

SUPPLEMENTARY MATERIAL

Rhabdastrenones A-D from the sponge *Rhabdastrella globostellata*

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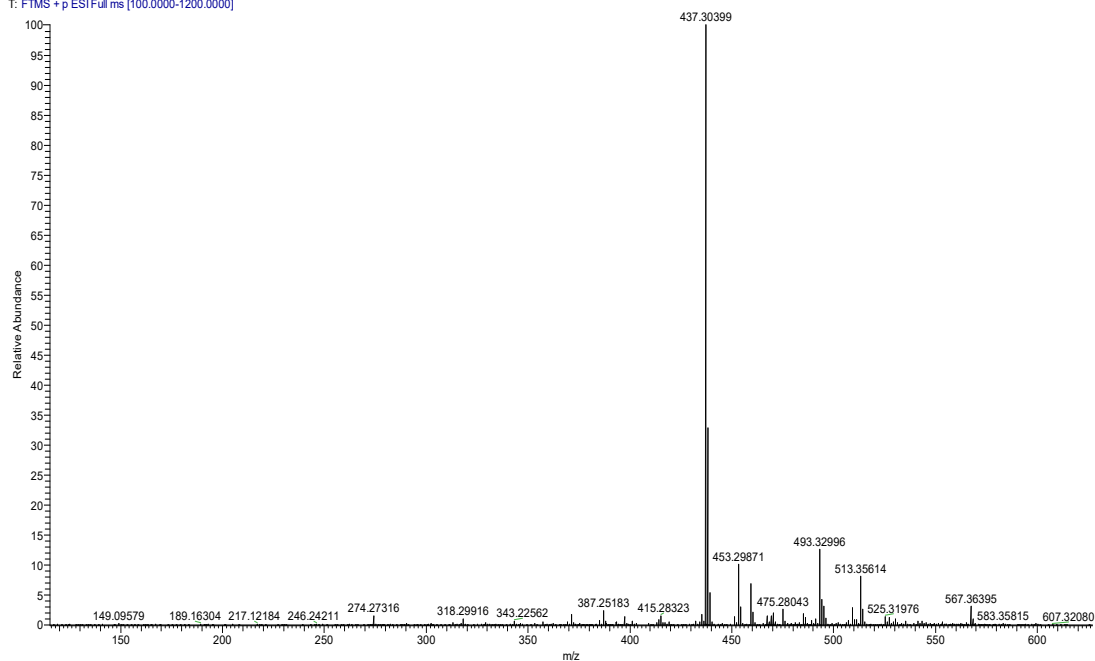


Figure S1. HR-ESI-MS of compound **1**

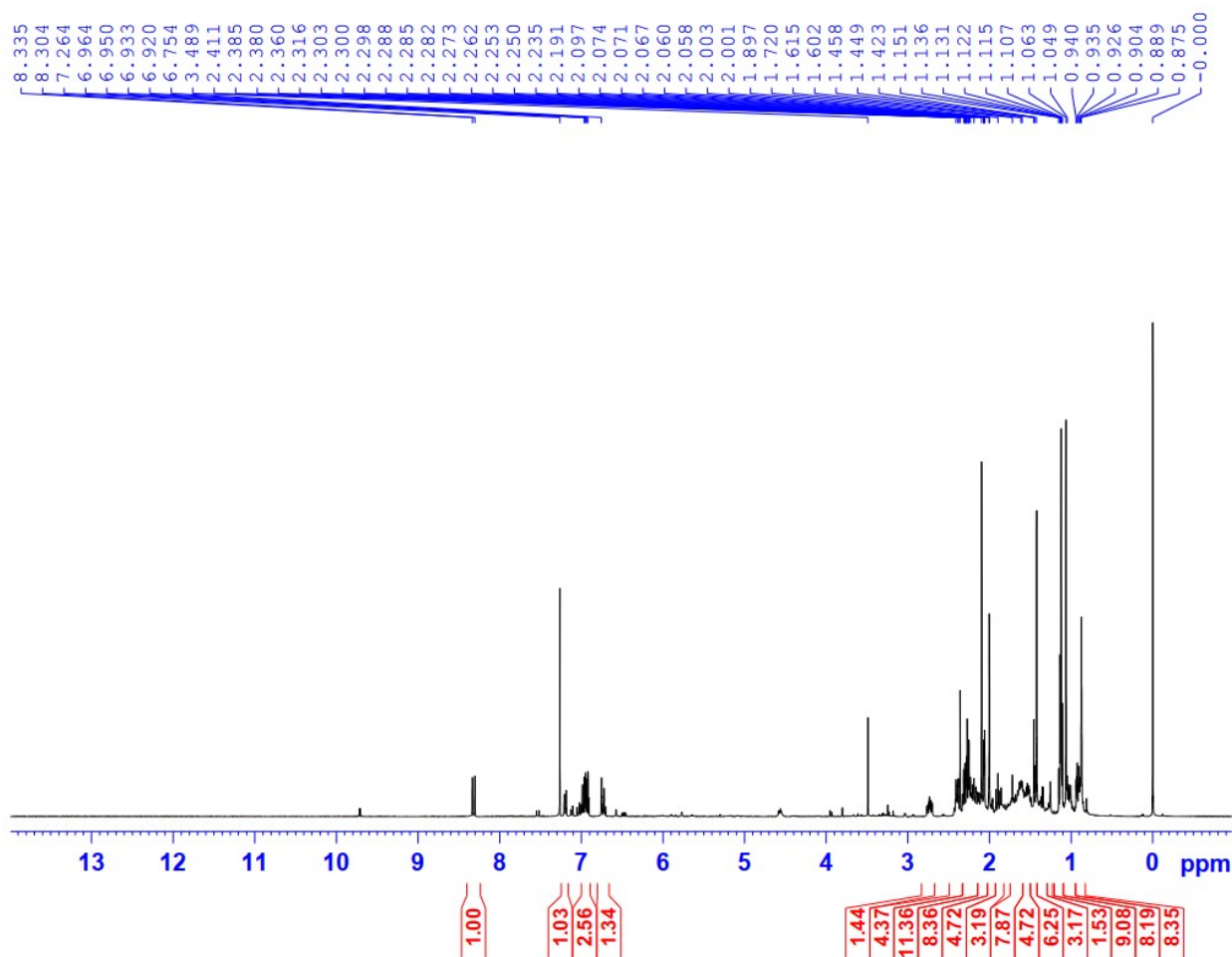


Figure S2. ¹H-NMR spectrum of compound **1** in CDCl₃

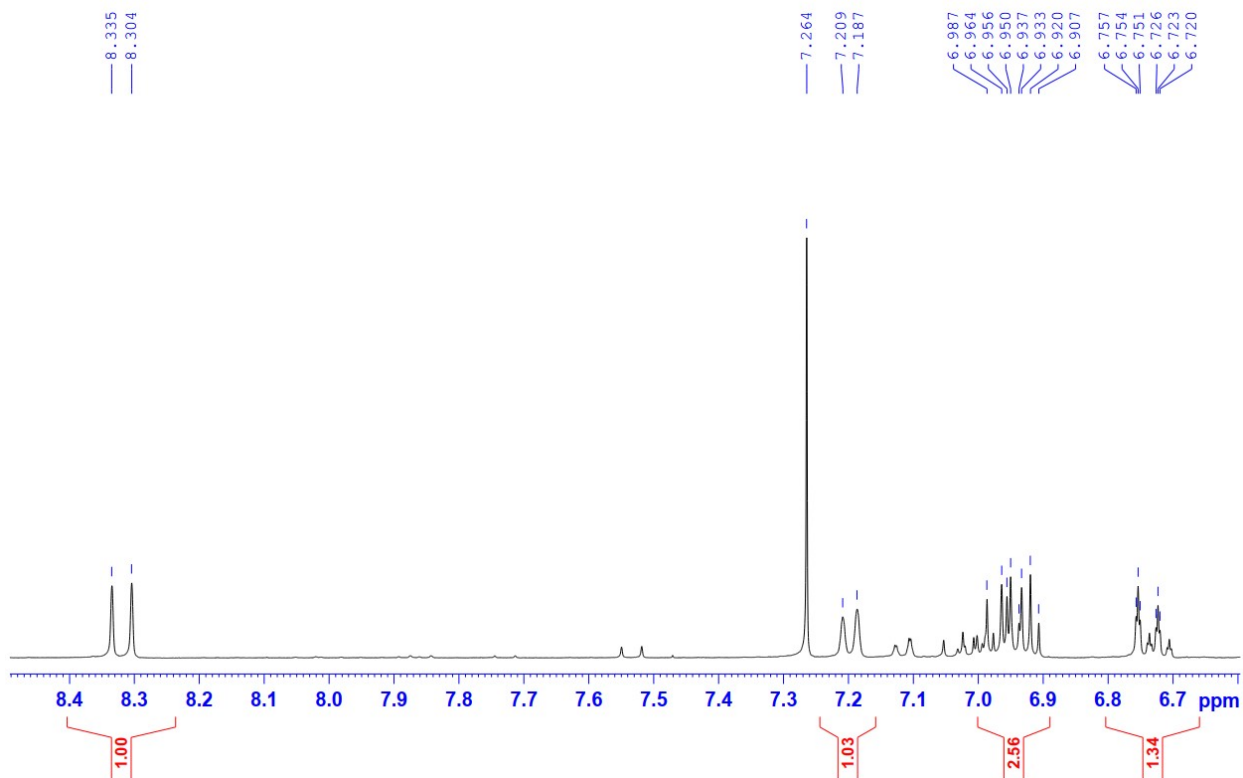


Figure S3. Expanded ^1H -NMR spectrum of compound **1**

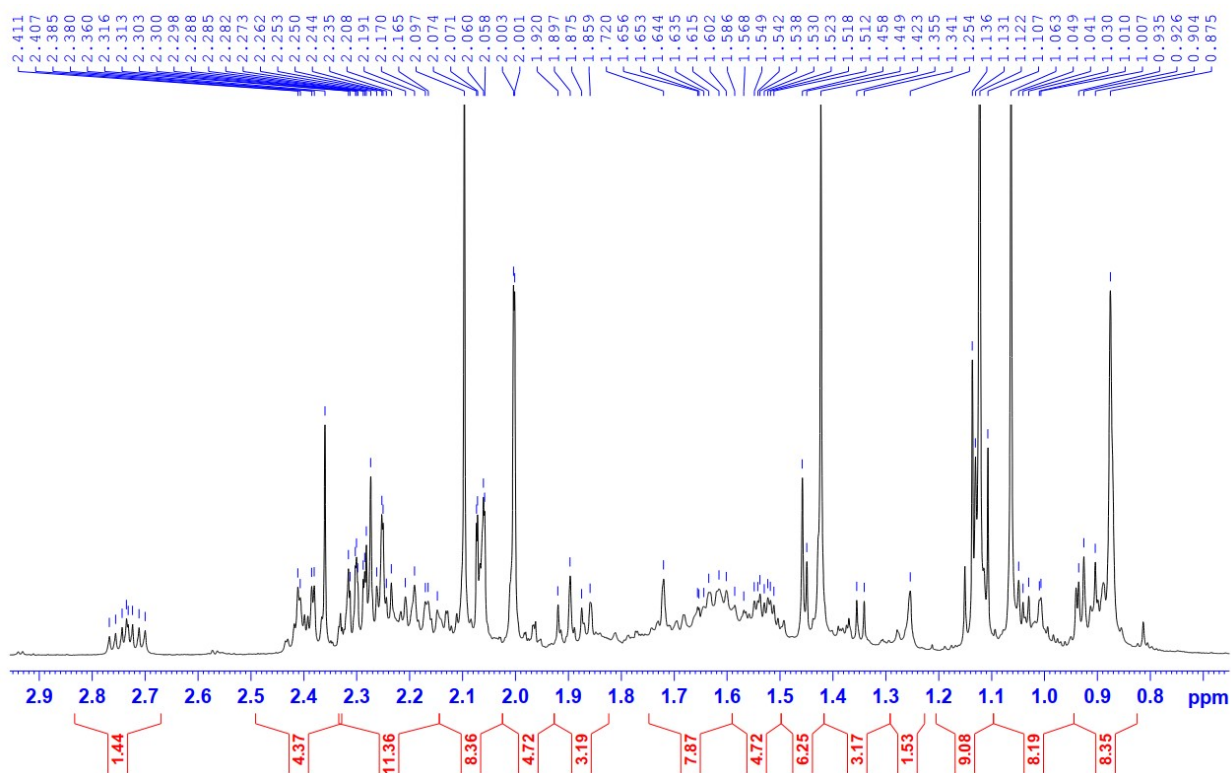


Figure S4. Expanded ^1H -NMR spectrum of compound **1**

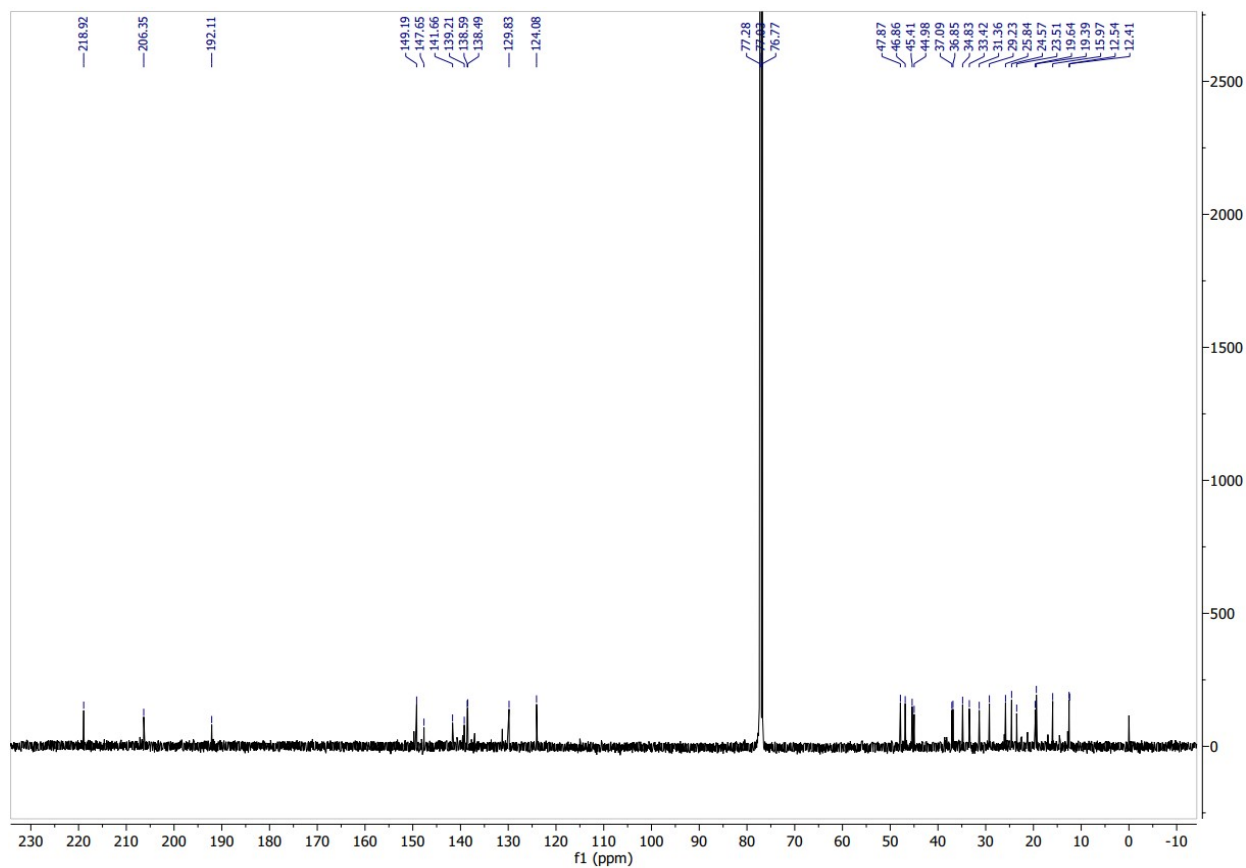


Figure S5. ^{13}C -NMR spectrum of compound **1** in CDCl_3

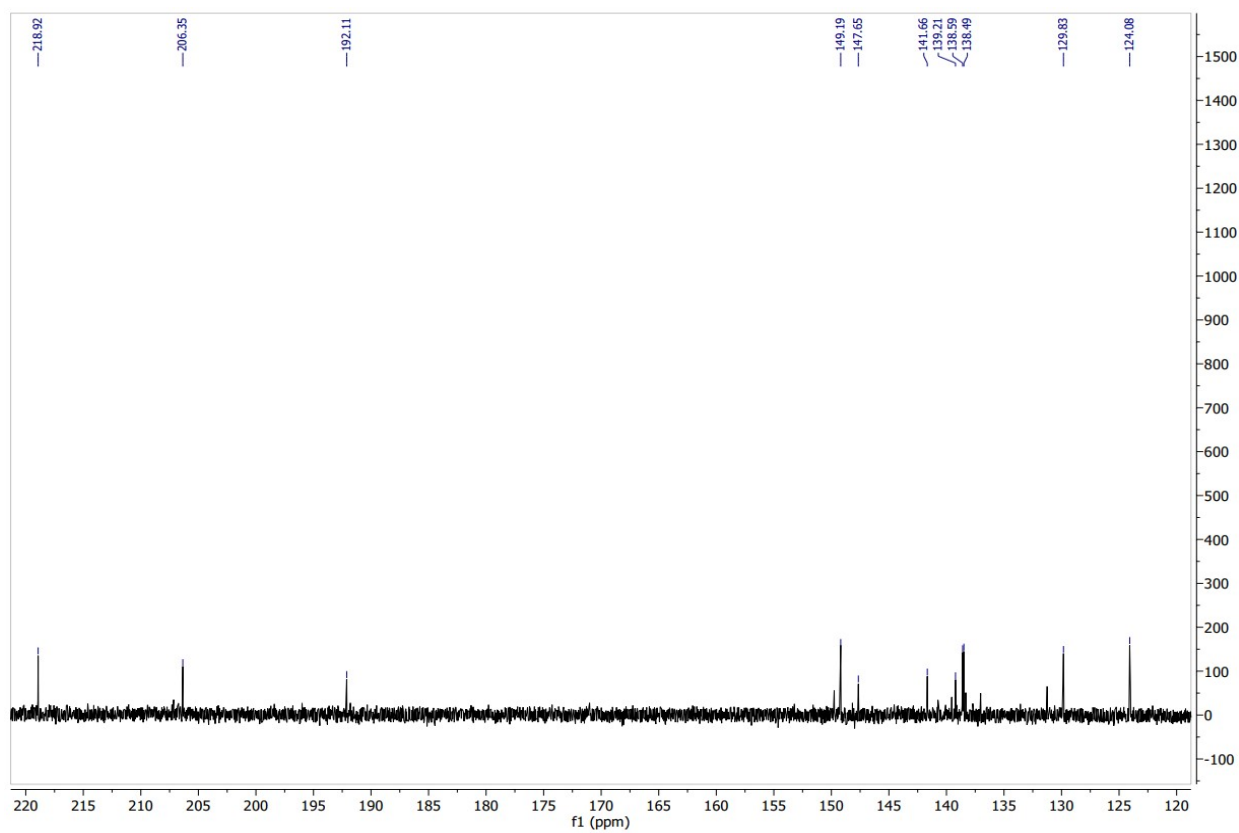


Figure S6. Expanded ^{13}C -NMR spectrum of compound **1**

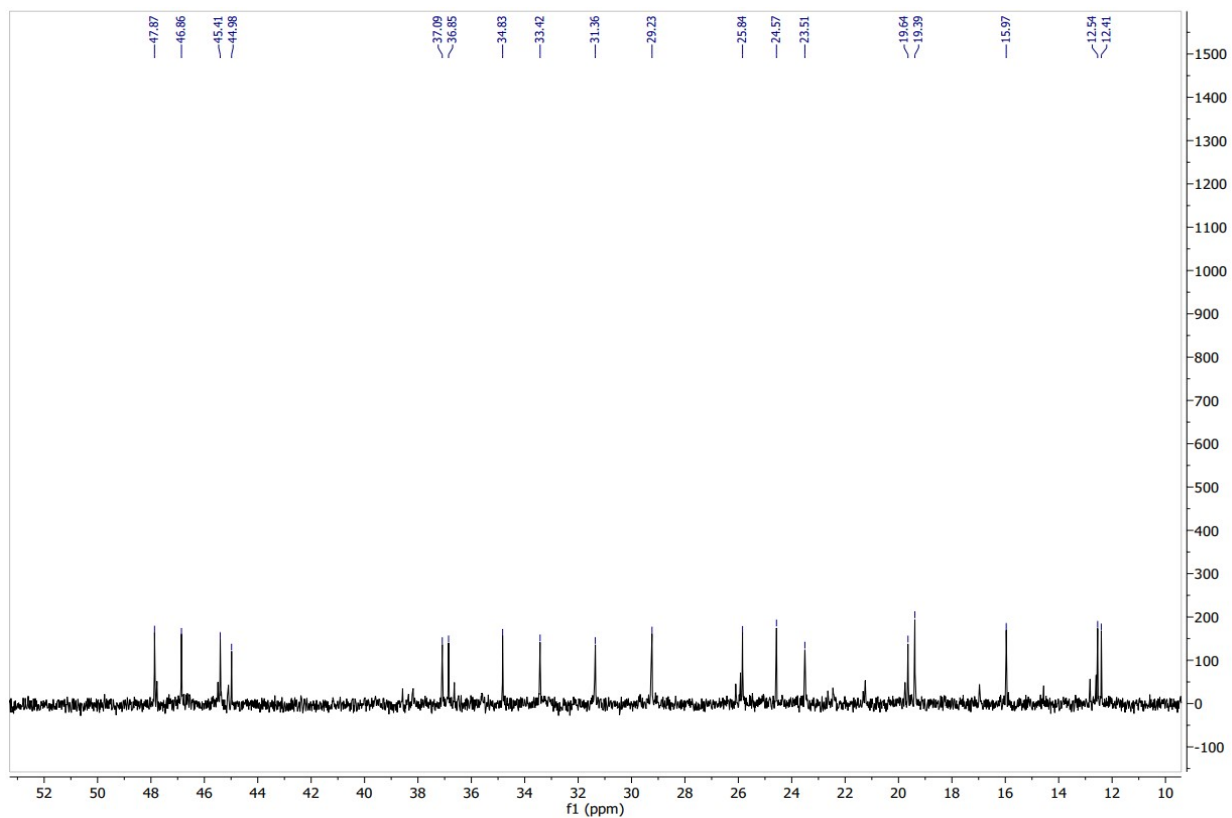


Figure S7. Expanded ^{13}C -NMR spectrum of compound 1

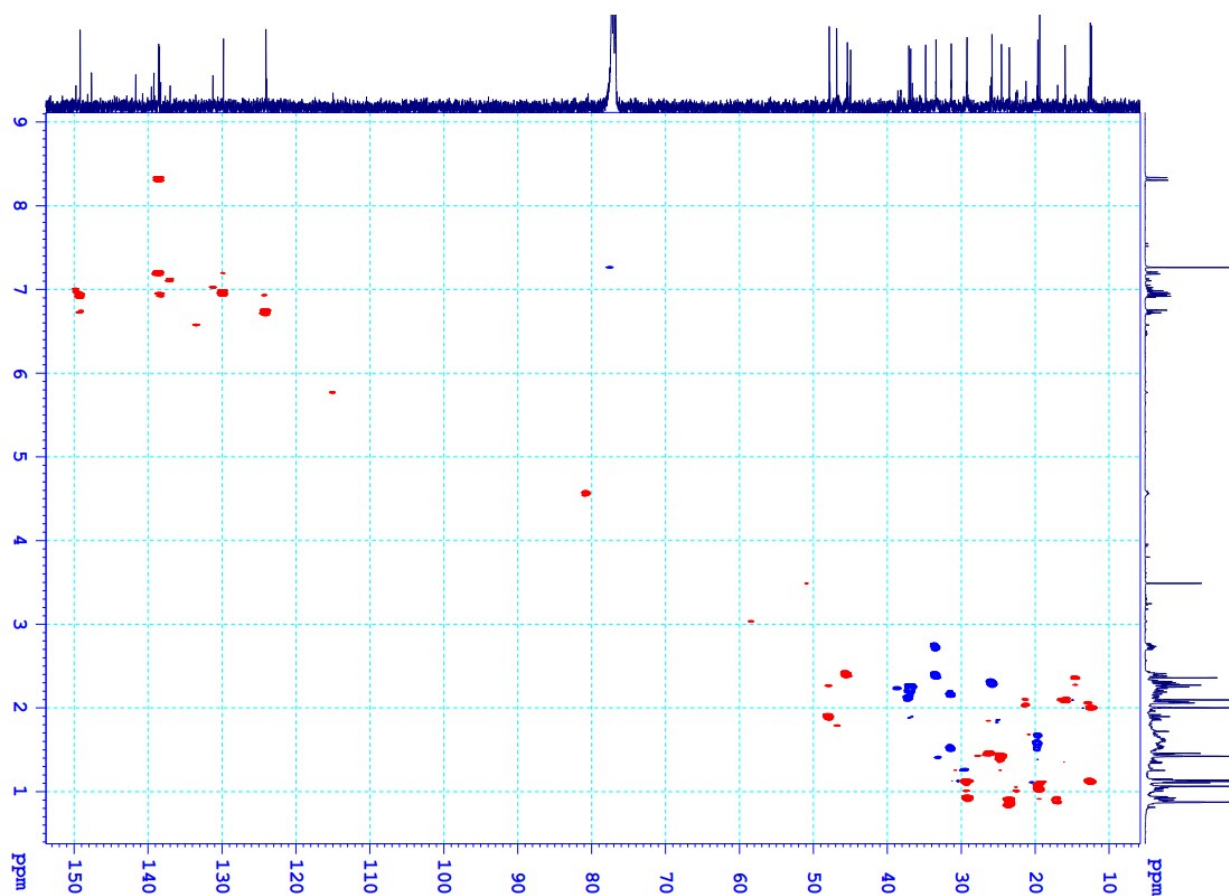


Figure S8. HSQC spectrum of compound 1

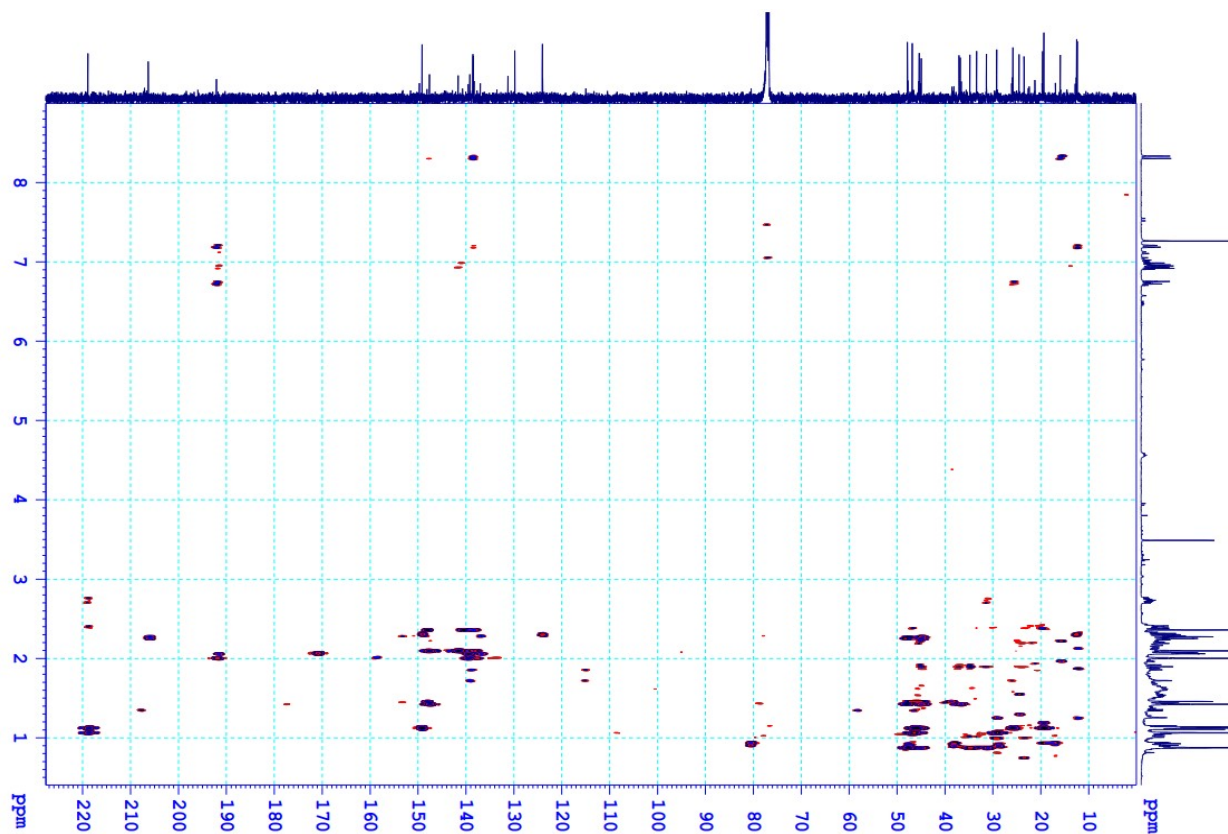


Figure S9. HMBC spectrum of compound **1**

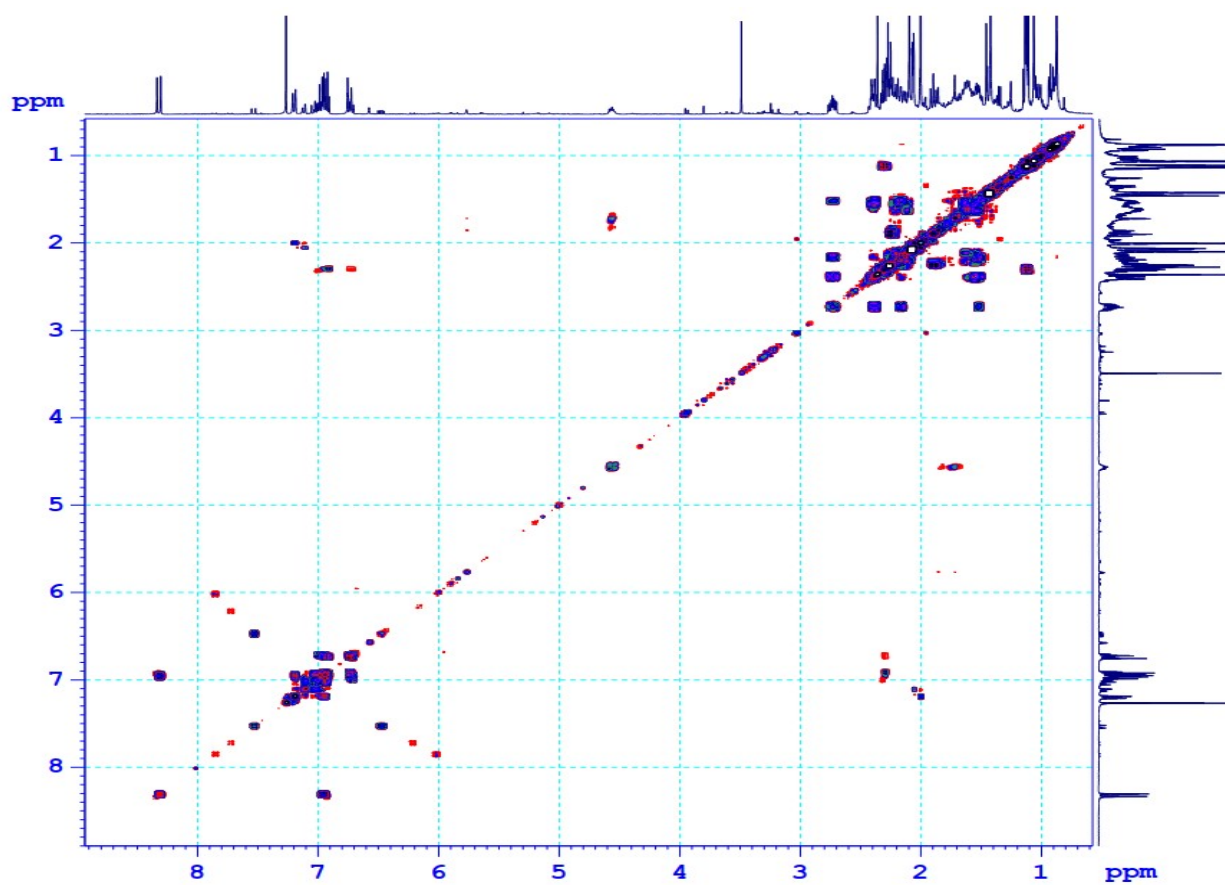


Figure S10. ^1H - ^1H COSY spectrum of compound **1**

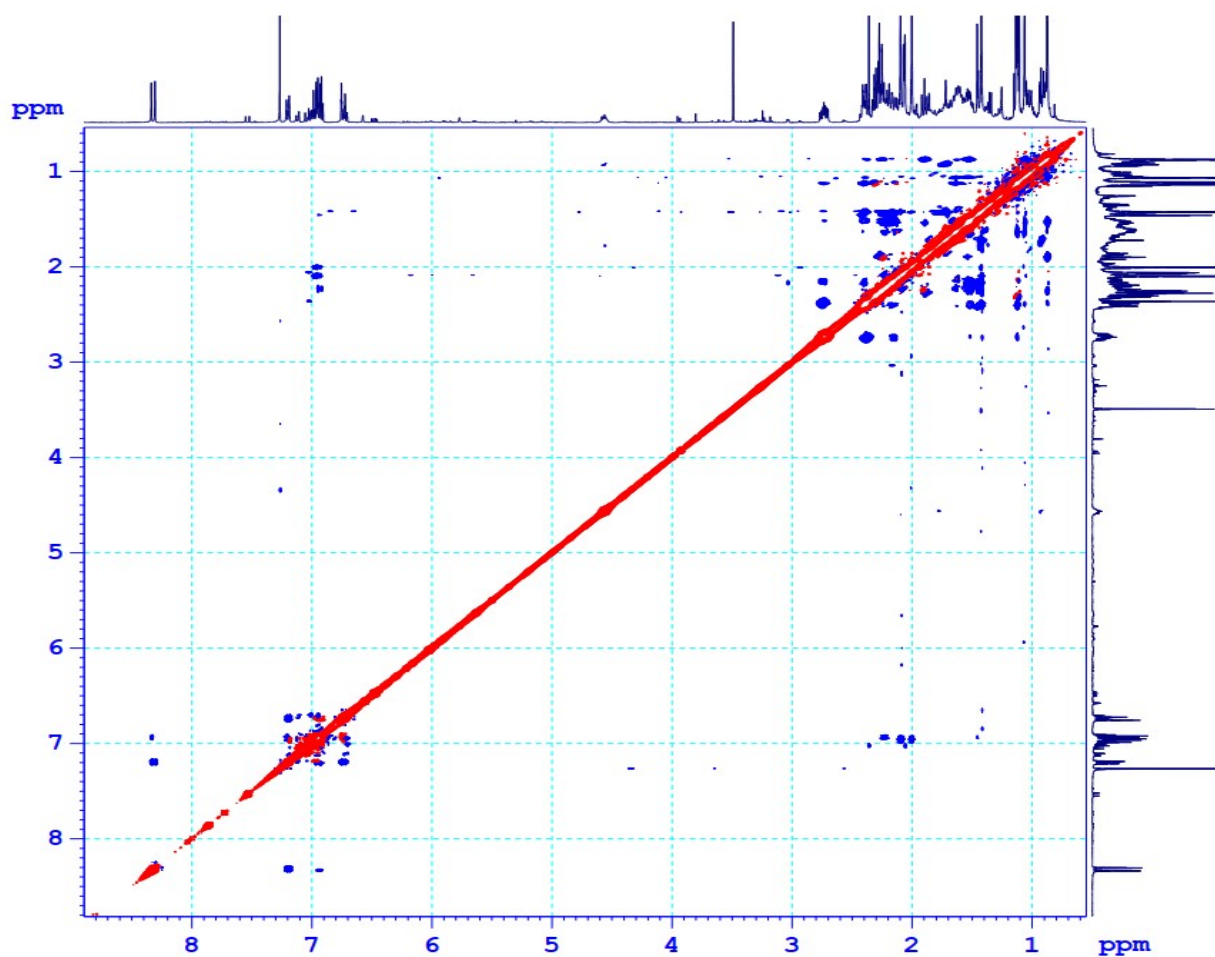


Figure S11. NOESY spectrum of compound **1**

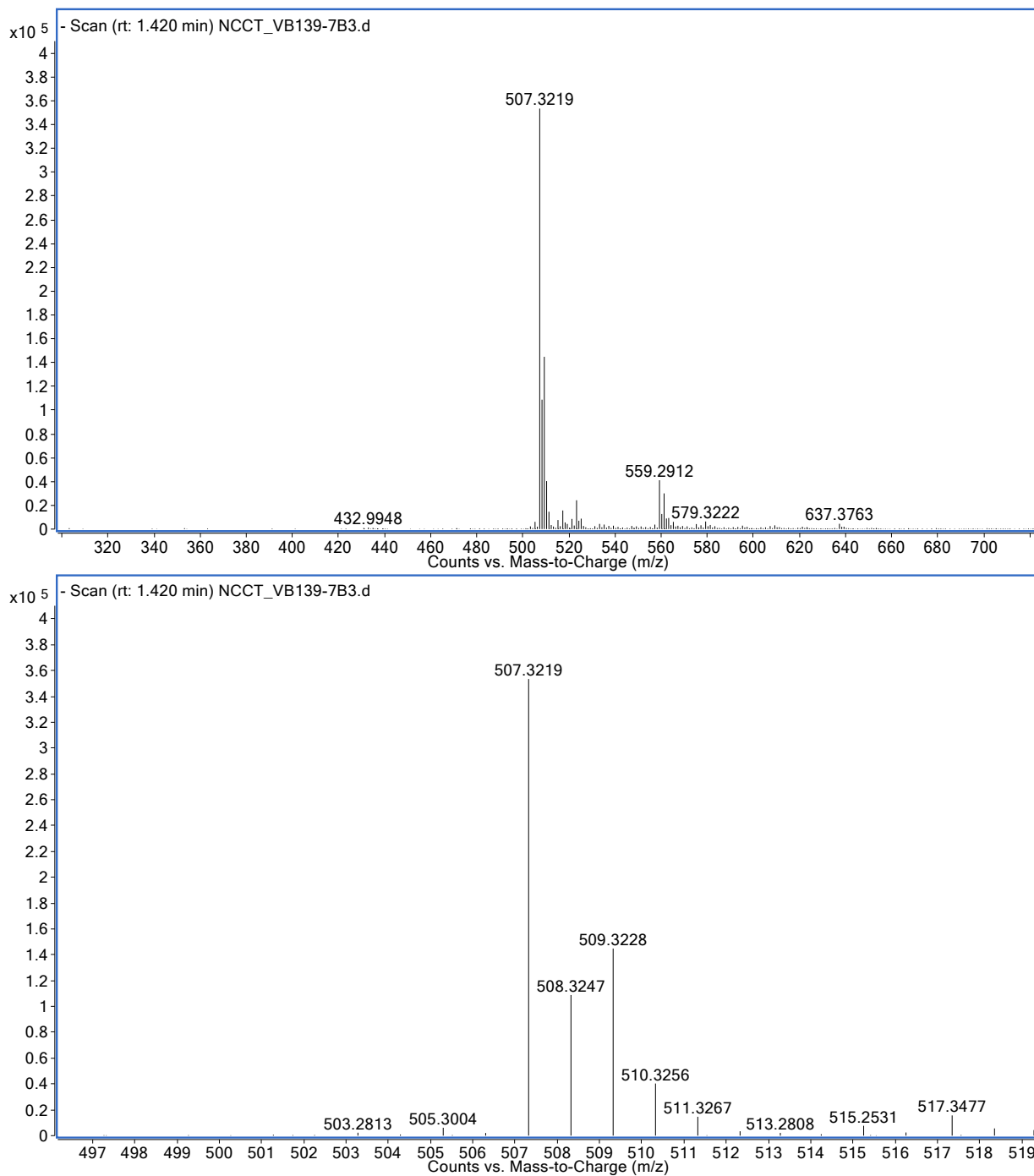


Figure S12. HRESIMS of compound **2**

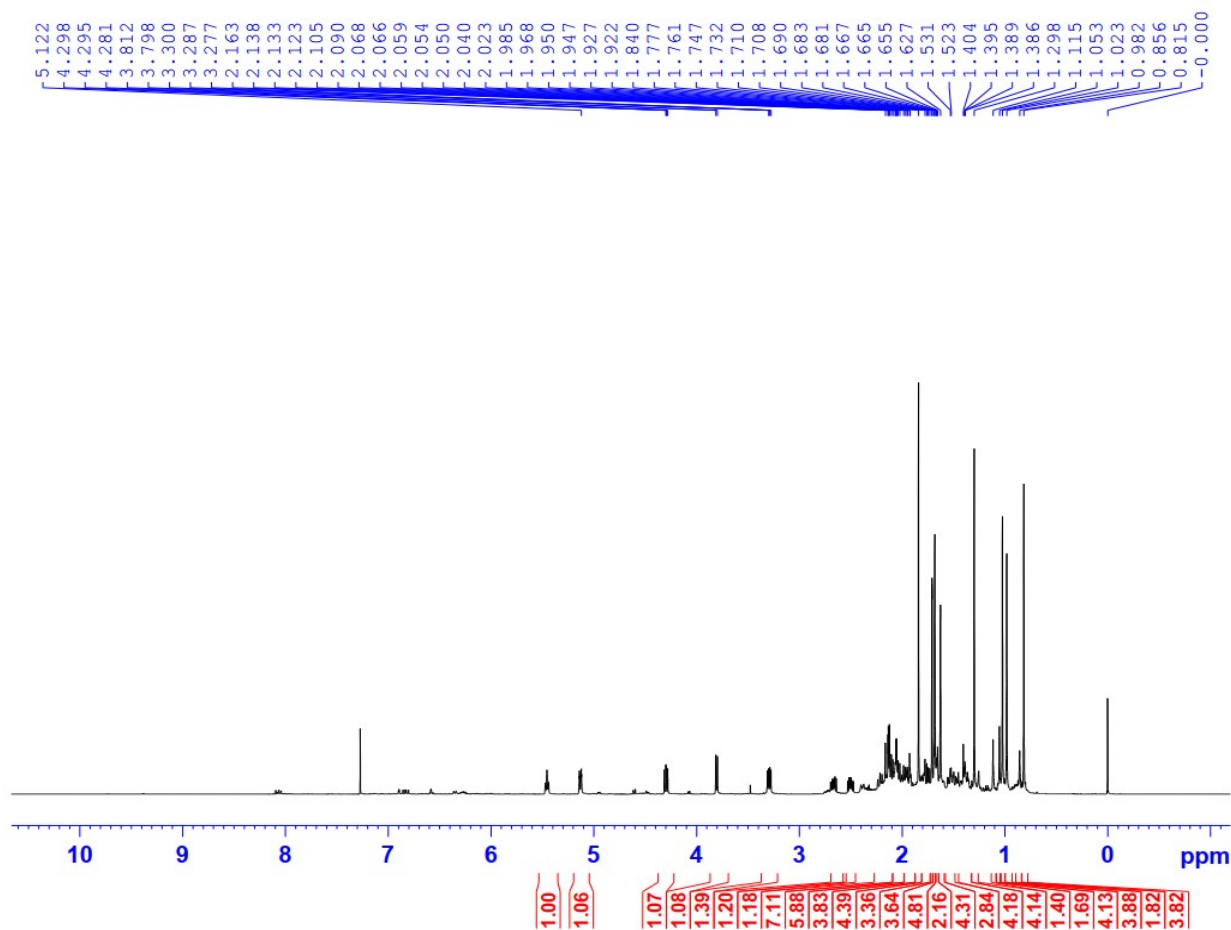


Figure S13. ^1H -NMR spectrum of compound **2** in CDCl_3

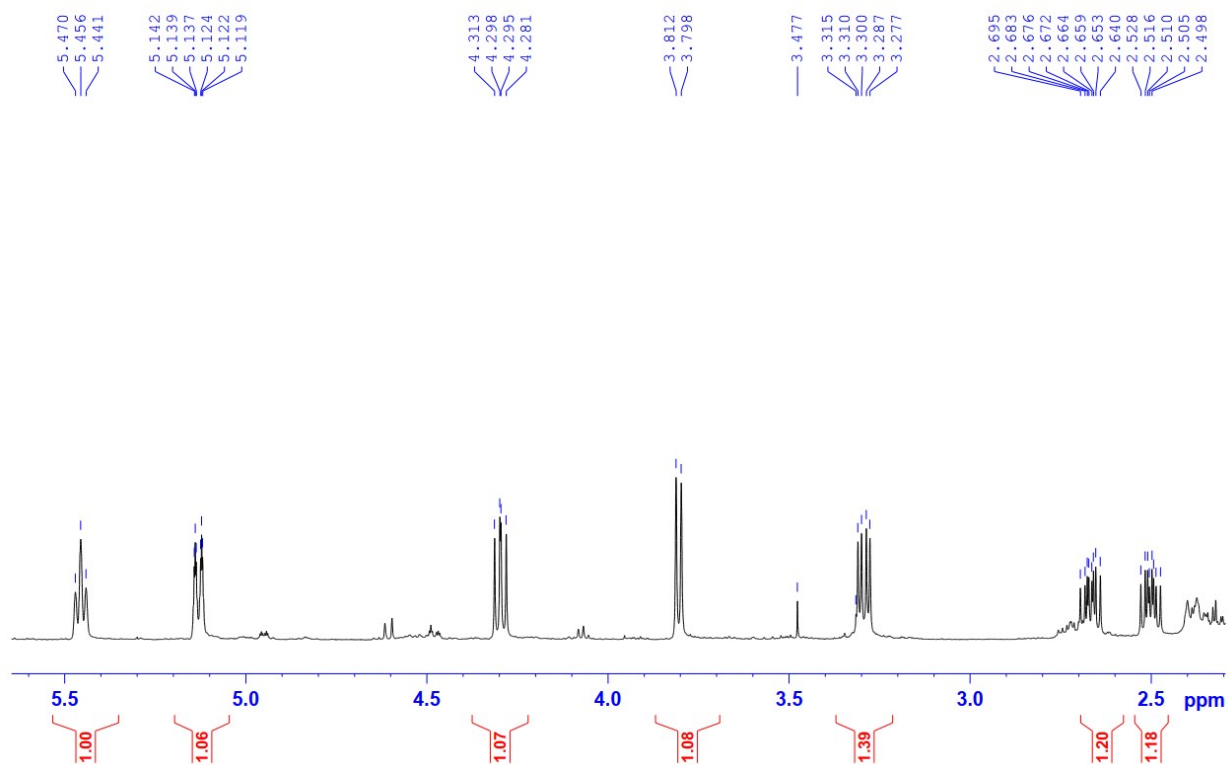


Figure S14. Expanded ^1H -NMR spectrum of compound **2**

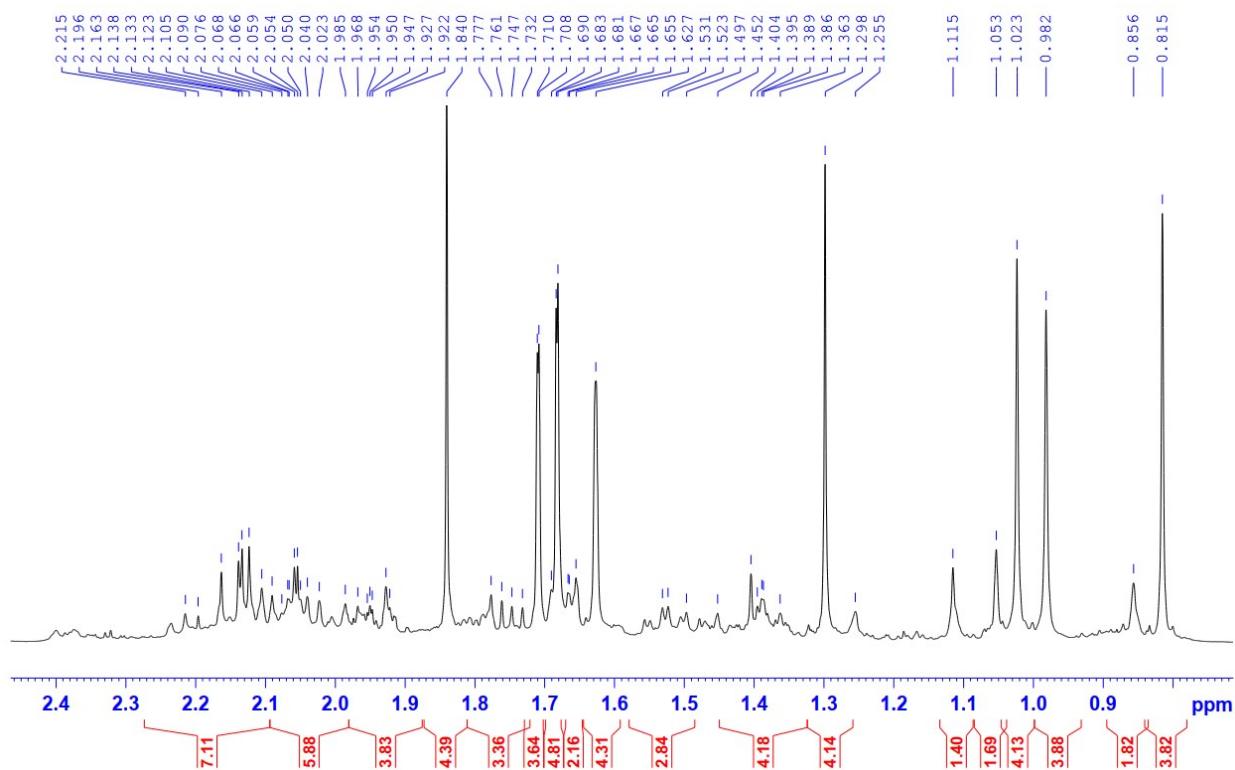


Figure S15. Expanded ^1H -NMR spectrum of compound **2**

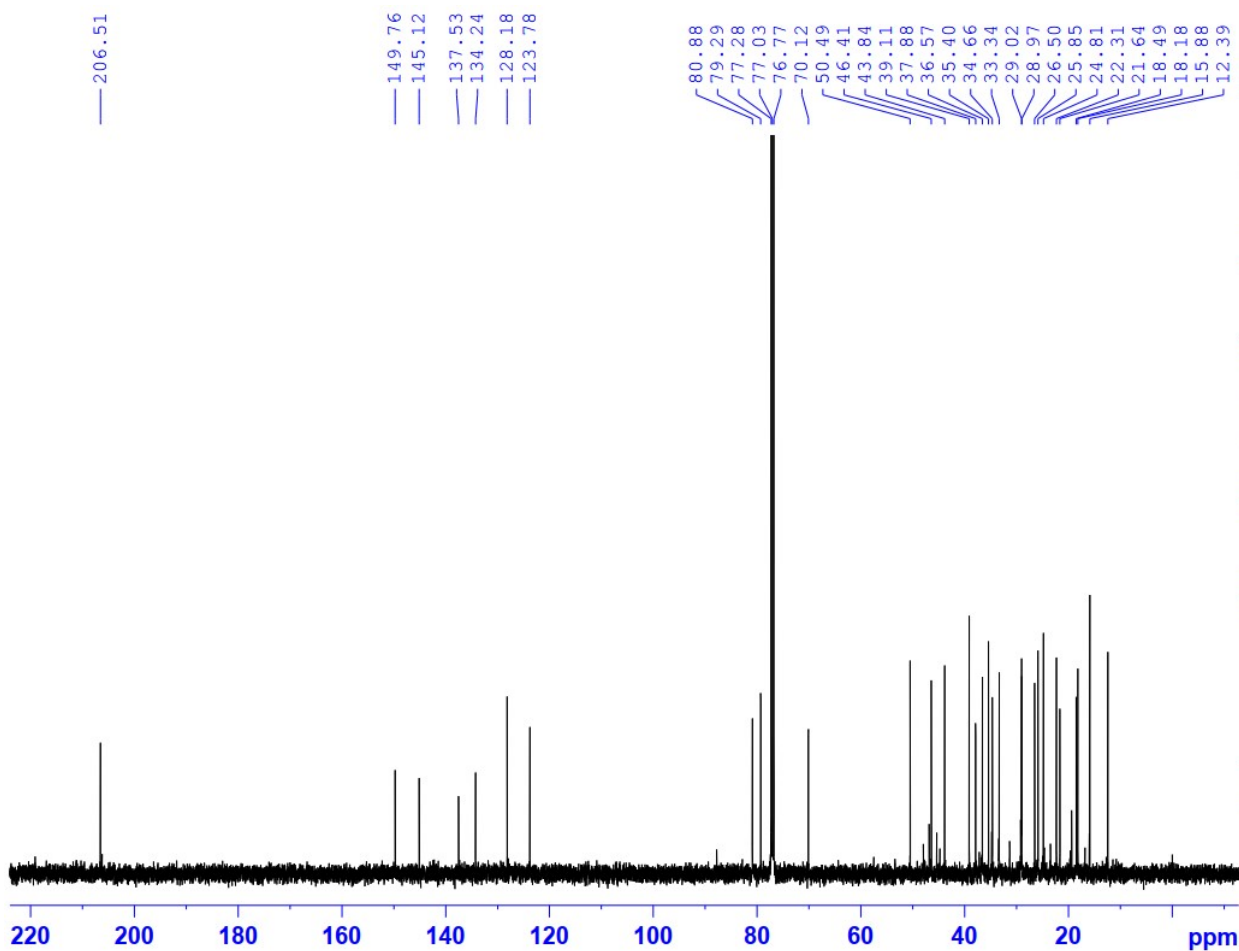


Figure S16. ^{13}C -NMR spectrum of compound **2** in CDCl_3

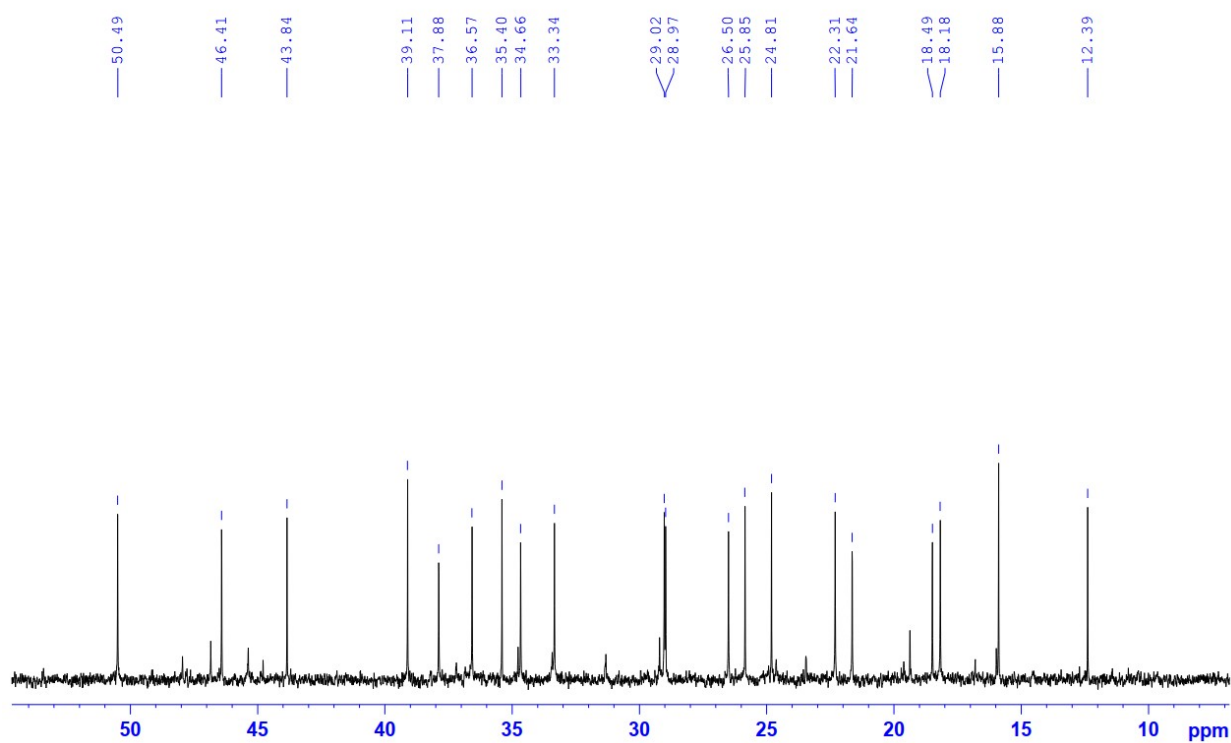


Figure S17. Expanded ^{13}C -NMR spectrum of compound 2

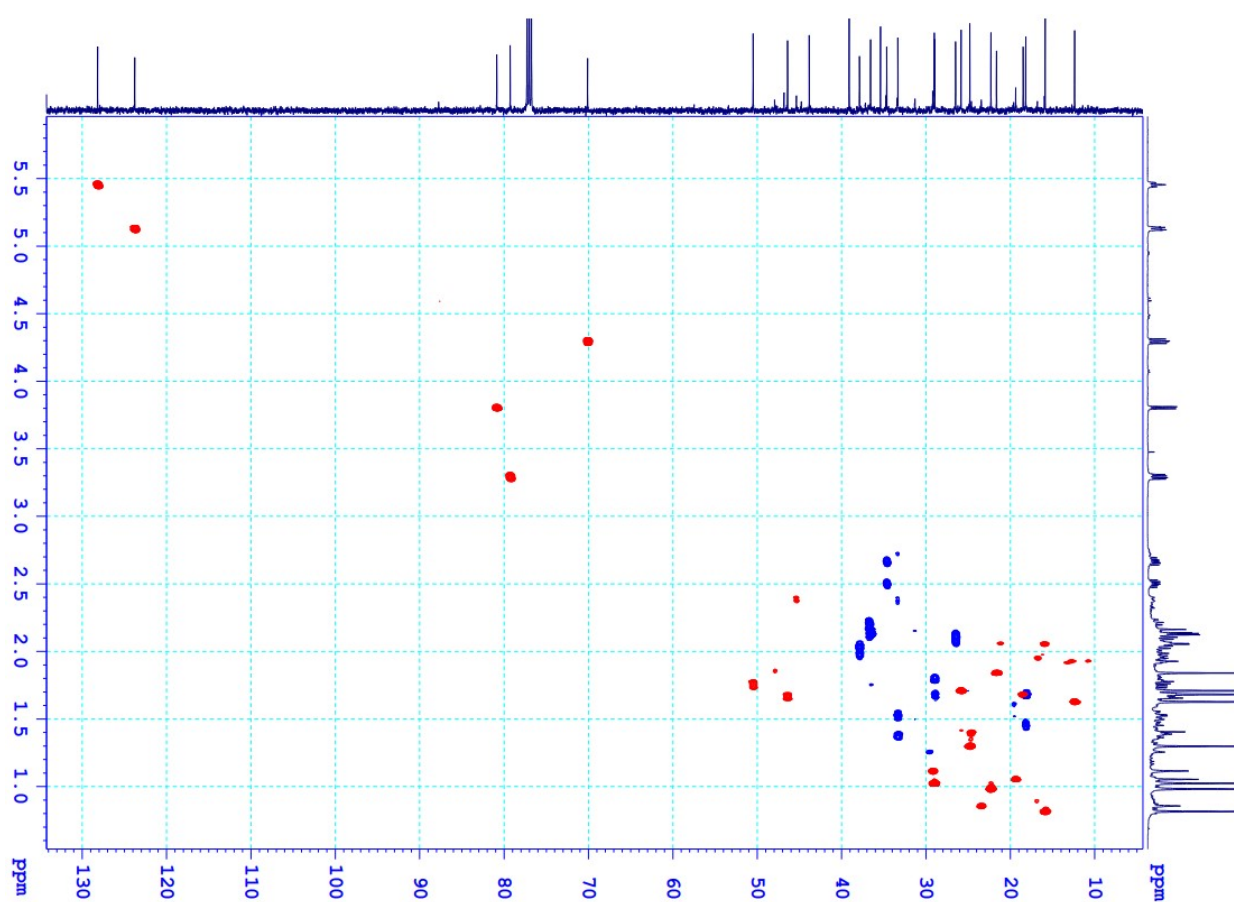


Figure S18. HSQC spectrum of compound 2

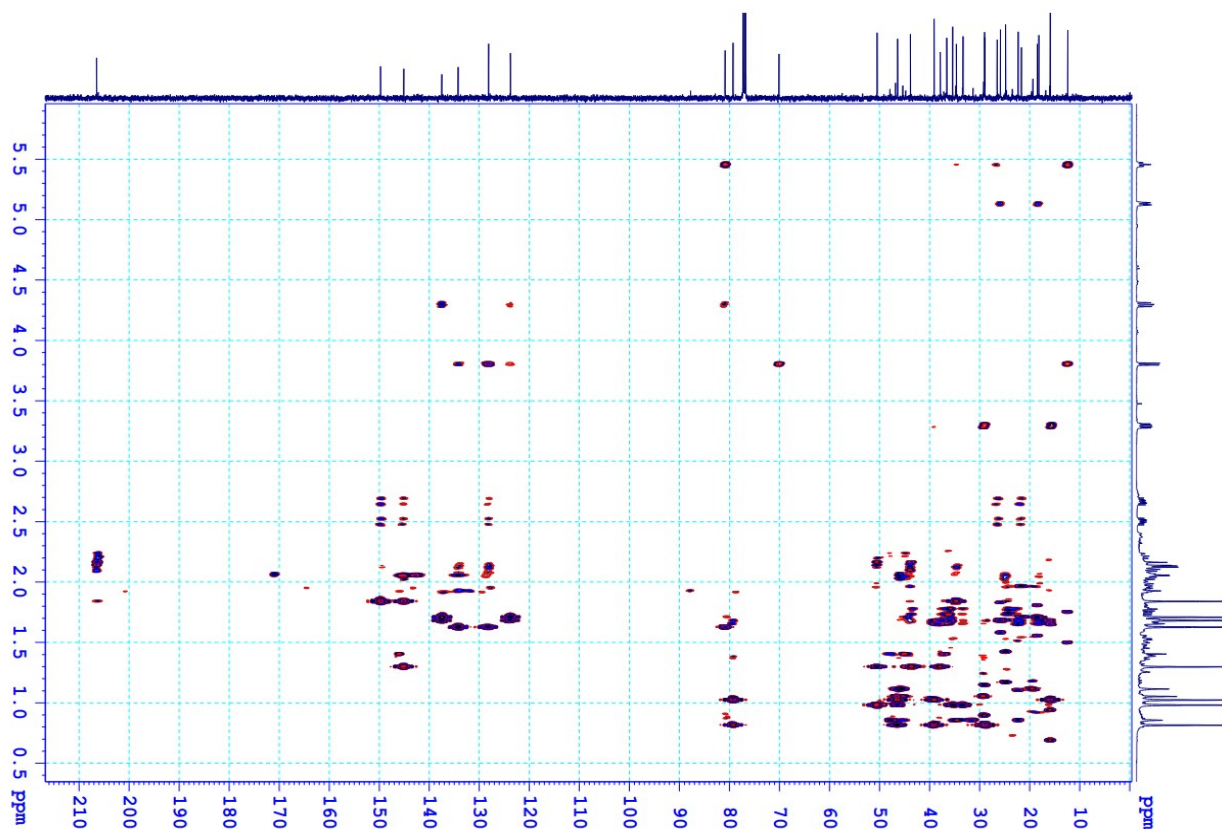


Figure S19. HMBC spectrum of compound 2

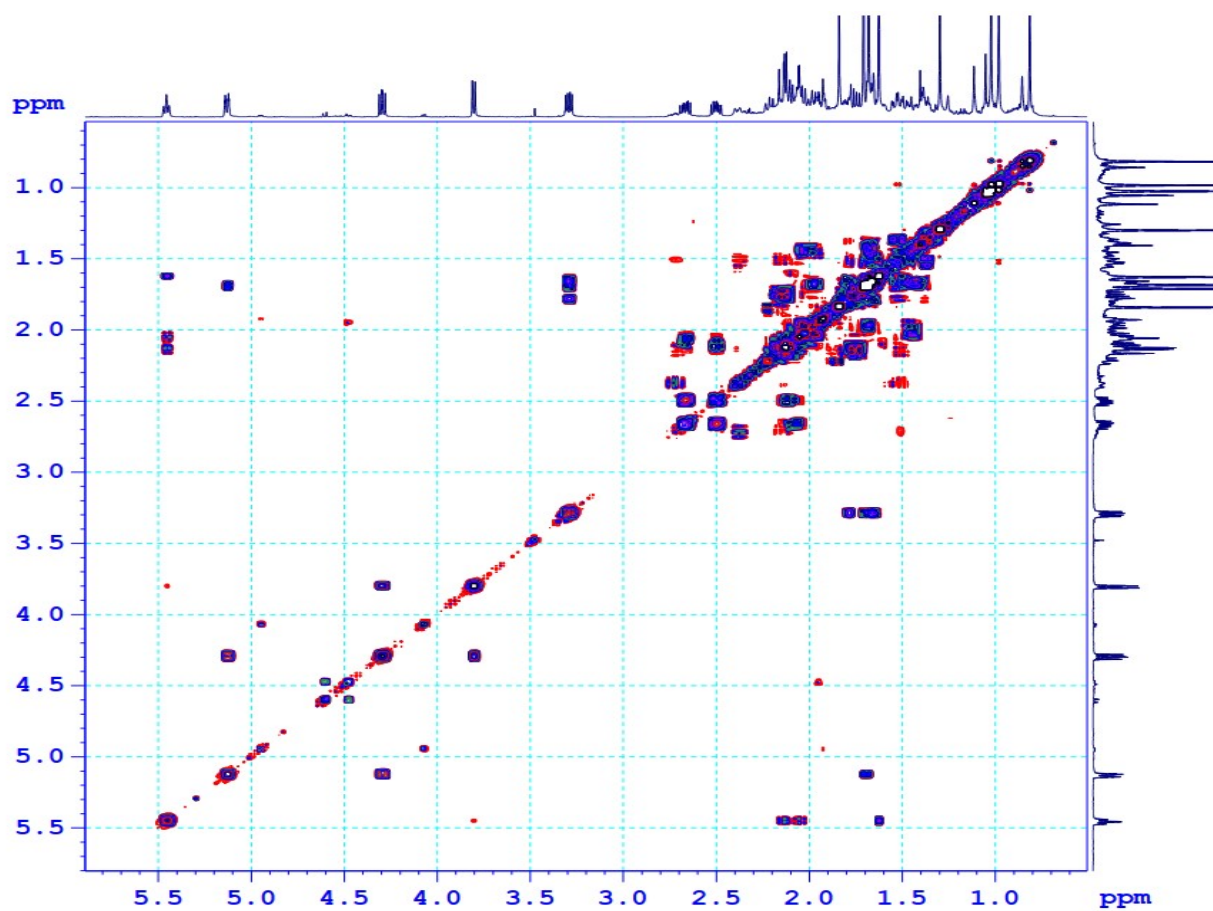


Figure S20. ^1H - ^1H COSY spectrum of compound 2

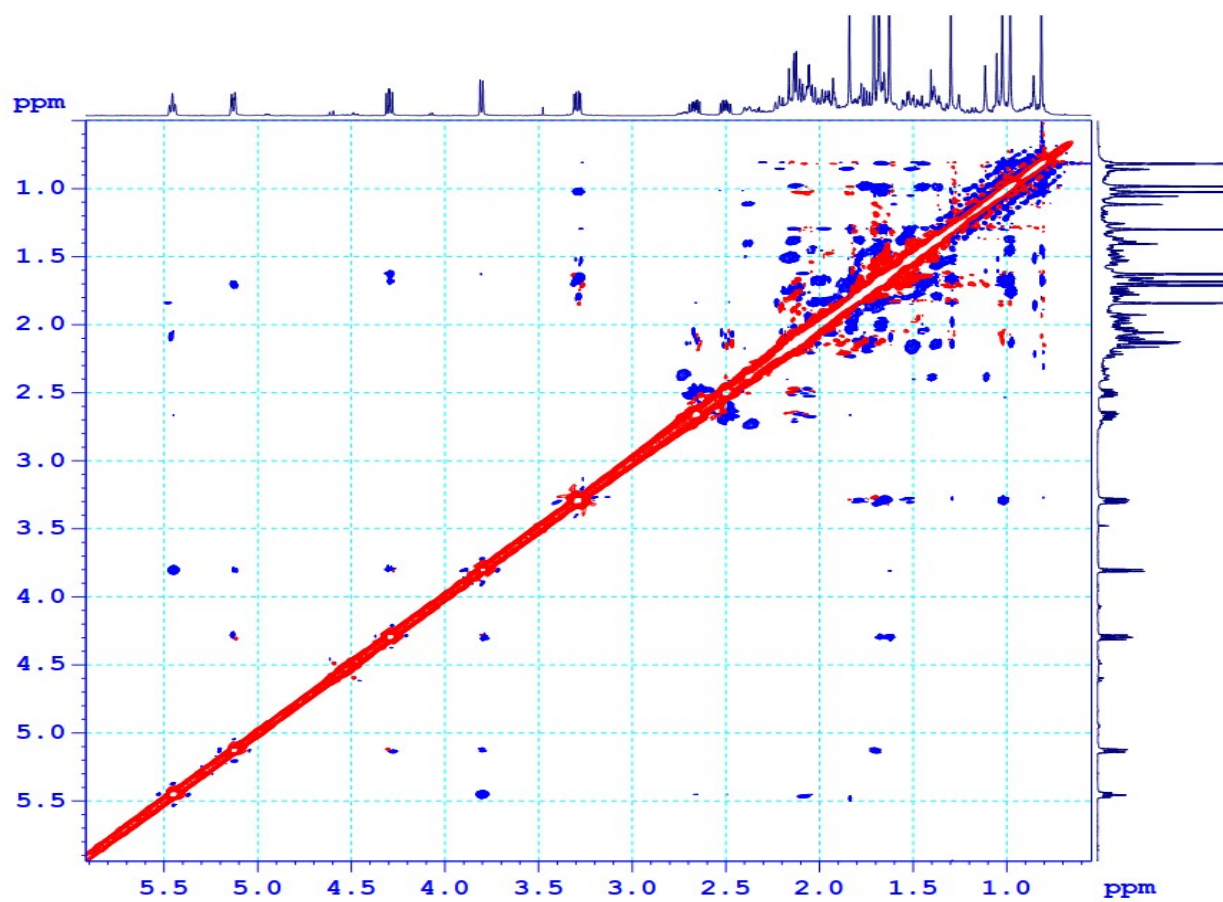


Figure S21. NOESY spectrum of compound **2**

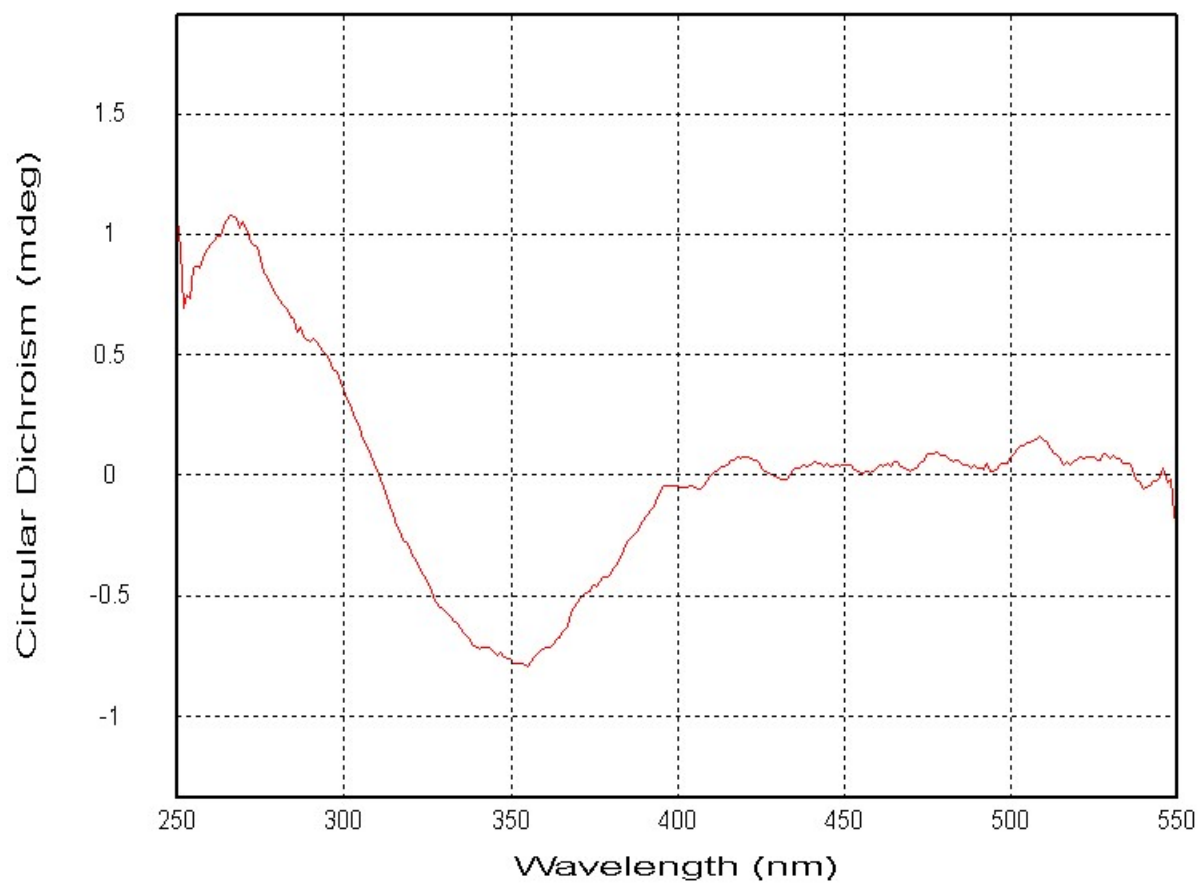


Figure S22. $\text{Mo}_2(\text{OAc})_4$ induced ECD spectrum of compound **2**

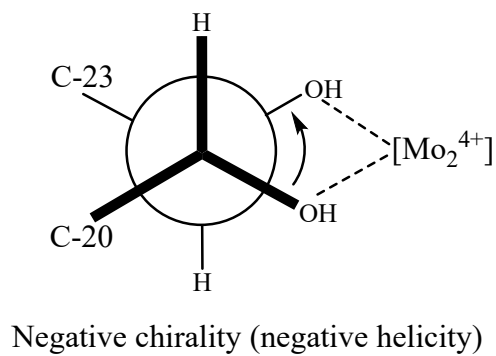


Figure S23. Favored conformation of the Mo_2^{4+} complex of compound **2**

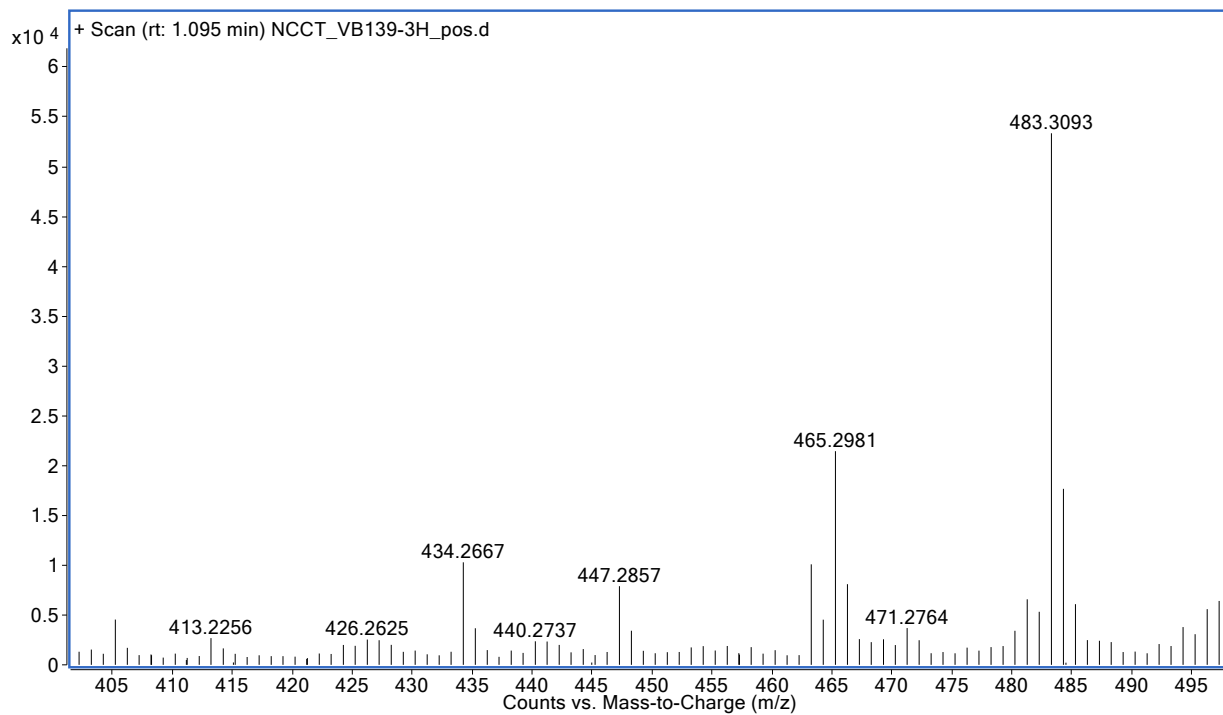


Figure S24. HRESIMS of compound **3**

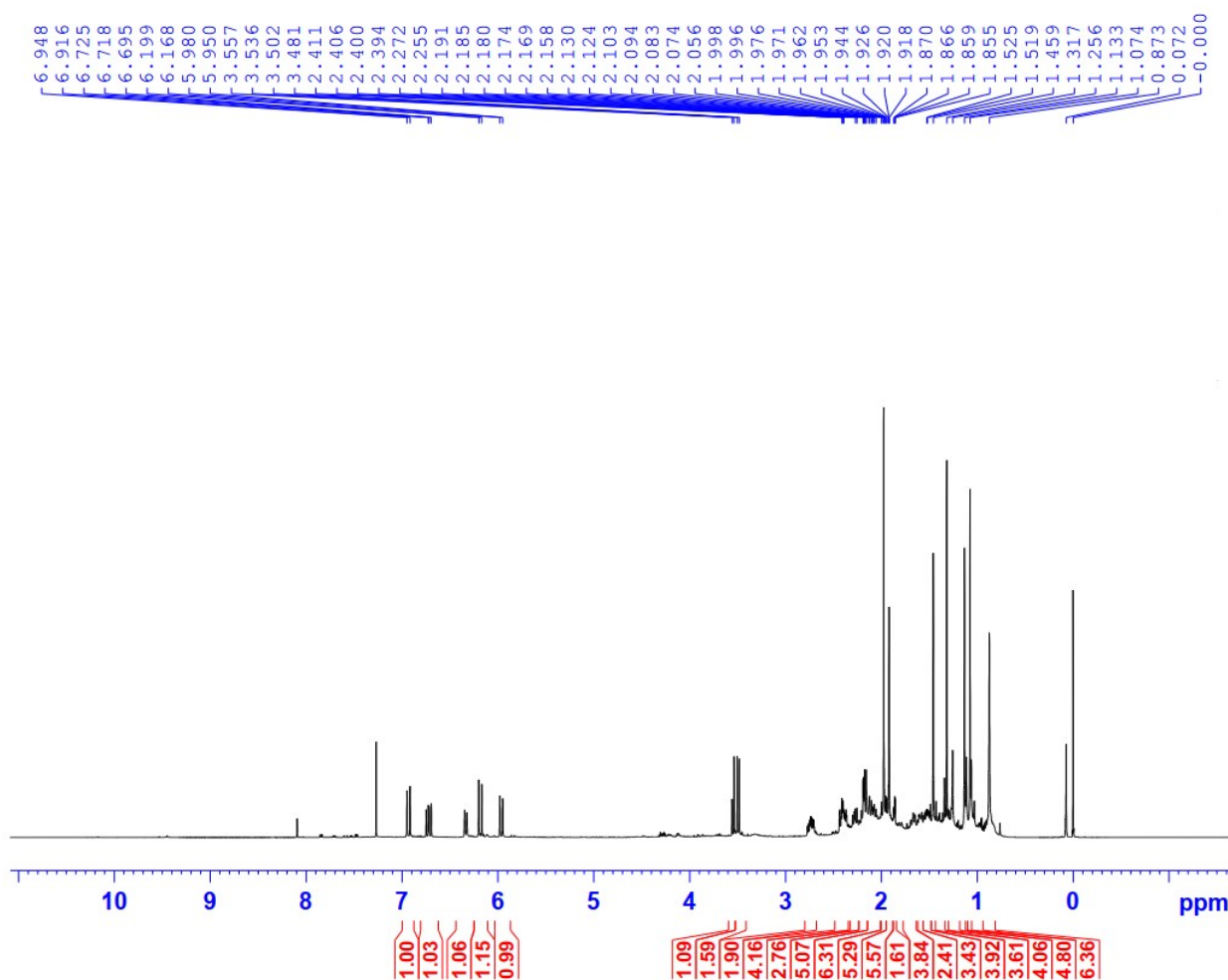


Figure S25. ^1H -NMR spectrum of compound **3** in CDCl_3

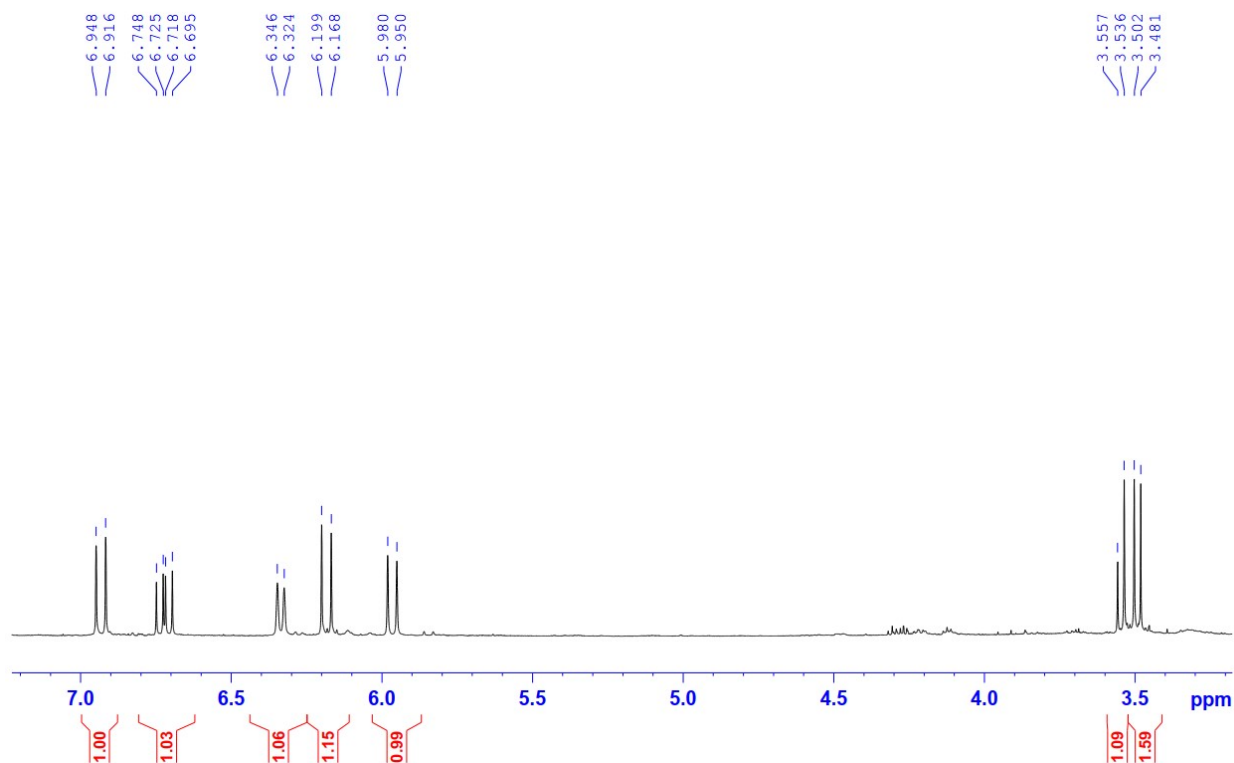


Figure S26. Expanded ^1H -NMR spectrum of compound **3**

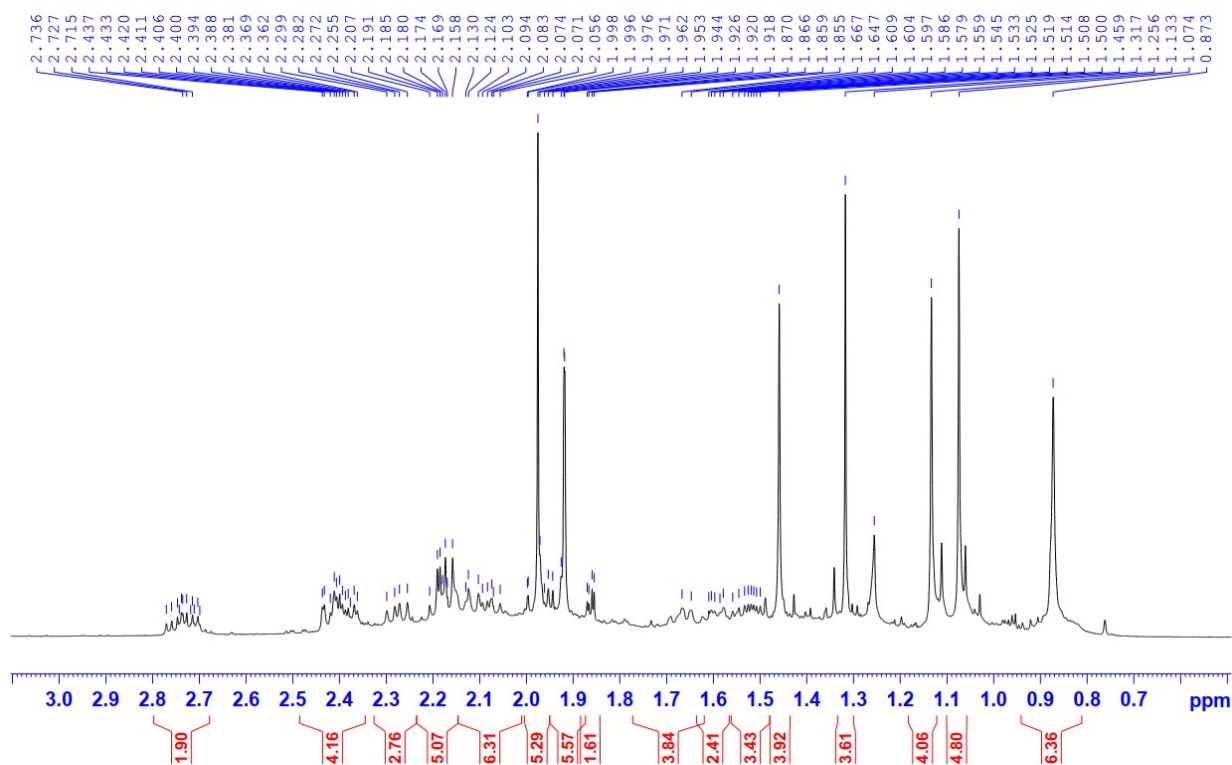


Figure S27. Expanded ^1H -NMR spectrum of compound **3**

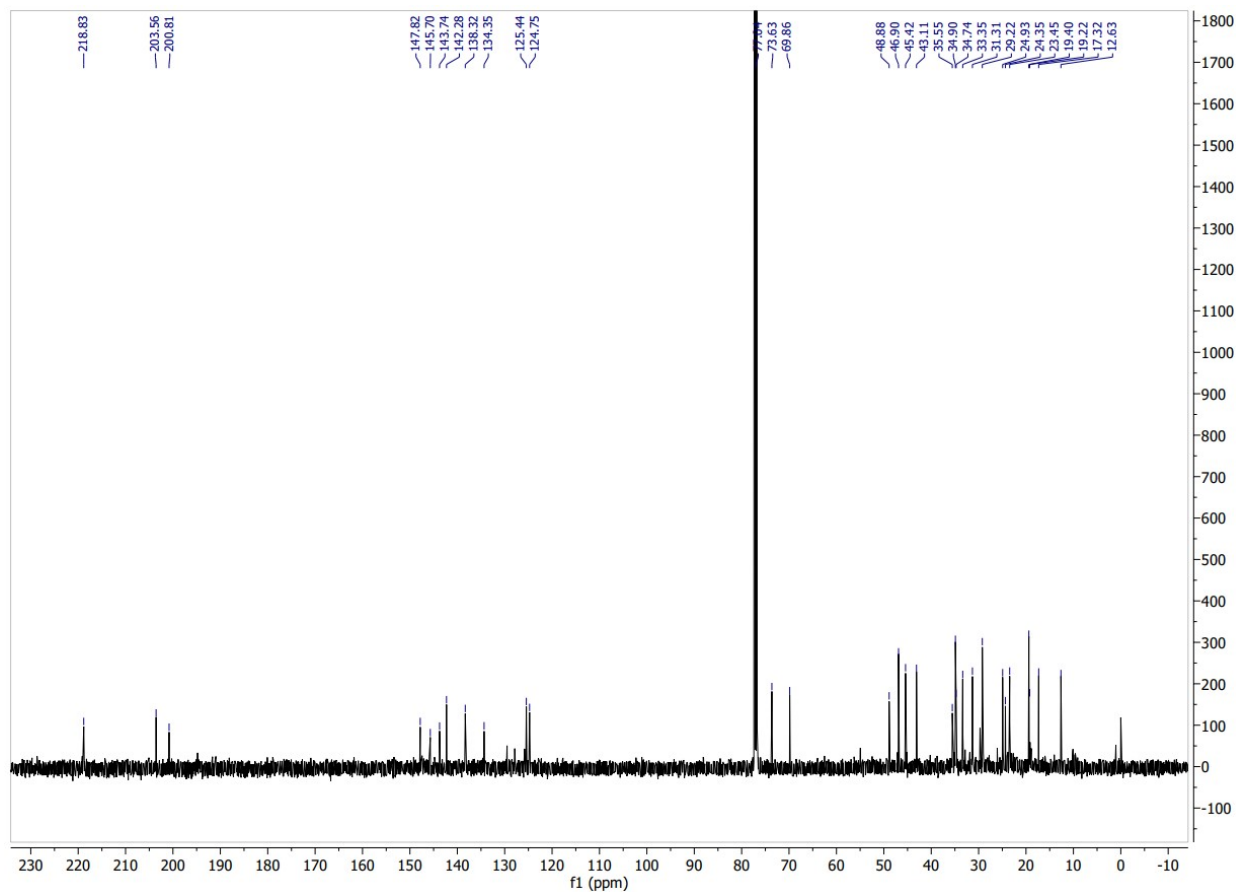


Figure S28. ^{13}C -NMR spectrum of compound **3** in CDCl_3

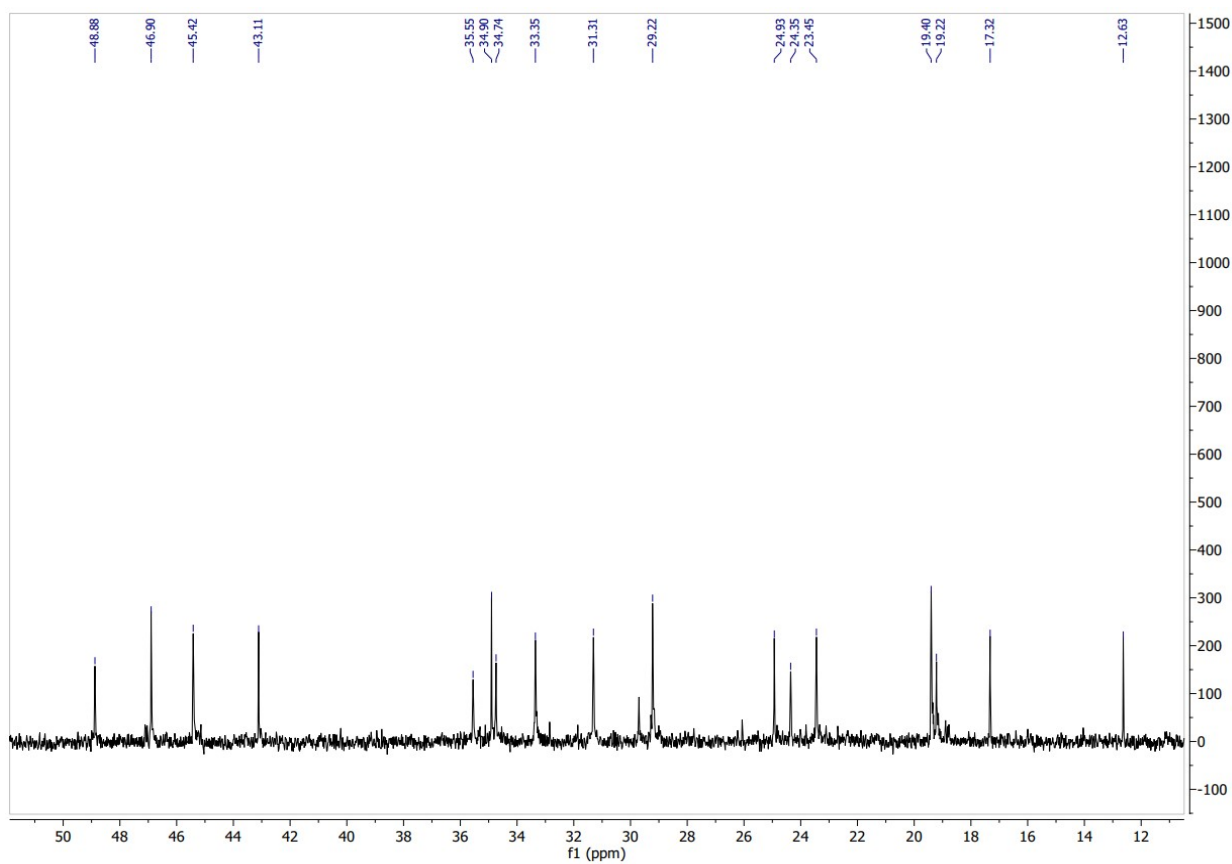


Figure S29. Expanded ^{13}C -NMR spectrum of compound **3** in CDCl_3

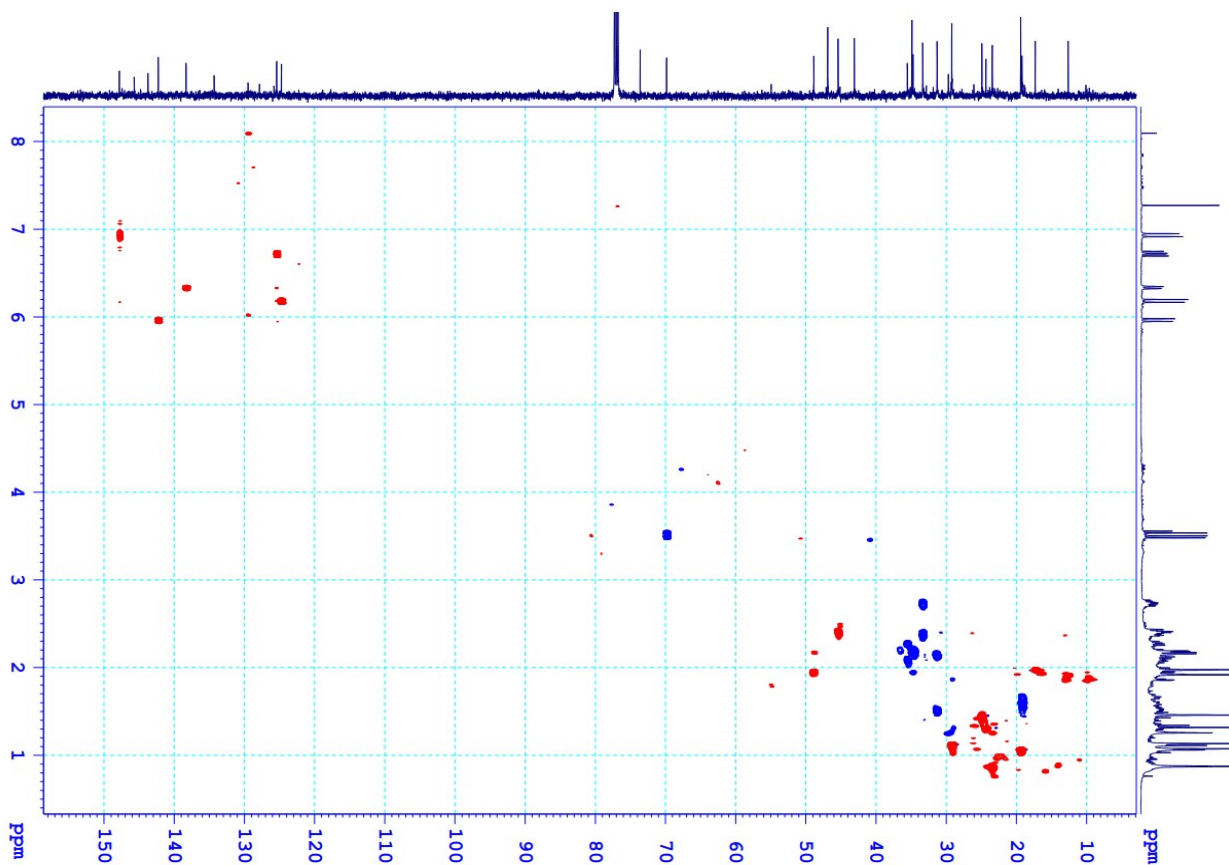


Figure S30. HSQC spectrum of compound 3

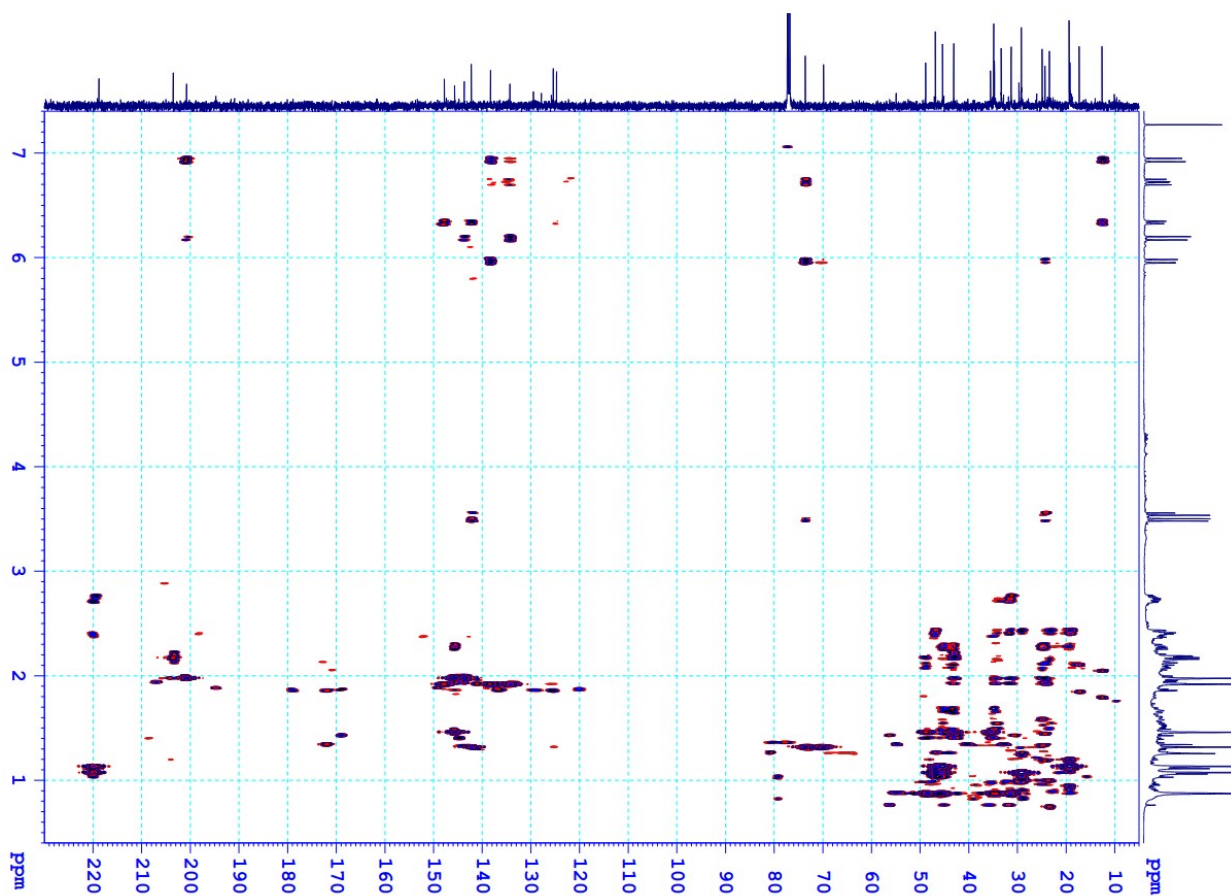


Figure S31. HMBC spectrum of compound 3

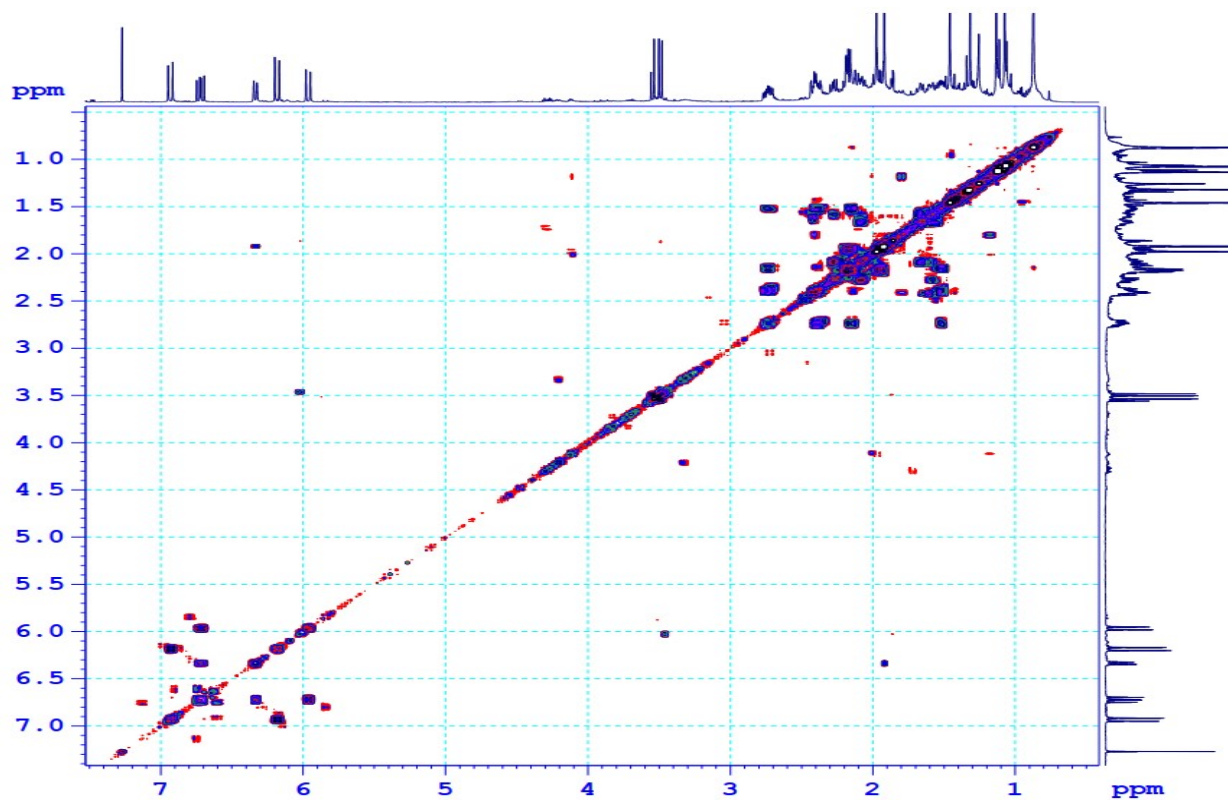


Figure S32. ^1H - ^1H COSY spectrum of compound **3**

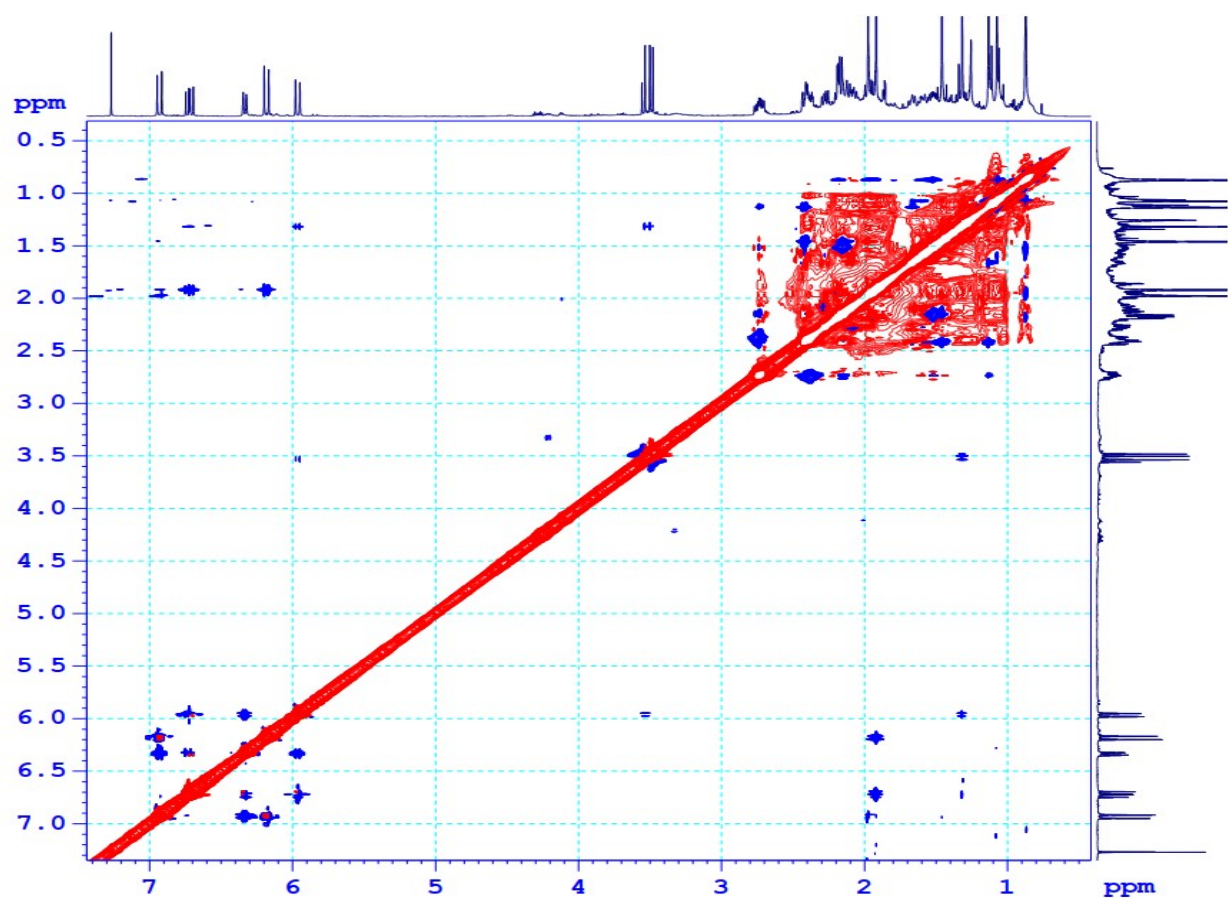


Figure S33. NOESY spectrum of compound **3**

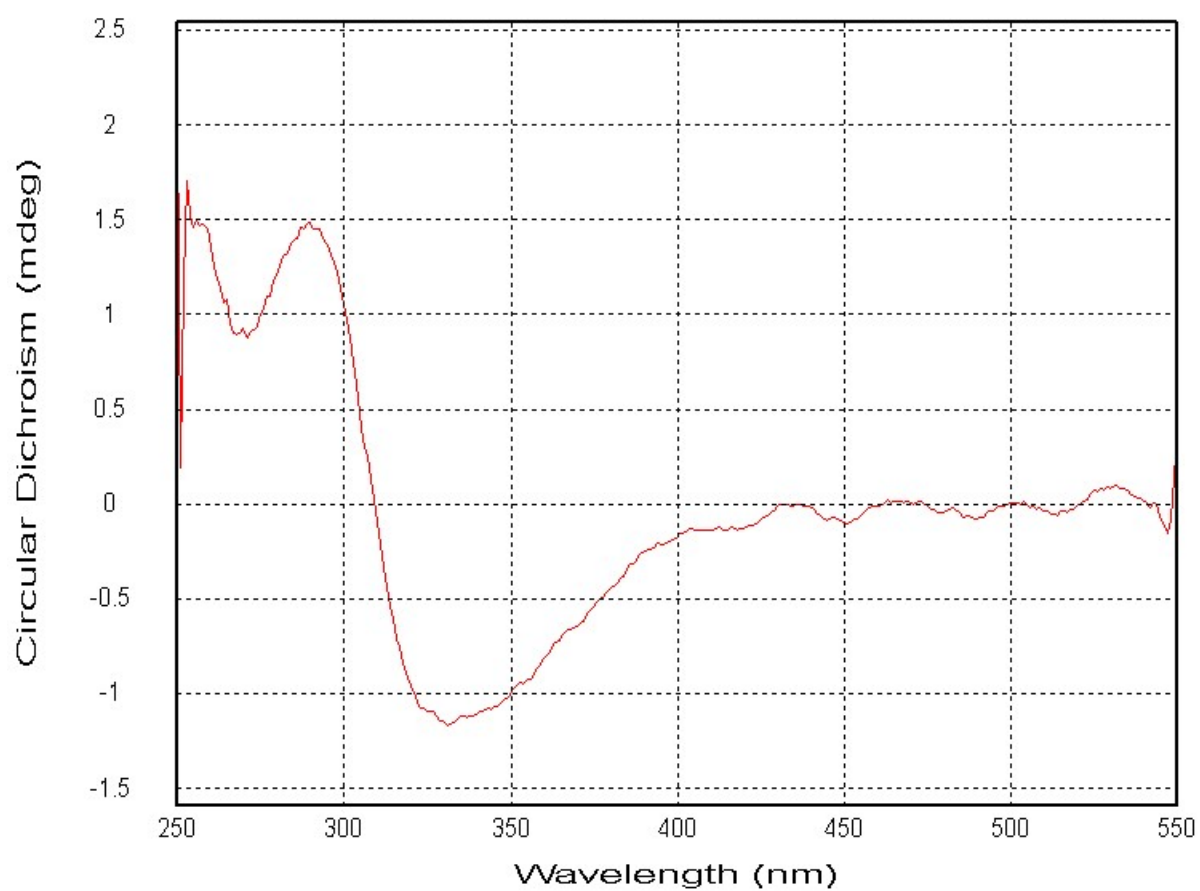
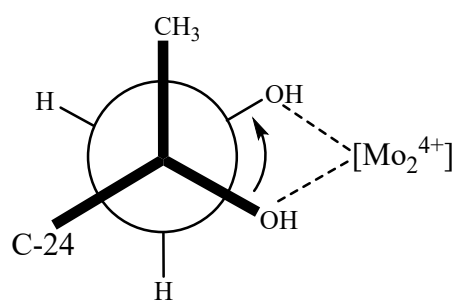


Figure S34. $\text{Mo}_2(\text{OAc})_4$ induced ECD spectrum of compound **3**



Negative chirality (negative helicity)

Figure S35. Favored conformation of the Mo_2^{4+} complex of compound **3**

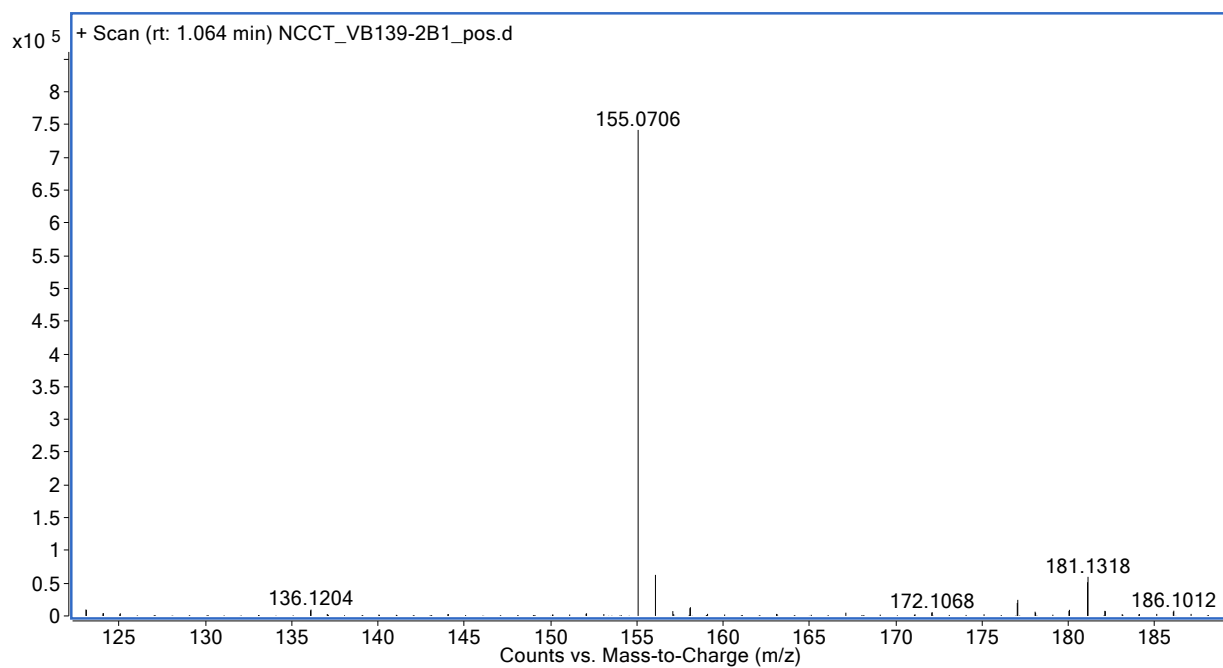


Figure S36. HRESIMS of compound **4**

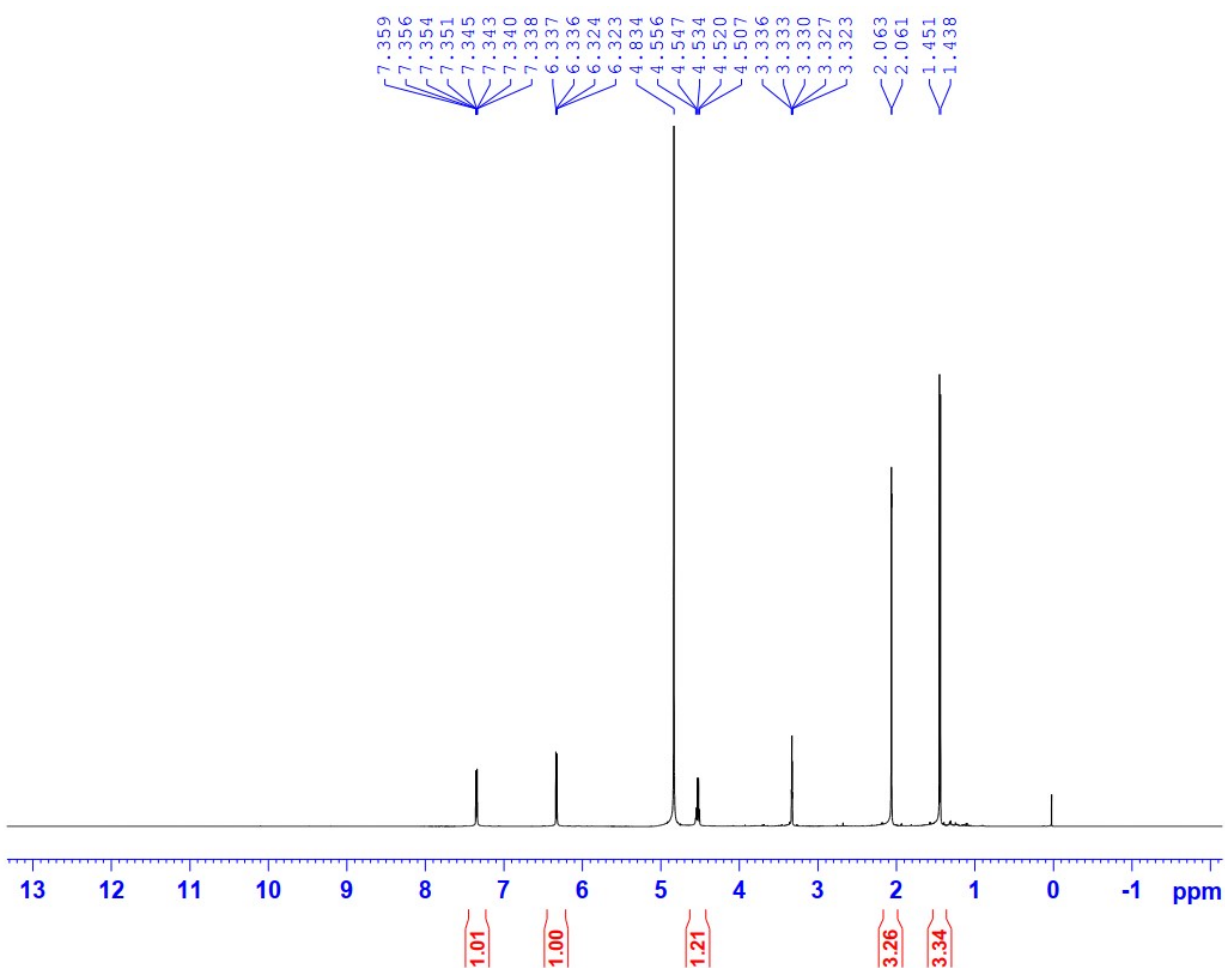


Figure S37. ¹H-NMR spectrum of compound **4** in CDCl₃

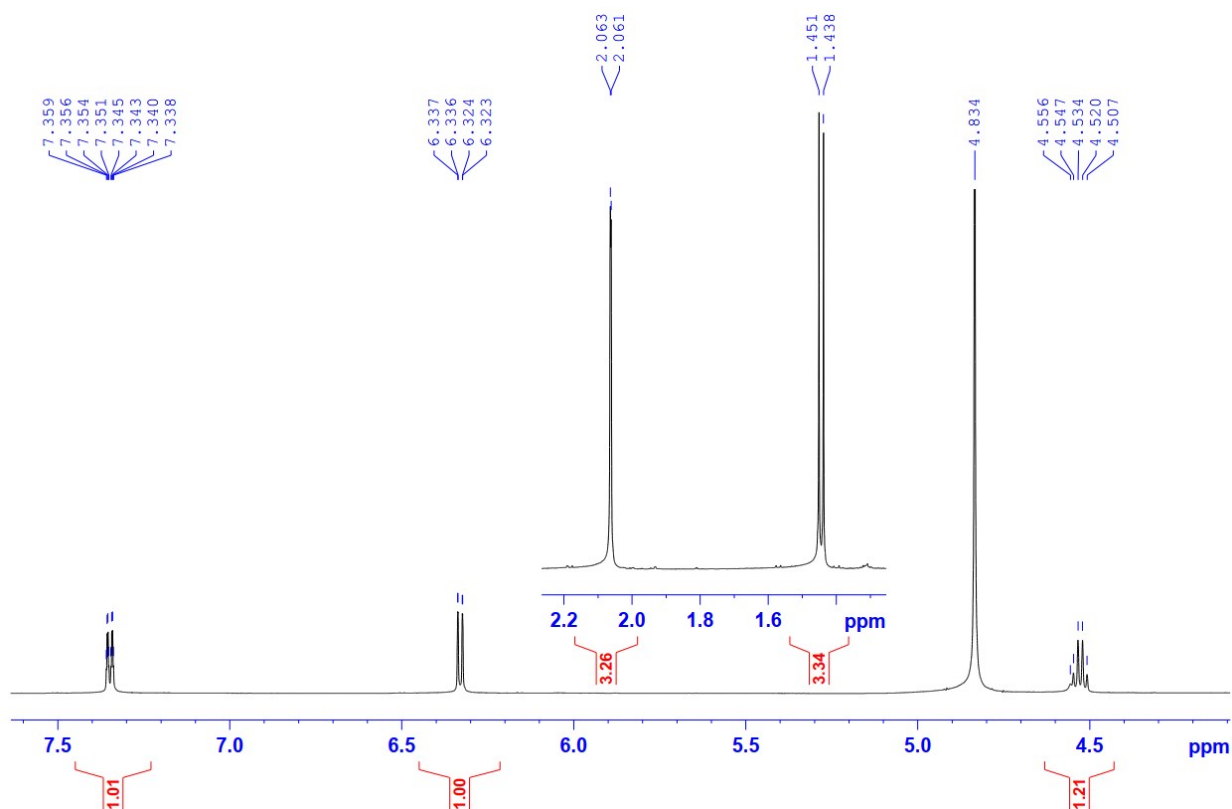


Figure S38. Expanded ^1H -NMR spectrum of compound **4** in CDCl_3

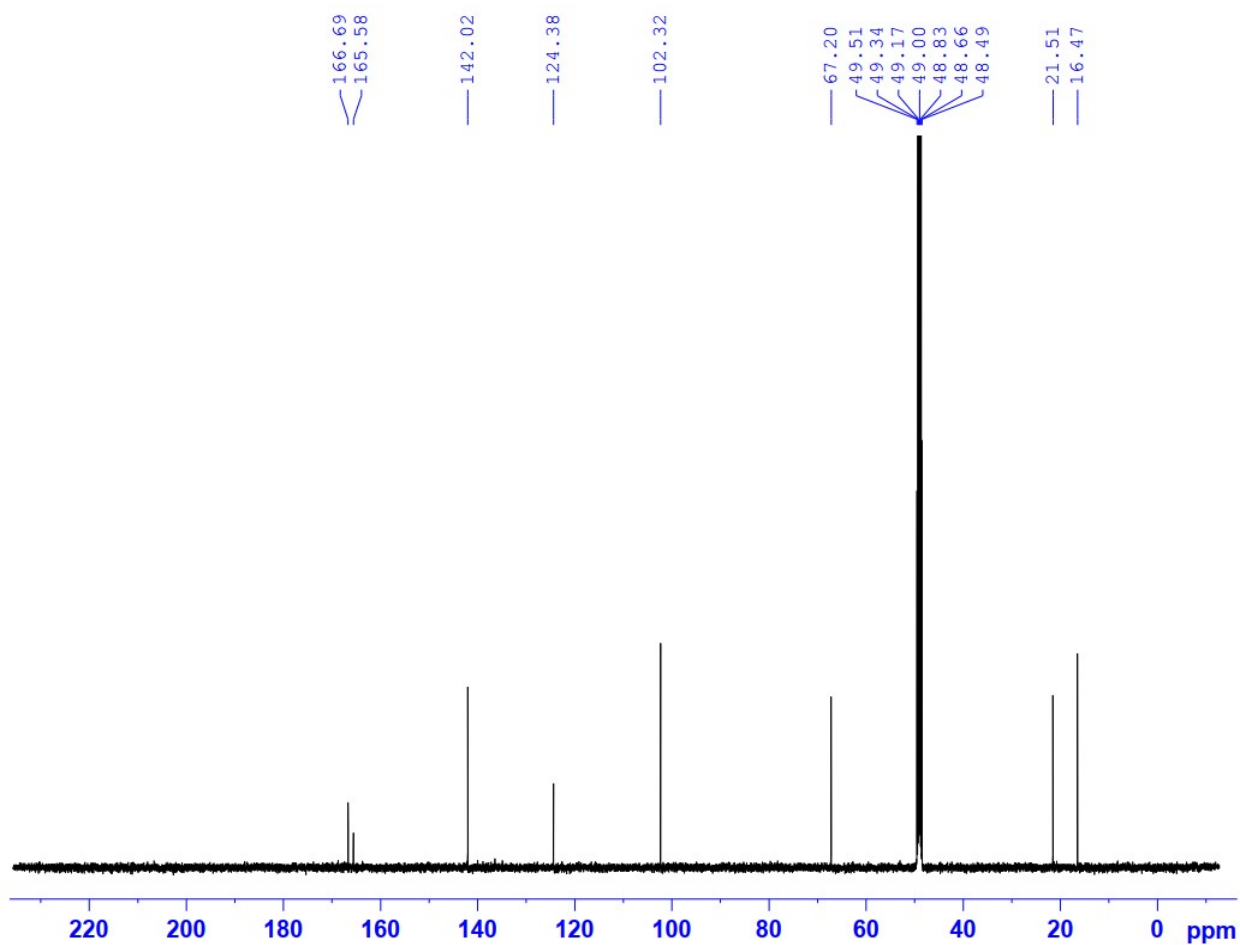


Figure S39. ^{13}C -NMR spectrum of compound **4** in CDCl_3

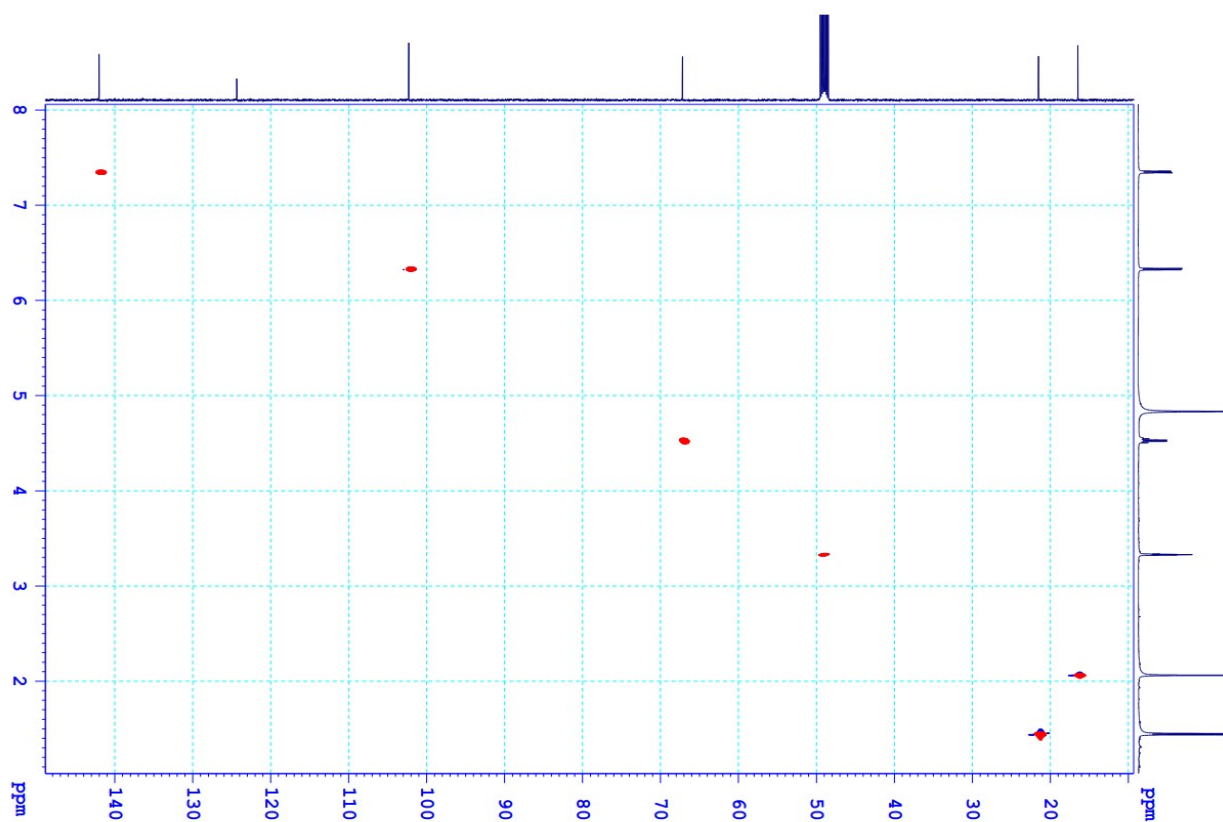


Figure S40. HSQC spectrum of compound 4

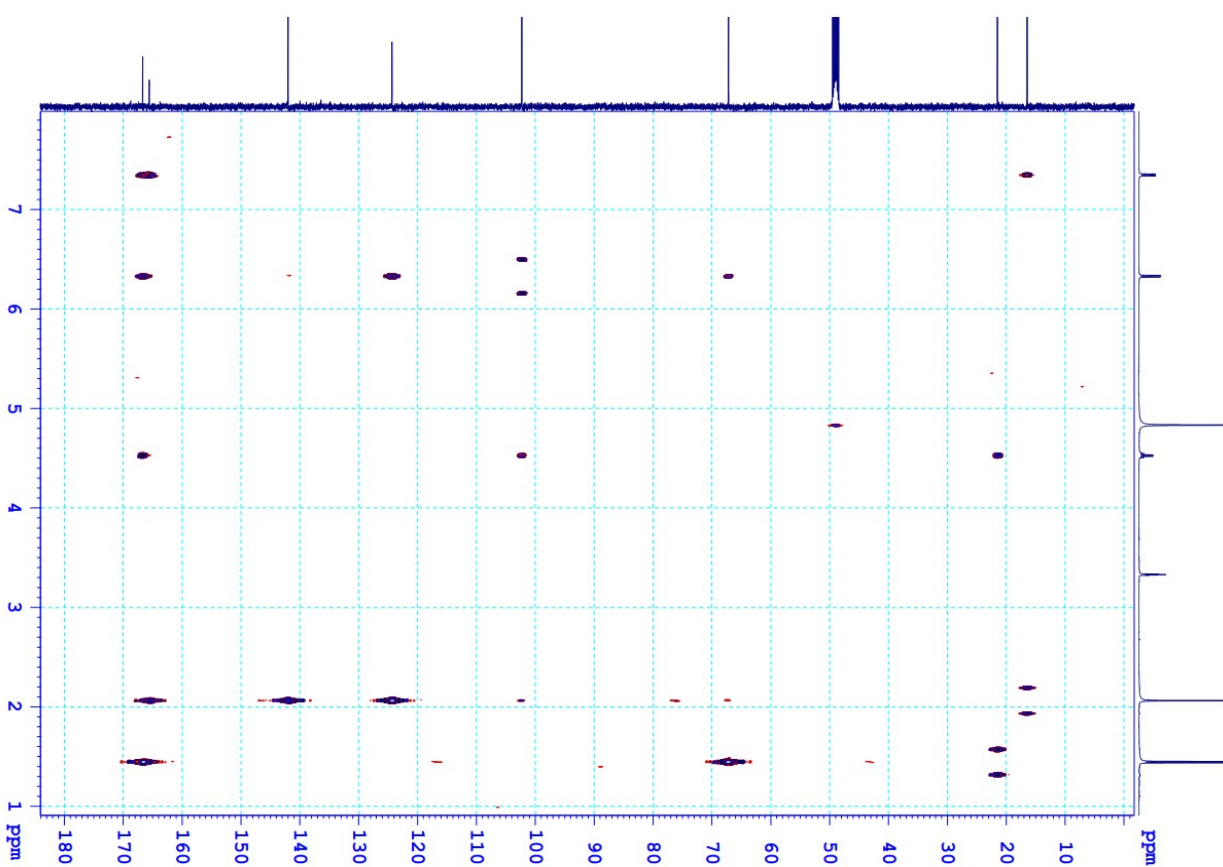


Figure S41. HMBC spectrum of compound 4

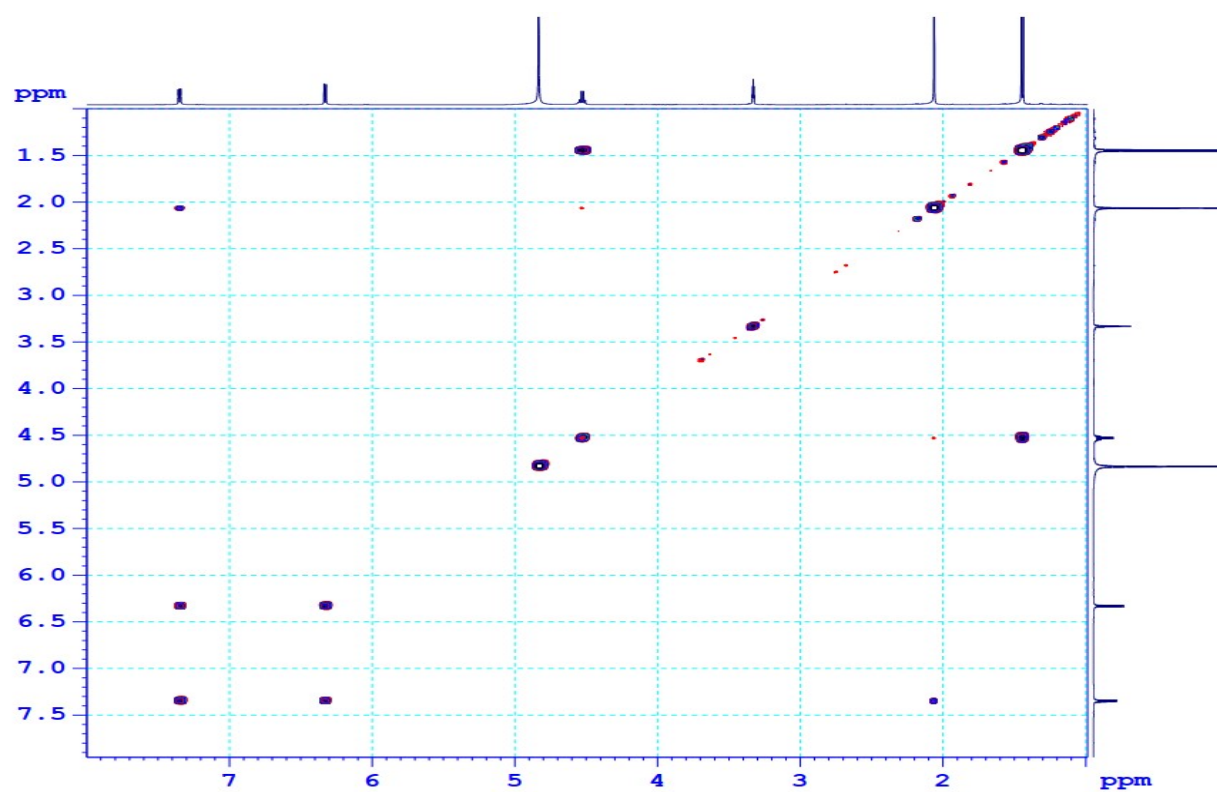


Figure S42. ^1H - ^1H COSY spectrum of compound **4**

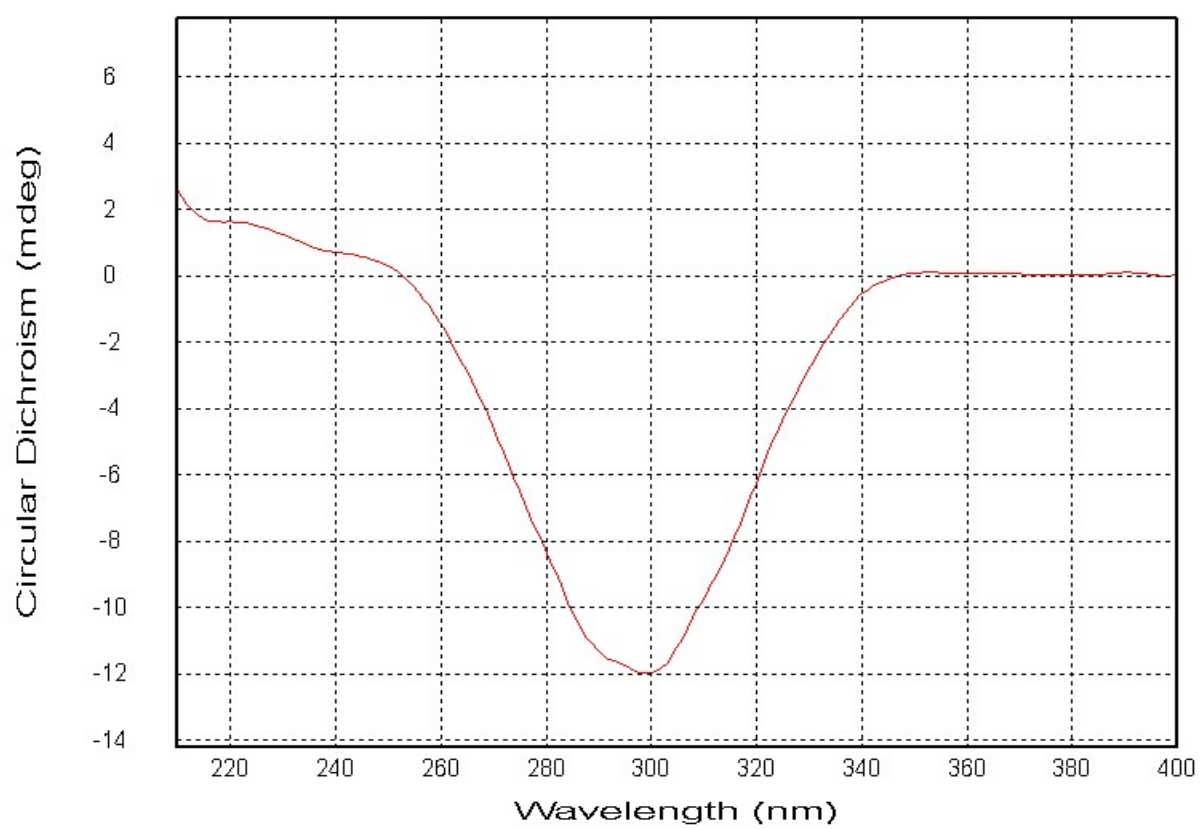


Figure S43. ECD spectrum of compound **4**

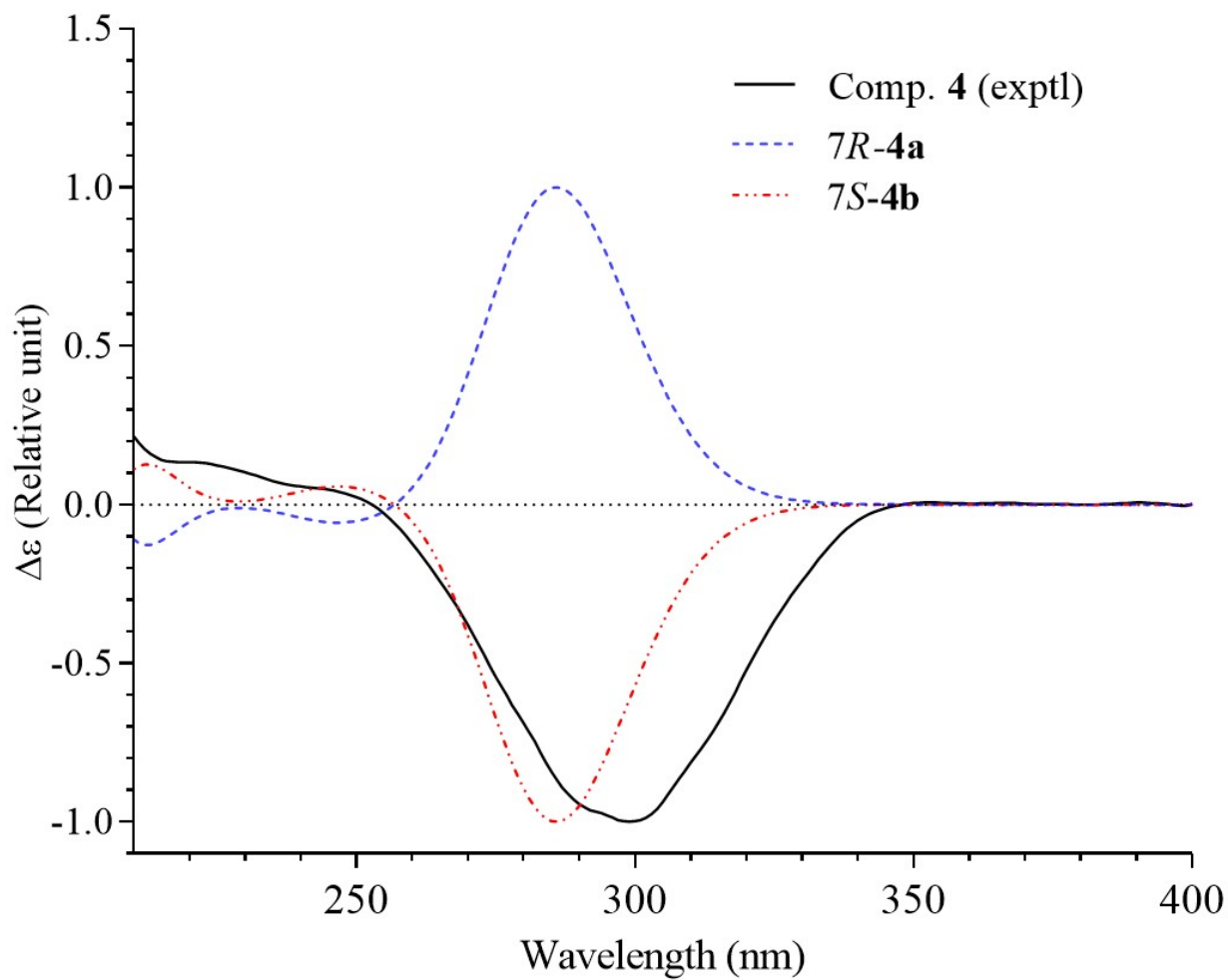


Figure S44. Comparison experimental ECD spectrum of compound **4** and TD-DFT calculation ECD spectra of enantiomers (**4a** and **4b**)