

Supplementary material

Discovery of guanidine derivatives from *Buthus martensii* Karsch with metal-binding and cholinesterase inhibition properties

Yu-Ming Liu ^{1,2,*}, Jing-Jing Fan ¹ and Li-Ning Wang ³

¹ Department of Pharmacy Engineering, Tianjin University of Technology, Tianjin 300384, PR China

² Tianjin Key Laboratory of Drug Targeting and Bioimaging, Tianjin University of Technology, Tianjin 300384, PR China

³ College of Traditional Chinese Medicine, Tianjin University of Traditional Chinese Medicine, Tianjin 300193, PR China

* *Corresponding author*. Department of Pharmacy Engineering, Tianjin University of Technology, Tianjin, 300384, PR China.

E-mail address: coumarin1968@hotmail.com (Y.-M. Liu).

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Figure S1. HR-ESI-MS spectrum of martensine A (1)

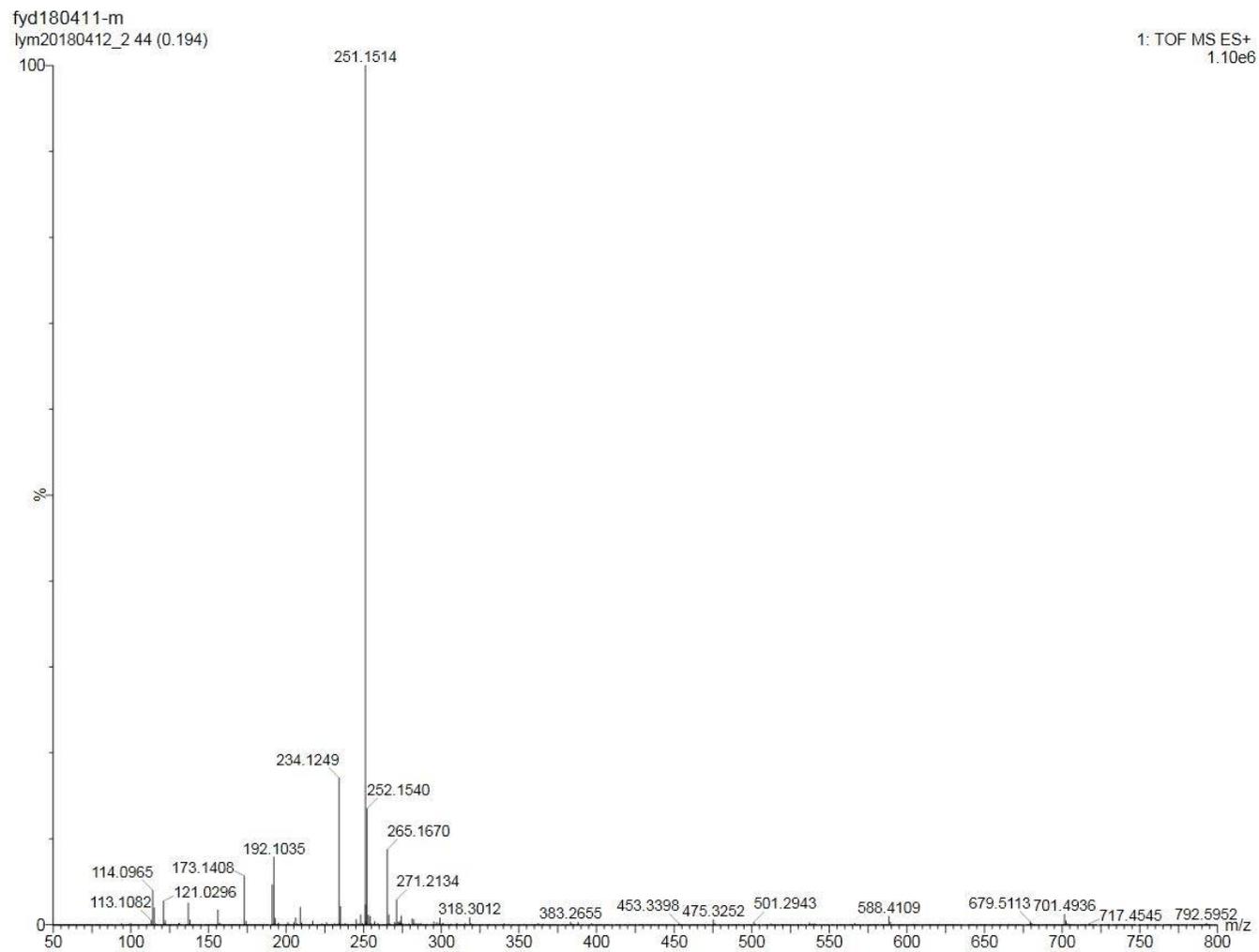


Figure S2. HR-ESI-MS⁺² spectrum ($M' = 251.1514 [M+H]^+$) of martensine A (1)

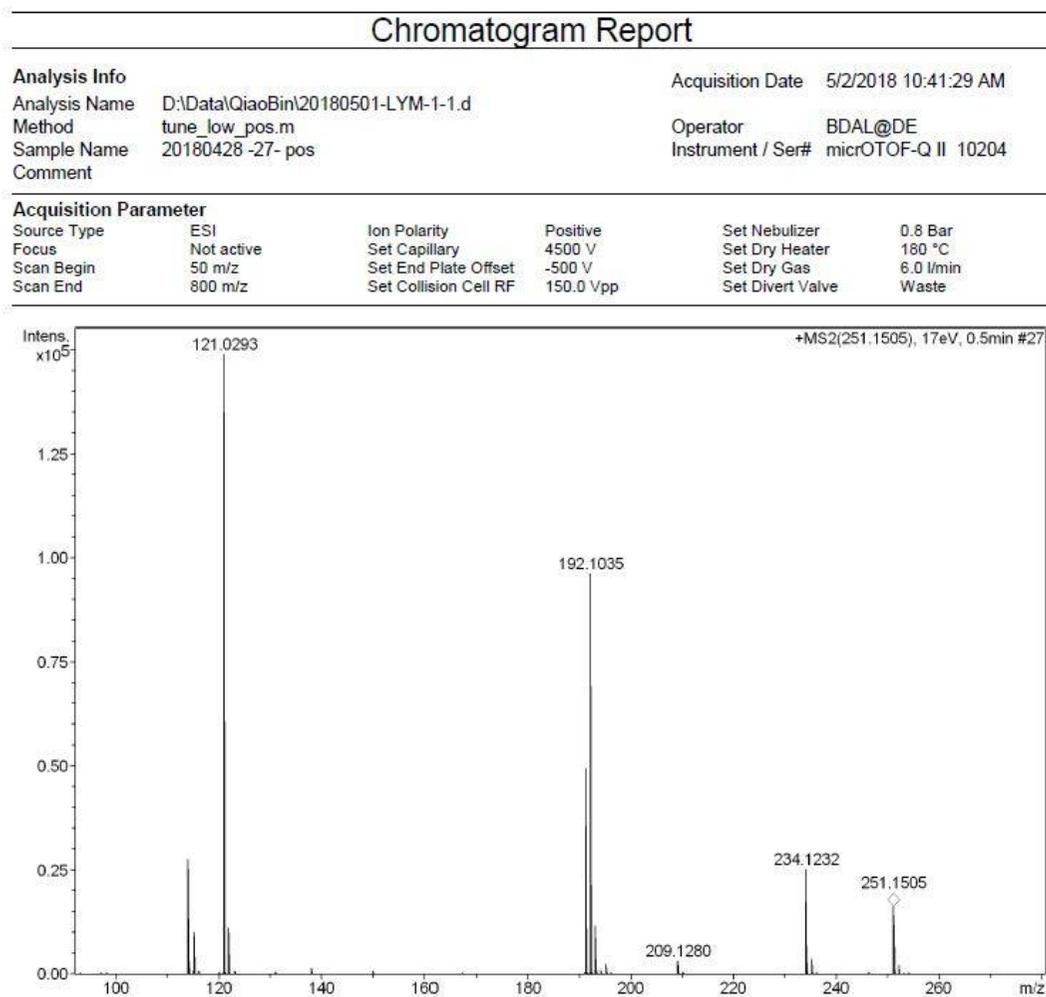


Figure S3. ¹H NMR spectrum (CD₃OD) of martensine A (1)

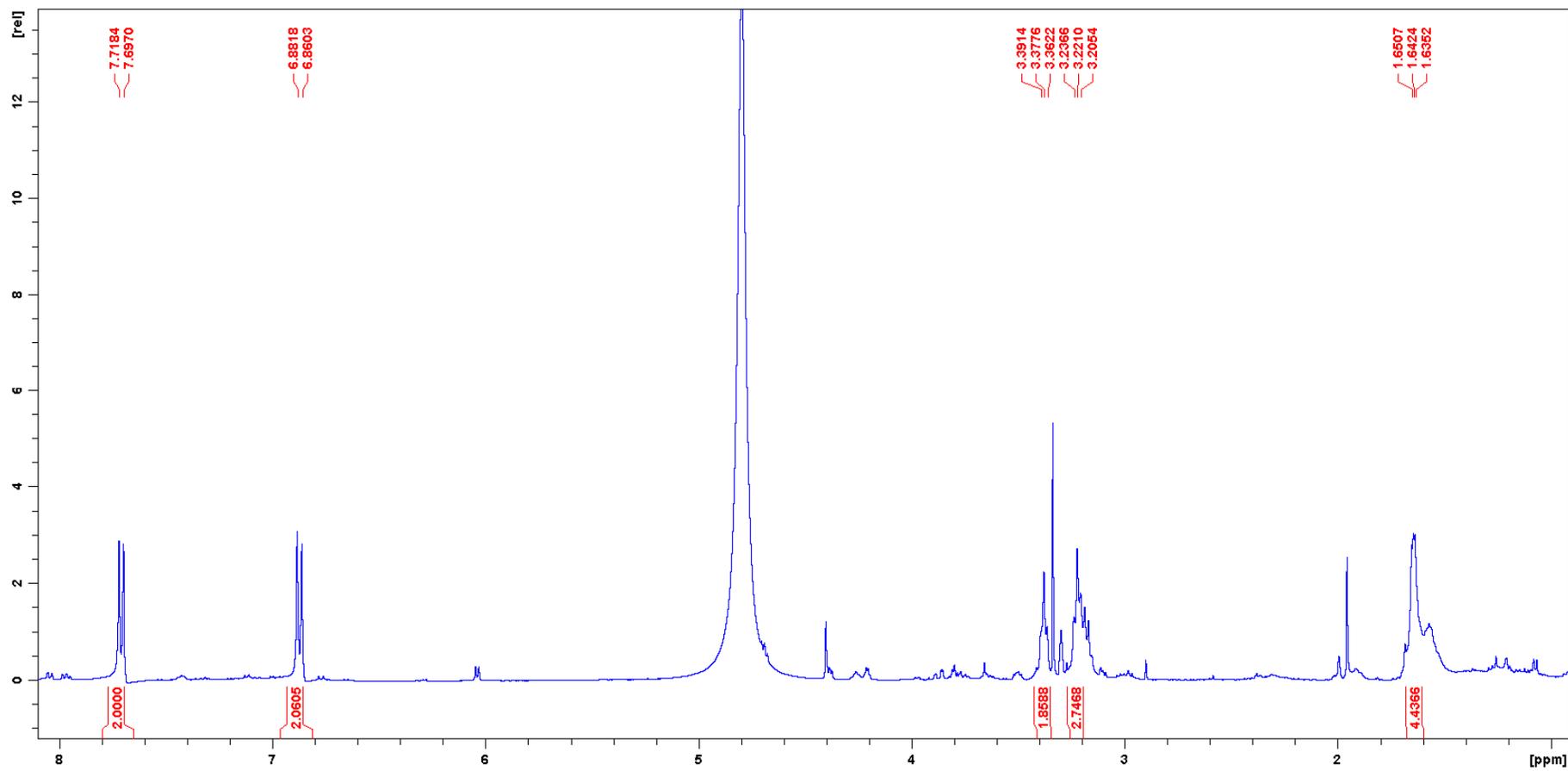


Figure S4. ^{13}C NMR spectrum (CD_3OD) of martensine A (**1**)

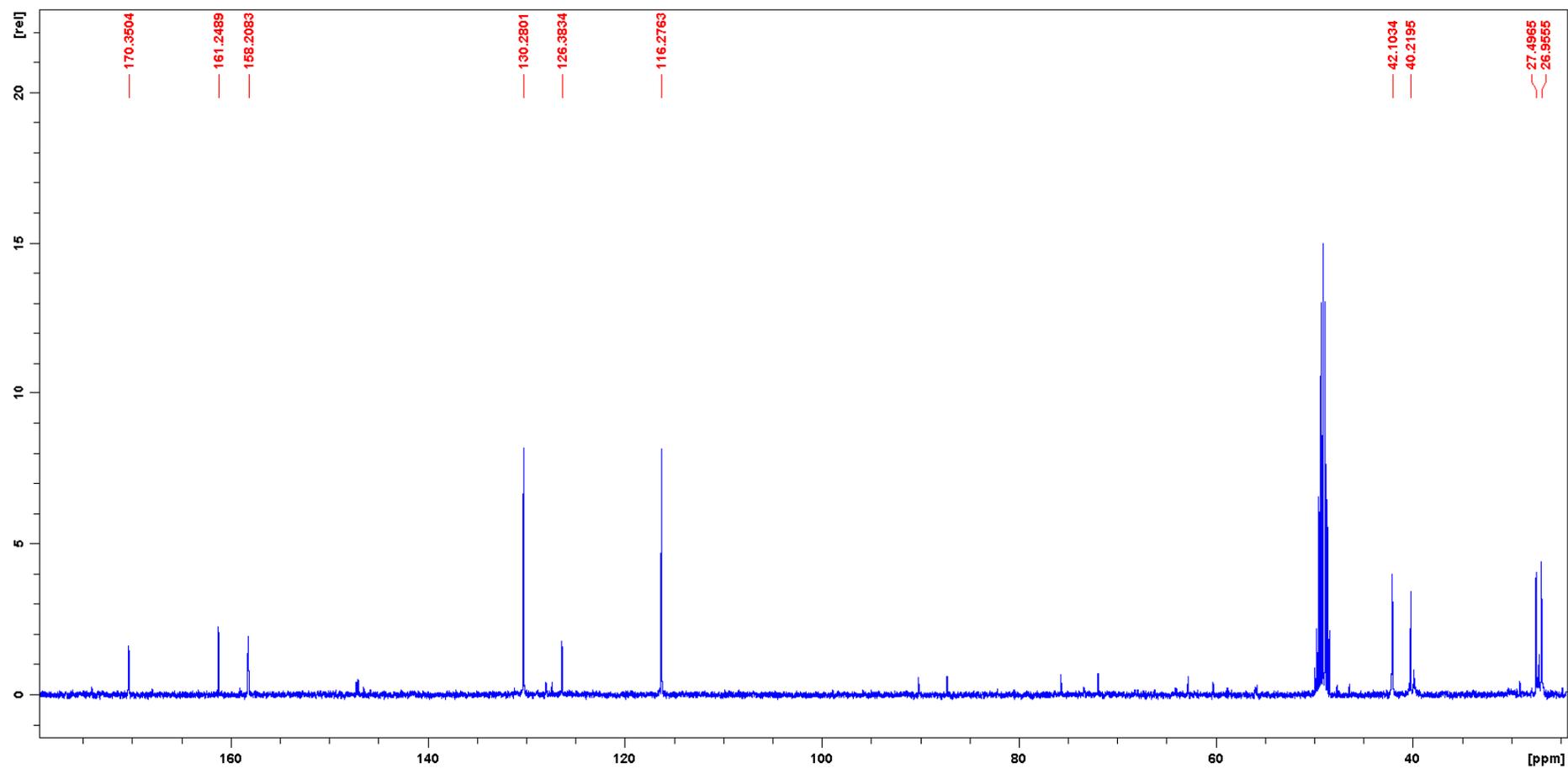


Figure S5. DEPT 135 spectrum of martensine A (1)

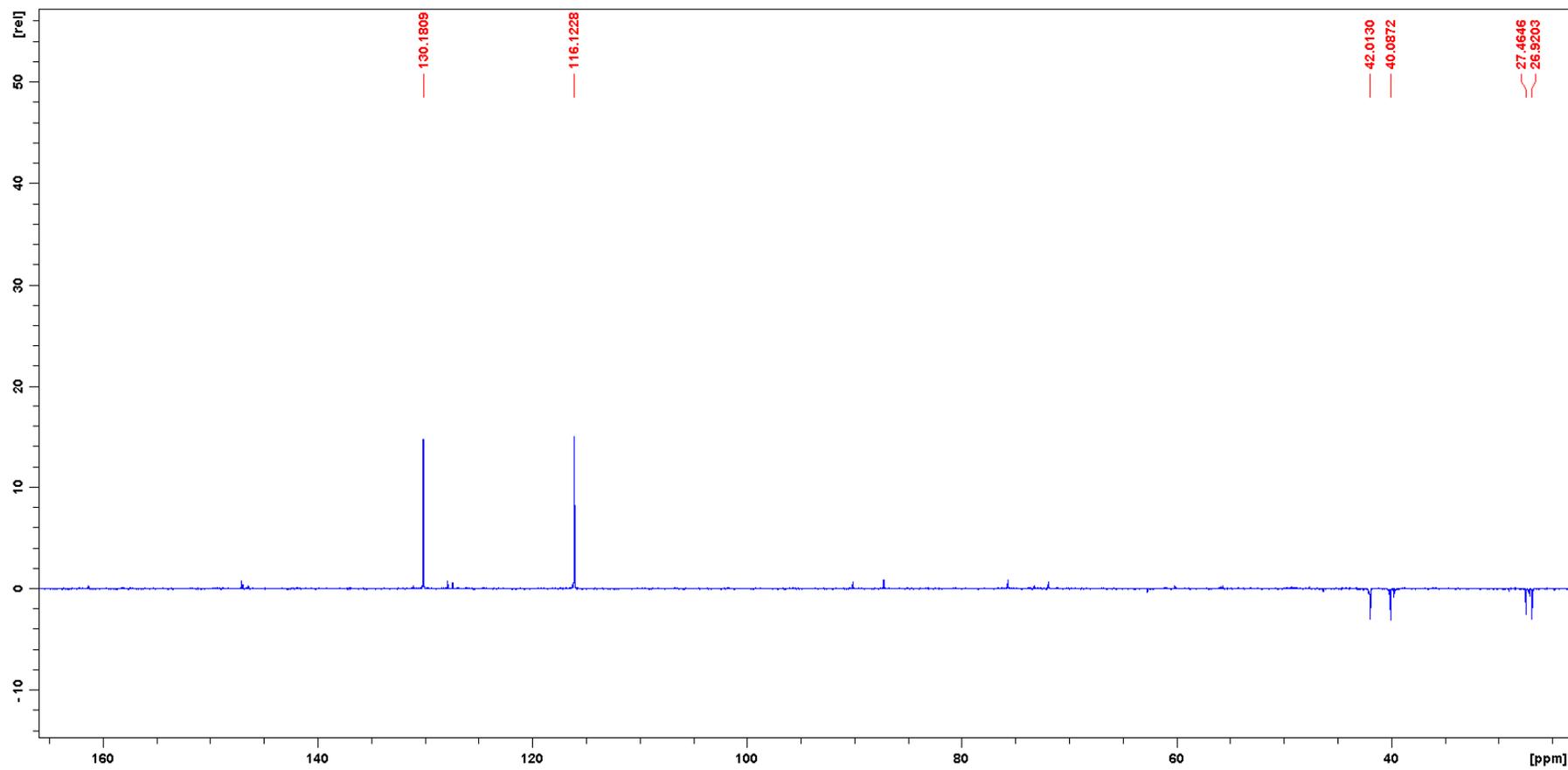


Figure S6. ^1H - ^1H COSY spectrum of martensine A (1)

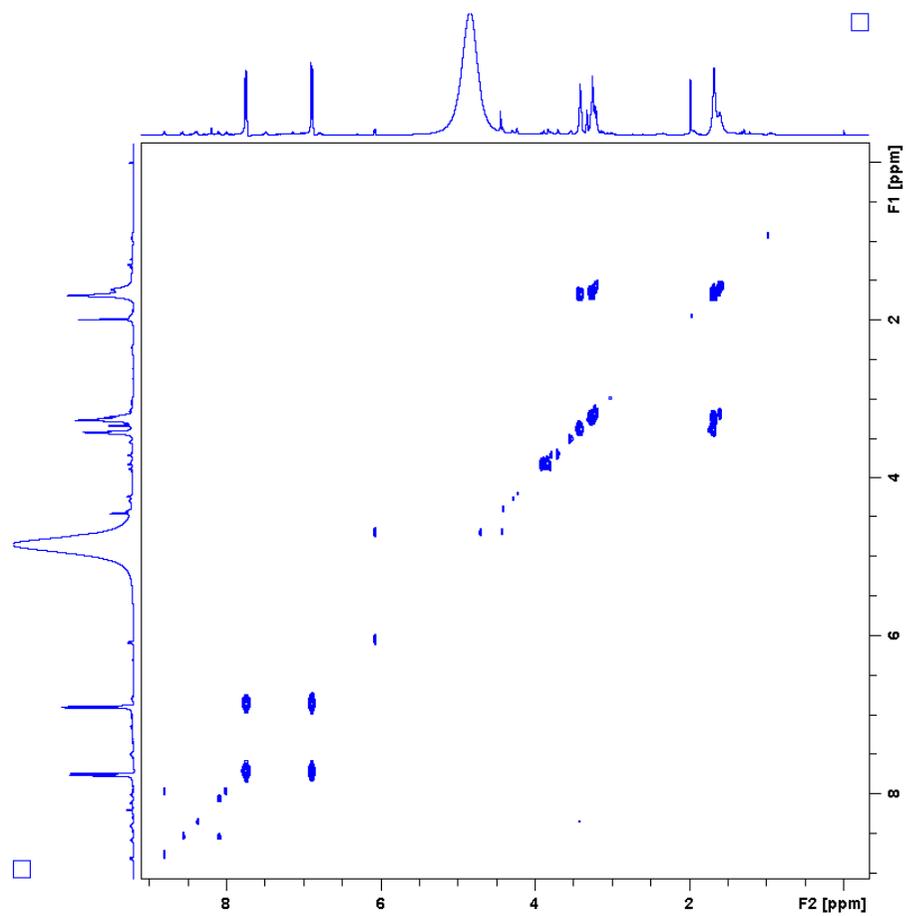


Figure S7. HSQC spectrum of martensine A (1)

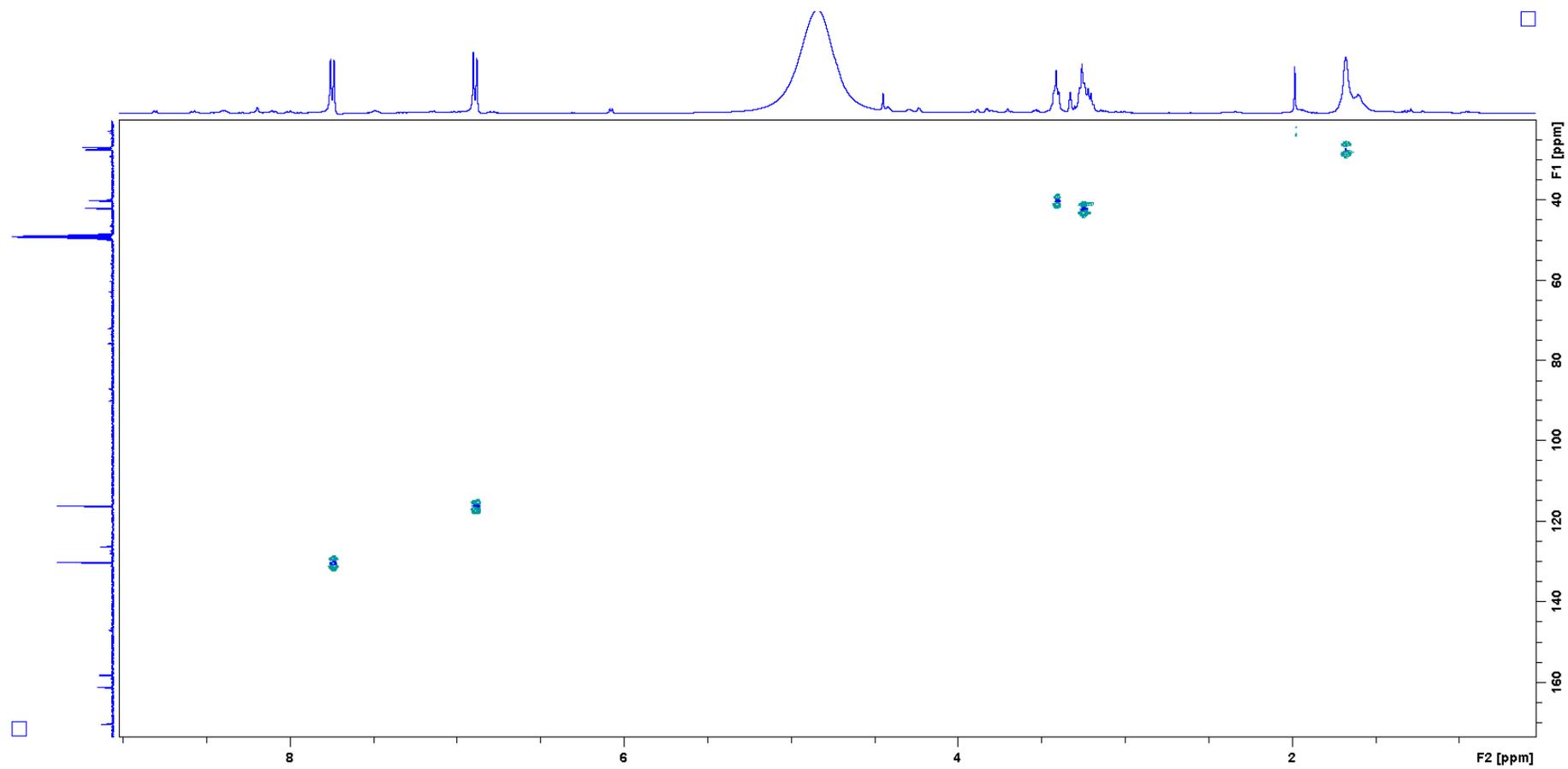


Figure S8. HMBC spectrum of martensine A (1)

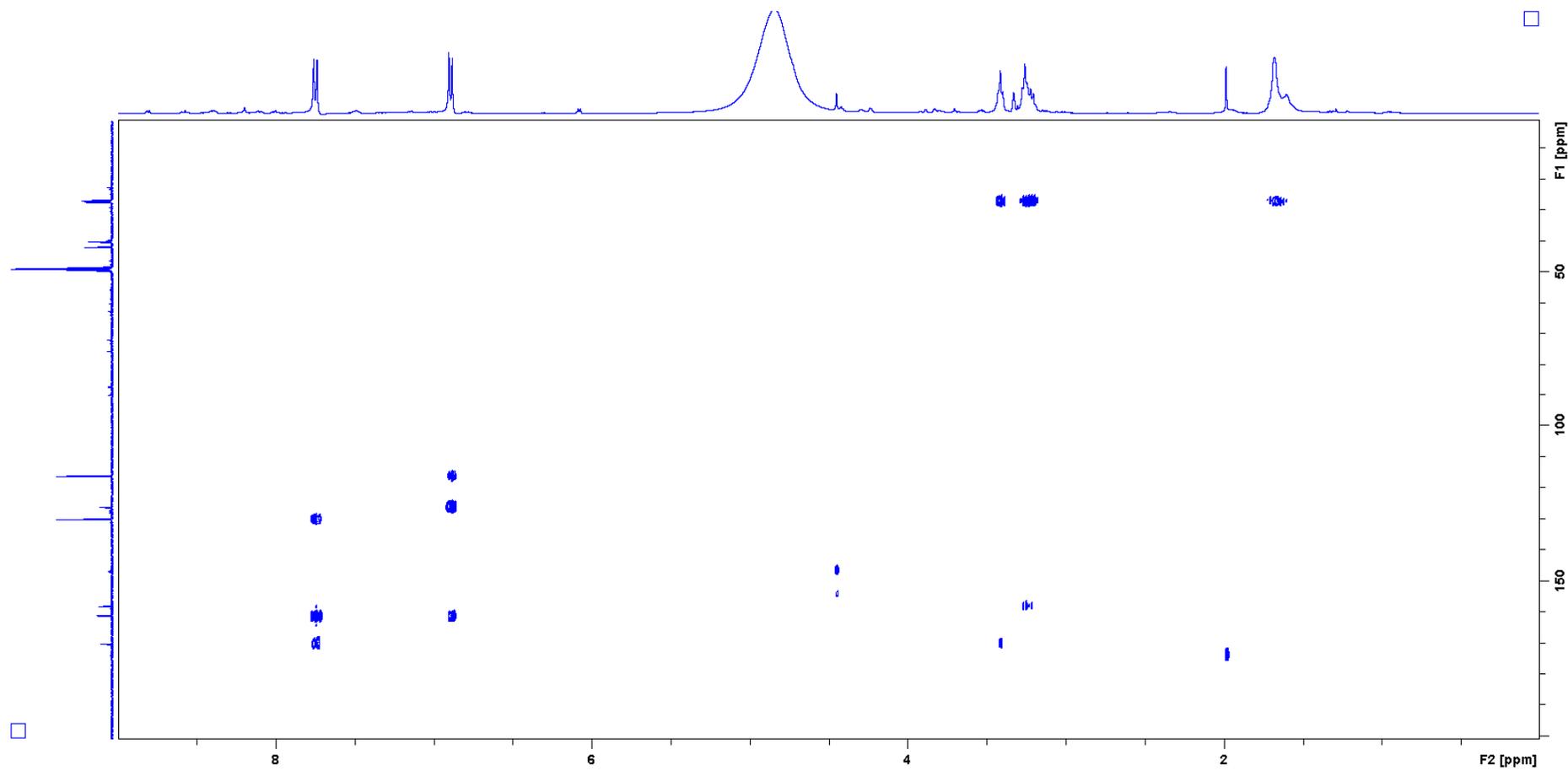


Figure S9. NOESY spectrum of martensine A (1)

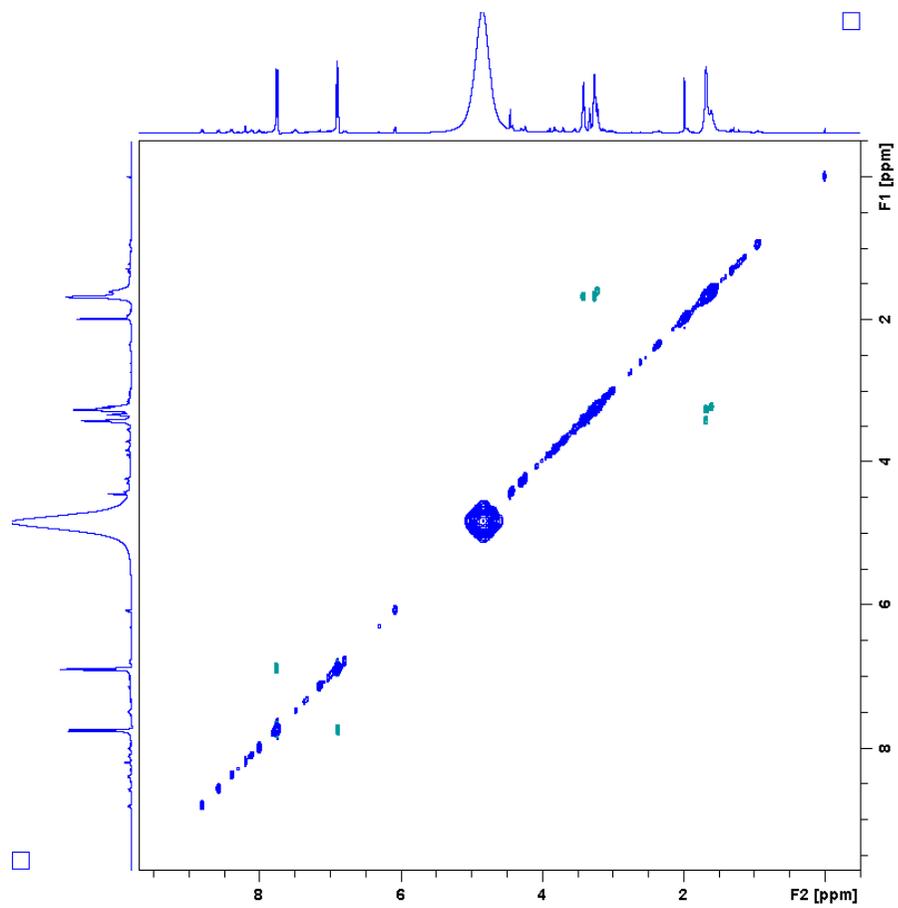


Figure S10. HR-ESI-MS spectrum of martensine B (2)

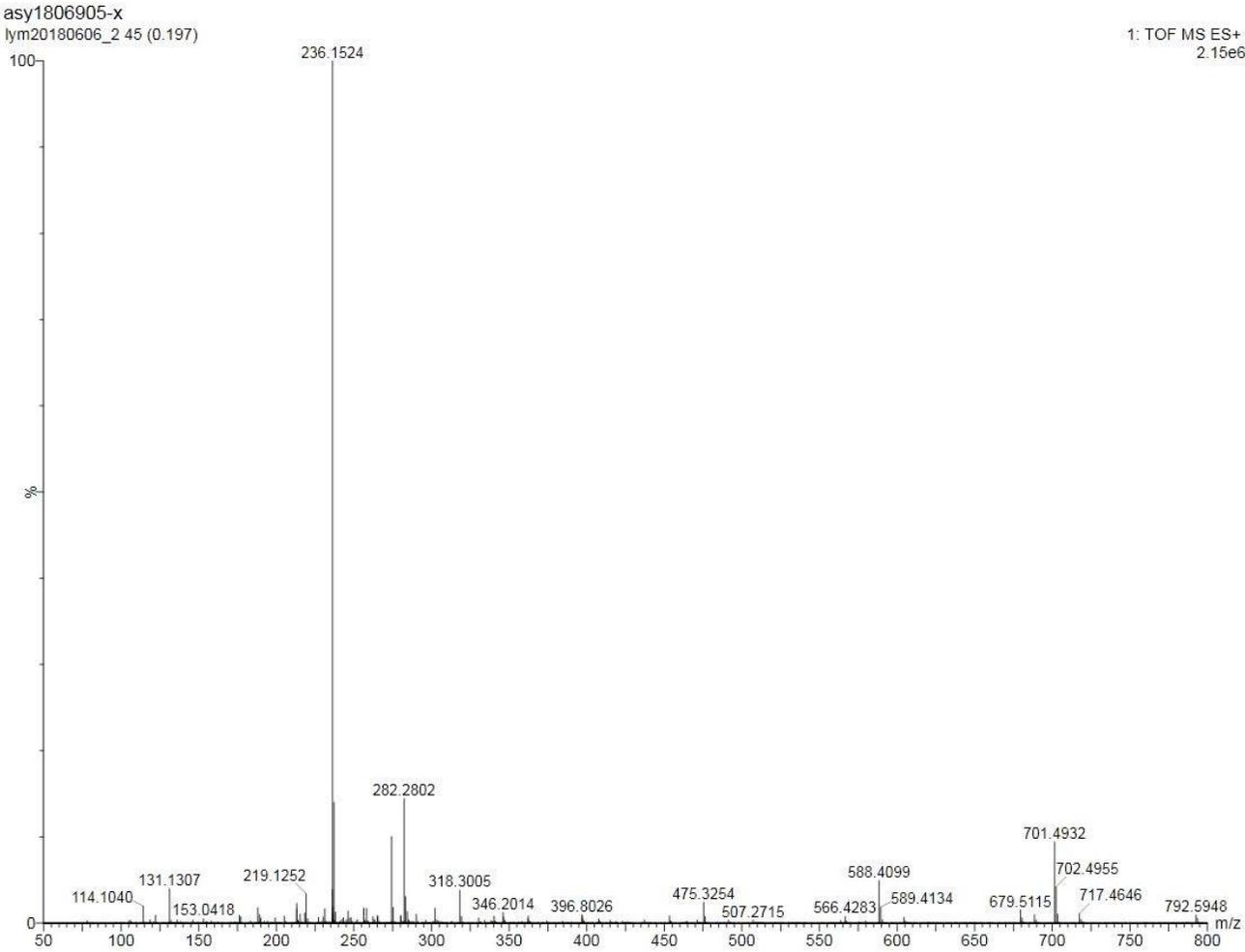


Figure S11. ¹H NMR spectrum (CD₃OD) of martensine B (2)

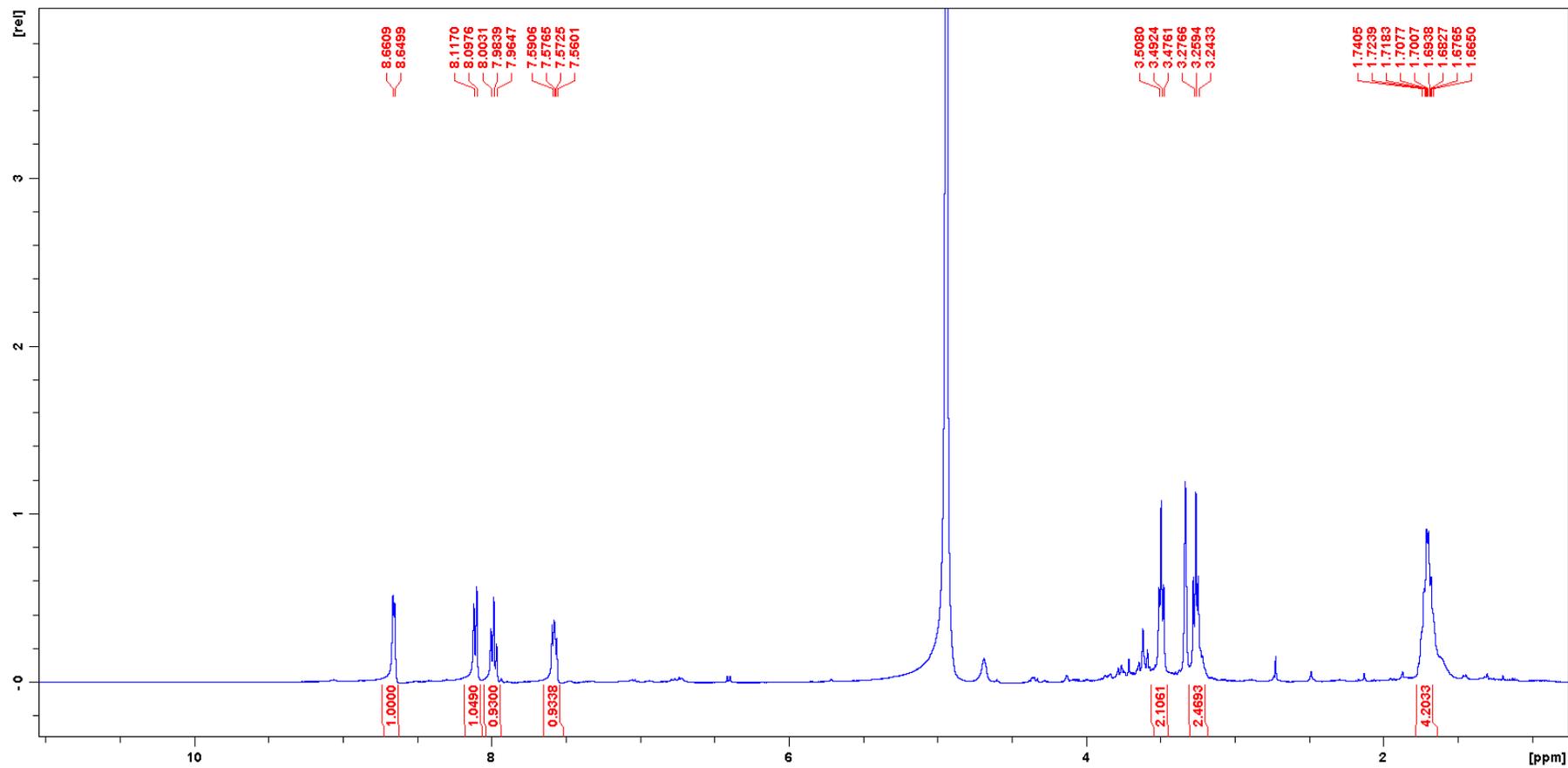


Figure S12. ^{13}C NMR spectrum (CD_3OD) of martensine B (**2**)

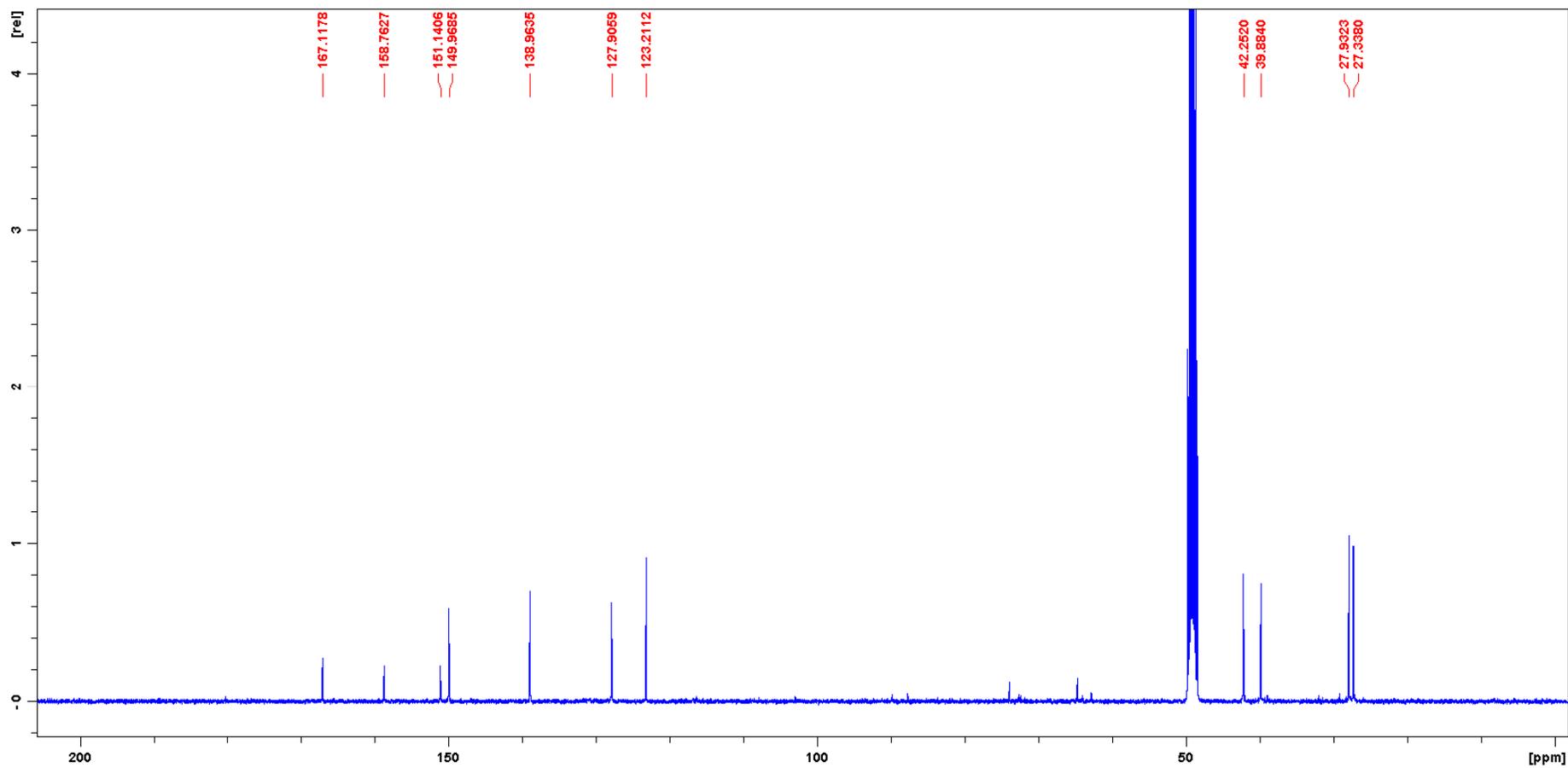


Figure S13. DEPT 135 spectrum of martensine B (2)

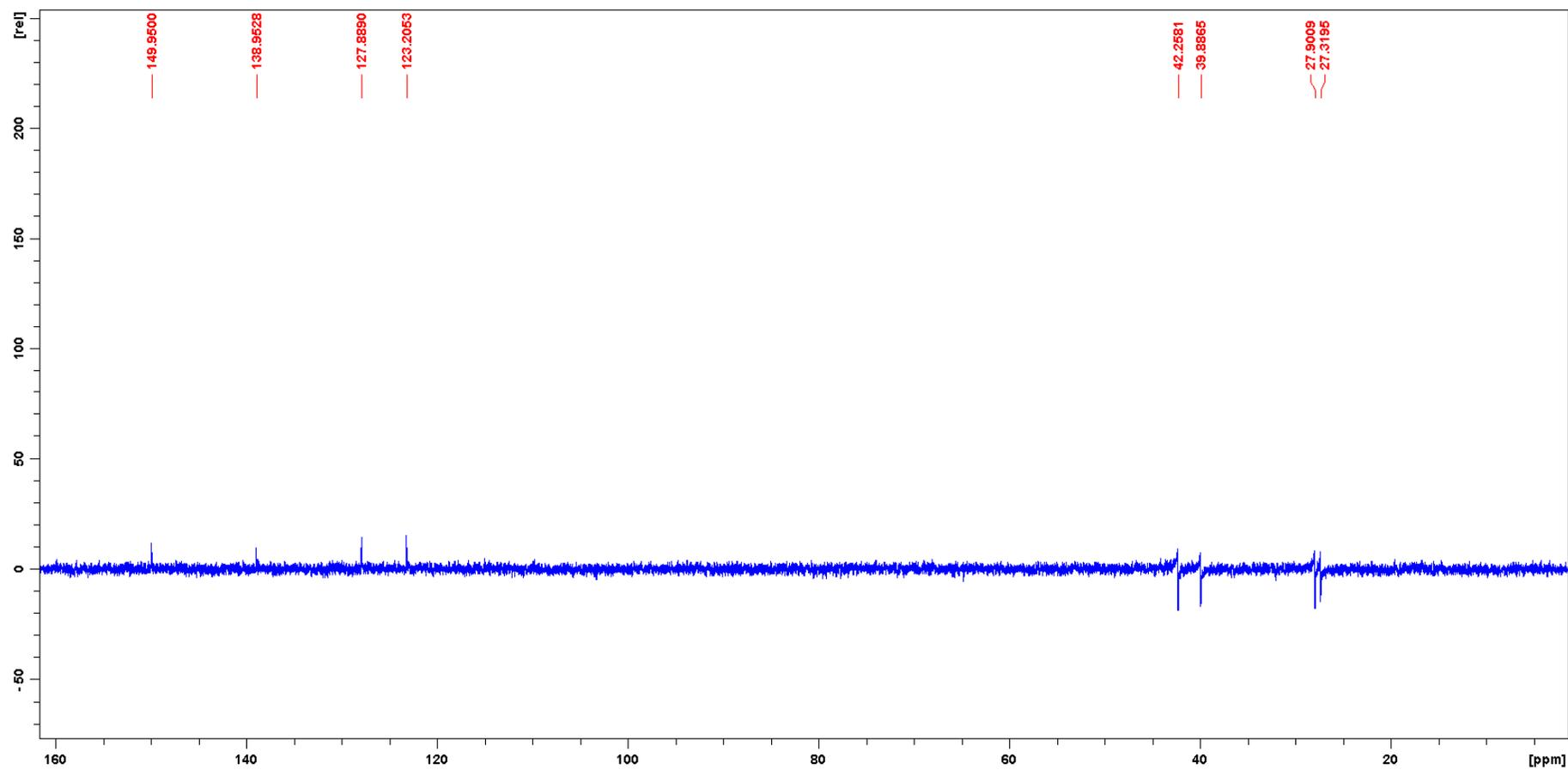


Figure S14. ^1H - ^1H COSY spectrum of martensine B (2)

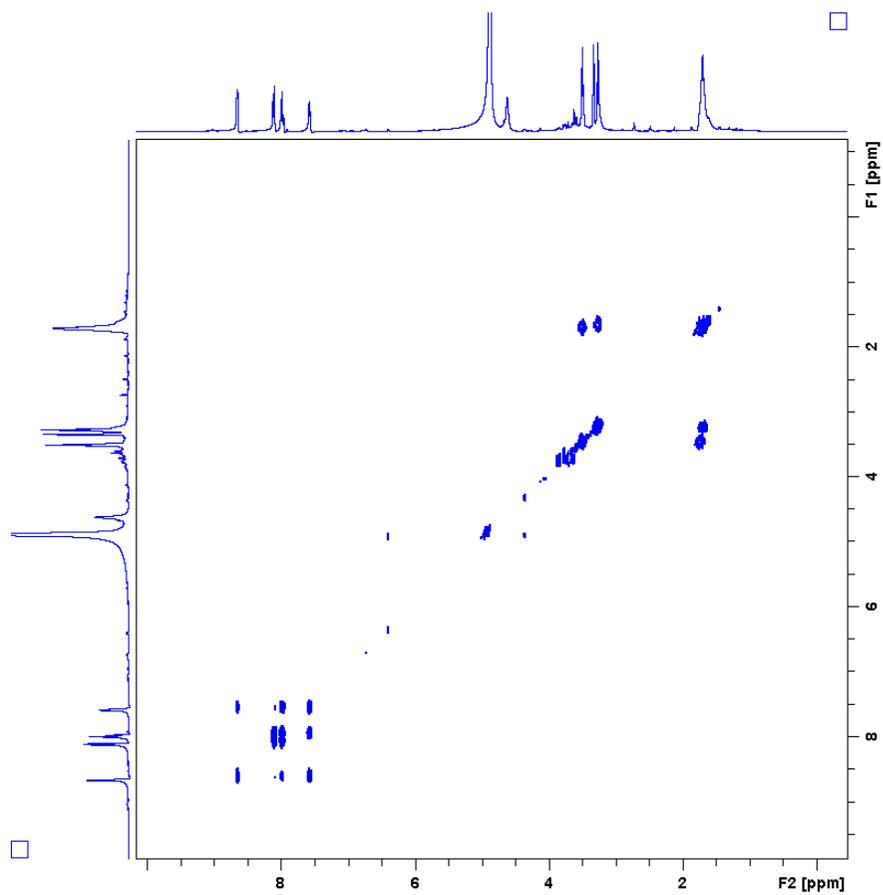


Figure S15. HSQC spectrum of martensine B (2)

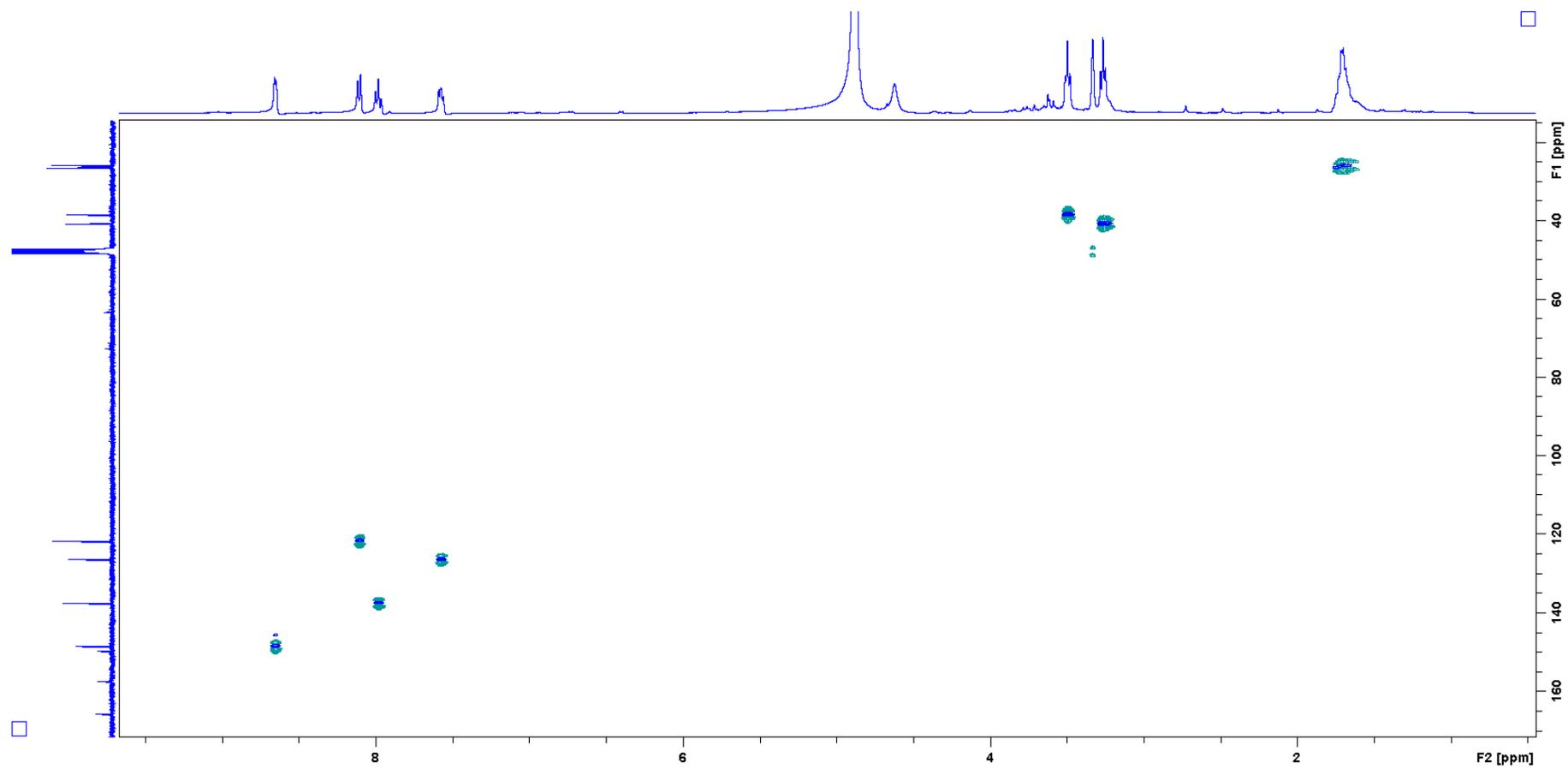


Figure S16. HMBC spectrum of martensine B (2)

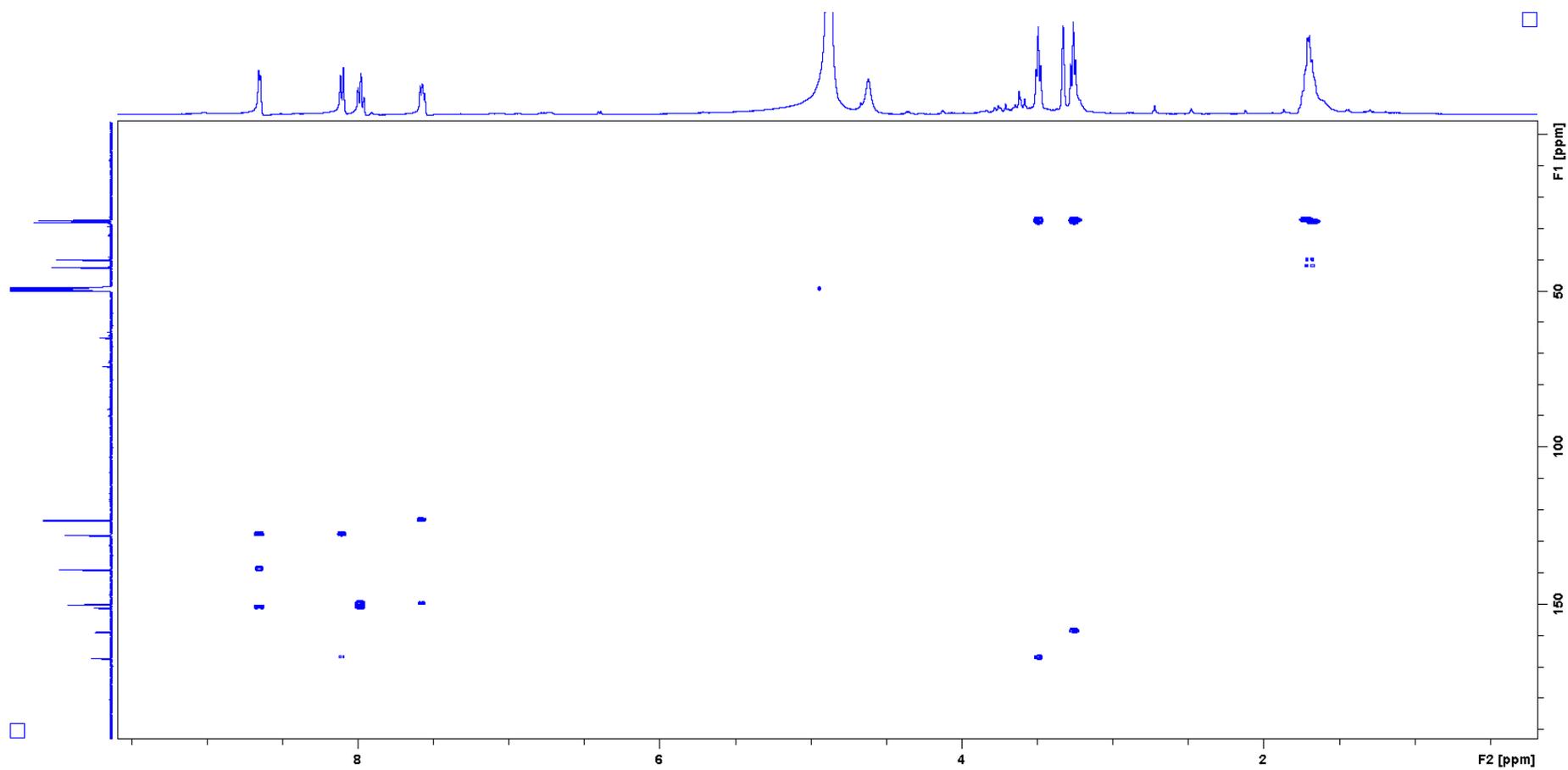


Figure S17. NOESY spectrum of martensine B (2)

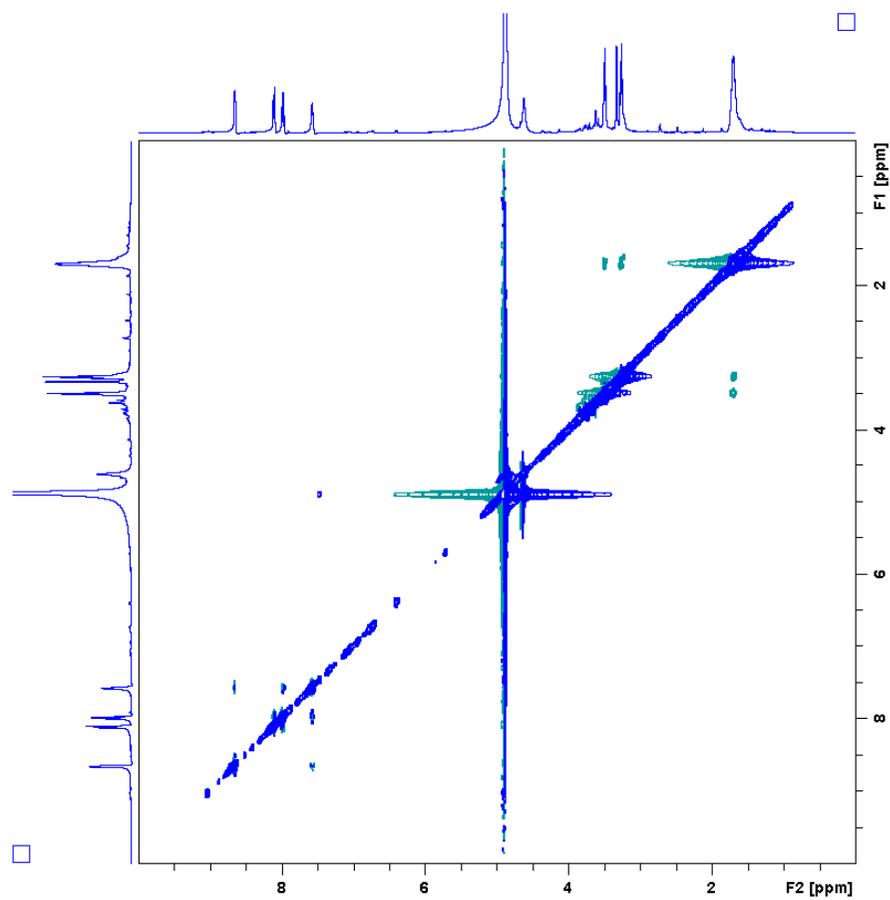


Figure S18. HR-ESI-MS spectrum of trigonelline (**3**)

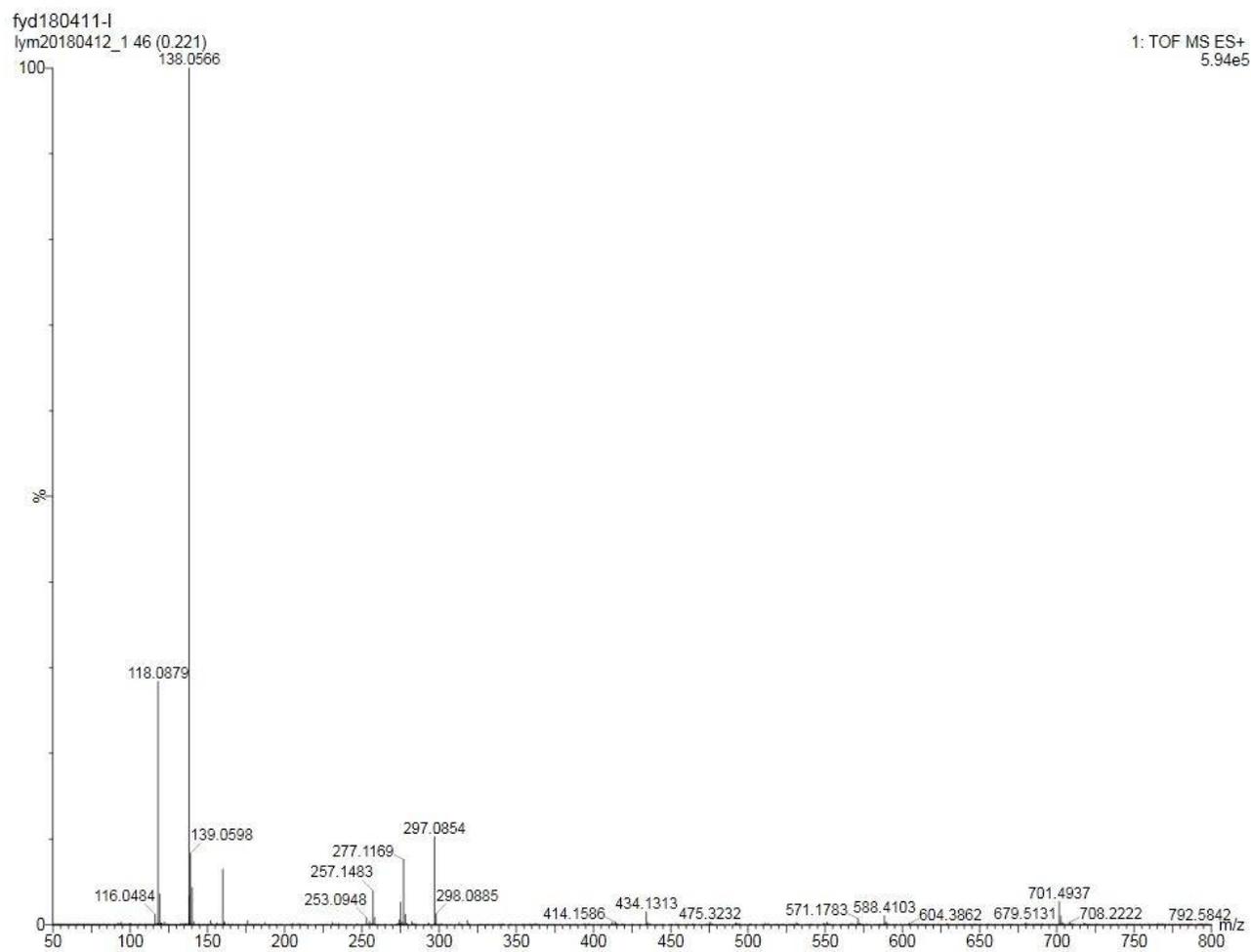


Figure S19. ¹H NMR spectrum (CD₃OD) of trigonelline (3)

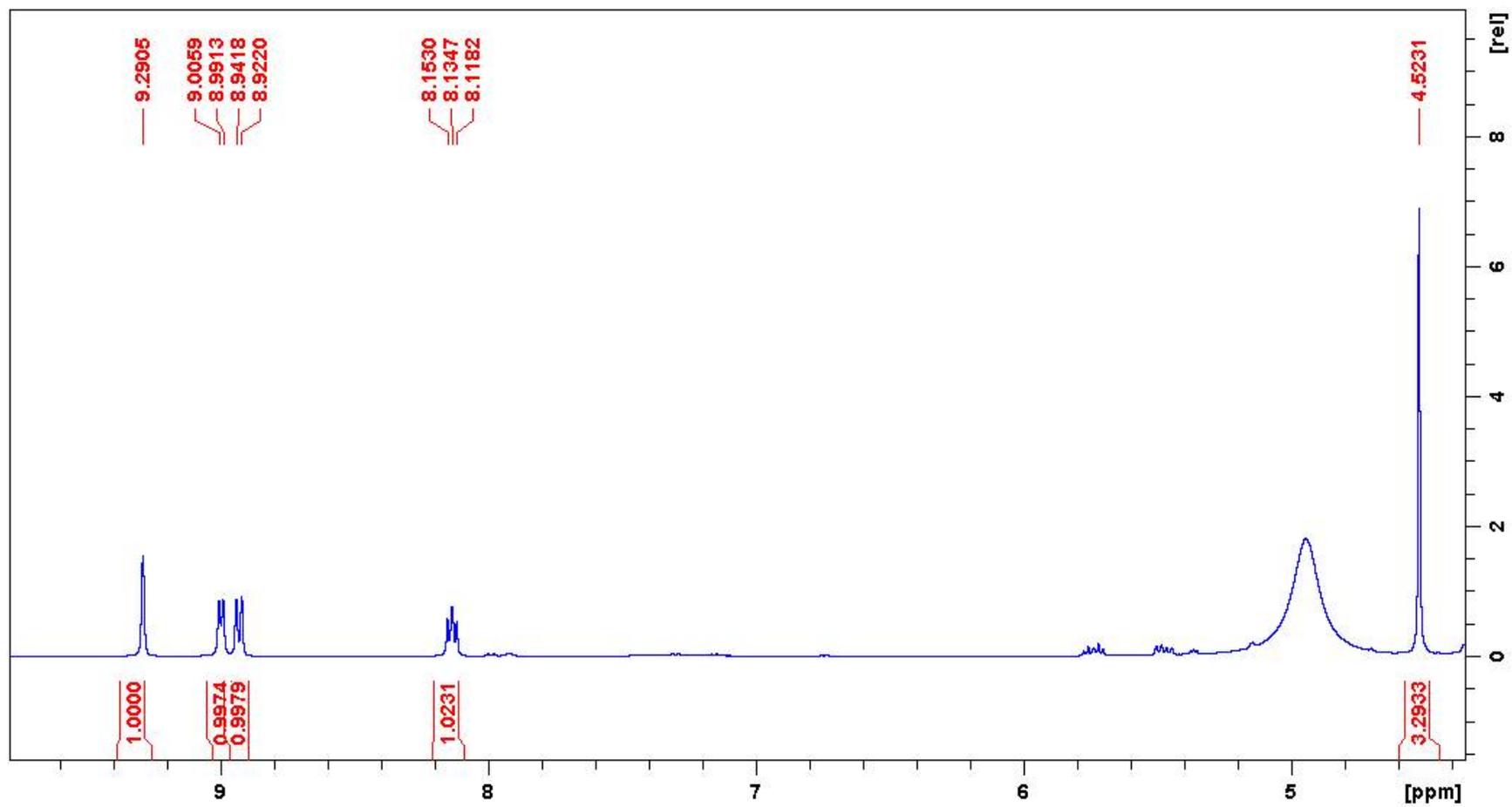


Figure S20. ^{13}C NMR spectrum (CD_3OD) of trigonelline (**3**)

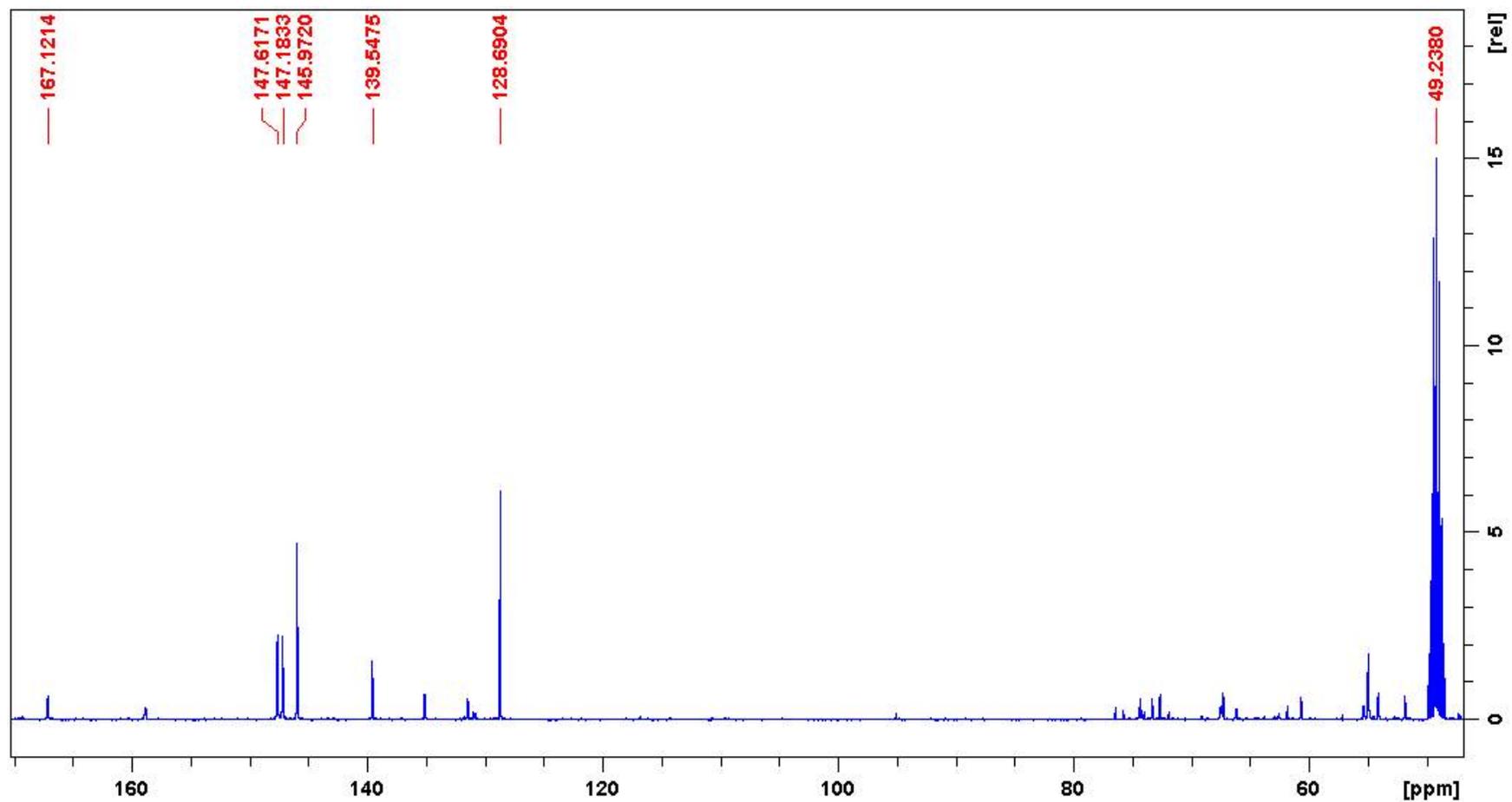


Figure S21. ^1H - ^1H COSY spectrum of trigonelline (3)

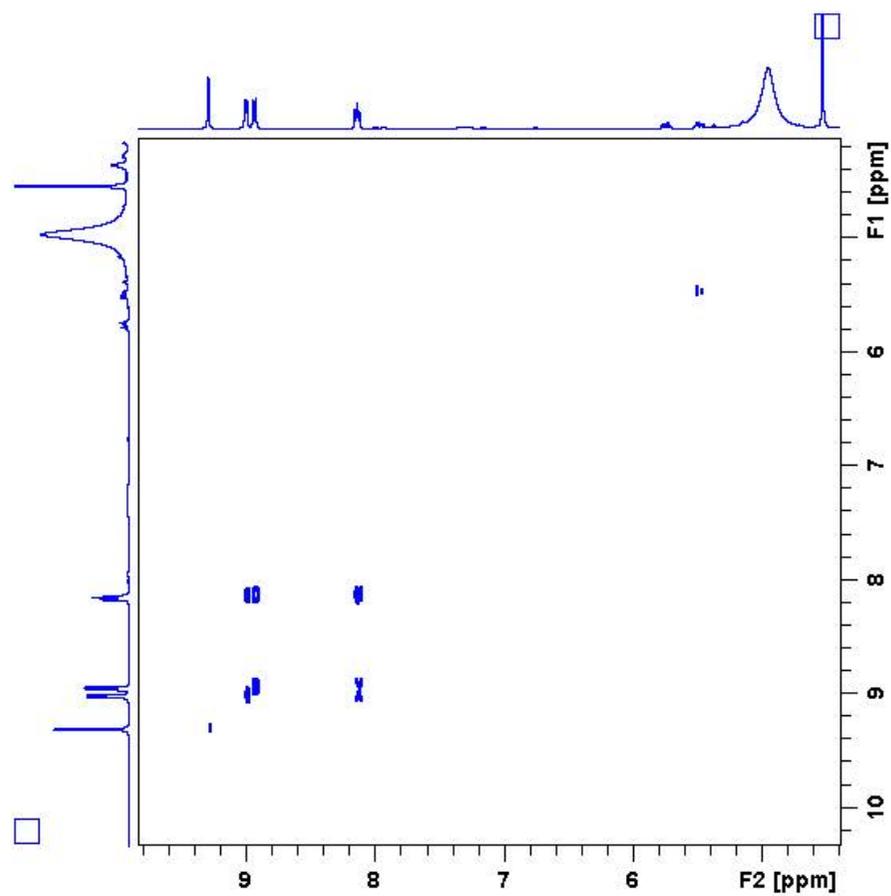


Figure S22. HSQC spectrum of trigonelline (3)

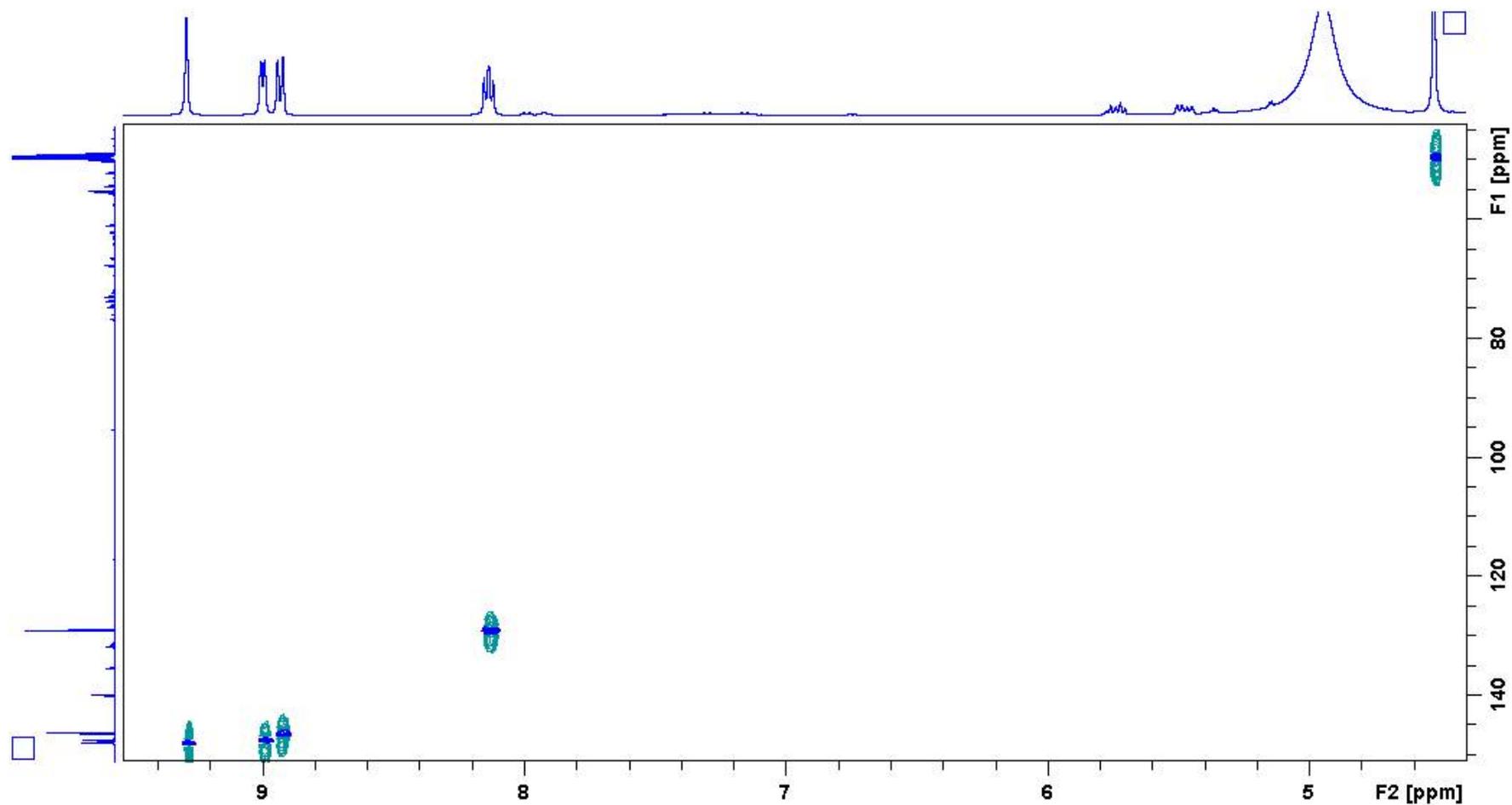


Figure S23. HMBC spectrum of trigonelline (3)

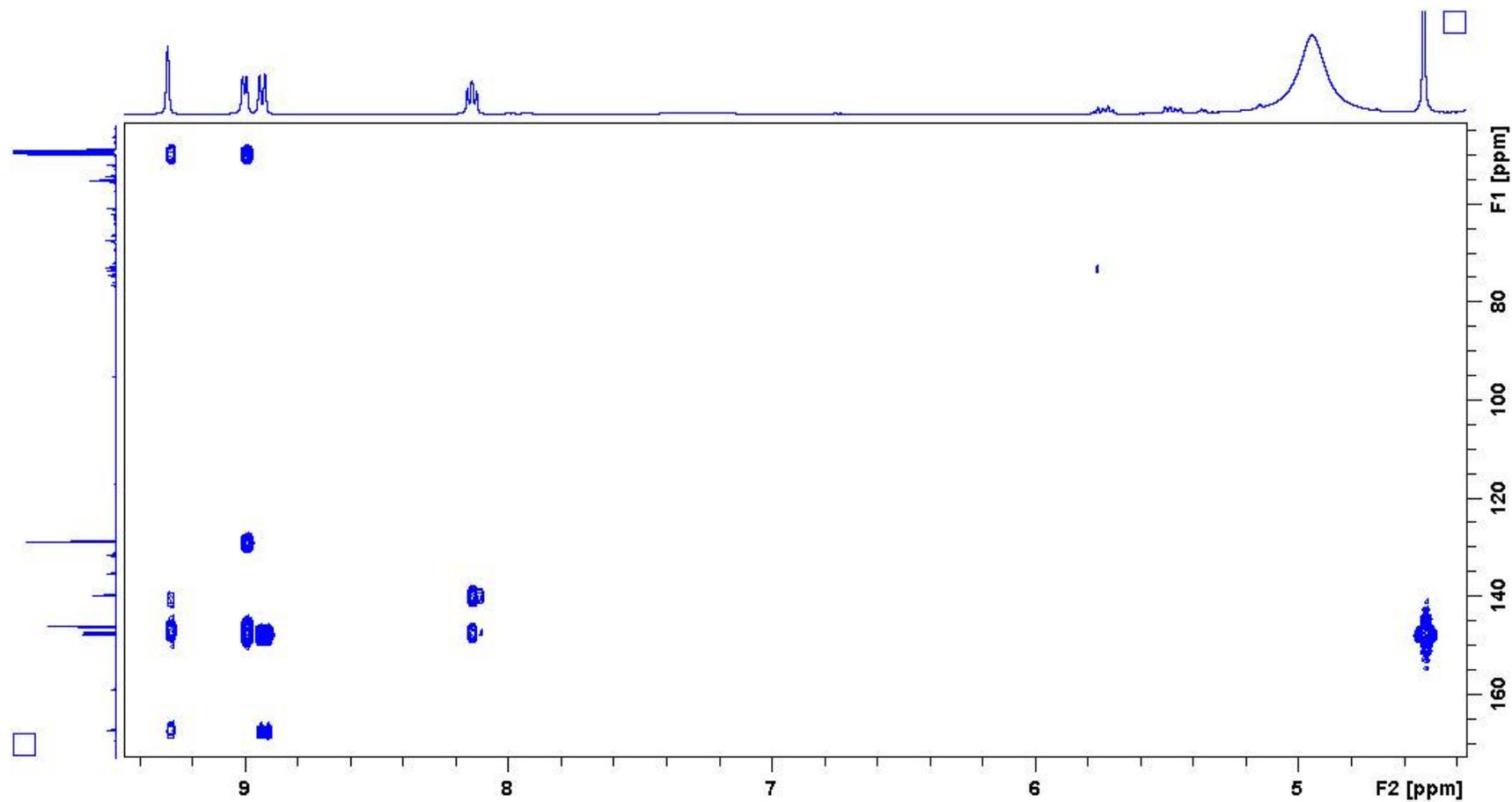


Figure S24. NOESY spectrum of trigonelline (**3**)

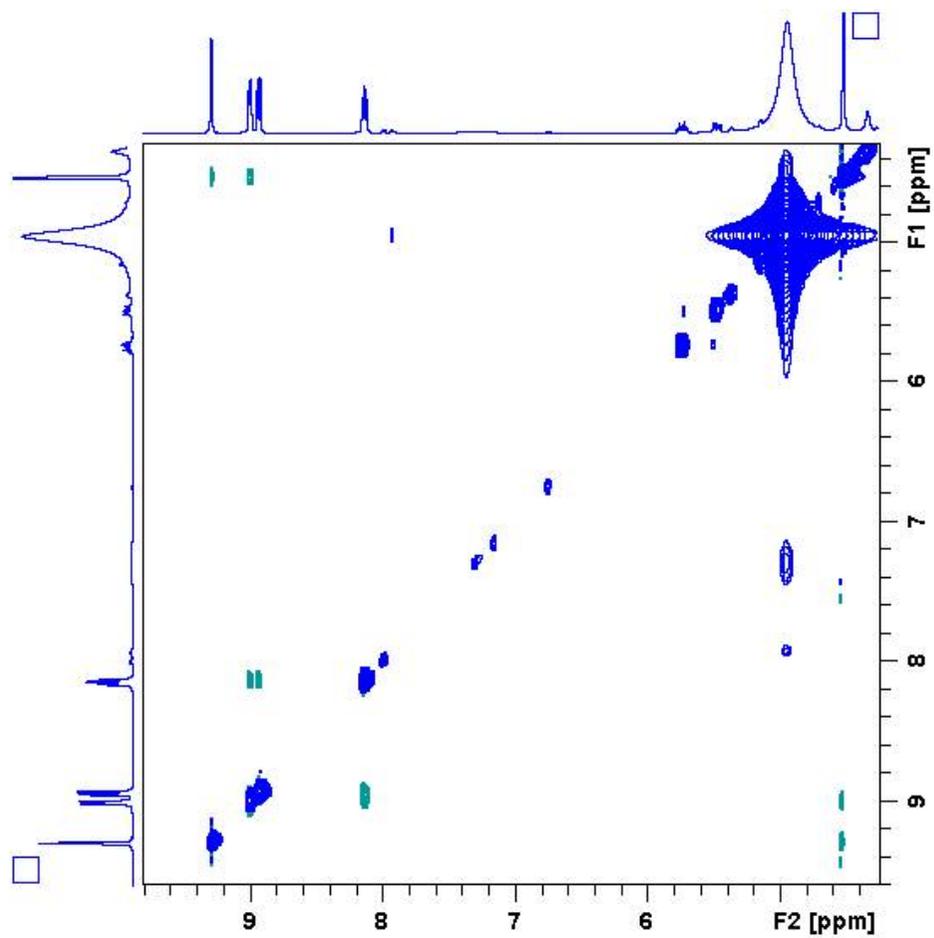


Figure S25. HR-ESI-MS spectrum of 3-methylbutyl hydrodisulfide (**4**)

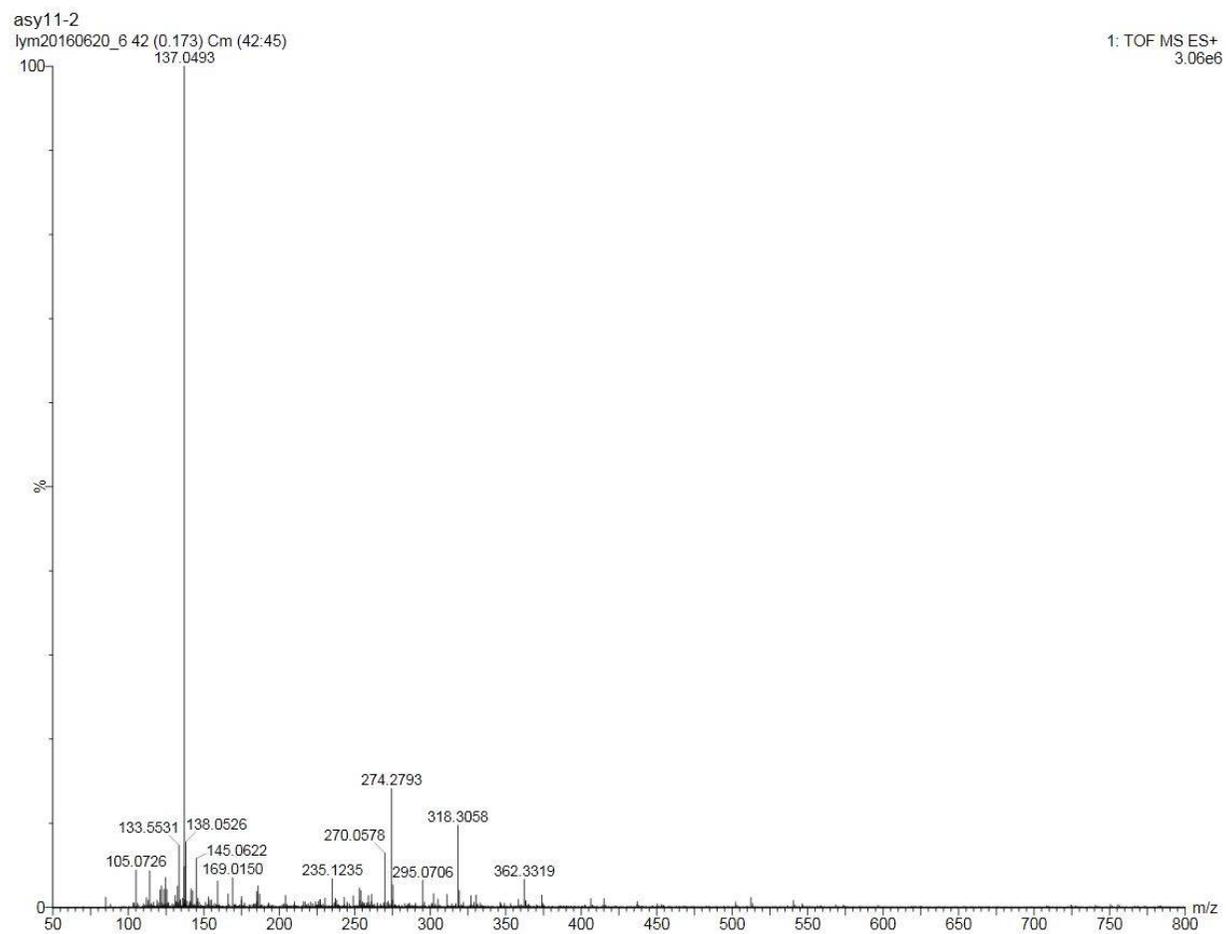


Figure S26. ^1H NMR spectrum (DMSO- d_6) of 3-methylbutyl hydrodisulfide (4)

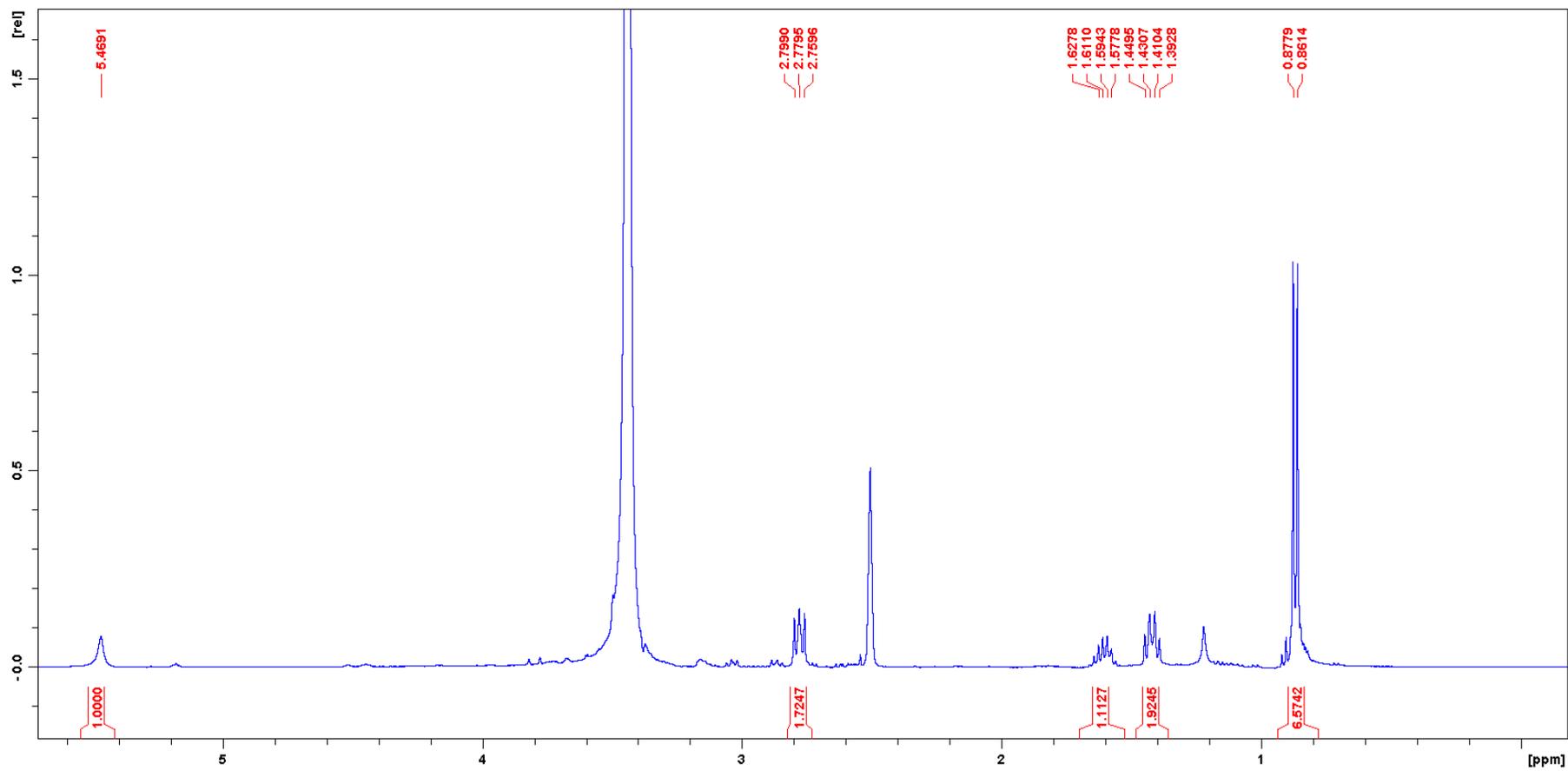
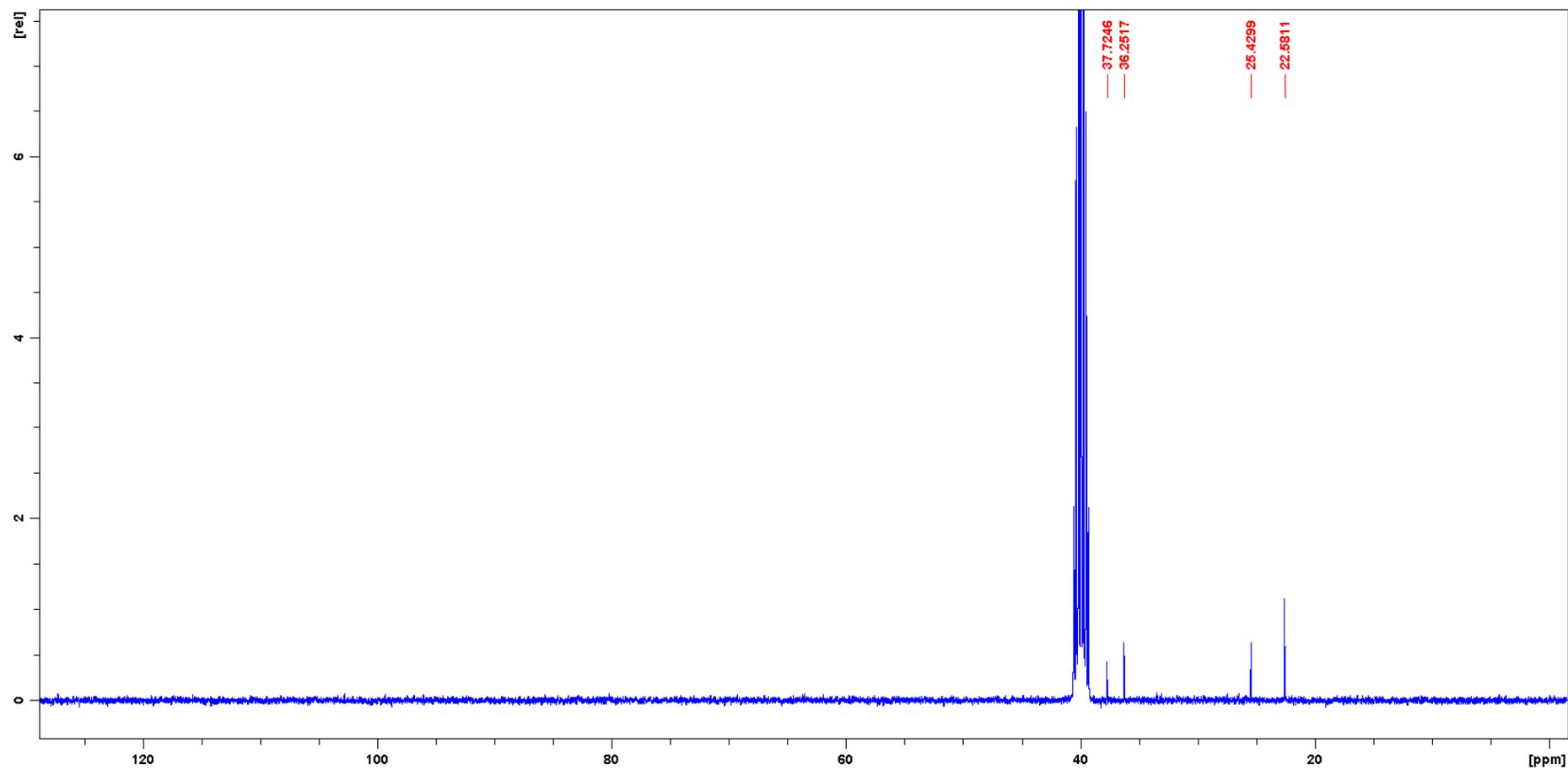


Figure S27. ^{13}C NMR spectrum (DMSO- d_6) of 3-methylbutyl hydrodisulfide (**4**)



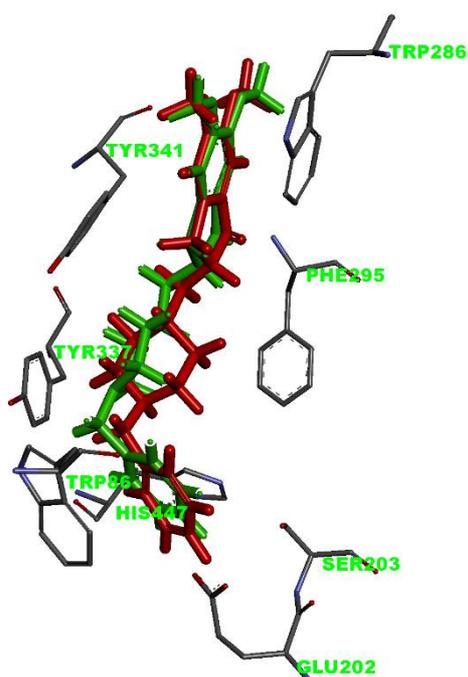


Fig. S28. Docking validation. Redocked donepezil (best-ranked docking solution) is reported in red sticks into the active site of AChE. Crystallographic donepezil is represented as green sticks.

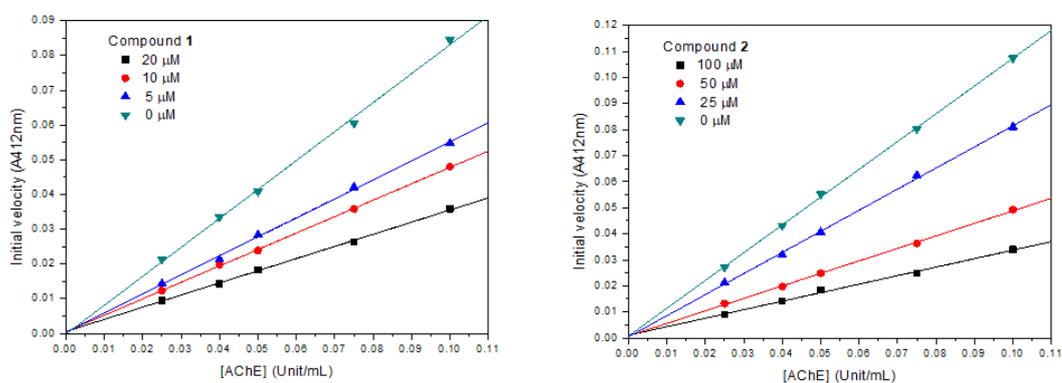


Fig. S29. Plots of initial velocity versus enzyme concentration for the inhibition of compounds 1 and 2 on the hydrolysis activity of AChE.