Supplementary Data

Manzamine Alkaloids from an *Acanthostrongylophora* sp. Sponge

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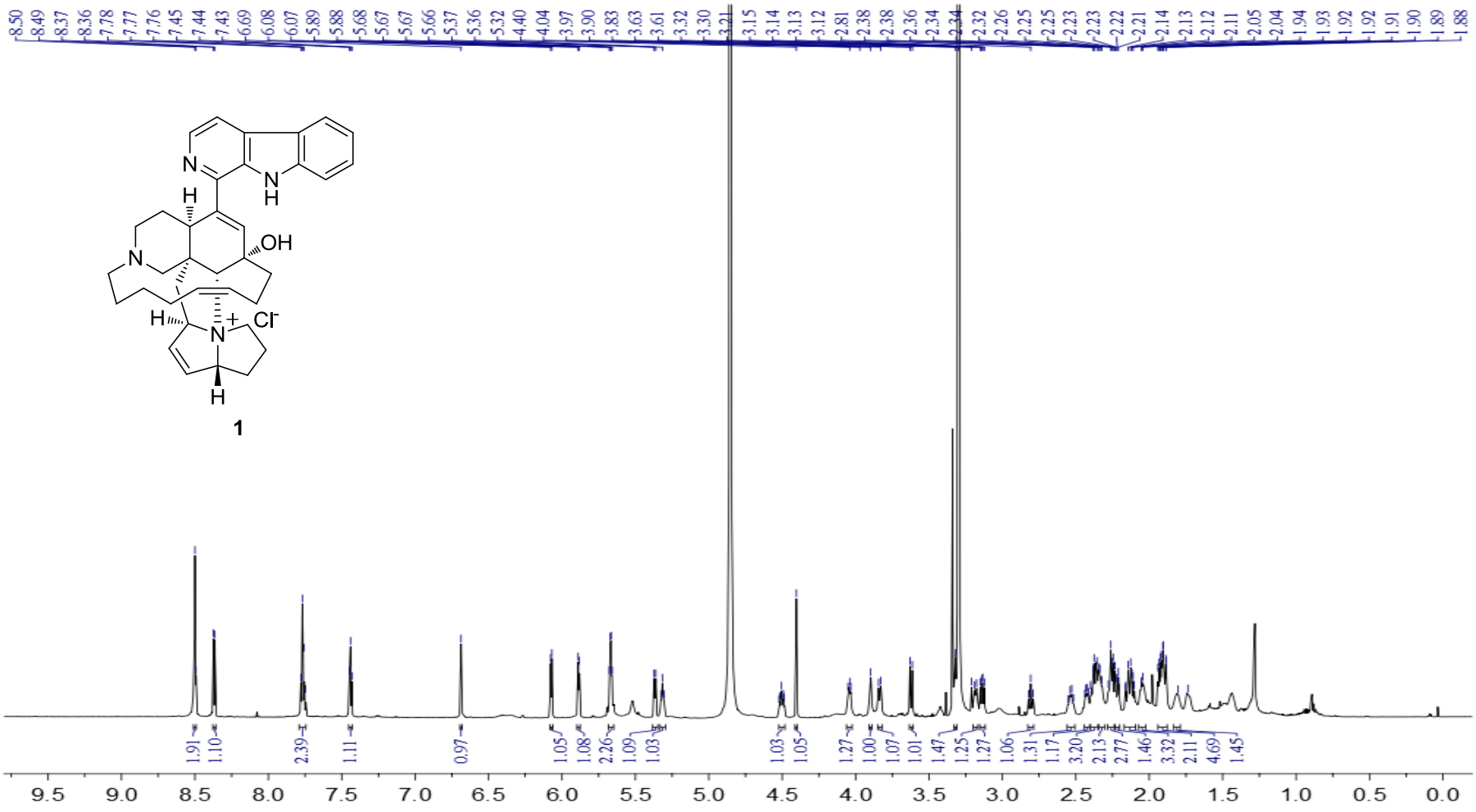
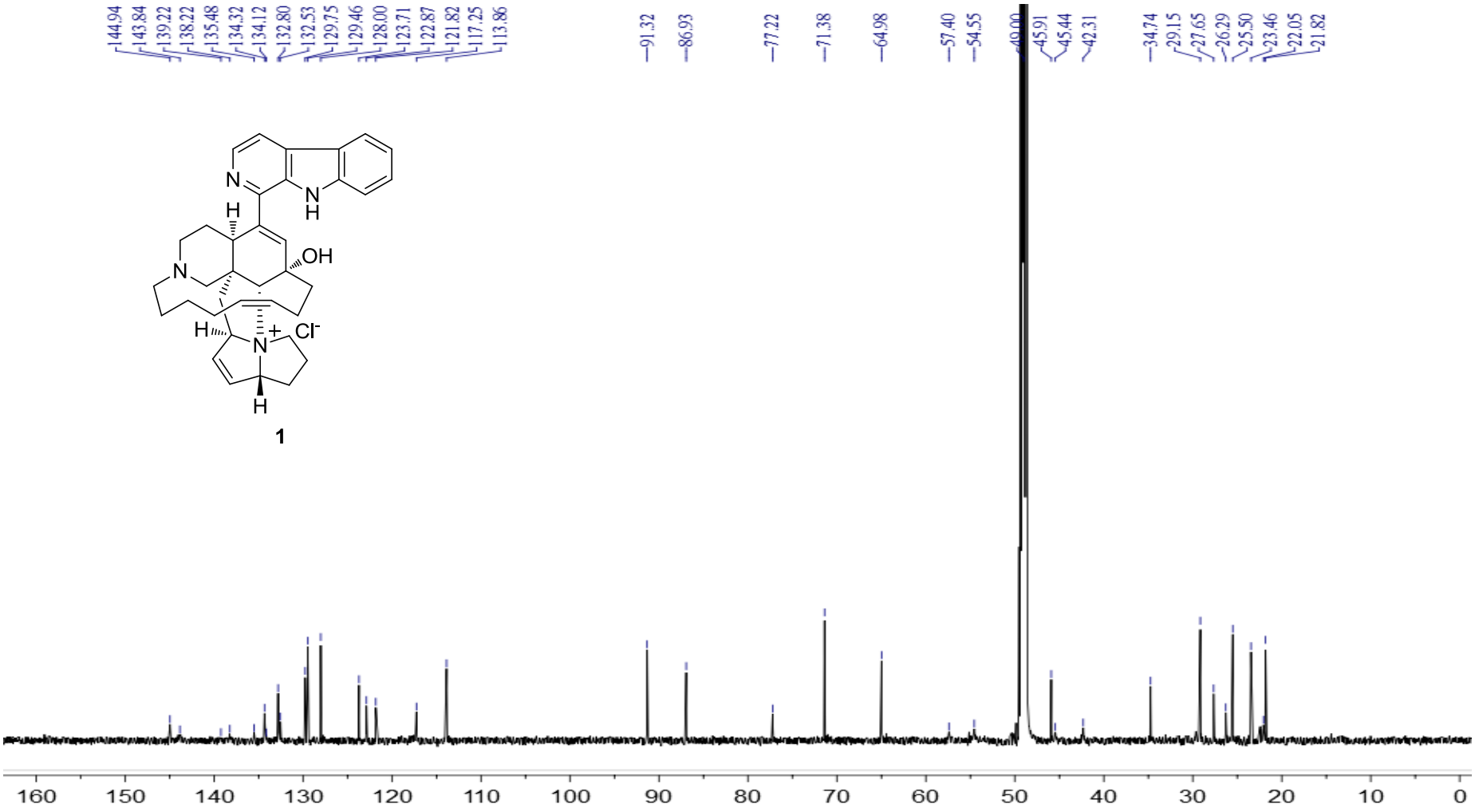


Figure S1. The ^{1}H NMR (800 MHz, CD_3OD) spectrum of **1**



1

Figure S2. The ^{13}C NMR (200 MHz, CD_3OD) spectrum of **1**

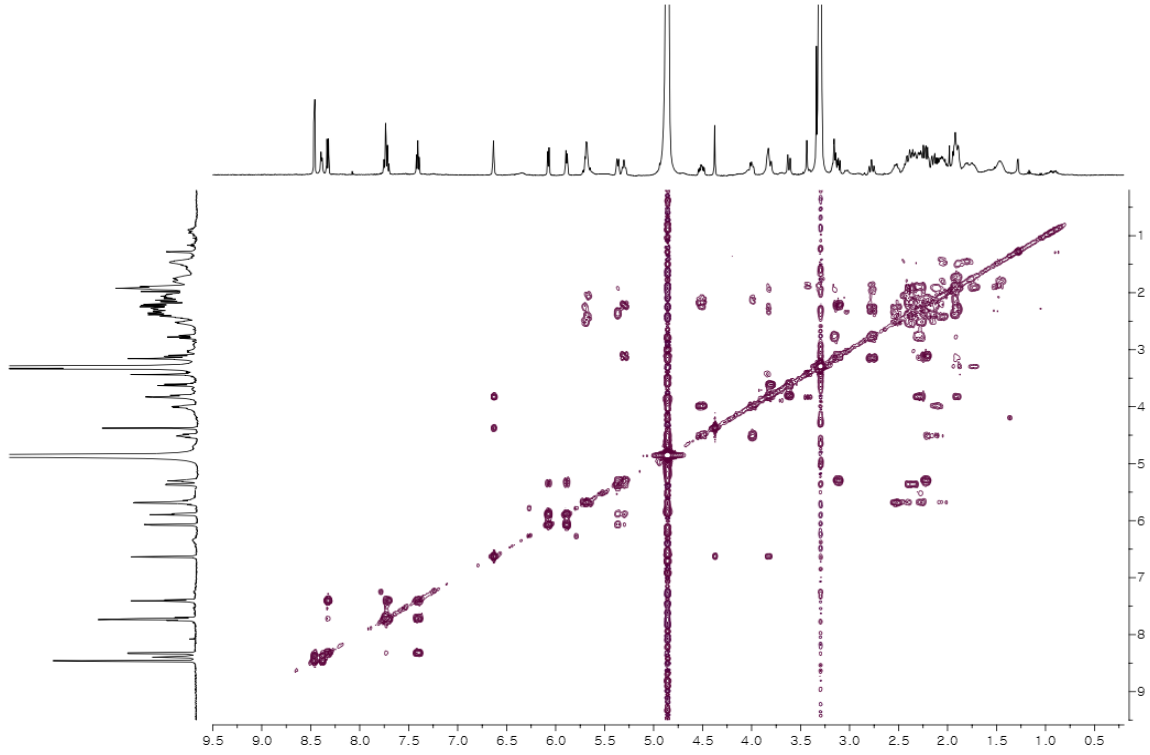


Figure S3. The COSY NMR (800 MHz, CD_3OD) spectrum of **1**

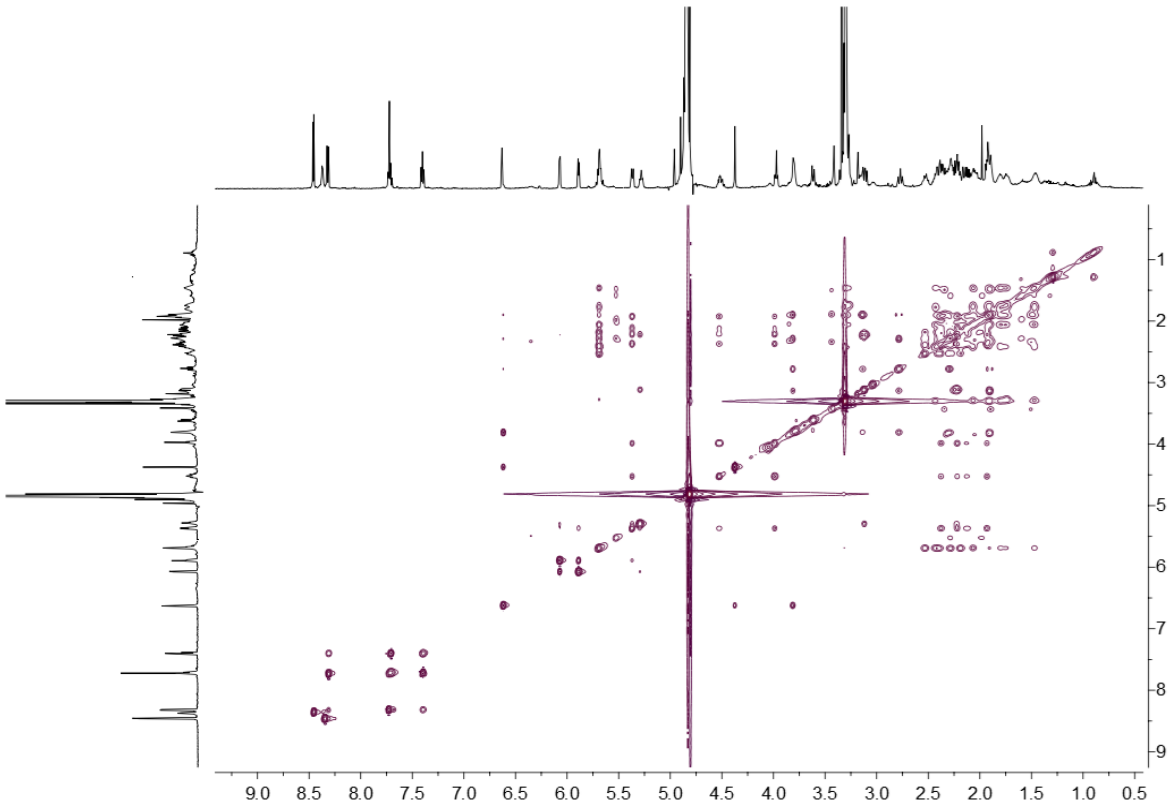


Figure S4. The TOCSY NMR (800 MHz, CD_3OD) spectrum of **1**

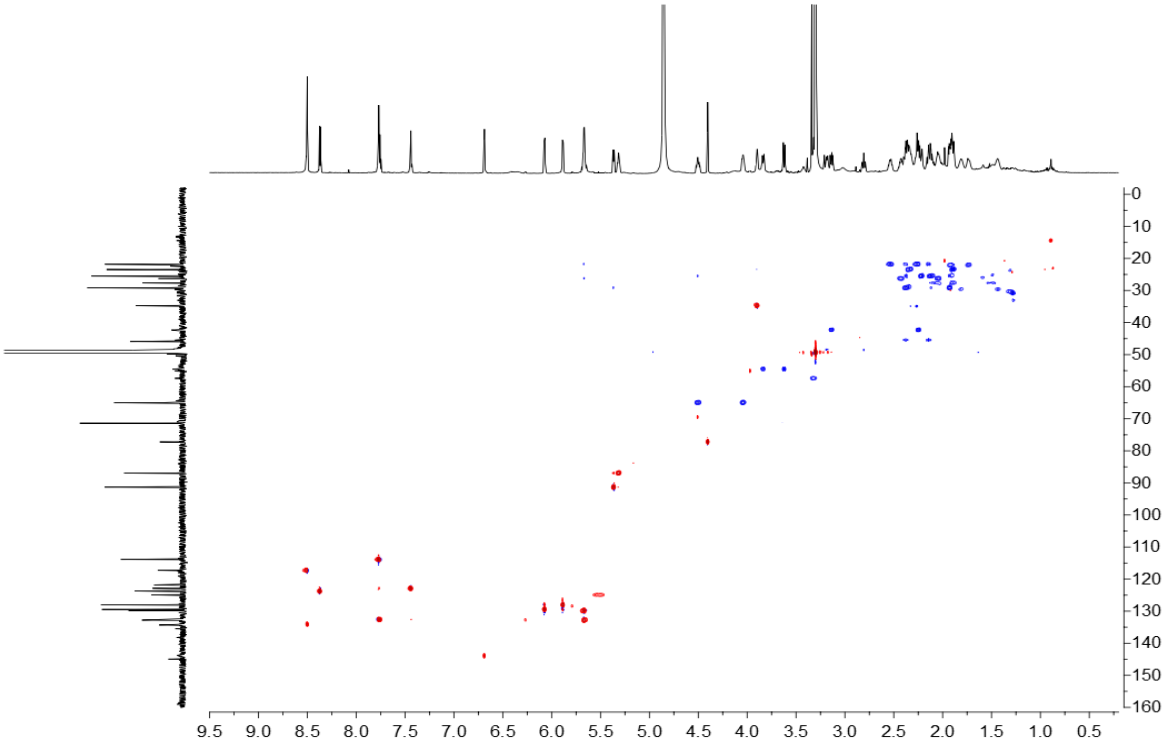


Figure S5. The eHSQC NMR (800 MHz, CD_3OD) spectrum of **1**

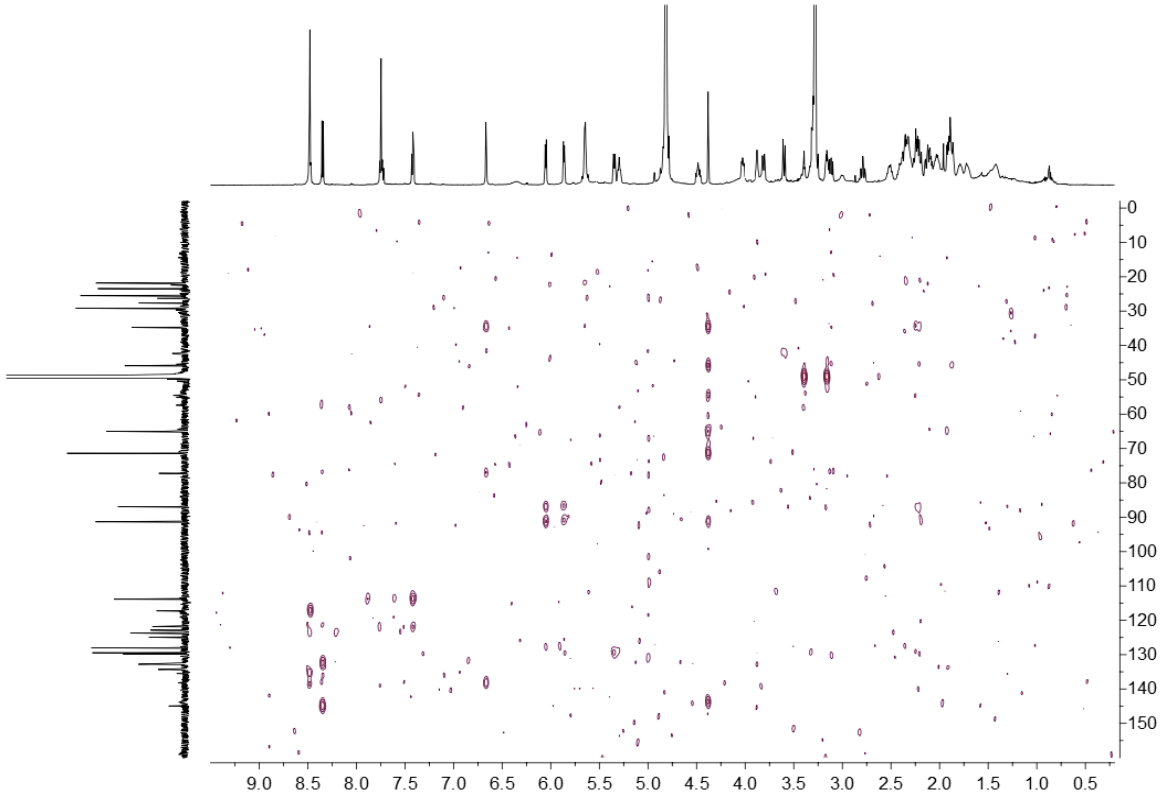


Figure S6. The HMBC NMR (800 MHz, CD_3OD) spectrum of **1**

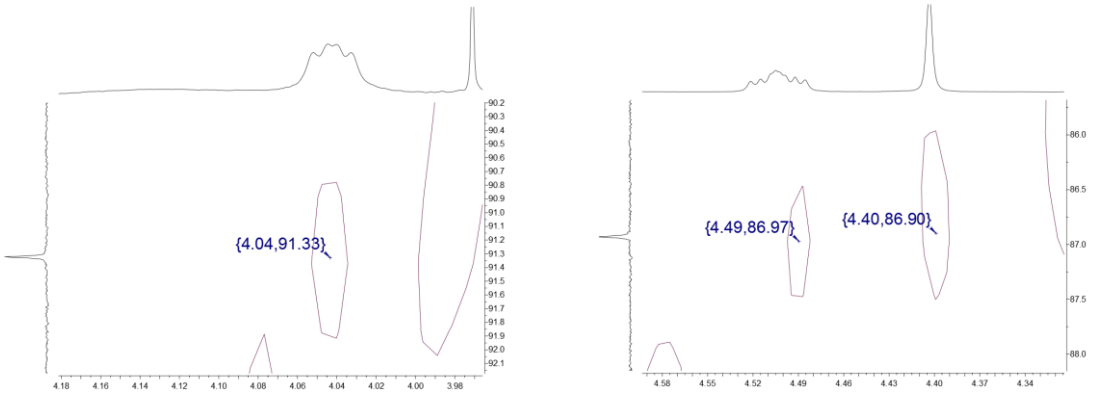


Figure S7. The expanded HMBC NMR (800 MHz, CD_3OD) spectrum of **1**

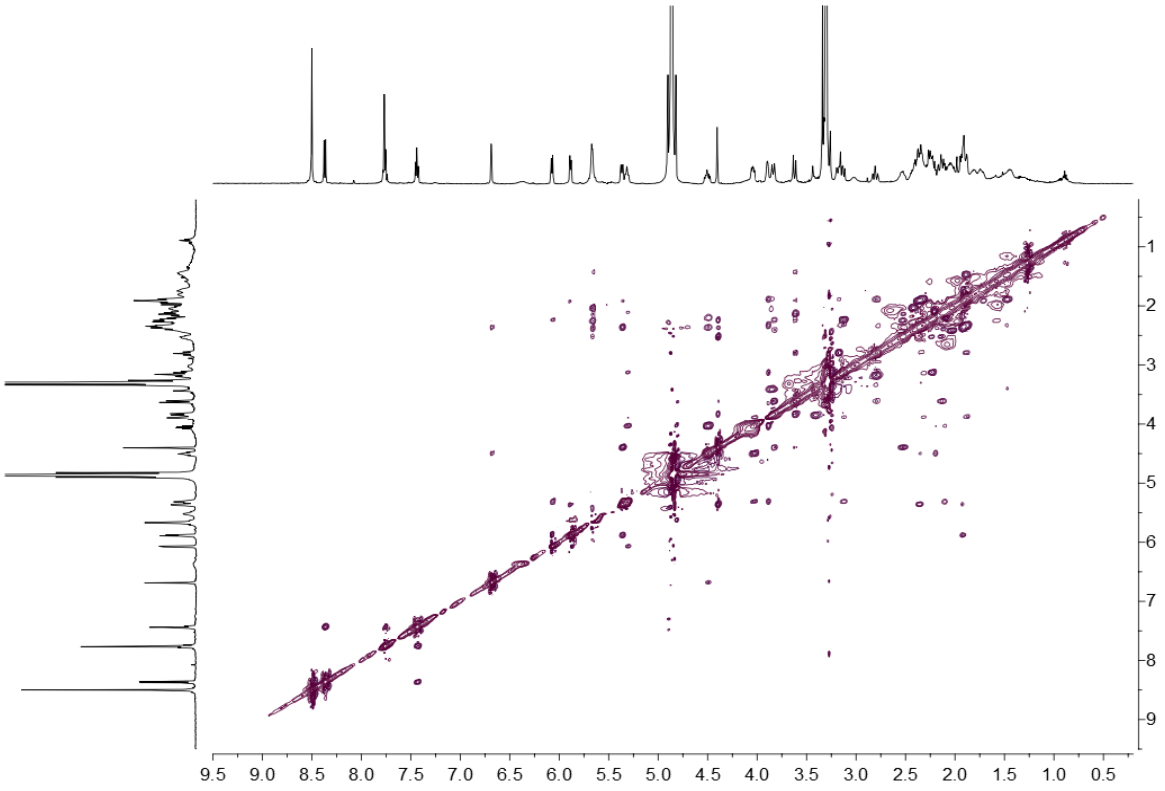


Figure S8. The ROESY NMR (800 MHz, CD_3OD) spectrum of **1**

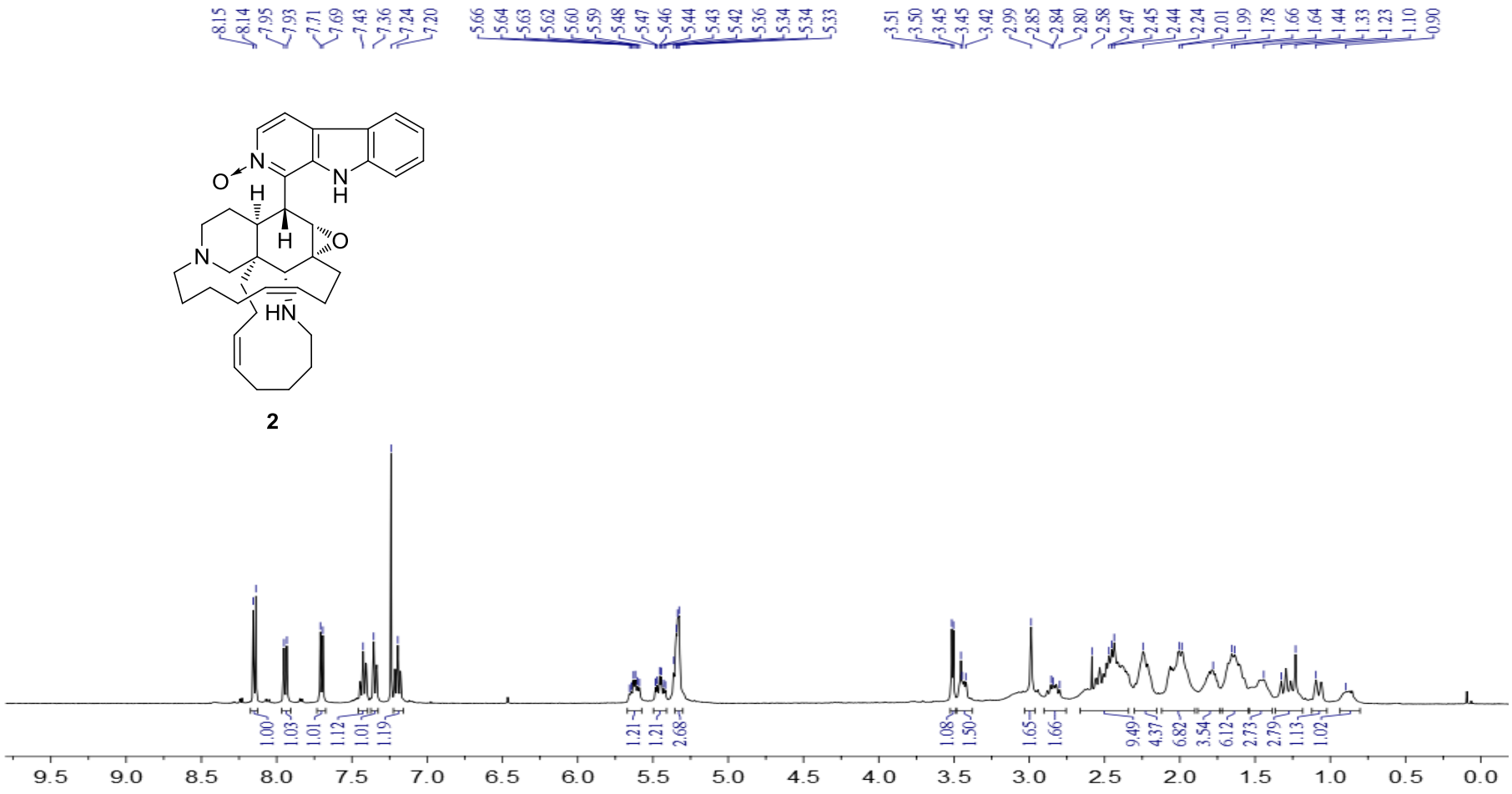


Figure S9. The ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **2**

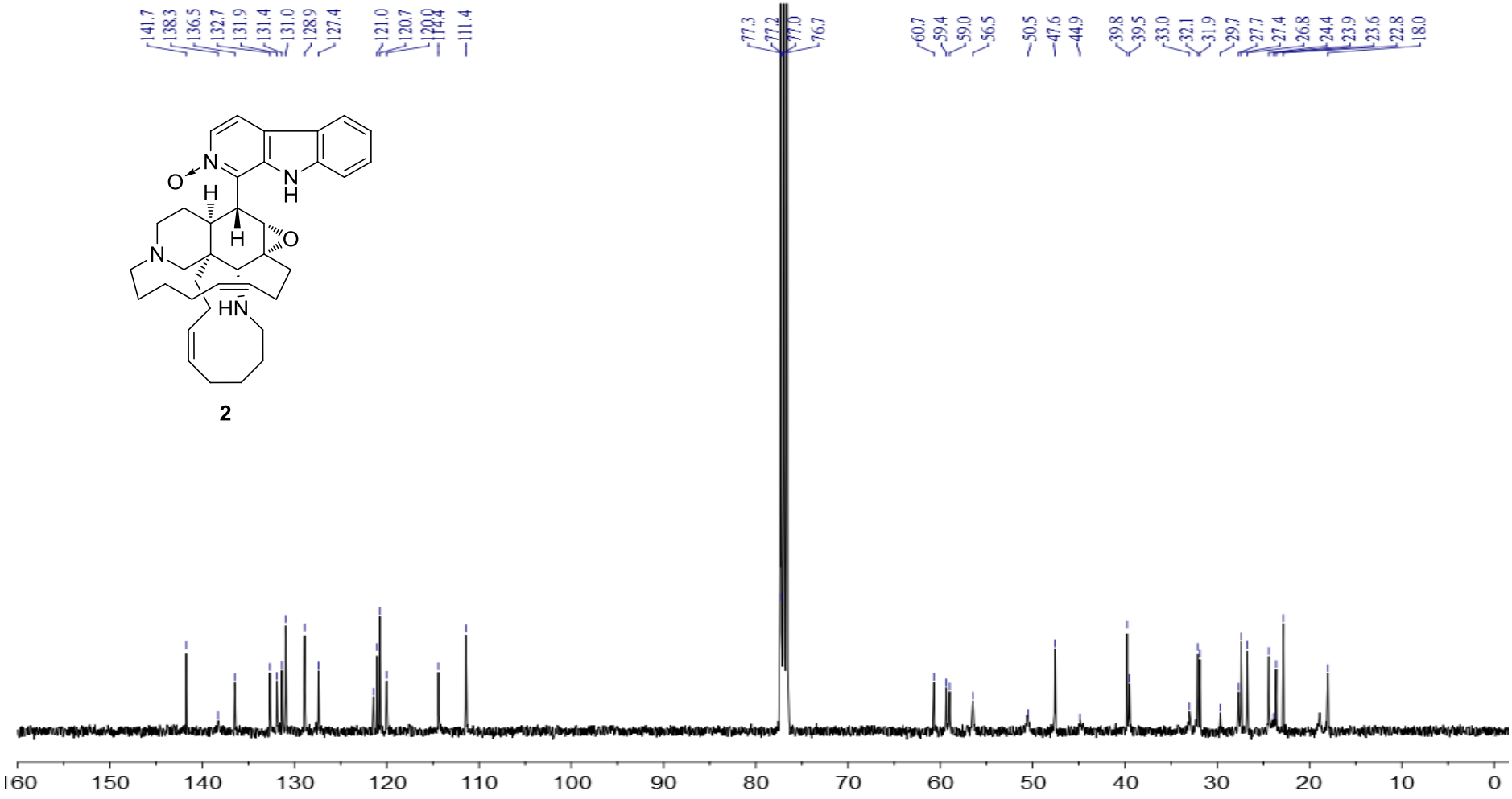


Figure S10. The ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **2**

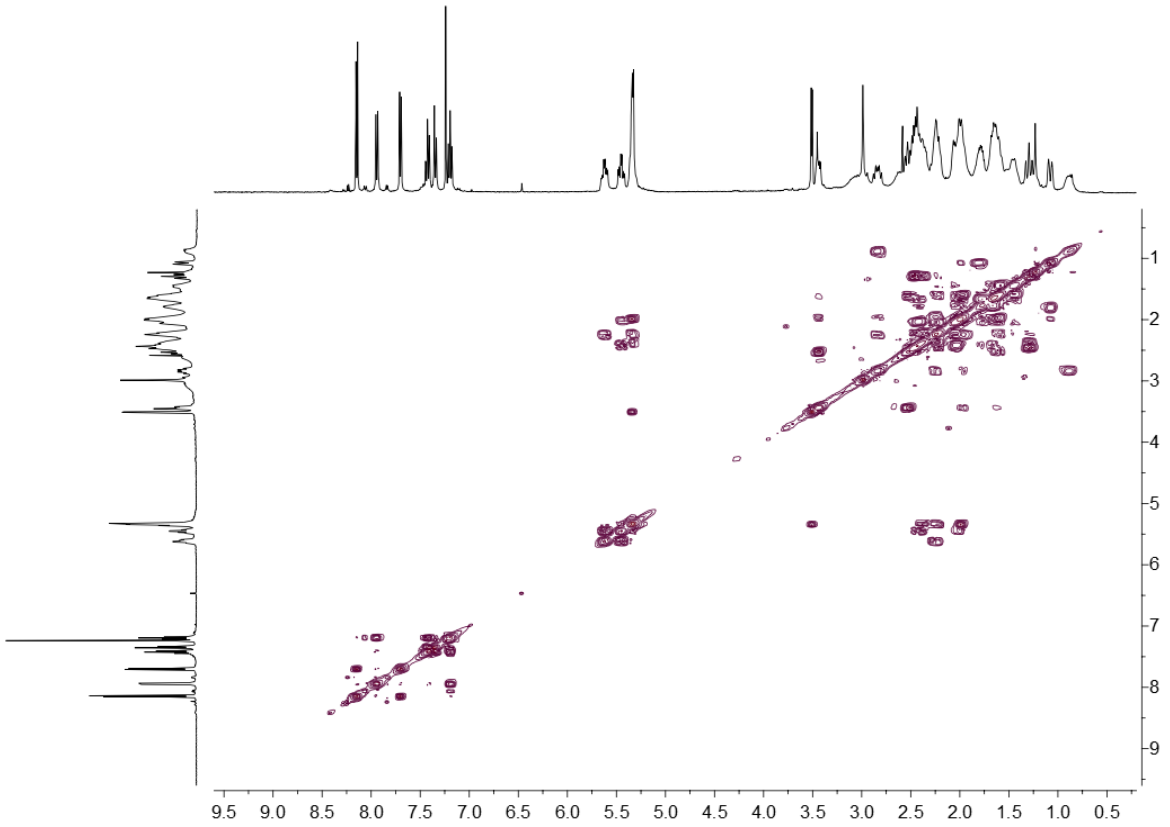


Figure S11. The COSY NMR (400 MHz, $CDCl_3$) spectrum of **2**

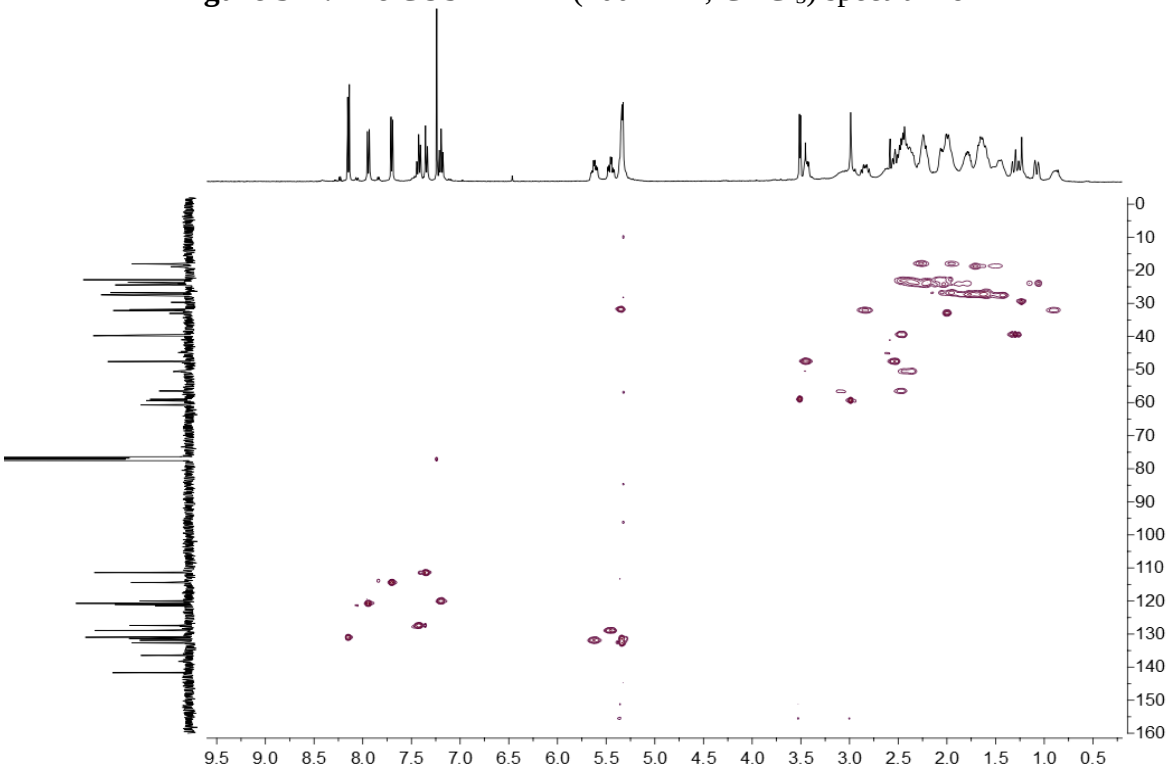


Figure S12. The HSQC NMR (400 MHz, $CDCl_3$) spectrum of **2**

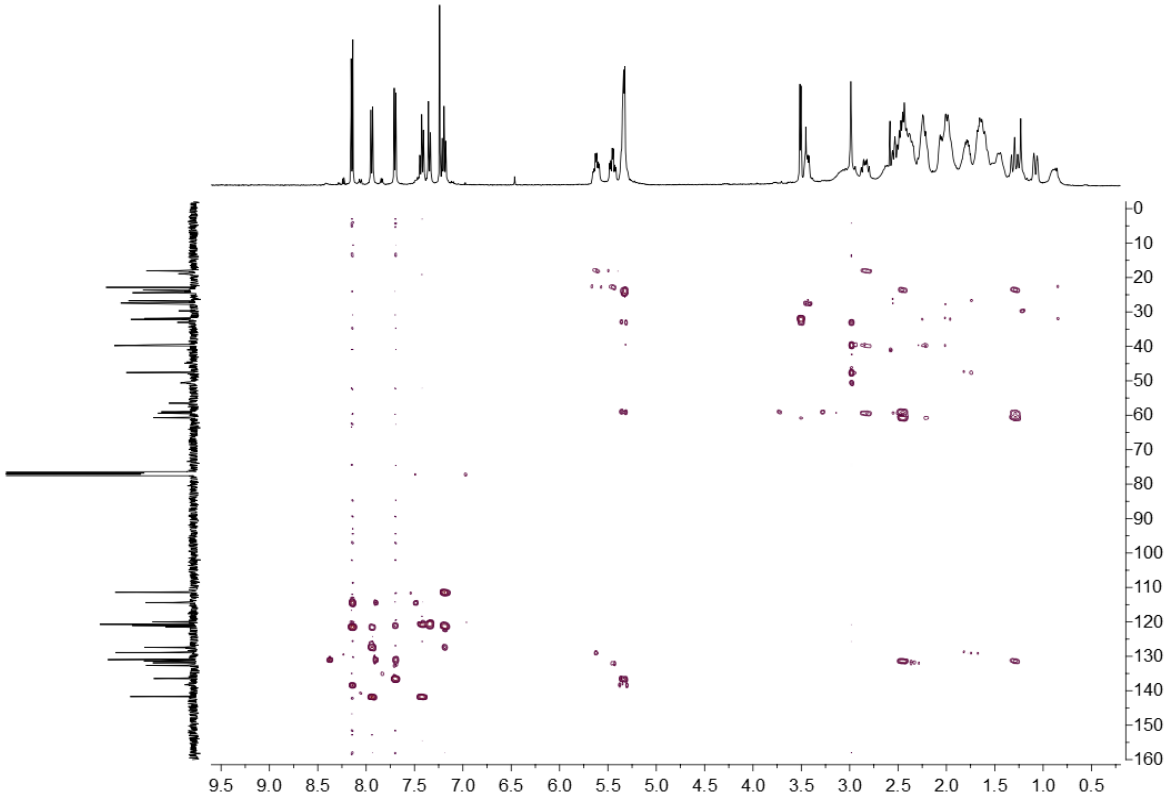


Figure S13. The HMBC NMR (400 MHz, $CDCl_3$) spectrum of **2**

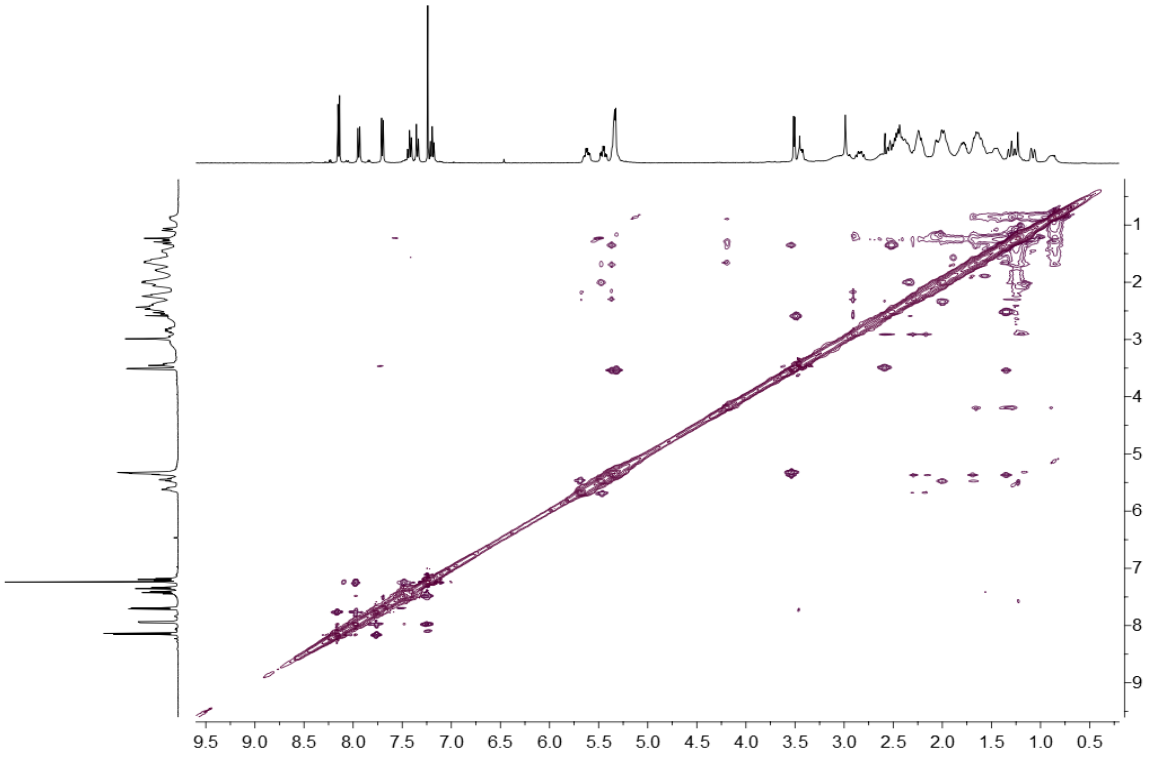


Figure S14. The ROESY NMR (400 MHz, $CDCl_3$) spectrum of **2**

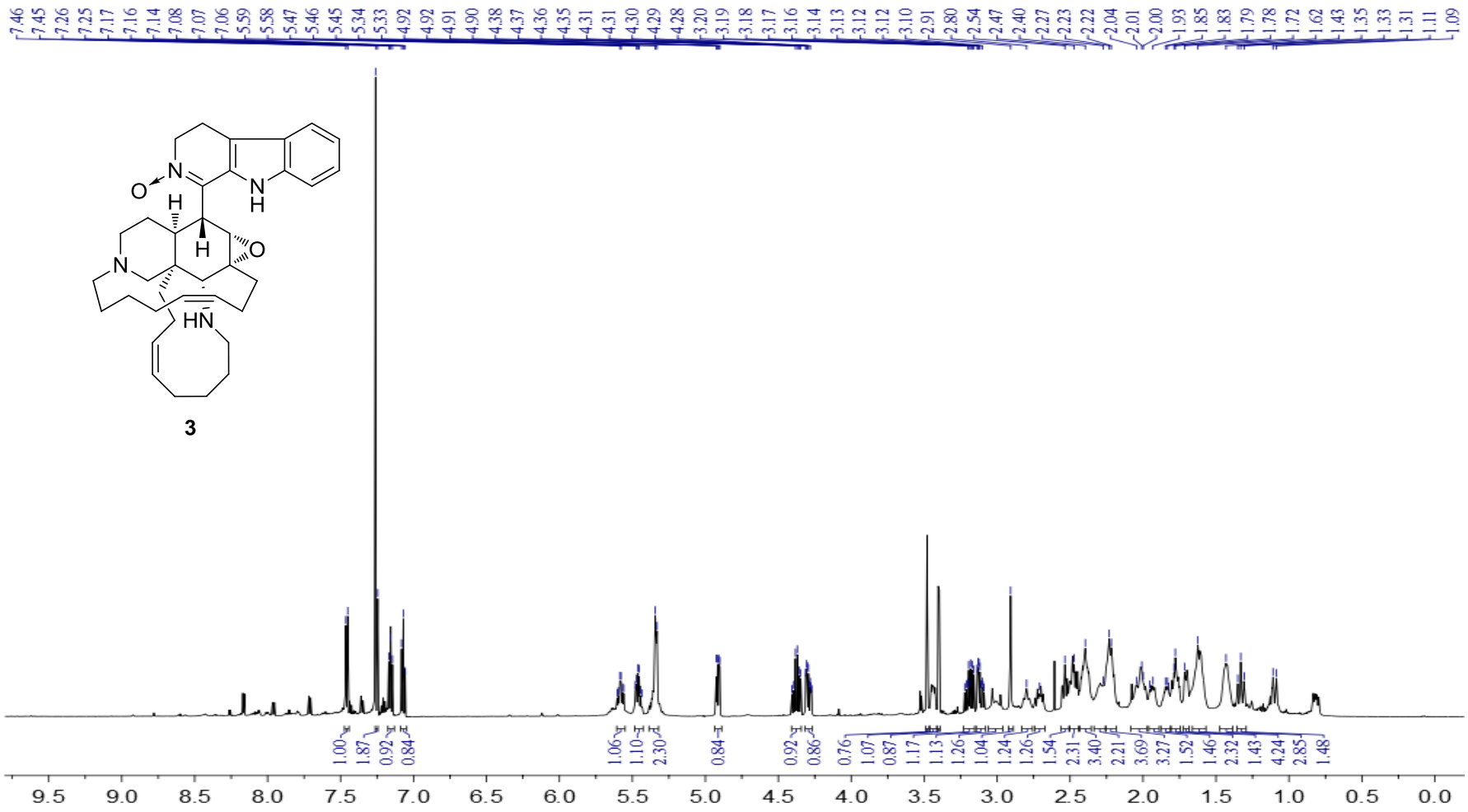


Figure S15. The ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **3**

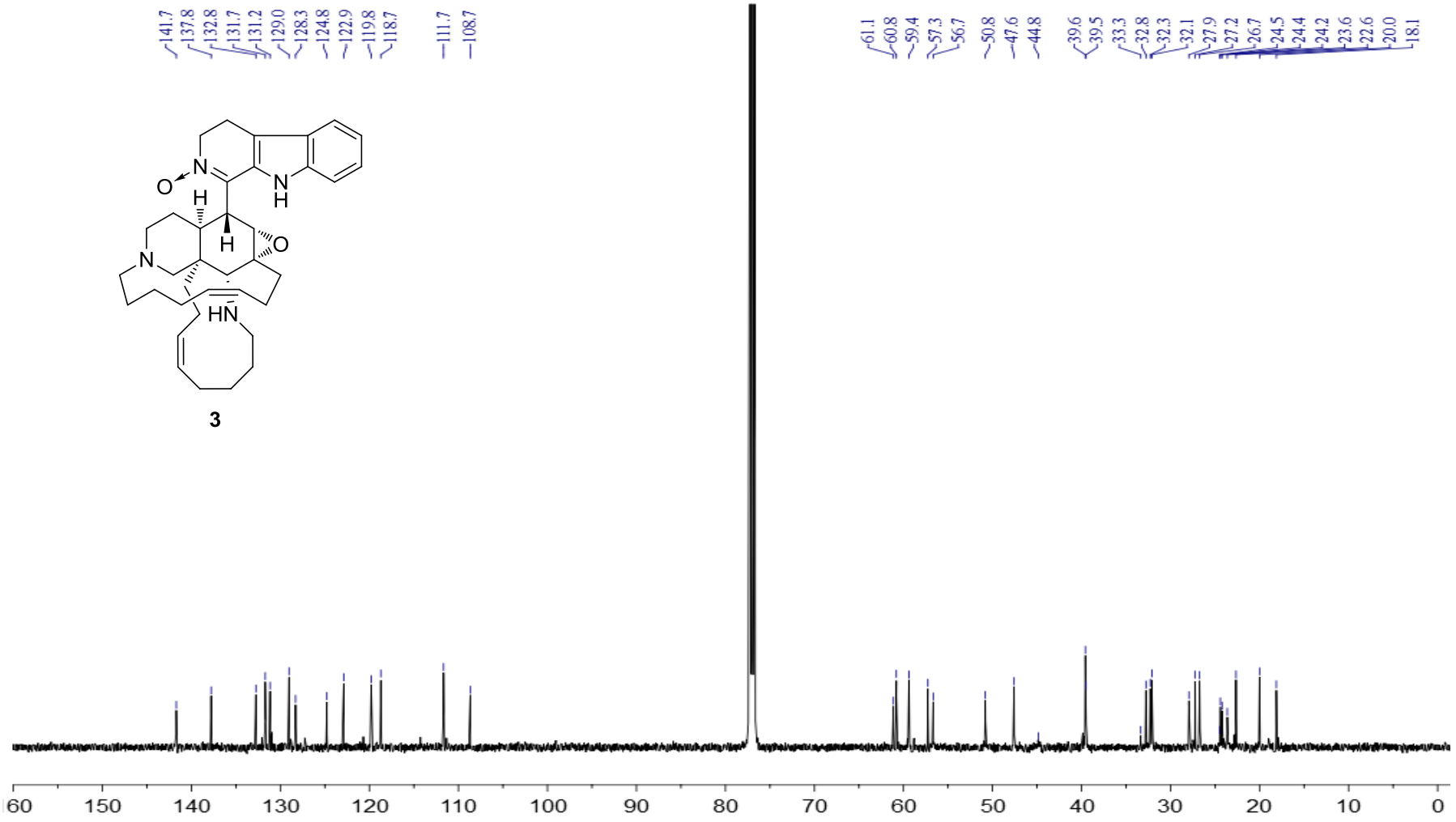


Figure S16. The ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of **3**

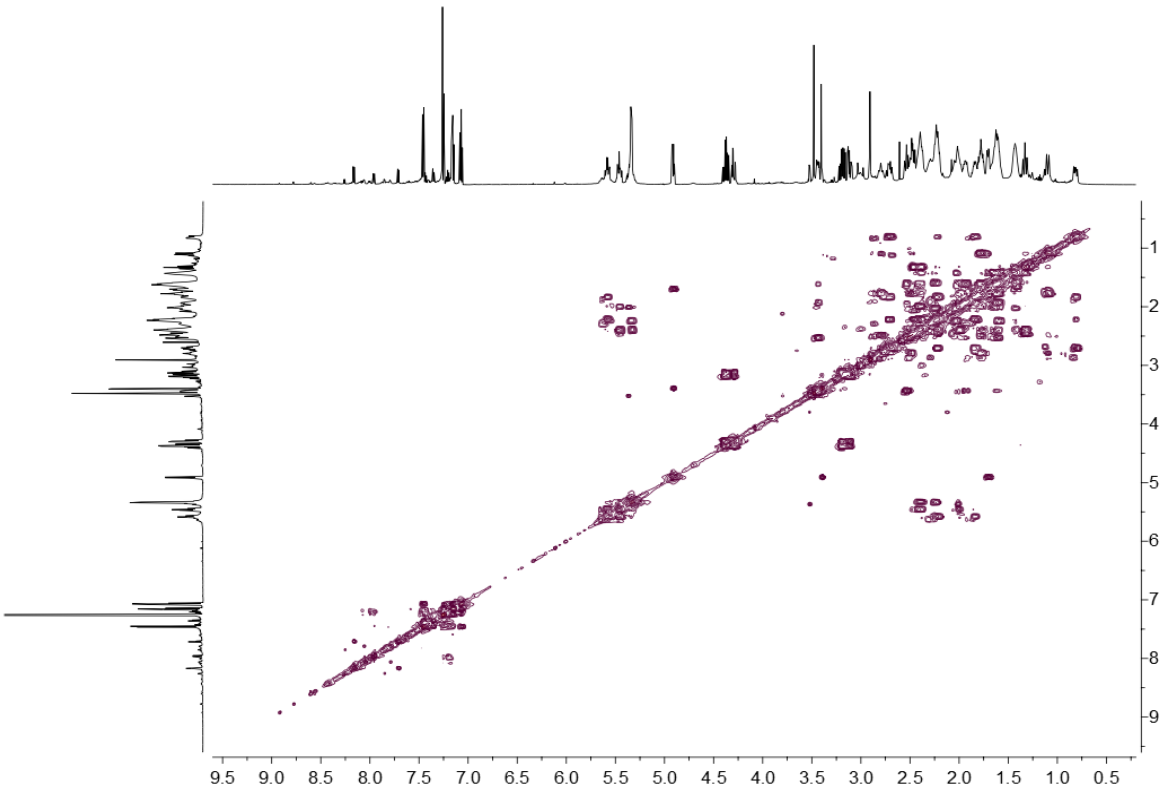


Figure S17. The COSY NMR (500 MHz, $CDCl_3$) spectrum of **3**

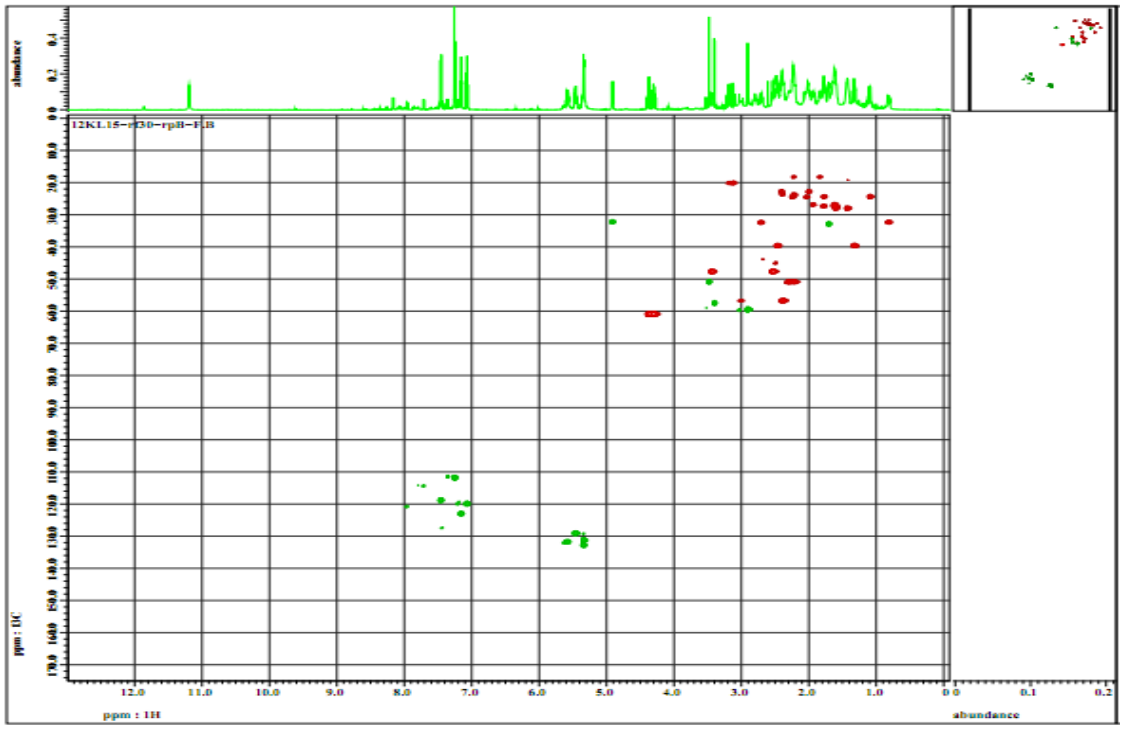


Figure S18. The eHSQC NMR (500 MHz, $CDCl_3$) spectrum of **3**

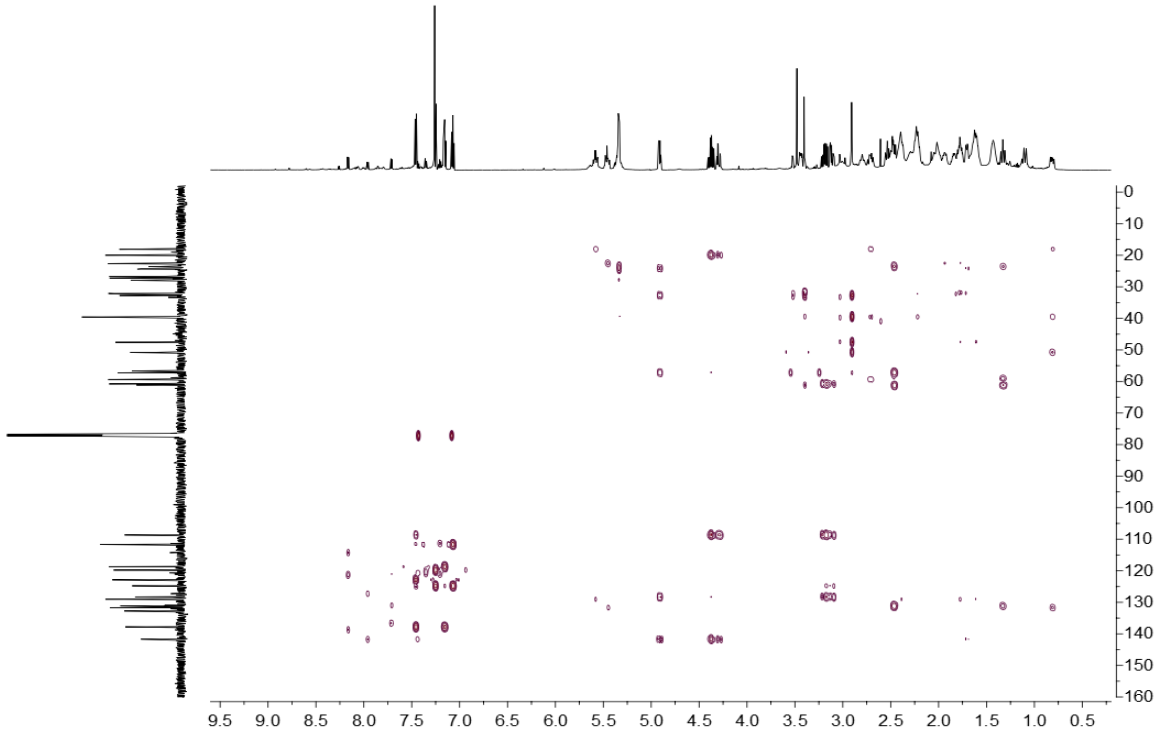


Figure S19. The HMBC NMR (500 MHz, $CDCl_3$) spectrum of **3**

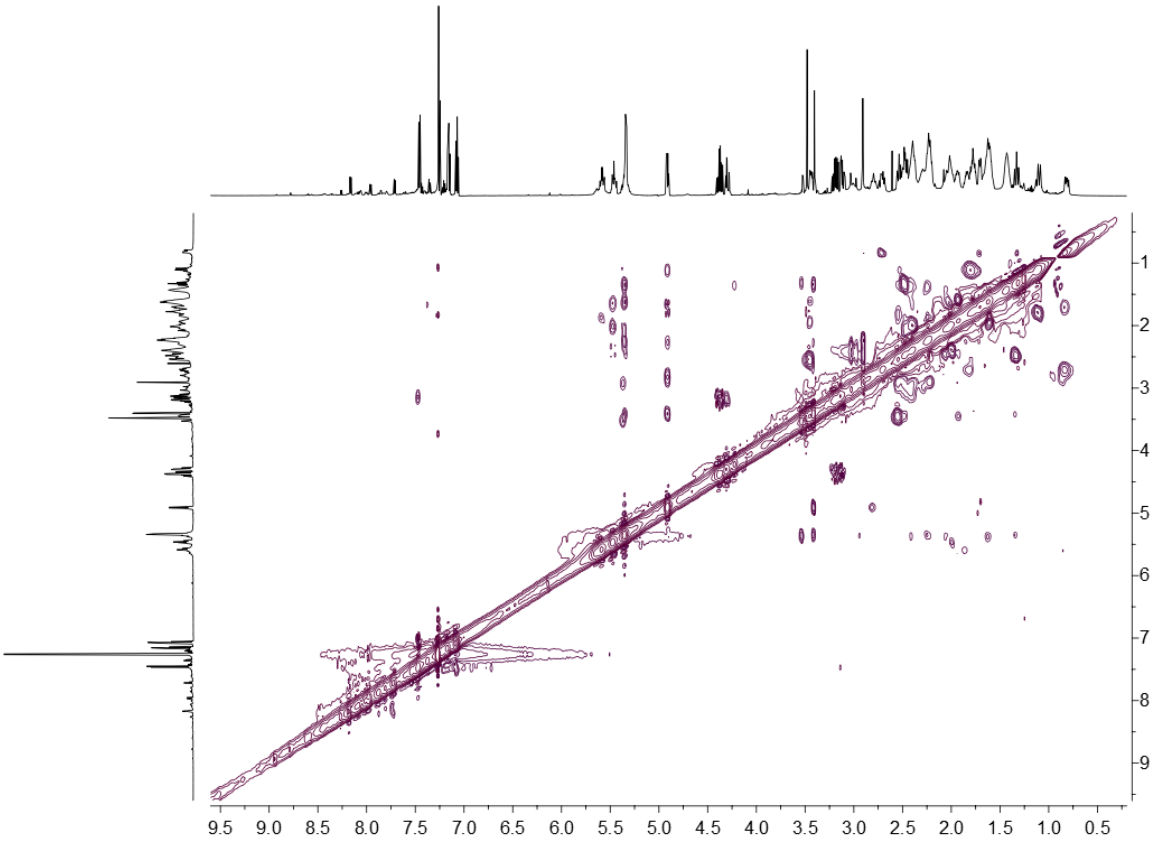


Figure S20. The ROESY NMR (500 MHz, $CDCl_3$) spectrum of **3**

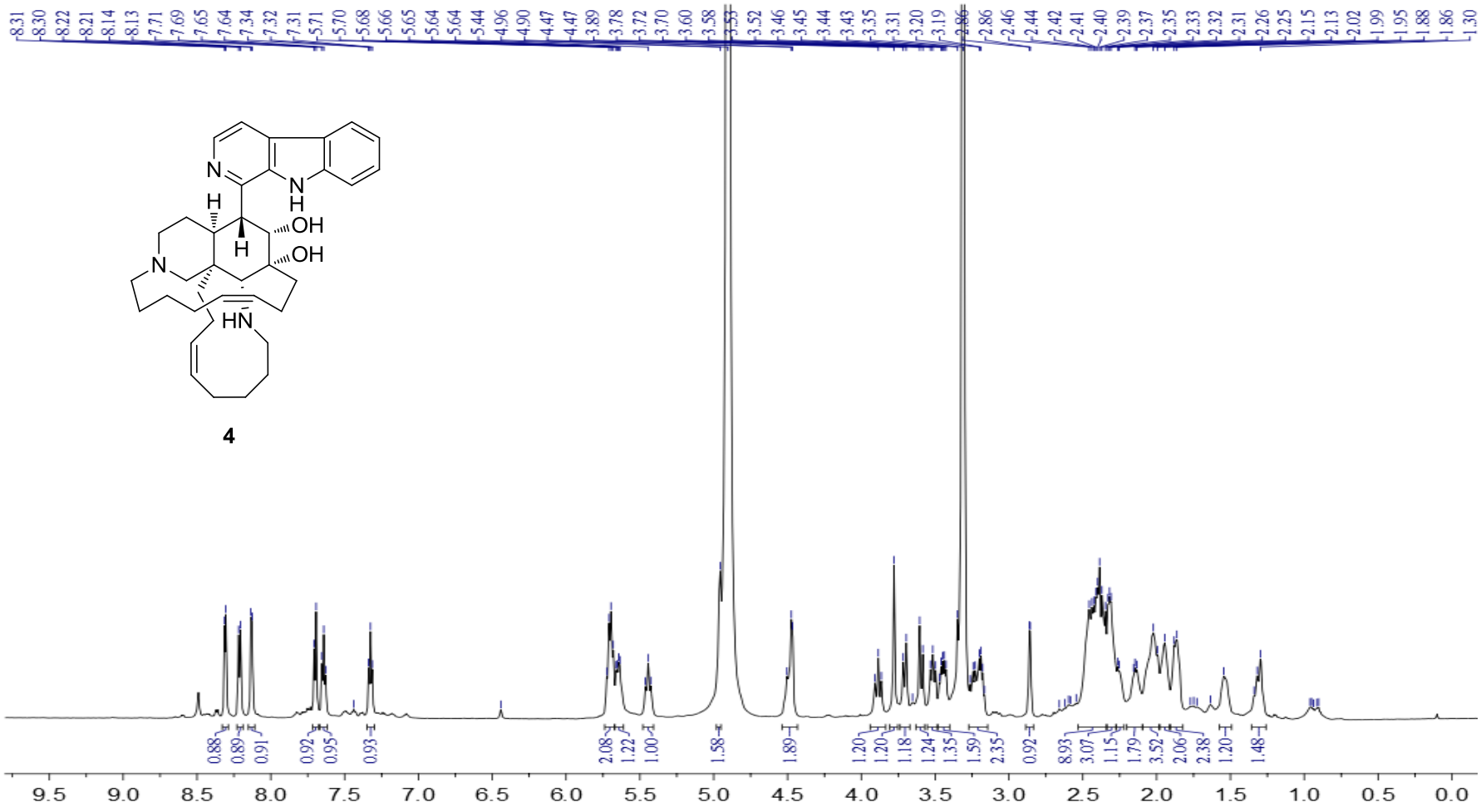


Figure S21. The ^{1}H NMR (600 MHz, CD_3OD) spectrum of **4**

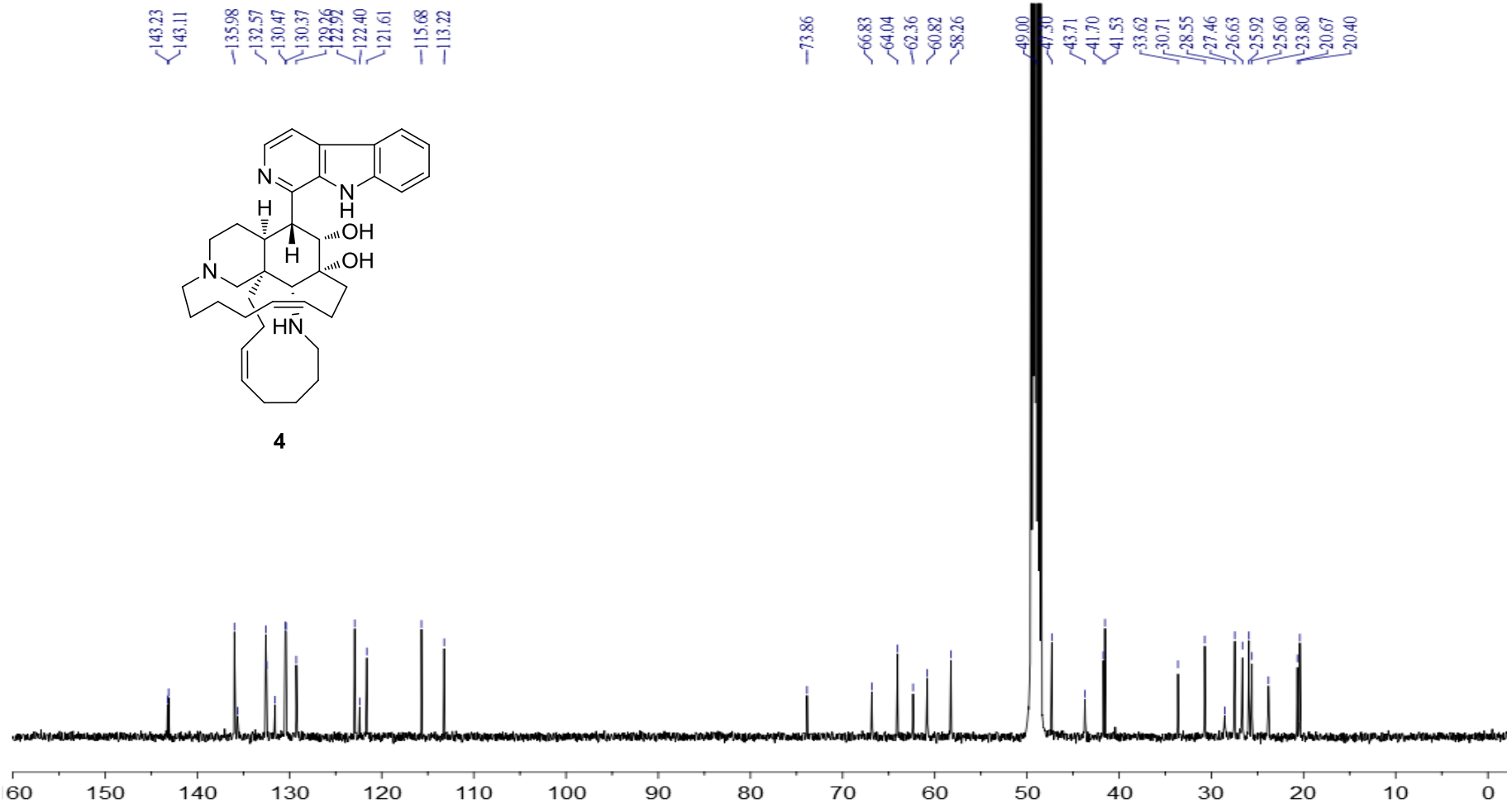


Figure S22. The ^{13}C NMR (150 MHz, CD_3OD) spectrum of **4**

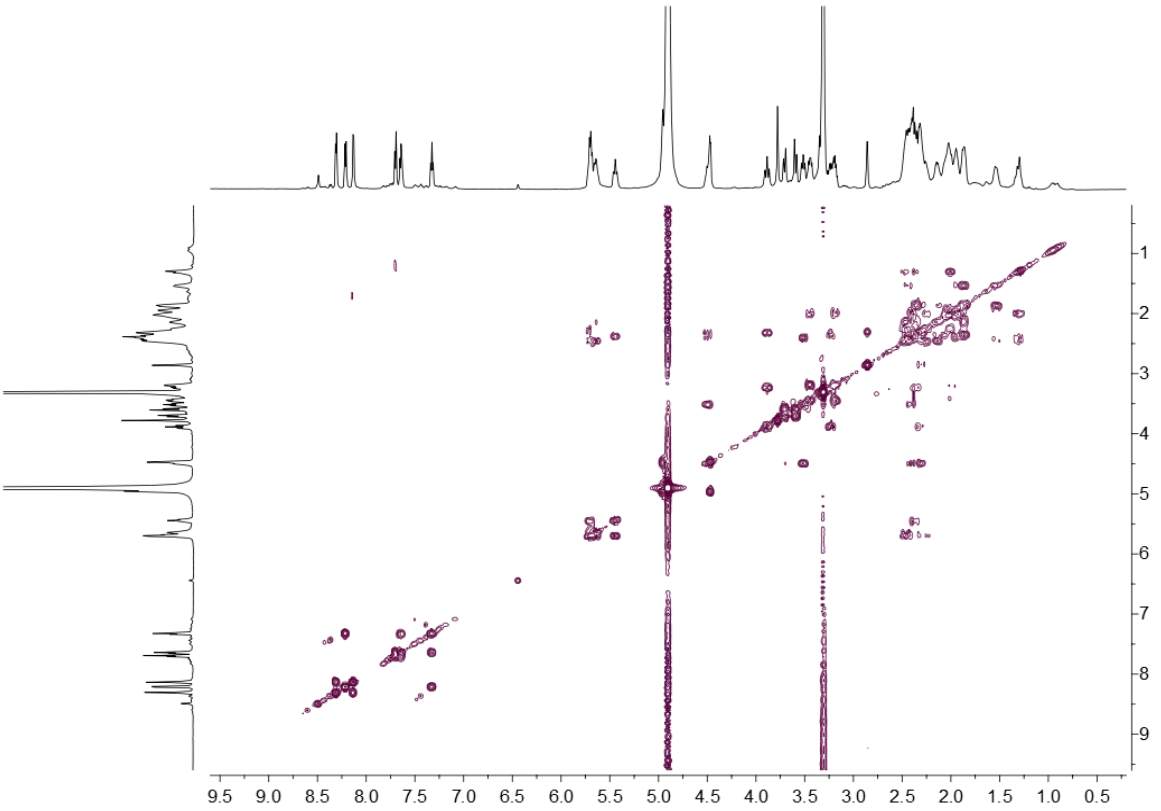


Figure S23. The COSY NMR (600 MHz, CD_3OD) spectrum of **4**

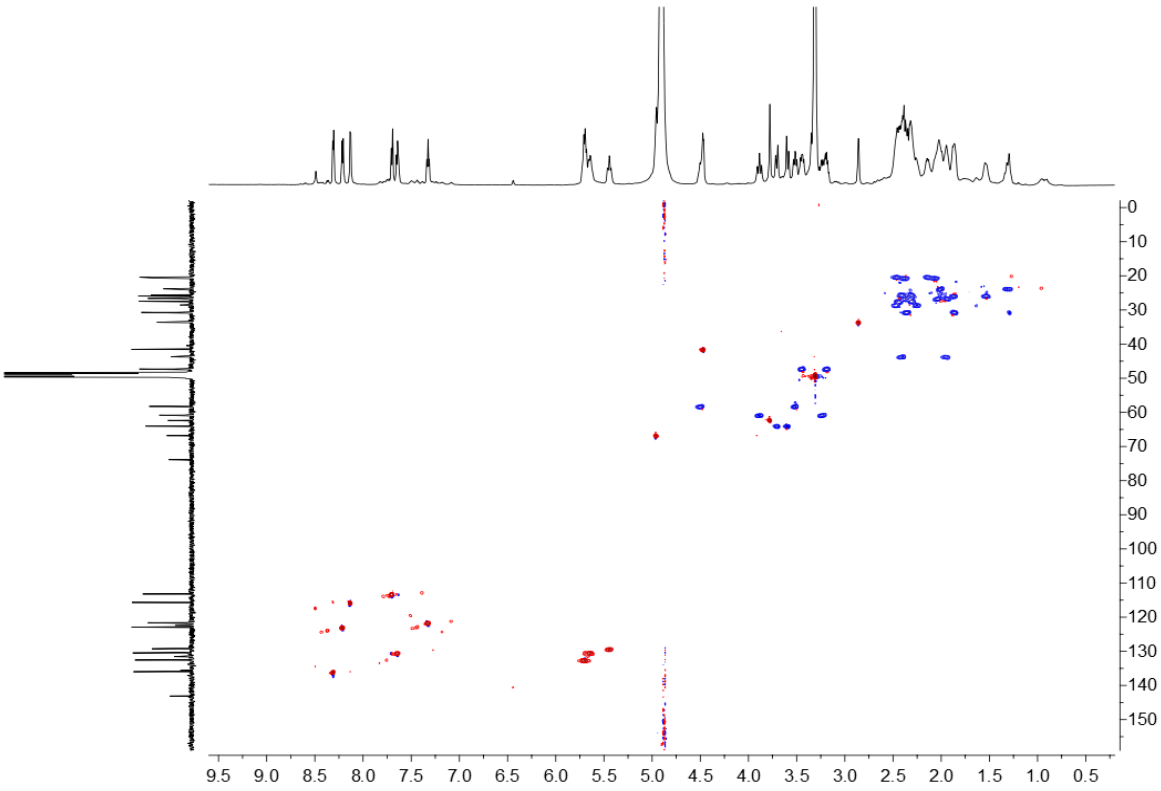


Figure S24. The eHSQC NMR (600 MHz, CD_3OD) spectrum of **4**

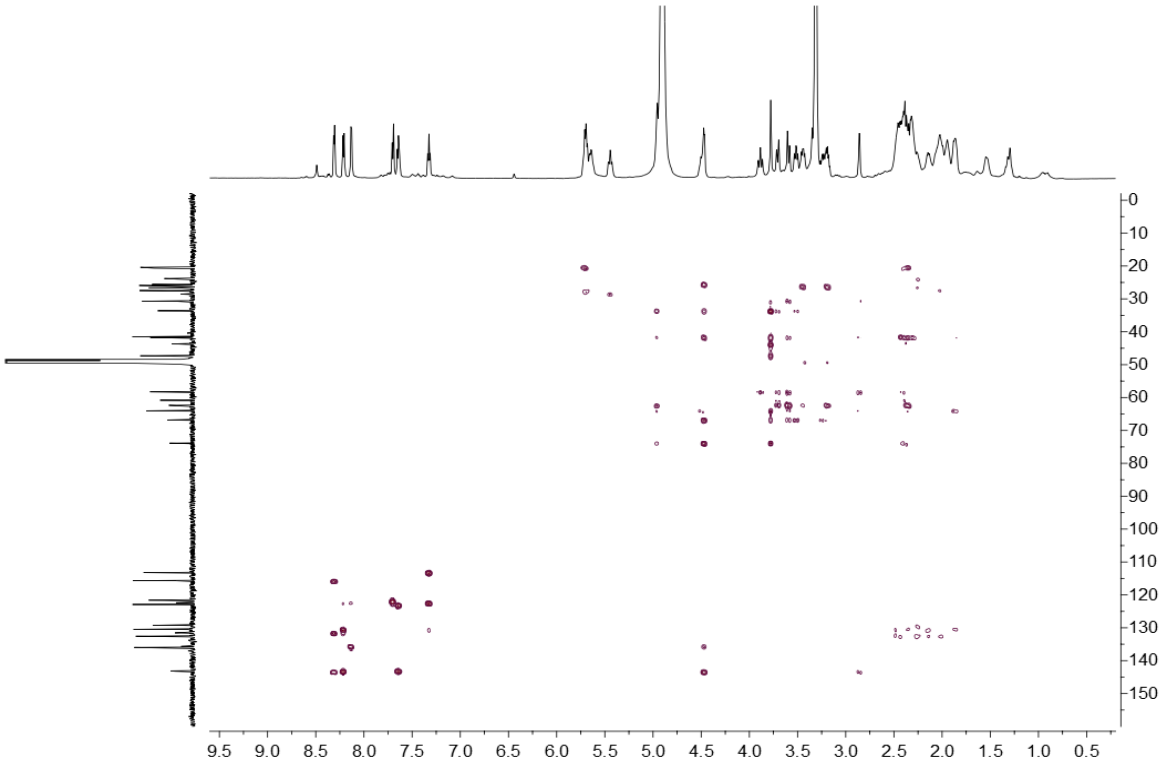


Figure S25. The HMBC NMR (600 MHz, CD_3OD) spectrum of **4**

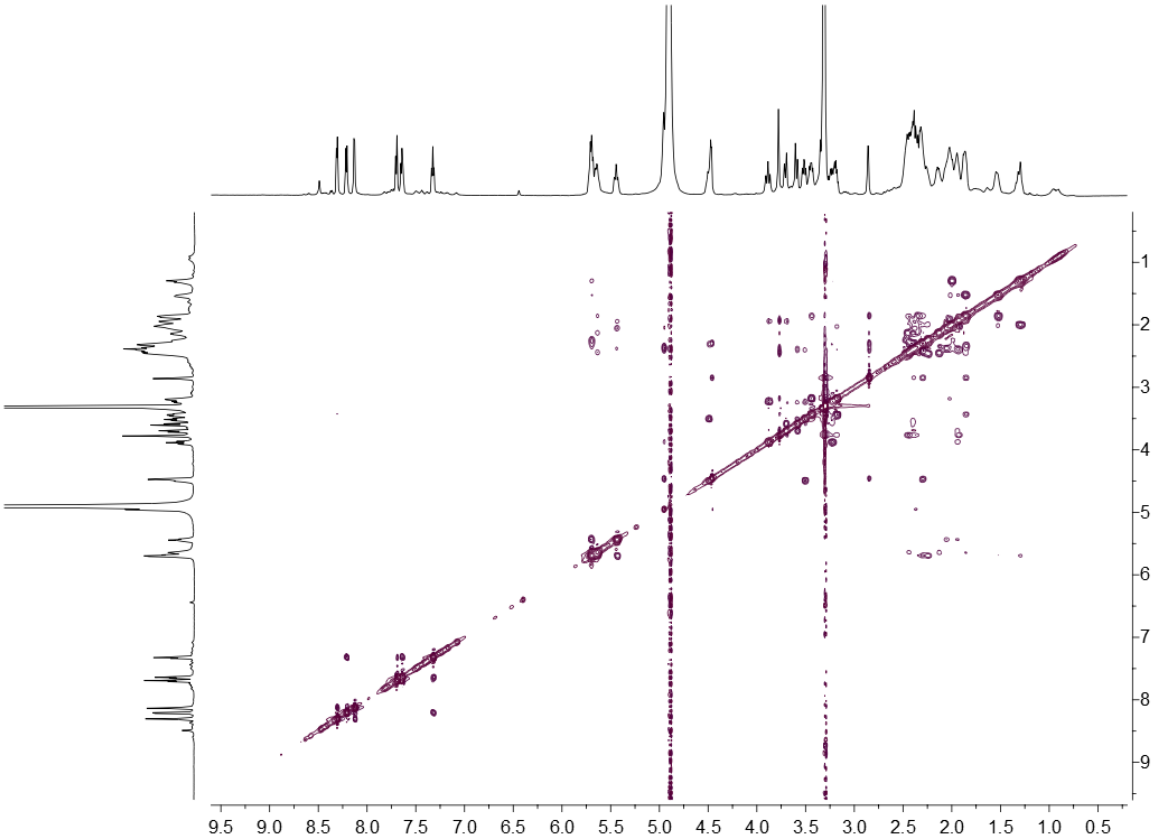


Figure S26. The ROESY NMR (600 MHz, CD_3OD) spectrum of **4**

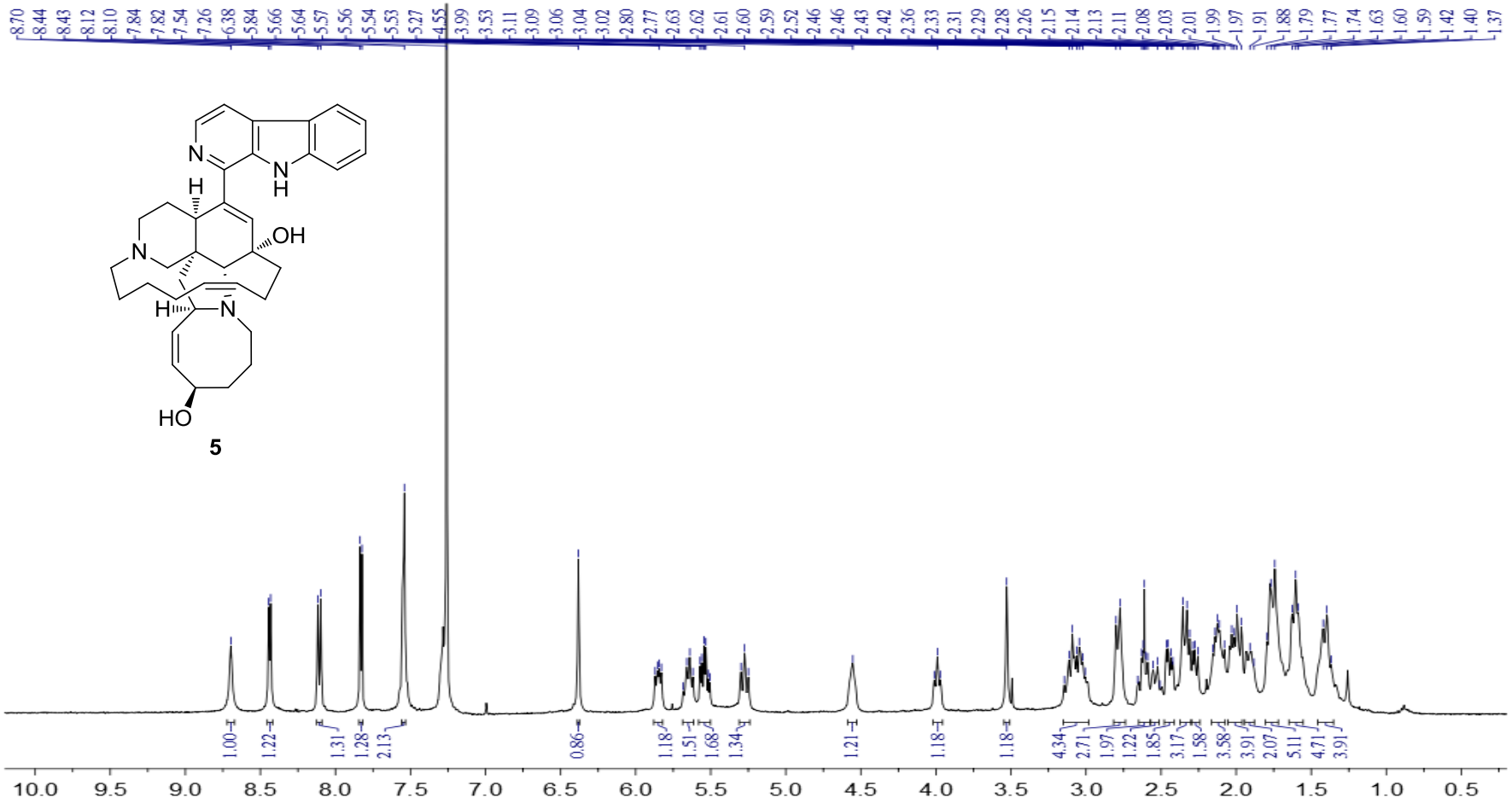


Figure S27. The ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **5**

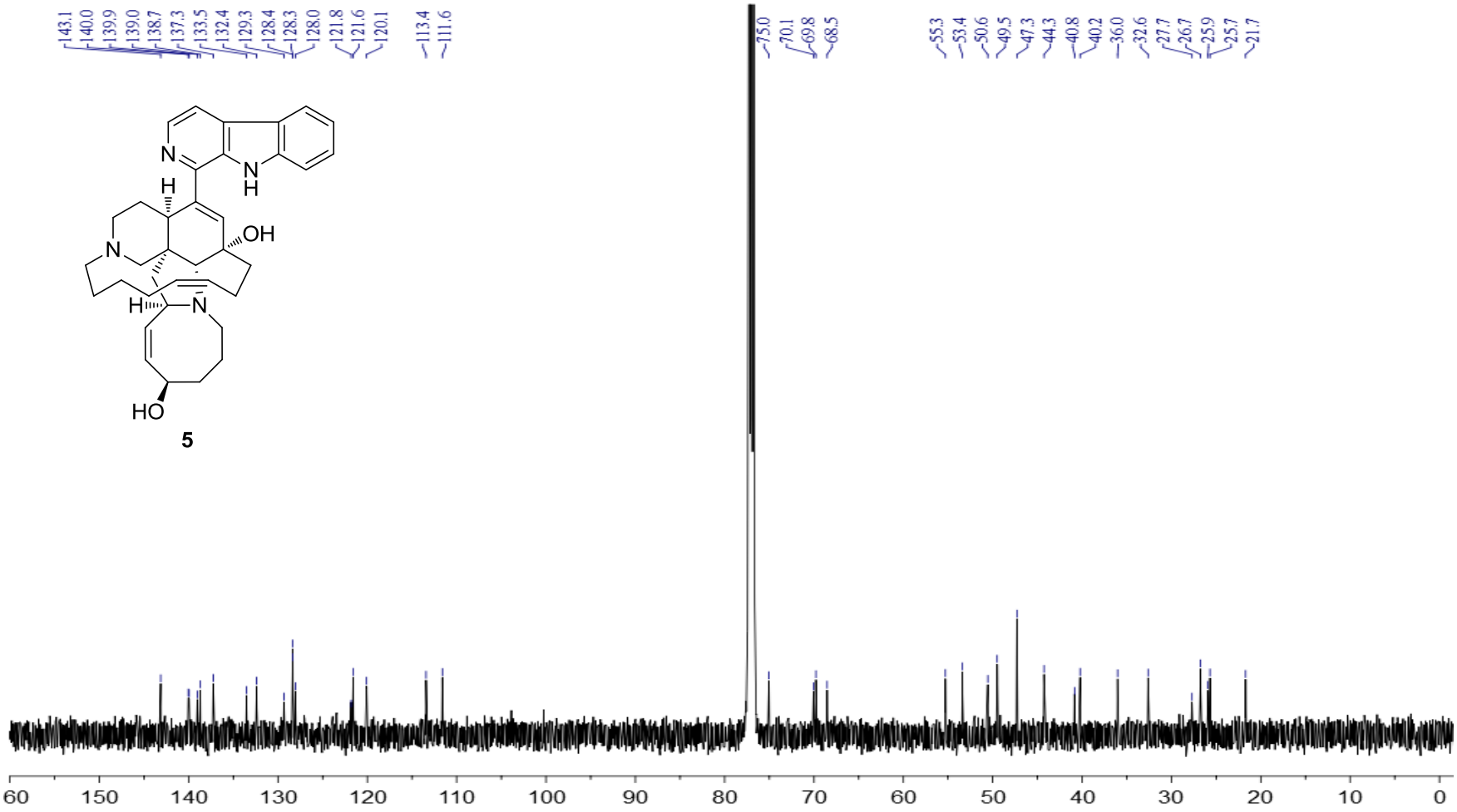


Figure S28. The ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **5**

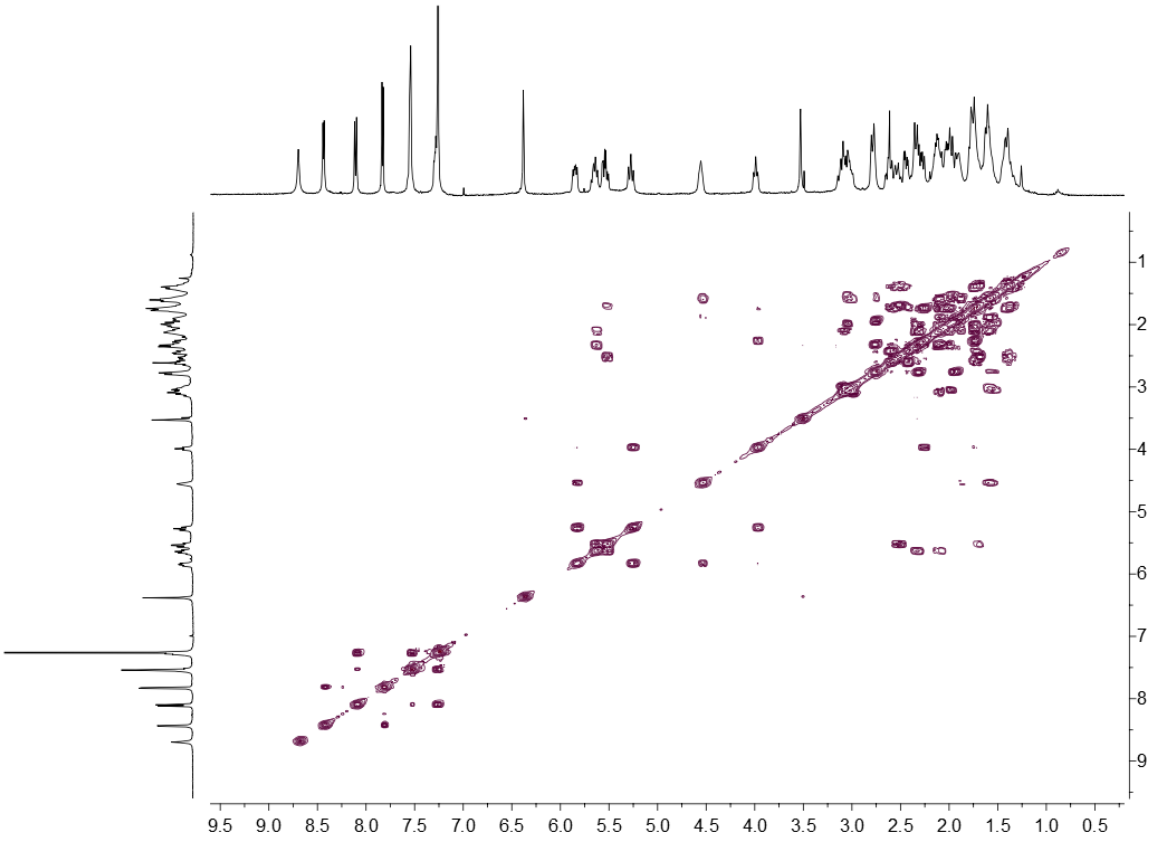


Figure S29. The COSY NMR (400 MHz, $CDCl_3$) spectrum of **5**

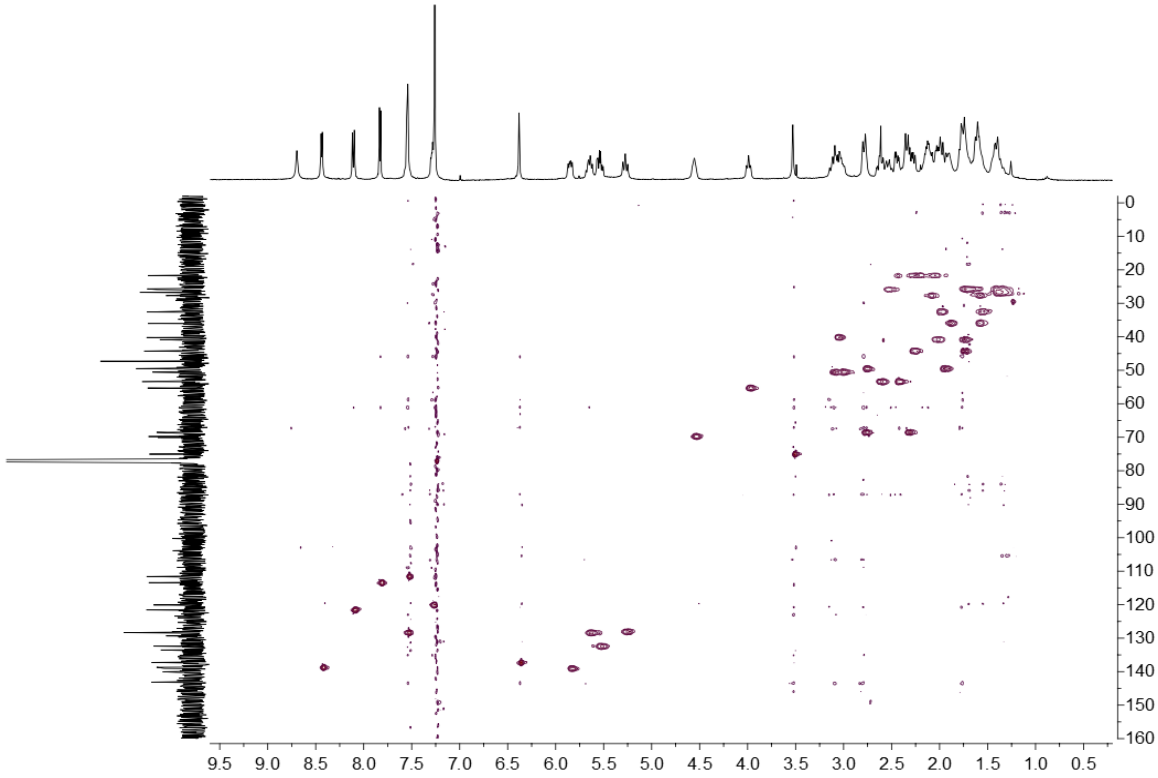


Figure S30. The HSQC NMR (400 MHz, $CDCl_3$) spectrum of **5**

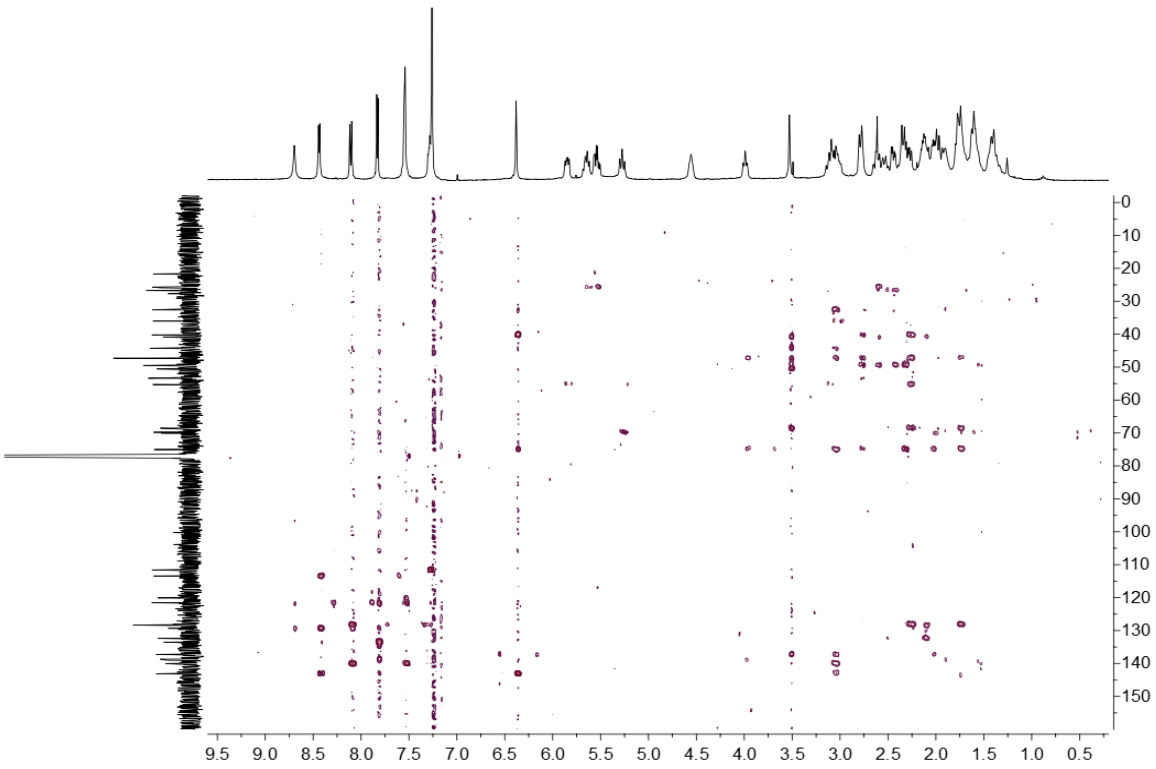


Figure S31. The HMBC NMR (400 MHz, $CDCl_3$) spectrum of **5**

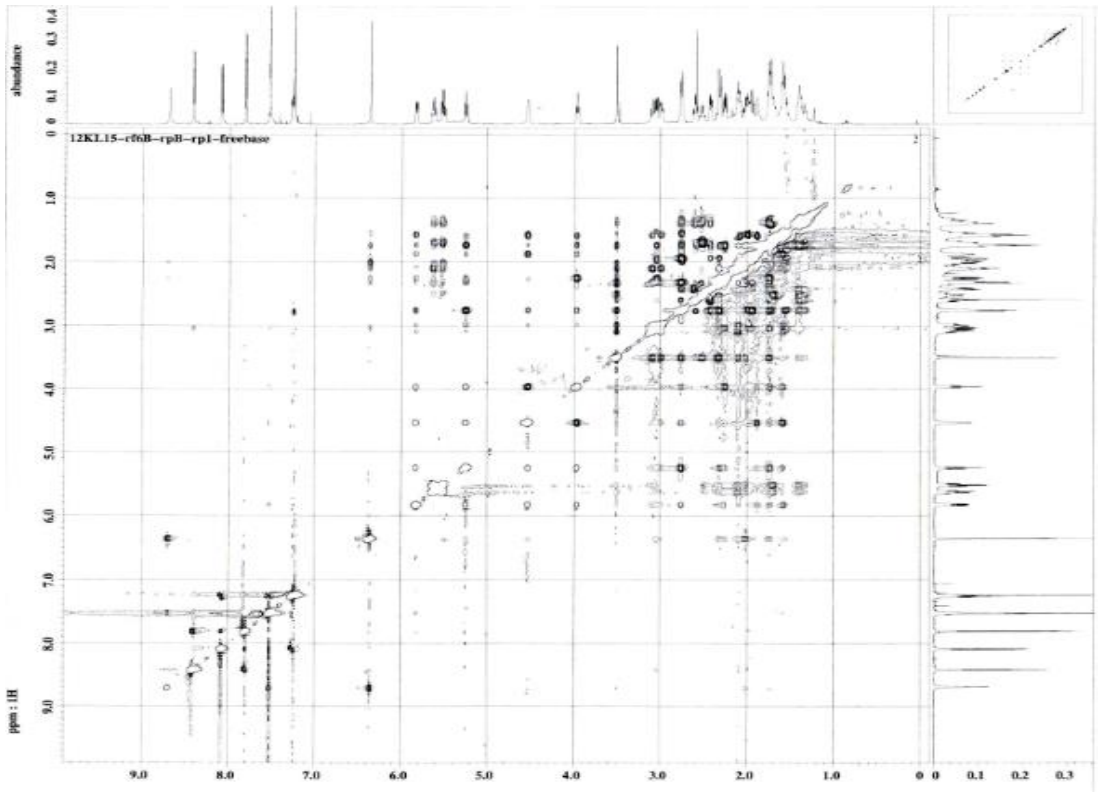


Figure S32. The ROESY NMR (400 MHz, $CDCl_3$) spectrum of **5**

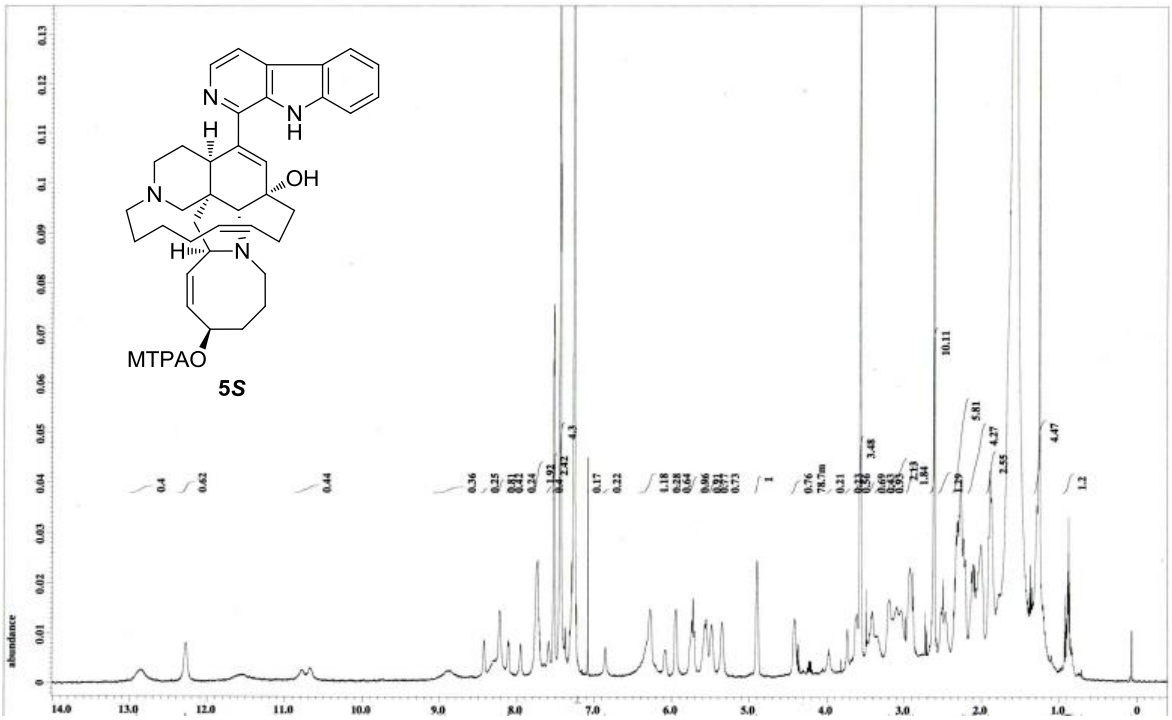


Figure S33. The ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of (*S*)-MTPA ester of **5** (**5*S***)

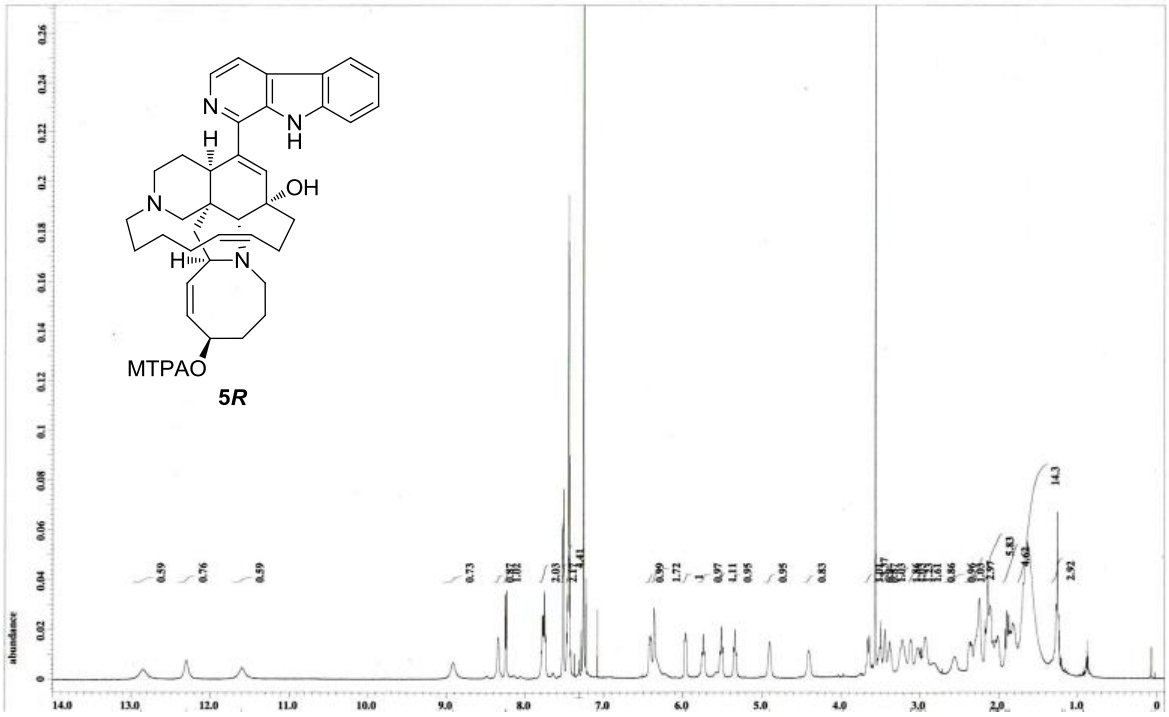


Figure S34. The ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of (*R*)-MTPA ester of **5** (**5*R***)

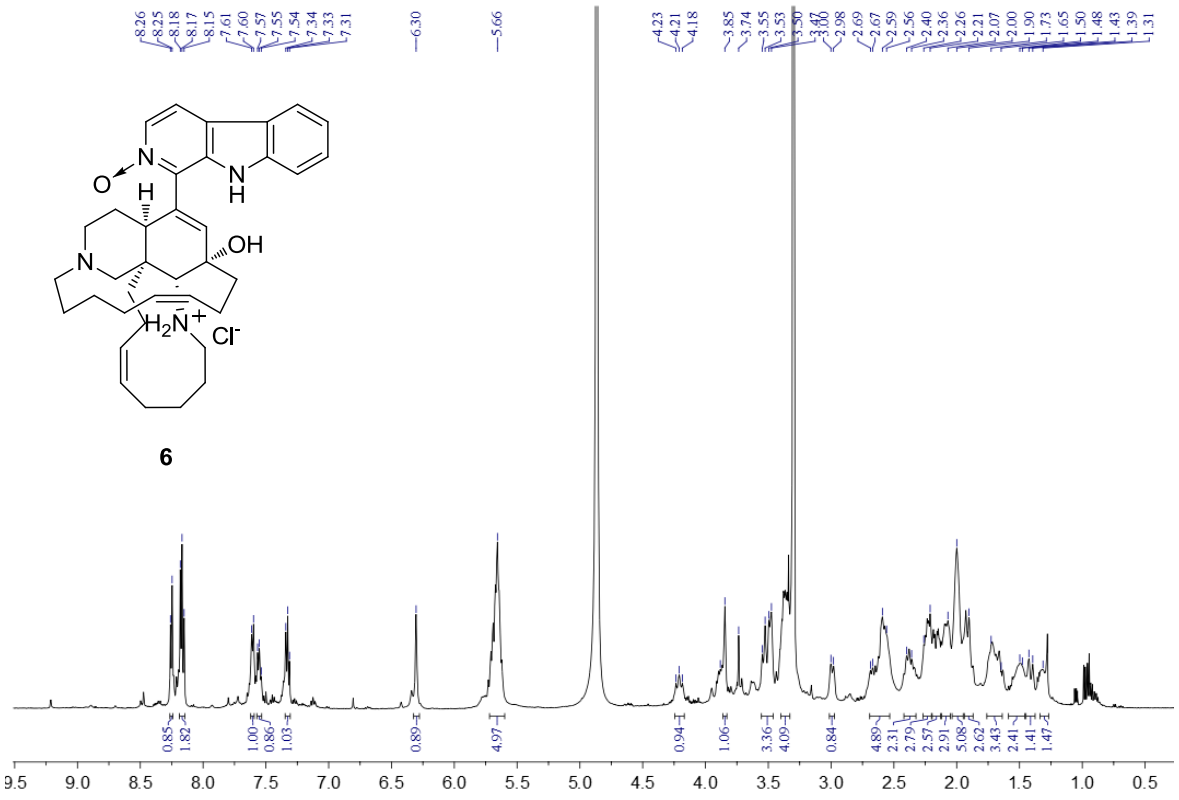


Figure S35. The ^{1}H NMR (500 MHz, CD_3OD) spectrum of **6**

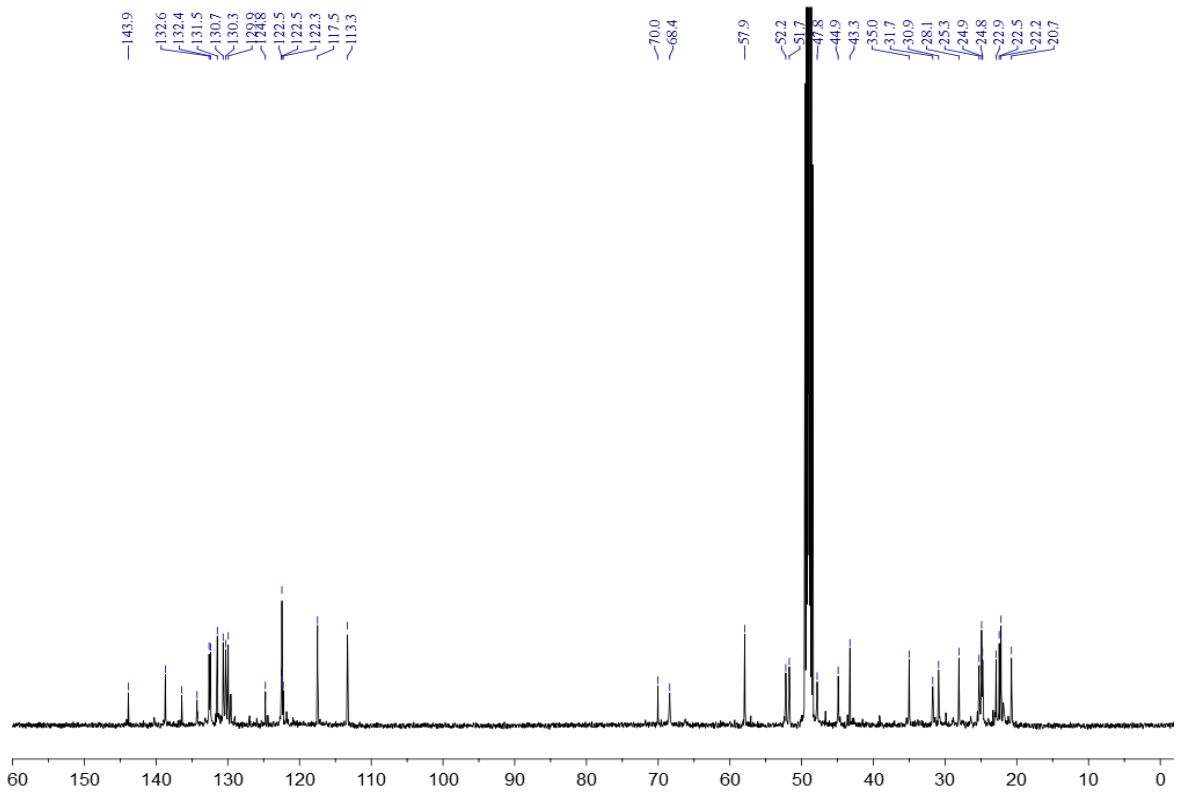


Figure S36. The ^{13}C NMR (125 MHz, CD_3OD) spectrum of **6**

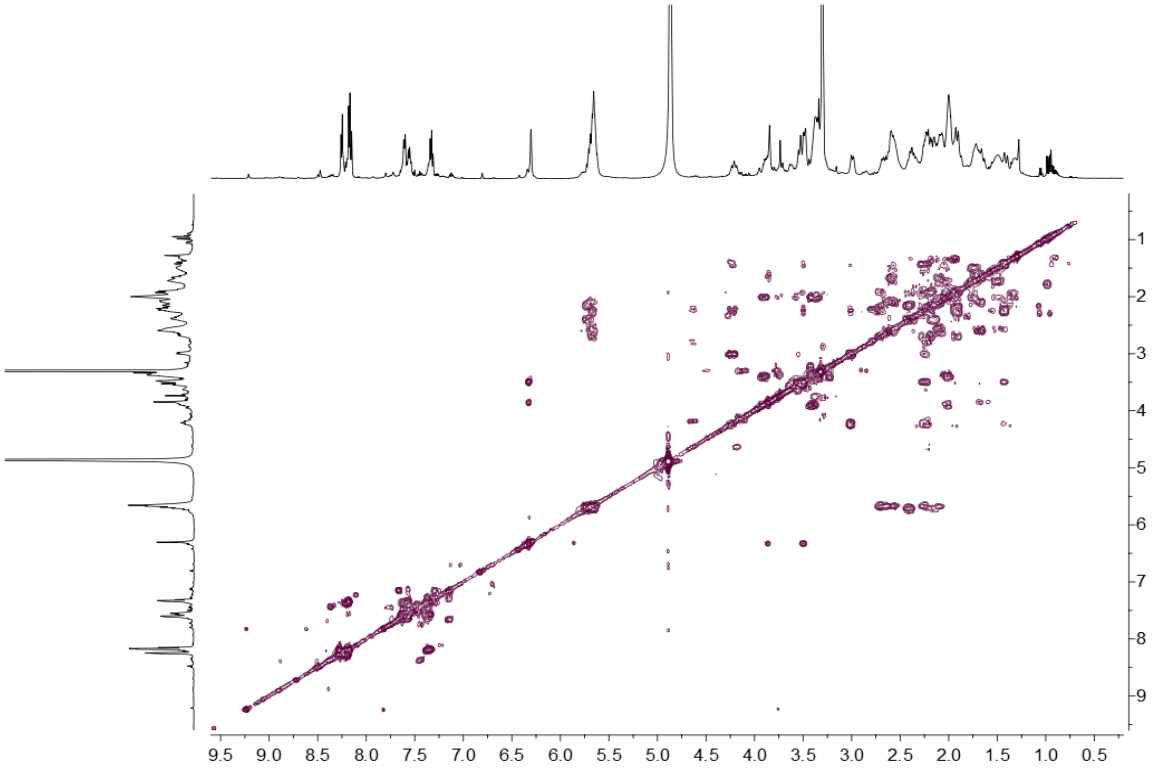


Figure S37. The COSY NMR (500 MHz, CD_3OD) spectrum of **6**

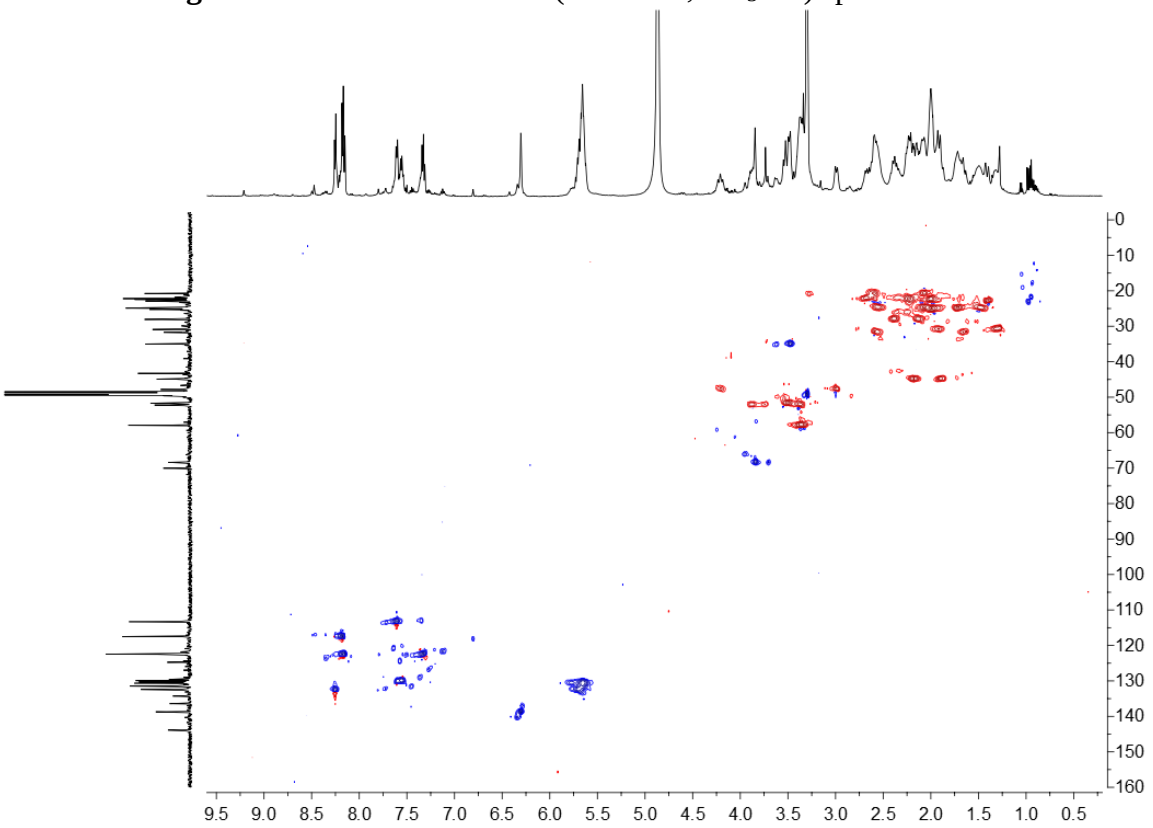


Figure S38. The eHSQC NMR (500 MHz, CD_3OD) spectrum of **6**

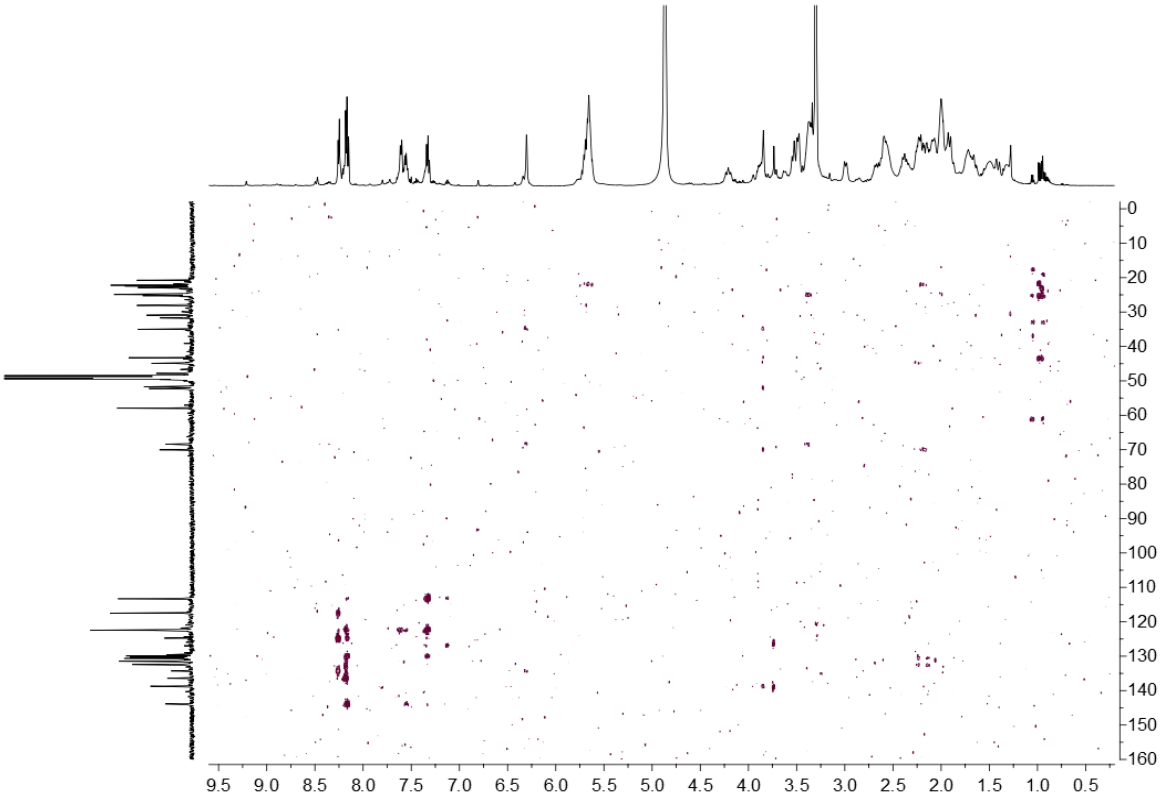


Figure S39. The HMBC NMR (500 MHz, CD_3OD) spectrum of **6**

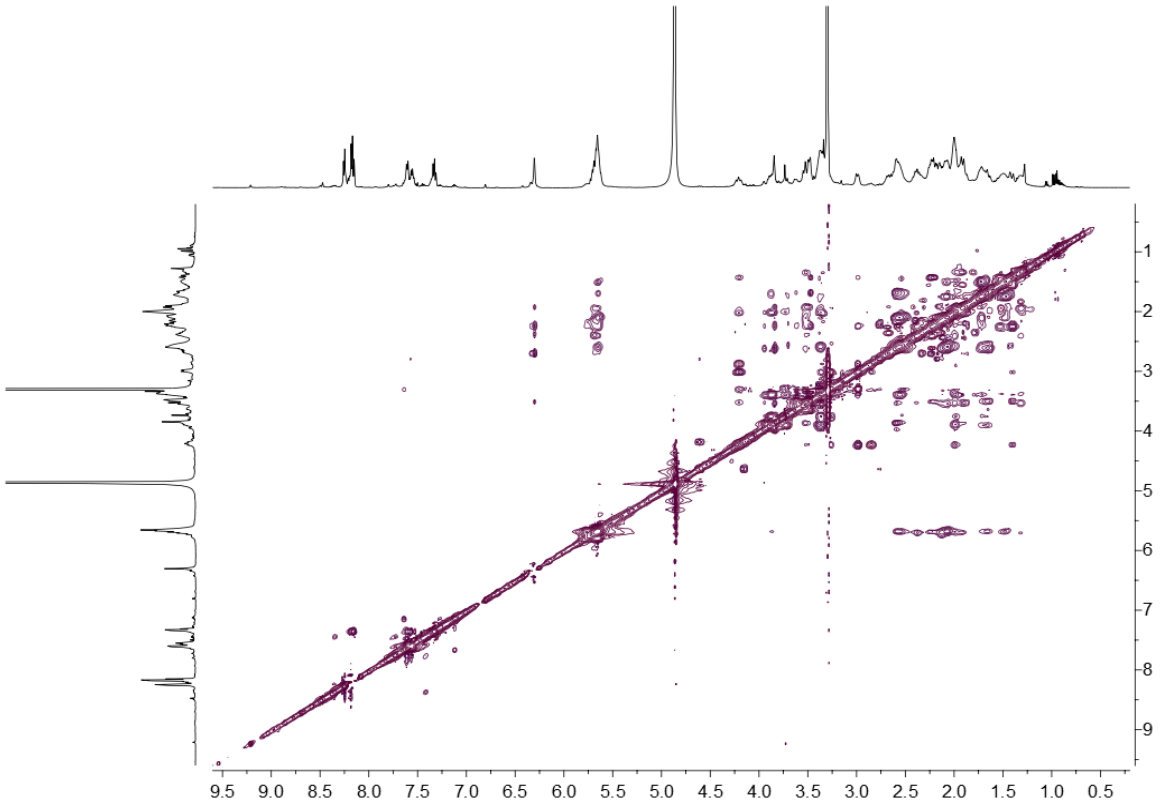


Figure S40. The ROESY NMR (500 MHz, CD_3OD) spectrum of **6**

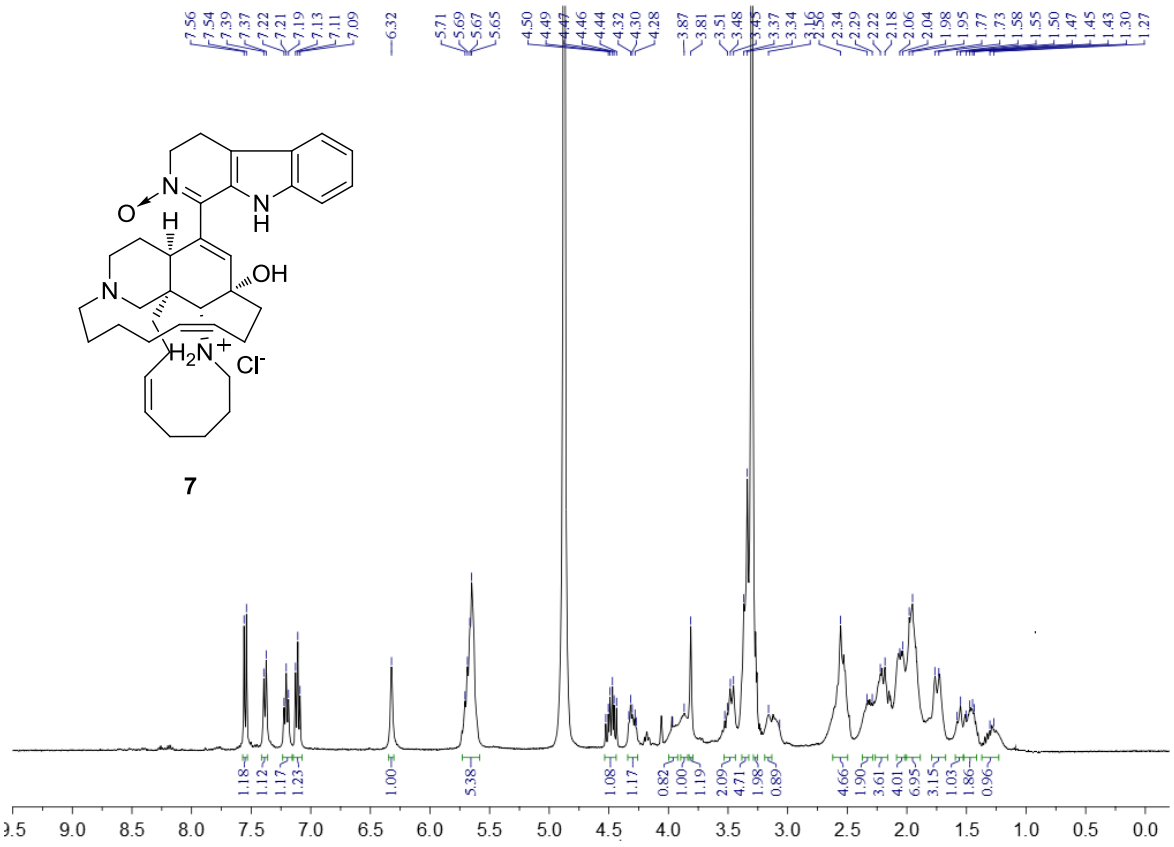


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Figure S41. The ^{1}H NMR (400 MHz, CD_3OD) spectrum of **7**

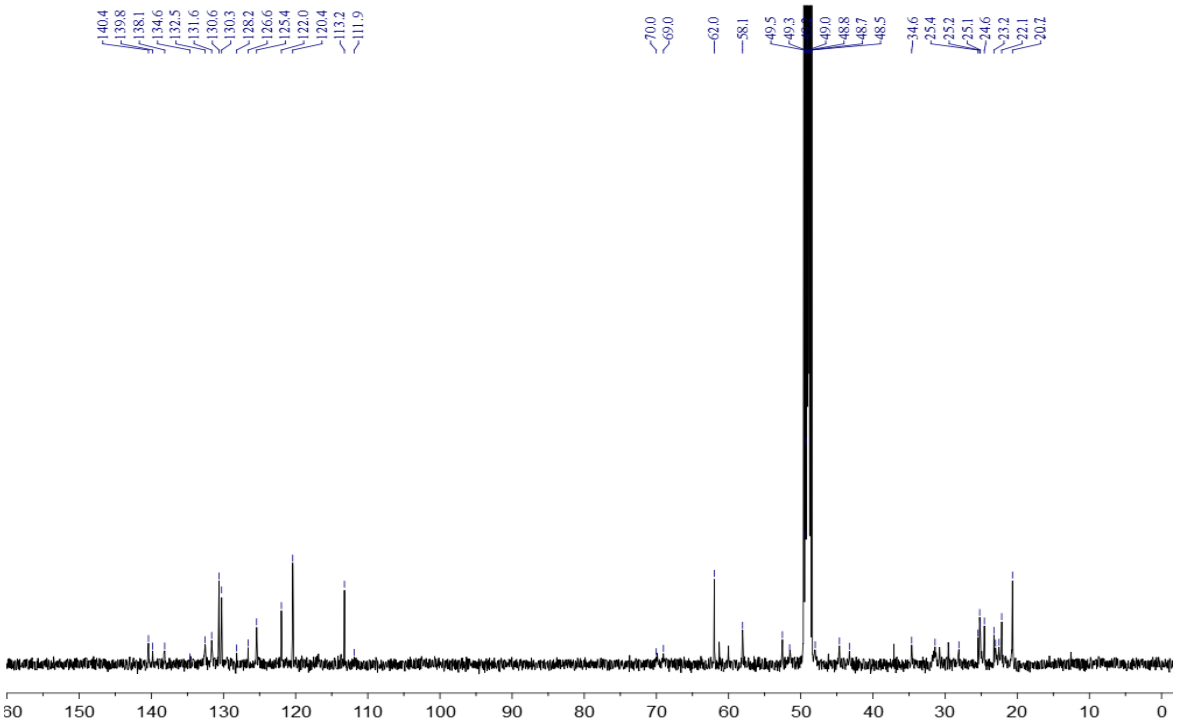


Figure S42. The ^{13}C NMR (100 MHz, CD_3OD) spectrum of **7**

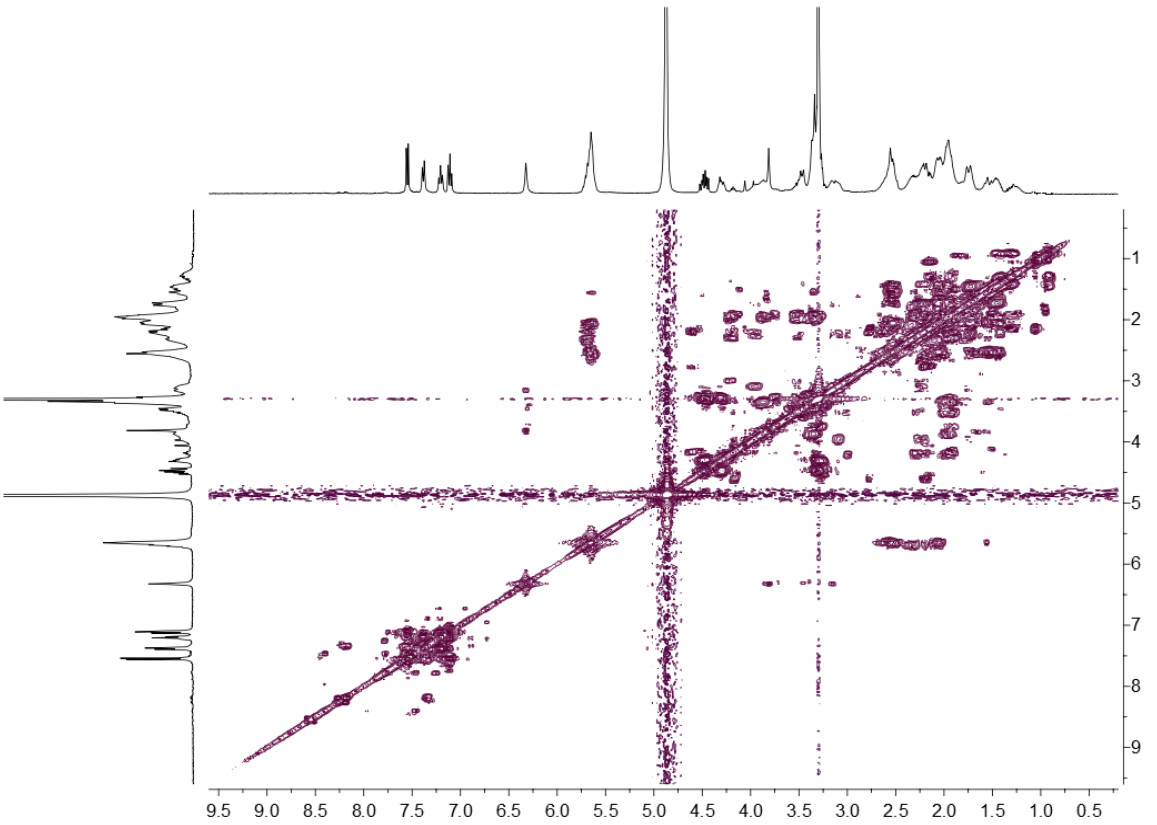


Figure S43. The COSY NMR (400 MHz, CD_3OD) spectrum of **7**

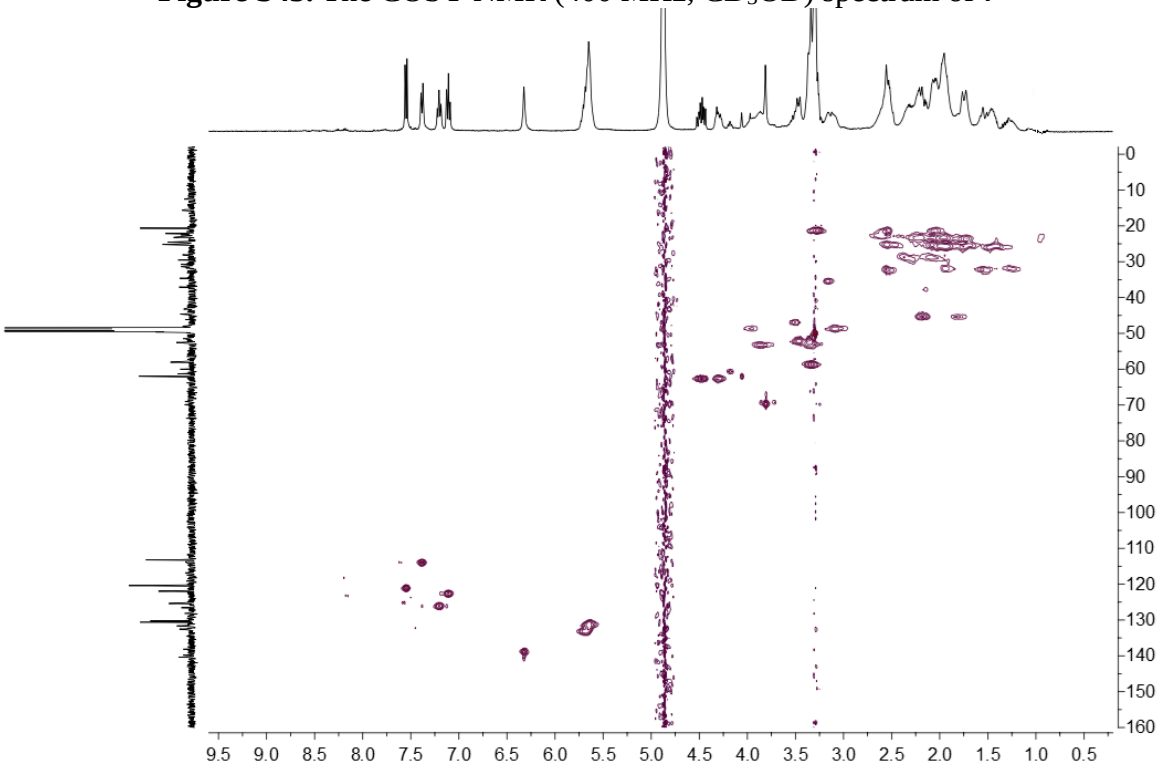


Figure S44. The HSQC NMR (400 MHz, CD_3OD) spectrum of **7**

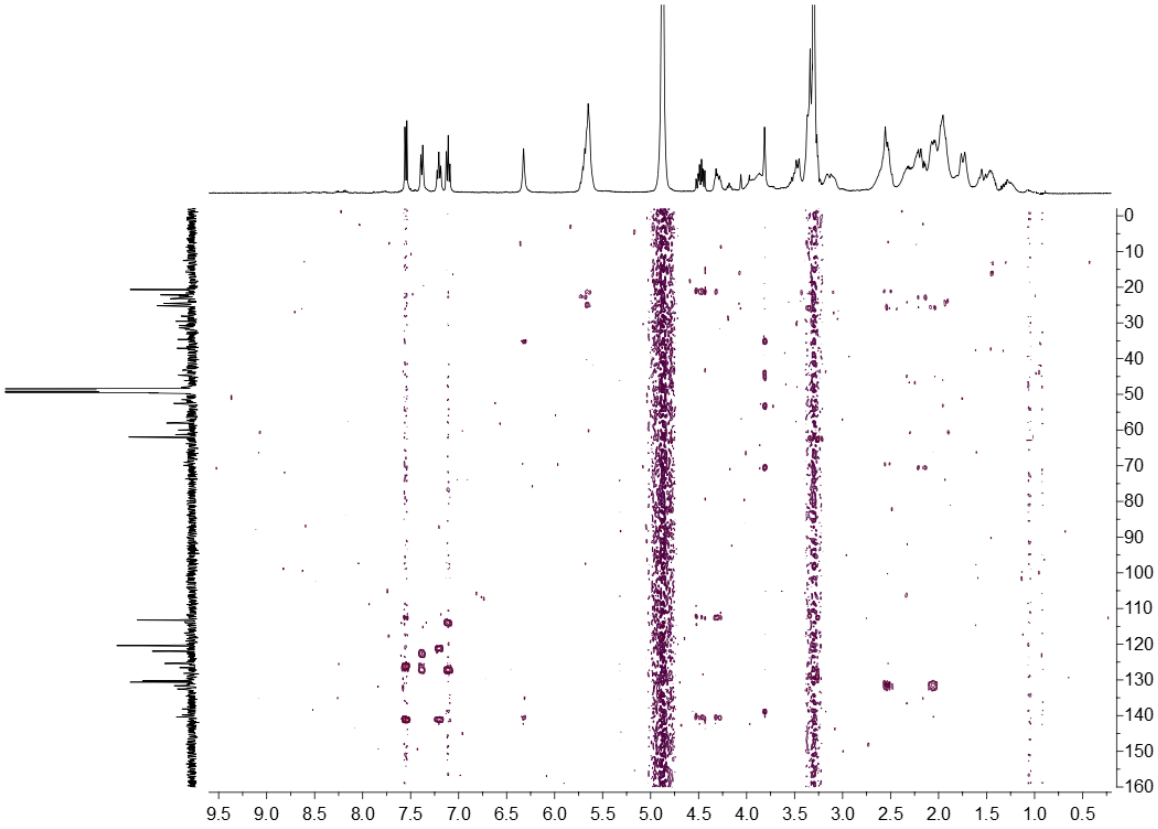


Figure S45. The HMBC NMR (400 MHz, CD_3OD) spectrum of **7**

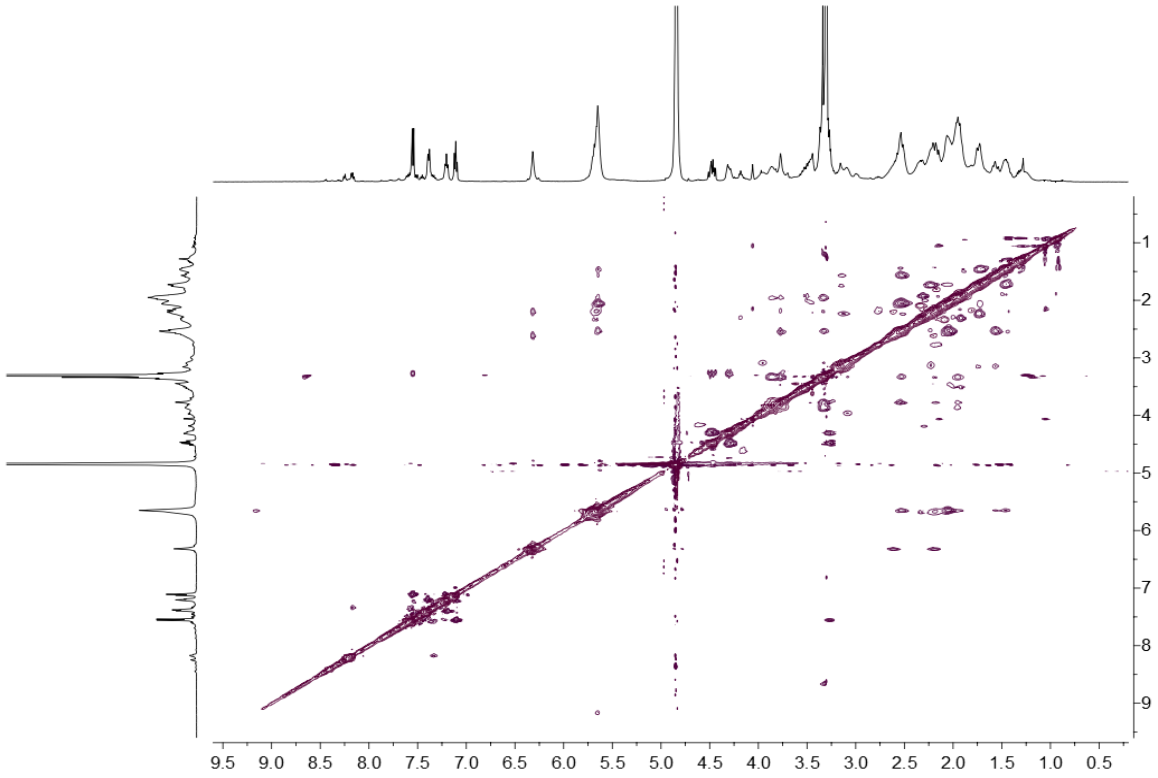
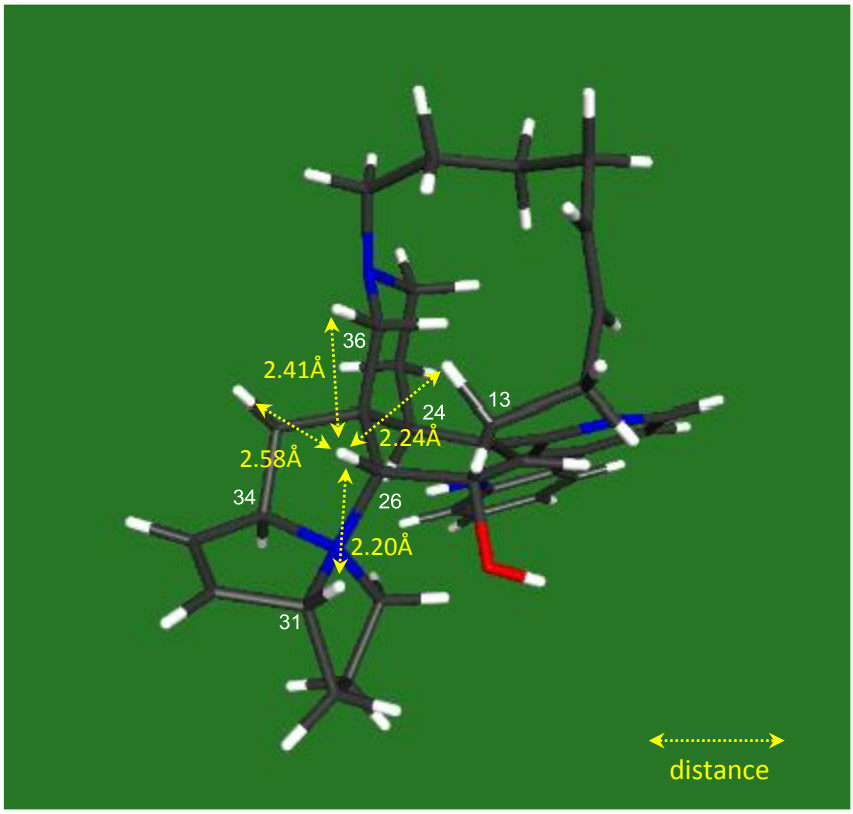


Figure S46. The ROESY NMR (400 MHz, CD_3OD) spectrum of **7**

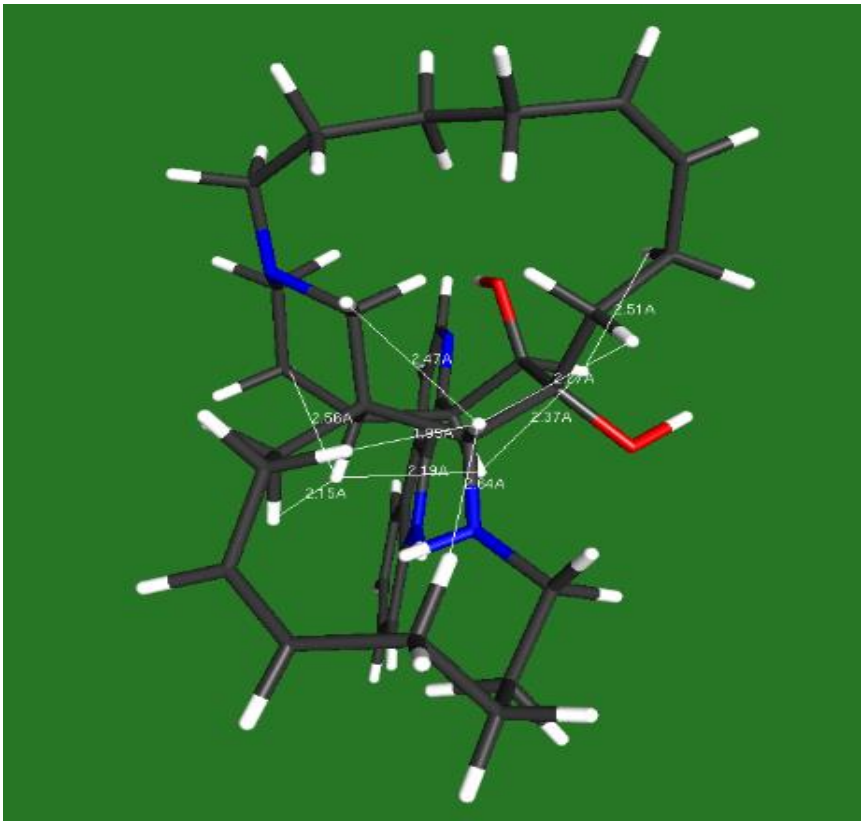


Kepulauamine A (**1**) : total energy = -1689.38544358226

kinetic energy = 1672.31095625132, potential energy = -2447.56326056390

The lowest energy conformation was calculated for (**1**) with 12*S*, 24*R*, 25*R*, 26*R*, 27*S*, 31*R*, and 34*R* configurations using TURBOMOLE 6.5. In the calculation, DFT settings (Functional B3-LYP / Gridsize M3), Geometry optimization options (Energy 10^{-6} Hartree, Gradient norm $\left| dE / dxyz \right| = 10^{-3}$ Hartree/Bohr)

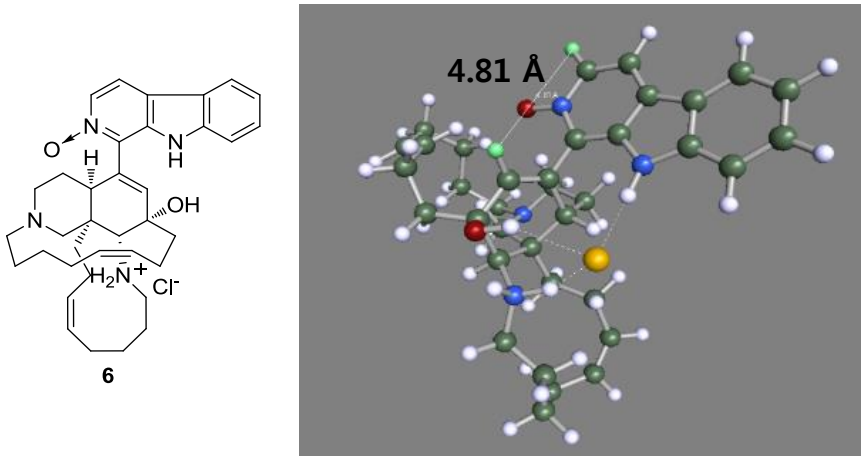
Figure S47. DFT calculation of compound **1**



11-Hydroxymanzamine J (**4**) : total energy = -1459.23192310491
kinetic energy = 1445.21230135345, potential energy = -2123.34342310311

The lowest energy conformation was calculated for (**4**) with 10*R*, 11*S*, 12*R*, 24*S*, 25*R*, and 26*R* configurations using TURBOMOLE 6.5. In the calculation, DFT settings (Functional B3-LYP / Gridsize M3), Geometry optimization options (Energy 10^{-6} Hartree, Gradient norm $\left| dE / dxyz \right| = 10^{-3}$ Hartree/Bohr)

Figure S48. DFT calculation of compound **4**



The lowest energy conformation was calculated for (**6**) with 12*S*, 24*R*, 25*R*, and 26*R* configurations using TURBOMOLE 4.2.1. In the calculation, DFT settings (Functional B3-LYP / Gridsize M3), Geometry optimization options (Energy 10^{-6} Hartree, Gradient norm $|dE / dxyz| = 10^{-3}$ Hartree/Bohr). 1) total energy = -2226.9503635370, kinetic energy = 2209.150029427, and potential energy = -4436.100392964. 2) total energy = -2226.95622032800, kinetic energy = 2208.42416678934, and potential energy = -4435.38038711734

Figure S49. DFT model study and ROESY NMR correlation of **6**