.266542	-1.520460	5.230003
H	6.858411	-2.894065	1.787721
H	5.264583	-2.979744	2.578337
H	5.424201	-3.356116	0.839215
H	-0.505168	3.955588	2.402711
H	-2.247781	3.571498	2.426672
H	-1.701980	5.199145	1.955043
H	-4.173723	2.257928	1.101323
H	-5.155339	2.799439	-0.276144
H	-3.840381	3.836004	0.331215
H	0.944571	4.429940	-0.087041
H	2.366831	4.292743	0.978840
H	2.277570	3.314967	-0.502513

B3LYP Energy = -1829.33375072 a.u.

(aR,1S,3S,3'S)-**21**, Conf L

C	-2.096674	-0.275759	-1.699204
C	-3.329272	-0.794122	-2.081043
C	-4.317082	-0.986555	-1.102248
C	-4.047192	-0.695611	0.232193
C	-2.802030	-0.176075	0.616767
C	-1.823443	0.032519	-0.363561
C	-2.562384	0.150085	2.076125
C	-3.867572	0.268548	2.858347
C	-3.657830	0.353405	4.358241
O	-4.674255	-0.886723	2.596663
C	-0.192402	1.924262	-0.230702
C	1.070395	2.464953	0.063432
C	2.056680	1.632476	0.600135
C	1.795359	0.269009	0.802103
C	0.545261	-0.263927	0.485679
C	-0.467702	0.570947	-0.024689
C	0.282763	-1.738547	0.708485
C	1.560258	-2.538136	0.935390
C	1.300827	-3.924976	1.493601
O	2.389758	-1.845012	1.878768
C	2.897866	-0.597589	1.386631
C	-5.138655	-0.929644	1.256419
C	4.083962	-0.837338	0.453828
C	5.319426	-1.163213	1.020461
C	6.424931	-1.450856	0.229302
C	6.274751	-1.410972	-1.146566
C	5.072681	-1.093608	-1.749717
C	3.978568	-0.805107	-0.936622
F	7.350188	-1.688326	-1.931097
O	-3.661109	-1.143201	-3.358171
C	-2.682647	-0.982491	-4.382528
O	-5.538903	-1.540510	-1.418314
C	-6.419523	-0.721405	-2.203307
O	1.315310	3.812439	-0.071607
C	1.342590	4.322958	-1.417281
O	3.275122	2.086759	1.028978
C	4.073852	2.914263	0.170689
O	-1.164014	2.740595	-0.769820
C	-1.794201	3.650628	0.146375
H	-1.325679	-0.108039	-2.437387
H	-1.955740	-0.632116	2.545663
H	-1.993762	1.077533	2.170175
H	-4.415713	1.158863	2.514997
H	-3.157242	-0.545720	4.723853
H	-3.039578	1.217755	4.608466
H	-4.613609	0.451137	4.874965
H	-0.261807	-2.153391	-0.142543
H	-0.366131	-1.866213	1.580971
H	2.105648	-2.631343	-0.012066
H	0.813523	-3.859032	2.468724
H	2.236748	-4.472939	1.610610
H	0.651514	-4.489403	0.821345
H	3.283142	-0.101002	2.277656

H	-5.938828	-0.187244	1.117161
H	-5.584666	-1.913389	1.115732
H	5.420596	-1.192233	2.098982
H	7.384928	-1.698010	0.663259
H	4.997399	-1.070716	-2.829012
H	3.036220	-0.544349	-1.400868
H	-2.390029	0.064938	-4.494296
H	-3.155988	-1.324749	-5.299546
H	-1.795851	-1.590377	-4.184213
H	-7.348696	-1.280020	-2.297926
H	-6.617062	0.227443	-1.696552
H	-6.002627	-0.531480	-3.192490
H	2.132842	3.836954	-1.995295
H	1.558421	5.385883	-1.331276
H	0.383382	4.177102	-1.912658
H	4.049724	2.543821	-0.856623
H	5.090449	2.840330	0.552106
H	3.741713	3.950140	0.200075
H	-1.061114	4.306482	0.618220
H	-2.490492	4.242233	-0.444641
H	-2.347990	3.102585	0.911915

B3LYP Energy = -1829.33351521 a.u.

(*aS*,1*R*,3*S*,3'*S*)-**21**, Conf A

C	2.001337	-1.476411	-0.921408
C	3.242787	-2.103141	-0.973950
C	4.342078	-1.484272	-0.358288
C	4.180041	-0.272979	0.309775
C	2.924528	0.345719	0.380238
C	1.833549	-0.259546	-0.254277
C	2.783749	1.658264	1.119903
C	3.970067	1.932982	2.039972
C	3.994809	3.354065	2.570121
O	5.189789	1.717256	1.318149
C	0.181149	1.434443	-1.065520
C	-1.078737	2.045957	-1.041082
C	-2.082945	1.523012	-0.223545
C	-1.823069	0.414175	0.595478
C	-0.535685	-0.133784	0.628279
C	0.469342	0.356192	-0.226735
C	-0.222523	-1.213933	1.640477
C	-1.212129	-1.174030	2.796670
C	-1.046044	-2.323683	3.772309
O	-2.537736	-1.257266	2.260293
C	-2.941536	-0.120868	1.488238
C	5.381695	0.349941	0.988474
C	-4.178686	-0.572608	0.732382
C	-5.445219	-0.168978	1.148684
C	-6.593131	-0.622845	0.504306
C	-6.446122	-1.495933	-0.557482
C	-5.206100	-1.928220	-0.996205
C	-4.073456	-1.459247	-0.340364
F	-7.559359	-1.946835	-1.195552
O	3.478788	-3.303258	-1.580984

C	2.386394	-3.977873	-2.200511
O	5.580854	-2.087223	-0.326117
C	6.271303	-2.181727	-1.582899
O	-1.332875	3.142856	-1.833308
C	-0.847728	4.388243	-1.301311
O	-3.304896	2.138922	-0.114081
C	-4.117419	2.223536	-1.299674
O	1.174054	1.970552	-1.853015
C	1.057800	1.696148	-3.258209
H	1.143483	-1.933377	-1.393898
H	2.698496	2.476659	0.396950
H	1.861157	1.662585	1.706234
H	3.942369	1.229202	2.885592
H	4.074751	4.065609	1.745477
H	3.079017	3.569959	3.124082
H	4.844871	3.501434	3.237815
H	0.795211	-1.083409	2.013865
H	-0.260613	-2.207440	1.181389
H	-1.103955	-0.220194	3.333172
H	-1.190703	-3.279322	3.264065
H	-1.774150	-2.248933	4.581092
H	-0.044442	-2.311163	4.206481
H	-3.238760	0.681631	2.176086
H	5.630222	-0.221079	1.895347
H	6.253111	0.309811	0.336373
H	-5.542125	0.515341	1.982952
H	-7.580637	-0.311212	0.818250
H	-5.135962	-2.614986	-1.829544
H	-3.096335	-1.789251	-0.670361
H	2.798758	-4.898755	-2.605478
H	1.959120	-3.383725	-3.012842
H	1.605192	-4.219419	-1.474905
H	7.245746	-2.612354	-1.360851
H	5.734012	-2.825513	-2.279007
H	6.404220	-1.189622	-2.023588
H	0.237705	4.364885	-1.190880
H	-1.317086	4.602346	-0.338129
H	-1.125767	5.156404	-2.020253
H	-5.060201	2.663150	-0.981470
H	-4.301704	1.226326	-1.704443
H	-3.646232	2.851788	-2.053212
H	1.899272	2.193460	-3.736378
H	1.119850	0.620529	-3.442818
H	0.121915	2.089833	-3.657775

B3LYP Energy = -1829.33591122 a.u.

(*aS*,1*R*,3*S*,3'*S*)-**21**, Conf B

C	1.988829	-1.330484	-1.139869
C	3.232973	-1.937145	-1.283443
C	4.342156	-1.373031	-0.634335
C	4.200914	-0.198164	0.100351
C	2.947744	0.413474	0.240780
C	1.836552	-0.163348	-0.385657
C	2.828829	1.679239	1.060500
C	4.041674	1.899116	1.960123



C	4.078405	3.282212	2.581893
O	5.237578	1.739305	1.186308
C	0.135668	1.565934	-1.004857
C	-1.132516	2.150433	-0.891353
C	-2.101972	1.543696	-0.089943
C	-1.797645	0.379509	0.630640
C	-0.501221	-0.145059	0.580041
C	0.467580	0.429355	-0.264218
C	-0.139857	-1.293712	1.496739
C	-1.086727	-1.348240	2.687459
C	-0.868730	-2.556617	3.578741
O	-2.428952	-1.420090	2.192794
C	-2.878630	-0.242774	1.512012
C	5.427743	0.399976	0.757542
C	-4.126241	-0.670018	0.758899
C	-4.032011	-1.461085	-0.386961
C	-5.172193	-1.912478	-1.042129
C	-6.408564	-1.559286	-0.528706
C	-6.544584	-0.780789	0.605646
C	-5.389103	-0.343338	1.247826
F	-7.529347	-1.993664	-1.164932
O	3.468113	-3.056963	-2.028398
C	2.374756	-3.656827	-2.718845
O	5.603210	-1.910737	-0.775025
C	5.820430	-3.183408	-0.146189
O	-1.430239	3.304357	-1.581012
C	-0.941456	4.509452	-0.966029
O	-3.330700	2.124418	0.104330
C	-4.181054	2.283767	-1.046391
O	1.095166	2.178458	-1.776726
C	0.921174	2.045787	-3.197042
H	1.120494	-1.753082	-1.625007
H	2.725328	2.539185	0.390355
H	1.922948	1.647833	1.671565
H	4.043247	1.140211	2.757184
H	4.125669	4.047042	1.803705
H	3.181689	3.454641	3.180462
H	4.950925	3.391340	3.227613
H	0.890253	-1.179436	1.840025
H	-0.188885	-2.251700	0.968441
H	-0.974060	-0.430192	3.282194
H	-1.011024	-3.479643	3.012681
H	-1.572737	-2.550794	4.411980
H	0.145320	-2.551942	3.983396
H	-3.174714	0.503062	2.261221
H	5.732208	-0.223585	1.611690
H	6.261445	0.415539	0.056860
H	-3.057430	-1.728540	-0.775677
H	-5.110407	-2.525525	-1.931710
H	-7.529476	-0.528607	0.976085
H	-5.477341	0.266769	2.138756
H	1.601897	-3.997201	-2.024250
H	2.790545	-4.513827	-3.243045
H	1.935459	-2.967328	-3.444617
H	6.872562	-3.418786	-0.294373
H	5.609586	-3.124830	0.925468

H	5.202946	-3.957686	-0.601691
H	0.147993	4.497331	-0.904064
H	-1.371545	4.632496	0.030843
H	-1.262459	5.329962	-1.604738
H	-3.740949	2.971681	-1.765888
H	-5.118279	2.686260	-0.668246
H	-4.366463	1.315952	-1.516669
H	-0.027294	2.479400	-3.517085
H	1.746596	2.586102	-3.655921
H	0.969145	0.994013	-3.490688

B3LYP Energy = -1829.33562322 a.u.

(*aS*,1*R*,3*S*,3'*S*)-**21**, Conf C

C	-2.124303	1.427610	-1.027471
C	-3.389052	2.006827	-1.009150
C	-4.412789	1.378800	-0.282133
C	-4.153727	0.205299	0.421238
C	-2.873955	-0.368096	0.414699
C	-1.859357	0.248337	-0.327273
C	-2.630702	-1.639510	1.200684
C	-3.718714	-1.888089	2.242090
C	-3.646665	-3.271286	2.860713
O	-5.003466	-1.755590	1.621528
C	-0.128242	-1.190116	-1.420698
C	1.165703	-1.721724	-1.495908
C	2.105358	-1.392593	-0.515940
C	1.801252	-0.458071	0.480206
C	0.501596	0.056292	0.560136
C	-0.471741	-0.313374	-0.385295
C	0.146799	0.965565	1.715442
C	1.103498	0.759823	2.882018
C	0.892490	1.744813	4.016517
O	2.442568	0.938890	2.406611
C	2.888191	-0.051932	1.473714
C	-5.273319	-0.418175	1.228052
C	4.132629	0.538577	0.833260
C	5.395464	0.159592	1.282505
C	6.549336	0.733244	0.755775
C	6.411022	1.699466	-0.223133
C	5.174299	2.110498	-0.690091
C	4.035720	1.522609	-0.150967
F	7.530515	2.267063	-0.748246
O	-3.716445	3.169001	-1.645384
C	-2.705447	3.841745	-2.392825
O	-5.666705	1.941136	-0.175839
C	-6.459186	1.947221	-1.374724
O	1.496868	-2.578969	-2.521588
C	2.252098	-1.970723	-3.584807
O	3.375268	-1.918235	-0.568688
C	3.477328	-3.331666	-0.323145
O	-1.050128	-1.446209	-2.405531
C	-1.493267	-2.805349	-2.554193
H	-1.322588	1.890305	-1.584876
H	-2.598696	-2.500142	0.523406
H	-1.656433	-1.600860	1.693560

H	-3.638093	-1.128944	3.034634
H	-3.773196	-4.038226	2.093442
H	-2.679350	-3.423100	3.343874
H	-4.429831	-3.399049	3.609273
H	-0.879469	0.779119	2.035522
H	0.190517	2.016488	1.409081
H	0.994907	-0.266161	3.263270
H	1.030499	2.768921	3.663553
H	1.603166	1.558877	4.822933
H	-0.118339	1.651058	4.418218
H	3.189316	-0.947950	2.033663
H	-5.472117	0.198085	2.117184
H	-6.194183	-0.448538	0.647261
H	5.485896	-0.598828	2.051089
H	7.534386	0.441478	1.095486
H	5.110966	2.872182	-1.456159
H	3.061359	1.833764	-0.506591
H	-2.331049	3.217528	-3.208450
H	-1.872673	4.144202	-1.752433
H	-3.182738	4.727398	-2.804985
H	-7.427023	2.359123	-1.095499
H	-6.002770	2.569055	-2.144664
H	-6.592484	0.929399	-1.752136
H	1.680816	-1.161104	-4.044906
H	2.430101	-2.753691	-4.319272
H	3.205771	-1.590233	-3.214735
H	4.540421	-3.562555	-0.336572
H	2.963590	-3.903545	-1.095796
H	3.063674	-3.579982	0.657952
H	-1.940507	-3.166059	-1.624755
H	-2.253082	-2.787124	-3.332784
H	-0.672981	-3.458357	-2.849218

B3LYP Energy = -1829.33406158 a.u.

(aS,1R,3S,3'S)-**21**, Conf D

C	2.130605	-1.122172	-1.385312
C	3.405748	-1.666415	-1.502049
C	4.428917	-1.183488	-0.670919
C	4.175812	-0.142700	0.218861
C	2.891842	0.409592	0.329500
C	1.865220	-0.092271	-0.479702
C	2.652443	1.525040	1.324447
C	3.759974	1.607816	2.371766
C	3.685017	2.862143	3.221376
O	5.031012	1.606741	1.710680
C	0.070316	1.477610	-1.246595
C	-1.235193	1.982734	-1.184359
C	-2.132440	1.463068	-0.248039
C	-1.775834	0.373961	0.554554
C	-0.466149	-0.117168	0.497767
C	0.466542	0.438351	-0.396627
C	-0.056625	-1.208013	1.462047
C	-0.964790	-1.215631	2.684272
C	-0.693977	-2.370038	3.631042
O	-2.320598	-1.340608	2.240882

C	-2.819391	-0.223420	1.494985
C	5.312996	0.366433	1.080463
C	-4.068458	-0.737077	0.798672
C	-3.981300	-1.516390	-0.354942
C	-5.121516	-2.042370	-0.951714
C	-6.349828	-1.778252	-0.370639
C	-6.478377	-1.015471	0.775052
C	-5.323037	-0.500359	1.356221
F	-7.470911	-2.286693	-0.950012
O	3.750238	-2.649581	-2.383508
C	2.753192	-3.141378	-3.276652
O	5.718167	-1.660443	-0.770987
C	5.927970	-3.009643	-0.326356
O	-1.617132	3.000074	-2.029762
C	-2.418719	2.576362	-3.147395
O	-3.412358	1.959984	-0.163238
C	-3.527120	3.304421	0.334943
O	0.951332	1.928491	-2.197823
C	1.361754	3.303454	-2.116068
H	1.326561	-1.483295	-2.010355
H	2.599257	2.488029	0.804570
H	1.688494	1.390140	1.820904
H	3.707604	0.722258	3.023163
H	3.784938	3.751790	2.595899
H	2.727394	2.913001	3.743336
H	4.483841	2.870962	3.964138
H	0.981560	-1.067203	1.766829
H	-0.109983	-2.190885	0.981061
H	-0.851254	-0.264606	3.225020
H	-0.836067	-3.324126	3.119268
H	-1.371354	-2.332551	4.485243
H	0.332032	-2.325533	4.001650
H	-3.125962	0.558011	2.203628
H	5.565191	-0.387120	1.841572
H	6.204682	0.523839	0.475198
H	-3.013726	-1.713967	-0.799145
H	-5.065493	-2.645325	-1.848560
H	-7.457128	-0.832743	1.198712
H	-5.405552	0.099715	2.254682
H	3.248359	-3.892215	-3.887466
H	2.369347	-2.345429	-3.919943
H	1.924598	-3.604562	-2.734111
H	6.997435	-3.193216	-0.409553
H	5.620811	-3.123478	0.717224
H	5.384100	-3.718803	-0.950497
H	-3.356260	2.133866	-2.806445
H	-1.869226	1.858876	-3.761189
H	-2.625798	3.471258	-3.730777
H	-3.099140	3.377253	1.338351
H	-4.592827	3.518640	0.379679
H	-3.033815	4.013681	-0.329486
H	2.096282	3.442167	-2.906579
H	0.519109	3.976809	-2.266972
H	1.831331	3.505344	-1.150483

B3LYP Energy = -1829.33375499 a.u.

(aS,1R,3S,3'S)-**21**, Conf E

C	1.967166	-1.543976	-0.816310
C	3.207178	-2.174932	-0.840225
C	4.311821	-1.522022	-0.270987
C	4.155703	-0.273504	0.326515
C	2.901426	0.349968	0.369498
C	1.804863	-0.289335	-0.221094
C	2.767220	1.702449	1.034510
C	3.961175	2.029442	1.927448
C	3.991456	3.479207	2.372853
O	5.175151	1.770138	1.210350
C	0.163926	1.387138	-1.088308
C	-1.091720	2.012132	-1.094846
C	-2.099396	1.524310	-0.254679
C	-1.857072	0.412769	0.568017
C	-0.578227	-0.148167	0.621589
C	0.442708	0.330497	-0.220531
C	-0.290592	-1.214452	1.655325
C	-1.294565	-1.140847	2.797957
C	-1.148893	-2.268491	3.802193
O	-2.613241	-1.229006	2.246334
C	-3.000335	-0.117334	1.429188
C	5.362622	0.385434	0.960296
C	-4.202698	-0.605146	0.638292
C	-4.044537	-1.415559	-0.485812
C	-5.147200	-1.915745	-1.169129
C	-6.410668	-1.593012	-0.704941
C	-6.610007	-0.797300	0.407828
C	-5.491282	-0.308661	1.076764
F	-7.495392	-2.075428	-1.369896
O	3.437208	-3.409523	-1.376276
C	2.340647	-4.115047	-1.952652
O	5.550707	-2.122968	-0.215074
C	6.229138	-2.290673	-1.470858
O	-1.383007	3.019788	-1.983829
C	-0.663944	4.256108	-1.819210
O	-3.368621	2.034867	-0.236267
C	-3.561515	3.451869	-0.123082
O	1.149724	1.858209	-1.929346
C	1.057090	1.393481	-3.286044
H	1.105664	-2.026220	-1.255761
H	2.674933	2.478116	0.266731
H	1.849991	1.739566	1.628091
H	3.939633	1.376562	2.813134
H	4.071354	4.140691	1.507500
H	3.078103	3.730291	2.915941
H	4.844013	3.663027	3.028217
H	0.724244	-1.089716	2.038599
H	-0.337946	-2.215969	1.215022
H	-1.185864	-0.175412	3.313393
H	-1.294017	-3.234735	3.314629
H	-1.886612	-2.170241	4.599723
H	-0.152772	-2.252428	4.248689
H	-3.335955	0.698048	2.084050
H	5.615182	-0.131891	1.897720

H	6.230053	0.304976	0.306702
H	-3.049757	-1.657100	-0.838761
H	-5.035944	-2.541628	-2.044862
H	-7.614437	-0.568680	0.739076
H	-5.629068	0.316988	1.950640
H	1.561559	-4.313264	-1.211825
H	2.749156	-5.058403	-2.306585
H	1.911806	-3.566513	-2.795643
H	7.203326	-2.713915	-1.234019
H	5.682311	-2.968807	-2.125705
H	6.363198	-1.325236	-1.966990
H	-1.053803	4.932047	-2.577500
H	0.405397	4.110885	-1.963762
H	-0.848101	4.677008	-0.827292
H	-3.436956	3.947379	-1.083753
H	-2.871929	3.880980	0.608318
H	-4.583332	3.582529	0.228699
H	0.107823	1.689684	-3.736749
H	1.880404	1.857768	-3.825261
H	1.164572	0.306791	-3.325874

B3LYP Energy = -1829.33368509 a.u.

(aS,1R,3S,3'S)-**21**, Conf F

C	-2.084508	1.461508	-0.869887
C	-3.345697	2.049542	-0.884604
C	-4.416799	1.373580	-0.279380
C	-4.207358	0.144847	0.342615
C	-2.931971	-0.434755	0.376254
C	-1.869117	0.228207	-0.248334
C	-2.739043	-1.767512	1.065881
C	-3.905637	-2.117578	1.985901
C	-3.878601	-3.558618	2.458612
O	-5.140311	-1.913114	1.286311
C	-0.176232	-1.391058	-1.123684
C	1.107944	-1.954060	-1.141165
C	2.071977	-1.473238	-0.250050
C	1.802724	-0.374278	0.573429
C	0.512486	0.166819	0.598975
C	-0.484945	-0.342059	-0.253097
C	0.187442	1.239595	1.615124
C	1.175404	1.206549	2.773333
C	0.999497	2.355543	3.748004
O	2.502109	1.298455	2.240086
C	2.914835	0.163042	1.471869
C	-5.379099	-0.540978	1.012937
C	4.156869	0.615183	0.723839
C	4.059101	1.422041	-0.409781
C	5.197593	1.891289	-1.055120
C	6.435266	1.541067	-0.543417
C	6.574708	0.748512	0.580621
C	5.420963	0.291674	1.211605
F	7.554493	1.992830	-1.171087
O	-3.626588	3.263188	-1.443974
C	-2.565038	3.991112	-2.056651
O	-5.674050	1.934056	-0.212406

C	-6.381279	2.051244	-1.457928
O	1.349087	-3.018991	-1.973502
C	2.378837	-2.839304	-2.962784
O	3.319844	-2.054834	-0.193551
C	3.353854	-3.370306	0.388319
O	-1.169021	-1.932685	-1.905572
C	-1.161000	-1.551209	-3.286335
H	-1.247986	1.962847	-1.335524
H	-2.630229	-2.554578	0.312126
H	-1.811649	-1.760153	1.644624
H	-3.891337	-1.447353	2.858803
H	-3.948084	-4.238857	1.607167
H	-2.948716	-3.767503	2.991345
H	-4.714141	-3.759121	3.130916
H	-0.829473	1.098626	1.986630
H	0.218095	2.234840	1.159118
H	1.072602	0.252110	3.309951
H	1.139365	3.311689	3.239400
H	1.725975	2.286132	4.558727
H	-0.003145	2.336908	4.179525
H	3.210564	-0.636299	2.164979
H	-5.631010	-0.013212	1.944796
H	-6.261125	-0.502703	0.375174
H	3.083904	1.687095	-0.798678
H	5.133447	2.515574	-1.936706
H	7.560619	0.498662	0.949897
H	5.511970	-0.330062	2.094341
H	-1.777385	4.228323	-1.336599
H	-3.010412	4.914042	-2.419874
H	-2.136402	3.439832	-2.898039
H	-5.872701	2.736729	-2.135595
H	-6.487561	1.071831	-1.932901
H	-7.366370	2.442065	-1.210642
H	3.359107	-2.721377	-2.502028
H	2.162893	-1.966999	-3.585111
H	2.360959	-3.736558	-3.577677
H	2.976859	-3.344807	1.413957
H	4.399221	-3.671565	0.393277
H	2.767330	-4.077760	-0.199339
H	-0.255293	-1.895704	-3.788688
H	-2.027085	-2.028865	-3.740115
H	-1.250860	-0.466294	-3.387188

B3LYP Energy = -1829.33360796 a.u.

(*aS*,1*R*,3*S*,3'*S*)-**21**, Conf G

C	1.969409	-1.349360	-1.062908
C	3.216252	-1.950015	-1.182990
C	4.320117	-1.367335	-0.553321
C	4.153923	-0.216069	0.220990
C	2.892176	0.372950	0.357769
C	1.791317	-0.191711	-0.307287
C	2.744896	1.618806	1.203114
C	3.942499	1.840530	2.122792
C	3.952162	3.215141	2.763849
O	5.152339	1.705470	1.365633

C	0.118054	1.548197	-0.958991
C	-1.150913	2.136040	-0.882108
C	-2.147820	1.525861	-0.117703
C	-1.870223	0.356010	0.604592
C	-0.574140	-0.171988	0.592718
C	0.422176	0.405376	-0.216295
C	-0.245898	-1.329673	1.510469
C	-1.233011	-1.394122	2.667453
C	-1.048074	-2.612651	3.552347
O	-2.557764	-1.457022	2.127027
C	-2.981561	-0.271666	1.443899
C	5.359758	0.373818	0.921522
C	-4.204257	-0.688186	0.645571
C	-5.481760	-0.353807	1.088977
C	-6.616021	-0.782036	0.404071
C	-6.443850	-1.559124	-0.726329
C	-5.191975	-1.919938	-1.195037
C	-4.073406	-1.477741	-0.497742
F	-7.543632	-1.984258	-1.404187
O	3.343235	-3.079648	-1.964936
C	3.572469	-4.299005	-1.239754
O	5.575440	-1.934746	-0.623737
C	6.207189	-1.883906	-1.915789
O	-1.422579	3.295675	-1.572805
C	-0.956673	4.494921	-0.929625
O	-3.381021	2.108650	0.037684
C	-4.192072	2.272295	-1.140704
O	1.103923	2.161037	-1.697023
C	0.974538	2.032648	-3.122958
H	1.129723	-1.807291	-1.571189
H	2.633508	2.489083	0.547898
H	1.831850	1.559960	1.801239
H	3.941527	1.070590	2.908872
H	4.002872	3.991257	1.997098
H	3.043553	3.368404	3.349499
H	4.812320	3.325559	3.425647
H	0.771677	-1.220581	1.890864
H	-0.277345	-2.282396	0.971390
H	-1.138437	-0.482805	3.275640
H	-1.174148	-3.528918	2.971704
H	-1.779421	-2.613531	4.361679
H	-0.048052	-2.615629	3.990542
H	-3.300331	0.467475	2.190517
H	5.639607	-0.264016	1.773258
H	6.216307	0.403277	0.249332
H	-5.598287	0.254960	1.977583
H	-7.612037	-0.523877	0.738960
H	-5.101760	-2.531831	-2.082971
H	-3.087139	-1.751845	-0.850675
H	2.733268	-4.509288	-0.571022
H	4.497812	-4.247764	-0.663582
H	3.646980	-5.088163	-1.985269
H	5.631037	-2.438380	-2.656932
H	6.325638	-0.847384	-2.242390
H	7.187578	-2.339236	-1.791715
H	0.130045	4.482725	-0.829808

H	-1.421161	4.608177	0.052885
H	-1.255782	5.321494	-1.571146
H	-5.138005	2.682747	-0.794144
H	-4.369352	1.305023	-1.615088
H	-3.723361	2.955631	-1.846398
H	0.037268	2.468942	-3.470979
H	1.814614	2.573402	-3.553979
H	1.029856	0.981668	-3.417945

B3LYP Energy = -1829.33335425 a.u.

(aS,1R,3S,3'S)-**21**, Conf H

C	1.963482	-1.407900	-1.043026
C	3.209281	-2.016824	-1.158822
C	4.319838	-1.410441	-0.551635
C	4.176995	-0.197041	0.117118
C	2.921735	0.415874	0.230896
C	1.809599	-0.199505	-0.356564
C	2.802081	1.723624	0.981885
C	4.017933	1.993874	1.863427
C	4.052122	3.406633	2.414798
O	5.210899	1.799804	1.093014
C	0.115348	1.507623	-1.046095
C	-1.151206	2.105988	-0.970964
C	-2.122014	1.541507	-0.135287
C	-1.832488	0.381267	0.600686
C	-0.543537	-0.157886	0.573631
C	0.440607	0.398039	-0.264940
C	-0.204384	-1.286883	1.522276
C	-1.166685	-1.301785	2.702133
C	-0.968137	-2.486615	3.628869
O	-2.502515	-1.379730	2.192785
C	-2.937021	-0.227112	1.460084
C	5.405137	0.440941	0.732941
C	-4.153585	-0.690389	0.676315
C	-5.434015	-0.439764	1.164305
C	-6.563038	-0.911547	0.500519
C	-6.382163	-1.644445	-0.657587
C	-5.127106	-1.920044	-1.172296
C	-4.014049	-1.437347	-0.493306
F	-7.477128	-2.110567	-1.317274
O	3.445025	-3.177564	-1.837816
C	2.351361	-3.816708	-2.491982
O	5.582748	-1.948499	-0.673239
C	5.814878	-3.176810	0.033683
O	-1.490054	3.162469	-1.783034
C	-0.789347	4.400759	-1.563374
O	-3.399512	2.021445	-0.040057
C	-3.620451	3.425622	0.153259
O	1.063547	2.056880	-1.882606
C	0.953127	1.661487	-3.259775
H	1.094692	-1.861057	-1.498749
H	2.693665	2.546413	0.267194
H	1.898600	1.721883	1.597245
H	4.026415	1.276847	2.698420
H	4.094589	4.131746	1.599294

H	3.157030	3.606066	3.007447
H	4.926425	3.550448	3.051225
H	0.822559	-1.173489	1.875375
H	-0.257554	-2.257689	1.018451
H	-1.054238	-0.368311	3.272590
H	-1.110559	-3.423614	3.086388
H	-1.682171	-2.453139	4.452878
H	0.040964	-2.477949	4.045639
H	-3.267996	0.537613	2.175429
H	5.718615	-0.136229	1.615876
H	6.233706	0.423838	0.026244
H	-5.557325	0.136225	2.073766
H	-7.561377	-0.718154	0.870363
H	-5.030174	-2.497450	-2.082358
H	-3.025702	-1.643002	-0.884970
H	1.580984	-4.120475	-1.778037
H	2.767964	-4.699946	-2.969895
H	1.908870	-3.168228	-3.252696
H	6.863312	-3.423062	-0.122771
H	5.629048	-3.046597	1.103680
H	5.187194	-3.978923	-0.354907
H	-1.206122	5.110339	-2.275185
H	0.279002	4.282999	-1.736516
H	-0.961174	4.762797	-0.546330
H	-3.548664	3.971315	-0.785269
H	-2.910503	3.835347	0.876207
H	-4.628955	3.511871	0.553747
H	1.746366	2.182404	-3.792165
H	1.096684	0.583075	-3.360199
H	-0.016912	1.947578	-3.671358

B3LYP Energy = -1829.33334384 a.u.

(aS,1R,3S,3'S)-**21**, Conf I

C	2.064898	-1.305213	-1.116020
C	3.329467	-1.874237	-1.233911
C	4.412064	-1.262821	-0.583053
C	4.223931	-0.081375	0.130530
C	2.950081	0.491199	0.246903
C	1.866242	-0.131533	-0.383438
C	2.779512	1.764733	1.045266
C	3.974413	2.039030	1.953801
C	3.958728	3.432657	2.552651
O	5.184210	1.905660	1.196674
C	0.124516	1.532644	-1.056931
C	-1.167110	2.074523	-0.980494
C	-2.092587	1.503239	-0.102115
C	-1.778447	0.345229	0.617833
C	-0.480236	-0.172685	0.555046
C	0.478125	0.420312	-0.287029
C	-0.105406	-1.315668	1.472995
C	-1.045839	-1.374912	2.669166
C	-0.815010	-2.580842	3.560473
O	-2.390942	-1.456389	2.182661
C	-2.852633	-0.284448	1.501181
C	5.422663	0.566699	0.792097

C	-4.096706	-0.721988	0.747218
C	-5.360157	-0.458237	1.271188
C	-6.512740	-0.907813	0.632805
C	-6.372687	-1.632854	-0.535793
C	-5.135442	-1.921900	-1.085524
C	-3.998303	-1.460878	-0.432065
F	-7.490691	-2.077808	-1.170339
O	3.608803	-3.000026	-1.954402
C	2.544162	-3.642968	-2.650708
O	5.691505	-1.761388	-0.701746
C	5.944604	-3.010852	-0.040834
O	-1.451840	3.205795	-1.705277
C	-2.515501	3.099557	-2.669515
O	-3.346580	2.055327	0.046005
C	-3.380658	3.316983	0.736977
O	1.086781	2.146414	-1.821320
C	0.981801	1.974094	-3.240215
H	1.216367	-1.763800	-1.603616
H	2.651887	2.610042	0.360879
H	1.869192	1.711066	1.648239
H	3.991800	1.293997	2.763803
H	3.990740	4.185753	1.762456
H	3.049291	3.585599	3.137192
H	4.818940	3.580657	3.207157
H	0.925425	-1.193156	1.810894
H	-0.151132	-2.275500	0.947618
H	-0.935764	-0.455394	3.262195
H	-0.954718	-3.505305	2.996164
H	-1.514114	-2.578781	4.397848
H	0.201352	-2.569216	3.959101
H	-3.156442	0.457289	2.251980
H	5.736207	-0.033539	1.659612
H	6.264085	0.598004	0.101218
H	-5.451827	0.110121	2.189125
H	-7.498192	-0.704156	1.030572
H	-5.070606	-2.494499	-2.001469
H	-3.023452	-1.678984	-0.849980
H	2.992693	-4.495435	-3.154926
H	2.095701	-2.978081	-3.393628
H	1.771301	-3.995004	-1.961950
H	5.351082	-3.814169	-0.477658
H	7.003502	-3.219005	-0.181446
H	5.729860	-2.931751	1.028785
H	-3.474320	2.913521	-2.186889
H	-2.306191	2.298314	-3.383066
H	-2.539708	4.053206	-3.192438
H	-2.957402	3.216033	1.739722
H	-4.430589	3.591820	0.812164
H	-2.835352	4.084274	0.185896
H	0.088012	2.459412	-3.634227
H	1.864934	2.443351	-3.668984
H	0.973667	0.912396	-3.500953

B3LYP Energy = -1829.33328584 a.u.

(aS,1R,3S,3'S)-**21**, Conf J

C	1.958721	-1.337049	-1.067773
C	3.205502	-1.935520	-1.197979
C	4.307259	-1.368909	-0.550983
C	4.158096	-0.180710	0.169308
C	2.901128	0.420904	0.295576
C	1.788156	-0.168046	-0.327798
C	2.769031	1.691359	1.105759
C	3.974341	1.928568	2.011040
C	3.996221	3.317788	2.619548
O	5.176685	1.770045	1.246775
C	0.088593	1.559360	-0.953898
C	-1.185999	2.132472	-0.858422
C	-2.166148	1.508025	-0.084134
C	-1.865809	0.339169	0.630650
C	-0.563923	-0.173301	0.601149
C	0.415808	0.418036	-0.218609
C	-0.210755	-1.328937	1.512327
C	-1.183167	-1.407496	2.680872
C	-0.972963	-2.625182	3.561292
O	-2.513459	-1.485738	2.156138
C	-2.959759	-0.304635	1.480305
C	5.376827	0.428515	0.831201
C	-4.185190	-0.735235	0.693559
C	-5.462381	-0.419898	1.151586
C	-6.597867	-0.861405	0.477205
C	-6.427080	-1.632579	-0.657439
C	-5.175434	-1.974876	-1.140411
C	-4.055709	-1.519573	-0.453506
F	-7.528100	-2.070721	-1.324987
O	3.316822	-3.105034	-1.921138
C	3.984701	-2.976247	-3.187204
O	5.567985	-1.917770	-0.657903
C	5.755339	-3.180673	0.004188
O	-1.479380	3.291510	-1.541439
C	-1.021453	4.493670	-0.897985
O	-3.404503	2.074897	0.088268
C	-4.230957	2.234489	-1.079899
O	1.056887	2.184693	-1.704526
C	0.903998	2.065656	-3.128719
H	1.114686	-1.799585	-1.564546
H	2.661202	2.543501	0.426729
H	1.859283	1.656162	1.710660
H	3.976149	1.177590	2.815410
H	4.043307	4.075471	1.834414
H	3.093970	3.489008	3.210050
H	4.863149	3.439559	3.270461
H	0.809884	-1.207797	1.880738
H	-0.236441	-2.281049	0.972009
H	-1.092715	-0.496083	3.289588
H	-1.094330	-3.541960	2.980506
H	-1.694715	-2.636415	4.379165
H	0.032120	-2.616543	3.987684
H	-3.280336	0.428877	2.231670
H	5.677929	-0.186721	1.692488
H	6.215917	0.442069	0.136677
H	-5.577815	0.184214	2.043501

H	-7.593731	-0.618099	0.823468
H	-5.086251	-2.583088	-2.030977
H	-3.069577	-1.779367	-0.817437
H	3.433128	-2.296611	-3.842545
H	3.998710	-3.971295	-3.627465
H	5.006765	-2.615444	-3.059816
H	6.799108	-3.449198	-0.145232
H	5.554393	-3.085481	1.074612
H	5.110042	-3.948494	-0.423538
H	0.066231	4.493796	-0.808281
H	-1.477973	4.597857	0.089243
H	-1.336088	5.319137	-1.533476
H	-3.781725	2.931739	-1.784660
H	-5.180062	2.625418	-0.719718
H	-4.396561	1.268398	-1.560886
H	-0.040428	2.500839	-3.458120
H	1.735049	2.612011	-3.570039
H	0.957553	1.016794	-3.431666

B3LYP Energy = -1829.33317067 a.u.

(*aS*,1*R*,3*S*,3'*S*)-**21**, Conf K

C	2.138936	0.455972	-1.678467
C	3.402124	0.223728	-2.212255
C	4.419083	-0.249534	-1.367964
C	4.153298	-0.499631	-0.024251
C	2.873963	-0.281896	0.508304
C	1.866347	0.210663	-0.330226
C	2.626369	-0.575530	1.973449
C	3.702457	-1.480210	2.567715
C	3.625503	-1.585973	4.078829
O	4.993581	-0.956113	2.233043
C	0.122683	1.760608	0.572482
C	-1.175319	2.043119	1.026288
C	-2.113663	1.008576	1.102287
C	-1.785328	-0.279577	0.651524
C	-0.487477	-0.551514	0.210050
C	0.476984	0.471928	0.166191
C	-0.126506	-1.967223	-0.181322
C	-1.070594	-2.967807	0.469900
C	-0.856669	-4.394634	0.000819
O	-2.414623	-2.605660	0.134134
C	-2.858481	-1.365994	0.697925
C	5.266299	-1.050223	0.842800
C	-4.131831	-1.023376	-0.056480
C	-5.375589	-1.275847	0.518264
C	-6.554840	-1.033429	-0.181107
C	-6.461914	-0.542708	-1.470257
C	-5.245961	-0.287026	-2.080597
C	-4.081192	-0.533780	-1.362126
F	-7.606519	-0.300717	-2.164808
O	3.734675	0.411282	-3.522535
C	2.729216	0.879973	-4.418339
O	5.671790	-0.555187	-1.854900
C	6.473659	0.560263	-2.276999
O	-1.511317	3.297100	1.484338

C	-1.571062	4.335379	0.488930
O	-3.345200	1.161464	1.678719
C	-4.204325	2.238106	1.273266
O	1.054331	2.770976	0.482962
C	1.540698	3.306179	1.726121
H	1.342953	0.825547	-2.308825
H	2.608677	0.358015	2.546197
H	1.645331	-1.036239	2.109809
H	3.612600	-2.484447	2.126814
H	3.763041	-0.604297	4.537203
H	2.652691	-1.975966	4.384629
H	4.399727	-2.255002	4.456903
H	0.903699	-2.184144	0.104071
H	-0.179223	-2.091912	-1.268526
H	-0.951201	-2.920134	1.562313
H	-1.006376	-4.468403	-1.078376
H	-1.558144	-5.069265	0.493514
H	0.158654	-4.722688	0.232041
H	-3.124152	-1.536288	1.749865
H	5.458316	-2.098688	0.571235
H	6.191689	-0.501399	0.673243
H	-5.429665	-1.660447	1.529697
H	-7.524911	-1.222660	0.259384
H	-5.218075	0.093019	-3.093453
H	-3.122331	-0.341350	-1.826928
H	1.892810	0.178611	-4.478839
H	3.210003	0.951472	-5.390879
H	2.359214	1.865312	-4.122663
H	7.437426	0.147010	-2.568046
H	6.020524	1.071123	-3.126328
H	6.614540	1.265928	-1.453336
H	-0.599177	4.488205	0.020213
H	-1.876087	5.238514	1.013424
H	-2.312254	4.090045	-0.275976
H	-3.929825	3.167791	1.767484
H	-5.208466	1.941853	1.570379
H	-4.177091	2.368789	0.189441
H	2.279452	4.059025	1.459651
H	0.736681	3.762255	2.304422
H	2.020510	2.524877	2.318905

B3LYP Energy = -1829.33254463 a.u.

(*aR*,1*R*,3*S*,3'*S*)-**21**, Conf A

C	2.923127	1.120526	0.774649
C	4.263241	0.753367	0.831247
C	4.681839	-0.396339	0.142203
C	3.768746	-1.137542	-0.602540
C	2.421154	-0.754319	-0.675264
C	2.000073	0.377175	0.033577
C	1.463490	-1.578720	-1.510871
C	2.193966	-2.484521	-2.498887
C	1.285373	-3.506340	-3.155613
O	3.224739	-3.200435	-1.806827
C	0.182964	1.887057	-0.791112

C	-1.136881	2.358073	-0.772885
C	-2.092616	1.704357	0.007002
C	-1.727799	0.611168	0.806229
C	-0.389103	0.206383	0.851978
C	0.570121	0.820429	0.024612
C	0.024090	-0.852505	1.850672
C	-0.983817	-0.945227	2.987670
C	-0.710051	-2.089927	3.945066
O	-2.282985	-1.161416	2.424439
C	-2.795094	-0.056681	1.671514
C	4.268613	-2.343619	-1.369970
C	-3.972919	-0.616365	0.893605
C	-5.277047	-0.361394	1.311698
C	-6.367285	-0.916450	0.646991
C	-6.123638	-1.739547	-0.436820
C	-4.842819	-2.025764	-0.877771
C	-3.769287	-1.457172	-0.201478
F	-7.179949	-2.288473	-1.094596
O	5.227508	1.444232	1.506338
C	4.854336	2.639871	2.187716
O	6.007481	-0.771684	0.112758
C	6.554535	-1.255127	1.350448
O	-1.491337	3.456117	-1.525326
C	-1.192294	4.719106	-0.905340
O	-3.376146	2.180359	0.106771
C	-4.168802	2.213420	-1.094617
O	1.131083	2.551851	-1.533317
C	1.021390	2.417002	-2.959645
H	2.579244	2.002841	1.294995
H	0.842879	-2.207221	-0.862354
H	0.777812	-0.924770	-2.054283
H	2.666545	-1.864063	-3.274923
H	0.844610	-4.163635	-2.402882
H	0.476929	-3.008068	-3.694519
H	1.844922	-4.119067	-3.863813
H	1.013411	-0.616262	2.246474
H	0.103195	-1.836064	1.375206
H	-0.990645	0.003409	3.543908
H	-0.740477	-3.044867	3.416225
H	-1.456142	-2.111732	4.740551
H	0.276372	-1.977397	4.399253
H	-3.179997	0.695782	2.372802
H	4.861867	-2.008561	-2.233499
H	4.924255	-2.950495	-0.746998
H	-5.450019	0.285073	2.163655
H	-7.383658	-0.720406	0.962304
H	-4.696220	-2.678393	-1.728399
H	-2.761077	-1.672145	-0.532555
H	4.449652	3.381744	1.494495
H	5.768632	3.023427	2.633853
H	4.123167	2.438818	2.975473
H	6.558211	-0.474013	2.110501
H	5.987641	-2.118715	1.709889
H	7.576121	-1.559482	1.131270
H	-1.534238	5.487506	-1.595903
H	-0.118083	4.824581	-0.741845

H	-1.725432	4.816617	0.043290
H	-4.213241	1.220439	-1.546471
H	-3.768165	2.930519	-1.808803
H	-5.167018	2.512348	-0.782446
H	1.141662	1.371823	-3.255860
H	0.064596	2.797438	-3.318395
H	1.833831	3.004803	-3.381907

B3LYP Energy = -1829.33508181 a.u.

(*aR*,1*R*,3*S*,3'*S*)-**21**, Conf B

C	2.862562	1.081118	0.842093
C	4.203346	0.721207	0.943307
C	4.663863	-0.391817	0.222440
C	3.792252	-1.104693	-0.596807
C	2.447922	-0.725816	-0.716564
C	1.983690	0.367970	0.022061
C	1.532908	-1.509073	-1.634064
C	2.310782	-2.384414	-2.613249
C	1.435891	-3.385429	-3.343471
O	3.311409	-3.121453	-1.898121
C	0.152539	1.751859	-0.972713
C	-1.177764	2.185267	-1.029786
C	-2.113109	1.659655	-0.136434
C	-1.748358	0.649658	0.762363
C	-0.410812	0.242766	0.833361
C	0.548530	0.792676	-0.036847
C	-0.003600	-0.741982	1.906414
C	-1.002582	-0.731242	3.055753
C	-0.730824	-1.796460	4.101454
O	-2.309349	-0.980406	2.525238
C	-2.820011	0.046526	1.667177
C	4.331990	-2.276806	-1.388853
C	-3.977252	-0.598735	0.923412
C	-5.282835	-0.413942	1.372749
C	-6.355070	-1.045862	0.749218
C	-6.091136	-1.871617	-0.327606
C	-4.807824	-2.088399	-0.799088
C	-3.752470	-1.445799	-0.161799
F	-7.130171	-2.493350	-0.948090
O	5.128254	1.385881	1.695925
C	4.710070	2.535886	2.426788
O	5.992675	-0.757003	0.238295
C	6.486063	-1.293363	1.476719
O	-1.556356	3.142362	-1.944337
C	-1.966958	2.613164	-3.217312
O	-3.425368	2.065826	-0.180076
C	-3.676168	3.427622	0.208157
O	1.059929	2.209567	-1.899267
C	1.491707	3.570635	-1.740862
H	2.485083	1.928167	1.397167
H	0.868611	-2.150824	-1.043605
H	0.891095	-0.824208	-2.192488
H	2.817335	-1.739214	-3.346128
H	0.965536	-4.069388	-2.633614
H	0.649572	-2.870579	-3.899196



H	2.027866	-3.972001	-4.047480
H	0.992693	-0.495039	2.275917
H	0.054389	-1.758687	1.501951
H	-0.993584	0.259989	3.532344
H	-0.770719	-2.790938	3.652320
H	-1.472557	-1.748158	4.899834
H	0.258812	-1.654421	4.540164
H	-3.228772	0.852091	2.292413
H	4.956367	-1.905972	-2.215020
H	4.966630	-2.903030	-0.763228
H	-5.471845	0.237256	2.217890
H	-7.372823	-0.904004	1.088192
H	-4.645244	-2.744092	-1.644436
H	-2.743037	-1.604911	-0.519811
H	4.329336	3.313833	1.759732
H	5.598010	2.901694	2.936505
H	3.945797	2.282774	3.166582
H	5.909519	-2.175145	1.770639
H	7.518638	-1.582520	1.291022
H	6.449889	-0.547471	2.270610
H	-2.243996	3.468839	-3.829863
H	-2.828760	1.952544	-3.099767
H	-1.144944	2.073451	-3.692163
H	-3.195819	4.126195	-0.476339
H	-3.324128	3.605223	1.228101
H	-4.755923	3.556241	0.170800
H	2.185056	3.764869	-2.556667
H	0.648315	4.259048	-1.801157
H	2.011541	3.696997	-0.787732

B3LYP Energy = -1829.33497895 a.u.

(aR,1R,3S,3'S)-**21**, Conf C

C	2.916653	1.061351	0.863118
C	4.241871	0.656451	0.983265
C	4.651269	-0.525790	0.346073
C	3.730793	-1.296469	-0.358934
C	2.393743	-0.889058	-0.475960
C	1.991277	0.301108	0.142660
C	1.430854	-1.744009	-1.273333
C	2.157588	-2.723872	-2.190464
C	1.236092	-3.759503	-2.806188
O	3.152224	-3.423985	-1.433013
C	0.243820	1.806630	-0.827773
C	-1.063161	2.309156	-0.885494
C	-2.061468	1.727977	-0.101739
C	-1.751584	0.677997	0.775013
C	-0.426365	0.245377	0.893046
C	0.576040	0.783051	0.063372
C	-0.076185	-0.759402	1.968080
C	-1.124376	-0.757789	3.072410
C	-0.911219	-1.847087	4.106481
O	-2.408900	-0.978383	2.477576
C	-2.866268	0.085128	1.635098
C	4.209888	-2.574716	-1.016127
C	-4.019981	-0.501479	0.840394

C	-3.785557	-1.410802	-0.192119
C	-4.839502	-1.999089	-0.882193
C	-6.132415	-1.662335	-0.519121
C	-6.406798	-0.770707	0.501211
C	-5.335853	-0.196734	1.181170
F	-7.169579	-2.229789	-1.191574
O	5.196055	1.328668	1.690594
C	4.821257	2.526208	2.367465
O	5.941803	-0.993928	0.467830
C	6.954138	-0.233676	-0.210414
O	-1.360557	3.364798	-1.718886
C	-1.075878	4.658115	-1.157699
O	-3.335995	2.236504	-0.076955
C	-4.083466	2.224588	-1.307389
O	1.231003	2.403244	-1.577739
C	1.177388	2.158346	-2.992020
H	2.582319	1.974484	1.334208
H	0.788334	-2.319896	-0.597912
H	0.766684	-1.111195	-1.866267
H	2.663119	-2.162239	-2.990380
H	0.759388	-4.356156	-2.025404
H	0.455045	-3.273975	-3.394796
H	1.794439	-4.430205	-3.460785
H	0.905144	-0.524573	2.384134
H	-0.007685	-1.771881	1.556129
H	-1.125996	0.223395	3.568955
H	-0.945351	-2.831889	3.635938
H	-1.684751	-1.803882	4.874378
H	0.061284	-1.727804	4.587972
H	-3.266109	0.887077	2.269772
H	4.850190	-2.329715	-1.876781
H	4.814557	-3.154130	-0.319692
H	-2.768447	-1.664703	-0.462978
H	-4.668745	-2.705089	-1.684318
H	-7.431884	-0.536383	0.756558
H	-5.533167	0.503903	1.983558
H	4.470868	3.287868	1.665891
H	5.721730	2.879279	2.864049
H	4.047026	2.334139	3.114995
H	7.885381	-0.780130	-0.074229
H	6.729643	-0.160032	-1.278313
H	7.048037	0.765085	0.216309
H	-1.666015	4.822665	-0.253070
H	-1.356908	5.388741	-1.913684
H	-0.012214	4.755306	-0.931647
H	-5.087666	2.551340	-1.046553
H	-4.126771	1.212547	-1.714992
H	-3.646173	2.901828	-2.038729
H	2.010029	2.708110	-3.426256
H	1.301542	1.092638	-3.200755
H	0.238681	2.514439	-3.417746

B3LYP Energy = -1829.33481287 a.u.

(aR,1R,3S,3'S)-**21**, Conf D

C	-2.848008	-1.073797	0.868630
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C	-4.177750	-0.706464	1.053842
C	-4.648475	0.469029	0.448236
C	-3.781913	1.272899	-0.288246
C	-2.442625	0.902065	-0.471986
C	-1.979944	-0.282074	0.111911
C	-1.536098	1.783315	-1.304489
C	-2.324727	2.767069	-2.164000
C	-1.454374	3.834753	-2.798913
O	-3.300085	3.429555	-1.348095
C	-0.221772	-1.586755	-1.092597
C	1.093754	-2.040682	-1.245566
C	2.072343	-1.636125	-0.335219
C	1.768447	-0.718736	0.677752
C	0.445406	-0.290193	0.840203
C	-0.557668	-0.723752	-0.045493
C	0.102005	0.587975	2.022478
C	1.138484	0.437253	3.127768
C	0.932733	1.398351	4.283386
O	2.432816	0.706970	2.576075
C	2.885421	-0.242726	1.604850
C	-4.319710	2.547647	-0.905111
C	4.041086	0.438041	0.891404
C	5.354864	0.136007	1.242257
C	6.428214	0.791218	0.645031
C	6.157718	1.759854	-0.303392
C	4.866631	2.095746	-0.673126
C	3.810414	1.426844	-0.065230
F	7.197544	2.406635	-0.896273
O	-5.079054	-1.411268	1.798478
C	-4.637048	-2.594562	2.458774
O	-5.945073	0.898049	0.634251
C	-6.963417	0.117685	-0.011288
O	1.407304	-2.904828	-2.270409
C	1.968120	-2.268706	-3.432430
O	3.368825	-2.075042	-0.469547
C	3.585679	-3.472518	-0.208337
O	-1.176844	-1.922141	-2.022978
C	-1.622626	-3.287482	-2.006115
H	-2.466576	-1.977188	1.322816
H	-0.862618	2.352582	-0.653261
H	-0.903105	1.166542	-1.946345
H	-2.853787	2.210589	-2.951941
H	-0.959597	4.430063	-2.028353
H	-0.687299	3.376503	-3.426316
H	-2.054216	4.502233	-3.419190
H	-0.888166	0.329335	2.400712
H	0.060080	1.641988	1.726195
H	1.118711	-0.596391	3.503195
H	0.986148	2.431763	3.934705
H	1.699010	1.251146	5.045698
H	-0.045517	1.238217	4.740849
H	3.284480	-1.119625	2.132912
H	-4.986515	2.299324	-1.744446
H	-4.911037	3.100159	-0.176071
H	5.549652	-0.625373	1.988168
H	7.451993	0.559633	0.907979

H	4.698757	2.862605	-1.417937
H	2.794874	1.679314	-0.343474
H	-4.293626	-3.346796	1.743426
H	-5.503104	-2.975684	2.994266
H	-3.837446	-2.376638	3.171715
H	-6.787816	0.072074	-1.089806
H	-7.004225	-0.891655	0.398802
H	-7.904578	0.629519	0.180034
H	2.168822	-3.062725	-4.148958
H	2.899219	-1.756594	-3.181993
H	1.256553	-1.559990	-3.862312
H	3.049305	-4.094176	-0.925065
H	3.272632	-3.724626	0.808578
H	4.657079	-3.634002	-0.307253
H	-2.360849	-3.374462	-2.800857
H	-0.795585	-3.972410	-2.194110
H	-2.093650	-3.522396	-1.047982

B3LYP Energy = -1829.33468082 a.u.

(aR,1R,3S,3'S)-**21**, Conf E

C	-2.867028	0.563271	-1.260797
C	-4.207927	0.196566	-1.194040
C	-4.676974	-0.455795	-0.042824
C	-3.812532	-0.710637	1.018777
C	-2.467159	-0.321947	0.957670
C	-1.995527	0.310240	-0.197711
C	-1.556806	-0.605041	2.133854
C	-2.337521	-0.938143	3.402943
C	-1.465035	-1.507373	4.505425
O	-3.345610	-1.911806	3.099949
C	-0.162415	1.980288	0.108839
C	1.169178	2.404649	-0.013279
C	2.106042	1.546961	-0.599637
C	1.729410	0.257473	-1.007178
C	0.394380	-0.144381	-0.900916
C	-0.559692	0.715810	-0.328112
C	-0.017256	-1.490192	-1.455765
C	0.978883	-1.972426	-2.500314
C	0.710009	-3.384487	-2.985535
O	2.286983	-1.963186	-1.917918
C	2.792675	-0.659154	-1.610499
C	-4.360214	-1.384860	2.258772
C	3.993612	-0.903217	-0.712817
C	5.284297	-0.831857	-1.232340
C	6.395159	-1.117229	-0.443048
C	6.186022	-1.485581	0.873008
C	4.919714	-1.578008	1.424625
C	3.824996	-1.285652	0.618557
F	7.262985	-1.767043	1.655149
O	-5.125490	0.436401	-2.175914
C	-4.697221	1.105325	-3.359615
O	-6.007555	-0.785157	0.102790
C	-6.492840	-1.840143	-0.743388
O	1.543331	3.682936	0.332289
C	1.506419	4.000587	1.735983

O	3.386661	1.934942	-0.887339
C	4.208402	2.503416	0.143433
O	-1.089131	2.813851	0.697593
C	-1.553304	3.899724	-0.121851
H	-2.483761	1.059267	-2.141231
H	-0.893924	-1.446193	1.899630
H	-0.912660	0.256492	2.322700
H	-2.837032	-0.027489	3.765329
H	-1.002767	-2.441974	4.180044
H	-0.672566	-0.802986	4.765997
H	-2.056516	-1.707413	5.399948
H	-1.013559	-1.420354	-1.894635
H	-0.078394	-2.237922	-0.656902
H	0.965915	-1.282873	-3.357147
H	0.755567	-4.089286	-2.152768
H	1.449658	-3.681486	-3.730279
H	-0.281442	-3.447974	-3.438298
H	3.152496	-0.196145	-2.539229
H	-4.978971	-0.671287	2.822634
H	-5.002299	-2.221994	1.988437
H	5.430439	-0.542162	-2.266008
H	7.401085	-1.060085	-0.837693
H	4.799744	-1.874890	2.458320
H	2.827767	-1.357535	1.034336
H	-5.580564	1.188826	-3.987940
H	-3.929954	0.532306	-3.887322
H	-4.316483	2.105421	-3.136201
H	-6.441784	-1.556383	-1.794505
H	-5.921343	-2.758313	-0.579848
H	-7.529897	-2.004624	-0.457443
H	1.847635	5.030337	1.819835
H	2.181538	3.347056	2.294324
H	0.496109	3.910264	2.133054
H	3.987714	3.559740	0.283811
H	5.235247	2.380523	-0.195358
H	4.076210	1.965047	1.084329
H	-0.727863	4.547657	-0.420947
H	-2.064753	3.517135	-1.008059
H	-2.259440	4.459718	0.487824

B3LYP Energy = -1829.33373011 a.u.

(aR,1R,3S,3'S)-**21**, Conf F

C	2.849117	0.705851	1.197736
C	4.173923	0.282376	1.254611
C	4.640404	-0.620644	0.286795
C	3.774708	-1.112809	-0.687043
C	2.441516	-0.684358	-0.742729
C	1.981872	0.231804	0.209757
C	1.535830	-1.214235	-1.832806
C	2.322668	-1.861912	-2.969080
C	1.445743	-2.639754	-3.931588
O	3.283218	-2.773956	-2.420869
C	0.217396	1.841794	-0.525973
C	-1.098148	2.329490	-0.535913
C	-2.074633	1.669120	0.217024

C	-1.752971	0.500438	0.925458
C	-0.433593	0.039429	0.947131
C	0.560836	0.705408	0.207460
C	-0.084392	-1.150210	1.813882
C	-1.111980	-1.331172	2.921738
C	-0.905238	-2.593162	3.738286
O	-2.411440	-1.417729	2.325613
C	-2.862194	-0.212881	1.697117
C	4.306929	-2.107438	-1.697846
C	-4.045276	-0.631253	0.840583
C	-5.346949	-0.362263	1.257339
C	-6.444179	-0.795632	0.517554
C	-6.210230	-1.511836	-0.641509
C	-4.932707	-1.808269	-1.085027
C	-3.852027	-1.362962	-0.331891
F	-7.273328	-1.941178	-1.374057
O	5.073549	0.679637	2.201640
C	4.634505	1.571827	3.223057
O	5.930600	-1.104022	0.323957
C	6.963931	-0.162231	-0.004528
O	-1.415577	3.502396	-1.182171
C	-1.359431	3.472262	-2.620158
O	-3.343803	2.153521	0.378438
C	-4.120875	2.527915	-0.769022
O	1.181336	2.480053	-1.277712
C	1.676111	3.713023	-0.728996
H	2.470342	1.401208	1.933177
H	0.843154	-1.956094	-1.418458
H	0.923181	-0.403757	-2.233618
H	2.865207	-1.079303	-3.520270
H	0.937333	-3.453749	-3.410090
H	0.689554	-1.985321	-4.369706
H	2.043134	-3.065911	-4.738754
H	0.909144	-1.016629	2.244035
H	-0.046588	-2.068607	1.217367
H	-1.083307	-0.456116	3.587351
H	-0.969548	-3.476363	3.099323
H	-1.664583	-2.674814	4.517259
H	0.077565	-2.581595	4.213615
H	-3.230750	0.471016	2.473174
H	4.984008	-1.596254	-2.398649
H	4.886050	-2.882142	-1.197020
H	-5.511917	0.199501	2.168866
H	-7.458379	-0.588080	0.832578
H	-4.793922	-2.376791	-1.995305
H	-2.846640	-1.591620	-0.662526
H	4.303352	2.526046	2.804457
H	5.498507	1.738873	3.861518
H	3.826739	1.132539	3.814334
H	7.009751	0.643140	0.728943
H	7.897788	-0.720949	0.005711
H	6.801718	0.254801	-1.002497
H	-1.634071	4.471169	-2.952811
H	-2.075538	2.747586	-3.016295
H	-0.356818	3.227277	-2.968661
H	-3.974626	1.817155	-1.585116

H	-3.870332	3.533211	-1.102051
H	-5.159907	2.491256	-0.447338
H	2.176149	3.532206	0.225358
H	2.398011	4.097312	-1.446888
H	0.869172	4.434909	-0.594190

B3LYP Energy = -1829.33357990 a.u.

(aR,1R,3S,3'S)-**21**, Conf G

C	2.909448	1.036384	0.796969
C	4.241461	0.639383	0.868834
C	4.656034	-0.483214	0.135091
C	3.748952	-1.167515	-0.669726
C	2.413436	-0.751004	-0.760247
C	1.994418	0.350206	-0.006152
C	1.459549	-1.501706	-1.665493
C	2.194568	-2.391052	-2.665013
C	1.278559	-3.360768	-3.386866
O	3.186438	-3.161723	-1.973050
C	0.189177	1.818753	-0.921414
C	-1.130645	2.294169	-0.934189
C	-2.085675	1.683358	-0.113849
C	-1.722881	0.657668	0.768231
C	-0.385453	0.252176	0.837007
C	0.569205	0.809429	-0.030588
C	0.023752	-0.746526	1.896270
C	-0.965372	-0.732454	3.053536
C	-0.690543	-1.799360	4.096773
O	-2.276766	-0.977134	2.532746
C	-2.792364	0.044606	1.670965
C	4.240215	-2.350295	-1.477139
C	-3.940825	-0.614811	0.926696
C	-5.259127	-0.353183	1.292432
C	-6.321619	-0.997549	0.663859
C	-6.035494	-1.915668	-0.329322
C	-4.738939	-2.211313	-0.715092
C	-3.694021	-1.552969	-0.076824
F	-7.064131	-2.552181	-0.950742
O	5.200469	1.275201	1.604012
C	4.829728	2.432135	2.349005
O	5.974146	-0.886003	0.123672
C	6.475501	-1.441733	1.350153
O	-1.470955	3.301521	-1.808024
C	-1.861791	4.547478	-1.201602
O	-3.388358	2.127366	-0.101407
C	-4.146787	1.952066	-1.313998
O	1.122686	2.271314	-1.819700
C	1.526369	3.645125	-1.748023
H	2.566909	1.892239	1.361252
H	0.788800	-2.129389	-1.067183
H	0.826435	-0.795546	-2.207336
H	2.706206	-1.754714	-3.402021
H	0.803222	-4.038165	-2.673948
H	0.496408	-2.819026	-3.922421
H	1.840252	-3.956884	-4.107467
H	1.025684	-0.511335	2.258007

H	0.068299	-1.761368	1.485487
H	-0.948740	0.258412	3.530476
H	-0.735955	-2.793444	3.647254
H	-1.427451	-1.749409	4.899524
H	0.302030	-1.660422	4.529783
H	-3.209221	0.848792	2.291423
H	4.860985	-1.993261	-2.312040
H	4.866773	-2.998503	-0.865900
H	-5.465577	0.367925	2.074177
H	-7.348893	-0.797600	0.938866
H	-4.558477	-2.939616	-1.494807
H	-2.674311	-1.773942	-0.366140
H	4.457219	3.224117	1.693896
H	5.737836	2.770317	2.842064
H	4.074036	2.196437	3.103289
H	7.495436	-1.760089	1.143429
H	6.476439	-0.698553	2.147461
H	5.879320	-2.307608	1.652146
H	-2.752291	4.425713	-0.585125
H	-2.069864	5.230029	-2.022893
H	-1.047875	4.948064	-0.591819
H	-4.197185	0.894998	-1.579363
H	-3.713742	2.519656	-2.136984
H	-5.146989	2.318434	-1.094222
H	2.438339	3.720283	-2.337218
H	0.767200	4.304745	-2.166971
H	1.741599	3.933133	-0.715696

B3LYP Energy = -1829.33284002 a.u.

(aR,1R,3S,3'S)-**21**, Conf H

C	2.888944	1.157937	0.850896
C	4.238323	0.829463	0.930165
C	4.711226	-0.277591	0.207437
C	3.842148	-1.013920	-0.593002
C	2.486612	-0.667214	-0.689581
C	2.010978	0.418924	0.053712
C	1.577349	-1.477250	-1.589937
C	2.362200	-2.323561	-2.588965
C	1.502518	-3.341534	-3.314006
O	3.391498	-3.039404	-1.894423
C	0.158558	1.848848	-0.830233
C	-1.180301	2.270833	-0.837925
C	-2.096154	1.647319	0.015283
C	-1.719871	0.561332	0.810833
C	-0.375020	0.175351	0.845969
C	0.566877	0.814526	0.022663
C	0.056520	-0.887118	1.832606
C	-0.949257	-1.012443	2.968806
C	-0.658091	-2.168285	3.907508
O	-2.247102	-1.237951	2.405159
C	-2.776343	-0.129215	1.670252
C	4.398136	-2.173029	-1.393057
C	-3.948876	-0.691147	0.885708
C	-5.249570	-0.518887	1.353328
C	-6.335073	-1.078694	0.685161

C	-6.089092	-1.820745	-0.454903
C	-4.811105	-2.022801	-0.947273
C	-3.742514	-1.452343	-0.265122
F	-7.140812	-2.372603	-1.118570
O	5.161245	1.520959	1.660593
C	4.730710	2.673844	2.380743
O	6.048459	-0.612357	0.200450
C	6.576561	-1.127869	1.433214
O	-1.538953	3.357176	-1.601421
C	-2.503969	3.116161	-2.642818
O	-3.401206	2.089026	0.065788
C	-3.590934	3.345766	0.739744
O	1.127372	2.474788	-1.567740
C	0.930993	2.651469	-2.977672
H	2.503702	2.007256	1.396797
H	0.948609	-2.144864	-0.989739
H	0.897247	-0.814699	-2.130107
H	2.840842	-1.660116	-3.324655
H	1.059475	-4.041841	-2.602600
H	0.695645	-2.843383	-3.855433
H	2.099273	-3.908237	-4.030115
H	1.041367	-0.639756	2.232197
H	0.152032	-1.862457	1.342983
H	-0.968524	-0.072919	3.540204
H	-0.677032	-3.115016	3.363610
H	-1.401932	-2.212926	4.704189
H	0.327834	-2.049800	4.361258
H	-3.170197	0.604957	2.386587
H	5.005845	-1.787426	-2.224875
H	5.052774	-2.786797	-0.775728
H	-5.424249	0.064724	2.249388
H	-7.349164	-0.946062	1.038504
H	-4.662985	-2.613518	-1.841781
H	-2.736680	-1.601451	-0.637313
H	4.321143	3.431868	1.708183
H	5.619351	3.066365	2.868976
H	3.985121	2.415824	3.137750
H	7.612583	-1.392995	1.231294
H	6.536010	-0.377597	2.222761
H	6.026997	-2.021416	1.743005
H	-2.645518	4.070012	-3.146631
H	-3.450518	2.768391	-2.230986
H	-2.121354	2.381134	-3.355515
H	-3.076720	4.154067	0.218054
H	-3.230218	3.286642	1.769999
H	-4.663165	3.530079	0.740812
H	1.924925	2.782962	-3.401816
H	0.467359	1.766355	-3.420244
H	0.322010	3.529394	-3.186333

B3LYP Energy = -1829.33275266 a.u.

(aR,1R,3S,3'S)-**21**, Conf I

C	2.851901	0.958069	0.934070
C	4.170141	0.545663	1.107022
C	4.625113	-0.584641	0.410312

C	3.753552	-1.302568	-0.404998
C	2.426005	-0.886815	-0.576238
C	1.978950	0.252263	0.101691
C	1.514003	-1.670991	-1.495359
C	2.295254	-2.599521	-2.420579
C	1.413606	-3.589215	-3.157952
O	3.239743	-3.351220	-1.646809
C	0.243819	1.636145	-1.045310
C	-1.059088	2.140511	-1.164588
C	-2.061145	1.649007	-0.320973
C	-1.758815	0.722667	0.686115
C	-0.436320	0.296595	0.854784
C	0.565650	0.730347	-0.030750
C	-0.097419	-0.595381	2.027940
C	-1.125283	-0.432780	3.138705
C	-0.921881	-1.392237	4.296227
O	-2.424389	-0.694528	2.595662
C	-2.877147	0.242191	1.611910
C	4.272348	-2.534268	-1.118184
C	-4.023932	-0.458807	0.903951
C	-3.780508	-1.535985	0.050096
C	-4.827978	-2.226723	-0.548494
C	-6.123762	-1.822488	-0.274790
C	-6.406856	-0.764930	0.569342
C	-5.342165	-0.090213	1.161199
F	-7.154499	-2.490540	-0.858582
O	5.073857	1.162741	1.923513
C	4.645720	2.291438	2.681026
O	5.908287	-1.059073	0.578082
C	6.956528	-0.246674	0.026727
O	-1.326824	3.053818	-2.157378
C	-1.735848	4.361377	-1.716589
O	-3.351068	2.119922	-0.414622
C	-4.061734	1.816398	-1.630781
O	1.208399	1.972665	-1.965245
C	1.764703	3.290181	-1.877463
H	2.482579	1.828621	1.457584
H	0.813215	-2.273633	-0.905701
H	0.911305	-0.985149	-2.094475
H	2.852090	-1.992796	-3.149946
H	0.889699	-4.234288	-2.449212
H	0.670510	-3.062498	-3.760015
H	2.011211	-4.217670	-3.819874
H	0.898333	-0.354344	2.402081
H	-0.073017	-1.648411	1.726048
H	-1.094554	0.601753	3.510871
H	-0.982978	-2.426239	3.950514
H	-1.684868	-1.238070	5.060475
H	0.058732	-1.237051	4.750295
H	-3.285234	1.122376	2.126217
H	4.958297	-2.233524	-1.924260
H	4.839032	-3.159188	-0.429074
H	-2.761757	-1.842470	-0.151075
H	-4.650110	-3.062426	-1.212504
H	-7.433805	-0.482508	0.760393
H	-5.546491	0.740016	1.826388

H	4.329994	3.112452	2.031547
H	5.510535	2.603733	3.261258
H	3.829960	2.028602	3.359764
H	7.881494	-0.798334	0.183152
H	6.802064	-0.093727	-1.045113
H	7.013633	0.717489	0.532254
H	-2.697640	4.327310	-1.204983
H	-1.814839	4.969690	-2.615142
H	-0.985854	4.792984	-1.048617
H	-5.064770	2.214855	-1.496735
H	-4.116055	0.736700	-1.777818
H	-3.586772	2.282628	-2.493591
H	2.576303	3.324579	-2.601653
H	1.026269	4.052086	-2.128381
H	2.165471	3.475019	-0.877469

B3LYP Energy = -1829.33265097 a.u.

(*aR*,1*R*,3*S*,3'*S*)-**21**, Conf J

C	2.870904	1.132156	0.888310
C	4.207488	0.781734	1.048790
C	4.683795	-0.383319	0.426748
C	3.816687	-1.191574	-0.303644
C	2.468831	-0.837766	-0.461923
C	1.999969	0.334403	0.141847
C	1.564135	-1.727444	-1.288221
C	2.355448	-2.682208	-2.177414
C	1.493532	-3.753622	-2.817979
O	3.352483	-3.341942	-1.387046
C	0.221279	1.718517	-0.940382
C	-1.102114	2.177276	-1.034071
C	-2.064446	1.665116	-0.158178
C	-1.748431	0.649553	0.748753
C	-0.418387	0.230967	0.868217
C	0.569403	0.760431	0.021034
C	-0.054073	-0.741982	1.967215
C	-1.097517	-0.723324	3.076351
C	-0.871123	-1.786838	4.134195
O	-2.384182	-0.967044	2.494291
C	-2.854581	0.072215	1.629183
C	4.364316	-2.451562	-0.942198
C	-4.008043	-0.541087	0.854227
C	-5.322171	-0.293580	1.244233
C	-6.393371	-0.891264	0.585869
C	-6.120031	-1.746476	-0.465249
C	-4.828364	-2.025749	-0.877751
C	-3.774338	-1.416263	-0.206774
F	-7.157521	-2.335207	-1.119457
O	5.111658	1.493579	1.782971
C	4.668528	2.677840	2.441804
O	5.988562	-0.798005	0.588754
C	6.988268	0.002671	-0.060903
O	-1.400306	3.194933	-1.909703
C	-2.339271	2.882968	-2.956105
O	-3.355647	2.147259	-0.195660
C	-3.525722	3.467598	0.349796

O	1.231517	2.242767	-1.702616
C	1.088592	2.266609	-3.129807
H	2.486213	2.032189	1.346111
H	0.918605	-2.323016	-0.632778
H	0.900535	-1.118125	-1.906101
H	2.863847	-2.104108	-2.963697
H	1.019222	-4.369503	-2.050817
H	0.710288	-3.298606	-3.427617
H	2.095691	-4.401050	-3.456975
H	0.926569	-0.489258	2.373591
H	0.020859	-1.763261	1.578187
H	-1.103973	0.269019	3.550344
H	-0.899589	-2.782483	3.686702
H	-1.641480	-1.732045	4.904564
H	0.102579	-1.648953	4.608274
H	-3.258722	0.883908	2.249428
H	5.019589	-2.184172	-1.784751
H	4.970022	-3.005866	-0.226443
H	-5.518634	0.379880	2.070009
H	-7.417445	-0.701009	0.879026
H	-4.658660	-2.703586	-1.704034
H	-2.758258	-1.624063	-0.517848
H	4.307708	3.421270	1.726127
H	5.538949	3.069848	2.962212
H	3.881389	2.457478	3.167749
H	7.938044	-0.500185	0.110849
H	6.797148	0.059567	-1.136296
H	7.022639	1.007248	0.361042
H	-3.310385	2.608666	-2.546060
H	-1.960333	2.068557	-3.578810
H	-2.430330	3.786038	-3.555999
H	-3.215412	3.492270	1.397712
H	-4.588559	3.689641	0.280880
H	-2.956273	4.204613	-0.217982
H	0.632625	1.341376	-3.491125
H	0.496945	3.120521	-3.455424
H	2.098454	2.345719	-3.528707

B3LYP Energy = -1829.33257105 a.u.

(*aR*,1*R*,3*S*,3'*S*)-**21**, Conf K

C	2.884034	1.159287	0.718066
C	4.226083	0.805469	0.802618
C	4.654598	-0.383722	0.190729
C	3.748481	-1.179118	-0.504956
C	2.397542	-0.812699	-0.602700
C	1.967443	0.362187	0.025927
C	1.448143	-1.701878	-1.379125
C	2.187444	-2.653185	-2.316005
C	1.289550	-3.721292	-2.910651
O	3.226804	-3.316796	-1.585341
C	0.156448	1.823856	-0.889533
C	-1.161037	2.308118	-0.908249
C	-2.120068	1.706246	-0.086837
C	-1.766763	0.631356	0.743591
C	-0.433975	0.217951	0.817400

C	0.536959	0.801536	-0.017787
C	-0.040523	-0.798003	1.866511
C	-1.059634	-0.825168	2.997742
C	-0.801306	-1.920100	4.015822
O	-2.354128	-1.064967	2.434293
C	-2.853260	-0.012317	1.600286
C	4.260782	-2.425845	-1.196040
C	-3.988608	-0.637937	0.807697
C	-3.735460	-1.431910	-0.310822
C	-4.771913	-2.057990	-0.994117
C	-6.065405	-1.877771	-0.535639
C	-6.357671	-1.103586	0.571844
C	-5.304001	-0.487602	1.241122
F	-7.086215	-2.483693	-1.200720
O	5.183588	1.545230	1.434034
C	4.799672	2.776297	2.042388
O	5.983312	-0.749425	0.188173
C	6.527587	-1.155922	1.454261
O	-1.547156	3.294767	-1.784797
C	-0.966215	4.597046	-1.584391
O	-3.438607	2.075707	-0.091573
C	-3.778451	3.456824	0.095791
O	1.098978	2.407670	-1.708927
C	1.029460	2.029907	-3.093659
H	2.532756	2.071549	1.178243
H	0.844875	-2.302004	-0.689044
H	0.745240	-1.094491	-1.953495
H	2.651901	-2.072641	-3.127069
H	0.855607	-4.337086	-2.119841
H	0.475926	-3.263914	-3.477185
H	1.855380	-4.369013	-3.581748
H	0.948480	-0.554914	2.259186
H	0.028991	-1.804137	1.439504
H	-1.064988	0.151350	3.503636
H	-0.829153	-2.900809	3.536406
H	-1.556805	-1.898773	4.802387
H	0.180073	-1.787477	4.475493
H	-3.282230	0.768437	2.242734
H	4.855174	-2.137751	-2.075597
H	4.918940	-2.988659	-0.535400
H	-2.718367	-1.562177	-0.658665
H	-4.587193	-2.672759	-1.865282
H	-7.382749	-0.988407	0.898688
H	-5.515103	0.123319	2.110794
H	4.389657	3.472381	1.306113
H	5.710339	3.193402	2.465248
H	4.069454	2.616762	2.840515
H	7.552174	-1.465718	1.257932
H	6.522823	-0.331534	2.167190
H	5.964499	-2.000685	1.861238
H	0.115887	4.567531	-1.702715
H	-1.217587	4.979406	-0.591724
H	-1.406500	5.241018	-2.342805
H	-3.657619	4.023393	-0.825476
H	-3.170950	3.901413	0.888396
H	-4.824175	3.465500	0.397764

H	1.236369	0.963681	-3.211283
H	0.052190	2.266272	-3.518027
H	1.800672	2.603053	-3.604232

B3LYP Energy = -1829.33254835 a.u.

(*aR*,1*R*,3*S*,3'*S*)-**21**, Conf L

C	2.871873	1.029765	0.959953
C	4.207696	0.655138	1.005885
C	4.643763	-0.423653	0.230487
C	3.745759	-1.086778	-0.609125
C	2.404068	-0.690643	-0.670769
C	1.960706	0.368813	0.137978
C	1.462479	-1.423176	-1.603901
C	2.209352	-2.242108	-2.653703
C	1.307978	-3.190993	-3.420475
O	3.218848	-3.027714	-2.007406
C	0.160626	1.949468	-0.579922
C	-1.155886	2.427360	-0.532651
C	-2.125262	1.711600	0.172674
C	-1.777852	0.546493	0.871973
C	-0.441982	0.130408	0.897212
C	0.530979	0.811464	0.141600
C	-0.047627	-1.018767	1.799180
C	-1.070948	-1.209430	2.909805
C	-0.816222	-2.438324	3.762154
O	-2.363380	-1.364727	2.311674
C	-2.859689	-0.190849	1.659787
C	4.256767	-2.224064	-1.468014
C	-4.031013	-0.666679	0.819283
C	-5.338939	-0.420481	1.230476
C	-6.424714	-0.904074	0.505219
C	-6.172771	-1.647635	-0.632728
C	-4.888129	-1.922785	-1.069809
C	-3.819168	-1.426102	-0.332432
F	-7.224332	-2.126773	-1.350043
O	5.066693	1.328927	1.849287
C	5.994039	2.207865	1.190871
O	5.965196	-0.817693	0.217300
C	6.451117	-1.411275	1.434722
O	-1.495552	3.593491	-1.182112
C	-1.173457	4.791994	-0.454067
O	-3.405951	2.188939	0.300428
C	-4.185430	2.327400	-0.901886
O	1.122845	2.669377	-1.249572
C	1.019800	2.675972	-2.682767
H	2.551042	1.862113	1.573880
H	0.818900	-2.099570	-1.030549
H	0.797619	-0.713023	-2.100722
H	2.704049	-1.558059	-3.359253
H	0.851137	-3.914017	-2.741274
H	0.511542	-2.638608	-3.923006
H	1.877161	-3.737075	-4.173945
H	0.937332	-0.826440	2.228216
H	0.031983	-1.954609	1.235383
H	-1.080174	-0.315594	3.550141

H	-0.846665	-3.341459	3.149004
H	-1.571910	-2.526402	4.543944
H	0.165261	-2.374752	4.236028
H	-3.247991	0.496441	2.423136
H	4.876686	-1.820160	-2.282118
H	4.890149	-2.890484	-0.883950
H	-5.518115	0.162673	2.125660
H	-7.443818	-0.714166	0.815412
H	-4.735278	-2.512629	-1.964079
H	-2.808270	-1.635182	-0.659152
H	6.647470	1.655557	0.513134
H	6.587282	2.670631	1.977064
H	5.457674	2.982237	0.635941
H	6.406793	-0.703295	2.262568
H	5.870739	-2.304006	1.682632
H	7.484387	-1.692921	1.242590
H	-1.509232	5.623447	-1.070611
H	-0.096855	4.867243	-0.290492
H	-1.698378	4.811580	0.503848
H	-4.265128	1.366196	-1.413765
H	-3.750264	3.071256	-1.566823
H	-5.173928	2.646679	-0.579015
H	1.130390	1.663440	-3.079559
H	0.069397	3.100459	-3.007093
H	1.840934	3.293123	-3.041610

B3LYP Energy = -1829.33234045 a.u.

(aR,1R,3S,3'S)-**21**, Conf M

C	2.869047	1.094608	0.820014
C	4.196376	0.709305	0.973811
C	4.621750	-0.502582	0.406561
C	3.713909	-1.320742	-0.260250
C	2.373697	-0.933856	-0.408899
C	1.956041	0.286511	0.136313
C	1.425622	-1.843349	-1.162097
C	2.169054	-2.859700	-2.024160
C	1.262679	-3.935874	-2.590818
O	3.166775	-3.508639	-1.225792
C	0.216853	1.743310	-0.915301
C	-1.085257	2.260413	-1.002960
C	-2.088141	1.723137	-0.189113
C	-1.792079	0.684790	0.707202
C	-0.473557	0.244253	0.850207
C	0.540119	0.758219	0.020273
C	-0.143988	-0.723143	1.964768
C	-1.201919	-0.663269	3.058622
C	-1.005838	-1.702995	4.145778
O	-2.481122	-0.906006	2.461748
C	-2.924898	0.108309	1.552421
C	4.211417	-2.627256	-0.844011
C	-4.037422	-0.538573	0.744797
C	-5.368302	-0.324237	1.095954
C	-6.403977	-0.954206	0.411576
C	-6.078159	-1.806896	-0.626674
C	-4.768559	-2.052156	-1.001883

C	-3.750633	-1.410964	-0.305007
F	-7.080850	-2.426875	-1.306177
O	5.138423	1.428058	1.651081
C	4.748001	2.657742	2.257855
O	5.915934	-0.949674	0.562919
C	6.925812	-0.217135	-0.148781
O	-1.414317	3.216144	-1.935568
C	-0.801225	4.508843	-1.772838
O	-3.396173	2.123312	-0.265113
C	-3.705421	3.517543	-0.127443
O	1.203049	2.256639	-1.730756
C	1.150898	1.830665	-3.102325
H	2.522576	2.029436	1.236456
H	0.790340	-2.393217	-0.458926
H	0.753203	-1.252915	-1.788402
H	2.673244	-2.334281	-2.849175
H	0.789454	-4.498244	-1.782978
H	0.478628	-3.489274	-3.205560
H	1.831652	-4.631685	-3.208985
H	0.837498	-0.485454	2.378945
H	-0.088894	-1.752435	1.594977
H	-1.201471	0.340539	3.507848
H	-1.039292	-2.709251	3.723084
H	-1.788144	-1.619842	4.901499
H	-0.038583	-1.564632	4.632770
H	-3.364678	0.930418	2.132745
H	4.857713	-2.421060	-1.710358
H	4.815105	-3.162945	-0.112560
H	-5.605497	0.348490	1.911617
H	-7.440737	-0.790009	0.674388
H	-4.557435	-2.727331	-1.820737
H	-2.721175	-1.591083	-0.588156
H	4.396342	3.376473	1.512911
H	5.641627	3.045895	2.740445
H	3.969923	2.500565	3.009584
H	6.709719	-0.206071	-1.220862
H	7.005134	0.804935	0.222035
H	7.861714	-0.744491	0.025373
H	-1.201449	5.132454	-2.569494
H	0.282462	4.444007	-1.858909
H	-1.068102	4.939459	-0.804274
H	-3.510057	4.060369	-1.050255
H	-3.135718	3.961306	0.693247
H	-4.767331	3.563660	0.106934
H	0.200292	2.102717	-3.563960
H	1.966319	2.341498	-3.610450
H	1.301319	0.750908	-3.174957

B3LYP Energy = -1829.33231506 a.u.

(aR,1R,3S,3'S)-**21**, Conf N

C	2.816990	0.917148	1.077046
C	4.154170	0.544810	1.141269
C	4.633336	-0.439255	0.271540
C	3.780755	-1.002765	-0.681543
C	2.441913	-0.604560	-0.761134



C	1.951796	0.351365	0.142757
C	1.546062	-1.220688	-1.813943
C	2.340834	-1.930015	-2.907450
C	1.475303	-2.793541	-3.804881
O	3.326390	-2.779106	-2.304167
C	0.134931	1.871694	-0.652802
C	-1.193225	2.313553	-0.657395
C	-2.140470	1.655512	0.129492
C	-1.791618	0.513578	0.860643
C	-0.455134	0.096121	0.884219
C	0.515942	0.775881	0.126203
C	-0.062969	-1.051183	1.788863
C	-1.081131	-1.231333	2.906249
C	-0.827122	-2.457185	3.763299
O	-2.378261	-1.384477	2.318082
C	-2.874523	-0.219008	1.650640
C	4.335773	-2.035685	-1.638923
C	-4.040531	-0.709477	0.810216
C	-5.346634	-0.548435	1.266457
C	-6.427573	-1.049927	0.546568
C	-6.171539	-1.722754	-0.633544
C	-4.887977	-1.911914	-1.116341
C	-3.823996	-1.400665	-0.382077
F	-7.218780	-2.217110	-1.347861
O	4.964691	1.121994	2.096851
C	5.944381	2.042136	1.587427
O	5.955272	-0.832533	0.281475
C	6.378643	-1.562158	1.447172
O	-1.549923	3.411251	-1.407500
C	-2.103598	3.094256	-2.696655
O	-3.448988	2.078735	0.134873
C	-3.691426	3.342341	0.777522
O	1.059168	2.467494	-1.478487
C	1.485750	3.785697	-1.097647
H	2.459968	1.666544	1.772839
H	0.865869	-1.942561	-1.347732
H	0.919576	-0.448345	-2.265503
H	2.861833	-1.176830	-3.516767
H	0.989691	-3.579756	-3.222659
H	0.701127	-2.189255	-4.281686
H	2.076981	-3.261943	-4.584911
H	0.925928	-0.868365	2.211799
H	0.004541	-1.987457	1.223481
H	-1.081638	-0.334111	3.542171
H	-0.864192	-3.362884	3.154387
H	-1.579409	-2.538775	4.549067
H	0.156886	-2.395289	4.232115
H	-3.270251	0.473355	2.406473
H	4.983464	-1.541352	-2.378039
H	4.951620	-2.759336	-1.106562
H	-5.529142	-0.019766	2.194487
H	-7.445822	-0.925372	0.890798
H	-4.731995	-2.447836	-2.043431
H	-2.814018	-1.542016	-0.746052
H	6.630518	1.546927	0.898411
H	6.493545	2.412139	2.450929

H	5.455108	2.878959	1.081606
H	5.785139	-2.472691	1.564533
H	7.419844	-1.827747	1.276337
H	6.293899	-0.951110	2.346191
H	-2.339548	4.045018	-3.170533
H	-3.013984	2.500859	-2.591171
H	-1.374128	2.554318	-3.304651
H	-3.175392	4.151295	0.260492
H	-3.372444	3.307315	1.822808
H	-4.766815	3.501315	0.732690
H	2.198110	4.103922	-1.856191
H	0.643137	4.476923	-1.069735
H	1.981556	3.759780	-0.123745

B3LYP Energy = -1829.33230346 a.u.

(*aR*,1*R*,3*S*,3'*S*)-**21**, Conf O

C	2.804926	0.914825	1.100024
C	4.143064	0.548848	1.179284
C	4.647243	-0.398837	0.284371
C	3.795450	-1.008790	-0.640161
C	2.448157	-0.639272	-0.715447
C	1.950650	0.336541	0.163272
C	1.558384	-1.291496	-1.751581
C	2.361460	-2.000104	-2.839441
C	1.509167	-2.892132	-3.721531
O	3.364519	-2.822429	-2.228298
C	0.150299	1.848698	-0.676127
C	-1.174946	2.297941	-0.703575
C	-2.135034	1.658046	0.082810
C	-1.801402	0.525984	0.835947
C	-0.467846	0.100520	0.881291
C	0.515822	0.763111	0.124526
C	-0.093780	-1.035023	1.808275
C	-1.124871	-1.189700	2.917543
C	-0.888705	-2.403590	3.796548
O	-2.416888	-1.343216	2.318628
C	-2.897664	-0.185567	1.626995
C	4.363644	-2.054340	-1.576680
C	-4.058949	-0.680332	0.782781
C	-5.369366	-0.482428	1.211137
C	-6.447061	-0.984605	0.486910
C	-6.183589	-1.695486	-0.668984
C	-4.895696	-1.921911	-1.123488
C	-3.835019	-1.409364	-0.385416
F	-7.227499	-2.191013	-1.387320
O	4.954959	1.169192	2.105946
C	5.365241	0.340258	3.206171
O	5.965327	-0.802744	0.330138
C	6.928579	0.176638	-0.096125
O	-1.516099	3.385496	-1.475183
C	-2.062446	3.050972	-2.763020
O	-3.440868	2.089099	0.066685
C	-3.682568	3.365096	0.684751
O	1.087462	2.426116	-1.500105
C	1.522763	3.744972	-1.130382

H	2.435473	1.660559	1.793226
H	0.898806	-2.021935	-1.269308
H	0.911065	-0.541007	-2.210352
H	2.865694	-1.245437	-3.460928
H	1.039534	-3.678288	-3.126334
H	0.722961	-2.309344	-4.205410
H	2.117350	-3.361233	-4.496103
H	0.892146	-0.852804	2.238289
H	-0.027336	-1.980937	1.259116
H	-1.125569	-0.282418	3.539114
H	-0.925492	-3.318413	3.201444
H	-1.649963	-2.467653	4.575233
H	0.090625	-2.341342	4.275062
H	-3.295420	0.522197	2.367360
H	5.008079	-1.570198	-2.325715
H	4.984602	-2.758529	-1.024323
H	-5.557789	0.075862	2.120424
H	-7.468495	-0.831911	0.809713
H	-4.733997	-2.487056	-2.032059
H	-2.821748	-1.579546	-0.727263
H	4.494561	0.003491	3.775628
H	5.993059	0.963031	3.840313
H	5.933876	-0.523750	2.858587
H	6.734486	0.481078	-1.127929
H	6.912907	1.052013	0.554068
H	7.900536	-0.309095	-0.038915
H	-2.287253	3.995353	-3.254725
H	-2.978206	2.466444	-2.654603
H	-1.332557	2.495179	-3.356041
H	-3.151534	4.161147	0.162939
H	-3.380550	3.344505	1.735464
H	-4.755685	3.532388	0.620140
H	2.242189	4.049340	-1.887917
H	0.685507	4.443136	-1.115294
H	2.012887	3.725343	-0.153577

B3LYP Energy = -1829.33217882 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf A

C	-0.493914	1.895754	-0.684918
C	-1.774998	2.457299	-0.761444
C	-2.878422	1.623850	-0.952479
C	-2.714750	0.235462	-1.013566
C	-1.434328	-0.320327	-0.929838
C	-0.310375	0.513776	-0.778098
O	-3.589840	-1.944133	-1.675384
C	-2.573024	-2.582427	-0.888354
C	-1.262091	-1.820690	-1.047342
C	-3.941934	-0.641325	-1.190034
C	-2.480240	-4.024860	-1.349421
C	-4.834232	-0.756543	0.045665
C	1.075227	-0.052526	-0.738068
C	1.771117	-0.211941	0.466276
C	3.056565	-0.768485	0.436936
C	3.626006	-1.182959	-0.764100

C	2.941711	-0.995257	-1.973987
C	1.667246	-0.438181	-1.943761
C	-6.131958	-1.248754	-0.123213
C	-6.985886	-1.419540	0.958918
C	-6.519954	-1.089165	2.220610
C	-5.246025	-0.598632	2.432721
C	-4.407105	-0.433939	1.332408
C	1.163191	0.184906	1.791005
C	1.846135	-0.519465	2.955973
O	3.266291	-0.328459	2.846535
C	3.841051	-0.982980	1.722161
C	1.426535	0.011881	4.312756
F	-7.348832	-1.248799	3.286486
O	4.905757	-1.688314	-0.734466
C	5.050506	-3.077847	-1.074517
O	3.596509	-1.374553	-3.108958
C	2.954142	-1.167192	-4.365189
C	5.289484	-0.472617	1.691693
O	6.214068	-1.084217	2.173775
O	5.386045	0.742685	1.150262
C	6.570453	2.718041	0.497204
C	6.705642	1.350478	1.126743
O	0.585572	2.712098	-0.440368
C	1.047968	3.480585	-1.562880
O	-1.941540	3.821245	-0.686190
C	-2.018456	4.339082	0.653570
C	-4.457955	2.963264	-2.142433
O	-4.153368	2.134777	-1.005787
H	-2.879825	-2.562119	0.164801
H	-0.540898	-2.174285	-0.306566
H	-0.834657	-2.058769	-2.027210
H	-4.551125	-0.217905	-1.989484
H	-1.701406	-4.551603	-0.794233
H	-3.427469	-4.541174	-1.188321
H	-2.237066	-4.071283	-2.413235
H	1.118021	-0.291550	-2.862896
H	-6.480579	-1.505382	-1.116582
H	-7.993053	-1.795083	0.834040
H	-4.921263	-0.347991	3.434054
H	-3.411416	-0.039355	1.487334
H	1.251490	1.267547	1.930231
H	0.095993	-0.048396	1.797539
H	1.637952	-1.597829	2.903598
H	3.915990	-2.058514	1.926312
H	1.941310	-0.523613	5.111405
H	0.350685	-0.112684	4.450612
H	1.664896	1.074119	4.396740
H	4.792697	-3.251419	-2.119066
H	6.097052	-3.321684	-0.905844
H	4.423750	-3.698336	-0.428459
H	3.653391	-1.524477	-5.117032
H	2.023294	-1.736068	-4.436437
H	2.749118	-0.107071	-4.535491
H	7.549264	3.200694	0.465748
H	6.191904	2.644040	-0.523161
H	5.895319	3.350518	1.075381

H	7.078430	1.407022	2.150255
H	7.371495	0.702130	0.555750
H	1.408198	2.819221	-2.354964
H	0.257183	4.127477	-1.945452
H	1.873809	4.086865	-1.196551
H	-2.867551	3.903966	1.185801
H	-1.093561	4.138880	1.197792
H	-2.160797	5.413664	0.558158
H	-5.510465	3.222694	-2.049922
H	-3.850102	3.867191	-2.143028
H	-4.300464	2.408375	-3.071341

B3LYP Energy = -2096.62250751 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf B

C	0.782920	-1.503033	1.512144
C	2.105078	-1.670669	1.943037
C	3.152262	-1.405251	1.059193
C	2.888647	-0.931754	-0.230652
C	1.566862	-0.765011	-0.655676
C	0.502331	-1.062298	0.215953
O	3.646992	-0.588908	-2.524265
C	2.522892	0.272708	-2.759474
C	1.290799	-0.305750	-2.072430
C	4.055606	-0.619031	-1.150096
C	2.356357	0.401354	-4.261973
C	4.829897	0.650765	-0.795521
C	-0.923307	-0.926227	-0.221127
C	-1.687664	0.197541	0.112855
C	-3.019523	0.263312	-0.314418
C	-3.572646	-0.749528	-1.097804
C	-2.792728	-1.858501	-1.462577
C	-1.483436	-1.941511	-0.998624
C	6.095015	0.829782	-1.363135
C	6.840055	1.976654	-1.119961
C	6.297840	2.948435	-0.295562
C	5.052840	2.811953	0.287392
C	4.323707	1.652709	0.030517
C	-1.104154	1.341159	0.909006
C	-1.893203	2.626595	0.700779
O	-3.284178	2.361951	0.945104
C	-3.871987	1.481763	-0.007221
C	-1.480520	3.747650	1.634676
F	7.019927	4.073532	-0.047519
O	-4.853746	-0.559072	-1.559846
C	-5.832745	-1.577565	-1.275214
O	-3.377839	-2.781912	-2.280781
C	-2.616537	-3.919594	-2.679943
C	-5.226636	1.131928	0.623734
O	-5.401201	0.271944	1.453089
O	-6.179029	1.965413	0.188543
C	-8.397164	2.866685	0.149885
C	-7.499562	1.827233	0.781400
O	-0.246930	-1.700153	2.401626
C	-0.566488	-3.071300	2.688582
O	2.371952	-2.125183	3.214294

C	2.378931	-1.101250	4.224554
C	4.918180	-2.864956	1.727073
O	4.462434	-1.526819	1.458548
H	2.744087	1.260775	-2.336939
H	0.487442	0.434624	-2.078309
H	0.926233	-1.154745	-2.660548
H	4.760668	-1.449836	-1.102809
H	1.499198	1.035991	-4.495999
H	3.246357	0.844387	-4.710708
H	2.192151	-0.579819	-4.712945
H	-0.871691	-2.793442	-1.259255
H	6.504088	0.061384	-2.008408
H	7.821785	2.118624	-1.552426
H	4.666526	3.592403	0.929751
H	3.352444	1.532587	0.492318
H	-1.103568	1.093529	1.975791
H	-0.062592	1.502533	0.621780
H	-1.782385	2.957159	-0.341963
H	-4.066384	2.028853	-0.937989
H	-2.069010	4.645457	1.441762
H	-0.425495	3.988950	1.491318
H	-1.629325	3.451620	2.675053
H	-6.790653	-1.151568	-1.566858
H	-5.635758	-2.480482	-1.848655
H	-5.843338	-1.803365	-0.207383
H	-3.273558	-4.504649	-3.318713
H	-1.728878	-3.625655	-3.246184
H	-2.317819	-4.522261	-1.818174
H	-9.398191	2.790164	0.578765
H	-8.021635	3.873848	0.335943
H	-8.474426	2.716476	-0.927935
H	-7.856962	0.813354	0.597624
H	-7.409115	1.966019	1.859474
H	0.291950	-3.590451	3.117205
H	-1.381077	-3.048566	3.409429
H	-0.899568	-3.583228	1.782144
H	3.142269	-0.350982	4.005471
H	1.398632	-0.626914	4.299639
H	2.616792	-1.599048	5.162484
H	4.368470	-3.306880	2.557397
H	4.812074	-3.489515	0.835767
H	5.971738	-2.777179	1.984048

B3LYP Energy = -2096.62241488 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf C

C	0.785254	-1.514567	1.503020
C	2.110413	-1.694617	1.919478
C	3.151074	-1.418263	1.031330
C	2.878050	-0.920918	-0.247598
C	1.553496	-0.740051	-0.657804
C	0.495108	-1.048776	0.217489
O	3.617824	-0.543220	-2.541719
C	2.497914	0.330032	-2.751067
C	1.267960	-0.252431	-2.063370
C	4.038803	-0.600018	-1.171939

C	2.318621	0.486756	-4.249497
C	4.825261	0.658022	-0.803089
C	-0.933422	-0.903950	-0.207218
C	-1.709313	0.191722	0.189581
C	-3.036229	0.275166	-0.249375
C	-3.572082	-0.693777	-1.093636
C	-2.805138	-1.807564	-1.465907
C	-1.488772	-1.893068	-1.023030
C	6.087400	0.836723	-1.377352
C	6.842502	1.974412	-1.122329
C	6.313384	2.937253	-0.279165
C	5.071877	2.800535	0.311199
C	4.332505	1.650560	0.042236
C	-1.146307	1.295310	1.052805
C	-1.953664	2.579059	0.911570
O	-3.341482	2.284016	1.140464
C	-3.921367	1.442691	0.150452
C	-1.557803	3.653894	1.905254
F	7.045225	4.053372	-0.019566
O	-4.891292	-0.566291	-1.465794
C	-5.142479	-0.357390	-2.865991
O	-3.424843	-2.743379	-2.241278
C	-2.703050	-3.922180	-2.592249
C	-5.242142	0.985153	0.789364
O	-5.337943	0.105937	1.609526
O	-6.261853	1.744738	0.369432
C	-8.549773	2.452595	0.355043
C	-7.567241	1.467488	0.946198
O	-0.236793	-1.725964	2.397694
C	-0.564676	-3.101331	2.654072
O	2.386181	-2.173154	3.179806
C	2.399587	-1.168848	4.209540
C	4.915631	-2.896618	1.662520
O	4.464274	-1.552678	1.415759
H	2.729706	1.308792	-2.312886
H	0.470264	0.494049	-2.047735
H	0.891735	-1.087216	-2.664258
H	4.738257	-1.436464	-1.145539
H	1.463961	1.131559	-4.464267
H	3.207568	0.931563	-4.698523
H	2.143482	-0.485069	-4.716318
H	-0.877517	-2.739295	-1.302888
H	6.486176	0.075313	-2.037209
H	7.822011	2.115955	-1.559933
H	4.696179	3.573667	0.968539
H	3.364028	1.530106	0.509806
H	-1.149984	0.986992	2.103445
H	-0.105371	1.487389	0.782651
H	-1.845799	2.966389	-0.111801
H	-4.164143	2.038197	-0.738084
H	-2.158457	4.552664	1.759914
H	-0.505973	3.916983	1.777664
H	-1.704381	3.299630	2.927584
H	-4.857581	-1.232896	-3.448628
H	-6.212826	-0.185698	-2.957618
H	-4.600641	0.521262	-3.226329

H	-3.391095	-4.525991	-3.178679
H	-1.822382	-3.687378	-3.196056
H	-2.398753	-4.479939	-1.702855
H	-9.542264	2.268844	0.770998
H	-8.265469	3.479314	0.590215
H	-8.609026	2.346240	-0.729180
H	-7.833135	0.435364	0.713972
H	-7.493720	1.564632	2.030006
H	-0.909337	-3.588478	1.738480
H	0.293479	-3.636832	3.062838
H	-1.373173	-3.089793	3.381892
H	3.160844	-0.413857	3.999454
H	1.419528	-0.696972	4.300759
H	2.644549	-1.684433	5.135947
H	5.973456	-2.817931	1.904421
H	4.375739	-3.344665	2.495936
H	4.792178	-3.510414	0.766029

B3LYP Energy = -2096.62235658 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf D

C	-0.817273	-1.928199	-1.140982
C	-2.157899	-2.196368	-1.455140
C	-3.171688	-1.631514	-0.679420
C	-2.856037	-0.863489	0.448413
C	-1.518840	-0.647105	0.790377
C	-0.488659	-1.165178	-0.016587
O	-3.529891	0.004234	2.630862
C	-2.379207	0.860920	2.635418
C	-1.184769	0.108940	2.058833
C	-3.987237	-0.337372	1.314421
C	-2.158667	1.313777	4.066741
C	-4.778857	0.818551	0.706676
C	0.951906	-0.960223	0.338595
C	1.669911	0.159990	-0.095997
C	3.017912	0.283560	0.266593
C	3.632528	-0.668665	1.078691
C	2.899115	-1.772176	1.543525
C	1.573284	-1.912524	1.147901
C	-6.086083	1.033687	1.152942
C	-6.843639	2.099998	0.684896
C	-6.270097	2.955446	-0.240837
C	-4.982909	2.779549	-0.711643
C	-4.242977	1.700938	-0.231390
C	1.026278	1.246169	-0.927975
C	1.780458	2.563089	-0.801145
O	3.166192	2.329230	-1.097883
C	3.823652	1.504470	-0.140999
C	1.293549	3.635292	-1.756496
F	-7.002881	4.000857	-0.707526
O	4.928311	-0.422219	1.467987
C	5.918251	-1.433058	1.193047
O	3.544507	-2.630735	2.385610
C	2.834251	-3.765075	2.879309
C	5.151017	1.153176	-0.826984
O	5.301347	0.256845	-1.622018

O	6.105638	2.025974	-0.483928
C	8.297242	2.981063	-0.617443
C	7.397418	1.882768	-1.136072
O	0.192972	-2.509608	-1.868095
C	0.329659	-2.087326	-3.235750
O	-2.478091	-3.008573	-2.520672
C	-2.415161	-4.416324	-2.229246
C	-5.038837	-1.486065	-2.182925
O	-4.495464	-1.909641	-0.919423
H	-2.590514	1.738714	2.011913
H	-0.366471	0.809695	1.879786
H	-0.817627	-0.601779	2.807724
H	-4.689440	-1.153801	1.484637
H	-1.276898	1.954557	4.130992
H	-3.020678	1.875573	4.428882
H	-2.007173	0.451804	4.720086
H	0.995961	-2.761309	1.485141
H	-6.519810	0.356668	1.879396
H	-7.857903	2.267688	1.022668
H	-4.573362	3.467686	-1.439491
H	-3.238803	1.547242	-0.604829
H	1.008920	0.959995	-1.985340
H	-0.013411	1.385891	-0.625229
H	1.703638	2.928823	0.232702
H	4.054292	2.097158	0.752711
H	1.862859	4.555949	-1.623029
H	0.239108	3.852306	-1.575226
H	1.406278	3.304496	-2.790963
H	5.884571	-1.718372	0.140010
H	6.877899	-0.970599	1.415176
H	5.770512	-2.306743	1.823731
H	3.536648	-4.298407	3.515056
H	1.966506	-3.463596	3.471795
H	2.512329	-4.419060	2.064893
H	9.277997	2.899980	-1.090046
H	7.887026	3.965276	-0.847863
H	8.430437	2.902461	0.462509
H	7.790837	0.891249	-0.908831
H	7.248523	1.950929	-2.214389
H	0.503144	-1.009944	-3.287648
H	1.201875	-2.608820	-3.623764
H	-0.552153	-2.348782	-3.820354
H	-2.705602	-4.931105	-3.142924
H	-1.401129	-4.708391	-1.949540
H	-3.111359	-4.672831	-1.427412
H	-4.912469	-0.408422	-2.308336
H	-4.568207	-2.016402	-3.009181
H	-6.100167	-1.721867	-2.143274

B3LYP Energy = -2096.62168880 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf E

C	0.521554	2.069497	-0.602576
C	1.824350	2.532567	-0.839657
C	2.902721	1.895939	-0.223608
C	2.682833	0.848349	0.679919

C	1.379627	0.429225	0.957302
C	0.288125	1.028266	0.300352
O	3.489697	-0.476617	2.568670
C	2.416359	-1.405502	2.362098
C	1.146973	-0.640774	2.002921
C	3.878261	0.229317	1.381696
C	2.276763	-2.223131	3.632560
C	4.750208	-0.654144	0.492472
C	-1.118977	0.606870	0.593530
C	-1.722209	-0.467364	-0.071994
C	-3.037971	-0.817667	0.262214
C	-3.727982	-0.128096	1.255240
C	-3.132381	0.964529	1.902884
C	-1.828046	1.312486	1.568326
C	4.263144	-1.319083	-0.633079
C	5.081009	-2.162167	-1.382497
C	6.395595	-2.323700	-0.988353
C	6.921606	-1.679410	0.118793
C	6.087033	-0.846178	0.853303
C	-0.985748	-1.272001	-1.119467
C	-1.611061	-2.648034	-1.310311
O	-3.019646	-2.487428	-1.541511
C	-3.724976	-1.997414	-0.407302
C	-1.046180	-3.410287	-2.493068
F	7.203719	-3.138585	-1.716594
O	-5.031351	-0.489756	1.509610
C	-5.294041	-1.070835	2.798236
O	-3.897774	1.617410	2.823131
C	-3.348977	2.763494	3.471648
C	-5.138238	-1.713646	-0.937354
O	-6.053414	-2.495503	-0.826114
O	-5.208010	-0.554275	-1.592989
C	-6.333270	1.136200	-2.860831
C	-6.489173	-0.206517	-2.184300
O	-0.548829	2.715785	-1.173430
C	-0.689149	2.584338	-2.597995
O	2.041453	3.603161	-1.678373
C	1.858158	4.888113	-1.057110
C	4.745201	2.312035	-1.710421
O	4.190155	2.347435	-0.382880
H	2.683179	-2.074770	1.534469
H	0.382740	-1.344077	1.665519
H	0.748404	-0.169964	2.908757
H	4.509175	1.037337	1.752394
H	1.458649	-2.939875	3.535984
H	3.195727	-2.774231	3.836215
H	2.067082	-1.572321	4.484158
H	-1.346490	2.147308	2.057023
H	3.236162	-1.174740	-0.943052
H	4.710086	-2.680034	-2.257275
H	7.958718	-1.826867	0.390077
H	6.483319	-0.335198	1.722855
H	-1.000375	-0.749170	-2.081924
H	0.064559	-1.381972	-0.841553
H	-1.476134	-3.239540	-0.393479
H	-3.845530	-2.807541	0.322923

H	-1.523893	-4.386385	-2.584809
H	0.027574	-3.561722	-2.366860
H	-1.210766	-2.855032	-3.418764
H	-6.339965	-1.369373	2.786150
H	-4.666419	-1.951713	2.957339
H	-5.124595	-0.345699	3.593945
H	-4.129042	3.129088	4.134741
H	-2.465003	2.503736	4.060181
H	-3.091894	3.541941	2.748875
H	-7.283061	1.425579	-3.314888
H	-6.048268	1.905866	-2.142333
H	-5.577412	1.094001	-3.646366
H	-6.767649	-0.990008	-2.890327
H	-7.237052	-0.179510	-1.390897
H	-0.837176	1.537075	-2.871929
H	-1.577064	3.153003	-2.865755
H	0.180051	2.986149	-3.118814
H	2.554559	5.014349	-0.224893
H	2.068374	5.631042	-1.823896
H	0.831410	5.003951	-0.704999
H	5.774478	2.649753	-1.609954
H	4.736206	1.291017	-2.098288
H	4.198758	2.972466	-2.381520

B3LYP Energy = -2096.62167486 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf F

C	-0.525739	-1.249901	1.608908
C	-1.810974	-1.707675	1.926103
C	-2.916437	-0.909592	1.626656
C	-2.750058	0.312649	0.965939
C	-1.465359	0.760963	0.643432
C	-0.340848	-0.016543	0.978160
O	-3.637027	2.509381	0.380612
C	-2.592907	2.662433	-0.592424
C	-1.290719	2.109253	-0.024656
C	-3.978883	1.139135	0.631186
C	-2.508963	4.137058	-0.939348
C	-4.835651	0.585951	-0.507256
C	1.048418	0.462055	0.689611
C	1.773496	-0.007567	-0.411717
C	3.065454	0.487514	-0.633138
C	3.612275	1.452830	0.208291
C	2.896183	1.904439	1.326609
C	1.615958	1.406828	1.548744
C	-4.362168	-0.326685	-1.448384
C	-5.168743	-0.764253	-2.496916
C	-6.457393	-0.274021	-2.584325
C	-6.969517	0.630122	-1.668861
C	-6.146993	1.053953	-0.632727
C	1.190419	-1.016785	-1.372935
C	1.907098	-0.989486	-2.716523
O	3.321448	-1.103379	-2.490162
C	3.883569	0.022366	-1.827889
C	1.508315	-2.126500	-3.636961
F	-7.254118	-0.697911	-3.601262

O	4.900114	1.872130	-0.036639
C	5.057043	3.239330	-0.452864
O	3.527552	2.809140	2.128731
C	2.849294	3.275263	3.293555
C	5.318619	-0.417764	-1.500384
O	6.266266	-0.137988	-2.196419
O	5.369004	-1.192395	-0.414244
C	6.934258	-3.057820	-0.716022
C	6.661561	-1.735453	-0.026321
O	0.560337	-2.057025	1.851688
C	0.962107	-2.162394	3.227273
O	-1.979844	-2.919555	2.556315
C	-2.062212	-4.045109	1.664433
C	-4.536712	-1.466914	3.290867
O	-4.194307	-1.337351	1.899007
H	-2.865938	2.098153	-1.492792
H	-0.544503	2.040362	-0.819881
H	-0.893923	2.823359	0.704832
H	-4.611893	1.183843	1.518218
H	-1.712499	4.311757	-1.665595
H	-3.449533	4.484240	-1.368914
H	-2.296955	4.728319	-0.045759
H	1.044249	1.745374	2.400995
H	-3.355208	-0.714450	-1.365771
H	-4.808008	-1.473806	-3.229985
H	-7.986909	0.985117	-1.767957
H	-6.532071	1.763388	0.090231
H	1.270021	-2.024031	-0.950229
H	0.126235	-0.820334	-1.522339
H	1.713682	-0.028605	-3.214679
H	3.987630	0.850518	-2.540081
H	2.042763	-2.059587	-4.585350
H	0.436451	-2.088618	-3.840787
H	1.738771	-3.088840	-3.175559
H	6.112484	3.364229	-0.684624
H	4.462150	3.438942	-1.348153
H	4.768900	3.924497	0.344255
H	3.535492	3.965220	3.778266
H	1.927407	3.802946	3.034747
H	2.620428	2.452444	3.975778
H	7.874911	-3.471483	-0.345472
H	6.139580	-3.775795	-0.508068
H	7.019721	-2.930105	-1.795322
H	7.430951	-0.998473	-0.251236
H	6.583883	-1.856980	1.052445
H	1.259525	-1.184006	3.613217
H	0.159513	-2.577640	3.838091
H	1.820141	-2.831222	3.241963
H	-2.910640	-3.936048	0.984939
H	-1.137704	-4.152611	1.093575
H	-2.208160	-4.922402	2.291453
H	-5.584233	-1.759686	3.315278
H	-3.926036	-2.227451	3.775894
H	-4.414724	-0.509082	3.803927

B3LYP Energy = -2096.62161168 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf G

C	0.837373	2.001297	-1.071170
C	2.184866	2.275883	-1.348601
C	3.181887	1.665849	-0.585163
C	2.842650	0.844605	0.497381
C	1.498533	0.621434	0.806021
C	0.485633	1.185342	0.008164
O	3.473883	-0.128247	2.647537
C	2.316984	-0.974648	2.596593
C	1.137420	-0.190548	2.031684
C	3.955027	0.266073	1.354333
C	2.068441	-1.484639	4.003948
C	4.740031	-0.871880	0.705528
C	-0.961712	0.968147	0.326862
C	-1.670205	-0.131642	-0.171712
C	-3.018841	-0.281639	0.177795
C	-3.640950	0.626538	1.029466
C	-2.938662	1.743609	1.505944
C	-1.601407	1.894262	1.153716
C	6.039166	-1.123545	1.156461
C	6.788785	-2.177651	0.649470
C	6.215654	-2.983639	-0.319872
C	4.936342	-2.770372	-0.796733
C	4.204419	-1.704732	-0.276992
C	-1.017217	-1.178030	-1.045906
C	-1.777418	-2.497207	-0.992767
O	-3.157842	-2.246382	-1.300426
C	-3.832060	-1.463390	-0.322280
C	-1.278264	-3.524319	-1.990410
F	6.940895	-4.016344	-0.824778
O	-4.975680	0.437971	1.310181
C	-5.303219	0.135691	2.677032
O	-3.637193	2.614612	2.288565
C	-2.975935	3.789588	2.755087
C	-5.125789	-1.029803	-1.029142
O	-5.197977	-0.134947	-1.834835
O	-6.145469	-1.827208	-0.687352
C	-8.412525	-2.589335	-0.810454
C	-7.423542	-1.571479	-1.331172
O	-0.157074	2.622521	-1.786722
C	-0.272623	2.265457	-3.174905
O	2.529866	3.136429	-2.366992
C	2.451735	4.529819	-2.015690
C	5.072519	1.569558	-2.060657
O	4.510799	1.947465	-0.790696
H	2.532526	-1.827594	1.941014
H	0.320140	-0.878638	1.804828
H	0.758485	0.487270	2.804877
H	4.664811	1.064649	1.570835
H	1.182020	-2.121869	4.026377
H	2.920601	-2.066552	4.357400
H	1.910588	-0.649251	4.689540
H	-1.038395	2.743643	1.513140
H	6.472985	-0.485254	1.917124
H	7.796950	-2.373239	0.990502

H	4.526896	-3.419809	-1.559344
H	3.206847	-1.521060	-0.654541
H	-0.984495	-0.842023	-2.088035
H	0.017641	-1.336670	-0.735529
H	-1.716842	-2.911776	0.023665
H	-4.108102	-2.100006	0.526981
H	-1.851288	-4.448785	-1.909421
H	-0.227062	-3.752459	-1.804235
H	-1.375399	-3.144264	-3.009359
H	-5.074913	0.978660	3.328495
H	-6.372431	-0.064321	2.693067
H	-4.762005	-0.752307	3.014980
H	-3.719334	4.338329	3.327888
H	-2.130453	3.541107	3.402129
H	-2.630617	4.406953	1.922044
H	-9.384456	-2.423277	-1.279048
H	-8.089759	-3.605035	-1.043859
H	-8.535039	-2.501407	0.270092
H	-7.726971	-0.549949	-1.098518
H	-7.287926	-1.649504	-2.410499
H	-0.446465	1.192086	-3.280058
H	-1.138000	2.806244	-3.551450
H	0.618946	2.552430	-3.732208
H	2.768046	5.085175	-2.896388
H	1.428437	4.806293	-1.754854
H	3.121908	4.752572	-1.182193
H	6.131681	1.810719	-2.000389
H	4.954702	0.495827	-2.222747
H	4.608605	2.124531	-2.874530

B3LYP Energy = -2096.62160619 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf H

C	0.679673	-0.909709	1.863332
C	1.980312	-0.942858	2.381768
C	3.066456	-0.986650	1.506274
C	2.863116	-0.948077	0.122598
C	1.562453	-0.913319	-0.390274
C	0.458513	-0.908730	0.483106
O	3.711817	-1.369794	-2.125760
C	2.622439	-0.609280	-2.669916
C	1.350925	-0.924027	-1.890019
C	4.070927	-0.966318	-0.797293
C	2.514980	-0.958399	-4.142383
C	4.872452	0.334914	-0.834797
C	-0.945659	-0.924852	-0.036353
C	-1.730165	0.233453	-0.075729
C	-3.043912	0.146663	-0.552352
C	-3.556896	-1.060035	-1.027827
C	-2.754734	-2.212050	-1.025308
C	-1.466648	-2.132685	-0.505356
C	6.155420	0.300052	-1.389335
C	6.927338	1.449829	-1.496937
C	6.393867	2.643089	-1.039097
C	5.132007	2.722710	-0.482647
C	4.375905	1.556327	-0.383578

C	-1.187364	1.571022	0.369360
C	-1.978734	2.722300	-0.235901
O	-3.375324	2.515678	0.031366
C	-3.922380	1.382010	-0.634122
C	-1.610032	4.077287	0.336196
F	7.142106	3.774284	-1.136233
O	-4.819814	-1.036085	-1.571193
C	-5.802158	-1.945511	-1.038024
O	-3.298845	-3.343735	-1.562191
C	-2.511778	-4.532444	-1.589732
C	-5.285317	1.197011	0.048055
O	-5.462525	0.592394	1.077846
O	-6.238105	1.860454	-0.620224
C	-7.722630	3.028712	0.946898
C	-7.574685	1.890803	-0.044205
O	-0.386855	-0.798896	2.723686
C	-0.749190	-2.000166	3.423526
O	2.182005	-0.966183	3.743062
C	2.264683	0.333425	4.353580
C	4.770494	-2.167102	2.691836
O	4.357687	-0.986962	1.979189
H	2.855526	0.458220	-2.570119
H	0.567548	-0.213365	-2.163972
H	0.987133	-1.910750	-2.195244
H	4.747240	-1.751849	-0.457431
H	1.683555	-0.418878	-4.600488
H	3.431847	-0.690684	-4.669109
H	2.342367	-2.029479	-4.268954
H	-0.841103	-3.013538	-0.480112
H	6.556991	-0.640928	-1.746167
H	7.922901	1.428139	-1.920468
H	4.752925	3.673714	-0.132101
H	3.390427	1.607632	0.060522
H	-1.225720	1.646874	1.461029
H	-0.136852	1.660645	0.083430
H	-1.833095	2.731116	-1.325598
H	-4.103278	1.629316	-1.687328
H	-2.199787	4.866099	-0.132461
H	-0.552902	4.285966	0.160648
H	-1.792800	4.099502	1.412405
H	-6.751837	-1.635733	-1.469600
H	-5.579645	-2.971629	-1.321967
H	-5.848336	-1.856897	0.048816
H	-3.135690	-5.288333	-2.060258
H	-1.602922	-4.394081	-2.181102
H	-2.245981	-4.858784	-0.580819
H	-8.754527	3.066027	1.303044
H	-7.069326	2.888657	1.808257
H	-7.487792	3.985401	0.478050
H	-8.229373	2.022697	-0.903549
H	-7.777563	0.926447	0.419251
H	-1.063741	-2.772304	2.716800
H	0.081079	-2.363183	4.030938
H	-1.587115	-1.736495	4.065386
H	2.425001	0.162784	5.416275
H	3.104574	0.898661	3.943217

H	1.334718	0.886751	4.208189
H	4.184419	-2.302327	3.600199
H	4.676288	-3.049853	2.053598
H	5.817492	-2.013468	2.944585

B3LYP Energy = -2096.62153607 a.u.

(*aS*,1*S*,3*S*,1'*S*,3'*S*)-**22**, Conf I

C	-0.460032	1.549868	-1.203098
C	-1.727913	2.091445	-1.449541
C	-2.849446	1.262421	-1.395405
C	-2.717522	-0.085910	-1.045911
C	-1.450168	-0.620607	-0.795170
C	-0.307483	0.196619	-0.887670
O	-3.648384	-2.342224	-1.034171
C	-2.643069	-2.740545	-0.089724
C	-1.314686	-2.092600	-0.463978
C	-3.966245	-0.945279	-0.965495
C	-2.586978	-4.256584	-0.099108
C	-4.863918	-0.659670	0.238035
C	1.065721	-0.357099	-0.666606
C	1.751855	-0.161824	0.537799
C	3.040817	-0.691143	0.677667
C	3.621295	-1.444141	-0.343402
C	2.916763	-1.671215	-1.535777
C	1.656111	-1.102200	-1.689247
C	-4.413993	-0.023734	1.394083
C	-5.258494	0.169957	2.485263
C	-6.561278	-0.281318	2.396630
C	-7.050487	-0.914410	1.266342
C	-6.190133	-1.098843	0.191301
C	1.128948	0.595532	1.687107
C	1.797331	0.250725	3.011026
O	3.217692	0.412811	2.868604
C	3.811134	-0.525607	1.977890
C	1.358694	1.138369	4.159488
F	-7.395511	-0.092565	3.453566
O	4.846722	-2.003292	-0.077732
C	5.915765	-1.819467	-1.023076
O	3.521380	-2.465607	-2.467766
C	2.833382	-2.730333	-3.688051
C	5.251560	-0.015747	1.828109
O	6.175779	-0.436489	2.482958
O	5.342463	0.997475	0.961129
C	6.492729	2.771119	-0.162982
C	6.635517	1.650930	0.841896
O	0.638741	2.376434	-1.195893
C	1.103346	2.802323	-2.486921
O	-1.858860	3.422966	-1.773282
C	-2.054235	4.290379	-0.642935
C	-4.398111	2.226445	-2.937128
O	-4.112622	1.763514	-1.604670
H	-2.944850	-2.400146	0.908610
H	-0.598856	-2.229711	0.350059
H	-0.897622	-2.619913	-1.328598
H	-4.561943	-0.766505	-1.861470



H	-1.818857	-4.612258	0.590603
H	-3.545928	-4.677605	0.205710
H	-2.349222	-4.624171	-1.099764
H	1.104005	-1.254319	-2.605756
H	-3.395168	0.337137	1.450122
H	-4.916038	0.664295	3.384889
H	-8.079537	-1.247542	1.233989
H	-6.557203	-1.594972	-0.699412
H	1.214825	1.673588	1.514977
H	0.061763	0.369668	1.747617
H	1.593098	-0.800426	3.260009
H	3.895470	-1.499881	2.474820
H	1.864411	0.851262	5.082221
H	0.281503	1.050899	4.314397
H	1.593457	2.183014	3.945218
H	5.820547	-2.506486	-1.860924
H	5.929831	-0.791643	-1.391937
H	6.832210	-2.022619	-0.472583
H	2.645651	-1.810463	-4.248175
H	3.492207	-3.375199	-4.264346
H	1.887730	-3.248003	-3.507245
H	7.449908	3.284920	-0.271445
H	6.197723	2.387158	-1.140639
H	5.748732	3.498300	0.164738
H	6.925965	2.020299	1.826178
H	7.371547	0.910277	0.526873
H	1.419365	1.941458	-3.081938
H	0.329268	3.358858	-3.016855
H	1.959953	3.447665	-2.303569
H	-2.965880	4.022325	-0.104250
H	-1.195524	4.243954	0.030161
H	-2.149827	5.297926	-1.042774
H	-5.445622	2.520305	-2.933920
H	-3.772882	3.079337	-3.198910
H	-4.248560	1.420453	-3.660659

B3LYP Energy = -2096.62152489 a.u.

(aS,1S,3S,1'S,3'S)-**22**, Conf J

C	0.712839	-0.696600	1.990899
C	2.024964	-0.664921	2.480246
C	3.091287	-0.808896	1.591193
C	2.856313	-0.930283	0.216969
C	1.544587	-0.953776	-0.267142
C	0.460560	-0.851082	0.625053
O	3.656356	-1.594672	-1.990642
C	2.552282	-0.899837	-2.589392
C	1.299687	-1.130514	-1.751759
C	4.043691	-1.048654	-0.722261
C	2.415919	-1.405881	-4.013146
C	4.840312	0.241305	-0.918937
C	-0.953885	-0.921928	0.139679
C	-1.741629	0.227213	0.002542
C	-3.052332	0.095408	-0.472666
C	-3.557686	-1.149234	-0.838182
C	-2.779779	-2.304456	-0.671812

C	-1.481017	-2.173454	-0.189909
C	6.117430	0.147543	-1.480156
C	6.882545	1.280301	-1.727397
C	6.348037	2.516307	-1.403975
C	5.091512	2.654842	-0.846834
C	4.342469	1.504911	-0.606026
C	-1.206936	1.602435	0.324531
C	-2.006732	2.690211	-0.380301
O	-3.401814	2.501958	-0.092017
C	-3.948288	1.310335	-0.643648
C	-1.645366	4.092749	0.069100
F	7.089466	3.631618	-1.638968
O	-4.861206	-1.216028	-1.276572
C	-5.050109	-1.598538	-2.649325
O	-3.372119	-3.489824	-0.995199
C	-2.632700	-4.693777	-0.801881
C	-5.292632	1.157258	0.085757
O	-5.415637	0.726523	1.205443
O	-6.294923	1.633422	-0.666074
C	-7.894089	2.889623	0.709849
C	-7.631423	1.628457	-0.089799
O	-0.335006	-0.495468	2.857523
C	-0.675802	-1.615329	3.691284
O	2.261325	-0.528689	3.829016
C	2.254059	0.830088	4.301001
C	4.825683	-1.837934	2.870372
O	4.392971	-0.753259	2.029614
H	2.782411	0.172663	-2.611016
H	0.507333	-0.455305	-2.083833
H	0.934169	-2.145772	-1.939488
H	4.729542	-1.792028	-0.313742
H	1.571862	-0.922174	-4.509001
H	3.320177	-1.192113	-4.584473
H	2.248335	-2.485137	-4.020748
H	-0.860815	-3.048750	-0.057965
H	6.520444	-0.826706	-1.730279
H	7.873840	1.213685	-2.156235
H	4.711363	3.638477	-0.604151
H	3.361940	1.603272	-0.158873
H	-1.247374	1.776235	1.404754
H	-0.156805	1.672892	0.031298
H	-1.862178	2.603598	-1.466808
H	-4.156844	1.462908	-1.709464
H	-2.238867	4.833886	-0.467639
H	-0.589144	4.290518	-0.123472
H	-1.829886	4.209139	1.138893
H	-4.512408	-0.918180	-3.315396
H	-4.717597	-2.622437	-2.818545
H	-6.118521	-1.521649	-2.839257
H	-3.296710	-5.499812	-1.103992
H	-1.732734	-4.713517	-1.422346
H	-2.356843	-4.825452	0.247559
H	-8.926647	2.883254	1.066161
H	-7.235177	2.951847	1.576060
H	-7.751221	3.778421	0.093282
H	-8.291114	1.559660	-0.952855

H	-7.744033	0.734401	0.521589
H	-1.000015	-2.461419	3.080137
H	0.169042	-1.907507	4.316635
H	-1.502115	-1.286515	4.317872
H	3.035996	1.412045	3.807476
H	1.279829	1.292187	4.130943
H	2.454776	0.783430	5.369452
H	5.877936	-1.654755	3.077540
H	4.261560	-1.861173	3.801950
H	4.719102	-2.791746	2.346424

B3LYP Energy = -2096.62151038 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf K

C	0.545688	2.048302	-0.039973
C	1.837584	2.577462	-0.154250
C	2.922750	1.846516	0.332248
C	2.730814	0.574017	0.881541
C	1.439971	0.046798	0.985712
C	0.334353	0.792450	0.535053
O	3.561396	-1.244009	2.281160
C	2.533886	-2.101470	1.762078
C	1.237561	-1.310732	1.626983
C	3.940025	-0.203709	1.369412
C	2.411664	-3.284864	2.703734
C	4.833588	-0.763821	0.262833
C	-1.062227	0.271766	0.676685
C	-1.742303	-0.309039	-0.400209
C	-3.041371	-0.793582	-0.199043
C	-3.638112	-0.730066	1.057403
C	-2.968087	-0.122452	2.129438
C	-1.680800	0.364965	1.926111
C	4.412194	-0.921720	-1.056281
C	5.250845	-1.480183	-2.018720
C	6.518774	-1.874320	-1.637065
C	6.979113	-1.732489	-0.338605
C	6.125366	-1.175063	0.604709
C	-1.102084	-0.442949	-1.761833
C	-1.780694	-1.521693	-2.596083
O	-3.197059	-1.279630	-2.604389
C	-3.811937	-1.451372	-1.333286
C	-1.323265	-1.545670	-4.041427
F	7.347229	-2.415703	-2.569353
O	-4.929006	-1.189115	1.185357
C	-5.114185	-2.355541	2.005270
O	-3.647940	-0.050167	3.309725
C	-3.015493	0.583203	4.419899
C	-5.240873	-0.925055	-1.540155
O	-6.178269	-1.647505	-1.785248
O	-5.291347	0.408539	-1.504938
C	-7.394852	1.204602	-0.517061
C	-6.568394	1.049918	-1.778511
O	-0.517693	2.741226	-0.569230
C	-0.957292	3.878871	0.190291
O	2.033106	3.820410	-0.711716
C	2.133468	3.817943	-2.146691

C	4.526983	3.489519	0.987204
O	4.207757	2.320042	0.211784
H	2.843845	-2.461822	0.773320
H	0.512642	-1.892662	1.052696
H	0.801057	-1.177242	2.622581
H	4.554851	0.464882	1.973265
H	1.623087	-3.959830	2.364899
H	3.348589	-3.841882	2.743796
H	2.166219	-2.946710	3.712922
H	-1.142125	0.829759	2.739698
H	3.421858	-0.597945	-1.348713
H	4.930654	-1.603776	-3.044957
H	7.981795	-2.047876	-0.081393
H	6.469512	-1.060053	1.625735
H	-1.162228	0.510350	-2.297732
H	-0.040735	-0.678427	-1.654421
H	-1.600822	-2.504686	-2.137460
H	-3.922008	-2.522642	-1.123401
H	-1.833292	-2.336220	-4.593282
H	-0.247811	-1.725905	-4.094506
H	-1.538026	-0.590500	-4.524891
H	-6.163978	-2.624992	1.912580
H	-4.493980	-3.180704	1.645149
H	-4.877005	-2.140796	3.047114
H	-2.100841	0.059406	4.710196
H	-2.784603	1.629085	4.201395
H	-3.732832	0.535261	5.235367
H	-8.307401	1.757766	-0.751044
H	-7.677250	0.234826	-0.107984
H	-6.843534	1.758620	0.243785
H	-6.292761	2.017144	-2.194812
H	-7.095151	0.469605	-2.534701
H	-0.151587	4.604744	0.308285
H	-1.773565	4.323976	-0.374845
H	-1.325368	3.563972	1.170135
H	1.210131	3.448283	-2.596837
H	2.296371	4.851998	-2.443781
H	2.978733	3.206778	-2.471510
H	3.927960	4.343627	0.673650
H	4.369711	3.295299	2.051699
H	5.581318	3.689037	0.807680

B3LYP Energy = -2096.62142704 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf L

C	-0.727347	-1.552762	-1.429824
C	-2.045455	-1.799887	-1.834649
C	-3.095125	-1.519888	-0.958291
C	-2.838865	-0.951955	0.294590
C	-1.521857	-0.701653	0.691922
C	-0.453093	-1.014516	-0.169302
O	-3.590742	-0.489829	2.569335
C	-2.504976	0.434812	2.732255
C	-1.254088	-0.132808	2.070380
C	-4.010268	-0.630376	1.204997
C	-2.330405	0.672116	4.220562

C	-4.843689	0.576935	0.775747
C	0.969462	-0.800436	0.246433
C	1.710866	0.296848	-0.207314
C	3.034850	0.443519	0.223872
C	3.599585	-0.461294	1.118646
C	2.866440	-1.575230	1.553060
C	1.554513	-1.726147	1.114462
C	-6.119893	0.725892	1.326820
C	-6.917406	1.820466	1.017591
C	-6.416209	2.770706	0.143757
C	-5.162104	2.662314	-0.425512
C	-4.380236	1.555203	-0.102375
C	1.114034	1.339080	-1.122450
C	1.877218	2.654400	-1.035672
O	3.273700	2.396983	-1.256698
C	3.885549	1.613077	-0.238794
C	1.444360	3.673964	-2.071232
F	-7.189151	3.844768	-0.168833
O	4.913956	-0.273140	1.482580
C	5.153574	0.033962	2.866438
O	3.512136	-2.445296	2.381852
C	2.818031	-3.612582	2.817476
C	5.208070	1.159386	-0.878263
O	5.313713	0.233313	-1.643491
O	6.205621	1.985082	-0.532050
C	8.330139	0.779751	-0.279591
C	7.516331	1.745754	-1.118239
O	0.300899	-1.772560	-2.315473
C	0.676071	-3.146856	-2.503249
O	-2.303755	-2.346287	-3.070830
C	-2.343281	-1.393016	-4.147455
C	-4.804250	-3.087492	-1.527500
O	-4.403414	-1.719440	-1.330498
H	-2.774664	1.381028	2.247148
H	-0.487062	0.643425	2.014053
H	-0.843645	-0.920190	2.711430
H	-4.677367	-1.493076	1.221842
H	-1.501914	1.360159	4.400933
H	-3.236007	1.102703	4.649737
H	-2.116165	-0.267836	4.734015
H	0.970114	-2.574803	1.440223
H	-6.496644	-0.025285	2.010931
H	-7.908006	1.938079	1.436913
H	-4.809257	3.424063	-1.108316
H	-3.401307	1.456944	-0.553079
H	1.133732	0.985256	-2.158568
H	0.065810	1.506684	-0.864381
H	1.757688	3.079233	-0.028637
H	4.126624	2.251827	0.619488
H	2.015001	4.597357	-1.964491
H	0.384535	3.906891	-1.951533
H	1.601259	3.283102	-3.078524
H	4.885591	-0.807105	3.505178
H	6.219318	0.235388	2.950200
H	4.590587	0.922248	3.166082
H	3.520831	-4.157480	3.442803

H	1.933368	-3.355172	3.406138
H	2.524829	-4.239030	1.971146
H	9.326390	0.675221	-0.715251
H	8.441715	1.148497	0.741310
H	7.864982	-0.205546	-0.249519
H	7.382145	1.378290	-2.134434
H	7.976218	2.731836	-1.149821
H	-0.163926	-3.732184	-2.880208
H	1.481361	-3.144187	-3.234712
H	1.040751	-3.573935	-1.565699
H	-2.572215	-1.958907	-5.048240
H	-3.125576	-0.650323	-3.973839
H	-1.376611	-0.898896	-4.260506
H	-4.254305	-3.542812	-2.350214
H	-4.649691	-3.665177	-0.612096
H	-5.866316	-3.057550	-1.761583

B3LYP Energy = -2096.62125425 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf M

C	-0.742088	0.587280	1.996565
C	-2.057081	0.533870	2.484515
C	-3.117400	0.745563	1.597789
C	-2.864896	0.980671	0.238123
C	-1.553672	1.016287	-0.239746
C	-0.477035	0.822509	0.646628
O	-3.641281	1.812108	-1.927520
C	-2.553751	1.121859	-2.559385
C	-1.300064	1.284178	-1.708934
C	-4.047801	1.222534	-0.684591
C	-2.403327	1.694687	-3.956315
C	-4.923286	-0.003110	-0.940713
C	0.942613	0.900778	0.179017
C	1.720964	-0.248451	-0.002555
C	3.047785	-0.108727	-0.427873
C	3.582176	1.147807	-0.712893
C	2.788775	2.296556	-0.565191
C	1.485461	2.157084	-0.098452
C	-6.244783	0.199868	-1.348666
C	-7.079809	-0.867874	-1.653858
C	-6.569719	-2.150764	-1.547094
C	-5.270620	-2.398092	-1.146690
C	-4.452438	-1.312122	-0.841874
C	1.159427	-1.630106	0.238639
C	1.957997	-2.694905	-0.500624
O	3.348754	-2.539353	-0.175697
C	3.917377	-1.330357	-0.667794
C	1.568191	-4.111702	-0.125871
F	-7.378324	-3.203560	-1.840962
O	4.858620	1.186872	-1.222515
C	5.833129	2.007413	-0.549240
O	3.355729	3.487861	-0.917314
C	2.582919	4.678172	-0.778606
C	5.272044	-1.259119	0.050383
O	5.440351	-0.831300	1.166857
O	6.233422	-1.811458	-0.699196

C	8.460654	-2.586007	-1.115205
C	7.556438	-1.916864	-0.105393
O	0.304947	0.378245	2.867138
C	0.665666	1.513048	3.672510
O	-2.313092	0.390989	3.828070
C	-1.968683	-0.878139	4.414593
C	-4.986992	-0.218229	2.803596
O	-4.424551	0.828096	1.998280
H	-2.806907	0.057006	-2.635188
H	-0.514840	0.621195	-2.080204
H	-0.923455	2.304767	-1.834177
H	-4.682716	1.982653	-0.228408
H	-1.571814	1.214582	-4.476244
H	-3.312587	1.533490	-4.536940
H	-2.207609	2.768175	-3.909757
H	0.864102	3.031108	0.035153
H	-6.628689	1.209969	-1.429860
H	-8.105171	-0.716088	-1.964668
H	-4.910920	-3.416002	-1.072086
H	-3.437678	-1.497724	-0.514371
H	1.172380	-1.857480	1.309838
H	0.115167	-1.668437	-0.080393
H	1.838290	-2.554853	-1.584461
H	4.111813	-1.429826	-1.742758
H	2.162931	-4.835218	-0.684828
H	0.513816	-4.284789	-0.349785
H	1.727831	-4.280844	0.940940
H	6.792883	1.737728	-0.985373
H	5.633311	3.064310	-0.710467
H	5.842204	1.785221	0.519331
H	3.226583	5.488380	-1.112130
H	1.687427	4.646235	-1.404585
H	2.295871	4.847931	0.262450
H	9.464654	-2.679864	-0.696839
H	8.099106	-3.584795	-1.363732
H	8.526027	-1.999955	-2.033059
H	7.901742	-0.914359	0.150375
H	7.475418	-2.494335	0.816339
H	1.487206	1.187073	4.306974
H	1.001614	2.338854	3.040886
H	-0.173970	1.835551	4.290997
H	-2.523850	-1.686328	3.931095
H	-0.899290	-1.068944	4.337481
H	-2.260465	-0.813780	5.460787
H	-4.702061	-0.108794	3.848136
H	-6.066202	-0.121443	2.702306
H	-4.679462	-1.198385	2.432285

B3LYP Energy = -2096.62094005 a.u.

(aS,1S,3S,1'S,3'S)-**22**, Conf N

C	-0.475079	1.534722	-1.252072
C	-1.750690	2.059952	-1.511481
C	-2.859825	1.211140	-1.438886
C	-2.693552	-0.138379	-1.091488
C	-1.421600	-0.647966	-0.827898

C	-0.295811	0.193827	-0.909837
O	-3.580518	-2.416861	-1.058129
C	-2.581092	-2.772362	-0.092204
C	-1.261431	-2.111413	-0.471901
C	-3.925915	-1.024793	-1.036387
C	-2.499539	-4.287030	-0.059752
C	-4.873089	-0.730379	0.126401
C	1.087397	-0.327856	-0.674730
C	1.777942	-0.065574	0.514768
C	3.067984	-0.587181	0.678257
C	3.647197	-1.378783	-0.310031
C	2.965412	-1.622907	-1.511191
C	1.687169	-1.098588	-1.674480
C	-6.202253	-1.149888	0.020554
C	-7.104145	-0.963669	1.060904
C	-6.653855	-0.349073	2.217232
C	-5.349672	0.082861	2.364599
C	-4.463289	-0.112146	1.307266
C	1.157714	0.745431	1.628036
C	1.841545	0.480255	2.962907
O	3.259920	0.641869	2.798512
C	3.848126	-0.346286	1.961300
C	1.407453	1.428836	4.063286
F	-7.528474	-0.159162	3.240799
O	4.933451	-1.825567	-0.110519
C	5.102998	-3.245724	0.038208
O	3.627787	-2.360315	-2.448366
C	2.983757	-2.609307	-3.696288
C	5.290756	0.142281	1.763082
O	6.219300	-0.257339	2.426003
O	5.376901	1.102830	0.841501
C	6.547445	2.734615	-0.461459
C	6.690241	1.681232	0.613163
O	0.616674	2.373545	-1.316832
C	1.123082	2.613480	-2.640553
O	-1.910300	3.354812	-1.946643
C	-1.606631	4.394176	-0.998118
C	-4.673976	2.818460	-1.262169
O	-4.129587	1.593802	-1.775006
H	-2.898714	-2.410697	0.893903
H	-0.547436	-2.221093	0.347991
H	-0.833459	-2.648370	-1.325078
H	-4.490647	-0.879935	-1.957796
H	-1.734576	-4.610891	0.648940
H	-3.455180	-4.716032	0.244376
H	-2.243109	-4.677267	-1.047096
H	1.141830	-1.275829	-2.590531
H	-6.538746	-1.631283	-0.890093
H	-8.135394	-1.282019	0.982343
H	-5.037872	0.561847	3.283532
H	-3.442406	0.232781	1.409127
H	1.231915	1.813133	1.396392
H	0.093380	0.513179	1.710697
H	1.646083	-0.556302	3.273140
H	3.933295	-1.289153	2.516051
H	1.920461	1.195388	4.997034

H	0.331630	1.346569	4.230103
H	1.636872	2.460667	3.789612
H	4.848465	-3.766642	-0.884549
H	6.153965	-3.400181	0.272572
H	4.488260	-3.621879	0.860263
H	3.688131	-3.196450	-4.280207
H	2.060313	-3.178850	-3.562197
H	2.765122	-1.676751	-4.222920
H	7.521296	3.188373	-0.655735
H	6.181306	2.297778	-1.391549
H	5.859128	3.521523	-0.149943
H	7.050282	2.102382	1.552750
H	7.369706	0.882301	0.313854
H	1.485767	1.683841	-3.085182
H	0.355244	3.056546	-3.277542
H	1.953556	3.307385	-2.528138
H	-2.252846	4.311845	-0.120272
H	-0.562366	4.352816	-0.691932
H	-1.807534	5.333890	-1.508445
H	-4.332778	3.674795	-1.840304
H	-5.754303	2.718831	-1.348339
H	-4.410037	2.950214	-0.210440

B3LYP Energy = -2096.62091544 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf O

C	0.729112	-1.395976	1.578576
C	2.043925	-1.580901	2.024819
C	3.102391	-1.394669	1.133992
C	2.858553	-0.975984	-0.178824
C	1.544115	-0.788971	-0.618046
C	0.467263	-1.013414	0.260309
O	3.633780	-0.760535	-2.482843
C	2.539302	0.126672	-2.758859
C	1.287330	-0.384023	-2.054820
C	4.037698	-0.744232	-1.107146
C	2.383054	0.200116	-4.266077
C	4.855297	0.512271	-0.806026
C	-0.951233	-0.862724	-0.194256
C	-1.693852	0.289626	0.086274
C	-3.019817	0.368740	-0.358069
C	-3.585640	-0.659736	-1.112043
C	-2.825484	-1.798236	-1.425564
C	-1.525517	-1.894332	-0.939071
C	6.123338	0.626126	-1.383941
C	6.908329	1.755118	-1.187097
C	6.403207	2.775765	-0.399007
C	5.156526	2.704652	0.191849
C	4.386952	1.562206	-0.018145
C	-1.091275	1.453950	0.836291
C	-1.835755	2.748050	0.539080
O	-3.235964	2.541837	0.784619
C	-3.849191	1.614823	-0.107245
C	-1.397672	3.912400	1.406136
F	7.164479	3.883975	-0.196144
O	-4.854485	-0.458049	-1.602088

C	-5.858411	-1.446764	-1.300512
O	-3.417978	-2.737126	-2.220810
C	-2.676020	-3.903987	-2.568512
C	-5.197801	1.330464	0.571337
O	-5.396234	0.457557	1.381096
O	-6.099130	2.251109	0.204000
C	-8.406931	1.411955	0.124714
C	-7.392057	2.253354	0.872636
O	-0.310646	-1.515841	2.470266
C	-0.667469	-2.859453	2.834146
O	2.291732	-1.975026	3.320038
C	2.314958	-0.900394	4.276065
C	4.815693	-2.870112	1.901565
O	4.407062	-1.537833	1.543202
H	2.790851	1.123452	-2.375455
H	0.506710	0.379247	-2.095813
H	0.899425	-1.245932	-2.608176
H	4.712969	-1.596575	-1.020824
H	1.546255	0.850075	-4.529746
H	3.287836	0.598436	-4.726949
H	2.191768	-0.792819	-4.678976
H	-0.930340	-2.769198	-1.158845
H	6.502936	-0.179833	-2.000791
H	7.892488	1.846449	-1.627634
H	4.799784	3.522026	0.804730
H	3.414078	1.493546	0.450694
H	-1.123644	1.265531	1.914620
H	-0.038837	1.566829	0.566499
H	-1.704422	3.008855	-0.520845
H	-4.053173	2.110344	-1.064436
H	-1.959789	4.812524	1.154217
H	-0.335519	4.115622	1.256269
H	-1.560965	3.684857	2.461440
H	-5.919064	-1.604921	-0.222126
H	-6.796016	-1.030344	-1.662184
H	-5.648157	-2.385727	-1.807139
H	-3.336225	-4.496701	-3.196874
H	-1.773837	-3.649139	-3.130732
H	-2.403438	-4.482557	-1.681948
H	-9.383486	1.515871	0.602887
H	-8.498030	1.741137	-0.911568
H	-8.133070	0.357112	0.137593
H	-7.256696	1.904307	1.895093
H	-7.680482	3.302938	0.885685
H	-1.001454	-3.417170	1.955477
H	0.172183	-3.372129	3.305489
H	-1.490654	-2.773704	3.540327
H	2.535995	-1.354002	5.240164
H	3.095956	-0.179235	4.023945
H	1.345022	-0.401457	4.319335
H	4.261366	-3.230306	2.767322
H	4.673367	-3.551452	1.058358
H	5.875395	-2.804746	2.139206

B3LYP Energy = -2096.62091453 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf P

C	-0.760287	-0.152776	2.109251	H	-3.410280	-1.222242	-0.994528
C	-2.083974	-0.356763	2.530023	H	1.166446	-2.237841	0.607208
C	-3.128291	0.157010	1.754709	H	0.116325	-1.555277	-0.625304
C	-2.850673	0.842632	0.562502	H	1.849811	-1.840366	-2.339543
C	-1.531579	1.027224	0.145824	H	4.183626	-0.774399	-2.042738
C	-0.471238	0.529637	0.926667	H	2.153485	-4.295843	-2.331733
O	-3.586329	2.378577	-1.193230	H	0.503342	-3.889256	-1.834979
C	-2.490042	1.941778	-2.008534	H	1.701280	-4.368211	-0.620144
C	-1.250666	1.783491	-1.136100	H	4.873534	3.395582	-1.364261
C	-4.016179	1.396782	-0.239226	H	6.238489	2.342648	-1.815048
C	-2.310855	2.965103	-3.114411	H	4.632005	2.063649	-2.530765
C	-4.884957	0.340030	-0.919523	H	3.418653	5.374772	1.288646
C	0.956556	0.752026	0.535256	H	1.858522	4.830772	0.628530
C	1.727835	-0.266984	-0.036643	H	2.408129	4.249939	2.225620
C	3.055396	0.005973	-0.388046	H	9.553659	-2.096980	-1.210594
C	3.596566	1.275864	-0.206661	H	8.282456	-2.734147	-2.262275
C	2.833655	2.289355	0.391758	H	8.631716	-0.996162	-2.242936
C	1.516898	2.014481	0.748101	H	7.838234	-0.866170	0.142260
C	-6.195671	0.681806	-1.264776	H	7.494225	-2.599301	0.124228
C	-7.022780	-0.209983	-1.936374	H	0.976853	1.114570	3.714071
C	-6.515747	-1.456635	-2.262060	H	-0.223672	0.228234	4.700208
C	-5.227238	-1.837362	-1.939275	H	1.432999	-0.406273	4.515880
C	-4.416823	-0.927973	-1.262596	H	-2.597868	-2.934381	3.124385
C	1.158873	-1.639132	-0.309744	H	-0.967705	-2.513839	3.718044
C	1.958729	-2.368227	-1.381232	H	-2.330761	-2.642341	4.860419
O	3.347488	-2.357890	-1.012689	H	-6.096250	-1.006906	2.464049
C	3.935402	-1.062341	-1.013934	H	-4.696977	-1.949733	1.907473
C	1.555828	-3.820087	-1.553157	H	-4.761793	-1.358172	3.591380
F	-7.316605	-2.338649	-2.917198	B3LYP Energy = -2096.62082184 a.u.			
O	4.916436	1.470198	-0.547217	(aS,1S,3S,1'S,3'S)-22, Conf Q			
C	5.166885	2.380766	-1.631346	C	0.745104	-1.822622	1.266327
O	3.457697	3.485965	0.589740	C	2.074346	-2.074892	1.636459
C	2.729119	4.537005	1.221057	C	3.113474	-1.593587	0.838714
C	5.252058	-1.260347	-0.246573	C	2.832994	-0.922963	-0.358480
O	5.342989	-1.313564	0.954951	C	1.507202	-0.723077	-0.751076
O	6.274277	-1.441820	-1.092229	C	0.451406	-1.158530	0.071671
C	8.564893	-1.893784	-1.626393	O	3.573092	-0.235335	-2.583814
C	7.574802	-1.708035	-0.499305	C	2.430345	0.626158	-2.685069
O	0.270057	-0.659356	2.870193	C	1.215377	-0.074689	-2.088154
C	0.624437	0.126936	4.020478	C	3.991671	-0.477791	-1.233123
O	-2.361643	-0.950400	3.739029	C	2.253955	0.973609	-4.151474
C	-2.035124	-2.347966	3.855565	C	4.777747	0.716156	-0.694611
C	-5.019497	-1.133809	2.558208	C	-0.977718	-0.974111	-0.336918
O	-4.442492	0.110527	2.135799	C	-1.691574	0.190276	-0.029982
H	-2.746878	0.973485	-2.456025	C	-3.029912	0.289819	-0.432228
H	-0.464240	1.279400	-1.703105	C	-3.637853	-0.730875	-1.162059
H	-0.863100	2.778774	-0.894292	C	-2.908017	-1.881681	-1.500638
H	-4.660111	1.955608	0.440452	C	-1.592881	-1.995486	-1.062664
H	-1.470763	2.688651	-3.754822	C	4.230753	1.661441	0.172958
H	-3.208897	3.025910	-3.730560	C	4.967122	2.768224	0.590752
H	-2.112758	3.952672	-2.692045	C	6.261528	2.909182	0.128253
H	0.909005	2.781764	1.206086	C	6.845555	1.992377	-0.729826
H	-6.577287	1.662165	-1.005111	C	6.091764	0.898254	-1.135673
H	-8.039953	0.047758	-2.200845	C	-1.053282	1.347631	0.704131
H	-4.869766	-2.822748	-2.208212				

C	-1.792638	2.651443	0.433882
O	-3.185814	2.458854	0.725096
C	-3.834149	1.547710	-0.156814
C	-1.313018	3.808645	1.288461
F	6.990782	3.982141	0.534017
O	-4.922106	-0.509772	-1.600981
C	-5.930978	-1.479155	-1.255738
O	-3.545573	-2.812734	-2.268388
C	-2.841508	-4.001204	-2.623904
C	-5.170727	1.265787	0.544074
O	-5.330051	0.444160	1.414231
O	-6.117330	2.105852	0.105489
C	-7.479550	2.939706	1.969003
C	-7.424565	2.048975	0.743248
O	-0.284785	-2.331518	2.020402
C	-0.467482	-1.759392	3.326298
O	2.352868	-2.790119	2.780261
C	2.330845	-4.217686	2.602309
C	4.951151	-1.358591	2.372294
O	4.428167	-1.864351	1.130434
H	2.631345	1.546352	-2.121936
H	0.393190	0.637982	-1.994835
H	0.871244	-0.844680	-2.787916
H	4.689606	-1.310747	-1.320255
H	1.383102	1.618161	-4.287207
H	3.132888	1.497169	-4.529903
H	2.108193	0.067728	-4.743806
H	-1.018389	-2.879278	-1.299852
H	3.220435	1.535794	0.540330
H	4.548968	3.504774	1.264311
H	7.864925	2.135122	-1.063666
H	6.533740	0.172908	-1.808523
H	-1.056751	1.166332	1.784394
H	-0.007202	1.449498	0.408408
H	-1.692796	2.913000	-0.629243
H	-4.051682	2.051940	-1.106089
H	-1.872741	4.715476	1.056291
H	-0.254047	4.000499	1.104841
H	-1.445206	3.581288	2.348186
H	-5.915365	-1.675767	-0.182171
H	-6.880366	-1.022938	-1.528933
H	-5.788821	-2.405048	-1.808458
H	-3.536431	-4.588278	-3.219223
H	-1.954800	-3.774438	-3.221608
H	-2.549916	-4.571344	-1.738117
H	-8.491690	2.927319	2.379453
H	-6.794225	2.590695	2.741707
H	-7.227144	3.969713	1.712862
H	-8.110536	2.391342	-0.029247
H	-7.648112	1.012306	0.990531
H	-1.326362	-2.267911	3.758859
H	0.411223	-1.915750	3.952077
H	-0.685125	-0.691732	3.247884
H	2.562928	-4.650840	3.573241
H	1.342912	-4.551203	2.278662
H	3.085334	-4.525143	1.874493

H	4.826300	-0.274804	2.424320
H	4.465361	-1.831103	3.224296
H	6.012294	-1.598336	2.365446

B3LYP Energy = -2096.62076943 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf R

C	-0.493348	-0.323379	1.965607
C	-1.763546	-0.595296	2.489441
C	-2.889993	-0.046339	1.875097
C	-2.758073	0.727128	0.716538
C	-1.488349	0.987212	0.191440
C	-0.342299	0.470490	0.825341
O	-3.699271	2.389252	-0.800074
C	-2.678448	2.079040	-1.760875
C	-1.354061	1.864274	-1.036932
C	-4.008969	1.288707	0.064810
C	-2.631292	3.221958	-2.757394
C	-4.872564	0.260964	-0.666754
C	1.033109	0.768331	0.314229
C	1.754290	-0.164064	-0.440769
C	3.044994	0.166097	-0.873071
C	3.593141	1.419967	-0.602167
C	2.853618	2.367472	0.122297
C	1.590928	2.018026	0.591236
C	-4.408200	-0.994216	-1.055274
C	-5.222955	-1.877713	-1.760457
C	-6.510709	-1.482808	-2.067303
C	-7.013584	-0.246438	-1.698050
C	-6.183204	0.618702	-0.996908
C	1.167564	-1.508191	-0.804790
C	1.871891	-2.116442	-2.009575
O	3.288101	-2.111654	-1.768328
C	3.851652	-0.805607	-1.719157
C	1.470245	-3.552542	-2.284597
F	-7.315559	-2.339057	-2.751194
O	4.823415	1.688950	-1.149199
C	5.868867	2.185703	-0.294139
O	3.428589	3.593445	0.299802
C	2.701969	4.590063	1.015157
C	5.290717	-1.054104	-1.244742
O	6.226080	-1.160221	-2.001858
O	5.361631	-1.215502	0.081524
C	6.807898	-3.108985	0.661338
C	6.643286	-1.601918	0.652614
O	0.611398	-0.908117	2.539487
C	1.041429	-0.329507	3.782218
O	-1.896273	-1.368284	3.620535
C	-1.951031	-2.783434	3.369603
C	-4.479144	0.214678	3.640102
O	-4.155049	-0.314333	2.341533
H	-2.959660	1.157547	-2.285553
H	-0.625424	1.433097	-1.727638
H	-0.952957	2.839334	-0.741033
H	-4.628699	1.732745	0.844821
H	-1.856215	3.042777	-3.505399

H	-3.588505	3.323150	-3.270505
H	-2.408980	4.162858	-2.249150
H	1.013093	2.729887	1.163240
H	-3.401630	-1.300209	-0.801482
H	-4.868854	-2.854484	-2.062981
H	-8.030249	0.023383	-1.952185
H	-6.560941	1.591245	-0.704328
H	1.255052	-2.196567	0.042395
H	0.101259	-1.404494	-1.018568
H	1.670925	-1.501691	-2.898555
H	3.943498	-0.408178	-2.737447
H	2.000203	-3.939507	-3.155735
H	0.397361	-3.614607	-2.476882
H	1.704829	-4.185111	-1.425970
H	5.743166	3.248340	-0.098654
H	5.884658	1.637721	0.650342
H	6.797365	2.009580	-0.833617
H	2.499075	4.275927	2.042456
H	3.340793	5.469698	1.026580
H	1.761143	4.832232	0.513988
H	7.744253	-3.367427	1.160918
H	5.988650	-3.586029	1.201088
H	6.841210	-3.508145	-0.352620
H	7.439233	-1.114717	0.091502
H	6.615038	-1.198979	1.663404
H	1.333049	0.713926	3.636907
H	0.255818	-0.396277	4.536119
H	1.907836	-0.904916	4.101877
H	-2.814084	-3.030287	2.746941
H	-1.032686	-3.125042	2.888017
H	-2.053734	-3.262851	4.341069
H	-5.523008	-0.037902	3.814002
H	-3.854097	-0.231447	4.412661
H	-4.361710	1.301676	3.648641

B3LYP Energy = -2096.62066153 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf S

C	-0.769446	-1.924555	-1.188515
C	-2.107963	-2.178503	-1.522410
C	-3.126797	-1.634039	-0.739133
C	-2.817498	-0.899859	0.413042
C	-1.482798	-0.696938	0.772130
C	-0.447169	-1.193577	-0.041431
O	-3.509673	-0.082663	2.609874
C	-2.354054	0.766184	2.646832
C	-1.158681	0.018981	2.066327
C	-3.954839	-0.390548	1.280961
C	-2.147048	1.185679	4.090301
C	-4.734366	0.783815	0.692707
C	0.991538	-0.996761	0.325596
C	1.695519	0.156444	-0.042163
C	3.036207	0.282083	0.345142
C	3.655245	-0.705691	1.105951
C	2.959255	-1.875563	1.445893
C	1.629624	-2.000512	1.057480

C	-4.187259	1.680264	-0.225356
C	-4.916934	2.773290	-0.688484
C	-6.205148	2.949638	-0.220713
C	-6.789415	2.080999	0.685856
C	-6.042120	1.000185	1.136836
C	1.045837	1.283226	-0.812004
C	1.781488	2.598708	-0.589897
O	3.171484	2.406993	-0.896004
C	3.844345	1.518004	-0.011632
C	1.283459	3.727882	-1.471194
F	-6.927955	4.009113	-0.670810
O	4.982767	-0.535653	1.428646
C	5.284365	-0.382946	2.826005
O	3.656595	-2.820745	2.138520
C	3.004759	-4.049776	2.454786
C	5.141697	1.176028	-0.761606
O	5.218517	0.372707	-1.658010
O	6.153447	1.941214	-0.329836
C	7.551175	2.694526	-2.201995
C	7.442469	1.791081	-0.989269
O	0.240442	-2.492201	-1.927110
C	0.417199	-1.989979	-3.262556
O	-2.417997	-2.953778	-2.617688
C	-2.369593	-4.370628	-2.371170
C	-4.981905	-1.448984	-2.255791
O	-4.449803	-1.899013	-0.996502
H	-2.552633	1.659018	2.040523
H	-0.330630	0.715626	1.919696
H	-0.810291	-0.717359	2.799529
H	-4.662568	-1.207284	1.424392
H	-1.263772	1.821602	4.178308
H	-3.010789	1.742629	4.455755
H	-2.005854	0.308764	4.725817
H	1.071030	-2.889701	1.311796
H	-3.182436	1.526431	-0.596986
H	-4.498804	3.471991	-1.401241
H	-7.804066	2.249746	1.021928
H	-6.484495	0.312526	1.847912
H	1.045302	1.065688	-1.885641
H	0.000981	1.390053	-0.514198
H	1.693683	2.890895	0.466425
H	4.114697	2.052564	0.906701
H	1.841192	4.644070	-1.273488
H	0.226054	3.919396	-1.278608
H	1.402687	3.470317	-2.525481
H	6.351801	-0.180892	2.883438
H	4.731110	0.460357	3.248266
H	5.050648	-1.293060	3.377702
H	3.745723	-4.650962	2.975768
H	2.143828	-3.888175	3.108936
H	2.684291	-4.571841	1.549782
H	8.553007	2.608084	-2.628609
H	6.829078	2.413942	-2.969007
H	7.386057	3.737365	-1.926735
H	8.165352	2.064634	-0.222899
H	7.577702	0.743823	-1.255008



H	0.653854	-0.923708	-3.241038
H	1.261863	-2.534768	-3.678467
H	-0.471891	-2.162276	-3.869395
H	-1.363940	-4.677761	-2.078006
H	-3.085997	-4.648951	-1.594730
H	-2.641209	-4.853427	-3.307791
H	-4.843109	-0.370956	-2.363378
H	-4.513018	-1.970747	-3.088318
H	-6.045951	-1.673498	-2.224645

B3LYP Energy = -2096.62059795 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf T

C	0.481905	1.963981	-0.783082
C	1.769833	2.419707	-1.100770
C	2.873620	1.874394	-0.443255
C	2.694231	0.930875	0.576070
C	1.405413	0.521774	0.927784
C	0.288462	1.025198	0.234462
O	3.563432	-0.160091	2.582833
C	2.508168	-1.128327	2.501120
C	1.215642	-0.434431	2.086384
C	3.915840	0.414234	1.316292
C	2.408825	-1.805065	3.855493
C	4.788117	-0.550162	0.514894
C	-1.103218	0.609788	0.600610
C	-1.706810	-0.523448	0.041869
C	-3.015574	-0.850795	0.420966
C	-3.697528	-0.090526	1.370864
C	-3.077185	1.025269	1.954838
C	-1.794403	1.372005	1.543552
C	4.297069	-1.334007	-0.529170
C	5.115580	-2.244303	-1.194692
C	6.435381	-2.352002	-0.799814
C	6.965465	-1.590255	0.228070
C	6.130165	-0.691653	0.879955
C	-0.977638	-1.410127	-0.942525
C	-1.580496	-2.807823	-0.985252
O	-2.993930	-2.692745	-1.211368
C	-3.697008	-2.094229	-0.127241
C	-1.018797	-3.676520	-2.093973
F	7.244423	-3.232030	-1.446607
O	-4.937526	-0.542188	1.750230
C	-6.046851	0.374299	1.729333
O	-3.782140	1.688912	2.917013
C	-3.192119	2.837013	3.523350
C	-5.107889	-1.877412	-0.691872
O	-6.015481	-2.657409	-0.525600
O	-5.186332	-0.781080	-1.452696
C	-6.297370	0.726387	-2.945423
C	-6.441930	-0.549761	-2.148477
O	-0.613879	2.525063	-1.394306
C	-0.779527	2.245674	-2.794347
O	1.946500	3.395455	-2.056786
C	1.780853	4.738058	-1.566798
C	4.675469	2.142212	-2.009145

O	4.147085	2.330445	-0.683625
H	2.775579	-1.878047	1.745932
H	0.462142	-1.185638	1.840557
H	0.820289	0.121513	2.943965
H	4.538455	1.269375	1.580220
H	1.606463	-2.545565	3.851710
H	3.343712	-2.310187	4.101648
H	2.195916	-1.069858	4.634571
H	-1.303644	2.234622	1.970971
H	3.265572	-1.232133	-0.840760
H	4.740686	-2.854894	-2.005623
H	8.006429	-1.699714	0.502636
H	6.530017	-0.089832	1.687508
H	-1.022888	-0.983019	-1.950464
H	0.080032	-1.474690	-0.679229
H	-1.423656	-3.302130	-0.015941
H	-3.814638	-2.826739	0.680589
H	-1.478590	-4.665333	-2.077393
H	0.059535	-3.795204	-1.971627
H	-1.208685	-3.222223	-3.068601
H	-6.940417	-0.246809	1.728317
H	-6.038505	1.019405	2.605059
H	-6.023561	0.984872	0.824105
H	-3.924017	3.200886	4.240233
H	-2.268664	2.578963	4.048155
H	-2.987967	3.616407	2.784603
H	-7.226619	0.924788	-3.483029
H	-6.091137	1.576142	-2.293101
H	-5.490896	0.643467	-3.675234
H	-6.643243	-1.410074	-2.788019
H	-7.241413	-0.482071	-1.409737
H	-0.906321	1.172782	-2.956977
H	-1.686992	2.763064	-3.098306
H	0.068206	2.612535	-3.372854
H	0.768709	4.887909	-1.185940
H	2.510009	4.952857	-0.782194
H	1.953875	5.396884	-2.415426
H	5.697993	2.512241	-1.976124
H	4.683092	1.080829	-2.266496
H	4.099328	2.701866	-2.744213

B3LYP Energy = -2096.62058368 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf U

C	0.556261	1.953561	-0.960404
C	1.861971	2.333618	-1.304469
C	2.942129	1.796520	-0.602238
C	2.723996	0.944421	0.487342
C	1.419367	0.615156	0.863528
C	0.324965	1.104363	0.126275
O	3.544652	-0.003767	2.583943
C	2.453101	-0.934352	2.582260
C	1.188867	-0.234434	2.095864
C	3.922040	0.440980	1.273011
C	2.321848	-1.479630	3.992205
C	4.748983	-0.628289	0.562122

C	-1.082825	0.772059	0.515655
C	-1.727388	-0.375992	0.038919
C	-3.044538	-0.631145	0.445926
C	-3.693420	0.222967	1.333091
C	-3.054906	1.384501	1.792857
C	-1.750547	1.639865	1.382745
C	4.224393	-1.470834	-0.417894
C	4.999036	-2.474142	-0.996535
C	6.309158	-2.615209	-0.580404
C	6.872277	-1.796358	0.384143
C	6.080352	-0.805075	0.950086
C	-1.034115	-1.358361	-0.878655
C	-1.699580	-2.727975	-0.835917
O	-3.106708	-2.564388	-1.071955
C	-3.780179	-1.876089	-0.024895
C	-1.177609	-3.687663	-1.887440
F	7.075435	-3.586995	-1.142282
O	-4.999670	-0.057763	1.662605
C	-5.253900	-0.412185	3.032530
O	-3.781677	2.192122	2.616686
C	-3.183207	3.398794	3.086563
C	-5.187456	-1.626228	-0.588269
O	-6.127379	-2.347980	-0.351174
O	-5.217355	-0.576328	-1.412298
C	-6.623121	-1.015475	-3.374585
C	-6.478034	-0.262220	-2.066762
O	-0.518447	2.502517	-1.617024
C	-0.672906	2.156884	-3.004023
O	2.080703	3.229510	-2.327594
C	1.966374	4.609337	-1.936013
C	4.751923	1.863188	-2.179115
O	4.233286	2.179160	-0.874271
H	2.694944	-1.760075	1.901452
H	0.412602	-0.978816	1.905281
H	0.805272	0.404999	2.898851
H	4.582326	1.287296	1.463093
H	1.490508	-2.185146	4.050573
H	3.234749	-1.996801	4.290328
H	2.136202	-0.667998	4.699076
H	-1.237618	2.527240	1.725044
H	3.201416	-1.342287	-0.747696
H	4.598243	-3.131046	-1.757343
H	7.904912	-1.934309	0.676728
H	6.505805	-0.158367	1.708370
H	-1.055604	-0.997211	-1.912696
H	0.018407	-1.453584	-0.603555
H	-1.564614	-3.167717	0.162615
H	-3.922613	-2.555314	0.824818
H	-1.680629	-4.652321	-1.810790
H	-0.105414	-3.845921	-1.756243
H	-1.348564	-3.286042	-2.888308
H	-6.304731	-0.689036	3.080960
H	-4.639134	-1.266183	3.329338
H	-5.061198	0.431285	3.695072
H	-3.936809	3.880363	3.704654
H	-2.295177	3.194260	3.690531

H	-2.917506	4.059081	2.257191
H	-7.543396	-0.701795	-3.872452
H	-5.785192	-0.803596	-4.040450
H	-6.676025	-2.091371	-3.206606
H	-7.292485	-0.487918	-1.380186
H	-6.431028	0.812999	-2.228597
H	-0.772764	1.075046	-3.119562
H	-1.591991	2.638140	-3.331240
H	0.167675	2.516547	-3.596886
H	2.174879	5.198518	-2.826803
H	0.957790	4.827226	-1.579224
H	2.696063	4.849239	-1.159257
H	5.792601	2.180132	-2.169287
H	4.703629	0.786431	-2.355565
H	4.206470	2.395011	-2.957062

B3LYP Energy = -2096.62053124 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf V

C	0.565702	2.053524	-0.750673
C	1.875720	2.490270	-0.996842
C	2.940144	1.881925	-0.329983
C	2.698886	0.889868	0.628920
C	1.388358	0.495302	0.909076
C	0.310956	1.064754	0.203878
O	3.464174	-0.326563	2.605354
C	2.391276	-1.262542	2.431703
C	1.131937	-0.515381	2.007317
C	3.878437	0.304425	1.385394
C	2.225042	-2.007998	3.742720
C	4.758144	-0.638218	0.566552
C	-1.102618	0.666095	0.497928
C	-1.700506	-0.440964	-0.117206
C	-3.020067	-0.771999	0.221444
C	-3.718361	-0.032085	1.171319
C	-3.130343	1.095960	1.762800
C	-1.821943	1.424400	1.424544
C	4.292119	-1.347363	-0.540454
C	5.114784	-2.241165	-1.223018
C	6.413079	-2.408599	-0.780532
C	6.918184	-1.721658	0.310686
C	6.079226	-0.837932	0.977982
C	-0.954365	-1.306657	-1.107177
C	-1.570865	-2.696282	-1.205343
O	-2.976351	-2.560628	-1.467467
C	-3.705458	-1.983272	-0.390328
C	-0.987345	-3.540423	-2.321773
F	7.226033	-3.273329	-1.442856
O	-5.022096	-0.383908	1.435308
C	-5.293283	-0.887227	2.754466
O	-3.905974	1.798683	2.636616
C	-3.365819	2.981700	3.223015
C	-5.095071	-1.713764	-0.988757
O	-6.022995	-2.477891	-0.863826
O	-5.116264	-0.598292	-1.722191
C	-7.289668	0.536255	-1.554078

C	-6.347287	-0.269898	-2.425960
O	-0.489751	2.681197	-1.368469
C	-0.625181	2.461122	-2.782305
O	2.111032	3.507626	-1.894708
C	1.967961	4.828509	-1.342430
C	4.807059	2.191401	-1.811240
O	4.232925	2.315582	-0.497118
H	2.670590	-1.977303	1.647540
H	0.371307	-1.233589	1.694226
H	0.717724	0.005092	2.878277
H	4.509737	1.128690	1.717885
H	1.407942	-2.728634	3.669339
H	3.138769	-2.547360	3.995531
H	1.998738	-1.310552	4.552125
H	-1.344166	2.284039	1.872169
H	3.278057	-1.198622	-0.888330
H	4.759742	-2.793569	-2.083136
H	7.943218	-1.875867	0.621291
H	6.459494	-0.293769	1.834403
H	-0.969702	-0.850713	-2.103207
H	0.095559	-1.390649	-0.819560
H	-1.445345	-3.218489	-0.246046
H	-3.864624	-2.740007	0.387811
H	-1.456862	-4.524532	-2.344692
H	0.086050	-3.673388	-2.173534
H	-1.146367	-3.058020	-3.288348
H	-6.337753	-1.191022	2.751970
H	-4.663155	-1.753847	2.971556
H	-5.133624	-0.114813	3.506434
H	-4.153366	3.383491	3.855610
H	-2.487662	2.758648	3.834718
H	-3.102403	3.717297	2.458824
H	-8.163714	0.825577	-2.142134
H	-7.630137	-0.045642	-0.697911
H	-6.804591	1.443497	-1.191540
H	-6.011959	0.304952	-3.287242
H	-6.809669	-1.194718	-2.767926
H	0.260578	2.799257	-3.320261
H	-0.807389	1.403740	-2.988417
H	-1.491301	3.040538	-3.094942
H	0.949313	4.988587	-0.983868
H	2.679060	4.982821	-0.527600
H	2.184456	5.523227	-2.151519
H	5.836668	2.530148	-1.717904
H	4.797791	1.147362	-2.131717
H	4.274072	2.809162	-2.532045

B3LYP Energy = -2096.62051940 a.u.

(aS,1S,3S,1'S,3'S)-22, Conf W

C	0.754381	1.992138	-1.022161
C	2.090282	2.321869	-1.295212
C	3.110452	1.735211	-0.544407
C	2.803636	0.880392	0.521642
C	1.469248	0.599806	0.825929
C	0.434703	1.141727	0.040622

O	3.474637	-0.120379	2.647725
C	2.350083	-1.007661	2.575555
C	1.140986	-0.253605	2.032677
C	3.938735	0.327416	1.365681
C	2.123746	-1.563603	3.969222
C	4.771363	-0.758108	0.687663
C	-1.003275	0.863939	0.355376
C	-1.673188	-0.245532	-0.174339
C	-3.015917	-0.451570	0.168844
C	-3.668199	0.407955	1.047765
C	-3.004645	1.533826	1.557806
C	-1.674211	1.742598	1.208906
C	6.088841	-0.949354	1.113799
C	6.882728	-1.956263	0.578772
C	6.335196	-2.776507	-0.393338
C	5.038846	-2.621941	-0.846628
C	4.262506	-1.602750	-0.299234
C	-0.984735	-1.247173	-1.072995
C	-1.695477	-2.594314	-1.042654
O	-3.083255	-2.389976	-1.350853
C	-3.791553	-1.641222	-0.369163
C	-1.157059	-3.586656	-2.054998
F	7.103321	-3.763494	-0.925448
O	-4.995491	0.164739	1.321613
C	-5.312787	-0.186508	2.679090
O	-3.732296	2.355349	2.366779
C	-3.108313	3.531305	2.879356
C	-5.079822	-1.222153	-1.095988
O	-5.158424	-0.294352	-1.862650
O	-6.074278	-2.078348	-0.824803
C	-8.243014	-0.929828	-0.722309
C	-7.346870	-1.872517	-1.501319
O	-0.262783	2.590976	-1.724483
C	-0.366945	2.258899	-3.119694
O	2.400041	3.214986	-2.296747
C	2.286915	4.596911	-1.911632
C	5.002755	1.734495	-2.020255
O	4.427324	2.071973	-0.744996
H	2.595867	-1.834690	1.897737
H	0.348254	-0.964829	1.790404
H	0.739870	0.390747	2.823076
H	4.613780	1.149582	1.603913
H	1.264936	-2.237951	3.974574
H	2.999740	-2.118310	4.307879
H	1.931270	-0.753712	4.676239
H	-1.141467	2.601494	1.591337
H	6.502377	-0.300757	1.877043
H	7.905118	-2.104813	0.900645
H	4.650459	-3.280357	-1.612546
H	3.250974	-1.464073	-0.658693
H	-0.970135	-0.890109	-2.108447
H	0.056845	-1.372362	-0.770096
H	-1.621649	-3.022054	-0.032641
H	-4.070155	-2.300481	0.461547
H	-1.696816	-4.532228	-1.990608
H	-0.098835	-3.780152	-1.869189

H	-1.265297	-3.194108	-3.068069
H	-6.374788	-0.421958	2.688469
H	-4.742554	-1.065490	2.992049
H	-5.112217	0.644670	3.354404
H	-3.868156	4.033230	3.473129
H	-2.254746	3.284153	3.516223
H	-2.783425	4.191799	2.071598
H	-9.209729	-0.854186	-1.225278
H	-8.413500	-1.301308	0.289409
H	-7.809564	0.068429	-0.662931
H	-7.150959	-1.500170	-2.505686
H	-7.776867	-2.870469	-1.564675
H	-1.252430	2.774792	-3.484248
H	0.512537	2.590630	-3.671261
H	-0.500840	1.182242	-3.246991
H	2.961868	4.819659	-1.082037
H	2.574735	5.181636	-2.783039
H	1.259731	4.837188	-1.630760
H	4.935574	0.658110	-2.193275
H	4.510723	2.275496	-2.827043
H	6.049434	2.025081	-1.960083

B3LYP Energy = -2096.62044233 a.u.

(*aR*,1*S*,3*S*,1'*S*,3'*S*)-**22**, Conf A

C	-0.973719	2.046342	0.660274
C	-2.251156	2.488750	0.289729
C	-3.103403	1.623626	-0.398024
C	-2.665612	0.345211	-0.766711
C	-1.373737	-0.073000	-0.436591
C	-0.522548	0.775842	0.295956
O	-2.887610	-1.585173	-2.248116
C	-2.010131	-2.331506	-1.391858
C	-0.883333	-1.426563	-0.906618
C	-3.599963	-0.541208	-1.571292
C	-1.510846	-3.524152	-2.185907
C	-4.772222	-1.118183	-0.780173
C	0.860146	0.346308	0.678077
C	1.954351	0.595670	-0.158129
C	3.221140	0.146761	0.235290
C	3.402620	-0.501703	1.453480
C	2.303798	-0.766566	2.283781
C	1.042589	-0.332952	1.885151
C	-4.729614	-1.335542	0.597203
C	-5.800720	-1.922069	1.268128
C	-6.916613	-2.282319	0.537054
C	-7.003392	-2.080283	-0.830147
C	-5.921868	-1.497579	-1.479112
C	1.811709	1.367472	-1.449647
C	3.142996	1.964452	-1.886662
O	4.131648	0.921315	-1.916754
C	4.441965	0.385957	-0.635975
C	3.103556	2.580342	-3.271650
F	-7.969648	-2.849552	1.183046
O	4.667508	-0.945645	1.768682

C	5.304458	-0.304689	2.886868
O	2.562368	-1.448129	3.436505
C	1.468253	-1.791793	4.283718
C	5.192770	-0.915386	-0.958115
O	4.661447	-1.949784	-1.279379
O	6.517224	-0.727338	-0.908653
C	8.796191	-1.424567	-1.148635
C	7.353900	-1.863168	-1.260668
O	-0.111739	2.913739	1.291612
C	-0.419937	3.213106	2.662699
O	-2.666085	3.762163	0.610658
C	-2.234569	4.775690	-0.314704
C	-5.307368	2.399717	0.164588
O	-4.339115	2.034579	-0.835658
H	-2.583575	-2.691502	-0.528529
H	-0.333016	-1.928219	-0.108389
H	-0.169360	-1.282225	-1.725271
H	-4.019958	0.057192	-2.380018
H	-0.816096	-4.115591	-1.586307
H	-2.343160	-4.163887	-2.482388
H	-0.990843	-3.191309	-3.086646
H	0.180829	-0.525793	2.508190
H	-3.856997	-1.038145	1.164266
H	-5.773752	-2.093916	2.336183
H	-7.897846	-2.370559	-1.365569
H	-5.973217	-1.335027	-2.549209
H	1.443147	0.716133	-2.249927
H	1.077910	2.165975	-1.326315
H	3.458355	2.721588	-1.155085
H	5.135470	1.058237	-0.116613
H	4.076627	2.996536	-3.535568
H	2.363542	3.382076	-3.307186
H	2.834309	1.827972	-4.015701
H	6.313837	-0.708176	2.930094
H	5.351053	0.777038	2.734733
H	4.777484	-0.525643	3.814820
H	1.900965	-2.338946	5.117548
H	0.959091	-0.900692	4.660708
H	0.750167	-2.431647	3.764271
H	9.450096	-2.259180	-1.408782
H	9.009104	-0.598770	-1.829041
H	9.033484	-1.109280	-0.131491
H	7.121768	-2.684265	-0.581277
H	7.100587	-2.177338	-2.273930
H	0.333583	3.924545	2.994605
H	-1.411822	3.656988	2.753798
H	-0.357442	2.308929	3.273901
H	-2.645164	5.715923	0.048007
H	-1.144861	4.836360	-0.339634
H	-2.619985	4.570088	-1.316000
H	-4.975297	3.266003	0.734518
H	-6.219187	2.637892	-0.378977
H	-5.496309	1.558686	0.835339

B3LYP Energy = -2096.62272909 a.u.

(*aR*,1*S*,3*S*,1'*S*,3'*S*)-**22**, Conf B

C	-1.014459	2.036786	0.793859	H	-5.885805	-1.267946	-2.698651
C	-2.291899	2.480161	0.423766	H	1.447007	0.904375	-2.139851
C	-3.117788	1.642096	-0.326987	H	1.078479	2.297925	-1.135949
C	-2.652620	0.393250	-0.758303	H	3.453435	2.850064	-0.927242
C	-1.360477	-0.023078	-0.427375	H	5.098705	1.173433	0.052901
C	-0.536210	0.795698	0.367582	H	4.084891	3.253051	-3.284574
O	-2.813277	-1.451609	-2.351617	H	2.367822	3.616105	-3.050062
C	-1.940764	-2.232738	-1.521939	H	2.853347	2.103910	-3.834861
C	-0.838803	-1.340558	-0.961815	H	4.615000	-2.882614	1.244399
C	-3.557033	-0.461271	-1.628875	H	6.027232	-2.347529	2.188121
C	-1.406483	-3.369865	-2.372532	H	4.465383	-2.613953	3.005318
C	-4.731086	-1.104684	-0.893352	H	1.875771	-2.229030	5.238164
C	0.845546	0.363673	0.749511	H	0.954592	-0.801091	4.712378
C	1.949693	0.663564	-0.055927	H	0.708750	-2.374704	3.903389
C	3.211567	0.185860	0.318997	H	9.555102	-1.767389	-1.640147
C	3.384533	-0.534379	1.500544	H	8.970658	-0.129966	-1.965247
C	2.282859	-0.791685	2.331907	H	9.137133	-0.698061	-0.294492
C	1.022101	-0.359781	1.930227	H	7.320745	-2.394022	-0.694768
C	-4.713978	-1.384983	0.473041	H	7.154691	-1.826299	-2.359654
C	-5.784260	-2.028996	1.090501	H	-0.457245	2.158622	3.426907
C	-6.873446	-2.382550	0.317132	H	0.226712	3.792029	3.256531
C	-6.934568	-2.118872	-1.040973	H	-1.512035	3.527770	2.966357
C	-5.854370	-1.479343	-1.636364	H	-1.194132	4.874269	-0.016814
C	1.813495	1.508381	-1.302198	H	-2.631861	4.658969	-1.059219
C	3.144865	2.131167	-1.699036	H	-2.716895	5.712487	0.374856
O	4.136425	1.093264	-1.774151	H	-5.038325	3.197569	0.853988
C	4.440005	0.504382	-0.514078	H	-6.252272	2.595581	-0.306269
C	3.112488	2.817890	-3.050475	H	-5.521043	1.476424	0.866272
F	-7.925699	-3.005613	0.910928	B3LYP Energy = -2096.62266221 a.u.			
O	4.669939	-0.883695	1.843033	(aR,1S,3S,1'S,3'S)-22, Conf C			
C	4.945898	-2.276463	2.089834	C	-0.845211	2.195211	0.398354
O	2.535110	-1.440556	3.506382	C	-2.135554	2.567048	-0.003749
C	1.443709	-1.720466	4.379870	C	-2.980332	1.608937	-0.566503
C	5.248286	-0.744085	-0.893194	C	-2.522322	0.303148	-0.784123
O	4.768714	-1.806573	-1.209236	C	-1.217872	-0.048789	-0.426561
O	6.558577	-0.474412	-0.902635	C	-0.374199	0.897977	0.184034
C	8.860674	-0.993391	-1.307665	O	-2.727490	-1.801065	-2.009596
C	7.449200	-1.532681	-1.351368	C	-1.822690	-2.418945	-1.083079
O	-0.178354	2.880249	1.488910	C	-0.706819	-1.440515	-0.734265
C	-0.515052	3.096734	2.868837	C	-3.451270	-0.694118	-1.454650
O	-2.734665	3.726190	0.808140	C	-1.312857	-3.692366	-1.731606
C	-2.283151	4.801982	-0.033804	C	-4.597049	-1.190396	-0.575391
C	-5.342658	2.352375	0.238750	C	1.019130	0.544219	0.604281
O	-4.352687	2.056872	-0.763212	C	2.106004	0.713757	-0.260901
H	-2.525037	-2.650026	-0.692496	C	3.386187	0.355743	0.183002
H	-0.298726	-1.878049	-0.179869	C	3.582719	-0.128341	1.473622
H	-0.108919	-1.139743	-1.754219	C	2.490481	-0.318665	2.332641
H	-3.974722	0.175170	-2.409283	C	1.218605	0.028483	1.887091
H	-0.716523	-3.986069	-1.792631	C	-4.530811	-1.220788	0.817579
H	-2.222578	-4.002168	-2.724778	C	-5.576657	-1.739775	1.578054
H	-0.871417	-2.977661	-3.240035	C	-6.691257	-2.223204	0.919676
H	0.158714	-0.565912	2.546517	C	-6.801065	-2.207616	-0.460681
H	-3.862442	-1.092084	1.073557	C	-5.744671	-1.688823	-1.198999
H	-5.777090	-2.249705	2.149863	C	1.932169	1.298087	-1.644438
H	-7.808958	-2.405820	-1.610268				

C	3.245199	1.843205	-2.191028
O	4.257845	0.830965	-2.063196
C	4.600214	0.548515	-0.712434
C	3.177355	2.226916	-3.656193
F	-7.719754	-2.726055	1.652482
O	4.857082	-0.495459	1.841975
C	5.481525	0.303298	2.861690
O	2.766392	-0.846133	3.559846
C	1.684908	-1.074623	4.460569
C	5.539044	-0.663040	-0.805798
O	6.743818	-0.564762	-0.802664
O	4.873820	-1.808415	-0.965878
C	4.714419	-4.183062	-1.227068
C	5.668476	-3.016456	-1.110962
O	0.007117	3.145467	0.912023
C	-0.289495	3.597387	2.243107
O	-2.571080	3.861828	0.168174
C	-2.172463	4.765552	-0.877981
C	-5.189891	2.407713	-0.062198
O	-4.230964	1.940210	-1.028346
H	-2.374741	2.679734	-0.171388
H	-0.133364	-1.828085	0.109961
H	-0.009646	-1.385144	-1.577914
H	-3.897208	-0.209601	-2.323502
H	-0.602802	-4.196162	-1.072669
H	-2.138530	-4.375108	-1.936454
H	-0.808460	-3.465465	-2.673317
H	0.362011	-0.105475	2.532395
H	-3.659459	-0.827211	1.324899
H	-5.531709	-1.766254	2.658925
H	-7.693935	-2.589507	-0.938070
H	-5.814496	-1.671677	-2.280219
H	1.555022	0.536268	-2.336150
H	1.189470	2.097549	-1.620147
H	3.551465	2.714903	-1.595731
H	5.217117	1.364280	-0.314902
H	4.136279	2.620979	-3.995058
H	2.414382	2.992192	-3.811084
H	2.924071	1.357710	-4.266663
H	6.502773	-0.061623	2.946017
H	5.494514	1.356864	2.570392
H	4.966338	0.188577	3.815254
H	2.130807	-1.501878	5.355264
H	1.176908	-0.141519	4.718734
H	0.962460	-1.781014	4.043261
H	5.284561	-5.107488	-1.338343
H	4.092137	-4.269873	-0.335333
H	4.065622	-4.074913	-2.097440
H	6.296246	-2.912730	-1.997070
H	6.318748	-3.105928	-0.240014
H	0.461465	4.347381	2.483042
H	-1.283932	4.042040	2.294171
H	-0.212716	2.769011	2.952259
H	-2.592643	5.735726	-0.620383
H	-1.084579	4.839362	-0.930791
H	-2.571470	4.438098	-1.840805

H	-4.868930	3.346561	0.386132
H	-6.117146	2.553884	-0.612087
H	-5.344847	1.654348	0.713230

B3LYP Energy = -2096.62262112 a.u.

(*aR*,1*S*,3*S*,1'*S*,3'*S*)-**22**, Conf D

C	-1.044216	2.171366	0.251043
C	-2.350185	2.469385	-0.159959
C	-3.141628	1.462303	-0.714551
C	-2.662801	0.151138	-0.802958
C	-1.363098	-0.145518	-0.381633
C	-0.538214	0.872343	0.133361
O	-2.824534	-2.071248	-1.797788
C	-1.939637	-2.578550	-0.786852
C	-0.837318	-1.558971	-0.521963
C	-3.571162	-0.923963	-1.371943
C	-1.406165	-3.911091	-1.278047
C	-4.719292	-1.342776	-0.454022
C	0.859699	0.581168	0.584816
C	1.924970	0.516980	-0.321616
C	3.206914	0.224103	0.162956
C	3.430060	0.031788	1.522907
C	2.358934	0.075043	2.428097
C	1.085526	0.356985	1.945217
C	-4.711874	-1.134740	0.924379
C	-5.760265	-1.581134	1.726195
C	-6.816449	-2.236466	1.123098
C	-6.866400	-2.460560	-0.242527
C	-5.809124	-2.008655	-1.022258
C	1.745005	0.789383	-1.797544
C	3.057021	1.213202	-2.445405
O	4.057747	0.225421	-2.149321
C	4.401901	0.146066	-0.771056
C	2.976143	1.326229	-3.955336
F	-7.847261	-2.671624	1.895936
O	4.706699	-0.284914	1.929813
C	5.371631	0.688229	2.753714
O	2.656489	-0.173637	3.735420
C	1.594696	-0.165397	4.687798
C	5.143060	-1.195280	-0.657126
O	4.602053	-2.272012	-0.596806
O	6.468277	-1.015016	-0.708294
C	8.739316	-1.773999	-0.754743
C	7.294475	-2.210913	-0.673184
O	-0.280137	3.140967	0.856967
C	0.179449	4.209354	0.013640
O	-2.836118	3.751545	-0.032789
C	-3.580455	3.983561	1.176115
C	-4.596658	2.595804	-2.231481
O	-4.436018	1.714674	-1.104936
H	-2.514410	-2.739732	0.133469
H	-0.283637	-1.844574	0.374873
H	-0.120187	-1.597460	-1.348658
H	-4.016652	-0.542845	-2.291725
H	-0.714059	-4.334965	-0.547798

H	-2.222671	-4.617872	-1.431738	C	-5.789816	-1.895800	-1.295353
H	-0.873366	-3.784195	-2.222929	C	-6.856063	-2.437691	-0.588638
H	0.246454	0.406658	2.624085	C	-6.821046	-2.382965	0.794532
H	-3.885702	-0.610780	1.387122	C	-5.770981	-1.809079	1.485170
H	-5.761119	-1.421822	2.796528	C	-4.713524	-1.269595	0.755872
H	-7.714914	-2.972232	-0.677469	C	1.741448	1.021786	-1.661751
H	-5.831851	-2.178819	-2.092189	C	3.046791	1.540067	-2.250437
H	1.382361	-0.105825	-2.314446	O	4.064528	0.544456	-2.056179
H	0.992553	1.565404	-1.949574	C	4.404331	0.334475	-0.689545
H	3.379762	2.174505	-2.020820	C	2.971250	1.818636	-3.738892
H	5.109706	0.946622	-0.524963	F	-7.860655	-2.907632	1.496736
H	3.937776	1.631005	-4.370094	O	4.721939	-0.316276	1.951722
H	2.226885	2.067826	-4.238812	C	5.027916	-1.569673	2.593472
H	2.696914	0.366803	-4.395289	O	2.648882	-0.369935	3.778245
H	4.867617	0.796127	3.713652	C	1.591961	-0.365003	4.735845
H	6.381444	0.313570	2.906662	C	5.227720	-0.960335	-0.720334
H	5.414887	1.655716	2.246254	O	4.761819	-2.074530	-0.713511
H	2.055731	-0.393610	5.645533	O	6.532600	-0.687884	-0.833198
H	1.113928	0.814968	4.740512	C	8.840252	-1.271770	-1.091631
H	0.847278	-0.928103	4.454566	C	7.435522	-1.818418	-0.977934
H	9.386053	-2.653167	-0.729681	O	-0.330632	3.047263	1.223490
H	8.933931	-1.233026	-1.681967	C	0.146466	4.196020	0.505144
H	9.003712	-1.131636	0.086555	O	-2.878669	3.725500	0.370970
H	7.080901	-2.748158	0.251728	C	-3.632937	3.821816	1.591867
H	7.013242	-2.849759	-1.511240	C	-4.603198	2.797781	-1.960421
H	0.827699	3.822335	-0.776757	O	-4.445677	1.802496	-0.932803
H	-0.657749	4.752945	-0.424074	H	-2.492250	-2.737111	-0.164797
H	0.754744	4.873518	0.655488	H	-0.274410	-1.854690	0.204334
H	-4.458454	3.335678	1.220320	H	-0.087497	-1.425220	-1.480654
H	-2.950102	3.817057	2.052588	H	-3.979800	-0.305580	-2.363742
H	-3.895773	5.024654	1.146840	H	-0.663397	-4.234038	-0.988563
H	-5.664824	2.629644	-2.435106	H	-2.163439	-4.438911	-1.907709
H	-4.229203	3.595857	-2.003497	H	-0.818828	-3.515170	-2.599542
H	-4.072374	2.197572	-3.104305	H	0.236476	0.203013	2.692226
B3LYP Energy = -2096.62196716 a.u.				H	-5.801353	-1.932523	-2.378355
(aR,1S,3S,1'S,3'S)-22, Conf E				H	-7.700223	-2.889972	-1.092438
C	-1.072958	2.141353	0.503060	H	-5.783887	-1.782375	2.566876
C	-2.378268	2.469058	0.112652	H	-3.891936	-0.807472	1.287832
C	-3.152836	1.521136	-0.557563	H	1.398403	0.182256	-2.276343
C	-2.657981	0.232844	-0.784600	H	0.973157	1.793967	-1.730724
C	-1.359220	-0.094651	-0.383270	H	3.348801	2.453541	-1.719016
C	-0.549872	0.869191	0.247367	H	5.062415	1.143472	-0.349792
O	-2.781643	-1.869547	-2.018363	H	3.929316	2.184315	-4.110383
C	-1.906147	-2.474336	-1.054202	H	2.210317	2.574288	-3.943296
C	-0.817330	-1.480284	-0.666163	H	2.711182	0.909480	-4.284744
C	-3.546568	-0.781239	-1.483009	H	4.669786	-2.403040	1.985987
C	-1.355364	-3.743700	-1.676151	H	6.113391	-1.607129	2.659320
C	-4.706039	-1.306780	-0.637777	H	4.592185	-1.616203	3.589029
C	0.848181	0.546563	0.675674	H	2.057870	-0.598260	5.690061
C	1.920637	0.591872	-0.223081	H	1.114655	0.616424	4.795323
C	3.201344	0.251663	0.233217	H	0.840712	-1.124603	4.503982
C	3.421272	-0.090629	1.566581	H	9.543523	-2.099496	-1.201609
C	2.350319	-0.094460	2.475154	H	8.938821	-0.621379	-1.961857
C	1.074252	0.203898	2.010102	H	9.114603	-0.706068	-0.200053
				H	7.319425	-2.467348	-0.109087
				H	7.142850	-2.381500	-1.865055

H	0.840953	3.894369	-0.283147
H	-0.680066	4.763968	0.077805
H	0.675758	4.808005	1.232685
H	-4.500127	3.158649	1.563595
H	-3.004541	3.577965	2.451464
H	-3.965759	4.855216	1.665862
H	-5.669952	2.847503	-2.168135
H	-4.243637	3.769788	-1.624225
H	-4.069876	2.497708	-2.866455

B3LYP Energy = -2096.62184912 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf F

C	-0.898546	2.259515	0.227557
C	-2.216225	2.536382	-0.160586
C	-3.004776	1.513638	-0.690357
C	-2.511566	0.207475	-0.773458
C	-1.201082	-0.068491	-0.371936
C	-0.379224	0.965077	0.115331
O	-2.661209	-2.026985	-1.742949
C	-1.756016	-2.512095	-0.739787
C	-0.661096	-1.477394	-0.504298
C	-3.415406	-0.883652	-1.318726
C	-1.215934	-3.845101	-1.222640
C	-4.546741	-1.306688	-0.382399
C	1.030715	0.697842	0.544361
C	2.082204	0.650076	-0.379087
C	3.378980	0.387326	0.086016
C	3.625375	0.203330	1.443202
C	2.568029	0.230001	2.365162
C	1.281923	0.485953	1.902219
C	-5.639836	-1.982953	-0.931706
C	-6.681625	-2.440211	-0.134440
C	-6.612782	-2.210765	1.229470
C	-5.552823	-1.544817	1.814149
C	-4.520195	-1.093293	0.994990
C	1.864113	0.901365	-1.854374
C	3.154723	1.318046	-2.547636
O	4.174972	0.354079	-2.240268
C	4.560411	0.357653	-0.871103
C	3.036714	1.380541	-4.057888
F	-7.628129	-2.651236	2.019369
O	4.911491	-0.092503	1.834020
C	5.584752	0.903425	2.623456
O	2.891967	-0.006854	3.668349
C	1.848472	0.002907	4.640711
C	5.475880	-0.868072	-0.735353
O	6.681204	-0.800902	-0.794360
O	4.786021	-2.005161	-0.626983
C	4.576722	-4.383734	-0.445842
C	5.554849	-3.236144	-0.550170
O	-0.133354	3.243743	0.807195
C	0.285346	4.316701	-0.051851
O	-2.715907	3.813331	-0.035396
C	-3.463015	4.039797	1.173014
C	-4.503632	2.616091	-2.188920

O	-4.309103	1.745212	-1.059618
H	-2.314577	-2.667960	0.191373
H	-0.091110	-1.745806	0.387692
H	0.043578	-1.517597	-1.341747
H	-3.876769	-0.517088	-2.236555
H	-0.508998	-4.253003	-0.497425
H	-2.027116	-4.562134	-1.355329
H	-0.699046	-3.724390	-2.177183
H	0.453253	0.525354	2.594424
H	-5.677677	-2.156950	-2.000601
H	-7.532670	-2.959891	-0.554675
H	-5.539007	-1.381238	2.883748
H	-3.691384	-0.560997	1.443286
H	1.487771	-0.002857	-2.345461
H	1.105168	1.672621	-1.998110
H	3.476008	2.296600	-2.163096
H	5.203552	1.225143	-0.677036
H	3.982851	1.688658	-4.504390
H	2.267405	2.099076	-4.347122
H	2.765097	0.402678	-4.460590
H	5.102100	1.022548	3.593206
H	6.602335	0.543250	2.757623
H	5.604226	1.861653	2.097710
H	2.329941	-0.207958	5.592339
H	1.358595	0.978912	4.689705
H	1.104349	-0.770241	4.432076
H	5.127371	-5.324701	-0.387944
H	3.959645	-4.293033	0.449148
H	3.923618	-4.422914	-1.318798
H	6.177909	-3.310259	-1.442348
H	6.209619	-3.177562	0.320168
H	0.912332	3.936441	-0.862362
H	-0.572264	4.848980	-0.462788
H	0.872917	4.988529	0.570530
H	-4.335574	3.384727	1.217310
H	-2.831678	3.879138	2.049906
H	-3.786707	5.078257	1.142819
H	-5.575705	2.631871	-2.373188
H	-4.147786	3.623302	-1.974625
H	-3.989192	2.219897	-3.068429

B3LYP Energy = -2096.62184399 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf G

C	-1.000639	2.077041	0.709090
C	-2.273712	2.498828	0.301090
C	-3.087364	1.623924	-0.420351
C	-2.613498	0.357751	-0.786305
C	-1.325193	-0.039238	-0.417801
C	-0.514500	0.817912	0.350110
O	-2.747157	-1.559697	-2.294139
C	-1.885209	-2.298883	-1.416328
C	-0.792990	-1.378265	-0.883915
C	-3.503180	-0.538496	-1.629574
C	-1.337090	-3.473440	-2.205010
C	-4.687525	-1.149932	-0.883281



C	0.860384	0.407402	0.778221
C	1.982079	0.682160	-0.011742
C	3.237104	0.228267	0.412696
C	3.385032	-0.442719	1.626411
C	2.264647	-0.675794	2.439439
C	1.011853	-0.267878	1.990650
C	-5.798554	-1.560799	-1.625659
C	-6.886454	-2.175892	-1.018683
C	-6.845763	-2.378028	0.350690
C	-5.769480	-1.986664	1.123876
C	-4.691061	-1.368301	0.494439
C	1.870723	1.474113	-1.294732
C	3.208214	2.086046	-1.688367
O	4.206243	1.051780	-1.694345
C	4.483565	0.522888	-0.402243
C	3.203981	2.711521	-3.069545
F	-7.905566	-2.976963	0.955700
O	4.663727	-0.766875	2.015138
C	4.945981	-2.145577	2.324561
O	2.491433	-1.277904	3.643722
C	1.380974	-1.526105	4.502613
C	5.312742	-0.732965	-0.704464
O	4.847430	-1.810290	-0.989175
O	6.621494	-0.449695	-0.677424
C	7.802060	-1.512484	-2.547536
C	7.554020	-1.502862	-1.051836
O	-0.175201	2.955220	1.372781
C	-0.530554	3.240332	2.735434
O	-2.722155	3.761647	0.618639
C	-2.286425	4.789527	-0.288733
C	-5.321642	2.354670	0.079323
O	-4.316580	2.015038	-0.893241
H	-2.480258	-2.678319	-0.576341
H	-0.260932	-1.877390	-0.071696
H	-0.054149	-1.211434	-1.675958
H	-3.909753	0.060066	-2.444992
H	-0.654106	-4.060132	-1.587359
H	-2.146997	-4.123696	-2.538308
H	-0.790964	-3.121155	-3.082636
H	0.134992	-0.455036	2.593893
H	-5.814064	-1.397893	-2.696816
H	-7.751195	-2.490886	-1.587884
H	-5.778061	-2.159364	2.192107
H	-3.849415	-1.046993	1.094289
H	1.525305	0.833660	-2.114048
H	1.129292	2.266464	-1.177713
H	3.495566	2.840194	-0.942387
H	5.120778	1.223830	0.150452
H	4.180579	3.138254	-3.301675
H	2.458120	3.506971	-3.121254
H	2.963319	1.962376	-3.826636
H	6.026807	-2.205000	2.435581
H	4.458887	-2.446182	3.249413
H	4.627110	-2.790269	1.503403
H	0.658354	-2.201013	4.036161
H	1.794419	-1.998663	5.390157

H	0.882527	-0.595613	4.786665
H	8.558533	-2.264249	-2.783485
H	6.893464	-1.759214	-3.097280
H	8.166891	-0.542151	-2.887498
H	8.460308	-1.262368	-0.499177
H	7.161697	-2.457191	-0.703973
H	-1.530734	3.670297	2.798175
H	-0.475020	2.332531	3.341812
H	0.202726	3.958862	3.095955
H	-1.197716	4.869899	-0.286207
H	-2.643283	4.584609	-1.300721
H	-2.722719	5.719560	0.070244
H	-5.026738	3.227043	0.660264
H	-6.222912	2.572182	-0.489871
H	-5.509577	1.507936	0.743149

B3LYP Energy = -2096.62177992 a.u.

(*aR*,1*S*,3*S*,1'*S*,3'*S*)-**22**, Conf H

C	-0.960933	2.097715	0.500018
C	-2.233806	2.506099	0.078443
C	-3.075493	1.586693	-0.549364
C	-2.630736	0.284453	-0.810609
C	-1.342510	-0.102913	-0.431426
C	-0.503336	0.803272	0.243749
O	-2.830044	-1.759821	-2.134674
C	-1.962223	-2.432282	-1.210178
C	-0.843301	-1.488041	-0.785372
C	-3.553101	-0.666498	-1.553488
C	-1.451364	-3.683729	-1.899313
C	-4.735040	-1.181032	-0.734461
C	0.871492	0.408328	0.687067
C	1.984340	0.590614	-0.141526
C	3.243533	0.186457	0.319507
C	3.398146	-0.352375	1.593889
C	2.279910	-0.554401	2.416023
C	1.027152	-0.164489	1.951588
C	-4.710519	-1.287170	0.656245
C	-5.789436	-1.821113	1.357865
C	-6.894700	-2.242290	0.643373
C	-6.963615	-2.150487	-0.736608
C	-5.874641	-1.618335	-1.415837
C	1.866679	1.243092	-1.499567
C	3.204456	1.806491	-1.960905
O	4.199303	0.772714	-1.870905
C	4.484678	0.367411	-0.537861
C	3.193711	2.290568	-3.397788
F	-7.955139	-2.759133	1.318787
O	4.657390	-0.755192	1.978197
C	5.258943	-0.020939	3.057938
O	2.512090	-1.134631	3.628376
C	1.400040	-1.395267	4.481859
C	5.271184	-0.940902	-0.714563
O	4.768754	-2.008925	-0.963297
O	6.589258	-0.716886	-0.622748
C	7.844344	-1.986637	-2.305309

C	7.483567	-1.844487	-0.839540
O	-0.109106	3.012284	1.075848
C	-0.440031	3.419096	2.413368
O	-2.653967	3.800016	0.292261
C	-2.234326	4.732381	-0.719712
C	-5.287794	2.393779	-0.073098
O	-4.306749	1.958984	-1.032220
H	-2.545624	-2.724293	-0.327892
H	-0.301134	-1.922166	0.056820
H	-0.120077	-1.407508	-1.604623
H	-3.963196	-0.136042	-2.413144
H	-0.765983	-4.225082	-1.244134
H	-2.279792	-4.345433	-2.155726
H	-0.918002	-3.423854	-2.816137
H	0.151406	-0.309240	2.568228
H	-3.845985	-0.942989	1.208943
H	-5.776483	-1.906557	2.436544
H	-7.850225	-2.485391	-1.258844
H	-5.912175	-1.542225	-2.496110
H	1.517826	0.519714	-2.245118
H	1.126533	2.044422	-1.464371
H	3.498971	2.630845	-1.296299
H	5.148959	1.101985	-0.066945
H	4.170031	2.689214	-3.676454
H	2.449259	3.078859	-3.524828
H	2.947770	1.469980	-4.074799
H	5.296383	1.046323	2.823584
H	4.712305	-0.176757	3.987675
H	6.271731	-0.405902	3.155803
H	1.813548	-1.865760	5.370413
H	0.889270	-0.471088	4.765410
H	0.688030	-2.076881	4.009261
H	8.567335	-2.796901	-2.423156
H	6.966347	-2.223384	-2.906703
H	8.294815	-1.068713	-2.686081
H	8.358003	-1.610069	-0.235163
H	7.009150	-2.745192	-0.453240
H	-0.400671	2.563479	3.092643
H	0.315969	4.145355	2.705060
H	-1.427622	3.879934	2.450436
H	-2.630012	4.443326	-1.696086
H	-2.642255	5.699615	-0.432926
H	-1.144976	4.791607	-0.761670
H	-6.195060	2.583786	-0.642610
H	-5.478943	1.605234	0.658003
H	-4.966235	3.303221	0.432002

B3LYP Energy = -2096.62172130 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf I

C	-0.884471	2.193348	0.296974
C	-2.162853	2.540148	-0.161867
C	-2.993445	1.549229	-0.687765
C	-2.530492	0.232910	-0.813773
C	-1.236786	-0.096235	-0.401006
C	-0.409015	0.886112	0.174559

O	-2.705487	-1.941148	-1.916364
C	-1.824599	-2.501787	-0.932335
C	-0.718042	-1.503003	-0.613031
C	-3.442530	-0.803471	-1.447213
C	-1.297351	-3.810263	-1.490979
C	-4.610389	-1.246184	-0.568497
C	0.973067	0.556681	0.647841
C	2.081517	0.691088	-0.195848
C	3.349034	0.345672	0.291491
C	3.512751	-0.090621	1.603709
C	2.399622	-0.241497	2.443604
C	1.139984	0.091473	1.954326
C	-4.574172	-1.202370	0.825365
C	-5.639468	-1.674234	1.589433
C	-6.742901	-2.186109	0.933671
C	-6.822949	-2.244065	-0.447532
C	-5.747473	-1.771279	-1.189348
C	1.944966	1.227362	-1.602523
C	3.272846	1.756065	-2.128717
O	4.279927	0.746428	-1.947311
C	4.585479	0.493845	-0.581674
C	3.244424	2.100797	-3.604807
F	-7.790353	-2.642990	1.669820
O	4.775478	-0.452872	2.013901
C	5.383972	0.376684	3.018475
O	2.643557	-0.721127	3.697046
C	1.539649	-0.910791	4.579344
C	5.500893	-0.739051	-0.623715
O	6.706594	-0.664264	-0.588621
O	4.808827	-1.871321	-0.773586
C	5.936244	-3.401267	-2.327778
C	5.556609	-3.113960	-0.888324
O	-0.045426	3.174086	0.774541
C	-0.371498	3.695494	2.072836
O	-2.601310	3.842758	-0.081067
C	-2.154025	4.687201	-1.156844
C	-5.212881	2.384480	-0.294855
O	-4.231861	1.847970	-1.201108
H	-2.399857	-2.709007	-0.021352
H	-0.167036	-1.839899	0.267047
H	0.001171	-1.496083	-1.439869
H	-3.866217	-0.372391	-2.354420
H	-0.607429	-4.274332	-0.783302
H	-2.117180	-4.504447	-1.680226
H	-0.764935	-3.637724	-2.428812
H	0.267943	-0.015692	2.583798
H	-3.711146	-0.787409	1.329969
H	-5.617989	-1.643087	2.670902
H	-7.707933	-2.645997	-0.923141
H	-5.794042	-1.811428	-2.271218
H	1.587434	0.442701	-2.278957
H	1.201984	2.026512	-1.624748
H	3.564380	2.643096	-1.548925
H	5.209564	1.307355	-0.191165
H	4.212587	2.484704	-3.928666
H	2.487381	2.862855	-3.799528

H	3.005373	1.216267	-4.198743
H	6.398669	0.004409	3.141211
H	5.416319	1.418517	2.688913
H	4.844740	0.302979	3.962725
H	1.962312	-1.301779	5.501488
H	1.027891	0.032901	4.786355
H	0.825858	-1.632570	4.173590
H	6.432031	-4.373052	-2.383176
H	5.051164	-3.432785	-2.964975
H	6.621642	-2.646644	-2.714059
H	6.433347	-3.052765	-0.245429
H	4.876181	-3.868379	-0.497803
H	-0.307471	2.906554	2.826780
H	0.371637	4.460607	2.288164
H	-1.368293	4.137953	2.078868
H	-2.586758	5.668895	-0.974787
H	-1.064990	4.761459	-1.162385
H	-2.506563	4.304355	-2.117418
H	-4.912377	3.363854	0.073754
H	-6.132852	2.467165	-0.869627
H	-5.370068	1.700754	0.542149

B3LYP Energy = -2096.62160191 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf J

C	-0.962418	2.029259	0.721359
C	-2.251320	2.469670	0.390576
C	-3.105461	1.620827	-0.314899
C	-2.659519	0.362410	-0.738617
C	-1.357469	-0.052452	-0.446540
C	-0.502986	0.778801	0.302054
O	-2.885935	-1.514867	-2.286367
C	-1.985451	-2.281318	-1.473068
C	-0.860145	-1.381915	-0.974542
C	-3.597994	-0.504756	-1.559383
C	-1.487570	-3.439396	-2.317539
C	-4.749298	-1.123987	-0.769377
C	0.891793	0.353663	0.642823
C	1.968738	0.658536	-0.197512
C	3.249618	0.218600	0.158761
C	3.461108	-0.476172	1.345984
C	2.379232	-0.802078	2.176743
C	1.104444	-0.375698	1.815221
C	-5.907747	-1.490394	-1.460577
C	-6.970630	-2.108741	-0.813733
C	-6.856039	-2.359973	0.543216
C	-5.730458	-2.014226	1.266442
C	-4.678604	-1.391177	0.598072
C	1.792972	1.481588	-1.452788
C	3.105679	2.124498	-1.880576
O	4.115034	1.104800	-1.968532
C	4.453861	0.522007	-0.715587
C	3.034269	2.799029	-3.236720
F	-7.890653	-2.962314	1.187131
O	4.739915	-0.901770	1.627754
C	5.372434	-0.296500	2.767903

O	2.667081	-1.531403	3.292965
C	1.591998	-1.931605	4.139735
C	5.232128	-0.744920	-1.105729
O	4.719552	-1.779631	-1.454273
O	6.551793	-0.512162	-1.085919
C	7.826873	-2.474875	-0.343467
C	7.436106	-1.588245	-1.509680
O	-0.099773	2.883543	1.369982
C	-0.381315	3.117602	2.759331
O	-2.676417	3.723714	0.769082
C	-2.262132	4.781416	-0.113789
C	-5.307703	2.348073	0.315063
O	-4.353574	2.032483	-0.715170
H	-2.539655	-2.678171	-0.613418
H	-0.291323	-1.906034	-0.204265
H	-0.161319	-1.199420	-1.798734
H	-4.039062	0.117838	-2.338072
H	-0.778023	-4.045034	-1.750366
H	-2.318513	-4.076203	-2.624032
H	-0.984794	-3.069210	-3.213501
H	0.255720	-0.612665	2.440988
H	-5.981078	-1.289082	-2.522771
H	-7.871932	-2.389041	-1.342951
H	-5.681663	-2.224754	2.326769
H	-3.798866	-1.104340	1.159591
H	1.426351	0.857437	-2.275354
H	1.045050	2.258760	-1.286158
H	3.415234	2.855767	-1.120786
H	5.138472	1.187297	-0.175838
H	3.994208	3.248345	-3.494321
H	2.276184	3.584432	-3.227619
H	2.771664	2.073861	-4.009562
H	4.856508	-0.566397	3.689074
H	6.389391	-0.682248	2.787814
H	5.397876	0.791324	2.661079
H	2.046319	-2.510000	4.940341
H	1.075398	-1.067246	4.565709
H	0.875509	-2.558030	3.602032
H	8.540773	-3.227158	-0.686550
H	8.300663	-1.891670	0.447728
H	6.959687	-2.989967	0.069672
H	6.941988	-2.156008	-2.296390
H	8.300061	-1.072985	-1.925599
H	0.368746	3.825661	3.106012
H	-1.377450	3.541327	2.891652
H	-0.291749	2.188564	3.328353
H	-2.678082	5.700576	0.294021
H	-1.173358	4.853391	-0.145159
H	-2.654582	4.617062	-1.119981
H	-6.231937	2.595413	-0.202843
H	-5.474613	1.480176	0.956756
H	-4.975313	3.196289	0.911360

B3LYP Energy = -2096.62157562 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf K

C	-0.877208	2.154714	0.544558
C	-2.175886	2.542273	0.186397
C	-3.019161	1.620191	-0.435394
C	-2.553234	0.338331	-0.753622
C	-1.242043	-0.027036	-0.436426
C	-0.398678	0.880377	0.231755
O	-2.752799	-1.667522	-2.134233
C	-1.835156	-2.346467	-1.264675
C	-0.723883	-1.388138	-0.851373
C	-3.480207	-0.612195	-1.490933
C	-1.321139	-3.562495	-2.012591
C	-4.615867	-1.183869	-0.645023
C	1.001930	0.507974	0.609373
C	2.076055	0.740798	-0.257076
C	3.362787	0.355688	0.142609
C	3.579289	-0.213005	1.394604
C	2.500251	-0.465287	2.254209
C	1.220975	-0.094457	1.850783
C	-5.768227	-1.632897	-1.296790
C	-6.814815	-2.217504	-0.594545
C	-6.690264	-2.350331	0.778221
C	-5.570676	-1.919207	1.463848
C	-4.535103	-1.332153	0.739707
C	1.887057	1.426115	-1.591105
C	3.191765	2.028851	-2.094978
O	4.210658	1.015312	-2.068822
C	4.564924	0.598628	-0.755929
C	3.110549	2.544260	-3.518562
F	-7.708621	-2.919448	1.475890
O	4.859798	-0.600964	1.715964
C	5.497986	0.124976	2.780472
O	2.795750	-1.072599	3.439152
C	1.727033	-1.374825	4.333284
C	5.459497	-0.629886	-0.985339
O	6.666386	-0.572260	-0.996888
O	4.743406	-1.725635	-1.251552
C	5.794179	-3.745087	-0.329852
C	5.462671	-2.948213	-1.576337
O	-0.025281	3.074552	1.111299
C	-0.309249	3.434960	2.472920
O	-2.620749	3.817138	0.456334
C	-2.245467	4.796424	-0.528551
C	-5.230671	2.355949	0.149410
O	-4.277175	1.974443	-0.858975
H	-2.377642	-2.680209	-0.371262
H	-0.141107	-1.833779	-0.042869
H	-0.033993	-1.264469	-1.693713
H	-3.935944	-0.066060	-2.317113
H	-0.599828	-4.108114	-1.400819
H	-2.142698	-4.235748	-2.260729
H	-0.828695	-3.260196	-2.939285
H	0.374016	-0.276911	2.496844
H	-5.849468	-1.524665	-2.371908
H	-7.711103	-2.561805	-1.093628
H	-5.513763	-2.037785	2.537947
H	-3.660164	-0.979829	1.270495

H	1.520101	0.715016	-2.339891
H	1.133524	2.210798	-1.503075
H	3.496932	2.844794	-1.424869
H	5.215164	1.353018	-0.296094
H	4.065436	2.971335	-3.827484
H	2.344164	3.317731	-3.596631
H	2.854835	1.733615	-4.203948
H	6.521469	-0.240974	2.822659
H	5.503347	1.196760	2.565230
H	4.998319	-0.059546	3.731328
H	2.187308	-1.858876	5.191018
H	1.212767	-0.467638	4.661852
H	1.007003	-2.057967	3.875107
H	6.262106	-4.688563	-0.620194
H	6.486911	-3.202754	0.313311
H	4.891373	-3.970804	0.239267
H	4.778532	-3.491508	-2.225655
H	6.359530	-2.687121	-2.136203
H	-1.309618	3.858842	2.566094
H	-0.209200	2.564296	3.126323
H	0.433500	4.180159	2.750437
H	-2.675558	5.740580	-0.200308
H	-1.159241	4.888463	-0.586692
H	-2.650649	4.530552	-1.507607
H	-4.908277	3.253823	0.674206
H	-6.161465	2.547114	-0.380364
H	-5.380379	1.539001	0.858695

B3LYP Energy = -2096.62148517 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf L

C	-0.887273	2.195939	0.517307
C	-2.179266	2.560633	0.113836
C	-2.997181	1.613257	-0.503916
C	-2.510833	0.327731	-0.773220
C	-1.205047	-0.015390	-0.411649
C	-0.388047	0.918439	0.252908
O	-2.654001	-1.718100	-2.101230
C	-1.754317	-2.362666	-1.188279
C	-0.662950	-1.382148	-0.774416
C	-3.408860	-0.653158	-1.506889
C	-1.210935	-3.595914	-1.885612
C	-4.559987	-1.214447	-0.674626
C	1.004434	0.569625	0.679847
C	2.107004	0.821552	-0.144127
C	3.381986	0.440156	0.294199
C	3.564201	-0.138001	1.550492
C	2.461312	-0.354251	2.391167
C	1.191276	-0.016917	1.932933
C	-4.521789	-1.305447	0.716721
C	-5.569832	-1.882722	1.430835
C	-6.658312	-2.362811	0.727931
C	-6.740200	-2.287857	-0.652437
C	-5.682104	-1.711545	-1.344130
C	1.951318	1.510299	-1.481164
C	3.261563	2.131803	-1.944520

O	4.294274	1.134378	-1.880487
C	4.610621	0.733652	-0.552035
C	3.218657	2.640962	-3.372061
F	-7.688555	-2.923012	1.415271
O	4.857928	-0.387610	1.937515
C	5.195884	-1.705395	2.405687
O	2.721936	-0.867577	3.629346
C	1.631430	-1.082850	4.521982
C	5.574230	-0.444243	-0.751708
O	6.776536	-0.328615	-0.726799
O	4.933175	-1.581417	-1.042066
C	4.823513	-3.868365	-1.744755
C	5.753366	-2.727646	-1.399839
O	-0.060436	3.139051	1.082544
C	-0.381970	3.528154	2.427750
O	-2.642722	3.837927	0.336735
C	-2.250962	4.793816	-0.664607
C	-5.229379	2.346568	0.000733
O	-4.246945	1.942005	-0.970163
H	-2.317286	-2.674968	-0.299676
H	-0.097579	-1.798564	0.061513
H	0.047727	-1.275043	-1.601808
H	-3.848928	-0.135402	-2.359408
H	-0.502663	-4.117409	-1.238550
H	-2.020618	-4.282800	-2.135519
H	-0.695885	-3.317370	-2.807441
H	0.328185	-0.186586	2.560799
H	-3.671001	-0.914833	1.259799
H	-5.546188	-1.956388	2.510204
H	-7.613357	-2.669218	-1.165387
H	-5.730155	-1.648087	-2.424811
H	1.614662	0.797376	-2.242395
H	1.185765	2.284962	-1.412792
H	3.532561	2.954311	-1.267867
H	5.203899	1.517014	-0.064574
H	4.176360	3.081680	-3.651698
H	2.443346	3.402132	-3.478079
H	2.997525	1.823878	-4.061937
H	6.279837	-1.772650	2.337374
H	4.874748	-1.850126	3.434828
H	4.740450	-2.466342	1.768170
H	2.070112	-1.483274	5.432569
H	1.114210	-0.147214	4.750033
H	0.918641	-1.805173	4.115087
H	5.412595	-4.744280	-2.023395
H	4.195158	-4.135820	-0.893859
H	4.179347	-3.607544	-2.585501
H	6.385551	-2.447104	-2.243019
H	6.401203	-2.969139	-0.556241
H	-0.294471	2.672862	3.102835
H	0.349443	4.283485	2.707710
H	-1.386684	3.948264	2.485086
H	-2.695779	5.742822	-0.371902
H	-1.164397	4.893237	-0.699221
H	-2.630400	4.499100	-1.645749
H	-4.931327	3.267034	0.500077

H	-6.149523	2.505255	-0.557572
H	-5.385366	1.553824	0.735687

B3LYP Energy = -2096.62144283 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf M

C	-1.017258	2.051213	0.779563
C	-2.305739	2.471555	0.420978
C	-3.125277	1.616557	-0.317438
C	-2.643918	0.373734	-0.748205
C	-1.341829	-0.019880	-0.428483
C	-0.523178	0.815848	0.354513
O	-2.789050	-1.478848	-2.333950
C	-1.895621	-2.242681	-1.510506
C	-0.803585	-1.330593	-0.963010
C	-3.542319	-0.498732	-1.607038
C	-1.350086	-3.372998	-2.362989
C	-4.698476	-1.159171	-0.858353
C	0.868797	0.407659	0.725598
C	1.961437	0.722330	-0.089590
C	3.235070	0.268072	0.276519
C	3.429795	-0.441585	1.461402
C	2.338567	-0.712220	2.302934
C	1.067183	-0.306357	1.908382
C	-5.822555	-1.554465	-1.589403
C	-6.885948	-2.210660	-0.982006
C	-6.807145	-2.470005	0.376027
C	-5.716631	-2.096114	1.137862
C	-4.663428	-1.435704	0.508470
C	1.802498	1.566081	-1.333519
C	3.116320	2.231078	-1.718705
O	4.134021	1.220769	-1.810934
C	4.451642	0.607489	-0.564553
C	3.067129	2.939378	-3.058486
F	-7.842784	-3.109395	0.981505
O	4.723074	-0.764087	1.799821
C	5.023423	-2.149356	2.058732
O	2.610408	-1.346098	3.481374
C	1.530641	-1.635972	4.365885
C	5.264858	-0.624620	-0.988987
O	4.798977	-1.711163	-1.234261
O	6.554148	-0.294706	-1.138124
C	8.119622	-2.118769	-0.627062
C	7.457020	-1.285444	-1.705892
O	-0.187691	2.912560	1.460423
C	-0.512121	3.131702	2.842859
O	-2.764741	3.712099	0.804144
C	-2.346031	4.789544	-0.052461
C	-5.355711	2.290905	0.268765
O	-4.371295	2.009292	-0.742609
H	-2.464930	-2.667672	-0.674589
H	-0.248055	-1.856563	-0.184071
H	-0.083864	-1.120511	-1.762284
H	-3.977970	0.128161	-2.385319
H	-0.644780	-3.976016	-1.787664
H	-2.158615	-4.019824	-2.706182

H	-0.829356	-2.974343	-3.236277	C	-5.615385	-1.727164	1.556543
H	0.212637	-0.523884	2.532991	C	-6.677233	-2.298746	0.882598
H	-5.867912	-1.346370	-2.651844	C	-6.752633	-2.318617	-0.500084
H	-7.760842	-2.513745	-1.542093	C	-5.716330	-1.742212	-1.223613
H	-5.695386	-2.314048	2.197608	C	1.938921	1.494768	-1.452991
H	-3.811156	-1.127336	1.100098	C	3.257352	2.114588	-1.896741
H	1.460750	0.954553	-2.176189	O	4.272776	1.097363	-1.895384
H	1.041955	2.330933	-1.167864	C	4.593994	0.624486	-0.593298
H	3.404908	2.944662	-0.934406	C	3.210070	2.698919	-3.294988
H	5.114305	1.267406	0.008556	F	-7.687850	-2.857249	1.601121
H	4.028828	3.401496	-3.285025	O	4.816773	-0.759186	1.794827
H	2.303657	3.719498	-3.044249	C	5.426828	-0.111951	2.924521
H	2.824874	2.233000	-3.855071	O	2.704010	-1.345940	3.417448
H	4.531283	-2.493792	2.965297	C	1.608557	-1.721582	4.249506
H	4.722992	-2.764915	1.208612	C	5.525562	-0.569485	-0.848580
H	6.103311	-2.196534	2.180880	O	6.730879	-0.485286	-0.814831
H	1.029635	-0.721743	4.694897	O	4.853010	-1.671306	-1.186282
H	0.802319	-2.305646	3.900784	C	4.677594	-3.958648	-1.871542
H	1.977586	-2.130509	5.224767	C	5.639234	-2.849487	-1.511506
H	8.859642	-2.778530	-1.085505	O	-0.010403	3.002494	1.241764
H	8.631746	-1.482809	0.096648	C	-0.295085	3.217225	2.634384
H	7.392548	-2.737539	-0.101382	O	-2.608913	3.793324	0.593707
H	6.899060	-1.905239	-2.406014	C	-1.975539	4.925158	-0.031819
H	8.187995	-0.692847	-2.253124	C	-4.604495	3.169553	-1.419328
H	-1.516825	3.542069	2.949718	O	-4.292947	1.943970	-0.739776
H	-0.427299	2.199126	3.406716	H	-2.440471	-2.674837	-0.369128
H	0.219210	3.845473	3.216553	H	-0.194244	-1.875019	-0.019018
H	-2.707589	4.632393	-1.071327	H	-0.062413	-1.288188	-1.661484
H	-2.790067	5.695105	0.356130	H	-3.973845	-0.023487	-2.260335
H	-1.258360	4.881713	-0.052721	H	-0.681103	-4.119048	-1.414862
H	-5.513219	1.413617	0.899975	H	-2.225247	-4.211918	-2.276726
H	-5.058867	3.142438	0.878913	H	-0.895757	-3.248161	-2.942265
H	-6.274756	2.517866	-0.267369	H	0.312641	-0.467214	2.471603
B3LYP Energy = -2096.62115145 a.u.				H	-3.756750	-0.693546	1.329194
(aR,1S,3S,1'S,3'S)-22, Conf N				H	-5.596748	-1.727260	2.638501
				H	-7.604931	-2.770601	-0.990302
				H	-5.759402	-1.751497	-2.306312
C	-0.854903	2.124855	0.595534	H	1.580343	0.830496	-2.247522
C	-2.141266	2.551817	0.229980	H	1.190470	2.280215	-1.335245
C	-2.993055	1.654518	-0.423048	H	3.549898	2.895477	-1.180731
C	-2.551909	0.358306	-0.727462	H	5.210238	1.370805	-0.076378
C	-1.254346	-0.040313	-0.400882	H	4.173540	3.134461	-3.562564
C	-0.394637	0.847932	0.270946	H	2.449572	3.480050	-3.351906
O	-2.792507	-1.632259	-2.117826	H	2.964733	1.923920	-4.024098
C	-1.888645	-2.340236	-1.256630	H	6.445084	-0.491297	2.974222
C	-0.761739	-1.408073	-0.826051	H	5.449079	0.971540	2.781133
C	-3.501168	-0.579861	-1.450241	H	4.895267	-0.353533	3.844825
C	-1.393608	-3.554530	-2.019731	H	2.043873	-2.270241	5.080975
C	-4.621174	-1.154941	-0.582970	H	1.078191	-0.845426	4.632063
C	0.993968	0.444338	0.661070	H	0.908150	-2.368975	3.715390
C	2.092648	0.730144	-0.157703	H	5.241049	-4.859529	-2.122397
C	3.367440	0.315315	0.250992	H	4.016041	-4.190490	-1.035705
C	3.547160	-0.343208	1.464179	H	4.068365	-3.685002	-2.734205
C	2.443460	-0.651870	2.272639	H	6.305800	-2.602043	-2.338637
C	1.177406	-0.245111	1.862591	H	6.250097	-3.104351	-0.644562
C	-4.587614	-1.153916	0.810443	H	0.432739	3.946279	2.984803

H	-1.304634	3.607218	2.773140
H	-0.175675	2.287859	3.196391
H	-2.469599	5.806441	0.371910
H	-0.911468	4.956747	0.198485
H	-2.117867	4.892700	-1.115074
H	-3.868029	3.378541	-2.198932
H	-5.578237	3.011596	-1.879329
H	-4.656128	4.005345	-0.724468

B3LYP Energy = -2096.62100273 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf O

C	-1.078735	2.200005	0.272861
C	-2.378416	2.464884	-0.178777
C	-3.127124	1.438343	-0.756445
C	-2.612779	0.139719	-0.829445
C	-1.319407	-0.123549	-0.368758
C	-0.536000	0.914361	0.170133
O	-2.690405	-2.087188	-1.824016
C	-1.821897	-2.571082	-0.787882
C	-0.754135	-1.523366	-0.492028
C	-3.477514	-0.958738	-1.421180
C	-1.240939	-3.889642	-1.262758
C	-4.639031	-1.405113	-0.533537
C	0.855669	0.659358	0.660258
C	1.947836	0.623411	-0.214877
C	3.221176	0.347185	0.301943
C	3.413250	0.148491	1.668279
C	2.321966	0.227589	2.548789
C	1.053917	0.460323	2.027848
C	-5.695566	-2.100784	-1.128433
C	-6.761359	-2.577718	-0.375669
C	-6.754063	-2.348362	0.989984
C	-5.731956	-1.663762	1.618782
C	-4.674377	-1.192578	0.843736
C	1.796358	0.897383	-1.694262
C	3.109647	1.361744	-2.309718
O	4.131334	0.404442	-1.987191
C	4.443288	0.347627	-0.598896
C	3.062452	1.473925	-3.821078
F	-7.793591	-2.808026	1.736435
O	4.705660	-0.021914	2.106415
C	5.005992	-1.210008	2.864532
O	2.593738	0.091586	3.879479
C	1.518660	0.202694	4.810070
C	5.283521	-0.931160	-0.477564
O	4.828907	-2.042954	-0.353893
O	6.587004	-0.648781	-0.598970
C	7.723729	-2.288786	-2.026758
C	7.525172	-1.761756	-0.619135
O	-0.360115	3.188119	0.903725
C	0.102238	4.268497	0.077183
O	-2.902456	3.733639	-0.068911
C	-3.649736	3.960694	1.138950
C	-4.565635	2.534318	-2.315820
O	-4.415528	1.657656	-1.184404

H	-2.418328	-2.747199	0.115846
H	-0.220431	-1.794081	0.421481
H	-0.012094	-1.544089	-1.297110
H	-3.907048	-0.590430	-2.353667
H	-0.557345	-4.294708	-0.513993
H	-2.034268	-4.617875	-1.436490
H	-0.687505	-3.749918	-2.193868
H	0.200966	0.519521	2.688203
H	-5.685227	-2.274561	-2.197972
H	-7.584358	-3.112479	-0.831394
H	-5.765972	-1.500906	2.688036
H	-3.875024	-0.645328	1.326244
H	1.471497	-0.005511	-2.222970
H	1.025209	1.651585	-1.860960
H	3.392997	2.331399	-1.876358
H	5.084029	1.197618	-0.334874
H	4.024973	1.805803	-4.212285
H	2.299952	2.194764	-4.122295
H	2.820296	0.507647	-4.268162
H	4.682629	-2.097900	2.317964
H	6.088662	-1.222573	2.972515
H	4.533905	-1.178568	3.843963
H	1.965587	0.074857	5.792887
H	1.043891	1.185481	4.752277
H	0.768968	-0.576553	4.649034
H	8.484590	-3.072354	-2.015076
H	6.801717	-2.715067	-2.422772
H	8.060647	-1.495166	-2.695257
H	8.444783	-1.339820	-0.218010
H	7.161108	-2.537956	0.052117
H	-0.732005	4.788389	-0.393837
H	0.633416	4.948449	0.740085
H	0.791844	3.899727	-0.686417
H	-4.505999	3.285112	1.196231
H	-3.011754	3.829020	2.015698
H	-3.999442	4.990179	1.094140
H	-5.628822	2.546361	-2.546292
H	-4.224464	3.541727	-2.079787
H	-4.011583	2.145920	-3.174613

B3LYP Energy = -2096.62099960 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf P

C	-0.996326	1.947295	0.861812
C	-2.268579	2.438139	0.529713
C	-3.117981	1.645791	-0.250246
C	-2.693644	0.387922	-0.701513
C	-1.408886	-0.070617	-0.404018
C	-0.547351	0.715586	0.382232
O	-2.938911	-1.421581	-2.319736
C	-2.069014	-2.242531	-1.525967
C	-0.932164	-1.390368	-0.974053
C	-3.643089	-0.437892	-1.550575
C	-1.584564	-3.377302	-2.408608
C	-4.797164	-1.083818	-0.783003
C	0.838417	0.254284	0.713056

C	1.924063	0.587199	-0.105558
C	3.197019	0.111448	0.232560
C	3.393363	-0.646725	1.383220
C	2.302831	-0.998994	2.191746
C	1.035448	-0.538865	1.845975
C	-5.881268	-1.575572	-1.516241
C	-6.948595	-2.208363	-0.891748
C	-6.915830	-2.342917	0.486211
C	-5.866433	-1.869787	1.249824
C	-4.806949	-1.237414	0.602207
C	1.764770	1.472969	-1.319641
C	3.088646	2.113749	-1.715143
O	4.081572	1.083205	-1.848825
C	4.408519	0.439233	-0.623220
C	3.030900	2.852159	-3.038291
F	-7.957004	-2.957957	1.108651
O	4.664155	-1.106397	1.647677
C	5.302179	-0.568449	2.818323
O	2.574798	-1.787957	3.270564
C	1.490510	-2.210632	4.094675
C	5.170894	-0.819875	-1.065042
O	4.649101	-1.826817	-1.476442
O	6.493699	-0.623434	-1.003117
C	8.778417	-1.281537	-1.294794
C	7.339565	-1.715226	-1.457688
O	-0.151777	2.719116	1.631718
C	-0.459184	2.749160	3.035192
O	-2.729010	3.631591	1.035217
C	-2.056174	4.822257	0.584629
C	-4.652136	3.291200	-1.142810
O	-4.404259	2.004643	-0.555868
H	-2.646414	-2.658420	-0.690831
H	-0.391051	-1.956878	-0.213828
H	-0.212687	-1.193527	-1.777012
H	-4.084002	0.219433	-2.300824
H	-0.899032	-4.022290	-1.855537
H	-2.425229	-3.980852	-2.753594
H	-1.058039	-2.983969	-3.280866
H	0.180167	-0.800391	2.452698
H	-5.890284	-1.464704	-2.594056
H	-7.792180	-2.587179	-1.453780
H	-5.880933	-1.989941	2.325153
H	-3.985902	-0.854070	1.193834
H	1.388237	0.895347	-2.171386
H	1.029651	2.253828	-1.116996
H	3.408253	2.803910	-0.921738
H	5.099697	1.070257	-0.051593
H	3.998140	3.298576	-3.272613
H	2.284803	3.647804	-2.993540
H	2.759580	2.168259	-3.845007
H	5.346017	0.522732	2.765230
H	4.778086	-0.874672	3.723385
H	6.312553	-0.971743	2.822466
H	1.932825	-2.834099	4.867668
H	0.986969	-1.359027	4.560090
H	0.765475	-2.798516	3.525910

H	9.438802	-2.083364	-1.630677
H	8.990443	-0.392415	-1.890418
H	9.007861	-1.065399	-0.250334
H	7.108751	-2.599452	-0.862330
H	7.093973	-1.931363	-2.498187
H	-1.455558	3.158132	3.210979
H	-0.390061	1.745879	3.462452
H	0.288883	3.390336	3.497117
H	-2.565140	5.654405	1.066539
H	-1.005324	4.812518	0.870612
H	-2.141703	4.922380	-0.500388
H	-4.652141	4.076727	-0.389612
H	-3.910144	3.513762	-1.913759
H	-5.636480	3.221607	-1.601880

B3LYP Energy = -2096.62099305 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf Q

C	-1.037349	2.208399	-0.024755
C	-2.339650	2.427843	-0.492791
C	-3.109248	1.342947	-0.915843
C	-2.614097	0.038765	-0.815339
C	-1.318201	-0.177720	-0.336730
C	-0.513738	0.913073	0.043809
O	-2.726548	-2.301067	-1.499856
C	-1.859076	-2.650198	-0.409639
C	-0.773636	-1.589319	-0.269024
C	-3.496355	-1.117650	-1.251181
C	-1.303103	-4.032163	-0.696394
C	-4.662183	-1.426578	-0.312107
C	0.879030	0.705694	0.552810
C	1.960119	0.527555	-0.319118
C	3.236056	0.318603	0.221404
C	3.438349	0.321973	1.598243
C	2.351698	0.480954	2.471429
C	1.084099	0.677651	1.934369
C	-5.727829	-2.181544	-0.810581
C	-6.799696	-2.540014	-0.002755
C	-6.789183	-2.130906	1.320149
C	-5.757987	-1.382252	1.853812
C	-4.694206	-1.032481	1.024628
C	1.802762	0.592957	-1.821362
C	3.121568	0.942255	-2.498870
O	4.126733	0.015735	-2.056236
C	4.447286	0.124844	-0.674011
C	3.068437	0.850920	-4.011573
F	-7.834736	-2.473462	2.119346
O	4.710806	0.080423	2.065378
C	5.353051	1.167458	2.753651
O	2.628391	0.422080	3.805358
C	1.551587	0.562901	4.730075
C	5.193316	-1.184038	-0.369556
O	4.654170	-2.242494	-0.159233
O	6.518787	-0.999863	-0.437146
C	7.606122	-2.895291	-1.555521
C	7.372178	-2.164015	-0.248173



O	-0.297266	3.264487	0.452970
C	0.179363	4.200224	-0.527070
O	-2.839061	3.709371	-0.554605
C	-3.656501	4.081448	0.569082
C	-4.540507	2.227227	-2.609451
O	-4.397936	1.524919	-1.361312
H	-2.452425	-2.686494	0.512309
H	-0.235813	-1.739390	0.669446
H	-0.038580	-1.732497	-1.067935
H	-3.923385	-0.871964	-2.224314
H	-0.615774	-4.336140	0.095520
H	-2.108730	-4.765242	-0.755588
H	-0.759235	-4.035987	-1.643439
H	0.233715	0.812106	2.587279
H	-5.720214	-2.496226	-1.847475
H	-7.629566	-3.120133	-0.384526
H	-5.789363	-1.078283	2.891888
H	-3.887680	-0.436658	1.431806
H	1.457977	-0.368692	-2.216986
H	1.044598	1.331365	-2.089066
H	3.426255	1.955669	-2.201256
H	5.146959	0.955933	-0.526454
H	4.034175	1.112275	-4.446015
H	2.315545	1.536206	-4.405691
H	2.810881	-0.163118	-4.323668
H	6.364791	0.830993	2.969807
H	5.392550	2.055466	2.116947
H	4.834609	1.401324	3.682928
H	1.997717	0.475514	5.717617
H	1.069155	1.539162	4.634256
H	0.808401	-0.227616	4.597246
H	8.302749	-3.719958	-1.388911
H	6.676616	-3.308423	-1.947618
H	8.038676	-2.228365	-2.302925
H	8.297819	-1.751641	0.149149
H	6.916624	-2.812171	0.498850
H	0.706953	4.974578	0.026211
H	0.874538	3.712891	-1.215644
H	-0.647424	4.642848	-1.082688
H	-3.975233	5.106296	0.389662
H	-4.531572	3.432564	0.643150
H	-3.078612	4.035313	1.494993
H	-4.170327	3.249016	-2.530166
H	-4.008232	1.700303	-3.405848
H	-5.605978	2.234437	-2.829207

B3LYP Energy = -2096.62094387 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf R

C	-1.017647	2.132695	0.446629
C	-2.332444	2.467448	0.096364
C	-3.136986	1.518029	-0.535580
C	-2.661184	0.222926	-0.763480
C	-1.351636	-0.110913	-0.404233
C	-0.514726	0.852928	0.188847
O	-2.847059	-1.892528	-1.966351

C	-1.938224	-2.493357	-1.030671
C	-0.829284	-1.502338	-0.694937
C	-3.583025	-0.793248	-1.413789
C	-1.419019	-3.771725	-1.661121
C	-4.709794	-1.300782	-0.514673
C	0.893617	0.524195	0.577404
C	1.939260	0.563871	-0.352983
C	3.235630	0.245225	0.073921
C	3.490692	-0.077626	1.403210
C	2.438275	-0.144366	2.328892
C	1.151648	0.167434	1.903192
C	-5.816514	-1.903720	-1.119324
C	-6.855806	-2.430116	-0.362548
C	-6.770415	-2.345257	1.016947
C	-5.696296	-1.756527	1.656139
C	-4.666442	-1.233273	0.877183
C	1.722839	0.978385	-1.790571
C	3.012022	1.498080	-2.413902
O	4.038645	0.507616	-2.240798
C	4.412942	0.294291	-0.884831
C	2.898867	1.767173	-3.901822
F	-7.783324	-2.854345	1.767967
O	4.781377	-0.406011	1.752508
C	5.441489	0.493480	2.659769
O	2.765734	-0.520062	3.598274
C	1.723838	-0.619370	4.567429
C	5.191675	-1.030117	-0.925195
O	4.678722	-2.121500	-0.953146
O	6.509434	-0.800228	-1.005669
C	7.800944	-2.459720	0.256816
C	7.391801	-1.953099	-1.112299
O	-0.242494	3.038935	1.131443
C	0.211247	4.181214	0.388180
O	-2.811753	3.731730	0.356221
C	-3.555527	3.843246	1.582398
C	-4.621570	2.786664	-1.908777
O	-4.439533	1.807059	-0.870187
H	-2.490859	-2.743835	-0.116645
H	-0.253943	-1.872618	0.156149
H	-0.132230	-1.457965	-1.538390
H	-4.049053	-0.325535	-2.281995
H	-0.704388	-4.260086	-0.995717
H	-2.239481	-4.463792	-1.855499
H	-0.916331	-3.554698	-2.606083
H	0.327208	0.137074	2.600934
H	-5.867413	-1.964027	-2.200069
H	-7.717409	-2.893311	-0.825206
H	-5.669561	-1.706656	2.736775
H	-3.826117	-0.760364	1.368918
H	1.371565	0.130715	-2.389115
H	0.948745	1.745636	-1.849195
H	3.322698	2.416269	-1.895601
H	5.104846	1.084225	-0.569088
H	3.847079	2.130976	-4.299579
H	2.132295	2.520778	-4.092200
H	2.626441	0.854098	-4.434913

H	4.950686	0.495886	3.632525
H	6.460114	0.125341	2.760995
H	5.459196	1.507076	2.250170
H	2.206532	-0.938293	5.487848
H	1.235919	0.345540	4.728223
H	0.978192	-1.362380	4.272977
H	8.499027	-3.291774	0.140607
H	8.297541	-1.675423	0.830260
H	6.936806	-2.813031	0.819411
H	6.888316	-2.725262	-1.691674
H	8.247519	-1.582041	-1.673472
H	-0.628658	4.752515	-0.007135
H	0.774090	4.793236	1.090149
H	0.870327	3.871530	-0.427005
H	-4.435501	3.197050	1.561524
H	-2.925621	3.588025	2.437634
H	-3.867507	4.883021	1.657781
H	-5.694235	2.845494	-2.080502
H	-4.239753	3.760020	-1.602056
H	-4.123222	2.465236	-2.827285

B3LYP Energy = -2096.62089225 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf S

C	-1.011793	1.906552	0.996663
C	-2.285509	2.418410	0.704085
C	-3.132909	1.687541	-0.135710
C	-2.699951	0.475751	-0.692919
C	-1.413502	-0.000541	-0.432946
C	-0.558412	0.717487	0.423195
O	-2.928001	-1.176509	-2.472402
C	-2.051555	-2.062907	-1.761071
C	-0.925454	-1.258893	-1.121184
C	-3.642618	-0.280438	-1.611669
C	-1.551513	-3.097740	-2.751429
C	-4.781943	-1.014365	-0.903306
C	0.816487	0.217361	0.742765
C	1.936576	0.647978	0.022939
C	3.189994	0.104023	0.330358
C	3.338669	-0.816535	1.367597
C	2.220813	-1.210531	2.119824
C	0.969420	-0.706607	1.778251
C	-5.849080	-1.477286	-1.678985
C	-6.900967	-2.184971	-1.111260
C	-6.870148	-2.423892	0.252629
C	-5.837623	-1.981938	1.056850
C	-4.793351	-1.273281	0.465896
C	1.825421	1.696136	-1.060612
C	3.164300	2.374617	-1.315707
O	4.159174	1.364269	-1.549207
C	4.436391	0.563780	-0.404908
C	3.159930	3.285987	-2.527531
F	-7.896206	-3.113476	0.819575
O	4.616696	-1.224786	1.669193
C	4.889973	-2.639593	1.677936
O	2.448282	-2.059059	3.165134

C	1.341072	-2.468893	3.964530
C	5.260850	-0.597223	-0.976806
O	4.794997	-1.582616	-1.496999
O	6.570314	-0.335637	-0.893290
C	8.887356	-0.805339	-1.274451
C	7.476486	-1.301103	-1.494375
O	-0.171267	2.619102	1.825355
C	-0.474272	2.533711	3.227795
O	-2.748362	3.566875	1.303154
C	-2.084051	4.791374	0.938790
C	-4.690478	3.393198	-0.864951
O	-4.423018	2.059123	-0.406685
H	-2.627019	-2.567705	-0.974751
H	-0.385202	-1.891669	-0.414777
H	-0.201778	-0.981644	-1.896219
H	-4.097289	0.437959	-2.294664
H	-0.866554	-3.792736	-2.261550
H	-2.385266	-3.667537	-3.163902
H	-1.020373	-2.613722	-3.573972
H	0.094352	-1.014441	2.332779
H	-5.856220	-1.284639	-2.745206
H	-7.731449	-2.542629	-1.705735
H	-5.853150	-2.184724	2.119693
H	-3.984955	-0.914391	1.089461
H	1.476628	1.245059	-1.996436
H	1.086595	2.446841	-0.775520
H	3.455196	2.947892	-0.424234
H	5.077144	1.124372	0.286650
H	4.136887	3.752136	-2.661756
H	2.414985	4.074286	-2.403502
H	2.918045	2.720199	-3.429604
H	4.576985	-3.090958	0.734565
H	5.969377	-2.728075	1.783624
H	4.392535	-3.129509	2.511966
H	1.754099	-3.125616	4.726160
H	0.860539	-1.613158	4.446054
H	0.603429	-3.018192	3.373604
H	9.592731	-1.510992	-1.717574
H	9.038417	0.168445	-1.742452
H	9.112002	-0.719855	-0.210326
H	7.306884	-2.271797	-1.027002
H	7.233890	-1.386877	-2.554361
H	-1.477531	2.909053	3.436321
H	-0.384512	1.501900	3.575716
H	0.263296	3.150984	3.736628
H	-2.595222	5.583136	1.482457
H	-1.032067	4.766246	1.219593
H	-2.174519	4.970337	-0.135709
H	-4.709642	4.099506	-0.037294
H	-3.947425	3.704667	-1.603334
H	-5.670166	3.352066	-1.337298

B3LYP Energy = -2096.62086968 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf T

C	-0.941585	2.267675	-0.007413
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C	-2.252724	2.483109	-0.452387
C	-3.022439	1.397204	-0.872992
C	-2.518725	0.095087	-0.790507
C	-1.214642	-0.117538	-0.332935
C	-0.410194	0.974588	0.043138
O	-2.625891	-2.238372	-1.495765
C	-1.742408	-2.592523	-0.420628
C	-0.661382	-1.526561	-0.283908
C	-3.400168	-1.062681	-1.224115
C	-1.182302	-3.968555	-0.727657
C	-4.549702	-1.389629	-0.271150
C	0.991779	0.770791	0.528284
C	2.061267	0.617816	-0.362567
C	3.348180	0.411022	0.154749
C	3.568609	0.388956	1.528819
C	2.493594	0.523727	2.420375
C	1.216818	0.721226	1.906138
C	-4.571482	-0.997711	1.066351
C	-5.620499	-1.363390	1.907464
C	-6.647247	-2.125817	1.384914
C	-6.667542	-2.533413	0.061612
C	-5.610469	-2.158862	-0.758238
C	1.873898	0.700600	-1.860997
C	3.178192	1.049496	-2.565953
O	4.193200	0.126683	-2.138688
C	4.547725	0.263071	-0.767602
C	3.094310	0.953559	-4.076862
F	-7.678335	-2.484077	2.195800
O	4.846673	0.142025	1.975573
C	5.502539	1.219711	2.666064
O	2.791287	0.441195	3.748488
C	1.730305	0.570985	4.692903
C	5.430715	-0.963334	-0.490294
O	6.637644	-0.928961	-0.538935
O	4.704880	-2.061948	-0.267084
C	5.684778	-4.018648	-1.377535
C	5.414601	-3.315348	-0.061741
O	-0.198522	3.322305	0.467741
C	0.245579	4.279416	-0.507319
O	-2.761380	3.761739	-0.493805
C	-3.566356	4.116514	0.644530
C	-4.485998	2.289685	-2.534866
O	-4.318932	1.574924	-1.296755
H	-2.323094	-2.641012	0.508802
H	-0.112221	-1.681156	0.647314
H	0.064953	-1.658369	-1.092792
H	-3.843174	-0.810467	-2.188387
H	-0.484265	-4.276610	0.053367
H	-1.984396	-4.705631	-0.784450
H	-0.650137	-3.960092	-1.681366
H	0.375117	0.838776	2.573375
H	-3.768652	-0.391106	1.464785
H	-5.644101	-1.060934	2.946183
H	-7.493650	-3.124606	-0.311220
H	-5.610513	-2.472302	-1.795517
H	1.514549	-0.255440	-2.257639

H	1.113451	1.444639	-2.105512
H	3.488222	2.064026	-2.277802
H	5.207045	1.131401	-0.646637
H	4.050233	1.215860	-4.531765
H	2.331622	1.635760	-4.457296
H	2.832563	-0.061988	-4.380678
H	5.524413	2.118005	2.043408
H	5.005193	1.436151	3.611112
H	6.520035	0.882615	2.851384
H	0.983651	-0.216767	4.562556
H	2.192775	0.470229	5.671611
H	1.247668	1.548944	4.617933
H	6.151253	-4.986543	-1.180698
H	4.756396	-4.191595	-1.923971
H	6.359502	-3.436412	-2.005443
H	6.335843	-3.109392	0.480940
H	4.746547	-3.896708	0.570960
H	0.787379	5.043934	0.045812
H	0.921166	3.808748	-1.226250
H	-0.598706	4.730036	-1.028917
H	-4.435757	3.460667	0.723634
H	-2.975747	4.065280	1.562102
H	-3.894644	5.140772	0.479714
H	-5.555013	2.293363	-2.736665
H	-4.119896	3.312523	-2.450832
H	-3.964427	1.773999	-3.345563

B3LYP Energy = -2096.62085627 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf U

C	-0.969577	2.068823	0.545532
C	-2.263250	2.474771	0.182578
C	-3.080292	1.581479	-0.516106
C	-2.653163	0.277455	-0.783336
C	-1.367845	-0.124376	-0.409766
C	-0.516304	0.779520	0.249873
O	-2.874563	-1.751022	-2.122432
C	-2.009155	-2.440780	-1.207147
C	-0.880548	-1.510691	-0.776075
C	-3.589062	-0.665105	-1.518946
C	-1.511593	-3.689897	-1.909662
C	-4.755260	-1.188511	-0.680899
C	0.873813	0.385278	0.643703
C	1.957916	0.592715	-0.216427
C	3.233512	0.187793	0.195709
C	3.432694	-0.374691	1.453314
C	2.343201	-0.601846	2.306627
C	1.073365	-0.212593	1.890269
C	-4.758676	-1.182684	0.713110
C	-5.826310	-1.714733	1.433294
C	-6.890186	-2.249944	0.733046
C	-6.929399	-2.273153	-0.651032
C	-5.853490	-1.738777	-1.348535
C	1.792614	1.273227	-1.555713
C	3.112833	1.849461	-2.050366
O	4.113169	0.817305	-2.013829

C	4.444538	0.388964	-0.698899
C	3.052923	2.361876	-3.476116
F	-7.939315	-2.767359	1.426203
O	4.706915	-0.774579	1.789115
C	5.336714	-0.051856	2.860532
O	2.618681	-1.203984	3.499113
C	1.536087	-1.495302	4.379968
C	5.227379	-0.913990	-0.923558
O	4.722492	-1.981582	-1.170300
O	6.546878	-0.691325	-0.882548
C	8.843372	-1.349299	-1.055310
C	7.412693	-1.829526	-1.143765
O	-0.090152	2.962109	1.109023
C	-0.341403	3.354153	2.464335
O	-2.647938	3.768229	0.440379
C	-3.792668	3.938163	1.296624
C	-4.365728	2.903292	-2.019696
O	-4.339396	1.959947	-0.932087
H	-2.593983	-2.734102	-0.326171
H	-0.342511	-1.957605	0.062134
H	-0.156219	-1.430430	-1.594359
H	-4.017175	-0.130537	-2.367372
H	-0.827875	-4.242669	-1.262358
H	-2.346287	-4.342686	-2.168586
H	-0.979601	-3.426074	-2.826188
H	0.218696	-0.376903	2.531061
H	-3.925203	-0.751894	1.252663
H	-5.835956	-1.712269	2.515371
H	-7.784203	-2.696004	-1.162378
H	-5.867933	-1.751662	-2.431993
H	1.419129	0.564650	-2.303512
H	1.053791	2.072870	-1.477934
H	3.427264	2.661597	-1.380012
H	5.122780	1.116719	-0.237019
H	4.018203	2.769803	-3.778865
H	2.302279	3.149760	-3.562252
H	2.787242	1.554034	-4.160992
H	5.357261	1.019188	2.641913
H	4.821420	-0.227157	3.804647
H	6.355393	-0.429047	2.920113
H	1.981237	-1.981501	5.244467
H	1.025262	-0.583215	4.700424
H	0.816502	-2.173363	3.913777
H	9.518715	-2.184773	-1.249515
H	9.042271	-0.570562	-1.793049
H	9.065255	-0.954802	-0.062598
H	7.194625	-2.603365	-0.406657
H	7.175402	-2.224041	-2.132518
H	-1.256474	3.940969	2.546266
H	-0.402070	2.477684	3.115092
H	0.506922	3.966282	2.764082
H	-4.694790	3.532129	0.840642
H	-3.623474	3.453835	2.261980
H	-3.898964	5.010896	1.442947
H	-3.899041	3.847289	-1.735297
H	-3.855510	2.492054	-2.894400

H -5.415703 3.065076 -2.253826  
 B3LYP Energy = -2096.62084443 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf V

C	-1.005399	2.037095	0.762326
C	-2.299347	2.454537	0.413440
C	-3.088528	1.617565	-0.380780
C	-2.634971	0.350436	-0.758504
C	-1.351139	-0.065442	-0.395672
C	-0.526452	0.785994	0.360790
O	-2.792856	-1.545525	-2.286708
C	-1.938436	-2.306055	-1.418512
C	-0.834200	-1.405291	-0.876764
C	-3.538684	-0.531312	-1.601659
C	-1.406237	-3.478479	-2.220891
C	-4.716237	-1.148376	-0.846843
C	0.862589	0.375310	0.740275
C	1.958222	0.677734	-0.075442
C	3.228460	0.223343	0.300370
C	3.416852	-0.476841	1.491644
C	2.322795	-0.736824	2.332108
C	1.054435	-0.327630	1.930800
C	-5.783831	-1.656891	-1.592747
C	-6.867491	-2.270784	-0.977593
C	-6.867768	-2.370029	0.403710
C	-5.835453	-1.879608	1.179773
C	-4.759246	-1.266452	0.541403
C	1.803228	1.501174	-1.333812
C	3.123433	2.136229	-1.747694
O	4.129825	1.111630	-1.811085
C	4.448250	0.548483	-0.542988
C	3.073994	2.800264	-3.109836
F	-7.924869	-2.966356	1.016767
O	4.708533	-0.803500	1.833549
C	5.004269	-2.188705	2.098710
O	2.589377	-1.364782	3.514957
C	1.506337	-1.643584	4.398993
C	5.276240	-0.692066	-0.904809
O	4.813480	-1.765721	-1.207987
O	6.582366	-0.402604	-0.915359
C	8.893796	-0.893349	-1.301011
C	7.490358	-1.453136	-1.346813
O	-0.147320	2.888996	1.414727
C	-0.430264	3.178360	2.789592
O	-2.712886	3.712170	0.781942
C	-3.868174	3.778493	1.638471
C	-4.370752	3.060197	-1.773311
O	-4.346021	2.012939	-0.785451
H	-2.538285	-2.685861	-0.582049
H	-0.309415	-1.920399	-0.069756
H	-0.092193	-1.239686	-1.666015
H	-3.955052	0.075196	-2.406574
H	-0.729120	-4.079848	-1.610983
H	-2.224513	-4.115477	-2.559349
H	-0.857444	-3.123524	-3.095796

H	0.197172	-0.535048	2.555210
H	-5.767412	-1.574064	-2.673031
H	-7.698539	-2.662113	-1.549602
H	-5.875477	-1.973027	2.257111
H	-3.950658	-0.870725	1.141950
H	1.440839	0.878526	-2.159588
H	1.058638	2.283304	-1.175380
H	3.425285	2.871917	-0.989278
H	5.097488	1.237939	0.010331
H	4.038868	3.244996	-3.356742
H	2.318218	3.587893	-3.117529
H	2.820359	2.069932	-3.880934
H	6.086824	-2.243809	2.193865
H	4.531751	-2.519754	3.020705
H	4.678474	-2.811089	1.263122
H	1.948887	-2.134975	5.261951
H	1.009366	-0.724712	4.721169
H	0.775484	-2.312377	3.936599
H	9.601214	-1.661135	-1.620244
H	8.995629	-0.036011	-1.967810
H	9.159695	-0.582432	-0.289671
H	7.370293	-2.308760	-0.681222
H	7.206093	-1.762314	-2.353404
H	-1.342856	3.765331	2.893459
H	-0.513470	2.255446	3.369762
H	0.415022	3.757496	3.155876
H	-4.755759	3.389971	1.140376
H	-3.693231	3.217462	2.560285
H	-4.004368	4.831560	1.875113
H	-5.419151	3.224915	-2.012452
H	-3.929366	3.979139	-1.385764
H	-3.835340	2.748313	-2.673627

B3LYP Energy = -2096.62079718 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf W

C	-0.934005	2.194921	0.426268
C	-2.254007	2.508461	0.075557
C	-3.047422	1.541722	-0.544345
C	-2.555363	0.250253	-0.758103
C	-1.240870	-0.062289	-0.398185
C	-0.414911	0.919057	0.181020
O	-2.717216	-1.883072	-1.932854
C	-1.799147	-2.459593	-0.991624
C	-0.701508	-1.450549	-0.672844
C	-3.465965	-0.785608	-1.392928
C	-1.266306	-3.740697	-1.605128
C	-4.583723	-1.295523	-0.484078
C	0.999459	0.613416	0.566962
C	2.041519	0.666543	-0.366940
C	3.345174	0.370375	0.056790
C	3.607233	0.054375	1.386486
C	2.558691	-0.025118	2.315627
C	1.266147	0.266081	1.893562
C	-4.534565	-1.214625	0.906922
C	-5.555174	-1.741327	1.695616

C	-6.626071	-2.347171	1.067050
C	-6.717185	-2.445456	-0.311191
C	-5.687043	-1.915294	-1.077797
C	1.809075	1.069340	-1.805781
C	3.086999	1.594684	-2.446920
O	4.126716	0.620157	-2.263528
C	4.519166	0.451357	-0.906556
C	2.959839	1.838149	-3.938055
F	-7.629861	-2.859945	1.827590
O	4.900774	-0.261075	1.733045
C	5.563877	0.651316	2.625379
O	2.896711	-0.392445	3.584692
C	1.862209	-0.488833	4.562028
C	5.424622	-0.790032	-0.934479
O	6.629174	-0.722726	-1.004070
O	4.719340	-1.923933	-0.961694
C	5.861584	-3.714354	0.274901
C	5.450451	-3.176788	-1.081796
O	-0.169047	3.117443	1.100294
C	0.263842	4.262187	0.348087
O	-2.749864	3.768631	0.323463
C	-3.488619	3.883887	1.552420
C	-4.552835	2.777189	-1.925791
O	-4.354291	1.809086	-0.879332
H	-2.346007	-2.703783	-0.072459
H	-0.119317	-1.802143	0.181556
H	-0.007971	-1.407975	-1.519435
H	-3.939777	-0.335523	-2.266176
H	-0.545676	-4.211836	-0.933670
H	-2.079030	-4.444728	-1.788591
H	-0.767670	-3.531307	-2.553999
H	0.444259	0.226280	2.593896
H	-3.697038	-0.728411	1.390374
H	-5.523975	-1.681007	2.775599
H	-7.576232	-2.921599	-0.765368
H	-5.742629	-1.985793	-2.157683
H	1.458150	0.214262	-2.394187
H	1.027761	1.829302	-1.862959
H	3.390384	2.524835	-1.945998
H	5.171404	1.282074	-0.610324
H	3.900732	2.206668	-4.348465
H	2.182675	2.579119	-4.135097
H	2.694591	0.913285	-4.454283
H	6.588310	0.296008	2.711965
H	5.563309	1.662696	2.210429
H	5.087202	0.652754	3.605301
H	2.353381	-0.794285	5.482519
H	1.368496	0.474269	4.715546
H	1.119706	-1.240202	4.280941
H	6.343084	-4.686330	0.145081
H	6.567062	-3.045478	0.767288
H	4.993066	-3.845964	0.921656
H	4.748549	-3.844196	-1.578416
H	6.312595	-3.016052	-1.727434
H	-0.586400	4.817684	-0.047460
H	0.819647	4.887154	1.044178

H	0.924763	3.957744	-0.467501
H	-4.359285	3.224917	1.543943
H	-2.850518	3.647845	2.407061
H	-3.815144	4.919875	1.617287
H	-4.184807	3.758592	-1.628154
H	-4.051689	2.455271	-2.842586
H	-5.626603	2.818599	-2.095609

B3LYP Energy = -2096.62074552 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf X

C	-0.848416	2.204297	0.301566
C	-2.152496	2.534724	-0.098897
C	-2.951672	1.544443	-0.677630
C	-2.496435	0.226674	-0.782150
C	-1.202307	-0.099001	-0.368070
C	-0.367645	0.898417	0.166779
O	-2.680321	-1.960279	-1.850602
C	-1.798909	-2.509574	-0.859600
C	-0.687369	-1.510303	-0.558498
C	-3.415167	-0.819608	-1.387559
C	-1.278644	-3.829129	-1.397919
C	-4.568583	-1.253171	-0.483356
C	1.034515	0.586612	0.591264
C	2.109579	0.736063	-0.292286
C	3.398804	0.410639	0.149901
C	3.615603	-0.021498	1.455701
C	2.535734	-0.189368	2.334710
C	1.254688	0.125301	1.891126
C	-4.567228	-1.071176	0.898747
C	-5.621935	-1.527642	1.686622
C	-6.678058	-2.166344	1.065831
C	-6.722084	-2.364197	-0.304122
C	-5.658826	-1.902689	-1.069779
C	1.912415	1.266156	-1.694330
C	3.212701	1.804209	-2.277063
O	4.238800	0.808878	-2.123221
C	4.600081	0.581620	-0.767065
C	3.122533	2.131464	-3.754630
F	-7.714630	-2.611105	1.824976
O	4.897856	-0.362029	1.822373
C	5.526831	0.483060	2.801087
O	2.831572	-0.665352	3.578413
C	1.762621	-0.873453	4.498696
C	5.549948	-0.623371	-0.826667
O	6.753702	-0.513883	-0.838641
O	4.894174	-1.779677	-0.941157
C	4.754410	-4.162157	-1.131847
C	5.698682	-2.984260	-1.057106
O	0.011468	3.181933	0.742644
C	-0.220595	3.702693	2.057145
O	-2.565971	3.840474	0.005201
C	-3.709967	4.084373	0.844428
C	-4.274308	2.653732	-2.315408
O	-4.220523	1.837718	-1.130126
H	-2.374438	-2.697802	0.055429

H	-0.137669	-1.835399	0.326859
H	0.032076	-1.519848	-1.385008
H	-3.855740	-0.405993	-2.295141
H	-0.589517	-4.284766	-0.684039
H	-2.101815	-4.522680	-1.574510
H	-0.746773	-3.674123	-2.339130
H	0.407440	0.006734	2.551631
H	-3.740701	-0.560060	1.375094
H	-5.627806	-1.388804	2.759788
H	-7.570923	-2.863112	-0.753018
H	-5.676942	-2.052044	-2.142868
H	1.534185	0.475467	-2.352300
H	1.162764	2.059340	-1.689437
H	3.515596	2.701090	-1.718860
H	5.213342	1.417899	-0.408406
H	4.073158	2.521017	-4.120946
H	2.350481	2.883597	-3.927670
H	2.869362	1.237569	-4.328508
H	6.550393	0.126520	2.893005
H	5.532777	1.522931	2.463992
H	5.019873	0.407882	3.762983
H	1.246157	0.062437	4.728520
H	1.044224	-1.602885	4.115352
H	2.223110	-1.262574	5.403353
H	5.331981	-5.084365	-1.221030
H	4.139767	-4.228701	-0.233087
H	4.097882	-4.084867	-1.999727
H	6.318798	-2.900809	-1.950699
H	6.356362	-3.042591	-0.189080
H	0.595794	4.393681	2.257611
H	-1.168337	4.239158	2.111363
H	-0.204565	2.899566	2.798772
H	-4.605709	3.609744	0.445406
H	-3.525809	3.717998	1.857779
H	-3.838458	5.164360	0.866771
H	-3.747956	2.165149	-3.139234
H	-5.328265	2.753800	-2.565427
H	-3.839474	3.637966	-2.137172

B3LYP Energy = -2096.62073045 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf Y

C	-0.959538	2.259257	0.347490
C	-2.279353	2.520832	-0.044180
C	-3.034890	1.505878	-0.633410
C	-2.506158	0.218740	-0.774588
C	-1.193345	-0.042271	-0.370996
C	-0.403997	0.986171	0.176908
O	-2.589645	-1.972694	-1.846302
C	-1.680538	-2.479102	-0.857507
C	-0.614808	-1.428492	-0.565398
C	-3.376616	-0.868571	-1.379081
C	-1.103572	-3.775504	-1.394354
C	-4.504889	-1.360666	-0.473509
C	1.008785	0.734380	0.605241
C	2.069314	0.761728	-0.308495

C	3.367209	0.494787	0.150427
C	3.611113	0.240388	1.499498
C	2.550358	0.250452	2.419647
C	1.259772	0.477102	1.954341
C	-5.586552	-2.020785	-1.063394
C	-6.622891	-2.538185	-0.296293
C	-6.559956	-2.385988	1.078590
C	-5.511218	-1.738653	1.703264
C	-4.484237	-1.225493	0.914046
C	1.854717	1.093628	-1.768388
C	3.133231	1.609283	-2.414881
O	4.185866	0.664312	-2.164996
C	4.556990	0.575854	-0.793613
C	3.026818	1.774466	-3.918342
F	-7.569898	-2.885996	1.839432
O	4.922514	0.082323	1.875797
C	5.284189	-1.085060	2.635311
O	2.873180	0.059326	3.732038
C	1.829861	0.095814	4.703698
C	5.516135	-0.621718	-0.757153
O	6.717604	-0.508977	-0.814539
O	4.869600	-1.792204	-0.744621
C	4.747981	-4.181960	-0.848887
C	5.681898	-2.993559	-0.852990
O	-0.230712	3.233353	0.987615
C	0.178850	4.355818	0.189723
O	-2.815278	3.776462	0.135349
C	-3.544612	3.937285	1.364740
C	-4.545826	2.641835	-2.093779
O	-4.340735	1.721505	-1.006339
H	-2.242570	-2.690722	0.060581
H	-0.044237	-1.723221	0.317924
H	0.096471	-1.410348	-1.398013
H	-3.838457	-0.472838	-2.284463
H	-0.390615	-4.196931	-0.682882
H	-1.895464	-4.506330	-1.563657
H	-0.584946	-3.600465	-2.339468
H	0.430147	0.488717	2.646259
H	-5.620221	-2.133412	-2.140628
H	-7.465439	-3.045350	-0.747790
H	-5.502039	-1.636229	2.780488
H	-3.664292	-0.706926	1.393868
H	1.525927	0.206399	-2.320906
H	1.062828	1.837446	-1.872804
H	3.412507	2.568692	-1.957015
H	5.167691	1.446117	-0.524054
H	3.967111	2.140971	-4.331834
H	2.238805	2.488557	-4.165126
H	2.788149	0.819575	-4.391125
H	4.816938	-1.976799	2.211572
H	6.366192	-1.165536	2.553267
H	4.993204	-0.980049	3.678175
H	2.315054	-0.065879	5.663090
H	1.327274	1.066335	4.710246
H	1.095787	-0.695798	4.530996
H	5.331128	-5.101052	-0.932928

H	4.171313	-4.226437	0.076231
H	4.054986	-4.138514	-1.690146
H	6.262073	-2.933505	-1.774571
H	6.379148	-3.018159	-0.014658
H	0.844181	4.032399	-0.614829
H	-0.682694	4.878321	-0.225724
H	0.723821	5.017853	0.859496
H	-4.393350	3.251098	1.403411
H	-2.890876	3.770285	2.223761
H	-3.904513	4.964158	1.375362
H	-5.616288	2.641661	-2.287940
H	-4.215956	3.645285	-1.826896
H	-4.014202	2.301228	-2.986301

B3LYP Energy = -2096.62071839 a.u.

(aR,1S,3S,1'S,3'S)-22, Conf Z

C	-0.924283	2.200101	0.455802
C	-2.206441	2.544596	0.005510
C	-3.006978	1.570629	-0.593485
C	-2.512076	0.275963	-0.796342
C	-1.215335	-0.048340	-0.388745
C	-0.416095	0.914658	0.255713
O	-2.620248	-1.826908	-2.036805
C	-1.742404	-2.428460	-1.074649
C	-0.662720	-1.428366	-0.677728
C	-3.390499	-0.737869	-1.509059
C	-1.180148	-3.690127	-1.702672
C	-4.561835	-1.263180	-0.681727
C	0.968509	0.586125	0.721930
C	2.083214	0.796638	-0.097446
C	3.349196	0.422725	0.371029
C	3.512257	-0.103406	1.652757
C	2.398312	-0.271226	2.489732
C	1.136105	0.053998	2.001463
C	-5.672485	-1.779559	-1.355626
C	-6.747617	-2.325211	-0.665225
C	-6.694348	-2.349649	0.718307
C	-5.617901	-1.849108	1.425546
C	-4.552436	-1.303291	0.712558
C	1.950019	1.433896	-1.461827
C	3.272177	2.025777	-1.930215
O	4.293843	1.021054	-1.819129
C	4.589858	0.659713	-0.474852
C	3.252183	2.485486	-3.374894
F	-7.741595	-2.879125	1.404353
O	4.799251	-0.351909	2.061915
C	5.116694	-1.650101	2.595129
O	2.640062	-0.730197	3.752926
C	1.536793	-0.899599	4.639730
C	5.522780	-0.550492	-0.625147
O	6.727316	-0.463387	-0.602101
O	4.844934	-1.680444	-0.859936
C	5.899954	-2.979772	-2.652508
C	5.607605	-2.881039	-1.168086
O	-0.114013	3.167293	1.004267

C	-0.469429	3.605414	2.325498
O	-2.677486	3.828502	0.165237
C	-2.259124	4.745898	-0.861161
C	-5.252217	2.319791	-0.176803
O	-4.245137	1.875889	-1.104331
H	-2.326620	-2.702835	-0.187275
H	-0.118348	-1.806083	0.189907
H	0.068784	-1.356711	-1.490670
H	-3.809328	-0.258836	-2.394272
H	-0.487573	-4.180110	-1.015253
H	-1.982314	-4.389686	-1.941477
H	-0.642490	-3.451888	-2.622915
H	0.264256	-0.084283	2.624949
H	-5.698160	-1.755270	-2.438668
H	-7.612210	-2.721058	-1.181696
H	-5.616901	-1.883023	2.507152
H	-3.710663	-0.896854	1.258136
H	1.615923	0.696065	-2.200151
H	1.191033	2.217478	-1.432202
H	3.543270	2.868610	-1.279121
H	5.199382	1.444147	-0.009899
H	4.217761	2.906896	-3.657274
H	2.486037	3.250061	-3.517062
H	3.031602	1.647206	-4.038983
H	4.785653	-1.741483	3.627294
H	4.657705	-2.435805	1.991005
H	6.200238	-1.733569	2.539588
H	1.961338	-1.259941	5.573472
H	1.021289	0.047740	4.817854
H	0.825782	-1.636543	4.256604
H	6.403845	-3.926525	-2.859462
H	4.976830	-2.949025	-3.233035
H	6.549979	-2.168788	-2.981558
H	6.523014	-2.877009	-0.578498
H	4.966584	-3.694931	-0.833993
H	0.256546	4.368974	2.597170
H	-1.474095	4.029274	2.341246
H	-0.402264	2.774913	3.033107
H	-2.711529	5.704931	-0.616773
H	-1.172032	4.845061	-0.870797
H	-2.612254	4.413674	-1.840148
H	-6.160083	2.445062	-0.763004
H	-5.420272	1.562246	0.591810
H	-4.971263	3.265223	0.284341

B3LYP Energy = -2096.62059567 a.u.



## 6. References

1. MacroModel; Schrödinger LLC, 2015. Available online: <https://newsite.schrodinger.com/platform/products/macromodel> (accessed on 12 July 2024).
2. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, V.; Barone, G.; Mennucci, B.; Petersson, G. A., et al. *Gaussian 09 Revisions C.01*; Gaussian, Inc.: Wallingford, CT, USA, 2010.
3. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, V.; Barone, G.; Mennucci, B.; Petersson, G. A., et al. *Gaussian 09 Revisions E.01*; Gaussian, Inc.: Wallingford, CT, USA, 2013.
4. Chai, J.-D.; Head-Gordon, M. Systematic optimization of long-range corrected hybrid density functionals. *J. Chem. Phys.* **2008**, *128*, 084106, <https://doi.org/10.1063/1.2834918>.
5. Stephens, P. J.; Harada, N. ECD cotton effect approximated by the Gaussian curve and other methods. *Chirality* **2010**, *22*, 229–233, <https://doi.org/10.1002/chir.20733>.
6. Varetto, U. *MOLEKEL 5.4*; Swiss National Supercomputing Centre: Manno, Switzerland, 2009.
7. Kerti, G.; Kurtán, T.; Illyés, T.-Z.; Kövér, K. E.; Sólyom, S.; Pescitelli, G.; Fujioka, N.; Berova, N.; Antus, S. Enantioselective Synthesis of 3-Methylisochromans and Determination of Their Absolute Configurations by Circular Dichroism. *Eur. J. Org. Chem.* **2007**, 296–305.
8. Inoue, K.; Makino, Y.; Itoh, N. Production of (R)-chiral alcohols by a hydrogen-transfer bioreduction with NADH-dependent *Leifsonia* alcohol dehydrogenase (LSADH). *Tetrahedron: Asymmetry* **2005**, *16*, 2539–2549, <https://doi.org/10.1016/j.tetasy.2005.06.036>.
9. Ren, X.; She, X.; Peng, K.; Su, Y.; Xie, X.; Pan, X.; Zhang, H. First Enantioselective Synthesis of the Neolignans Rhaphidecursinol A and Virolongin B. *J. Chin. Chem. Soc.* **2004**, *51*, 969–974, <https://doi.org/10.1002/jccs.200400144>.
10. González-Liste, P. J.; León, F.; Arribas, I.; Rubio, M.; García-Garrido, S. E.; Cadierno, V.; Pizzano, A. Highly Stereoselective Synthesis and Hydrogenation of (Z)-1-Alkyl-2-arylvinyl Acetates: a Wide Scope Procedure for the Preparation of Chiral Homobenzylic Esters. *ACS Catal.* **2016**, *6*, 3056–3060, <https://doi.org/10.1021/acscatal.6b00282>.
11. Parsons, S.; Flack, H. D.; Wagner, T. Use of intensity quotients and differences in absolute structure refinement. *Acta Crystallogr., Sect. B: Struct. Sci., Cryst. Eng. Mater.* **2013**, *69*, 249–259, <https://doi.org/10.1107/S2052519213010014>.
12. Sheldrick, G. A short history of SHELX. *Acta Crystallogr., Sect. A: Found. Adv.* **2008**, *64*, 112–122, <https://doi.org/10.1107/S0108767307043930>.

13. Westrip, S. publCIF: software for editing, validating and formatting crystallographic information files. *J. Appl. Crystallogr.* **2010**, *43*, 920–925, <https://doi.org/10.1107/S0021889810022120>.
14. Edgington, P. R.; McCabe, P.; Macrae, C. F.; Pidcock, E.; Shields, G. P.; Taylor, R.; Towler, M.; Van De Streek, J. Mercury: visualization and analysis of crystal structures. *J. Appl. Crystallogr.* **2006**, *39*, 453–457, <https://doi.org/10.1107/S002188980600731X>.
15. Spek, A. Single-crystal structure validation with the program PLATON. *J. Appl. Crystallogr.* **2003**, *36*, 7–13, <https://doi.org/10.1107/S0021889802022112>.