Supporting Information for

2-Unsubstituted Imidazole *N*-oxides as Novel Precursors of Chiral 3-Alkoxyimidazol-2-ylidenes Derived from *trans*-1,2-Diaminocyclohexane and Other Chiral Amino Compounds

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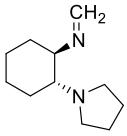
Content:



(*R*,*R*)-**4a**

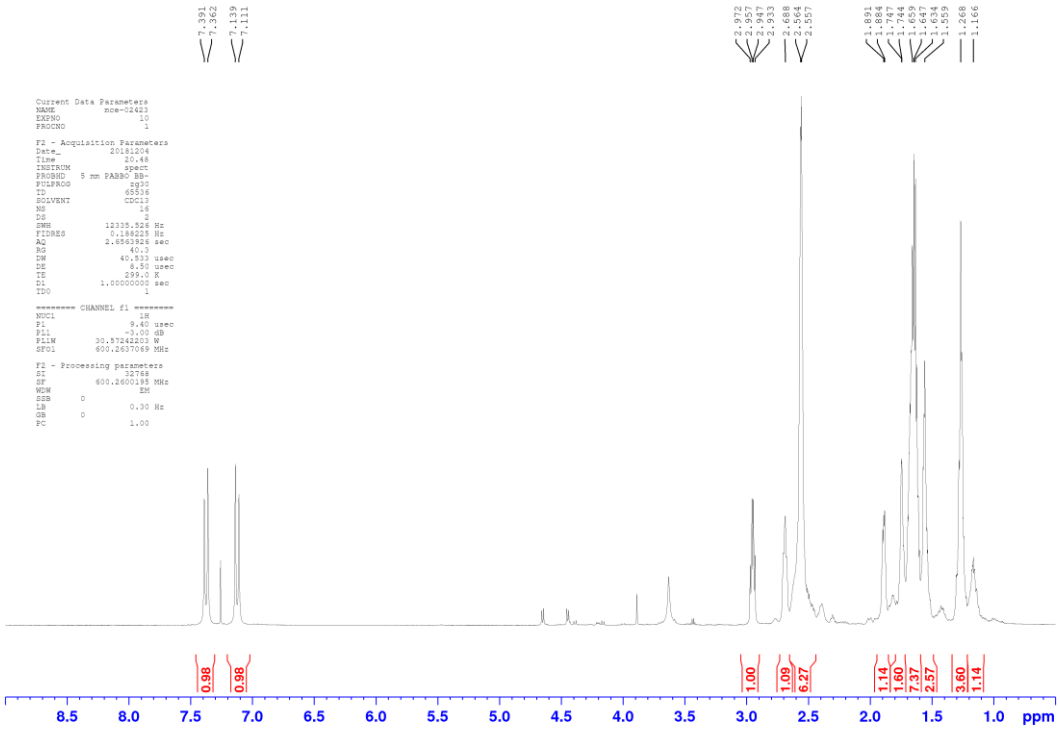


Figure S1. ^{1}H NMR of (*R*,*R*)-**4a** ($CDCl_3$, 600 MHz).

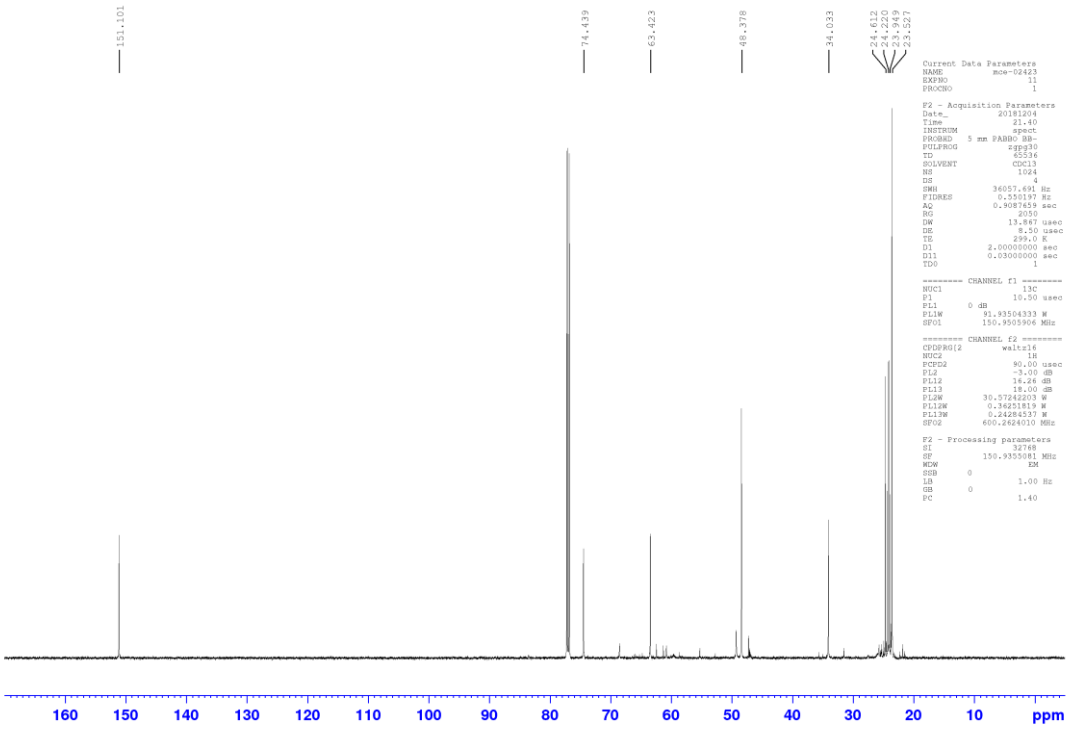
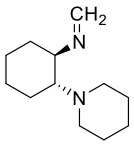


Figure S2. ^{13}C NMR of (*R*,*R*)-**4a** ($CDCl_3$, 151 MHz).



(*R*,*R*)-**4b**

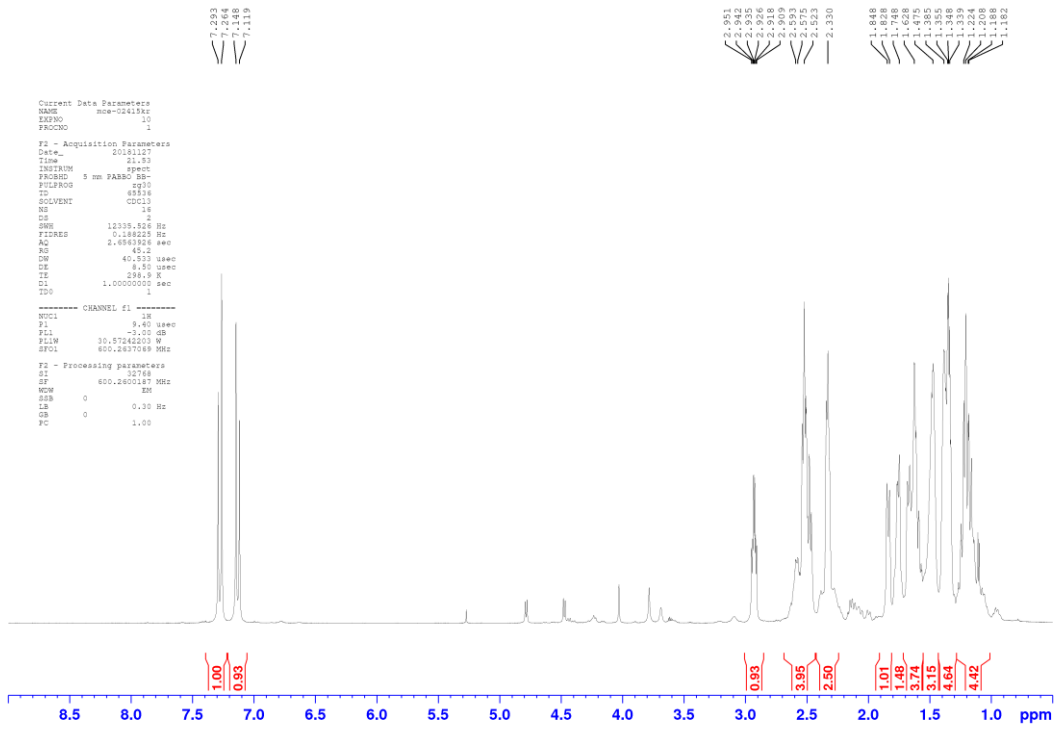


Figure S3. ^{1}H NMR of (*R*,*R*)-**4b** ($CDCl_3$, 600 MHz).

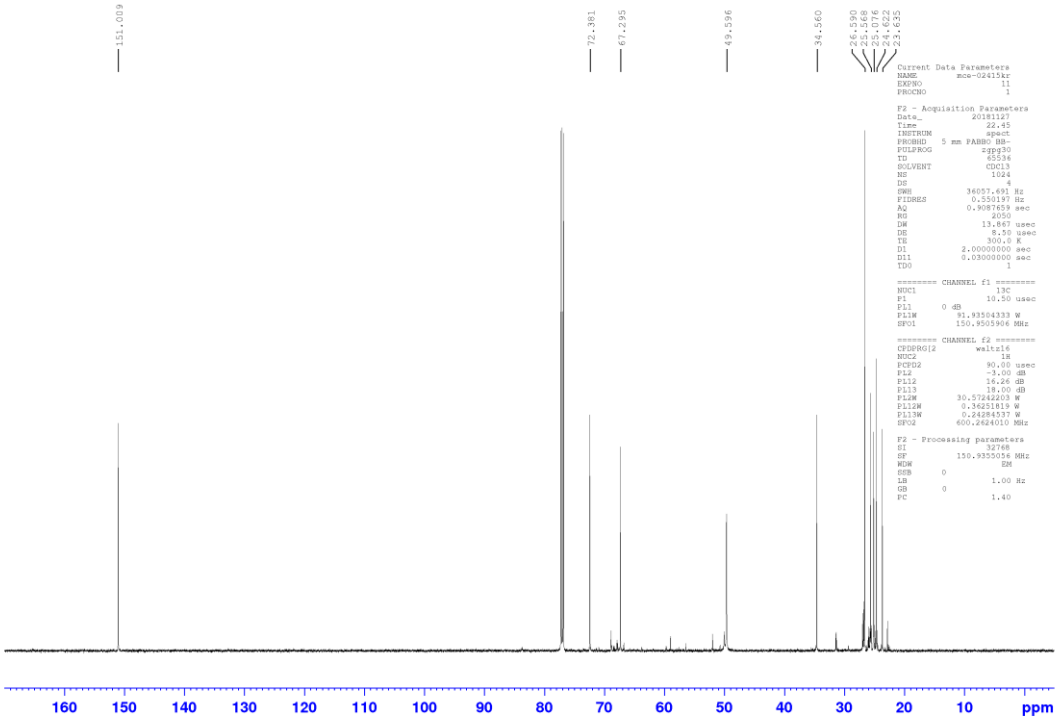


Figure S4. ^{13}C NMR of (*R*,*R*)-**4b** ($CDCl_3$, 151 MHz).

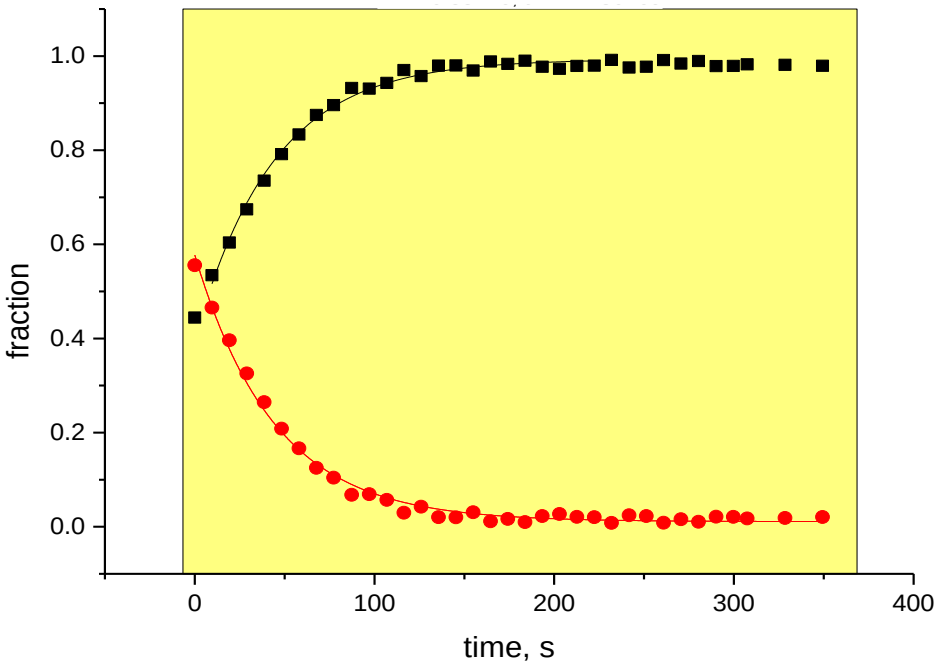


Figure S5. Kinetics of triazine-formaldimine **4b**/**4'b** equilibration after dissolution in $CDCl_3$ monitored by ^1H NMR integration. Content of triazine is shown in red dots, and the content of monomeric formaldimine in black squares. Decay curves were fitted with $t_{1/2}$ value of 30 s.

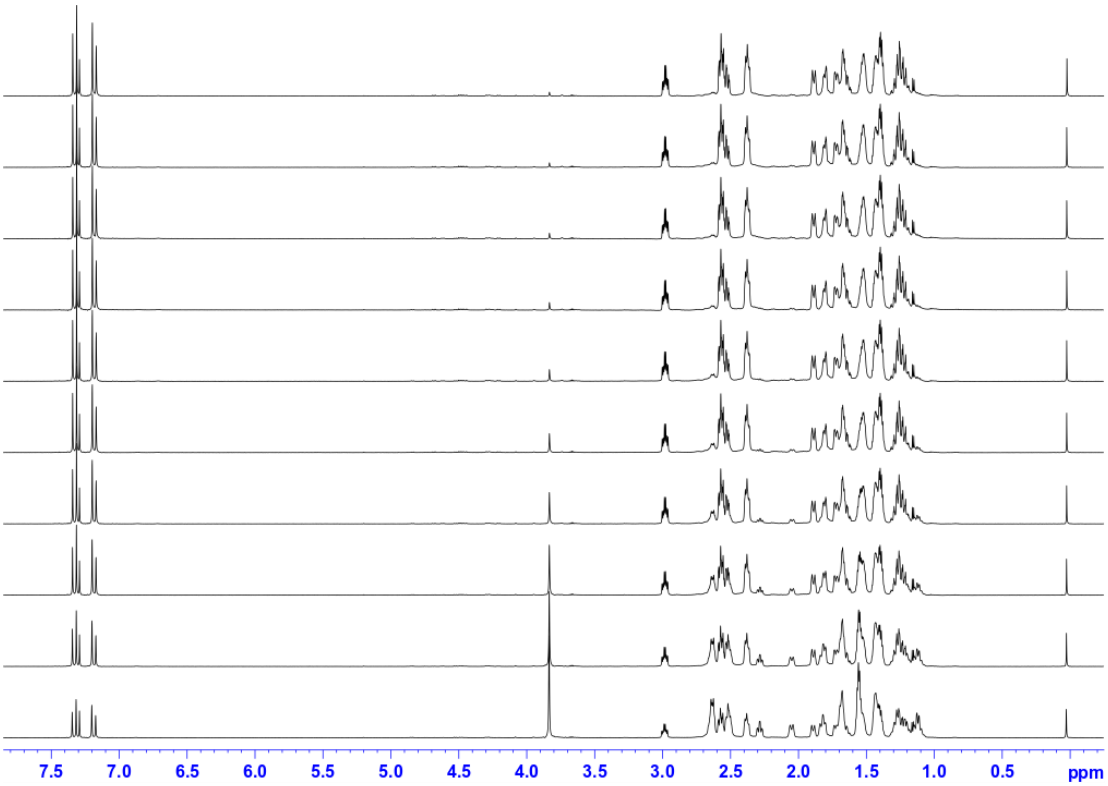


Figure S6. Overlays of NMR spectra (600 MHz, $CDCl_3$, NS=1) of **4b**/**4'b** taken at various intervals after dissolution and placing in the instrument and initiating measurement (accounting for approx. 15-20 s). Shown spectra bottom to top were collected after consecutive 19.3 s increments.

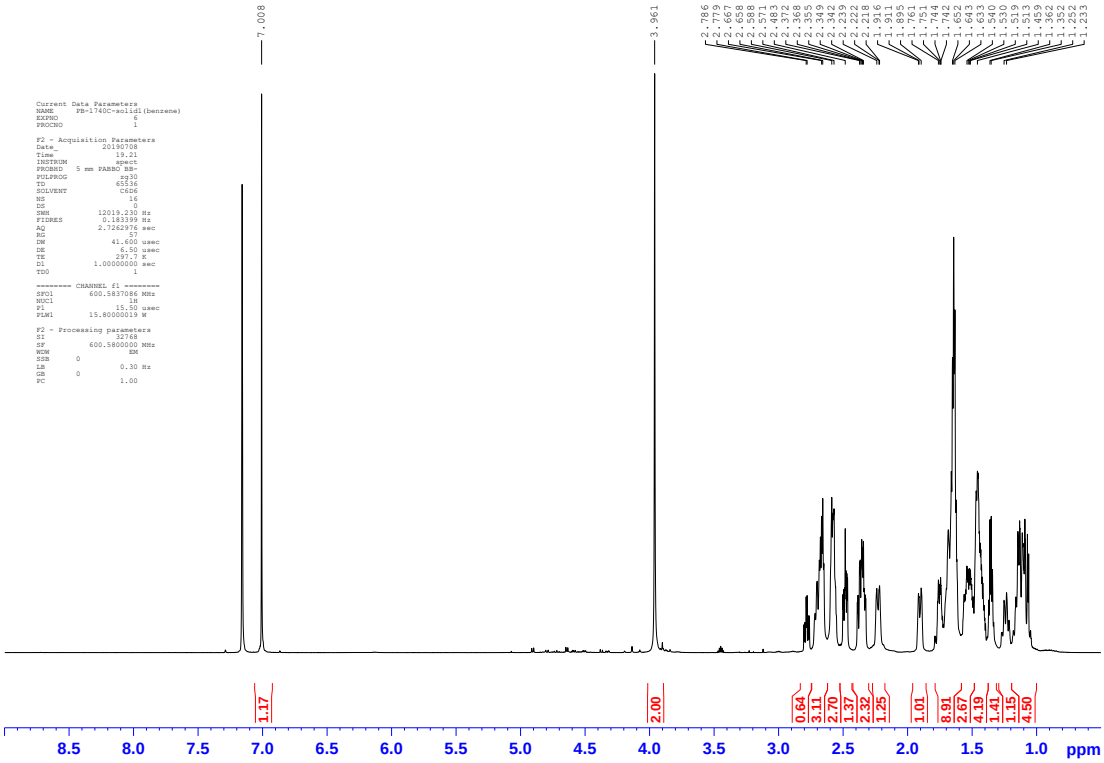


Figure S7. ^{1}H NMR spectrum of **4b**/**4'b** in benzene-d_6: triazine to monomeric formaldimine ratio is established at 1:0.6.

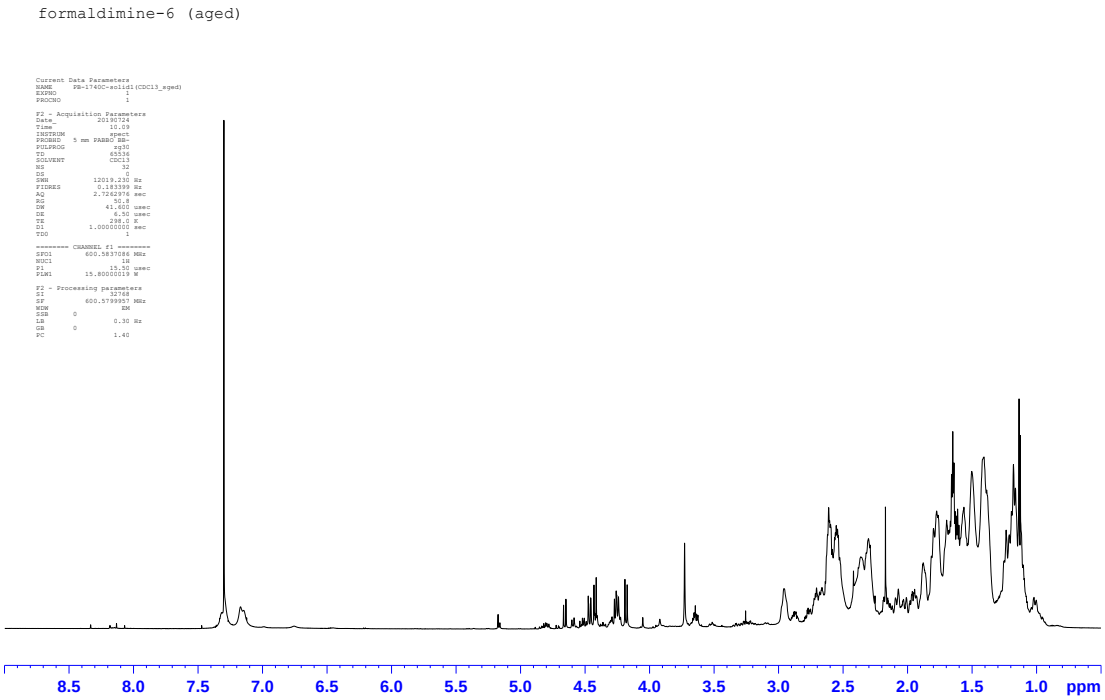
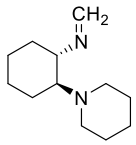


Figure S8. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of a sample of formaldimine **4b** following storage in the $CDCl_3$ solution for 16 days. Unidentified products account for approx. 75% of the material.



(*S*,*S*)-**4b**

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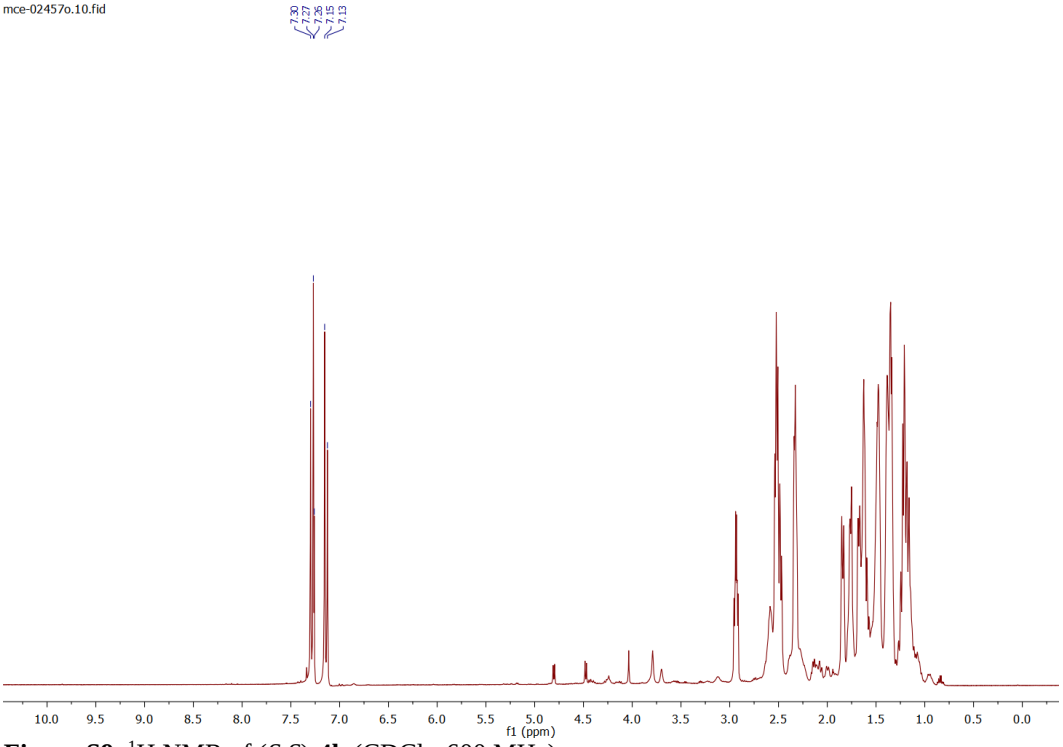

Figure S9. ^{1}H NMR of (*S*,*S*)-**4b** ($CDCl_3$, 600 MHz).

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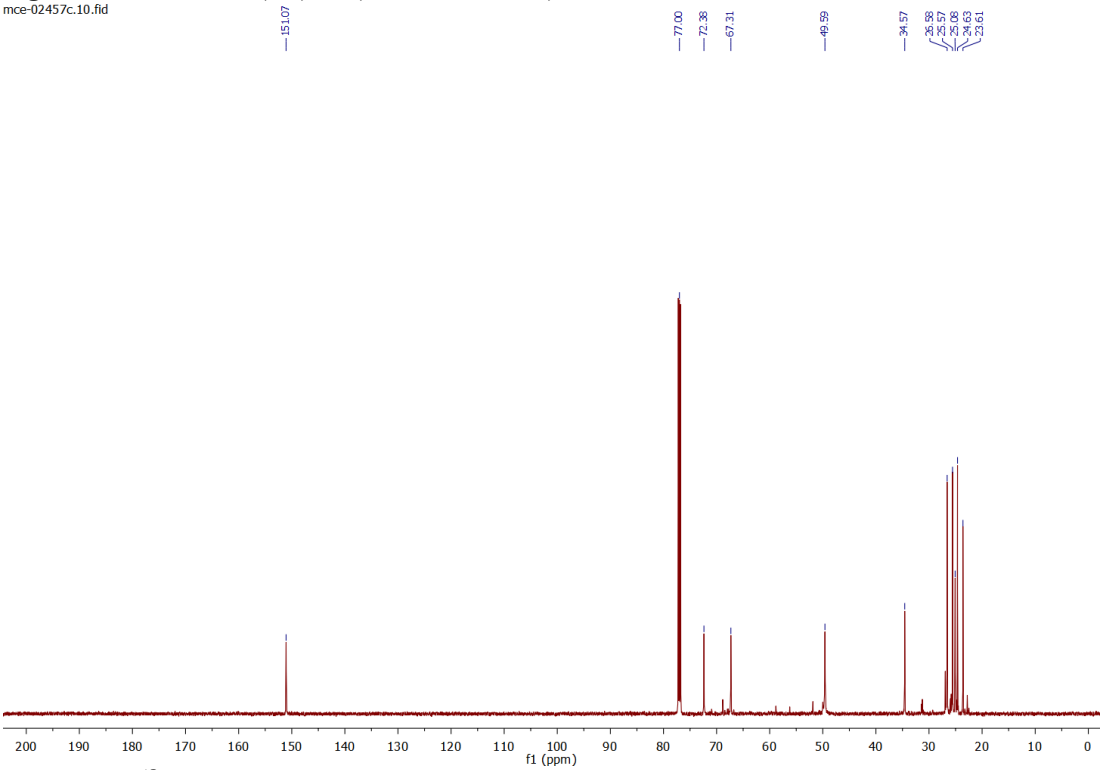
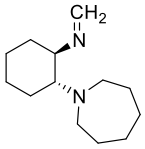


Figure S10. ^{13}C NMR of (*S*,*S*)-**4b** ($CDCl_3$, 151 MHz).



(*R*,*R*)-**4c**

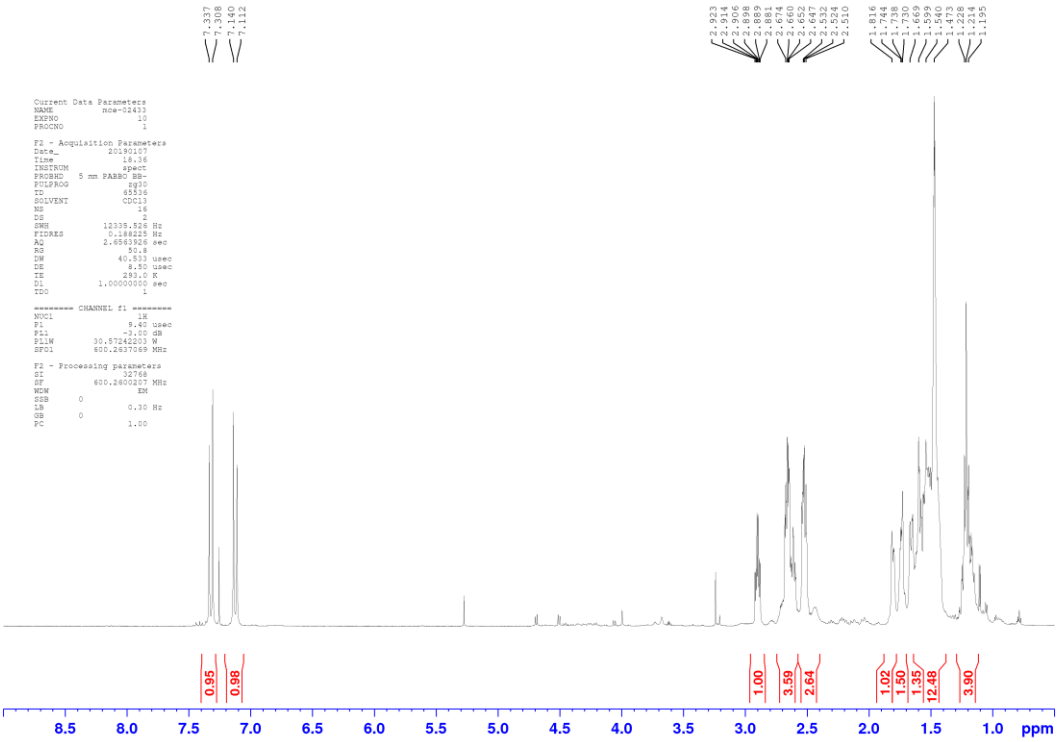


Figure S11. ^{1}H NMR of (*R*,*R*)-**4c** ($CDCl_3$, 600 MHz).

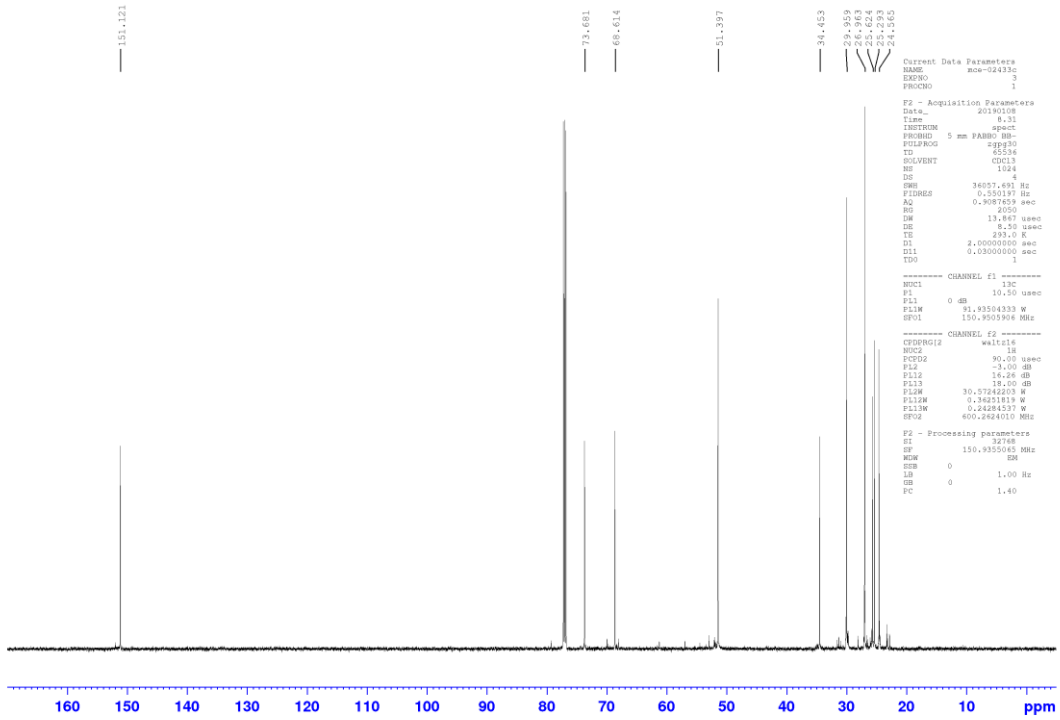
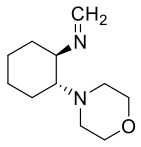


Figure S12. ^{13}C NMR of (*R*,*R*)-**4c** ($CDCl_3$, 151 MHz).



(*R*,*R*)-**4d**

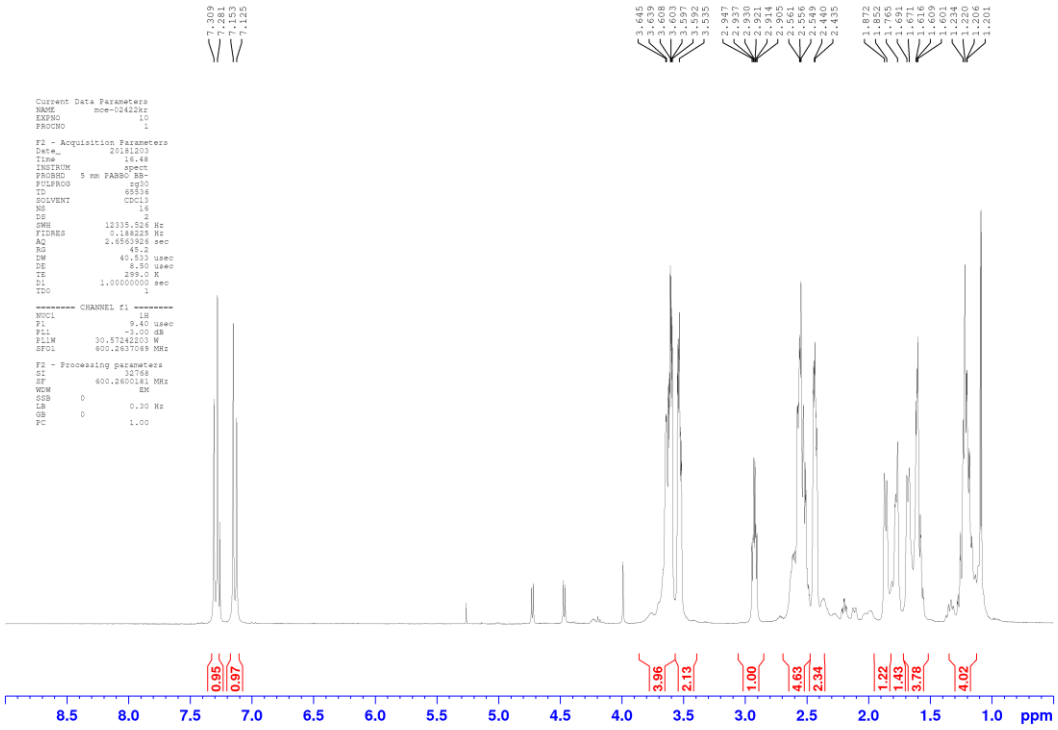


Figure S13. ^{1}H NMR of (*R*,*R*)-**4d** ($CDCl_3$, 600 MHz).

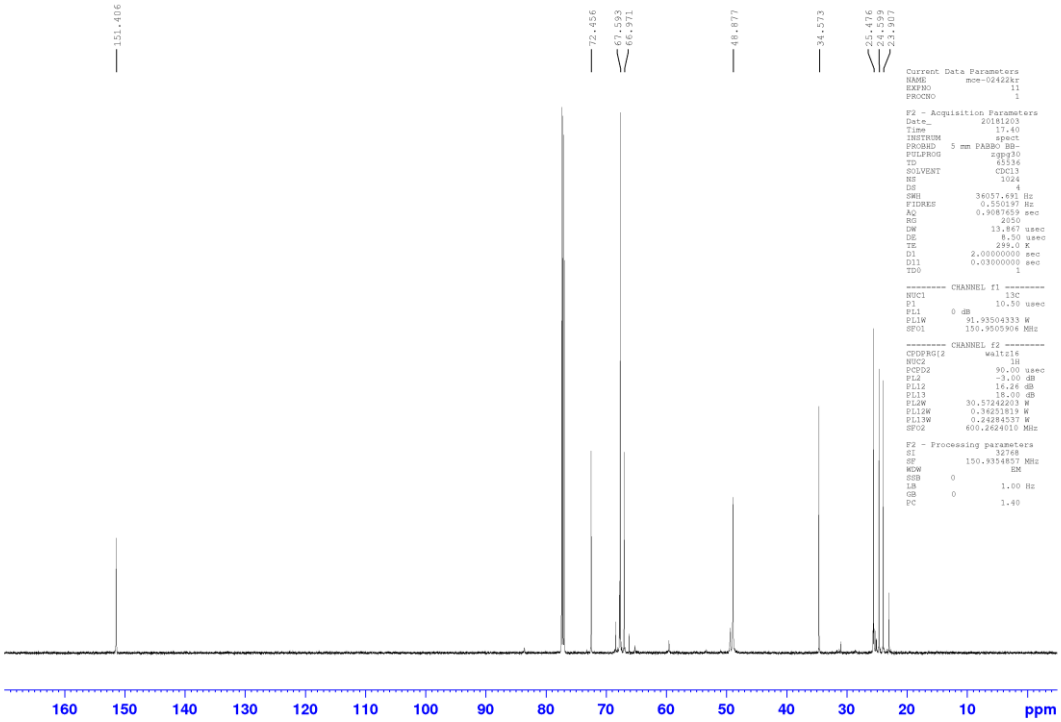


Figure S14. ^{13}C NMR of (*R*,*R*)-**4d** ($CDCl_3$, 151 MHz).

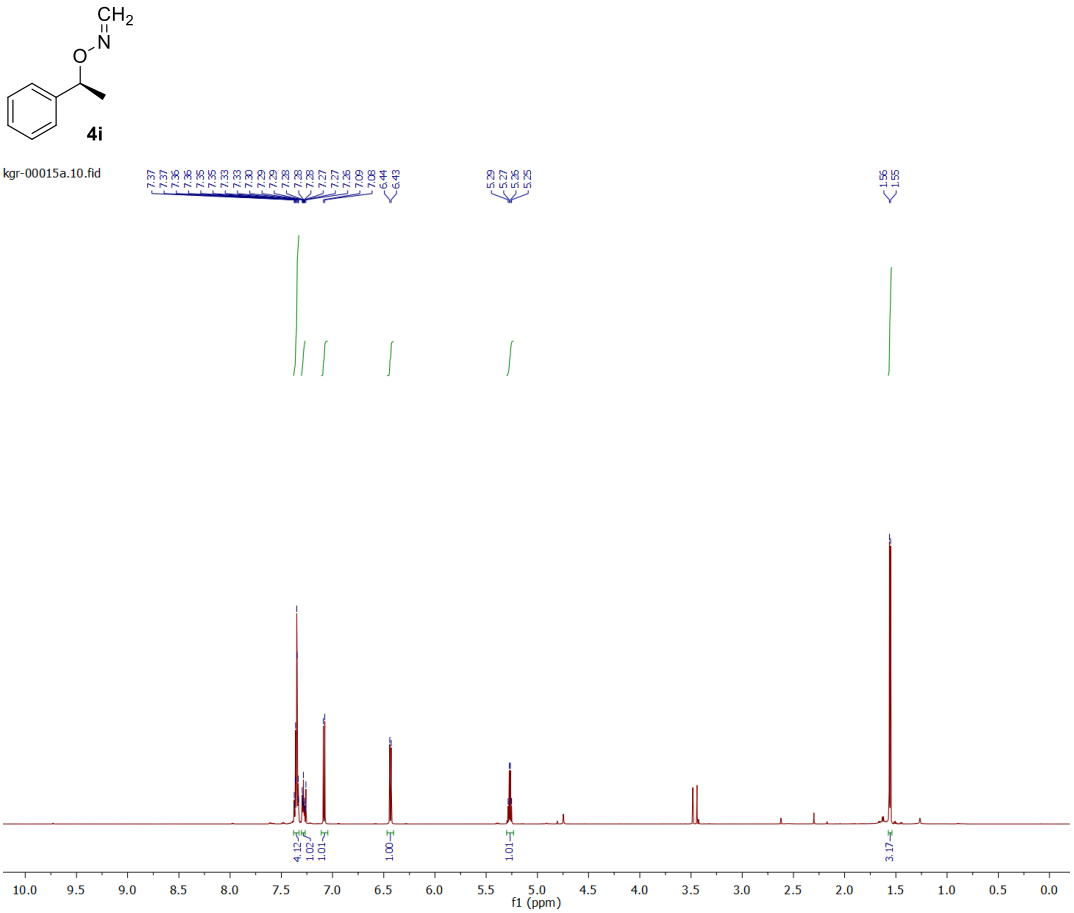


Figure S15. ^{1}H NMR of **4i** ($CDCl_3$, 600 MHz).

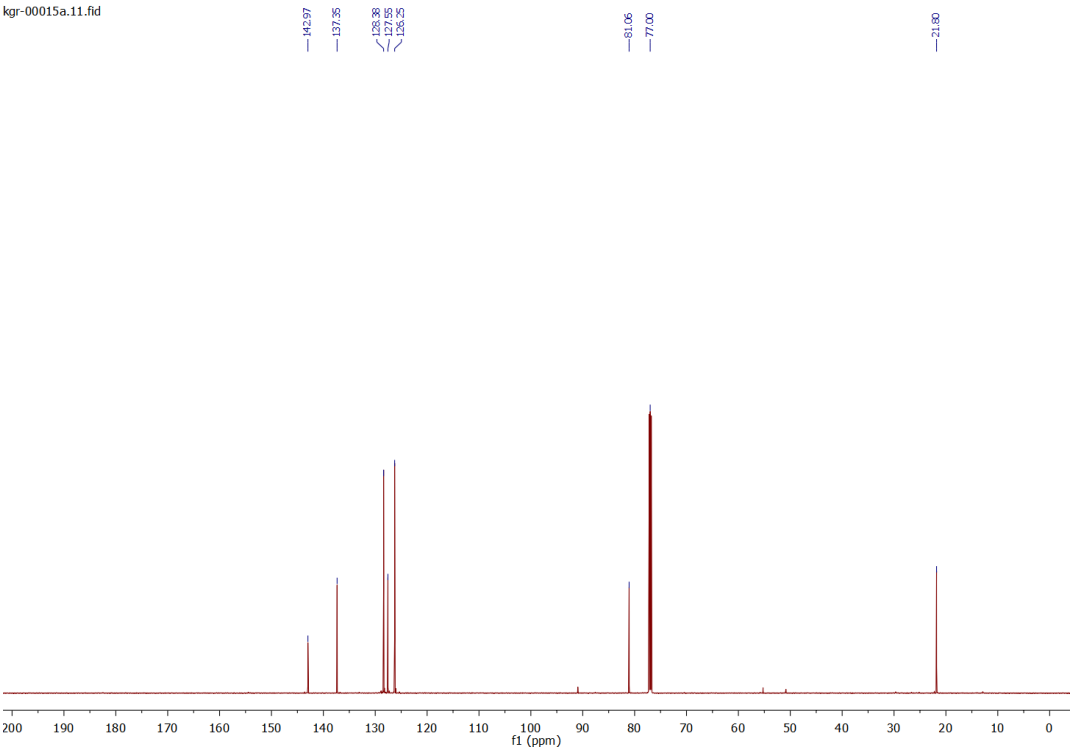
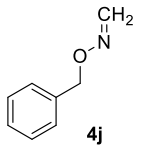


Figure S16. ^{13}C NMR of **4i** ($CDCl_3$, 151 MHz).



4j

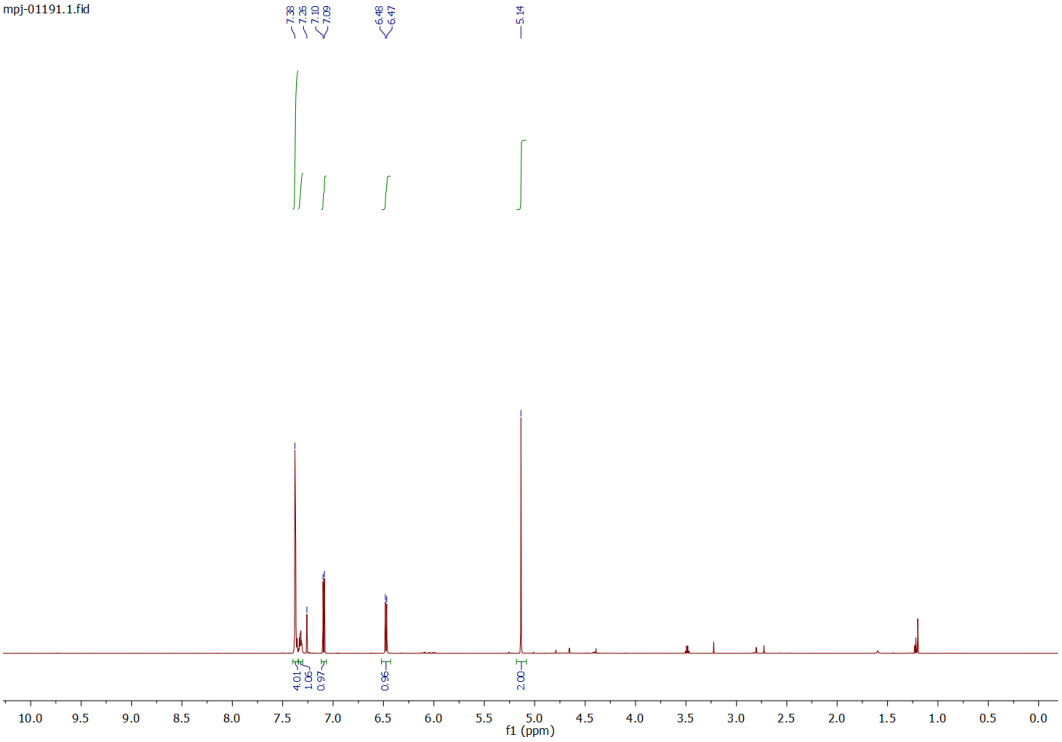


Figure S17. ^{1}H NMR of **4j** ($CDCl_3$, 600 MHz).

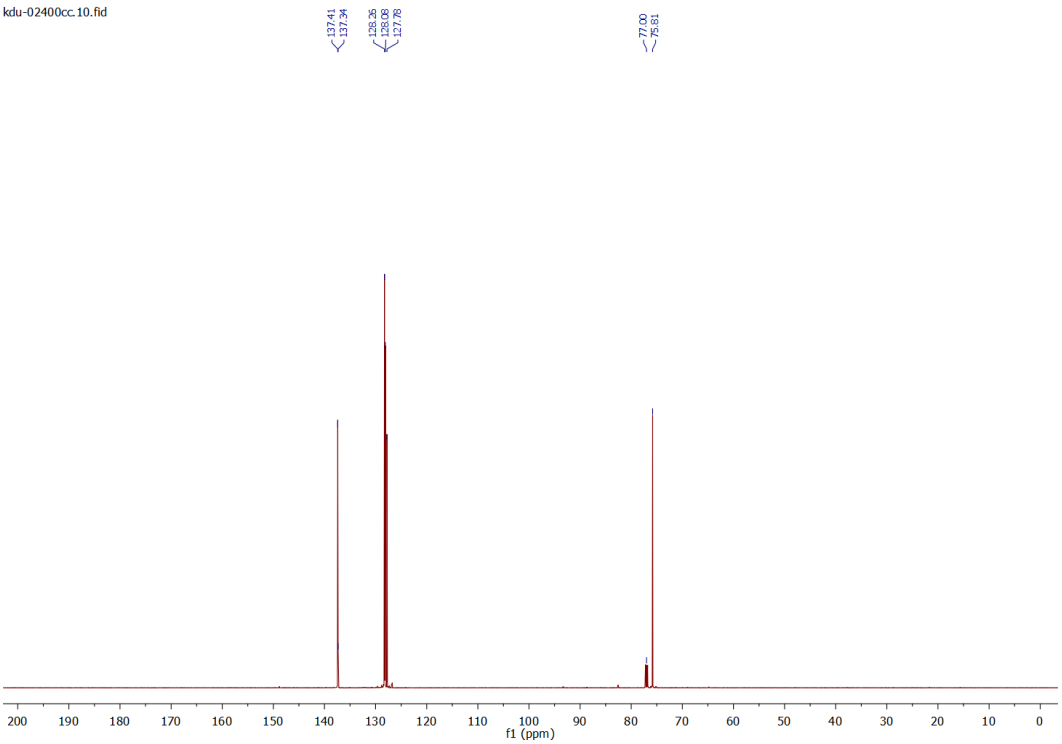
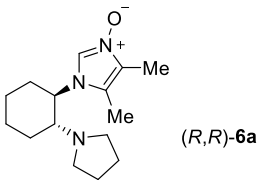


Figure S18. ^{13}C NMR of **4j** ($CDCl_3$, 151 MHz).



(*R*,*R*)-**6a**

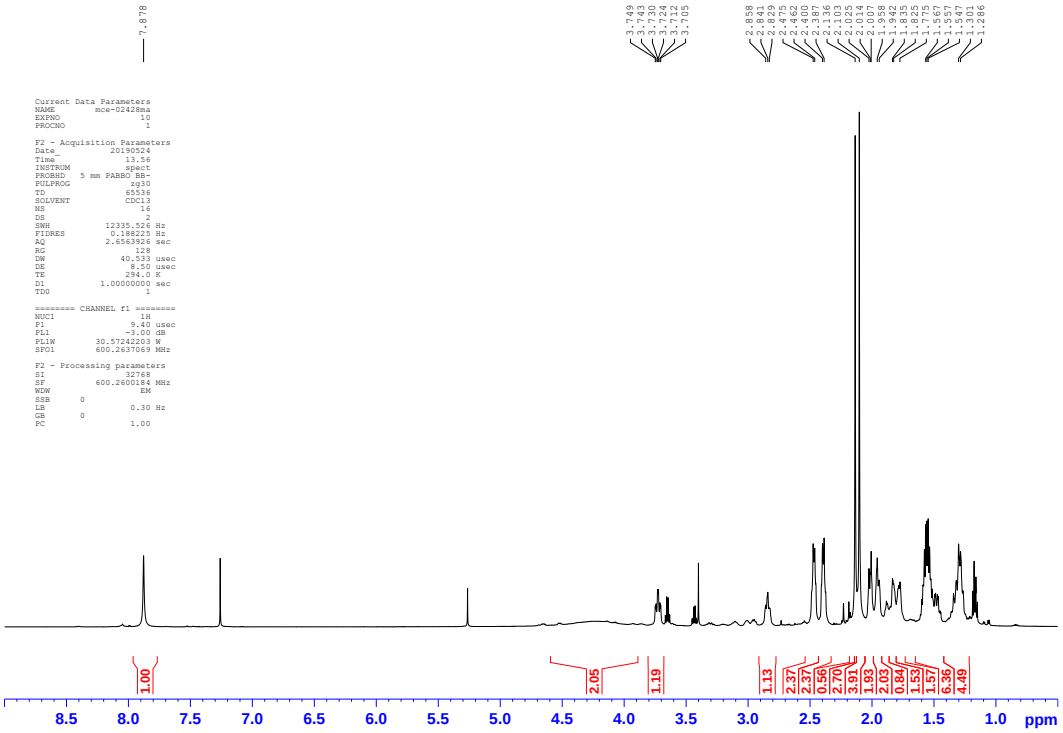


Figure S19. ^{1}H NMR of (*R*,*R*)-**6a** ($CDCl_3$, 600 MHz).

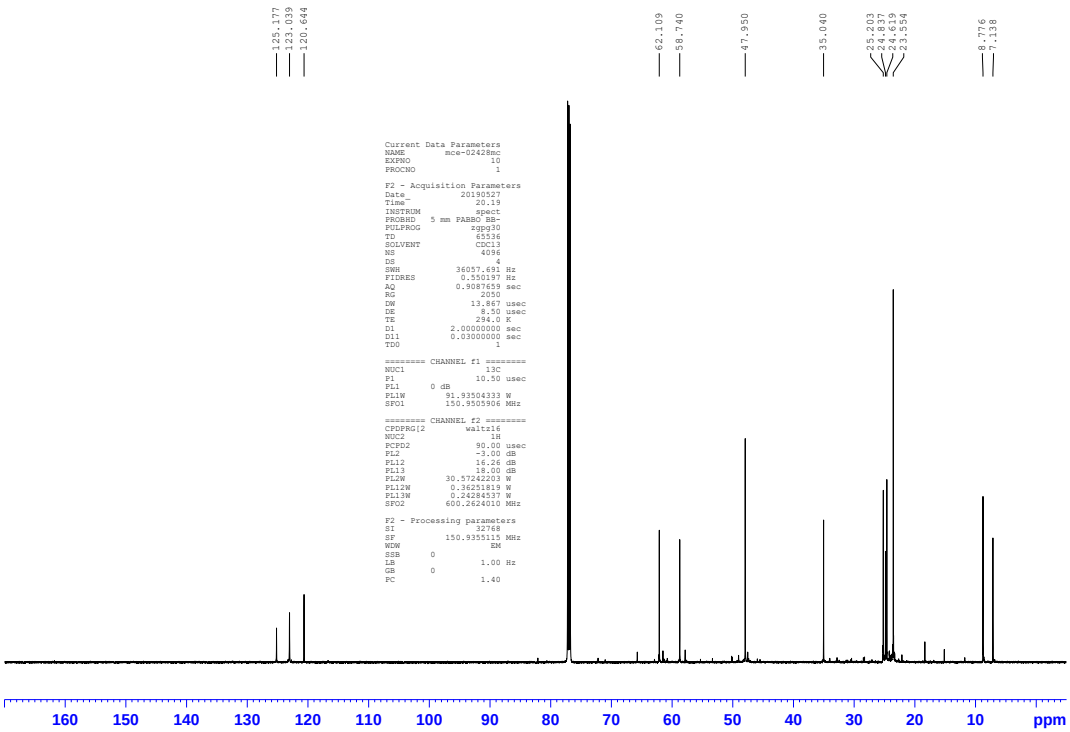


Figure S20. ^{13}C NMR of (*R*,*R*)-**6a** ($CDCl_3$, 151 MHz).

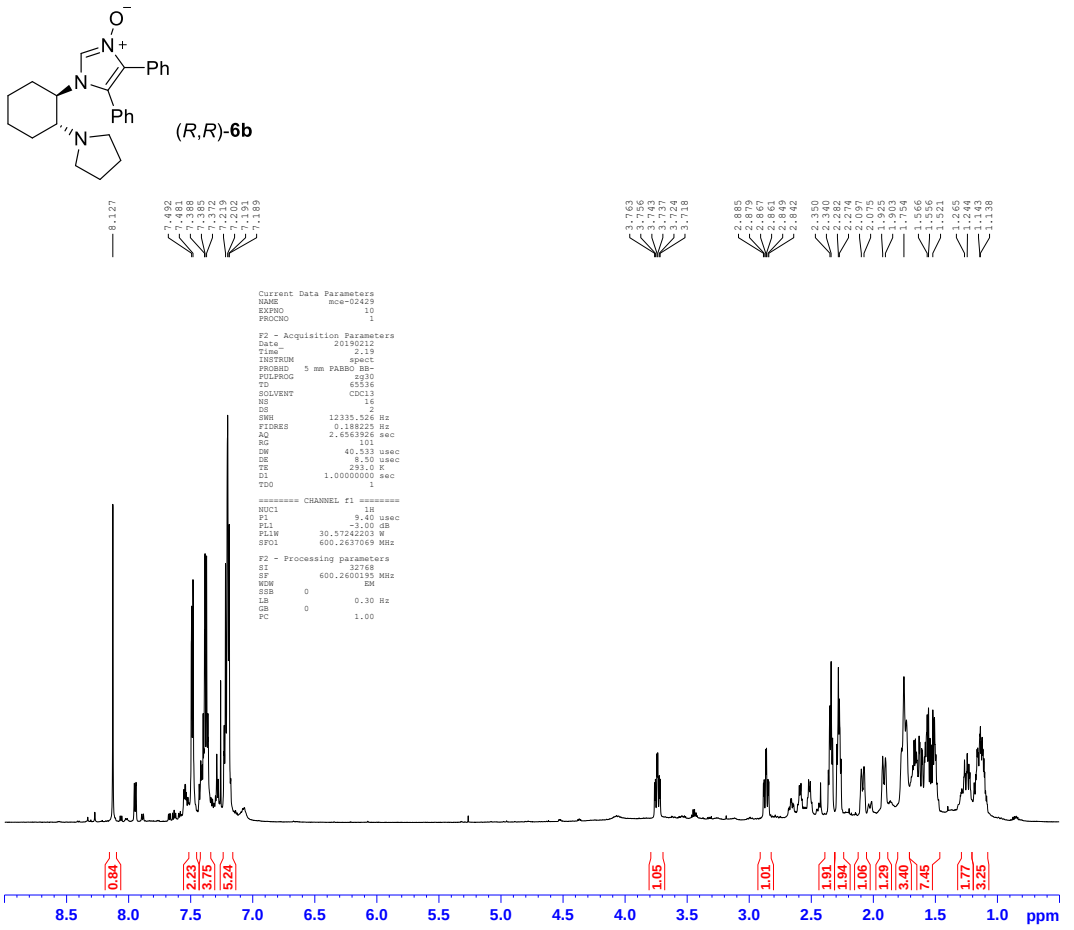


Figure S21. ^{1}H NMR of (*R*,*R*)-**6b** ($CDCl_3$, 600 MHz).

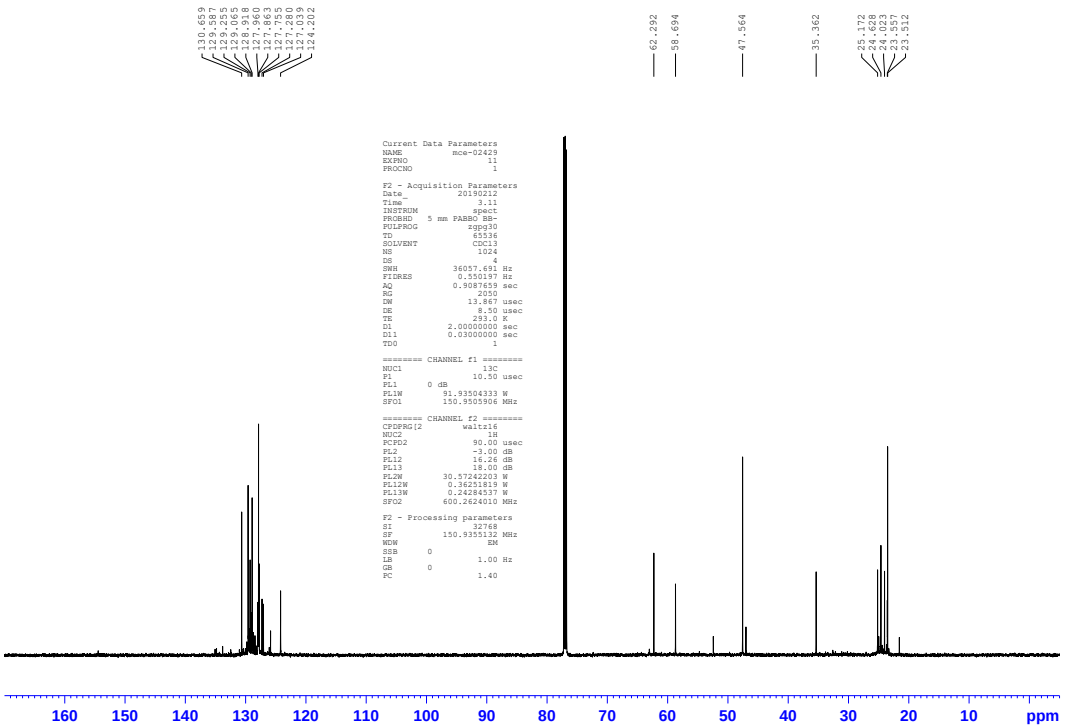
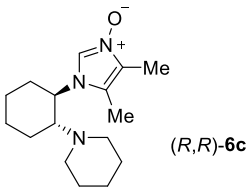


Figure S22. ^{13}C NMR of (*R*,*R*)-**6b** ($CDCl_3$, 151 MHz).



(*R*,*R*)-**6c**

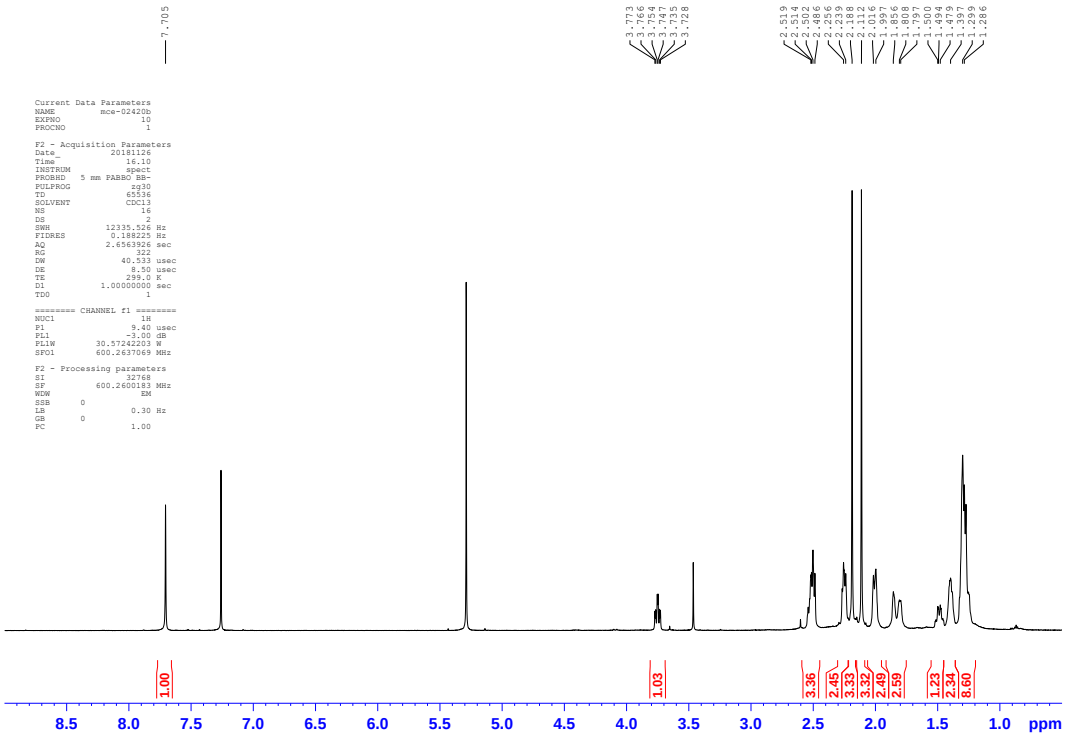


Figure S23. ^{1}H NMR of (*R*,*R*)-**6c** ($CDCl_3$, 600 MHz).

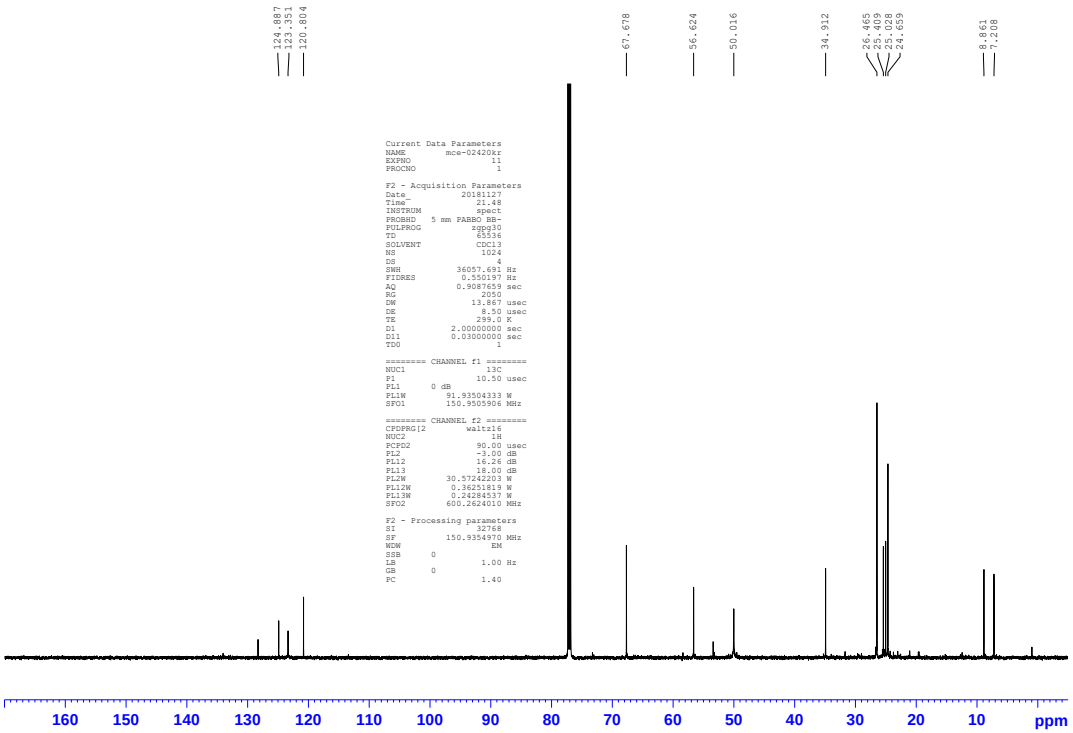


Figure S24. ^{13}C NMR of (*R*,*R*)-**6c** ($CDCl_3$, 151 MHz).

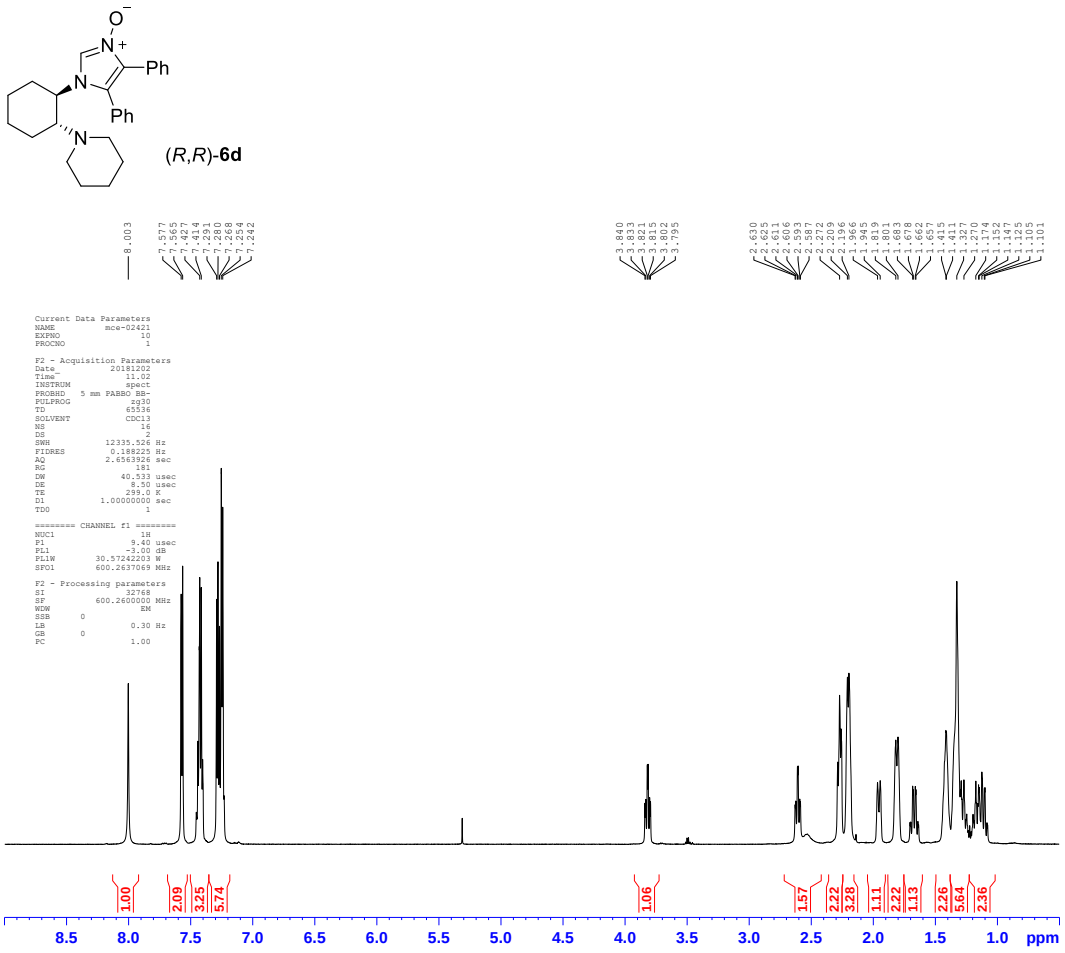


Figure S25. ^{1}H NMR of (*R*,*R*)-**6d** ($CDCl_3$, 600 MHz).

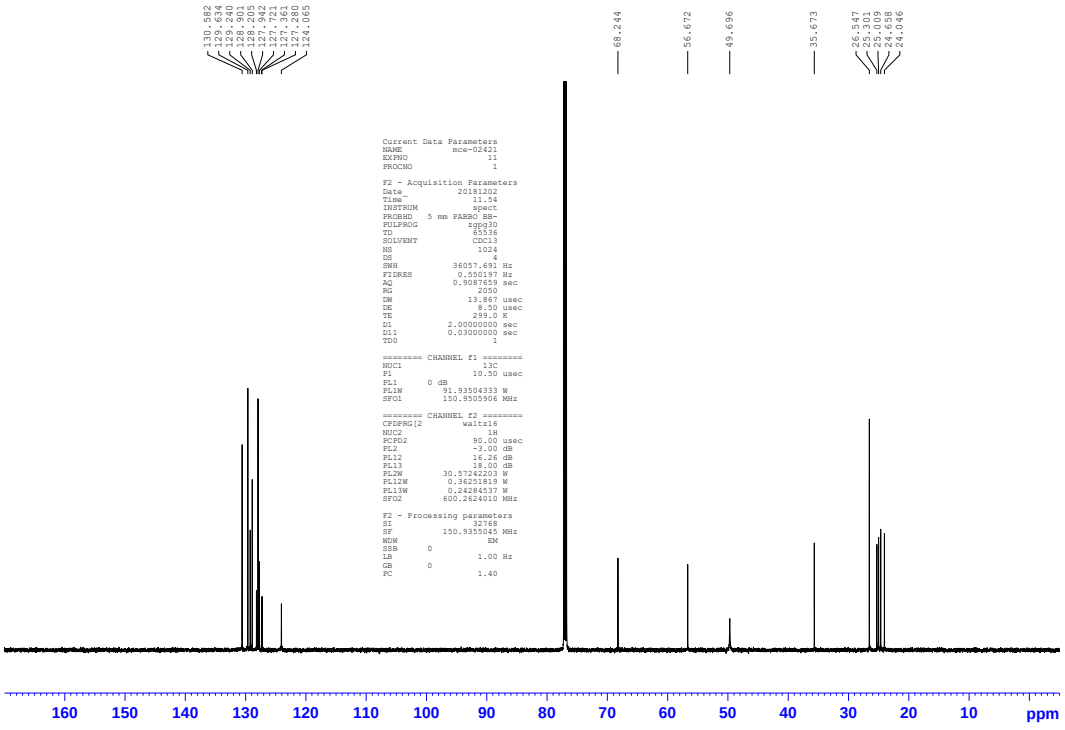
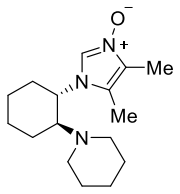


Figure S26. ^{13}C NMR of (*R*,*R*)-**6d** ($CDCl_3$, 151 MHz).



(*S*,*S*)-**6c**

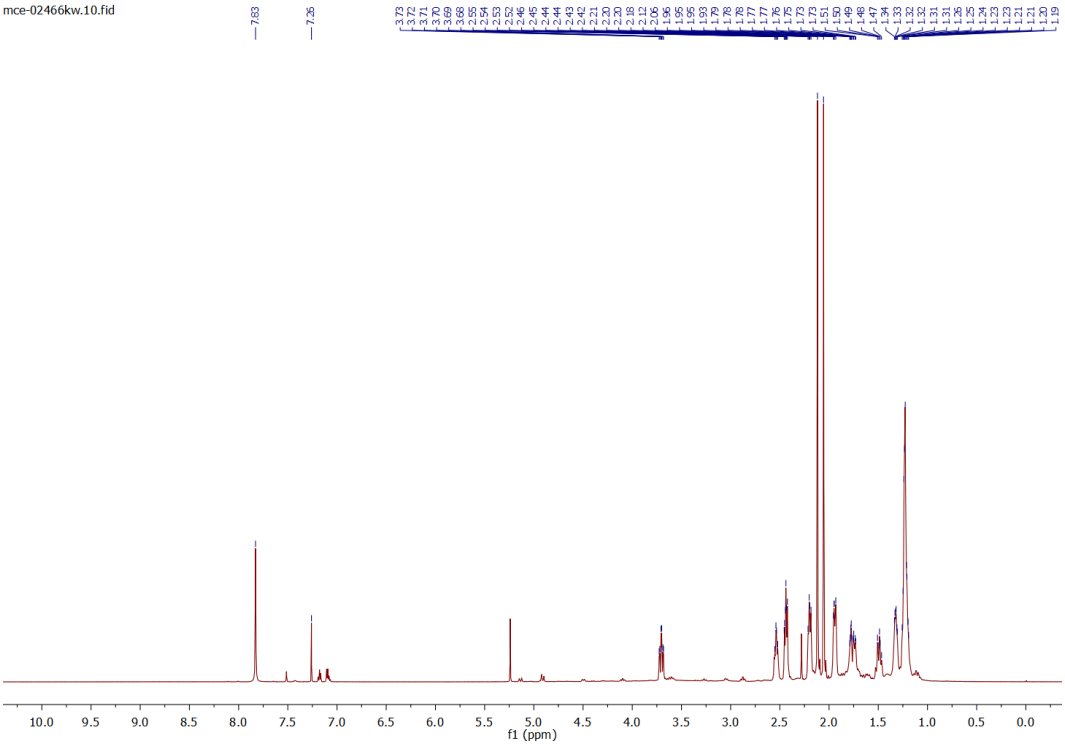


Figure S27. ^{1}H NMR of (*S*,*S*)-**6c** ($CDCl_3$, 600 MHz).

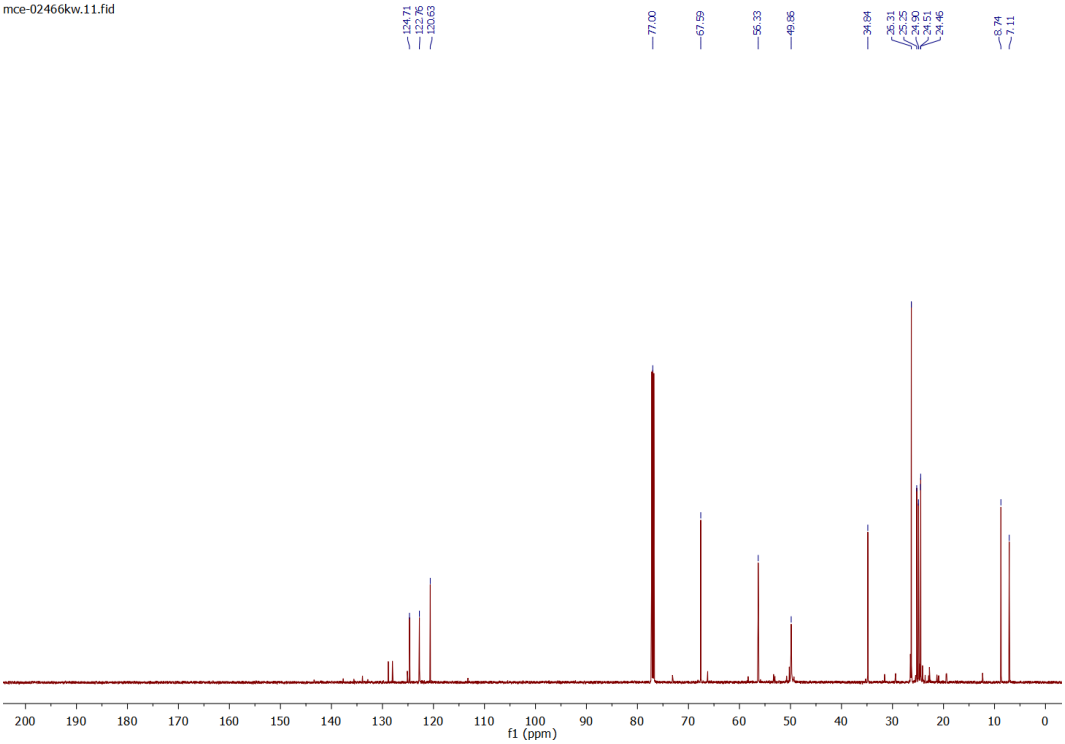
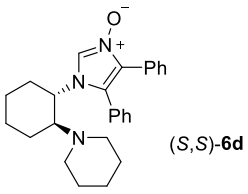


Figure S28. ^{13}C NMR of (*S*,*S*)-**6c** ($CDCl_3$, 151 MHz).



(*S*,*S*)-**6d**

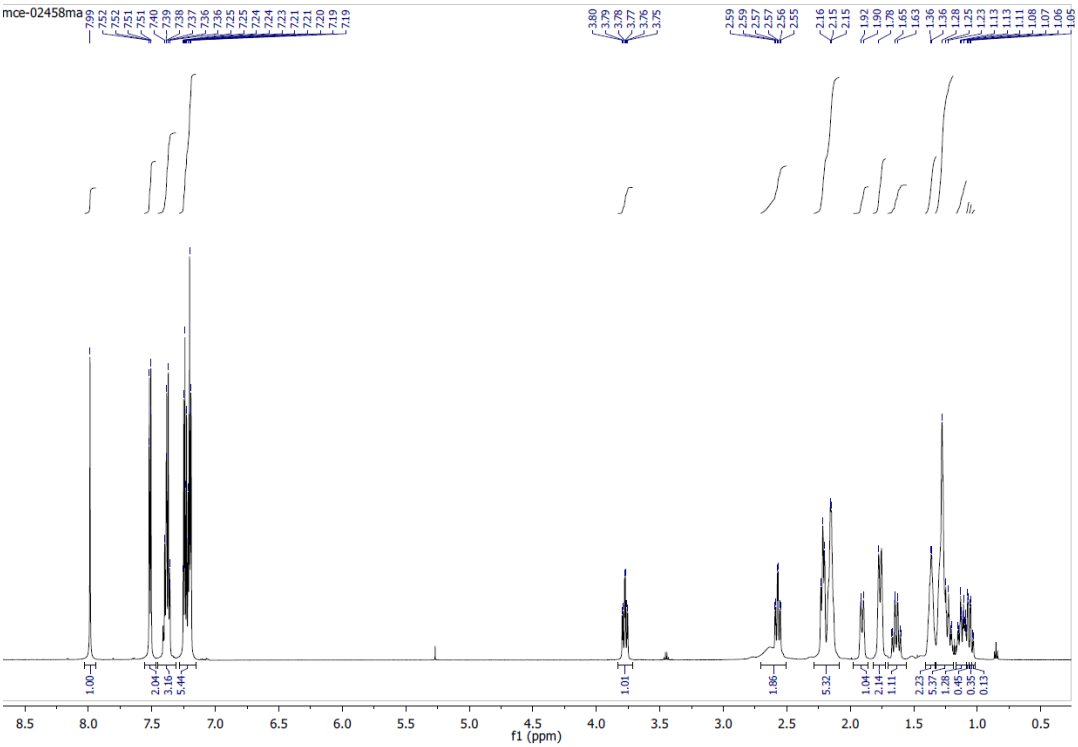


Figure S29. ^{1}H NMR of (*S*,*S*)-**6d** ($CDCl_3$, 600 MHz).

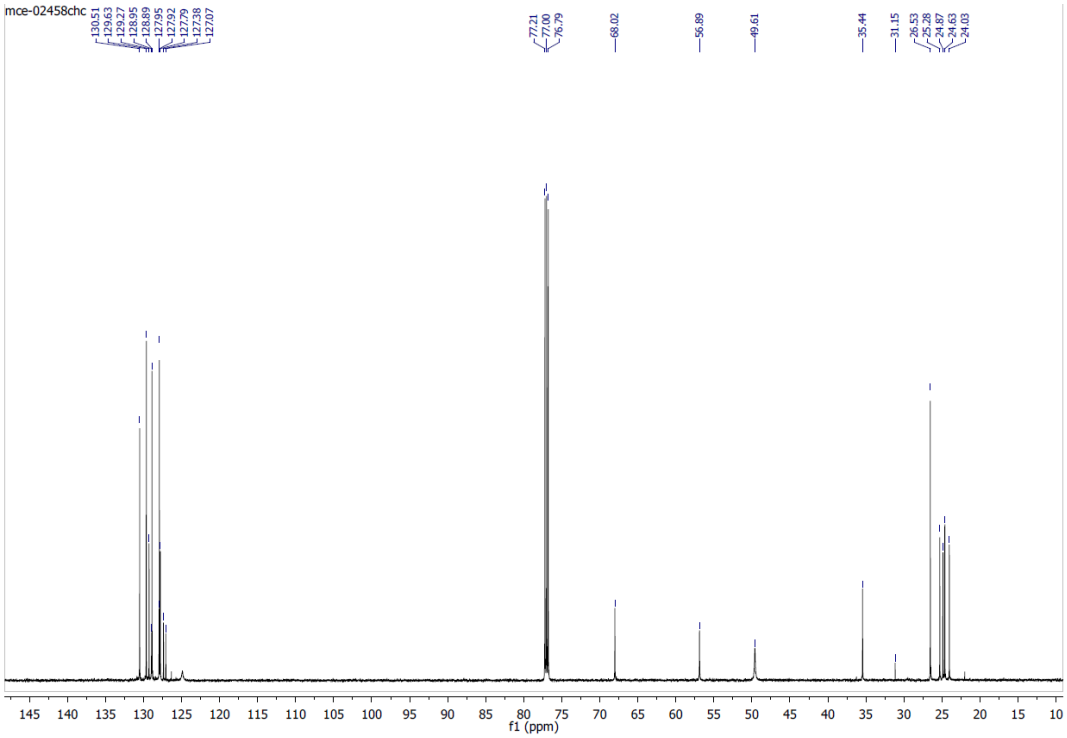
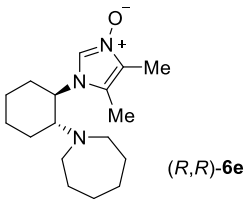


Figure S30. ^{13}C NMR of (*S*,*S*)-**6d** ($CDCl_3$, 151 MHz).



(*R*,*R*)-**6e**

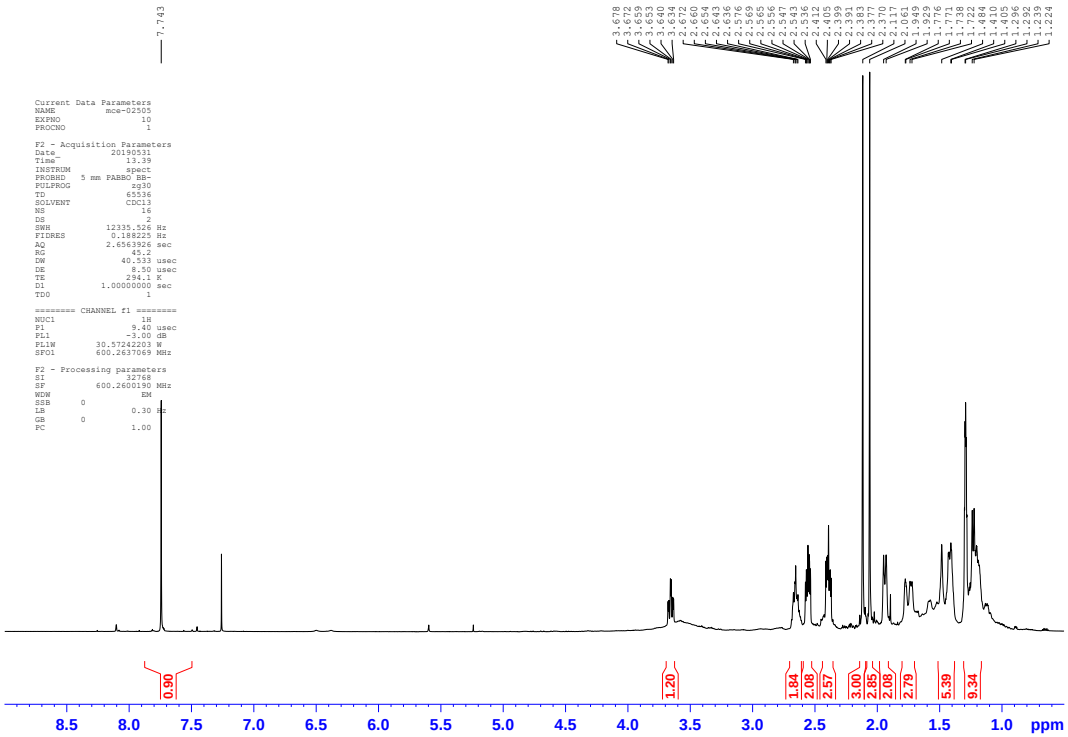


Figure S31. ^{1}H NMR of (*R*,*R*)-**6e** ($CDCl_3$, 600 MHz).

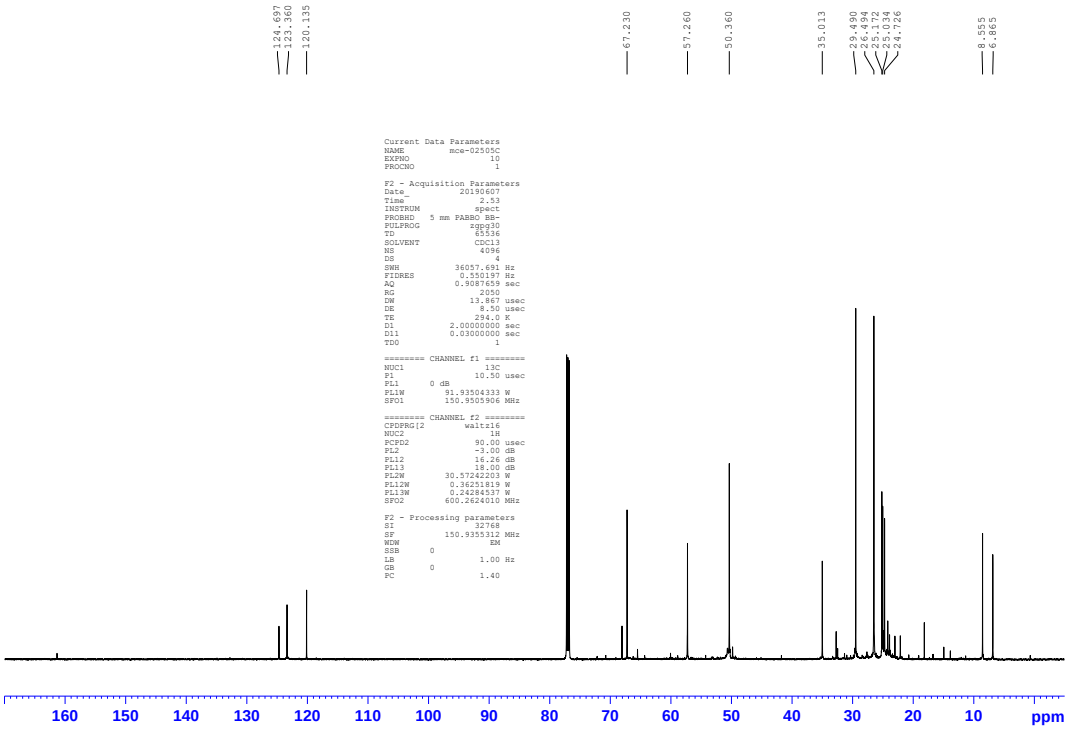


Figure S32. ^{13}C NMR of (*R*,*R*)-**6e** ($CDCl_3$, 151 MHz).

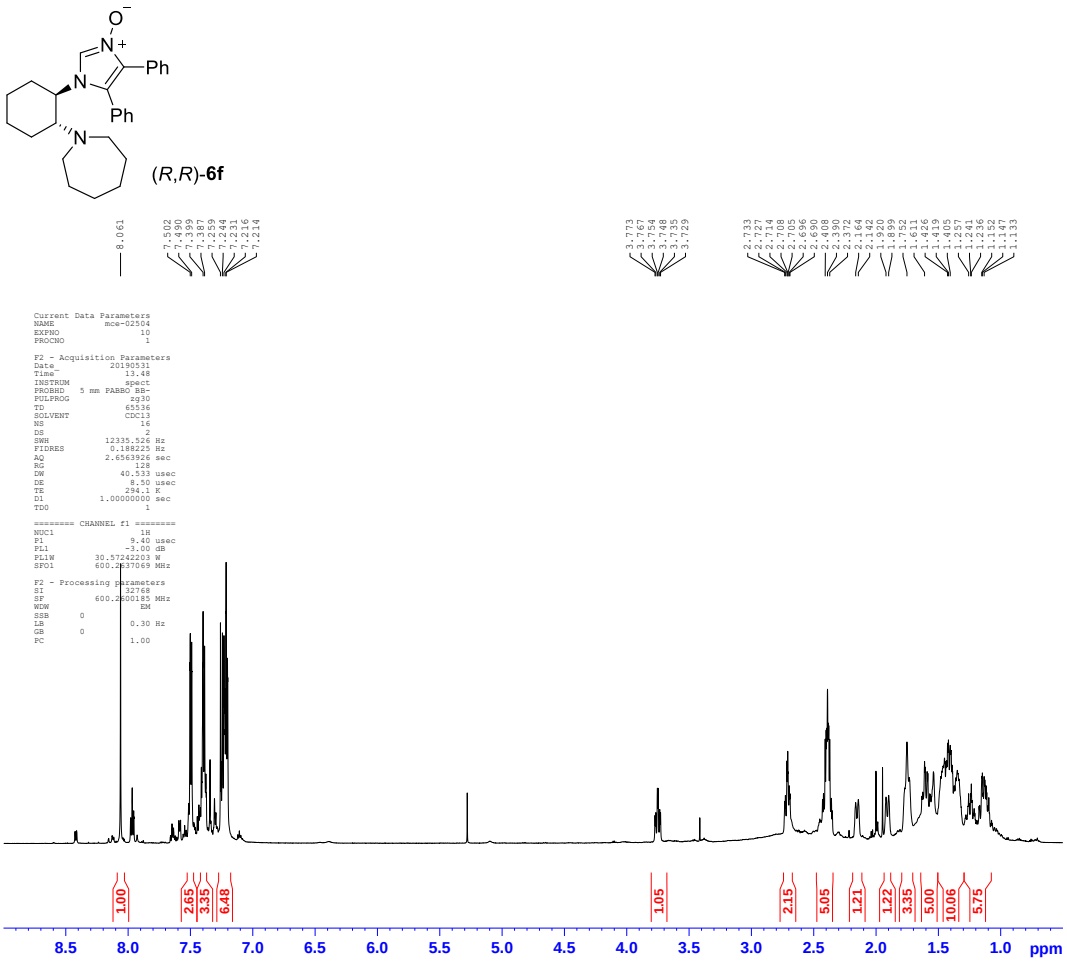


Figure S33. ^{1}H NMR of (*R*,*R*)-**6f** ($CDCl_3$, 600 MHz).

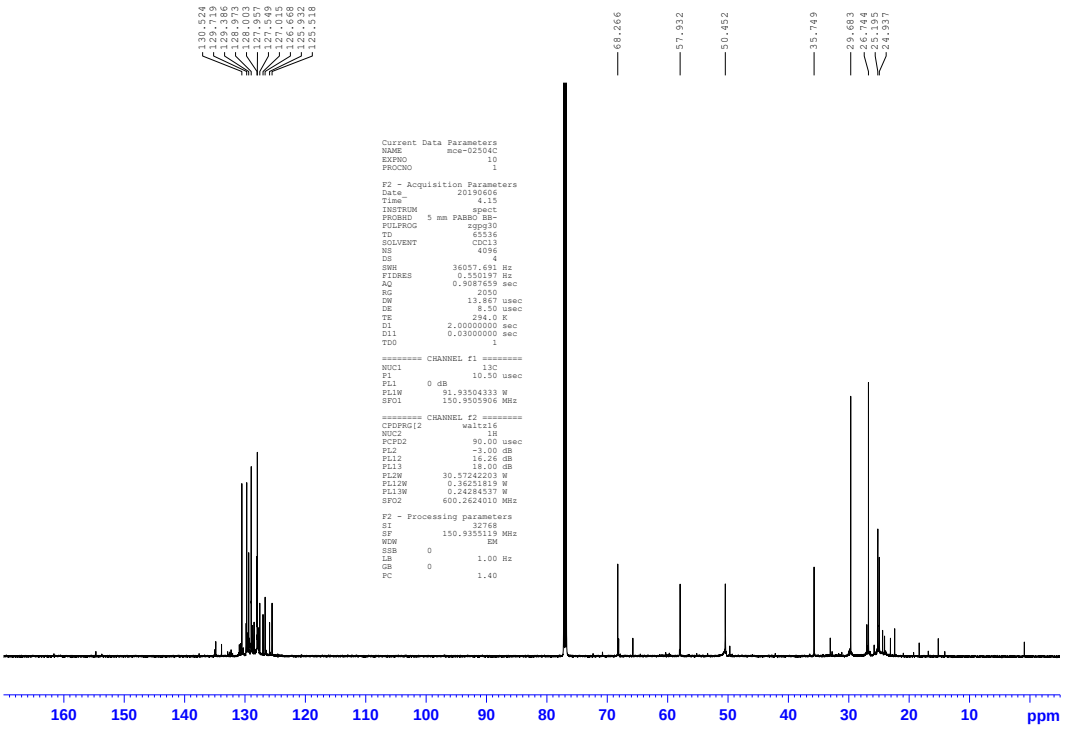
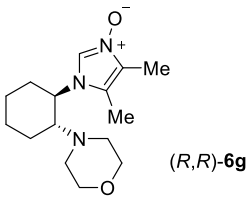


Figure S34. ^{13}C NMR of (*R*,*R*)-**6f** ($CDCl_3$, 151 MHz).



(*R*,*R*)-**6g**

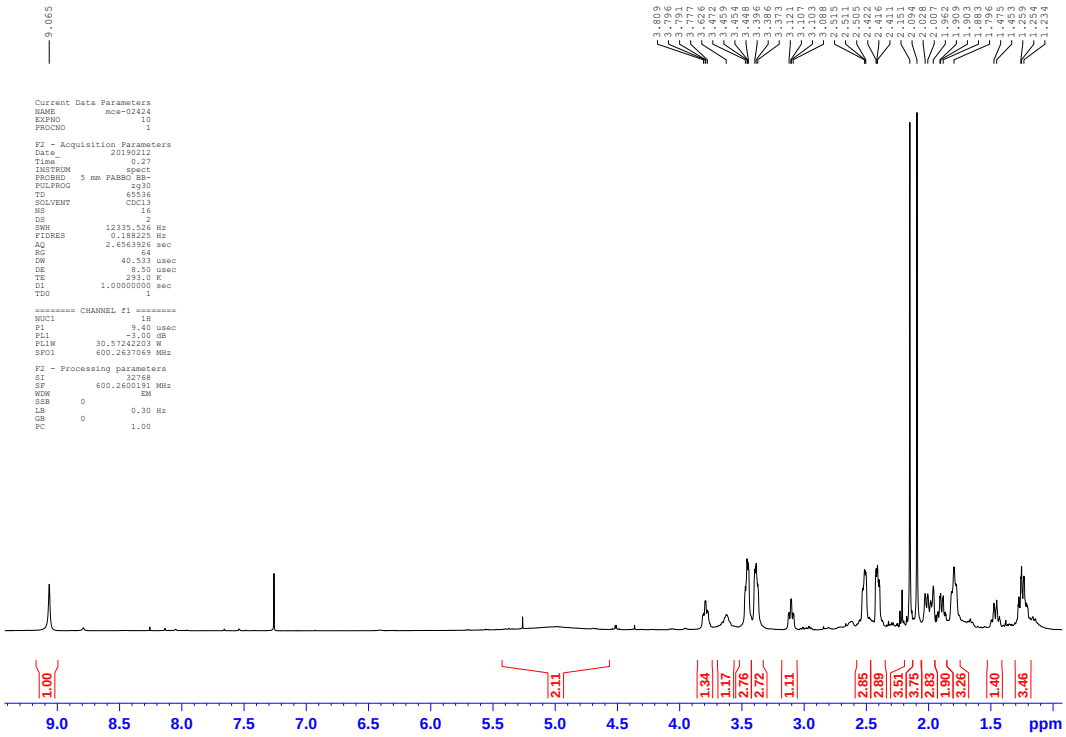


Figure S35. ^{1}H NMR of (*R*,*R*)-**6g** ($CDCl_3$, 600 MHz).

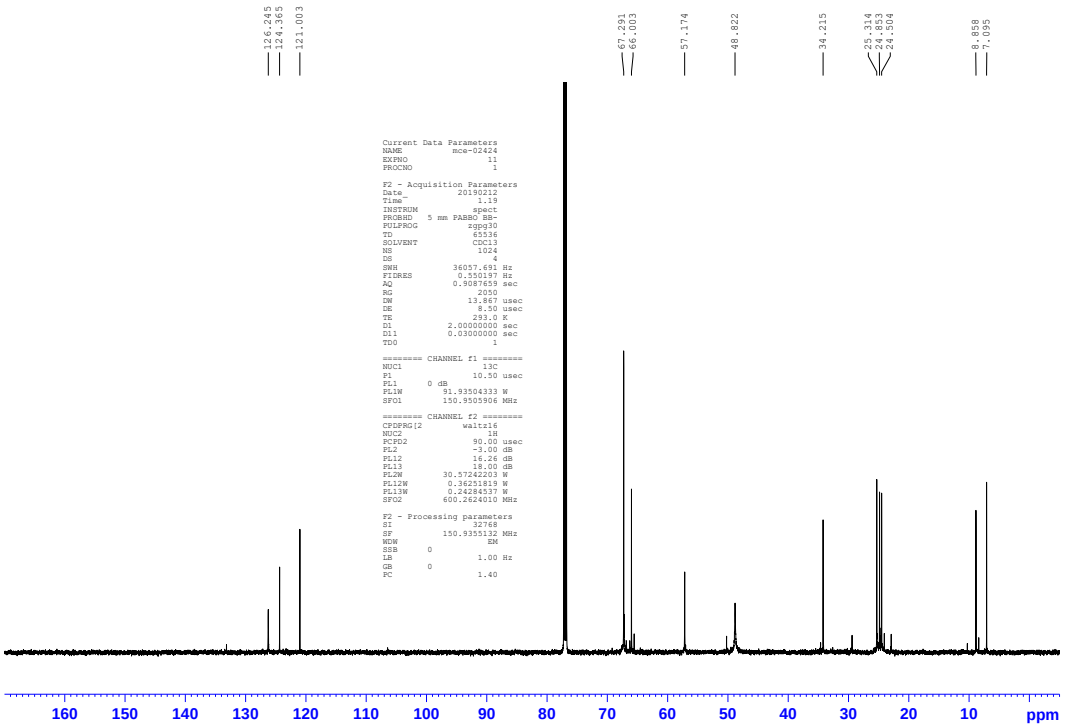
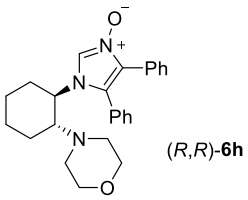


Figure S36. ^{13}C NMR of (*R*,*R*)-**6g** ($CDCl_3$, 151 MHz).



(*R*,*R*)-**6h**

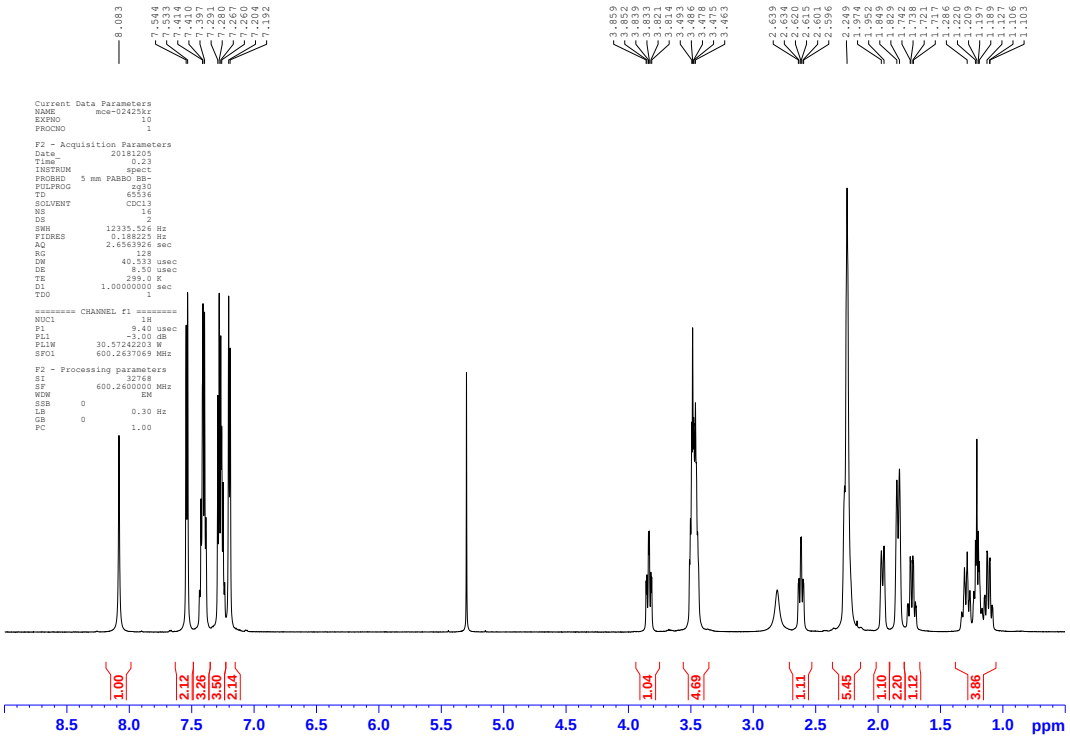


Figure S37. ^{1}H NMR of (*R*,*R*)-**6h** ($CDCl_3$, 600 MHz).

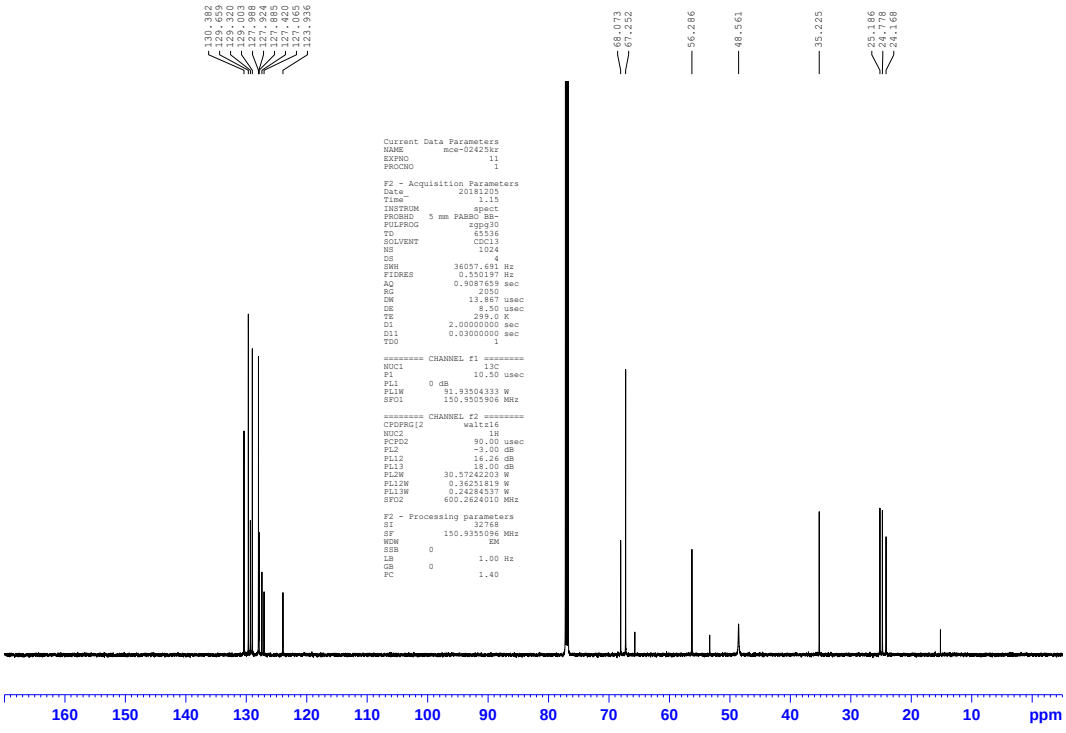
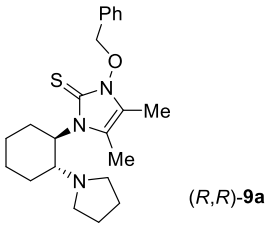


Figure S38. ^{13}C NMR of (*R*,*R*)-**6h** ($CDCl_3$, 151 MHz).



(*R*,*R*)-**9a**

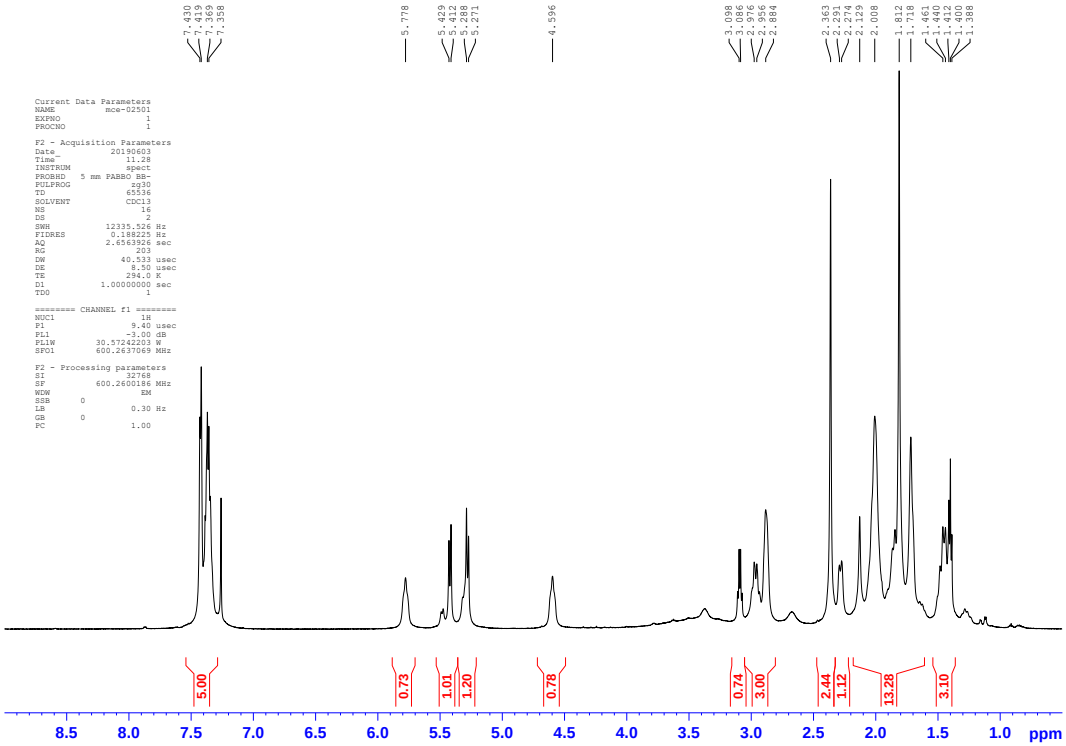


Figure S39. ^{1}H NMR of (*R*,*R*)-**9a** ($CDCl_3$, 600 MHz).

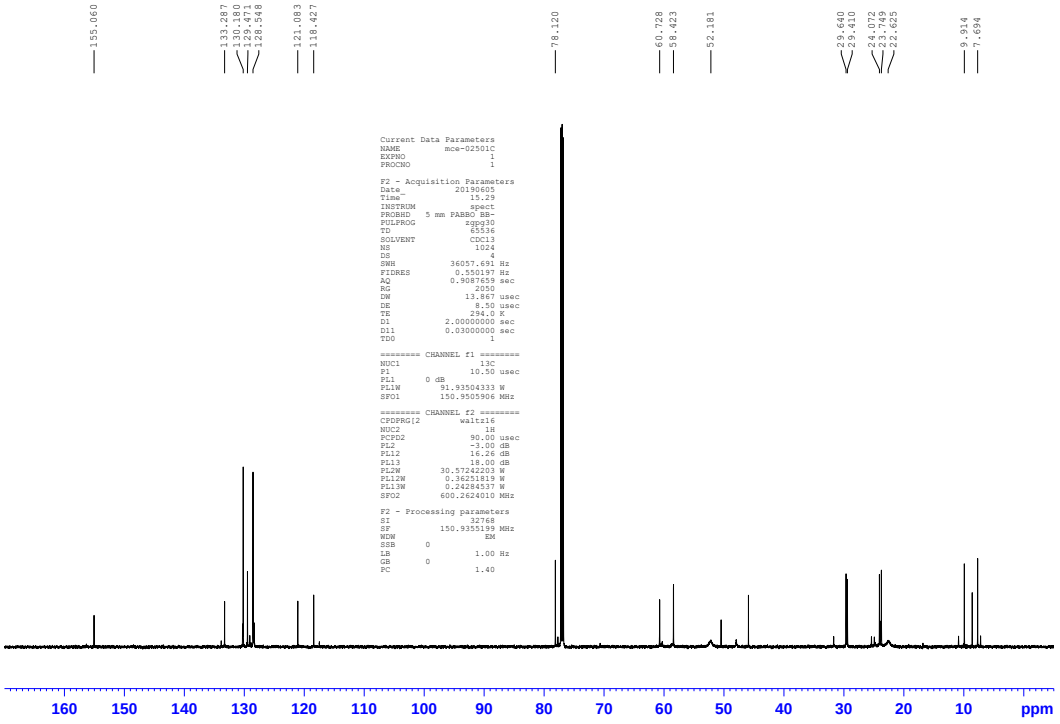


Figure S40. ^{13}C NMR of (*R*,*R*)-**9a** ($CDCl_3$, 151 MHz).

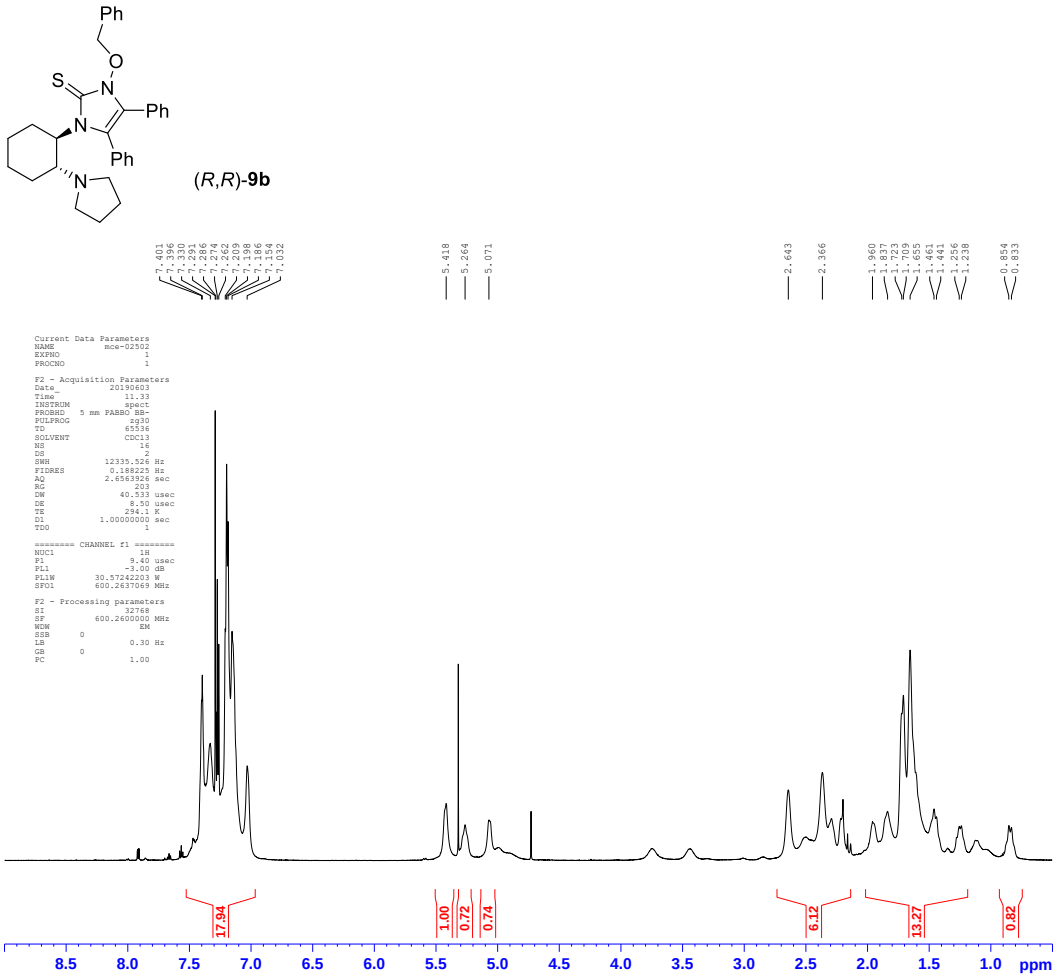


Figure S41. ^{1}H NMR of (*R*,*R*)-**9b** ($CDCl_3$, 600 MHz).

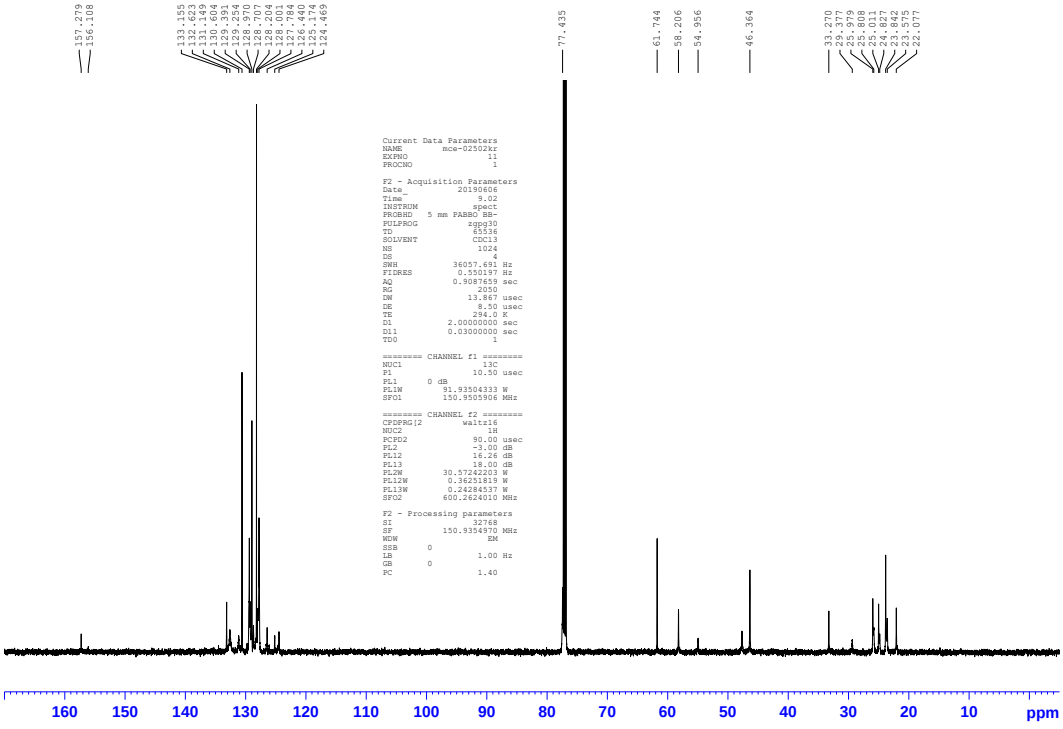
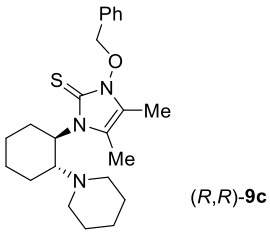


Figure S42. ^{13}C NMR of (*R*,*R*)-**9b** ($CDCl_3$, 151 MHz).



(*R*,*R*)-**9c**

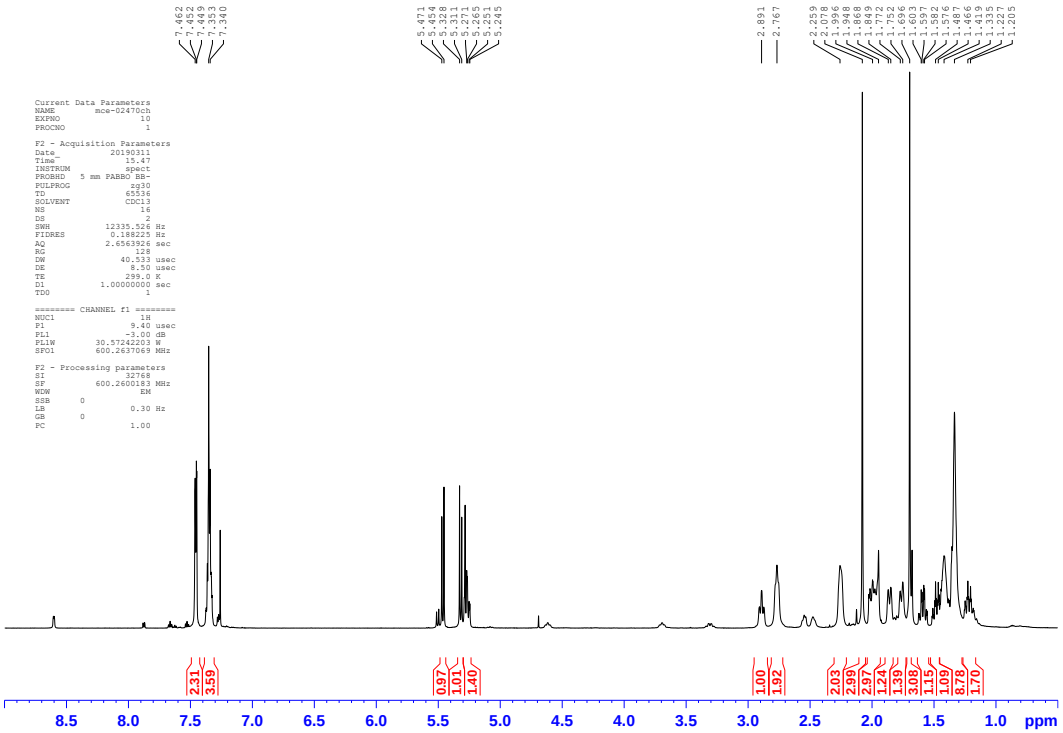


Figure S43. ^{1}H NMR of (*R*,*R*)-**9c** ($CDCl_3$, 600 MHz).

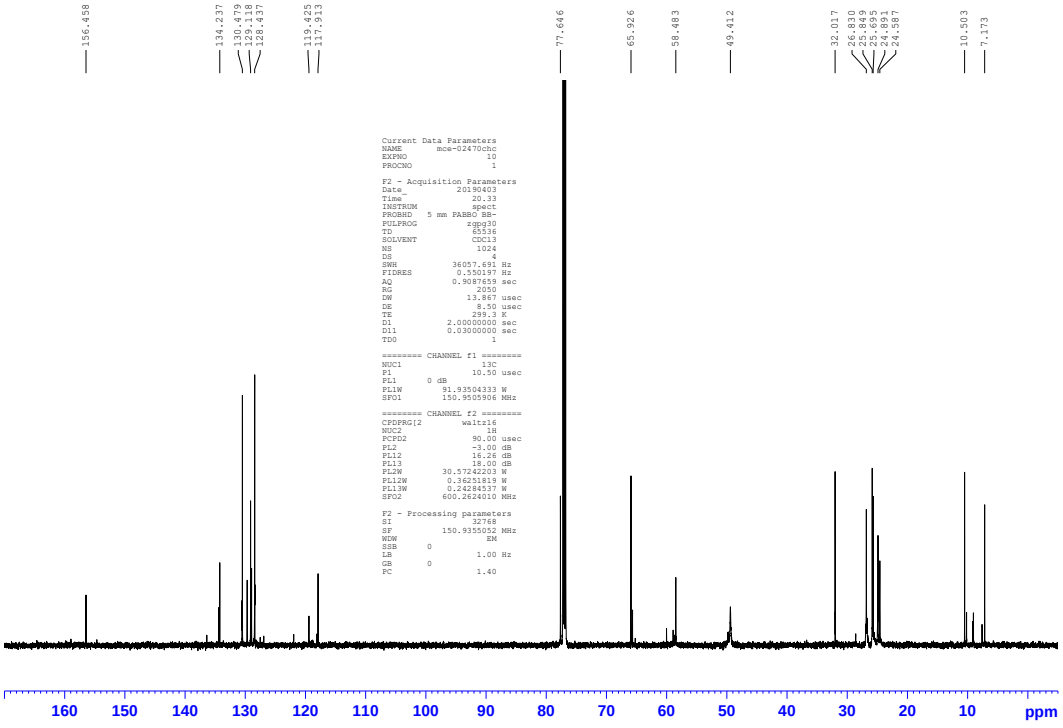


Figure S44. ^{13}C NMR of (*R*,*R*)-**9c** ($CDCl_3$, 151 MHz).

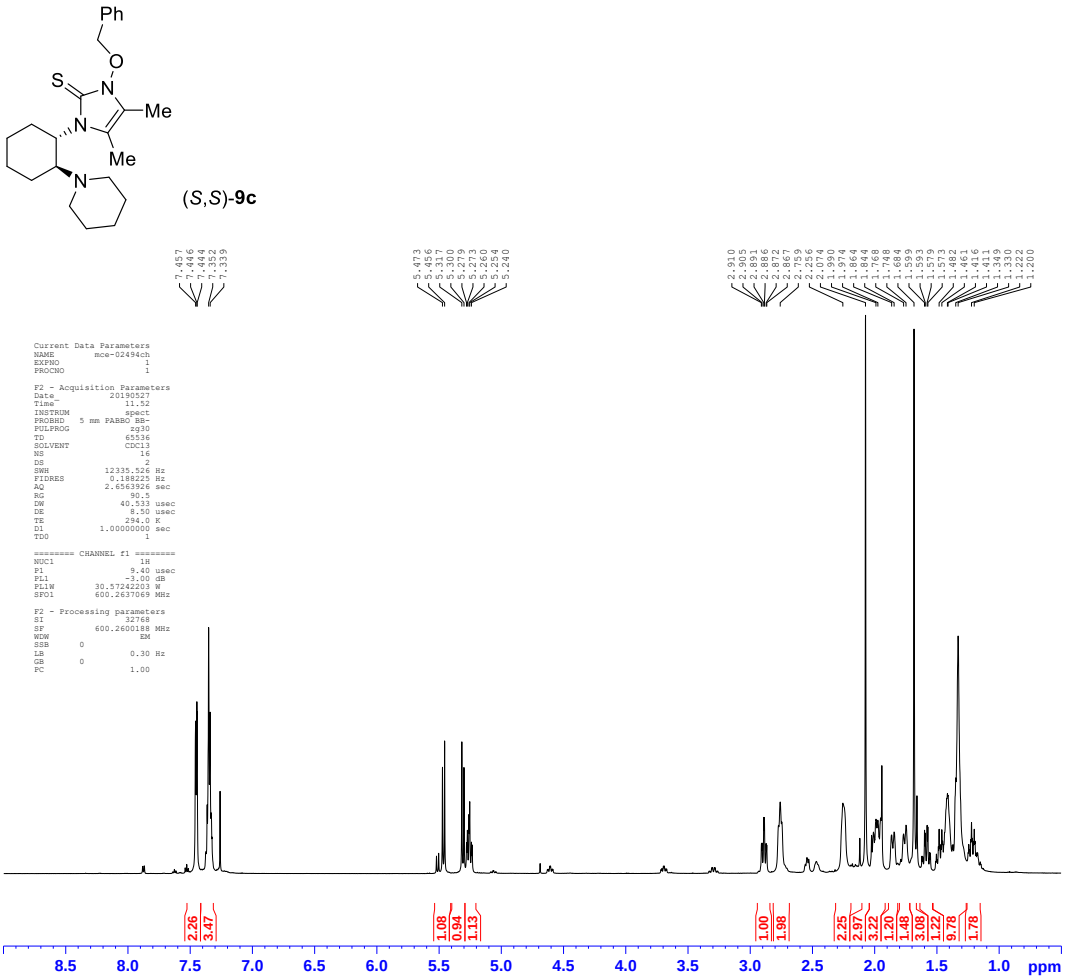


Figure S45. ^{1}H NMR of (*S*,*S*)-**9c** ($CDCl_3$, 600 MHz).

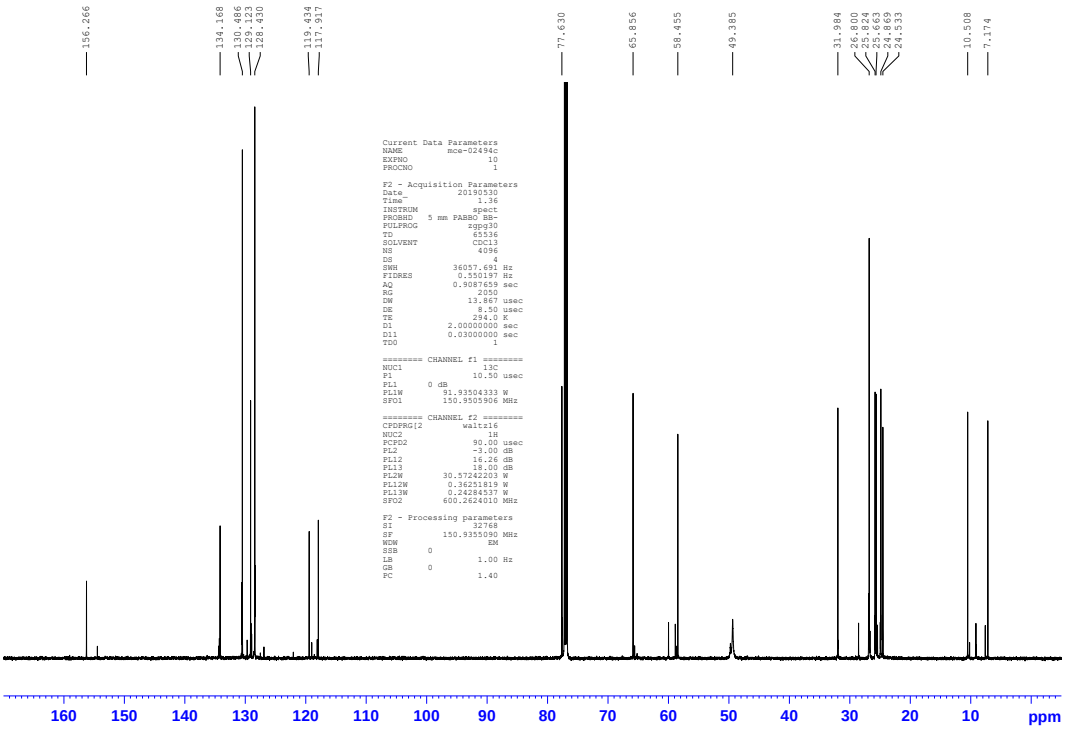


Figure S46. ^{13}C NMR of (*S*,*S*)-**9c** ($CDCl_3$, 151 MHz).

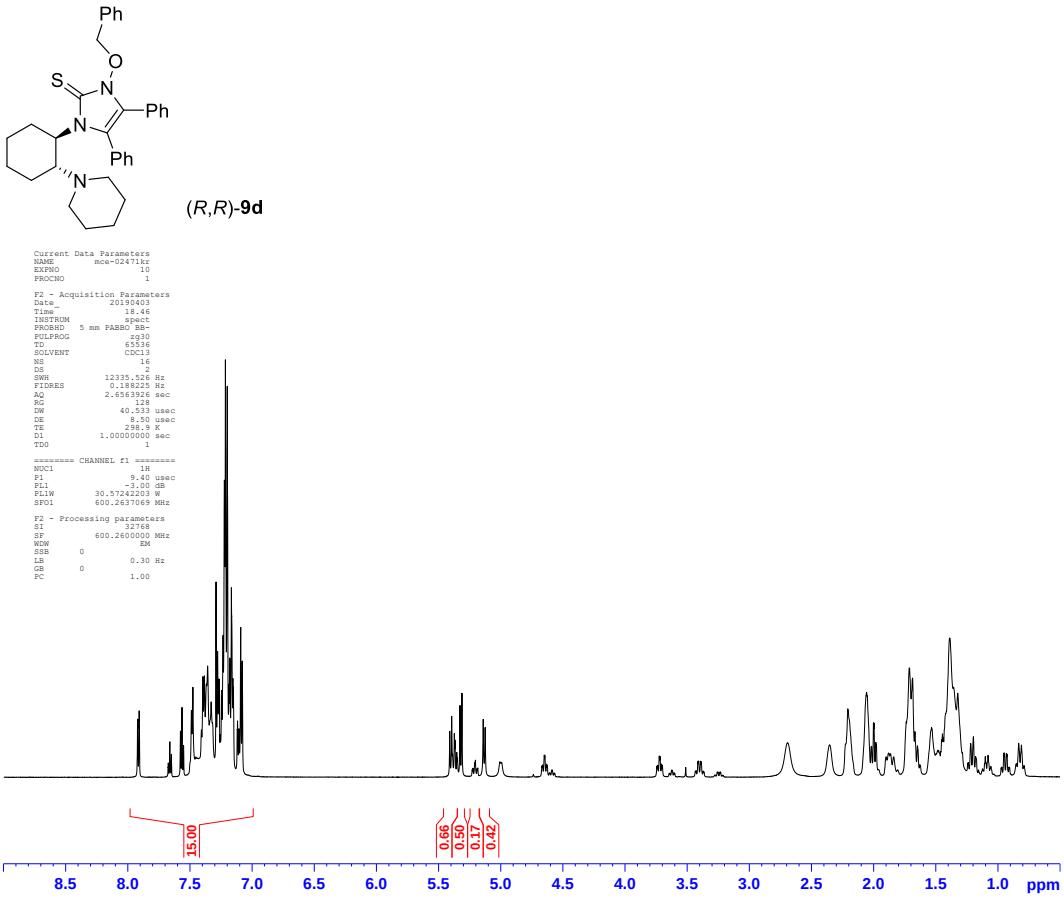


Figure S47. ^{1}H NMR of (*R*,*R*)-**9d** ($CDCl_3$, 600 MHz).

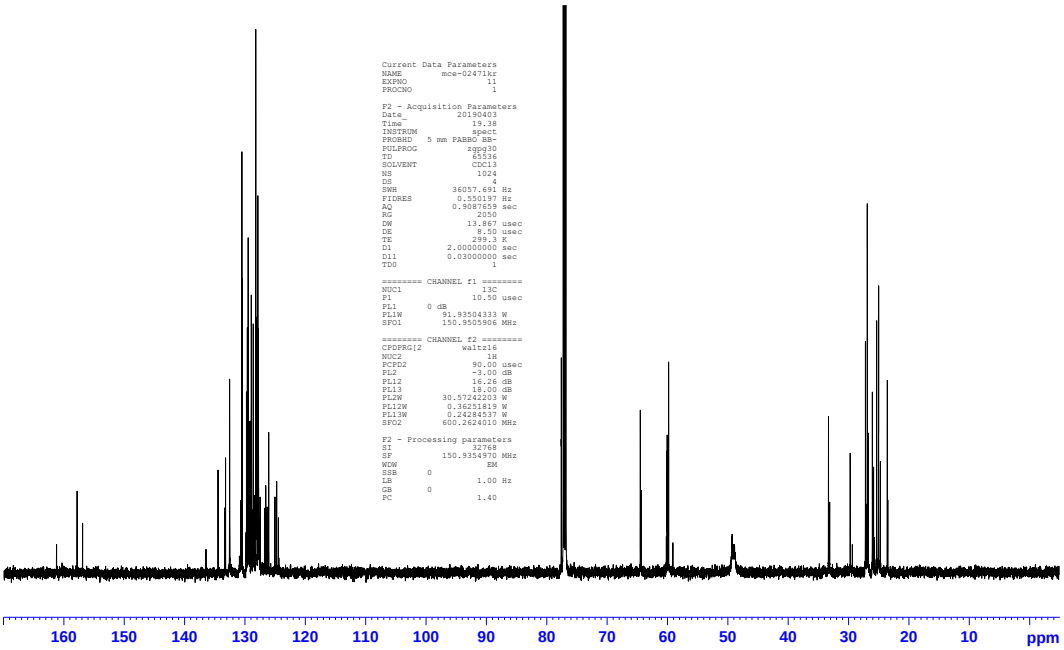
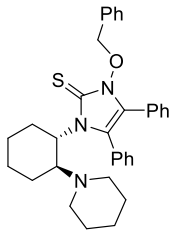


Figure S48. ^{13}C NMR of (*R*,*R*)-**9d** ($CDCl_3$, 151 MHz).



(*S*,*S*)-**9d**

mce-02503.10.fid

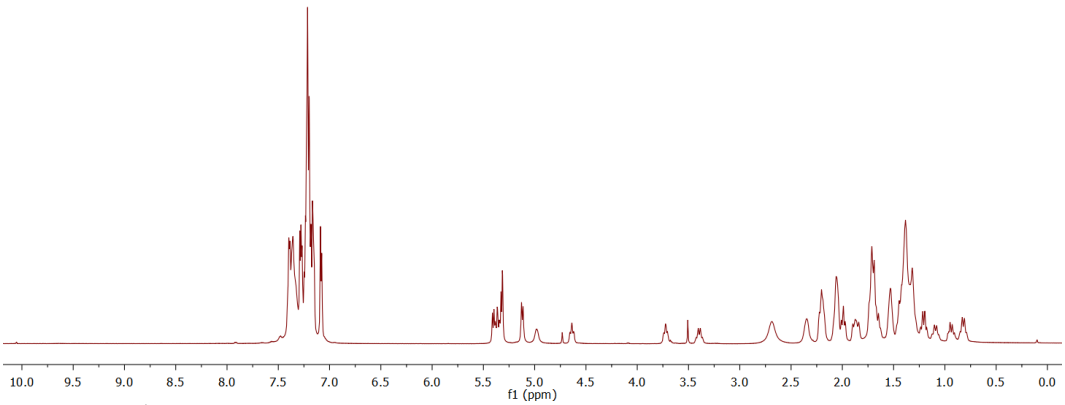


Figure S49. ^{1}H NMR of (*S*,*S*)-**9d** ($CDCl_3$, 600 MHz).

mce-02503C.1.fid
13C.stan

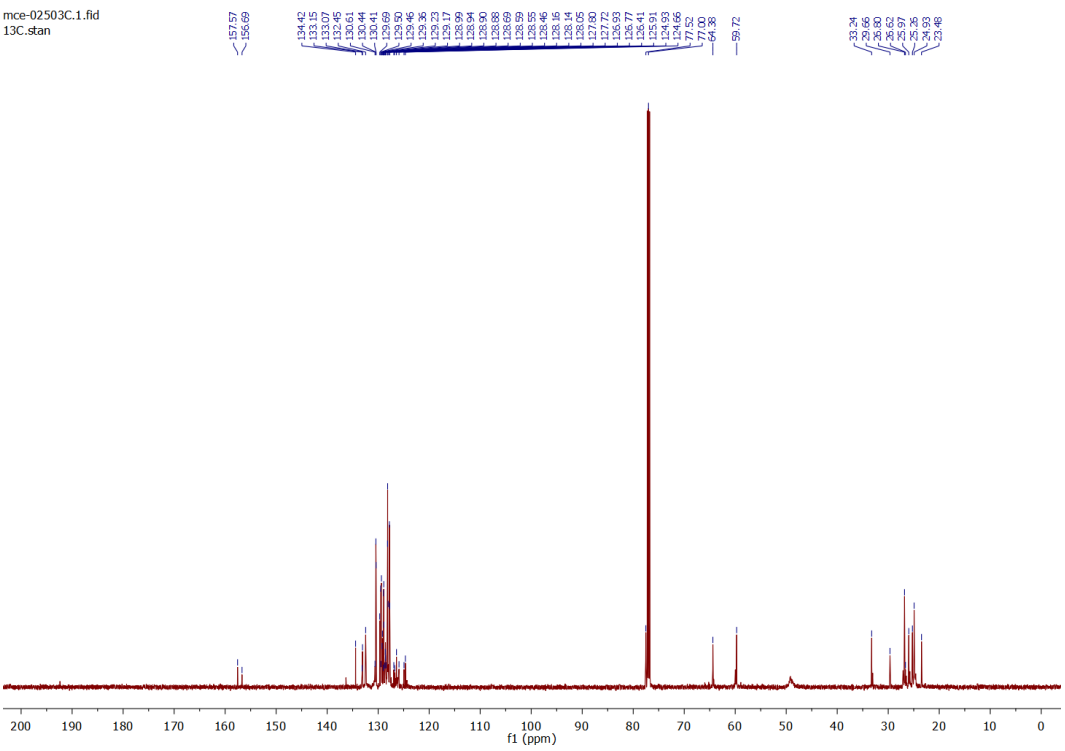
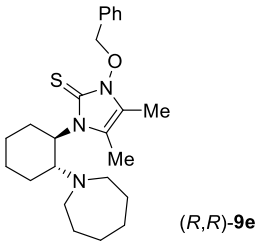


Figure S50. ^{13}C NMR of (*S*,*S*)-**9d** ($CDCl_3$, 151 MHz).



(*R*,*R*)-**9e**

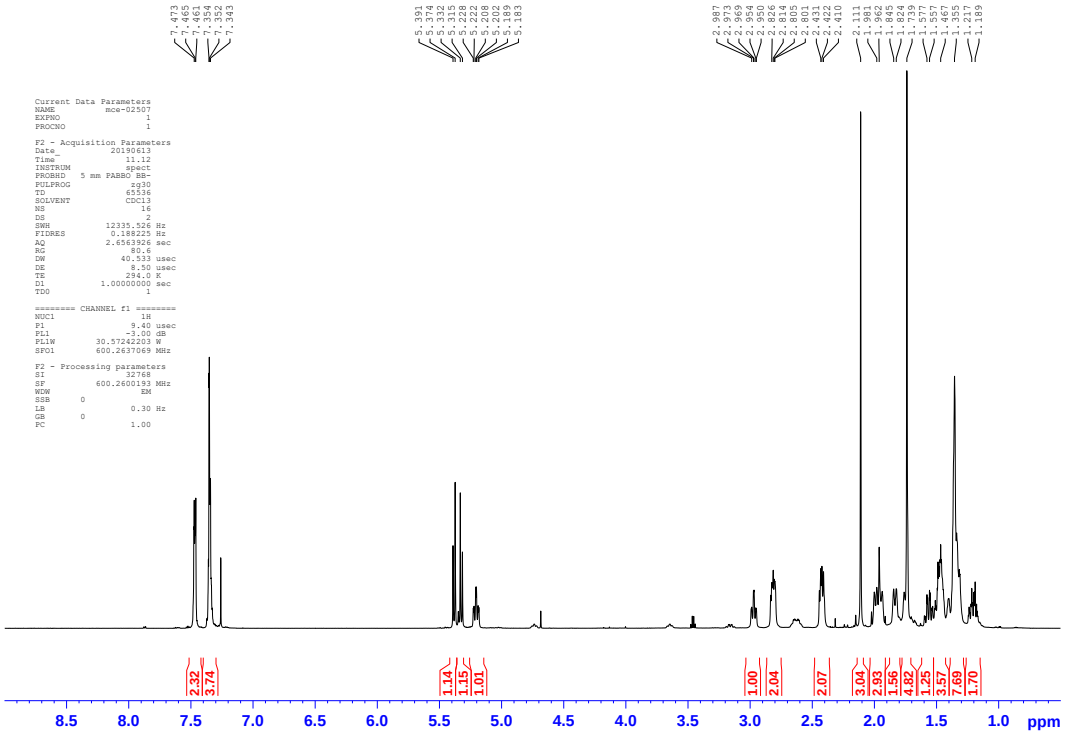


Figure S51. ^{1}H NMR of (*R*,*R*)-**9e** ($CDCl_3$, 600 MHz).

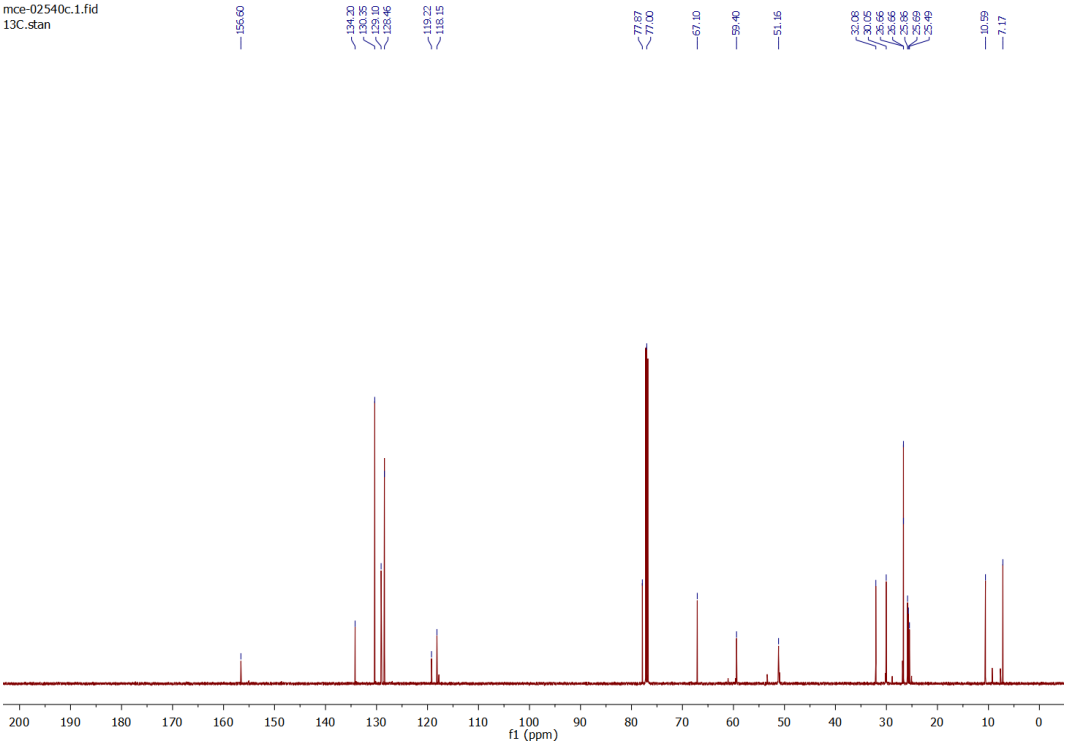


Figure S52. ^{13}C NMR of (*R*,*R*)-**9e** ($CDCl_3$, 151 MHz).

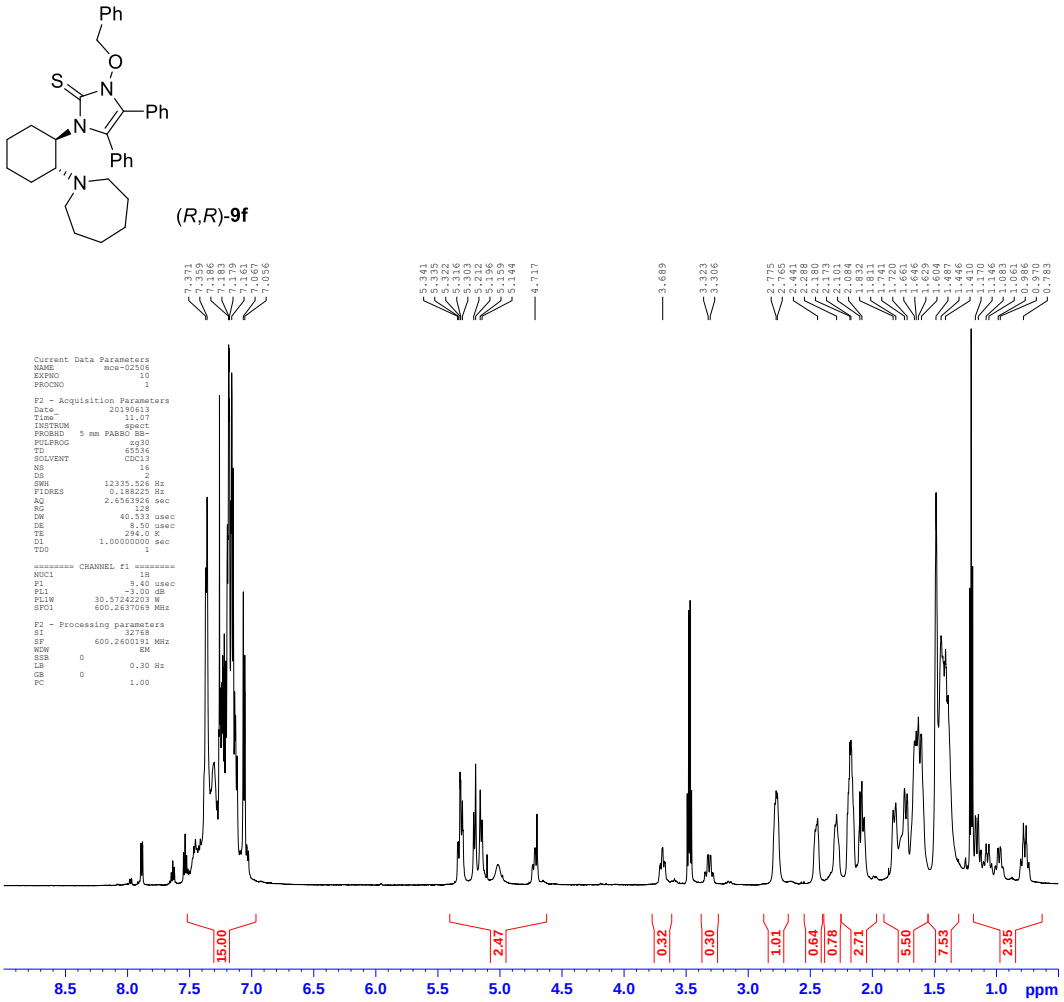


Figure S53. ^{1}H NMR of (*R*,*R*)-**9f** ($CDCl_3$, 600 MHz).

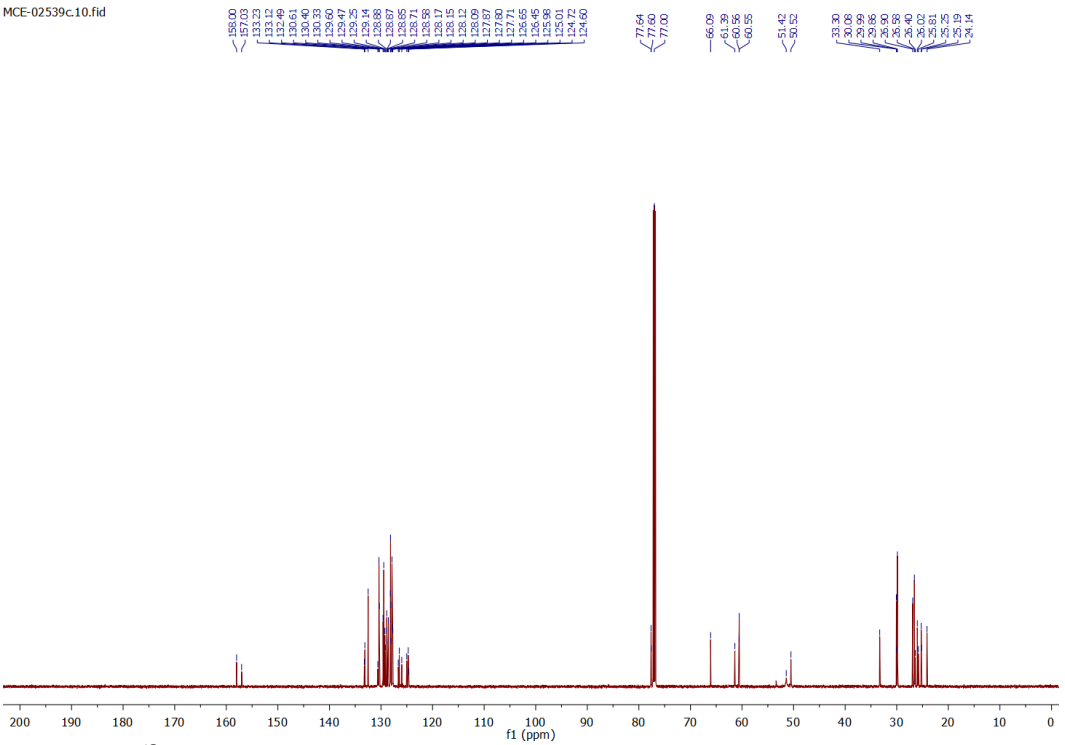
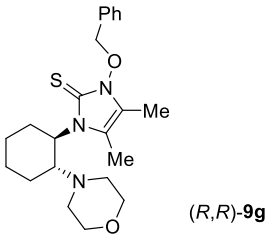


Figure S54. ^{13}C NMR of (*R*,*R*)-**9f** ($CDCl_3$, 151 MHz).



(*R*,*R*)-**9g**

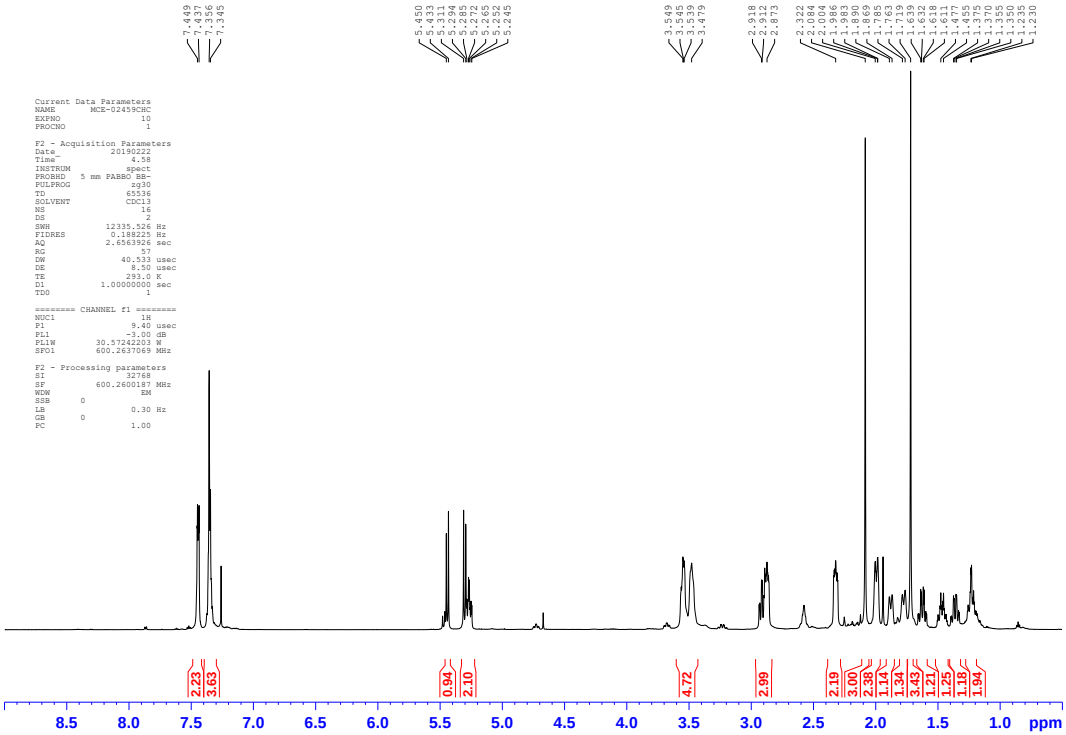


Figure S55. ^{1}H NMR of (*R*,*R*)-**9g** ($CDCl_3$, 600 MHz).

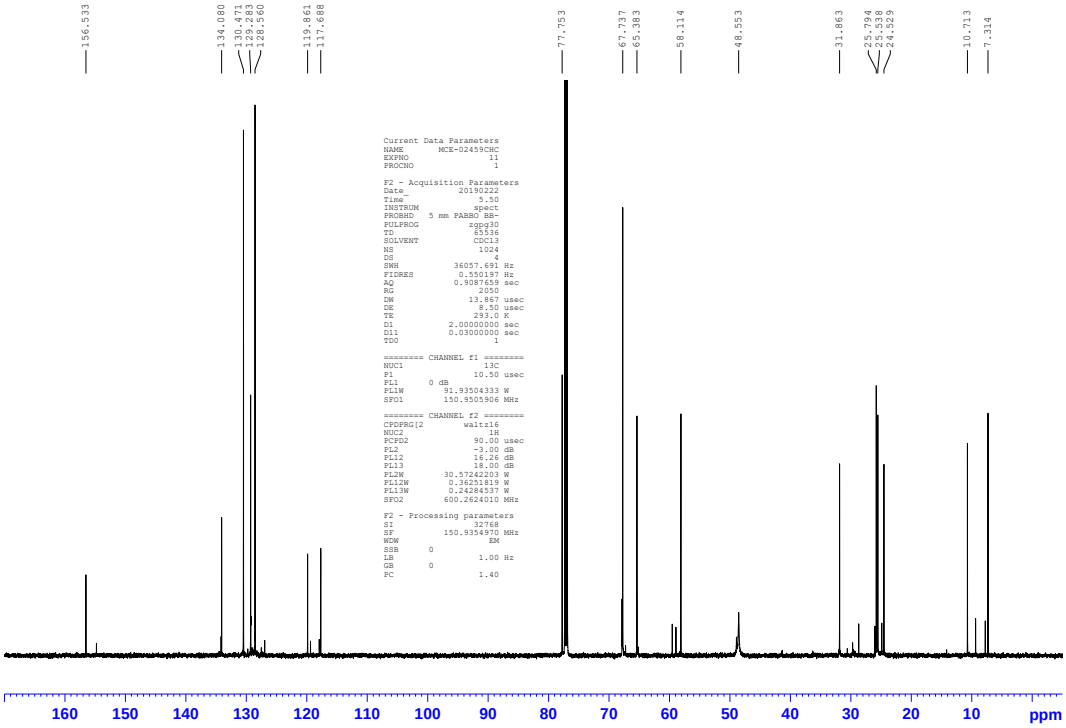


Figure S56. ^{13}C NMR of (*R*,*R*)-**9g** ($CDCl_3$, 151 MHz).

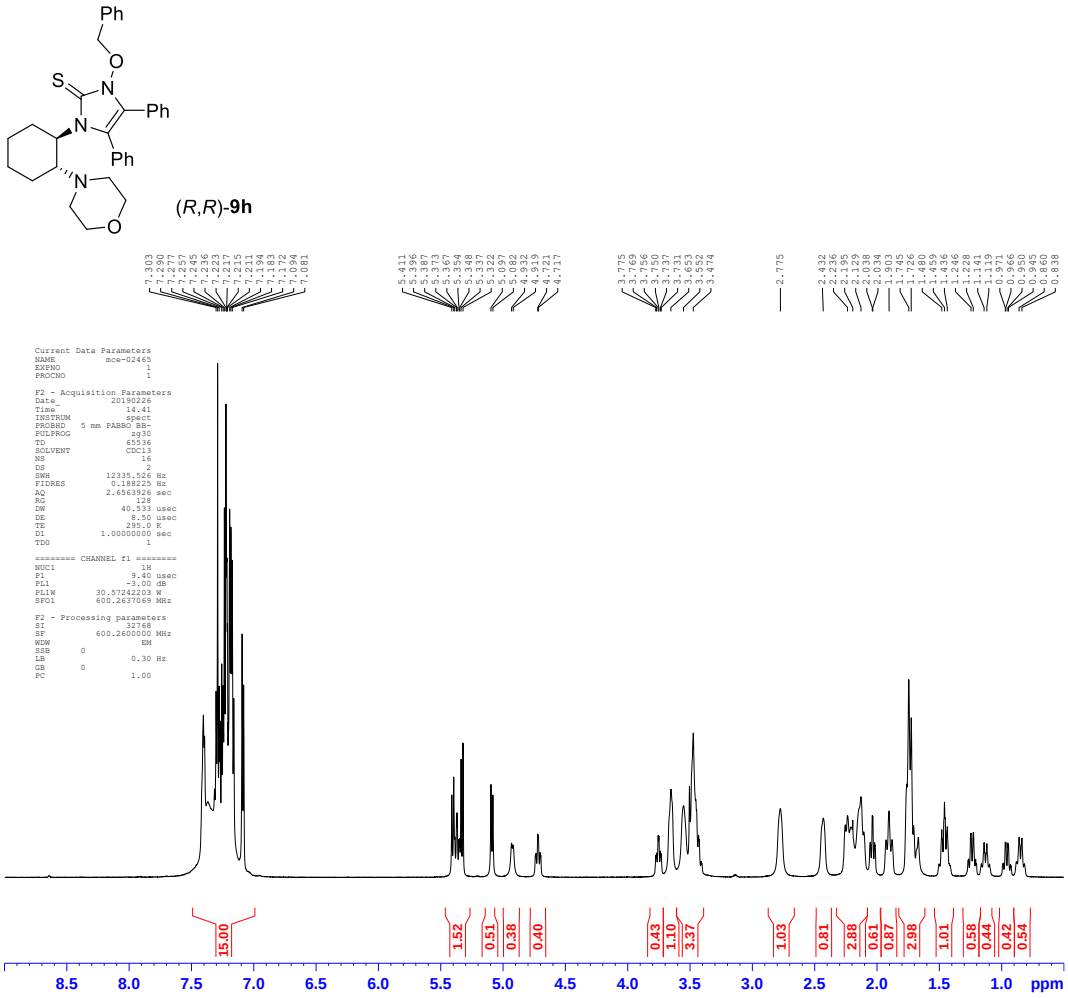


Figure S57. ^{1}H NMR of (*R*,*R*)-**9h** ($CDCl_3$, 600 MHz).

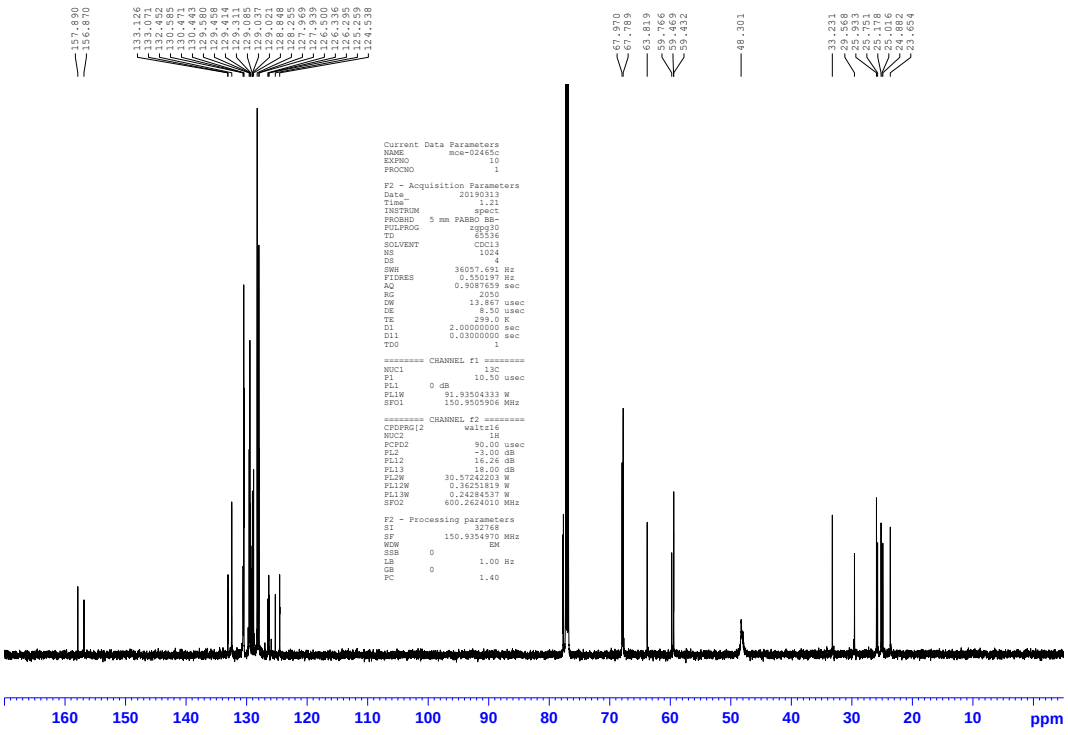
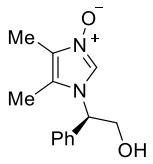


Figure S58. ^{13}C NMR of (*R*,*R*)-**9h** ($CDCl_3$, 151 MHz).



10b

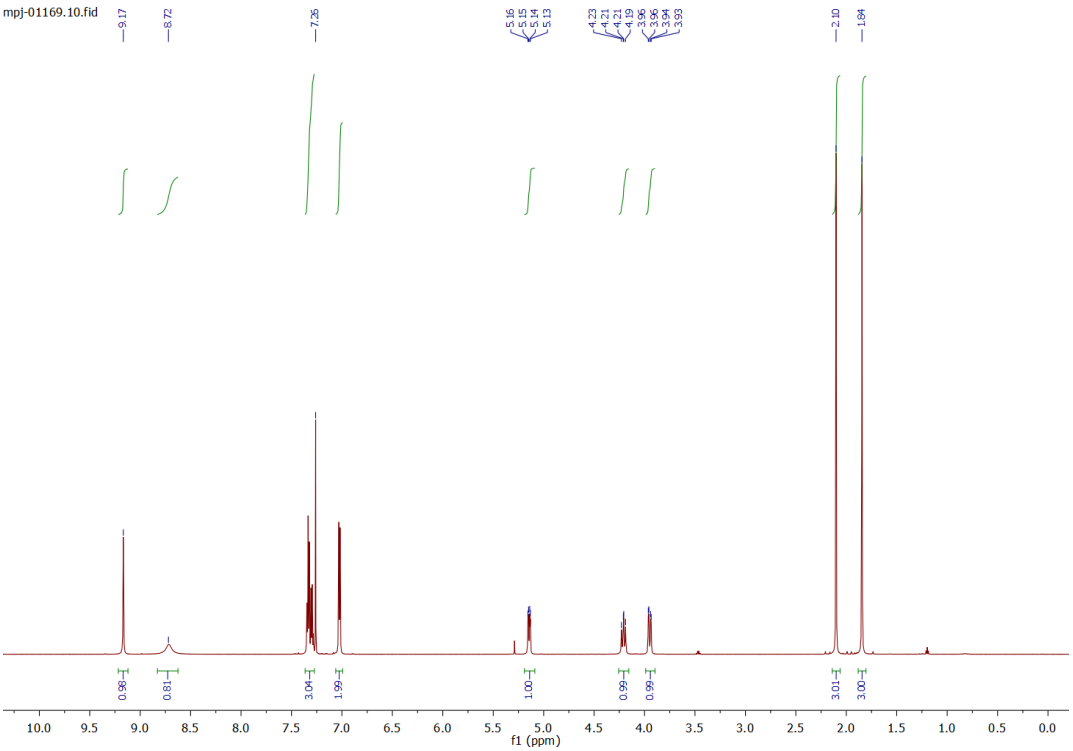


Figure S59. ^{1}H NMR of **10b** ($CDCl_3$, 600 MHz).

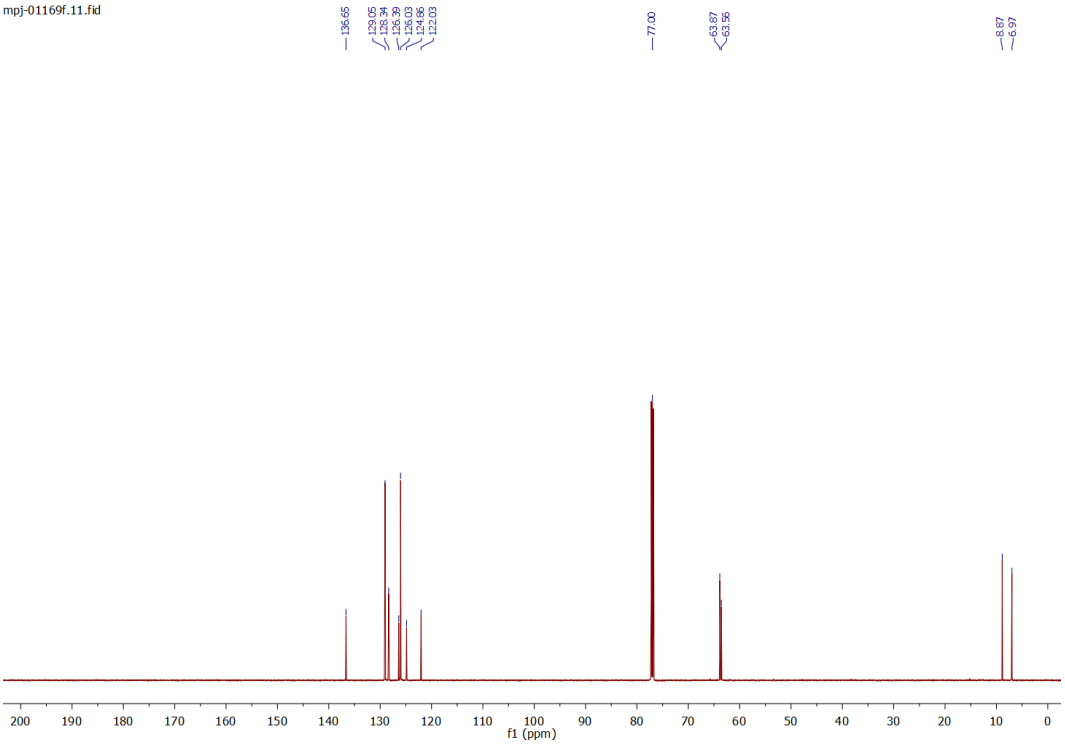
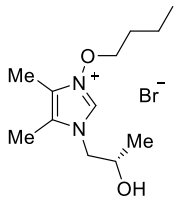


Figure S60. ^{13}C NMR of **10b** ($CDCl_3$, 151 MHz).



11a

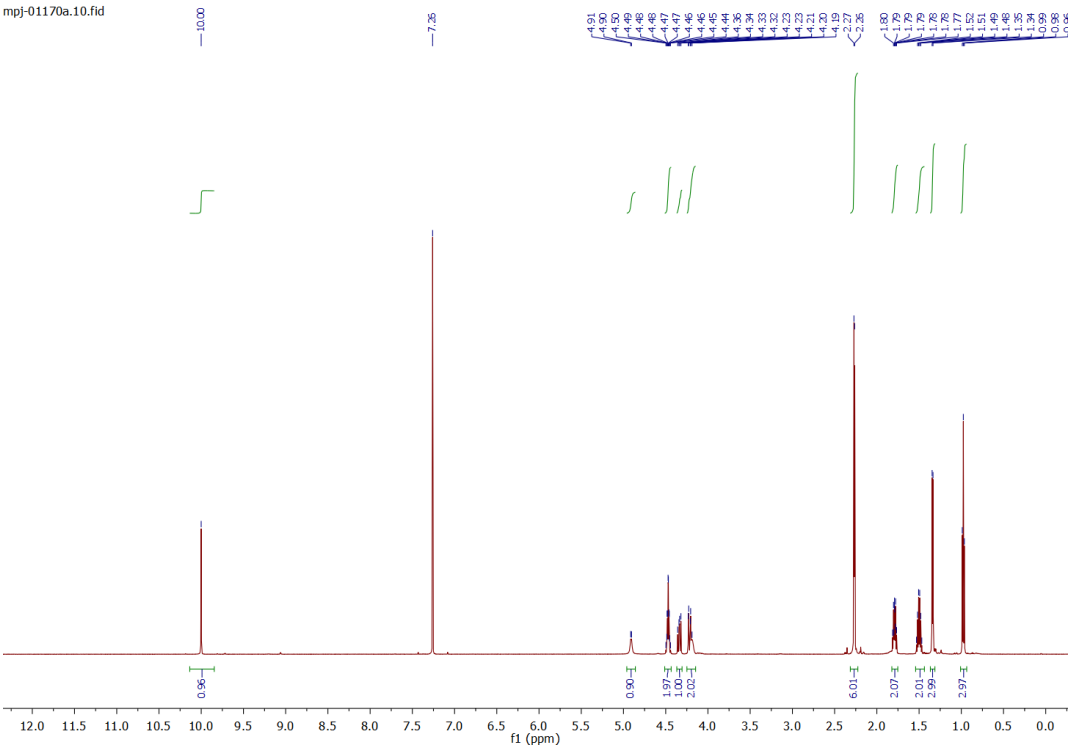


Figure S61. ^{1}H NMR of **11a** ($CDCl_3$, 600 MHz).

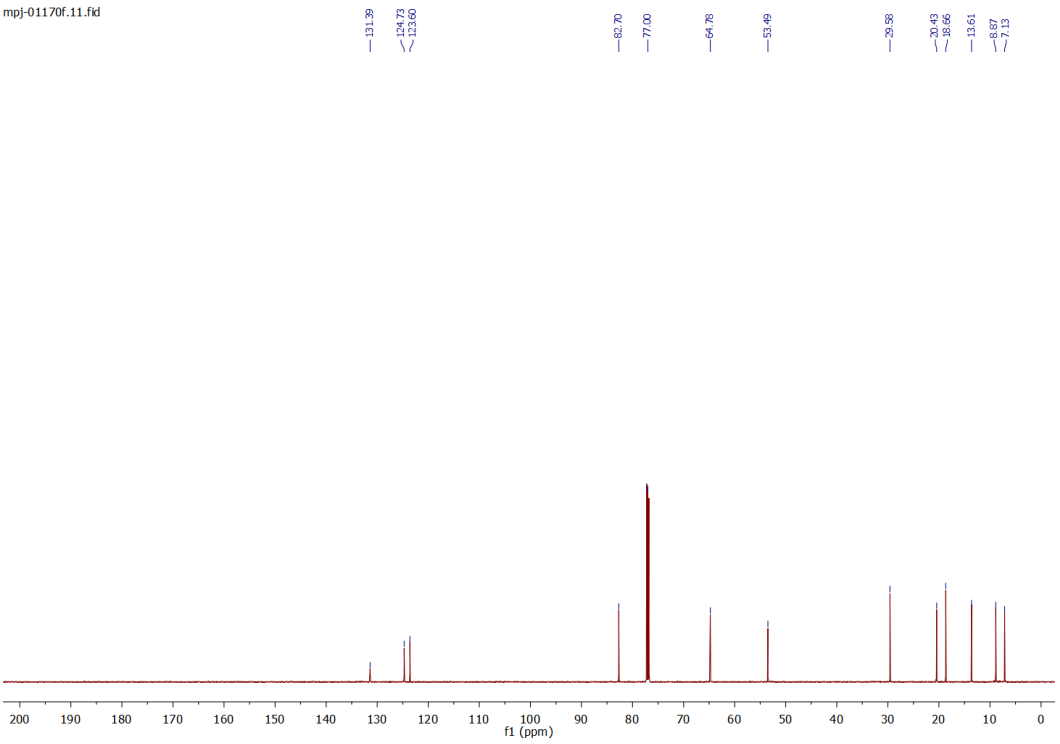
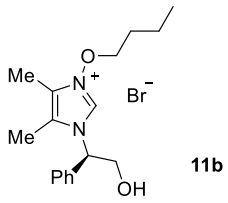


Figure S62. ^{13}C NMR of **11a** ($CDCl_3$, 151 MHz).



11b

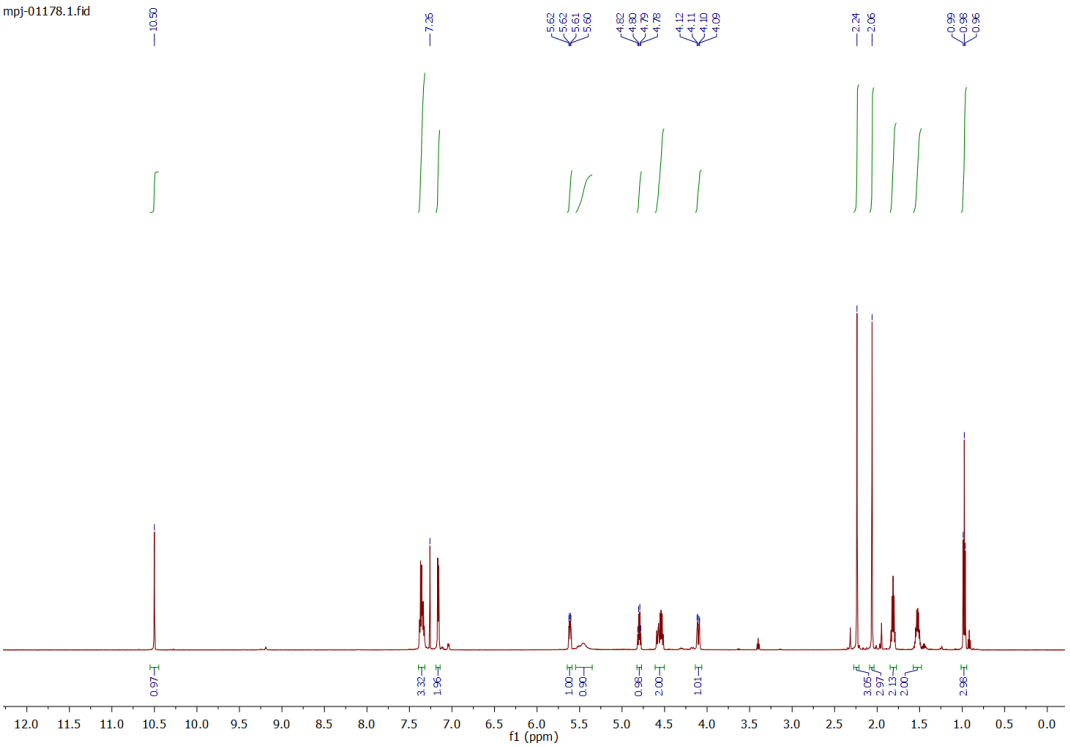


Figure S63. ^{1}H NMR of **11b** ($CDCl_3$, 600 MHz).

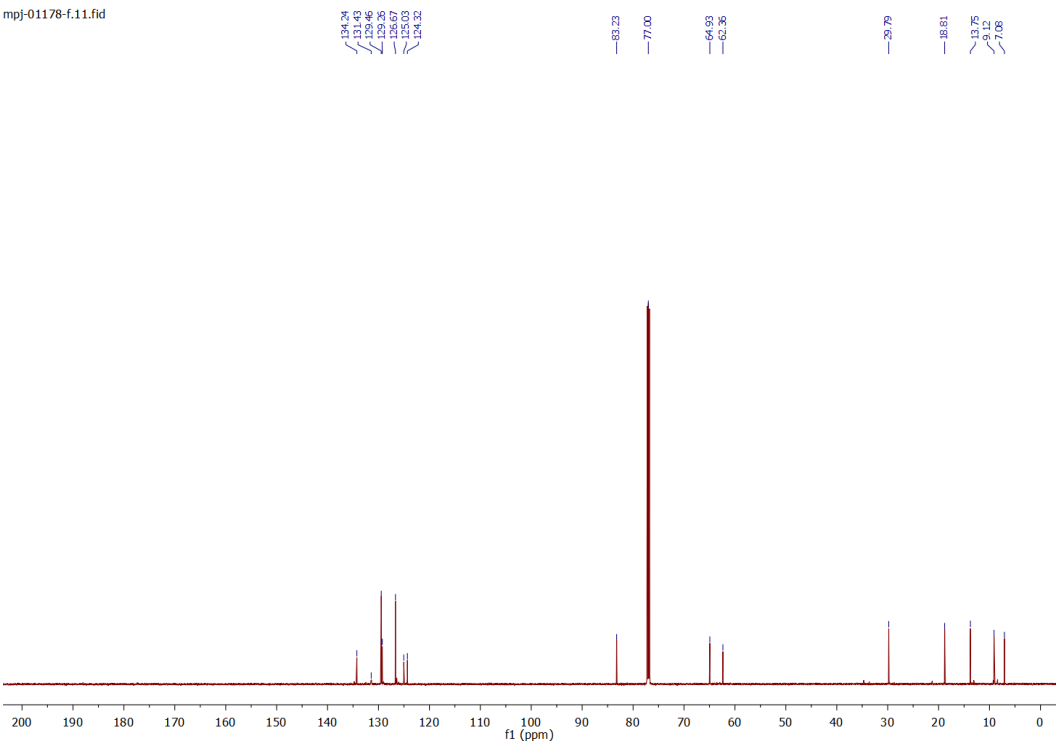
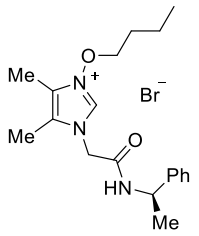


Figure S64. ^{13}C NMR of **11b** ($CDCl_3$, 151 MHz).



11d

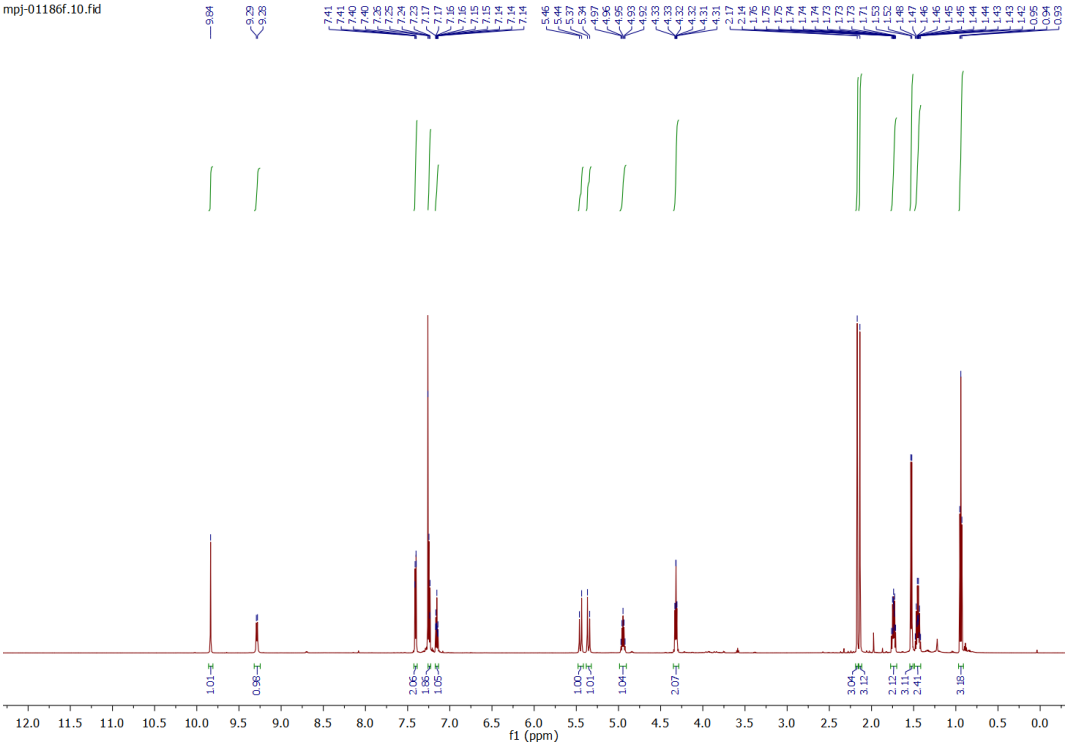


Figure S65. ^{1}H NMR of **11d** ($CDCl_3$, 600 MHz).

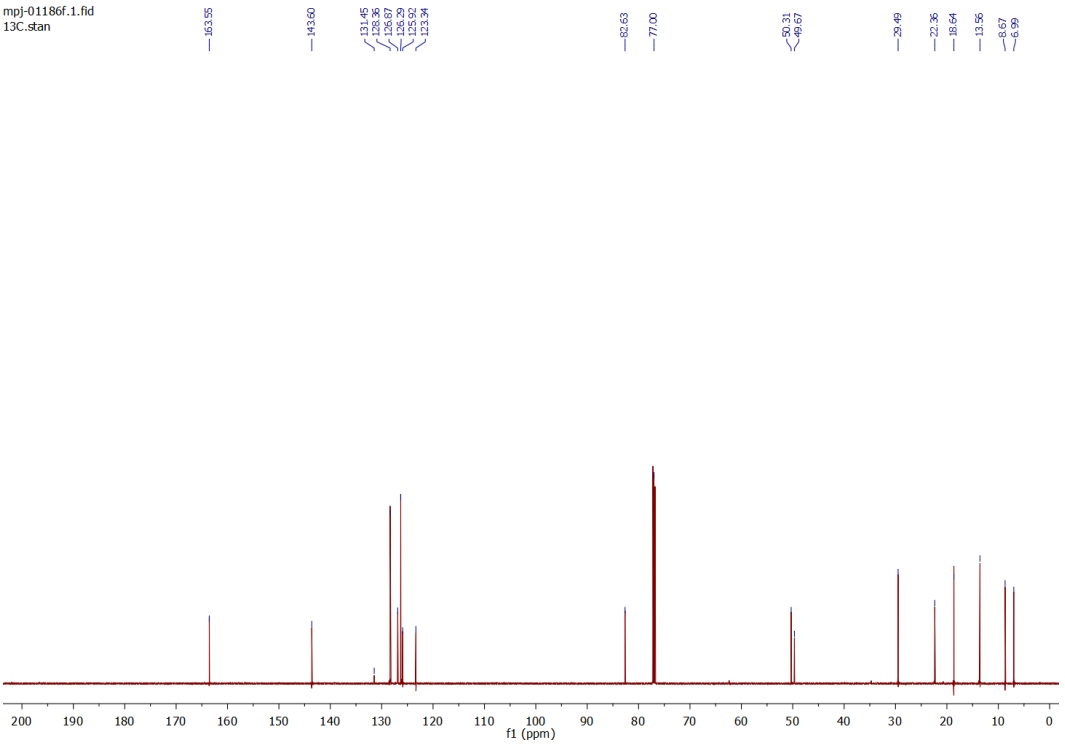
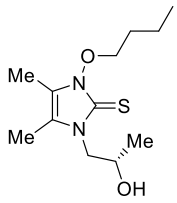


Figure S66. ^{13}C NMR of **11d** ($CDCl_3$, 151 MHz).



13a

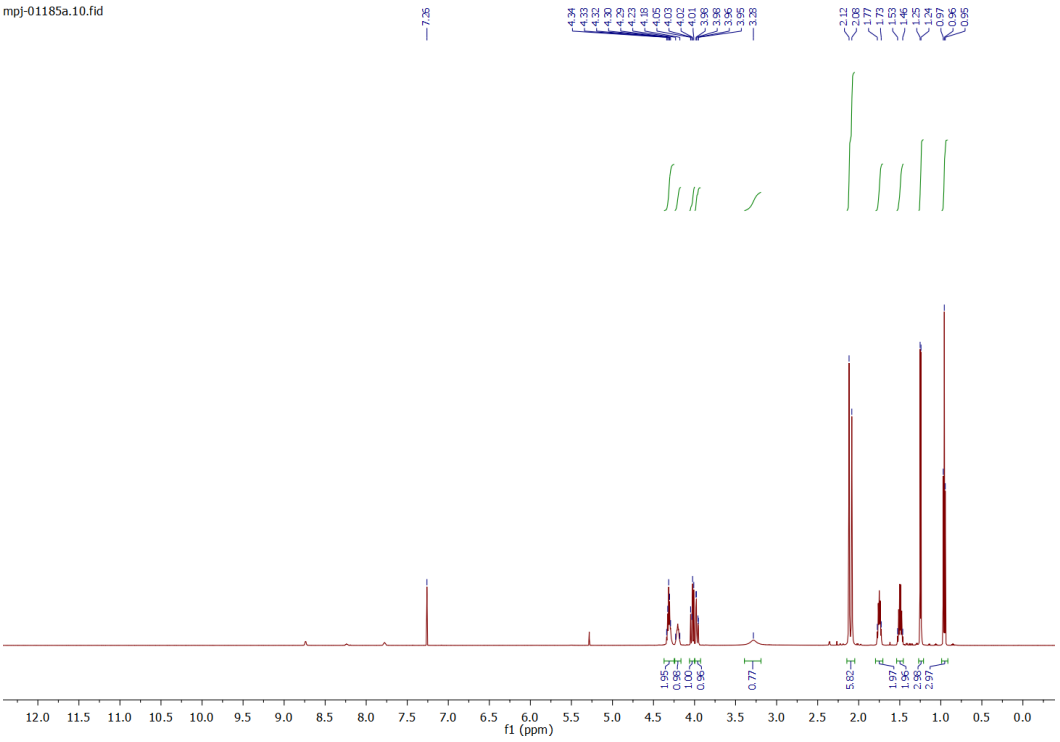


Figure S67. ^{1}H NMR of **13a** ($CDCl_3$, 600 MHz).

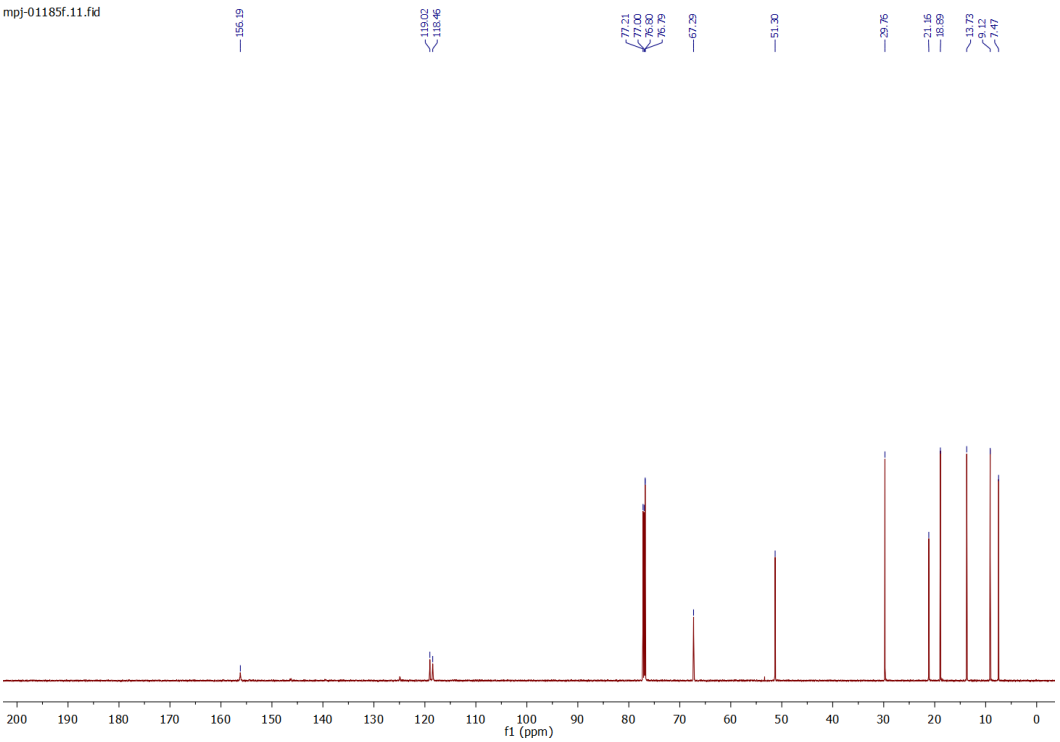
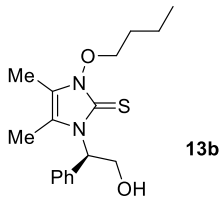


Figure S68. ^{13}C NMR of **13a** ($CDCl_3$, 151 MHz).



13b

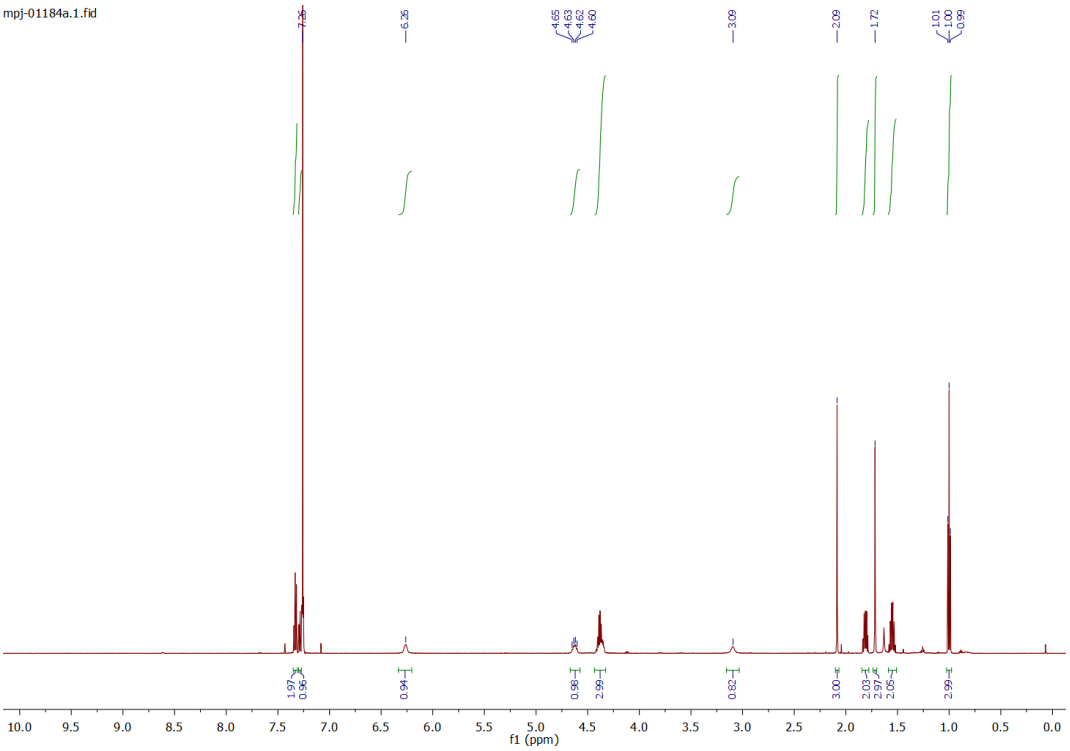


Figure S69. ^{1}H NMR of **13b** ($CDCl_3$, 600 MHz).

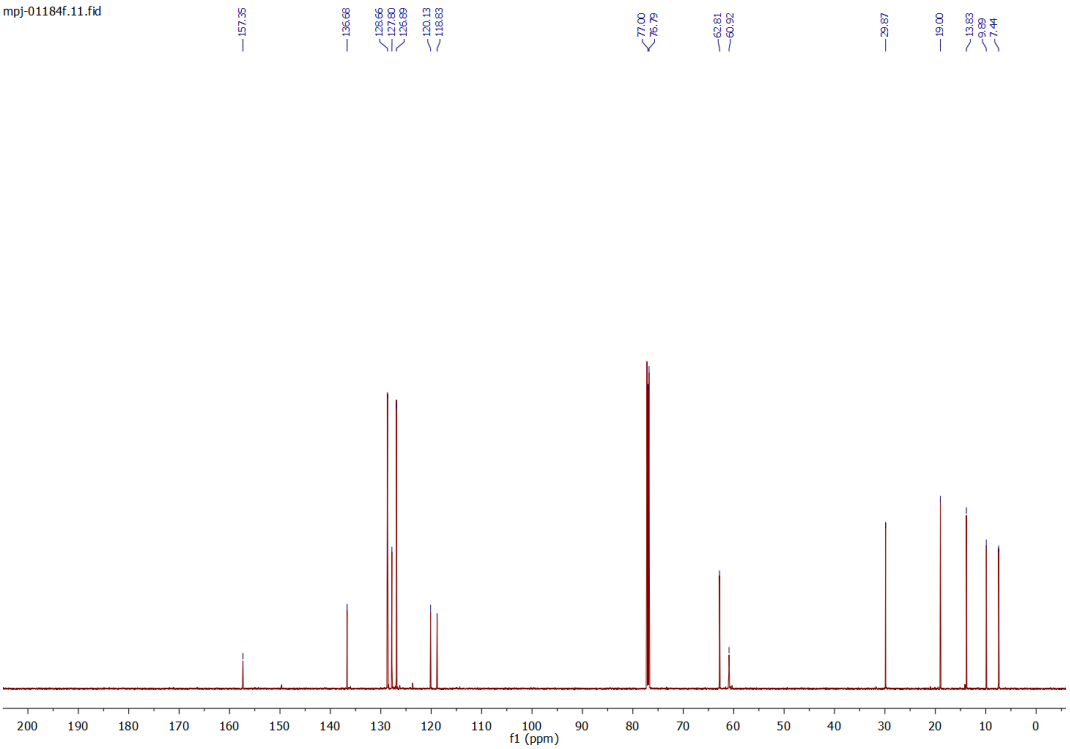
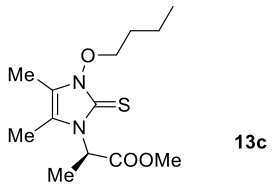


Figure S70. ^{13}C NMR of **13b** ($CDCl_3$, 151 MHz).



13c

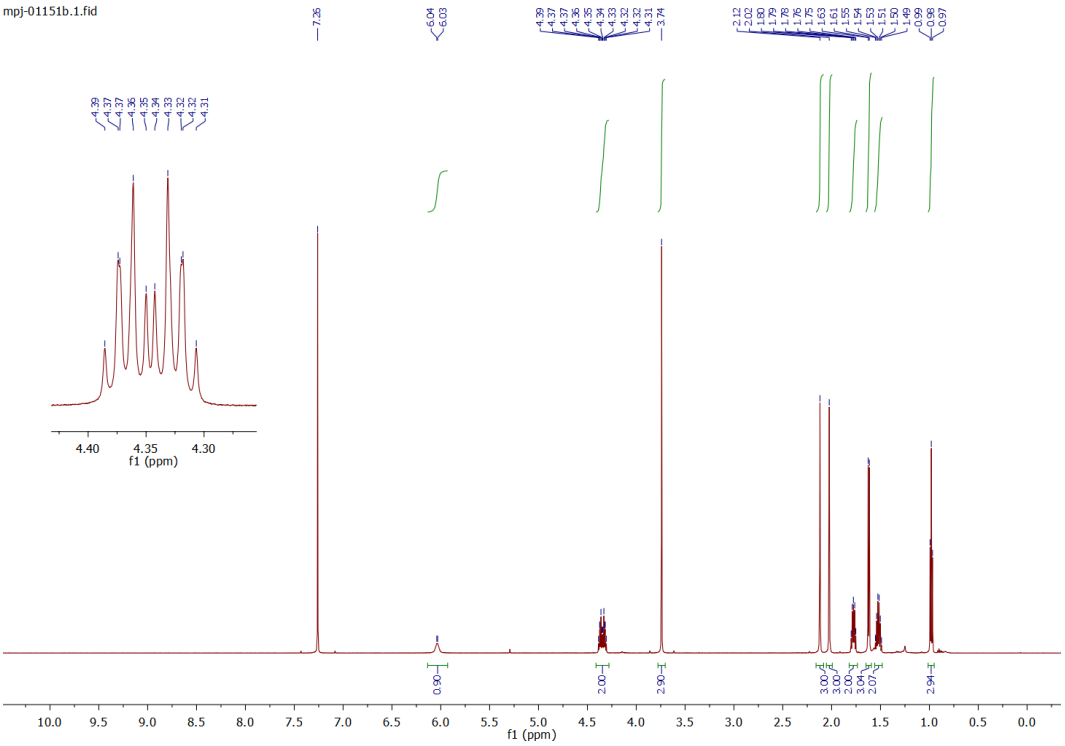


Figure S71. ^{1}H NMR of **13c** ($CDCl_3$, 600 MHz).

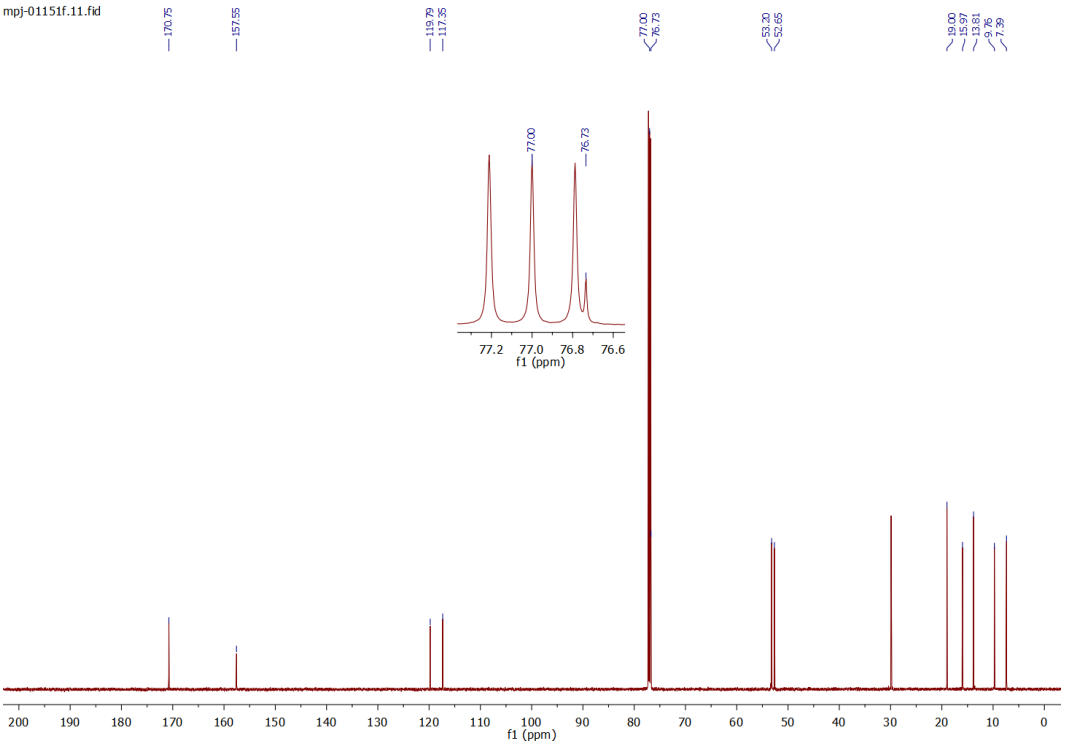


Figure S72. ^{13}C NMR of **13c** ($CDCl_3$, 151 MHz).

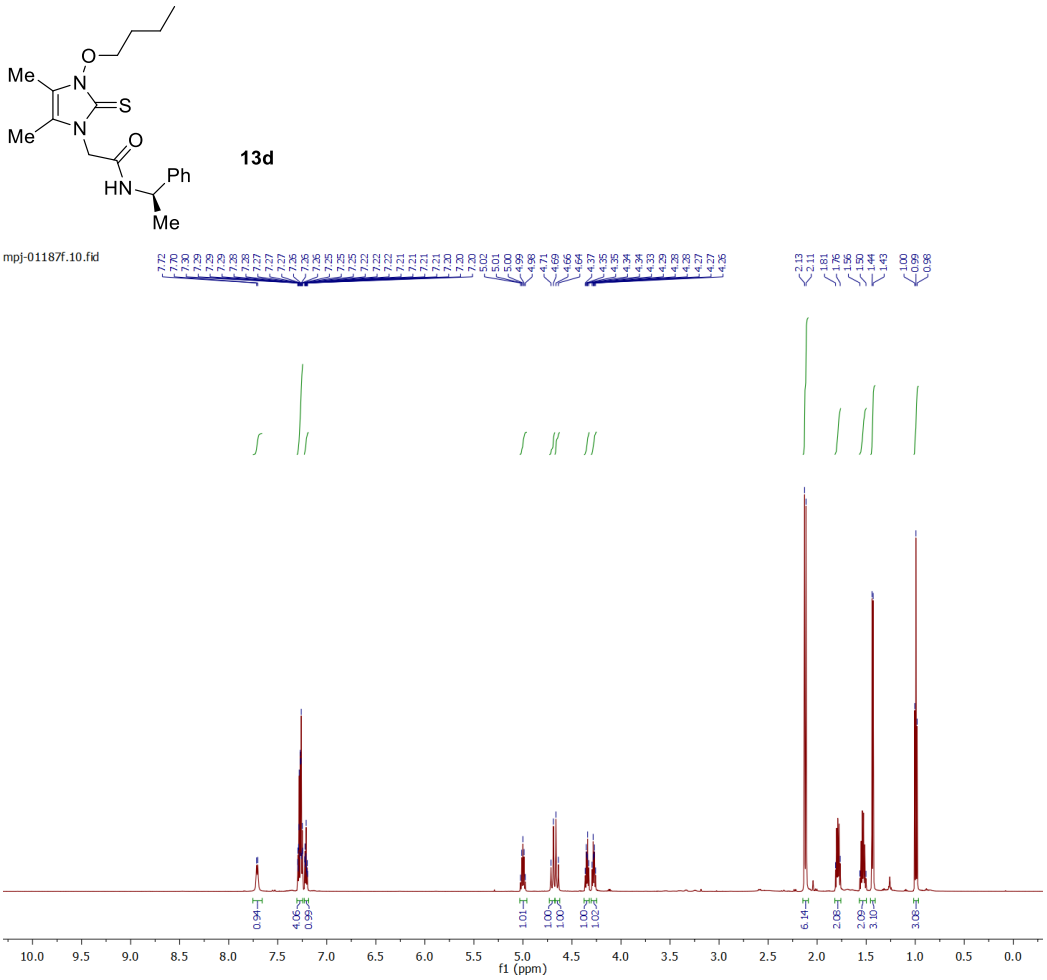


Figure S73. ^{1}H NMR of **13d** ($CDCl_3$, 600 MHz).

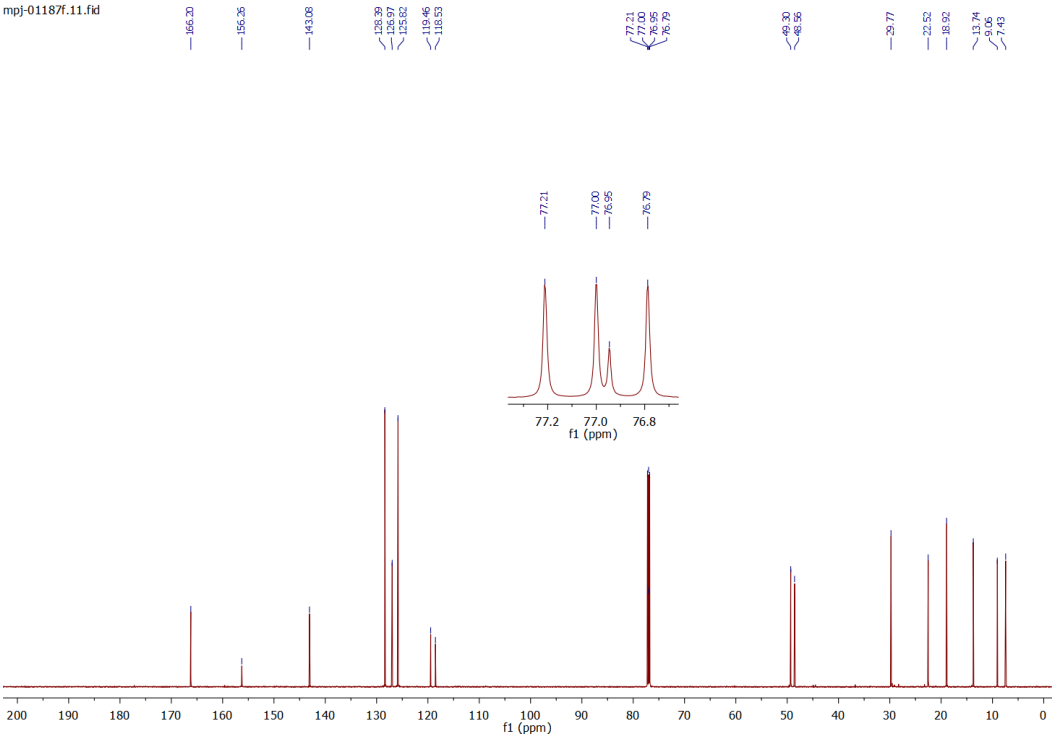


Figure S74. ^{13}C NMR of **13d** ($CDCl_3$, 151 MHz).

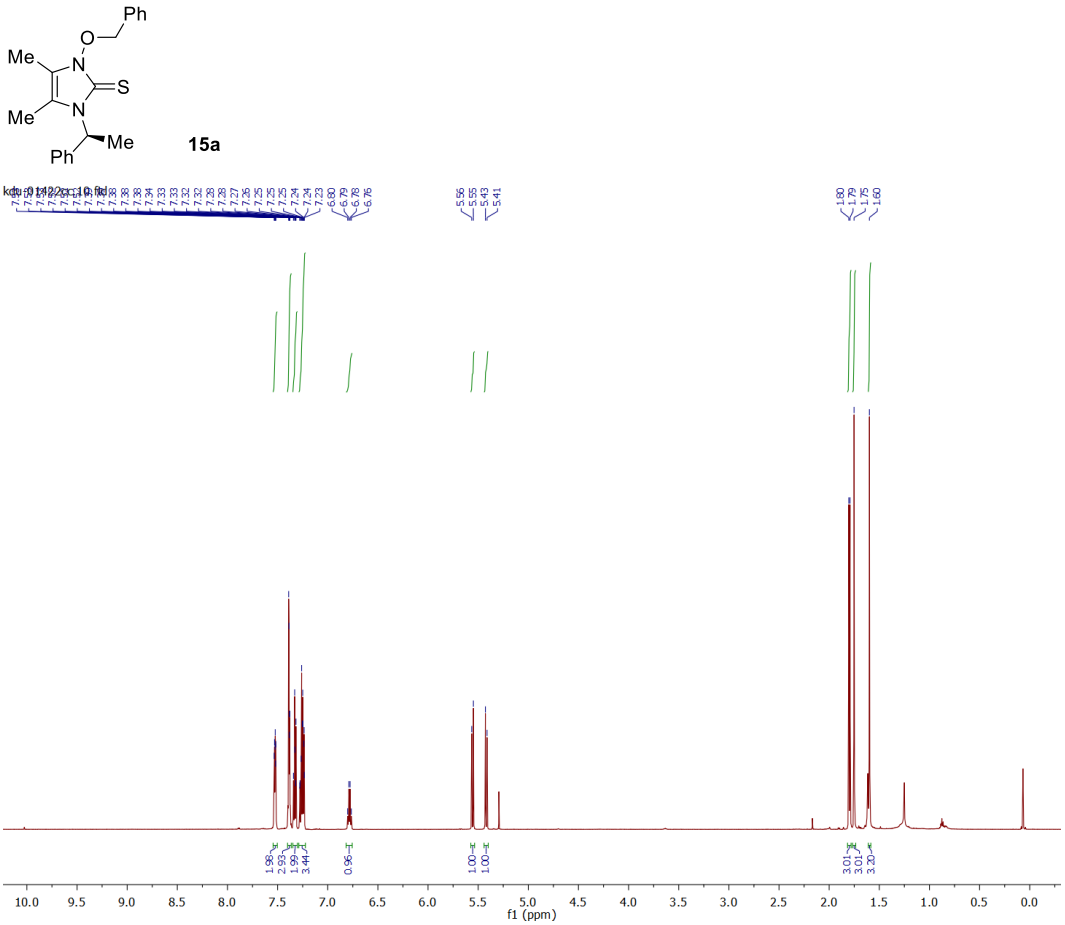


Figure S75. ^{1}H NMR of **15a** ($CDCl_3$, 600 MHz).

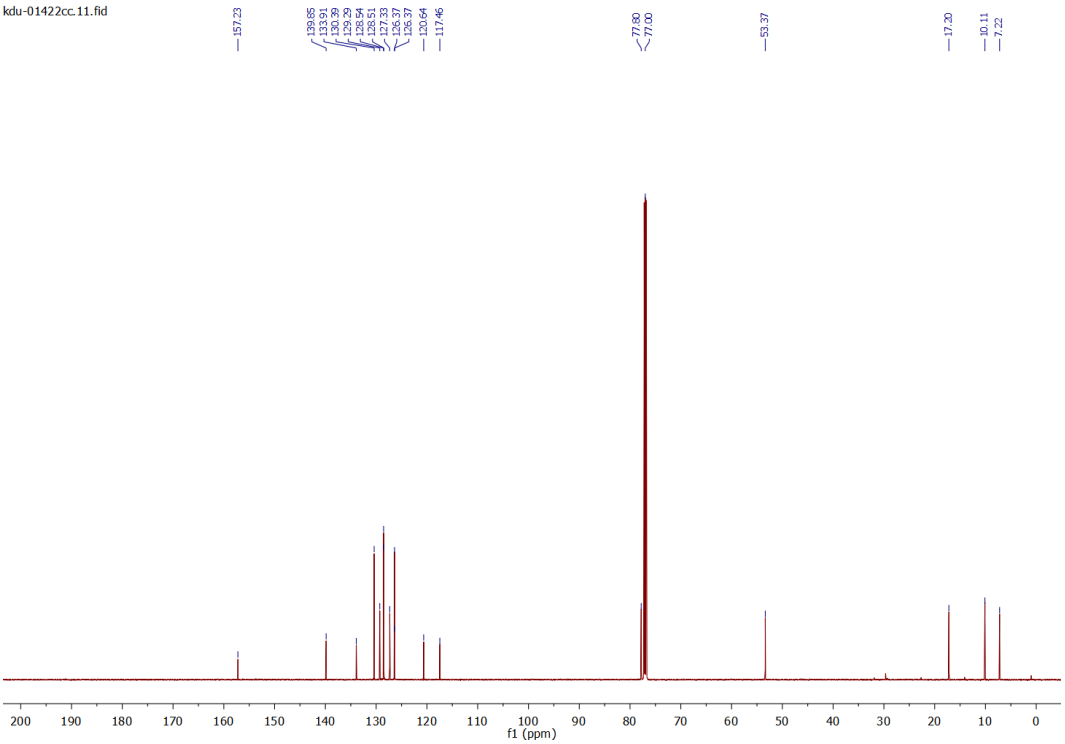


Figure S76. ^{13}C NMR of **15a** ($CDCl_3$, 151 MHz).

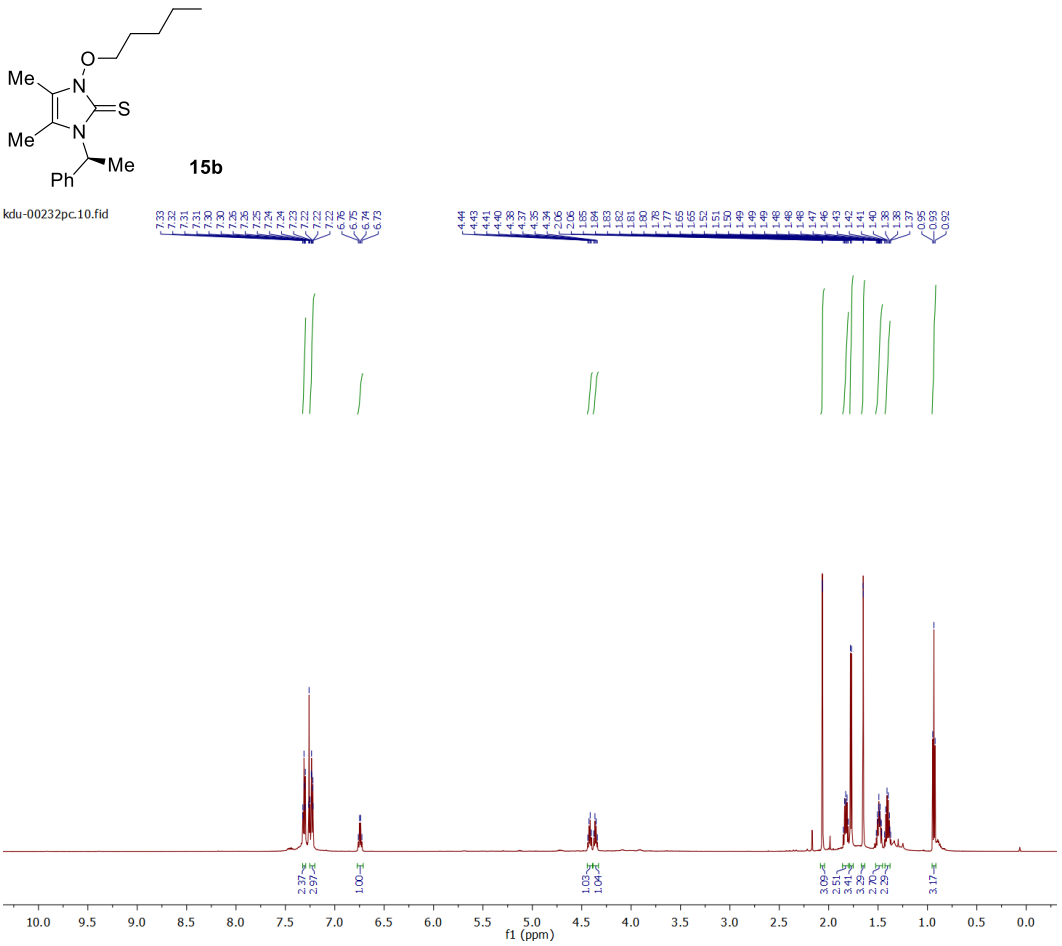


Figure S77. ^{1}H NMR of **15b** ($CDCl_3$, 600 MHz).

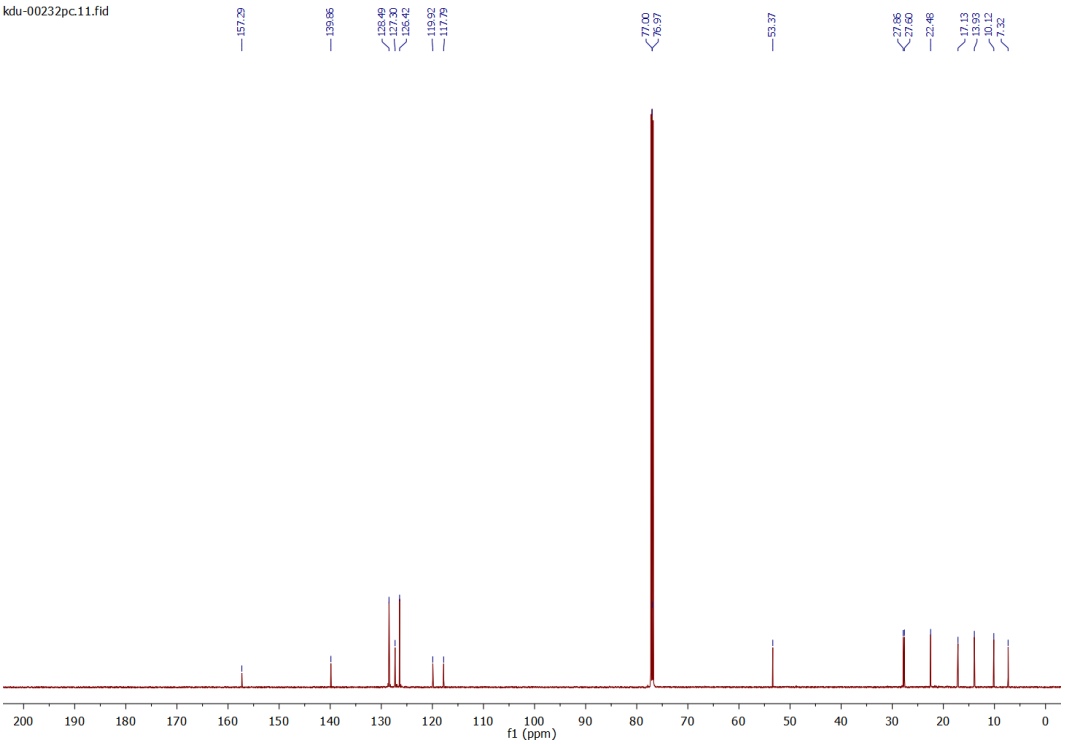
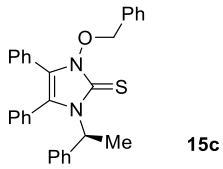


Figure S78. ^{13}C NMR of **15b** ($CDCl_3$, 151 MHz).



15c

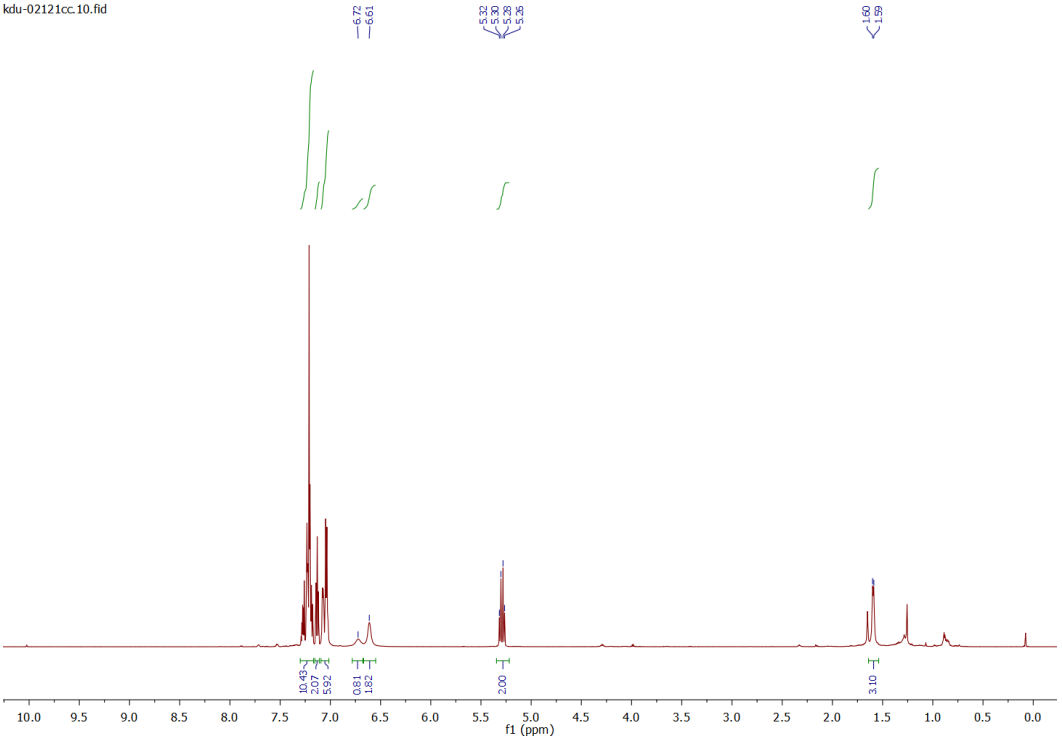


Figure S79. ^{1}H NMR of **15c** ($CDCl_3$, 600 MHz).

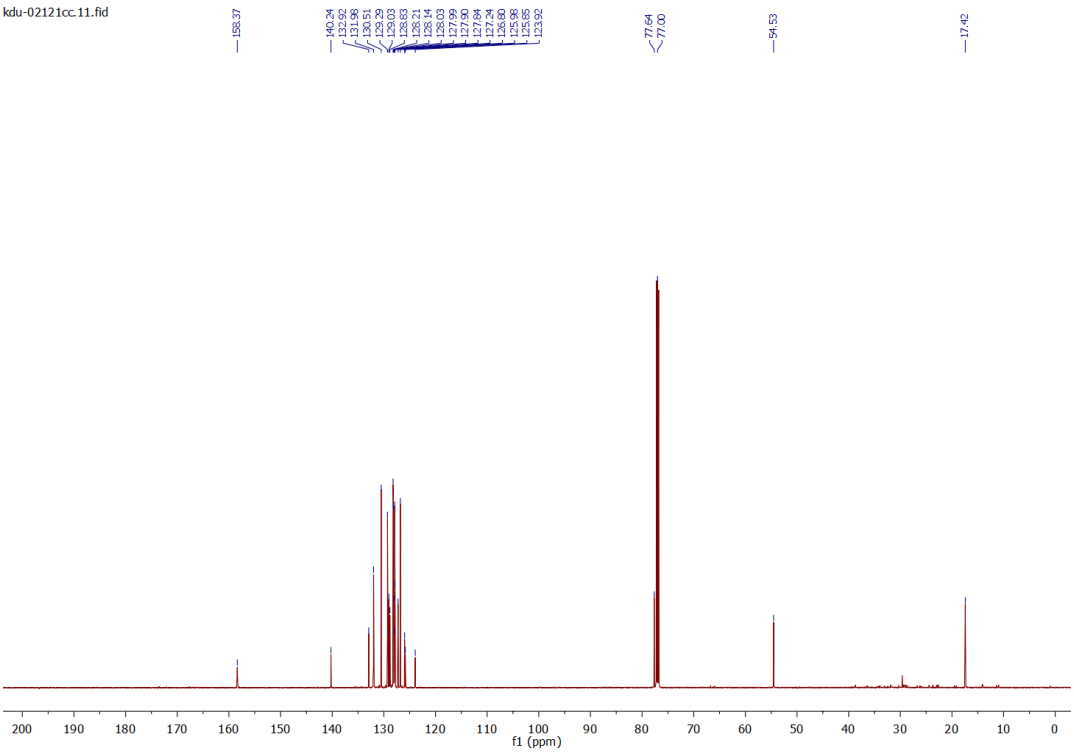


Figure S80. ^{13}C NMR of **15c** ($CDCl_3$, 151 MHz).

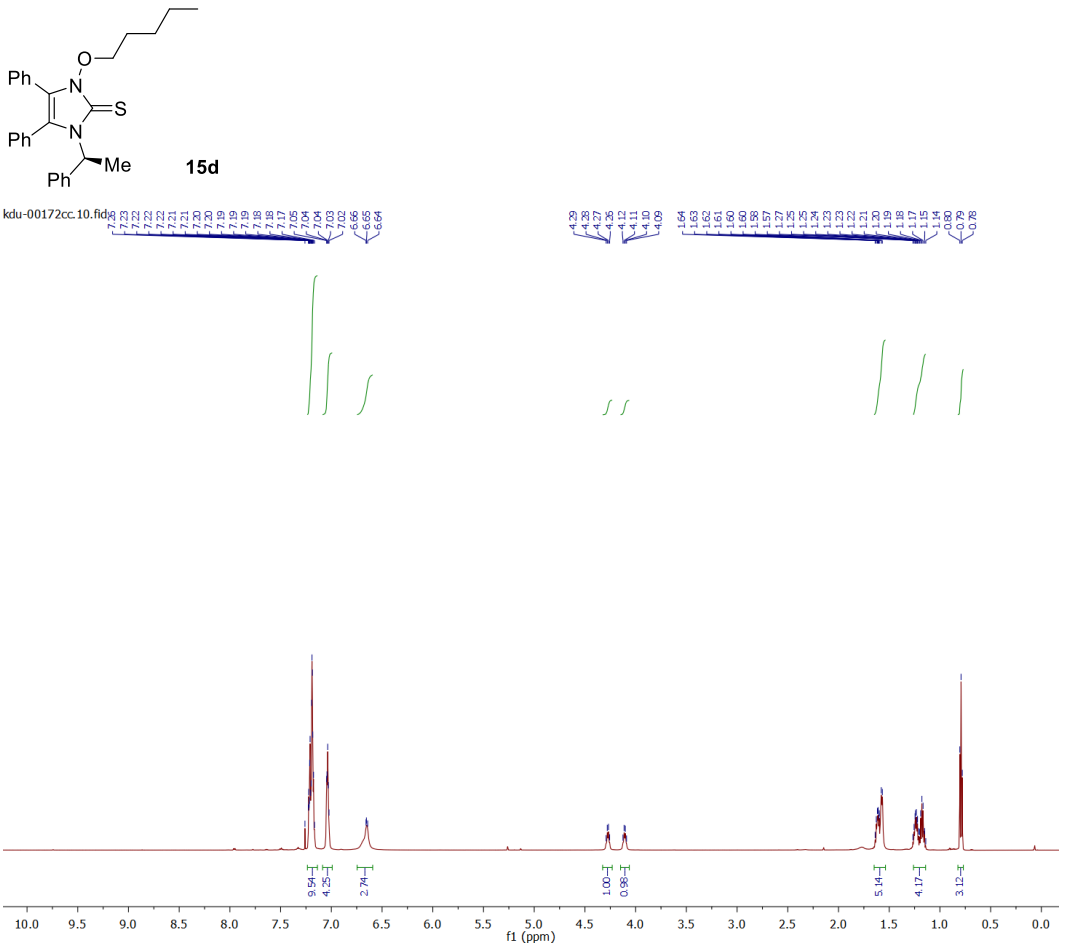


Figure S81. ^{1}H NMR of **15d** ($CDCl_3$, 600 MHz).

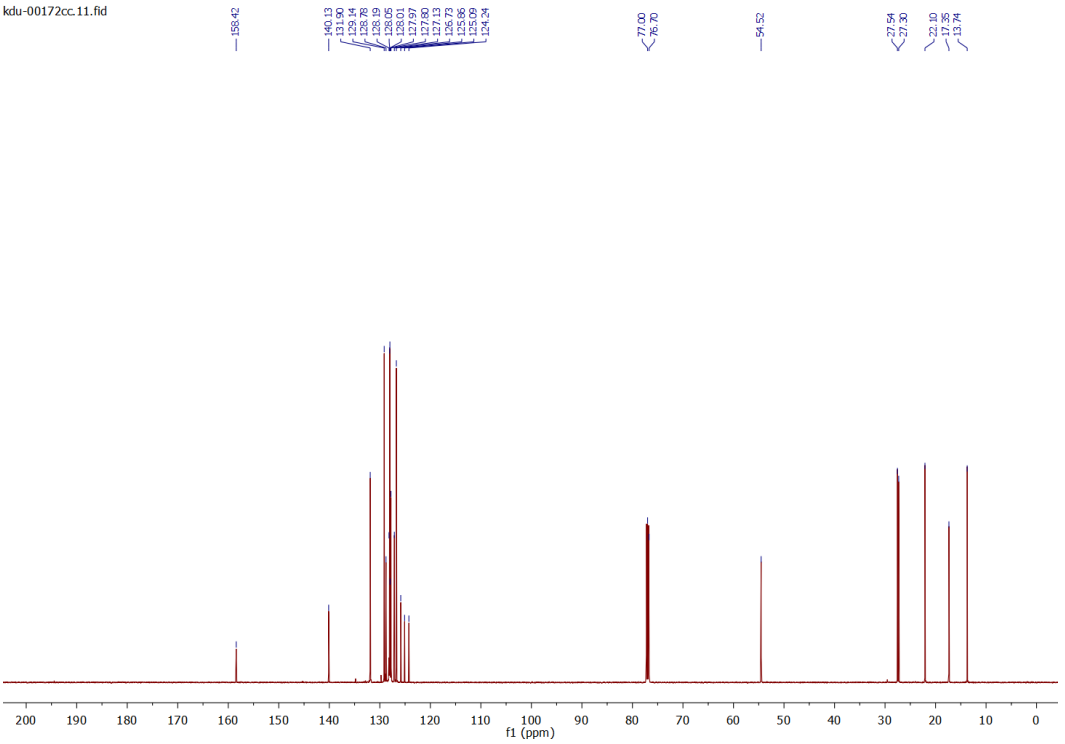


Figure S82. ^{13}C NMR of **15d** ($CDCl_3$, 151 MHz).