

Supplementary Material

Cytotoxic phenanthrene, dihydrophenanthrene, and dihydrostilbene derivatives and other aromatic compounds from *Combretum laxum*

Eder Bisoli¹, Talita Vilalva Freire¹, Nidia Cristiane Yoshida¹, Walmir Silva Garcez¹, Lyara Meira Marinho Queiróz², Maria de Fátima Cepa Matos², Renata Trentin Perdomo² and Fernanda Rodrigues Garcez^{1,*}

¹Institute of Chemistry, Universidade Federal de Mato Grosso do Sul, Campo Grande, MS, Brazil; ²Laboratory of Molecular Biology and Cell Culture, School of Pharmaceutical Sciences, Food Technology, and Nutrition, Universidade Federal de Mato Grosso do Sul, Campo Grande, MS, Brazil; *Correspondence: fernanda.garcez@ufms.br.

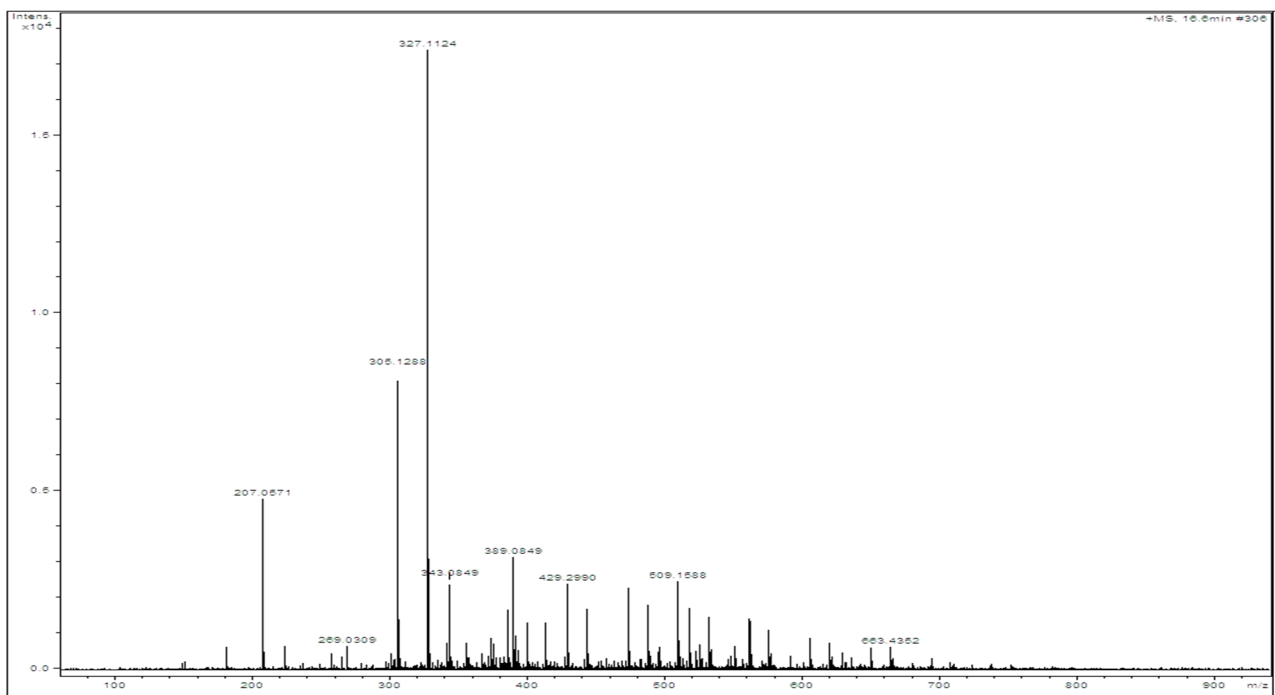


Figure S1. HRESIMS (positive mode) of compound 1.

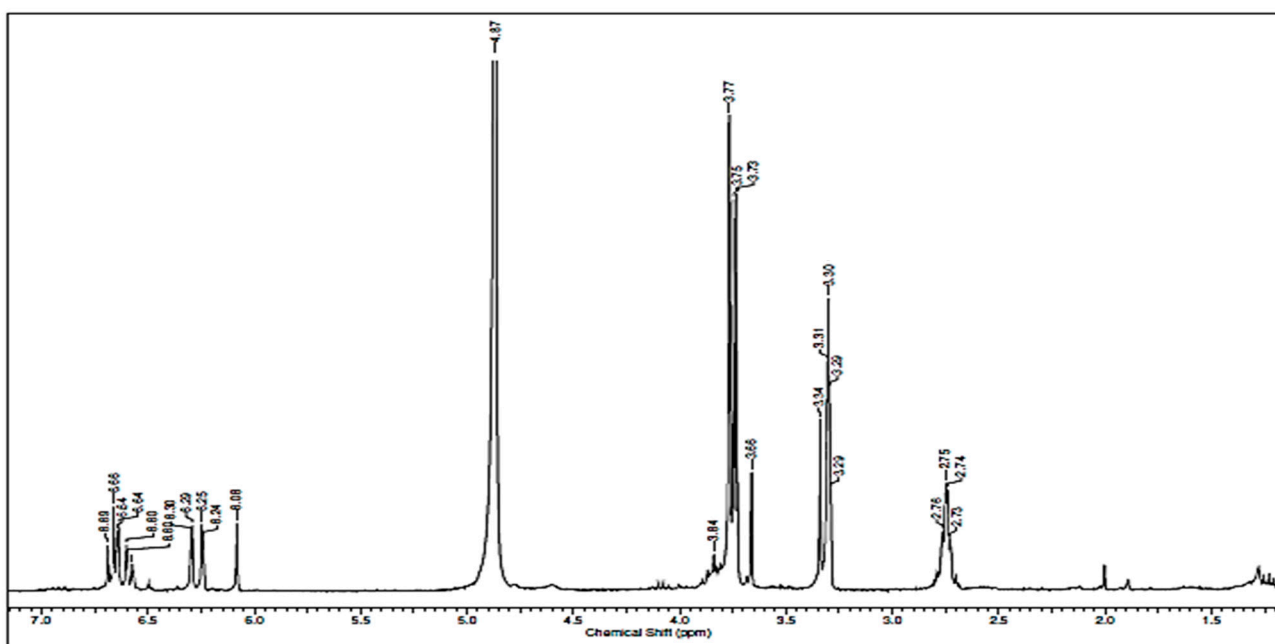


Figure S2. ¹H NMR spectrum (300 MHz, CD₃OD) of compound 1.

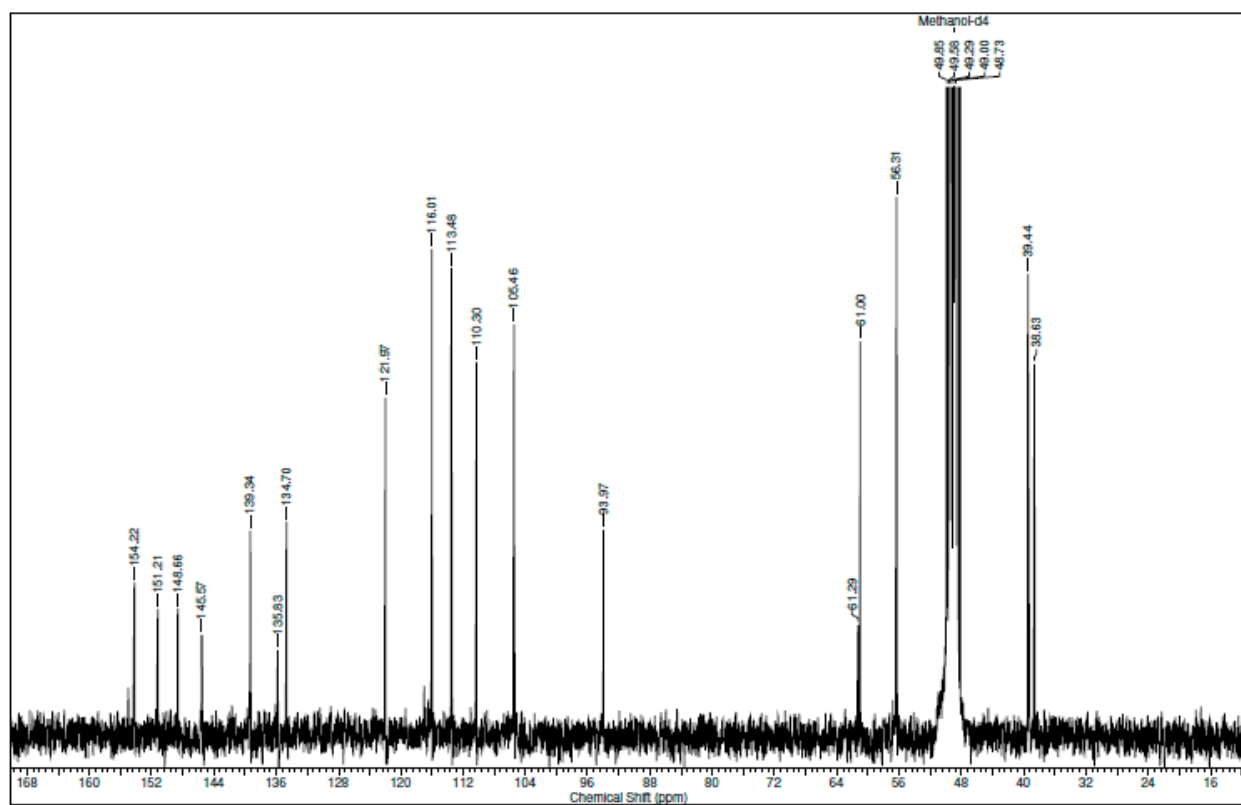


Figure S3. ^{13}C NMR spectrum (75 MHz, CD_3OD) of compound 1.

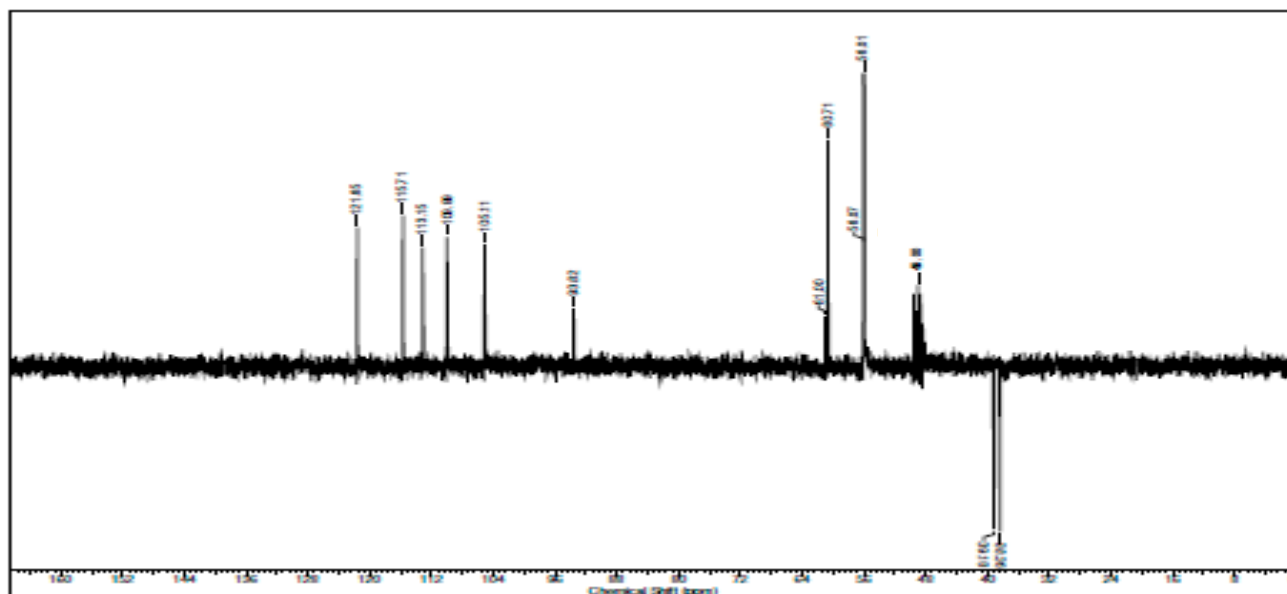


Figure S4. DEPT-135 spectrum (CD_3OD) of compound 1.

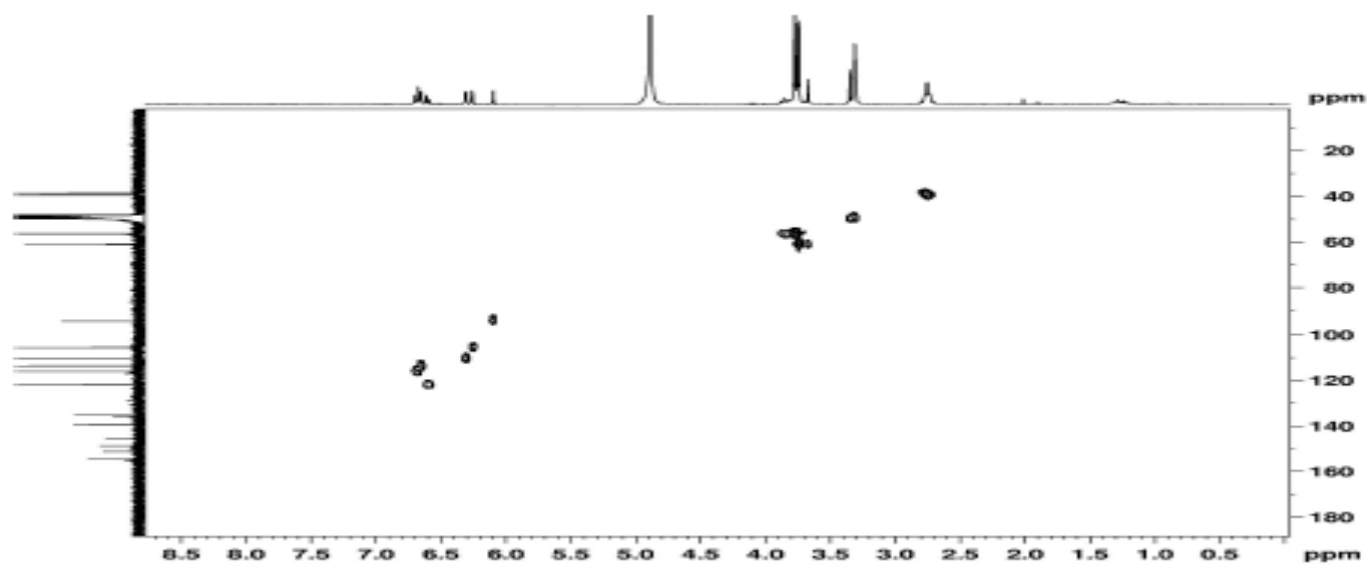


Figure S5. HSQC spectrum (CD_3OD) of compound 1.

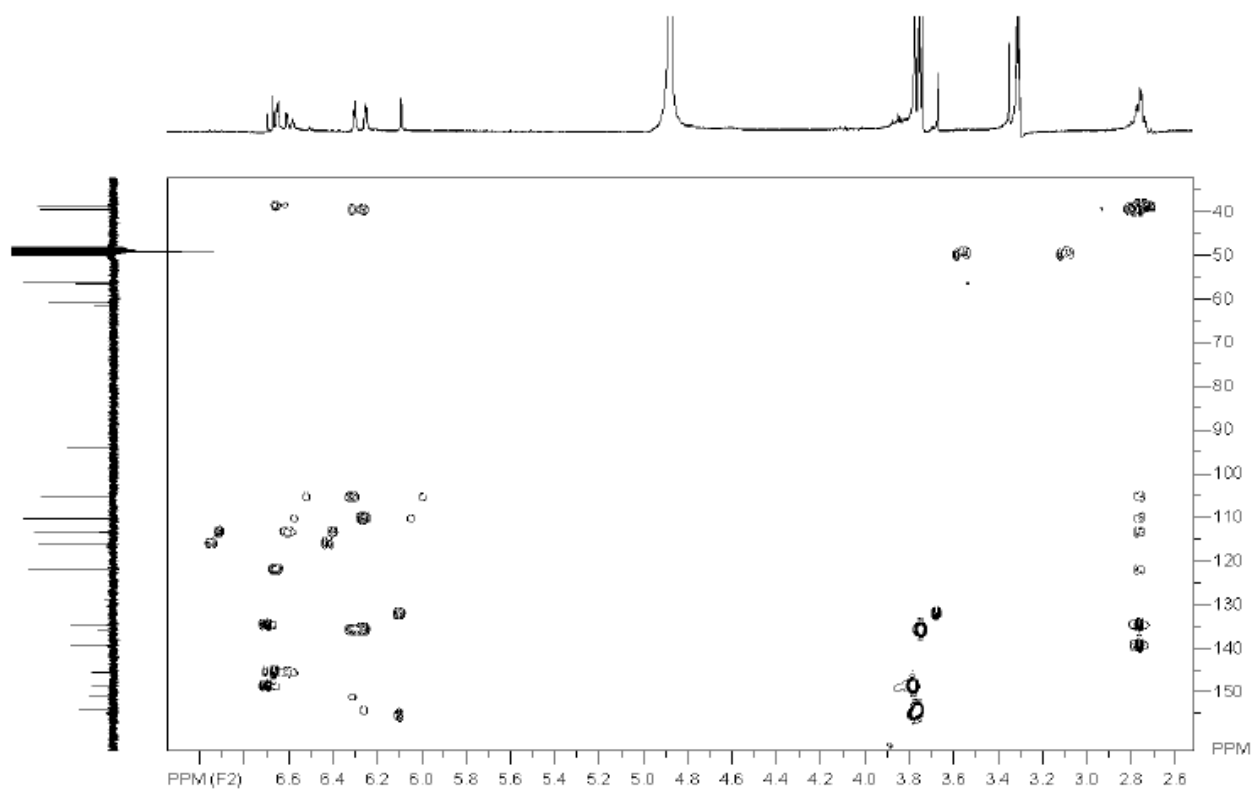


Figure S6. HMBC spectrum (CD_3OD) of compound 1.

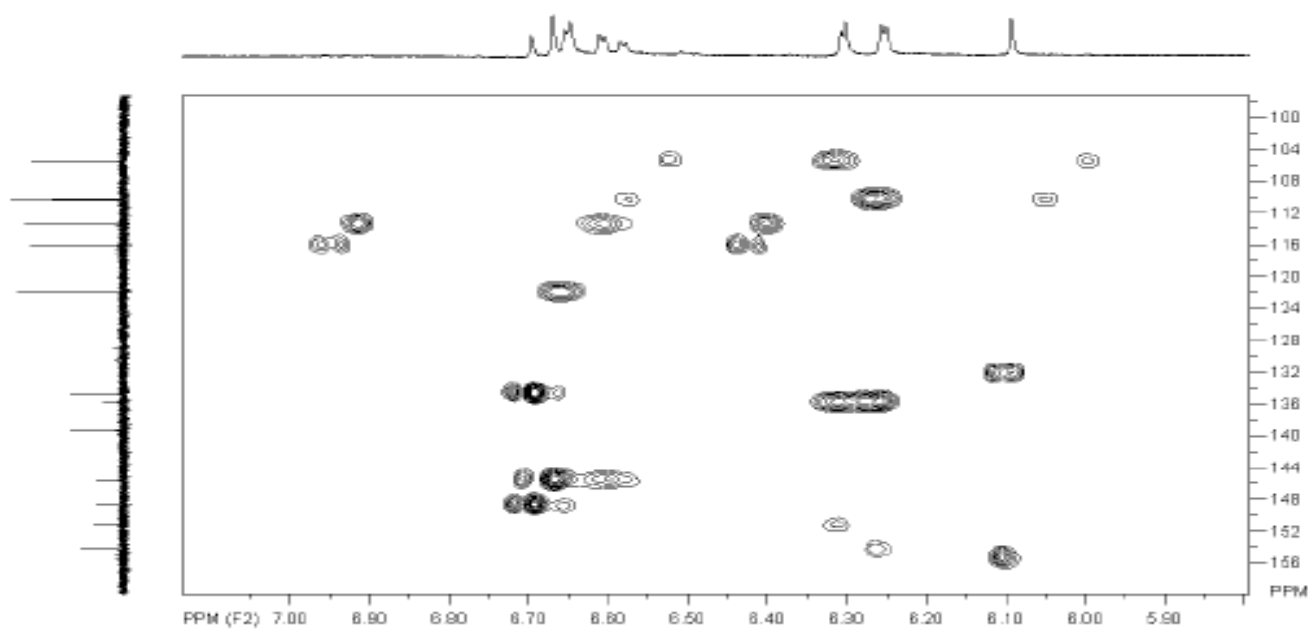


Figure S7. HMBC spectrum (expansion) of compound 1.

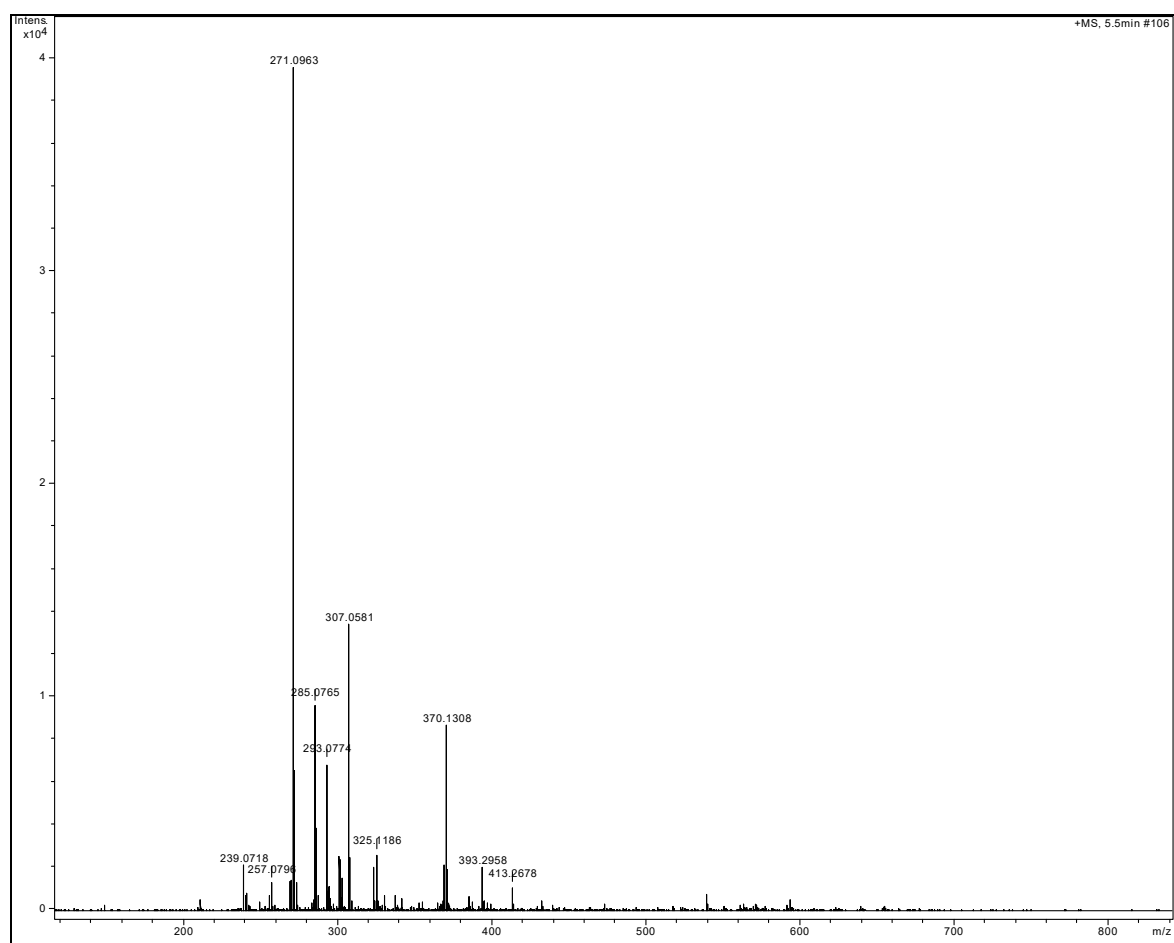


Figure S8. HRESIMS (positive mode) of compound 2.

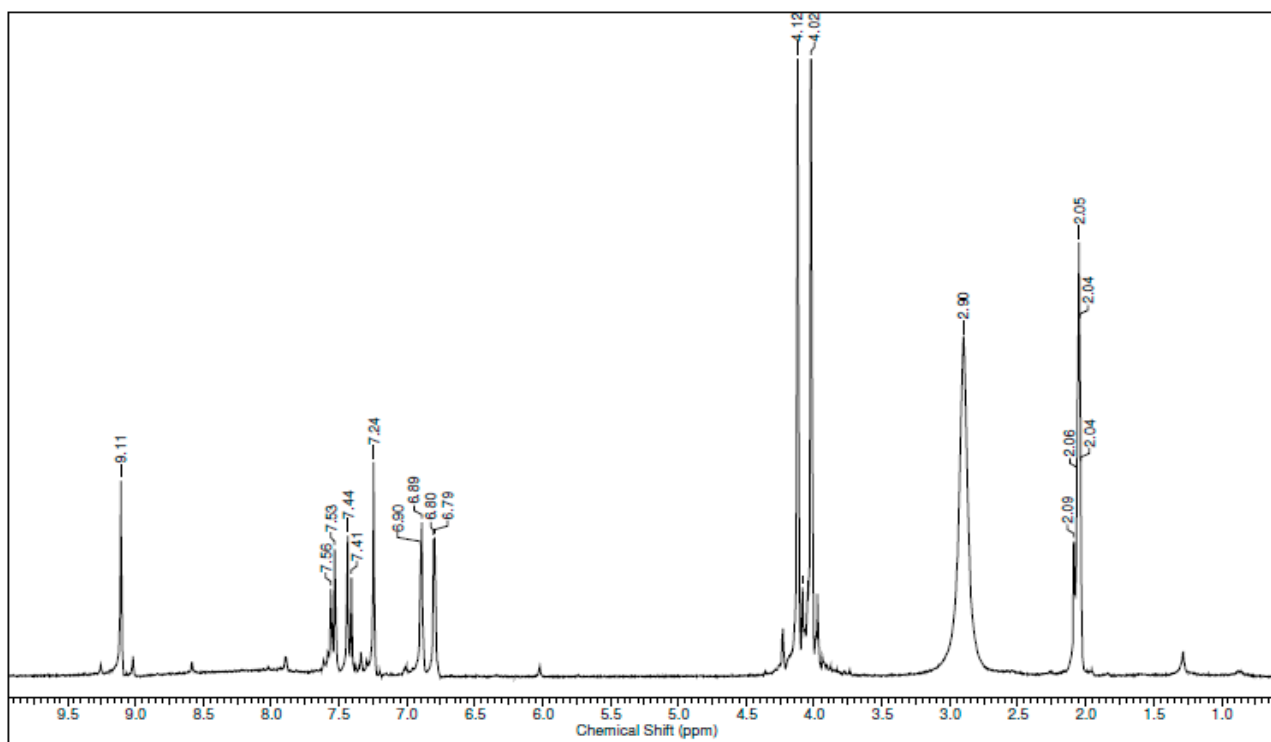


Figure S9. ^1H NMR spectrum (300 MHz, acetone- d_6) of compound 2.

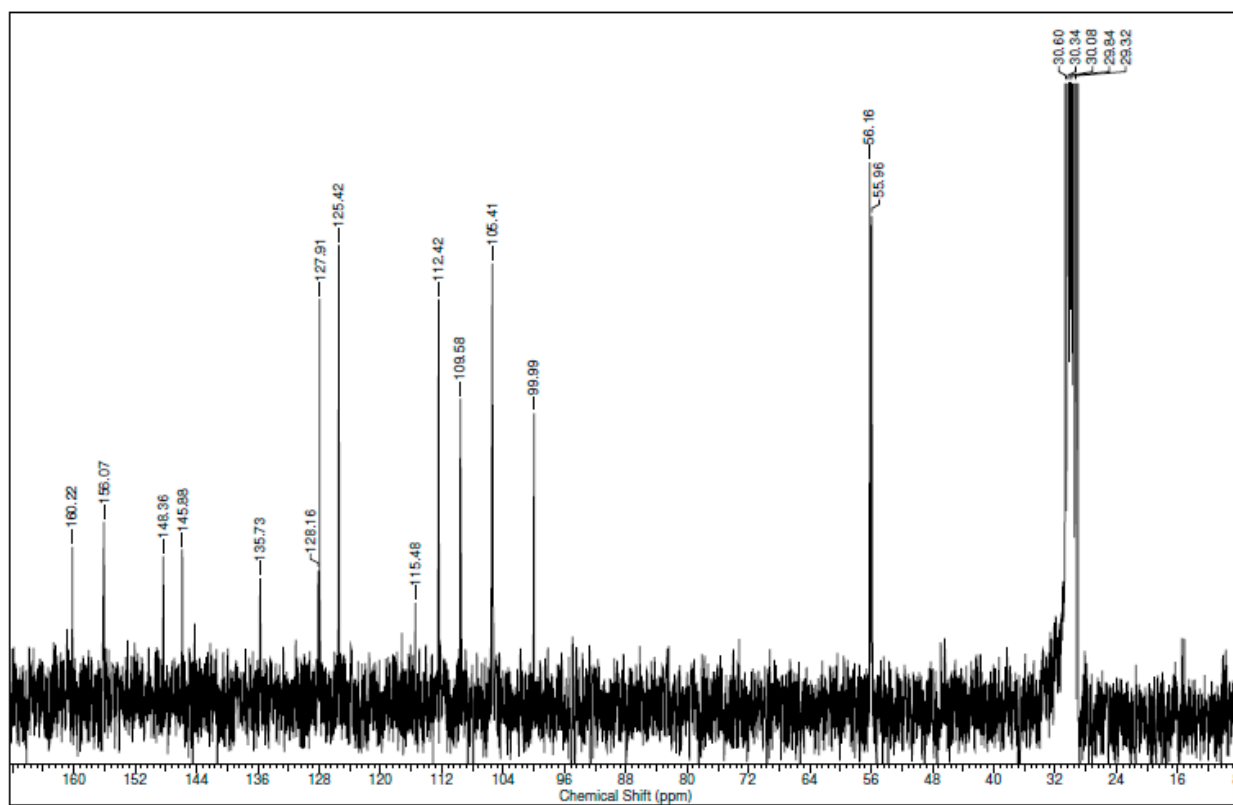


Figure S10. ^{13}C NMR spectrum (75 MHz, acetone- d_6) of compound 2.

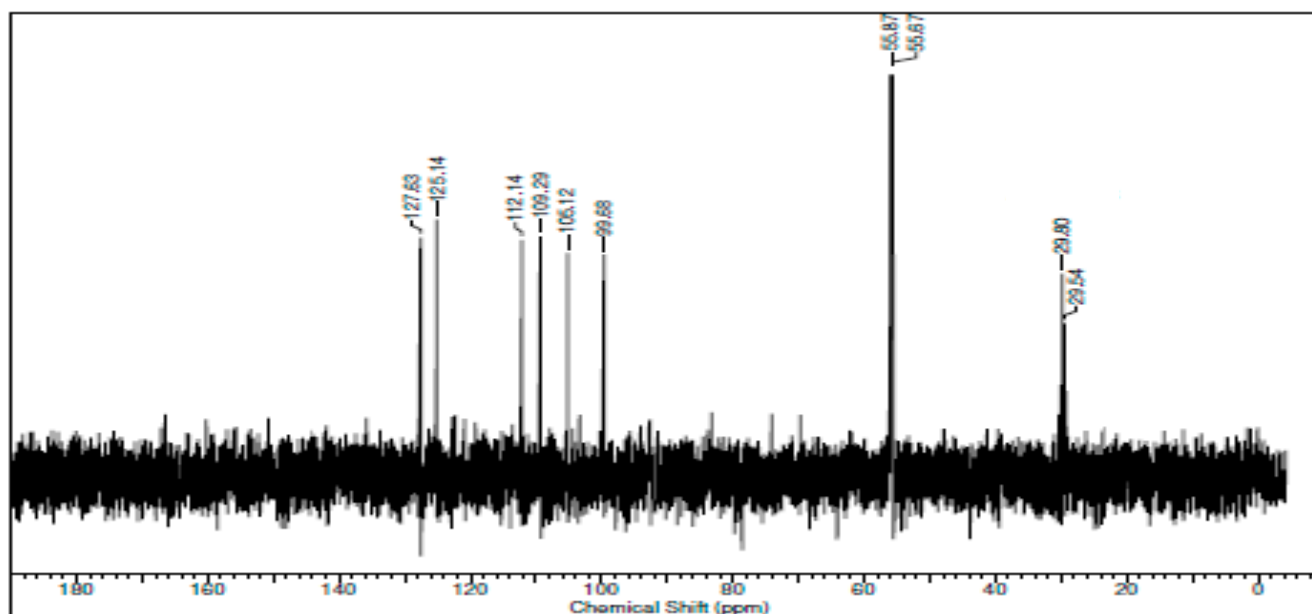


Figure S11. DEPT-135 spectrum (acetone- d_6) of compound 2.

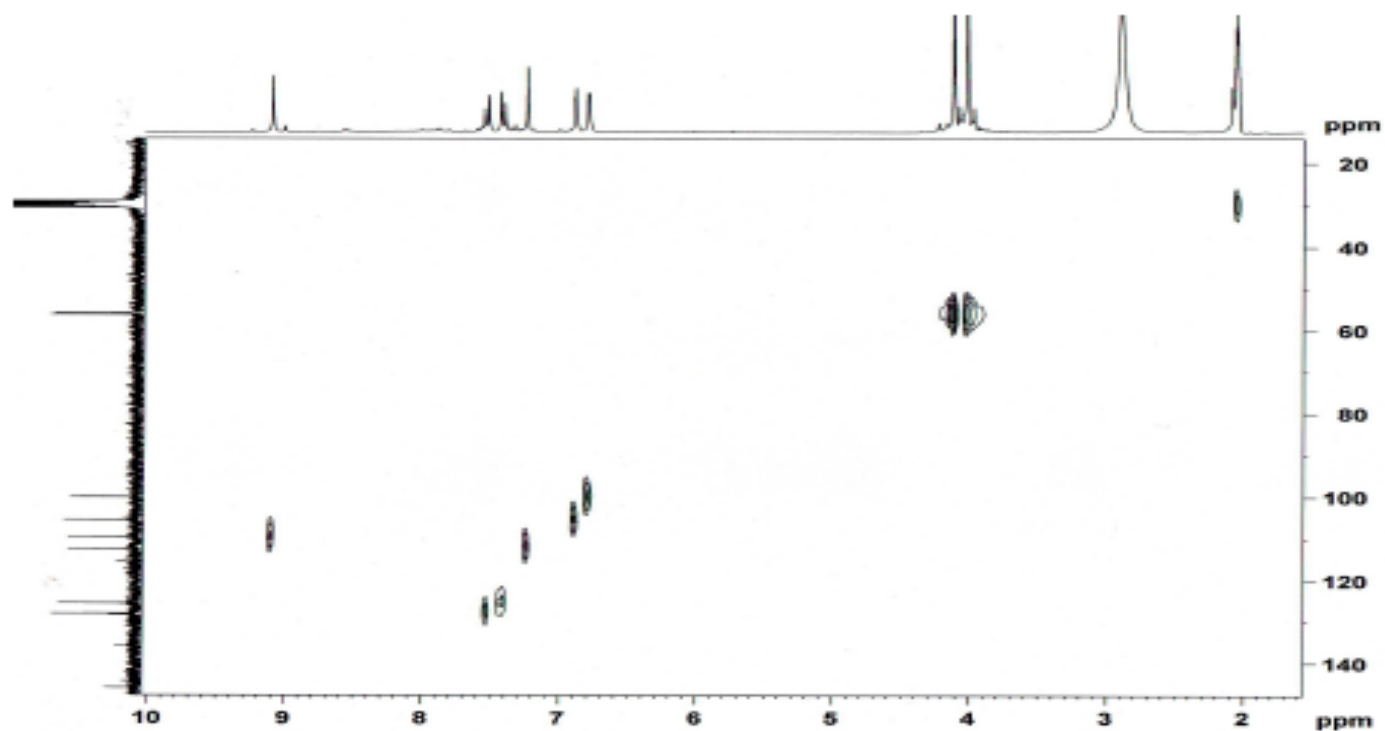


Figure S12. HSQC spectrum (acetone- d_6) of compound 2.

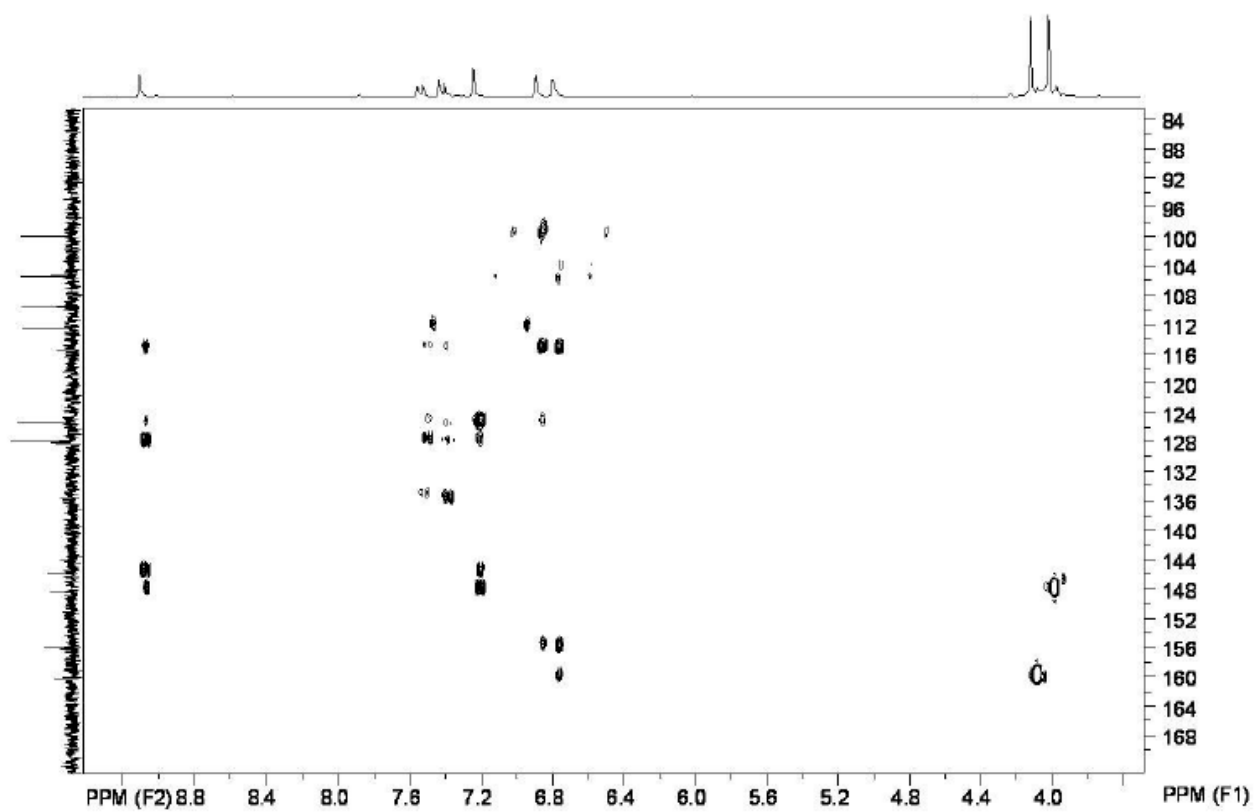


Figure S13. HMBC spectrum (acetone-d₆) of compound 2.

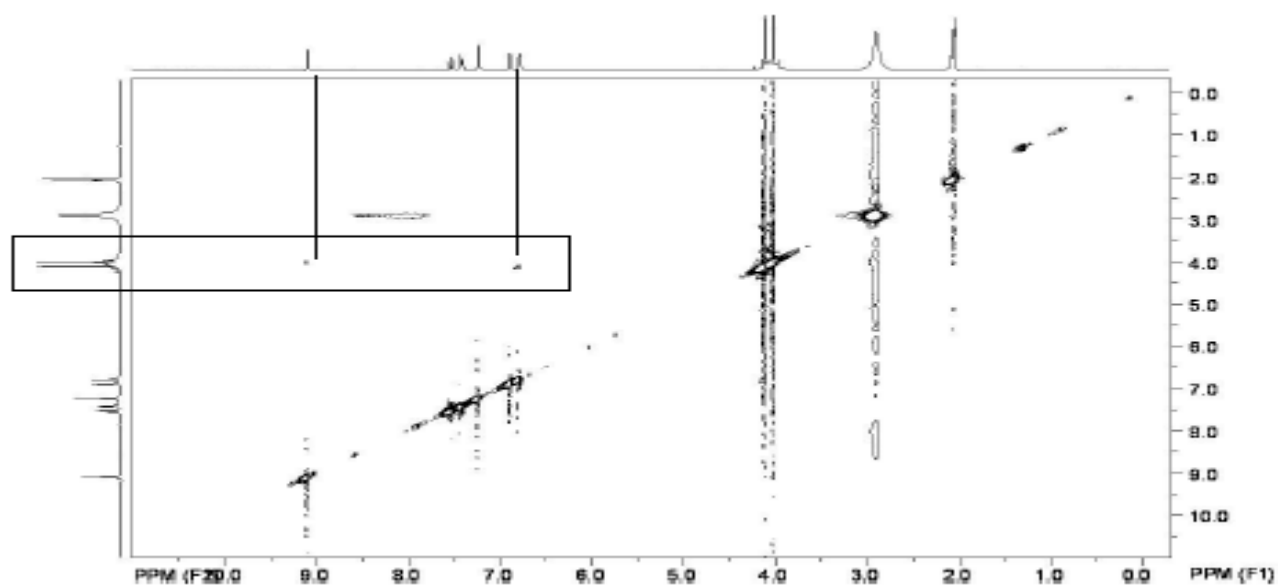


Figure S14. NOESY spectrum (300 MHz, acetone-d₆) of compound 2.

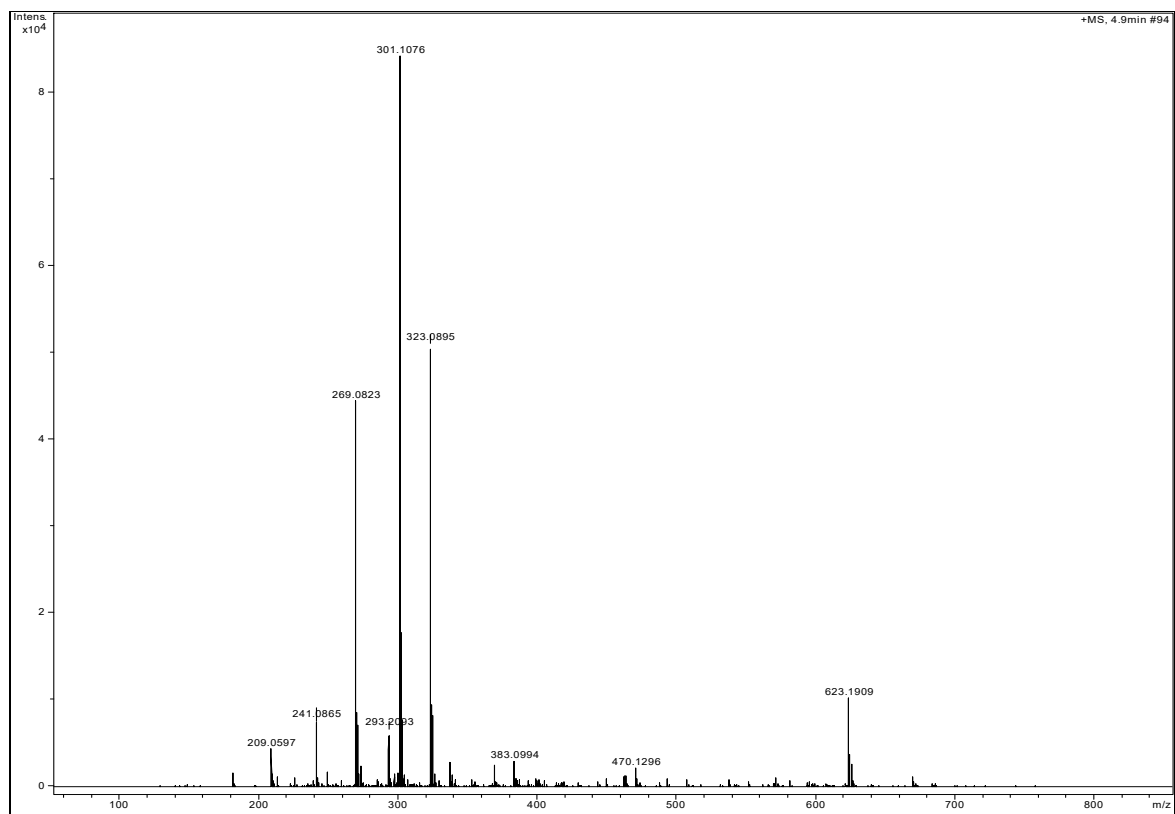


Figure S15. HRESIMS (positive mode) of compound 3.

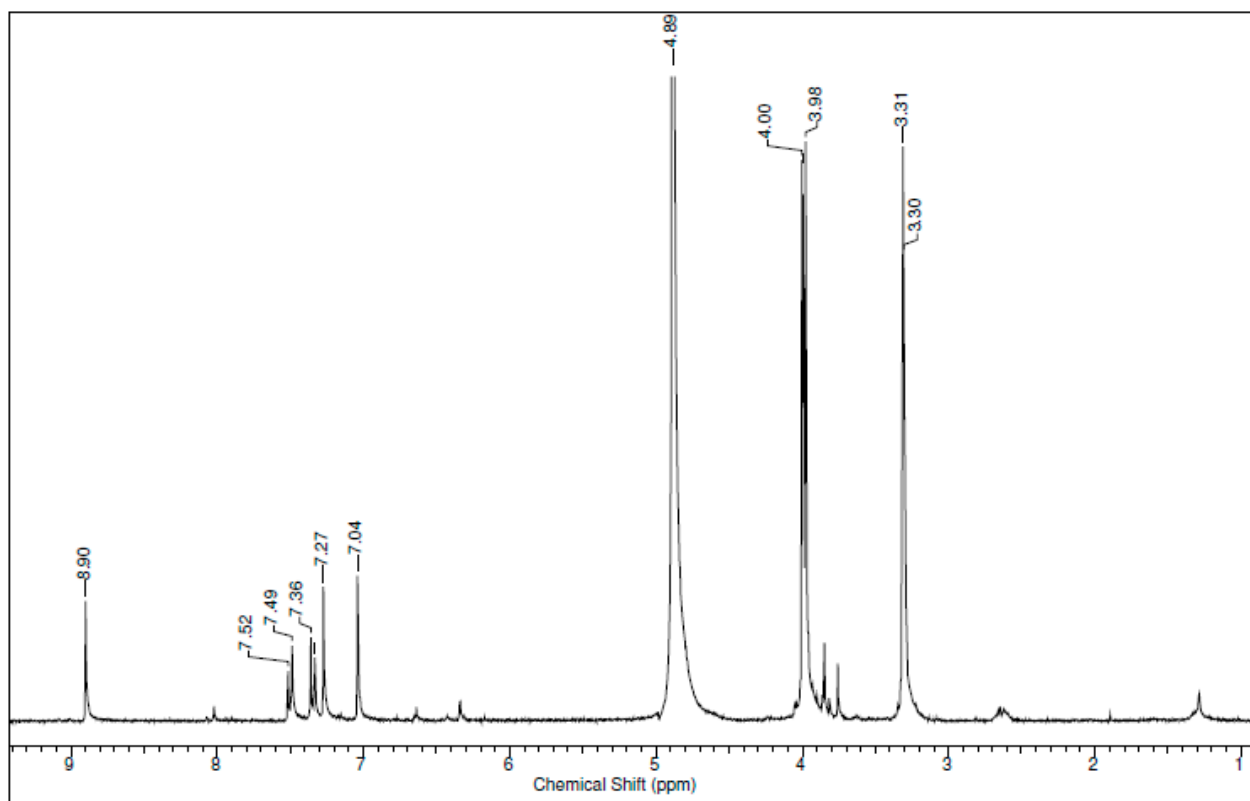


Figure S16. ¹H NMR spectrum (300 MHz, CD₃OD) of compound 3.

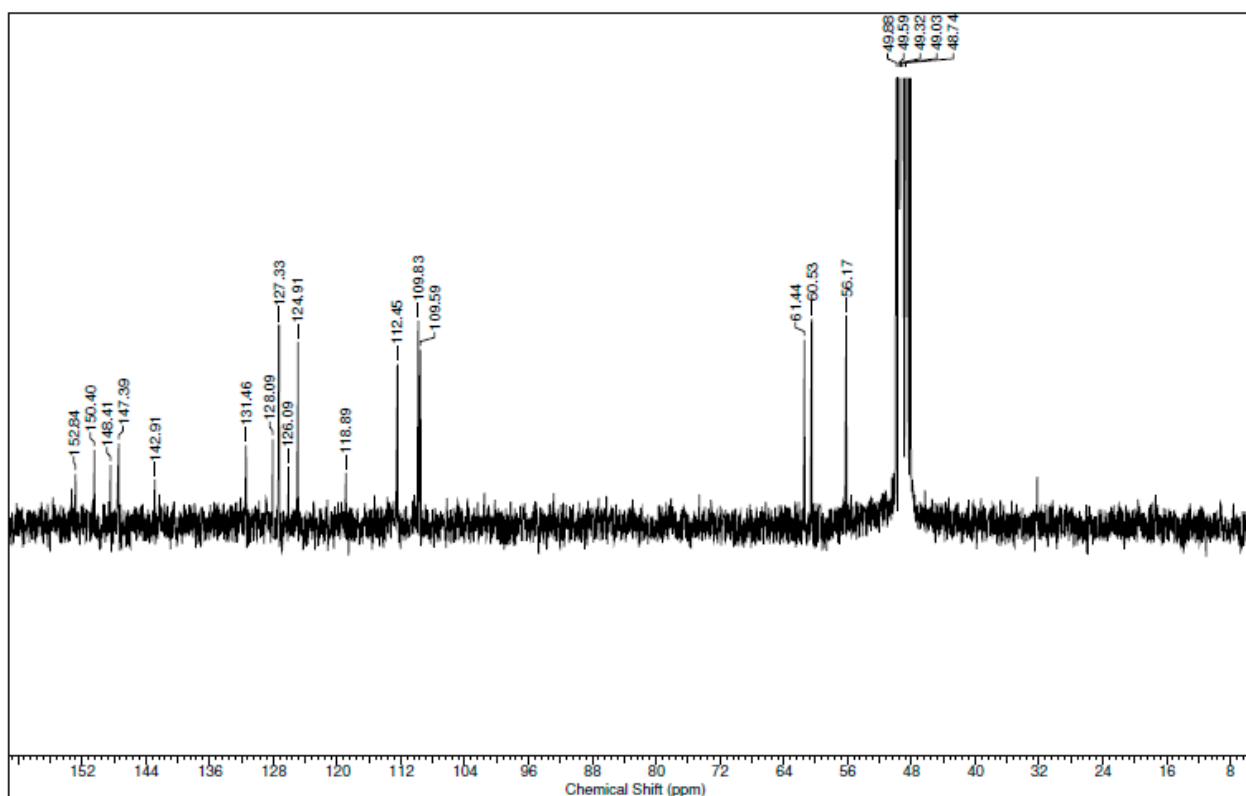


Figure S17. ^{13}C NMR spectrum (75 MHz, CD_3OD) of compound 3.

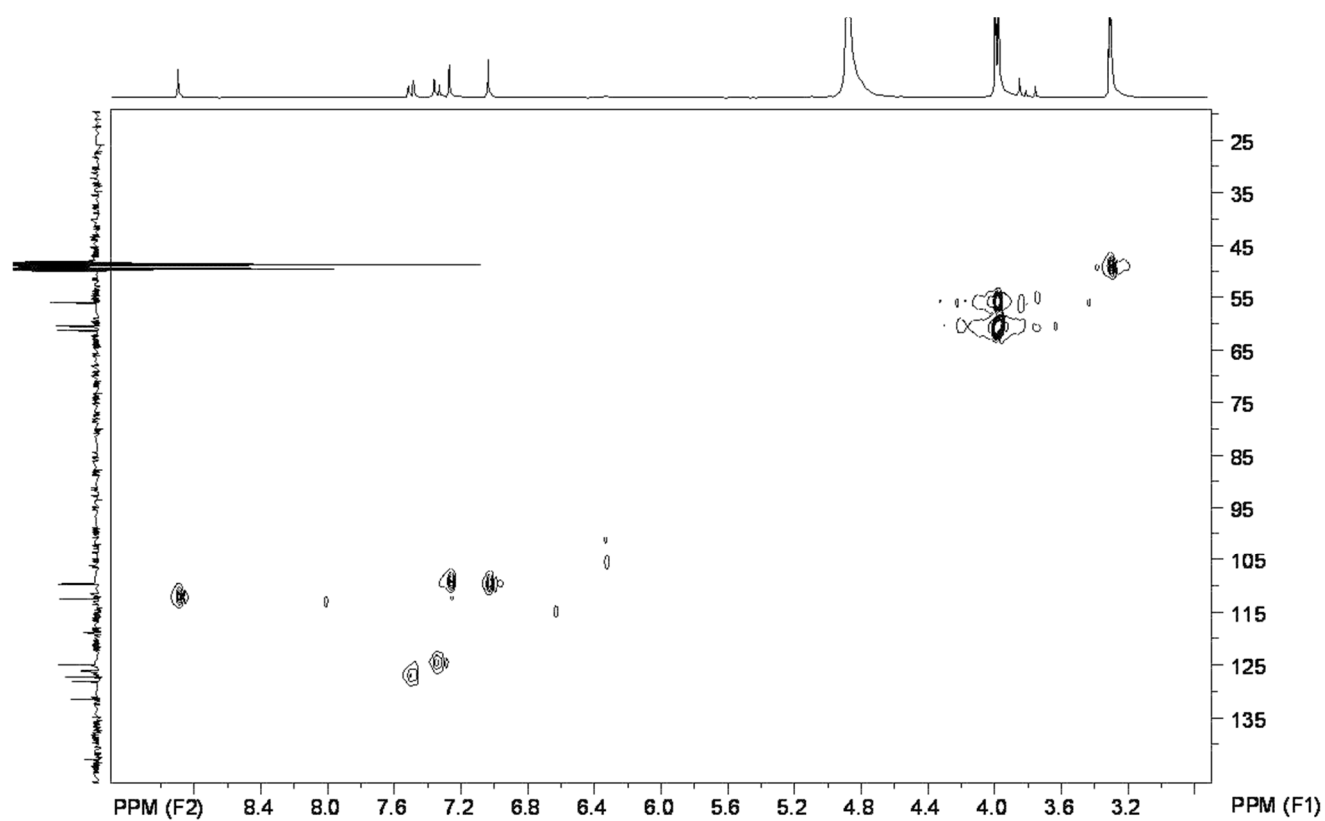


Figure S18. HSQC spectrum (CD_3OD) of compound 3.

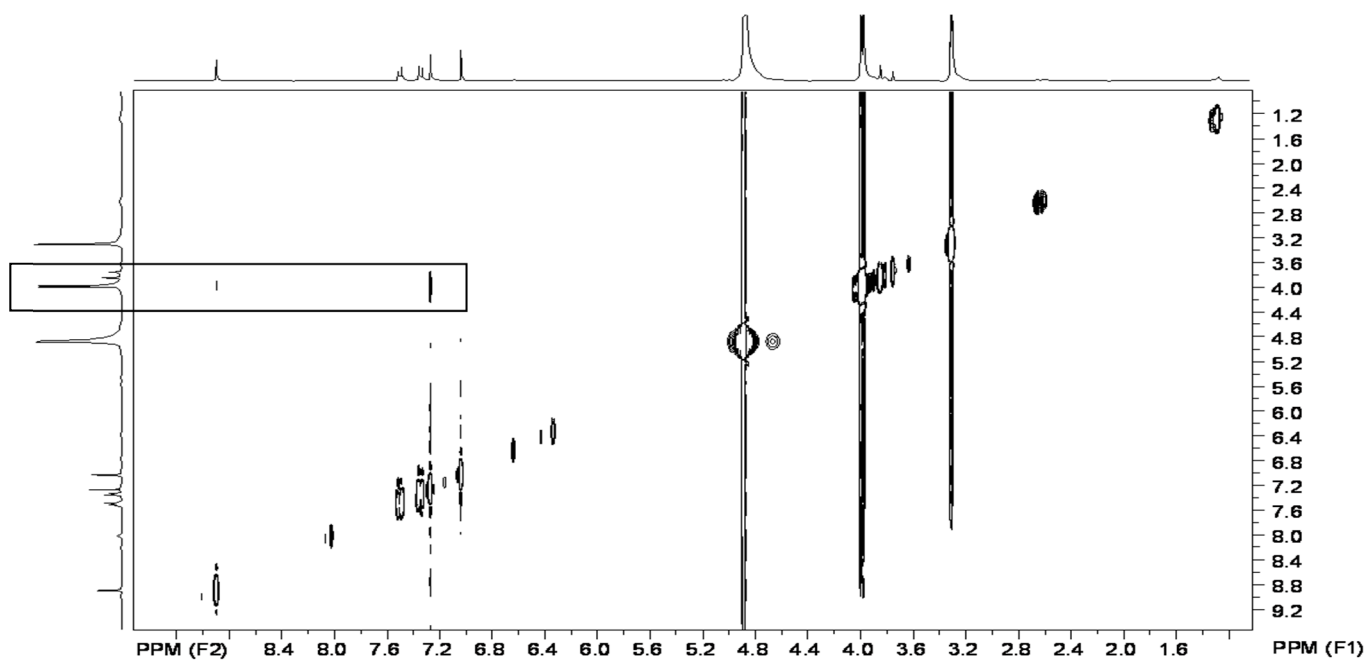


Figure S19. NOESY spectrum (300 MHz, CD₃OD) of compound 3.

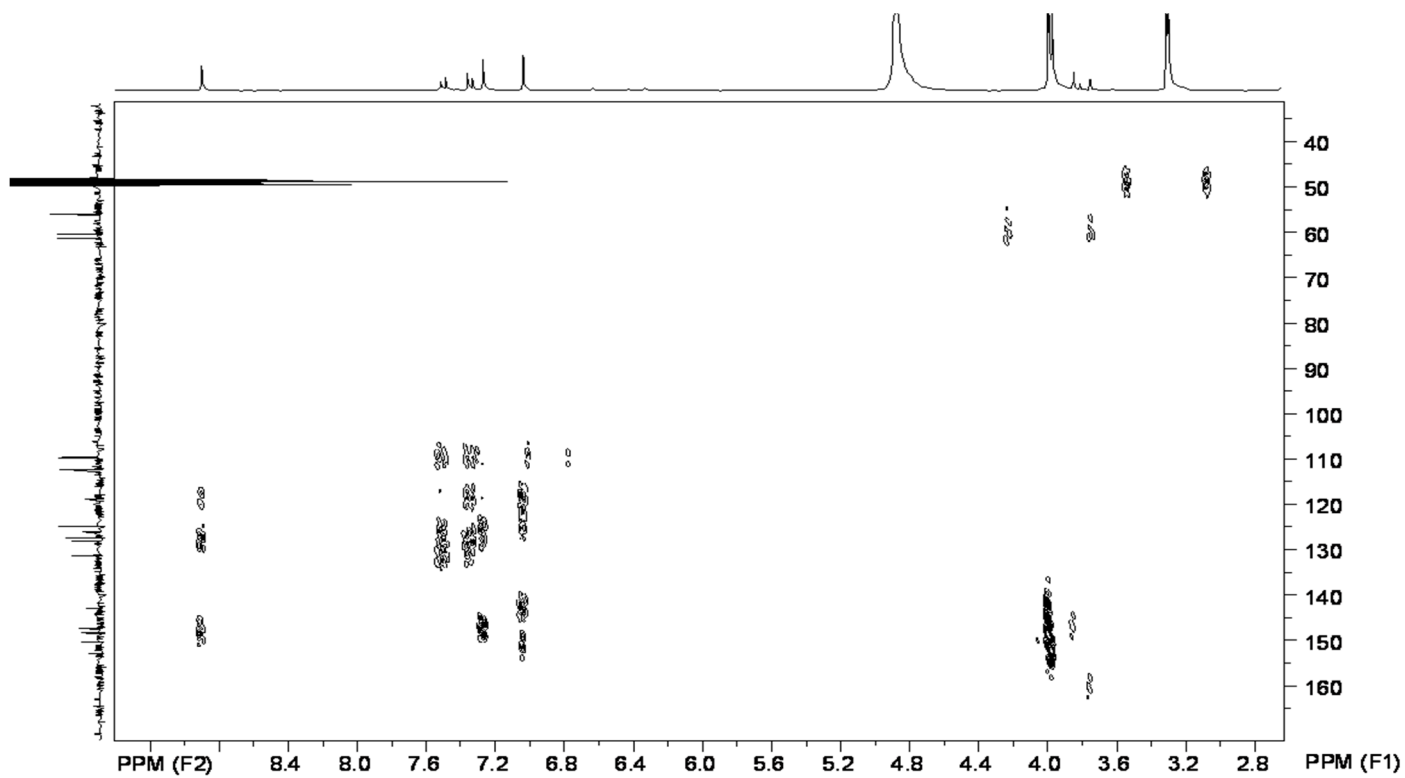


Figure S20. HMBC spectrum (CD₃OD) of compound 3.

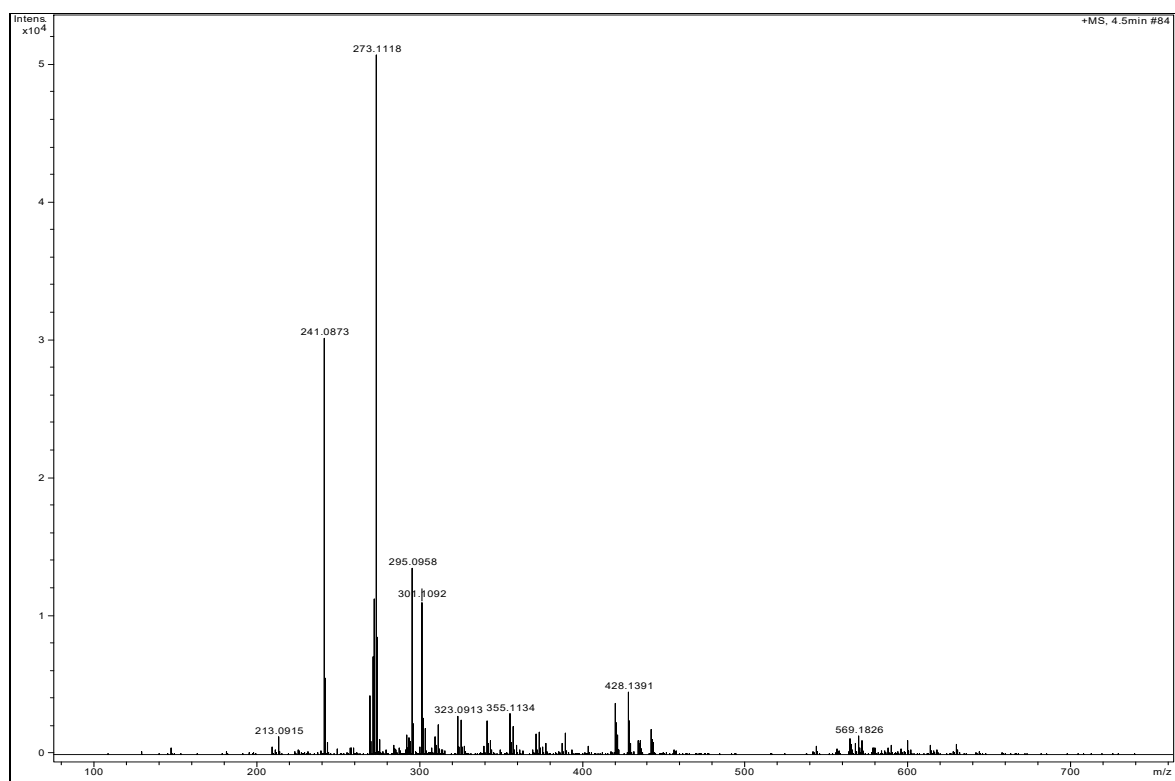


Figure S21. HRESIMS (positive mode) of compound 4.

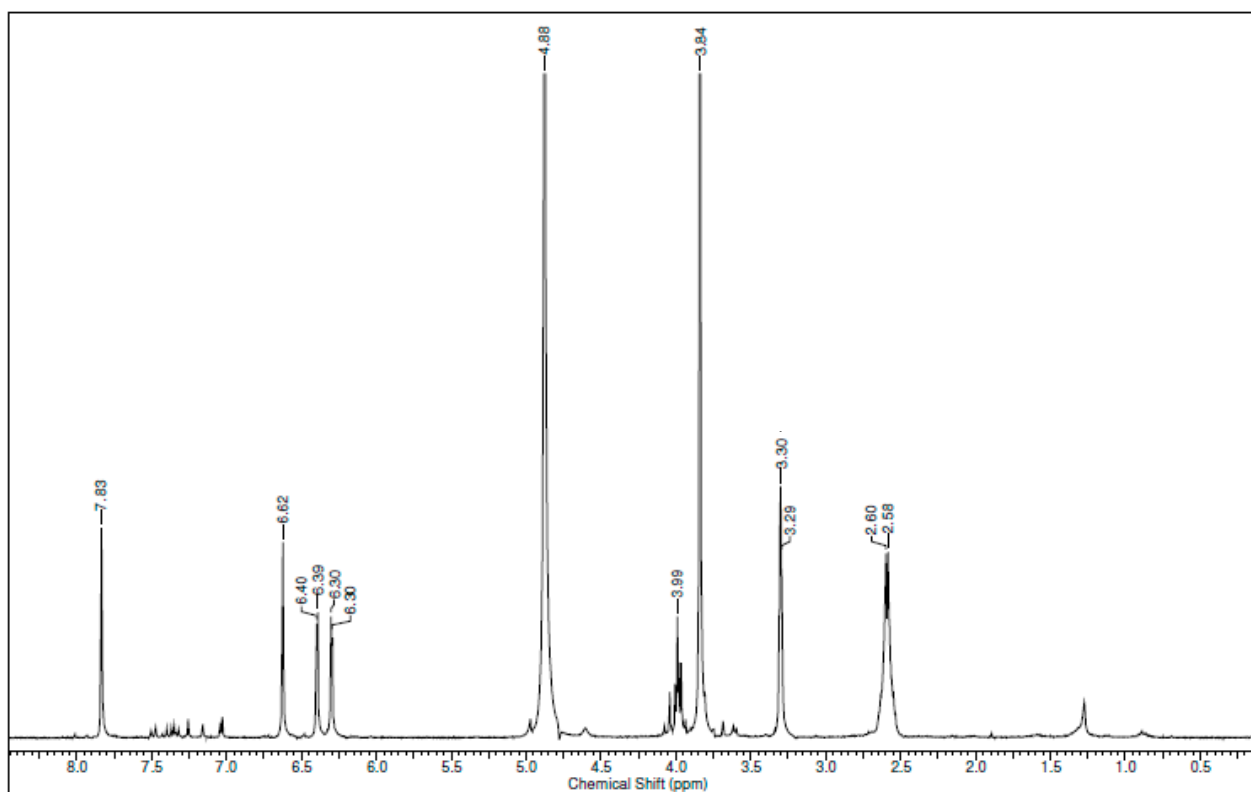


Figure S22. ^1H NMR spectrum (300 MHz, CD_3OD) of compound 4.

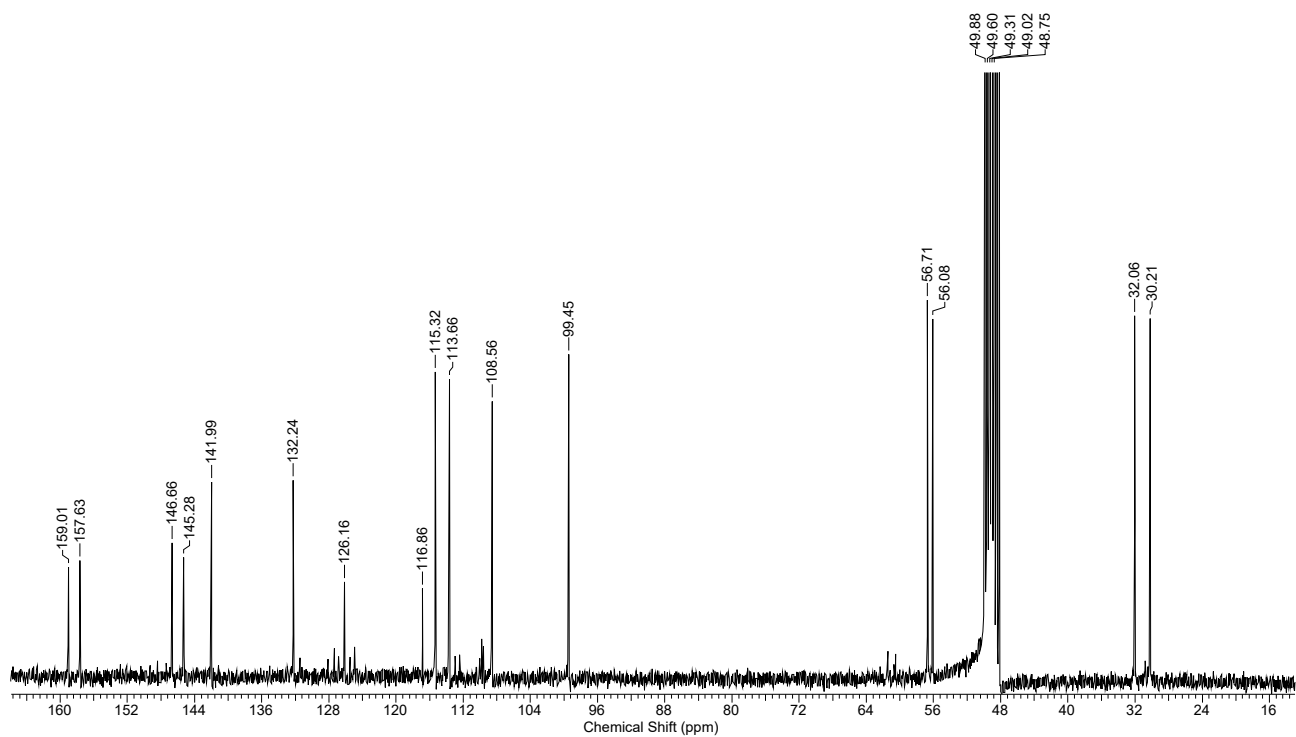


Figure S23 ^{13}C NMR spectrum (75 MHz, CD_3OD) of compound 4.

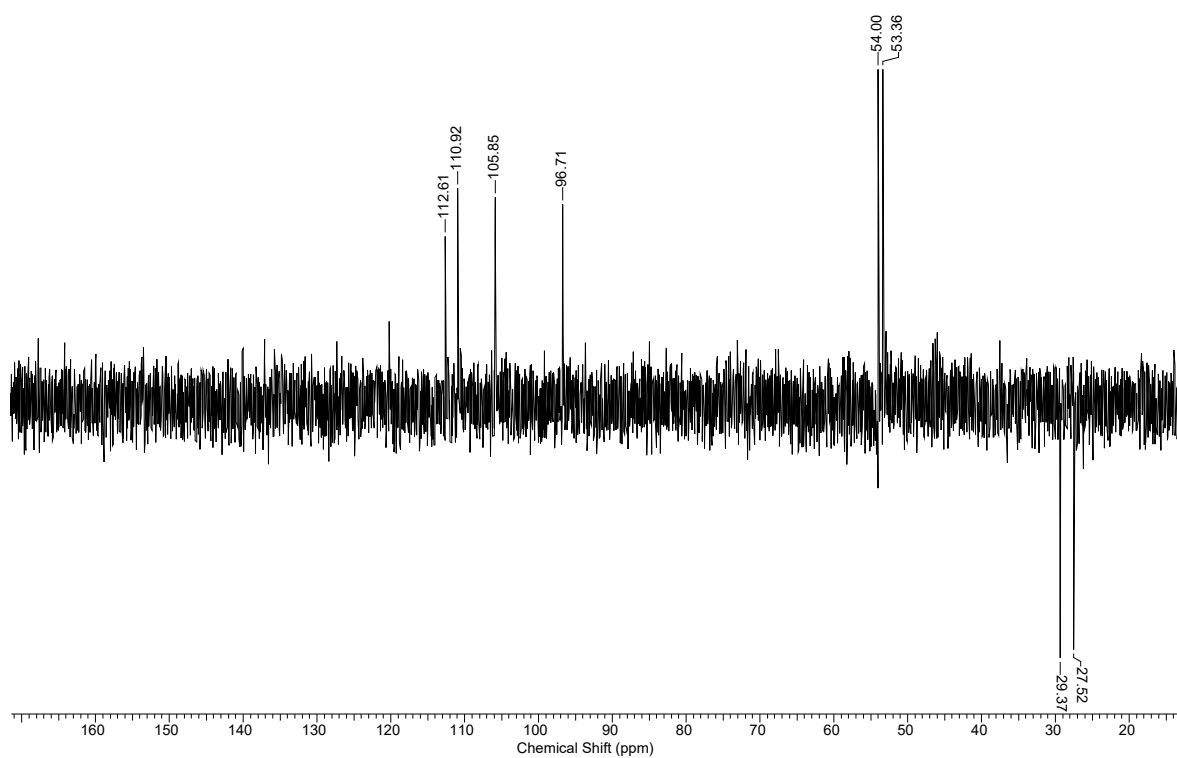


Figure S24. DEPT-135 spectrum (CD_3OD) of compound 4.

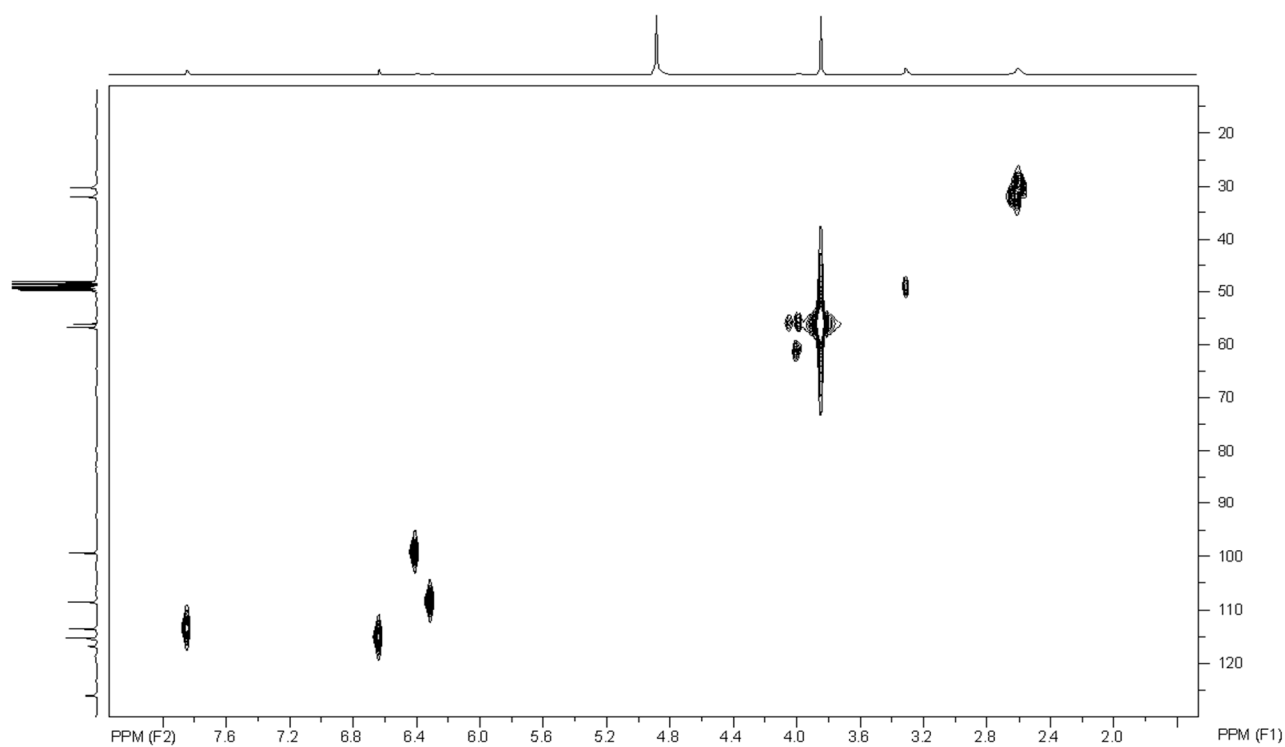


Figure S25. HSQC spectrum (CD_3OD) of compound 4.

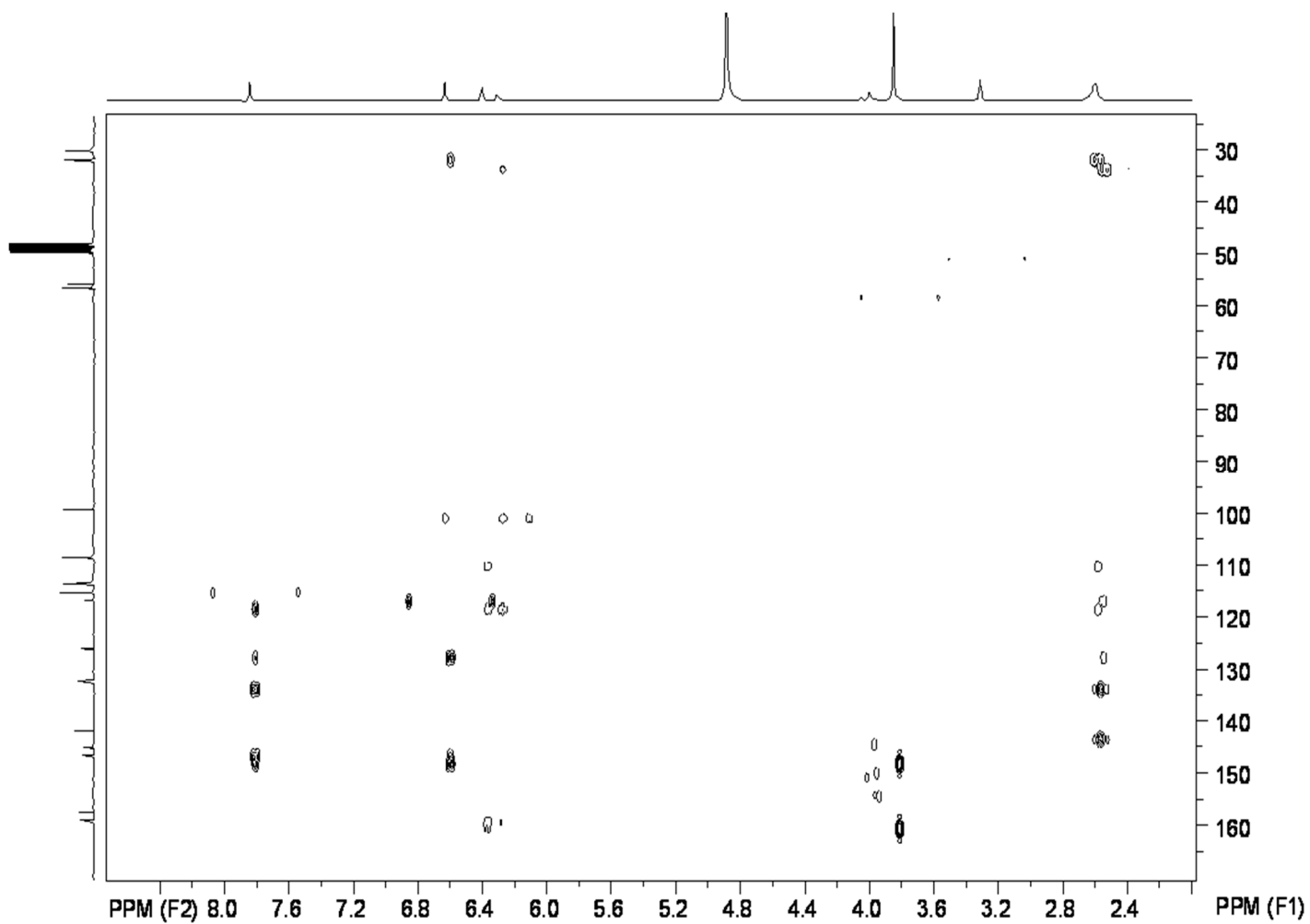


Figure S26. HMBC spectrum (CD_3OD) of compound 4.

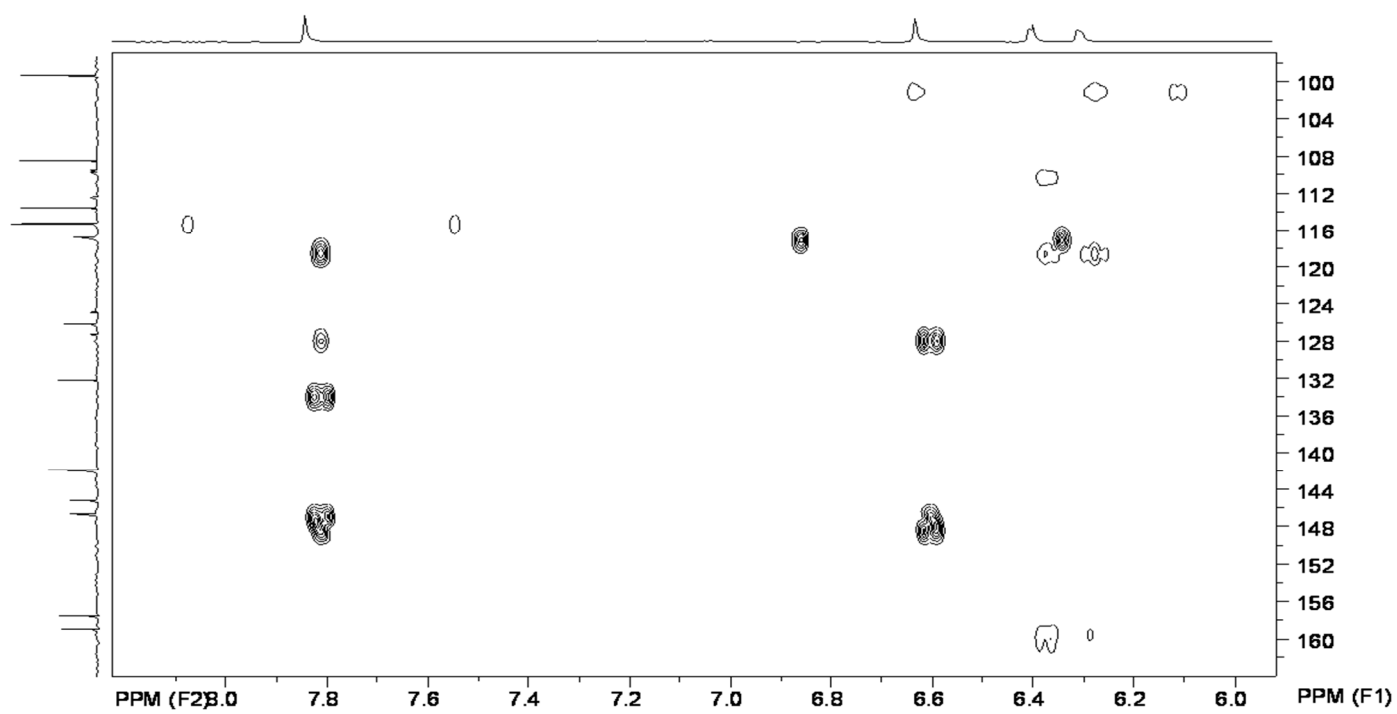


Figure S27. HMBC spectrum (expansion) of compound 4.

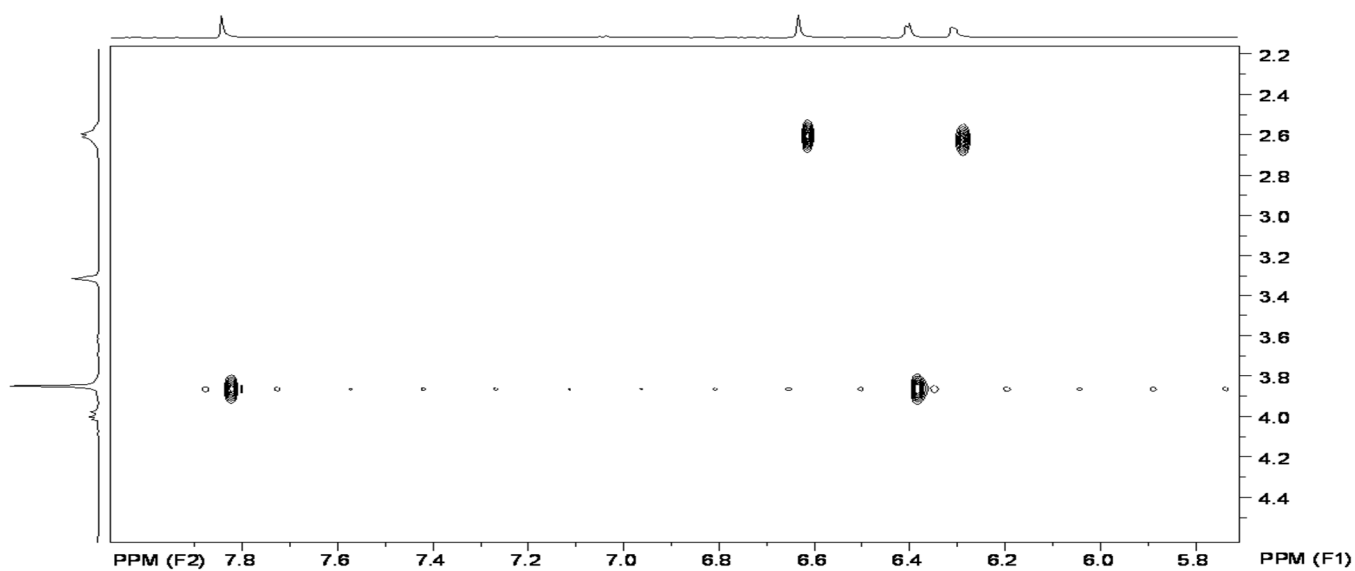


Figure S28. NOESY spectrum (300 MHz, CD₃OD) of compound 4.

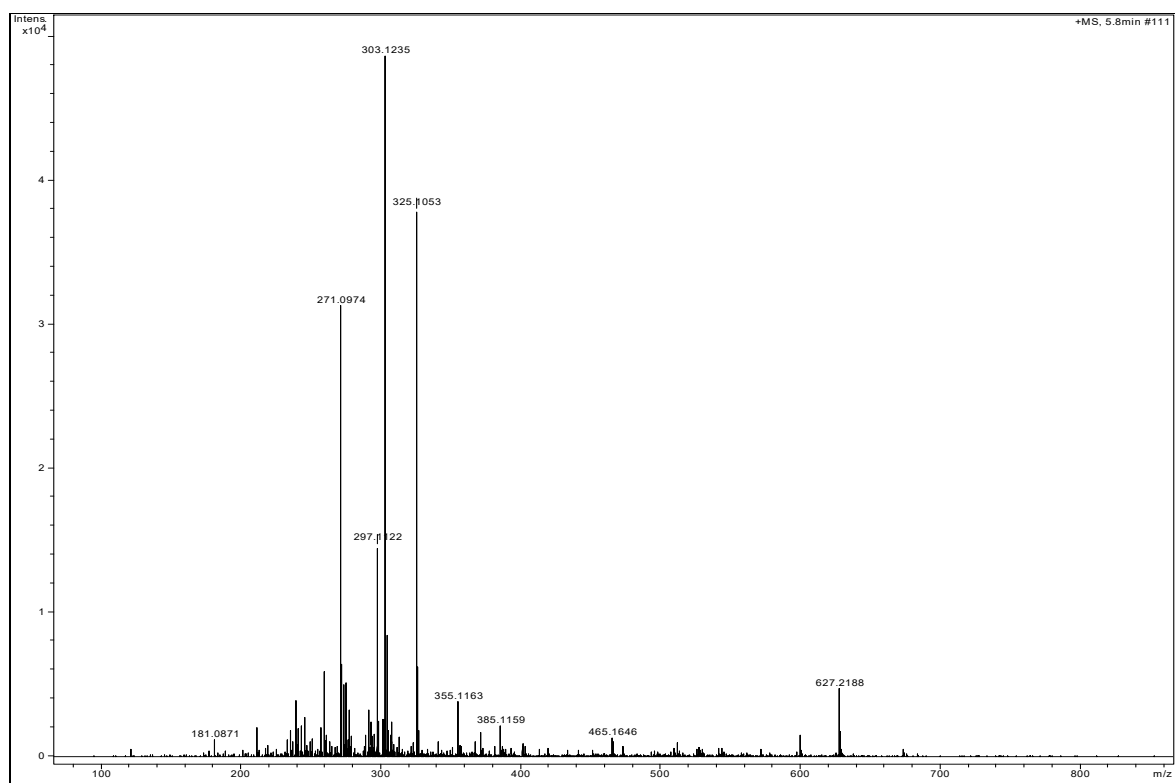


Figure S29. HRESIMS (positive mode) of compound 5.

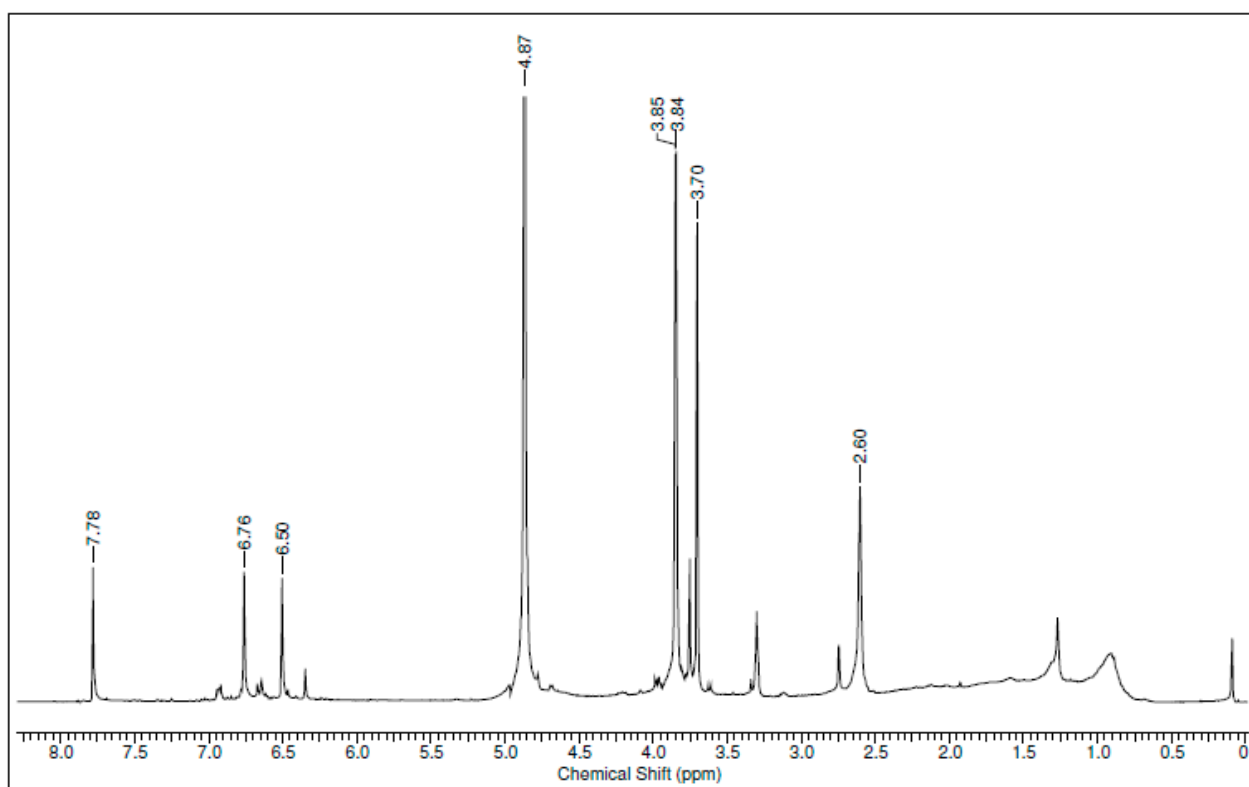


Figure S30. ^1H NMR spectrum (300 MHz, CD_3OD) of compound 5.

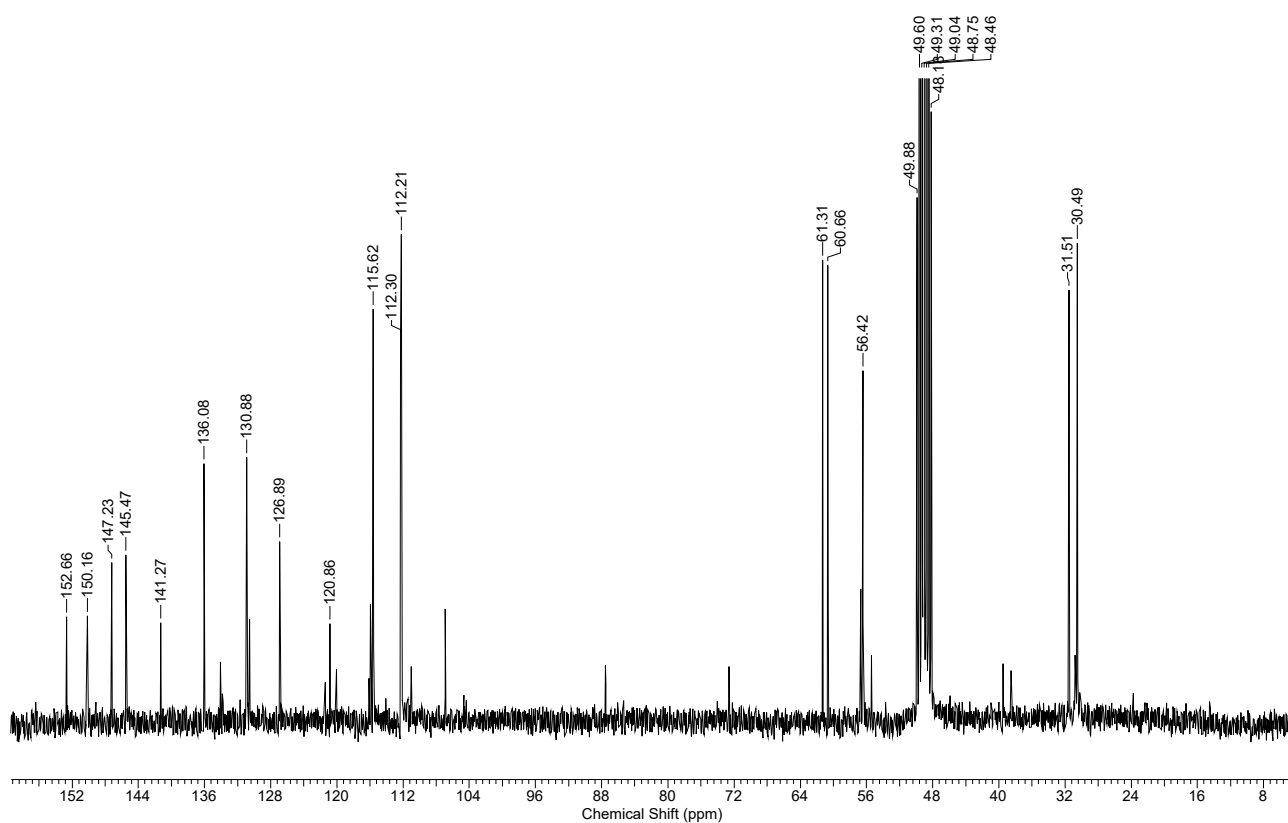


Figure S31. ^{13}C NMR spectrum (75 MHz, CD_3OD) of compound 5.

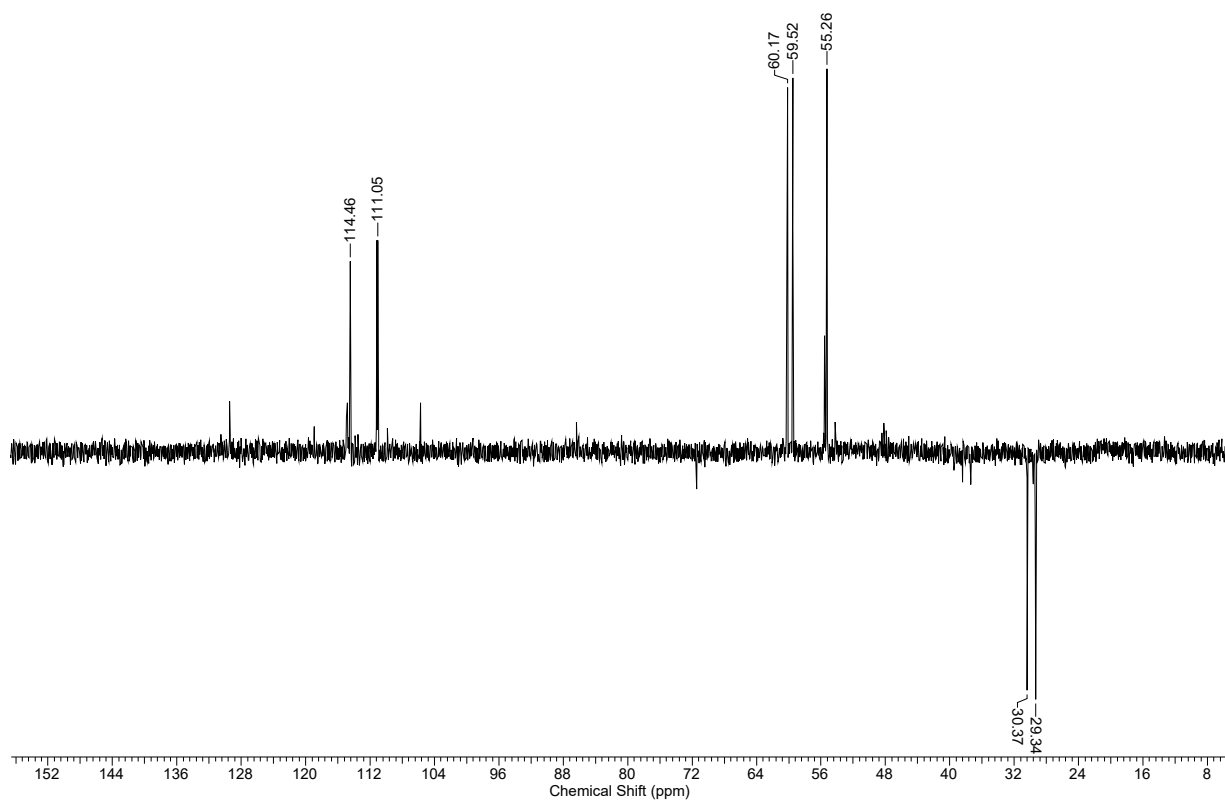


Figure S32. DEPT-135 spectrum (CD_3OD) of compound 5.

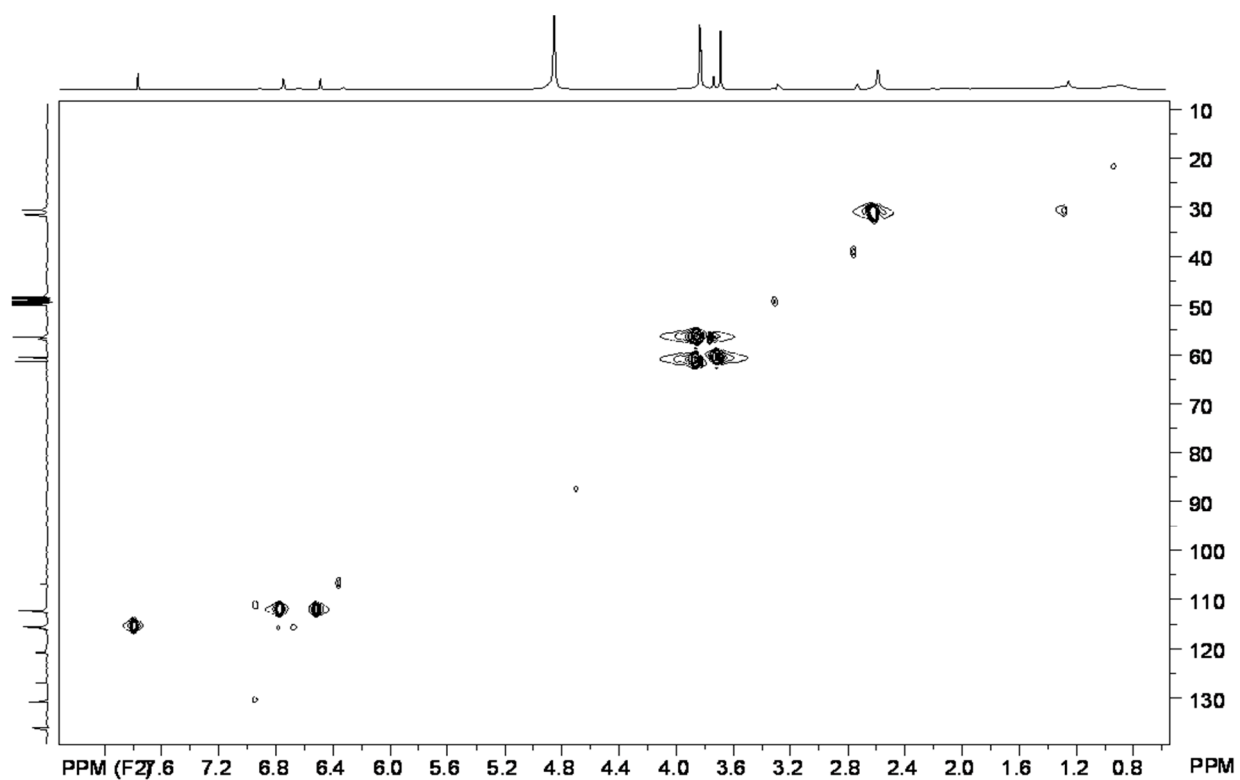


Figure S33. HSQC spectrum (CD_3OD) of compound 5.

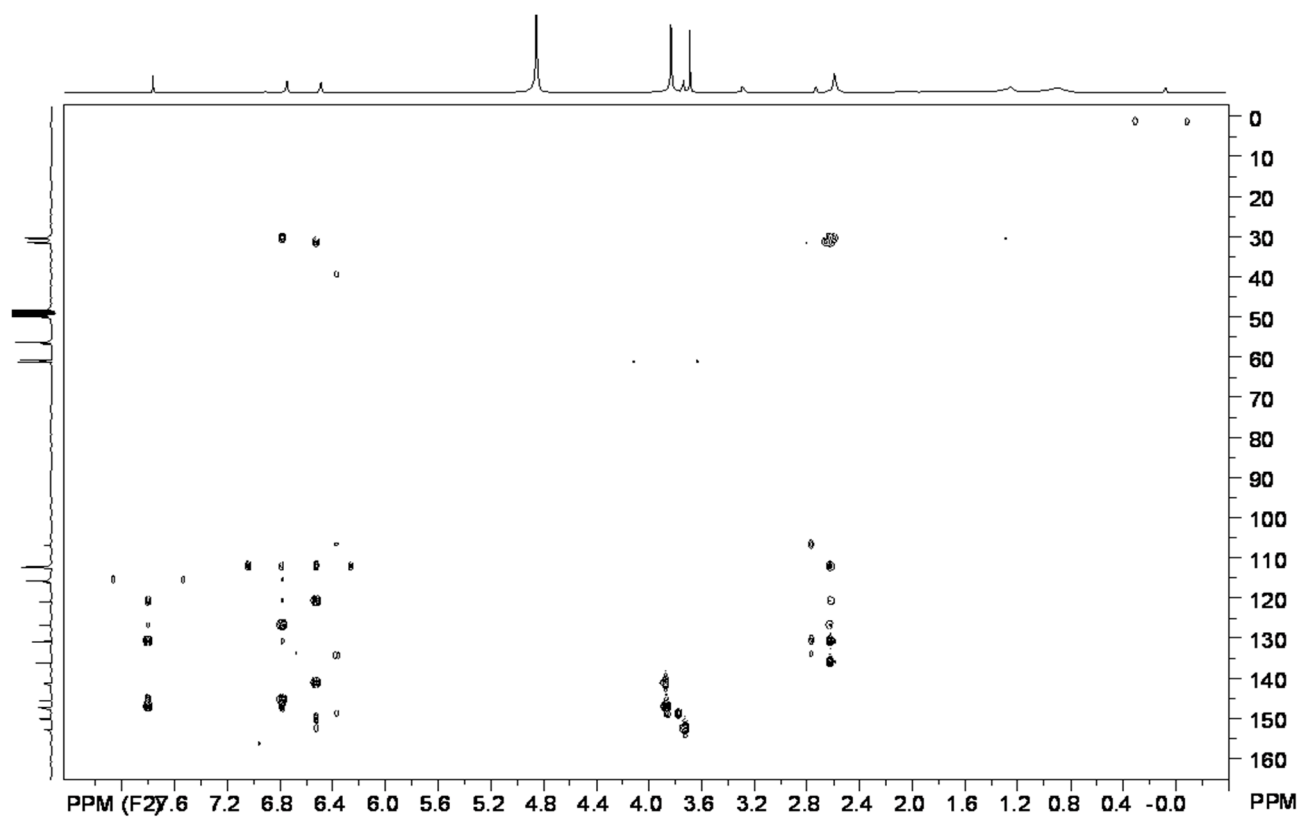


Figure S34. HMBC spectrum (CD_3OD) of compound 5.

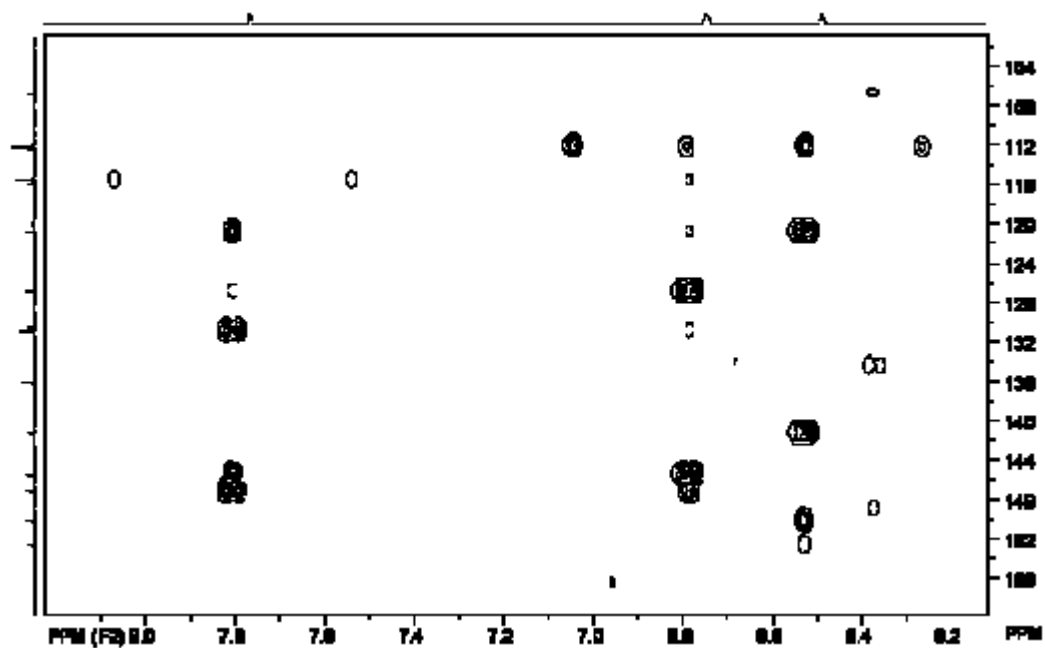


Figure S35. HMBC spectrum (expansion) of compound 5.

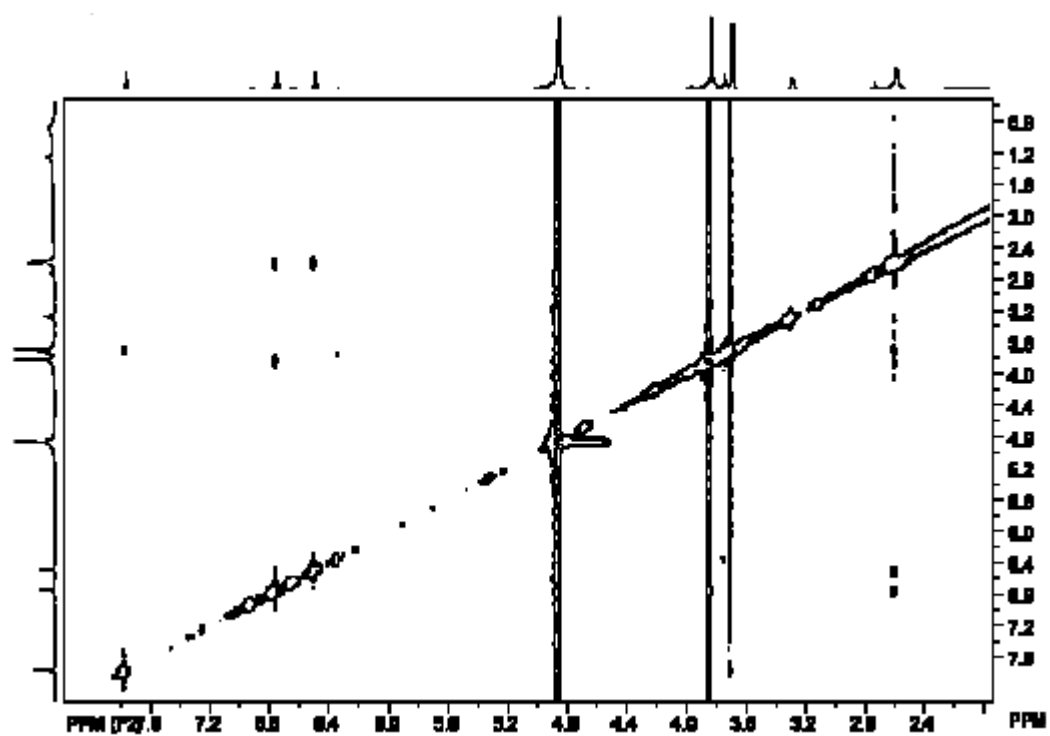


Figure S36. NOESY spectrum (300 MHz, CD₃OD) of compound 5.

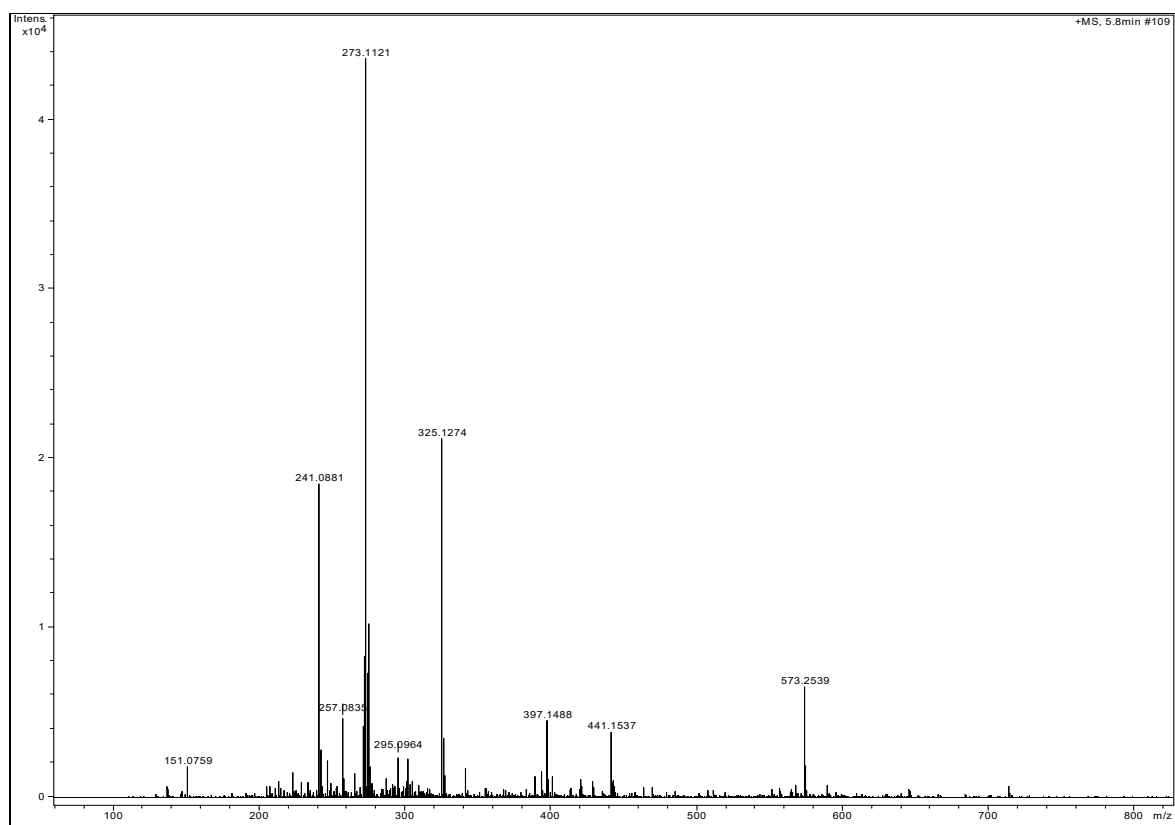


Figure S37. HRESIMS (positive mode) of compound 6.

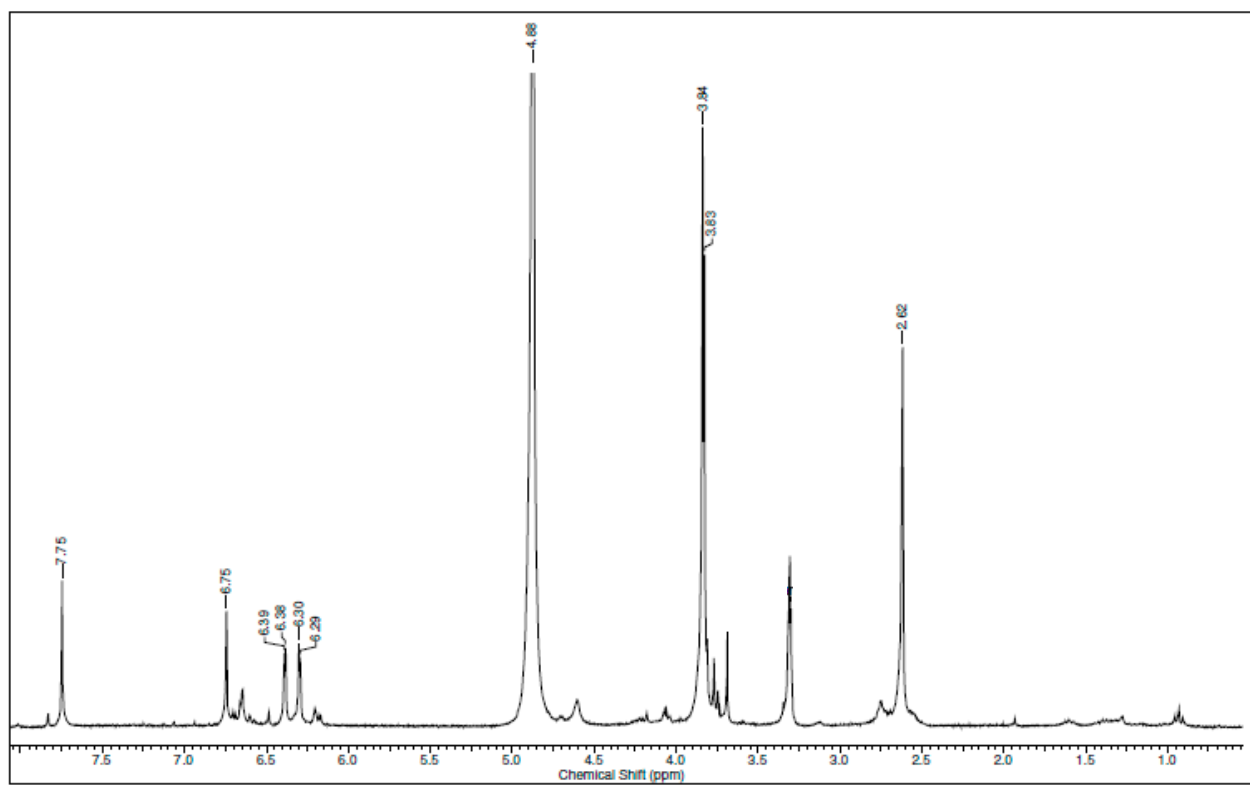


Figure S38. ¹H NMR spectrum (300 MHz, CD₃OD) of compound 6.

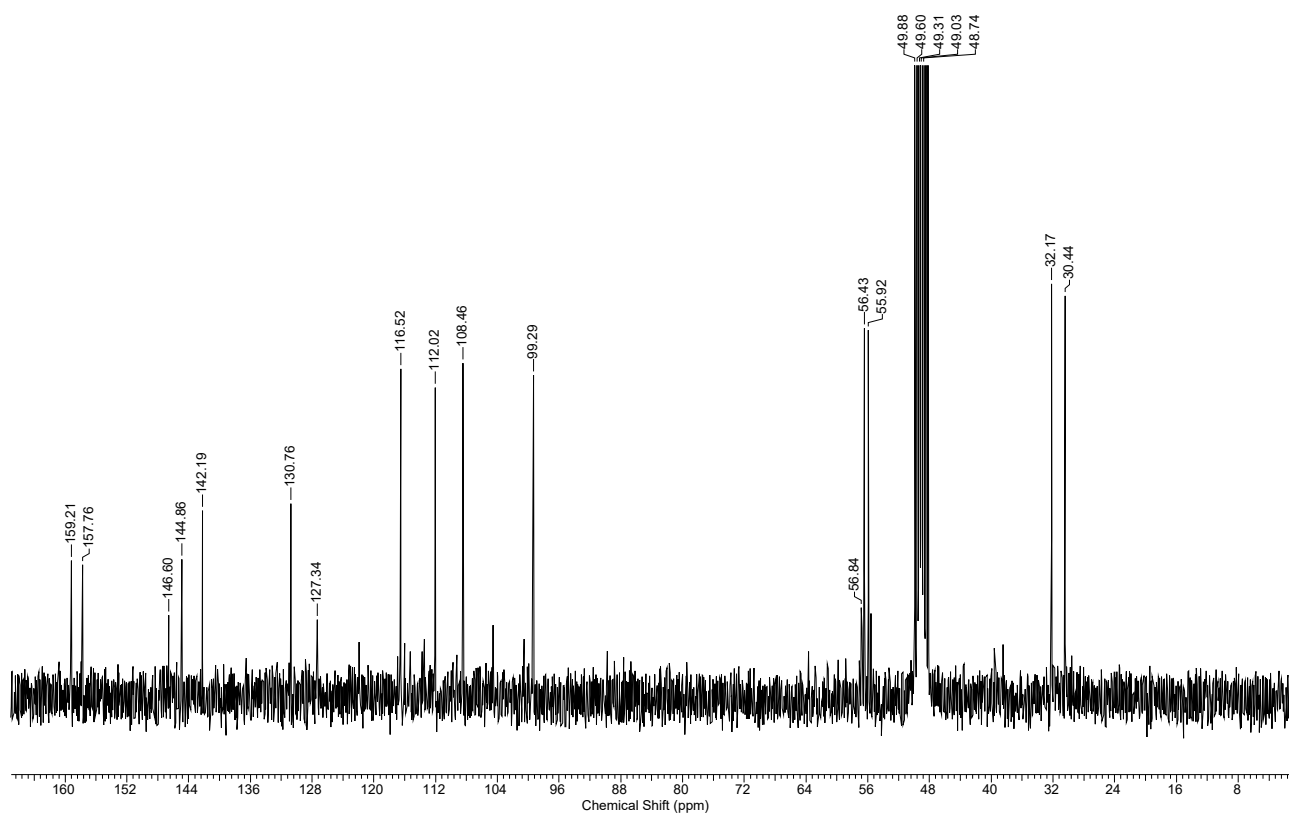


Figure S39. ^{13}C NMR spectrum (75 MHz, CD_3OD) of compound 6.

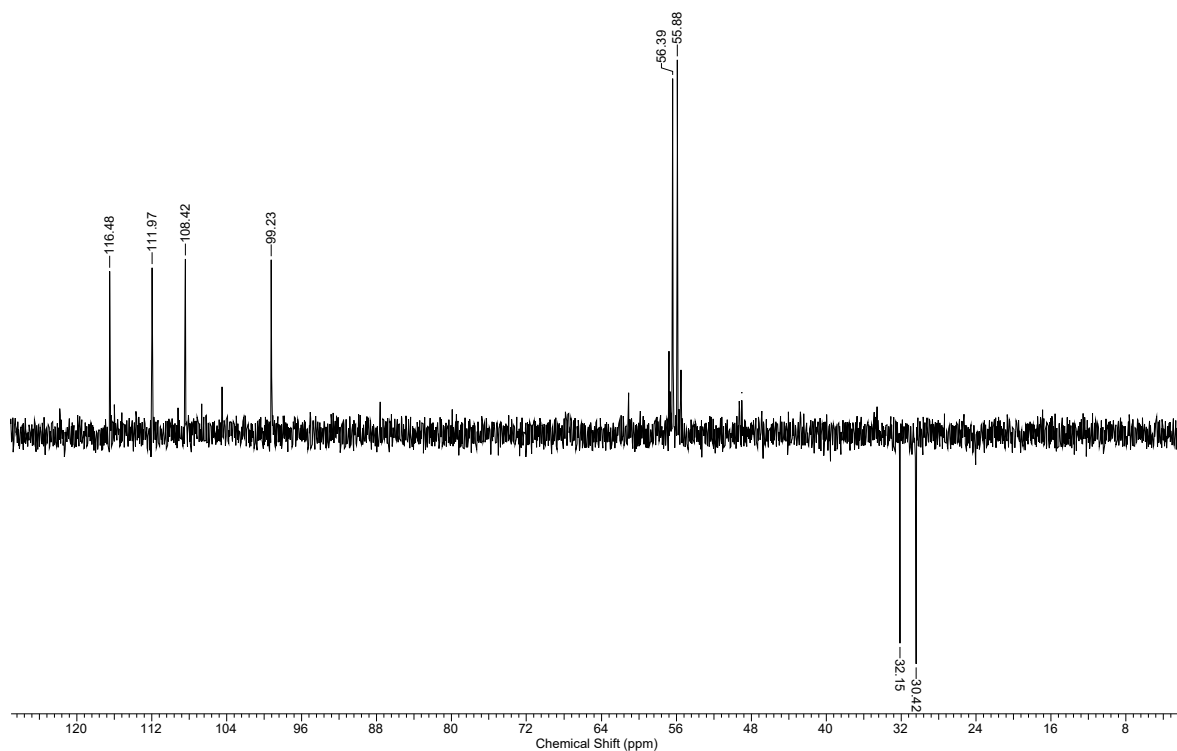


Figure S40. DEPT-135 spectrum (CD_3OD) of compound 6.

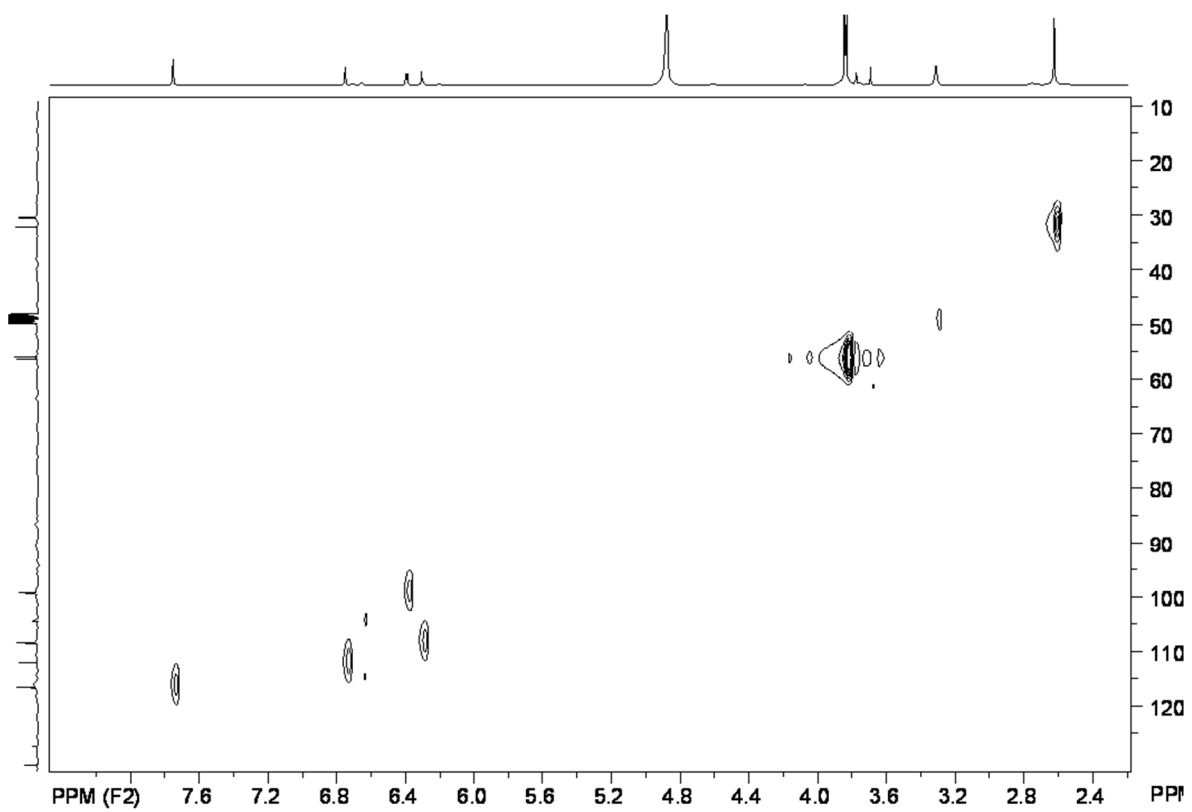


Figure S41. HSQC spectrum (CD₃OD) of compound 6.

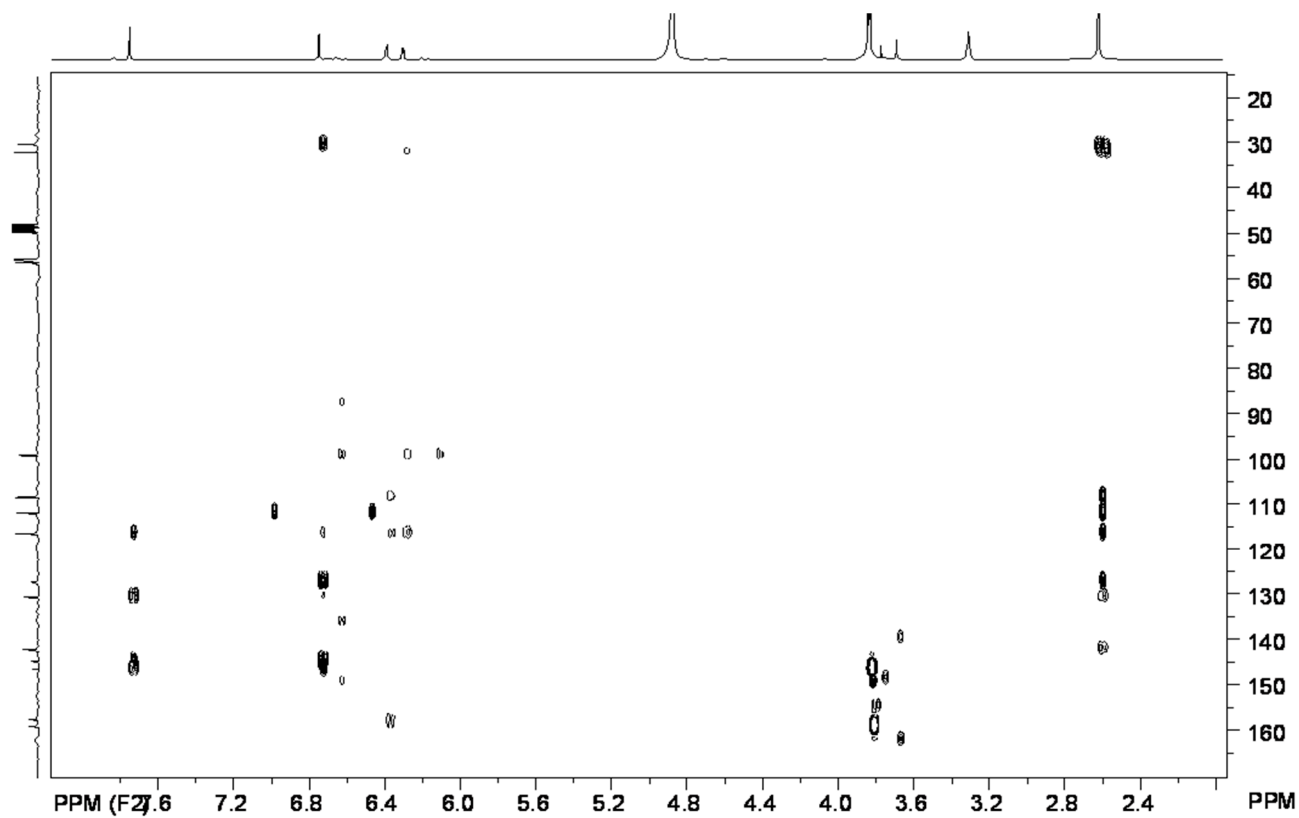


Figure S42. HMBC spectrum (CD₃OD) of compound 6.

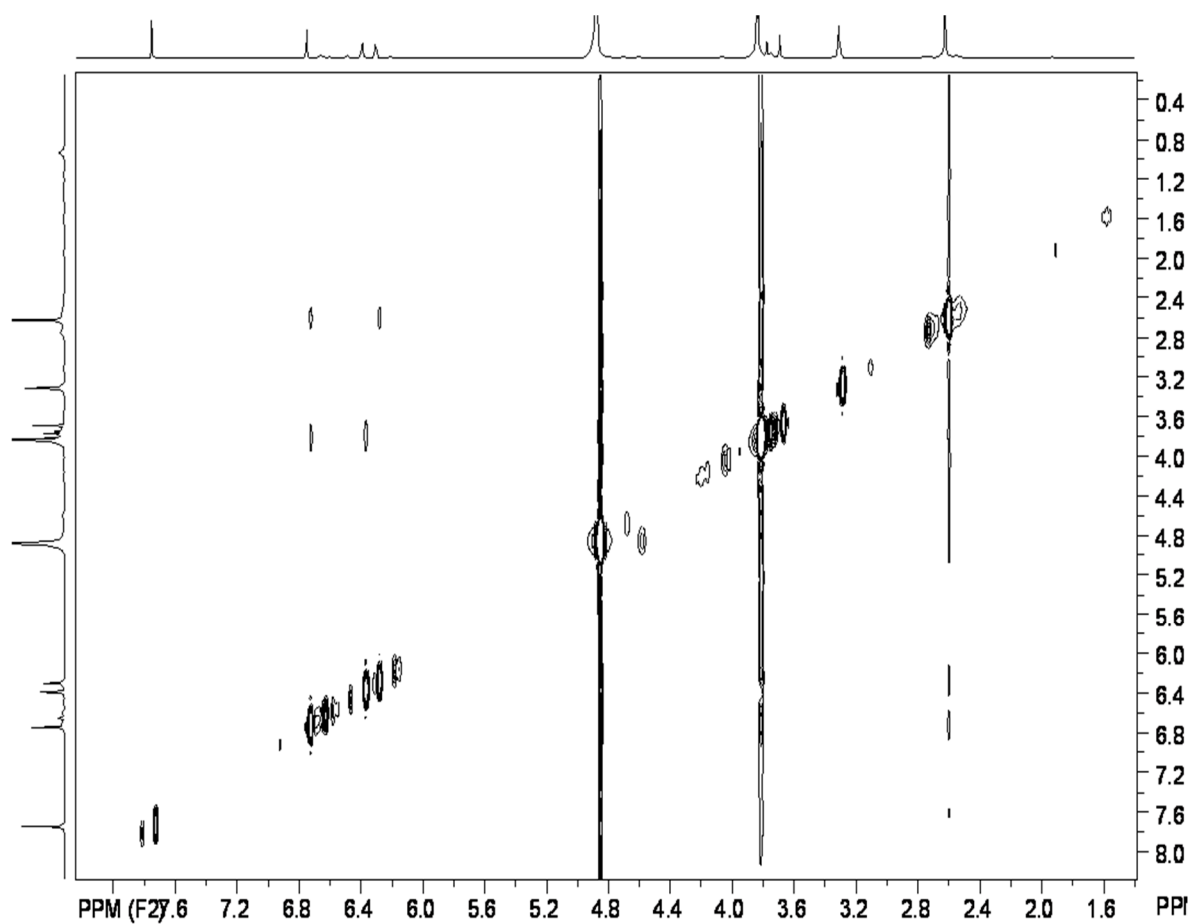


Figure S43. NOESY spectrum (CD_3OD) of compound 6.

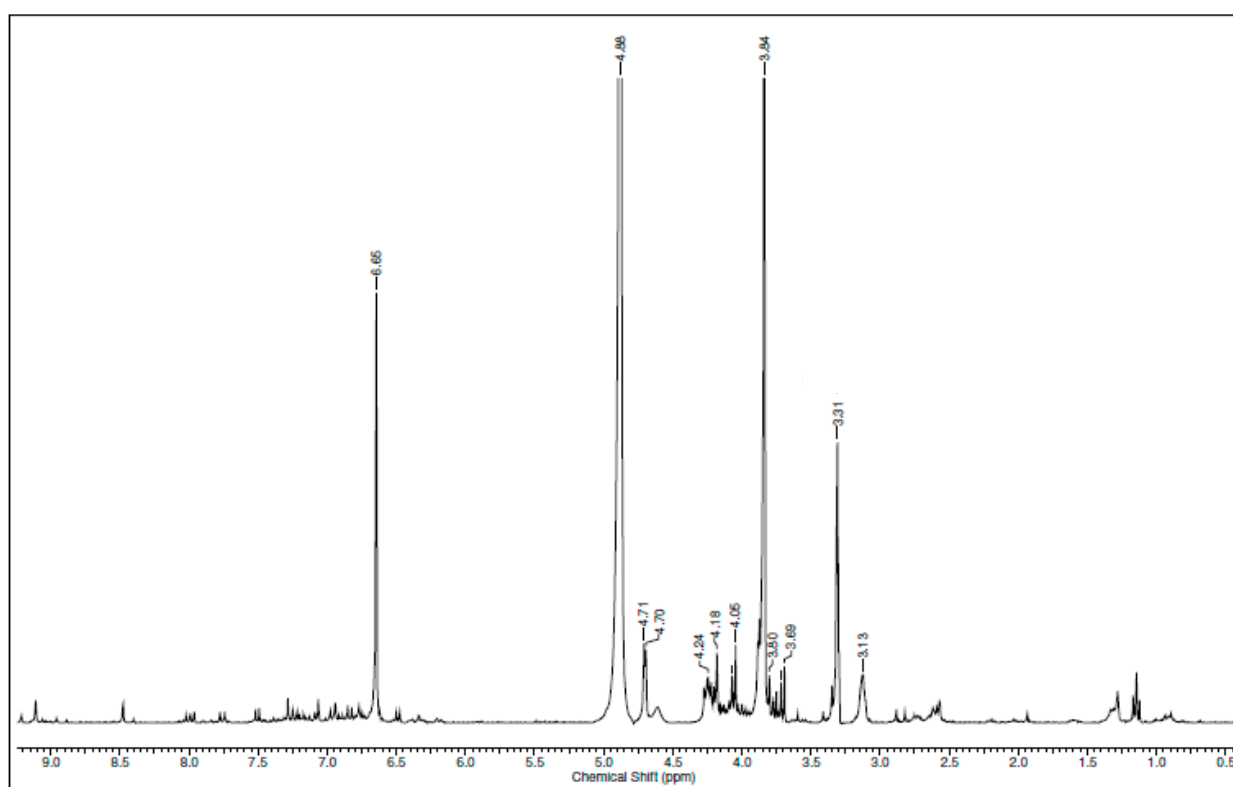


Figure S44. ^1H NMR spectrum (300 MHz, CD_3OD) of compound 7.

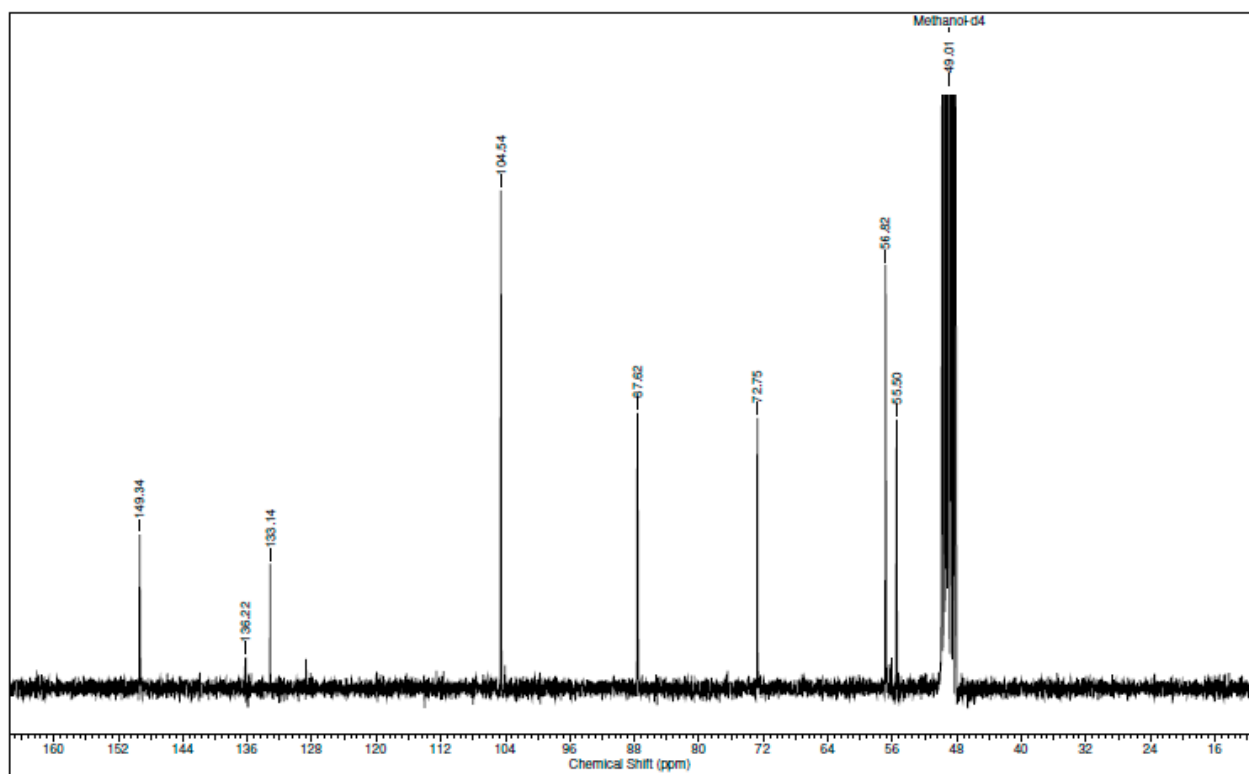


Figure S45. ^{13}C NMR spectrum (75 MHz, CD_3OD) of compound 7.

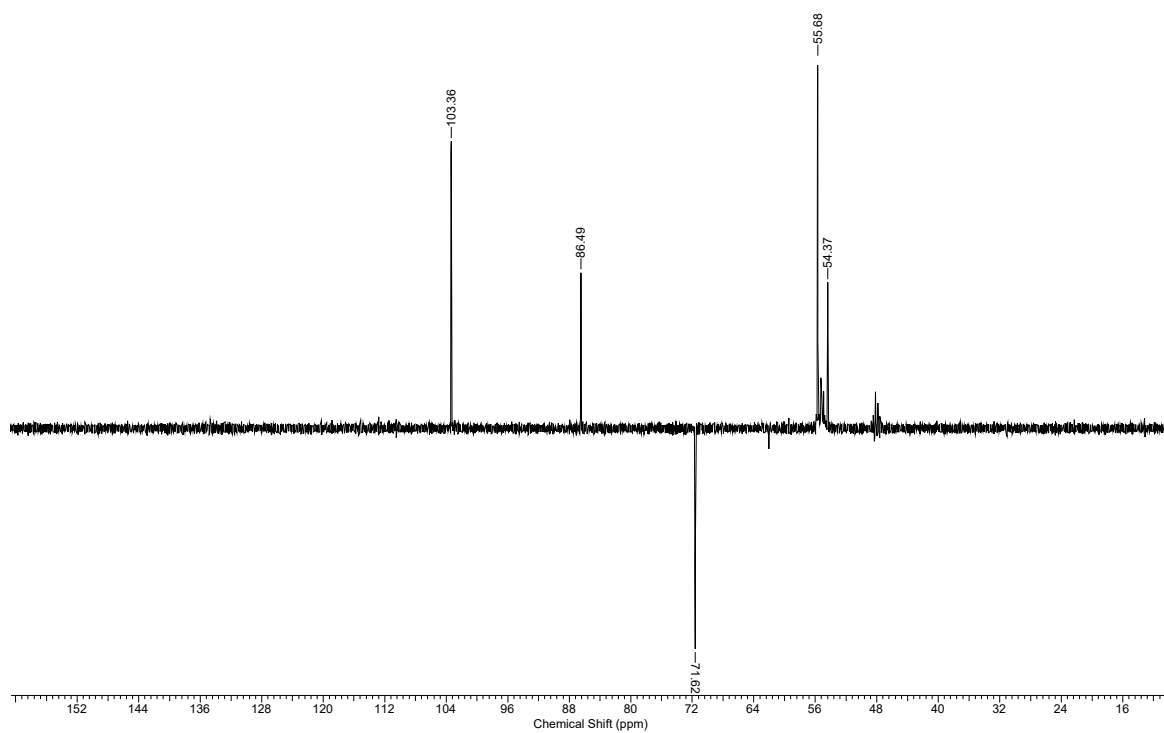


Figure S46. DEPT-135 spectrum (CD_3OD) of compound 7.

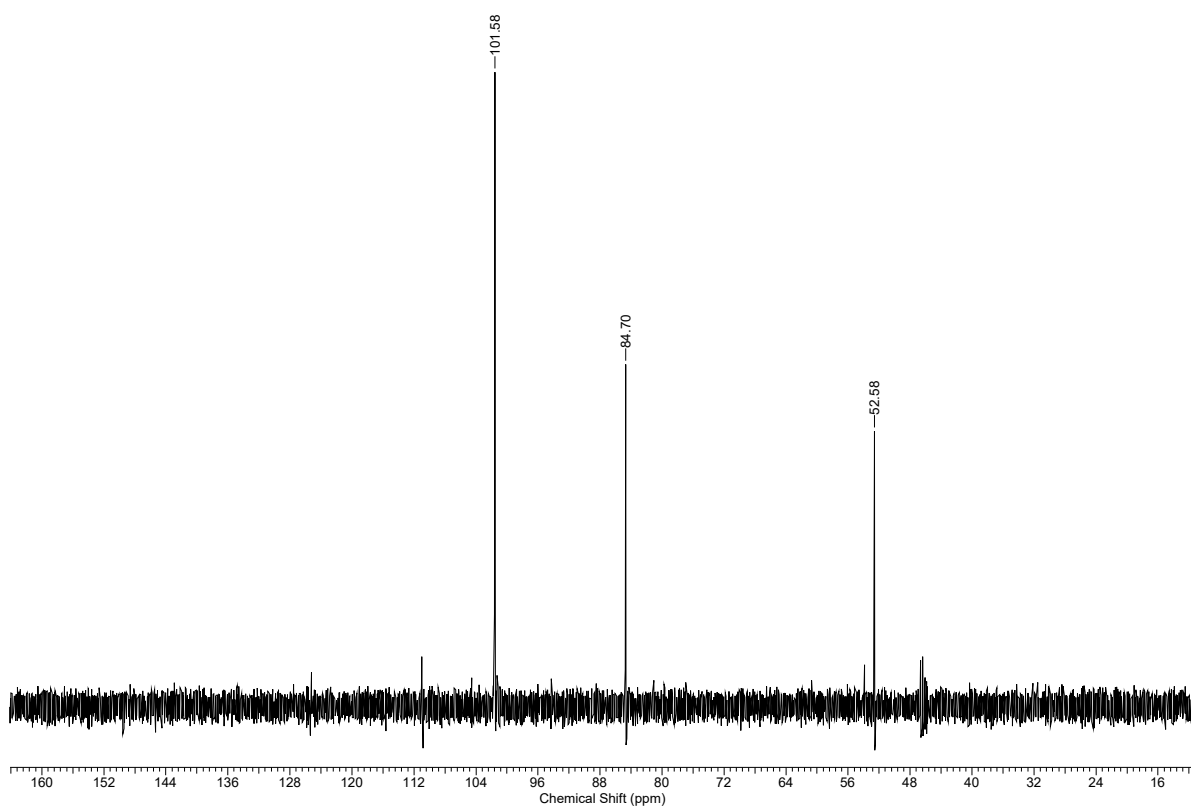


Figure S47. DEPT-90 spectrum (CD₃OD) of compound 7.

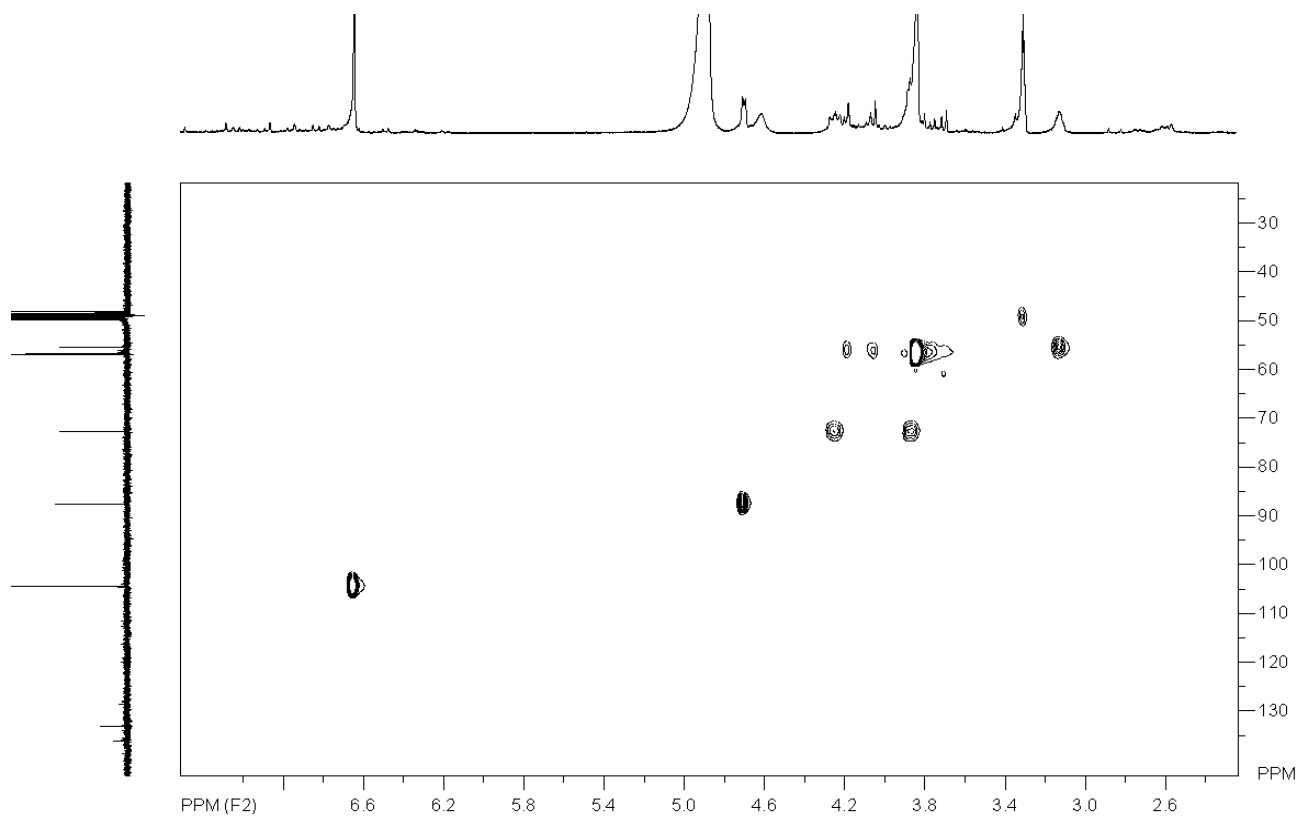


Figure S48. HSQC spectrum (CD₃OD) of compound 7.

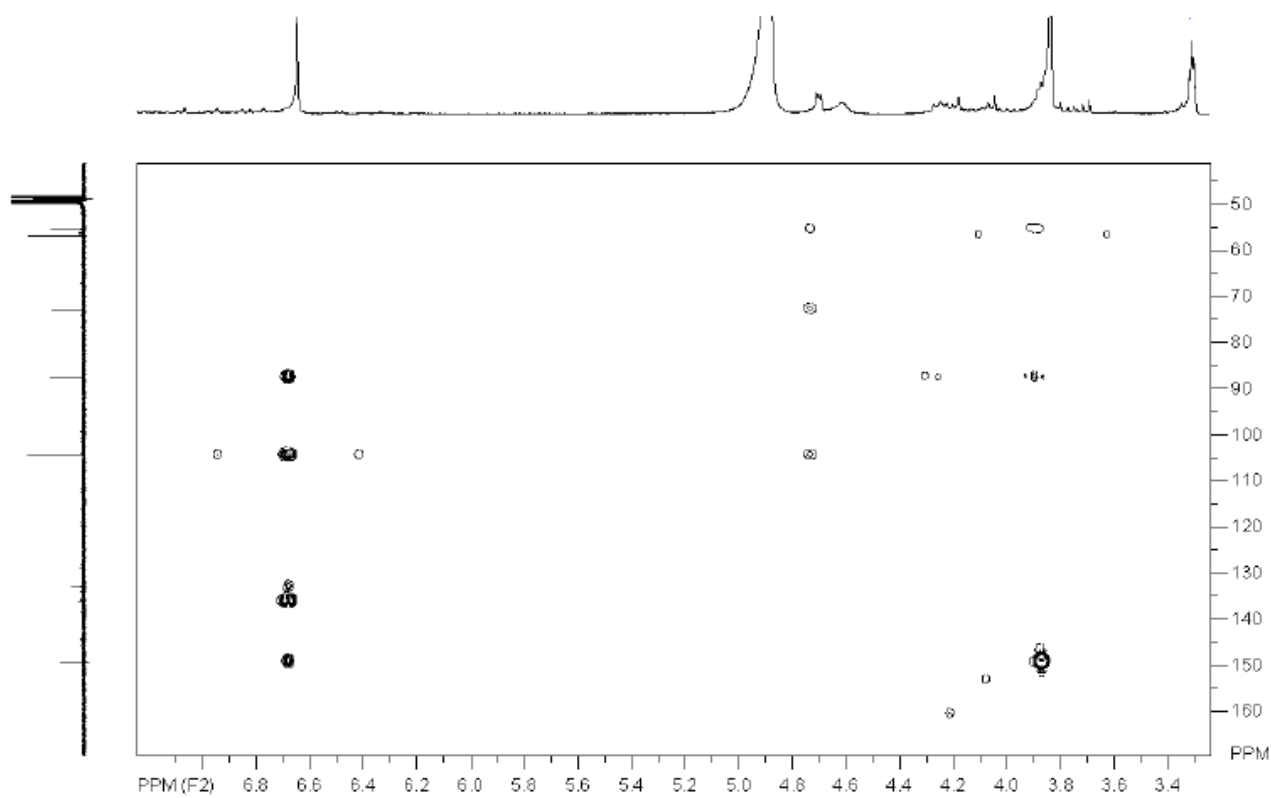


Figure S49. HMBC spectrum (CD_3OD) of compound 7.

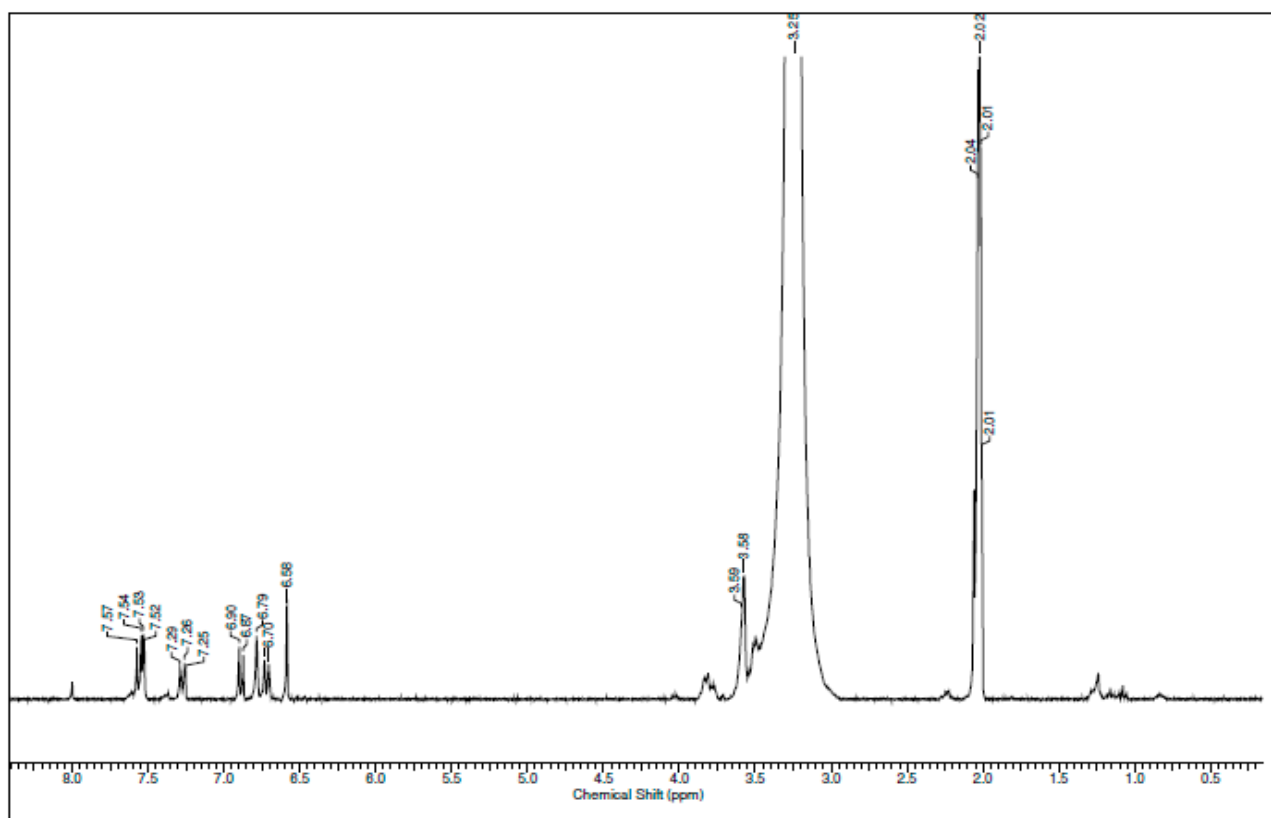


Figure S50. ^1H NMR spectrum (300 MHz, acetone- d_6) of compound 8.

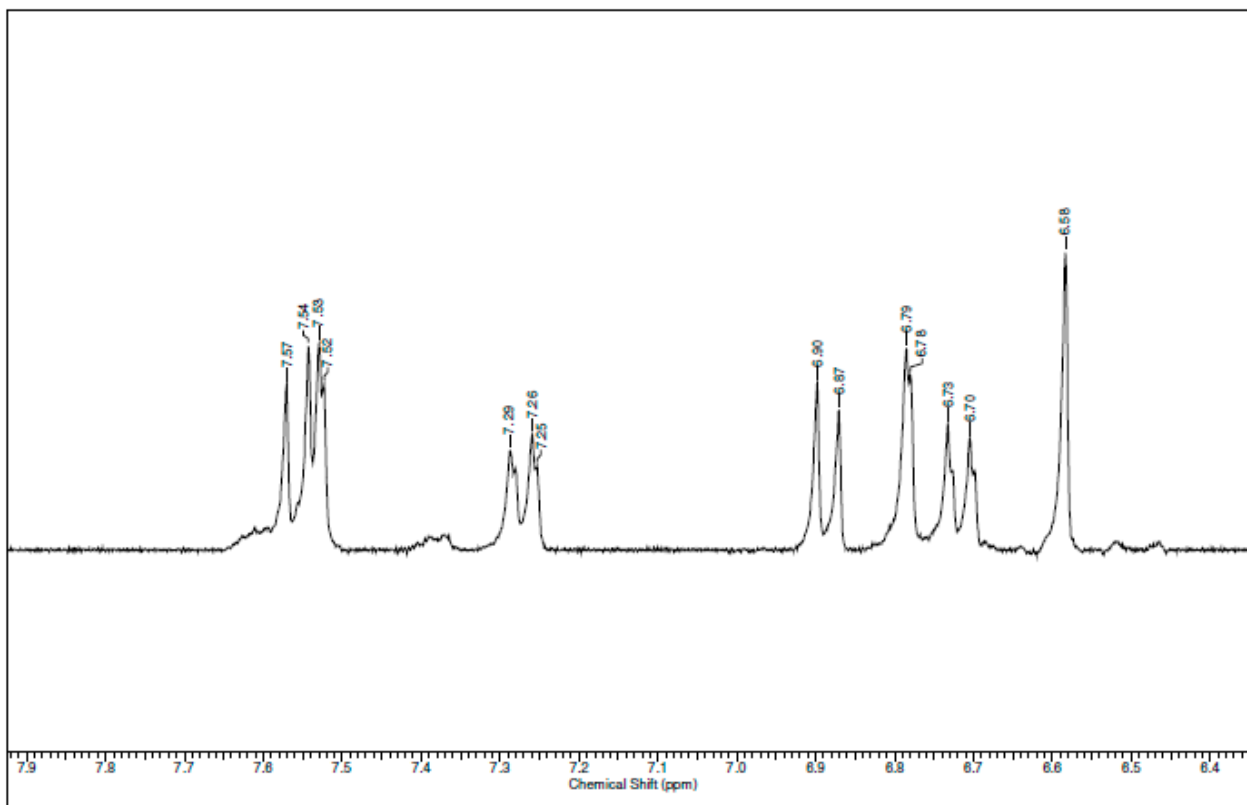


Figure S51. ^1H NMR spectrum (expansion) of compound 8.

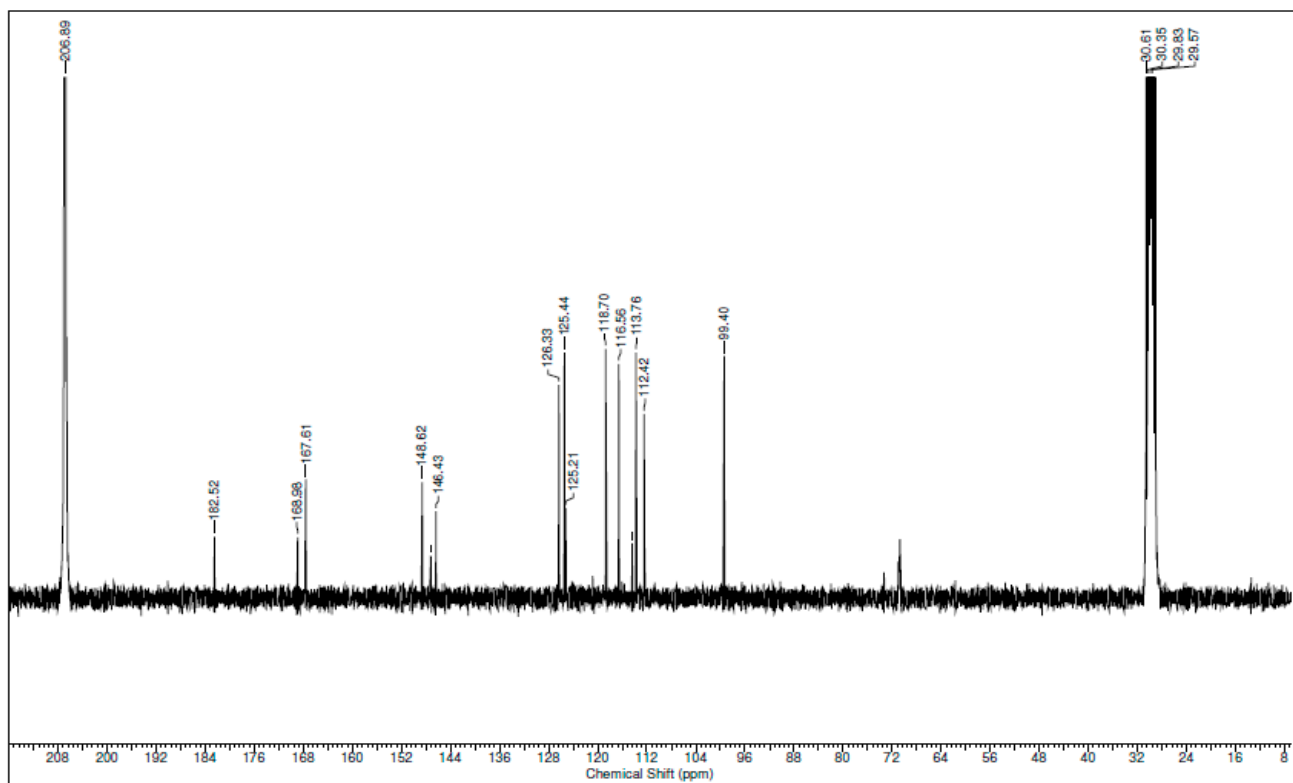


Figure S52. ^{13}C NMR spectrum (75 MHz, acetone- d_6) of compound 8.

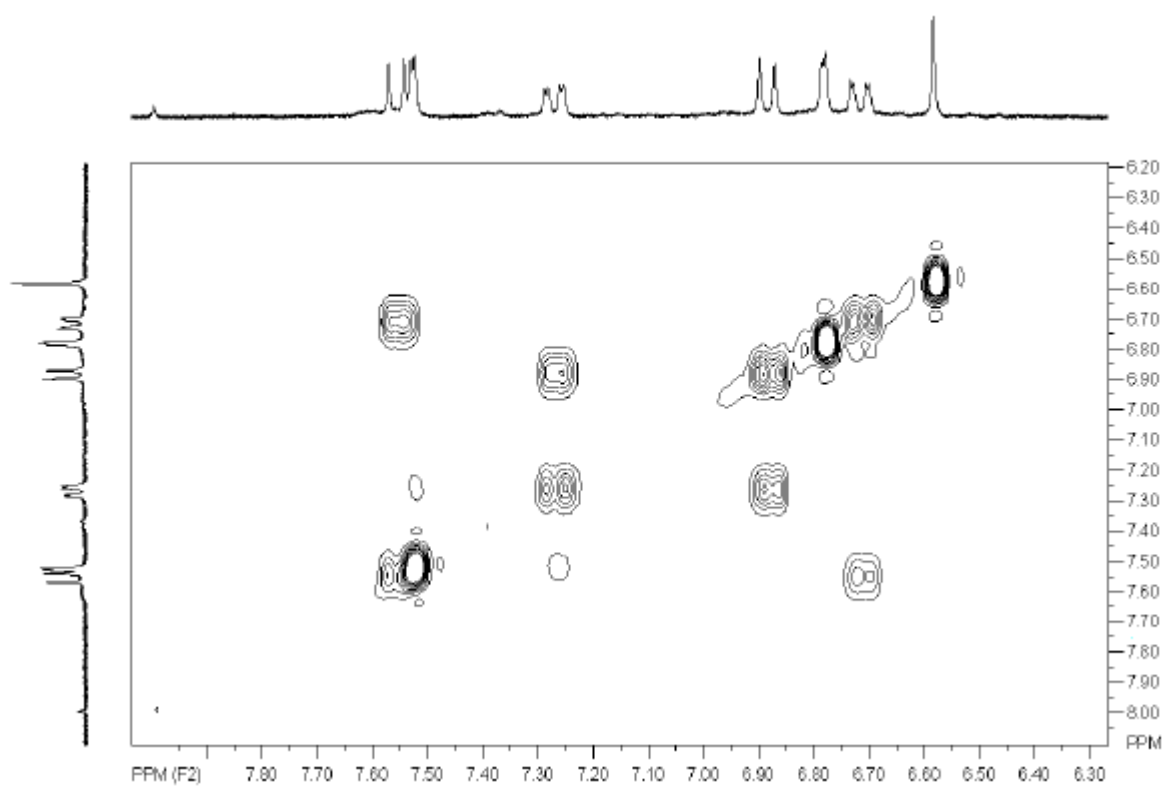


Figure S53. ^1H - ^1H COSY spectrum (300 MHz, acetone- d_6) of compound 8.

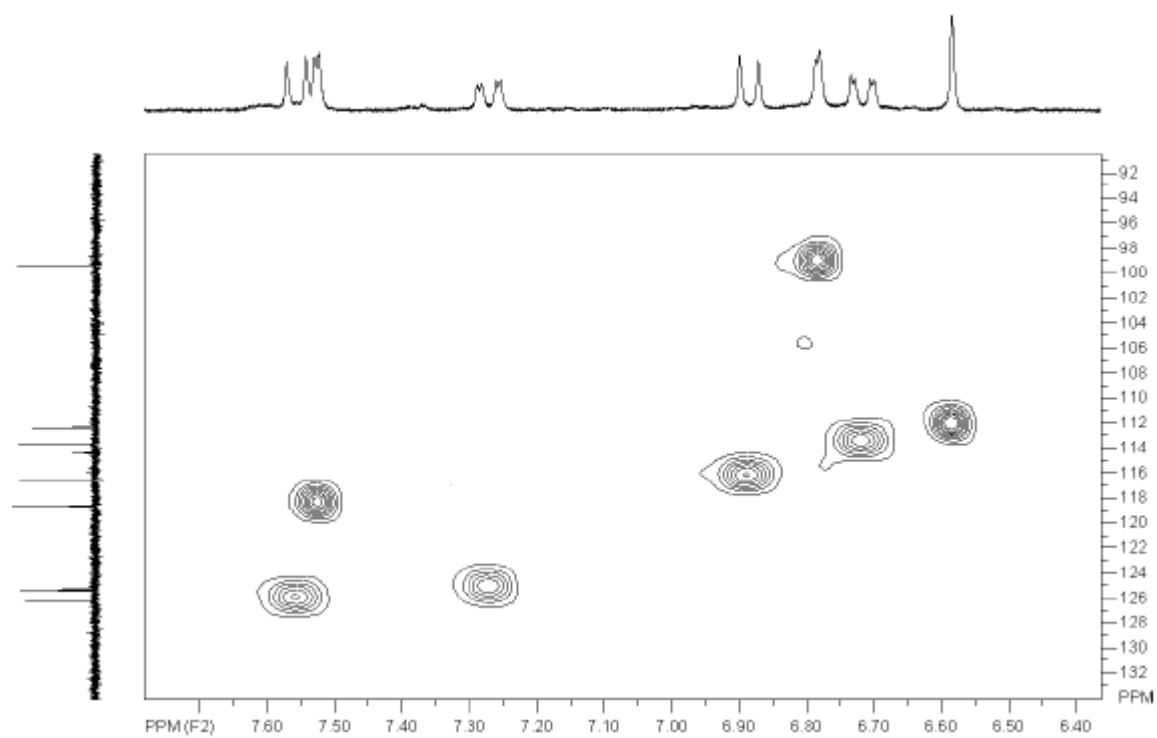


Figure S54. HSQC spectrum (acetone- d_6) of compound 8.

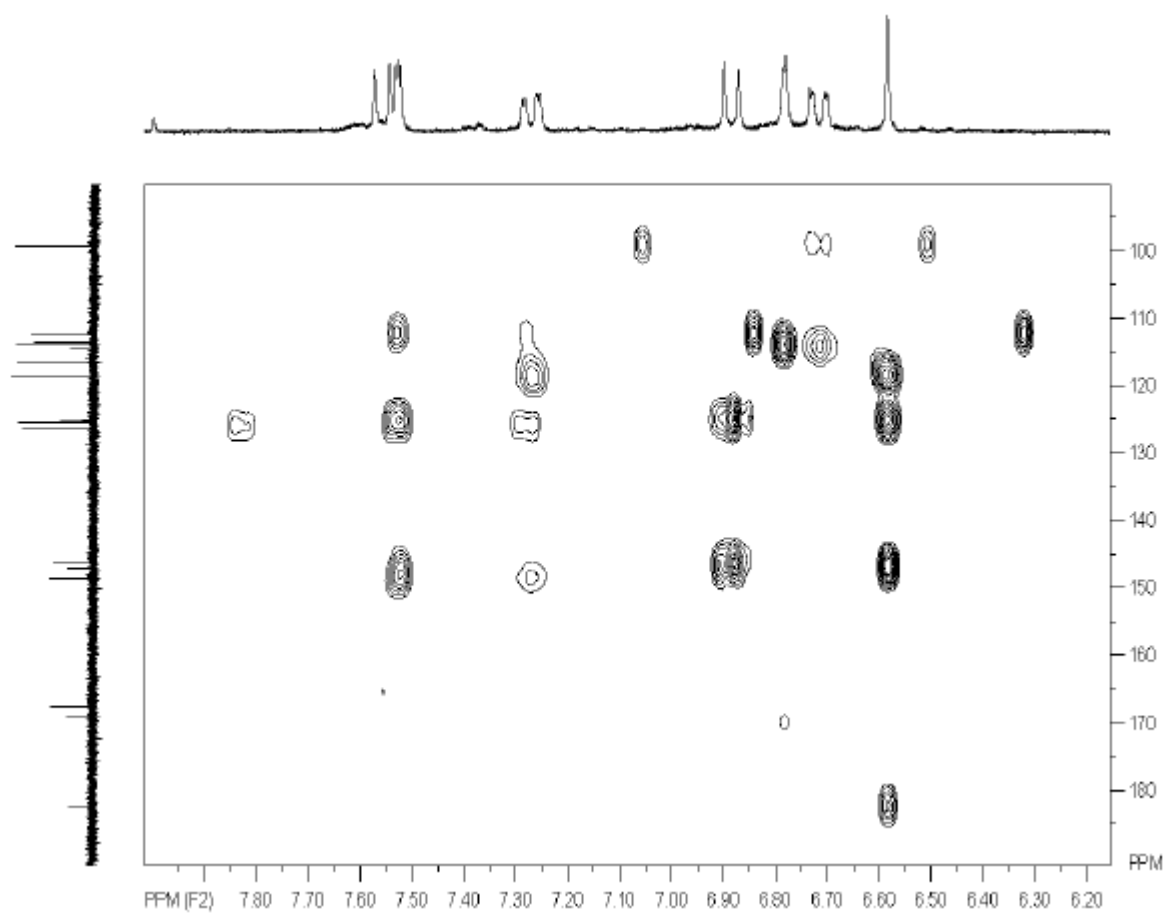


Figure S55. HMBC spectrum (acetone-d₆) of compound 8.

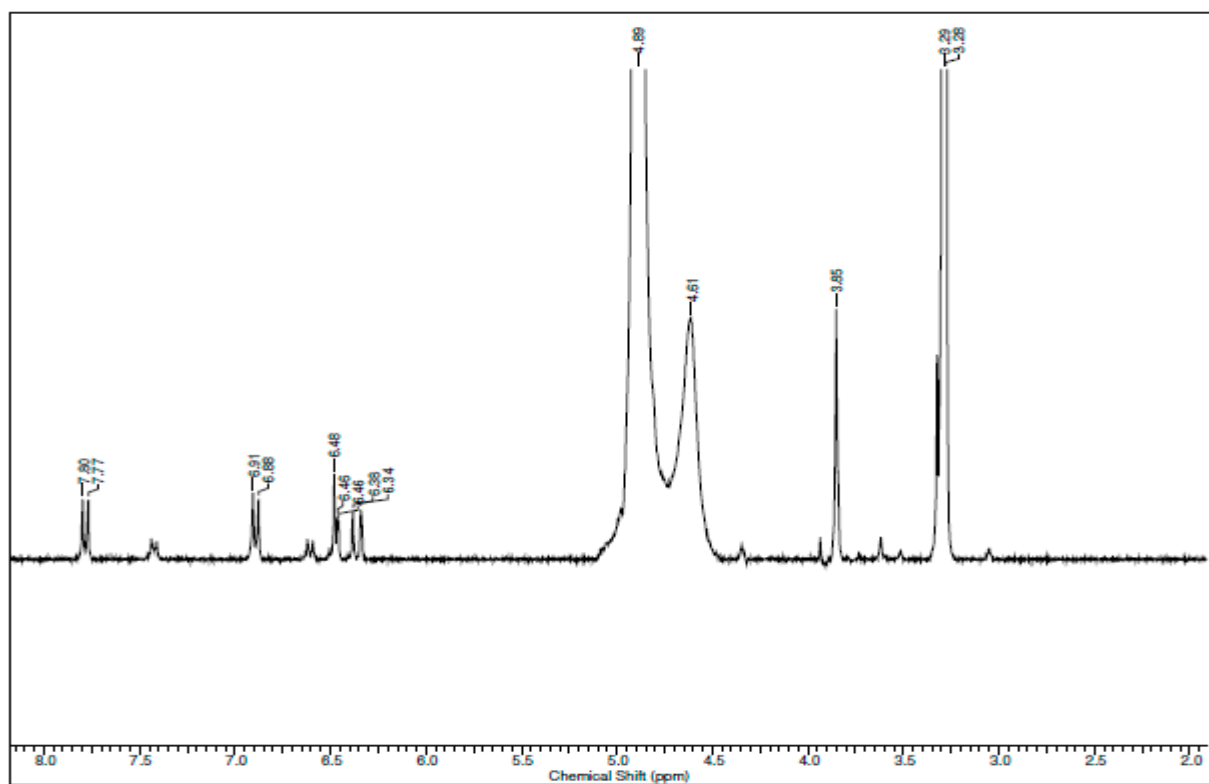


Figure S56. ¹H NMR spectrum (300 MHz, CD₃OD) of compound 9.

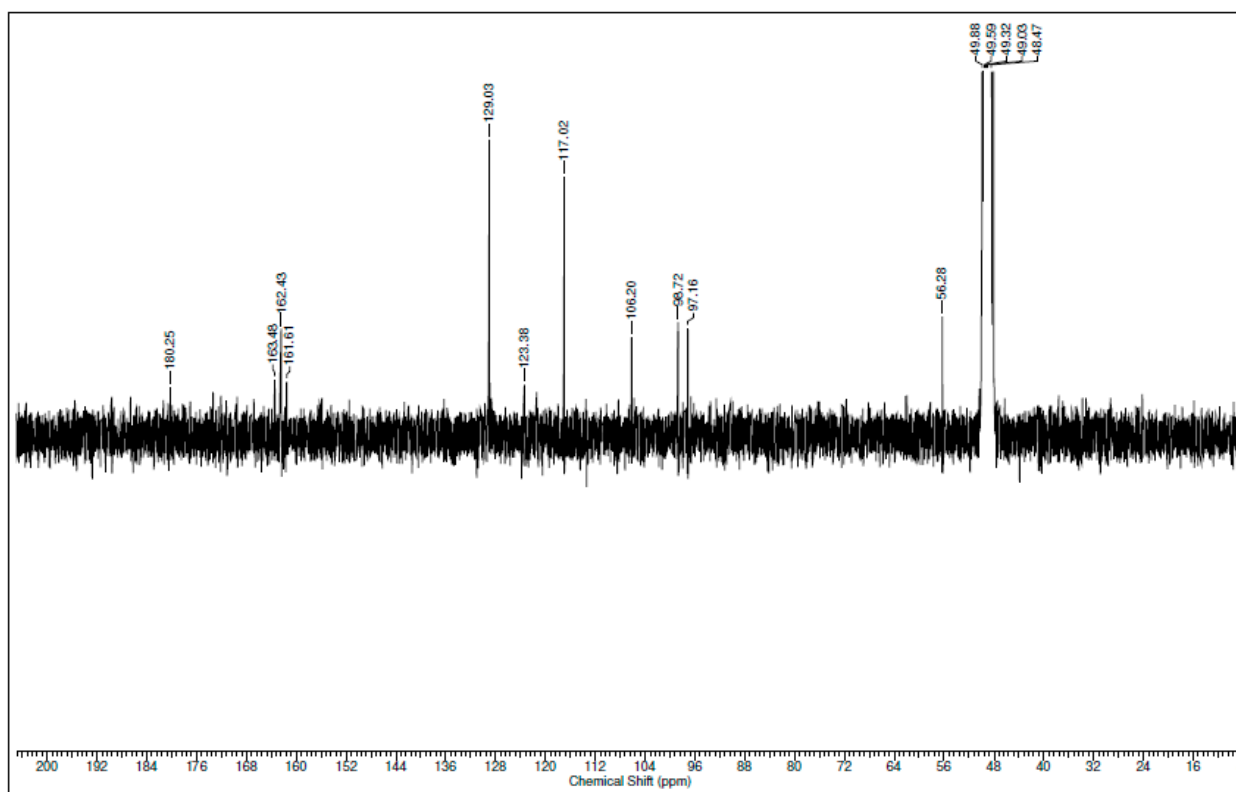


Figure S57. ^{13}C NMR spectrum (75 MHz, CD_3OD) of compound 9.

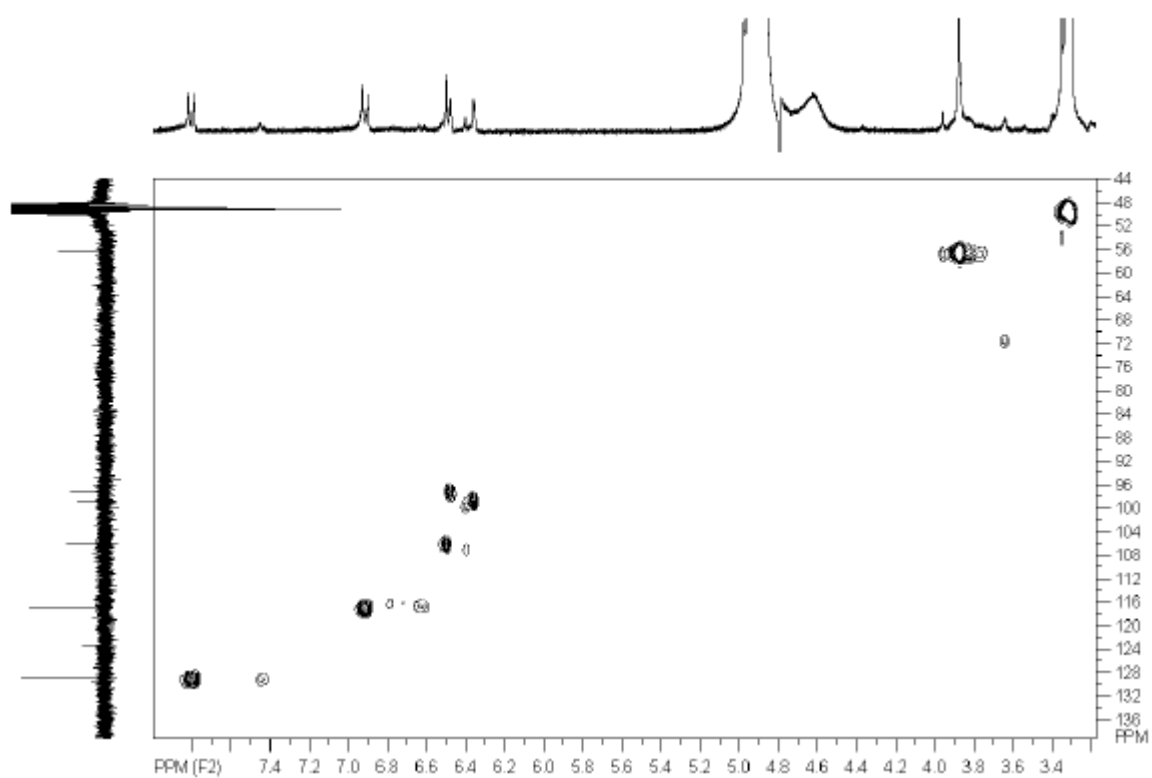


Figure S58. HSQC spectrum (CD_3OD) of compound 9.

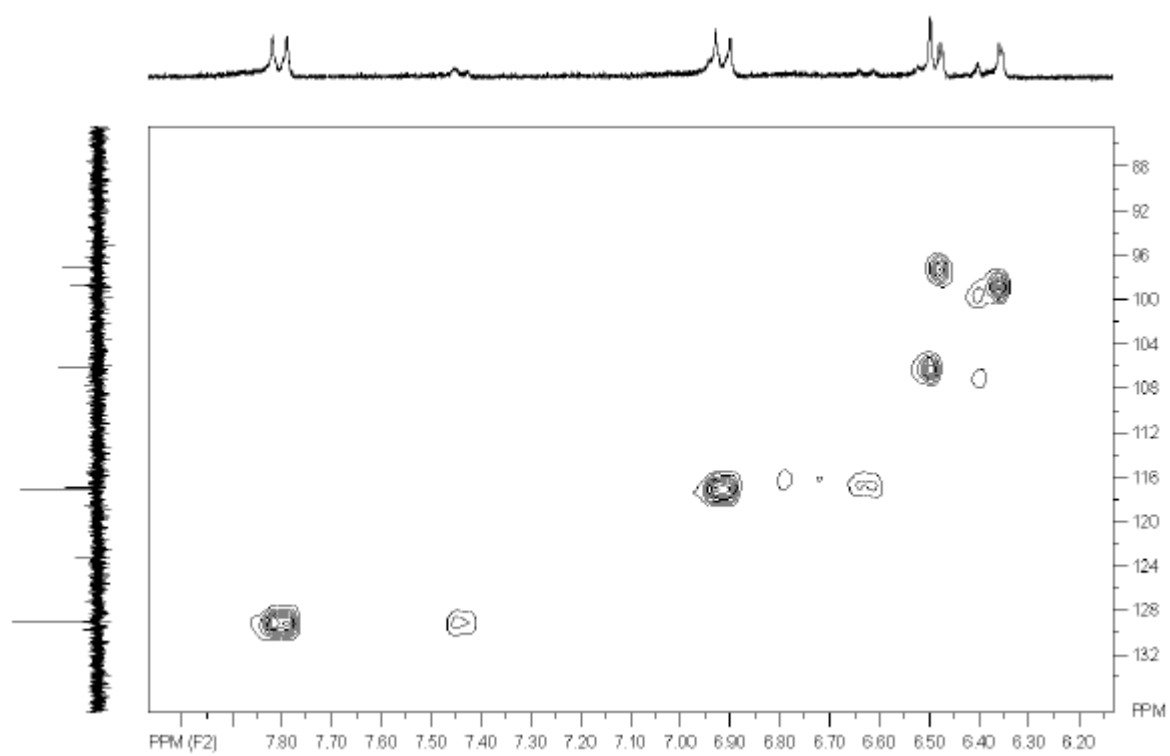


Figure S59. HSQC spectrum (expansion) of compound 9.

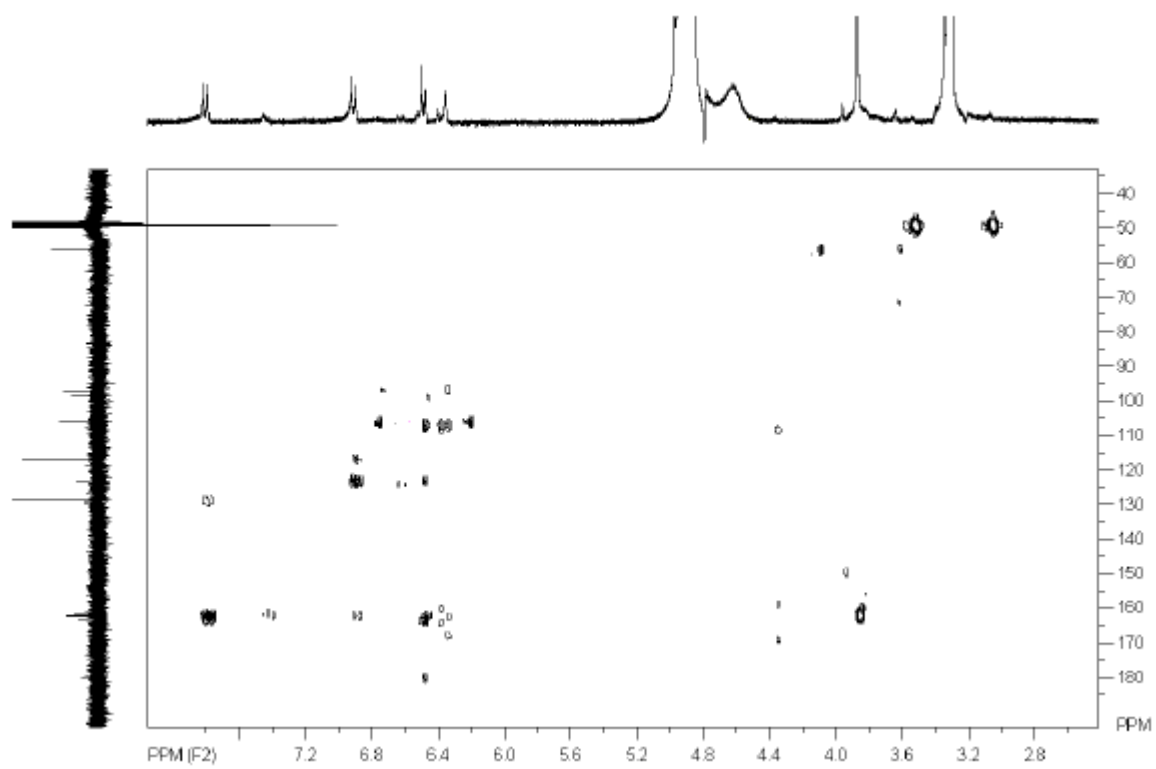


Figure S60. HMBC spectrum (CD_3OD) of compound 9.

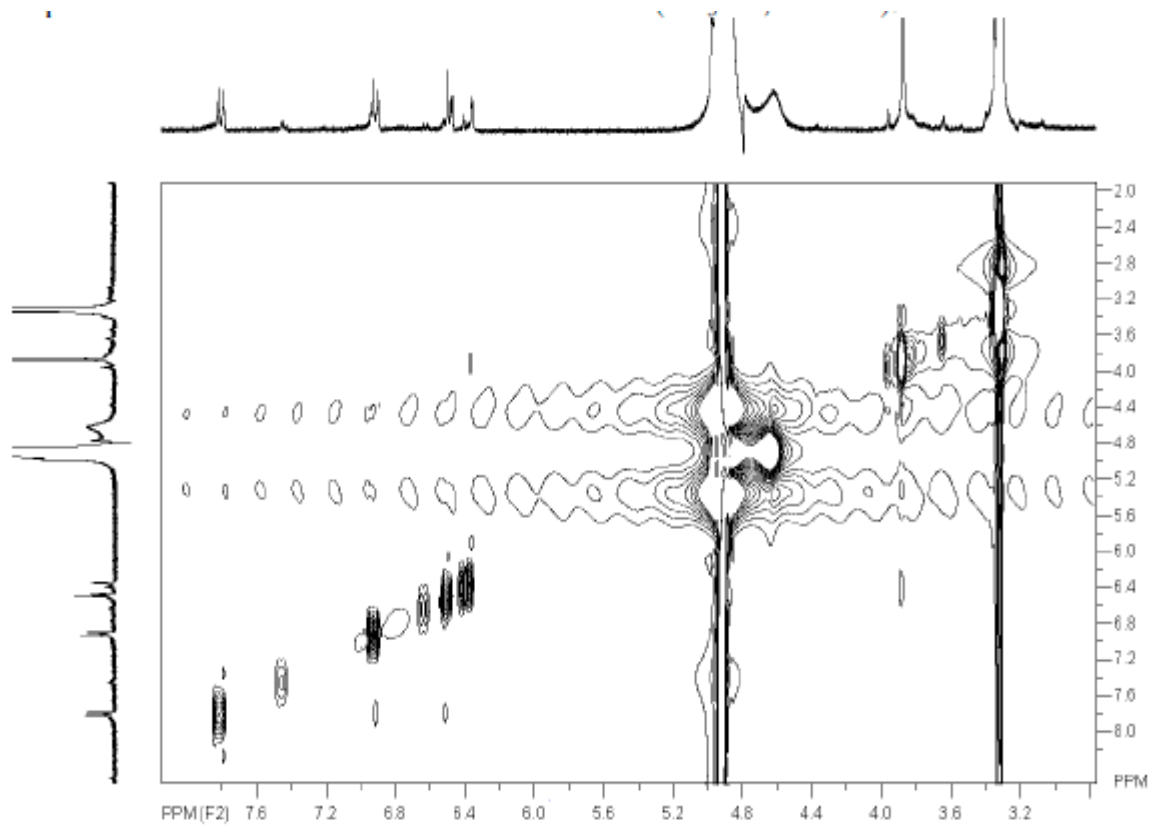


Figure S61. NOESY spectrum (300 MHz, CD₃OD) of compound 9.

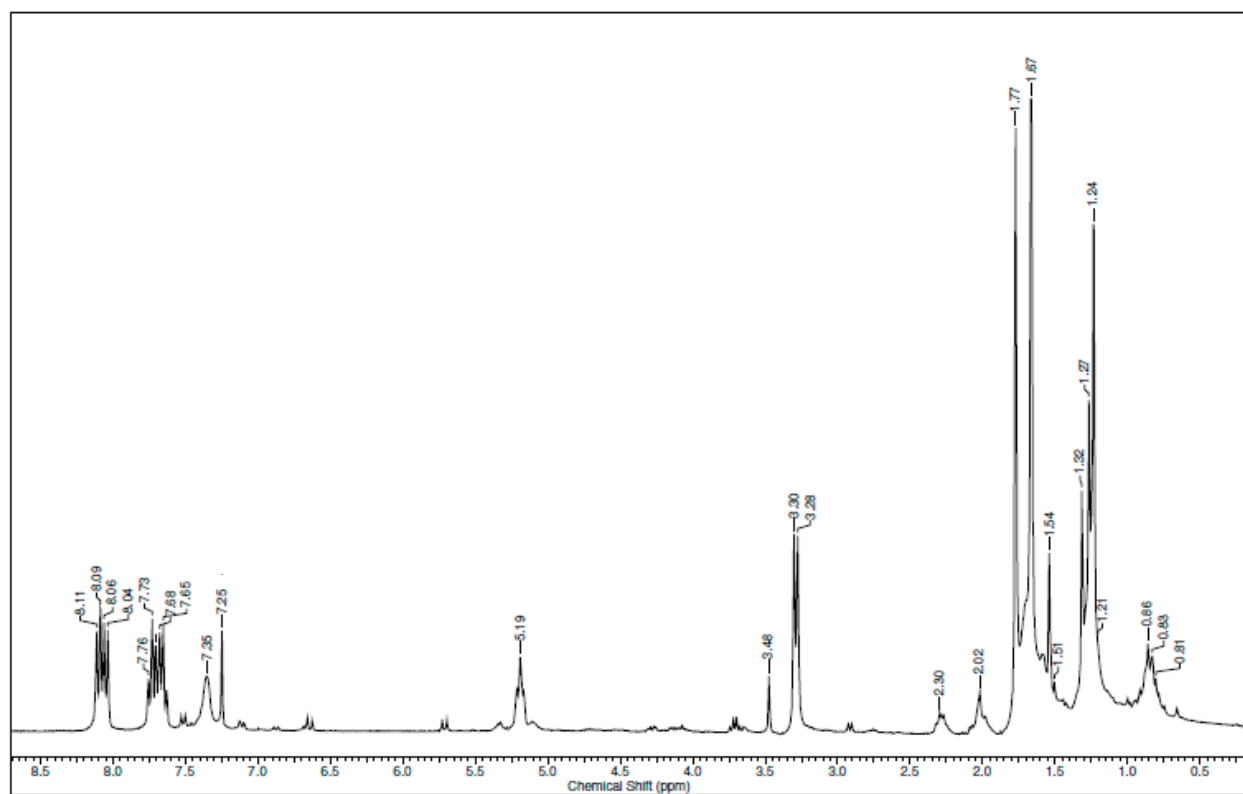


Figure S62. ¹H NMR spectrum (300 MHz, CDCl₃) of compound 10.

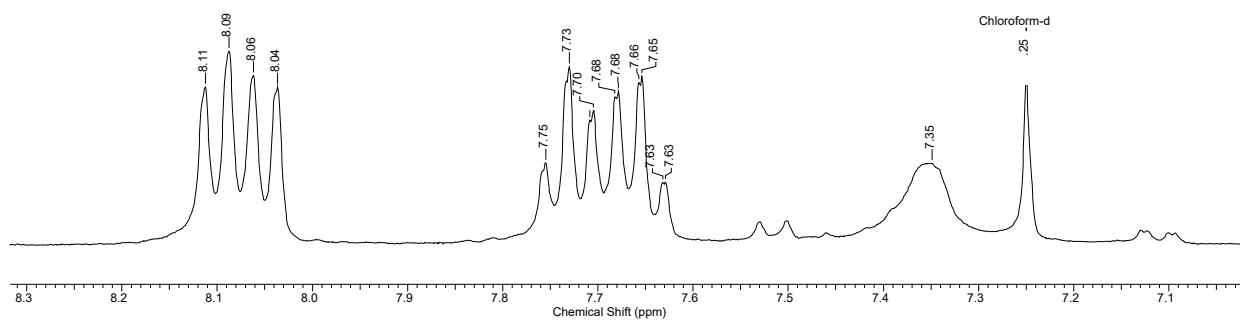


Figure S63. ^1H NMR spectrum (expansion) of compound **10**.

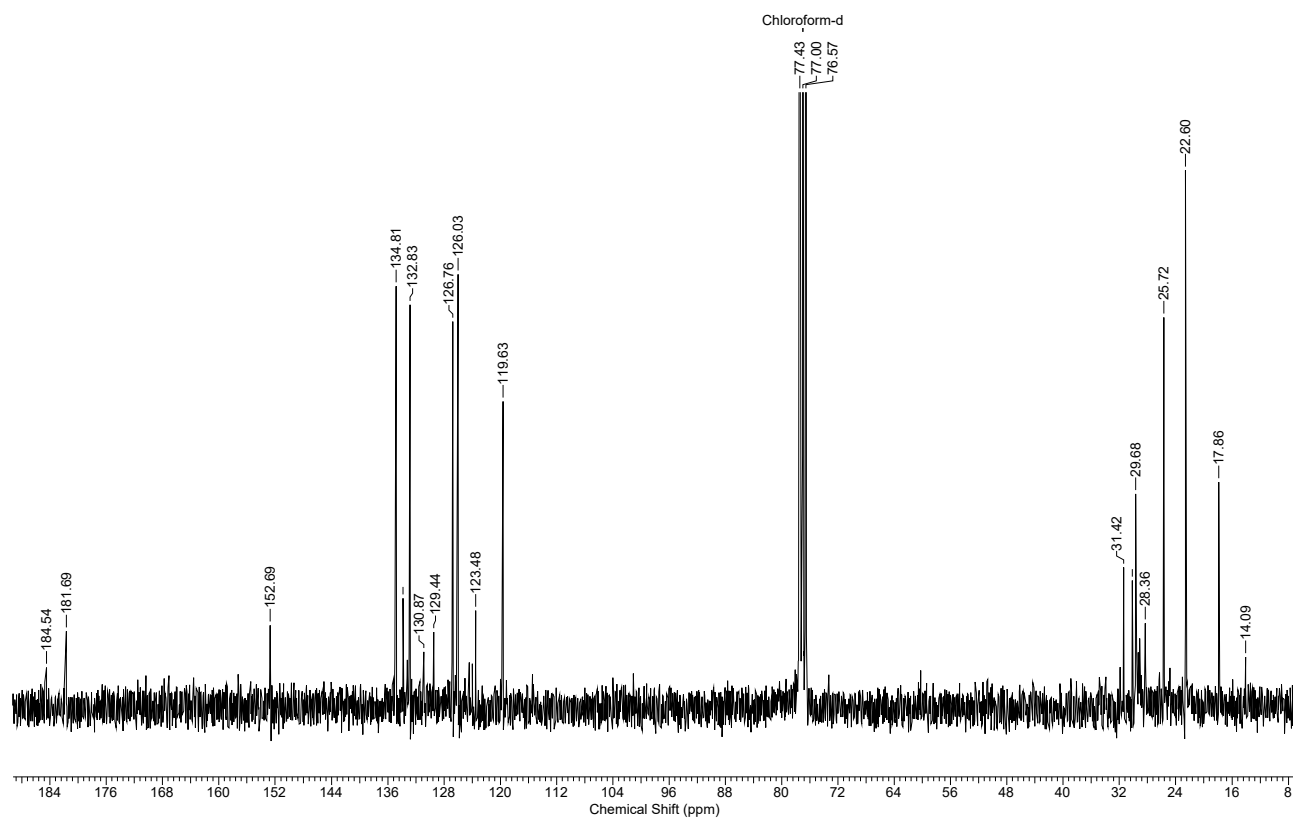


Figure S64. ^{13}C NMR spectrum (75 MHz, CDCl_3) of compound **10**.

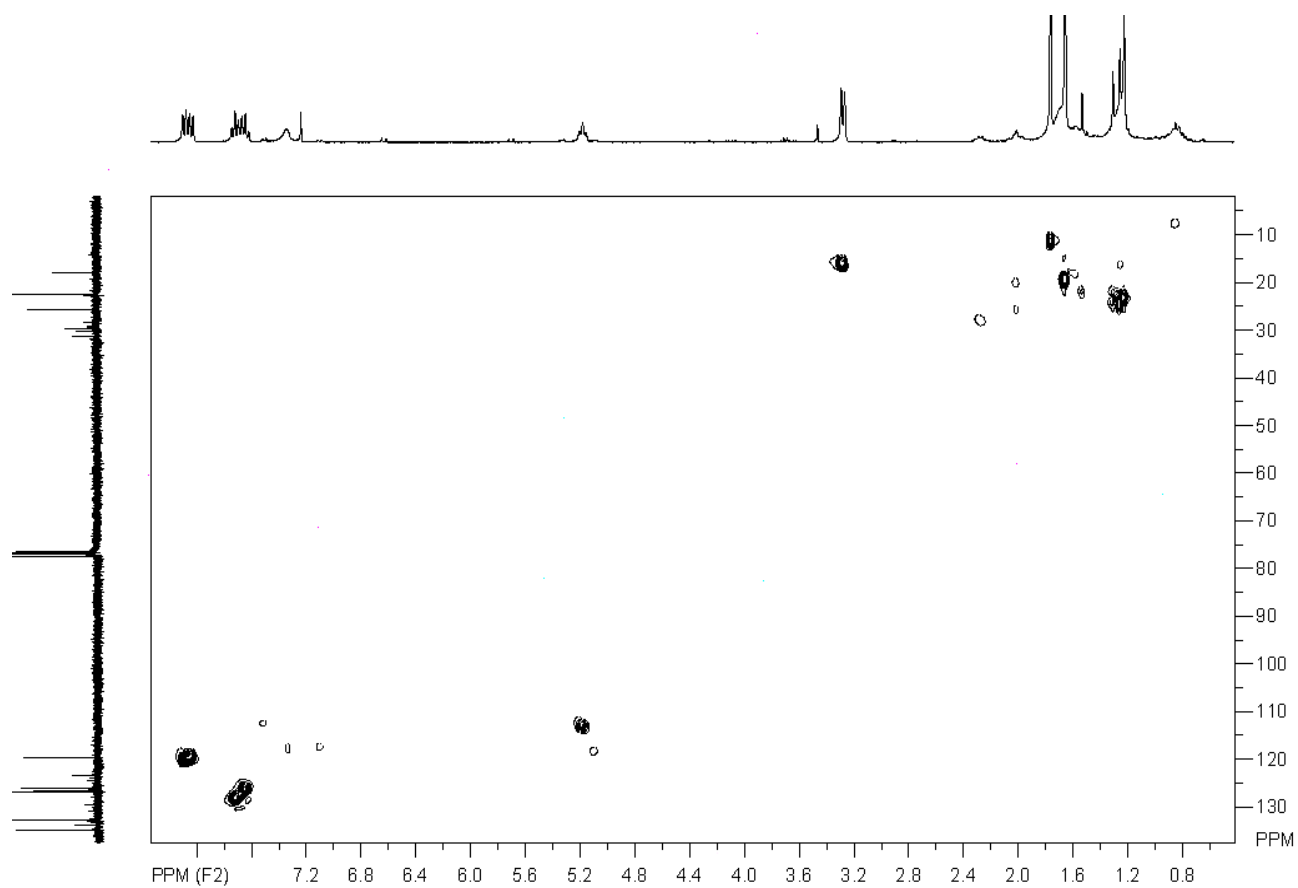


Figure S65. HSQC spectrum (CDCl_3) of compound **10**.

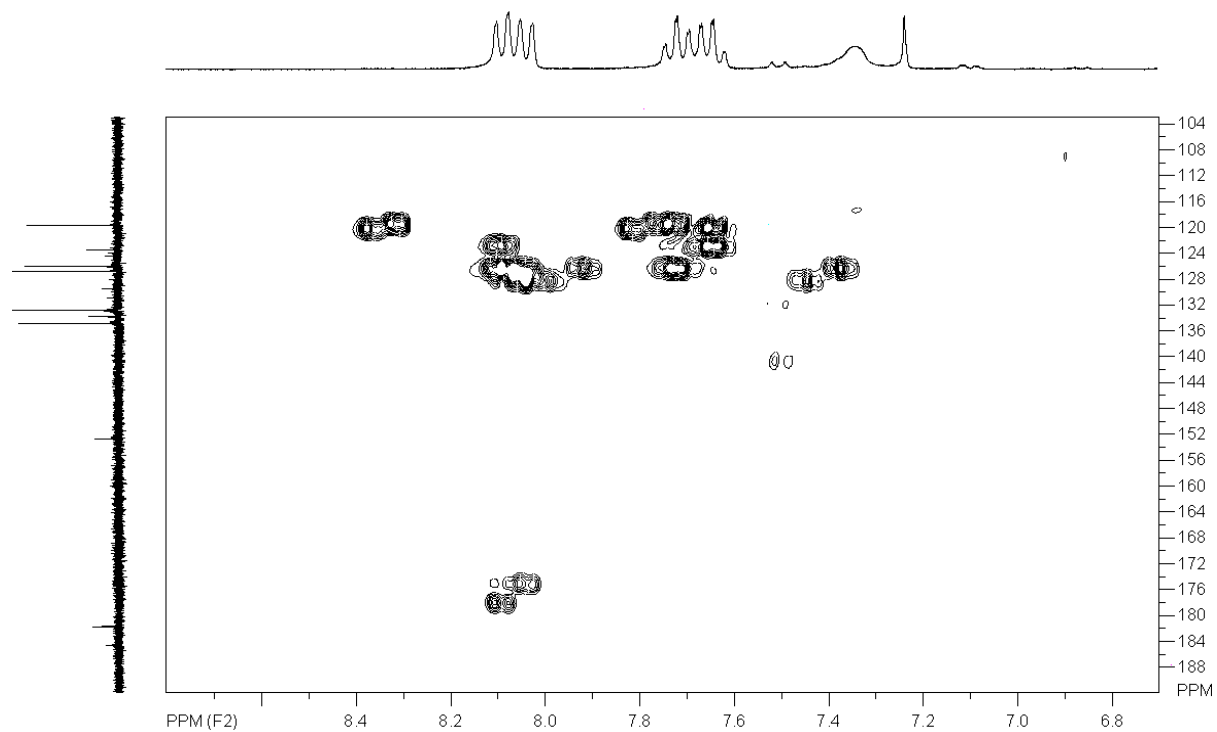


Figure S66. HMBC spectrum (expansion, CDCl_3) of compound **10**.

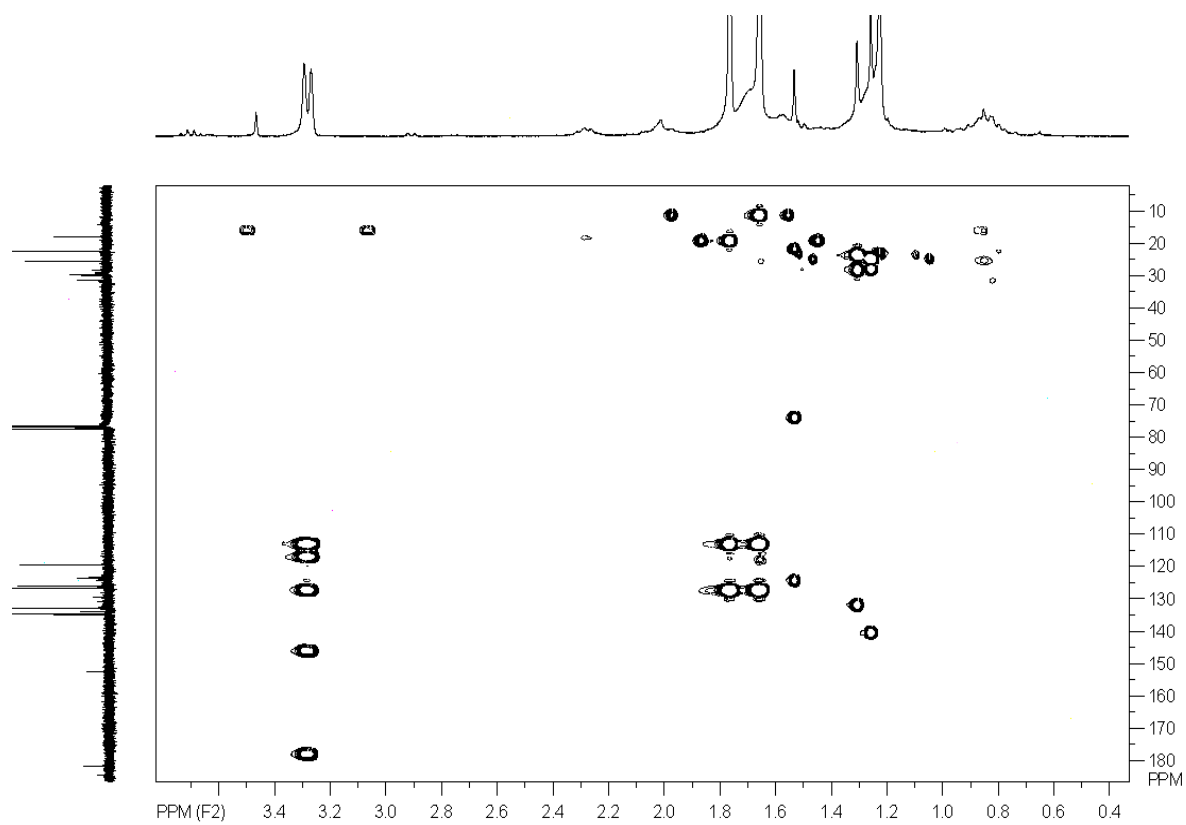


Figure S67. HMBC spectrum (expansion, CDCl_3) of compound 10.

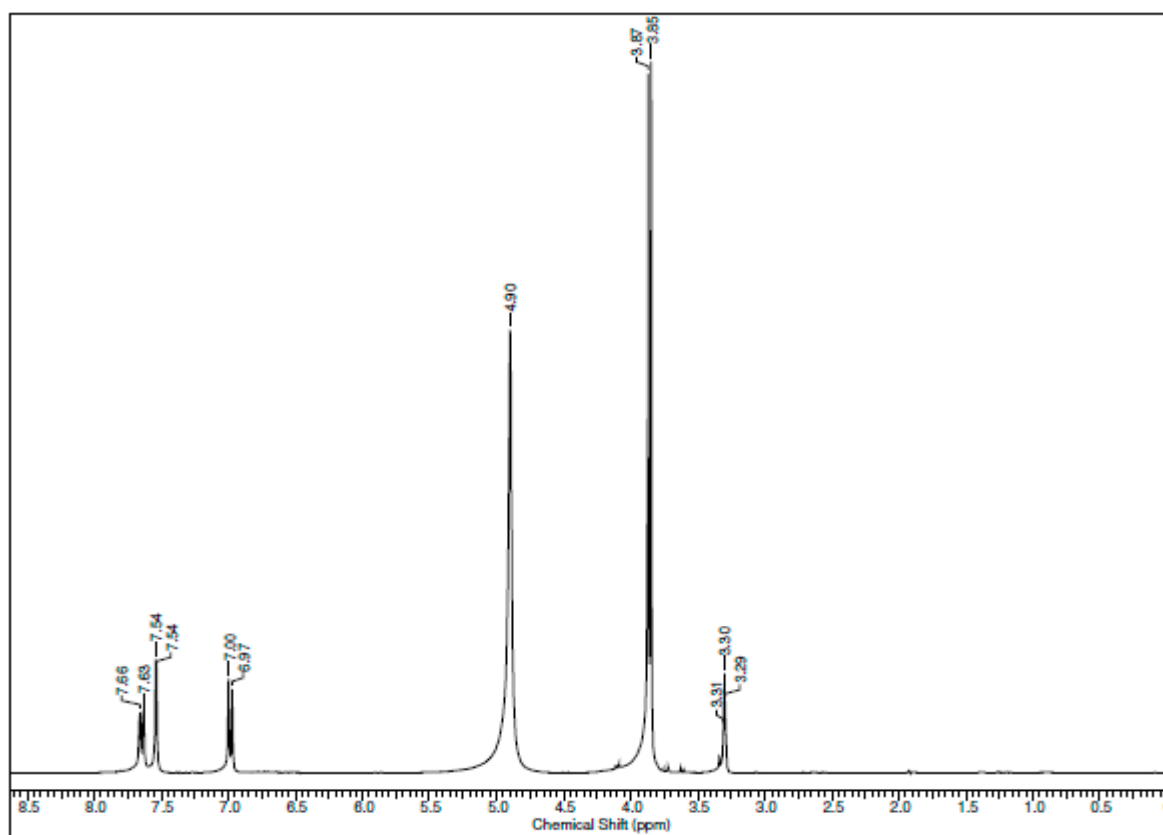


Figure S68. ^1H NMR spectrum (300 MHz, CD_3OD) of compound 11.

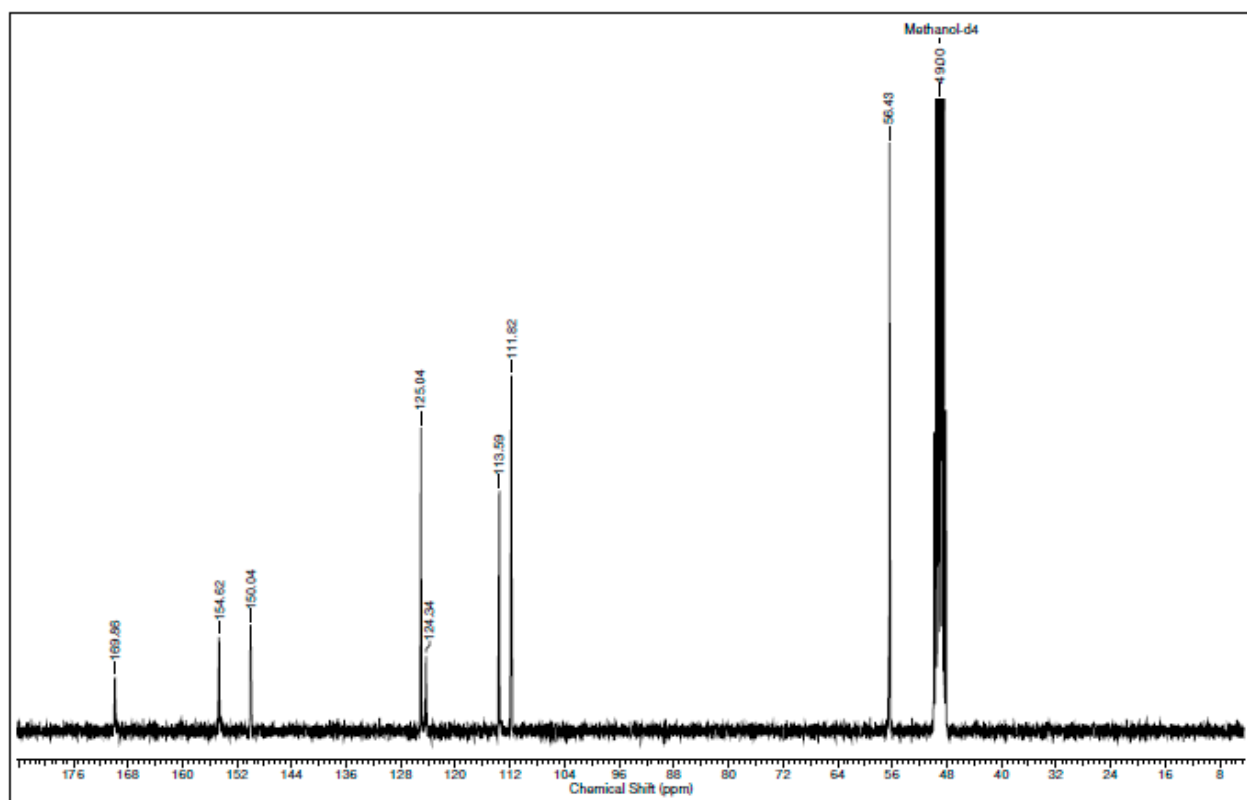


Figure S69. ^{13}C NMR spectrum (75 MHz, CD_3OD) of compound 11.

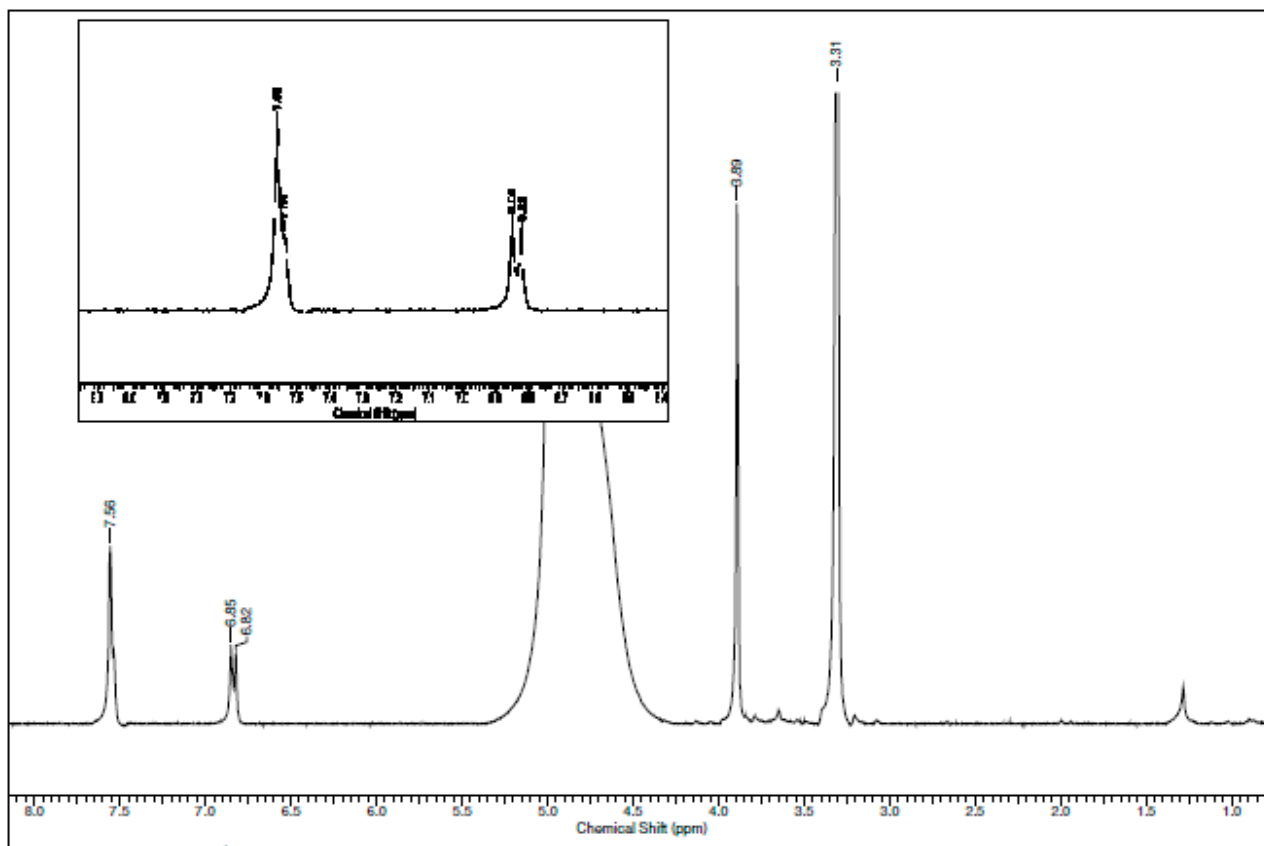


Figure S70. ^1H NMR spectrum (300 MHz, CD_3OD) of compound 12.

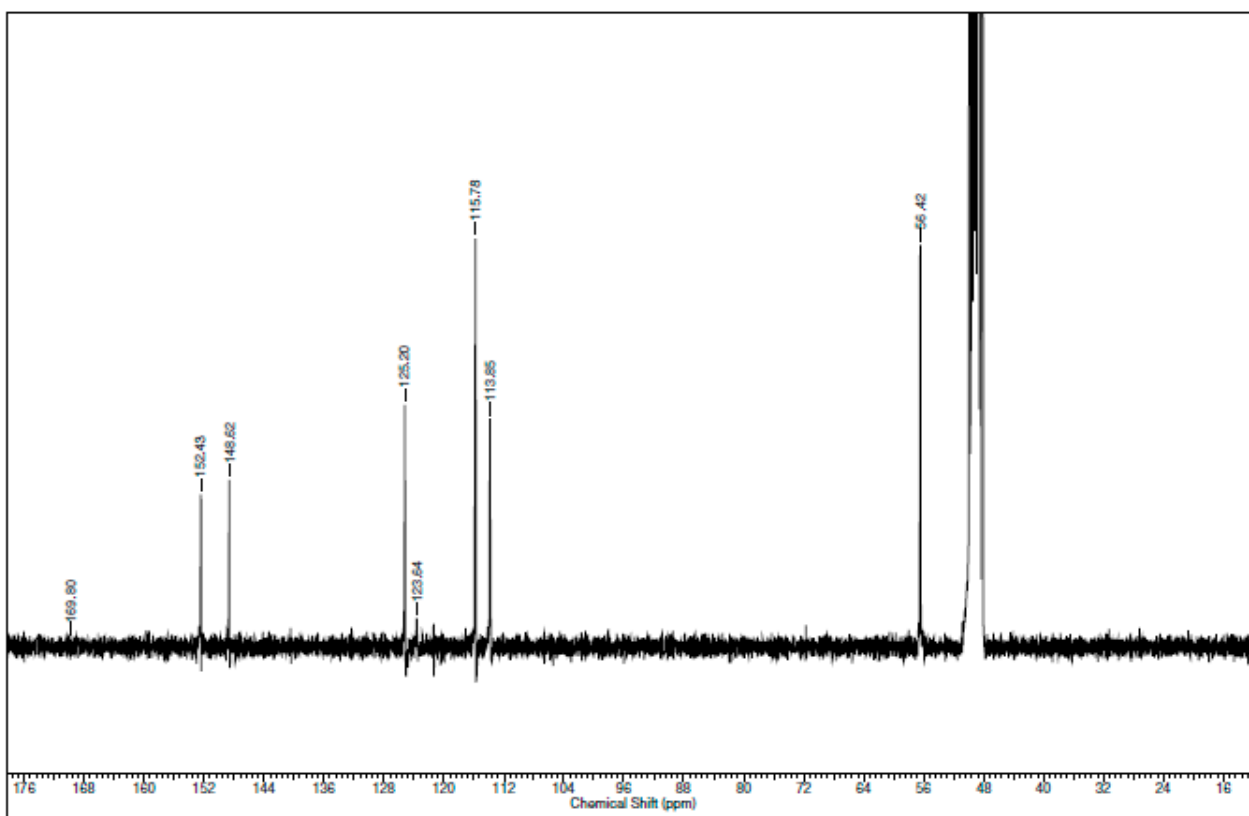


Figure S71. ^{13}C NMR spectrum (75 MHz, CD_3OD) of compound 12.

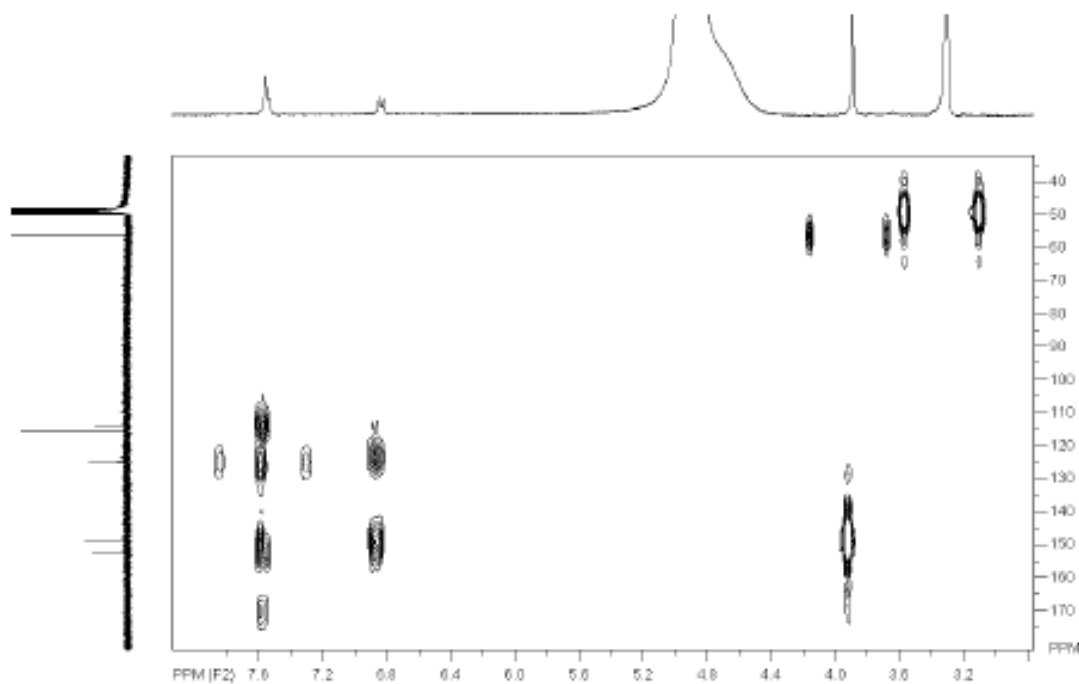


Figure S72. HSQC spectrum (CD_3OD) of compound 12.

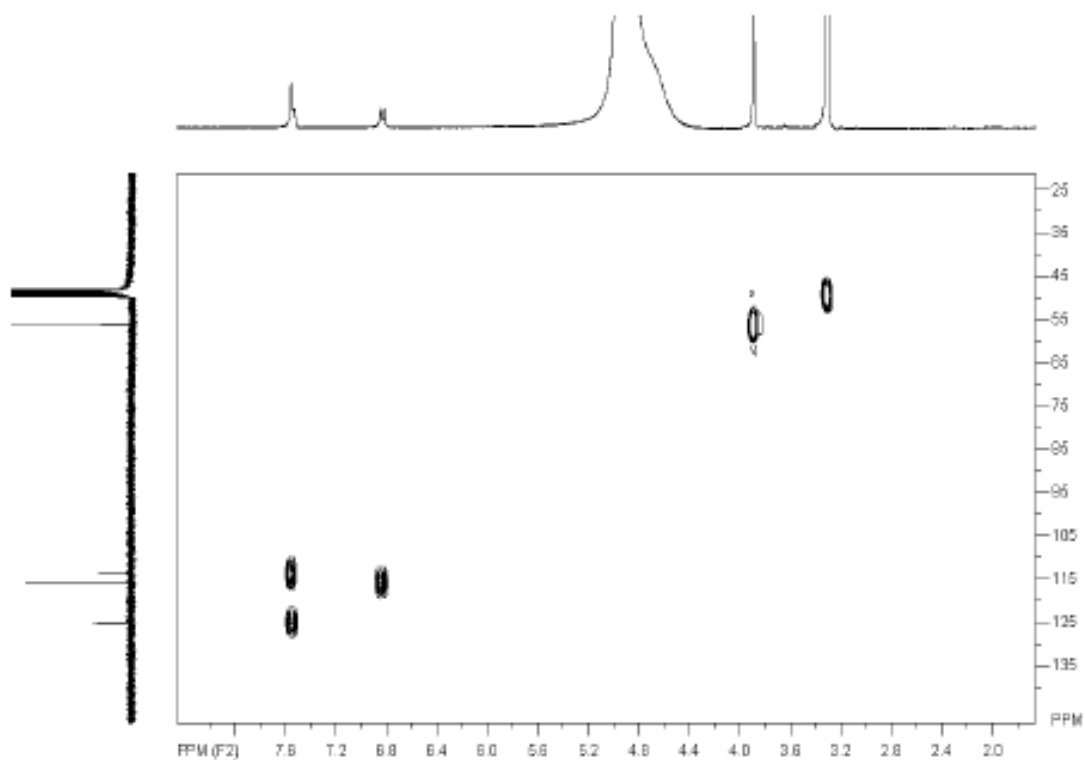


Figure S73. HMBC spectrum (CD₃OD) of compound 12.

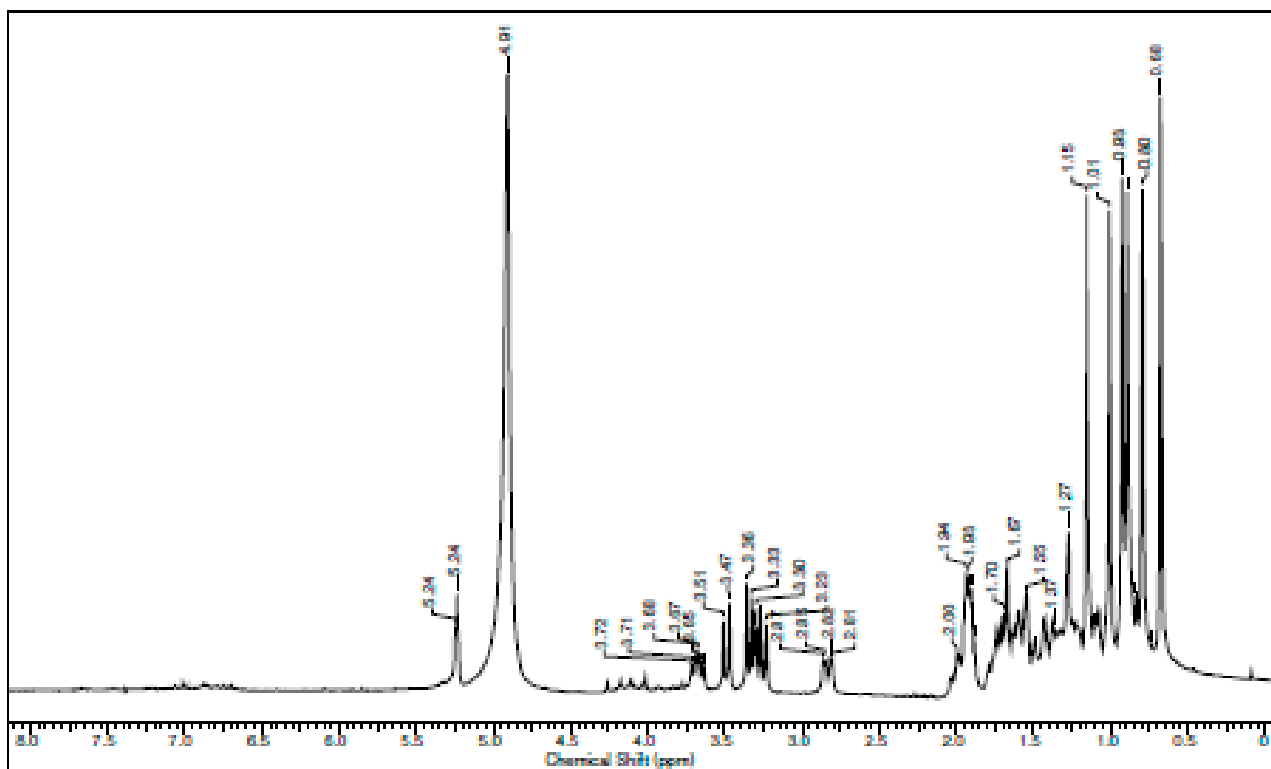


Figure S74. ¹H NMR spectrum (300 MHz, CD₃OD) of compound 13.

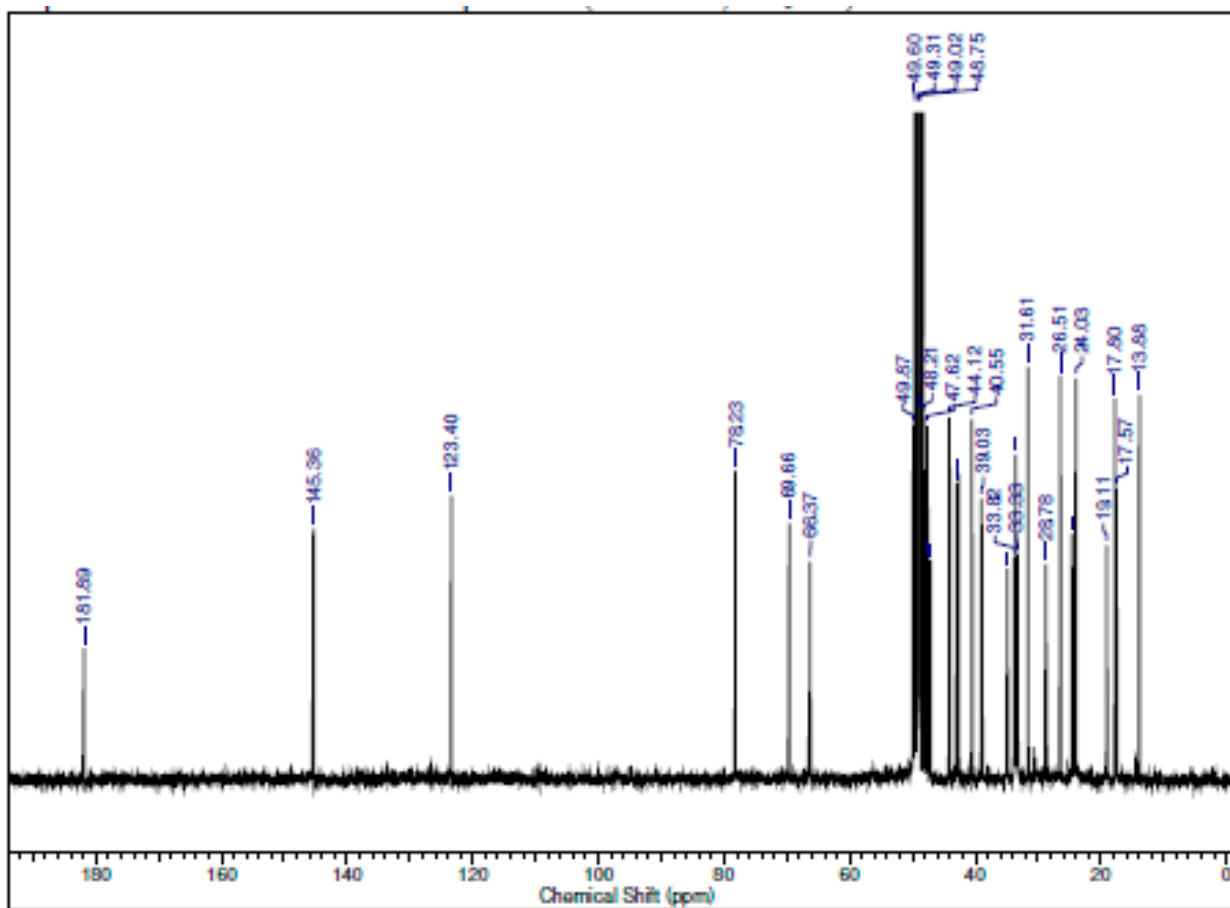


Figure S75. ^{13}C NMR spectrum (75 MHz, CD_3OD) of compound 13.

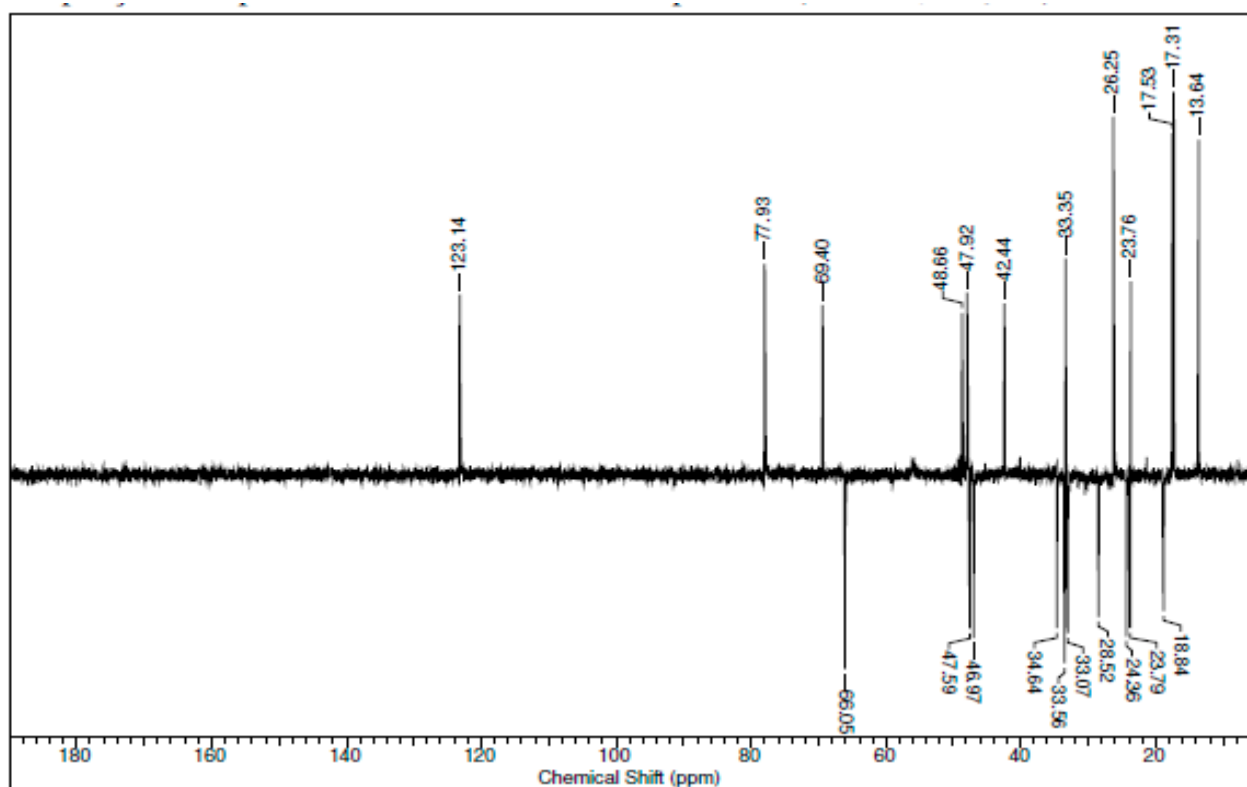


Figure S76. DEPT-135 spectrum (CD_3OD) of compound 13.

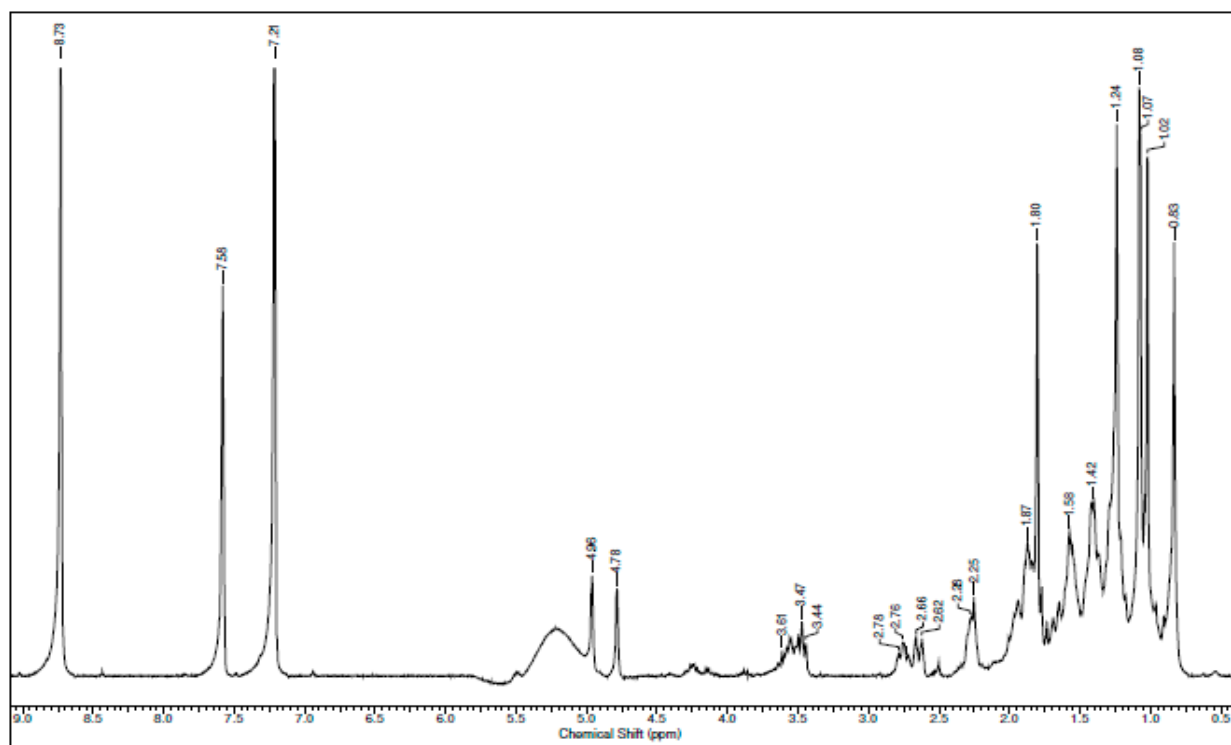


Figure S77. ^1H NMR spectrum (300 MHz, pyridine- d_5) of compound 14.

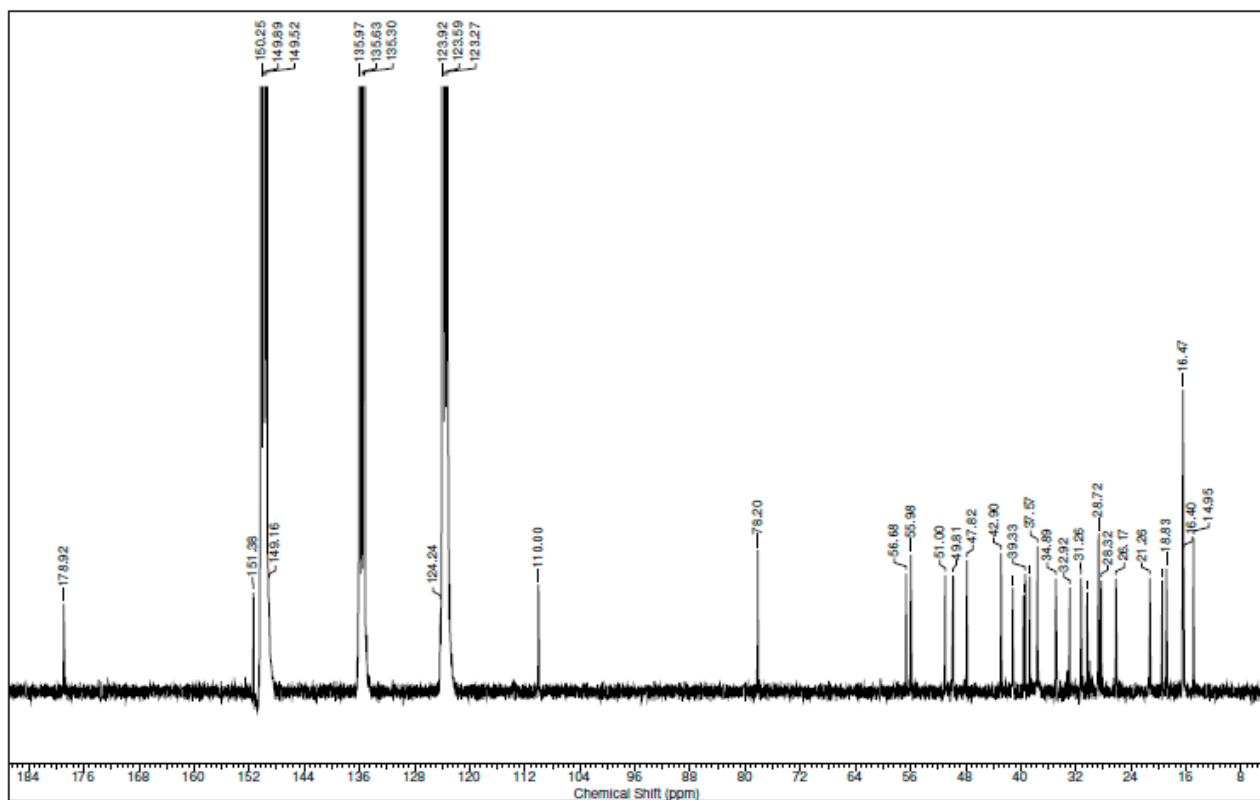


Figure S78. ^{13}C NMR spectrum (75 MHz, pyridine- d_5) of compound 14.

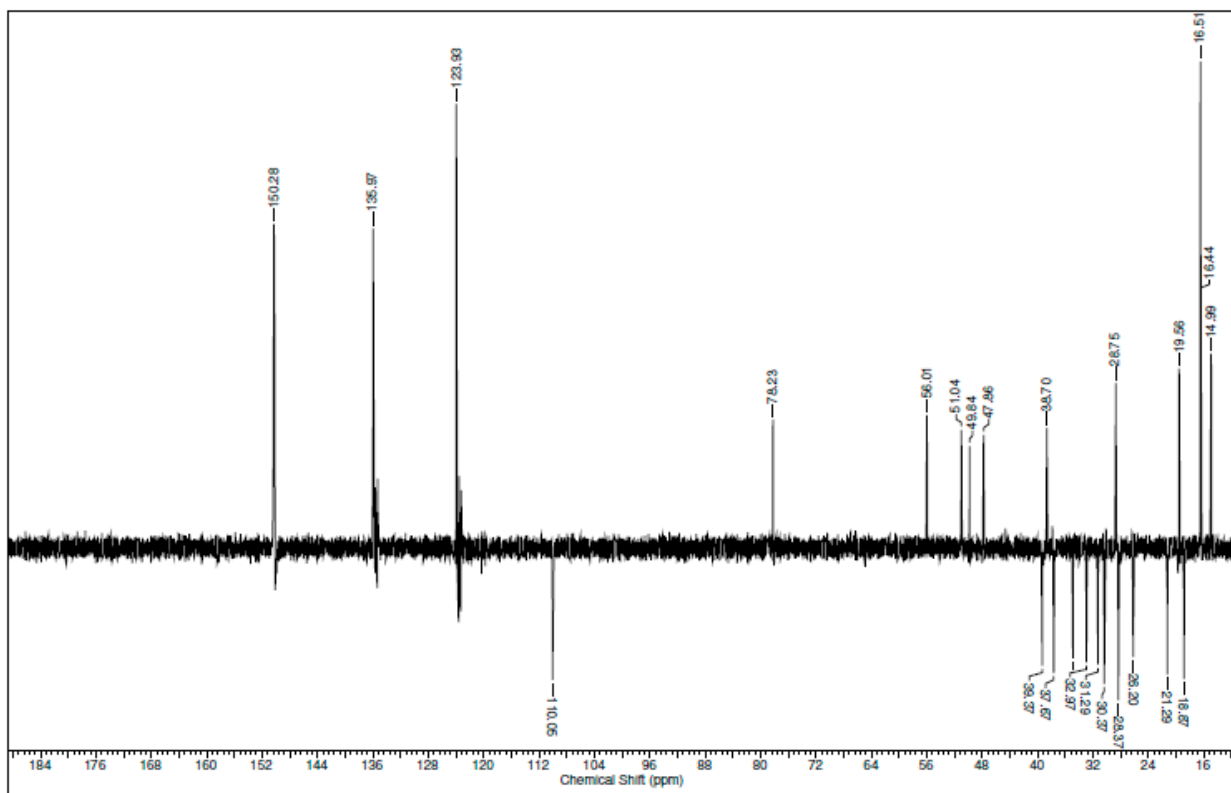


Figure S79. DEPT-135 spectrum (pyridine- d_5) of compound 14.

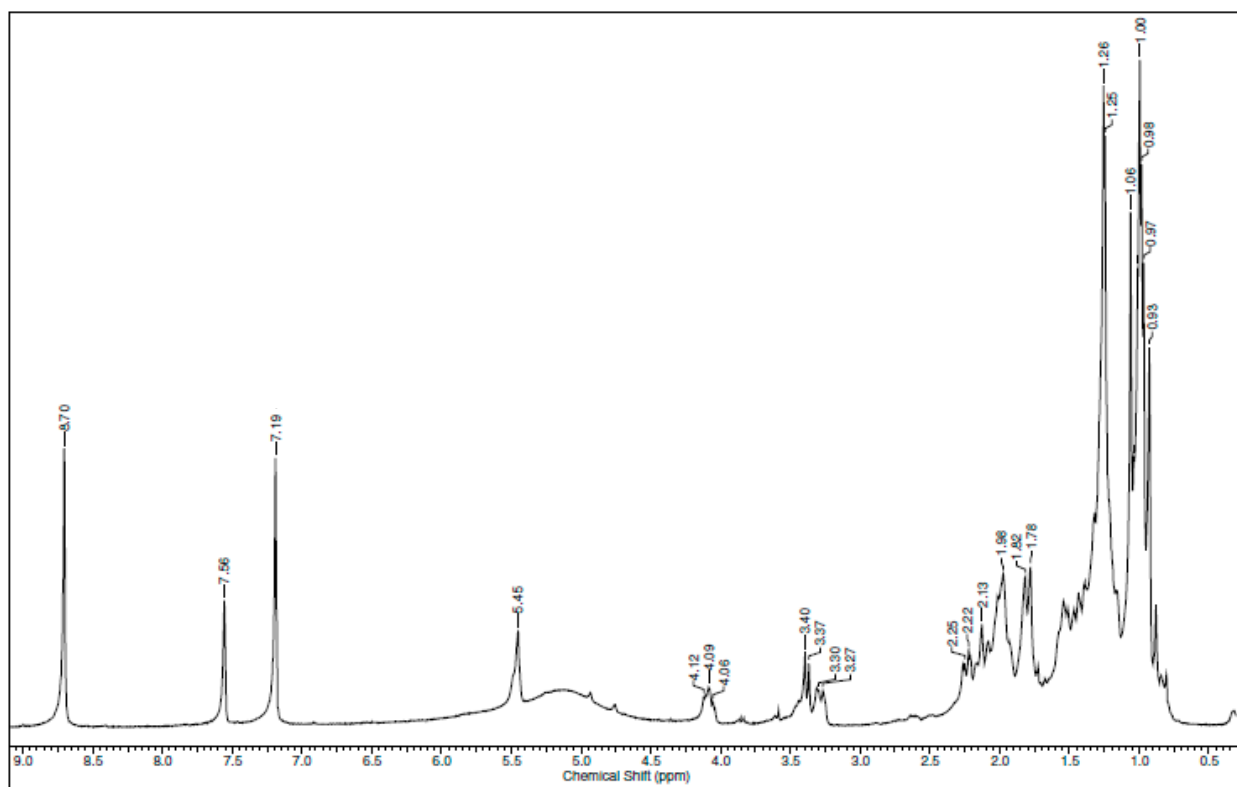


Figure S80. ^1H NMR spectrum (300 MHz, pyridine- d_5) of compound 15.

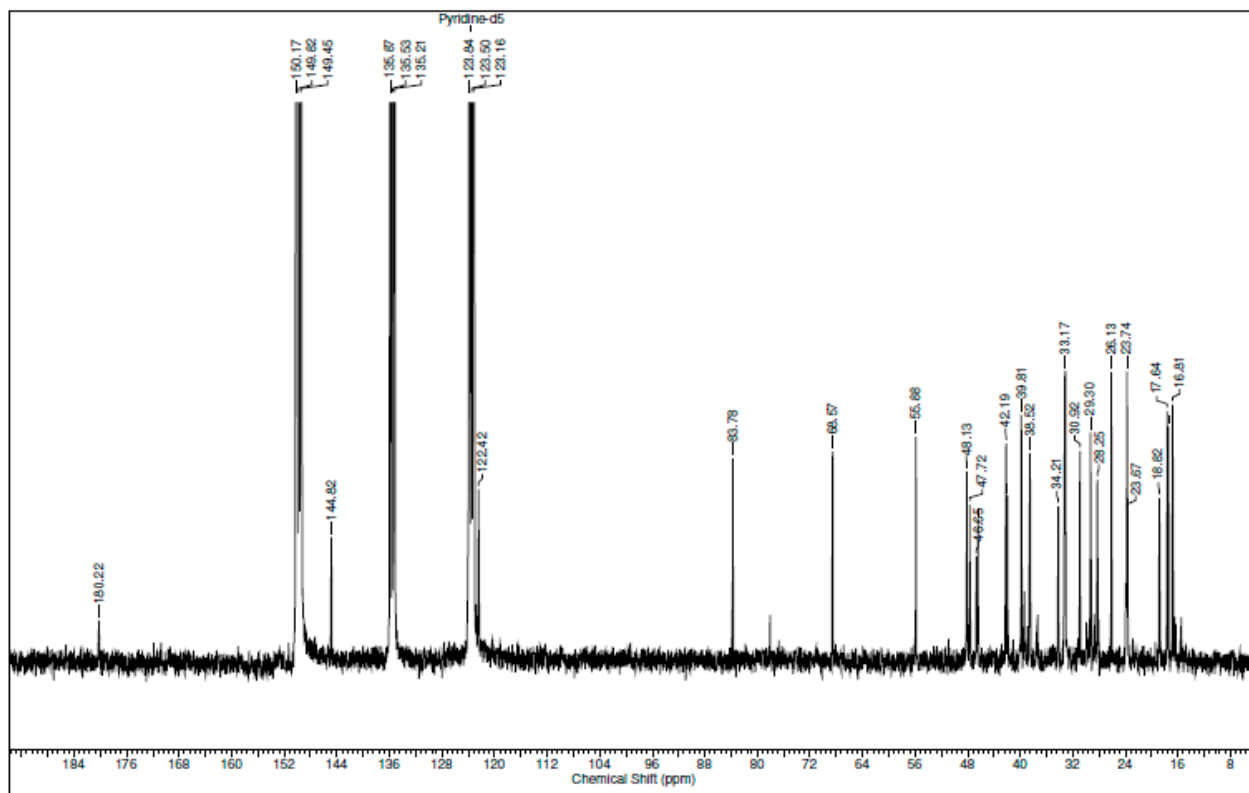


Figure S81. ¹³C NMR spectrum (75 MHz, pyridine-d₅) of compound 15.

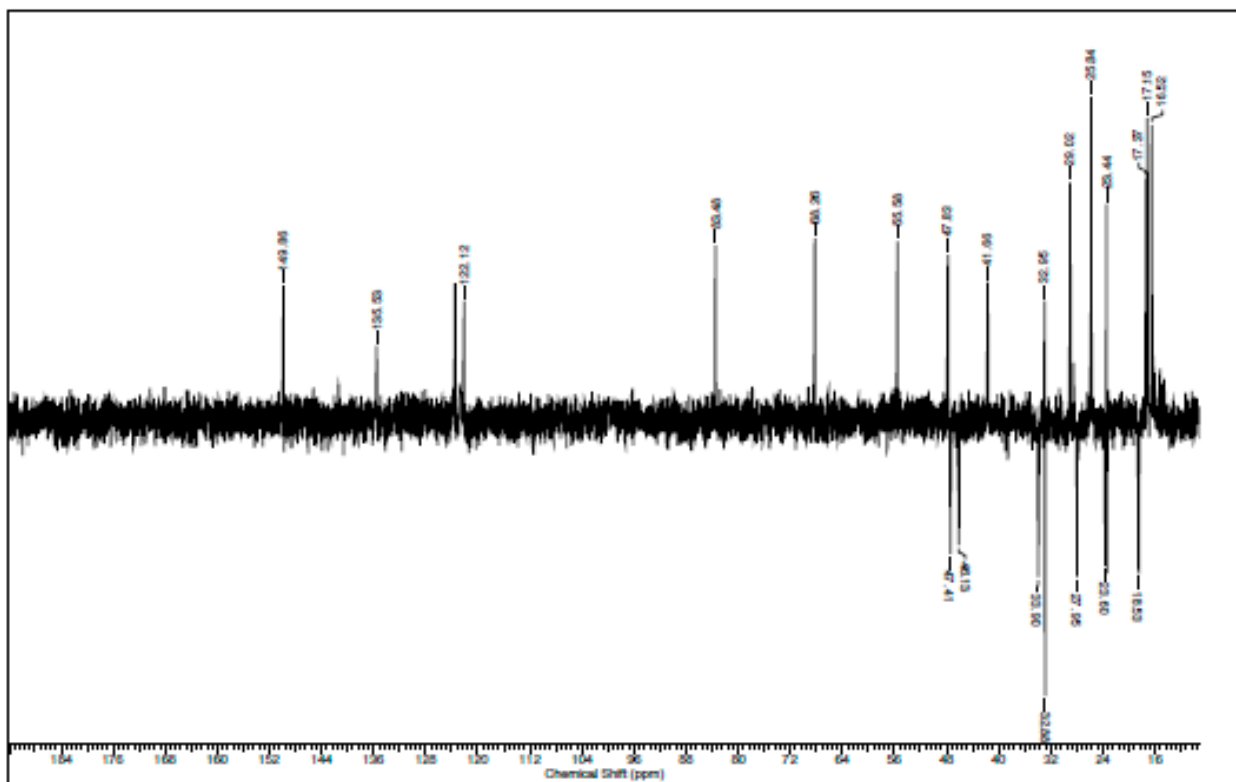


Figure S82. DEPT-135 spectrum (pyridine-d₅) of compound 15.