molecules

MDPI

Supplementary material

An unprecedented 4,8-Cycloeudesmane, further new Sesquiterpenoids, a Triterpene, Steroids and a Lignan from the resin of *Commiphora myrrha* and their anti-inflammatory activity *in vitro*

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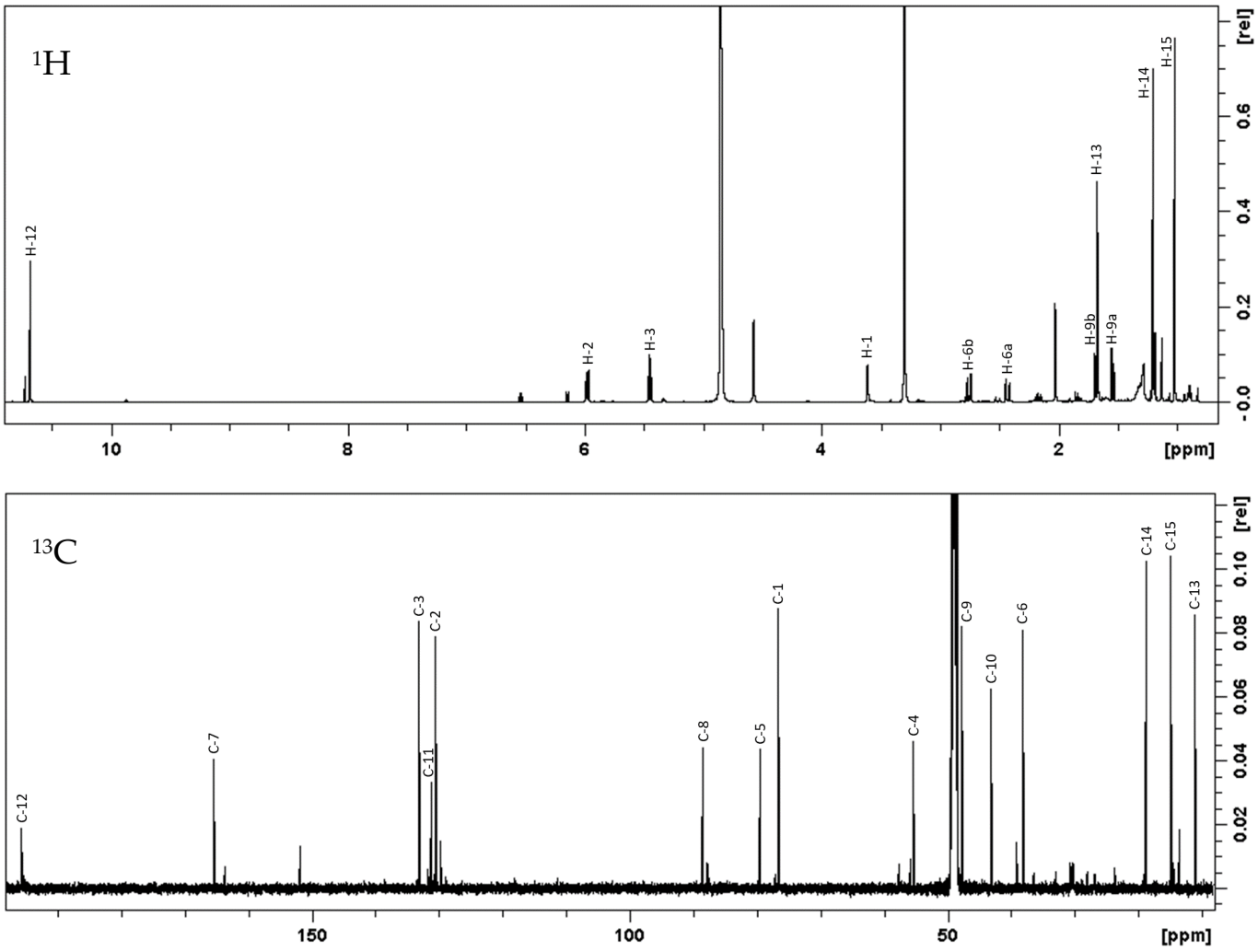


Figure S1. ^{1}H (600 MHz) and ^{13}C NMR (151 MHz) spectrum of compound **1** in CD_3OD.

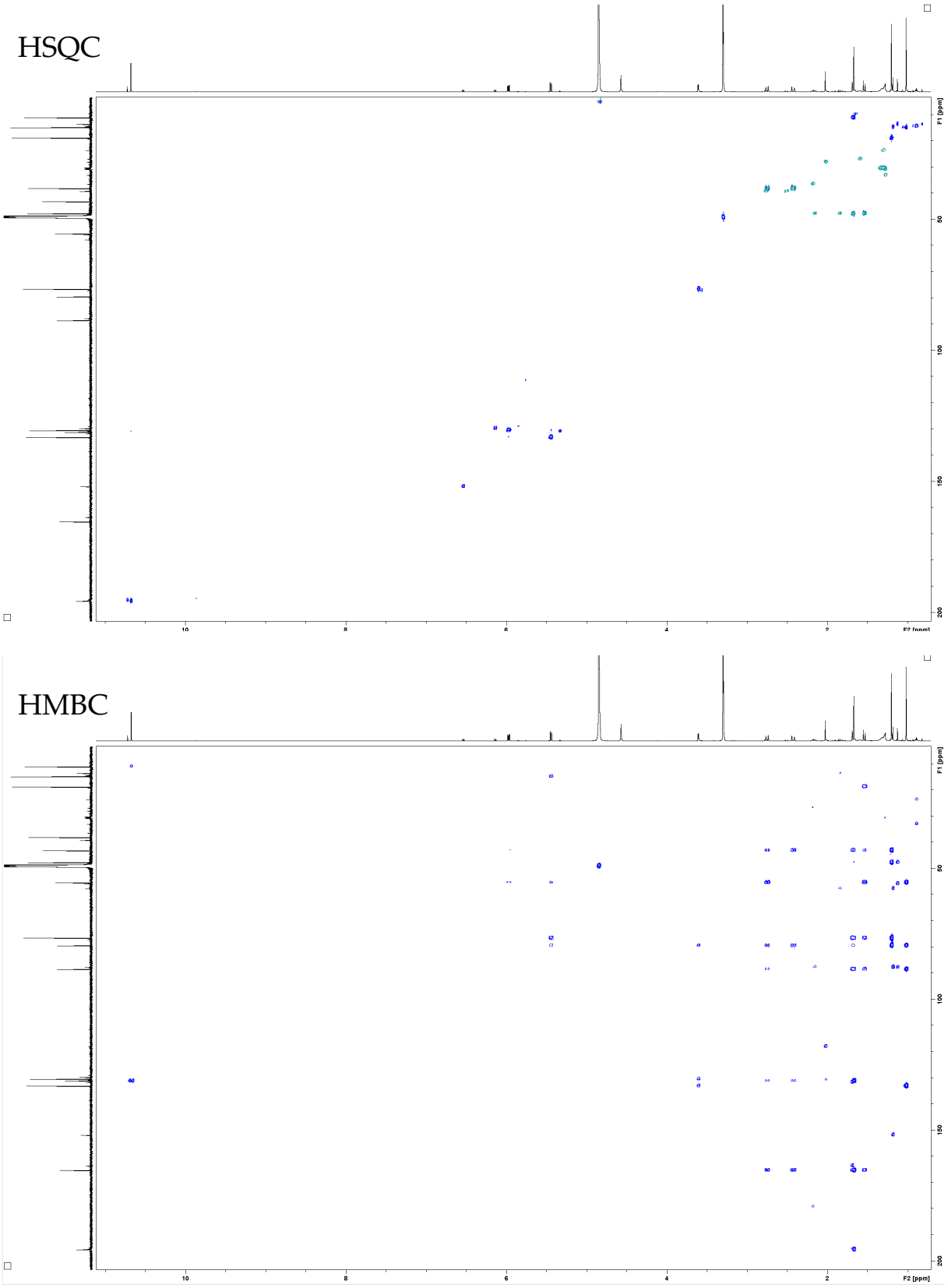


Figure S2. HSQC and HMBC spectrum of compound **1** in CD_3OD.

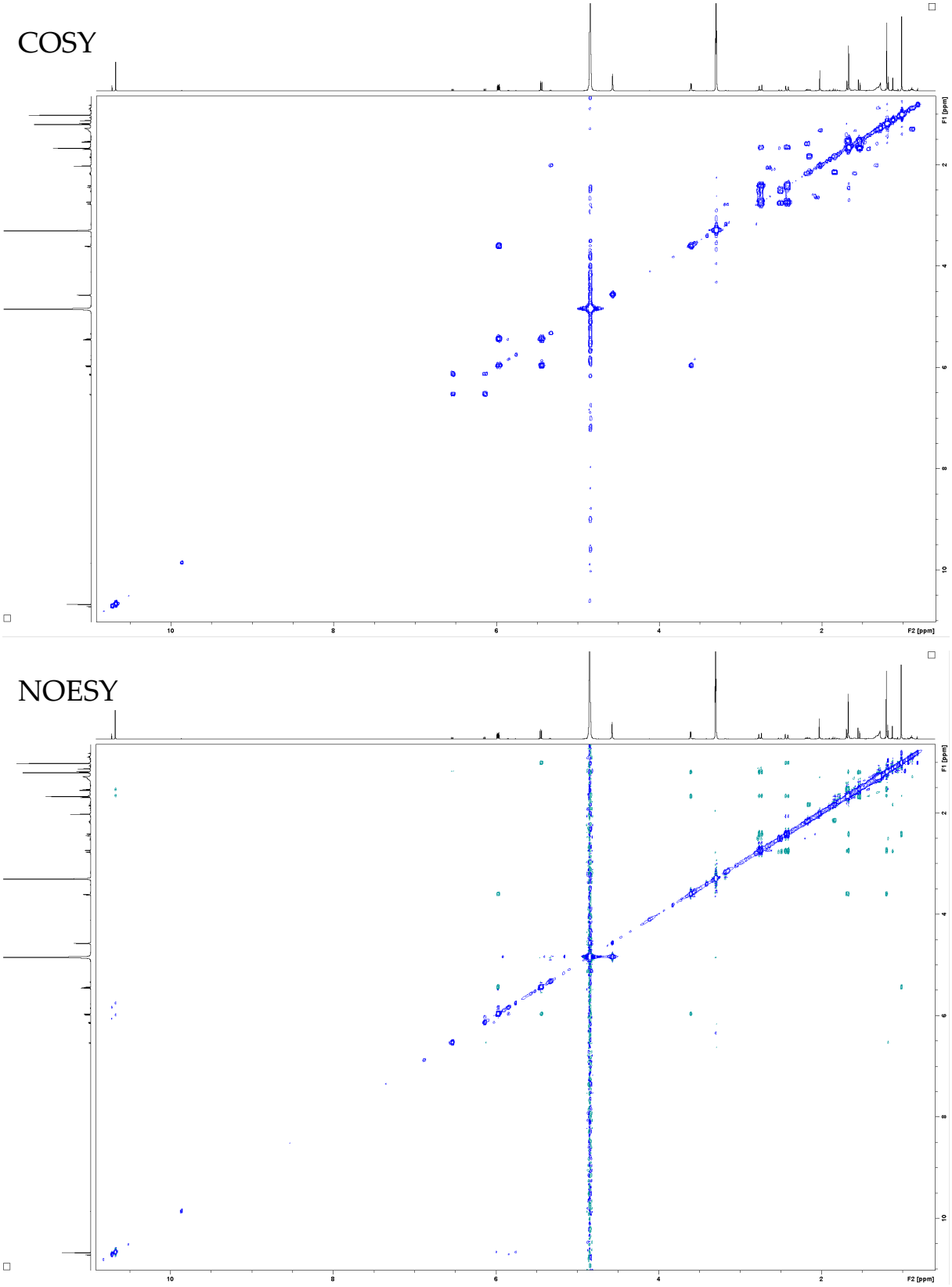


Figure S3. COSY and NOESY spectrum of compound **1** in CD_3OD.

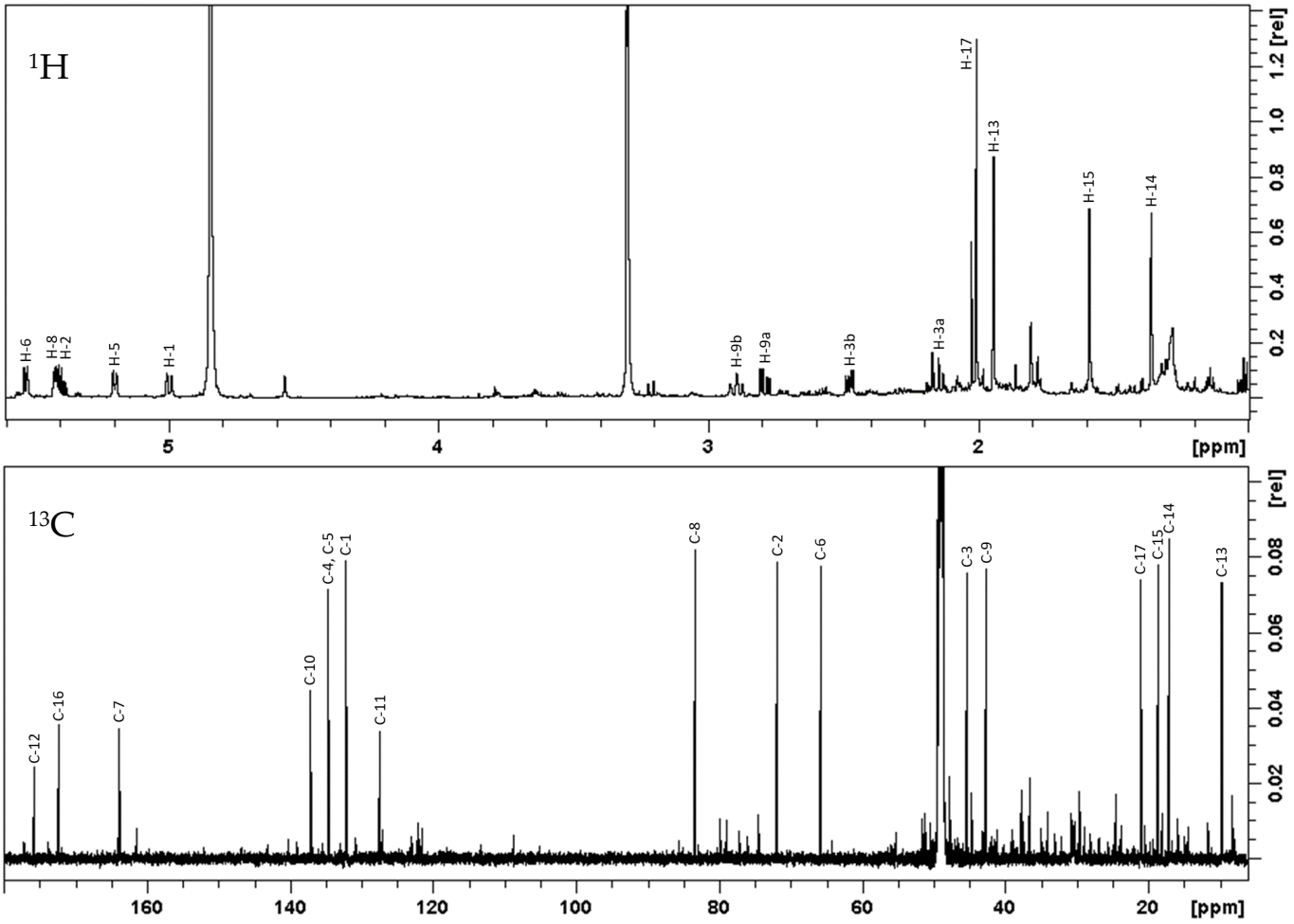


Figure S4. ^{1}H (600 MHz) and ^{13}C NMR (151 MHz) spectrum of compound **2** in CD_3OD.

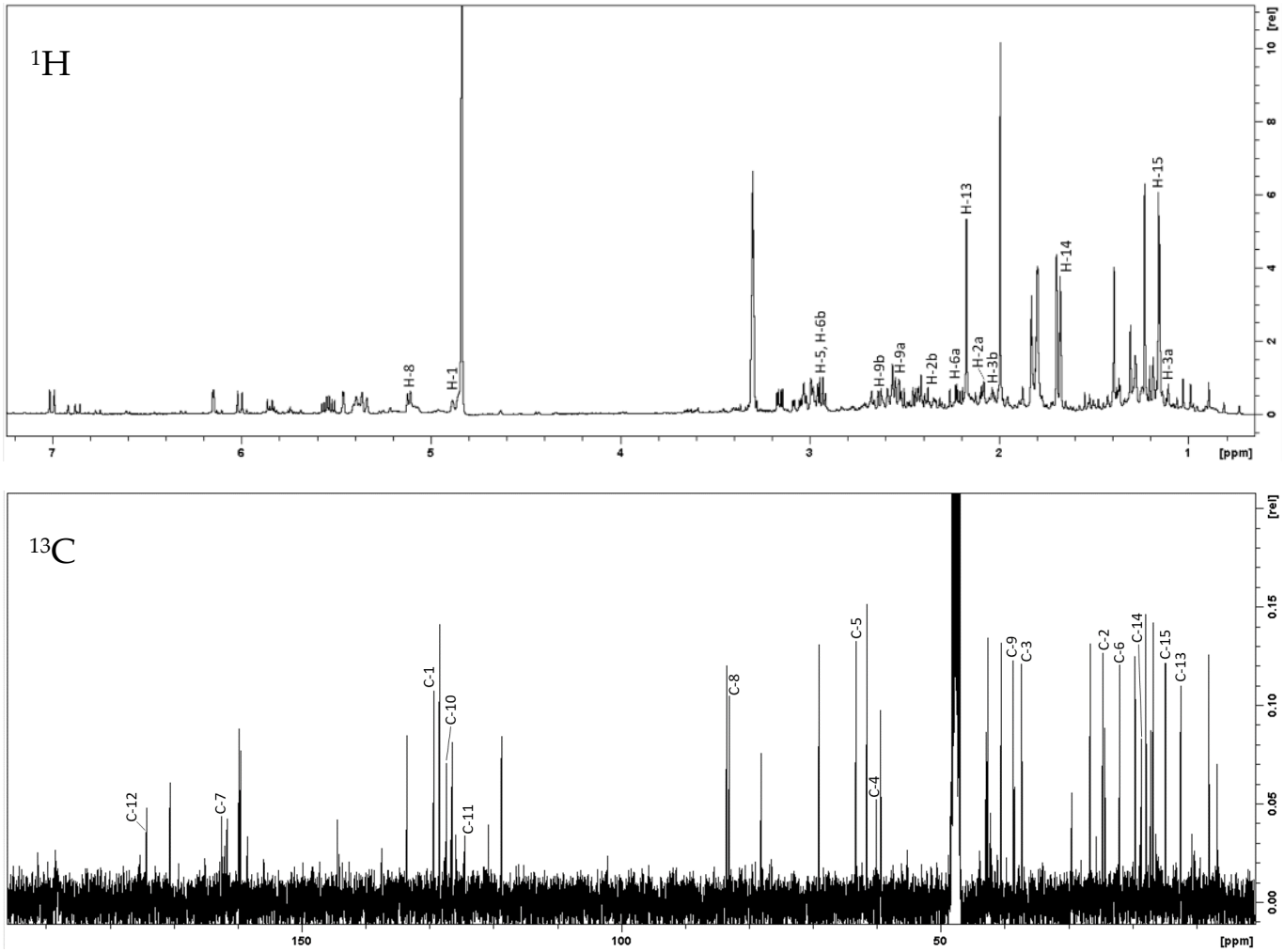


Figure S5. ^{1}H (400 MHz) and ^{13}C NMR (101 MHz) spectrum of the mixture of compounds **3**, **4** and **22** in CD_3OD. Signals of compound **3** are labelled.

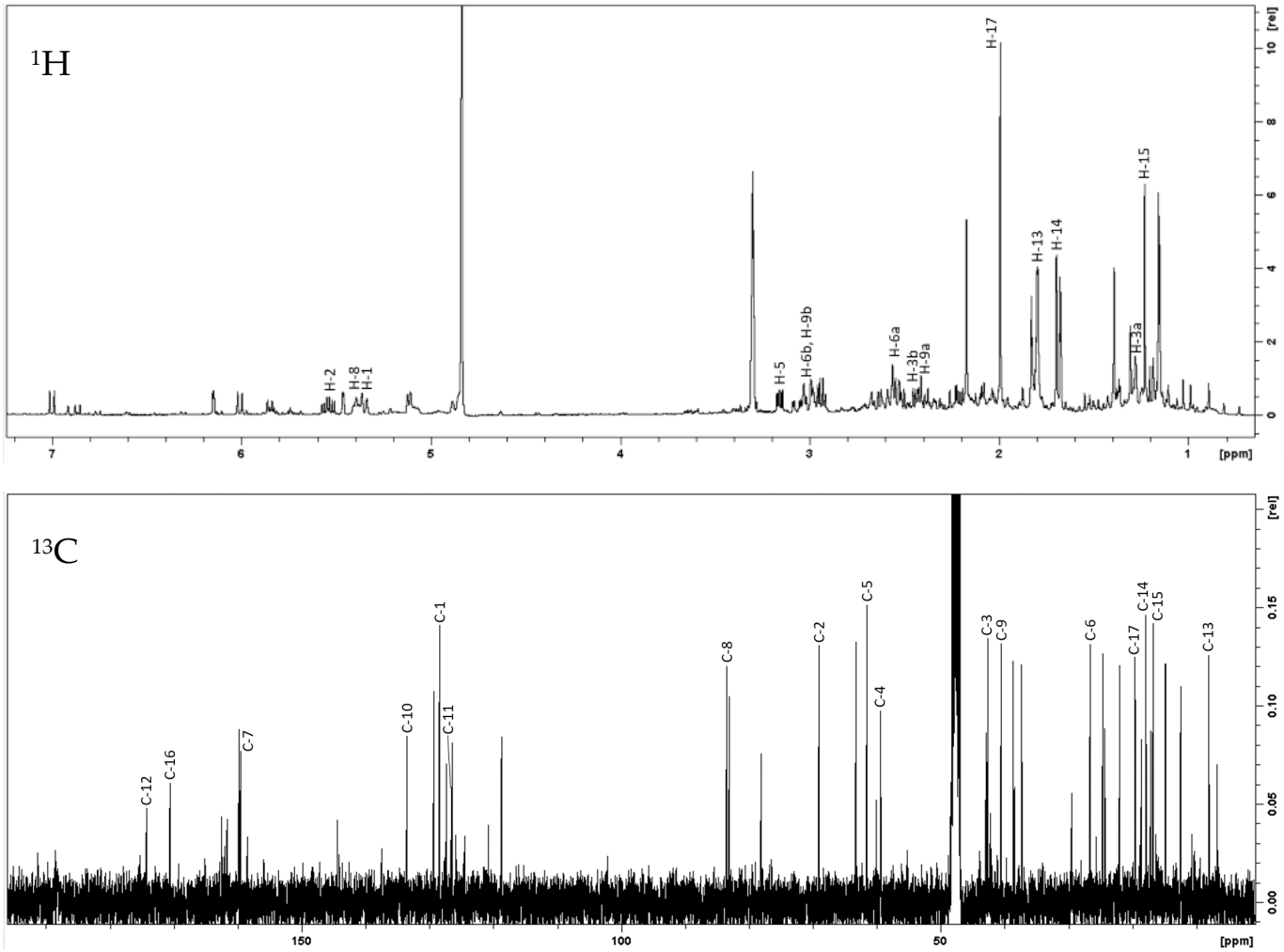


Figure S6. ^{1}H (400 MHz) and ^{13}C NMR (101 MHz) spectrum of the mixture of compounds **3**, **4** and **22** in CD_3OD. Signals of compound **4** are labelled.

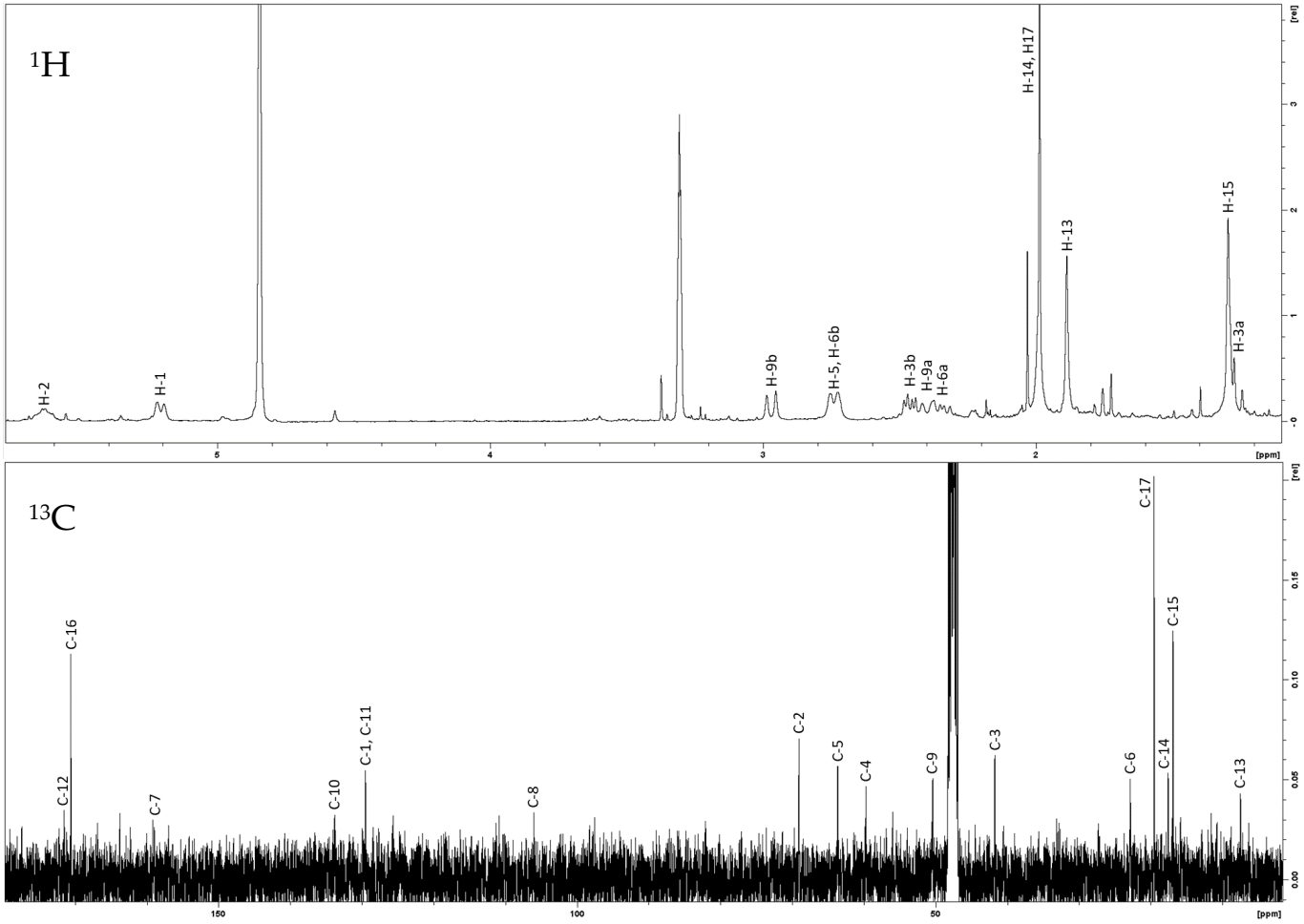


Figure S7. ^{1}H (400 MHz) and ^{13}C NMR (101 MHz) spectrum of compound **5** in CD_3OD.

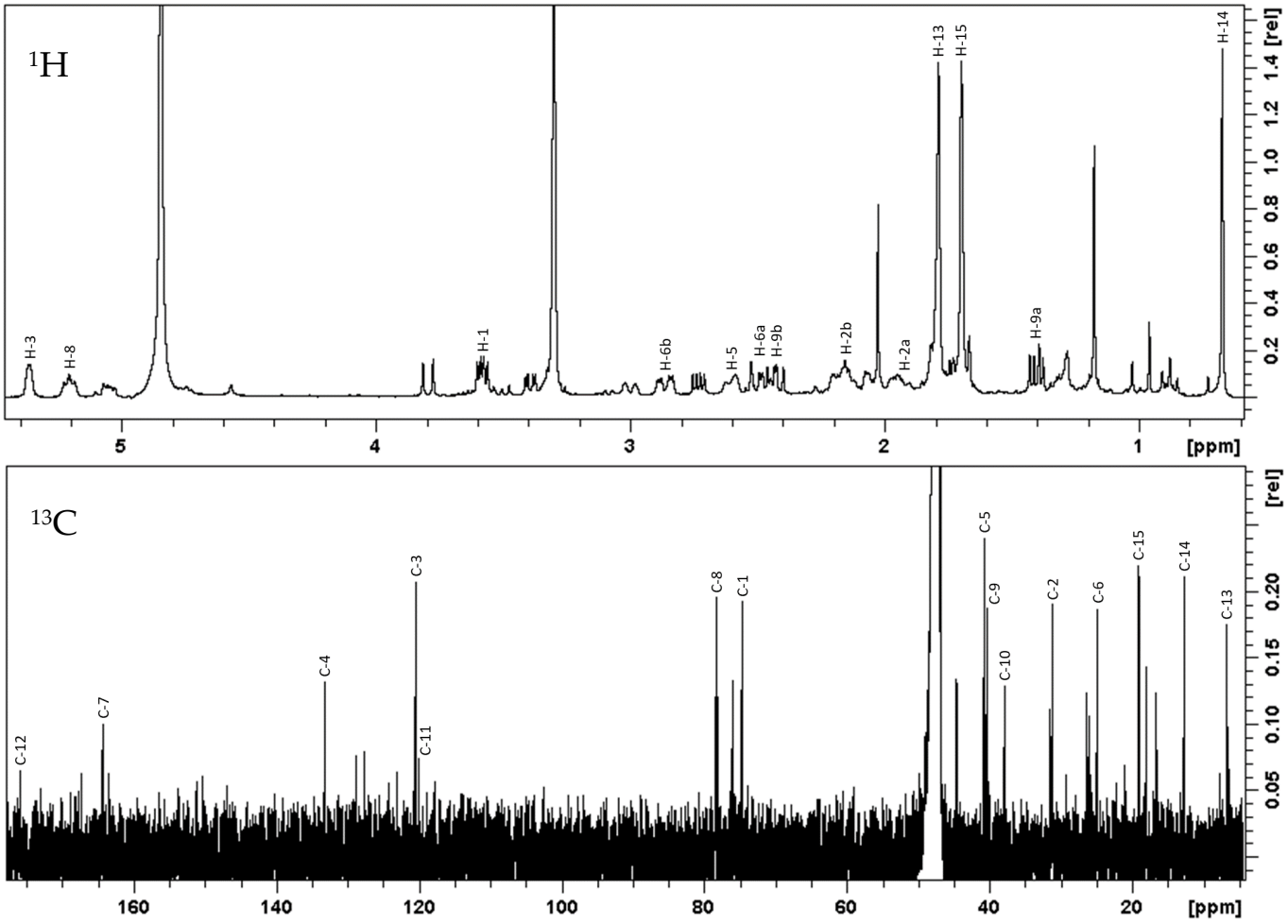


Figure S8. ^{1}H (400 MHz) and ^{13}C NMR (101 MHz) spectrum of compound **6** in CD_3OD.

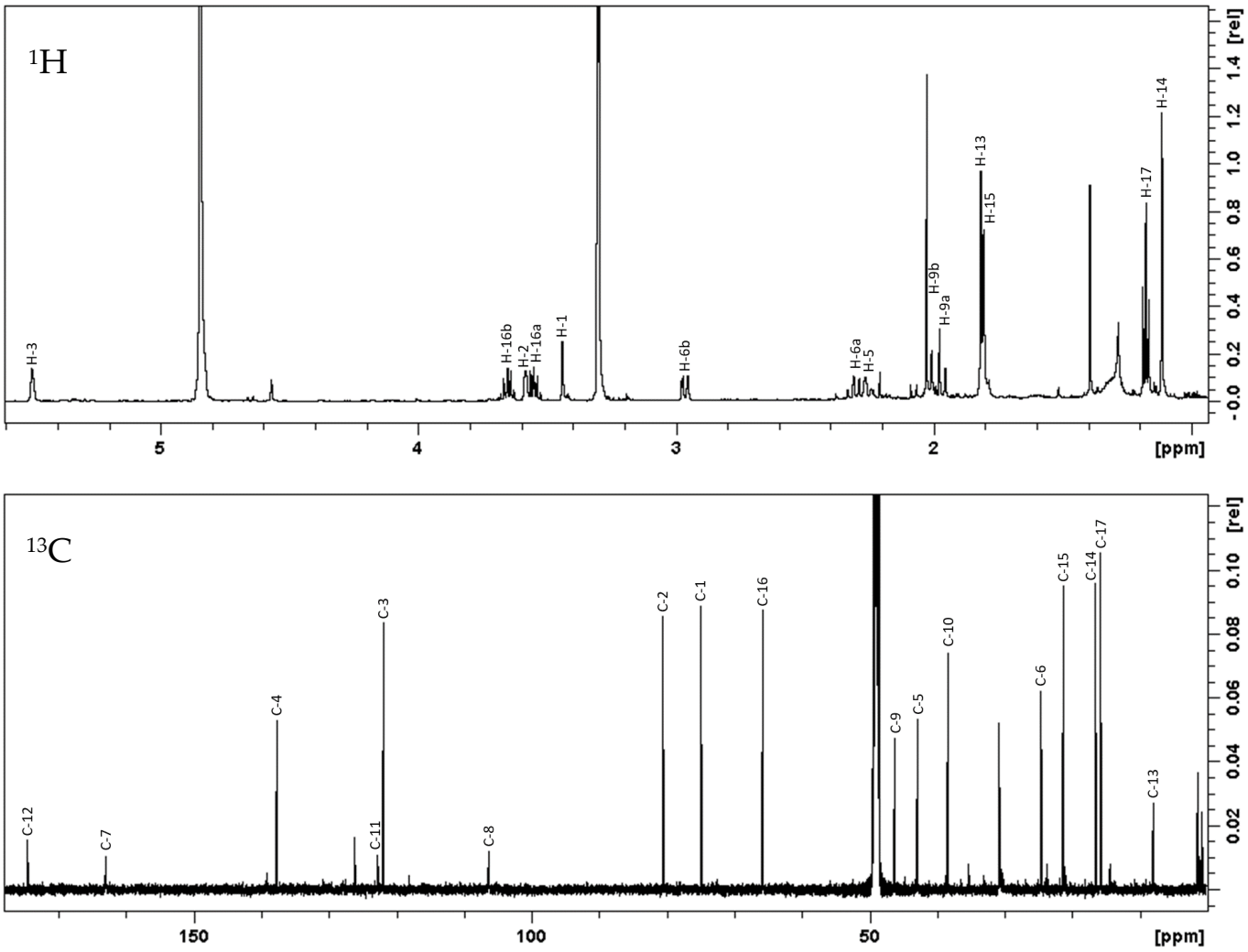


Figure S9. ^{1}H (600 MHz) and ^{13}C NMR (151 MHz) spectrum of compound **7** in CD_3OD.

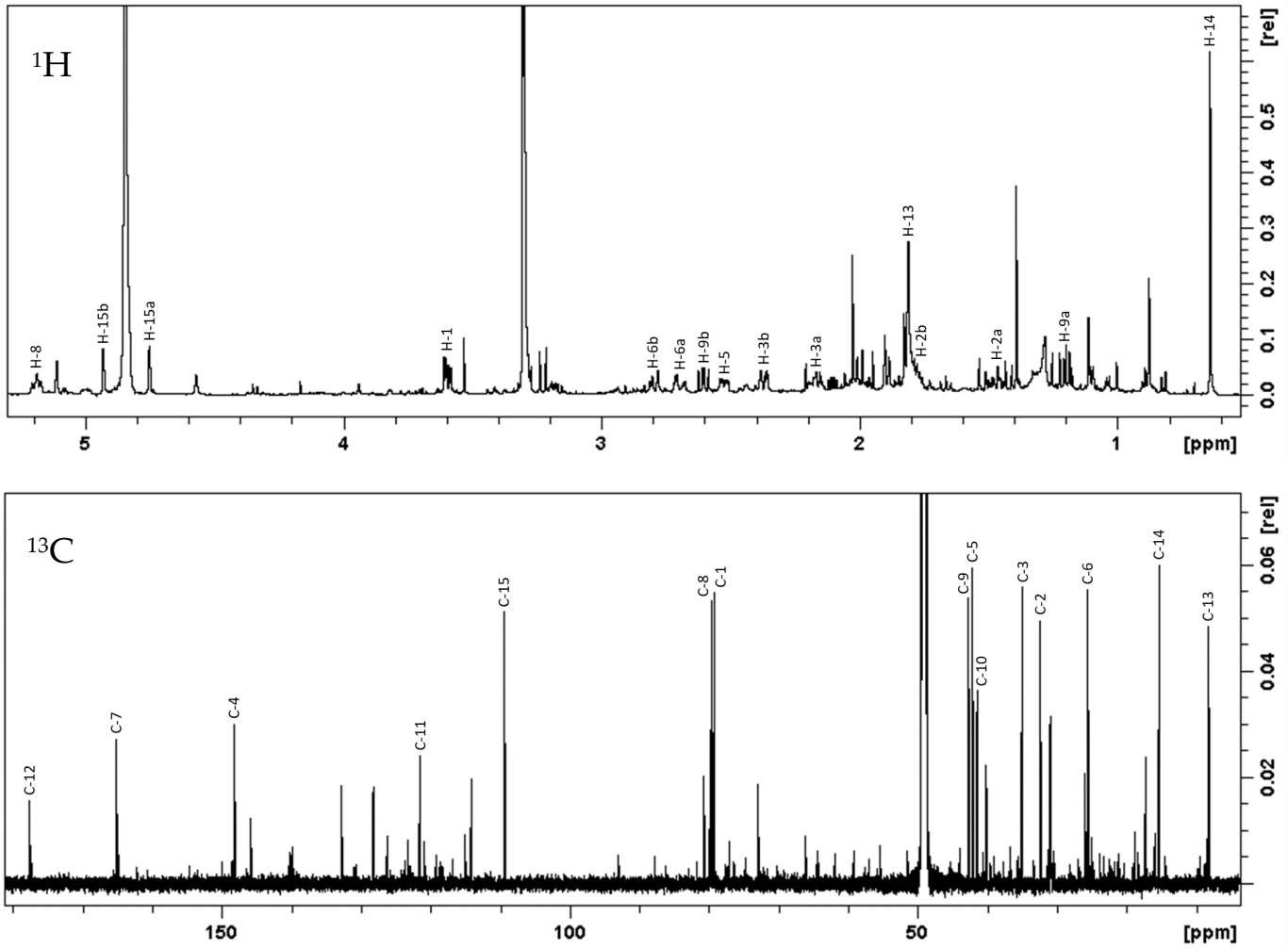


Figure S10. ^{1}H (600 MHz) and ^{13}C NMR (151 MHz) spectrum of compound **8** in CD_3OD.

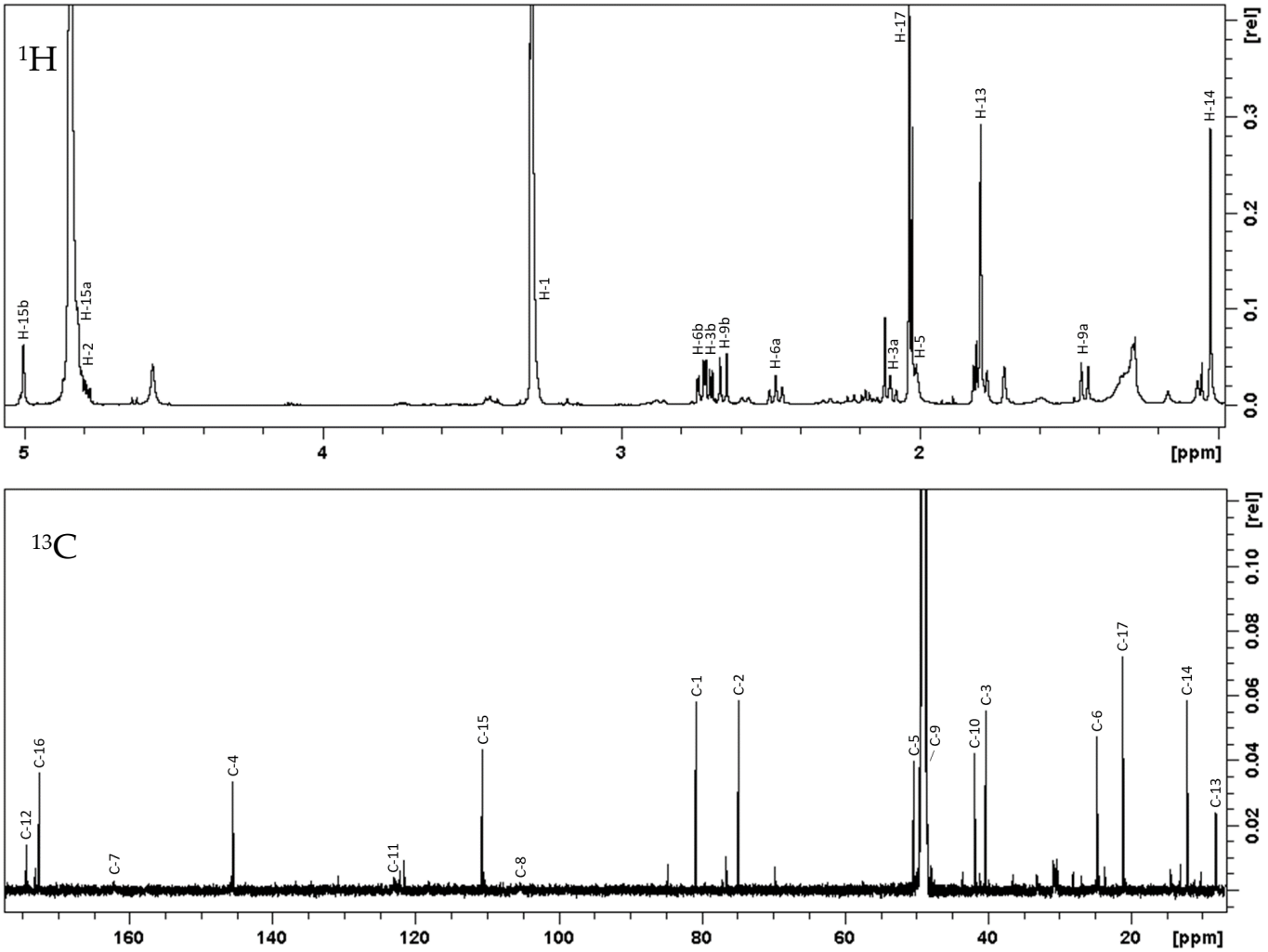


Figure S11. ^{1}H (600 MHz) and ^{13}C NMR (151 MHz) spectrum of compound **9** in CD_3OD.

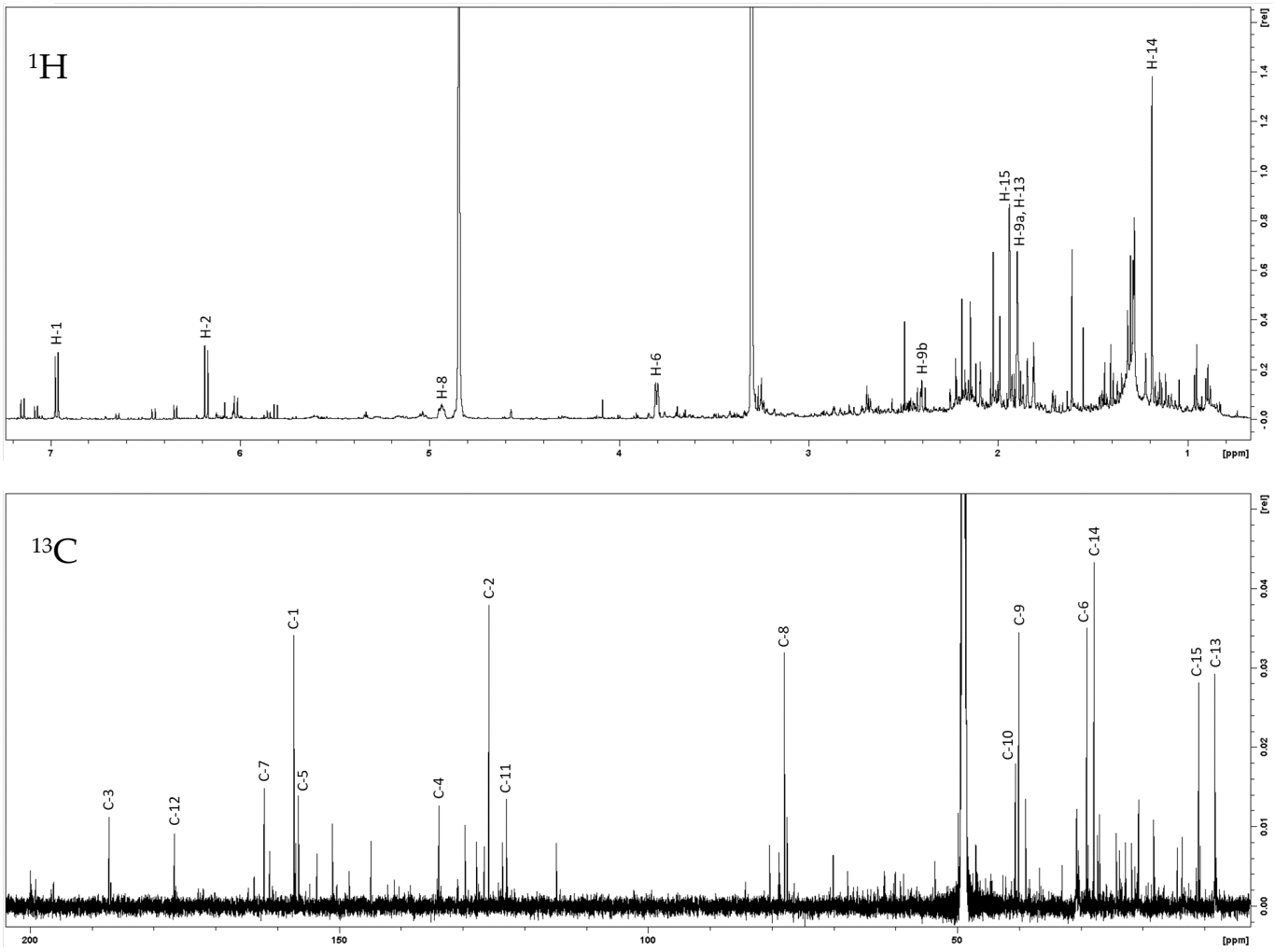


Figure S12. ^{1}H (600 MHz) and ^{13}C NMR (151 MHz) spectrum of compound **10** in CD_3OD.

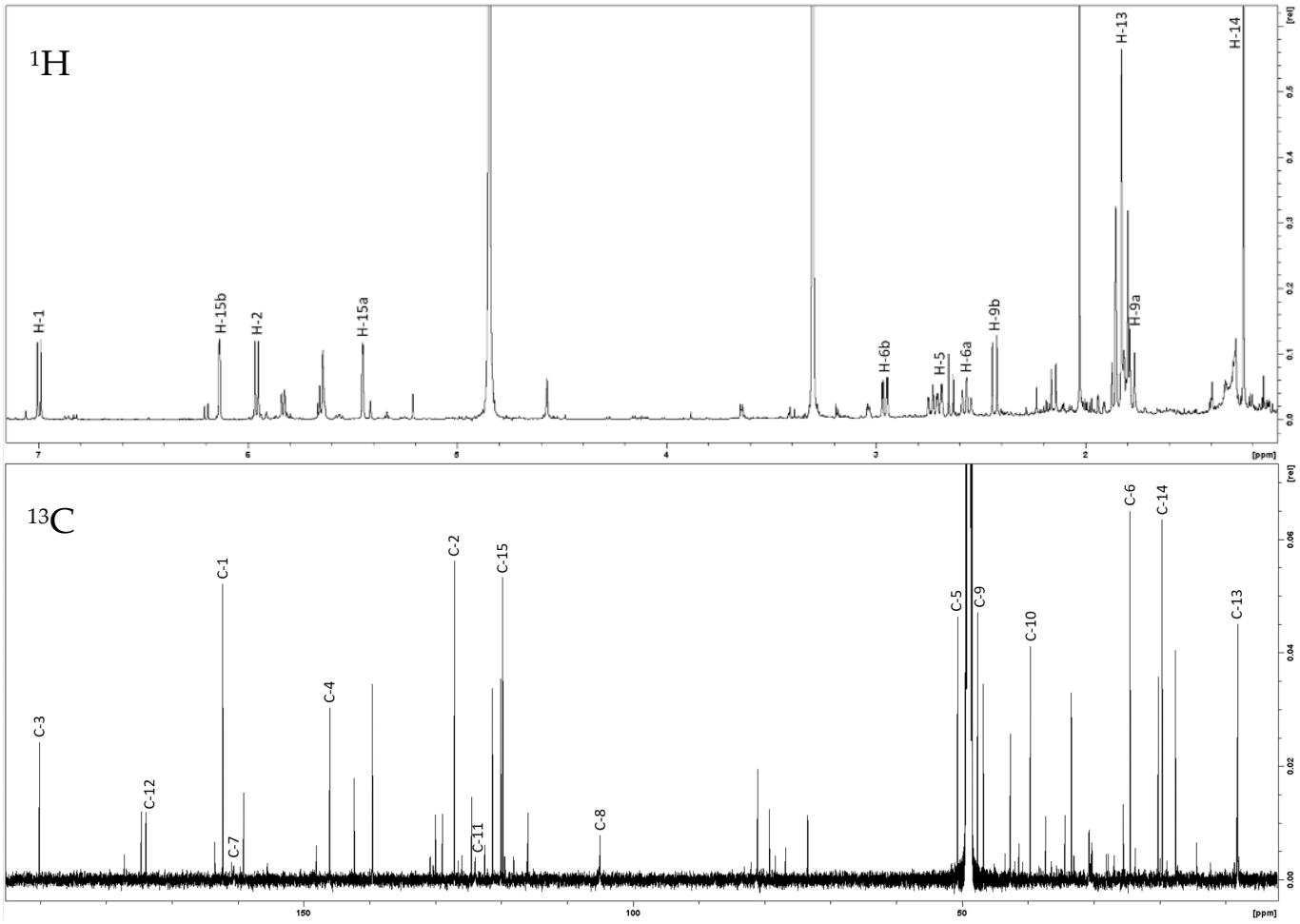


Figure S13. ^{1}H (600 MHz) and ^{13}C NMR (151 MHz) spectrum of compound **11** in CD_3OD.

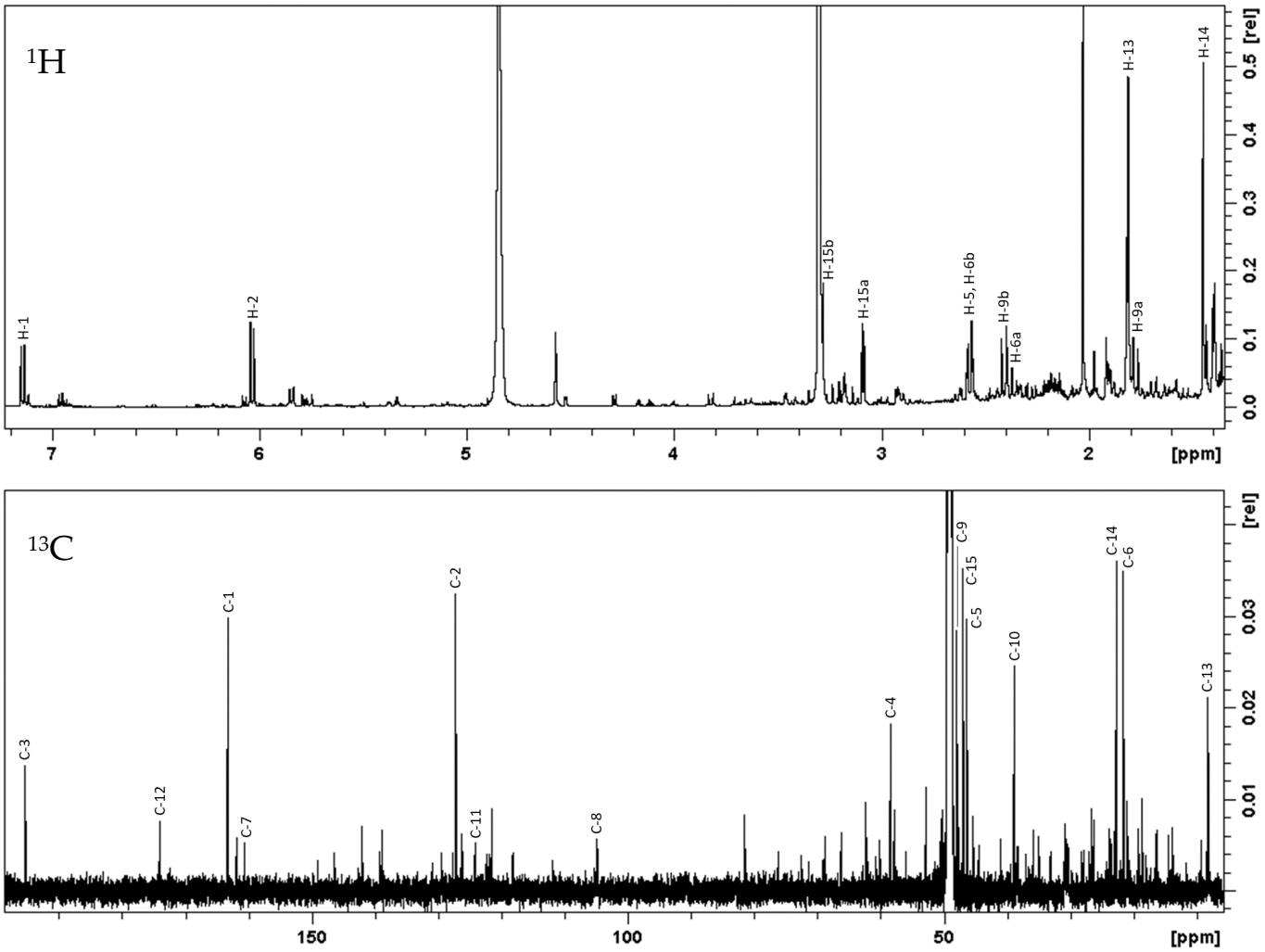


Figure S14. ^{1}H (600 MHz) and ^{13}C NMR (151 MHz) spectrum of compound **12** in CD_3OD.

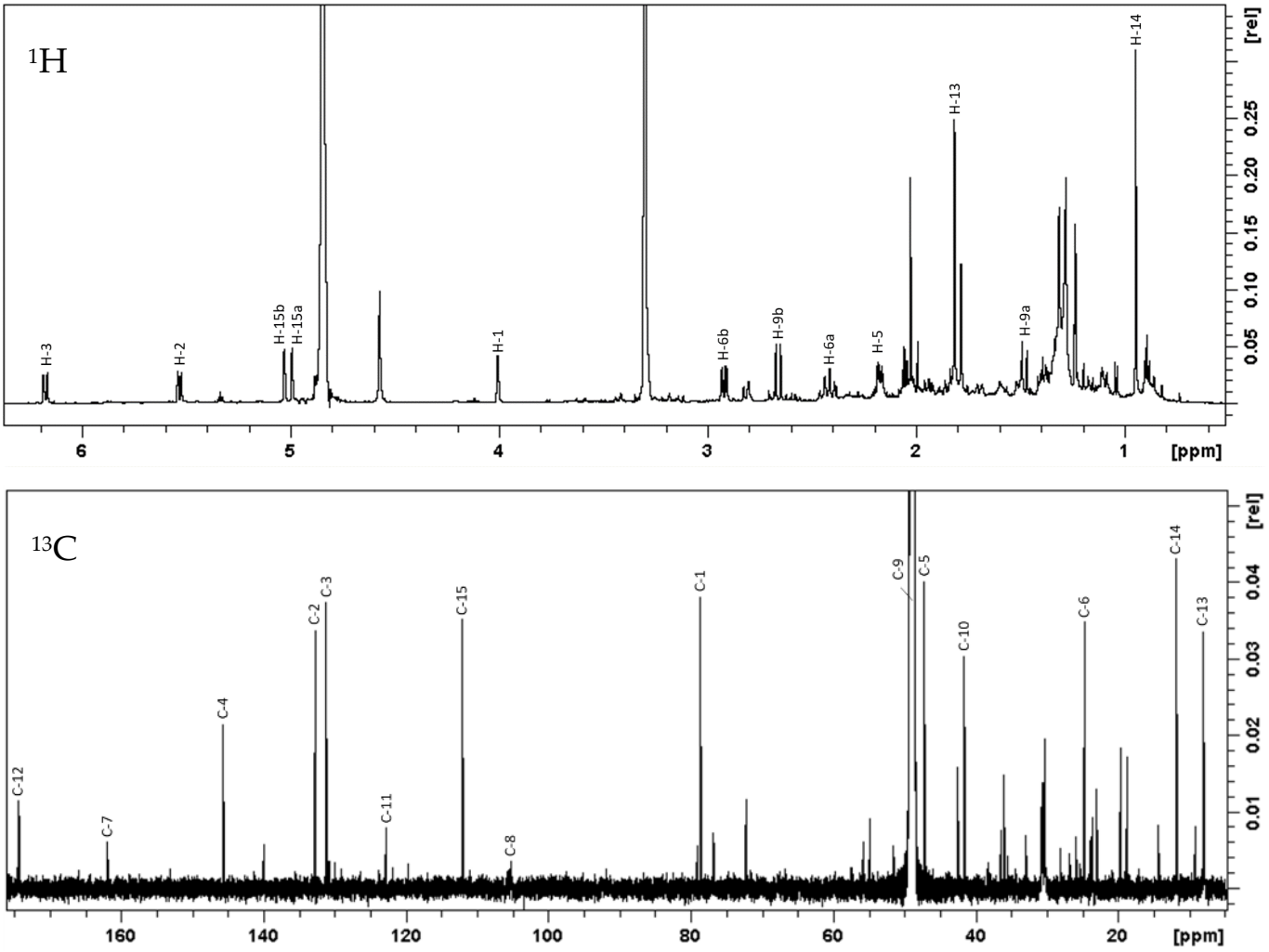


Figure S15. ^{1}H (600 MHz) and ^{13}C NMR (151 MHz) spectrum of compound **13** in CD_3OD.

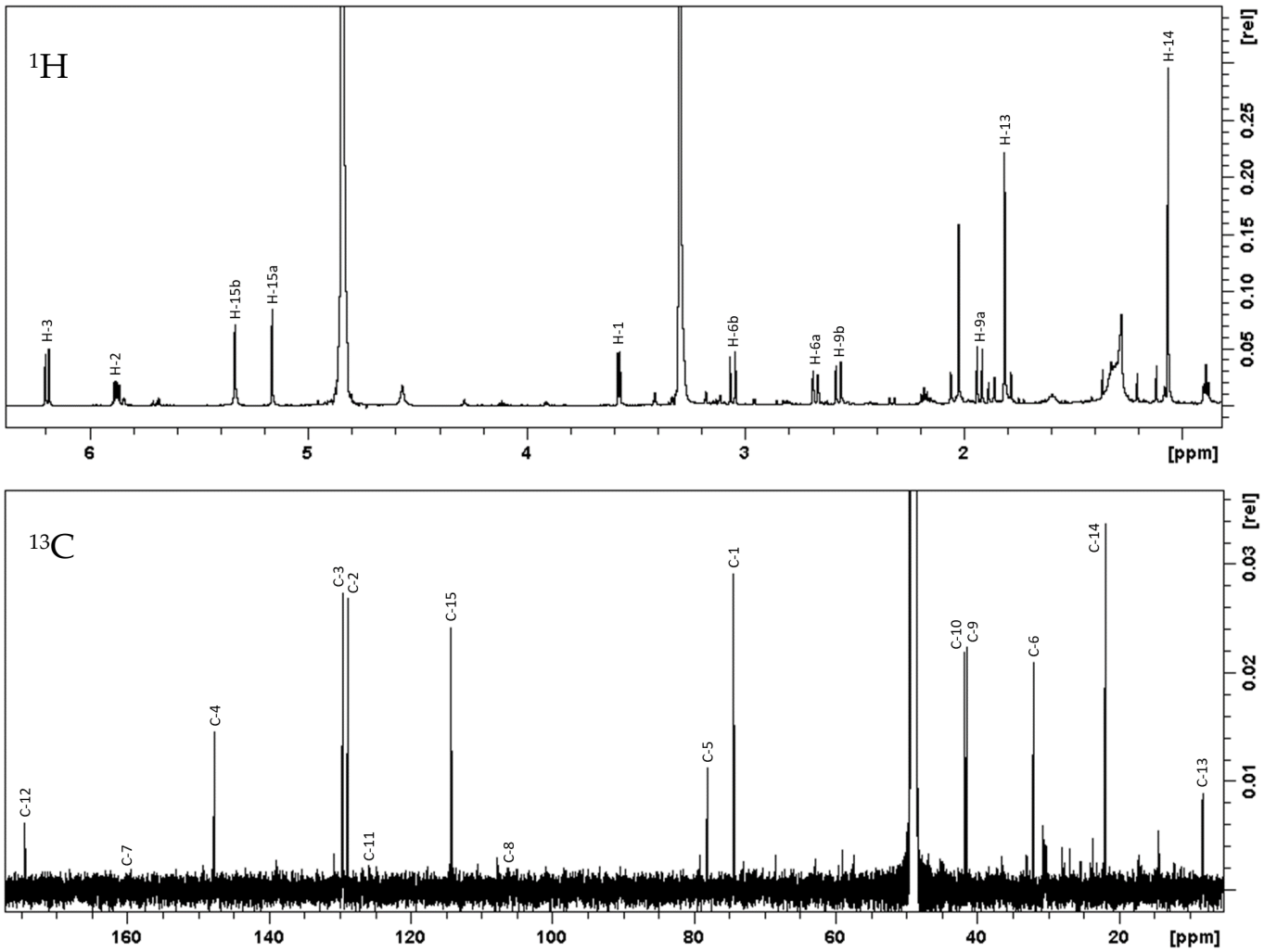


Figure S16. ^{1}H (600 MHz) and ^{13}C NMR (151 MHz) spectrum of compound **14** in CD_3OD.

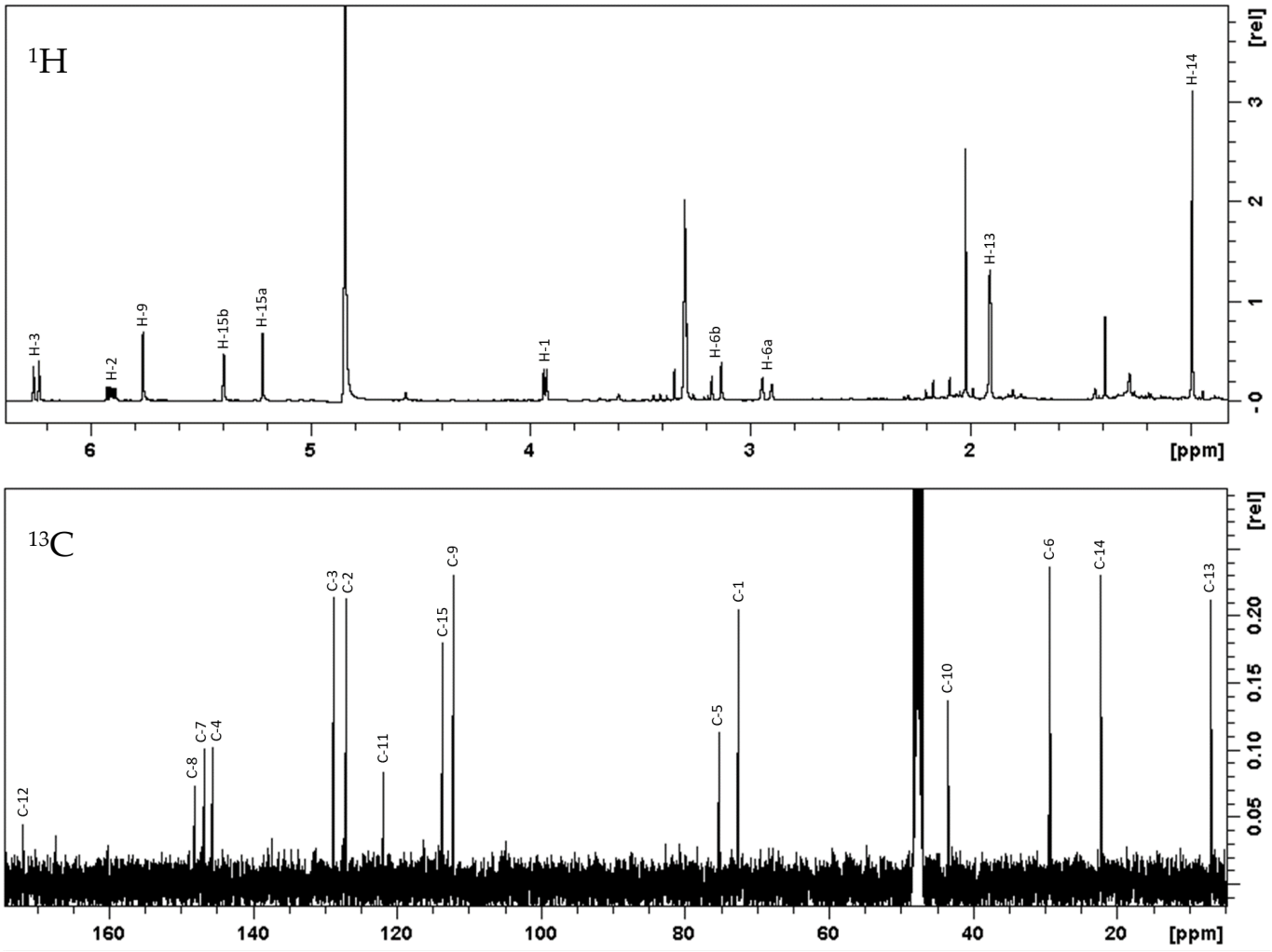


Figure S17. ^{1}H (400 MHz) and ^{13}C NMR (101 MHz) spectrum of compound **15** in CD_3OD.

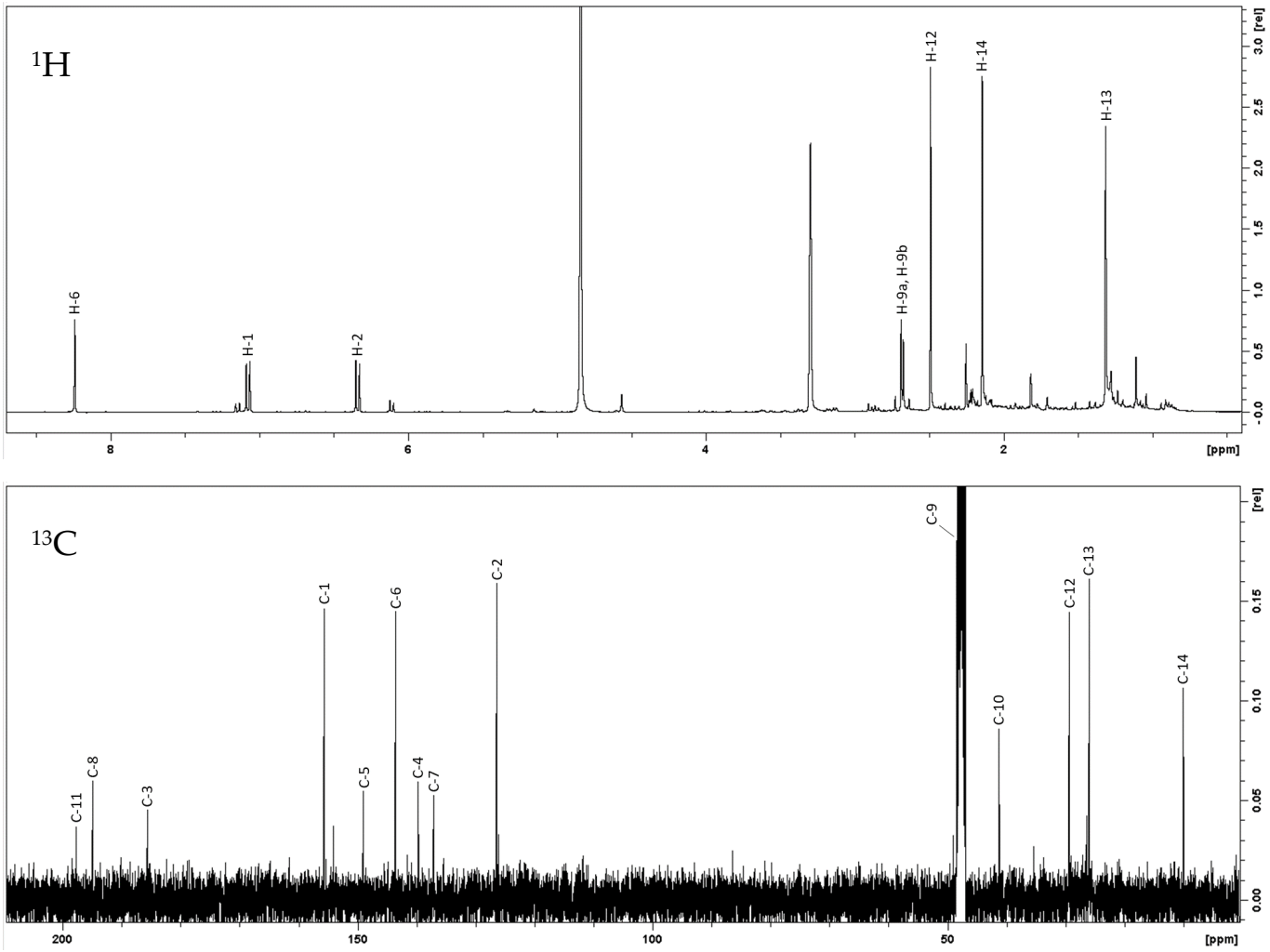


Figure S 18. ^{1}H (400 MHz) and ^{13}C NMR (101 MHz) spectrum of compound **16** in CD_3OD.

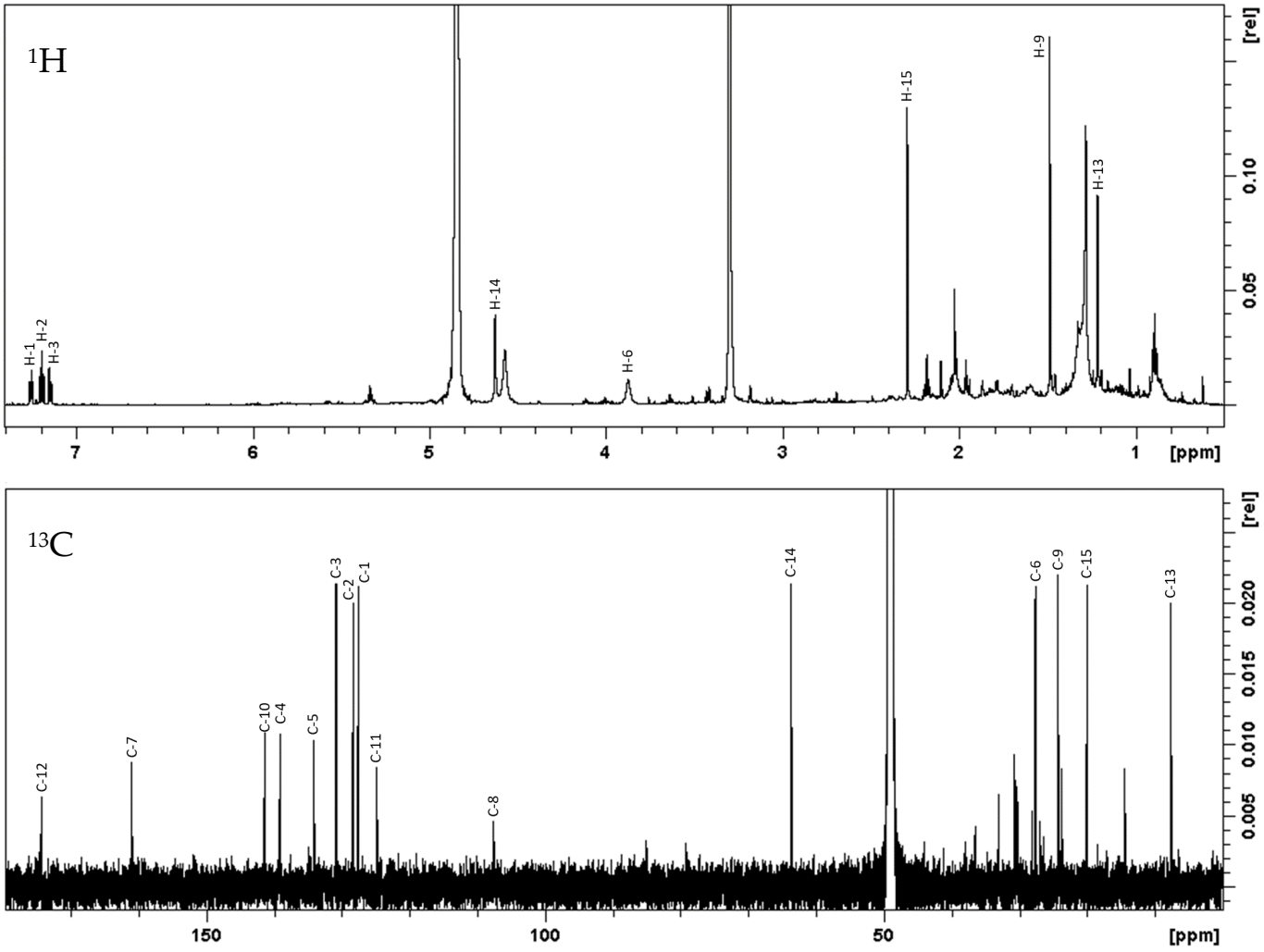


Figure S19. ^{1}H (600 MHz) and ^{13}C NMR (151 MHz) spectrum of compound **17** in CD_3OD.

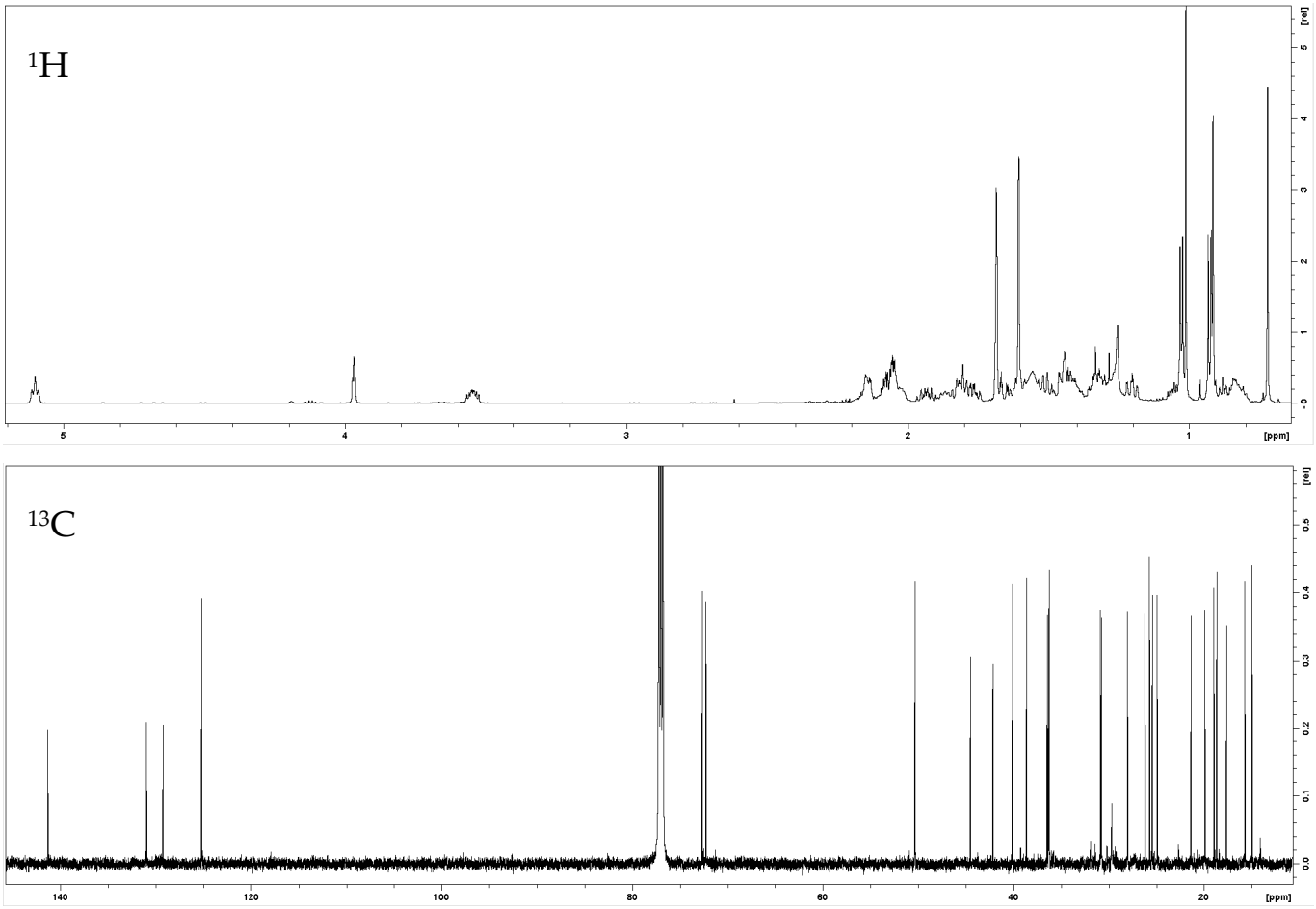


Figure S20. ^{1}H (600 MHz) and ^{13}C NMR (151 MHz) spectrum of compound **38** in $CDCl_3$.

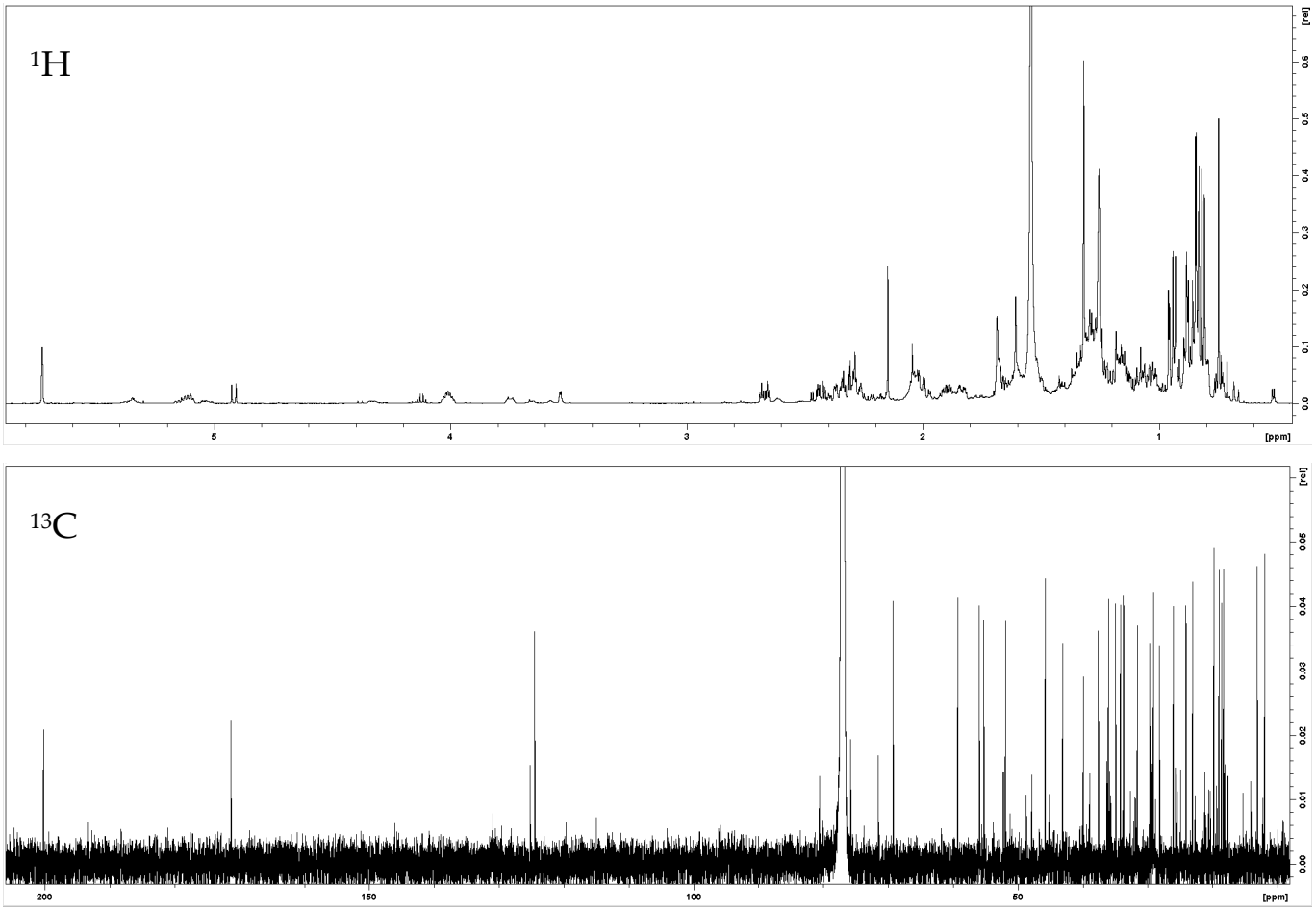


Figure S21. ^{1}H (600 MHz) and ^{13}C NMR (151 MHz) spectrum of compound **39** in $CDCl_3$.

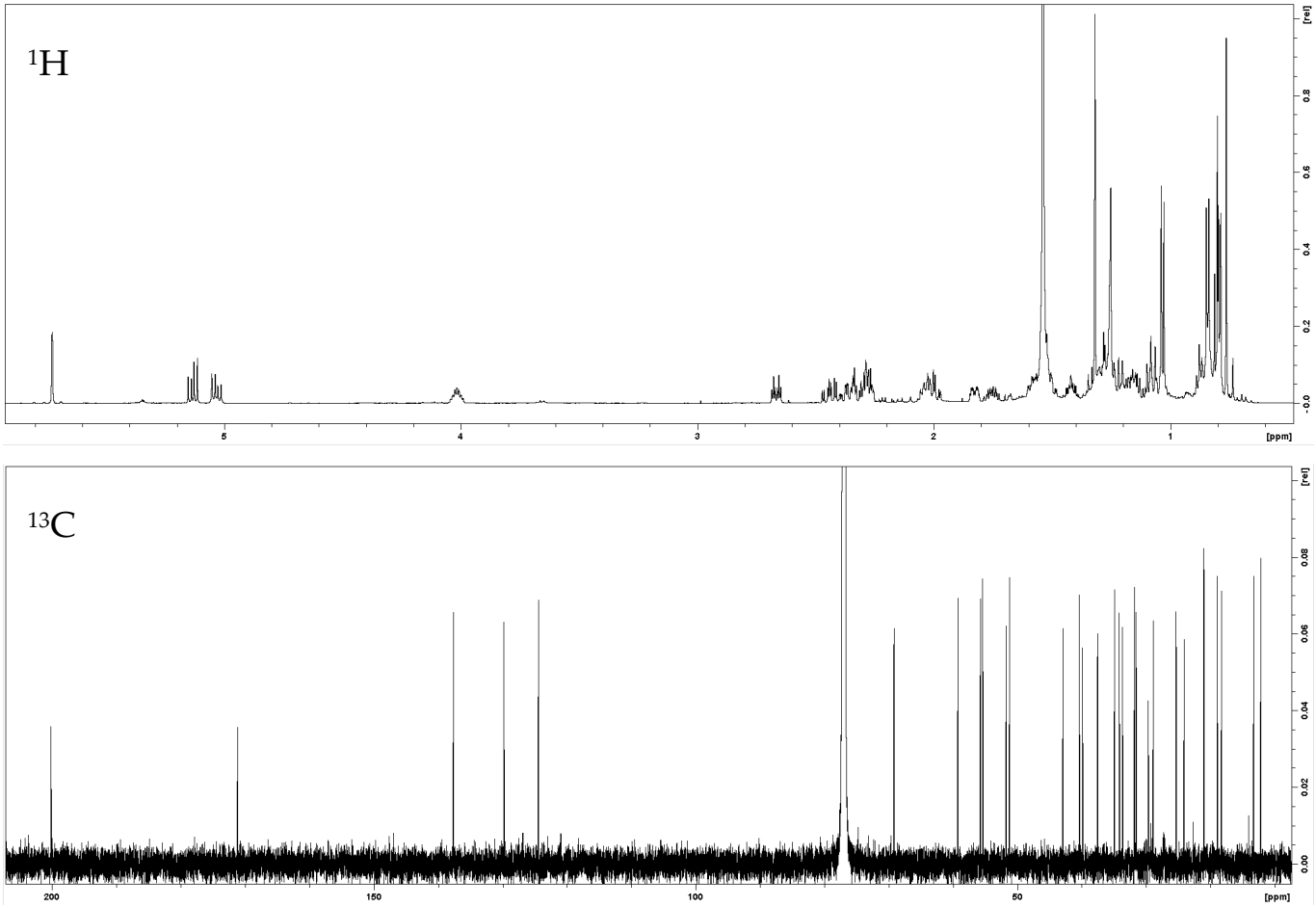


Figure S22. ^{1}H (600 MHz) and ^{13}C NMR (151 MHz) spectrum of compound **40** in $CDCl_3$.

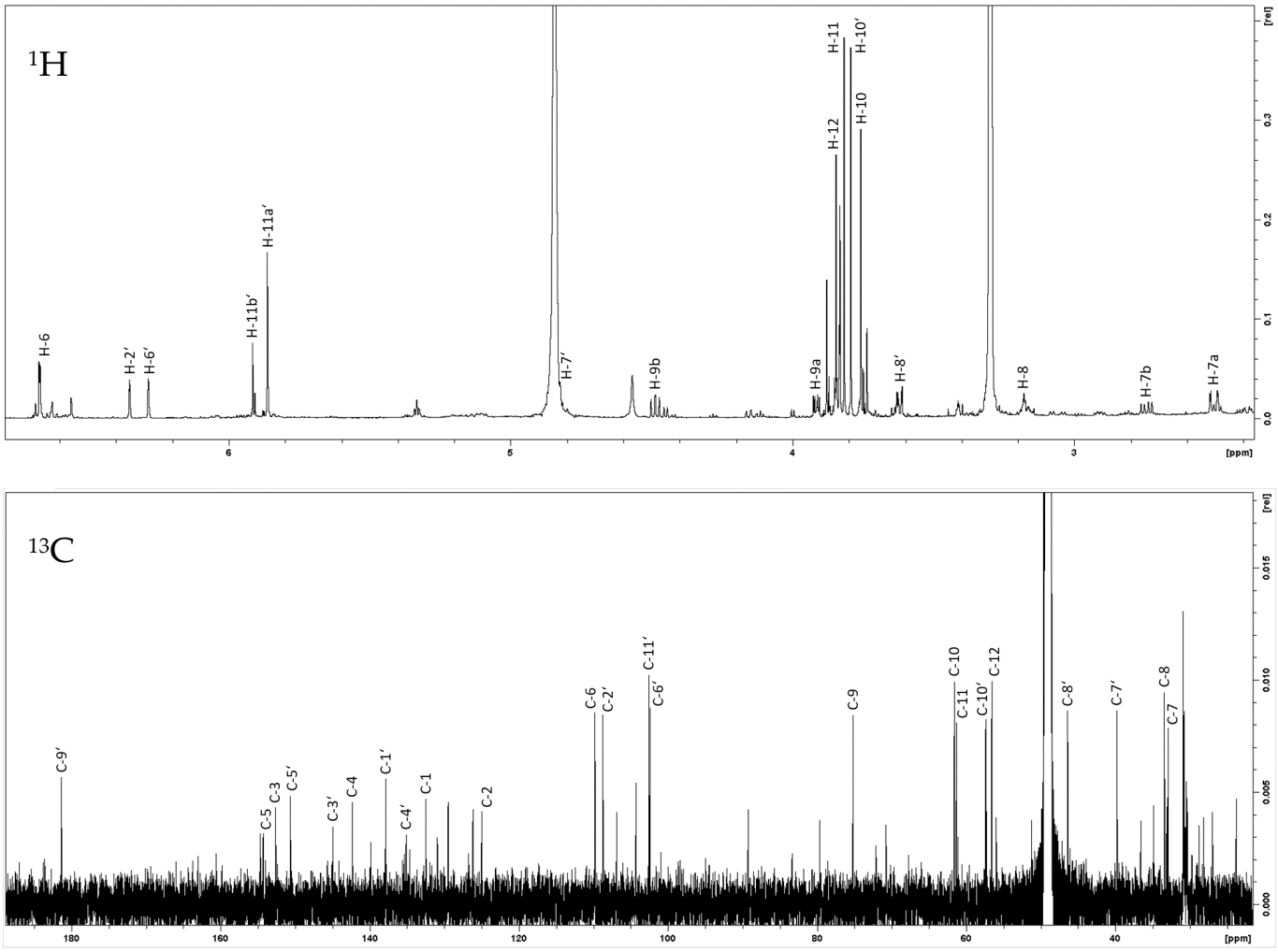


Figure S23. ^{1}H (600 MHz) and ^{13}C NMR (151 MHz) spectrum of compound **43** in CD_3OD.

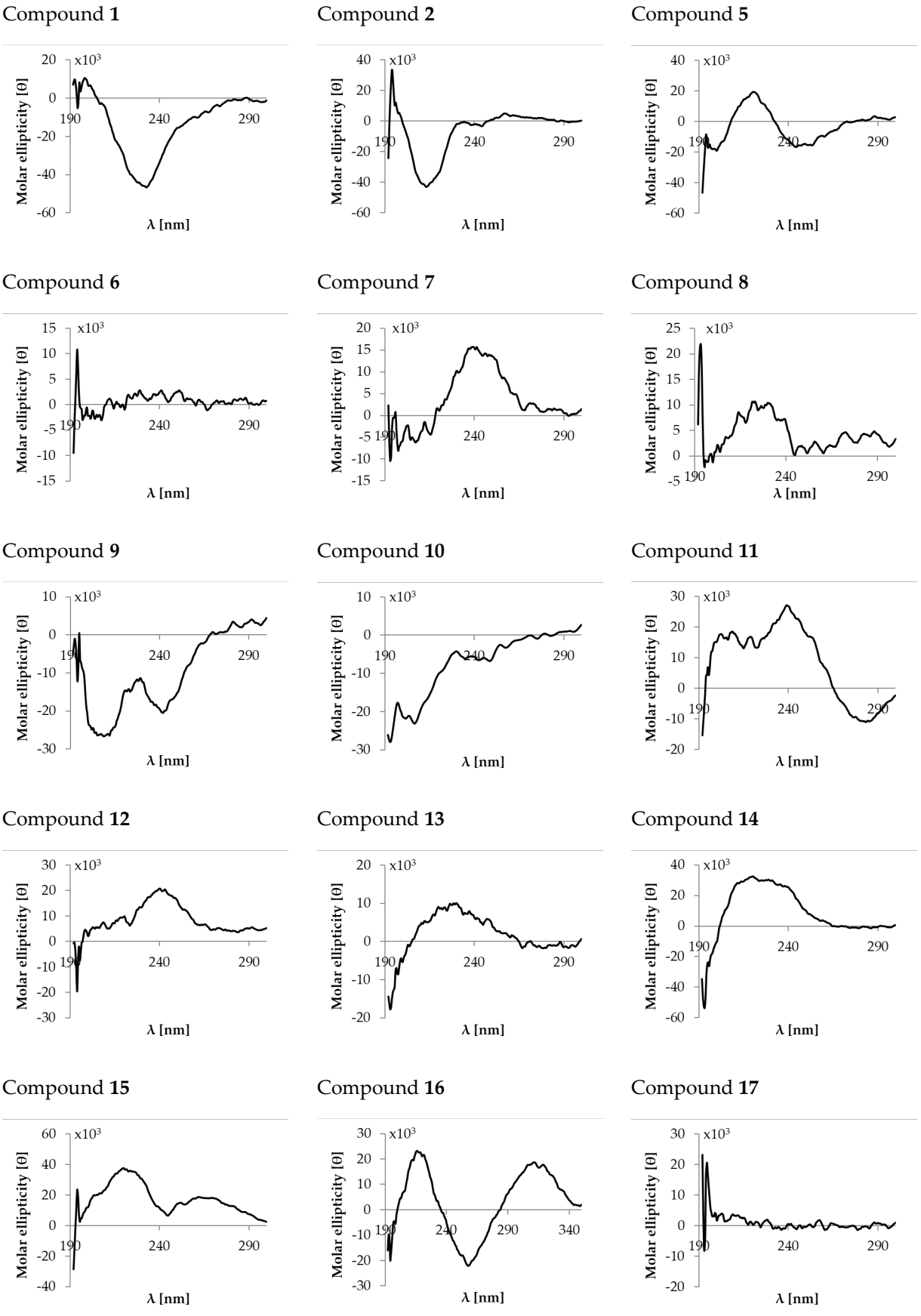
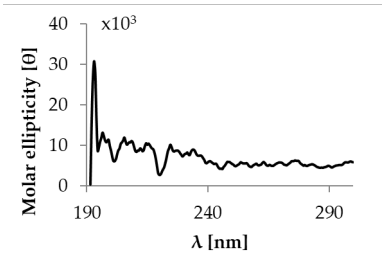
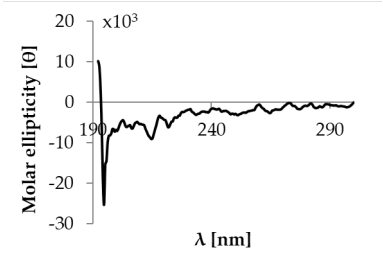


Figure S24. CD spectra of compounds **1**, **2**, **5–17** in MeOH, [θ] in [(°cm^2) x dmol^{-1}].

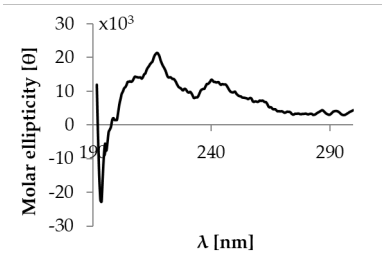
Compound **19**



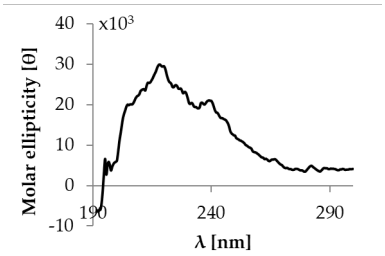
Compound (–)-**21**



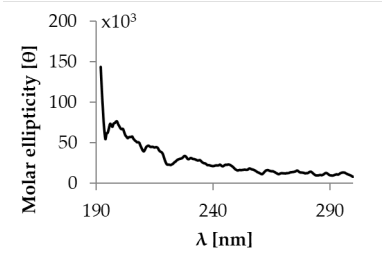
Compound **23**



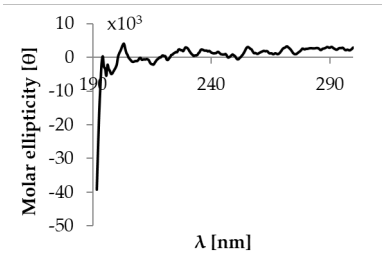
Compound **24**



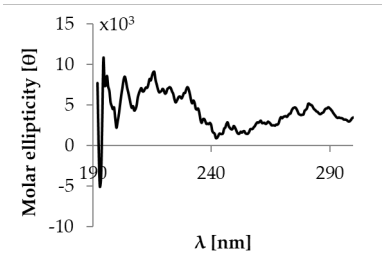
Compound **25**



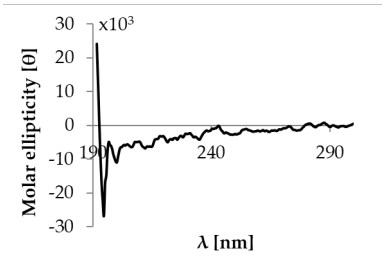
Compound **26**



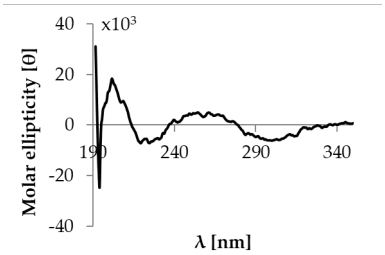
Compound **27**



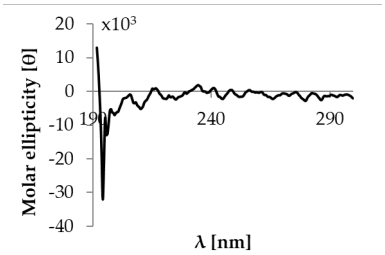
Compound **28**



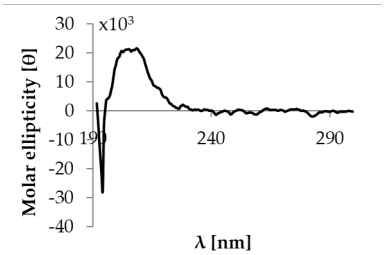
Compound **29**



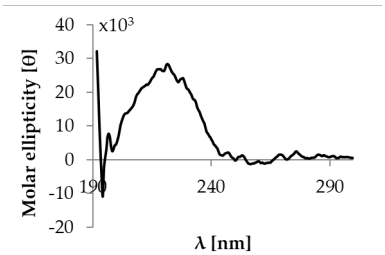
Compound **36**



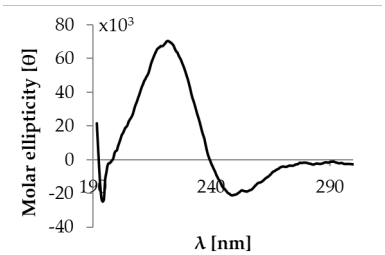
Compound **38**



Compound **39**



Compound **40**



Compound **41**

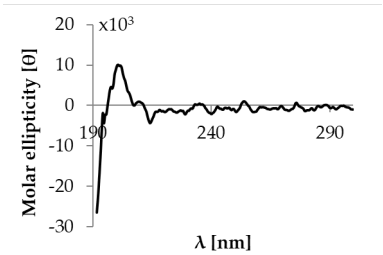


Figure S25. CD spectra of **19**, (–)-**21**, **23**–**29**, **36** and **38**–**41** in MeOH, [θ] in [(°cm^2) x dmol^{-1}].

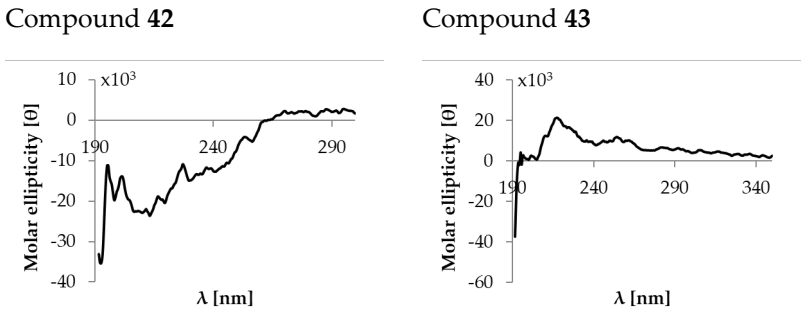


Figure S26. CD spectra of compounds **42** and **43** in MeOH, [θ] in [(°cm²) x dmol⁻¹].

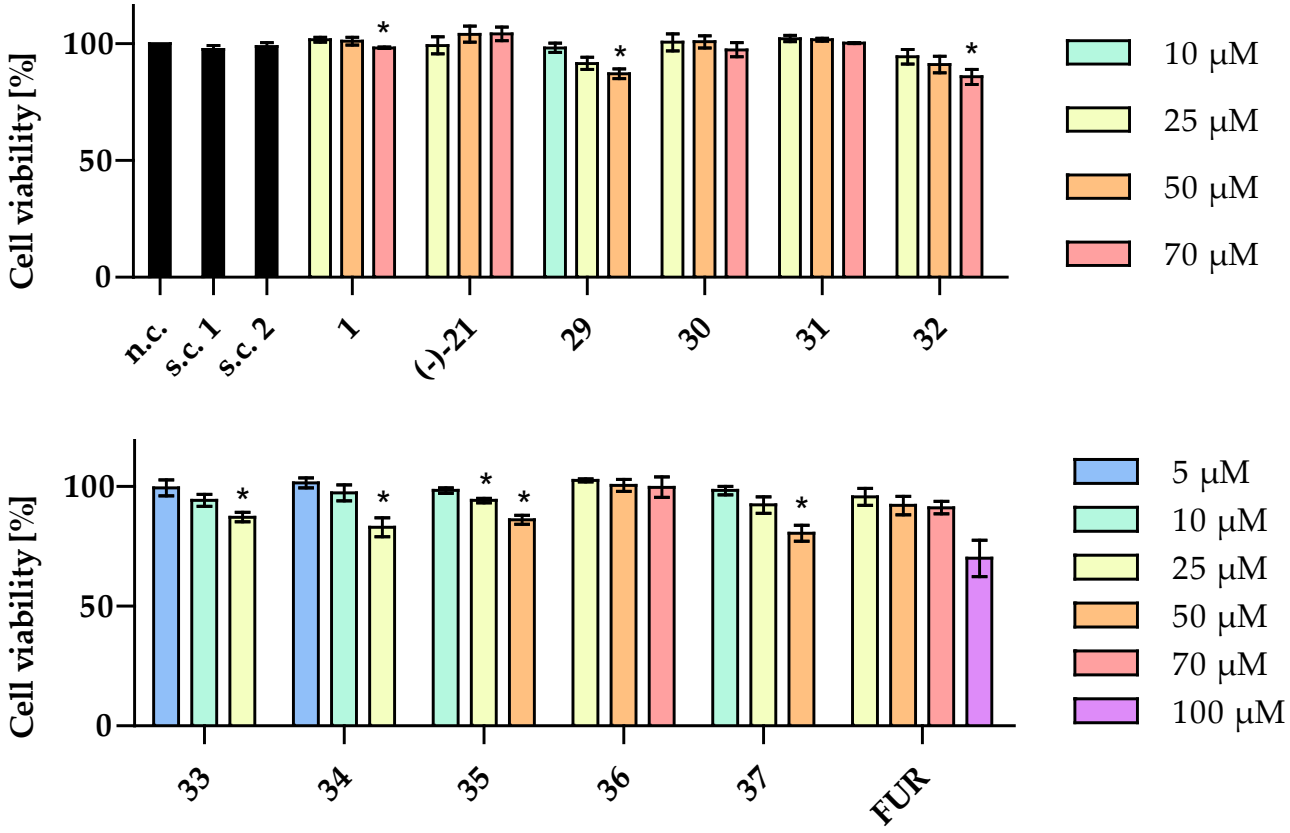


Figure S27. Influence of compounds **1**, (–)-**21**, **29**–**37** and furanoeudesma-1,3-diene (FUR) on the viability of RAW 264.7 cells in the MTT assay. The test was performed including a negative control (n.c., medium only) and two solvent controls (s.c. 1: 0.1% DMSO, s.c. 2: 0,14% DMSO, v/v). Data are presented as mean ± SEM, * $p < 0.05$ vs. n.c. (student's t-test, n=3).

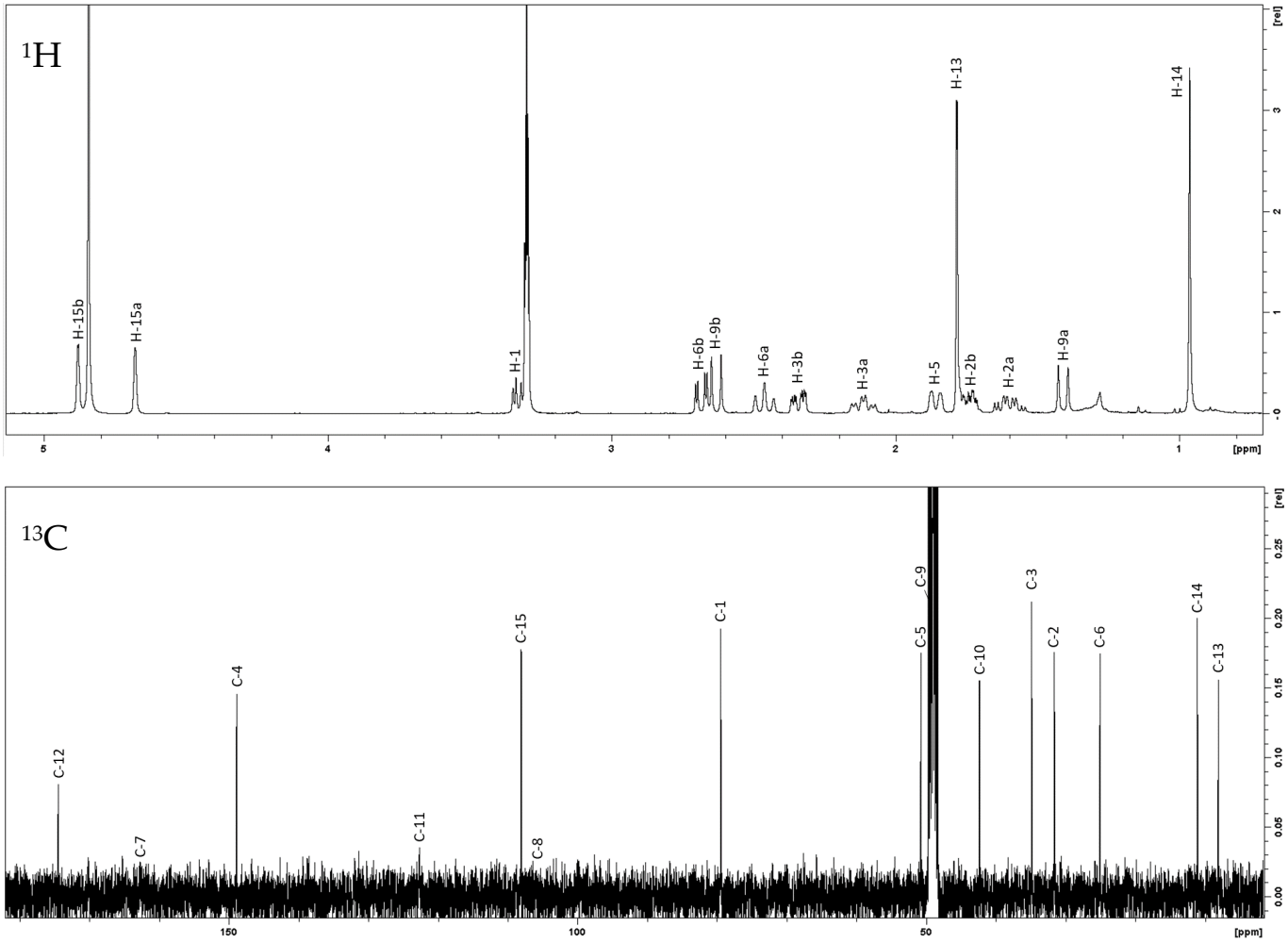


Figure S28. ^{1}H (400 MHz) and ^{13}C NMR (101 MHz) spectrum of compound (–)-**21** in CD_3OD.

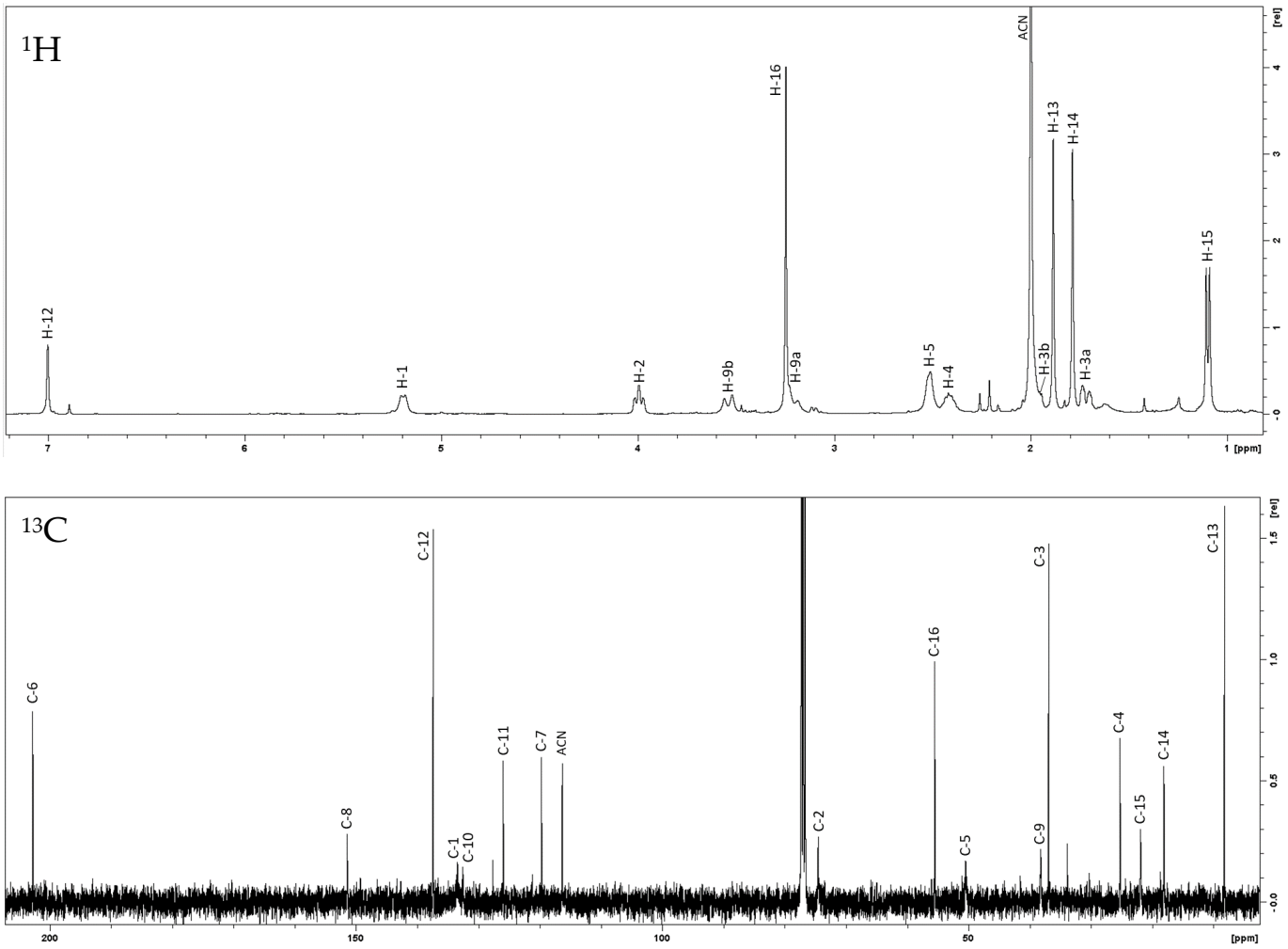


Figure S29. ^{1}H (400 MHz) and ^{13}C NMR (101 MHz) spectrum of compound **29** in $CDCl_3$.

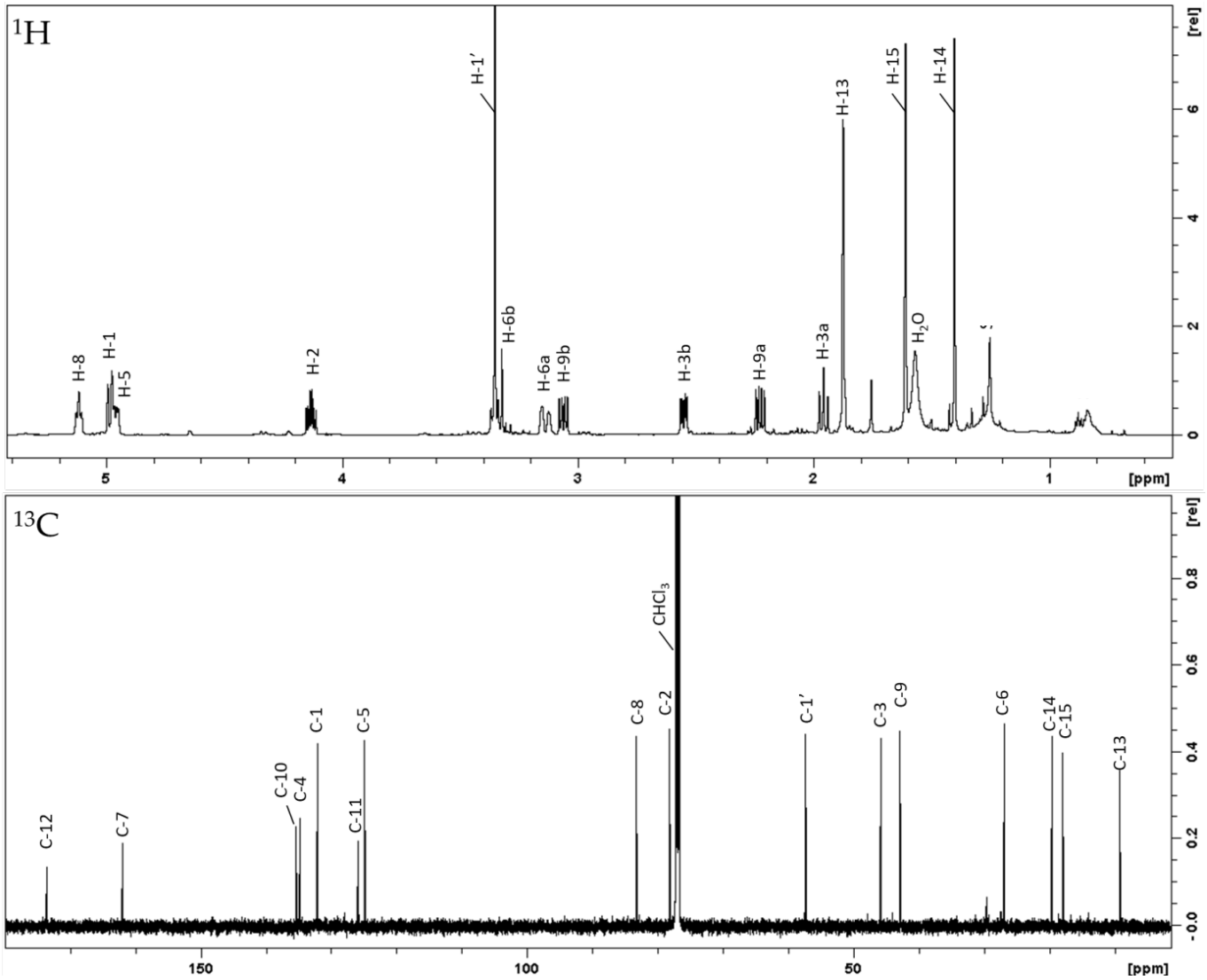


Figure S30. ^{1}H (600 MHz) and ^{13}C NMR (151 MHz) spectrum of compound **30** in $CDCl_3$.

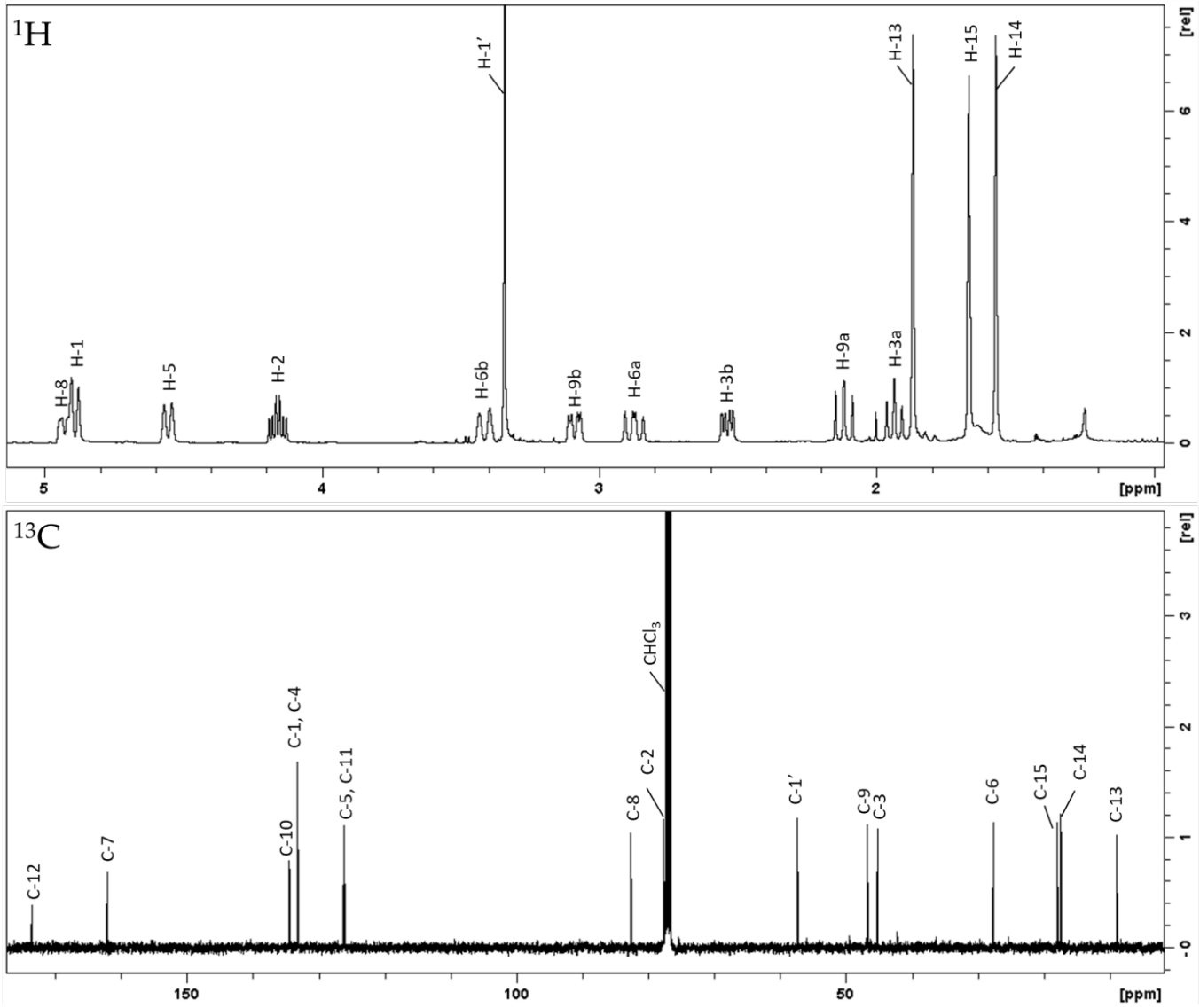


Figure S31. ^{1}H (400 MHz) and ^{13}C NMR (101 MHz) spectrum of compound **31** in $CDCl_3$.

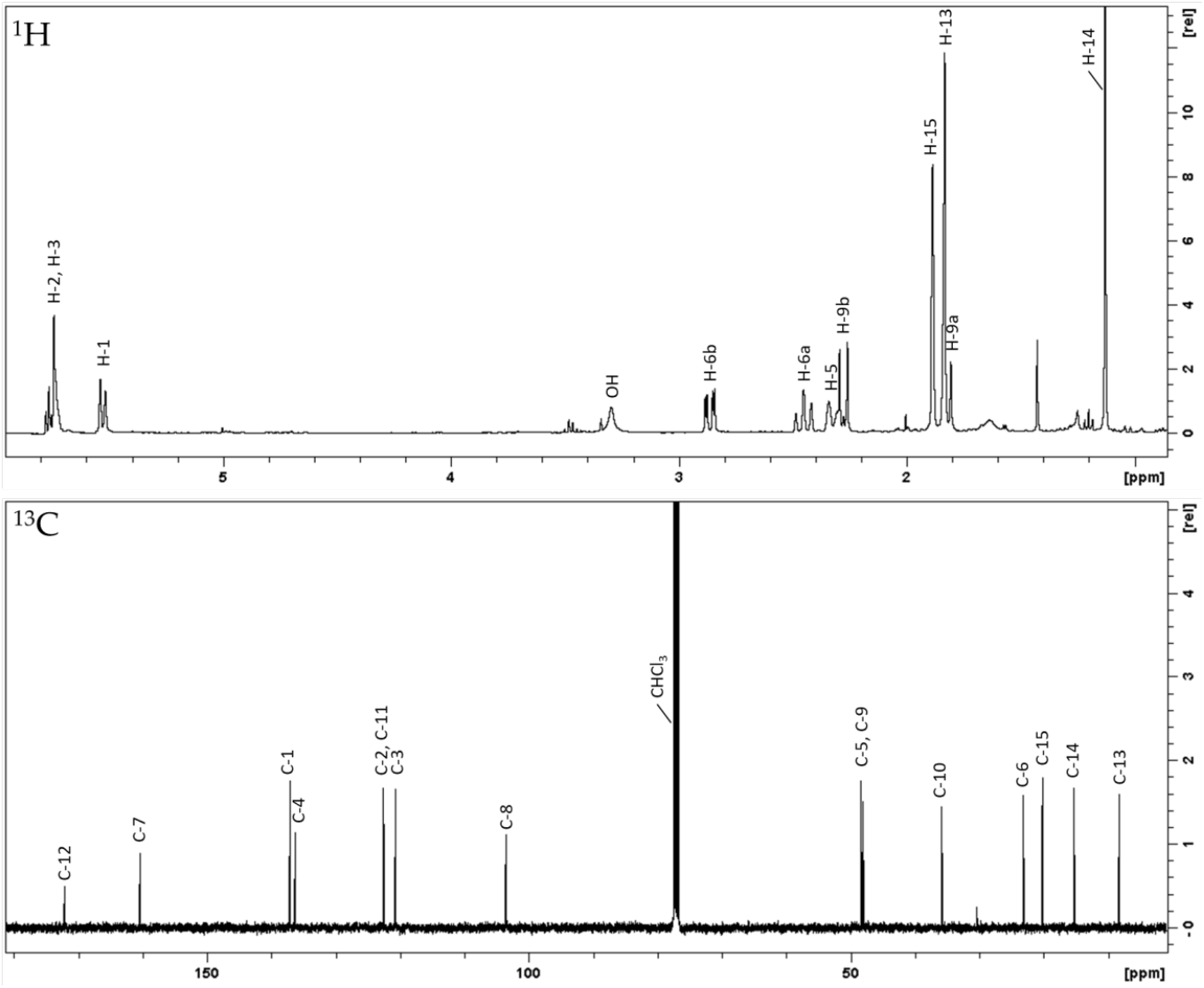


Figure S32. ^{1}H (400 MHz) and ^{13}C NMR (101 MHz) spectrum of compound **32** in $CDCl_3$.

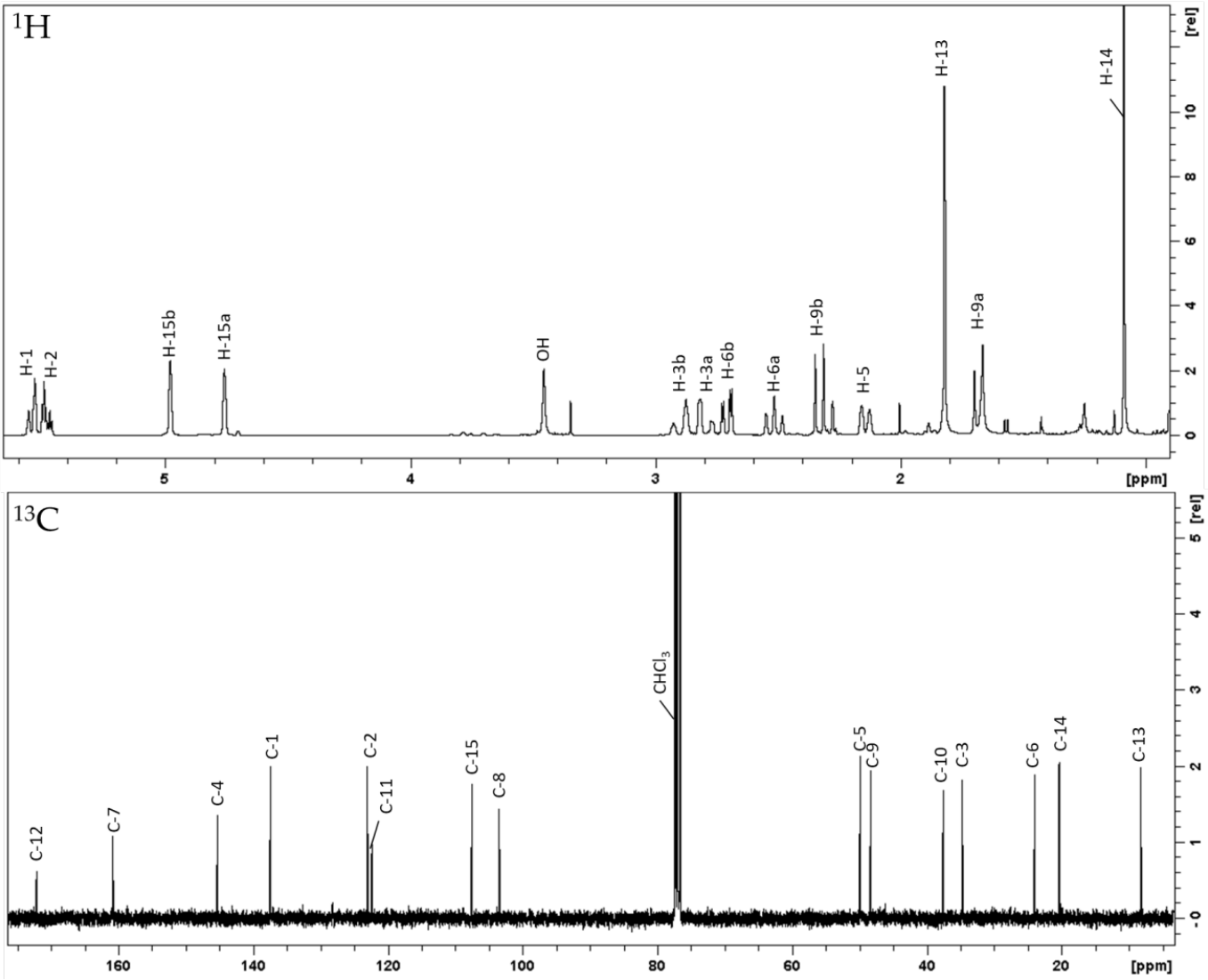


Figure S33. ^{1}H (400 MHz) and ^{13}C NMR (101 MHz) spectrum of compound **33** in $CDCl_3$.

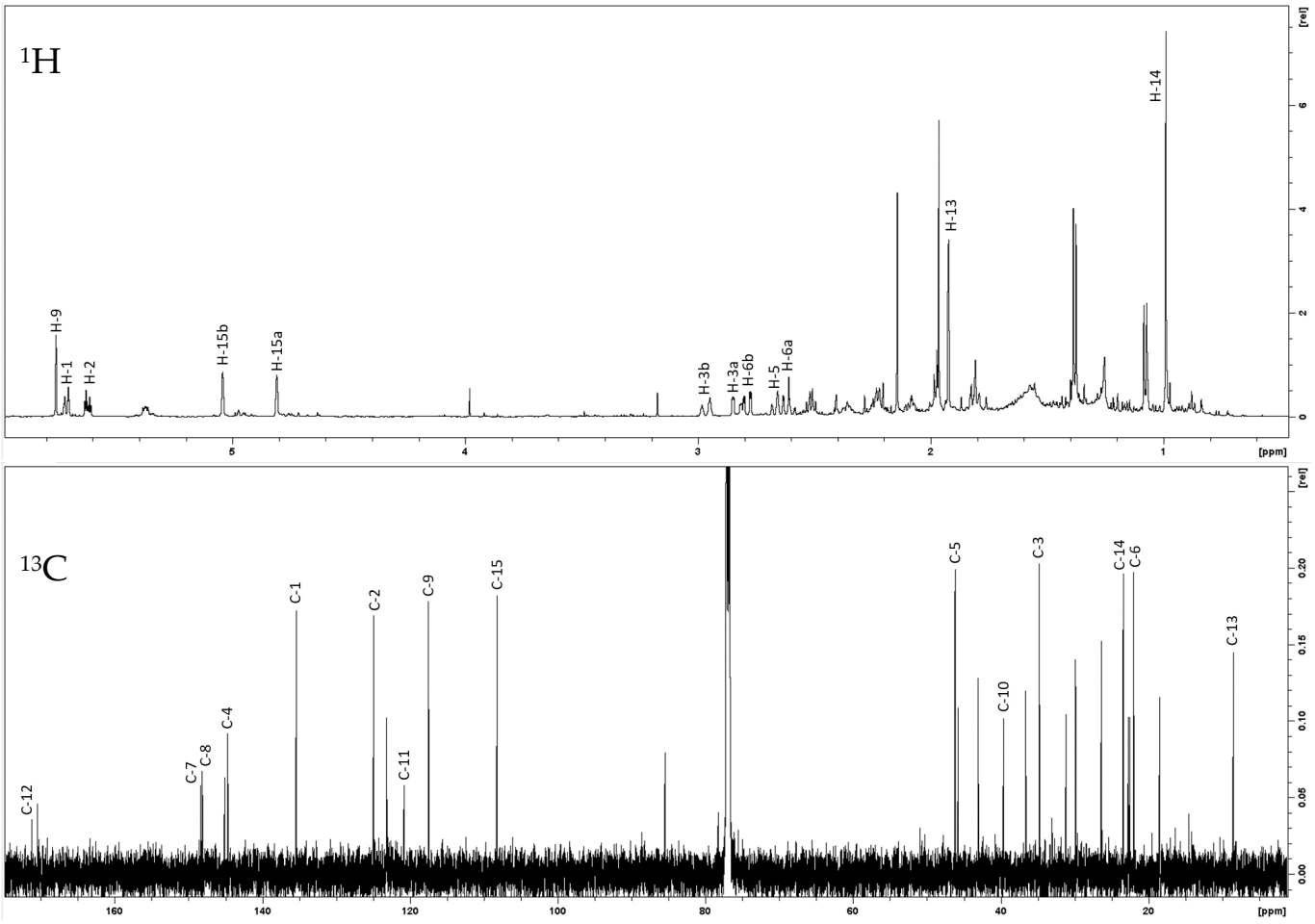


Figure S34. ^{1}H (600 MHz) and ^{13}C NMR (151 MHz) spectrum of compound **34** in $CDCl_3$.

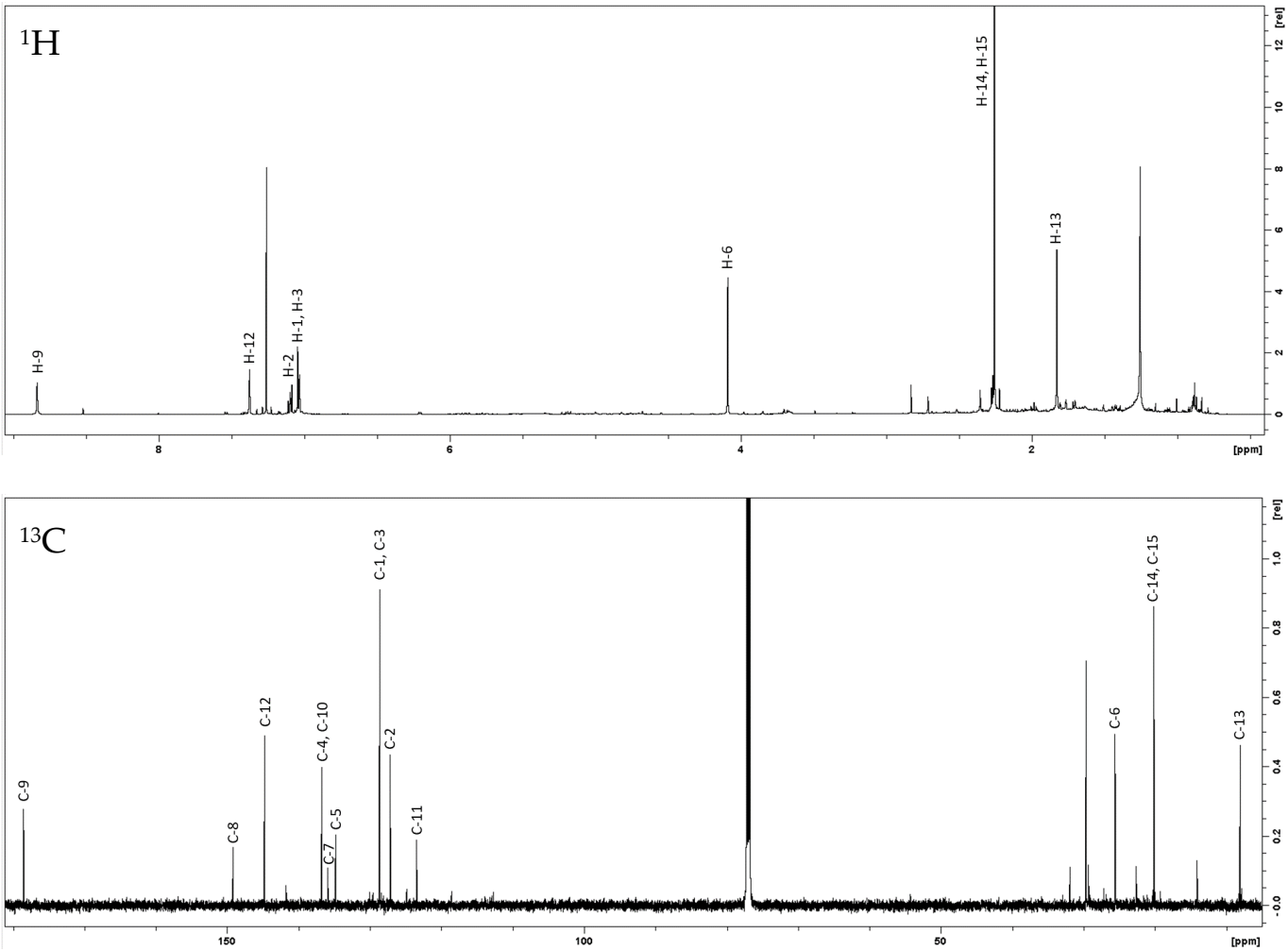


Figure S35. ^{1}H (600 MHz) and ^{13}C NMR (151 MHz) spectrum of compound **35** in $CDCl_3$.

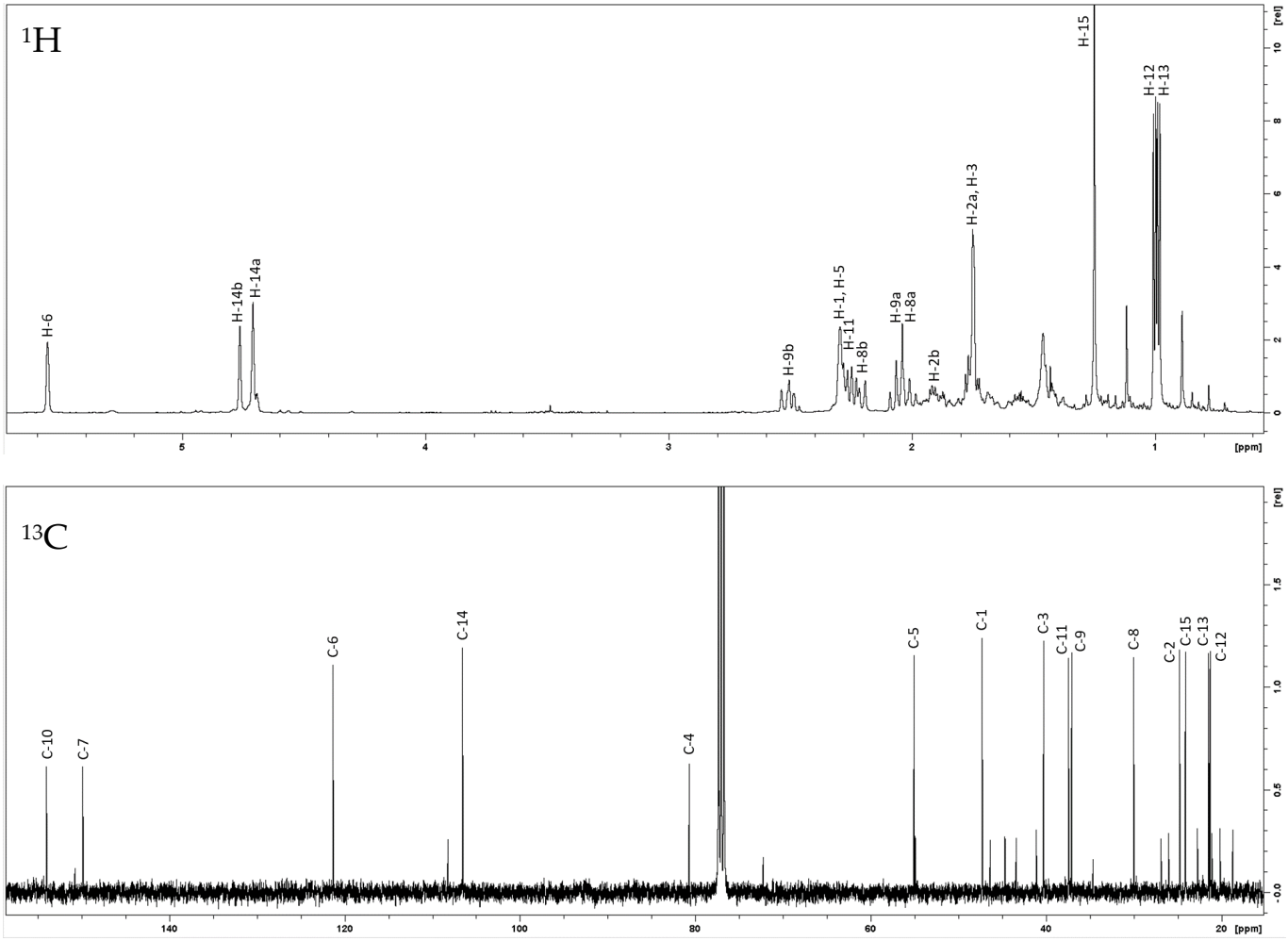


Figure S36. ^{1}H (400 MHz) and ^{13}C NMR (101 MHz) spectrum of compound **36** in $CDCl_3$.

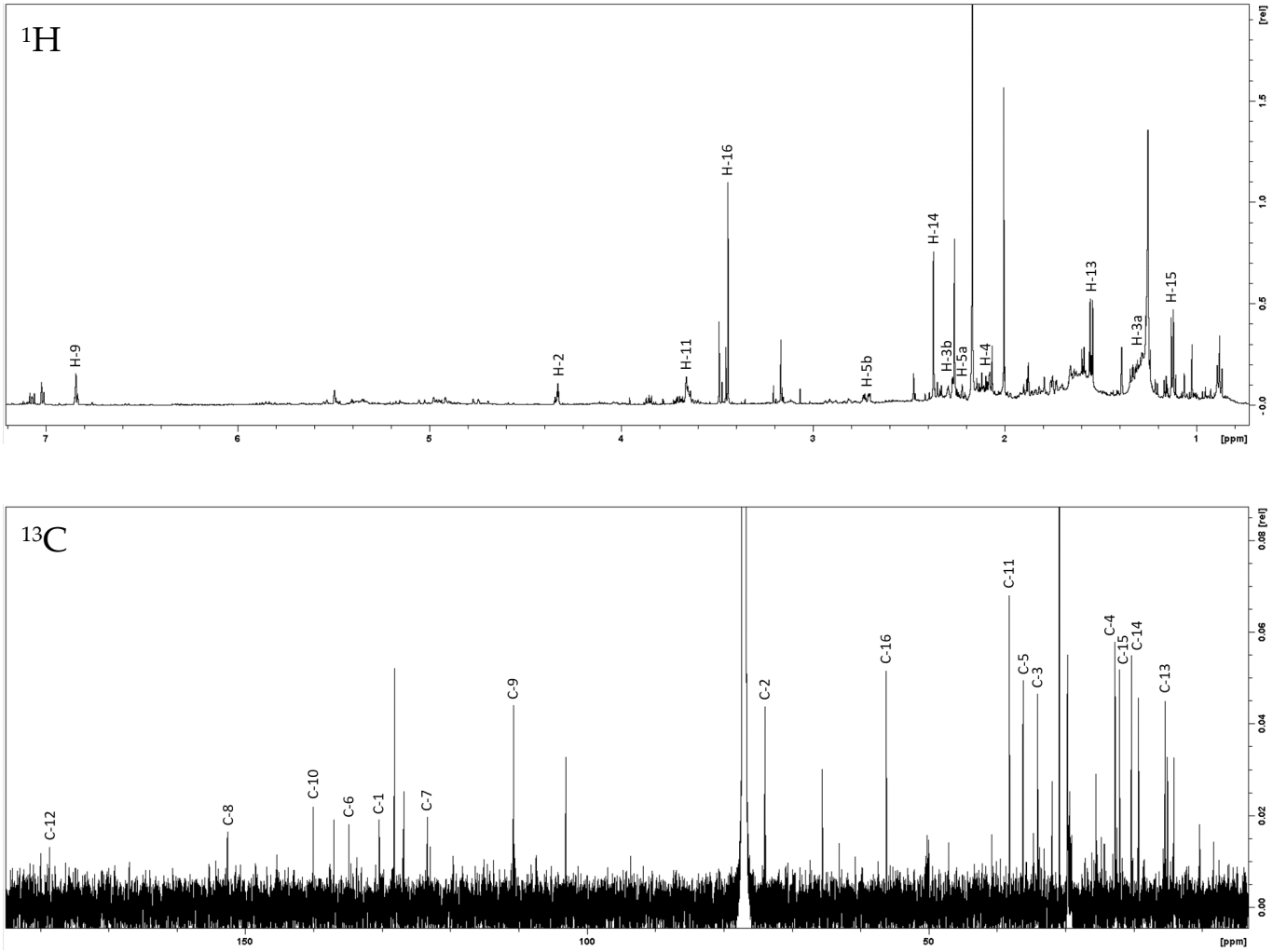


Figure S37. ^{1}H (600 MHz) and ^{13}C NMR (151 MHz) spectrum of compound **37** in $CDCl_3$.

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