

Supplementary material

Article

Synthesis and anticholinesterase evaluation of cassine, spectaline and analogues

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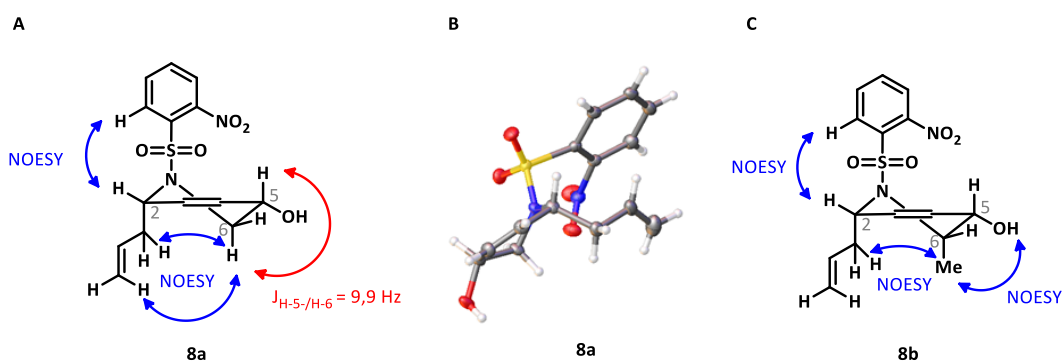


Figure S1. NOESY correlations (S1A and S1C) and coupling constants (S1A) observed by ^1H RMN spectroscopy. B: Crystal structure of intermediate **8a**.

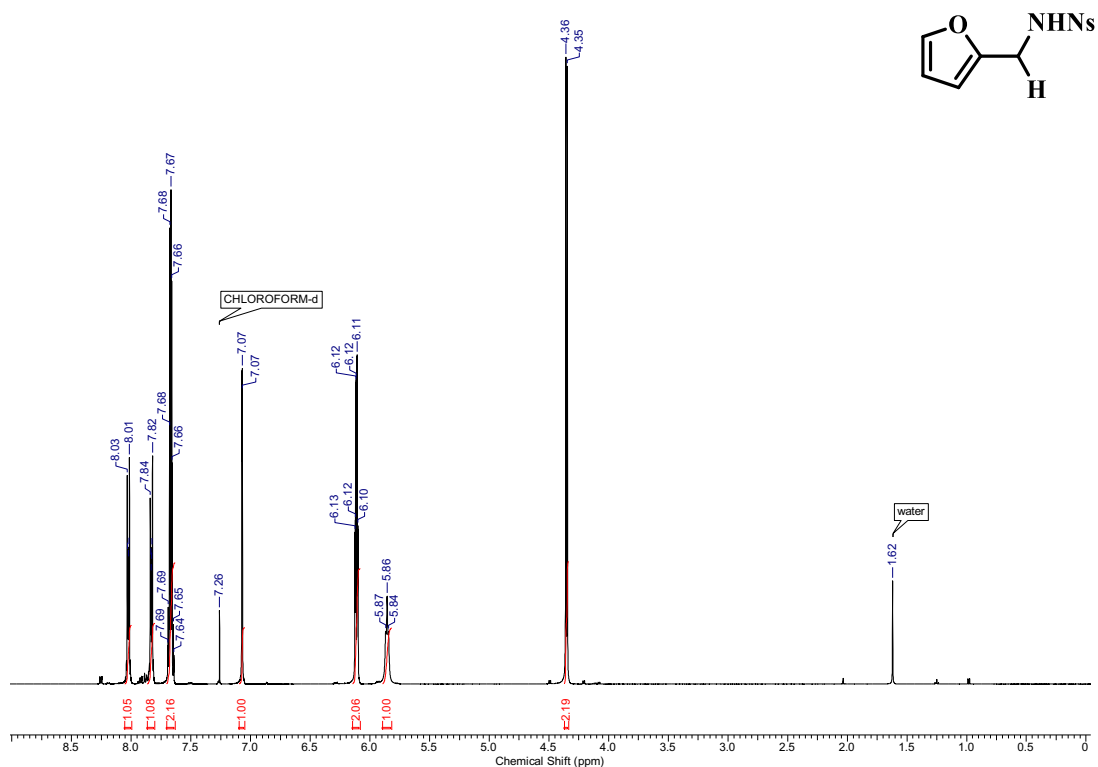


Figure S2. ¹H NMR spectra of compound **5a** (CDCl₃, 500 MHz).

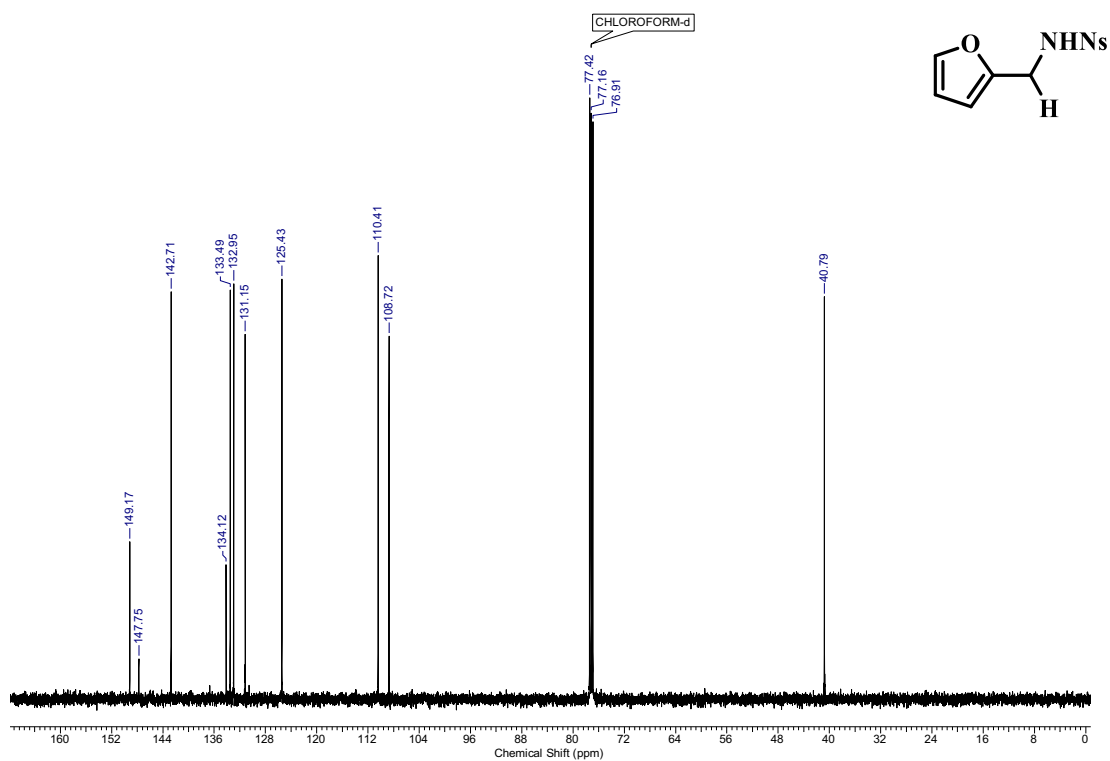


Figure S3. ¹³C NMR spectra of compound **5a** (CDCl₃, 126 MHz).

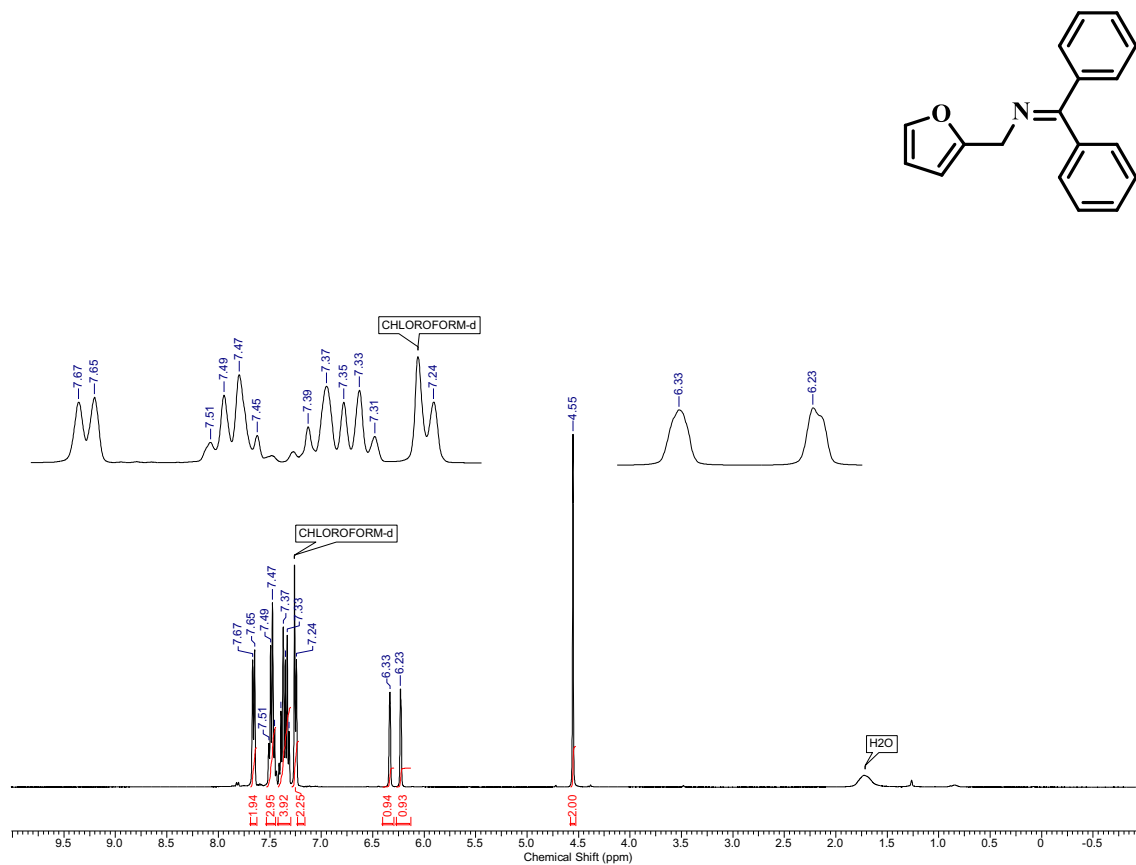


Figure S4. ¹H NMR spectra of compound **S-I** (CDCl₃, 400 MHz).

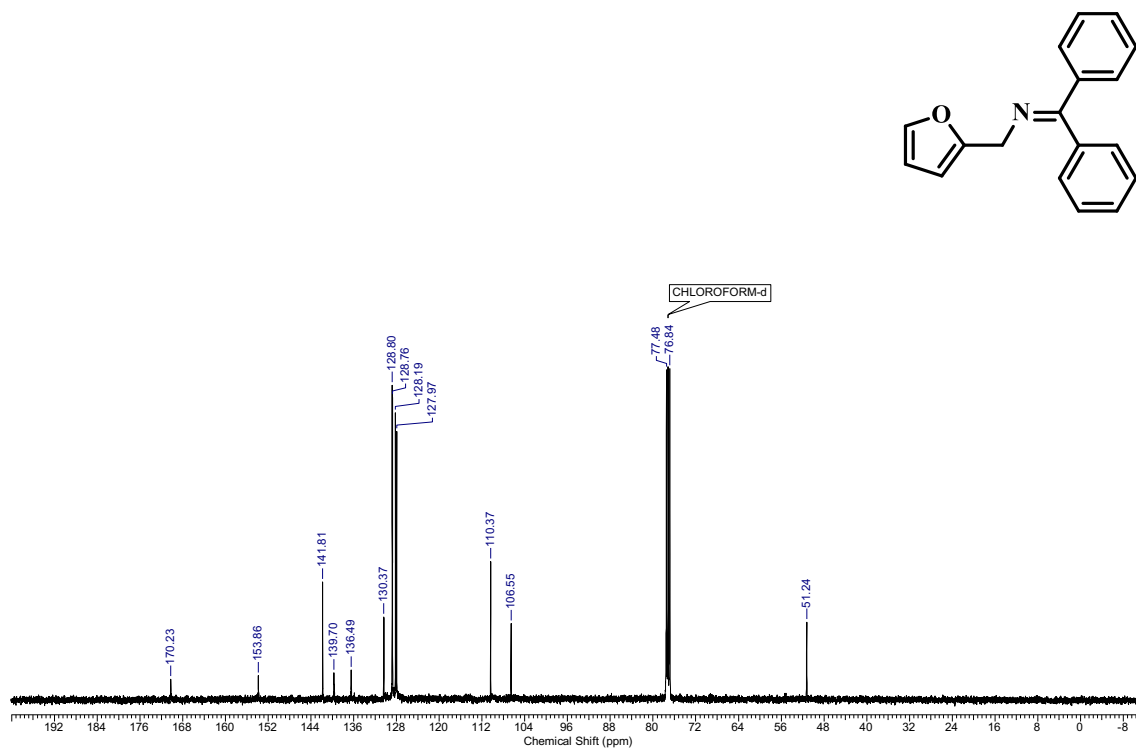


Figure S5. ¹³C NMR spectra of compound **S-I** (CDCl₃, 101 MHz).

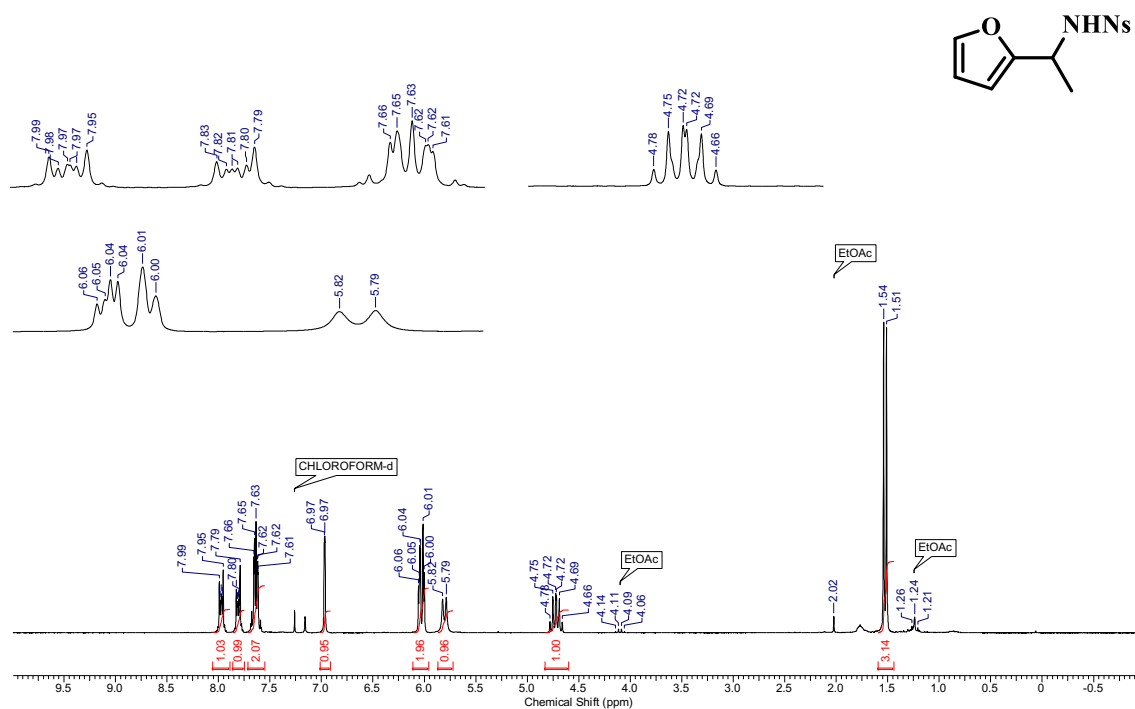


Figure S6. ^1H NMR spectra of compound **5b** (CDCl_3 , 250 MHz).

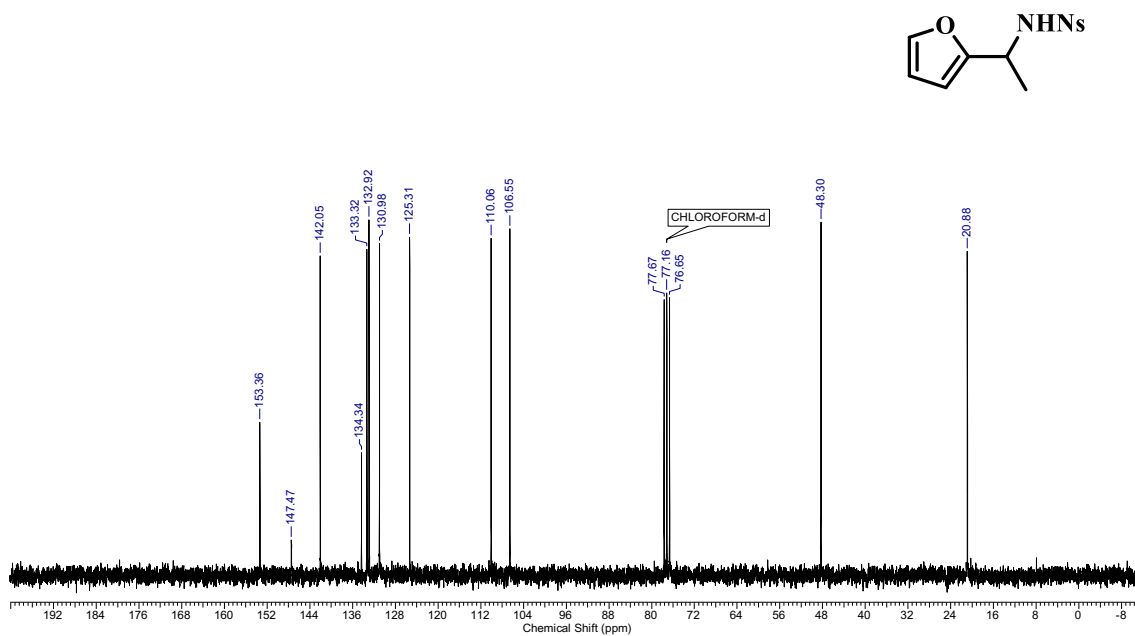


Figure S7. ^{13}C NMR spectra of compound **5b** (CDCl_3 , 63 MHz).

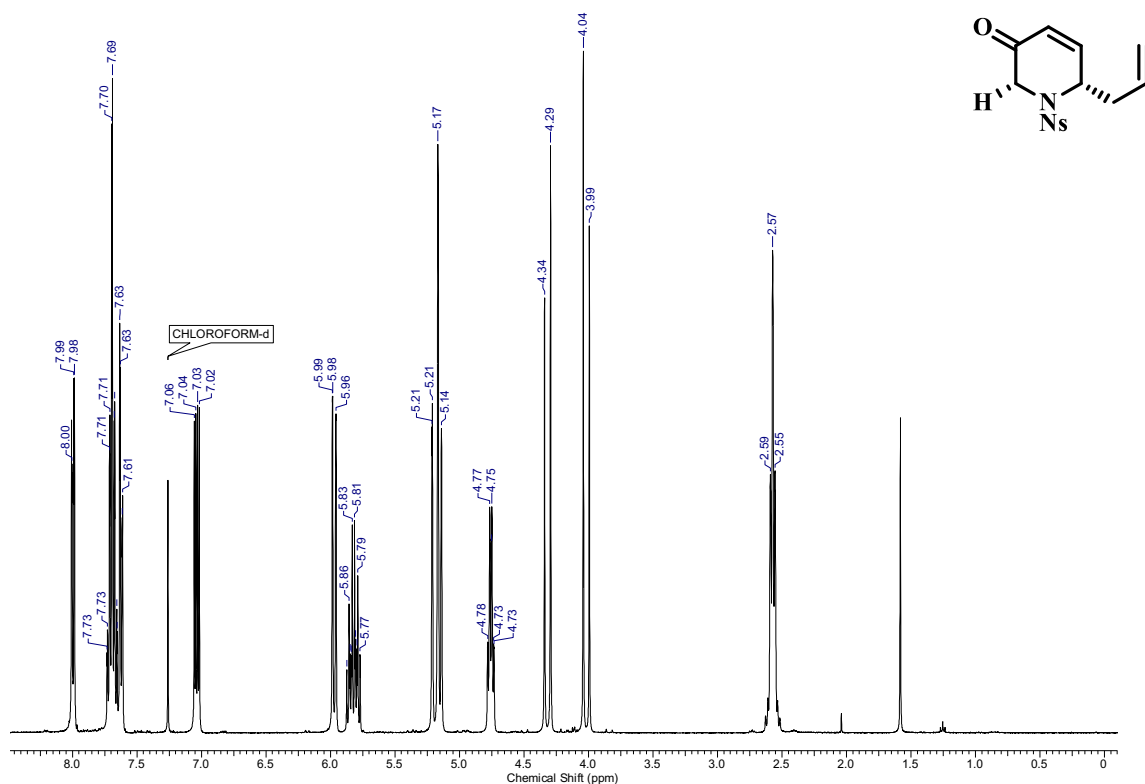


Figure S8. ¹H NMR spectra of compound **7a** (CDCl₃, 400 MHz).

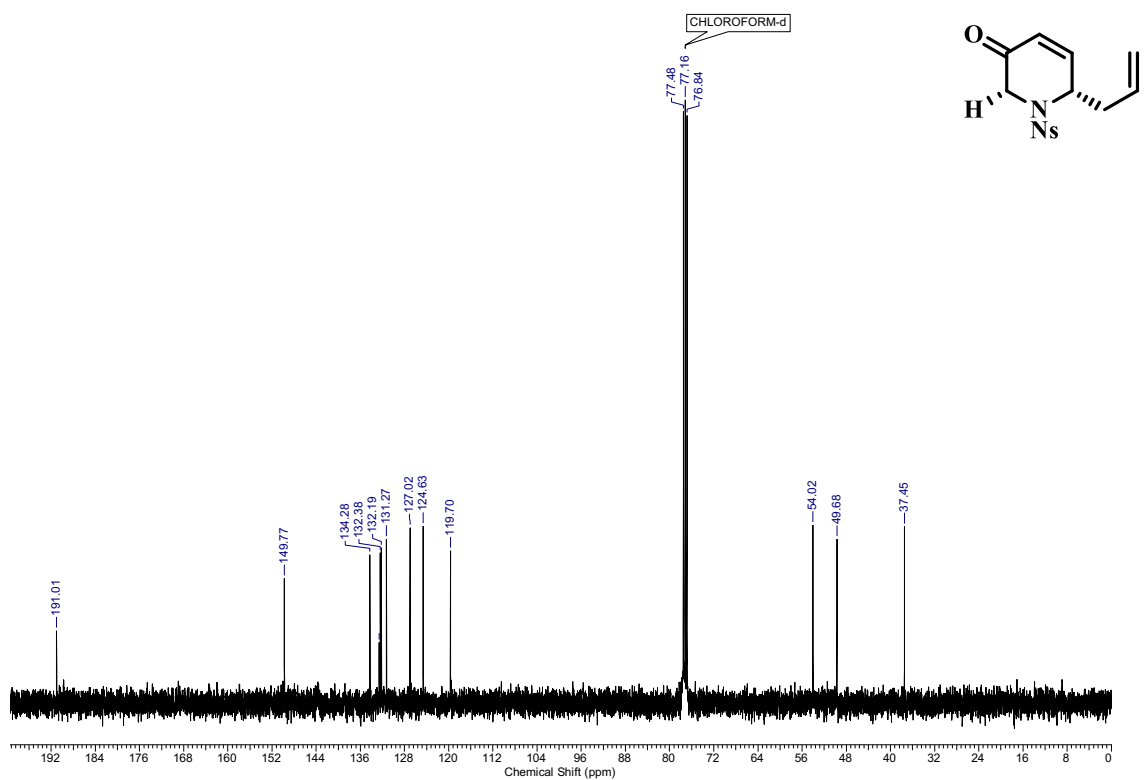


Figure S9. ¹³C NMR spectra of compound **7a** (CDCl₃, 101 MHz).

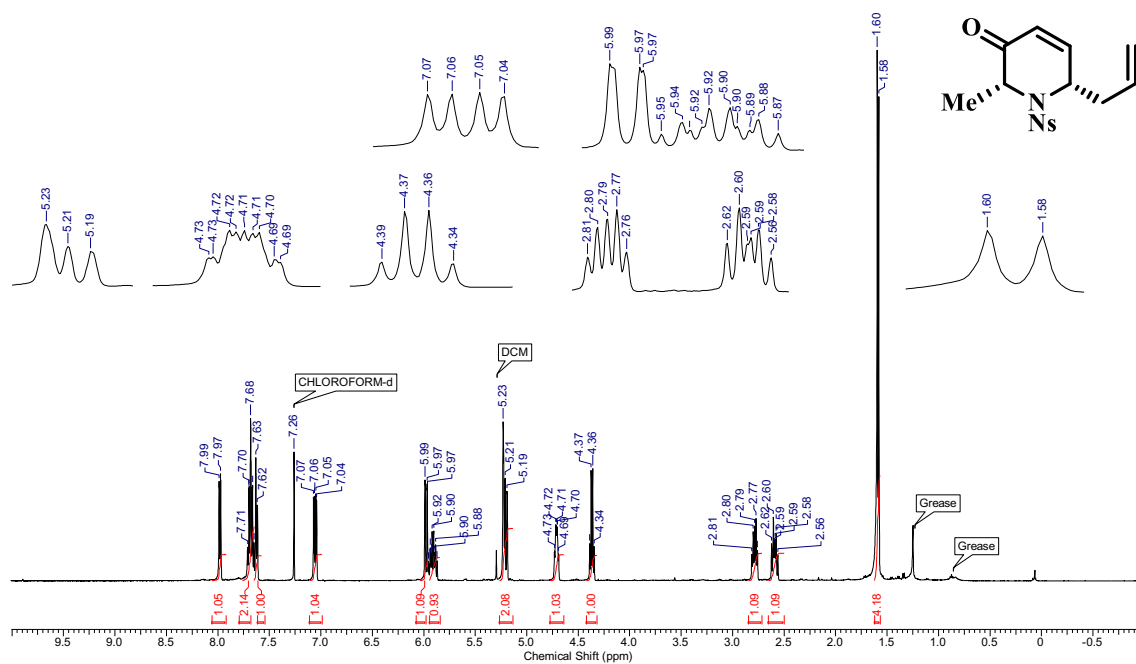


Figure S10. ¹H NMR spectra of compound **7b** (CDCl₃, 500 MHz).

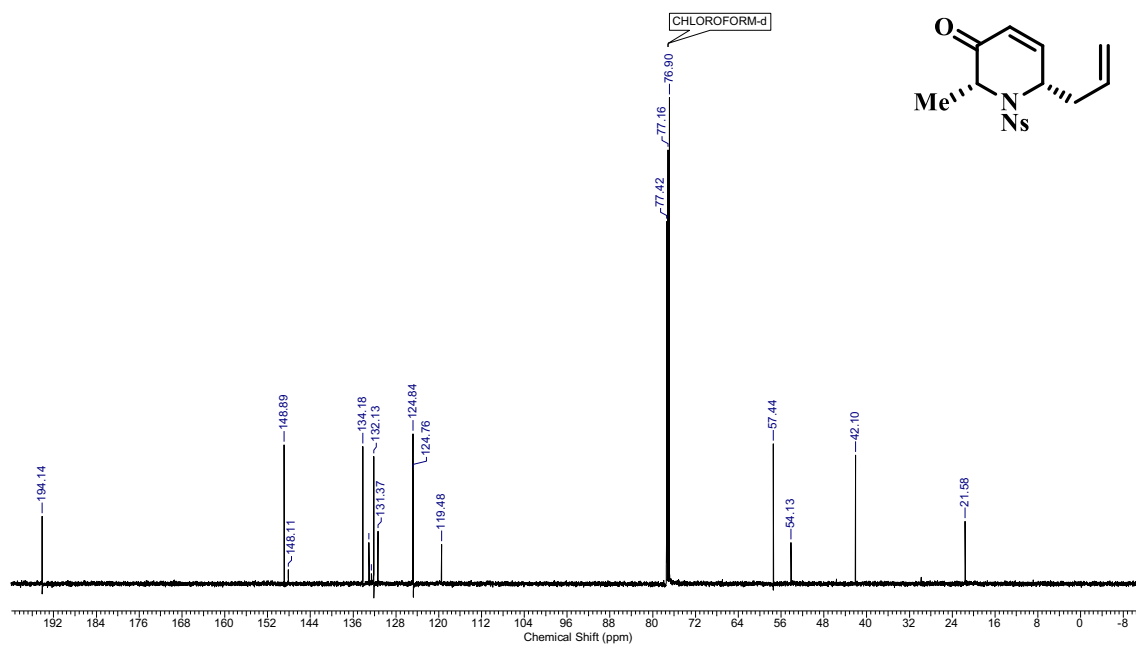


Figure S11. ¹³C NMR spectra of compound **7b** (CDCl₃, 126 MHz).

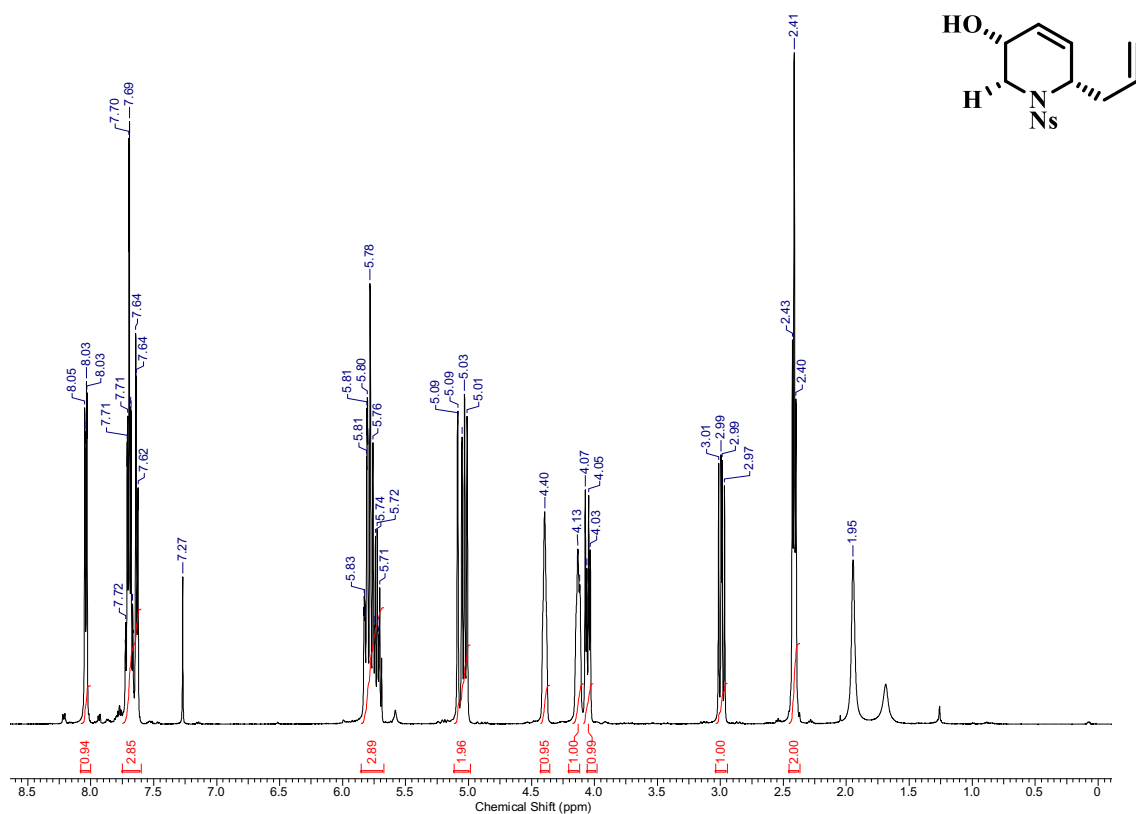


Figure S12. ¹H NMR spectra of compound **8a** (CDCl₃, 500 MHz).

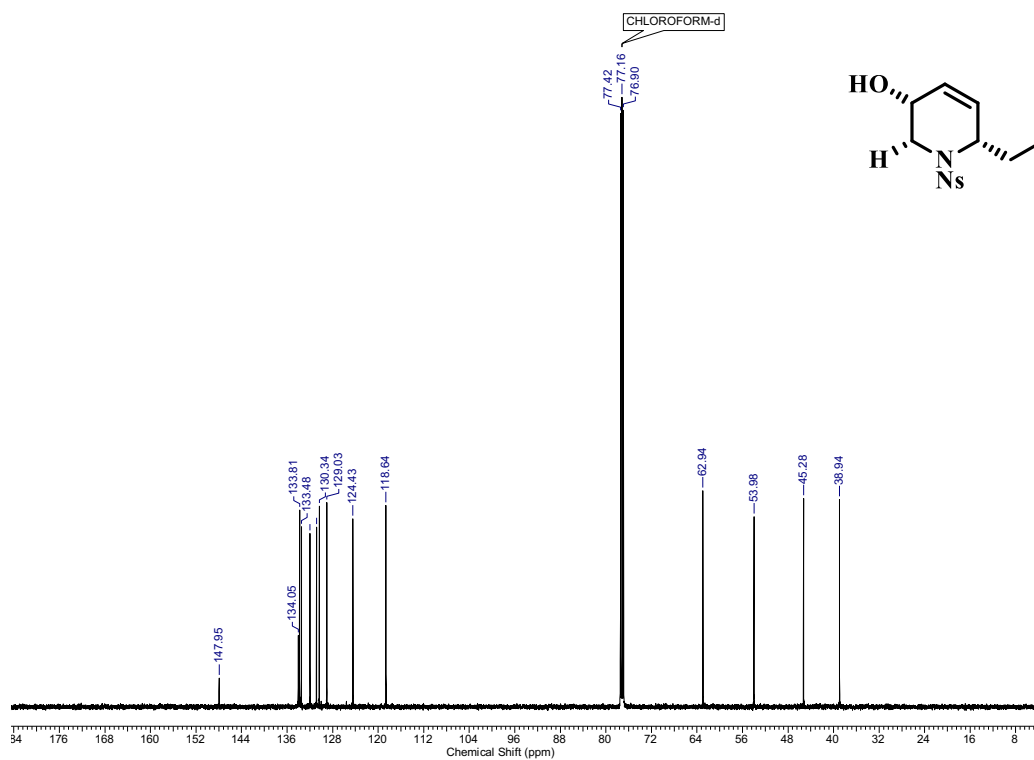


Figure S13. ¹³C NMR spectra of compound **8a** (CDCl₃, 126 MHz).

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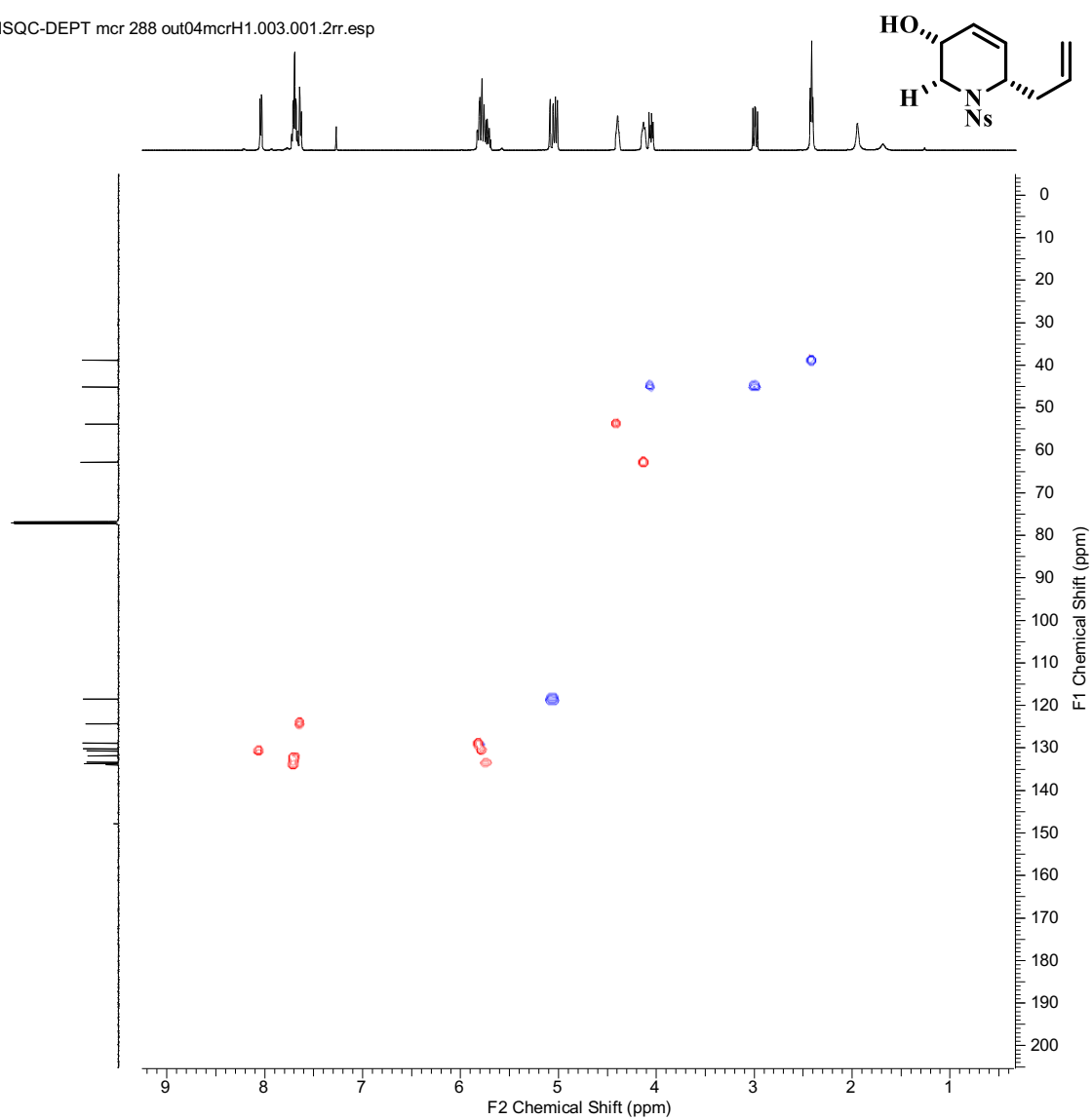


Figure S14. HSQC NMR spectra of compound **8a** (CDCl₃, 500MHz).

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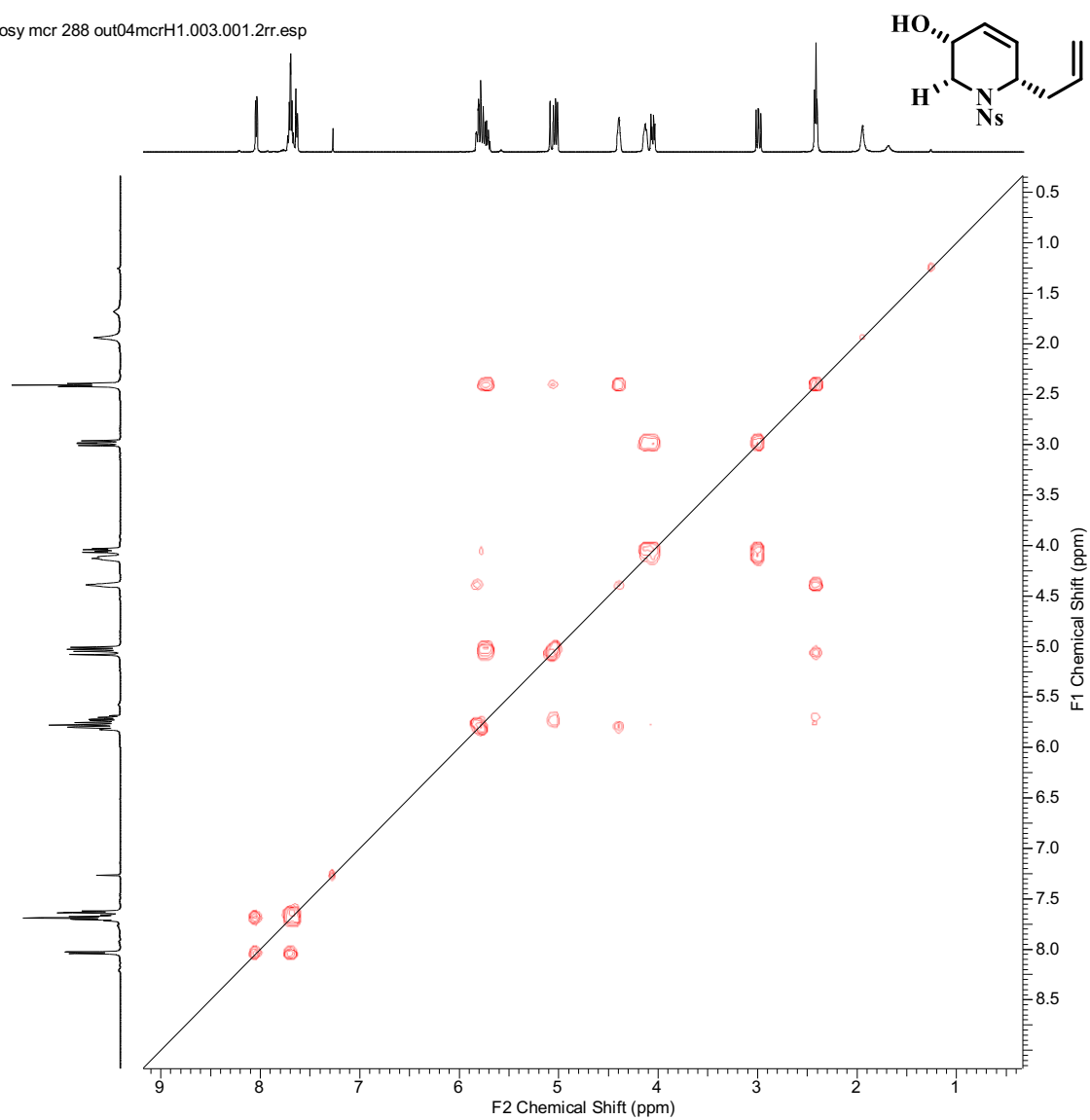


Figure S15. COSY NMR spectra of compound **8a** (CDCl₃, 500MHz).

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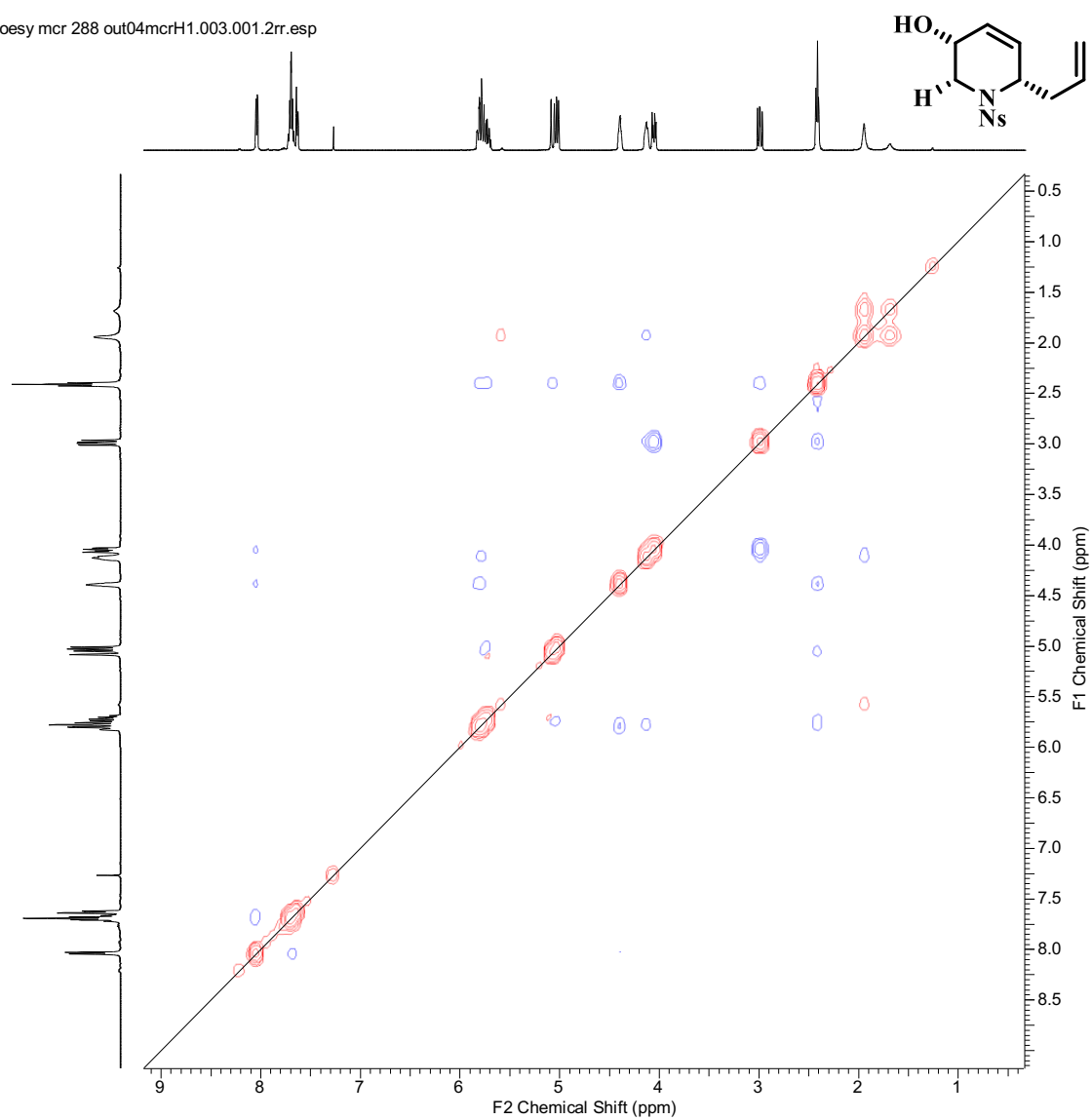


Figure S16. NOESY NMR spectra of compound **8a** (CDCl₃, 500MHz).

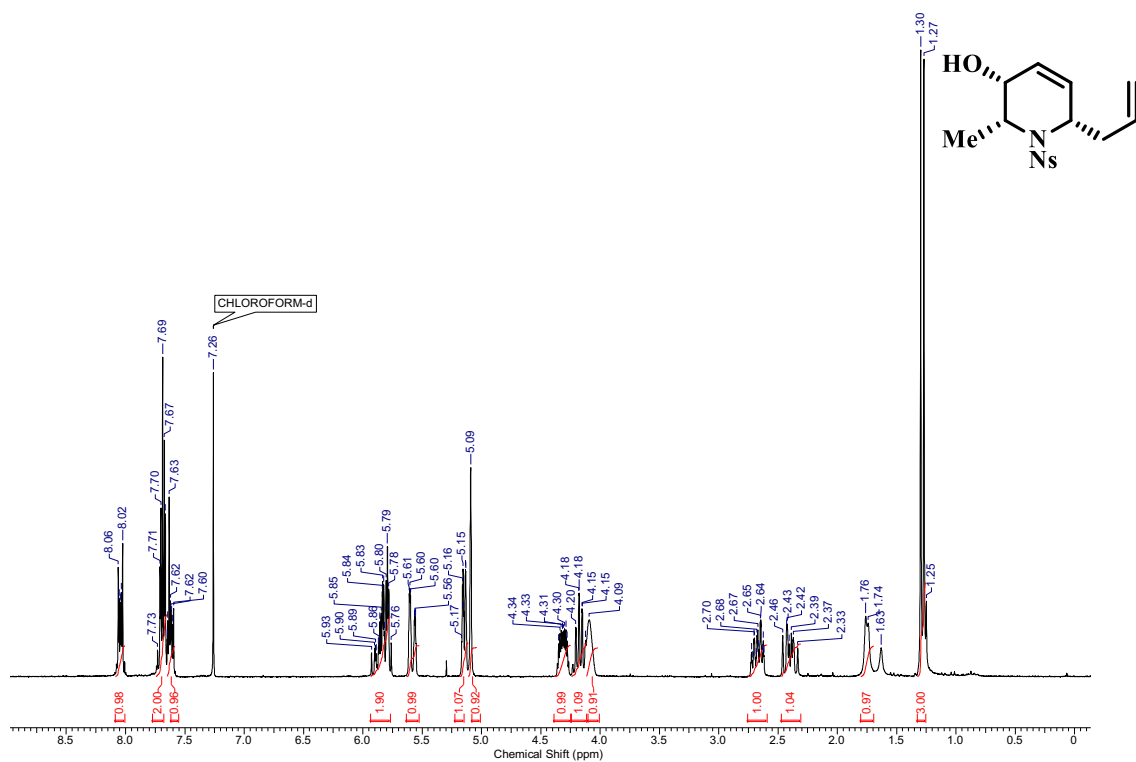


Figure S17. ¹H NMR spectra of compound **8b** (CDCl₃, 250 MHz).

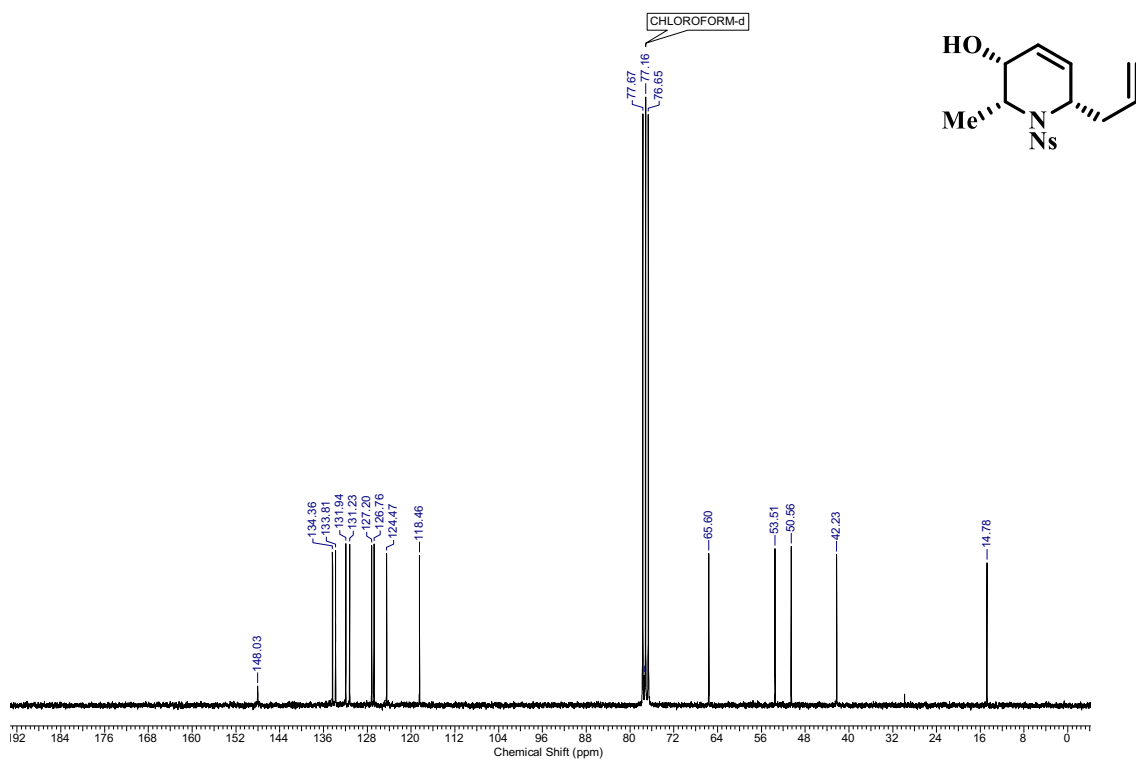


Figure S18. ¹³C NMR spectra of compound **8b** (CDCl₃, 63 MHz).

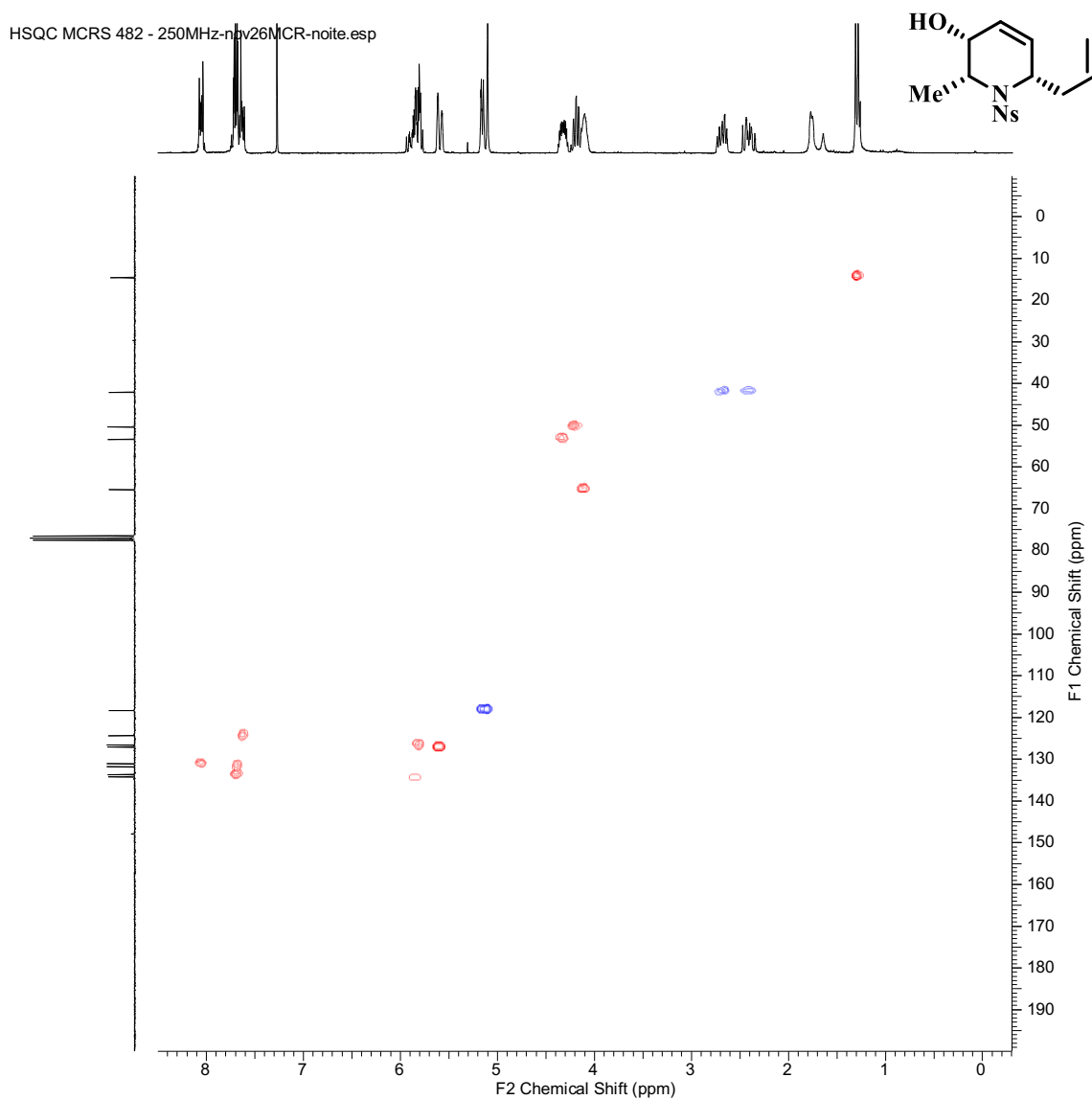


Figure S19. HSQC NMR spectra of compound **8b** (CDCl₃, 500MHz).

COSY MCRS 482 - 250MHz-nov26MCR-noite.esp

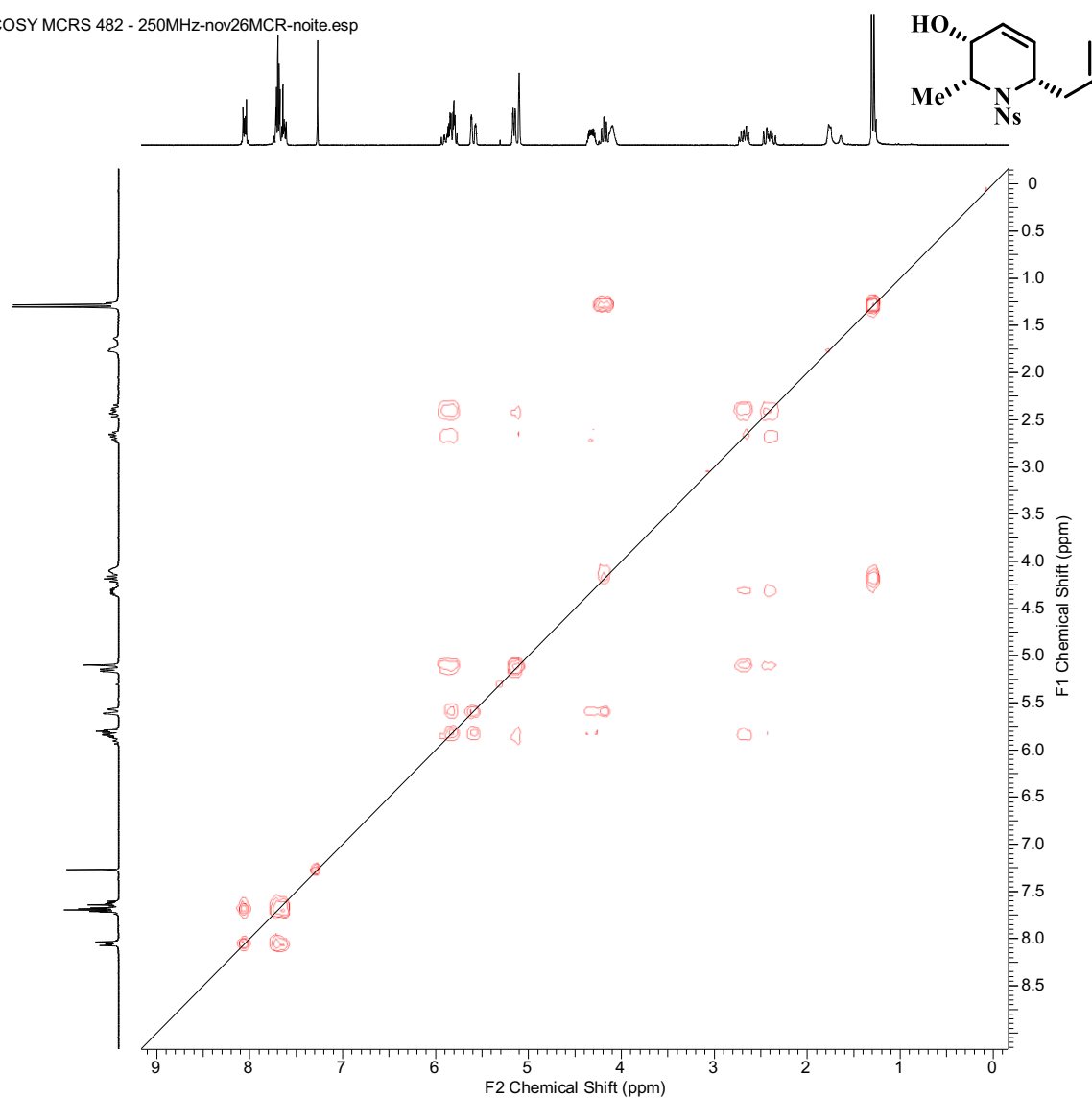


Figure S20. COSY NMR spectra of compound **8b** (CDCl₃, 500MHz).

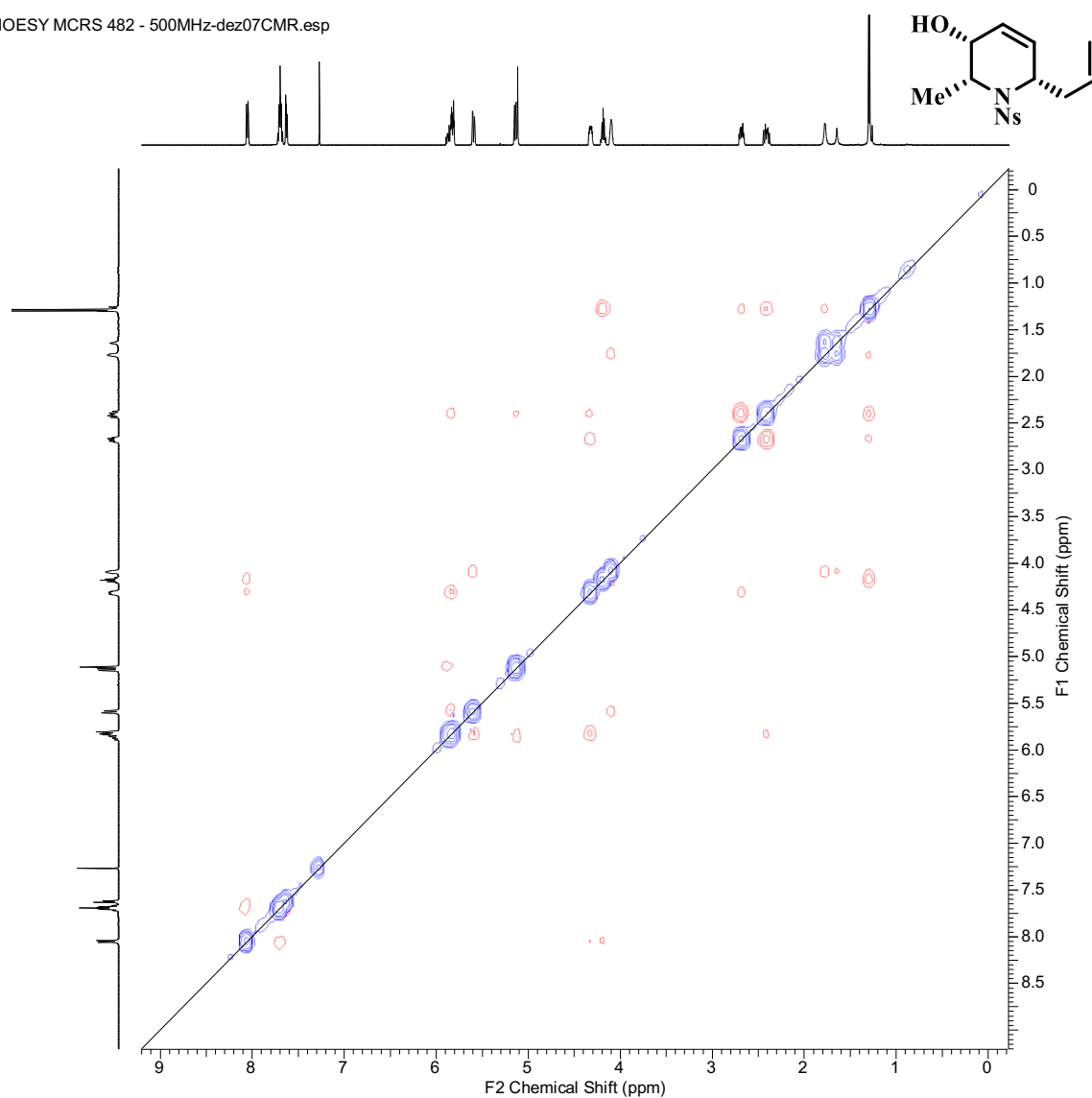


Figure S21. NOESY NMR spectra of compound **8b** (CDCl₃, 500MHz).

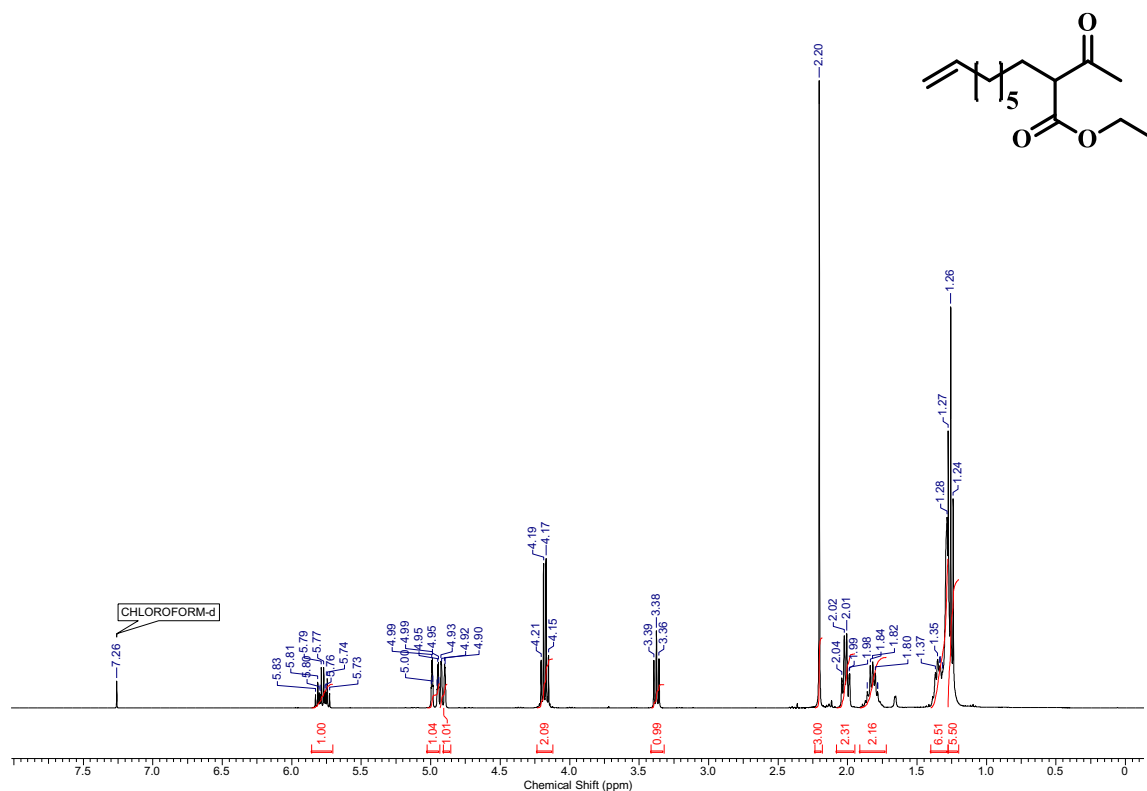


Figure S22. ¹H NMR spectra of compound S-IV (CDCl₃, 400 MHz)

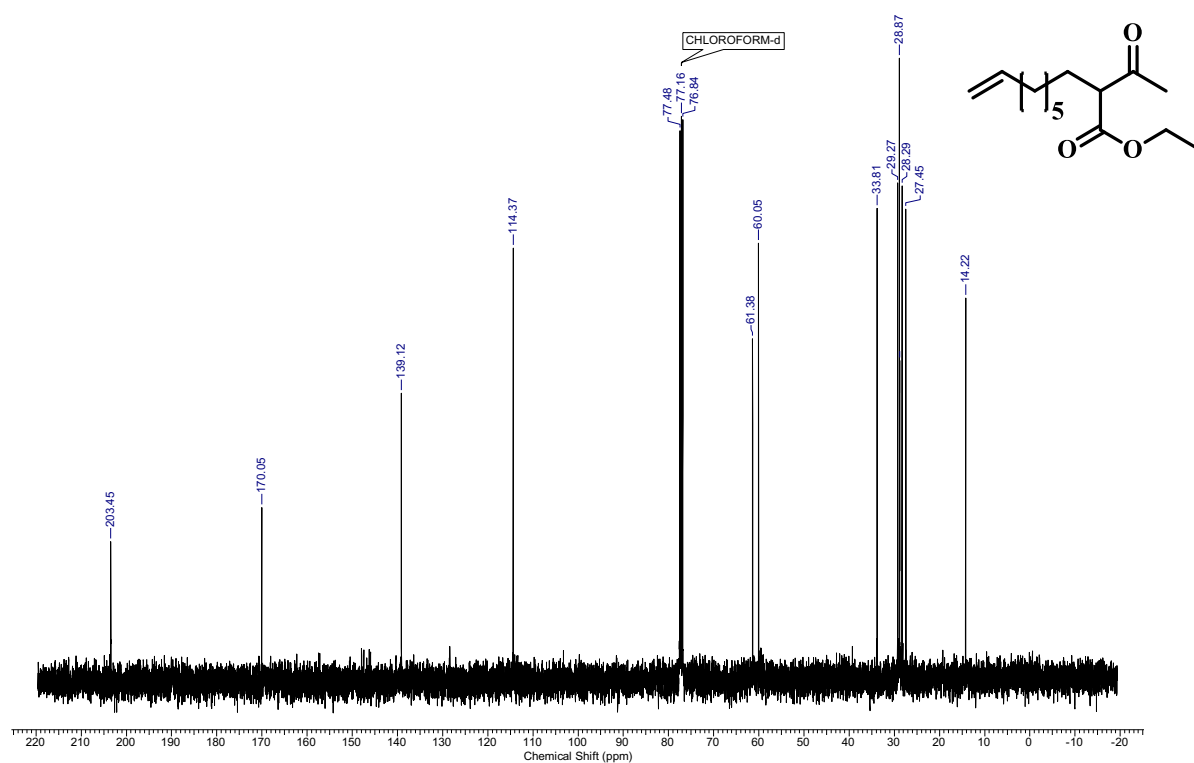


Figure S23. ¹³C NMR spectra of compound S-IV (CDCl₃, 101 MHz).

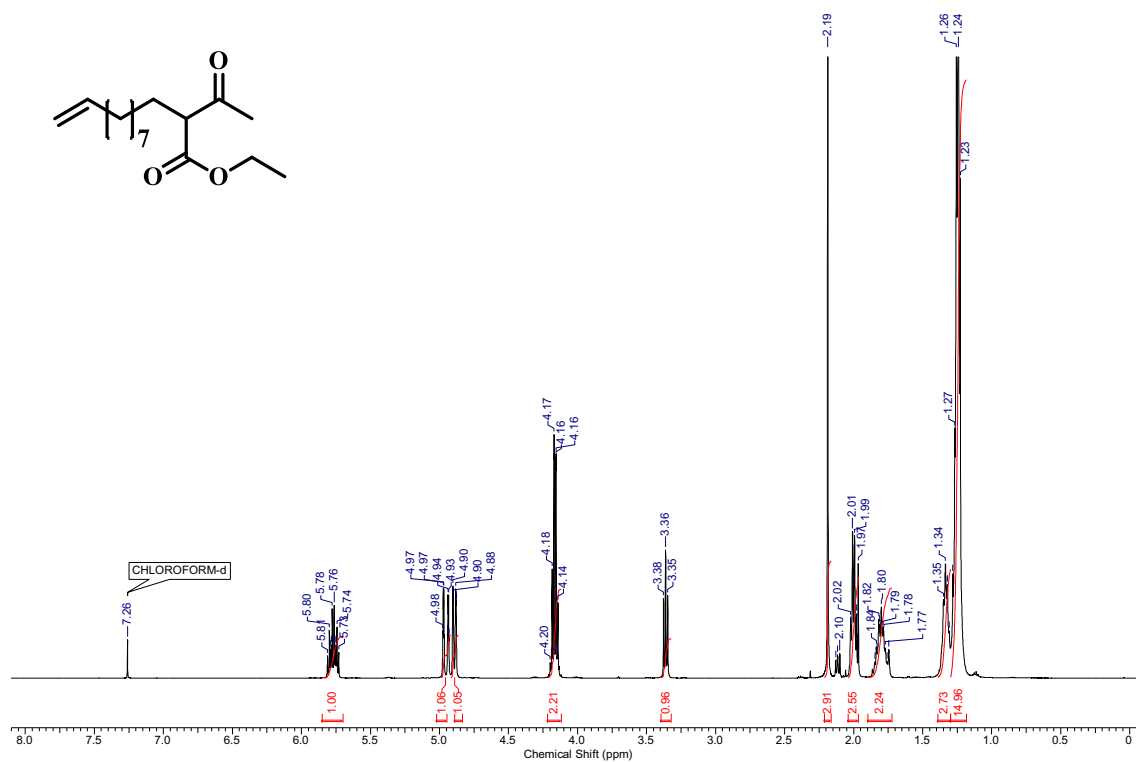


Figure S24. ¹H NMR spectra of compound S-V (CDCl₃, 500 MHz)

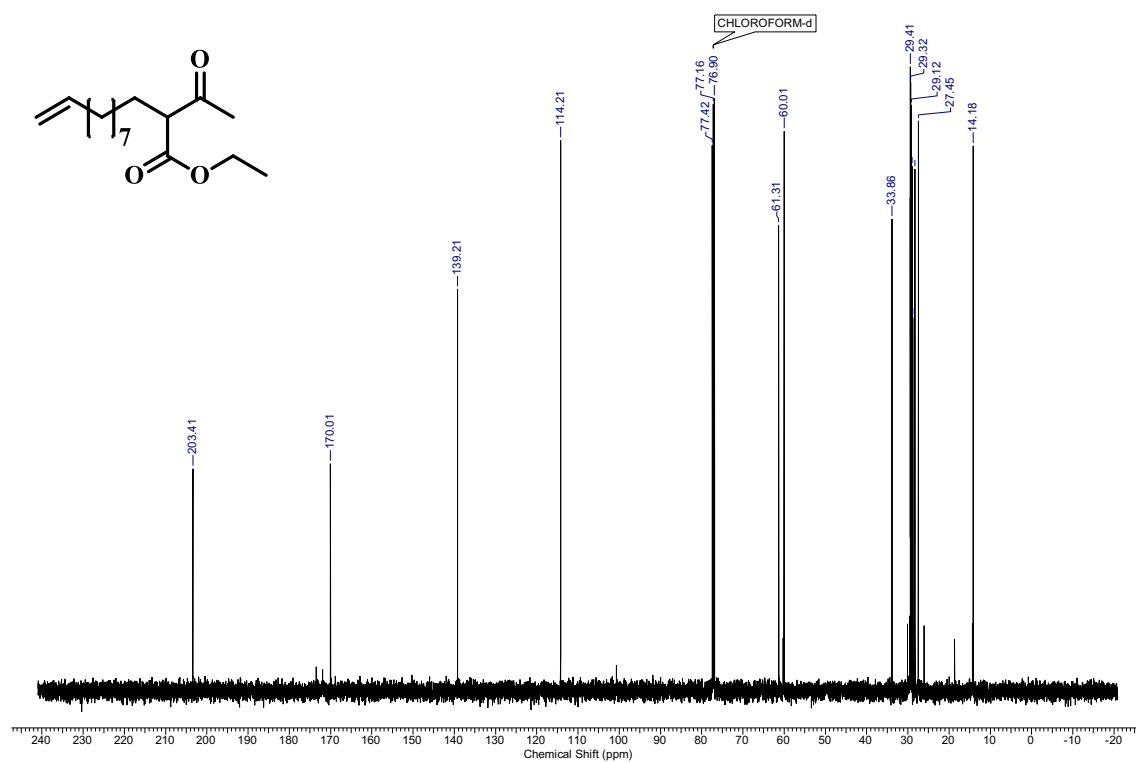


Figure S25. ¹³C NMR spectra of compound S-V (CDCl₃, 126 MHz).

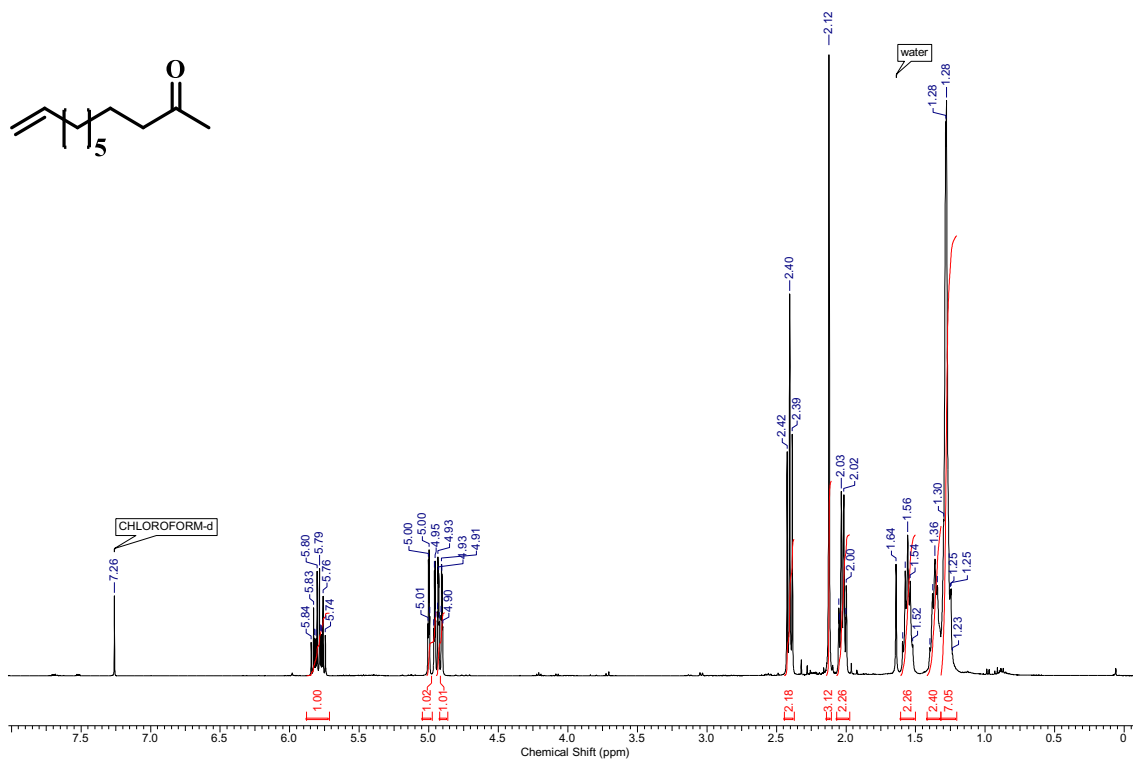


Figure S26. ¹H NMR spectra of compound **B** (CDCl₃, 400 MHz)

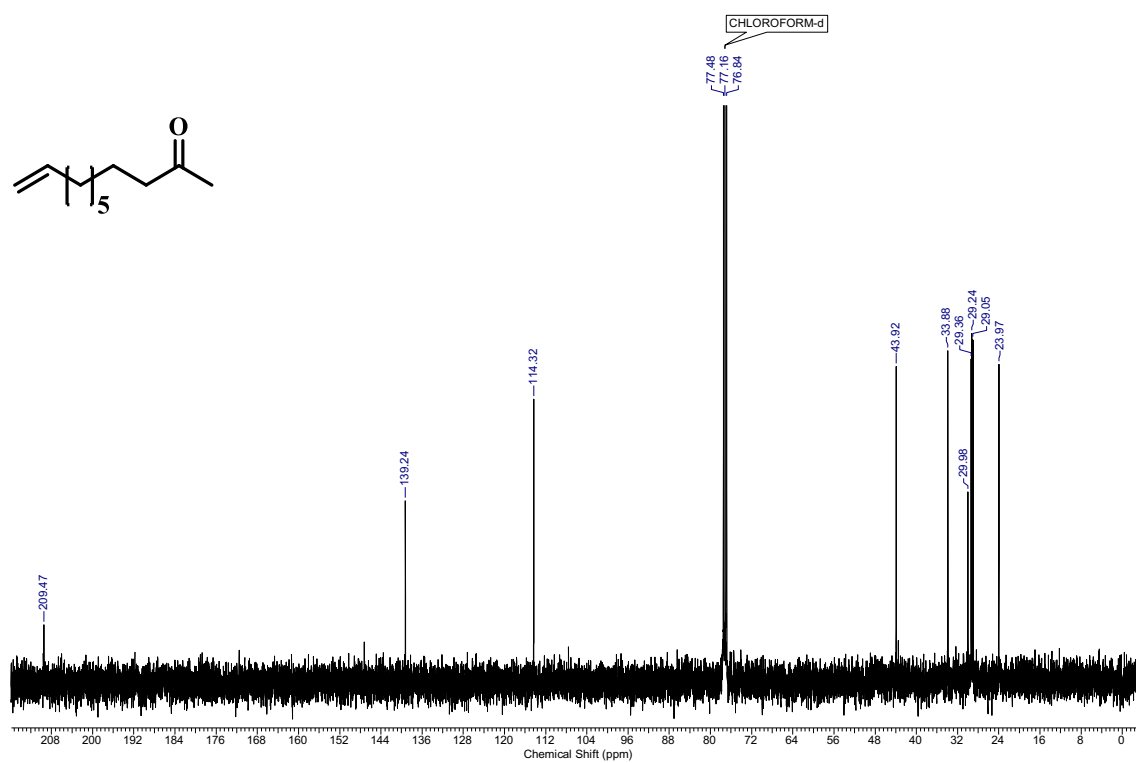


Figure S27. ¹³C NMR spectra of compound **B** (CDCl₃, 101 MHz).

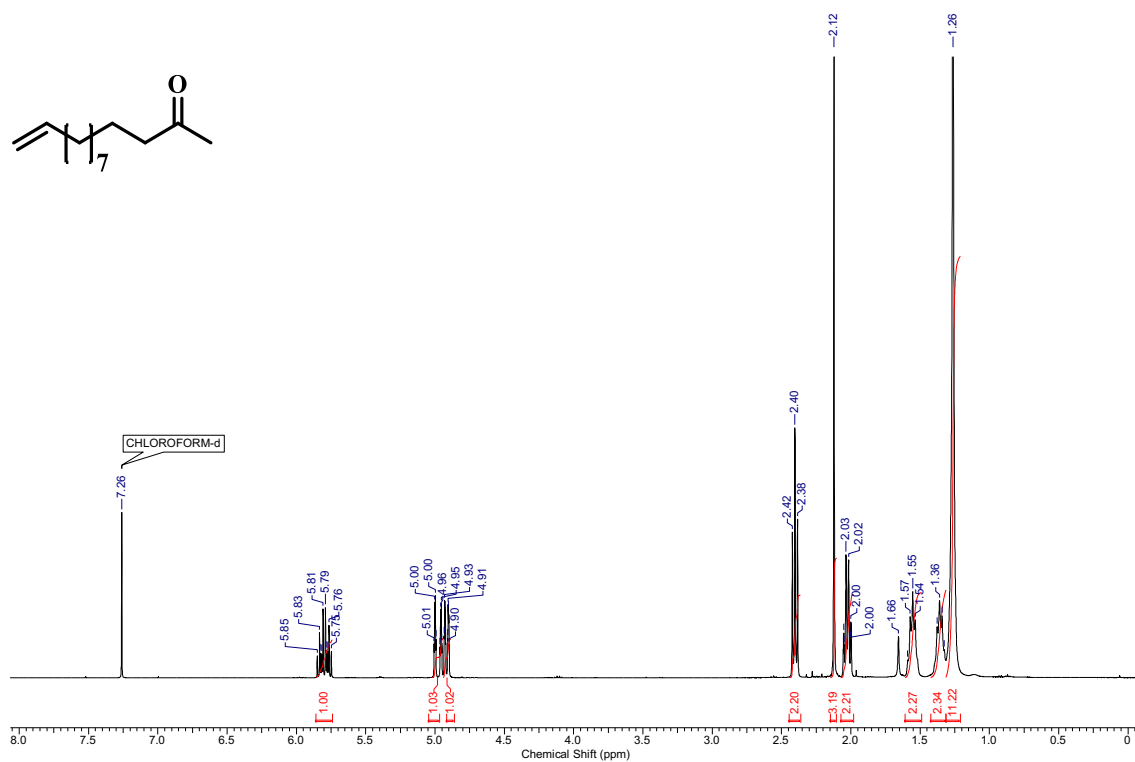


Figure S28. ¹H NMR spectra of compound C (CDCl₃, 400 MHz)

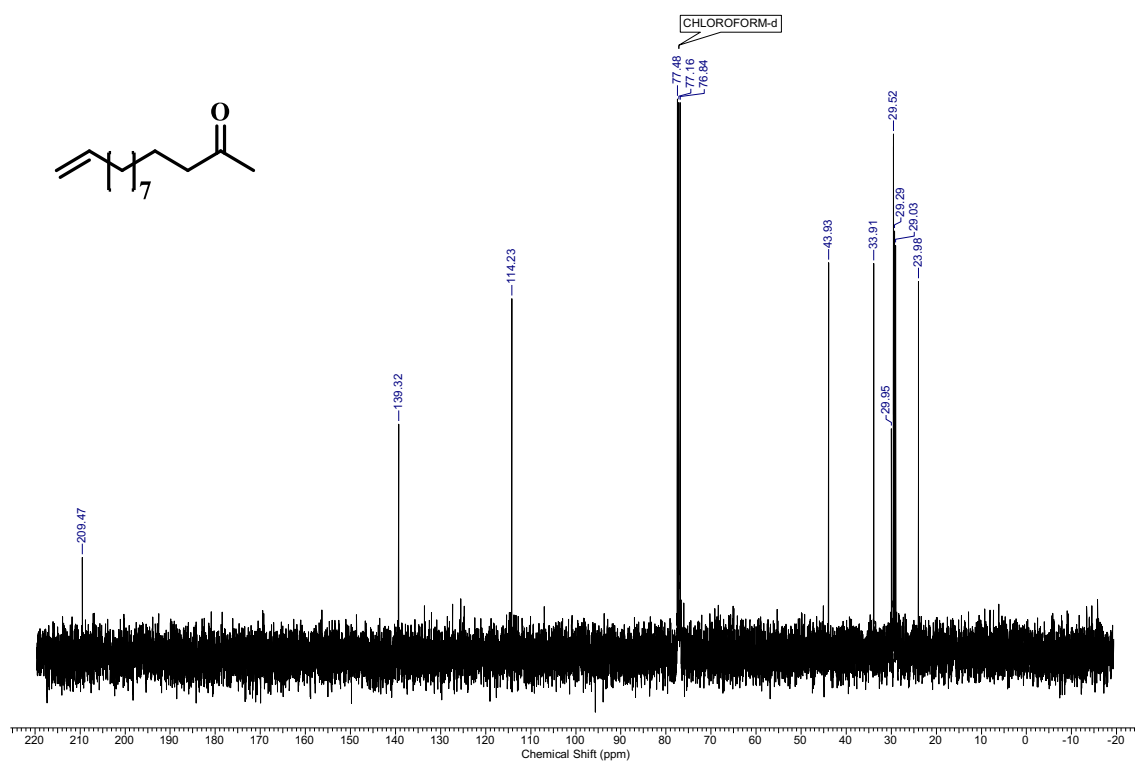


Figure S29. ¹³C NMR spectra of compound C (CDCl₃, 101 MHz).

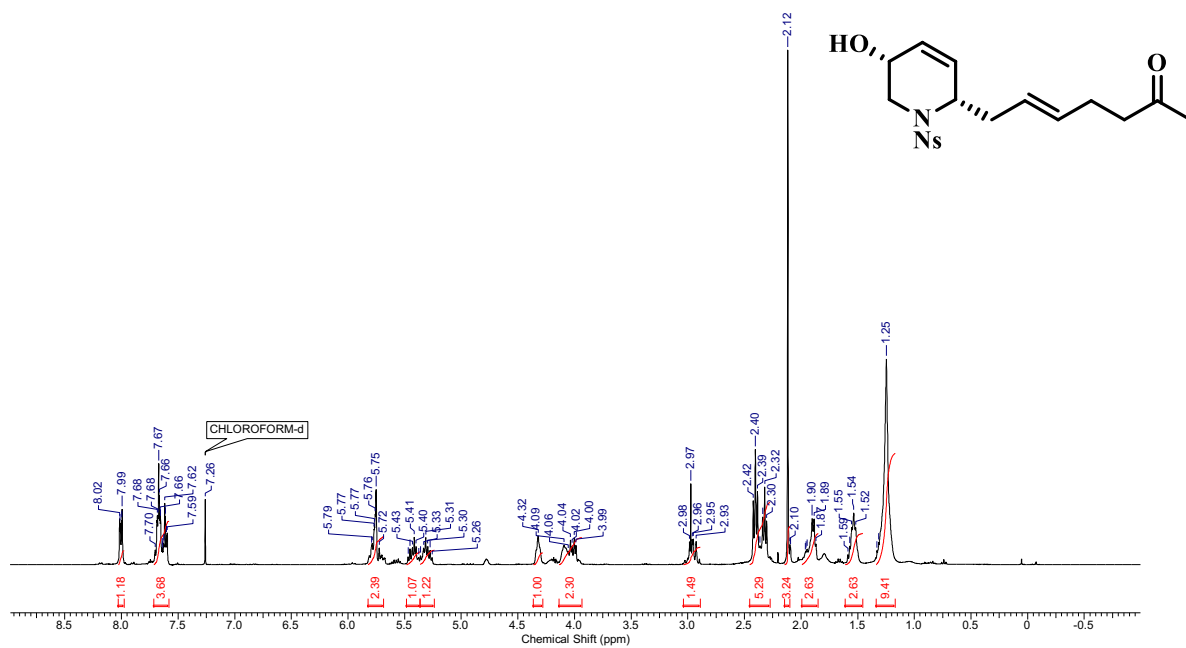


Figure S30. ¹H NMR spectra of compound **9a** (CDCl₃, 400 MHz)

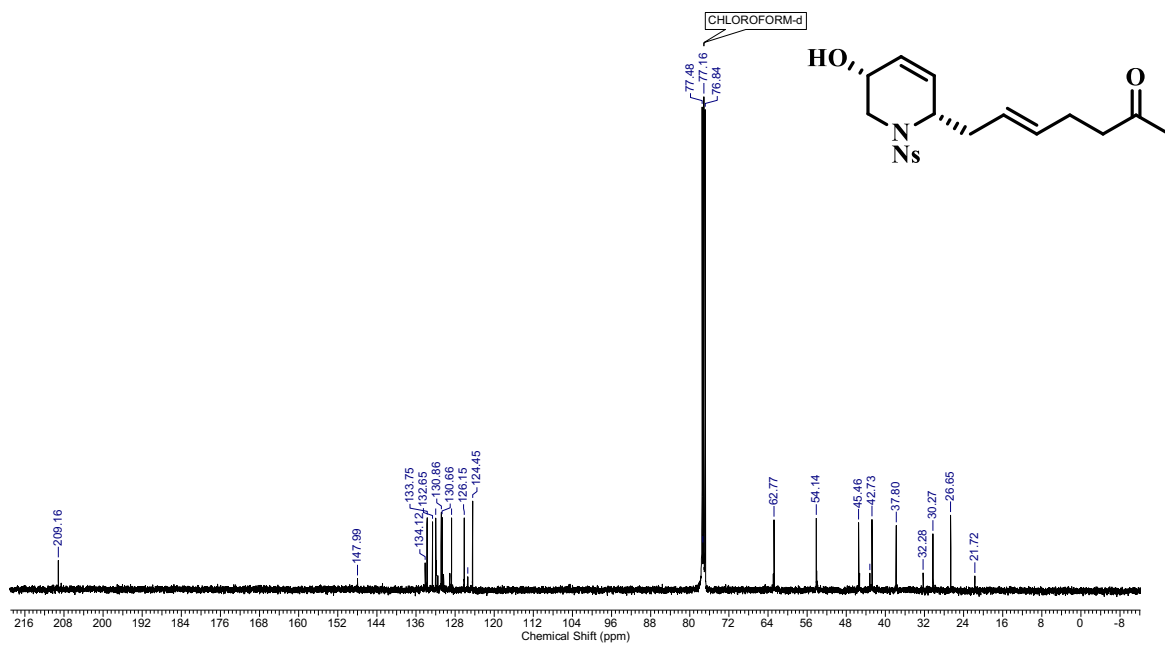


Figure S31. ¹³C NMR spectra of compound **9a** (CDCl₃, 101 MHz).

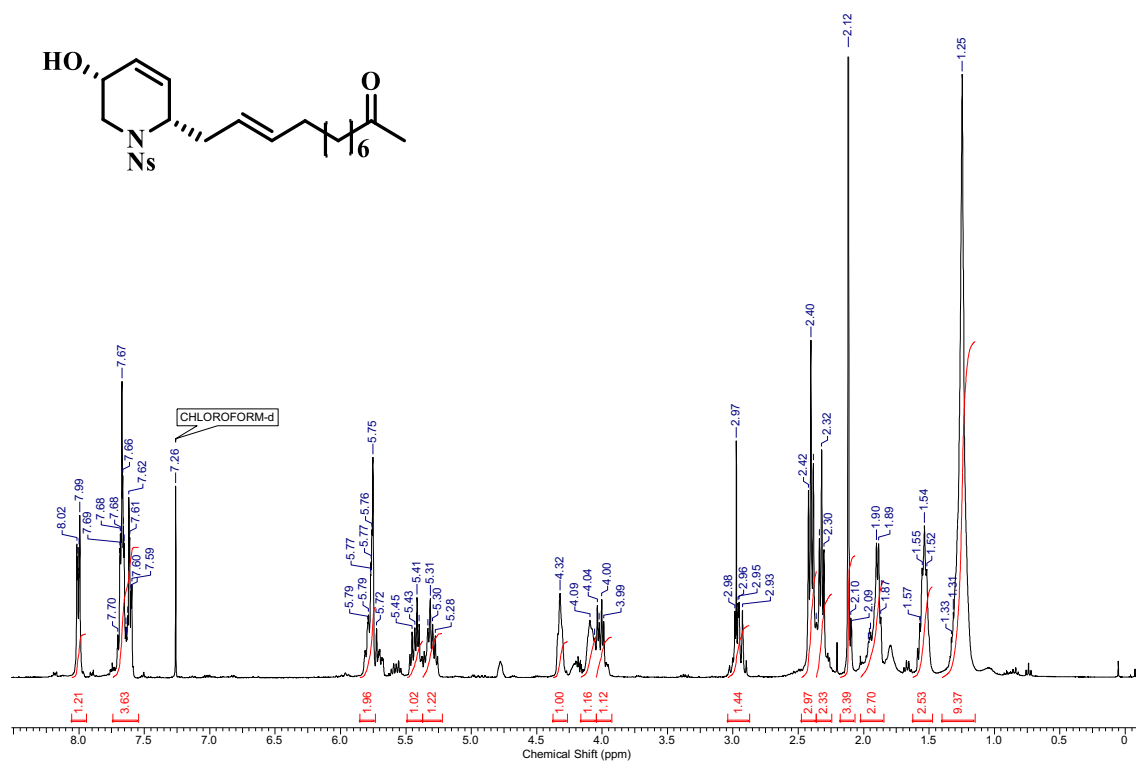


Figure S32. ¹H NMR spectra of compound **9b** (CDCl₃, 400 MHz)

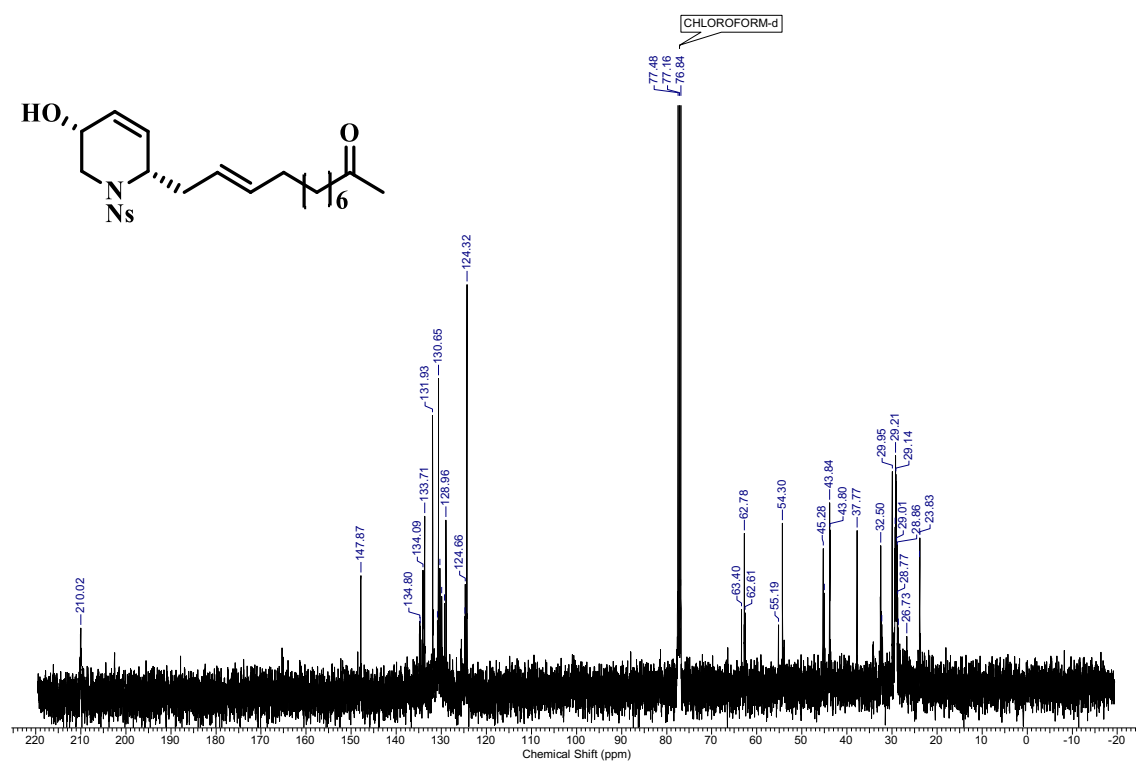


Figure S33. ¹³C NMR spectra of compound **9b** (CDCl₃, 101 MHz)

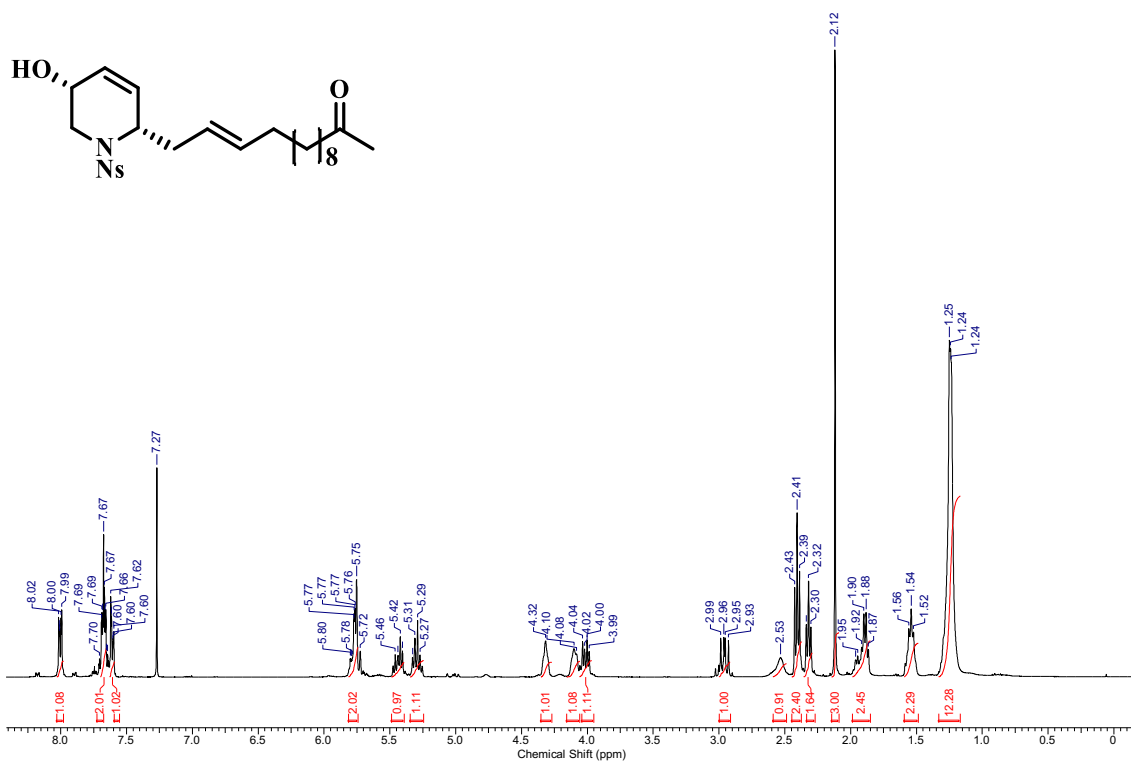


Figure S34. ¹H NMR spectra of compound **9c** (CDCl₃, 400 MHz)

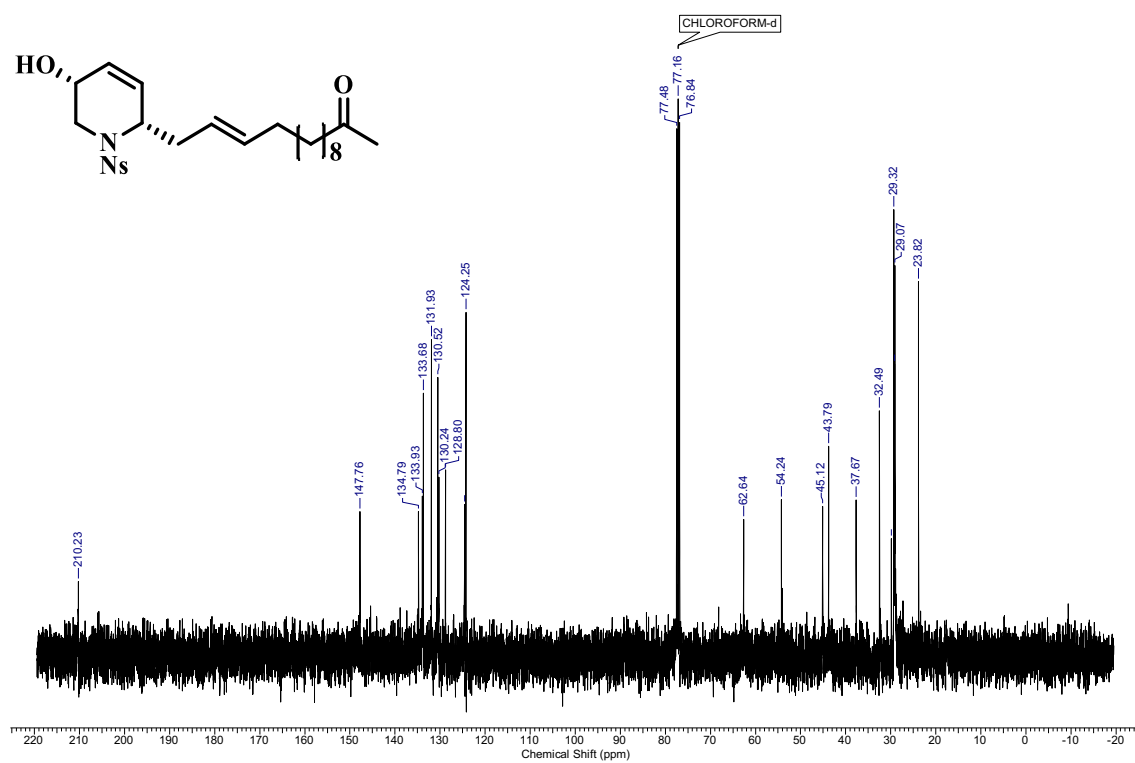


Figure S35. ¹³C NMR spectra of compound **9c** (CDCl₃, 101 MHz)

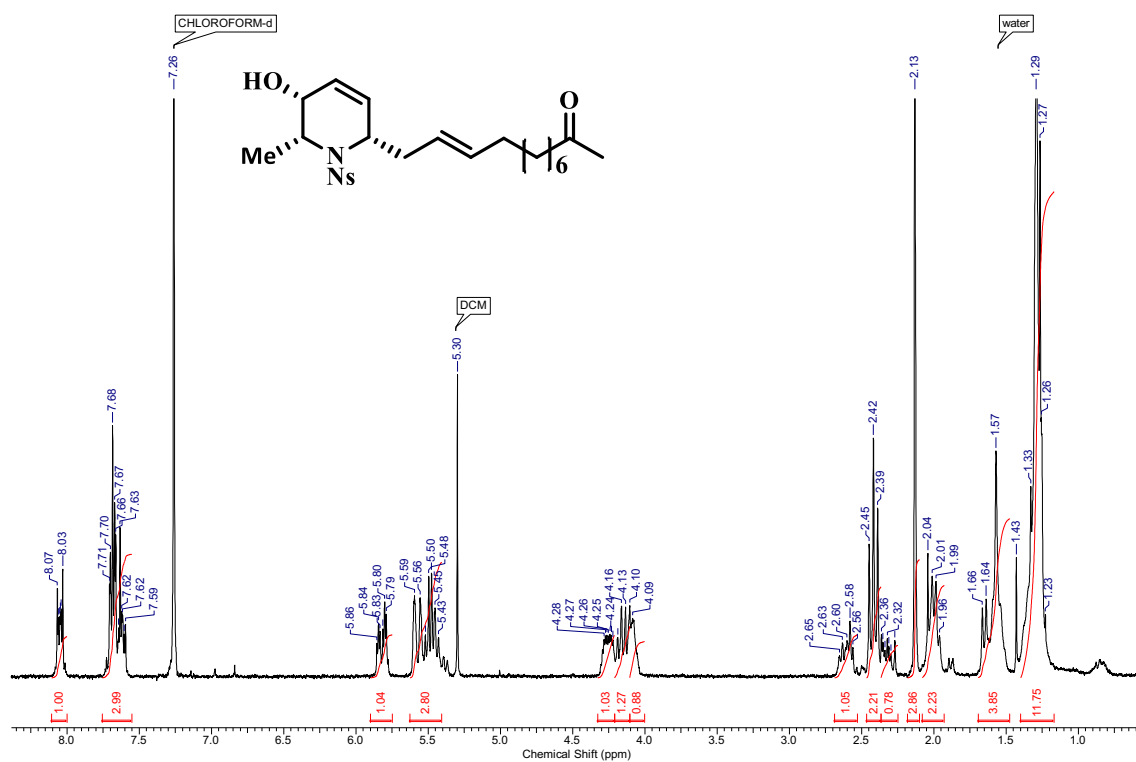


Figure S36. ¹H NMR spectra of compound **9d** (CDCl₃, 250 MHz)

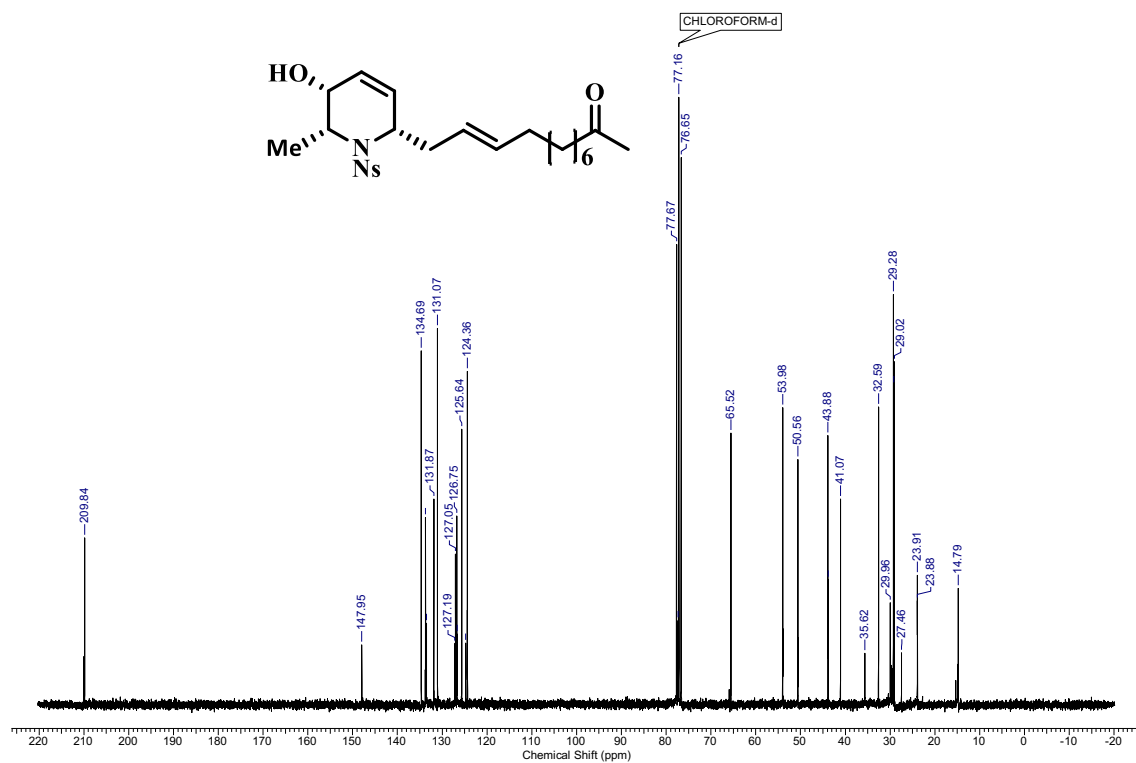


Figure S37. ¹³C NMR spectra of compound **9d** (CDCl₃, 63 MHz)

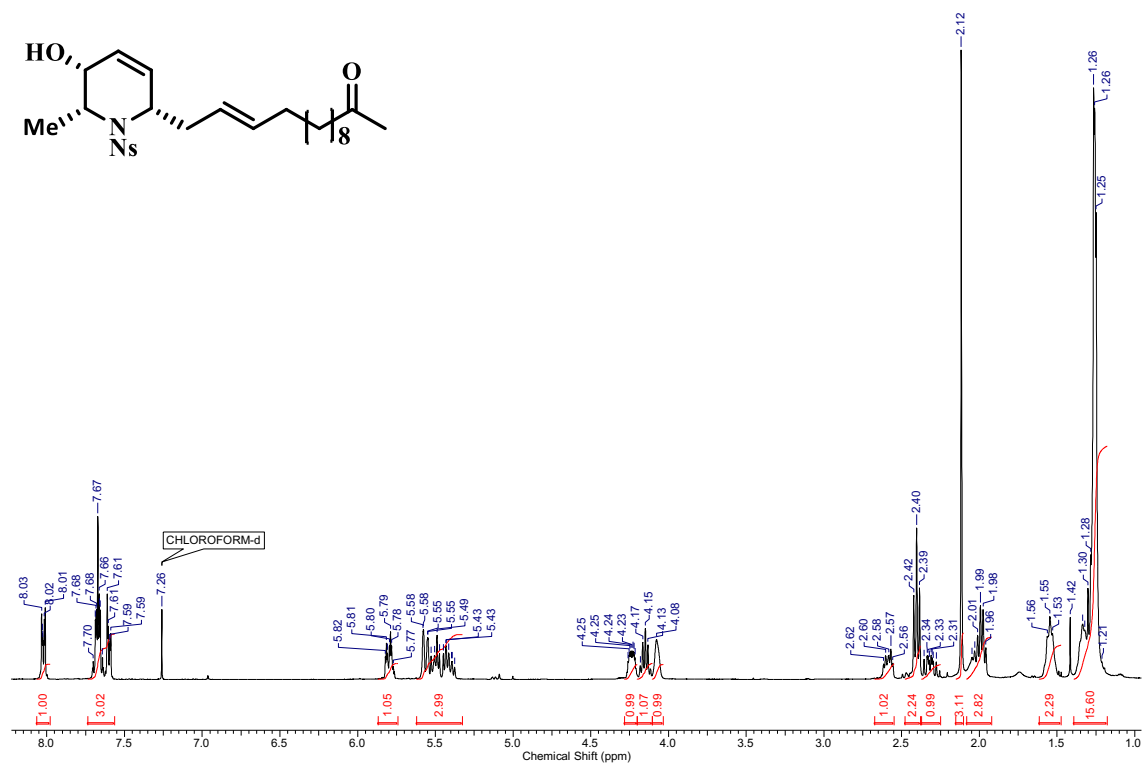


Figure S38. ¹H NMR spectra of compound **9e** (CDCl₃, 400 MHz)

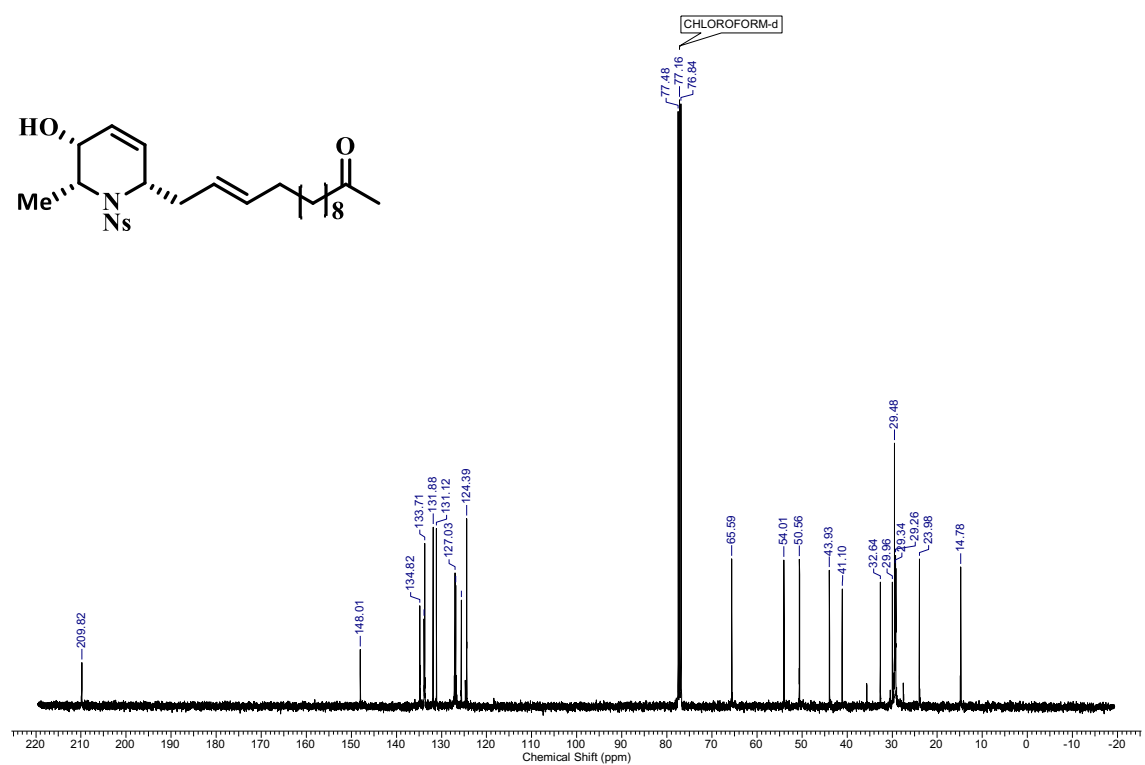


Figure S39. ¹³C NMR spectra of compound **9e** (CDCl₃, 101 MHz)

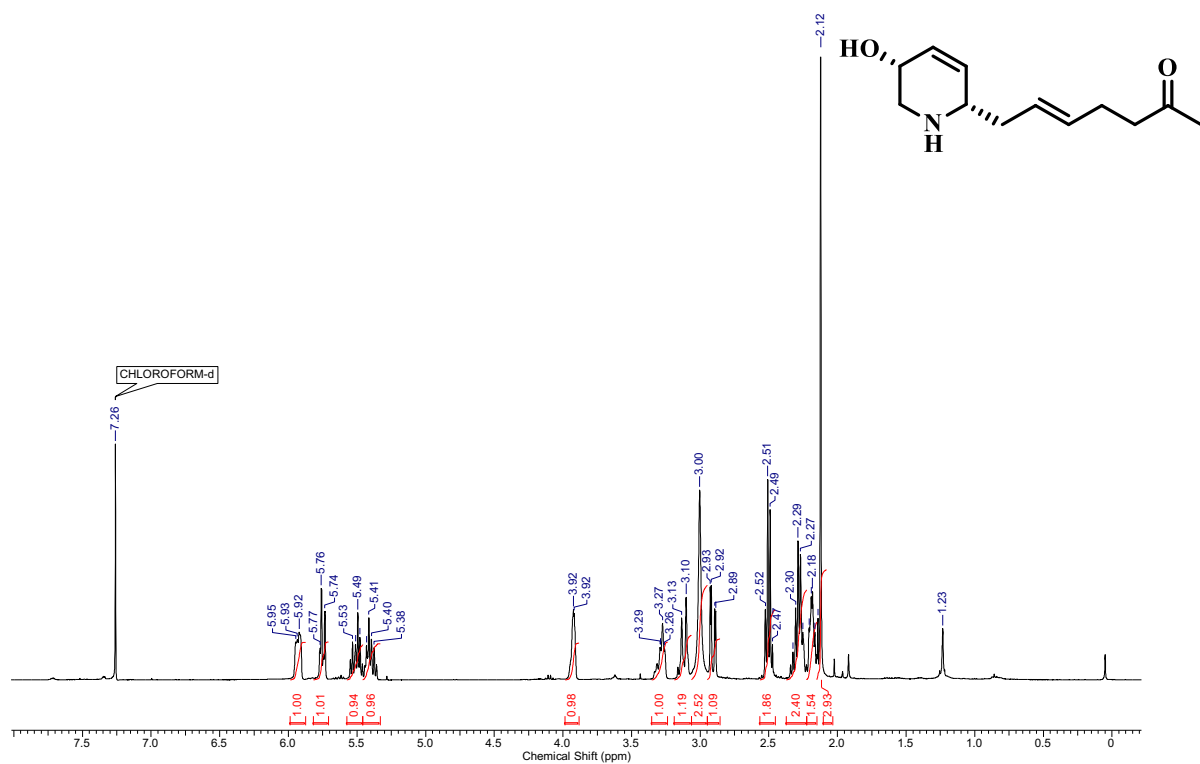


Figure S40. ¹H NMR spectra of compound **10a** (CDCl₃, 400 MHz)

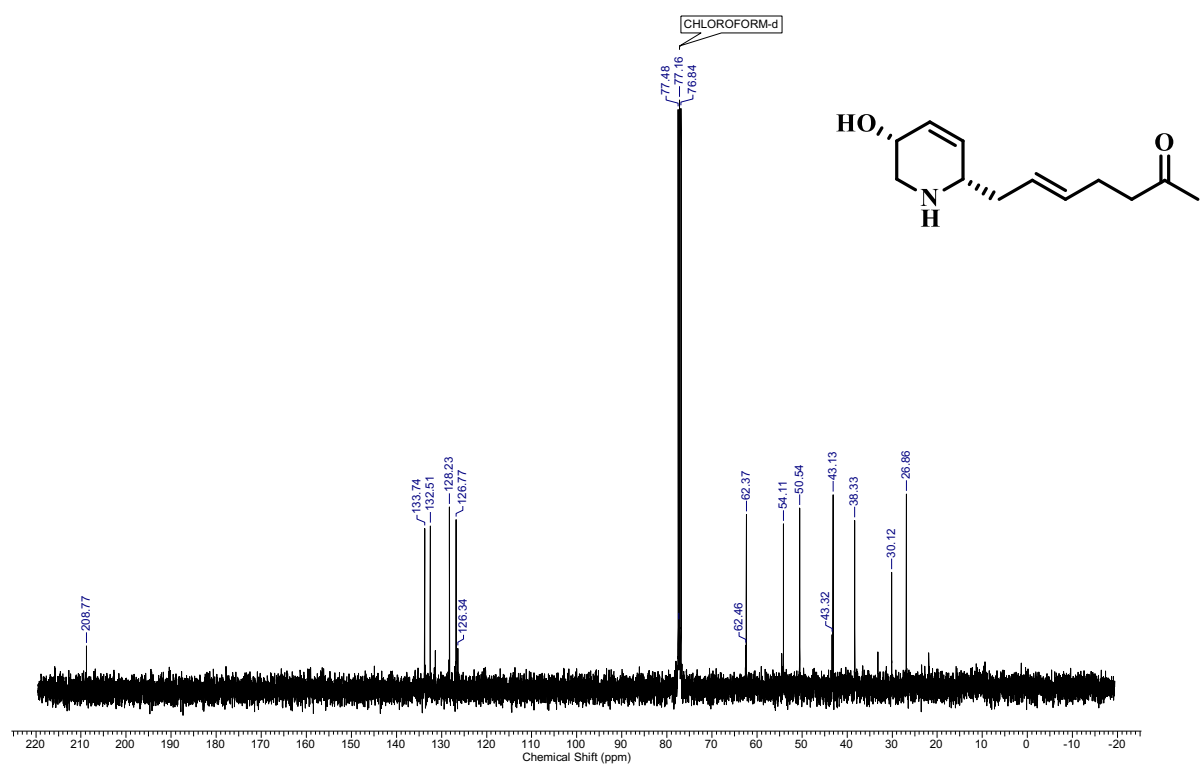


Figure S41. ¹³C NMR spectra of compound **10a** (CDCl₃, 101 MHz)

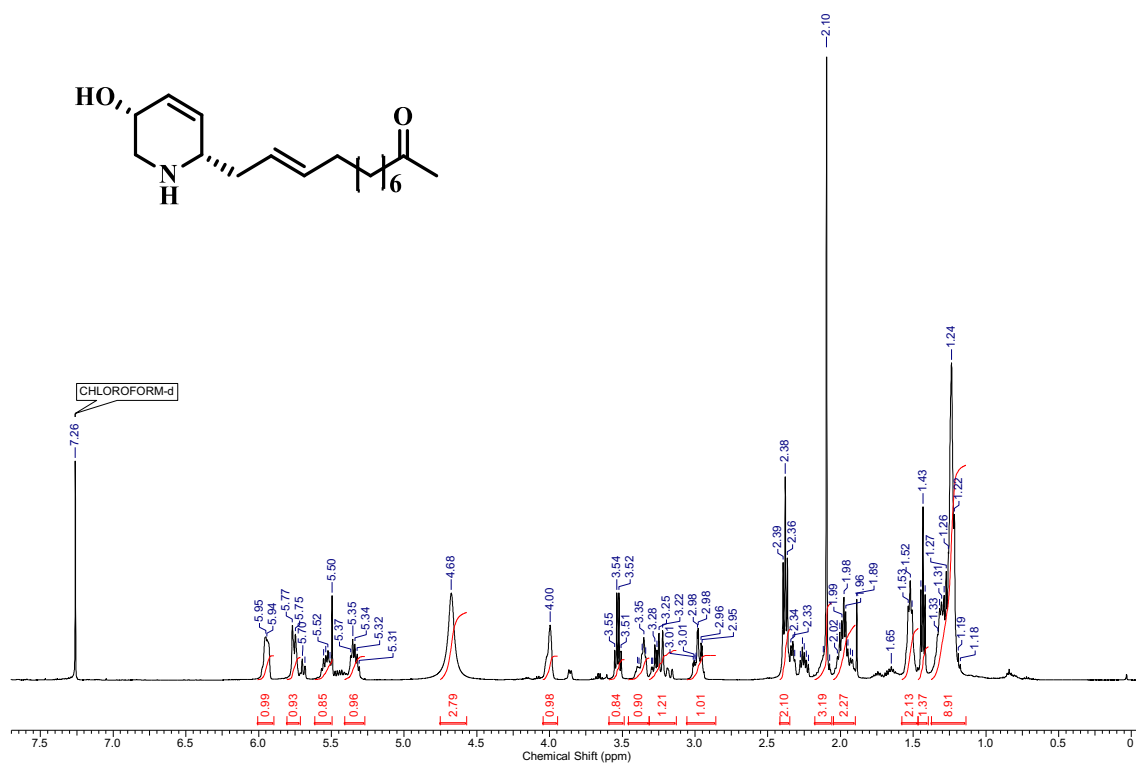


Figure S42. ¹H NMR spectra of compound **10b** (CDCl₃, 500 MHz)

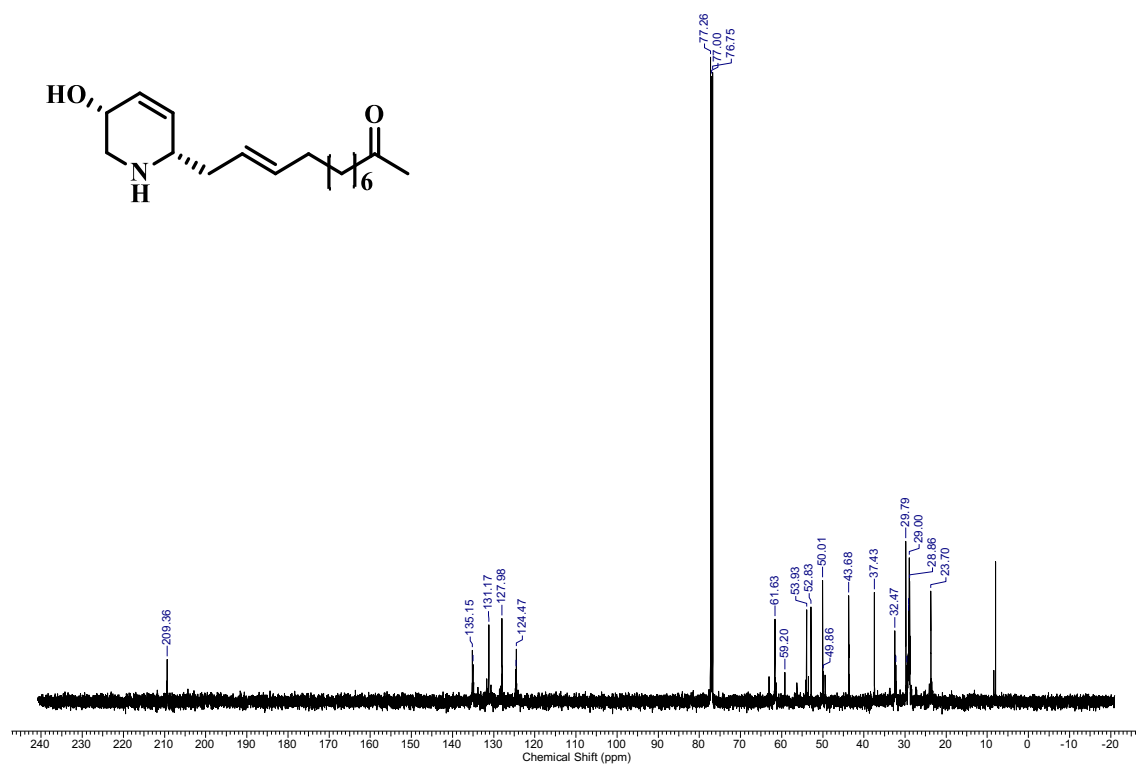


Figure S43. ¹³C NMR spectra of compound **10b** (CDCl₃, 126 MHz)

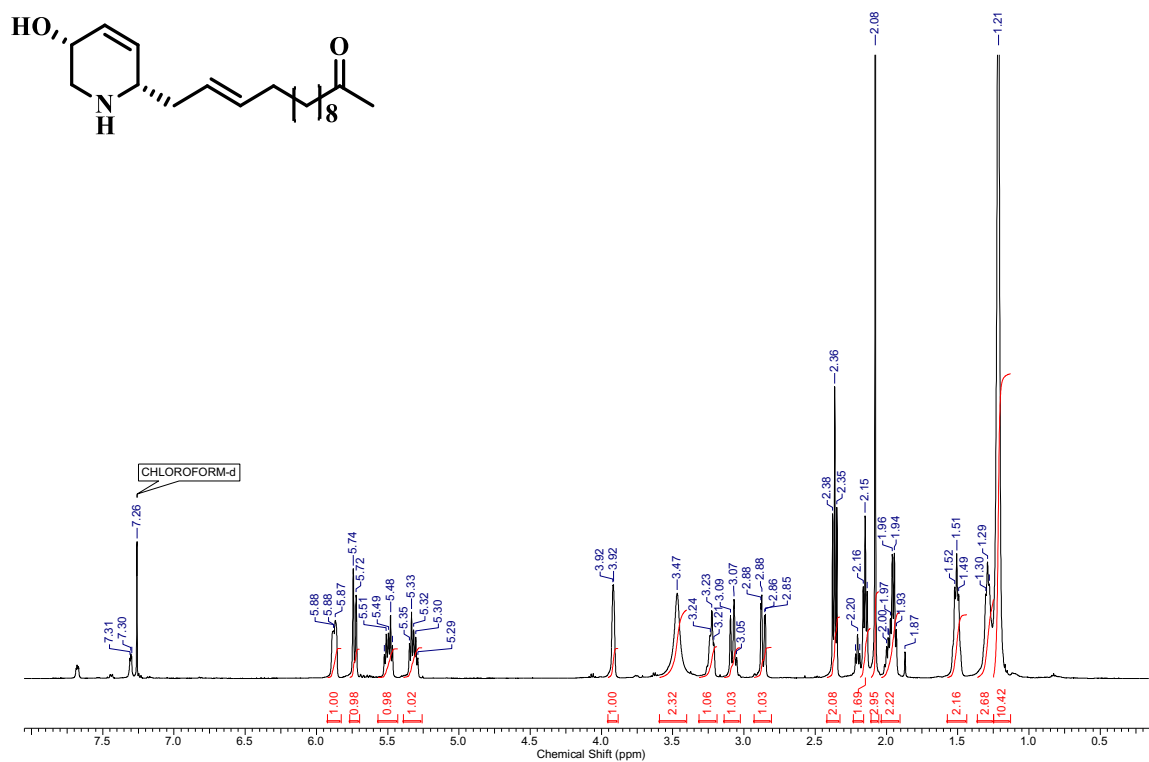


Figure S44. ¹H NMR spectra of compound **10c** (CDCl₃, 500 MHz)

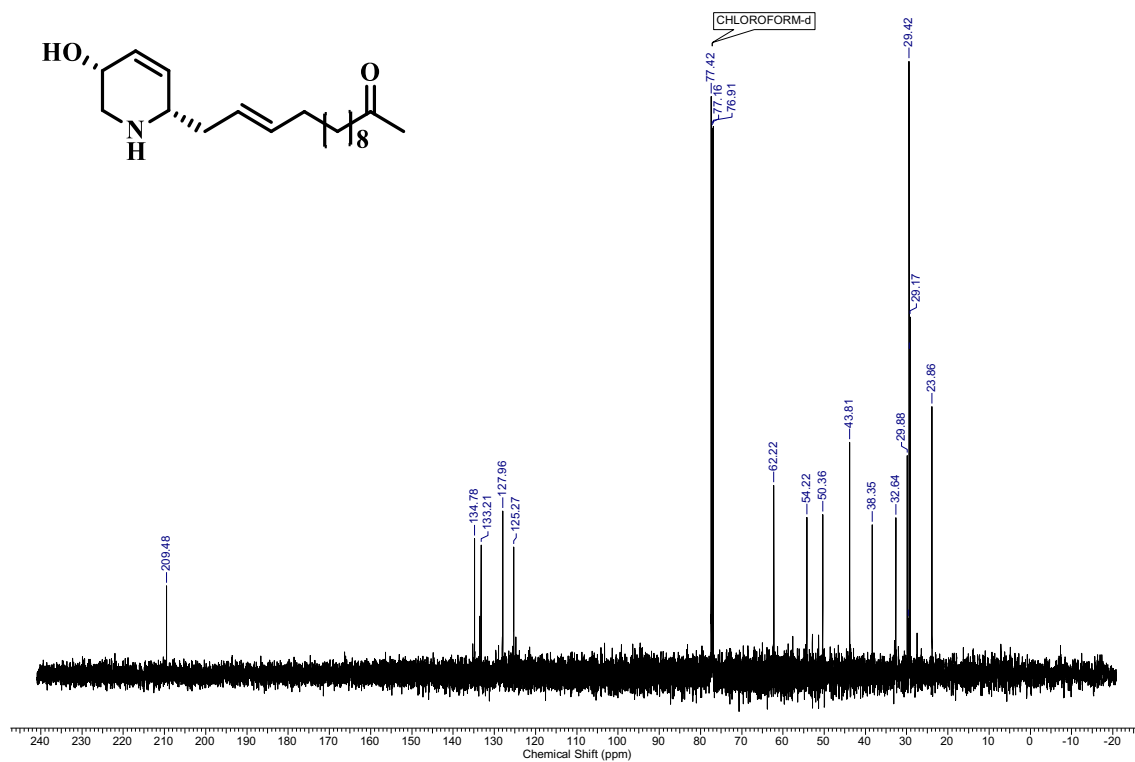


Figure S45. ¹³C NMR spectra of compound **10c** (CDCl₃, 126 MHz)

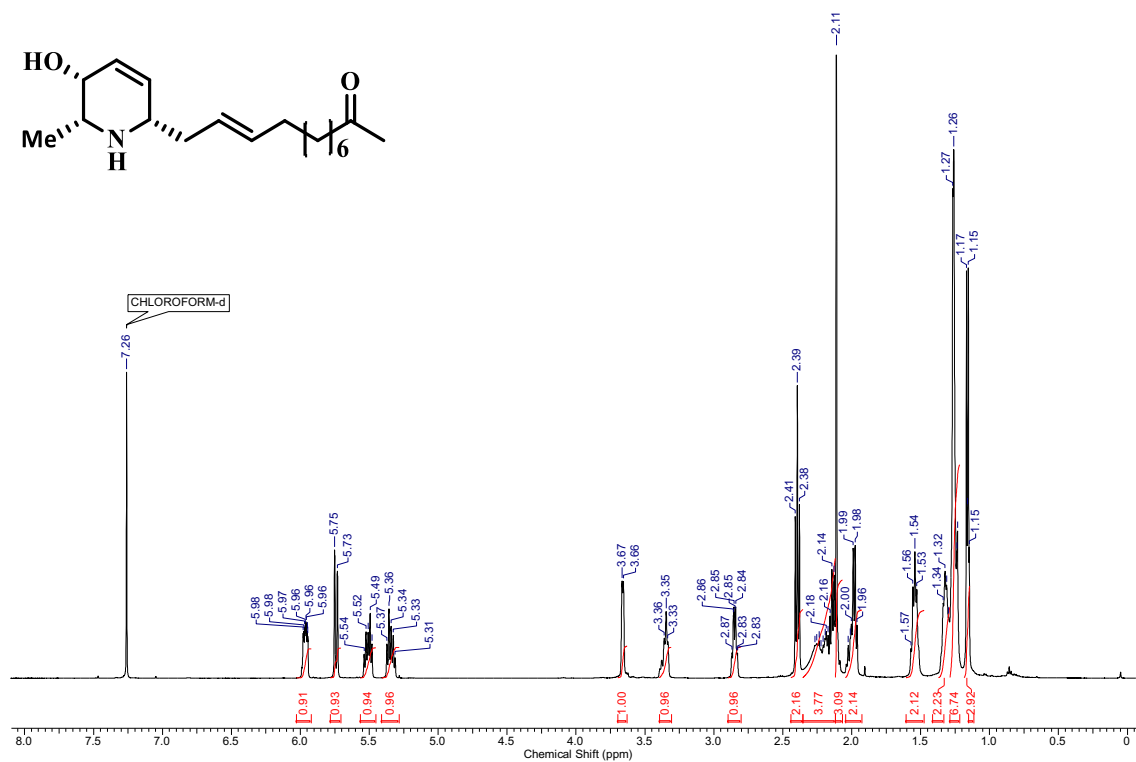


Figure S46. ¹H NMR spectra of compound **10d** (CDCl₃, 500 MHz)

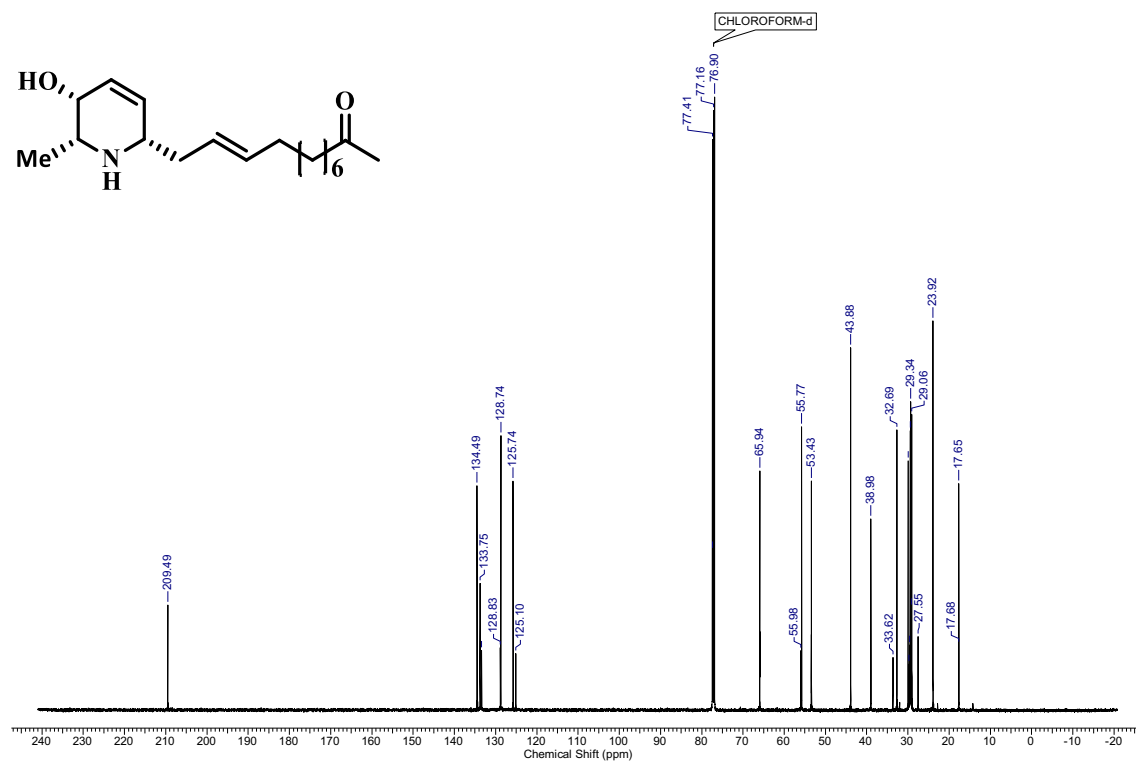


Figure S47. ¹³C NMR spectra of compound **10d** (CDCl₃, 126 MHz)

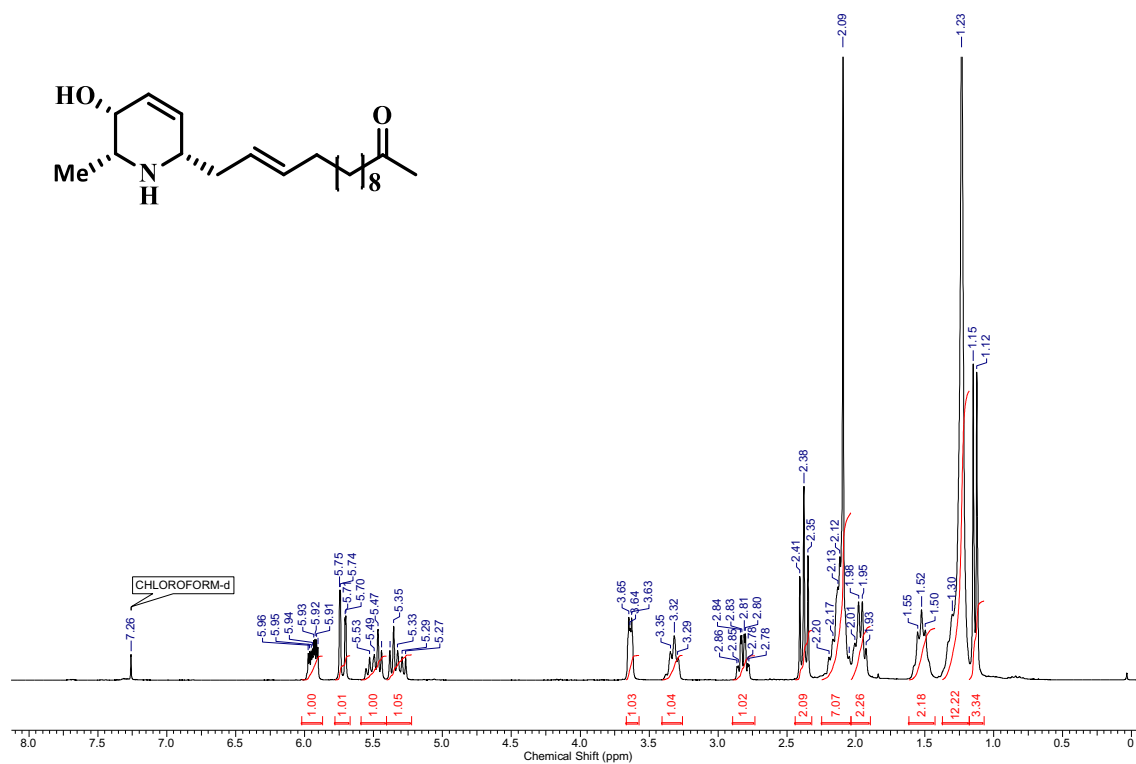


Figure S48. ¹H NMR spectra of compound **10e** (CDCl₃, 250 MHz)

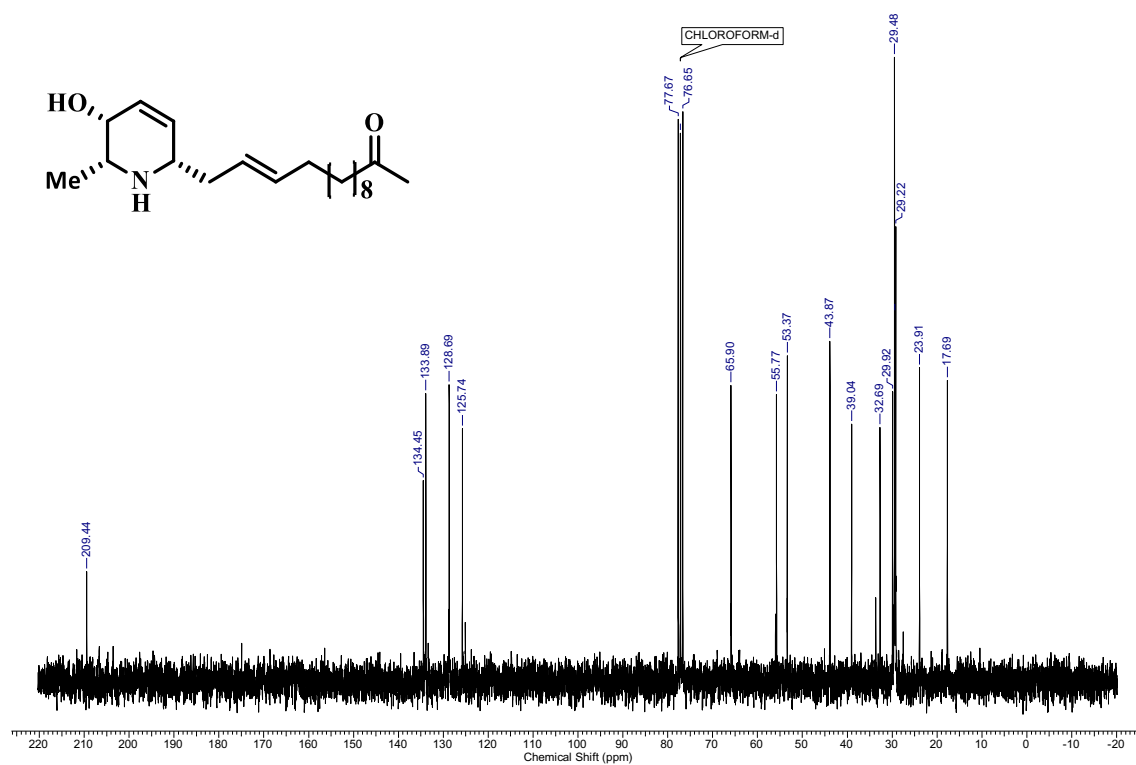


Figure S49. ¹³C NMR spectra of compound **10e** (CDCl₃, 63 MHz)

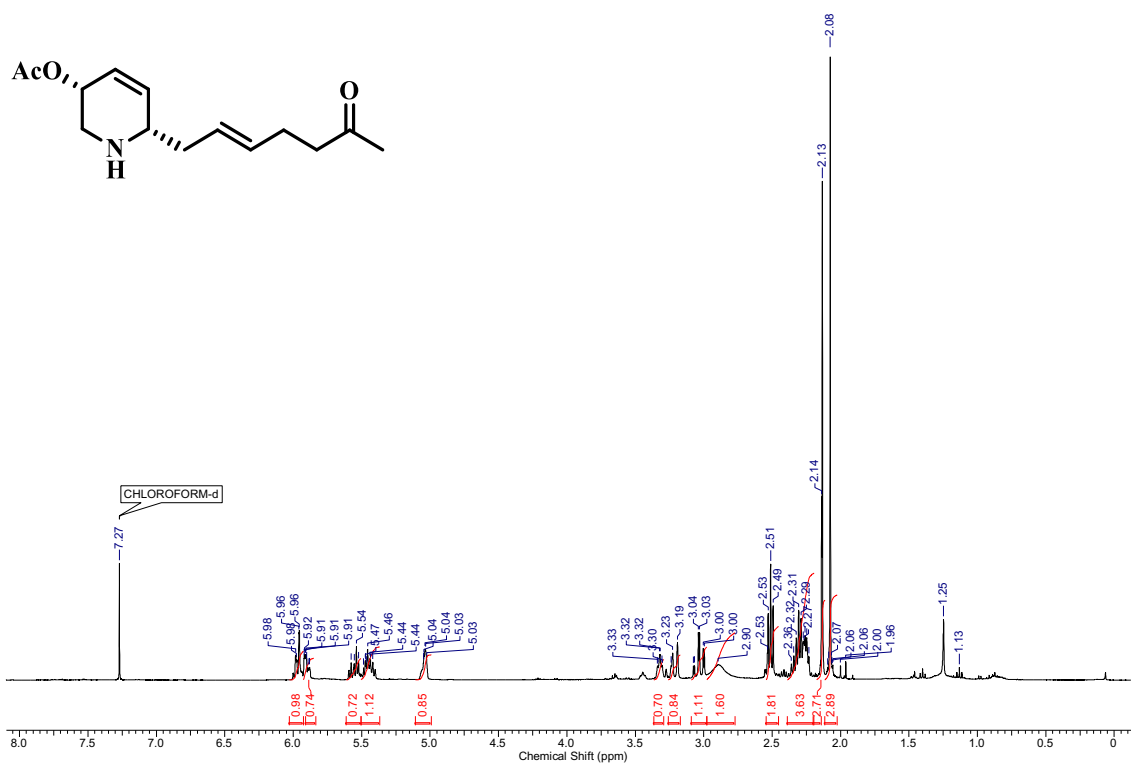


Figure S50. ¹H NMR spectra of compound **11a** (CDCl₃, 400 MHz)

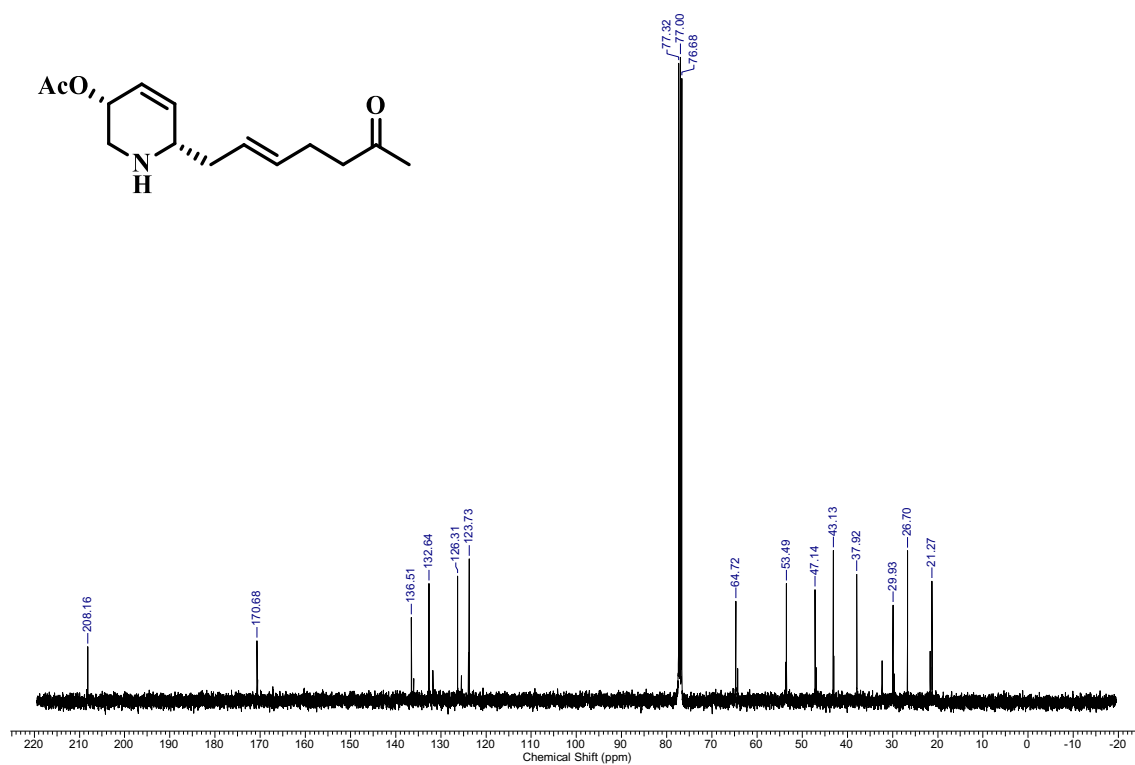


Figure S51. ¹³C NMR spectra of compound **11a** (CDCl₃, 101 MHz)

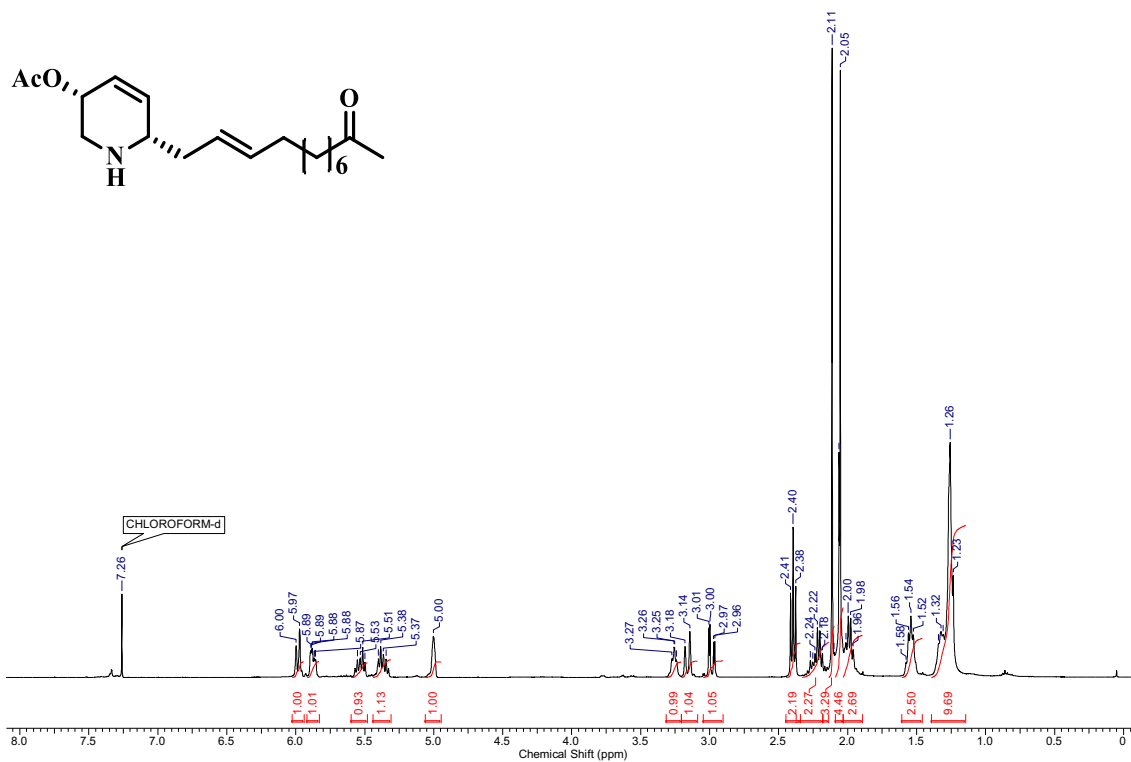


Figure S52. ^1H NMR spectra of compound **11b** (CDCl_3 , 400 MHz)

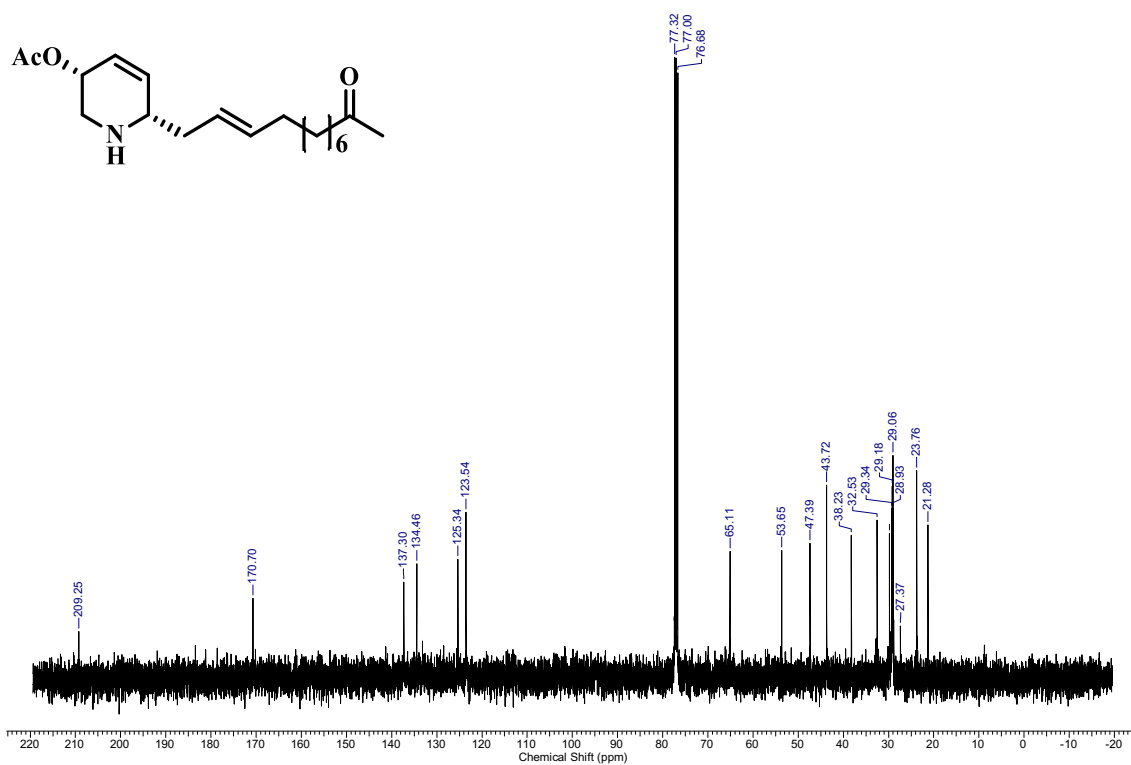


Figure S53. ^{13}C NMR spectra of compound **11b** (CDCl_3 , 101 MHz)

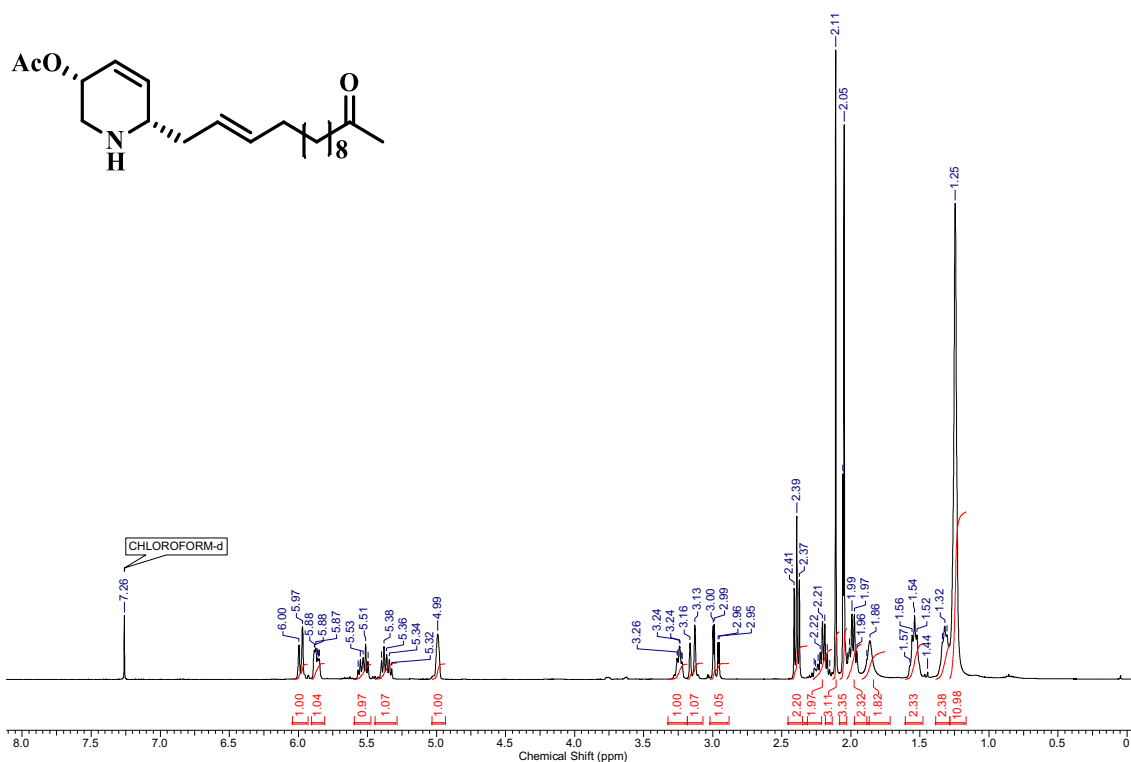


Figure S54. ¹H NMR spectra of compound **11c** (CDCl₃, 400 MHz)

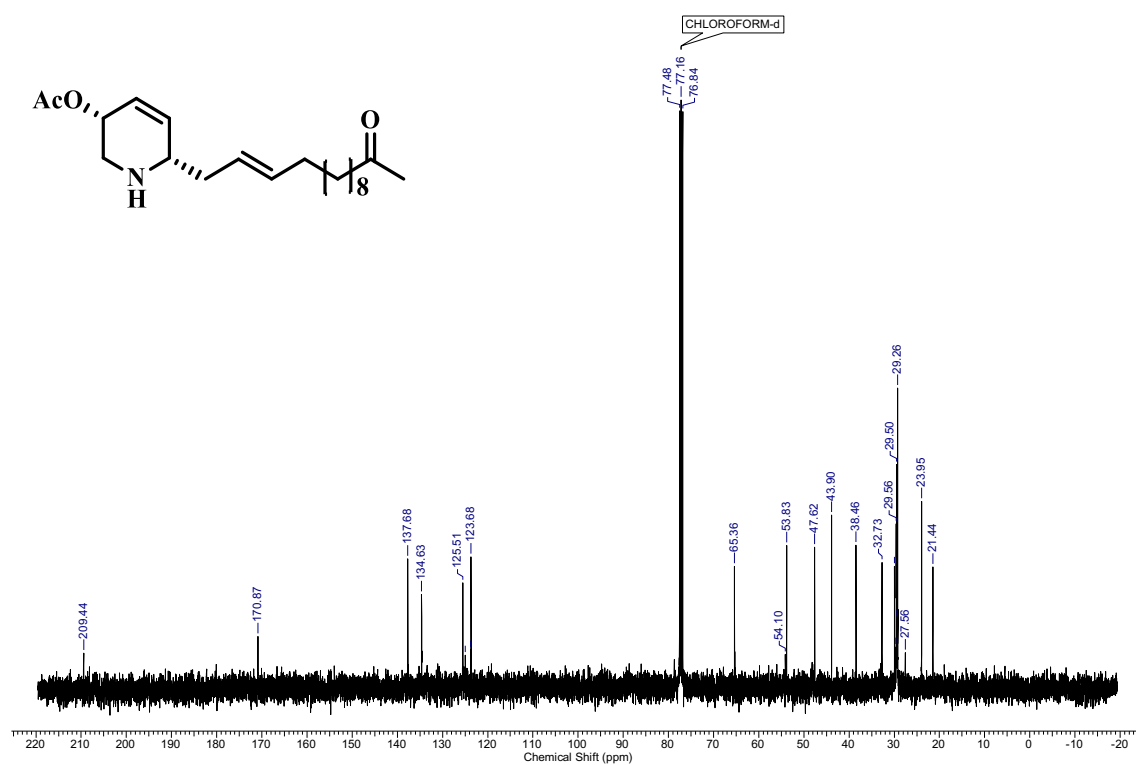


Figure S55. ¹³C NMR spectra of compound **11c** (CDCl₃, 101 MHz)

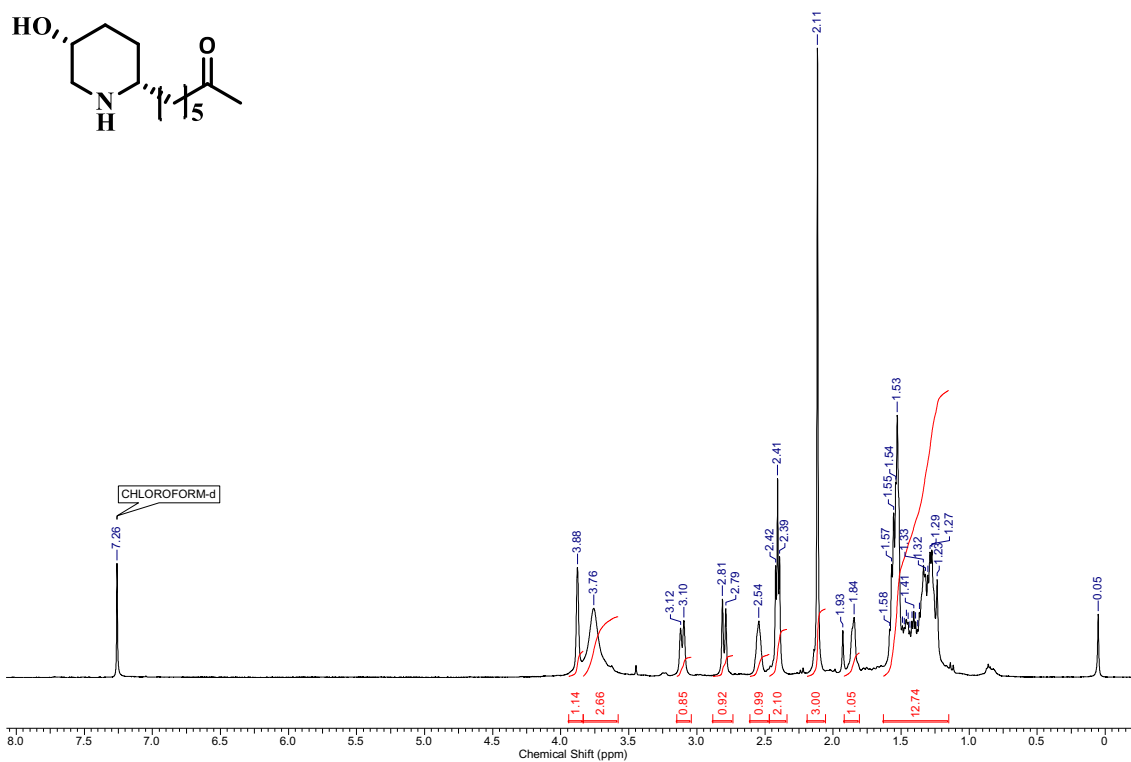


Figure S56. ¹H NMR spectra of compound **12a** (CDCl₃, 500 MHz)

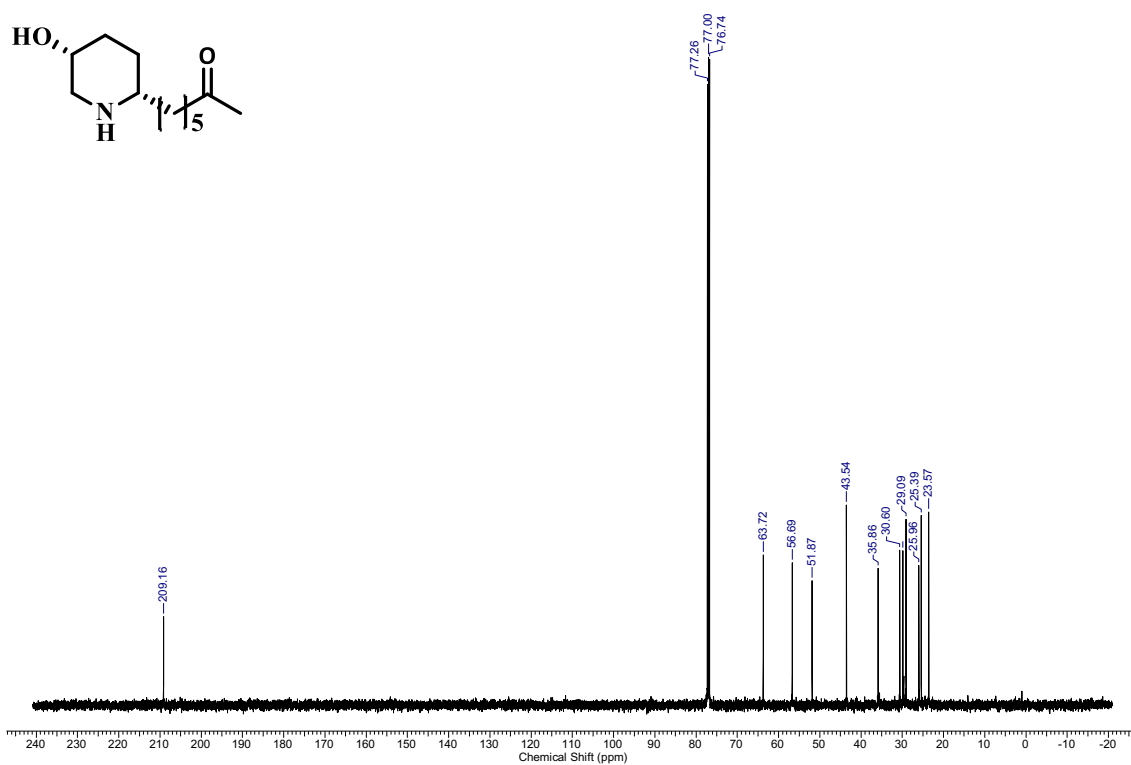


Figure S57. ¹³C NMR spectra of compound **12a** (CDCl₃, 126 MHz)

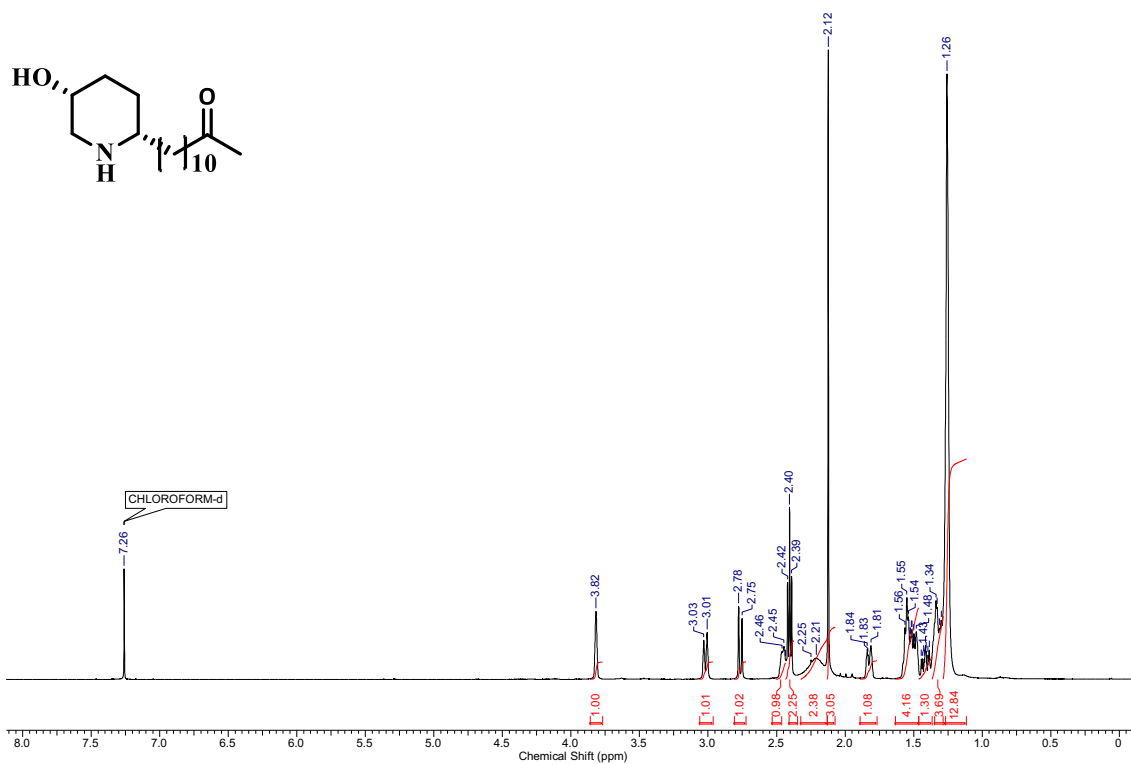


Figure S58. ^1H NMR spectra of compound **12b** (CDCl_3 , 500 MHz)

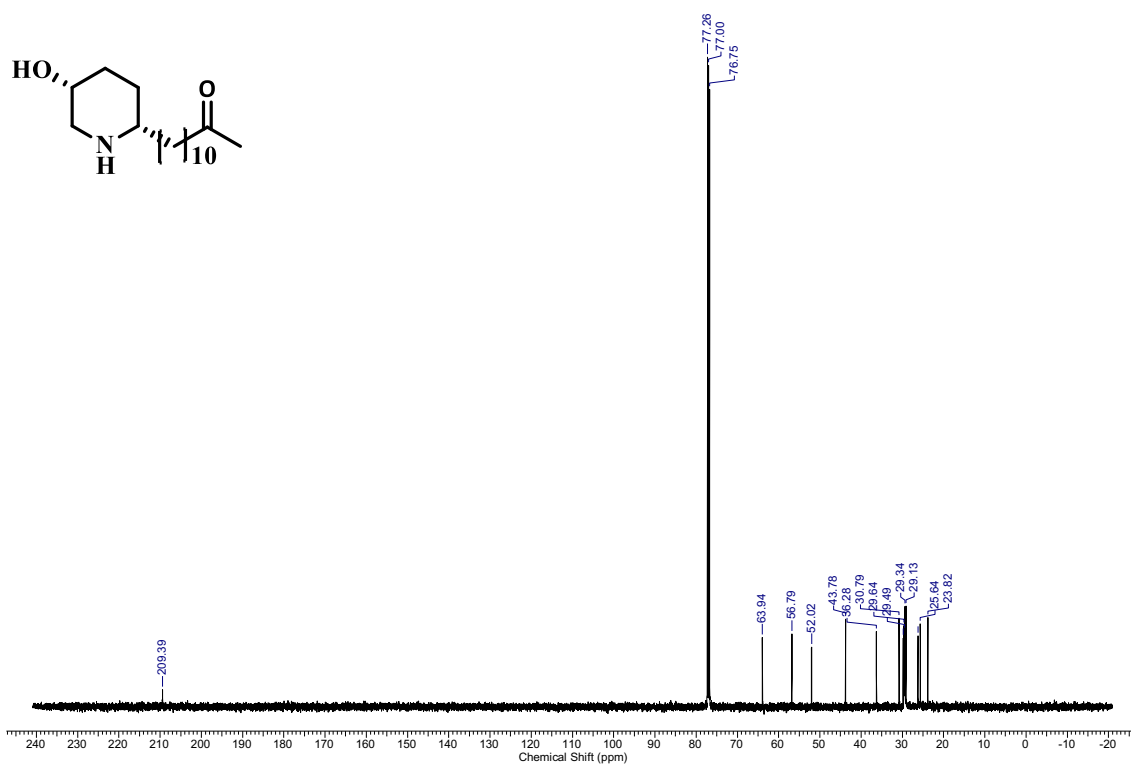


Figure S59. ^{13}C NMR spectra of compound **12b** (CDCl_3 , 126 MHz)

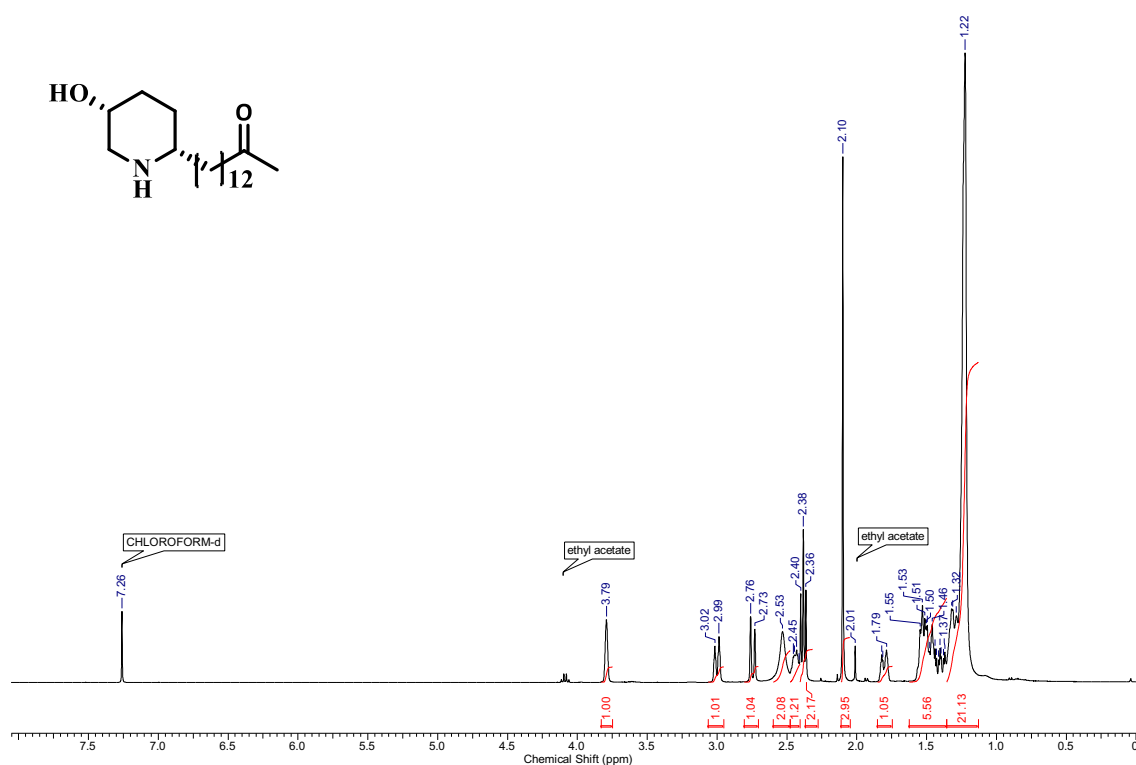


Figure S60. ¹H NMR spectra of compound **12c** (CDCl₃, 400 MHz)

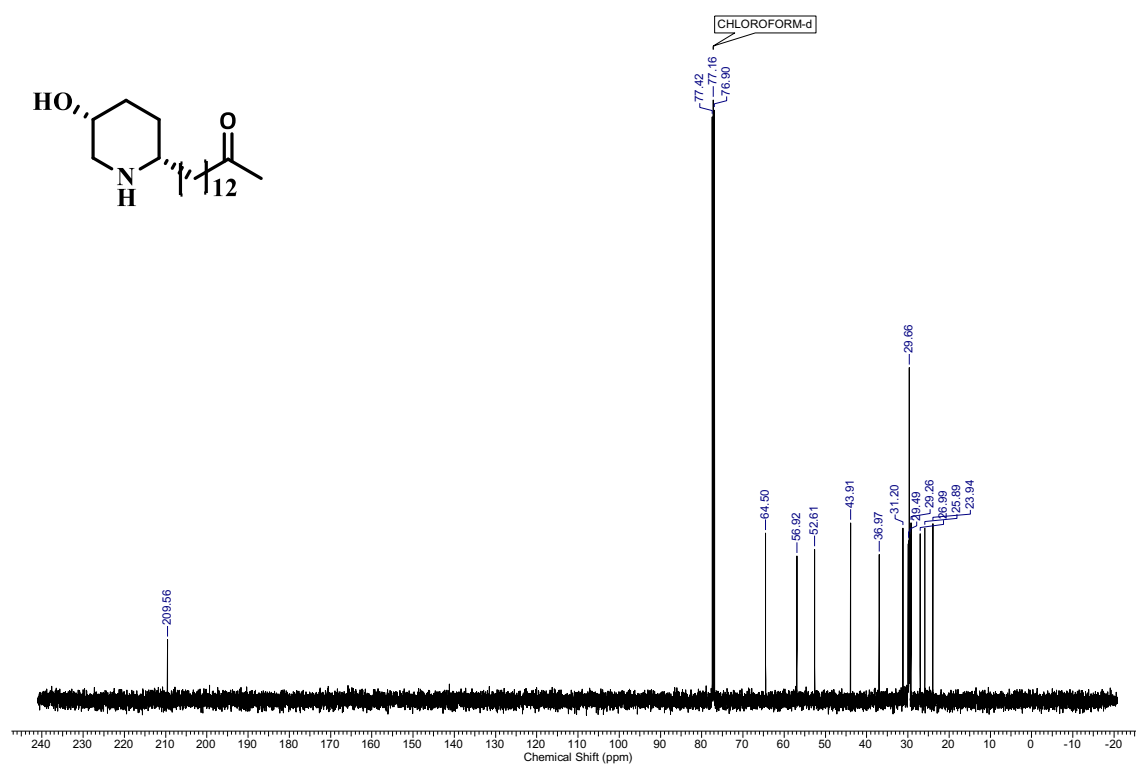


Figure S61. ¹³C NMR spectra of compound **12c** (CDCl₃, 101 MHz)

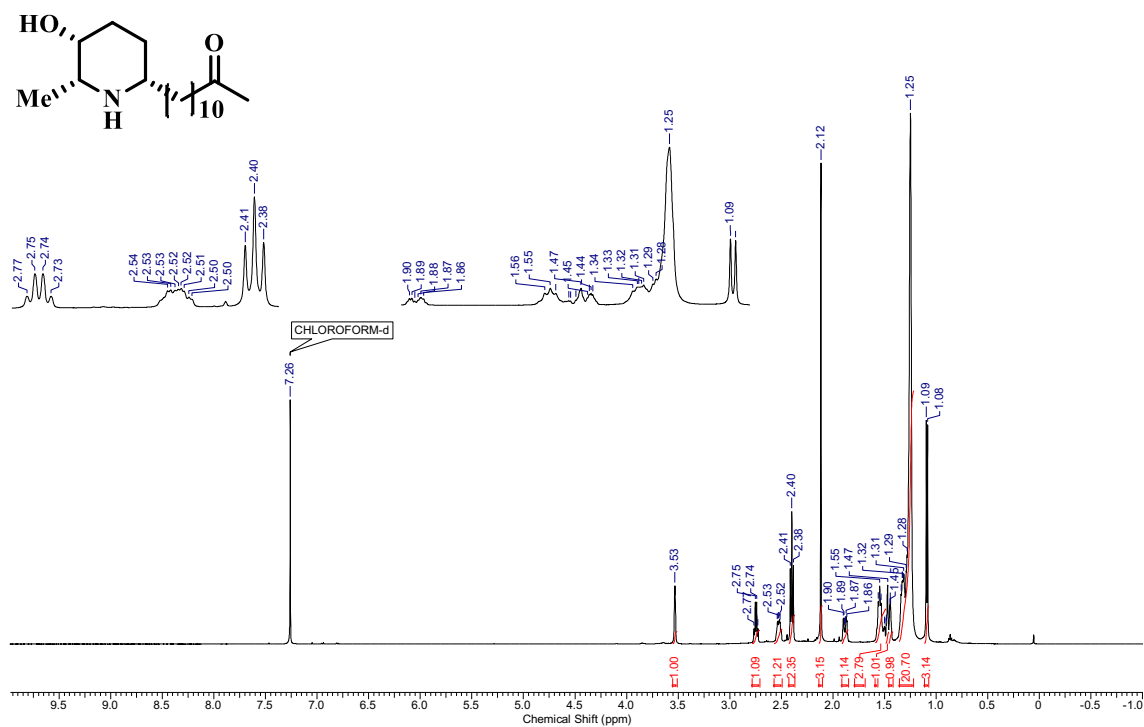


Figure S62. ¹H NMR spectra of compound **1** (\pm -cassine) (CDCl₃, 500 MHz)

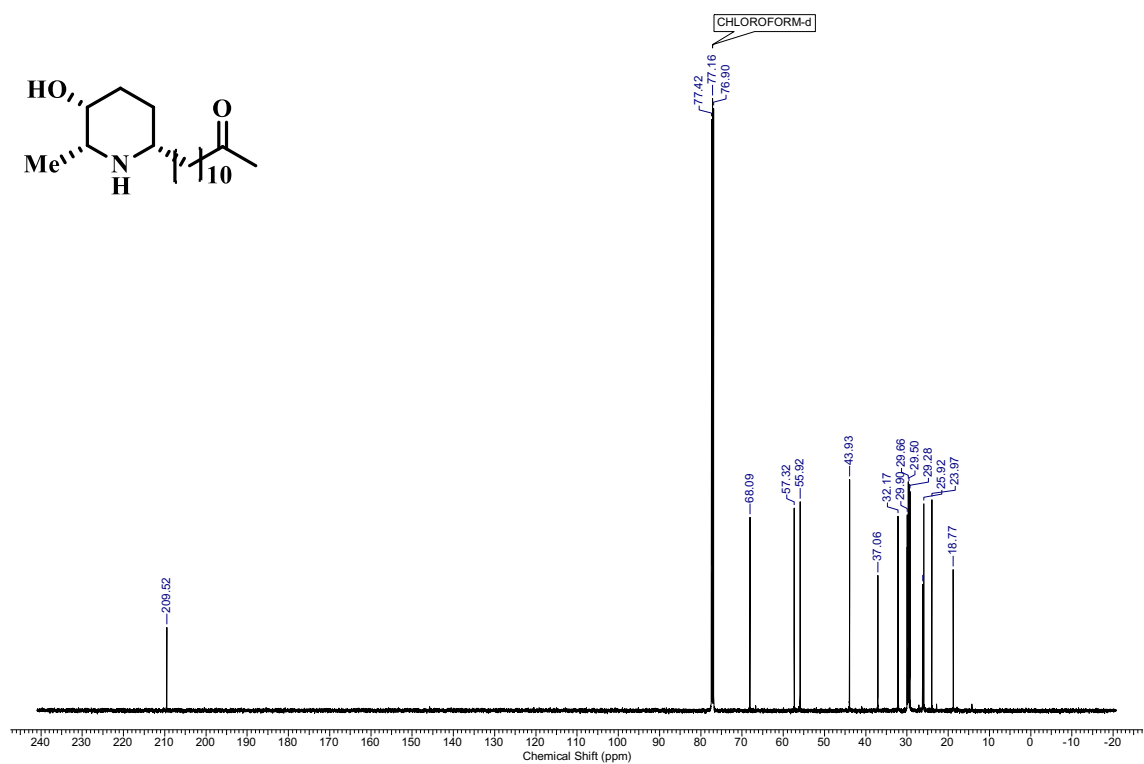


Figure S63. ¹³C NMR spectra of compound **1** (\pm -cassine) (CDCl₃, 126 MHz)

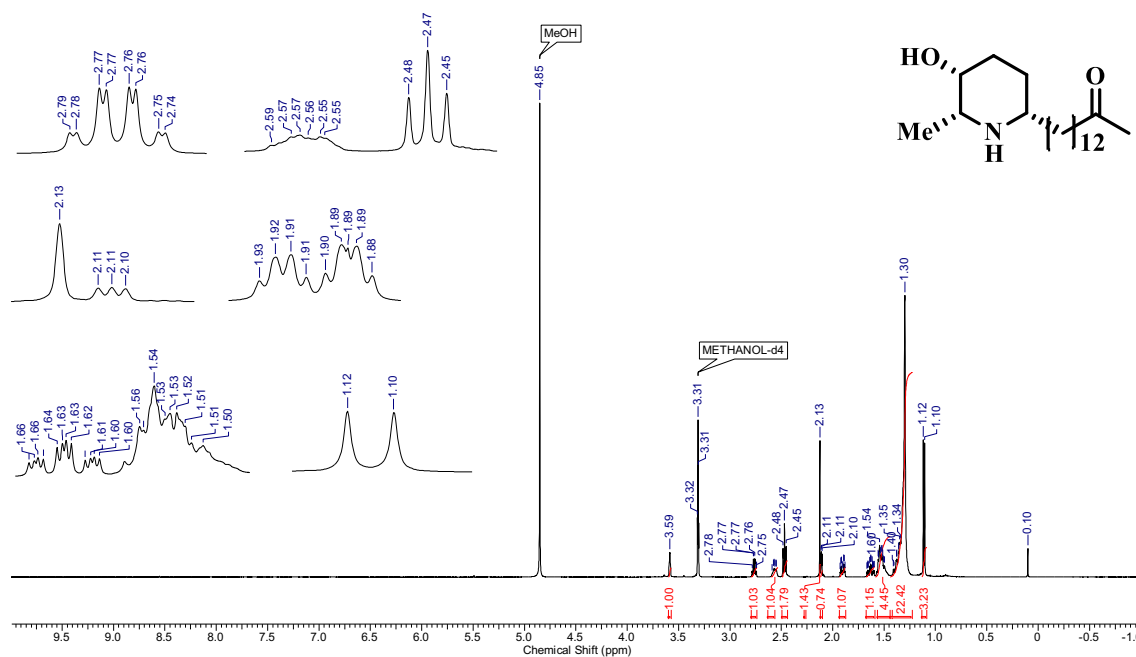


Figure S64. ¹H NMR spectra of compound 3 (±-spectaline) (MeOD, 500 MHz)

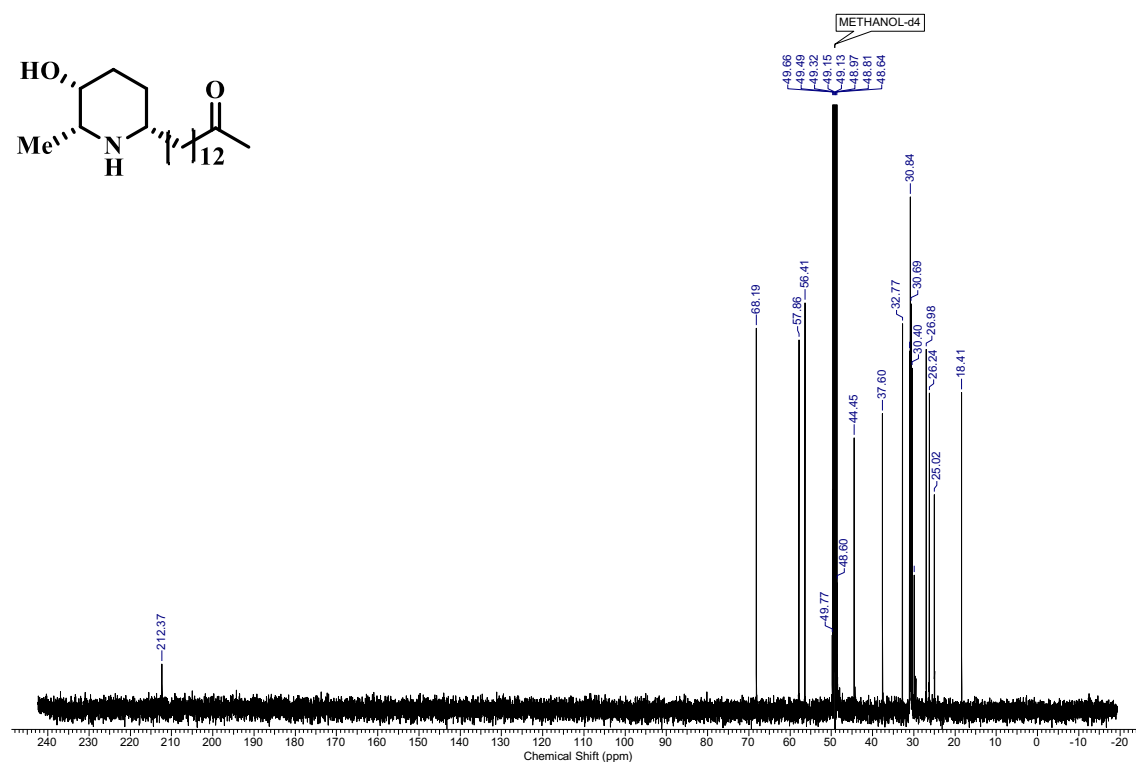


Figure S65. ¹³C NMR spectra of compound 3 (±-spectaline) (MeOD, 126 MHz)

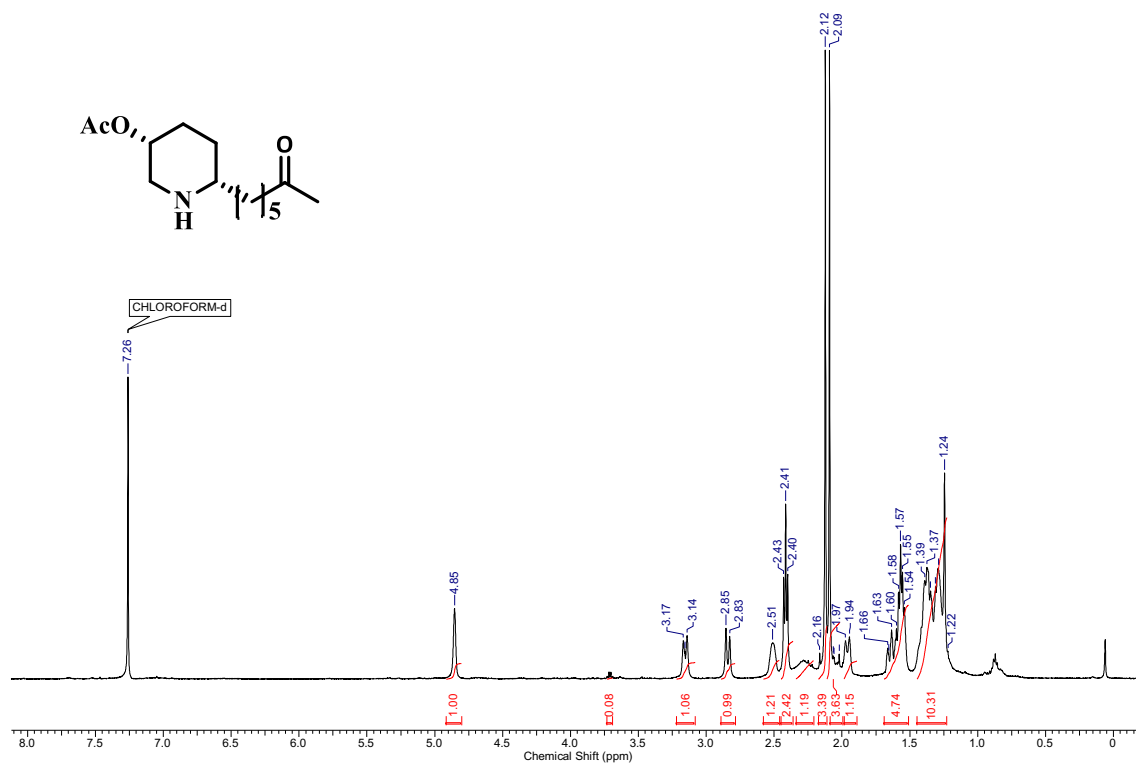


Figure S66. ¹H NMR spectra of compound **13a** (CDCl₃, 400 MHz)

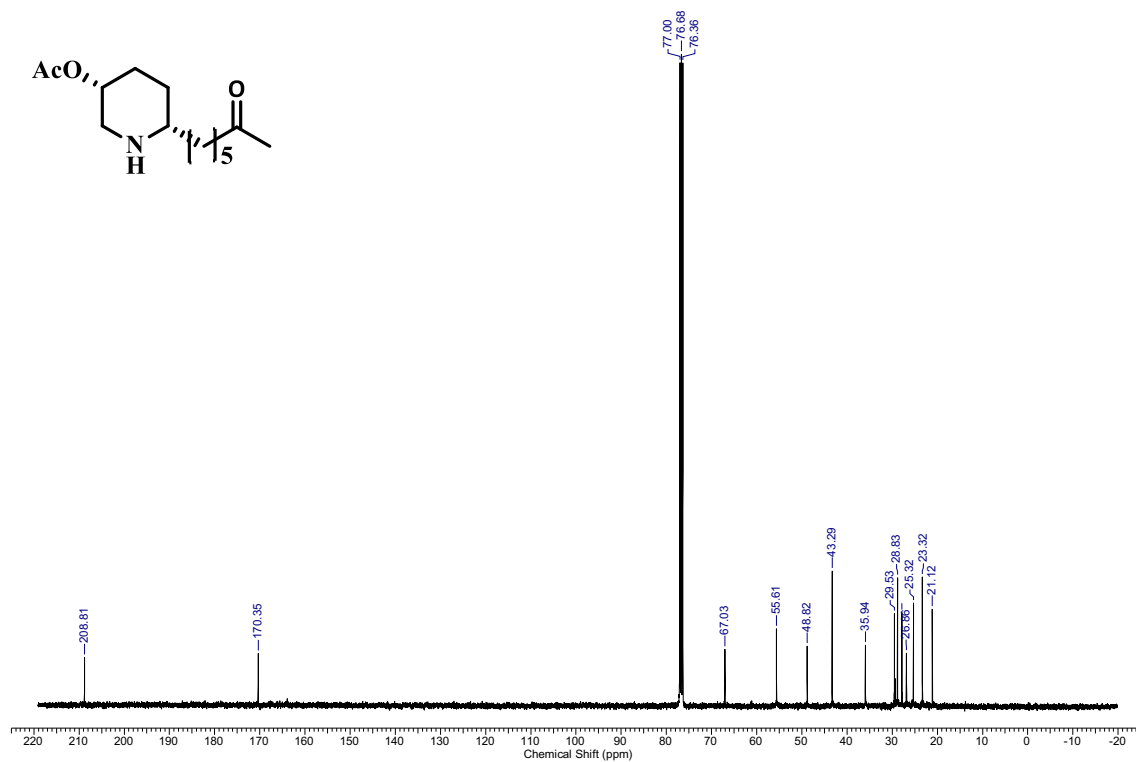


Figure S67. ¹³C NMR spectra of compound **13a** (CDCl₃, 101 MHz)

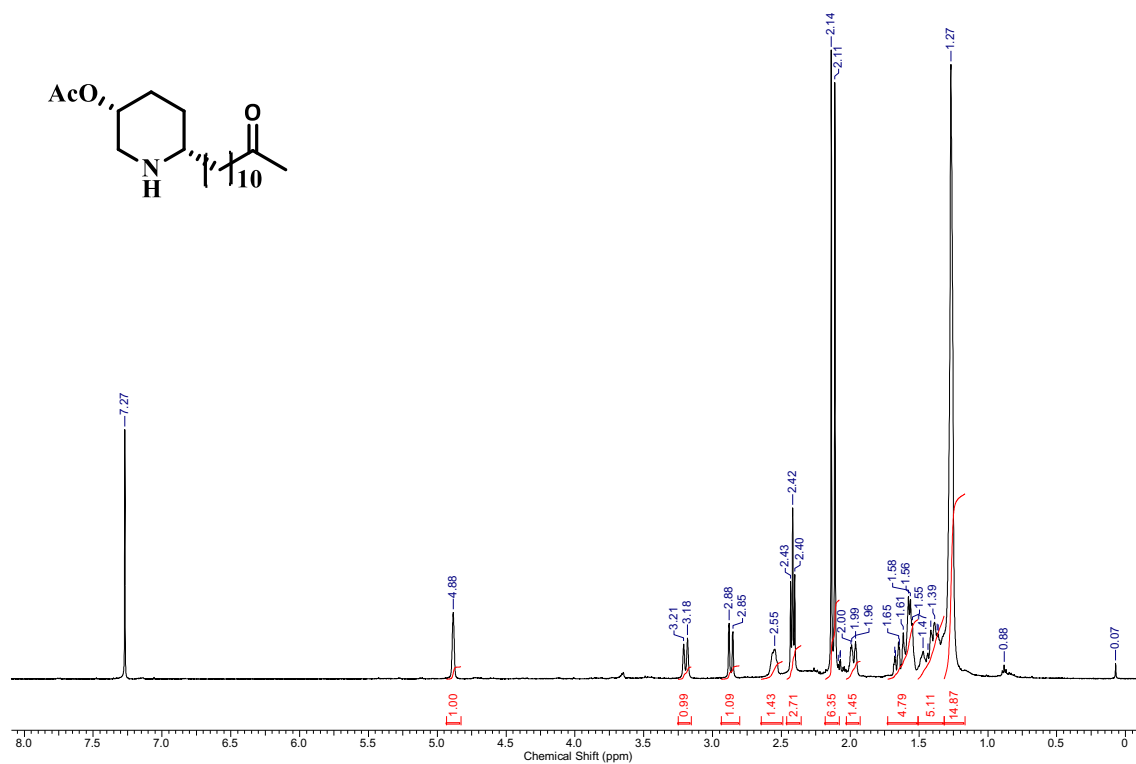


Figure S68. ¹H NMR spectra of compound **13b** (CDCl₃, 500 MHz)

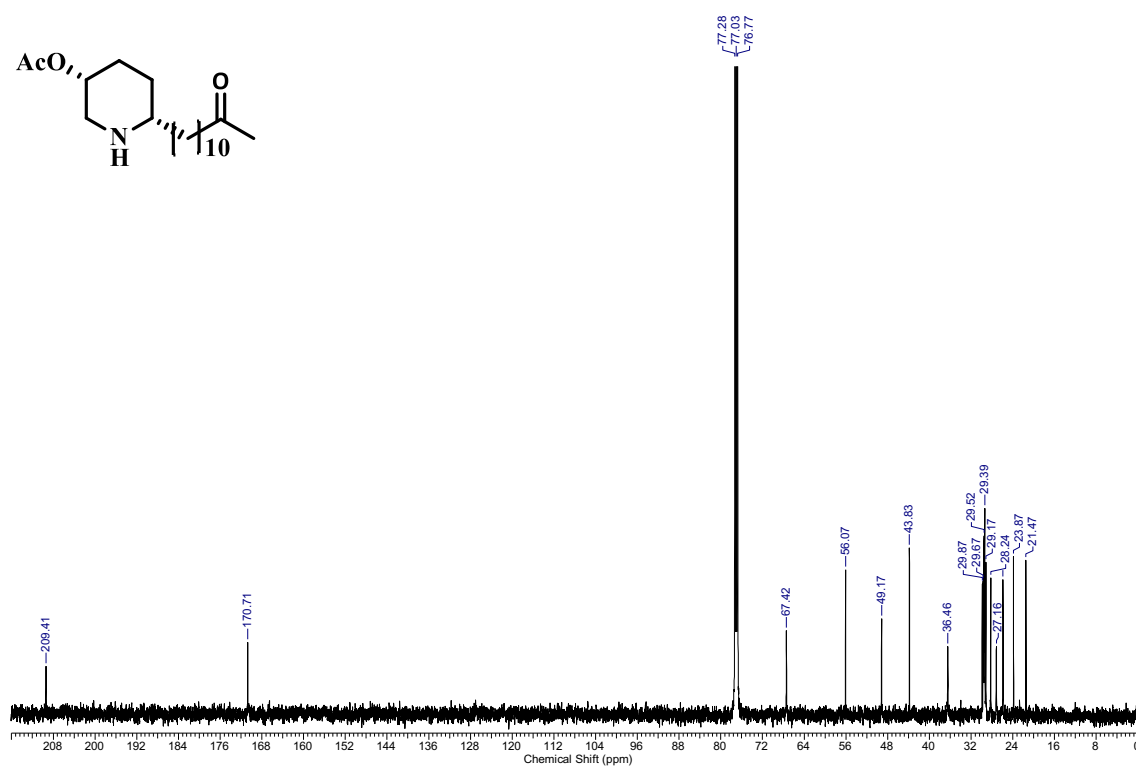


Figure S69. ¹³C NMR spectra of compound **13b** (CDCl₃, 126 MHz)

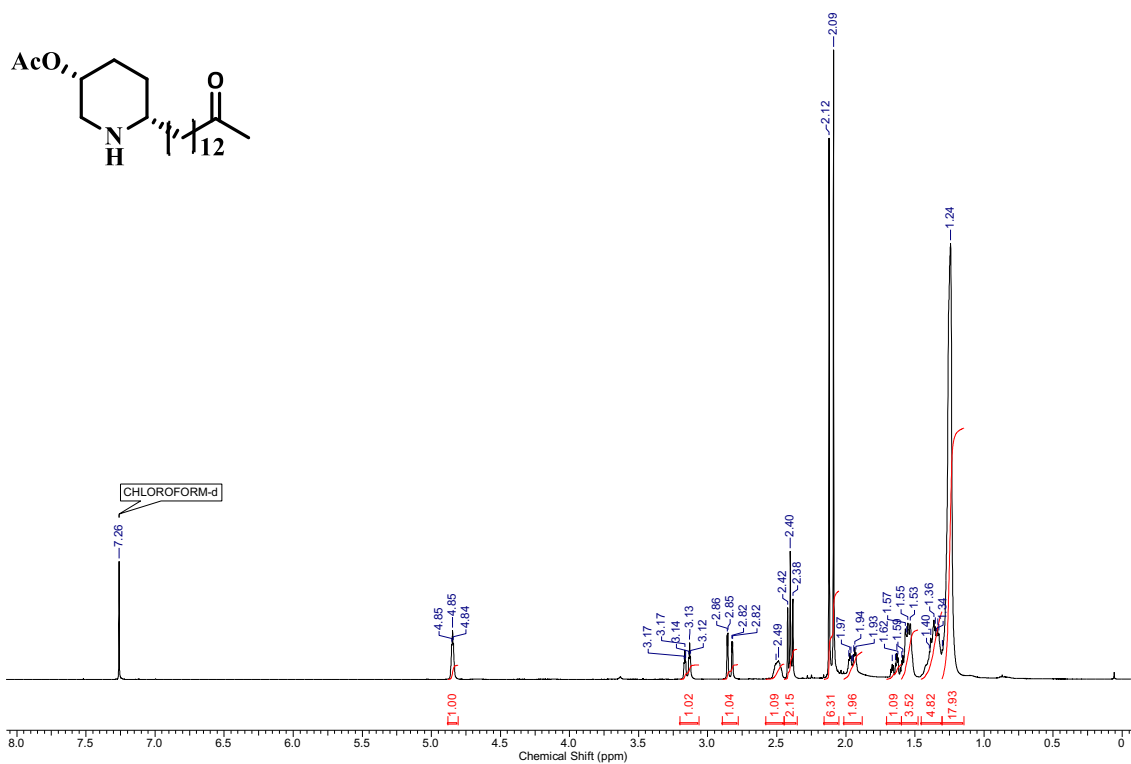


Figure S70. ^1H NMR spectra of compound **13c** (CDCl₃, 400 MHz)

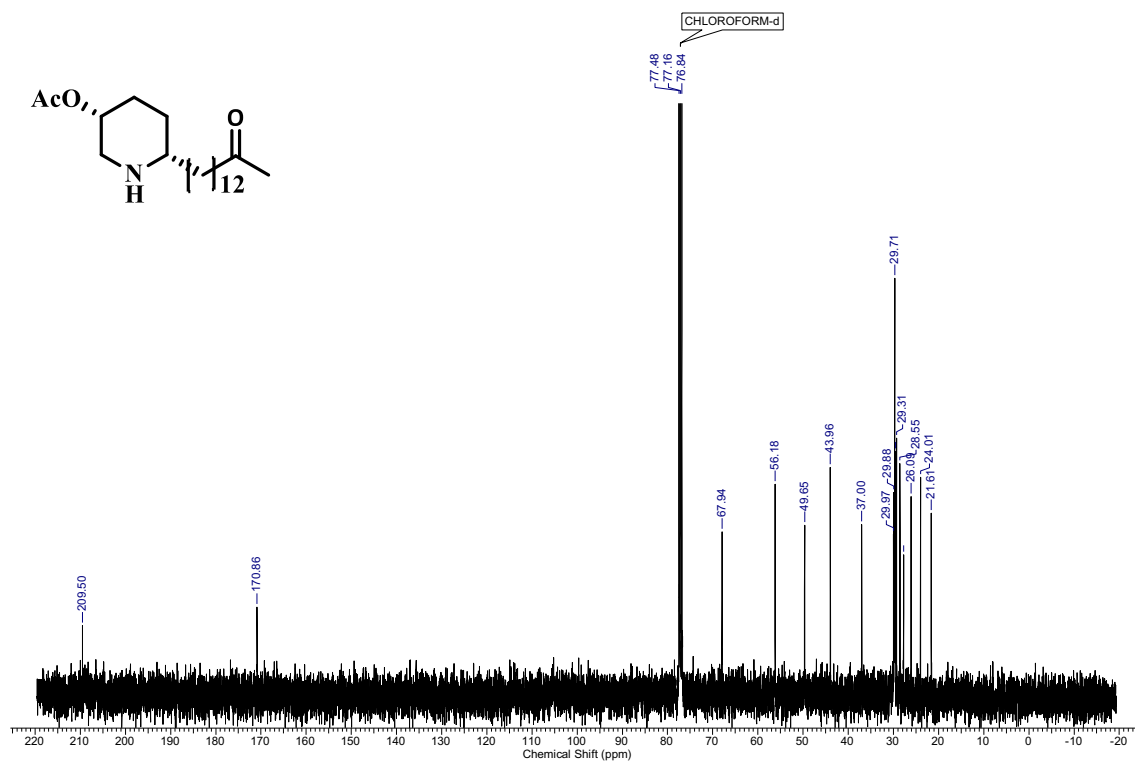


Figure S71. ^{13}C NMR spectra of compound **13c** (CDCl₃, 101 MHz)

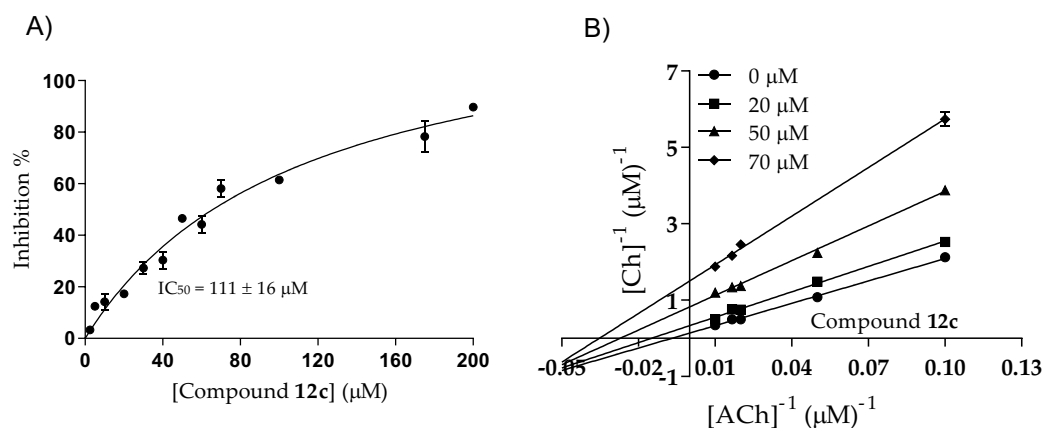


Figure S72. Dose-response inhibition curve (A) and Lineweaver-Burk reciprocal plots (B) for compound **12c** BChE_{hu}-ICER using the on-flow dual parallel enzyme assay. Results obtained from three independent experiments (n = 3) expressed by mean ± SEM).

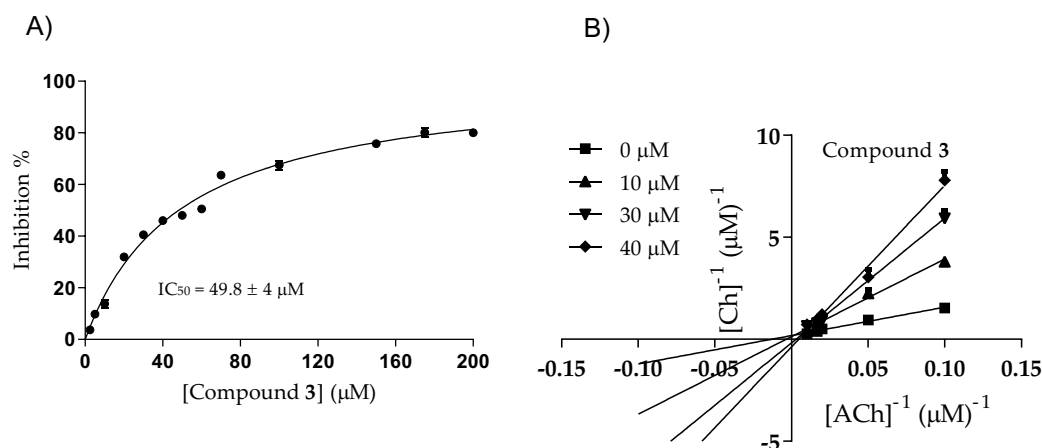


Figure S73. Dose-response inhibition curve (A) and Lineweaver-Burk reciprocal plots (B) for compound **3** BChE_{hu}-ICER using the on-flow dual parallel enzyme assay. Results obtained from three independent experiments (n = 3) expressed by mean ± SEM).