

Supplementary Material

**Pyrazolines as potential anti-alzheimer's agents: DFT, molecular docking,
enzyme inhibition and pharmacokinetic studies**

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Figure 1. ^1H NMR (400 MHz, CDCl_3) of compound **1a**.

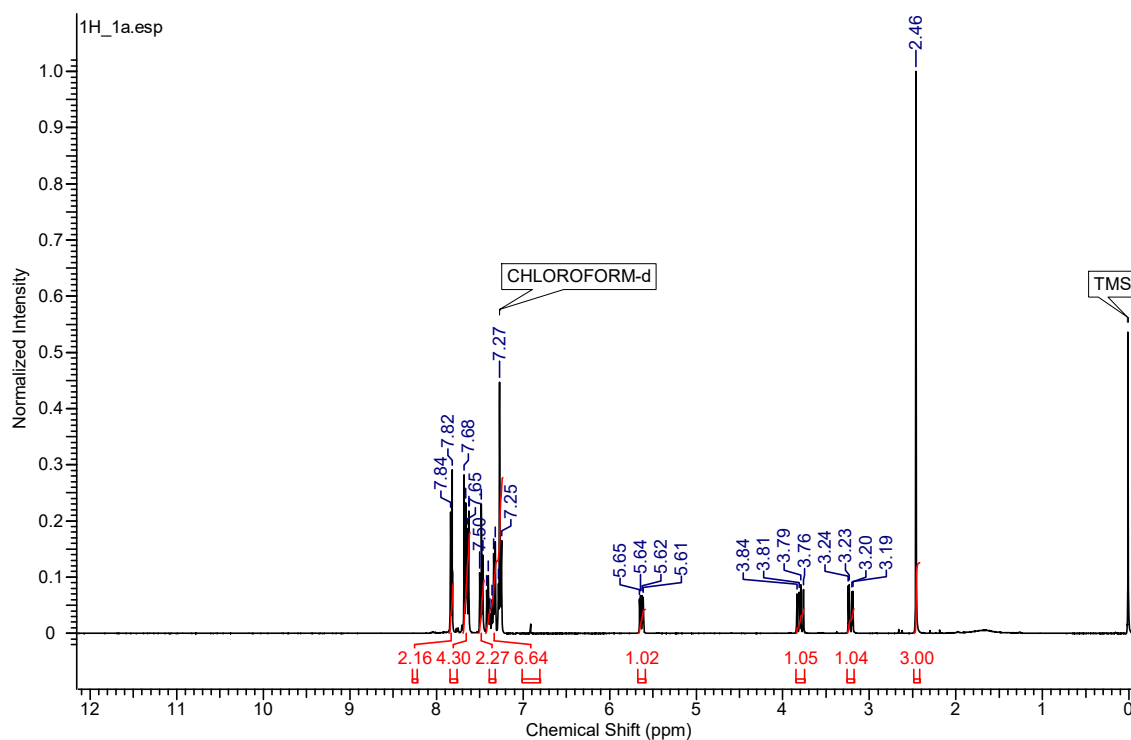


Figure 2. ^{13}C NMR (100 MHz, CDCl_3) of compound **1a**.

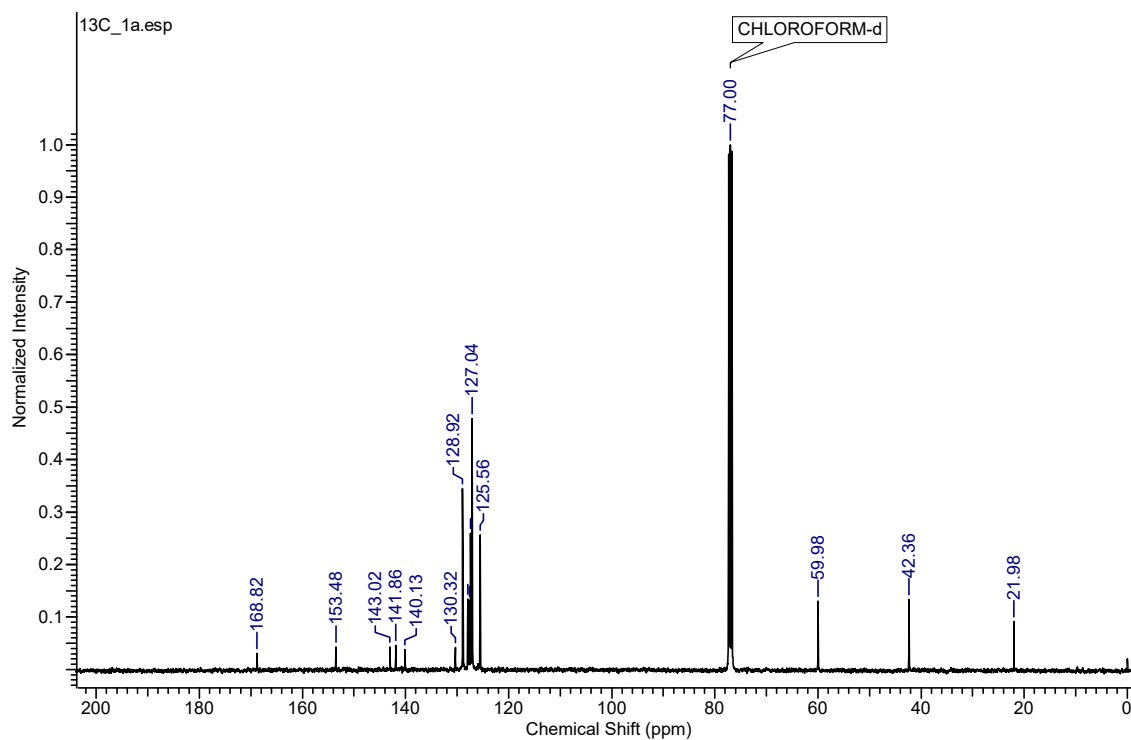


Figure 3. HR-ESI-MS of compound **1a**.

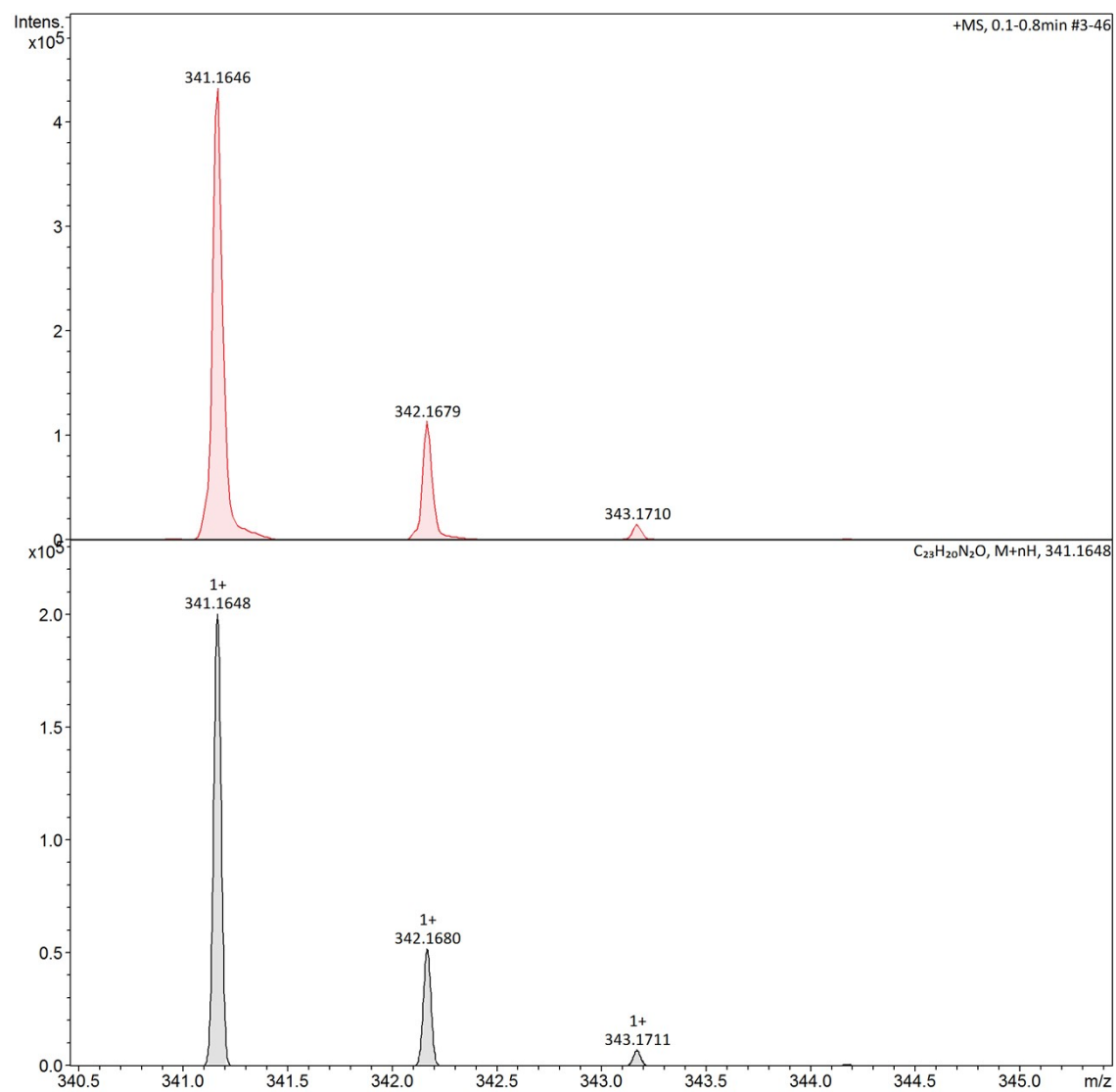


Figure 4. ^1H NMR (200 MHz, CDCl_3) of compound **1b**.

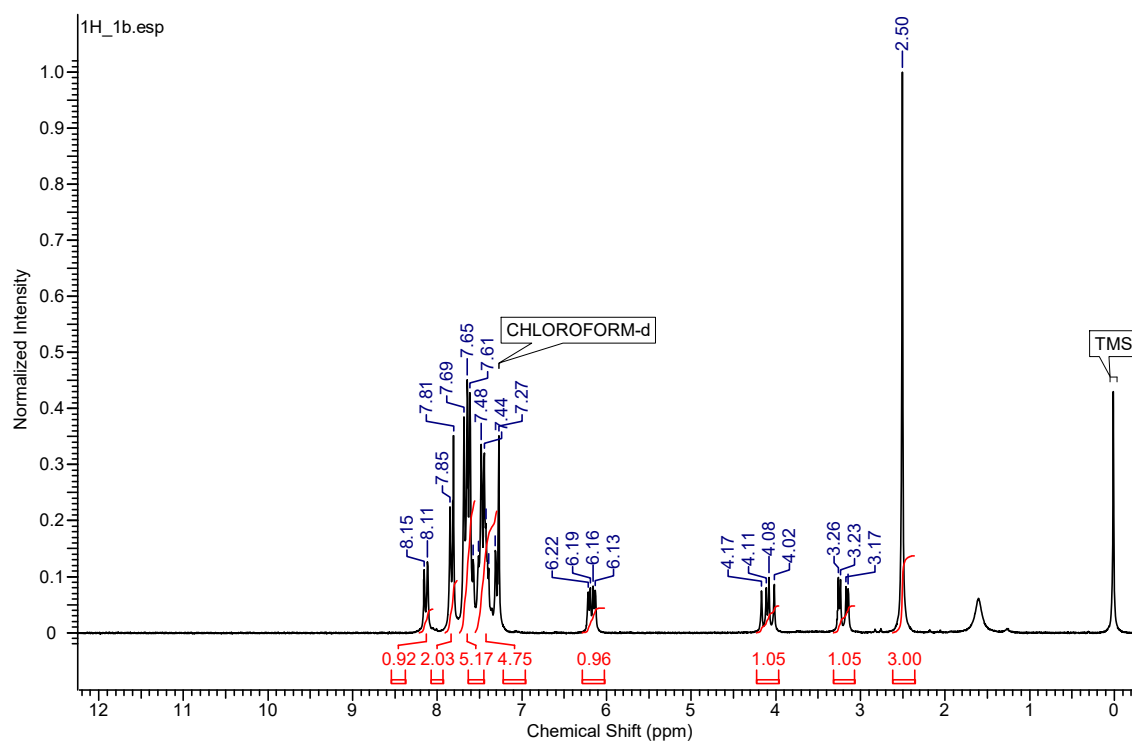


Figure 5. ^{13}C NMR (50 MHz, CDCl_3) of compound **1b**.

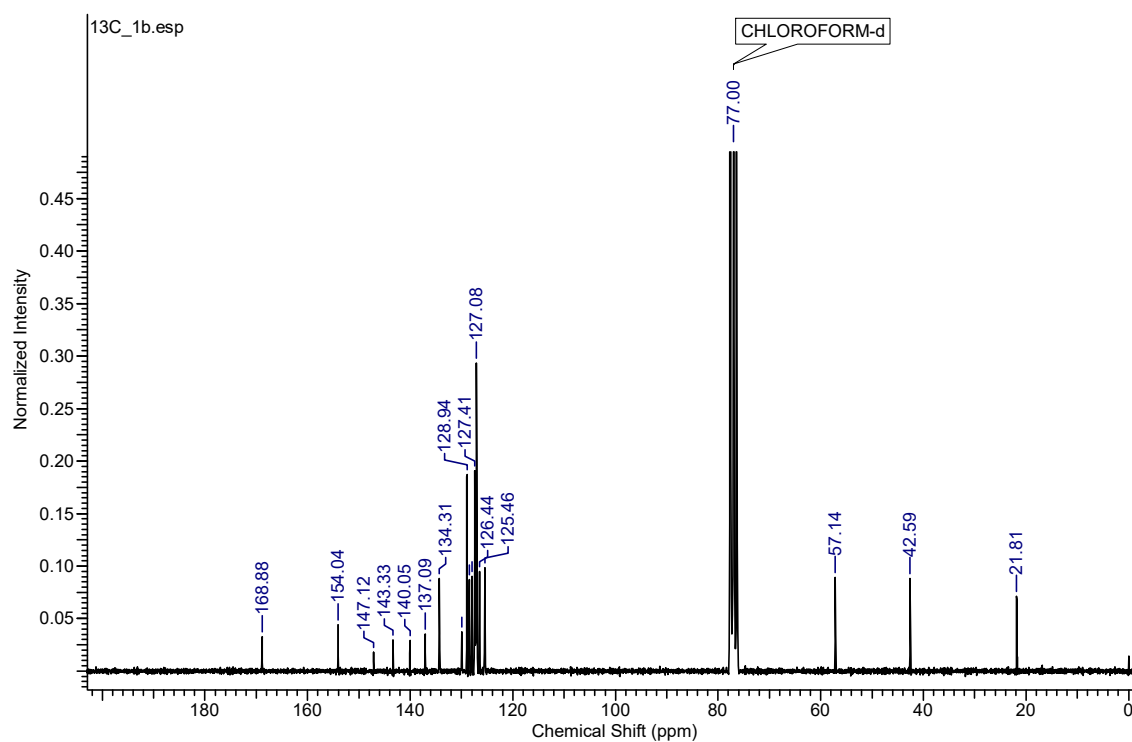


Figure 6. HR-ESI-MS of compound **1b**.

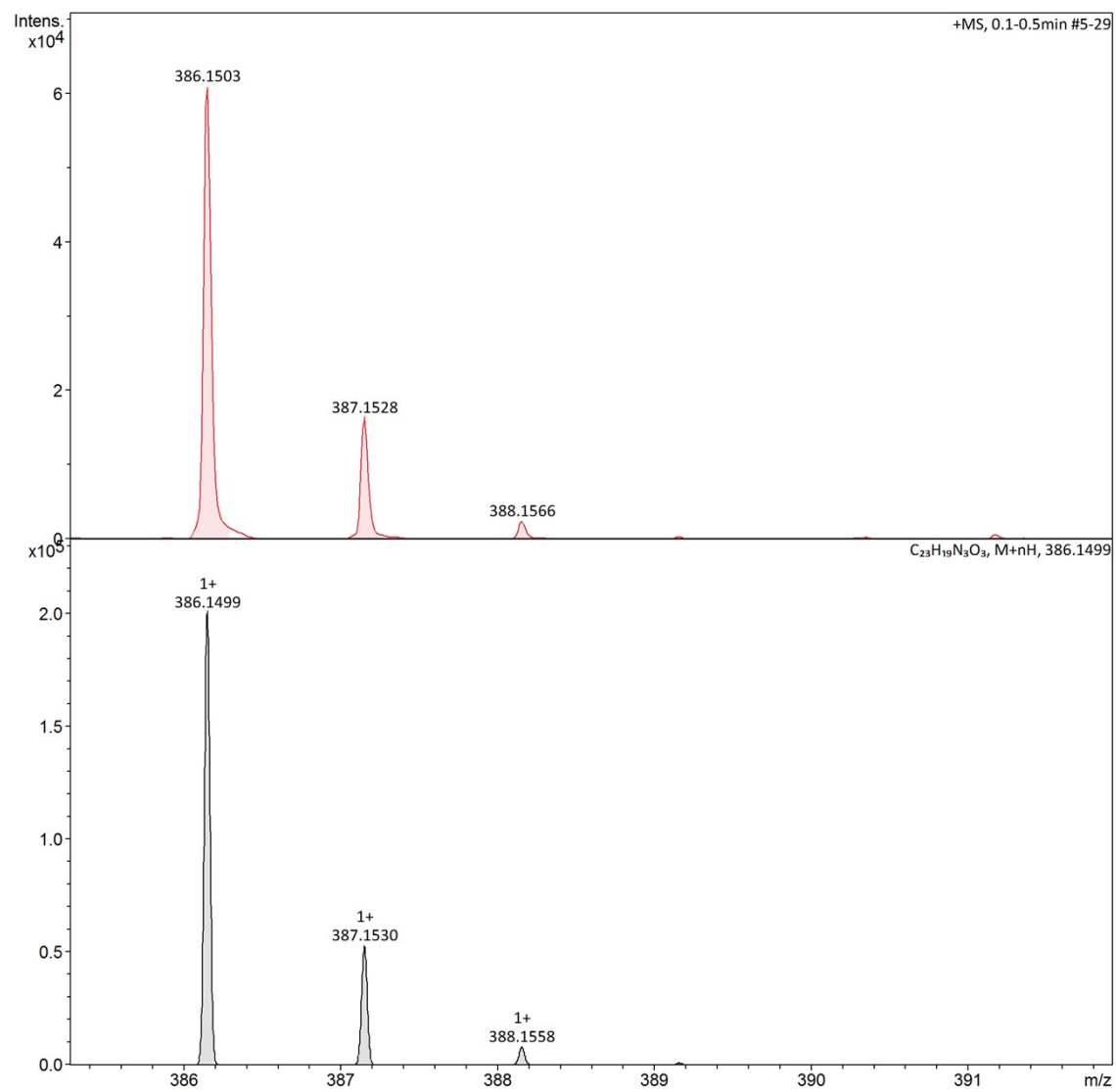


Figure 7. ^1H NMR (200 MHz, CDCl_3) of compound **1c**.

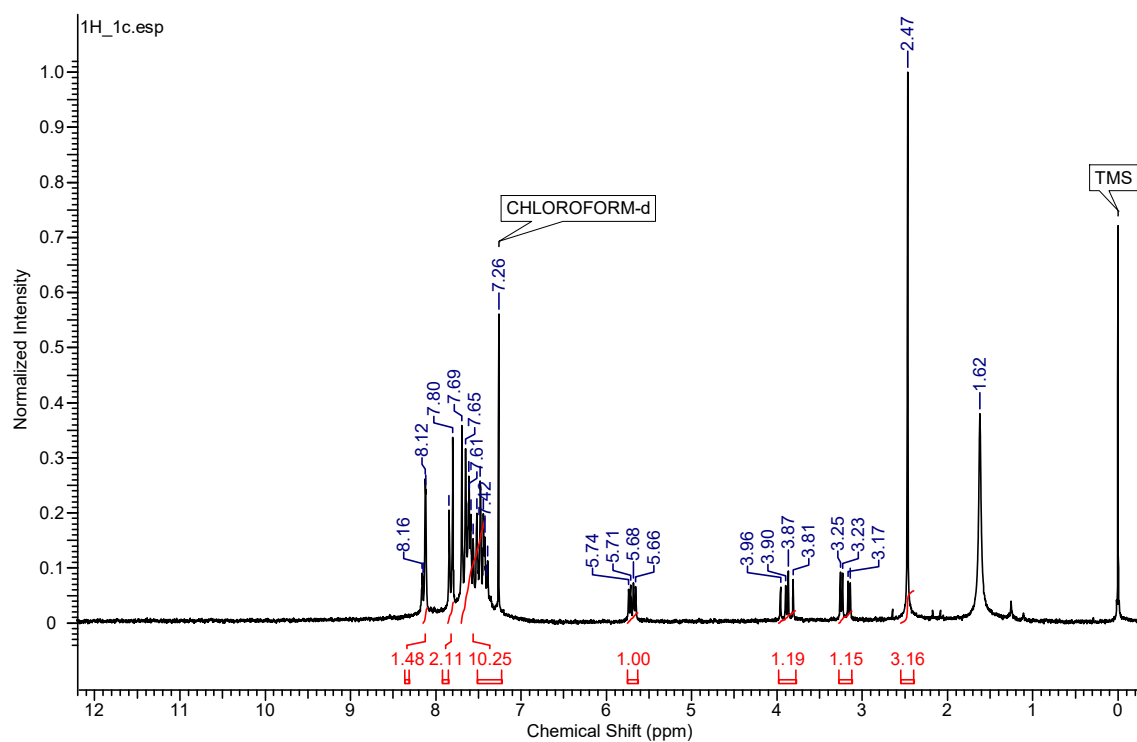


Figure 8. ^{13}C NMR (100 MHz, CDCl_3) of compound **1c**.

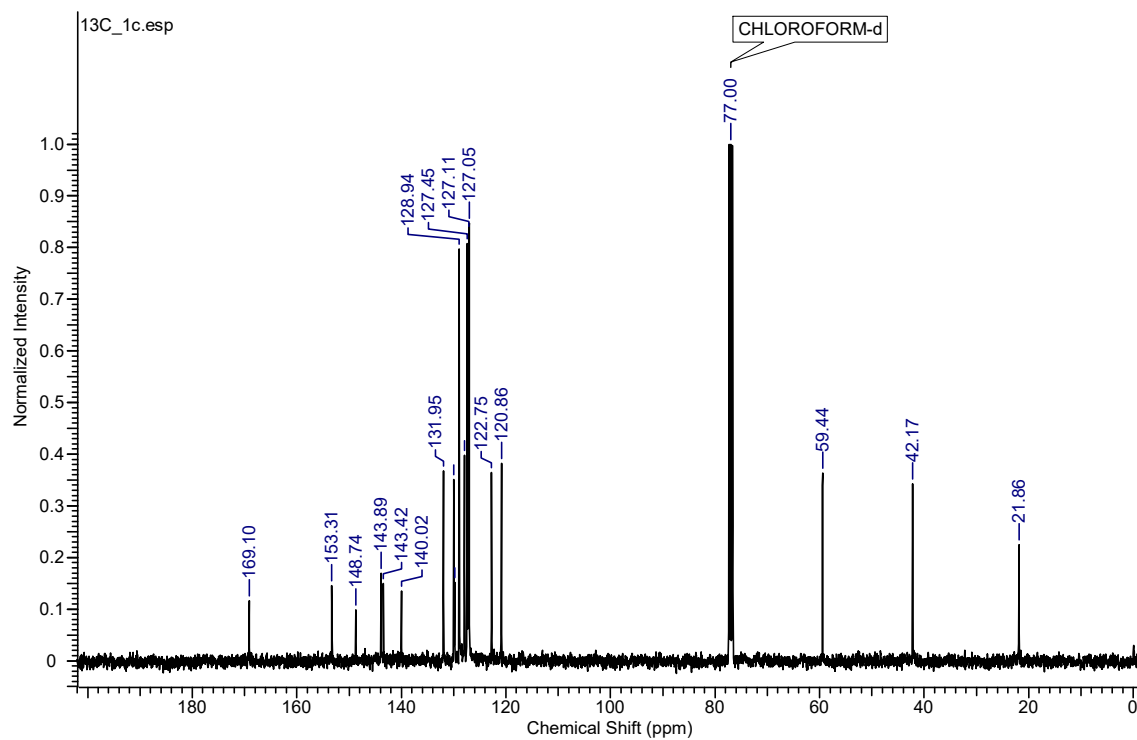


Figure 9. HR-ESI-MS of compound **1c**.

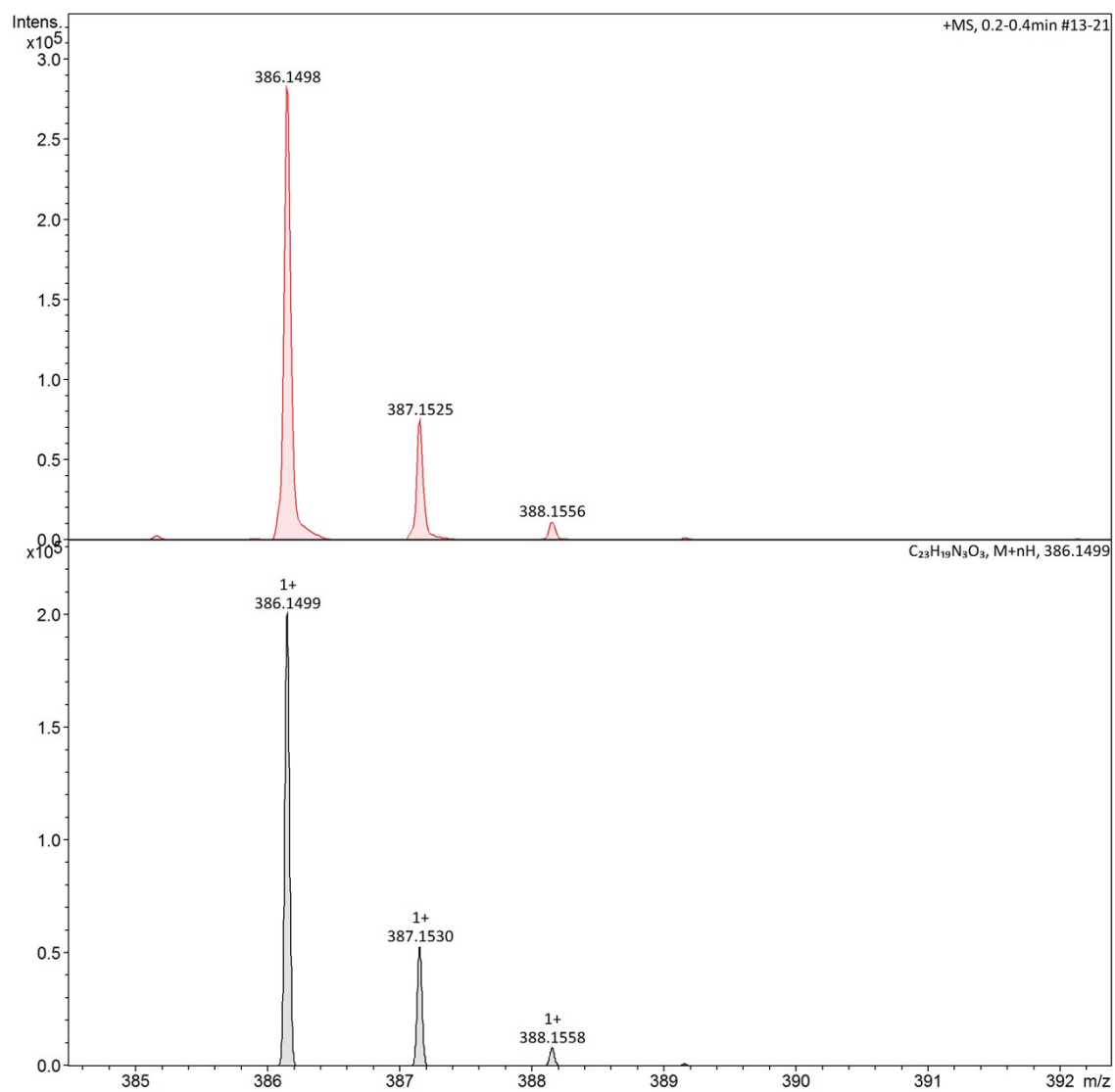


Figure 10. ^1H NMR (200 MHz, CDCl_3) of compound **1d**.

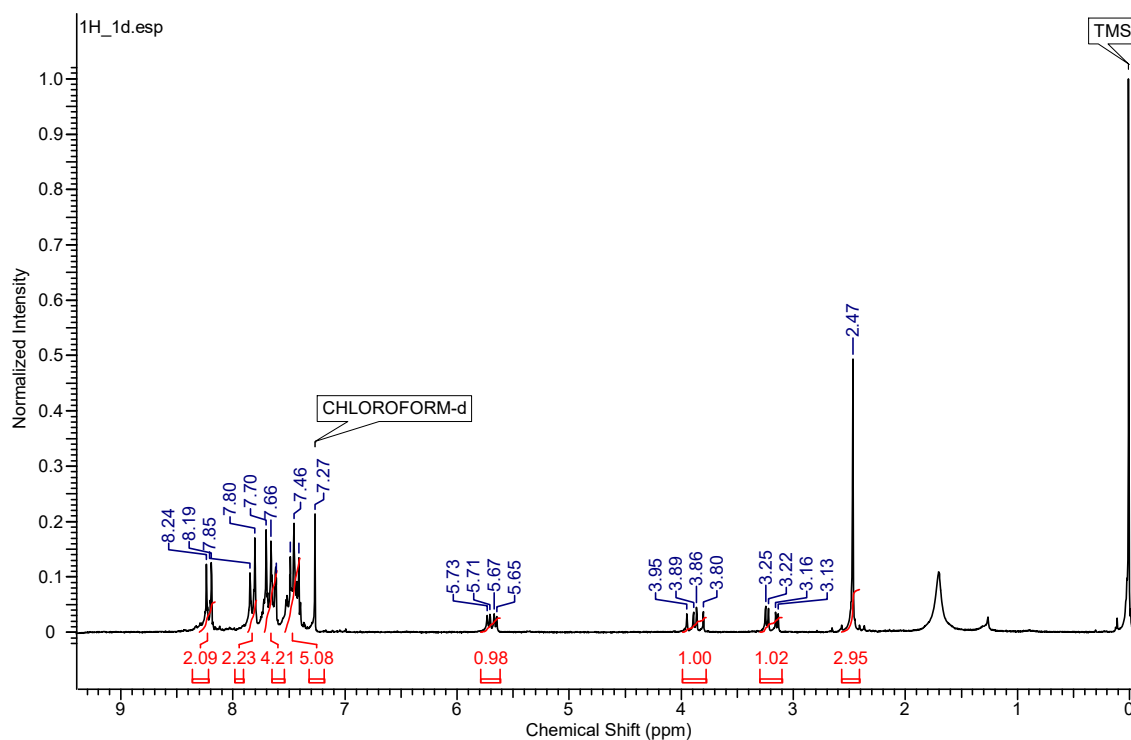


Figure 11. ^{13}C NMR (100 MHz, CDCl_3) of compound **1d**.

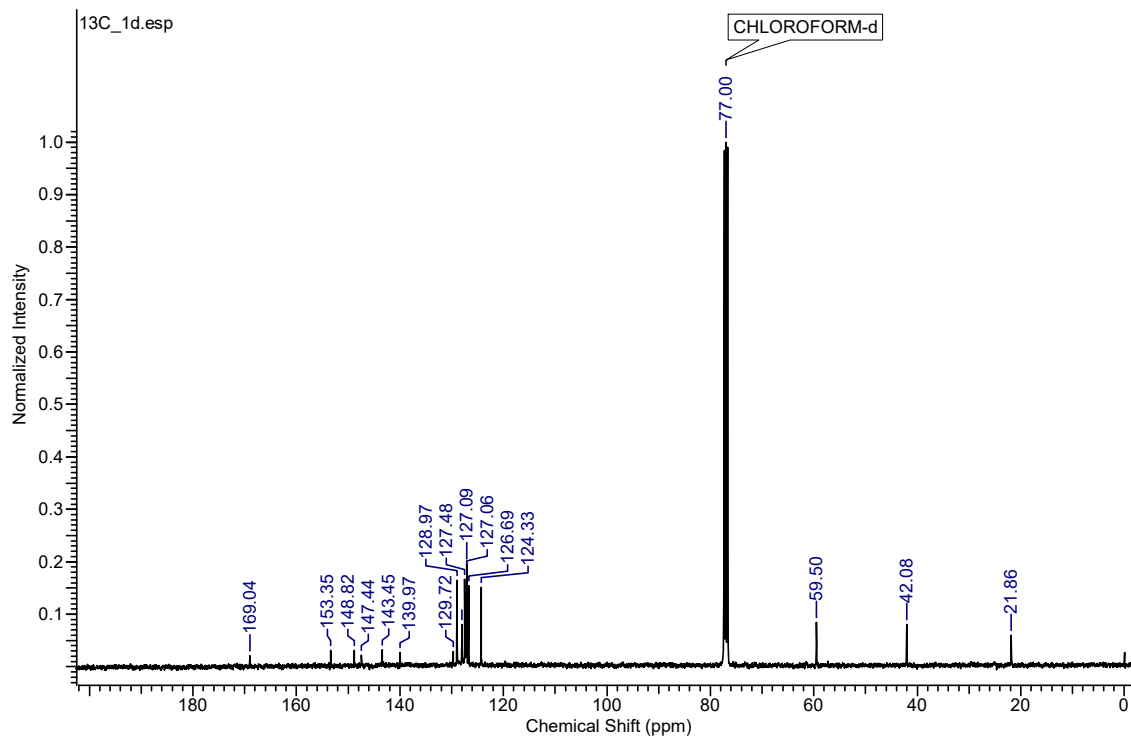


Figure 12. HR-ESI-MS of compound **1d**.

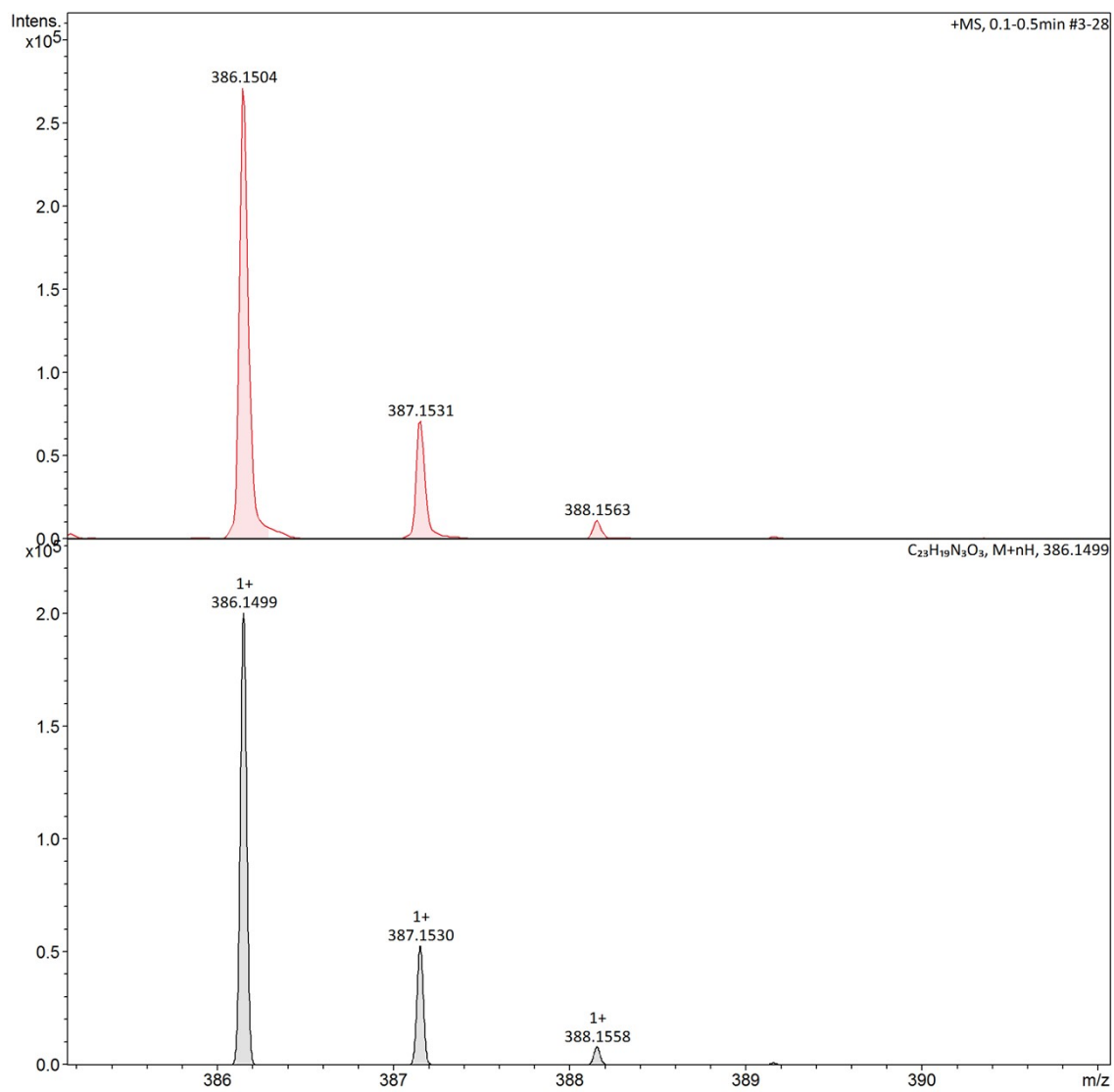


Figure 13. ^1H NMR (200 MHz, CDCl_3) of compound **1e**.

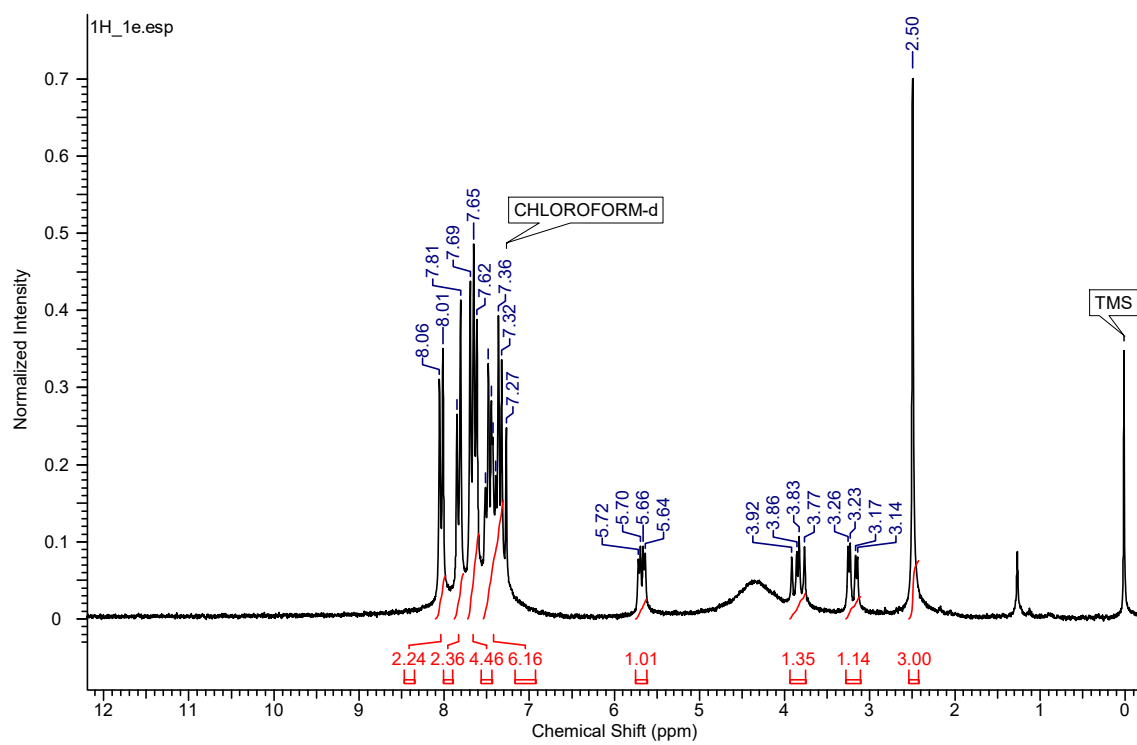


Figure 14. HR-ESI-MS of compound **1e**.

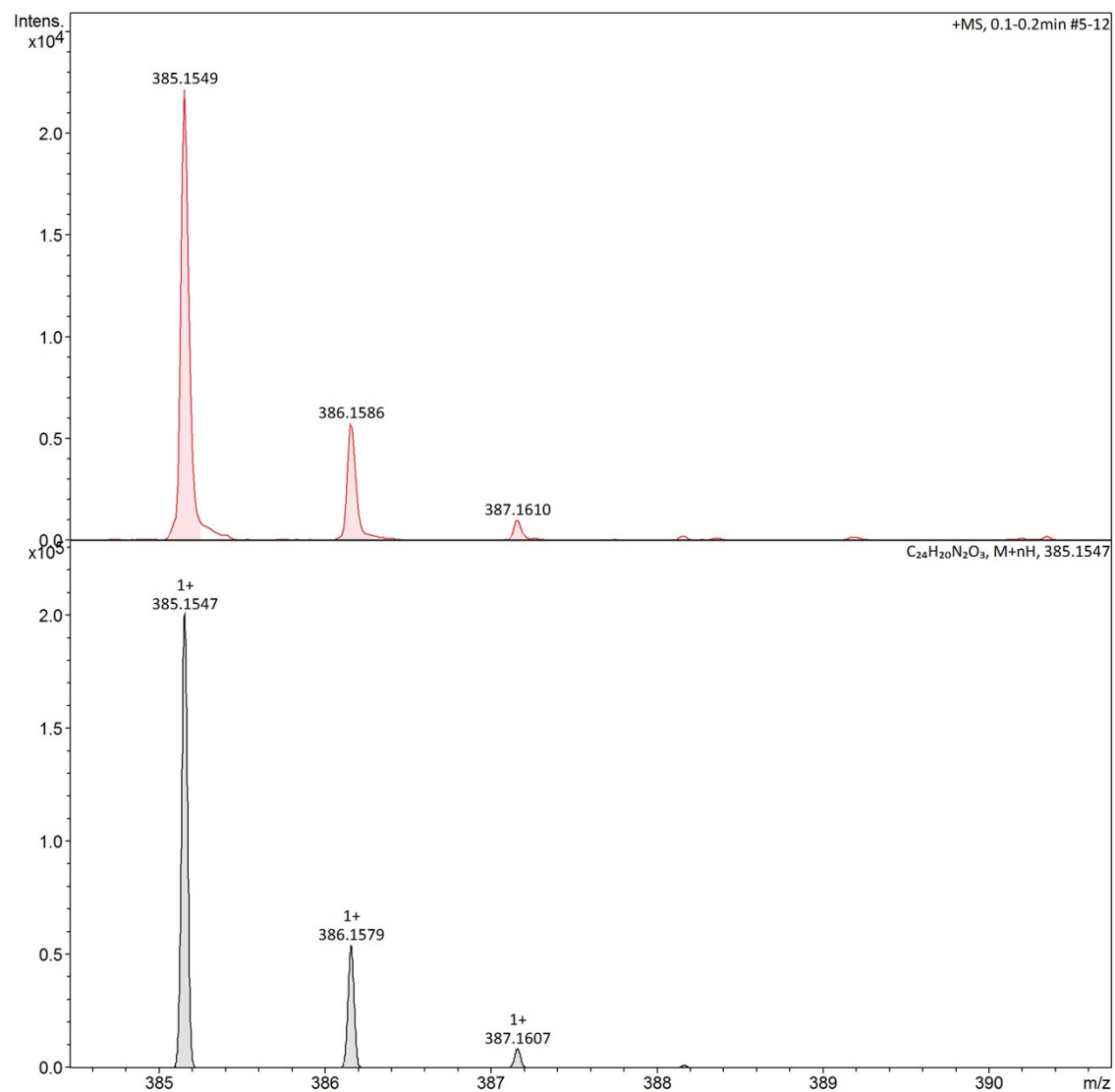


Figure 15. ^1H NMR (200 MHz, CDCl_3) of compound **1f**.

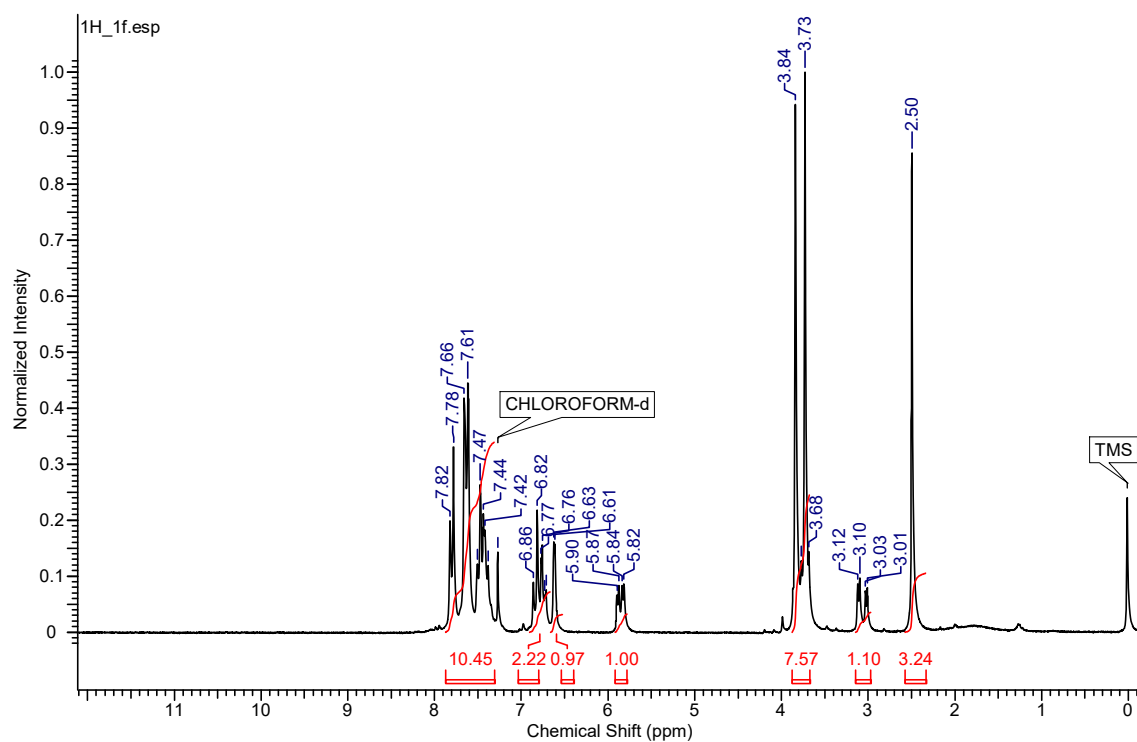


Figure 16. ^{13}C NMR (50 MHz, CDCl_3) of compound **1f**.

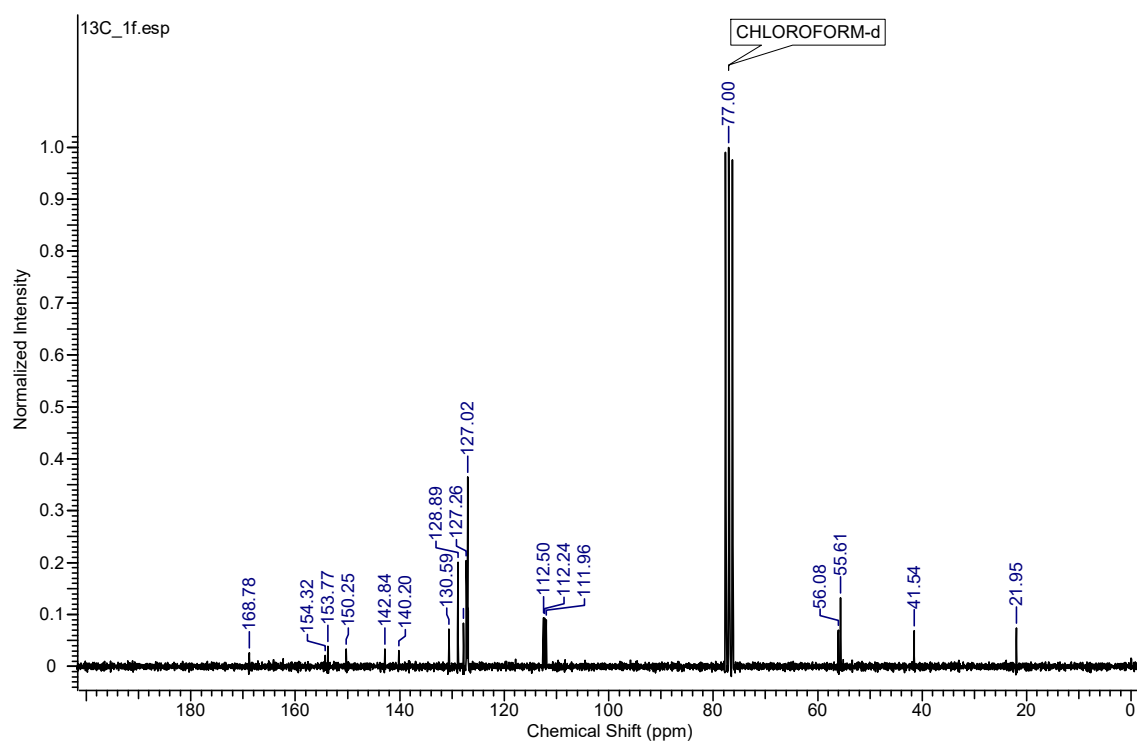


Figure 17. HR-ESI-MS of compound **1f**.

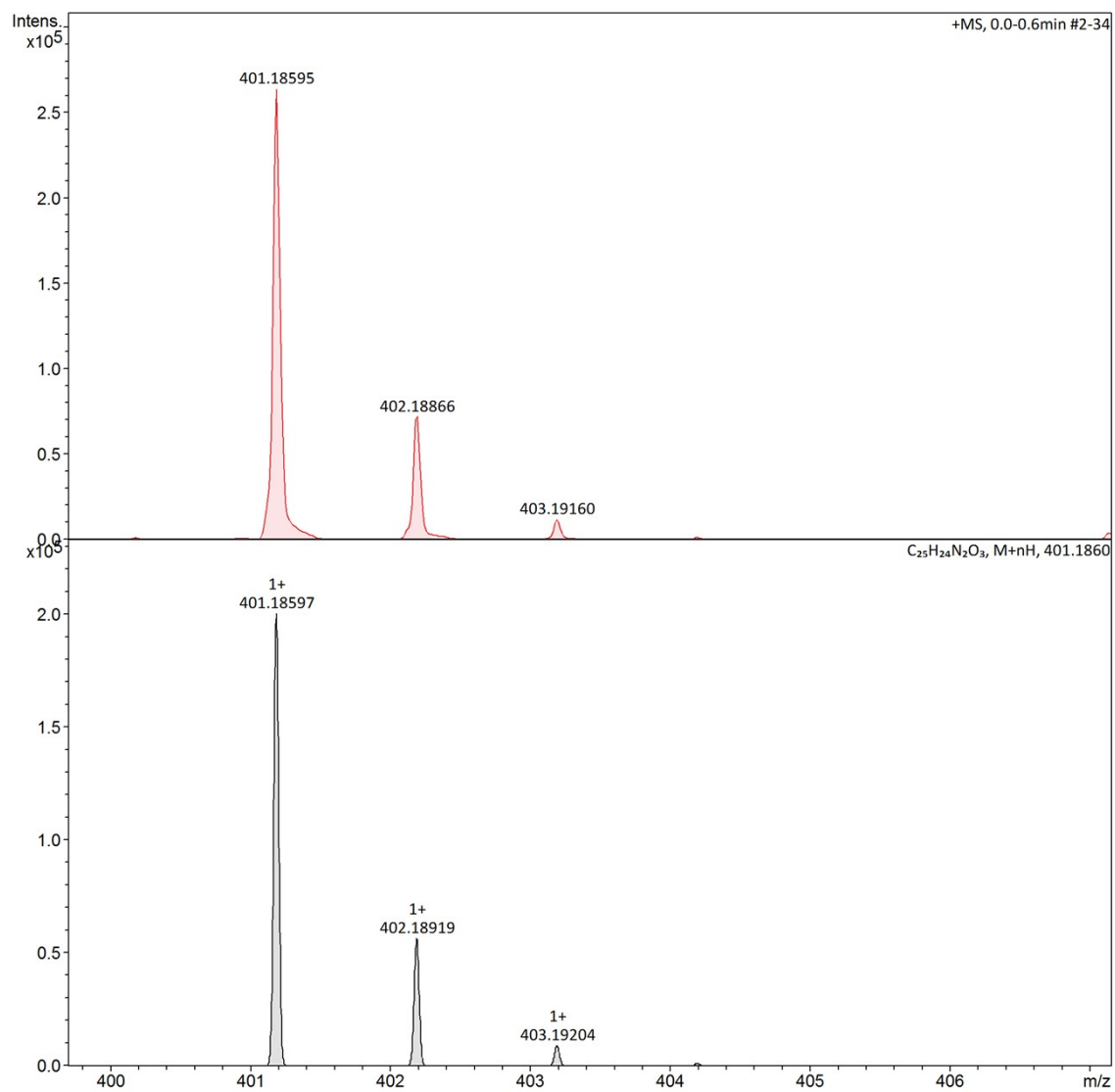


Figure 18. ^1H NMR (200 MHz, CDCl_3) of compound **1g**.

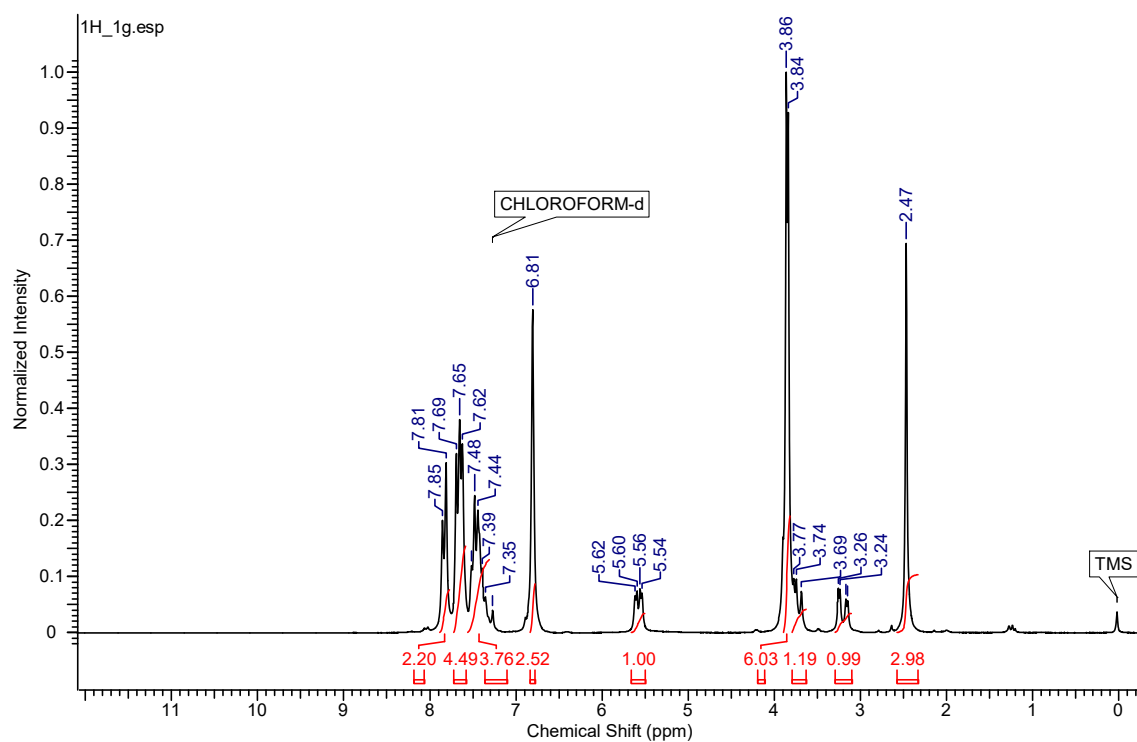


Figure 19. ^{13}C NMR (50 MHz, CDCl_3) of compound **1g**.

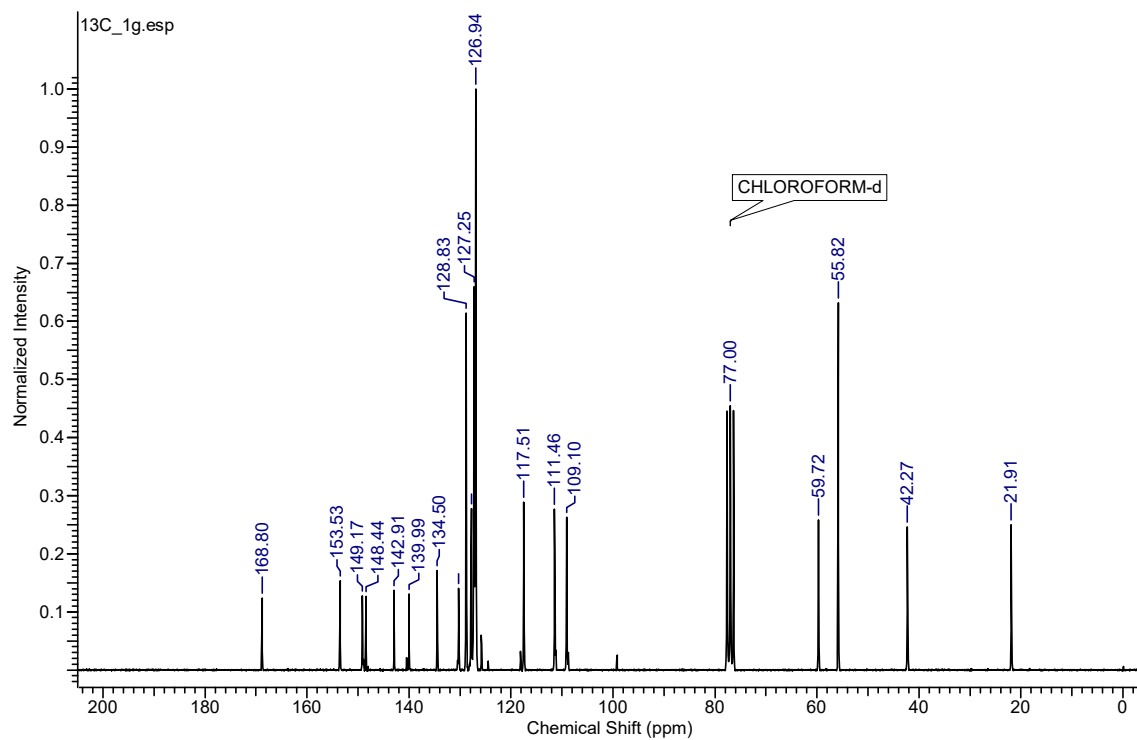


Figure 20. HR-ESI-MS of compound **1g**.

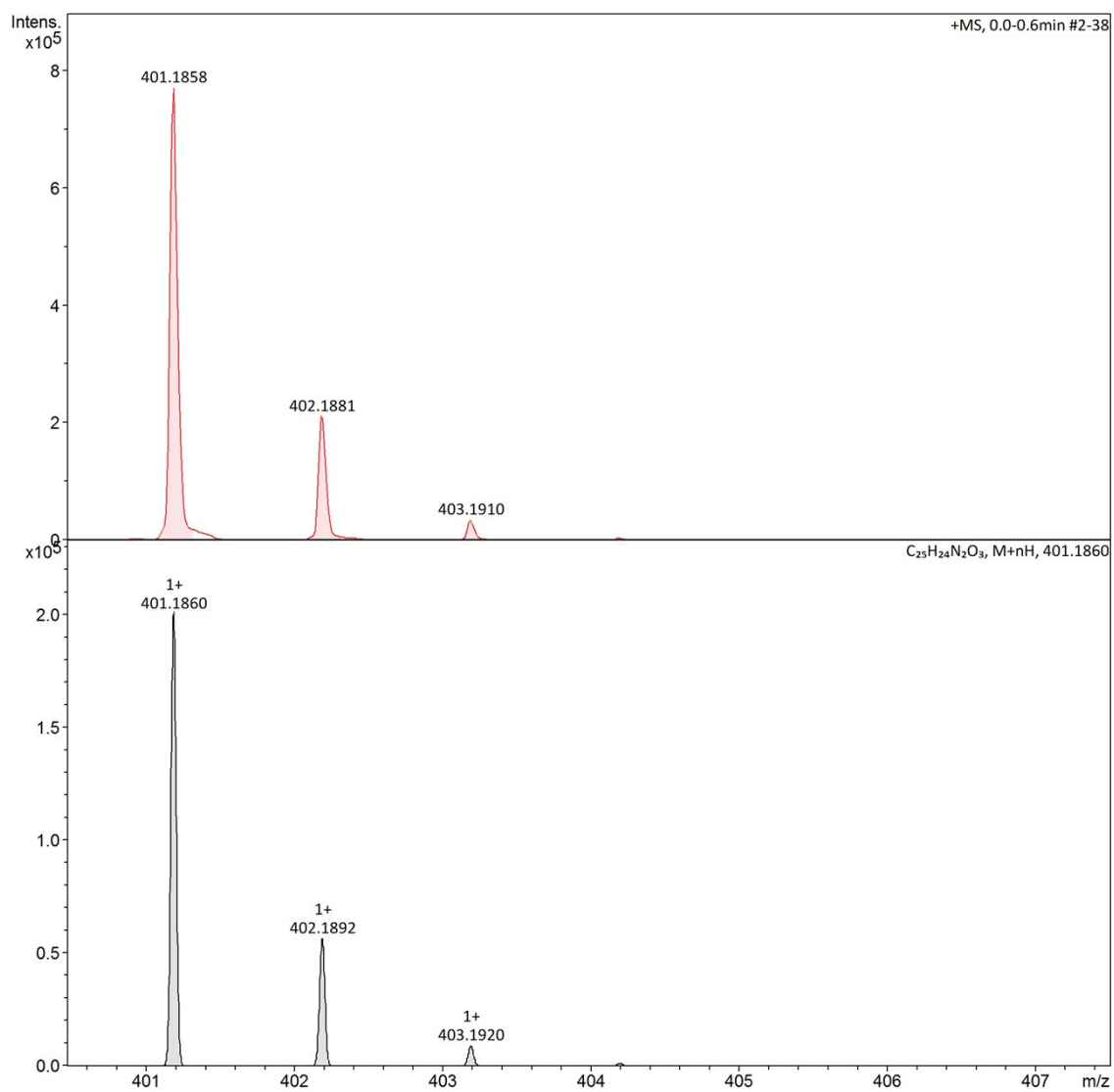


Figure 21. ^1H NMR (200 MHz, CDCl_3) of compound **1h**.

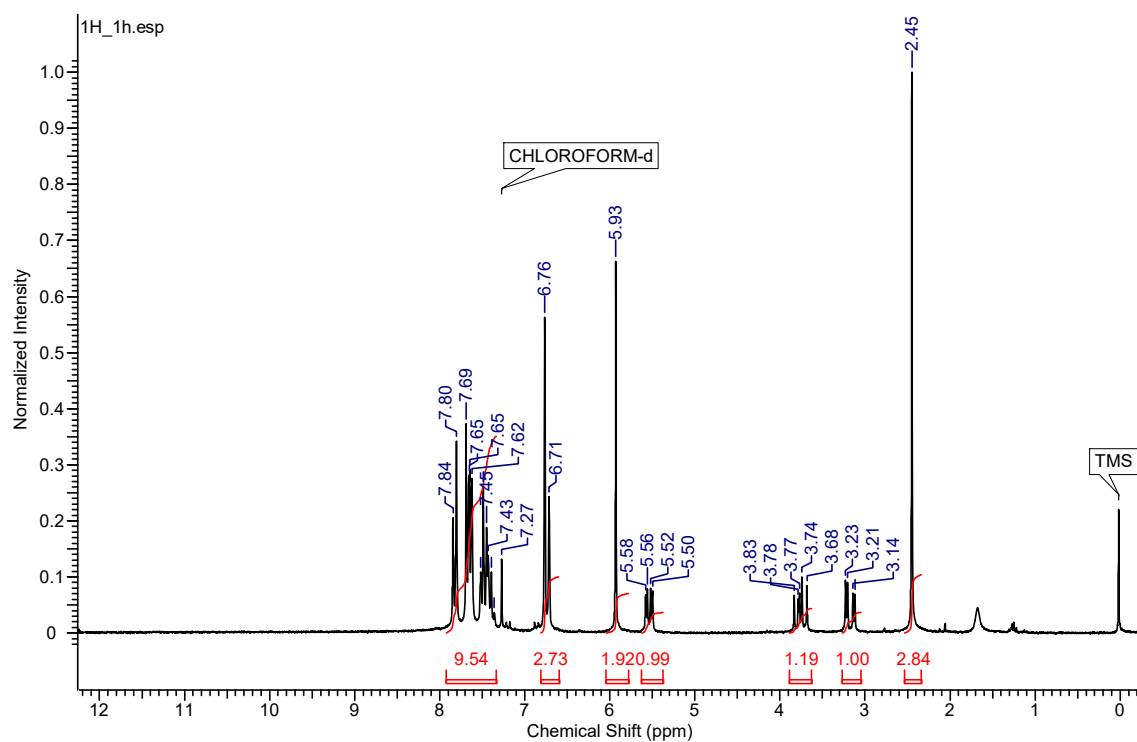


Figure 22. ^{13}C NMR (50 MHz, CDCl_3) of compound **1h**.

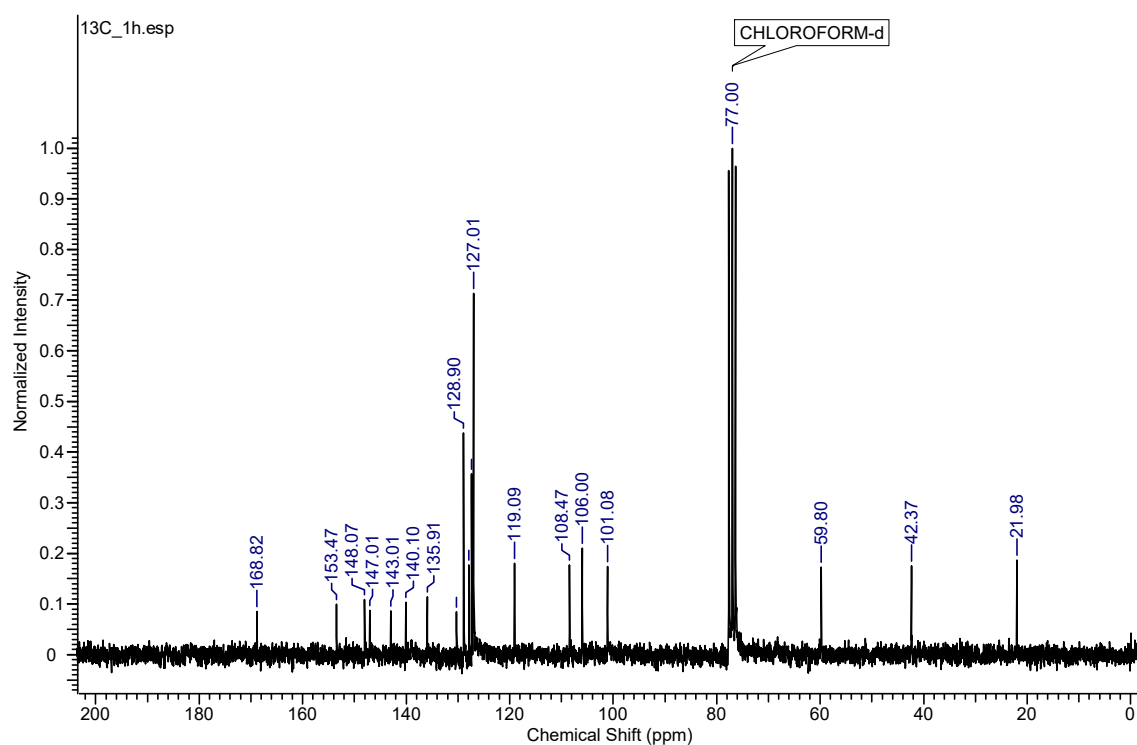


Figure 23. HR-ESI-MS of compound **1h**.

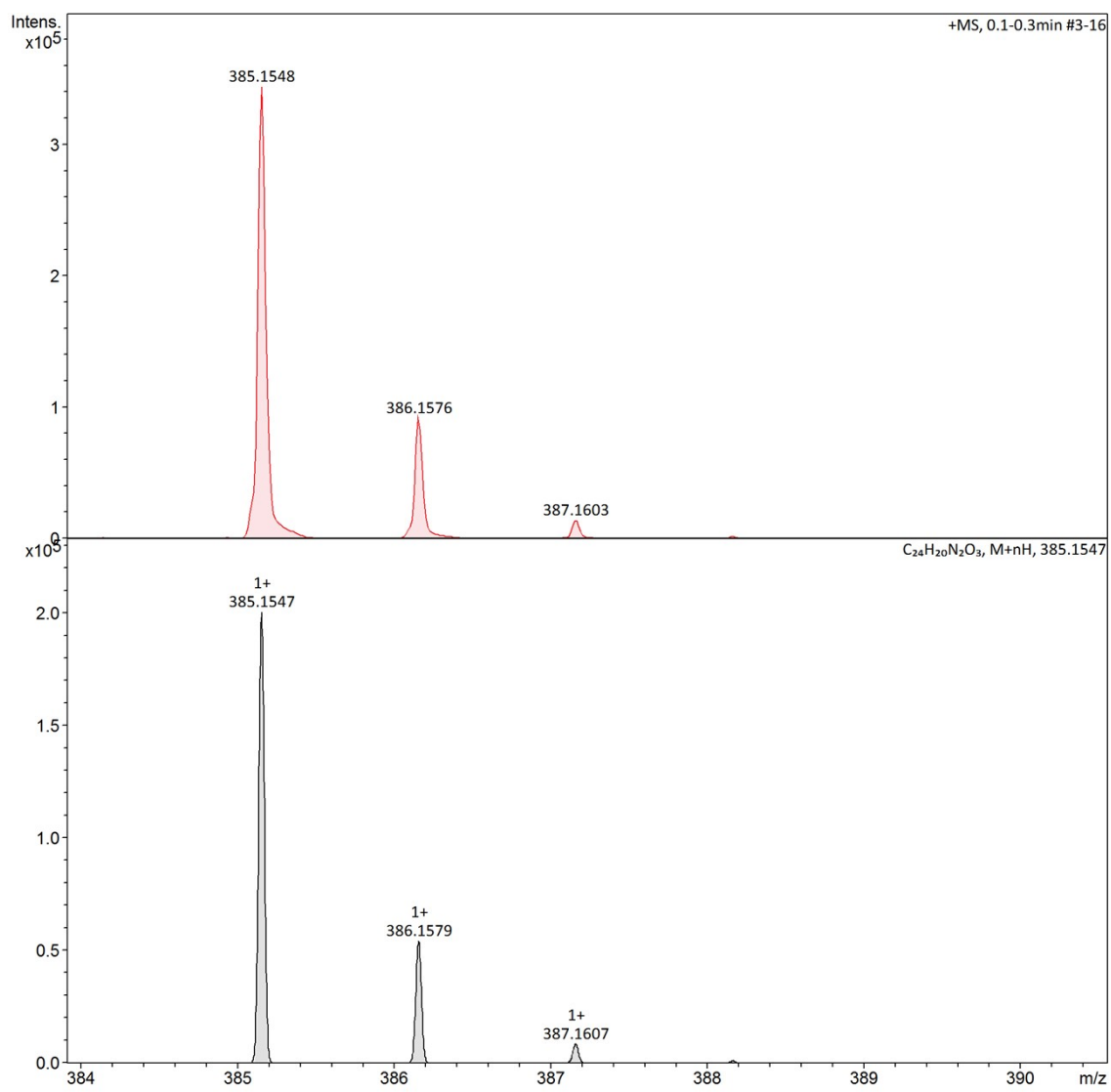


Figure 24. ^1H NMR (200 MHz, CDCl_3) of compound **1i**.

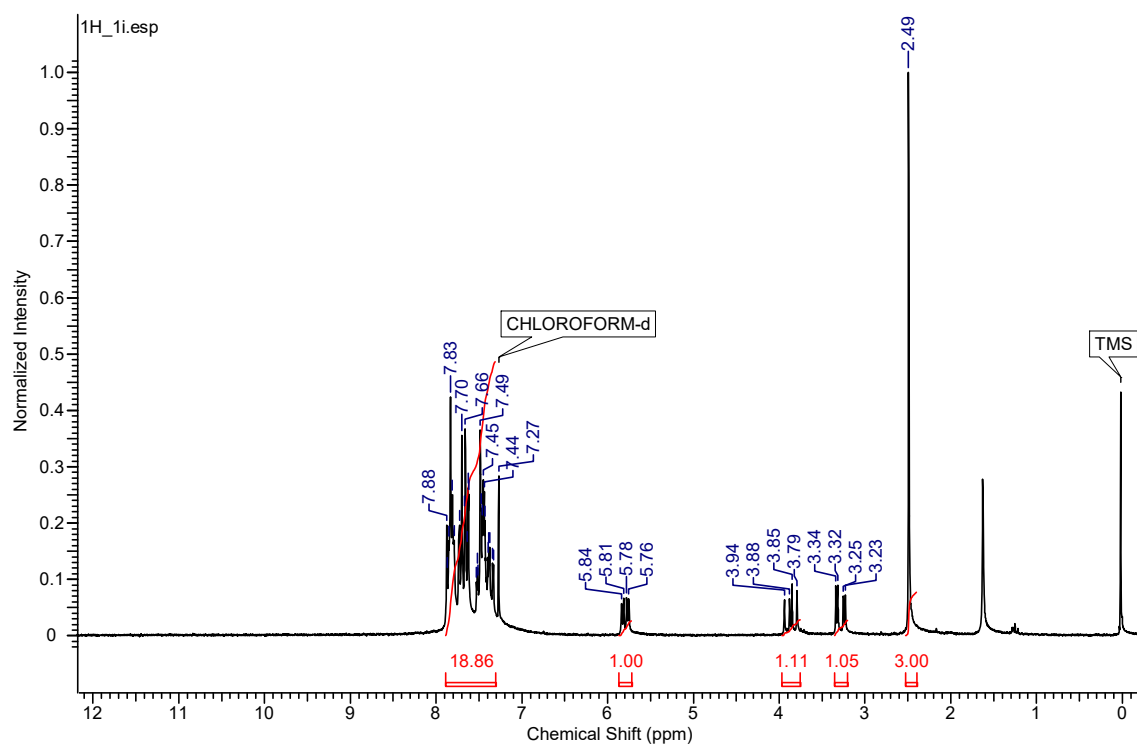


Figure 25. ^{13}C NMR (50 MHz, CDCl_3) of compound **1i**.

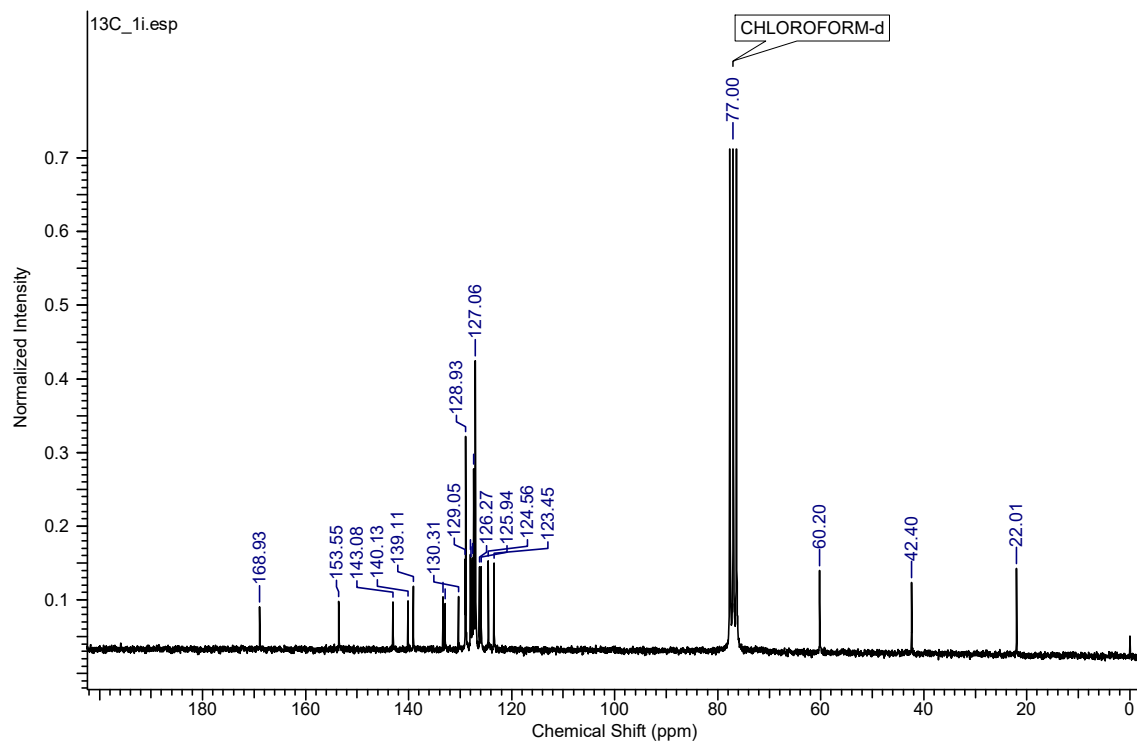


Figure 26. HR-ESI-MS of compound **1i**.

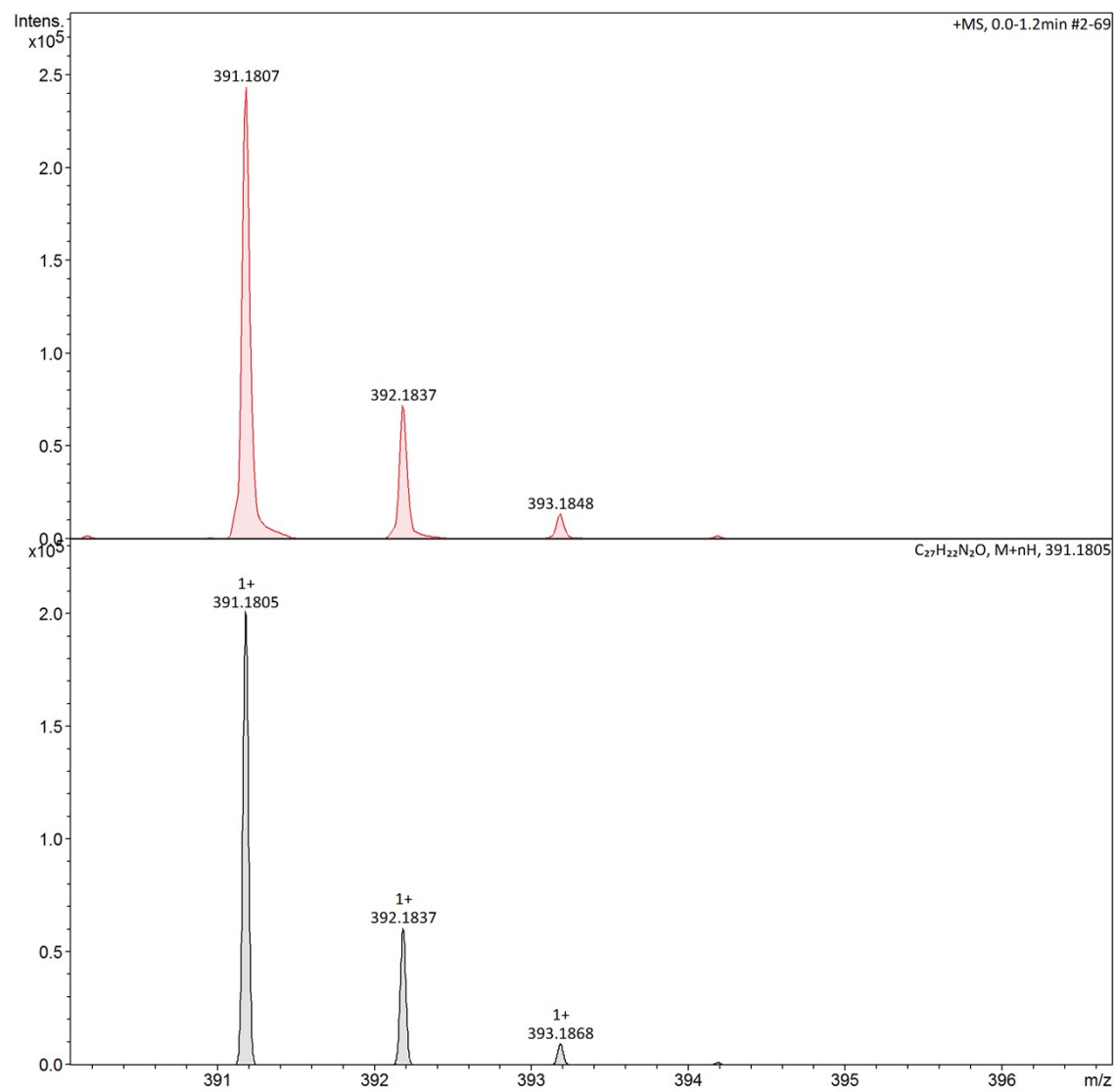


Figure 27. ^1H NMR (200 MHz, CDCl_3) of compound **2a**.

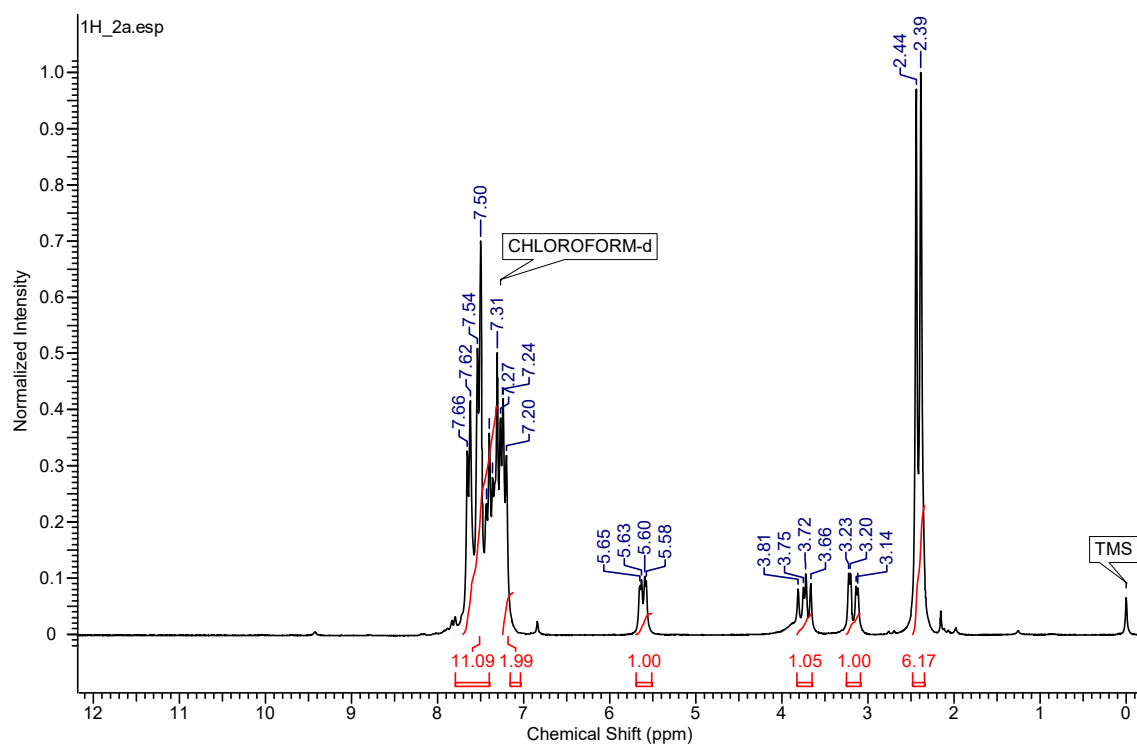


Figure 28. ^{13}C NMR (50 MHz, CDCl_3) of compound **2a**.

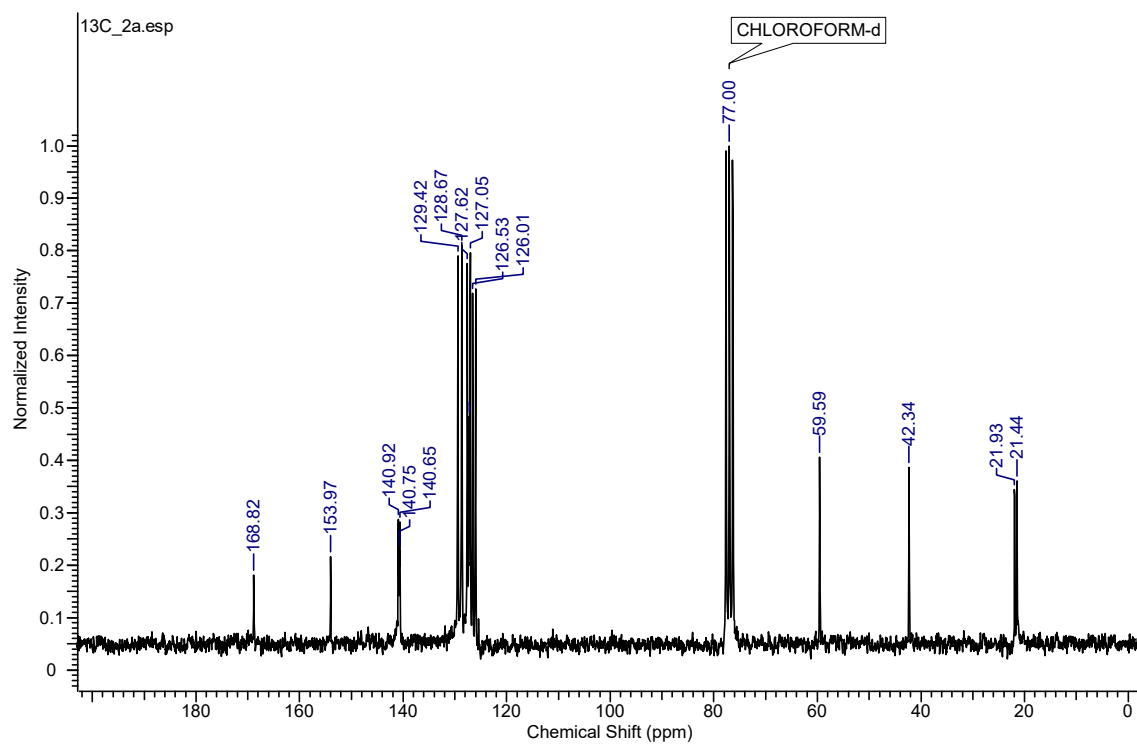


Figure 29. HR-ESI-MS of compound **2a**.

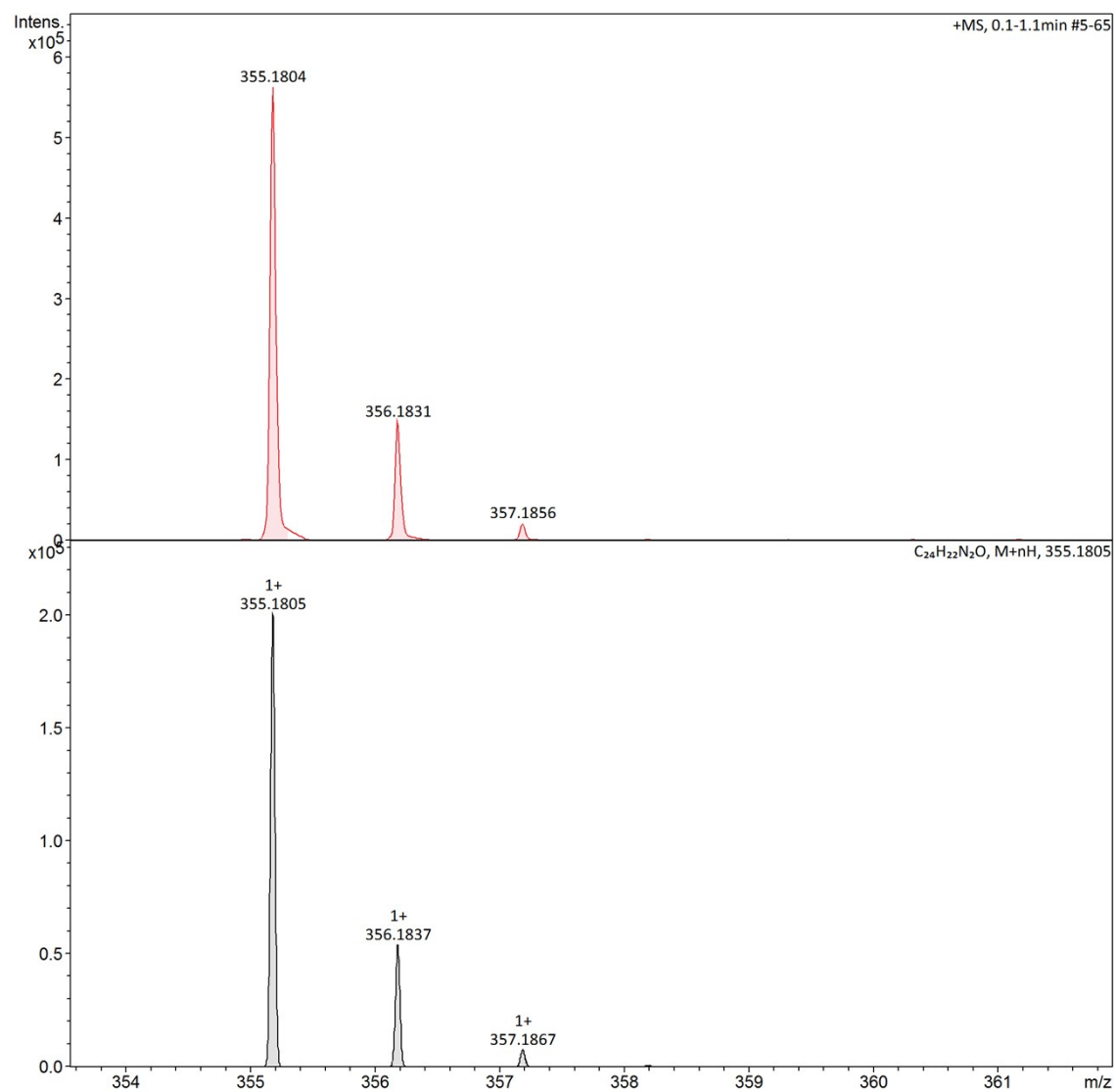


Figure 30. ^1H NMR (400 MHz, CDCl_3) of compound **2b**.

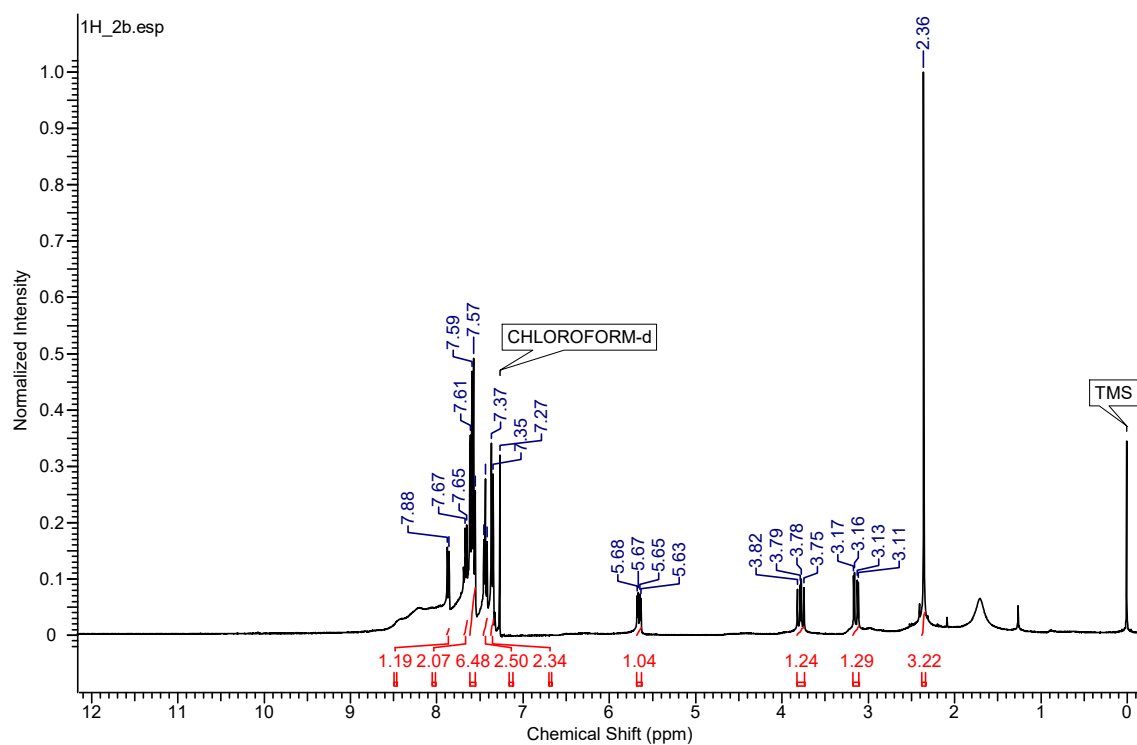


Figure 31. ^{13}C NMR (100 MHz, CDCl_3) of compound **2b**.

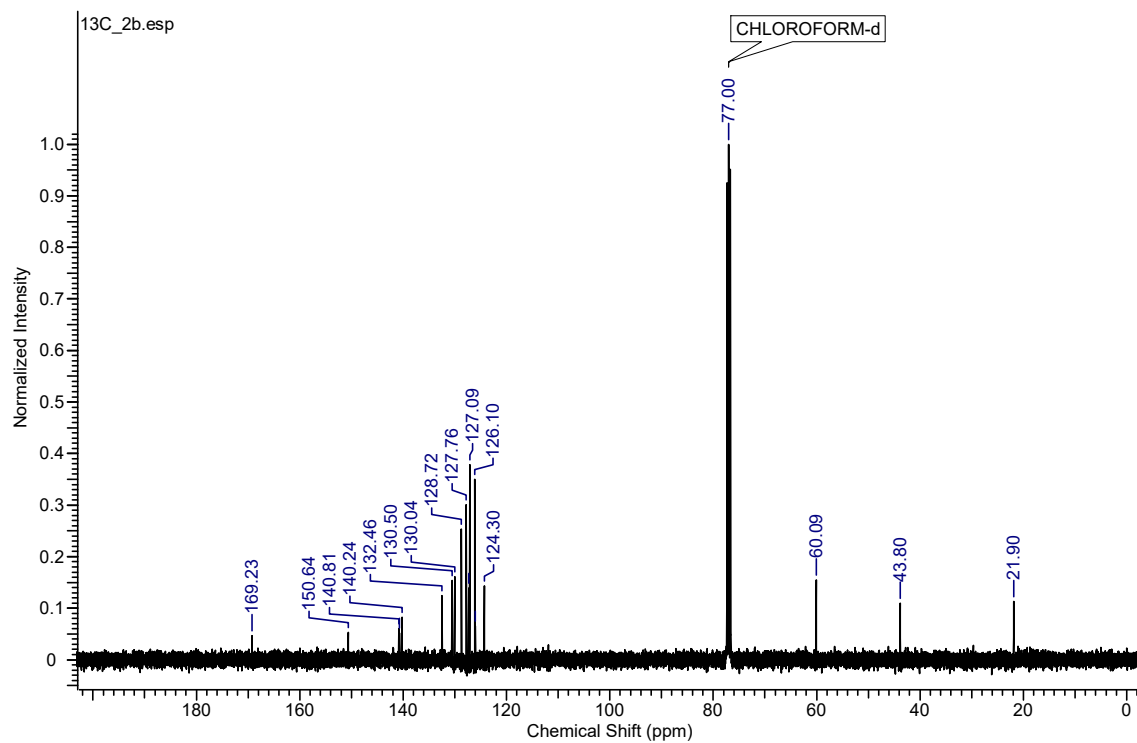


Figure 32. HR-ESI-MS of compound **2b**.

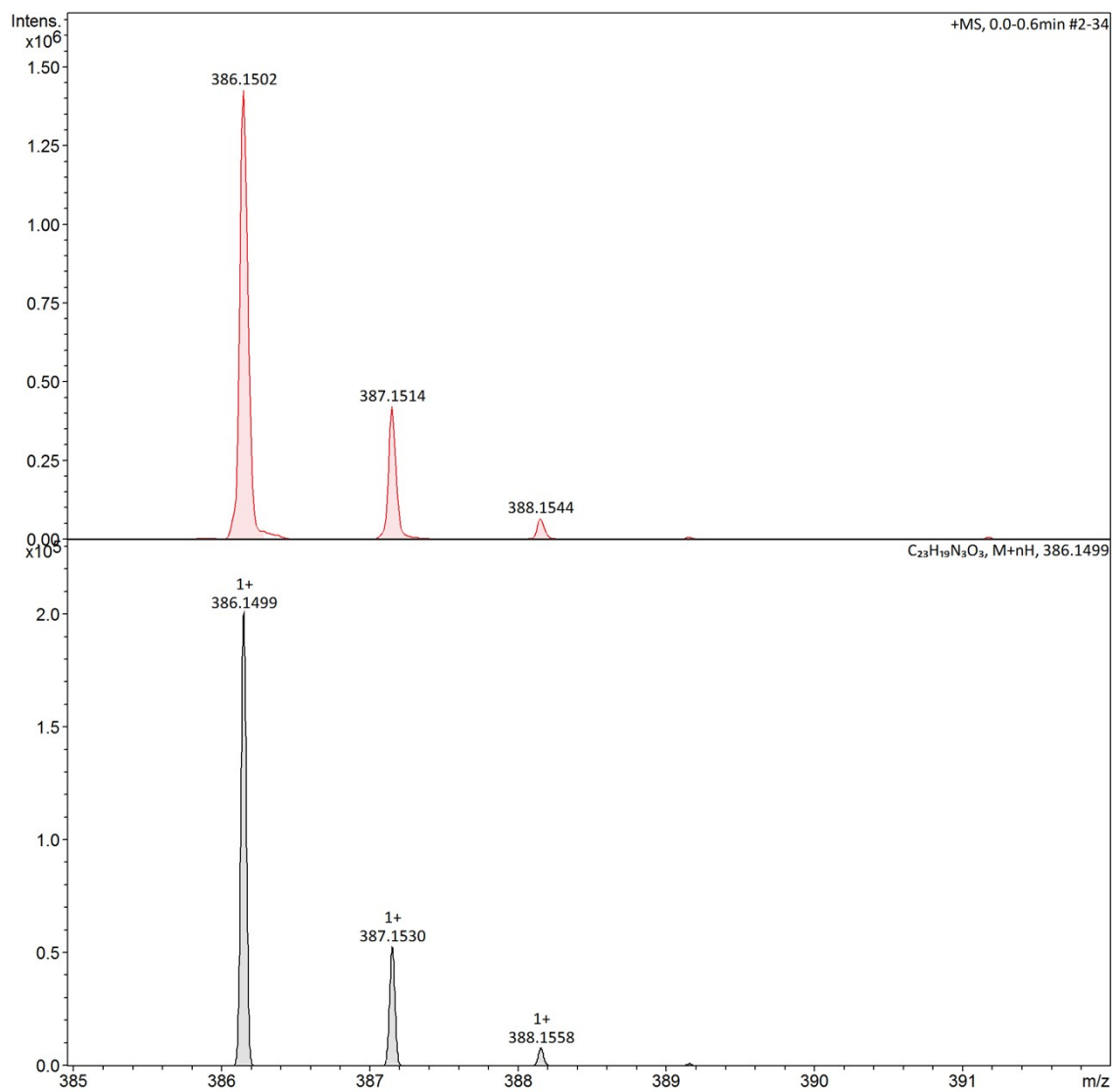


Figure 33. ^1H NMR (400 MHz, CDCl_3) of compound **2c**.

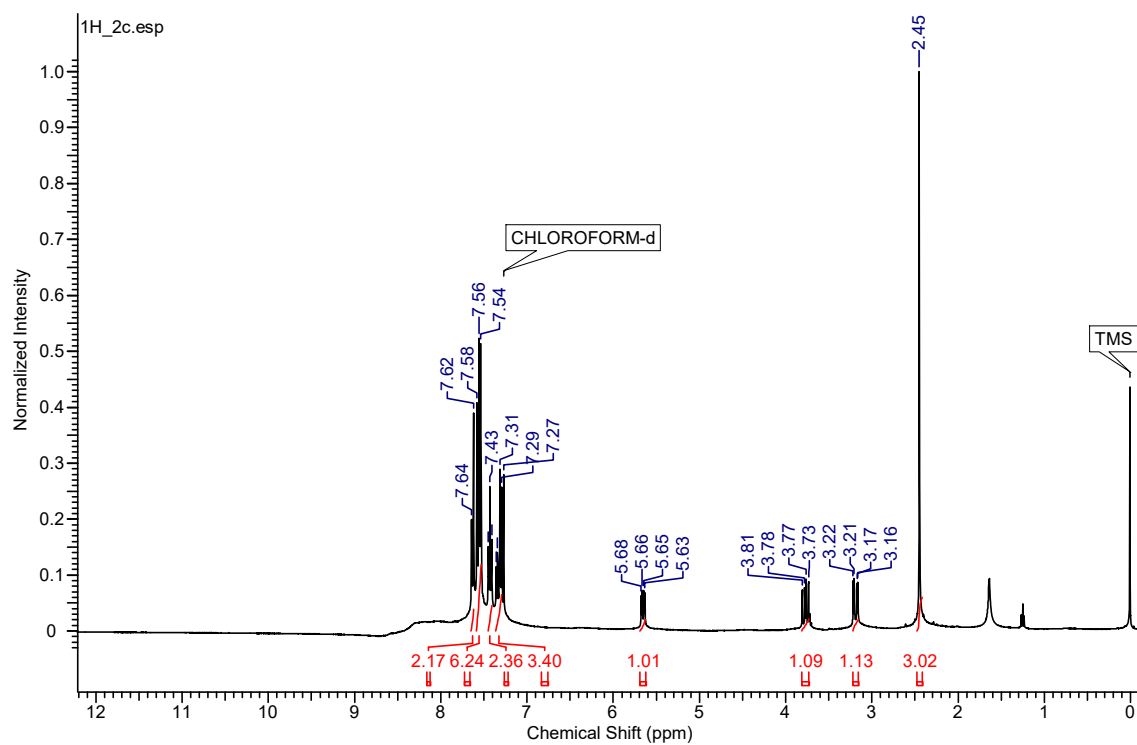


Figure 34. ^{13}C NMR (100 MHz, CDCl_3) of compound **2c**.

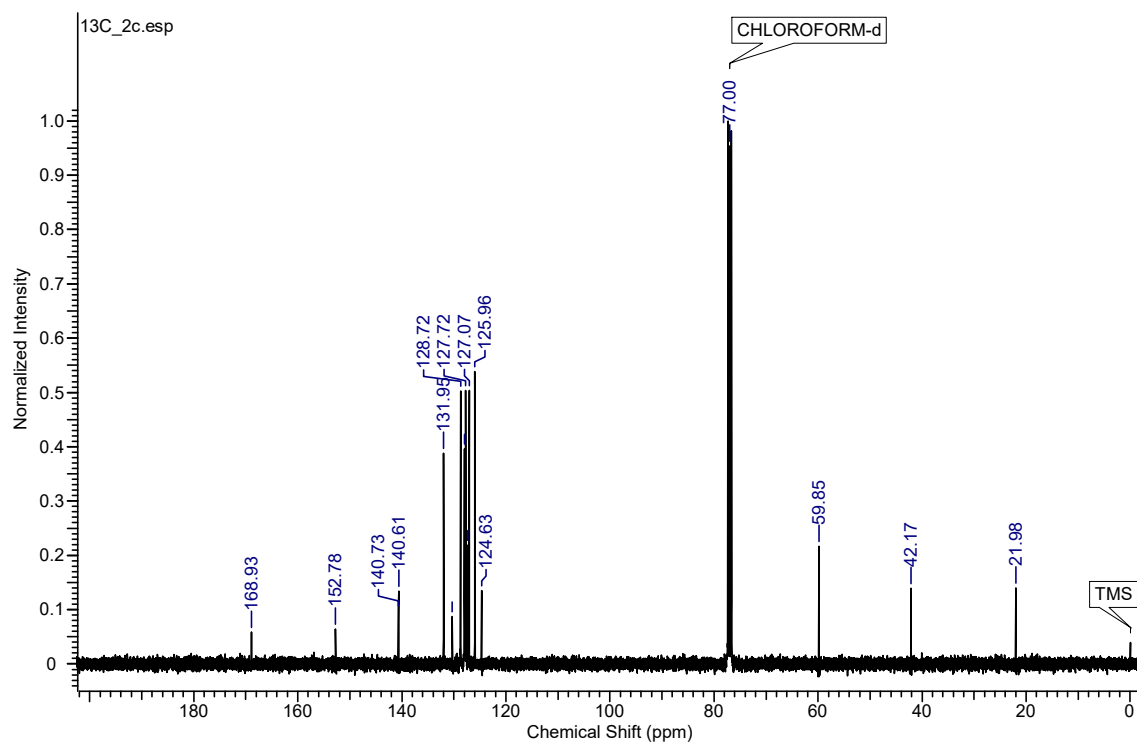


Figure 35. HR-ESI-MS of compound 2c.

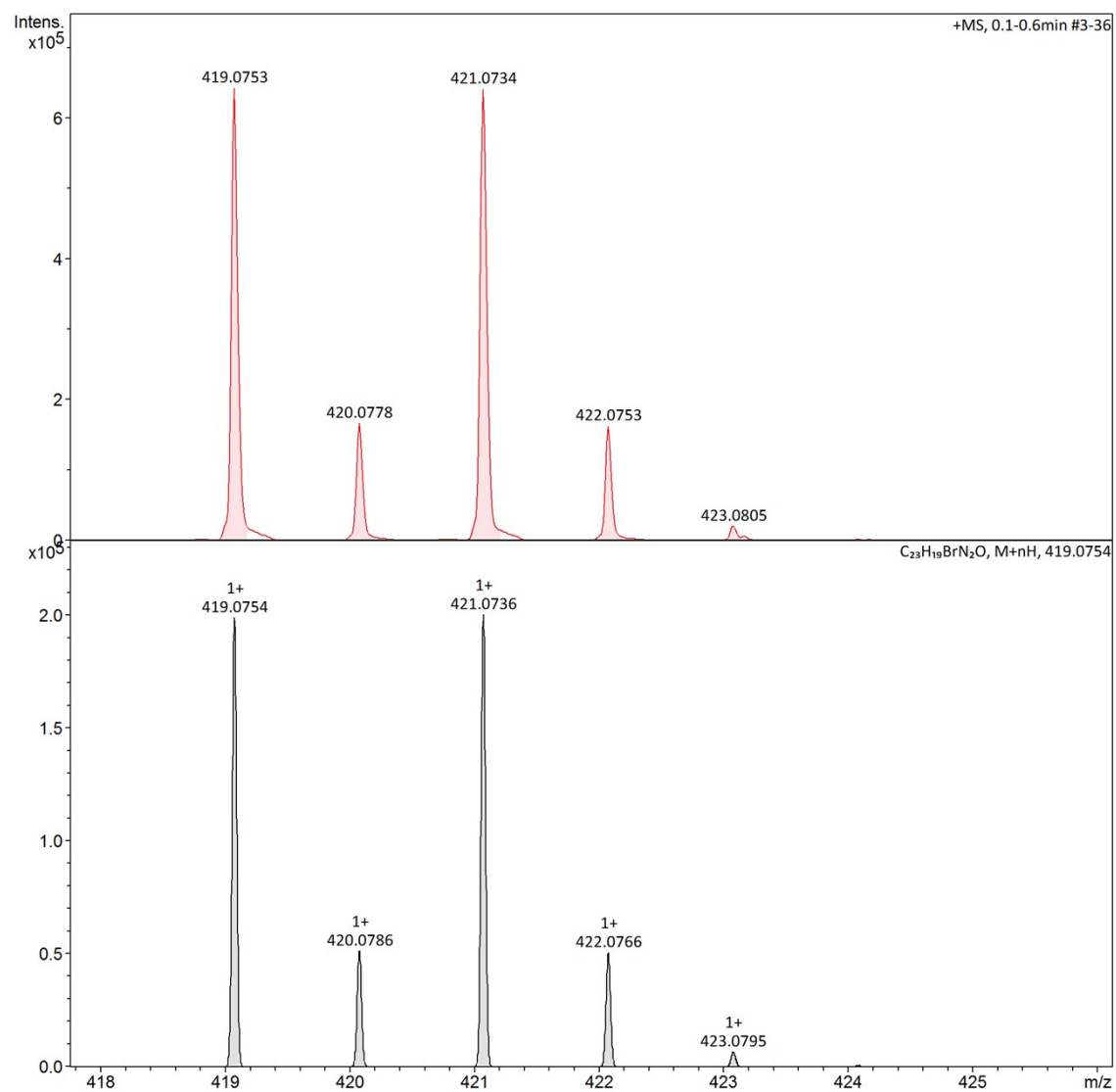


Figure 36. ^1H NMR (200 MHz, CDCl_3) of compound **2d**.

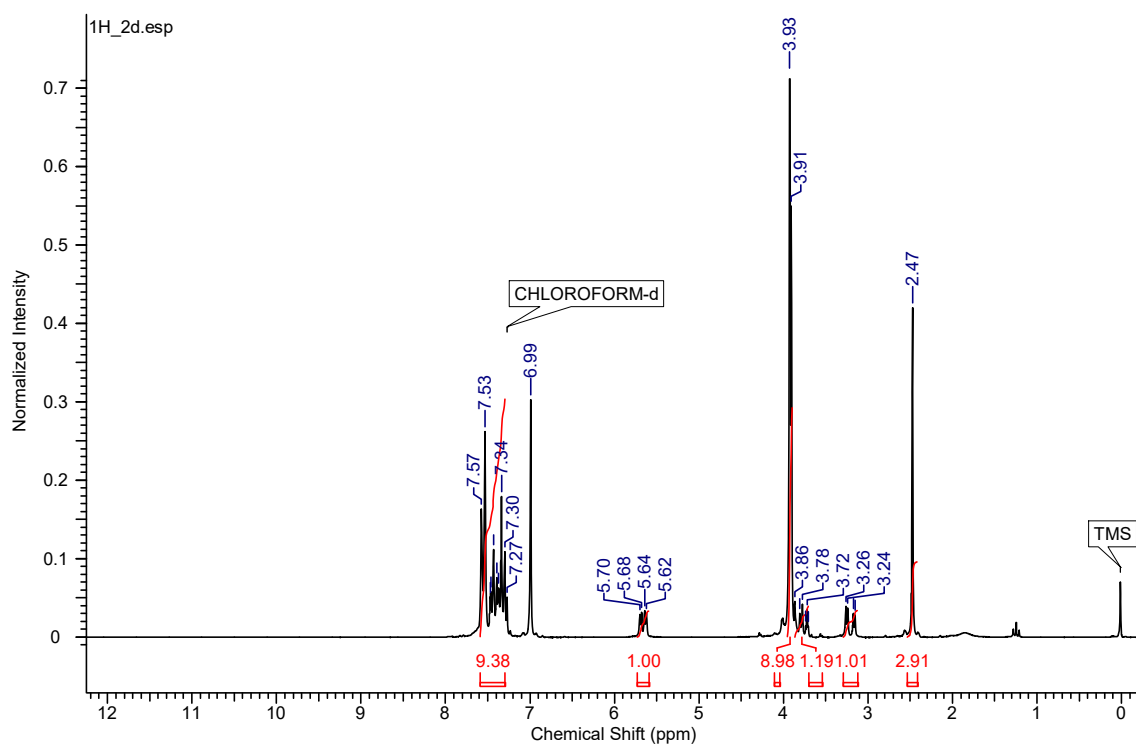


Figure 37. ^{13}C NMR (50 MHz, CDCl_3) of compound **2d**.

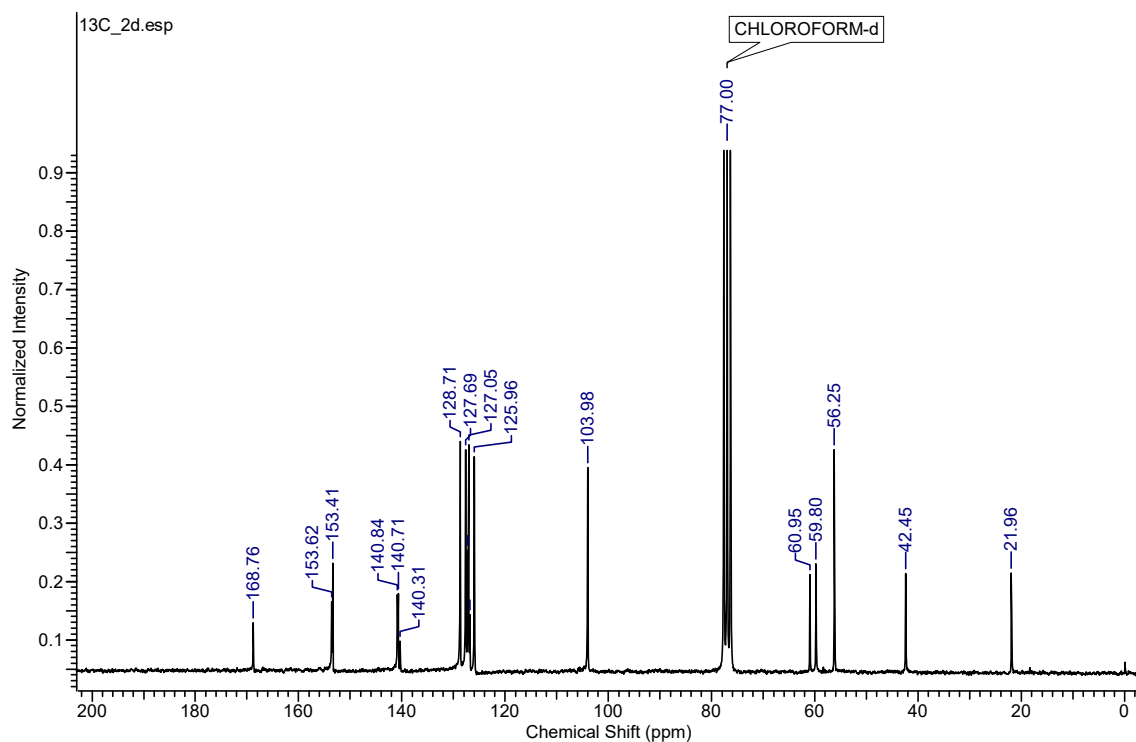


Figure 38. HR-ESI-MS of compound **2d**.

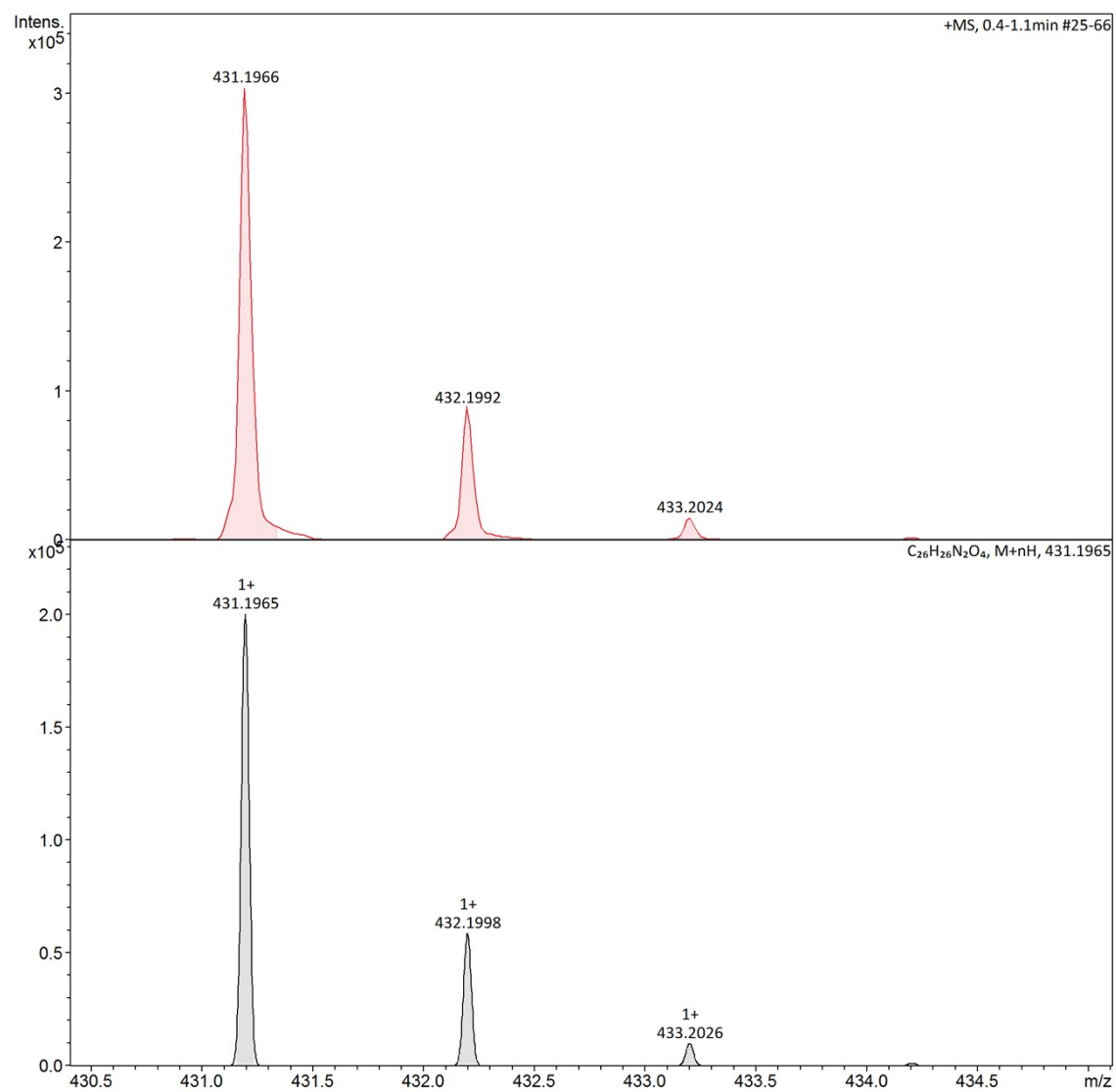


Figure 39. ^1H NMR (200 MHz, CDCl_3) of compound **2e**.

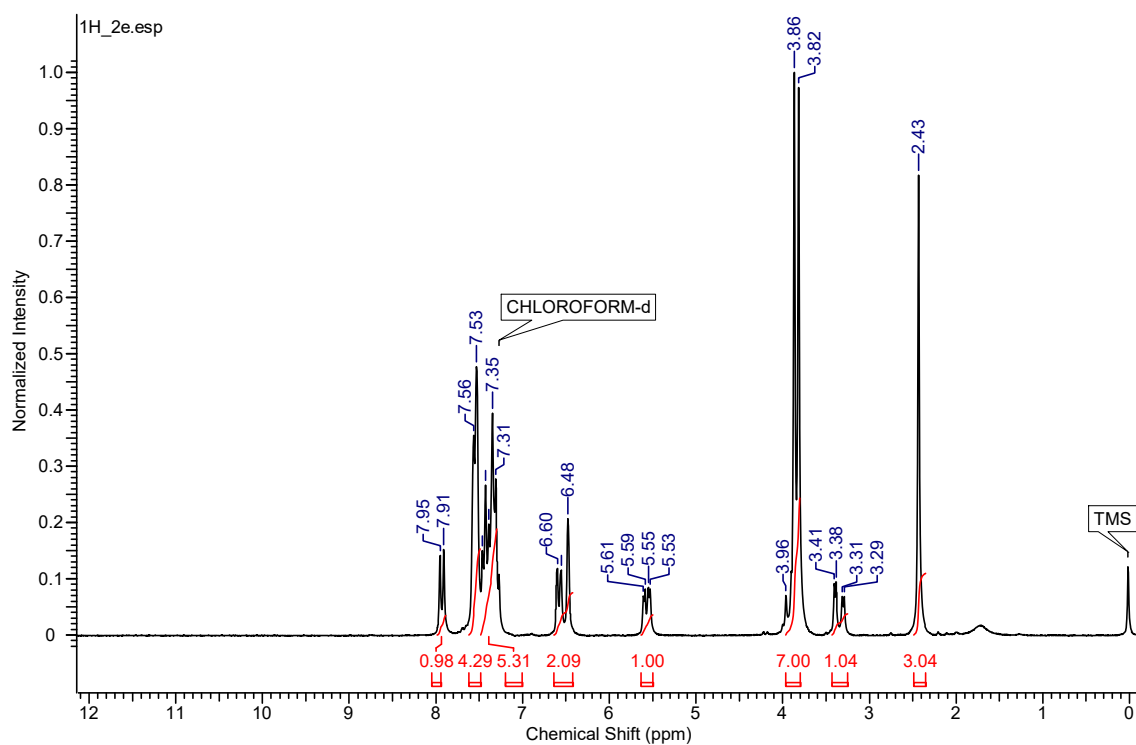


Figure 40. ^{13}C NMR (50 MHz, CDCl_3) of compound **2e**.

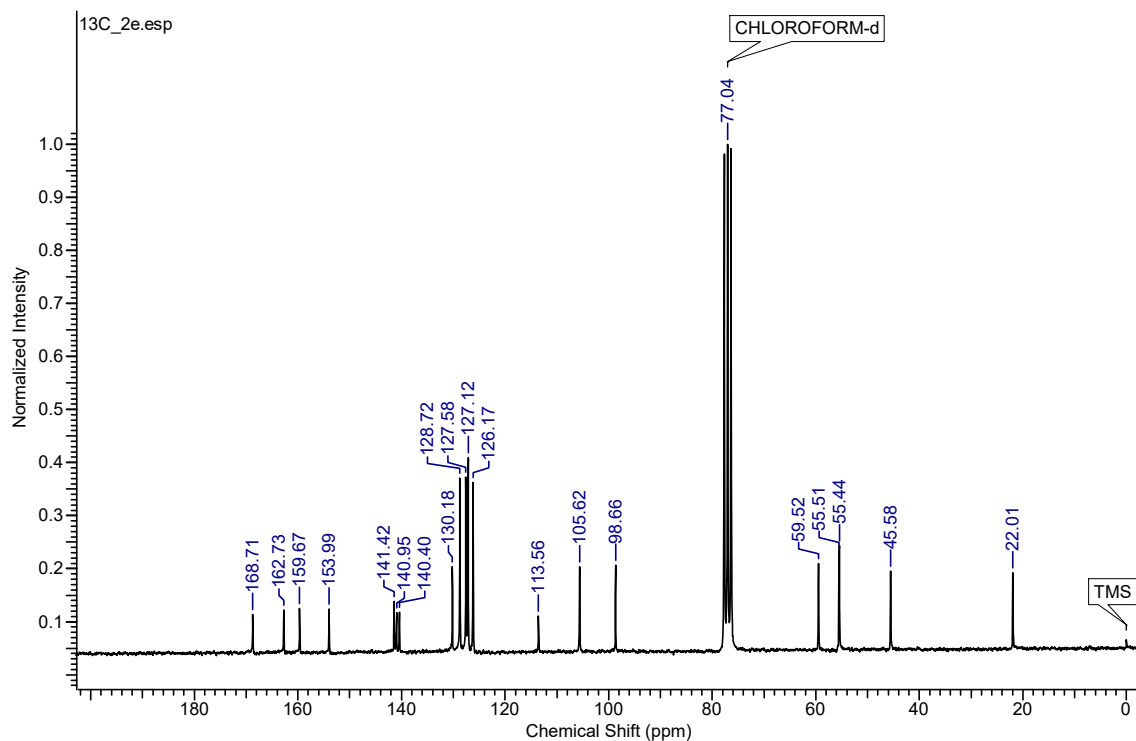


Figure 41. HR-ESI-MS of compound 2e.

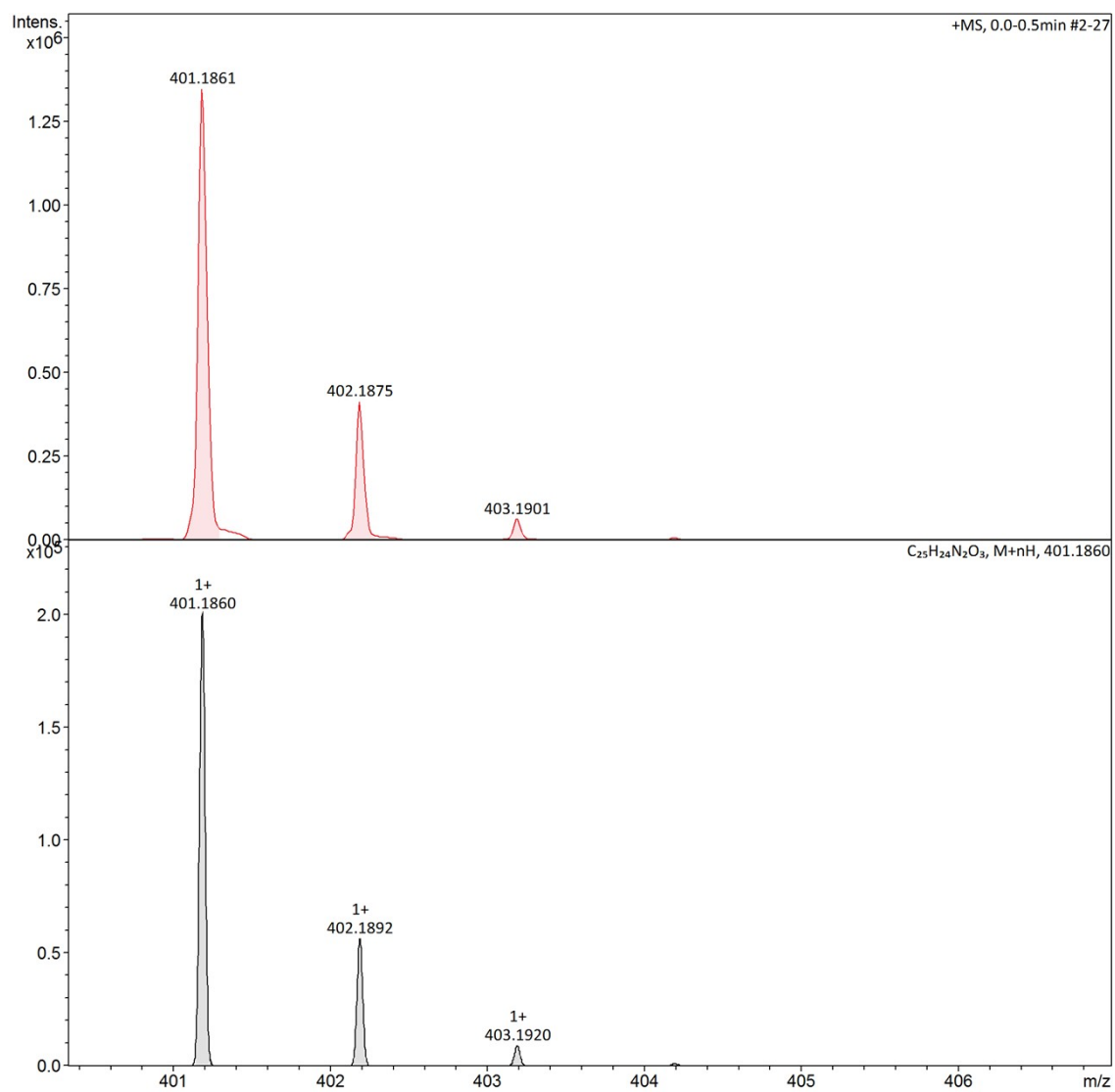


Figure 42. ^1H NMR (200 MHz, CDCl_3) of compound **2f**.

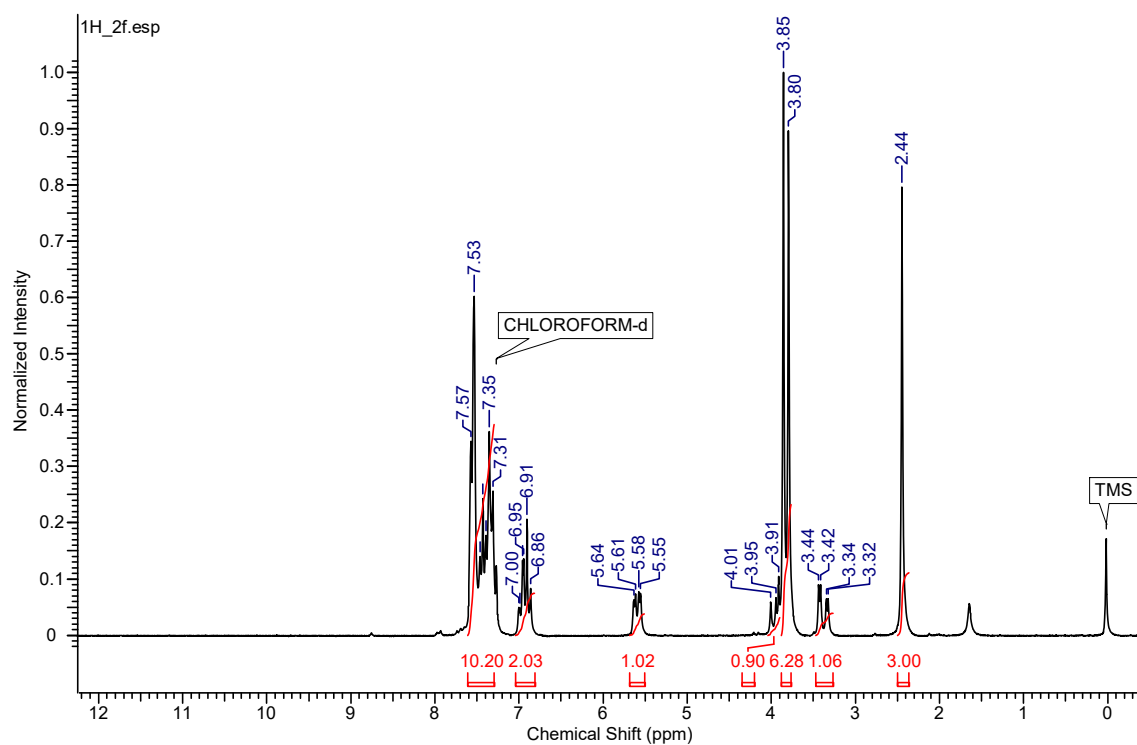


Figure 43. ^{13}C NMR (50 MHz, CDCl_3) of compound **2f**.

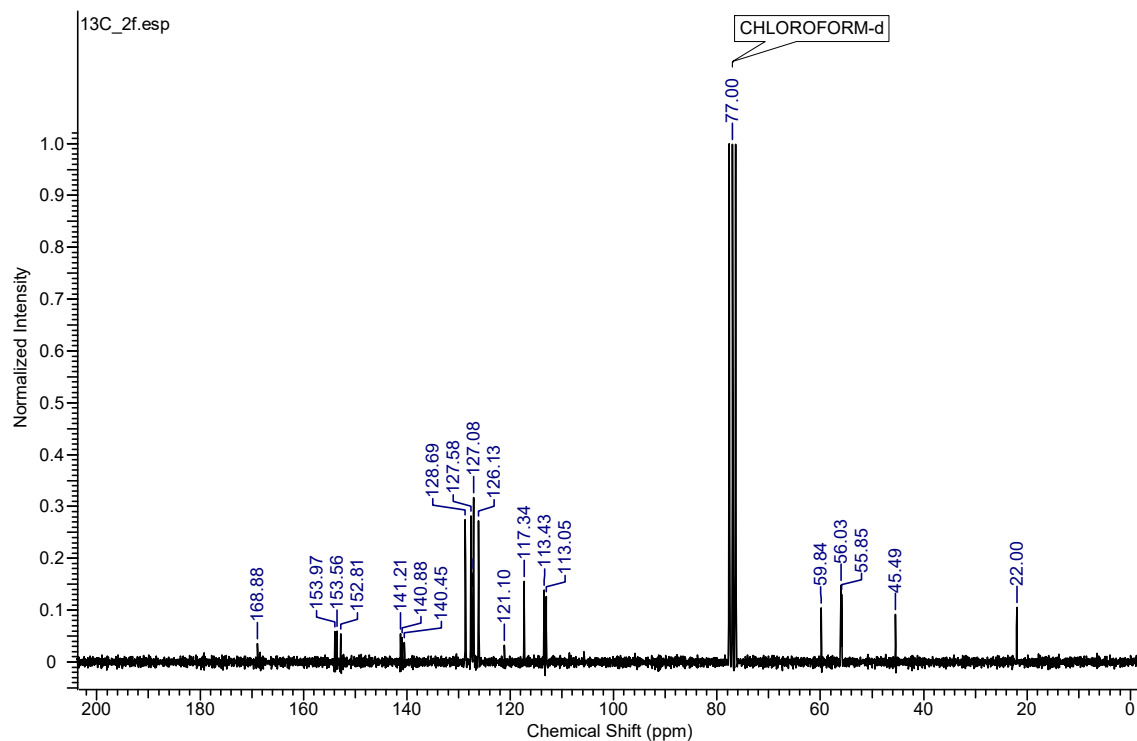


Figure 44. HR-ESI-MS of compound **2f**.

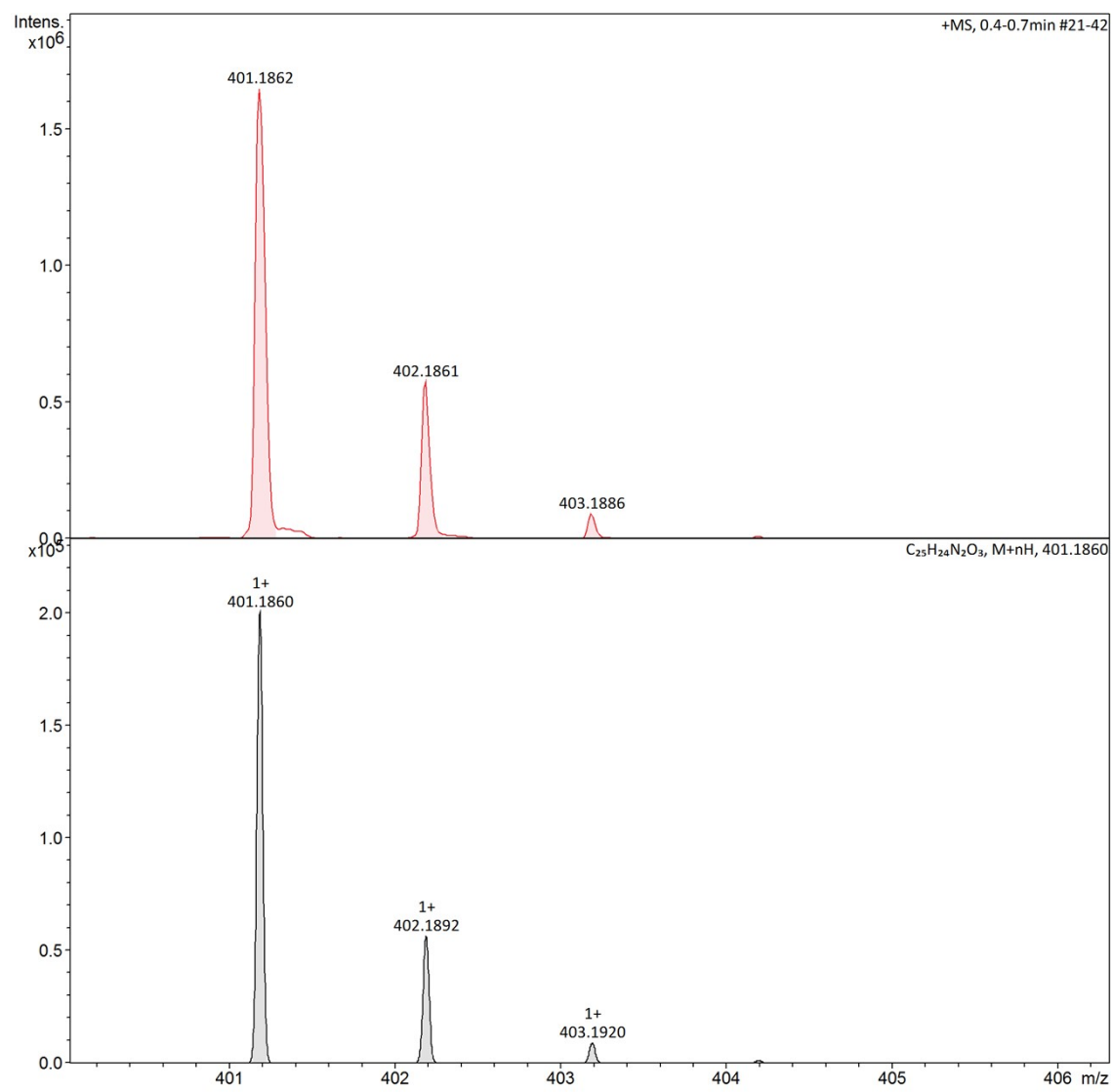


Figure 45. ^1H NMR (200 MHz, CDCl_3) of compound **2g**.

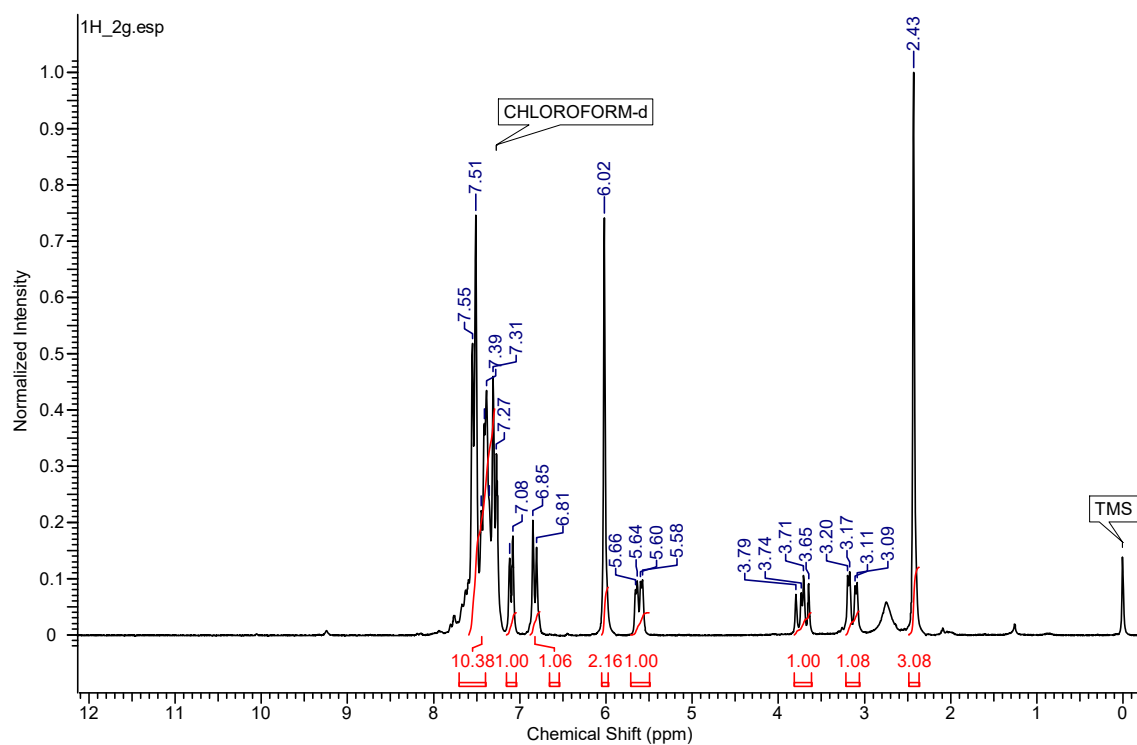


Figure 46. ^{13}C NMR (50 MHz, CDCl_3) of compound **2g**.

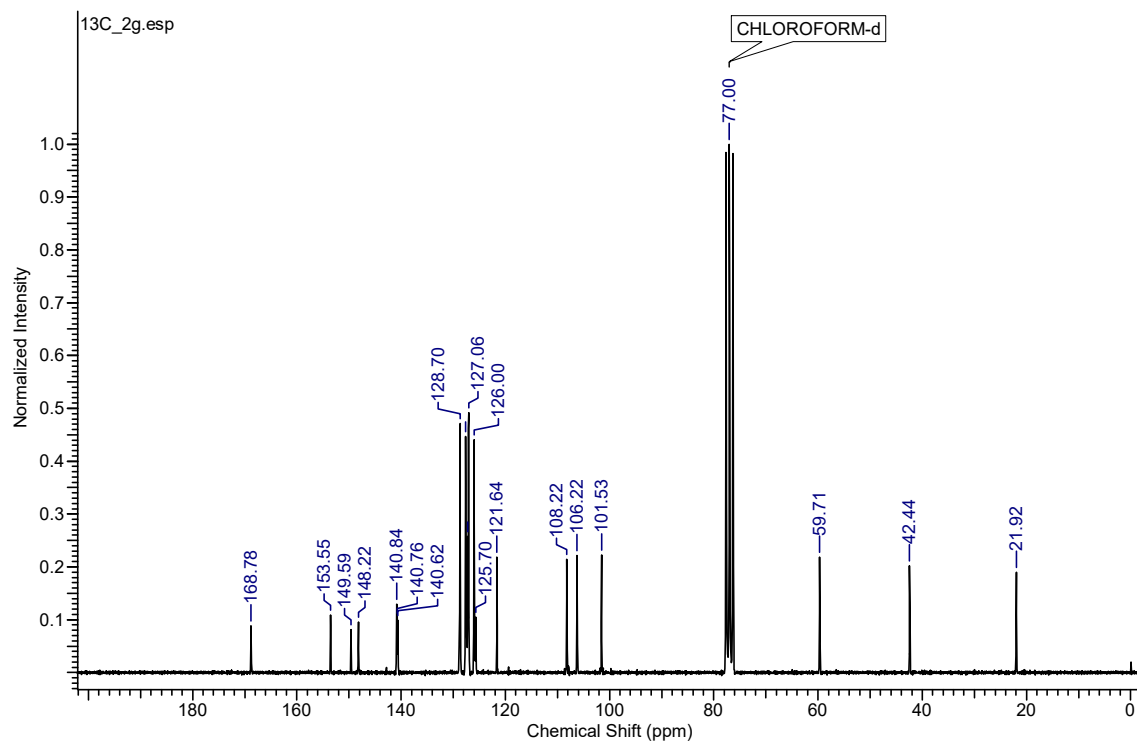


Figure 47. HR-ESI-MS of compound **2g**.

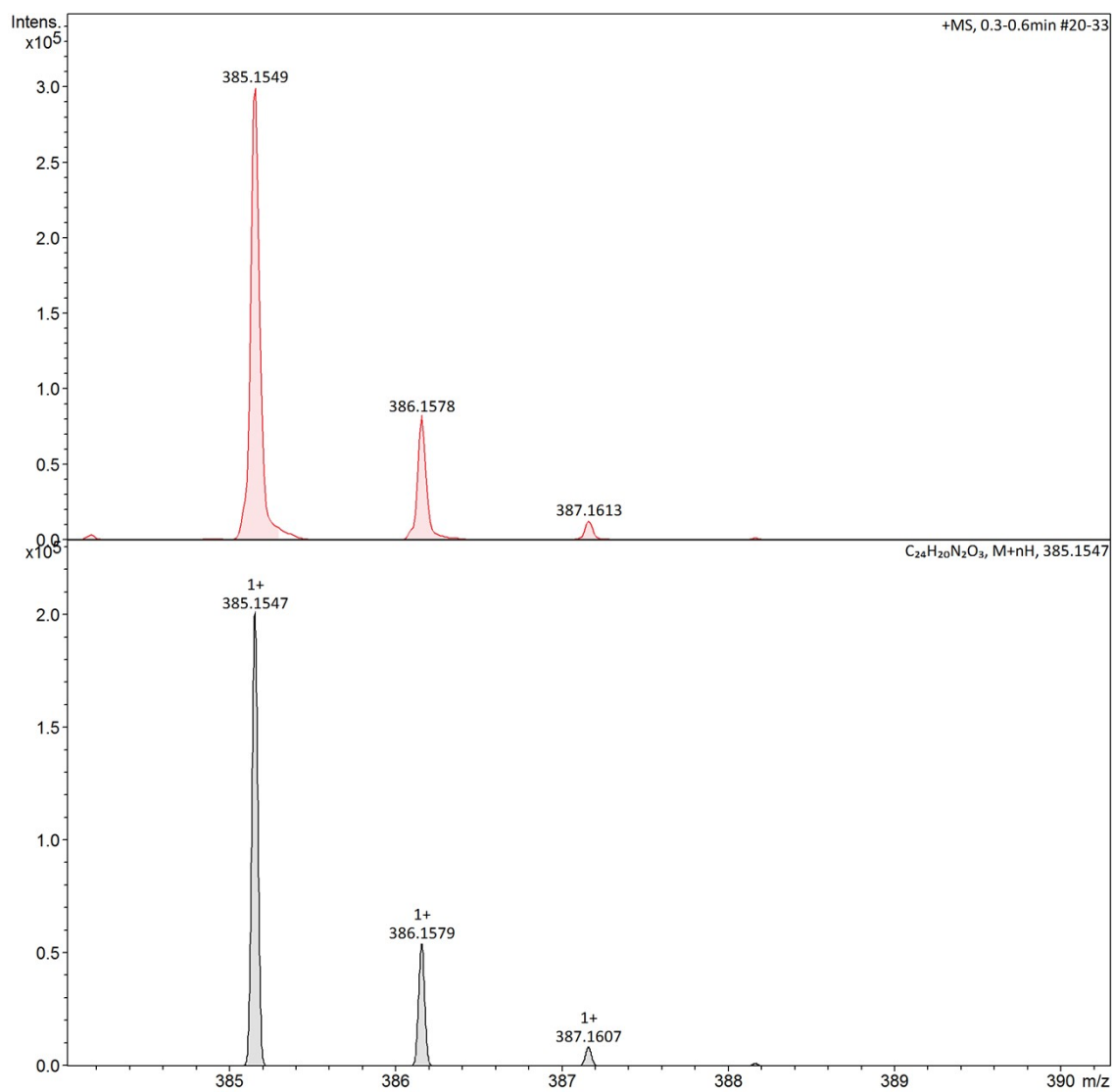


Figure 48. ^1H NMR (200 MHz, CDCl_3) of compound **2h**.

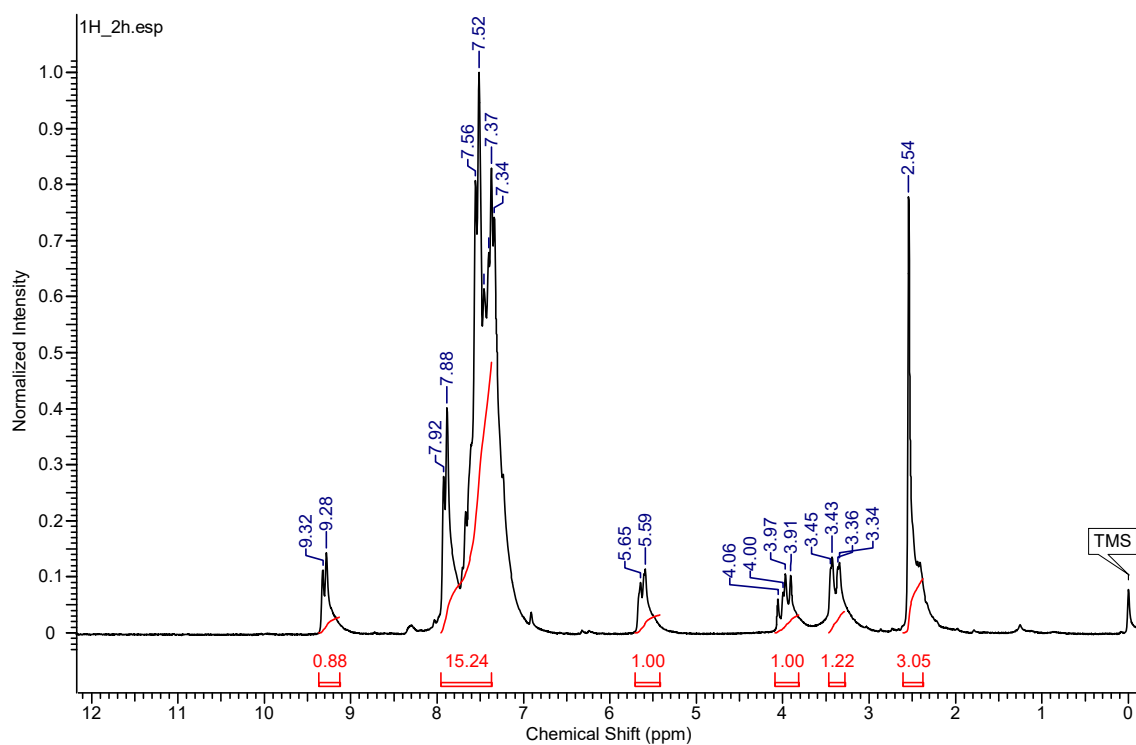


Figure 49. ^{13}C NMR (50 MHz, CDCl_3) of compound **2h**.

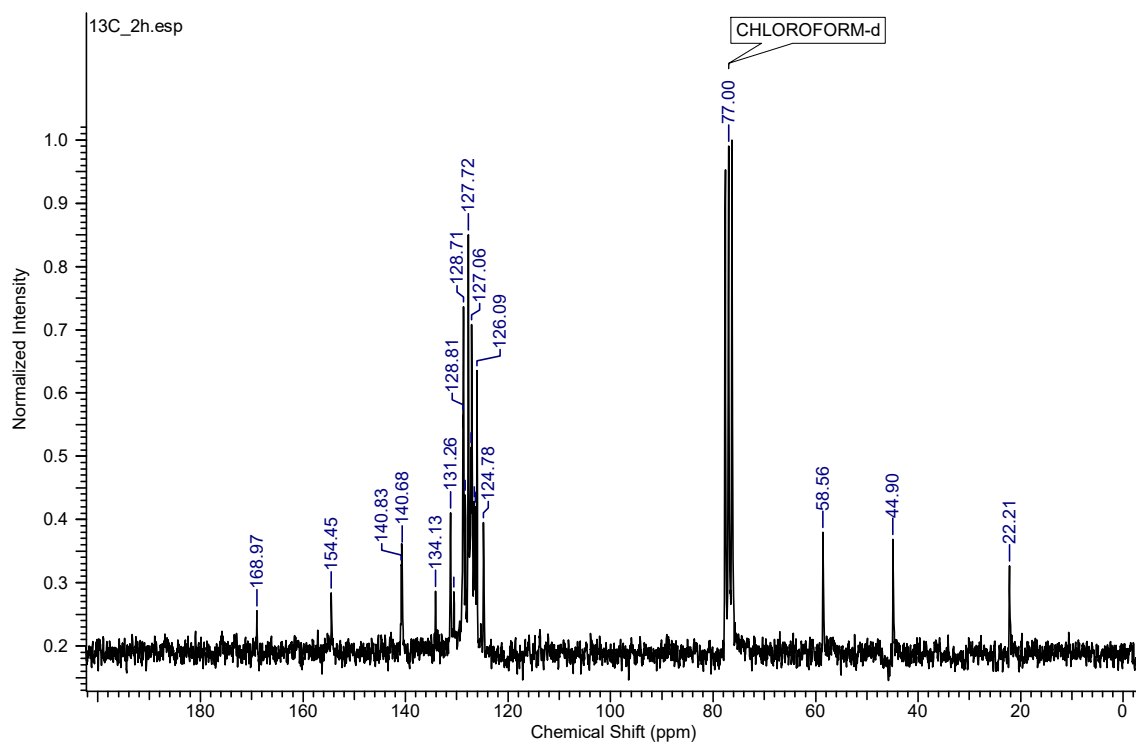


Figure 50. HR-ESI-MS of compound **2h**.

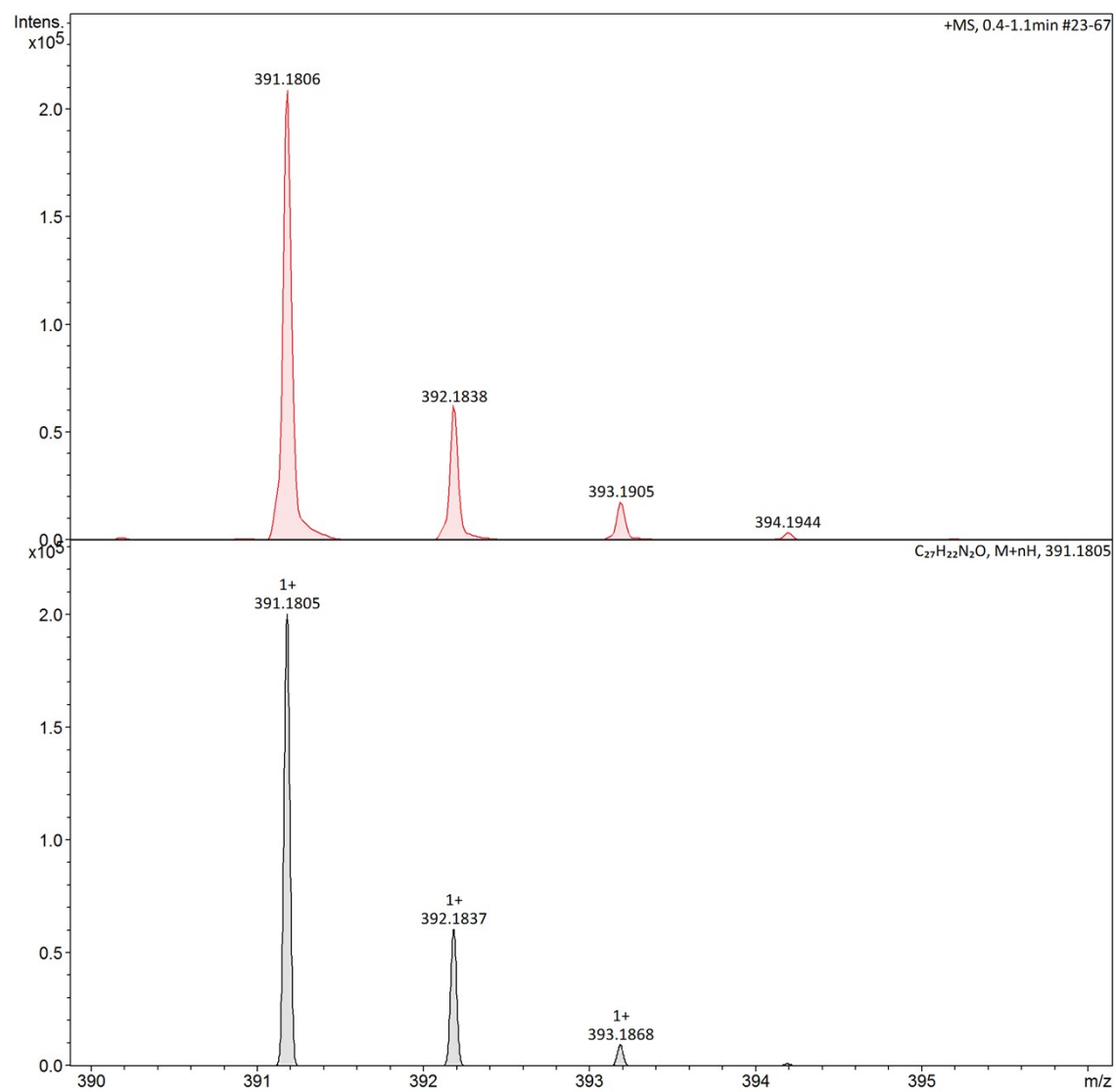


Figure 51. ^1H NMR (200 MHz, CDCl_3) of compound **2i**.

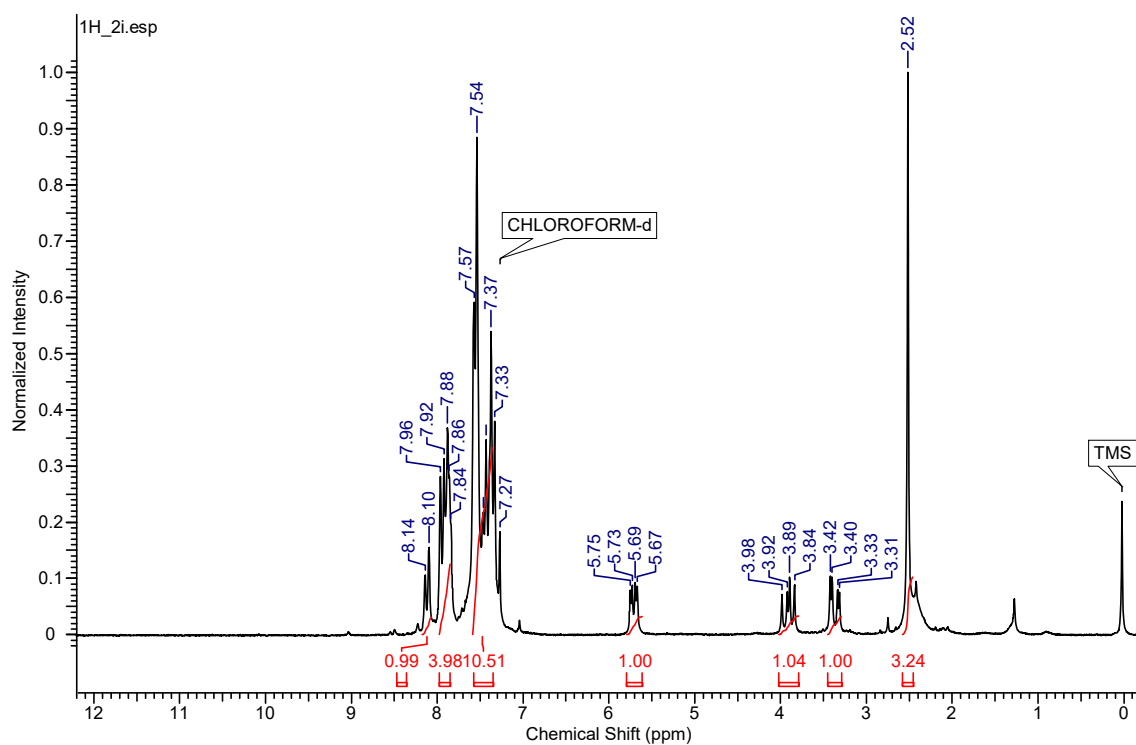


Figure 52. ^{13}C NMR (50 MHz, CDCl_3) of compound **2i**.

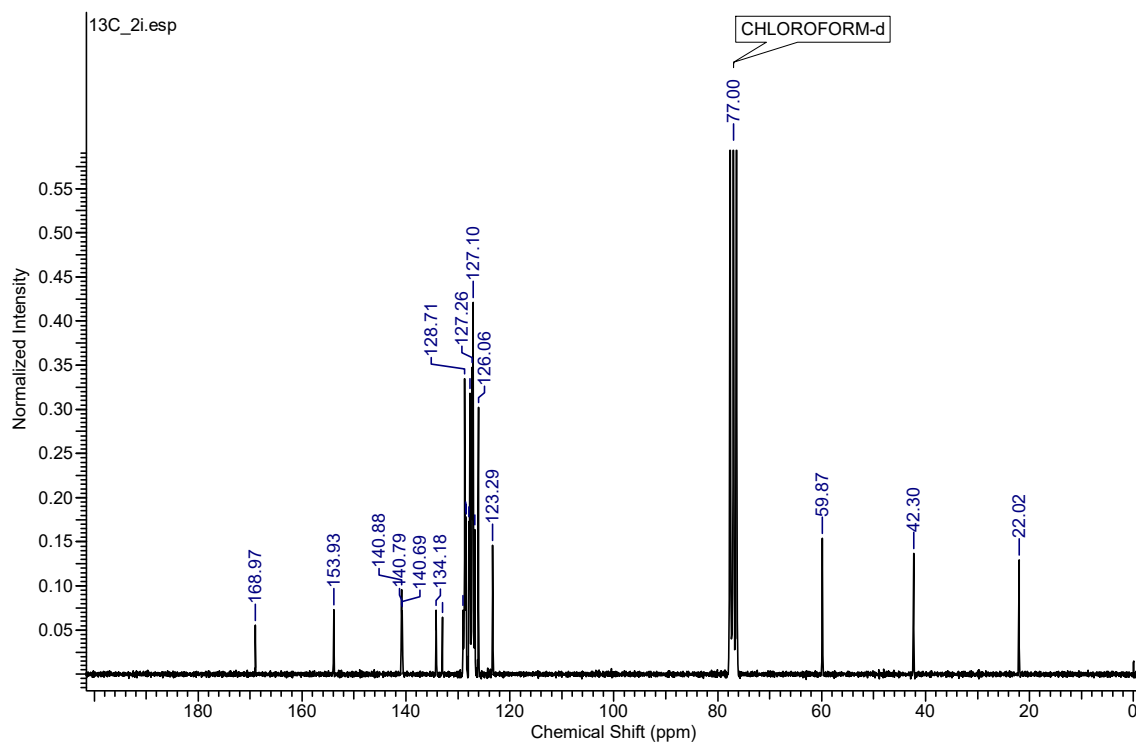


Figure 53. HR-ESI-MS of compound **2i**.

