

SUPPLEMENTARY INFORMATION

A Versatile Stereocontrolled Synthesis of 2-Deoxyiminosugar C-Glycosides and their Evaluation as Glycosidases Inhibitors

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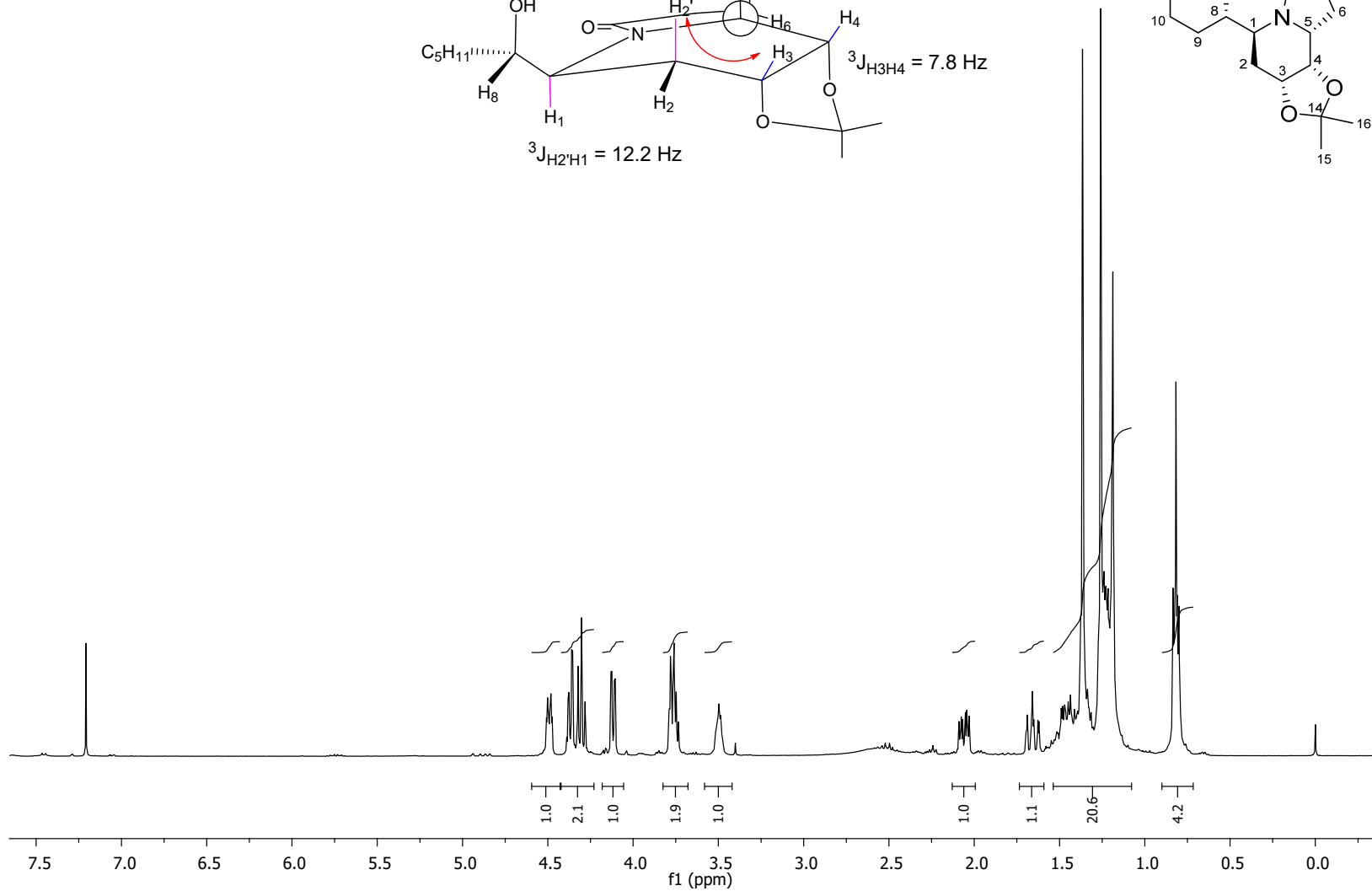
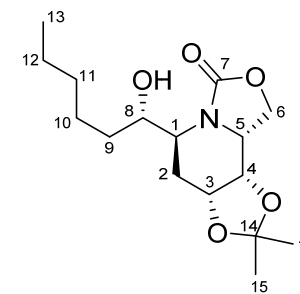
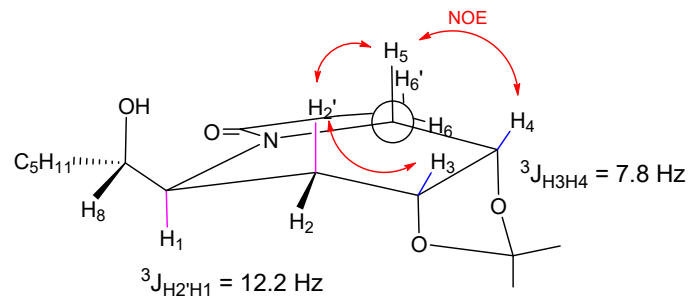
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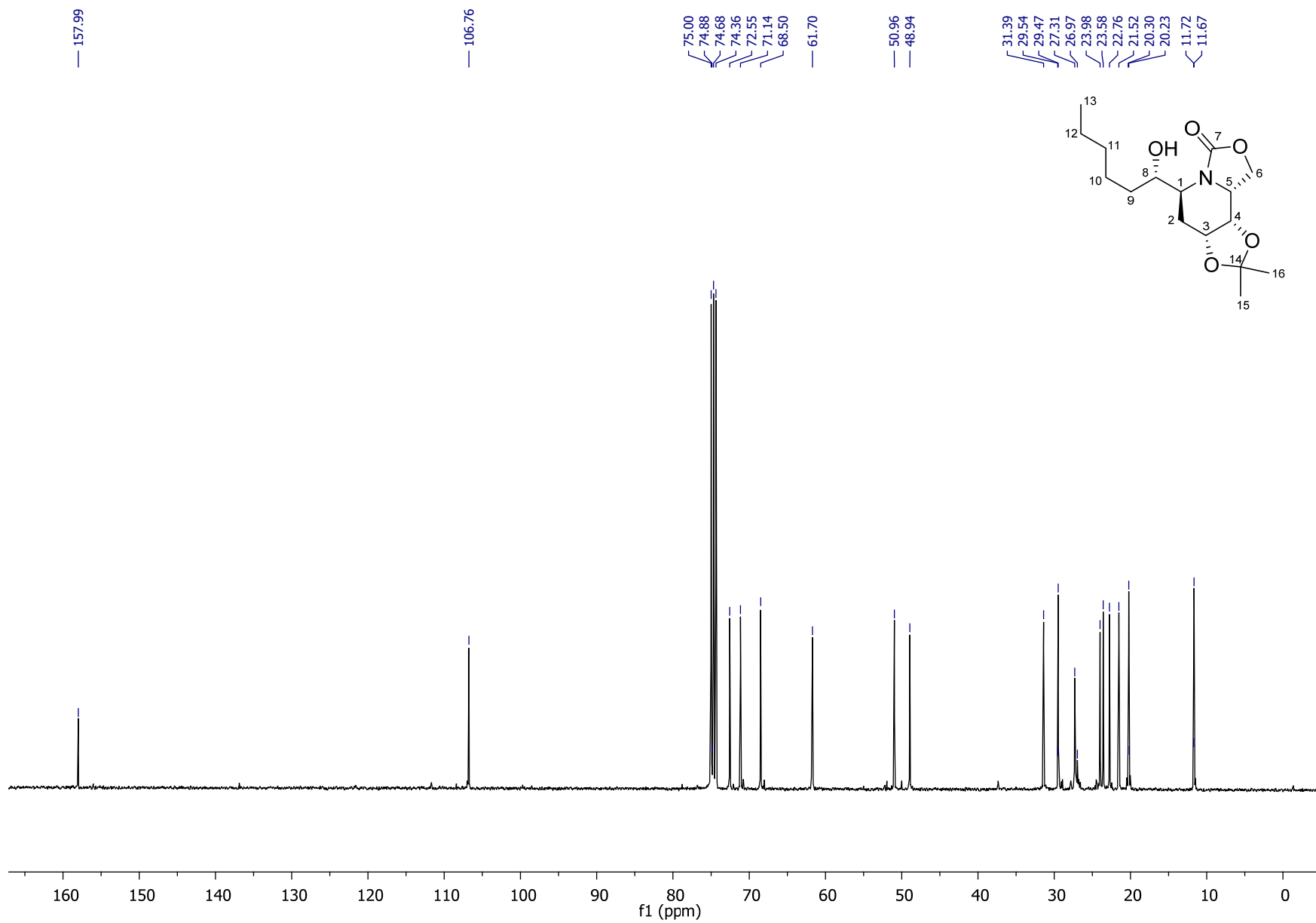
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1-NMR spectra and NOESY analysis

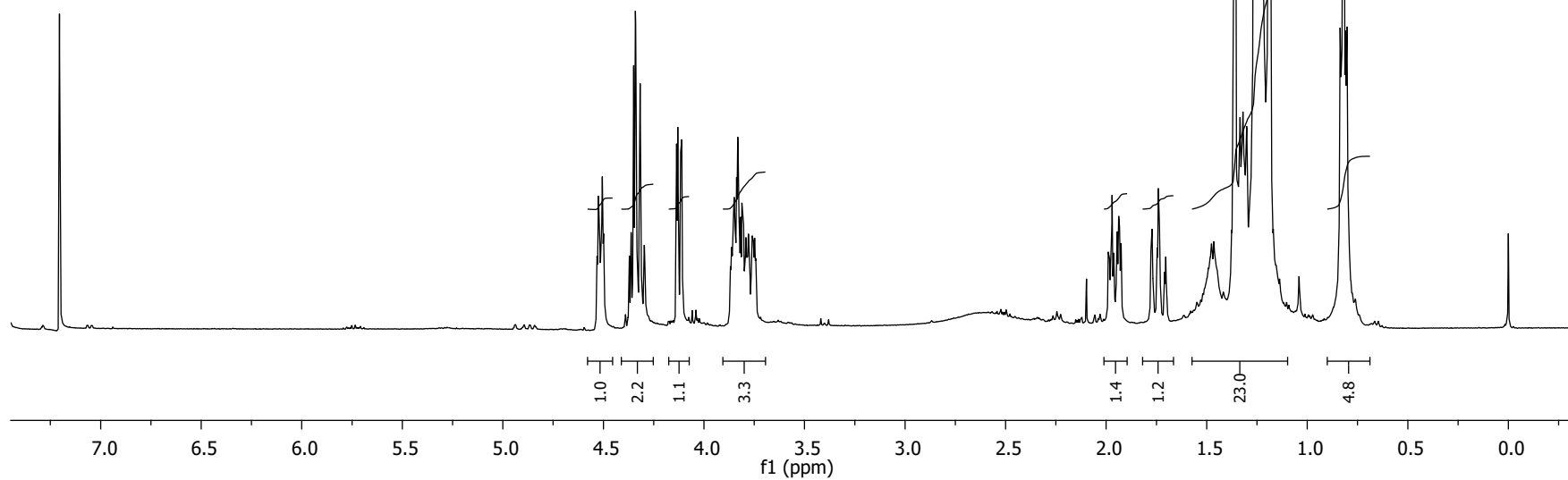
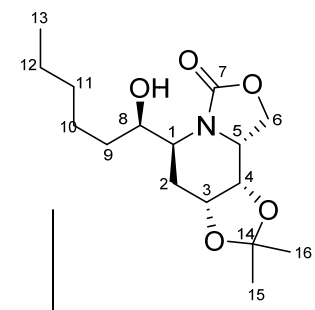
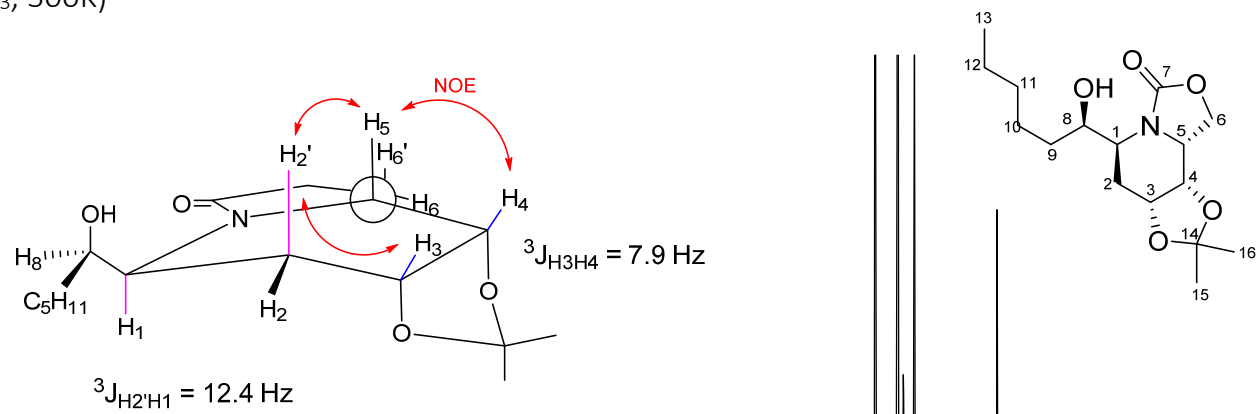
¹H NMR of compound 3 (400 MHz, CDCl₃, 300K)



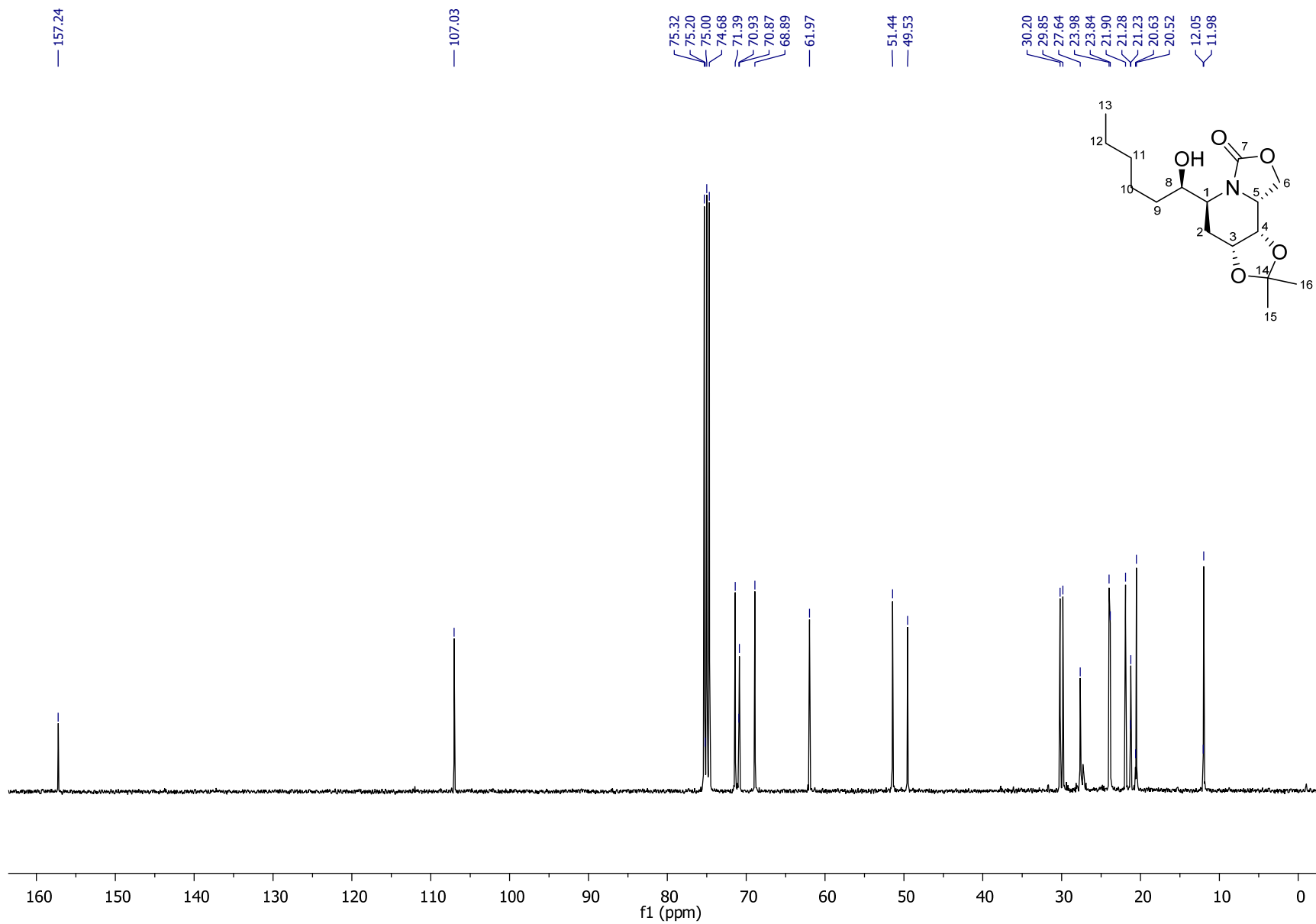
^{13}C NMR of compound **3** (100 MHz, CDCl_3 , 300K)



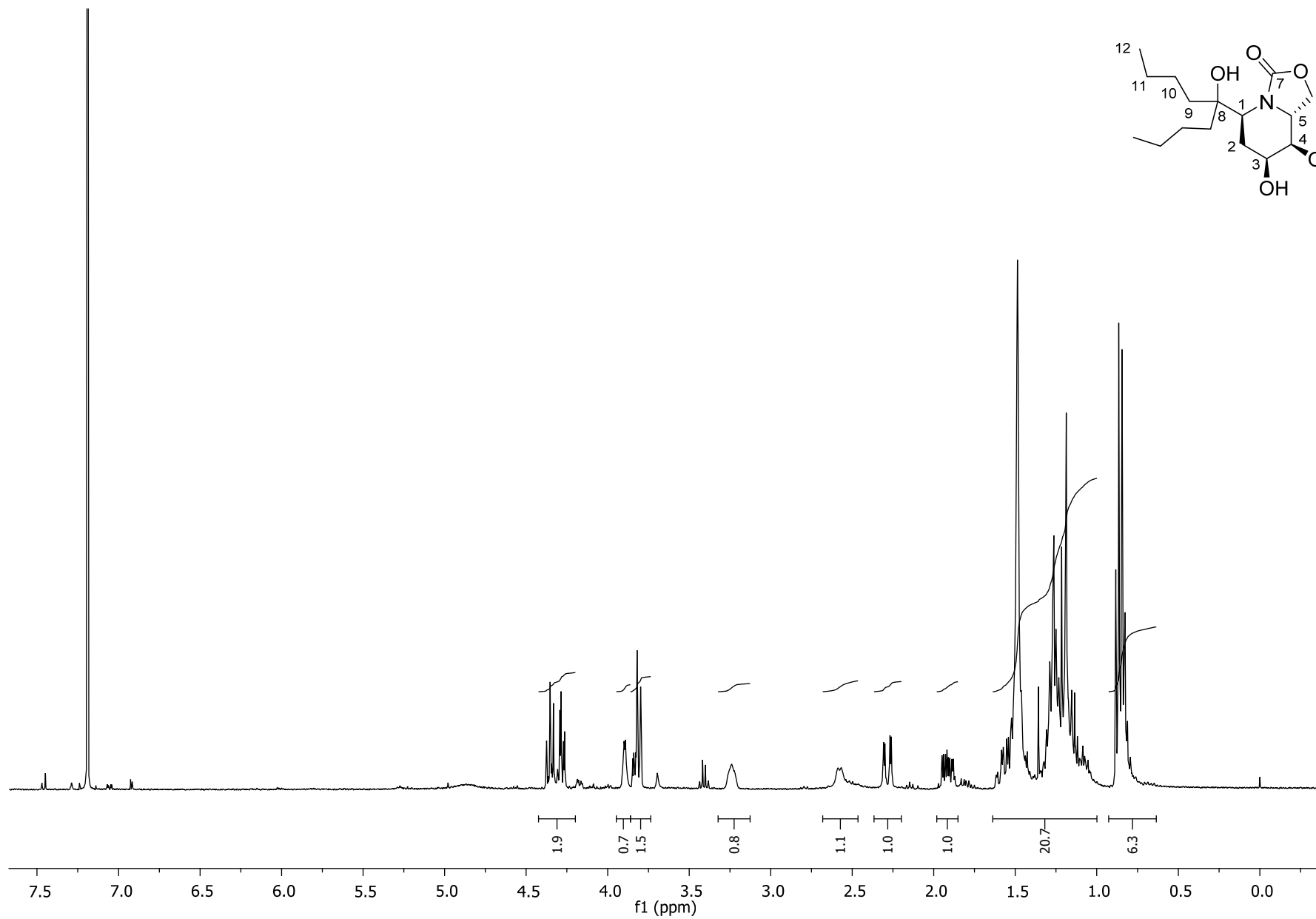
^1H NMR of compound **4** (400 MHz, CDCl_3 , 300K)



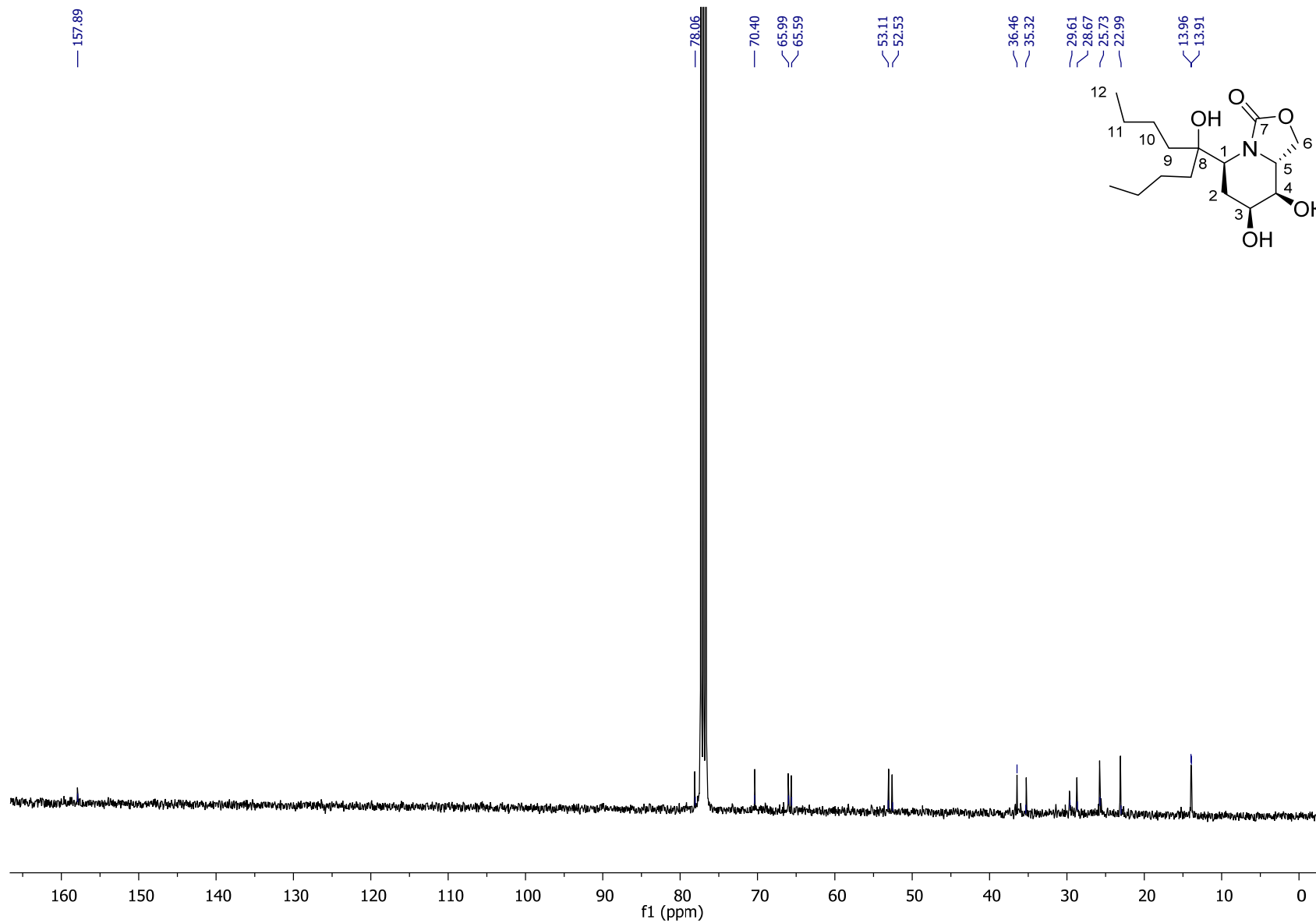
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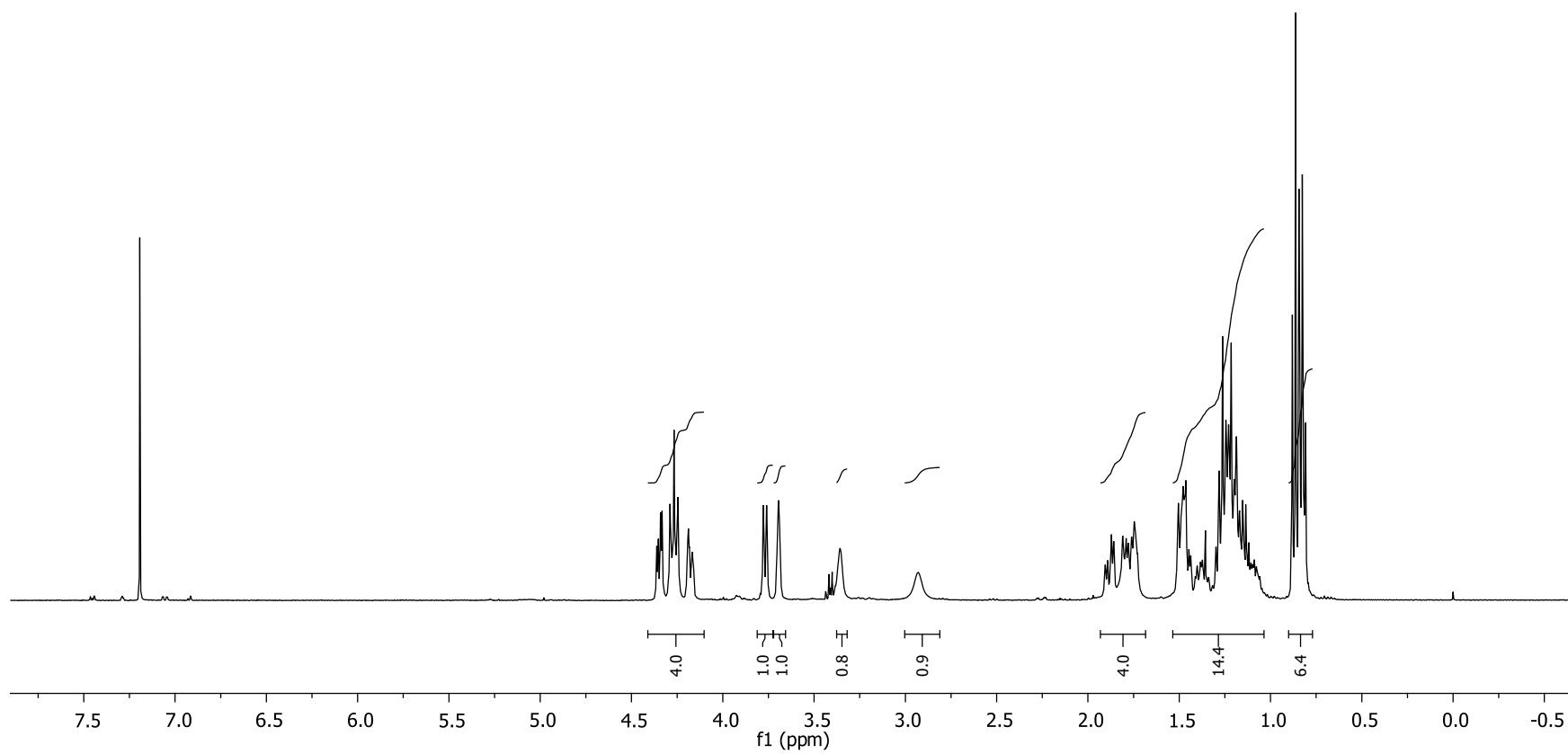
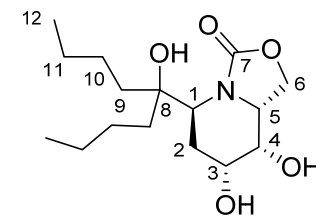
^1H NMR of compound **5-*exo*** (400 MHz, CDCl_3 , 300K)



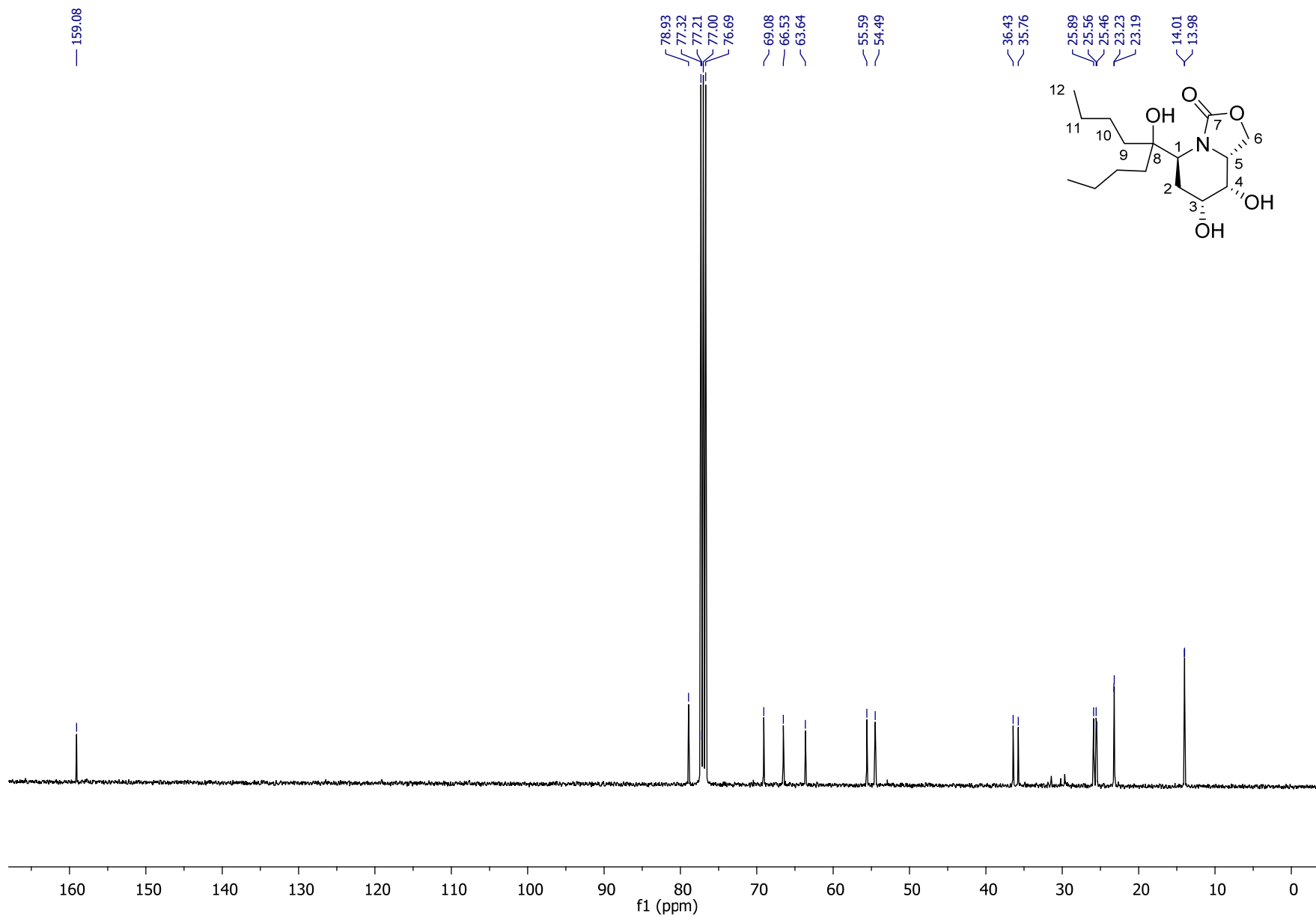
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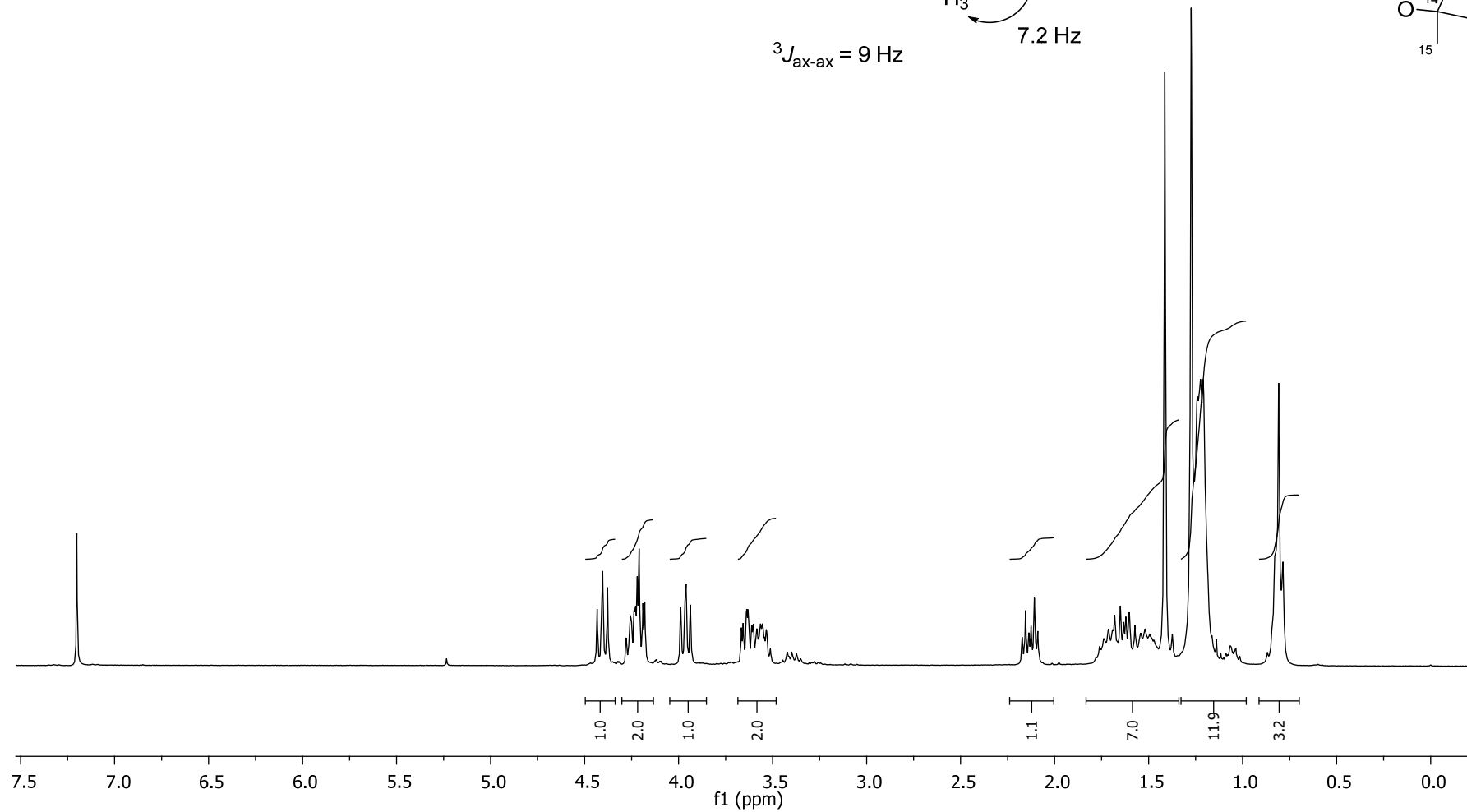
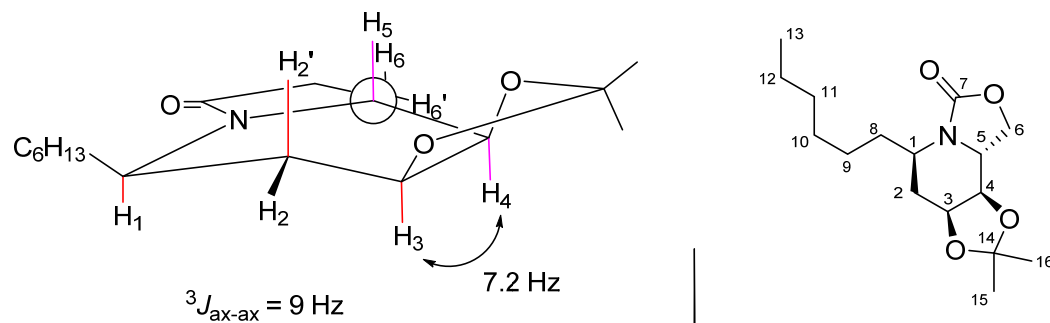
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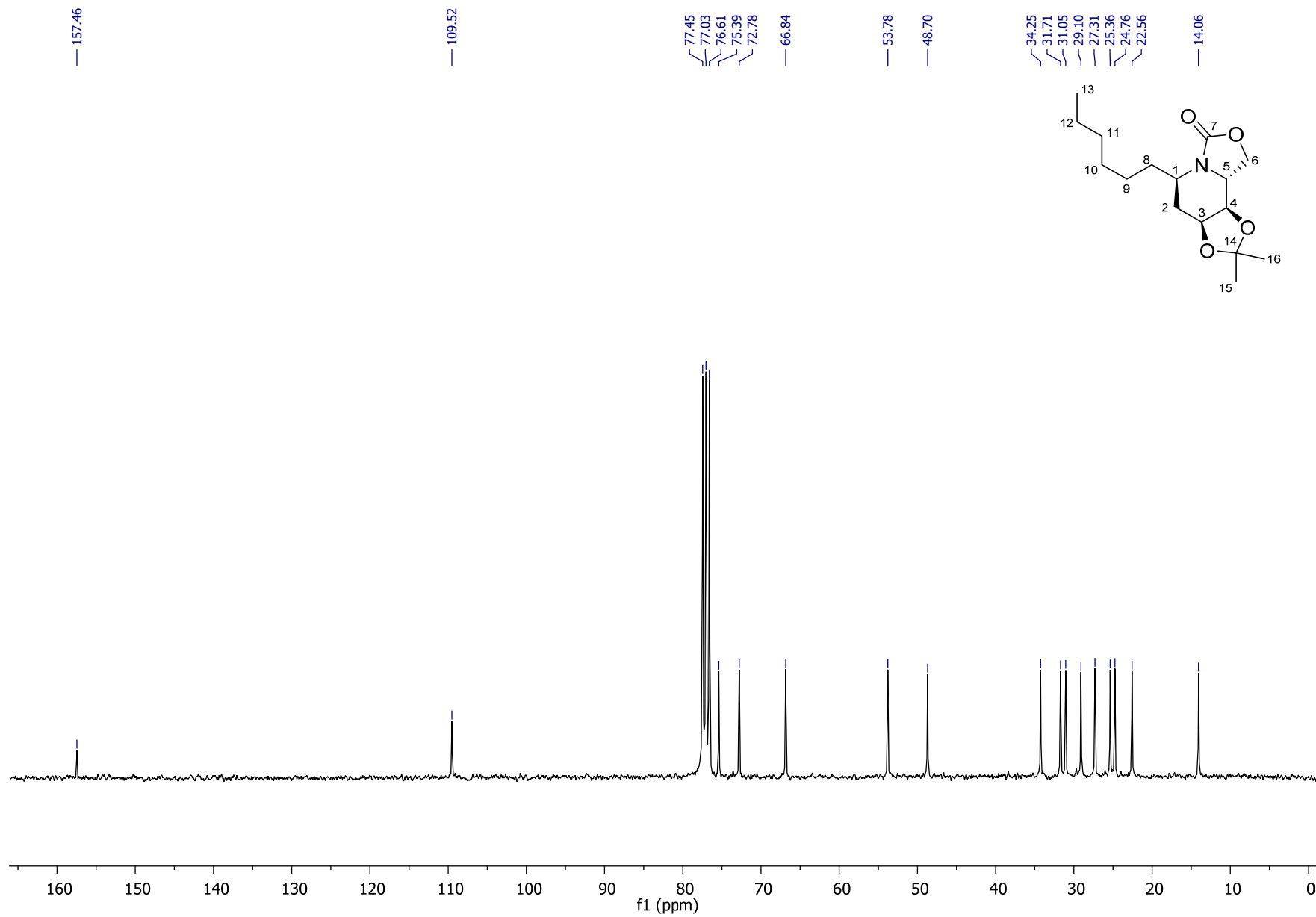
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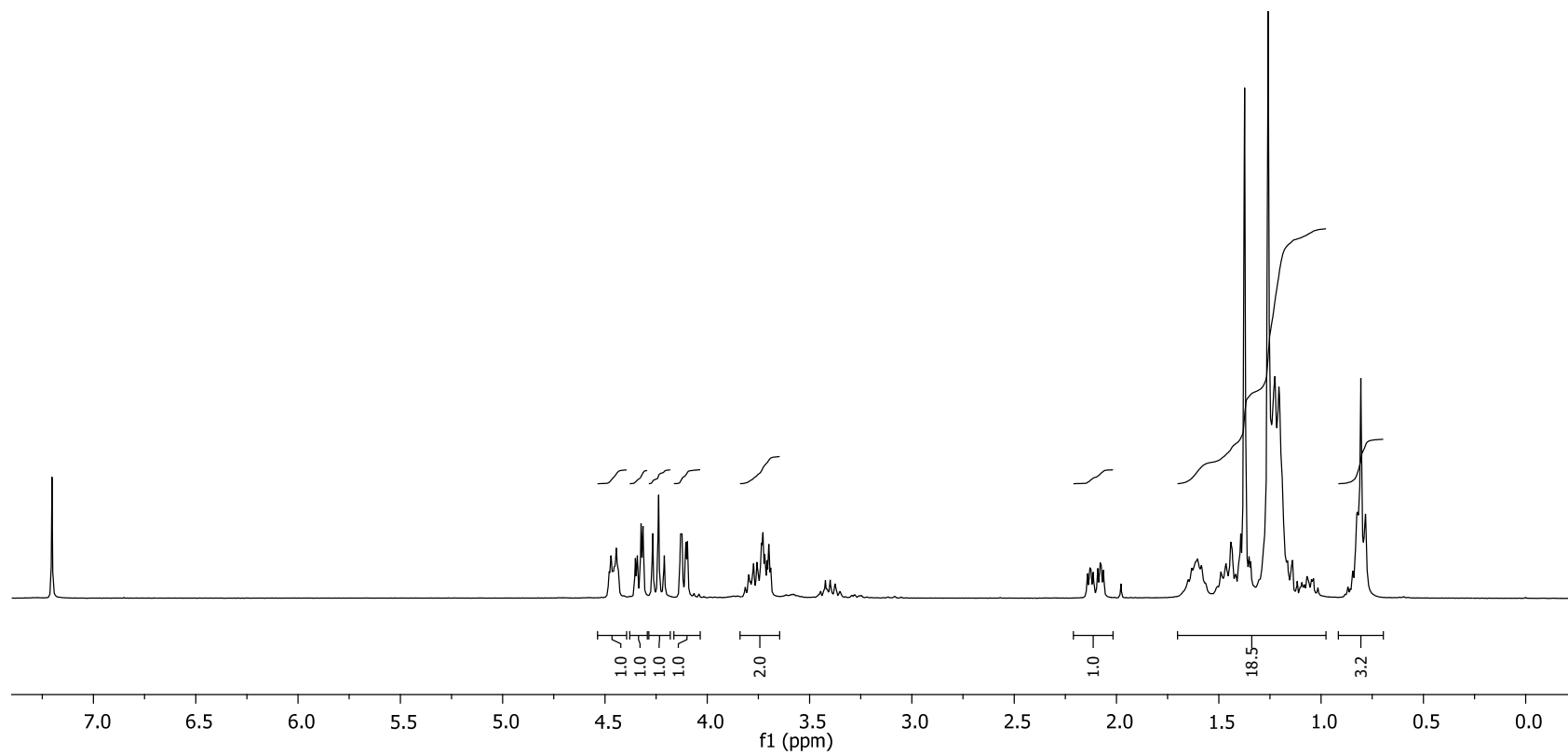
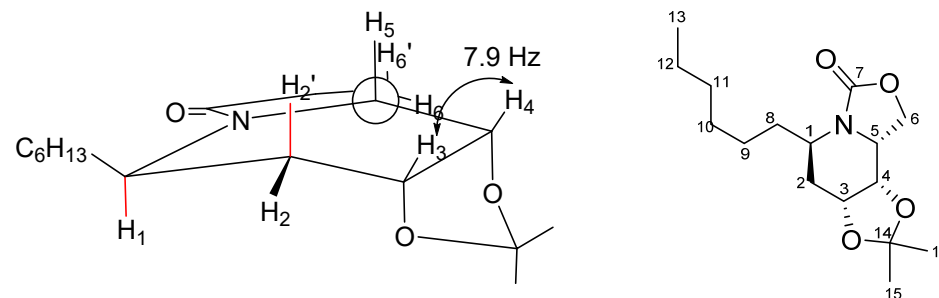
^1H NMR of compound **6-exo** (300 MHz, CDCl_3 , 300K)



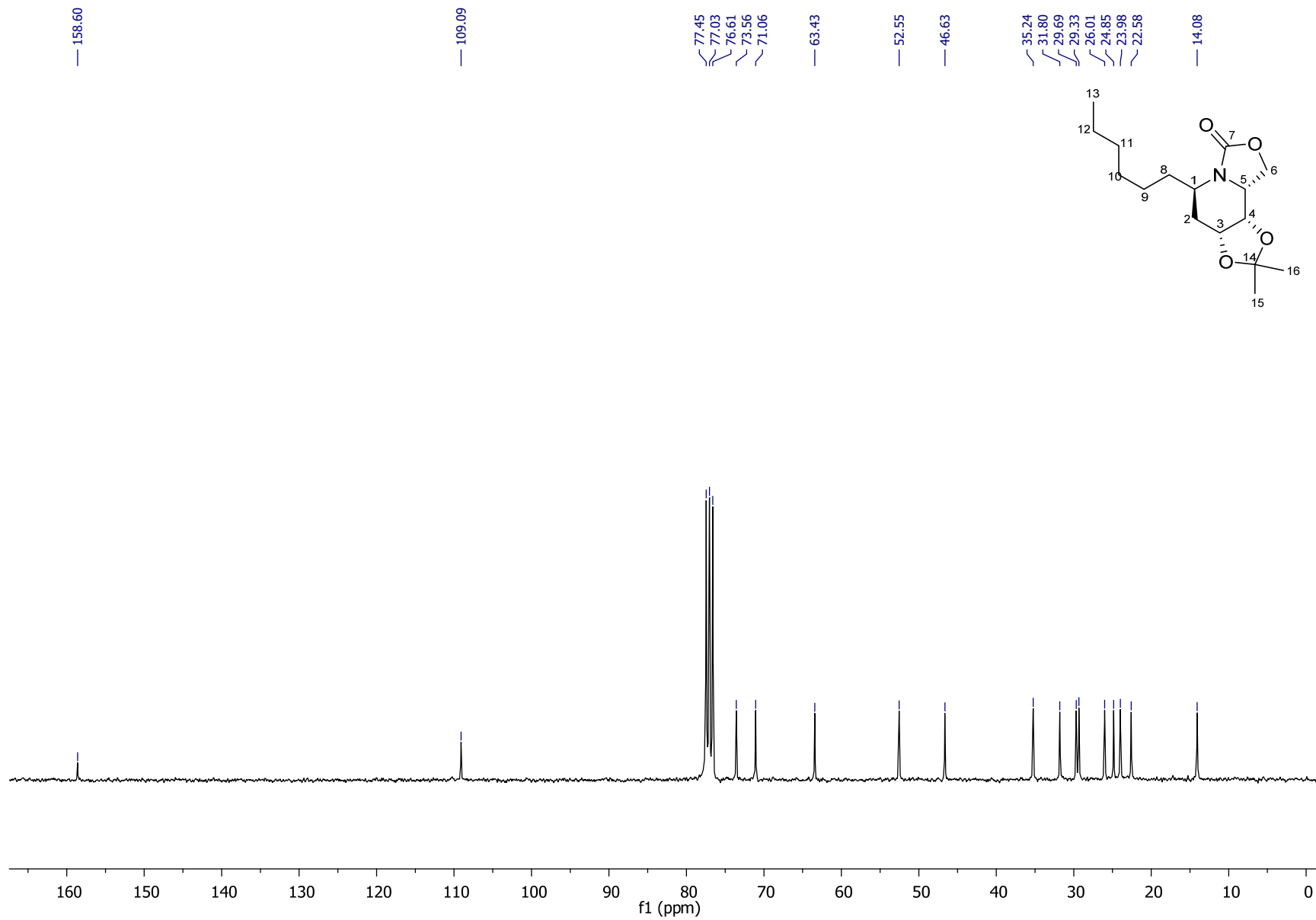
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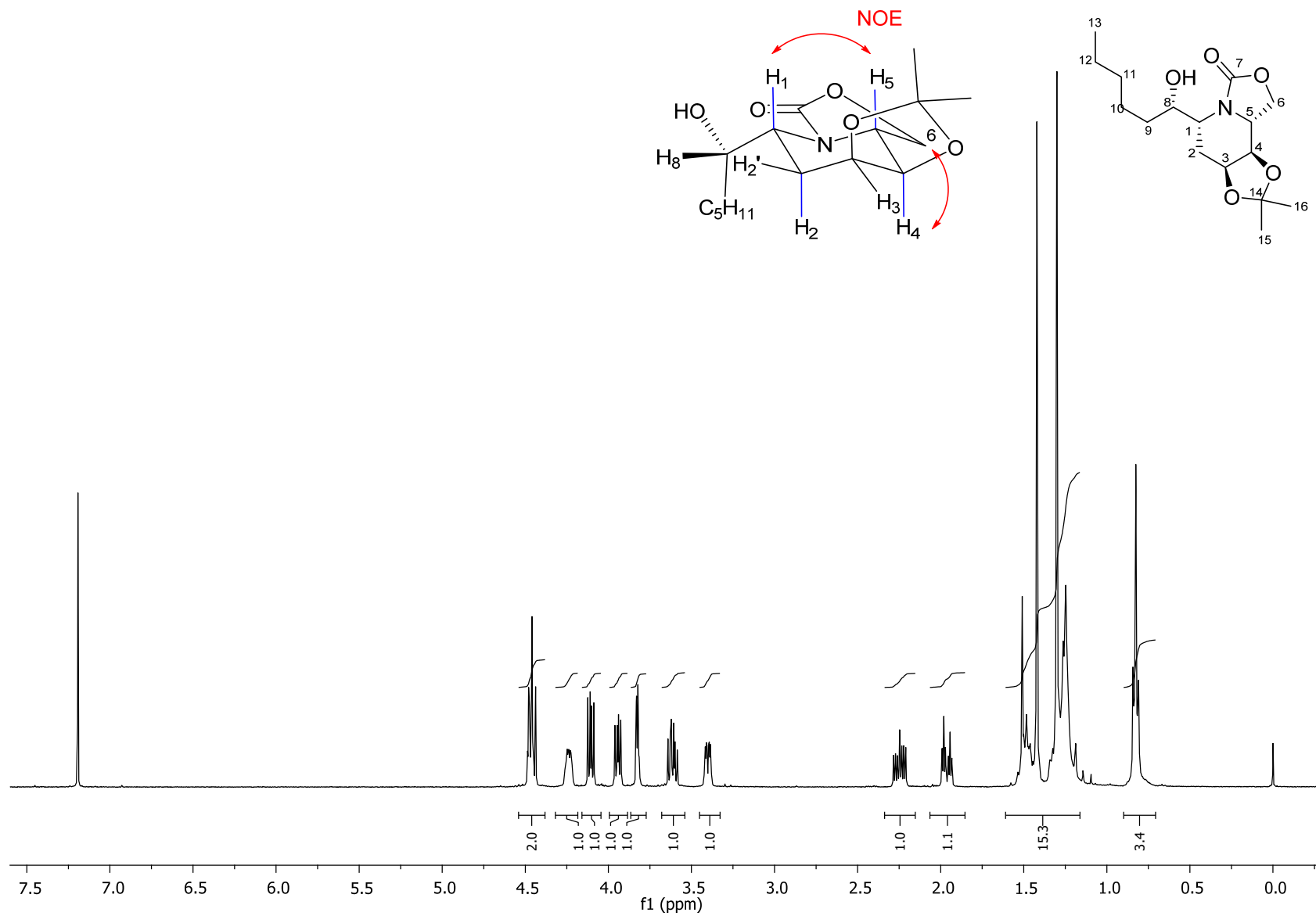
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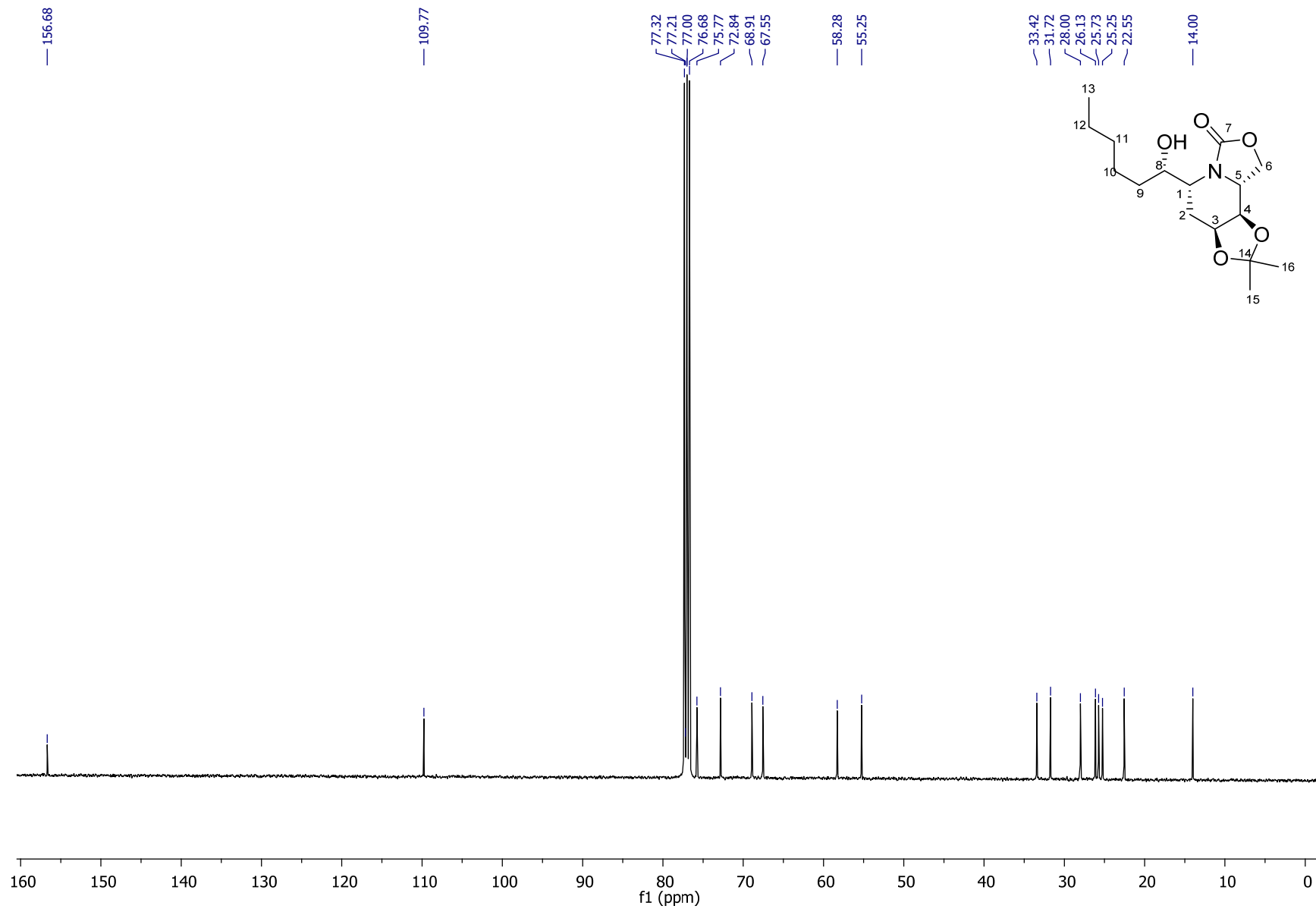
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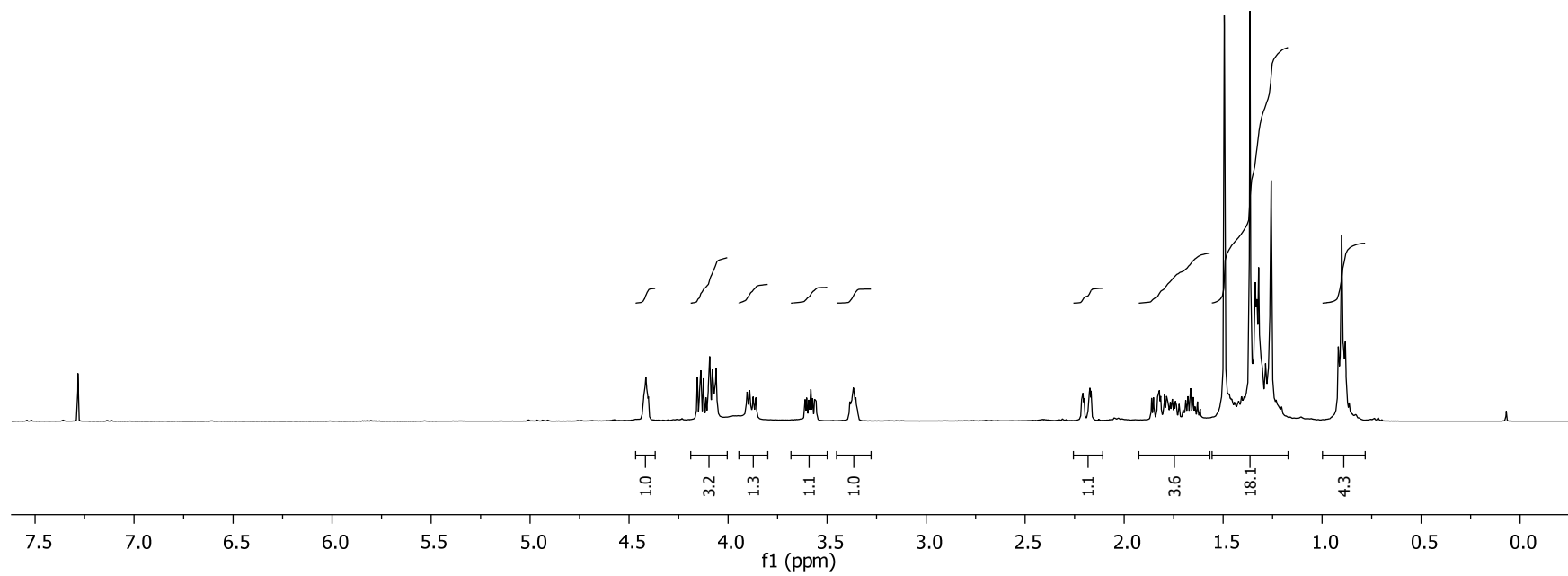
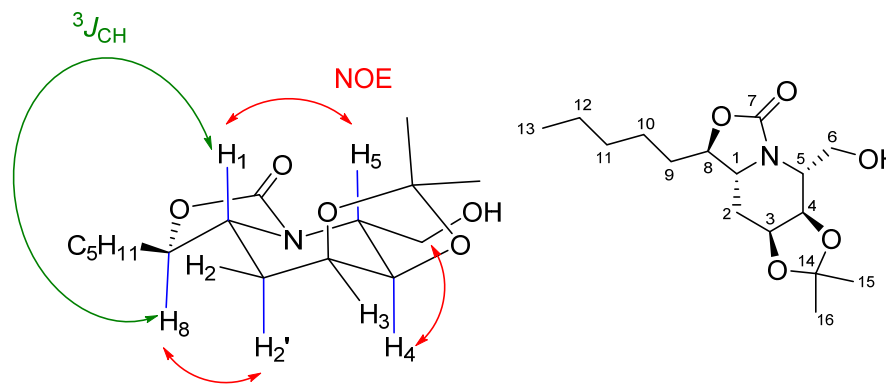
^1H NMR of compound **9** (400 MHz, CDCl_3 , 300K)



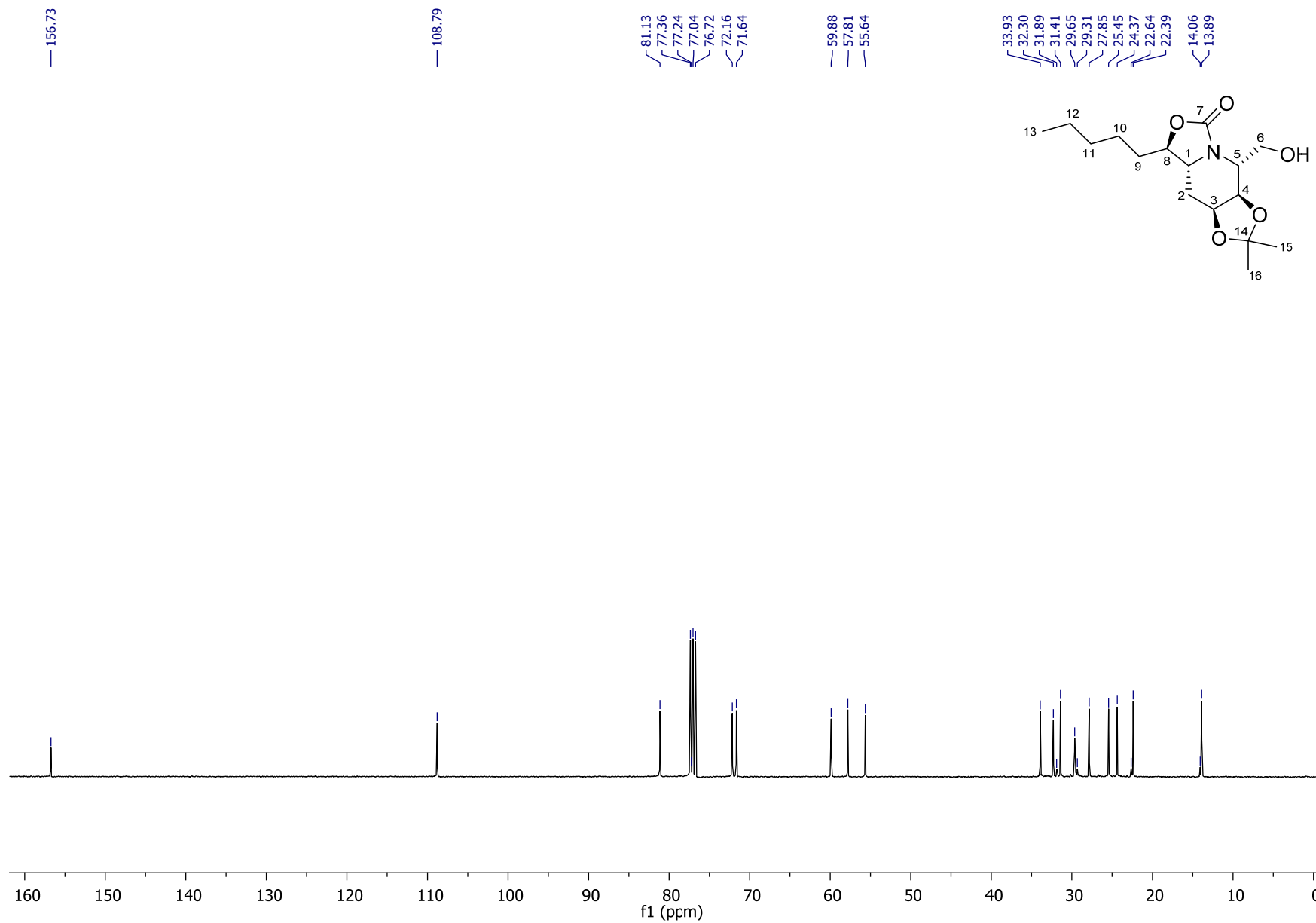
^{13}C NMR of compound **9** (100 MHz, CDCl_3 , 300K)



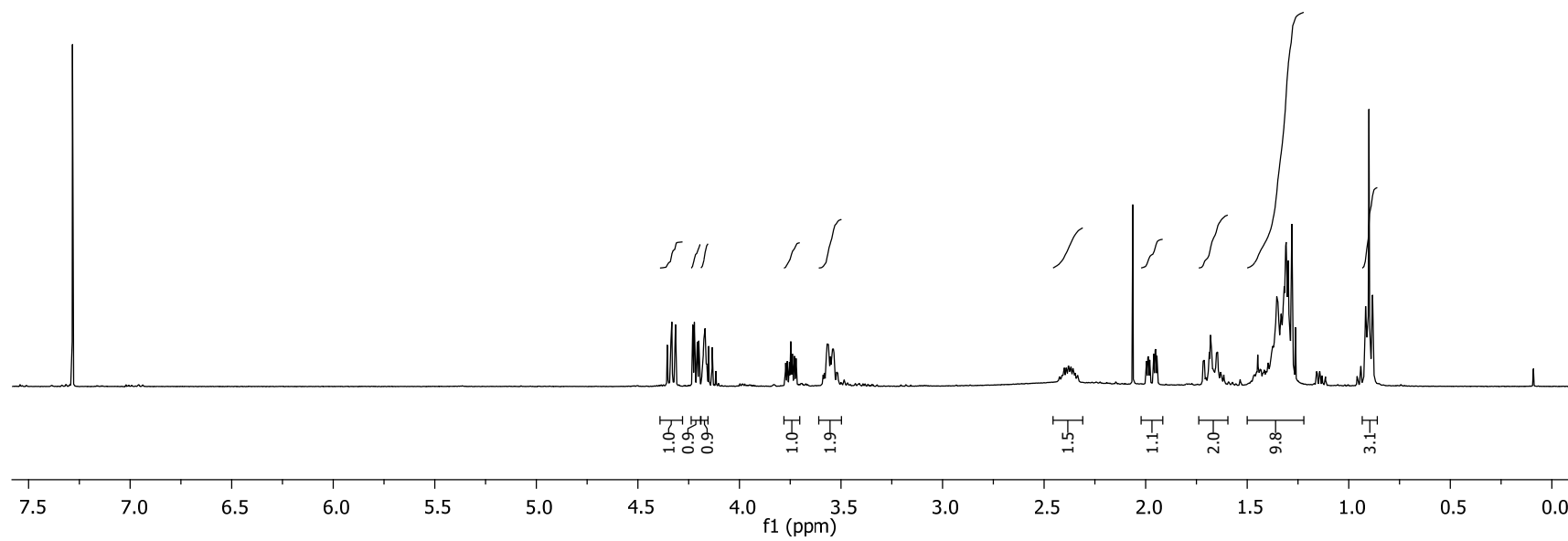
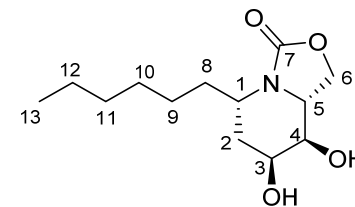
^1H NMR of compound **10** (400 MHz, CDCl_3 , 300K)



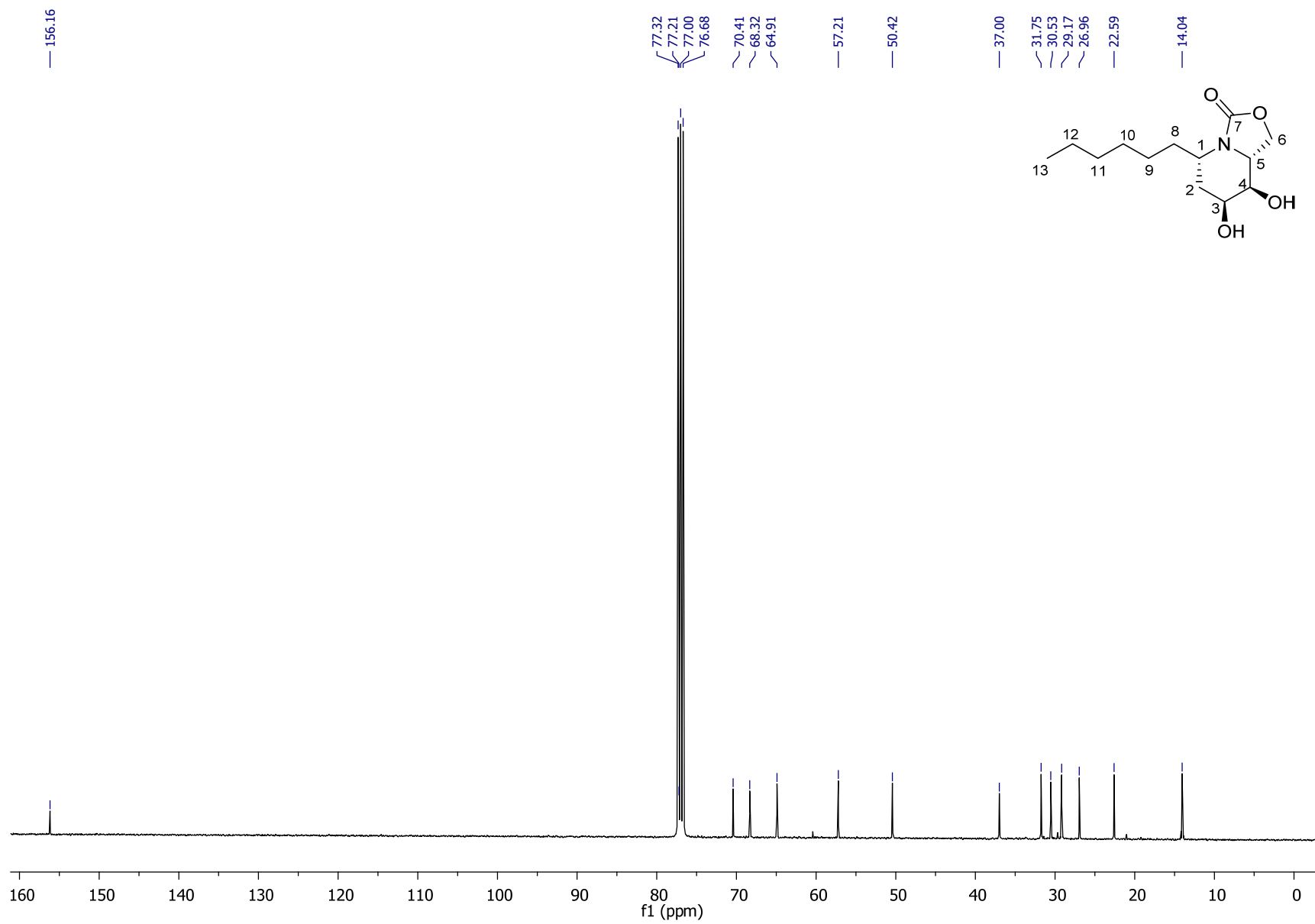
^{13}C NMR spectrum of compound **10** (100 MHz, CDCl_3 , 300K)



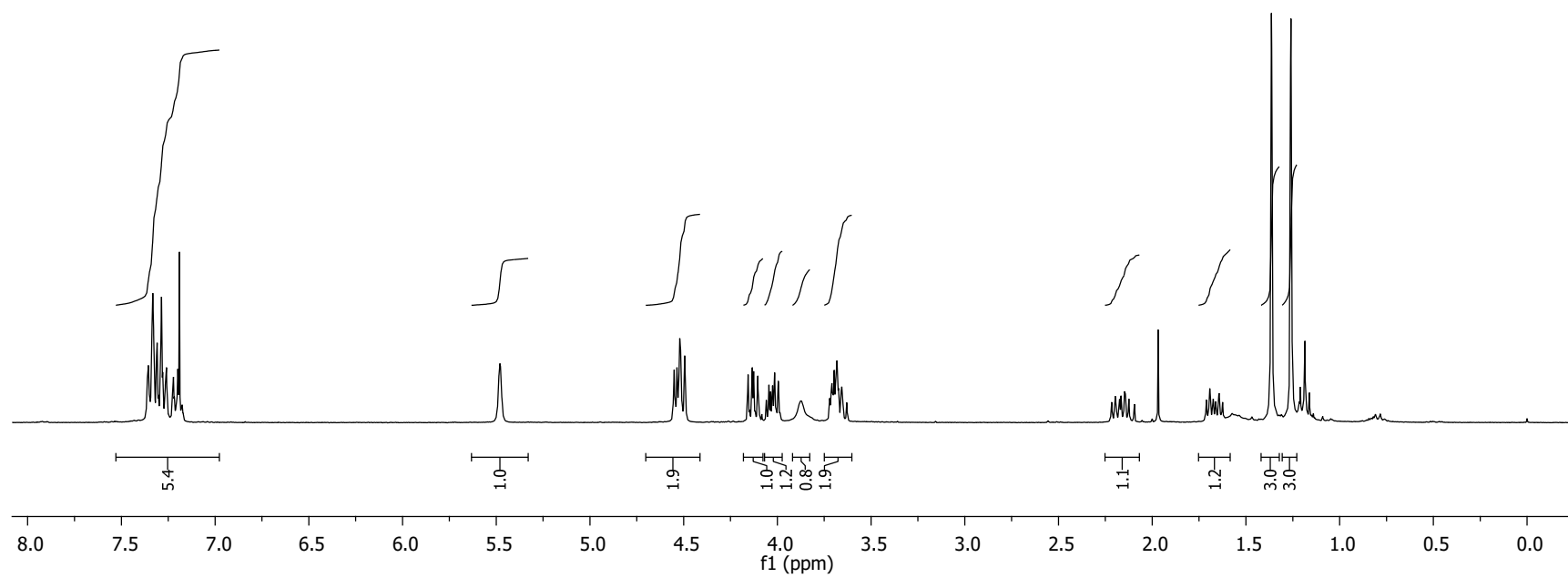
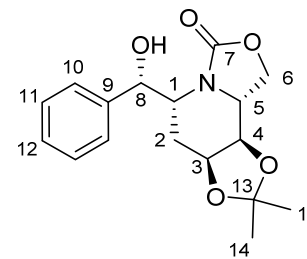
^1H NMR of compound **11** (400 MHz, CDCl_3 , 300K)



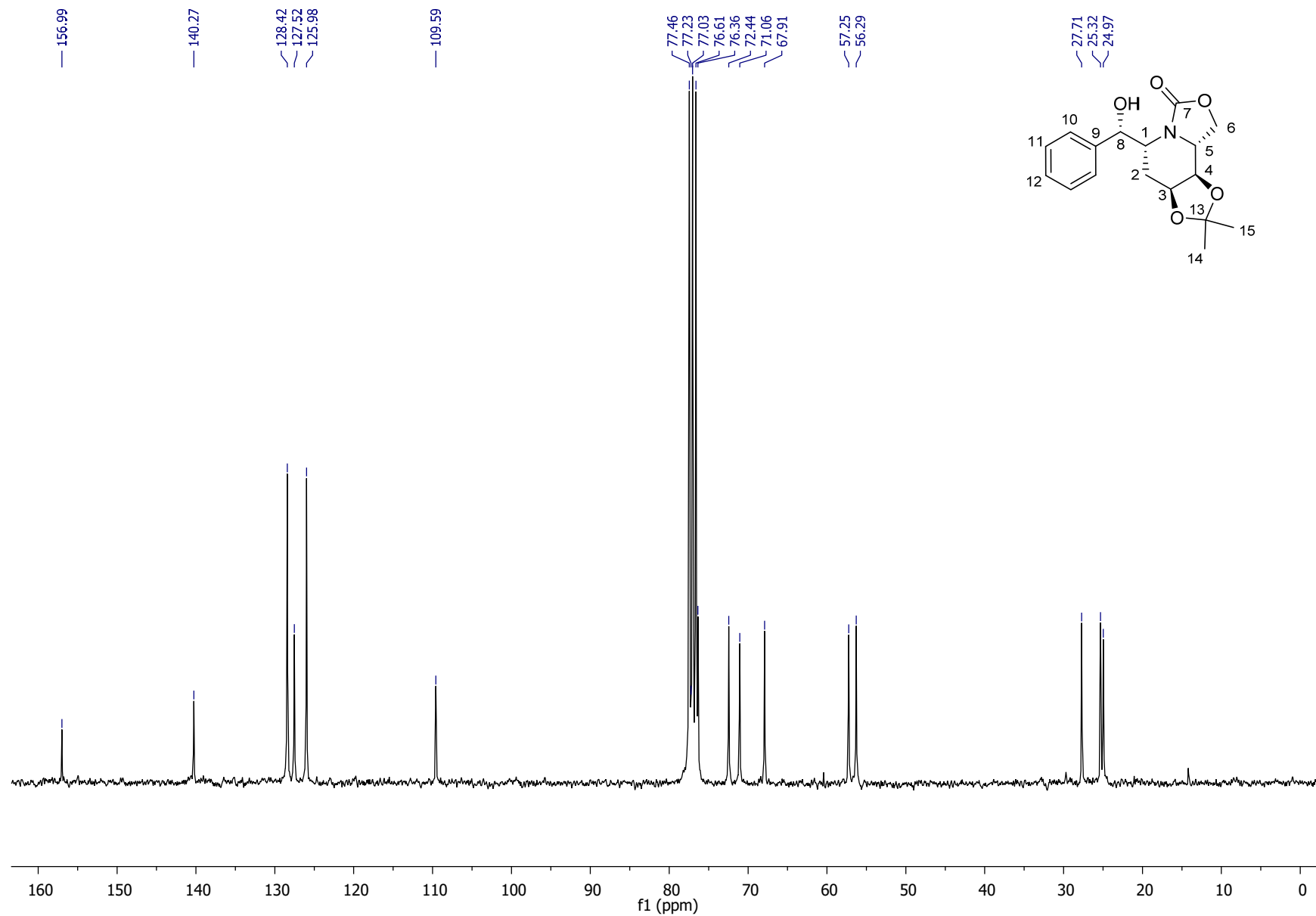
^{13}C NMR compound **11** (100 MHz, CDCl_3 , 300K)



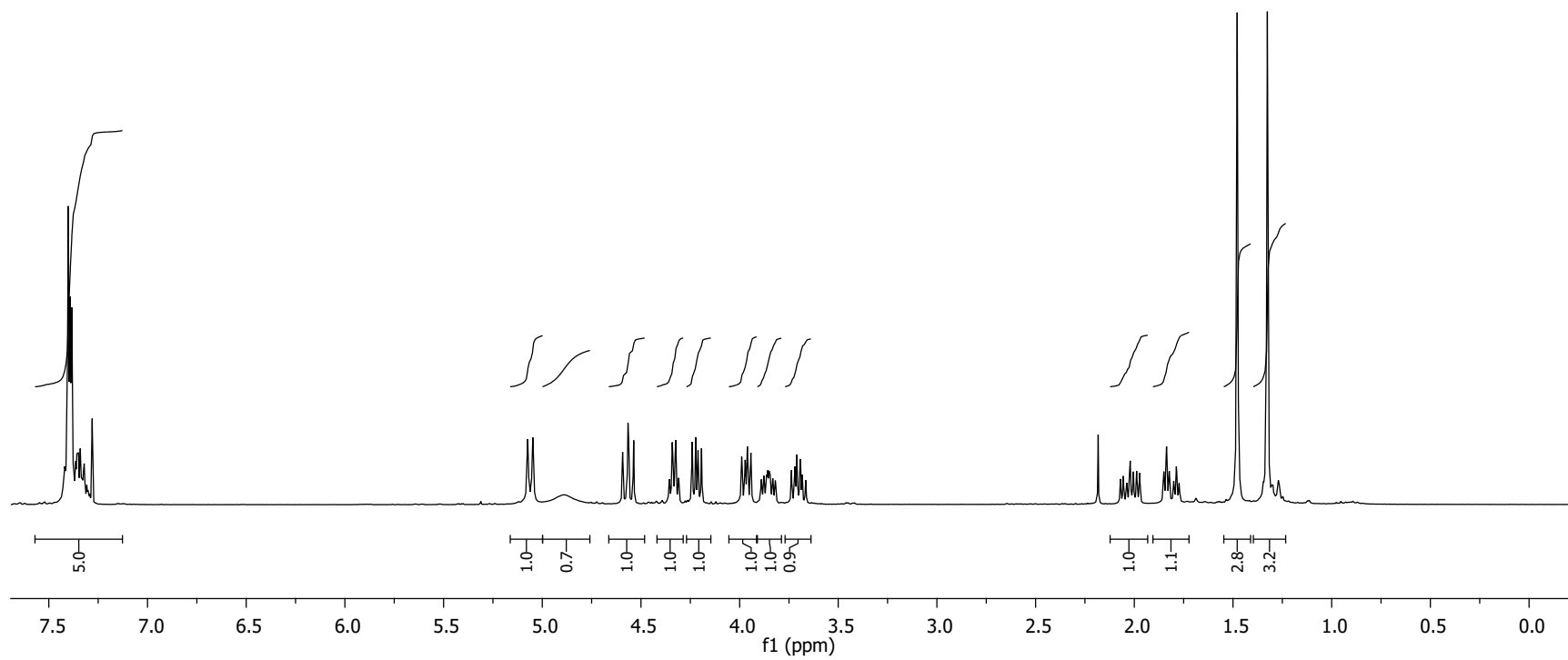
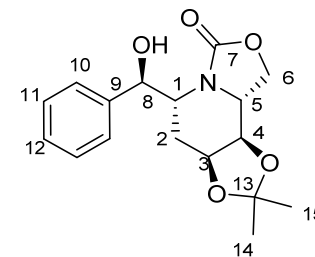
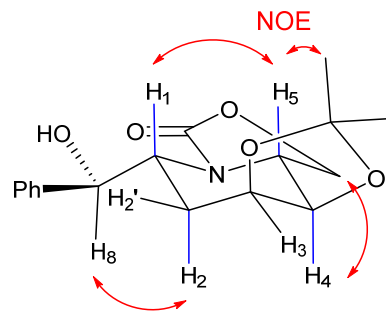
^1H NMR of compound **12** (300 MHz, CDCl_3 , 300K)



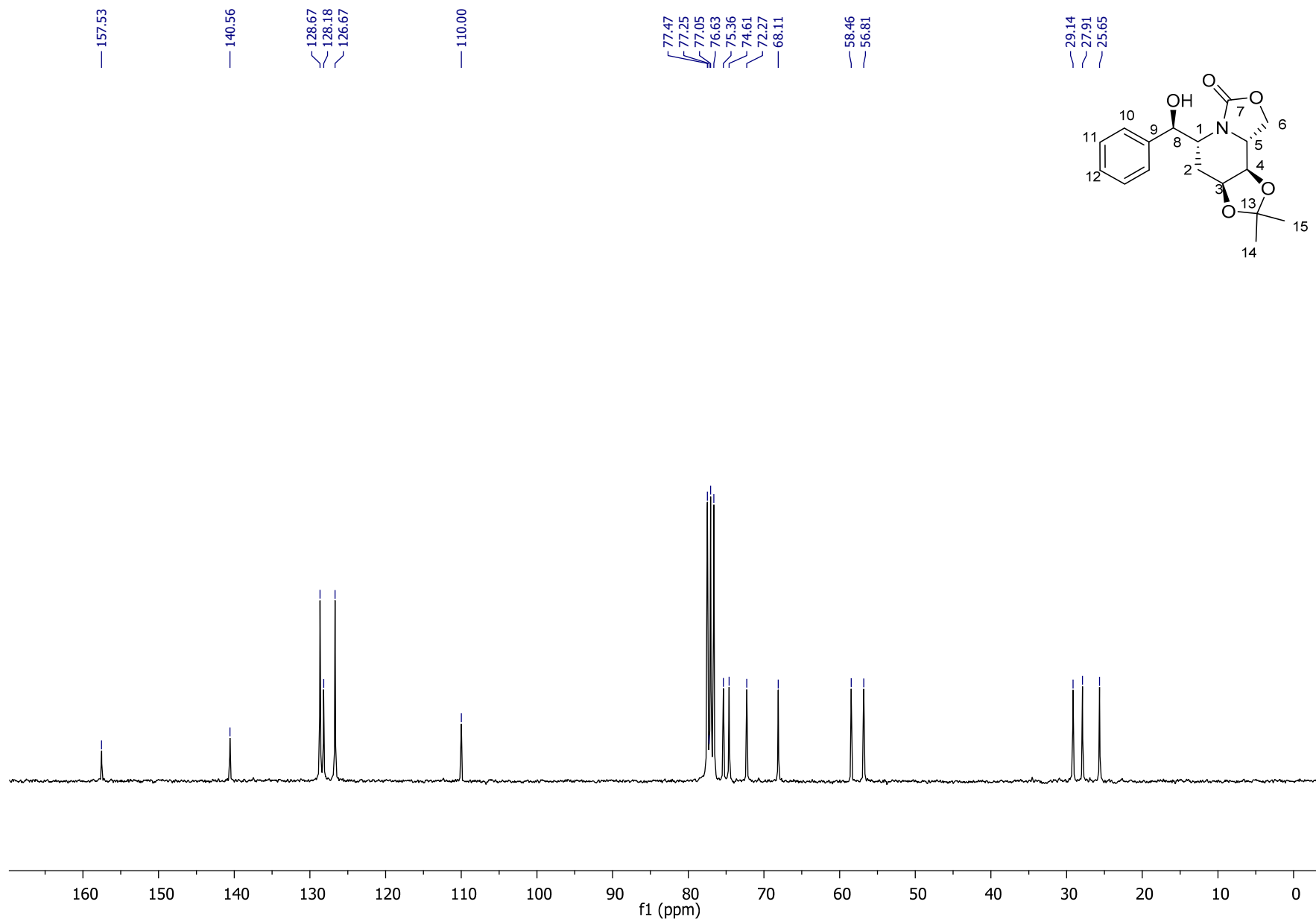
^{13}C NMR of compound **12** (75 MHz, CDCl_3 , 300K)



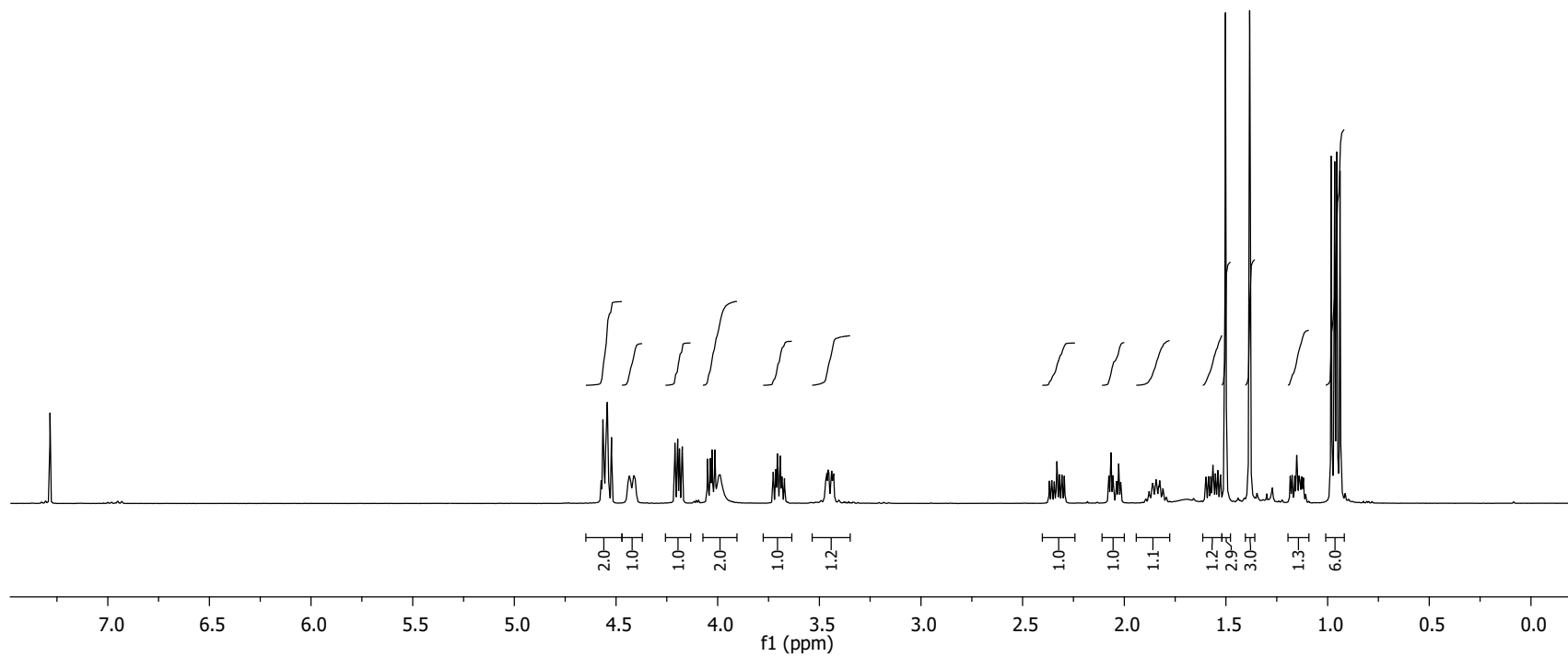
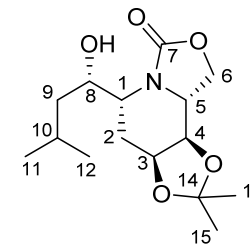
^1H NMR of compound **13** in (300 MHz, CDCl_3 , 300K)



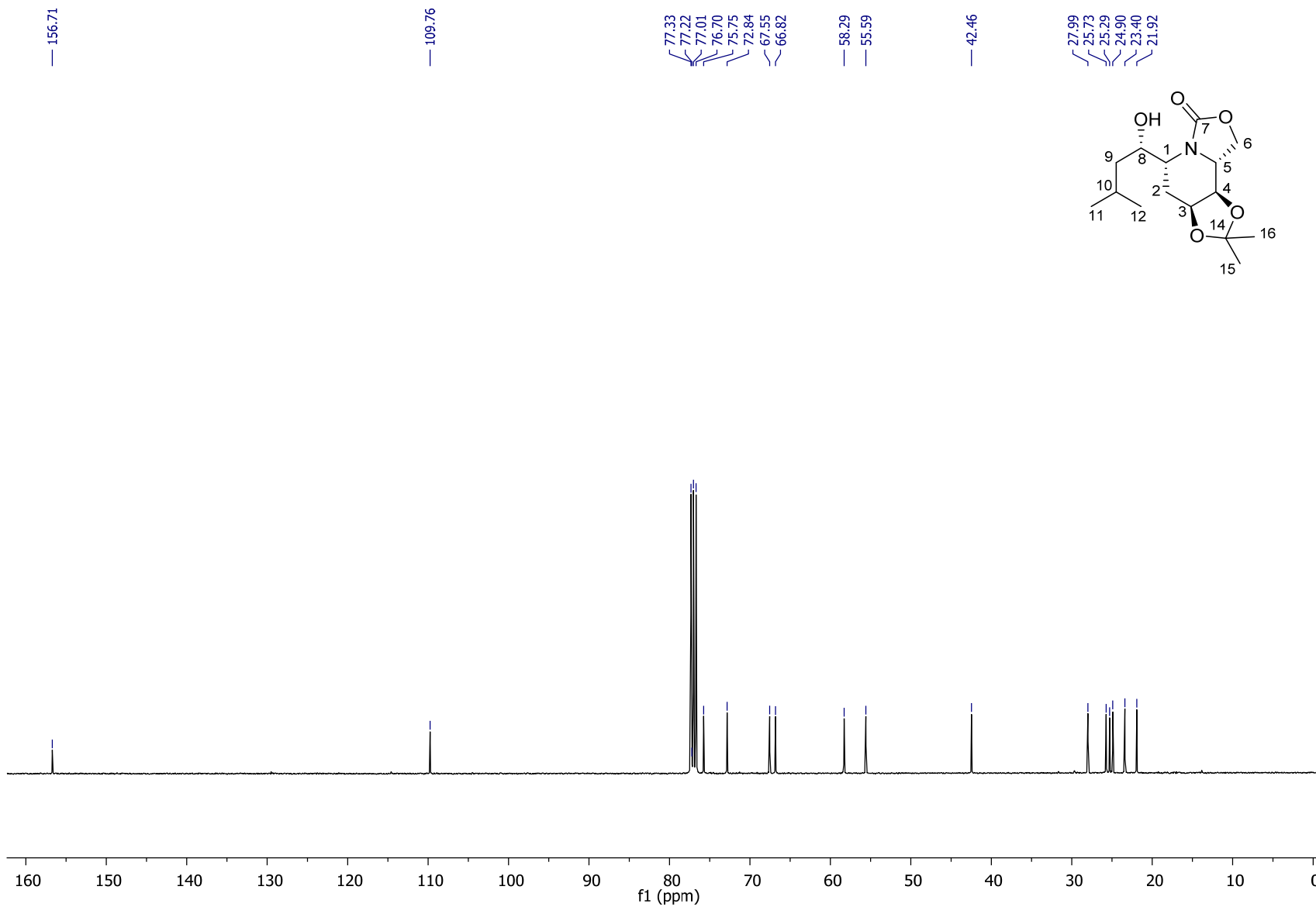
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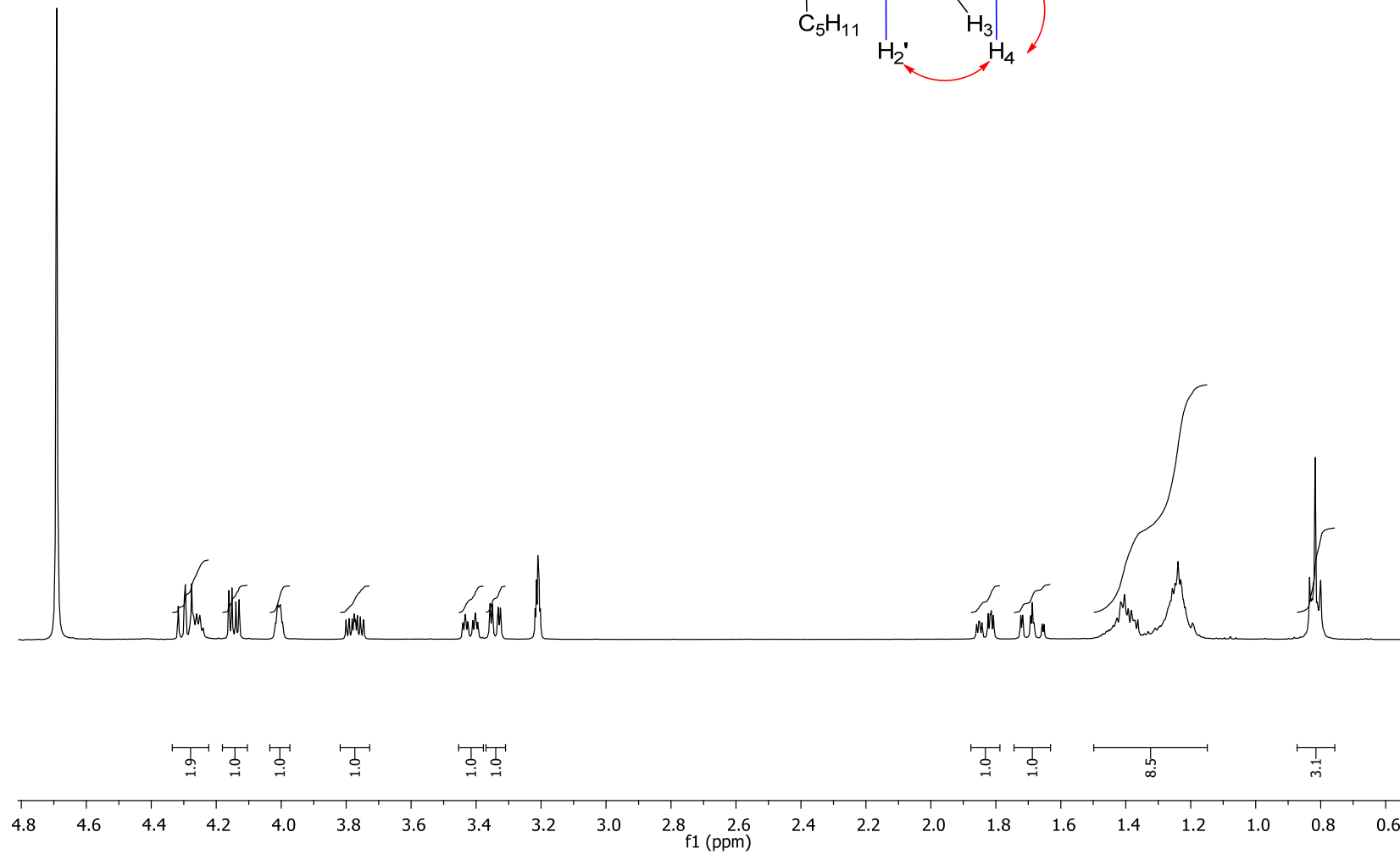
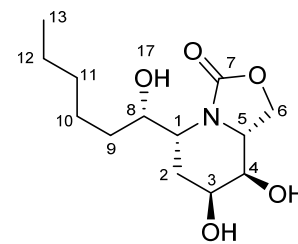
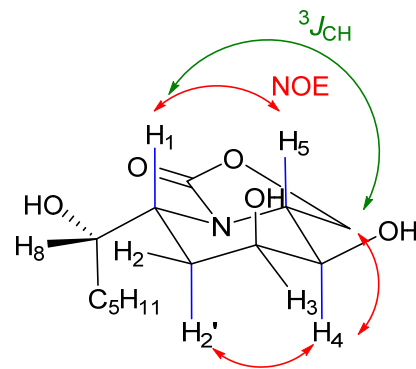
^1H NMR of compound **14** (400 MHz, CDCl_3 , 300K)



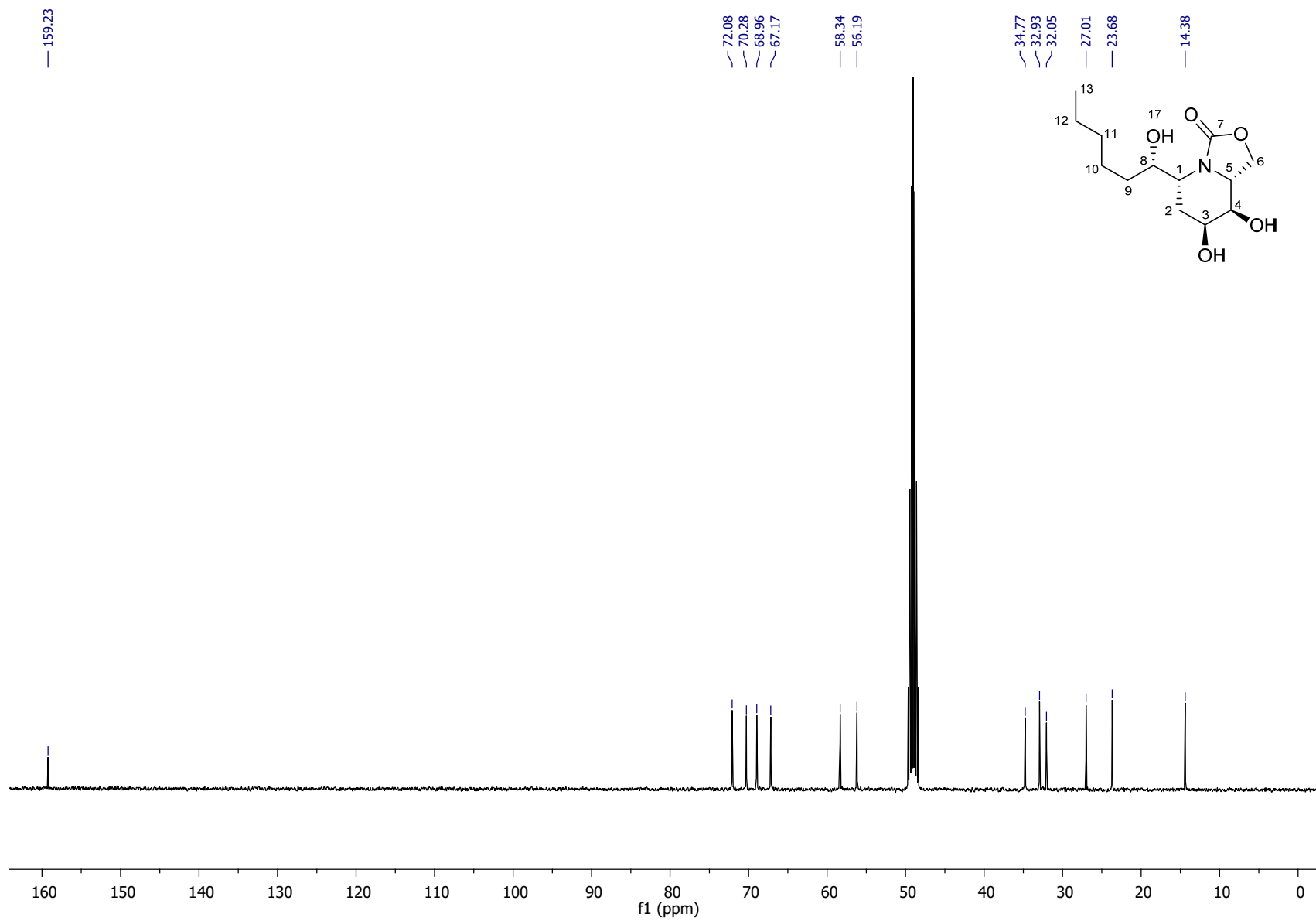
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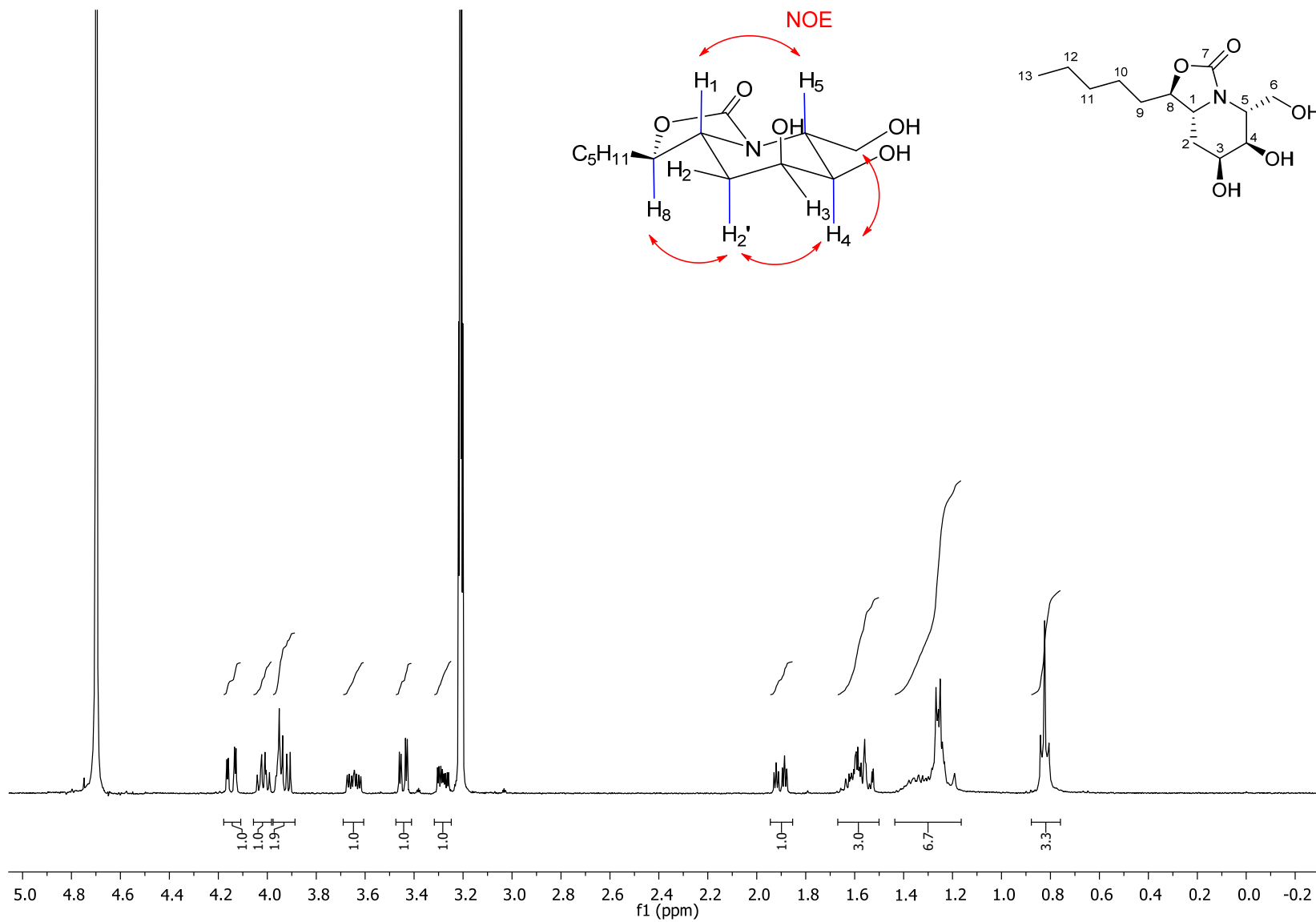
^1H NMR of compound **15** (400 MHz, CD_3OD , 300K)



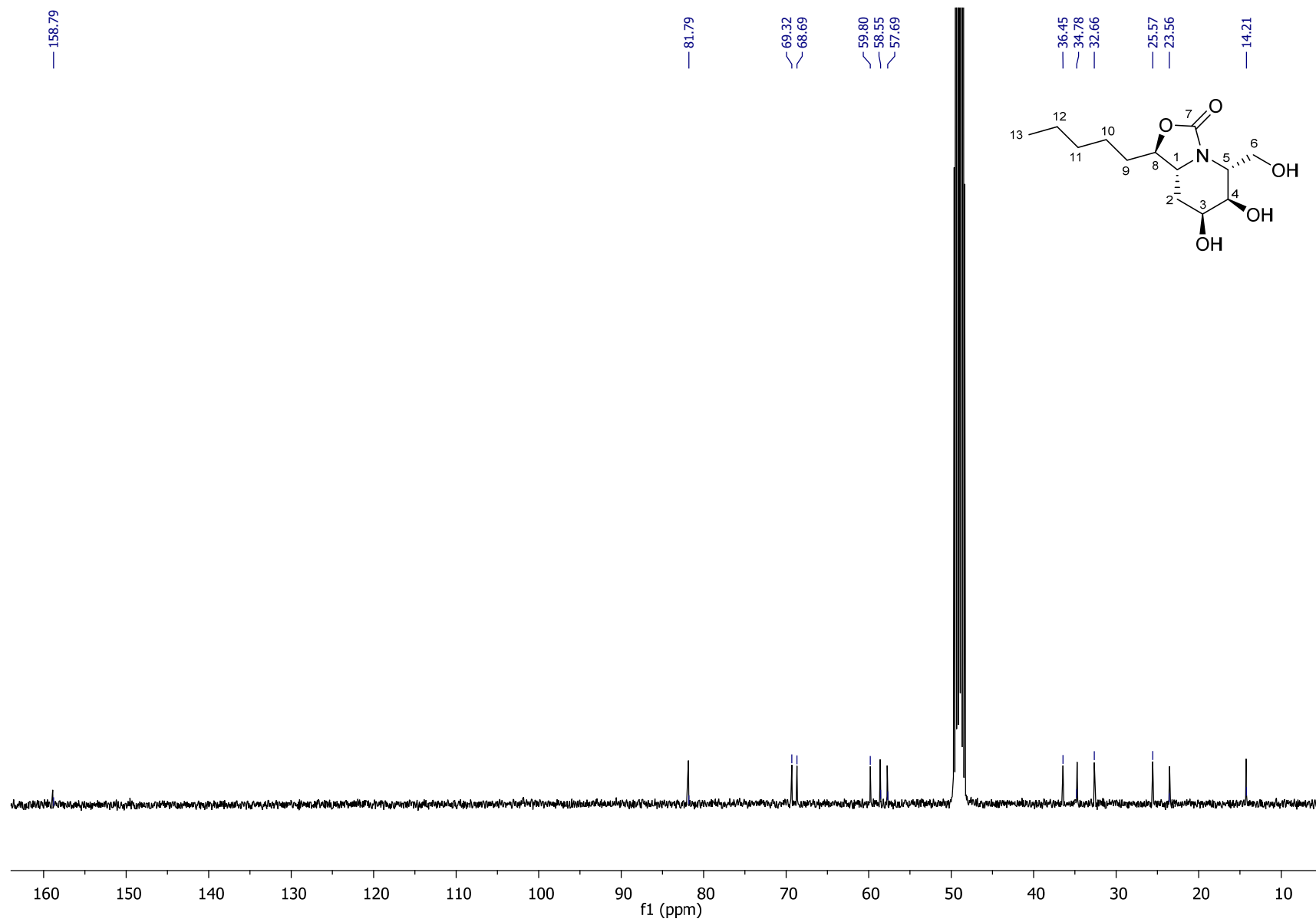
^{13}C NMR of compound **15** (100 MHz, CD_3OD , 300K)



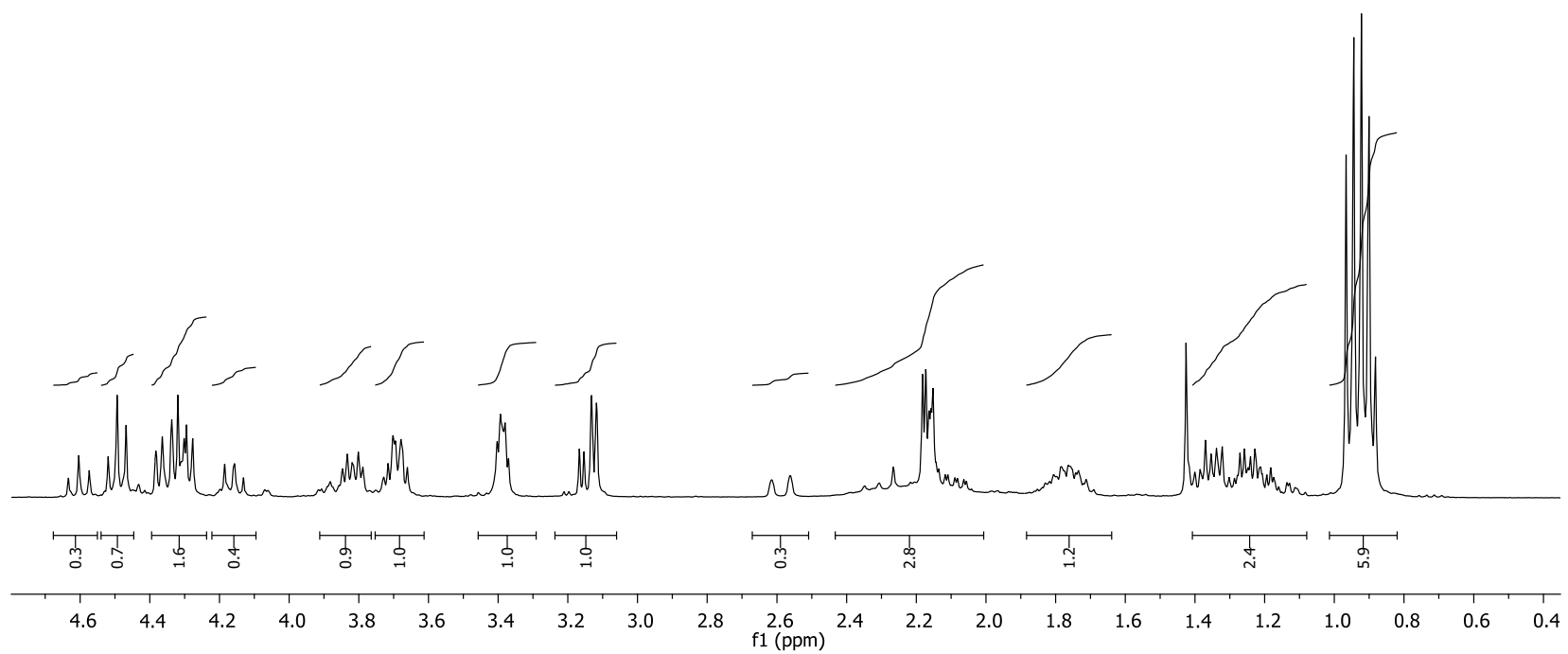
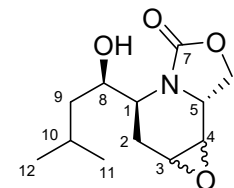
^1H NMR of compound **16** (400 MHz, CD_3OD , 300K)



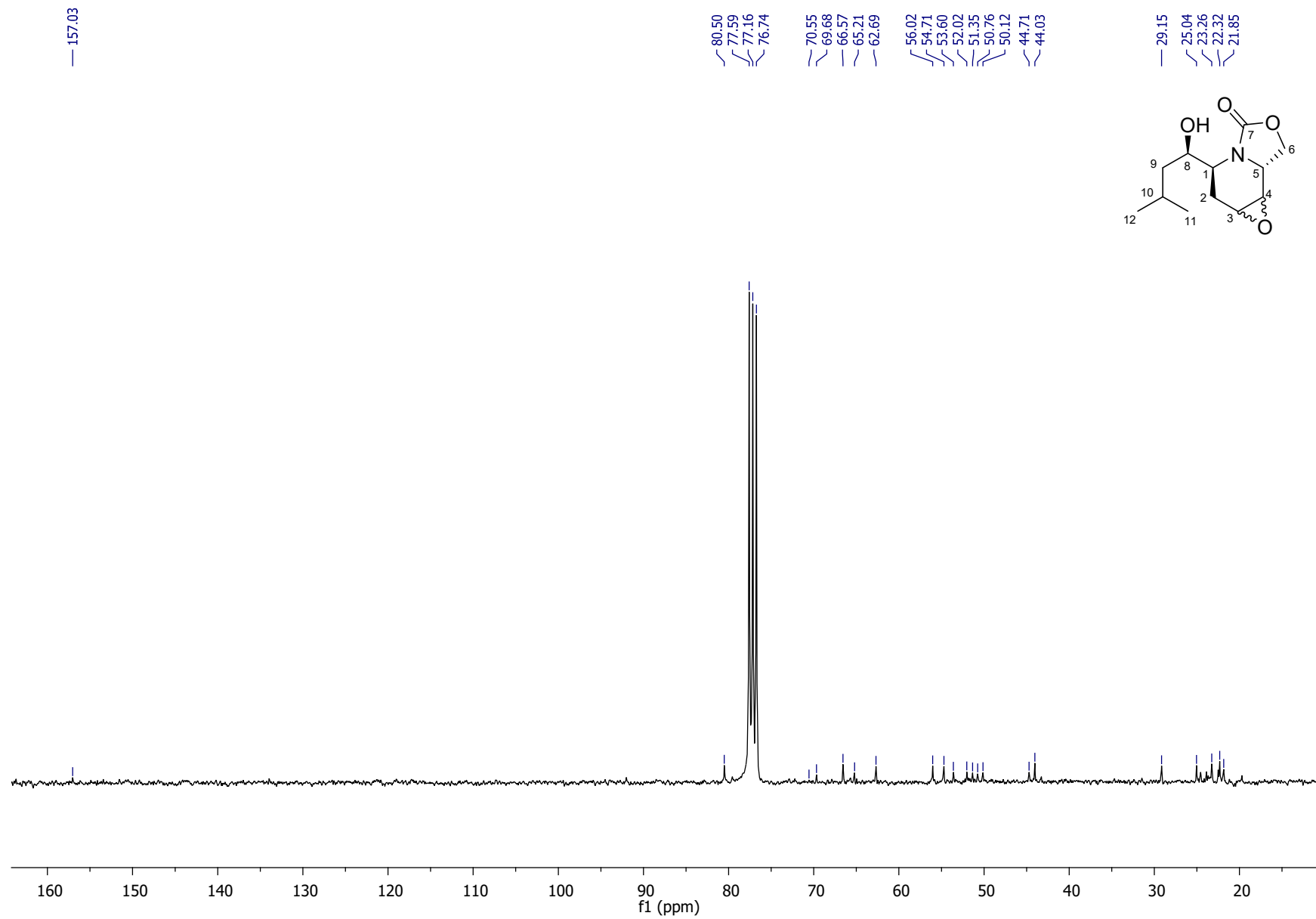
^{13}C NMR of compound **16** (100 MHz, CD_3OD , 300K)



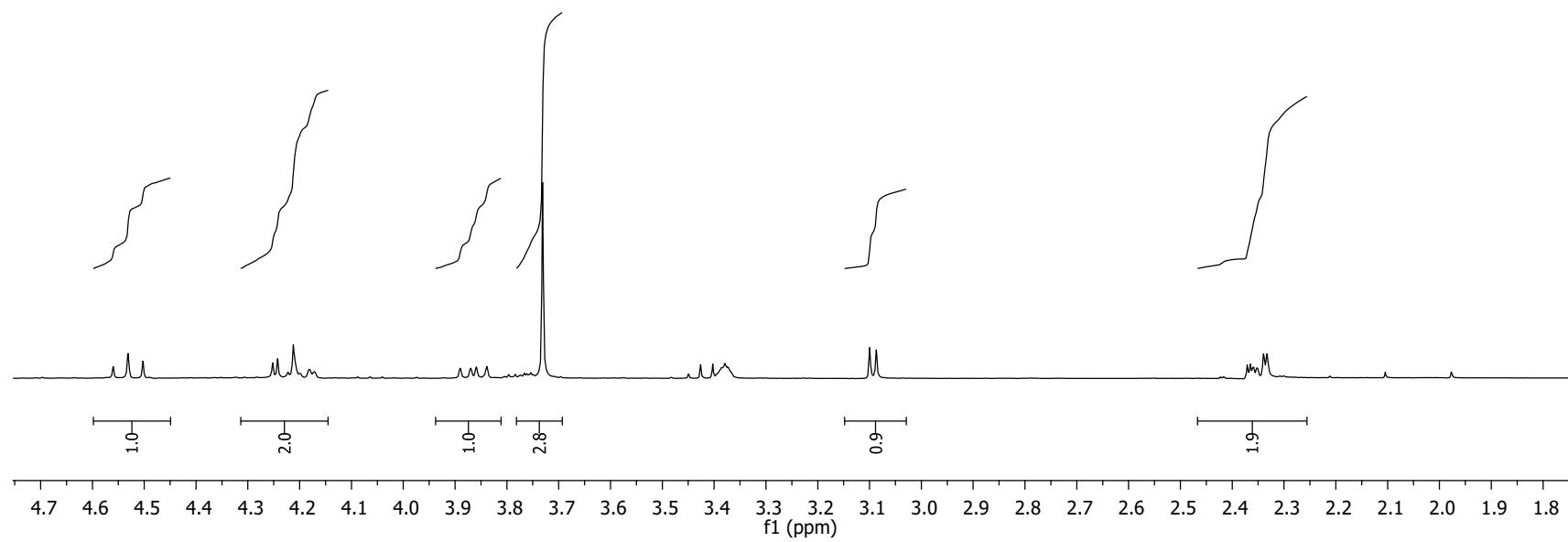
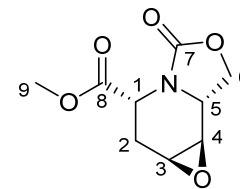
^1H NMR of compound **17** (*dr* = 67/33) in (300 MHz, CDCl_3 , 300K)



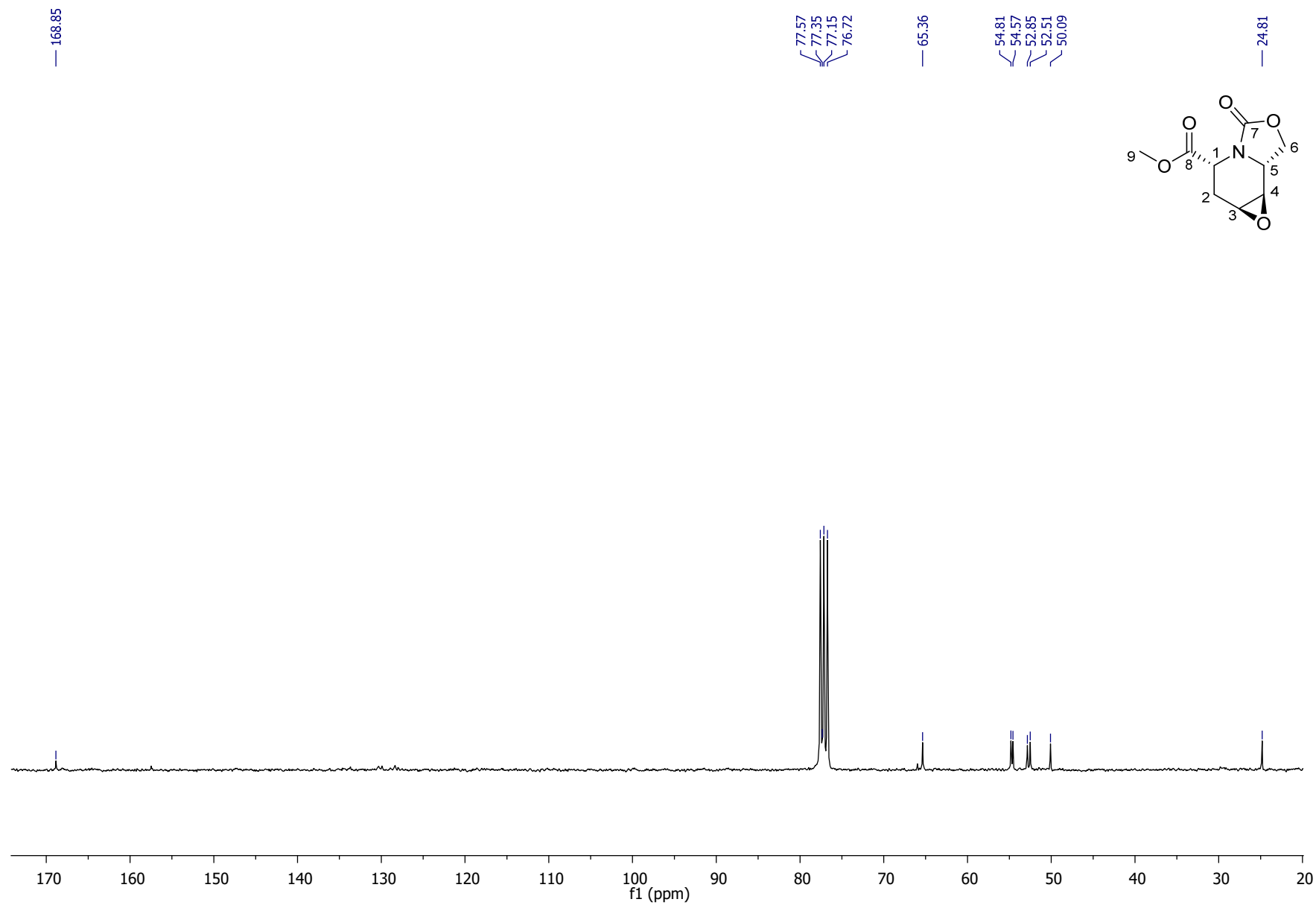
^{13}C NMR of compound **17** (*dr* = 67/33) (75 MHz, CDCl_3 , 300K)



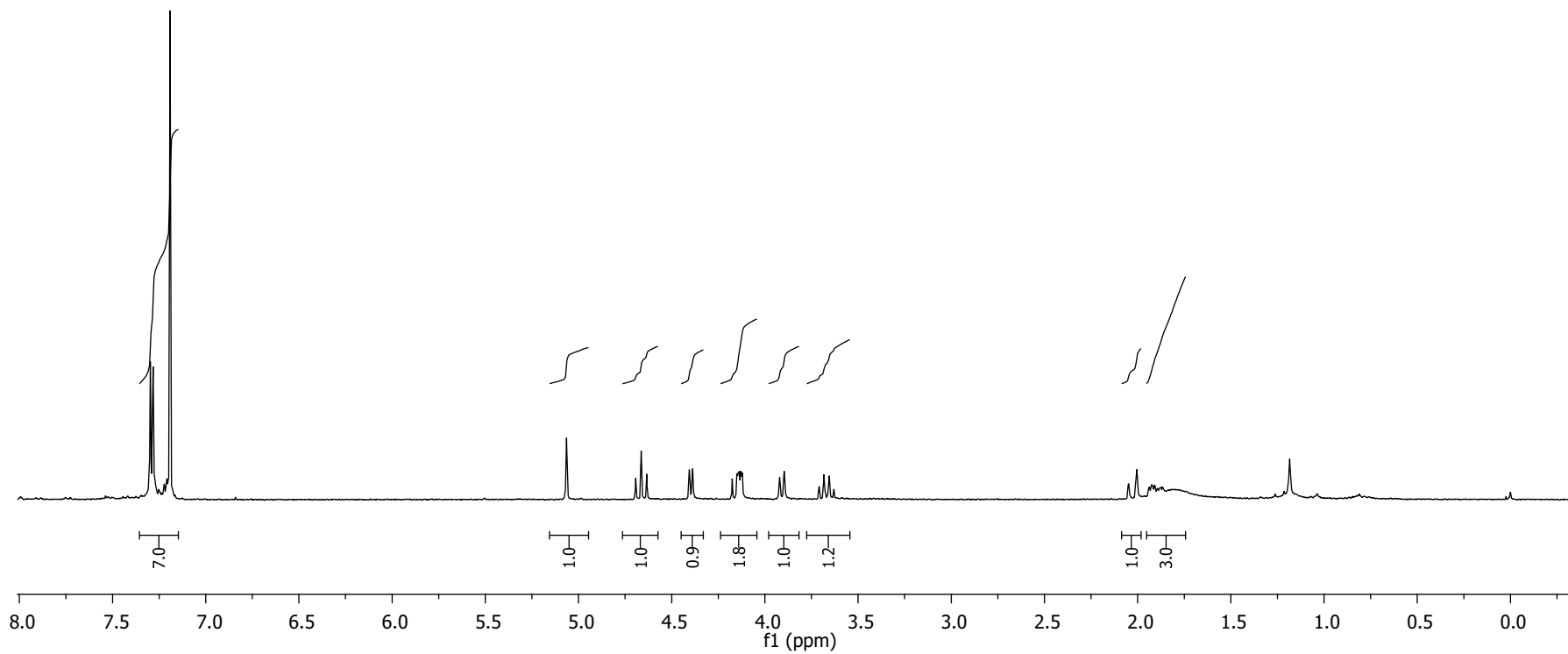
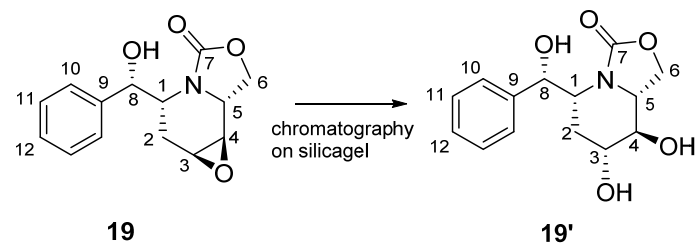
^1H NMR of compound **18** in (300 MHz, CDCl_3 , 300K)



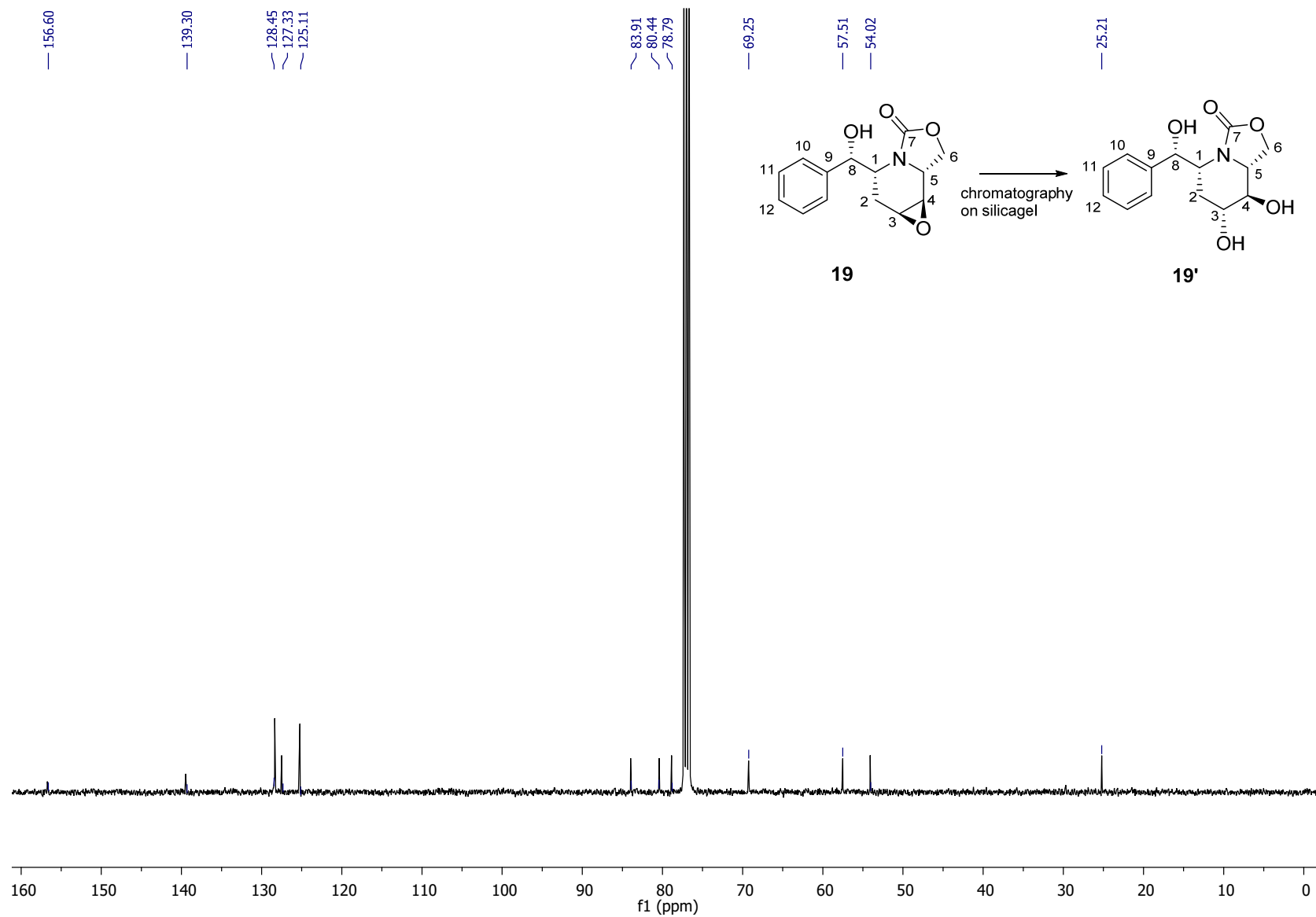
^{13}C NMR of compound **18** (75 MHz, CDCl_3 , 300K)



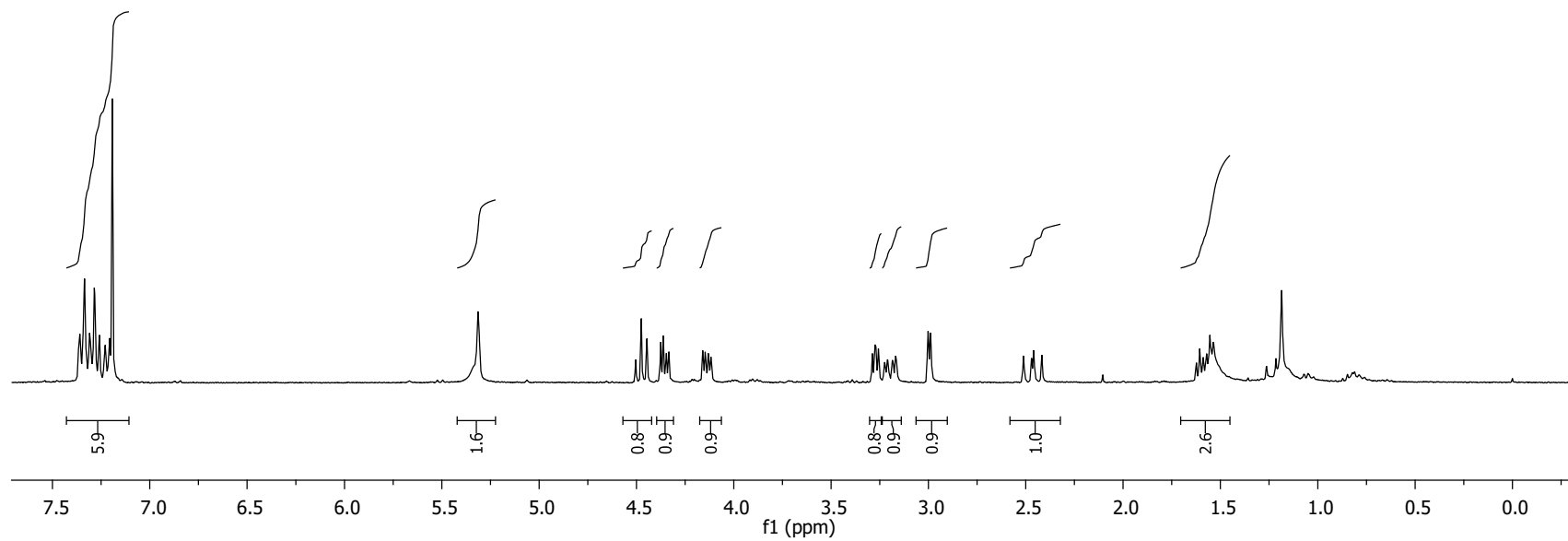
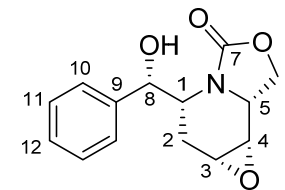
^1H NMR of compound **19'** (400 MHz, CDCl_3 , 300K) obtained from **19-exo**



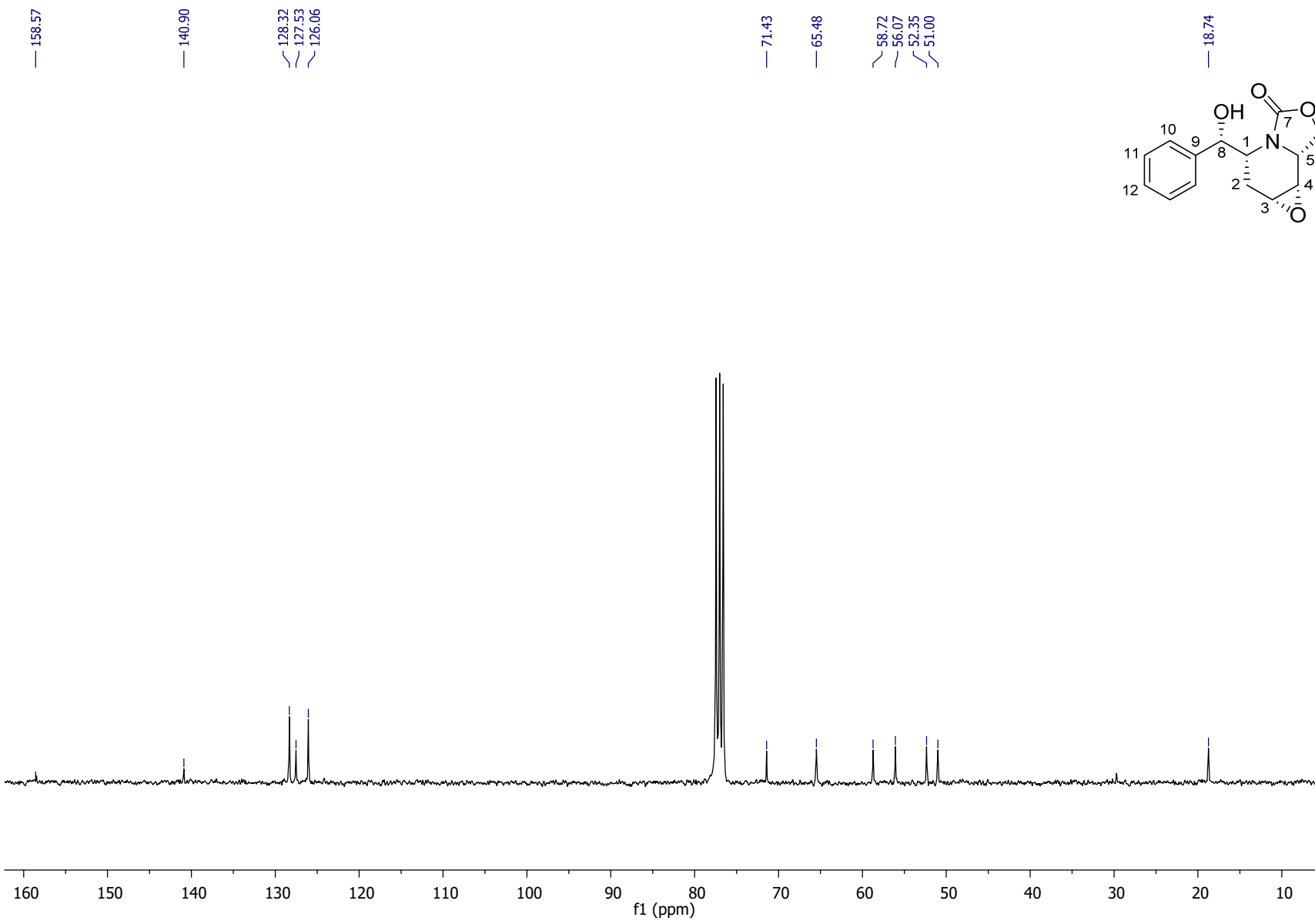
^{13}C NMR of compound **19'** (100 MHz, CDCl_3 , 300K) obtained from **19-exo**



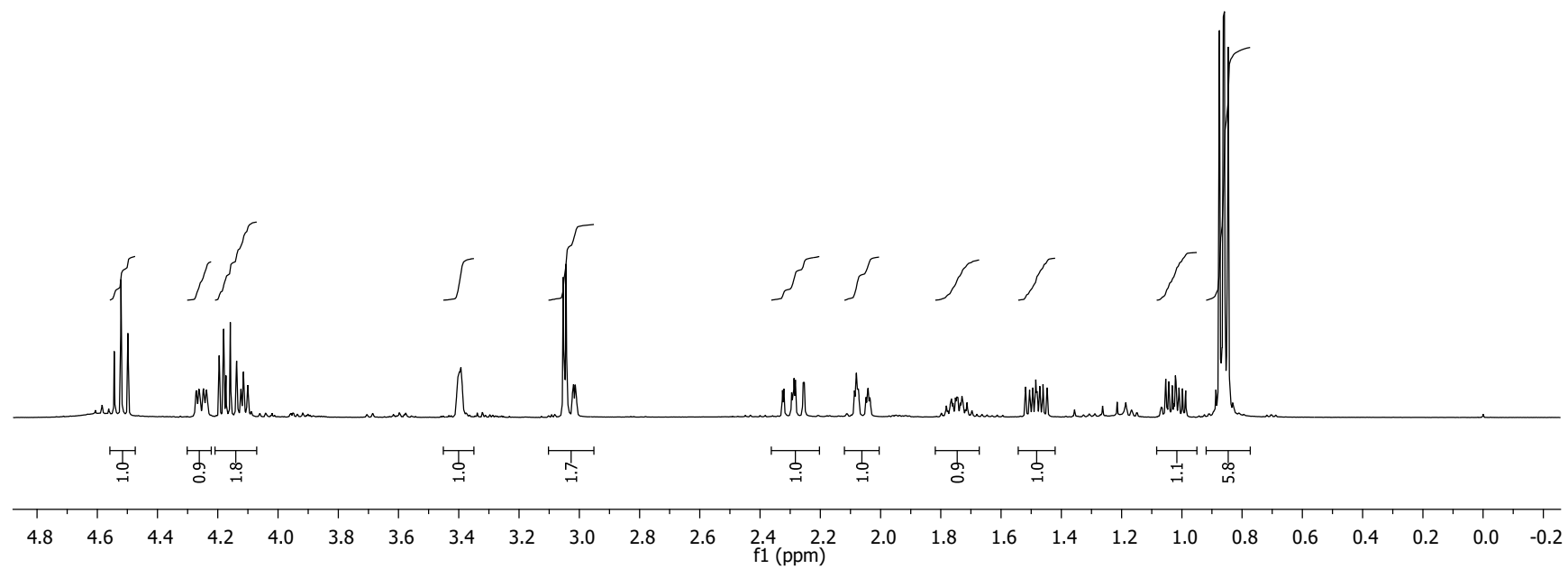
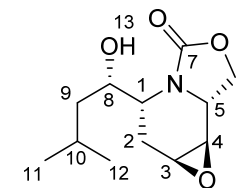
^1H NMR compound **19-endo** (300 MHz, CDCl_3 , 300K)



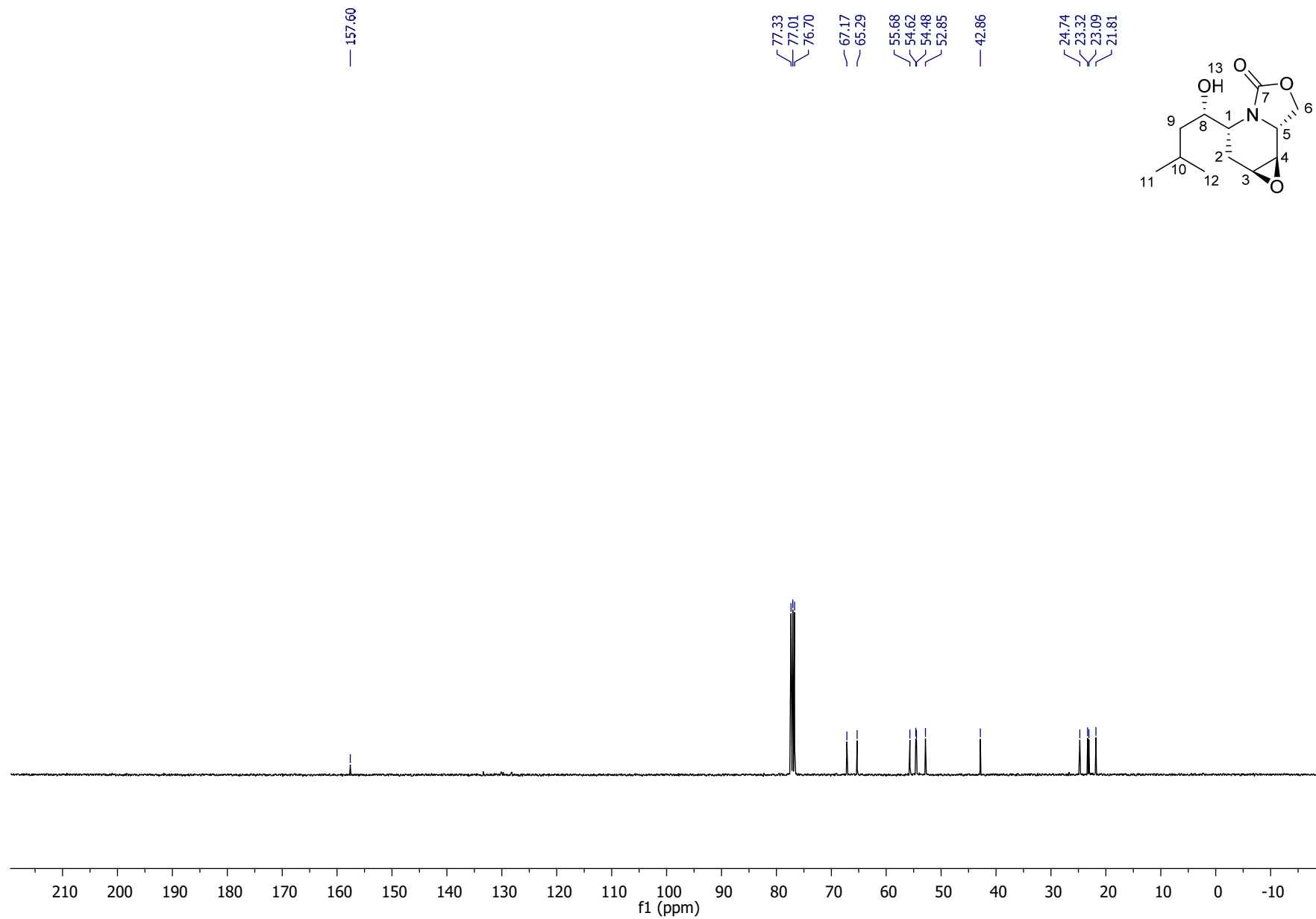
^{13}C NMR compound **19-endo** (75 MHz, CDCl_3 , 300K)



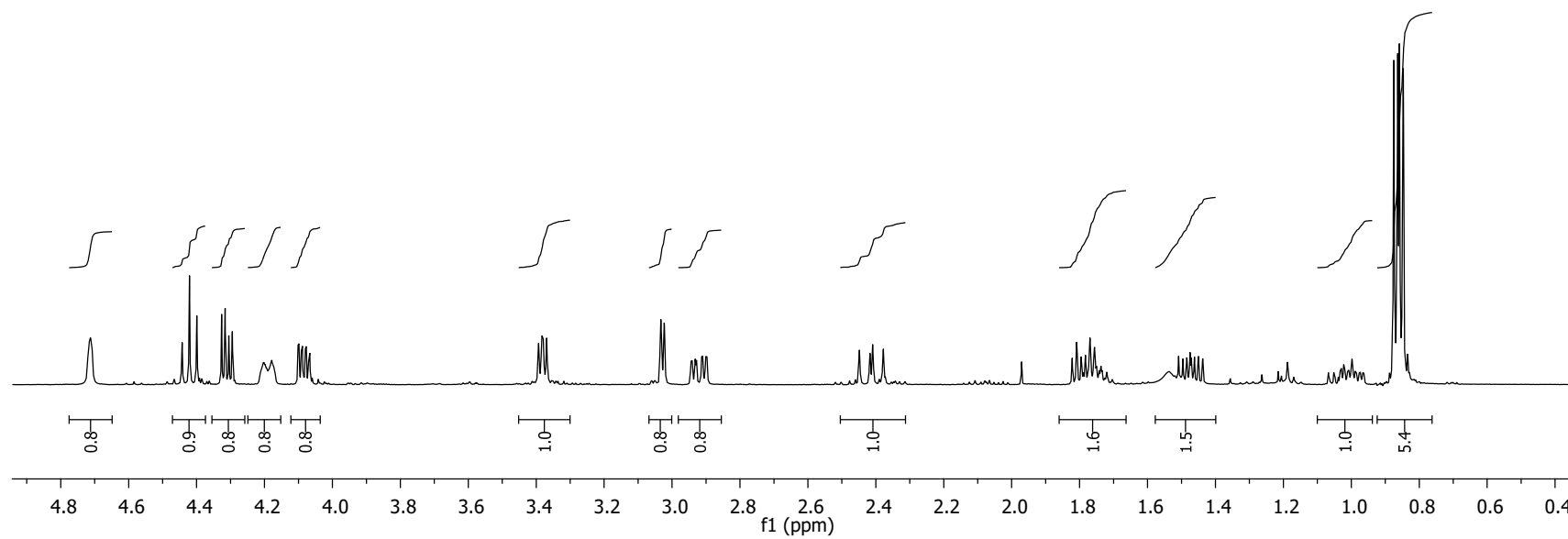
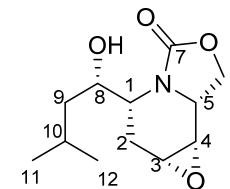
^1H NMR of compound **20-*exo*** (400 MHz, CDCl_3 , 300K)



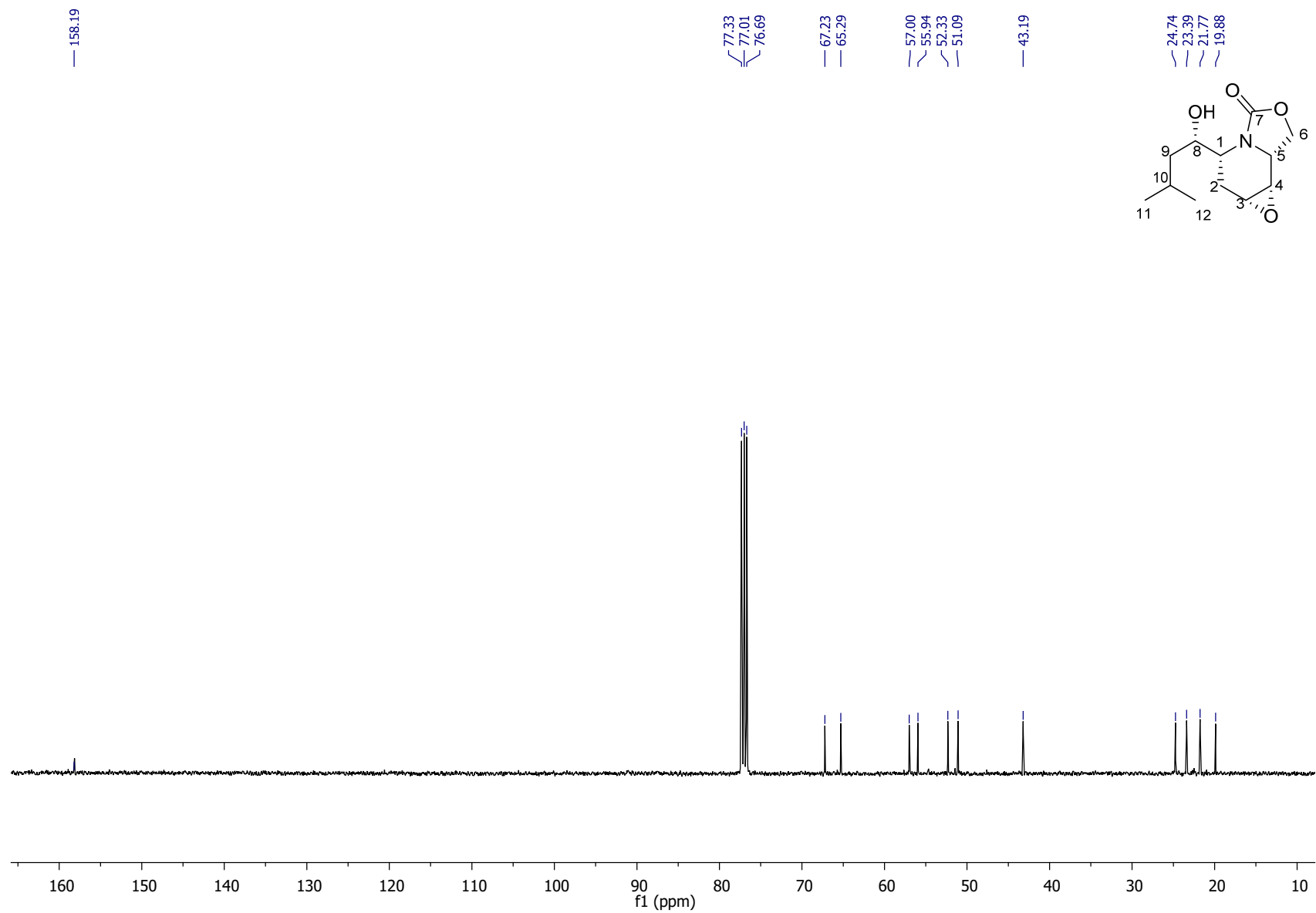
^{13}C NMR of compound **20-exo** (100 MHz, CDCl_3 , 300K)



^1H NMR of compound **20-endo** (300 MHz, CDCl_3 300K)



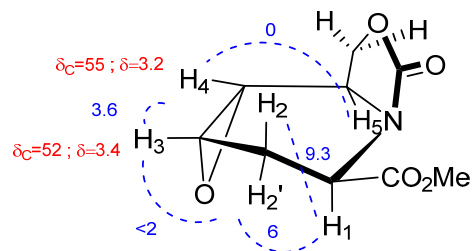
^{13}C NMR of compound **20-endo** (100 MHz, CDCl_3 , 300K)



Discrimination between *exo* and *endo* epoxides

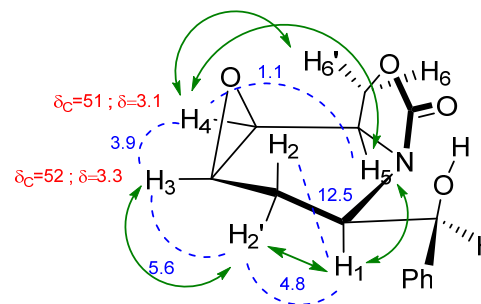
Having in hand the radiocrystallographic structure of **18-*exo***, the assignment of the *exo* or *endo* epoxide was established on the basis of NMR spectra, including chemical shift of epoxide carbons in ^{13}C NMR spectrometry and meaningful vicinal coupling constants or meaningful NOE effects as indicated on the following schemes.

Major (18-*exo*)

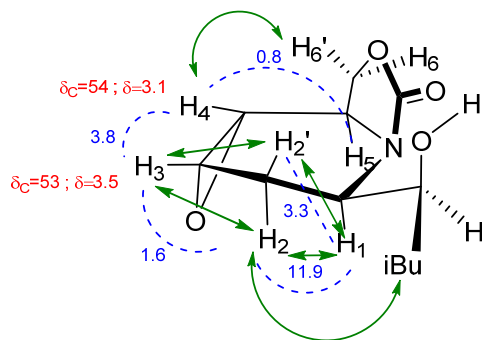


Conformation and configuration corroborated by radiocrystallographic structure

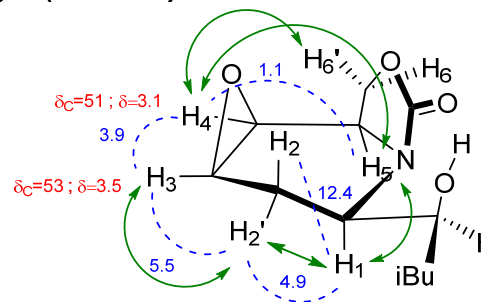
Major (19-*endo*)



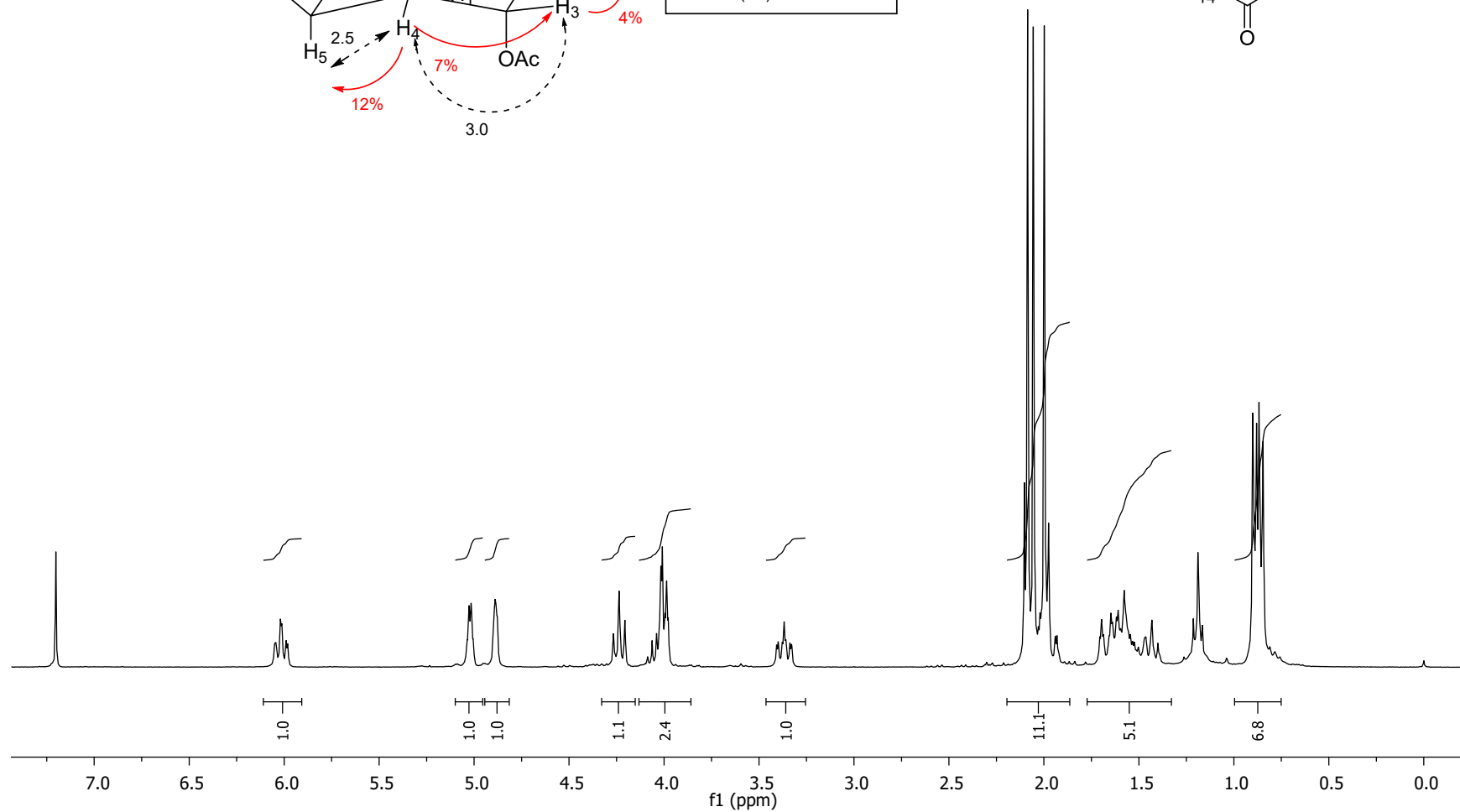
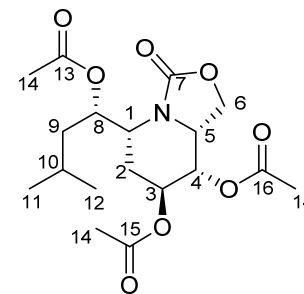
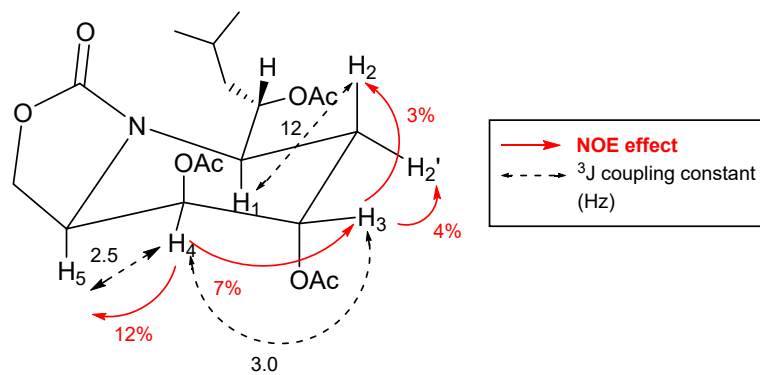
Minor (20-*exo*)



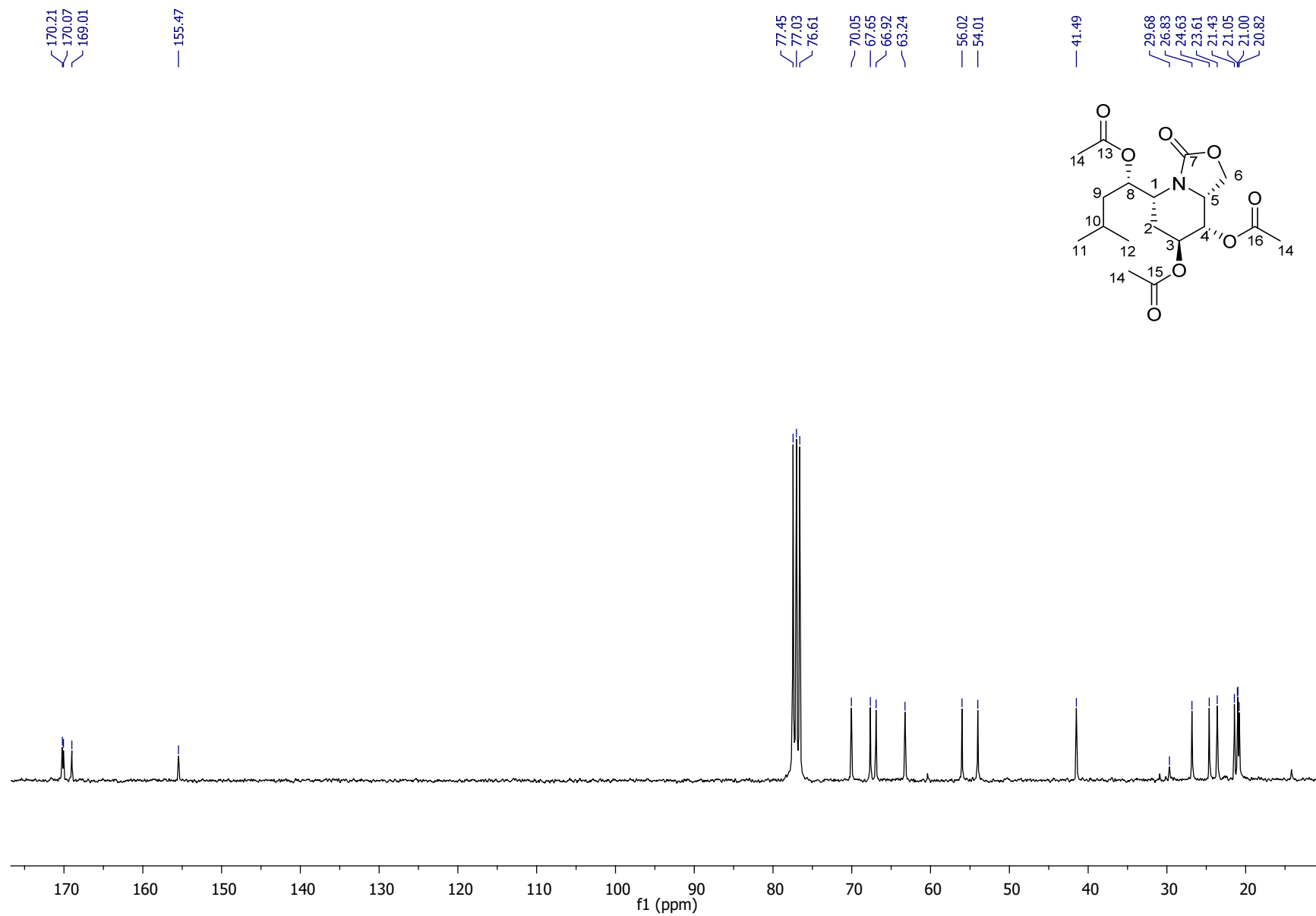
Major (20-*endo*)



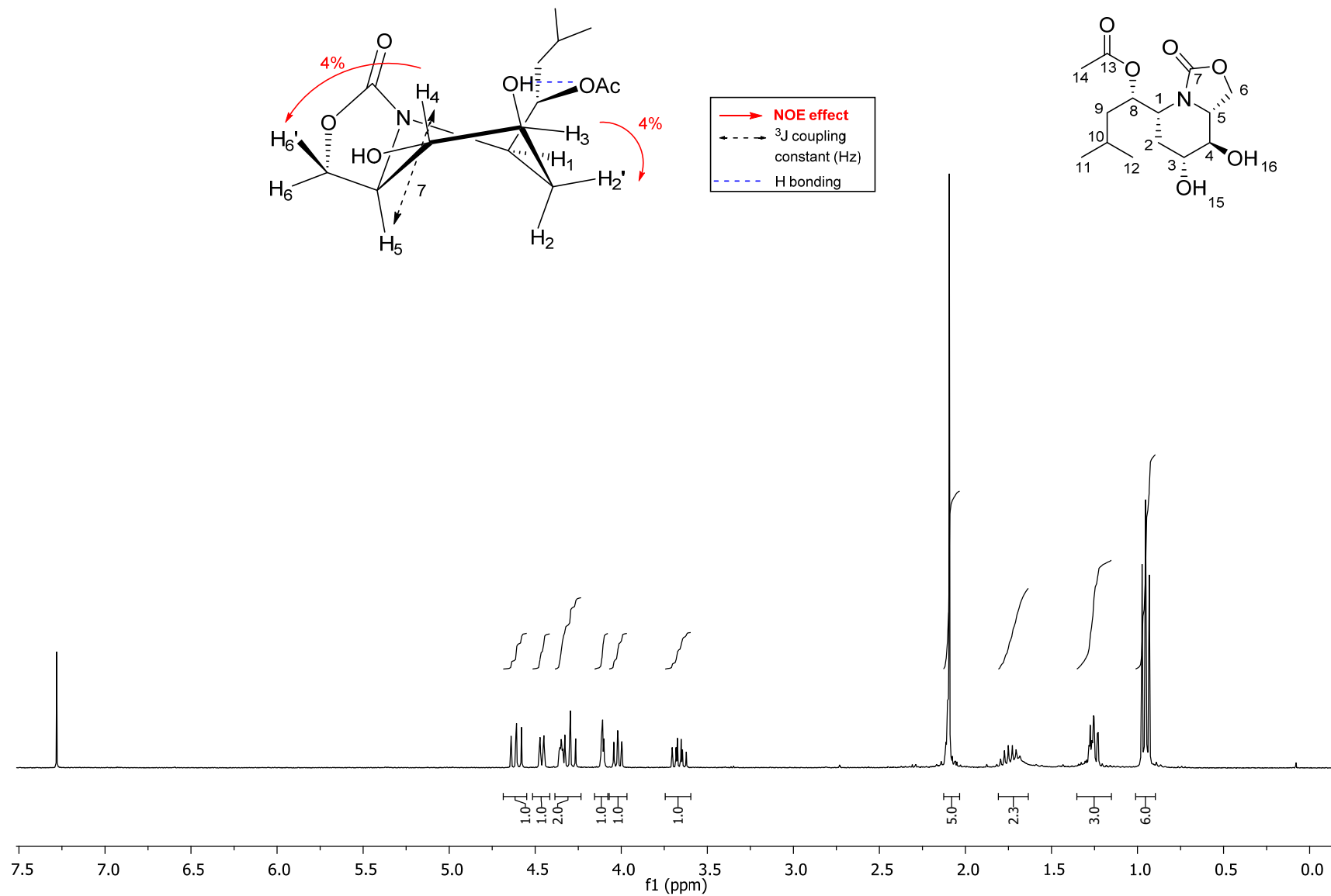
^1H NMR of compound **21** (300 MHz, CDCl_3 , 300K)



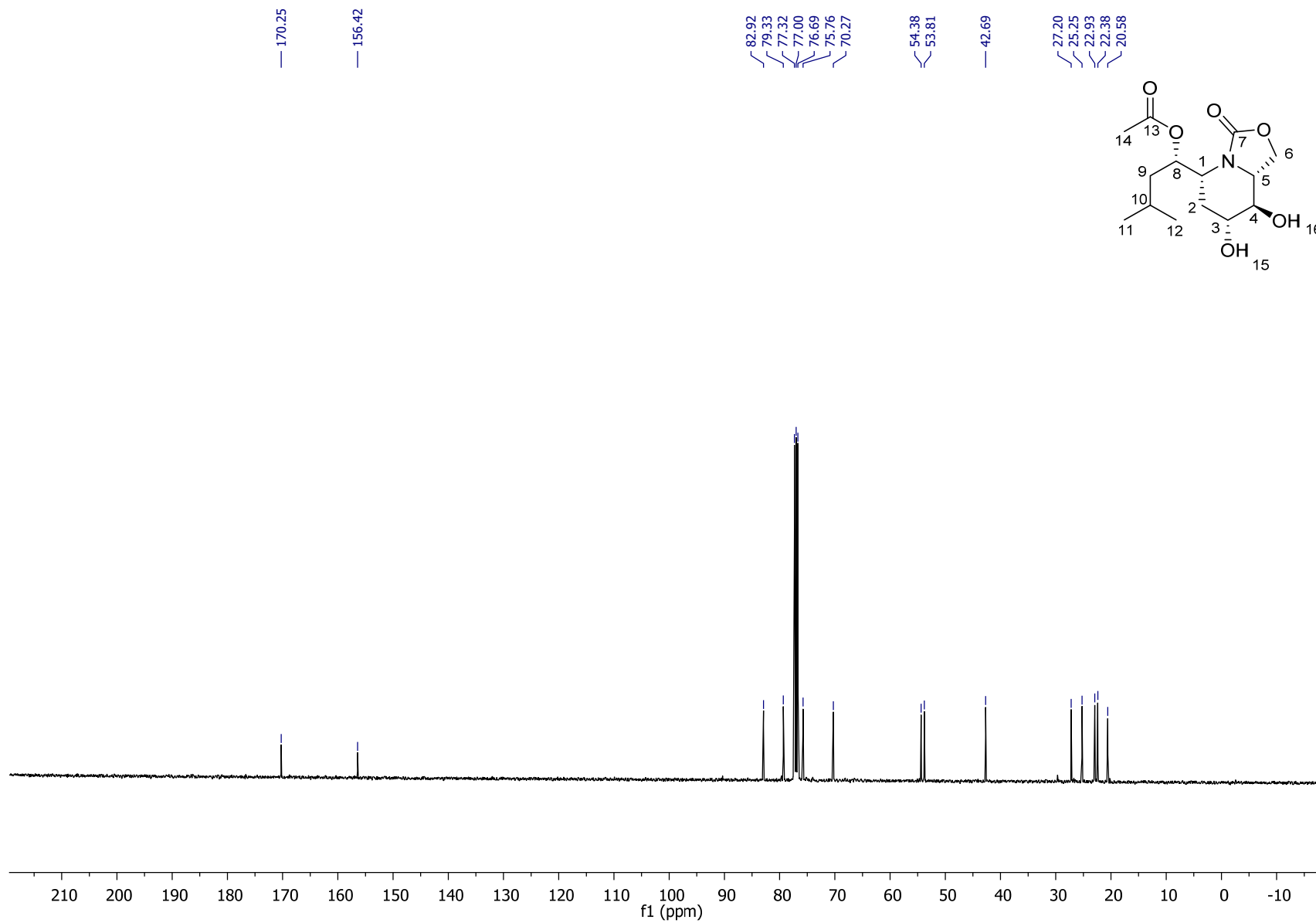
^{13}C NMR of compound **21** (75 MHz, CDCl_3 , 300K)



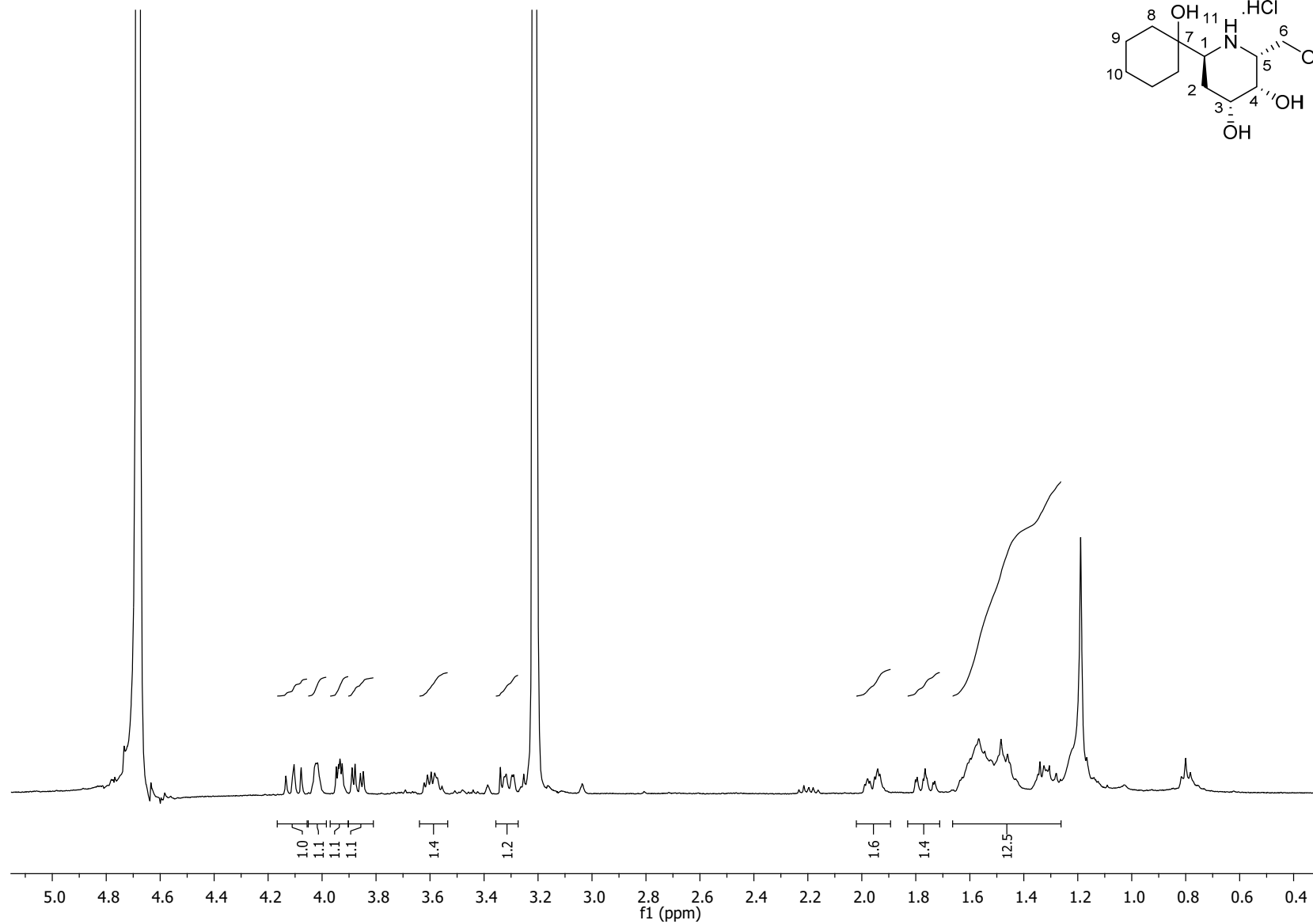
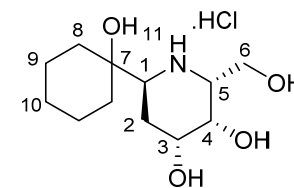
^1H NMR spectrum of compound **22** (400 MHz, CDCl_3 , 300K)



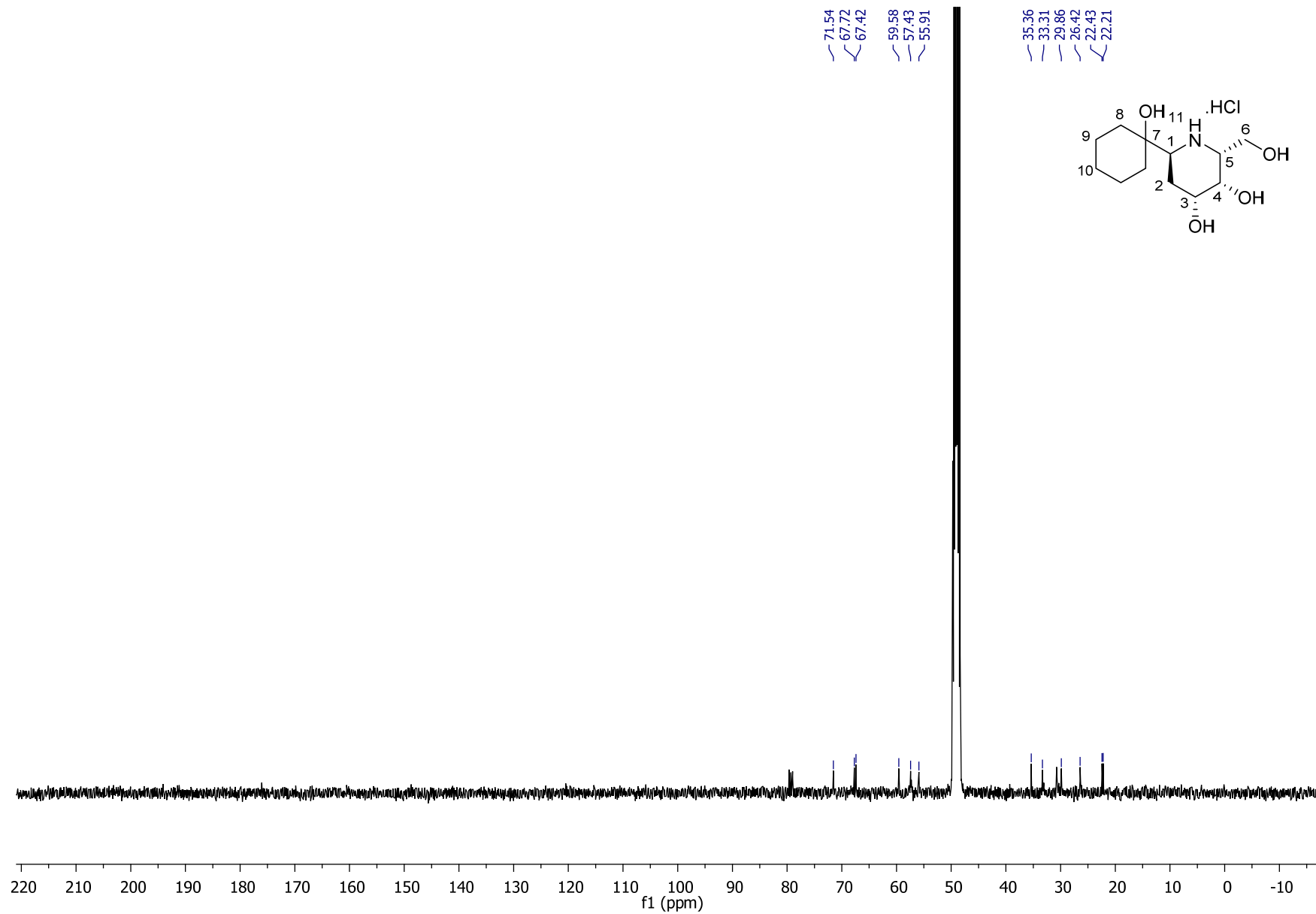
^{13}C NMR of compound **22** (100 MHz, CDCl_3 , 300K)



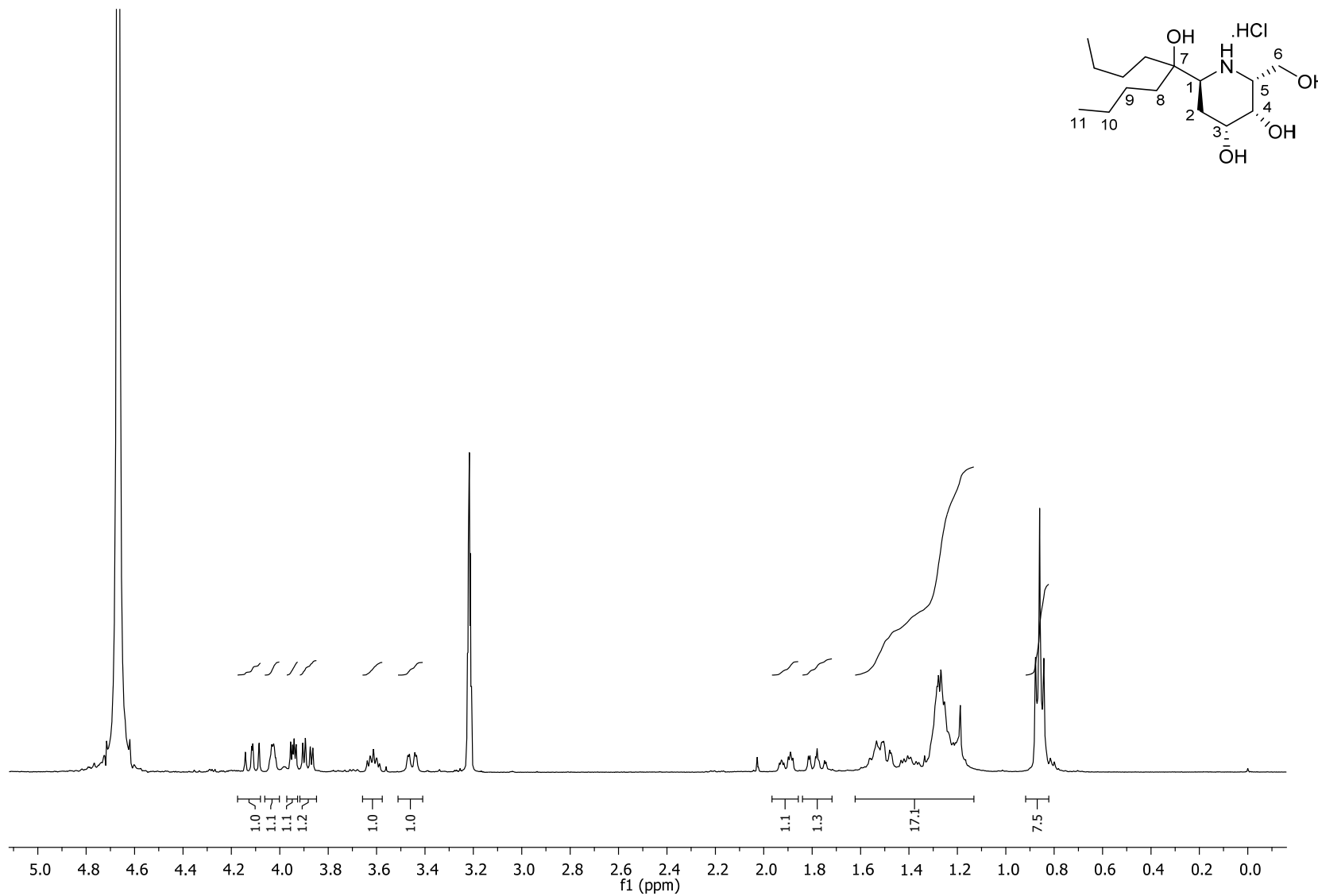
^1H NMR of compound **23** (400 MHz, CD_3OD , 300K)



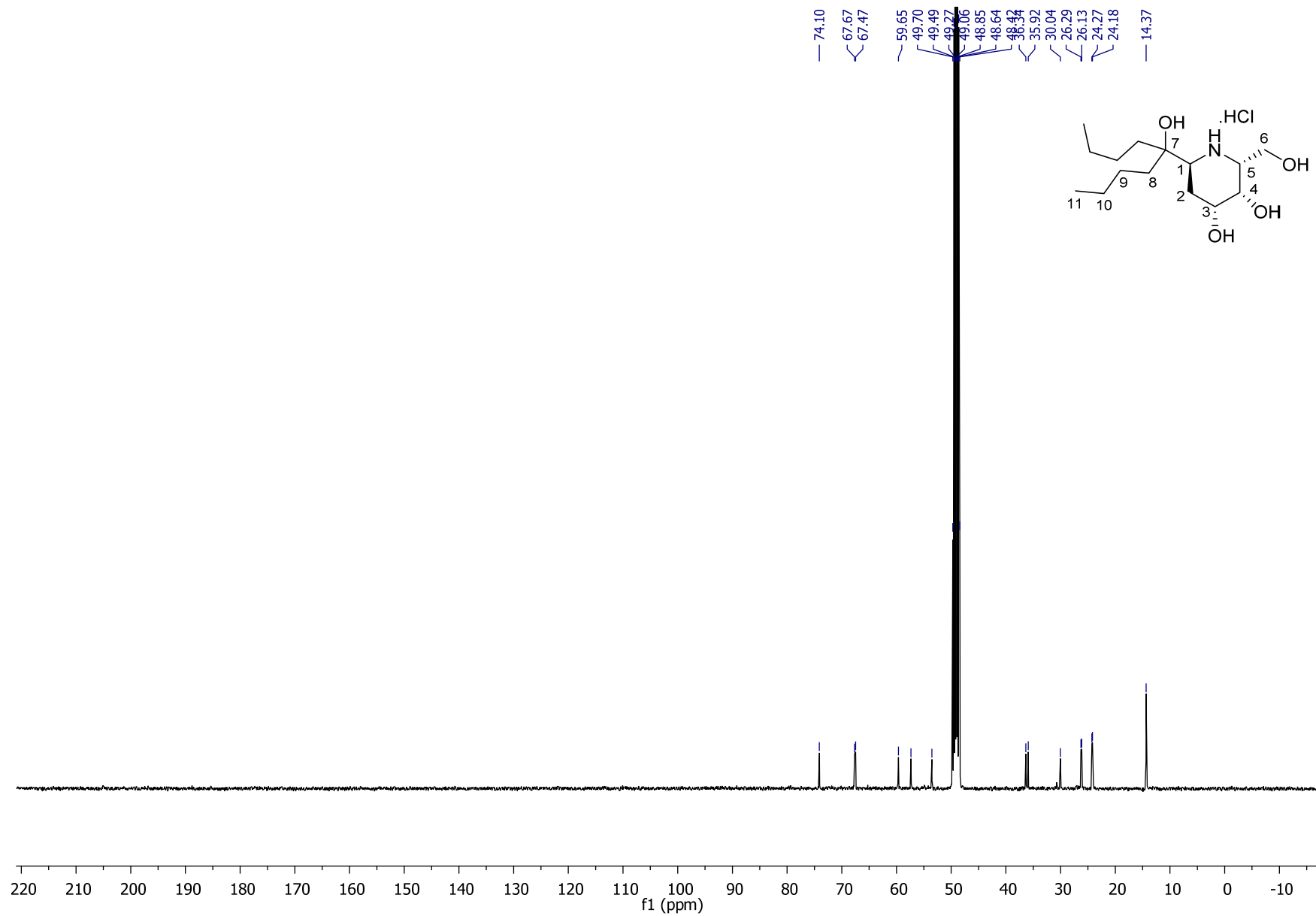
^{13}C NMR of compound **23** (100 MHz, CD_3OD , 300K)



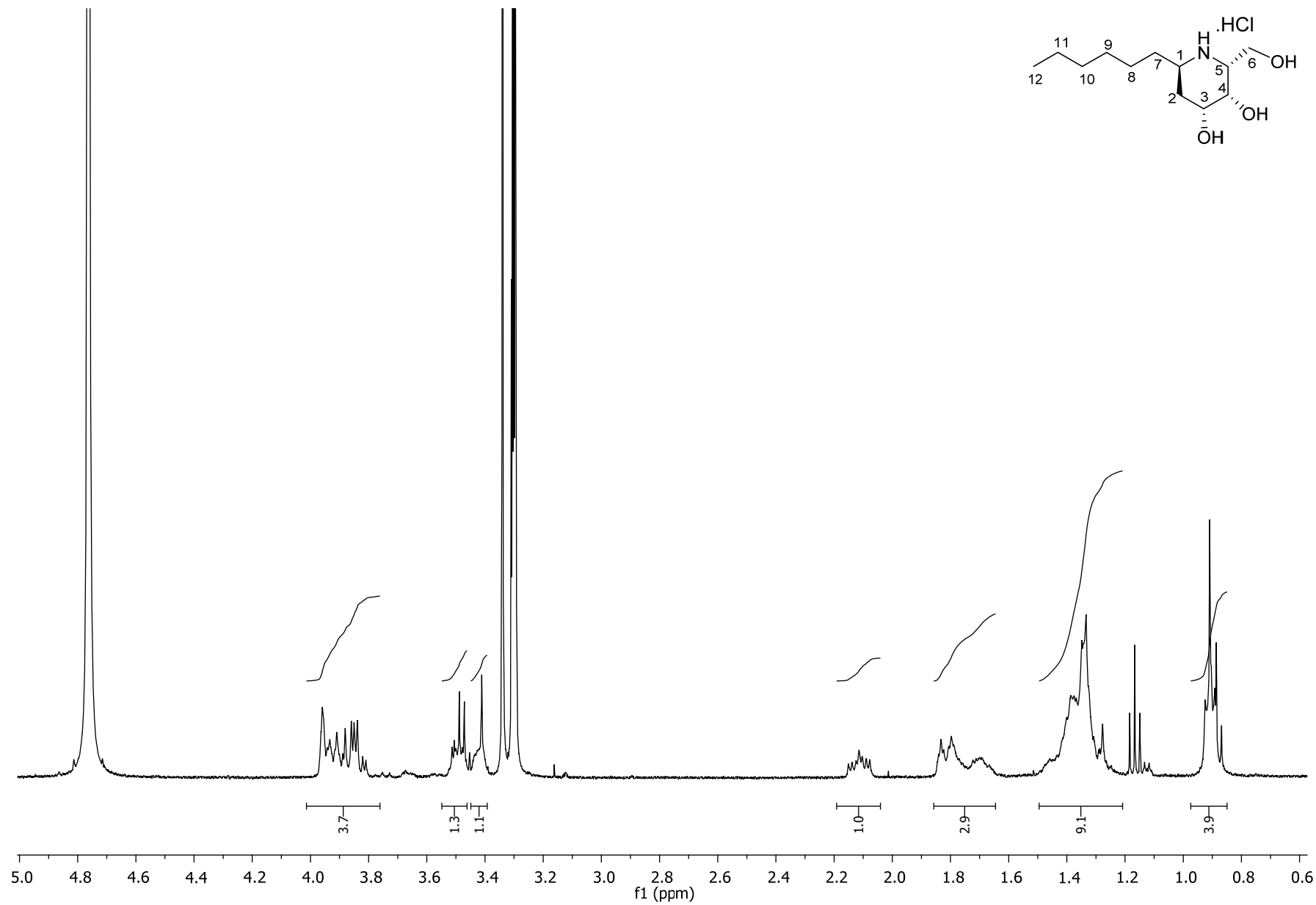
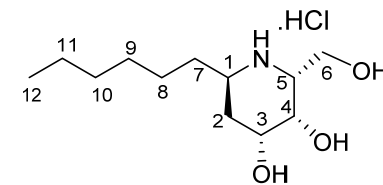
^1H NMR spectrum of compound **24** (400 MHz, CH_3OD , 300K)



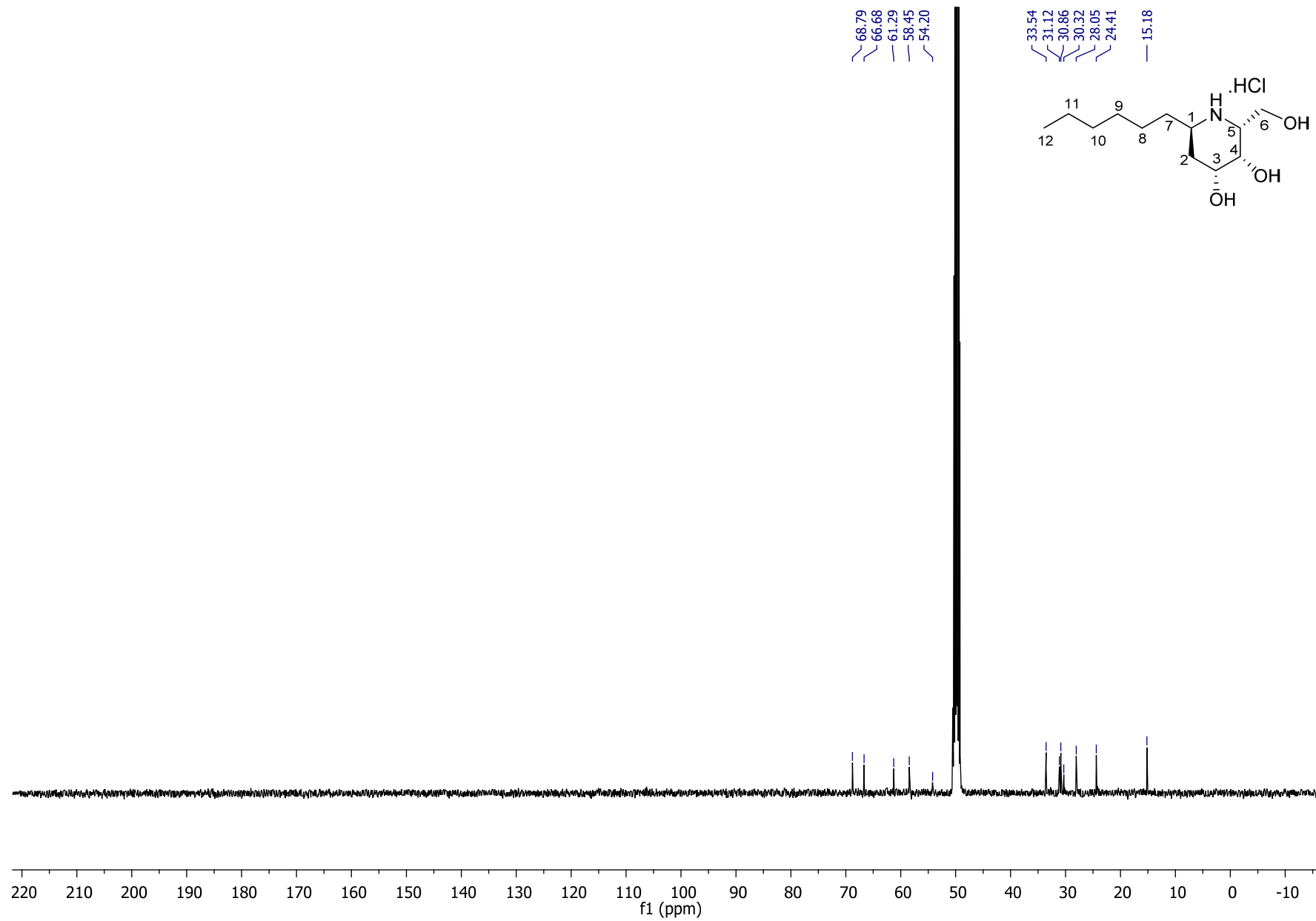
^{13}C NMR of compound **24** (100 MHz, CH_3OD , 300K)



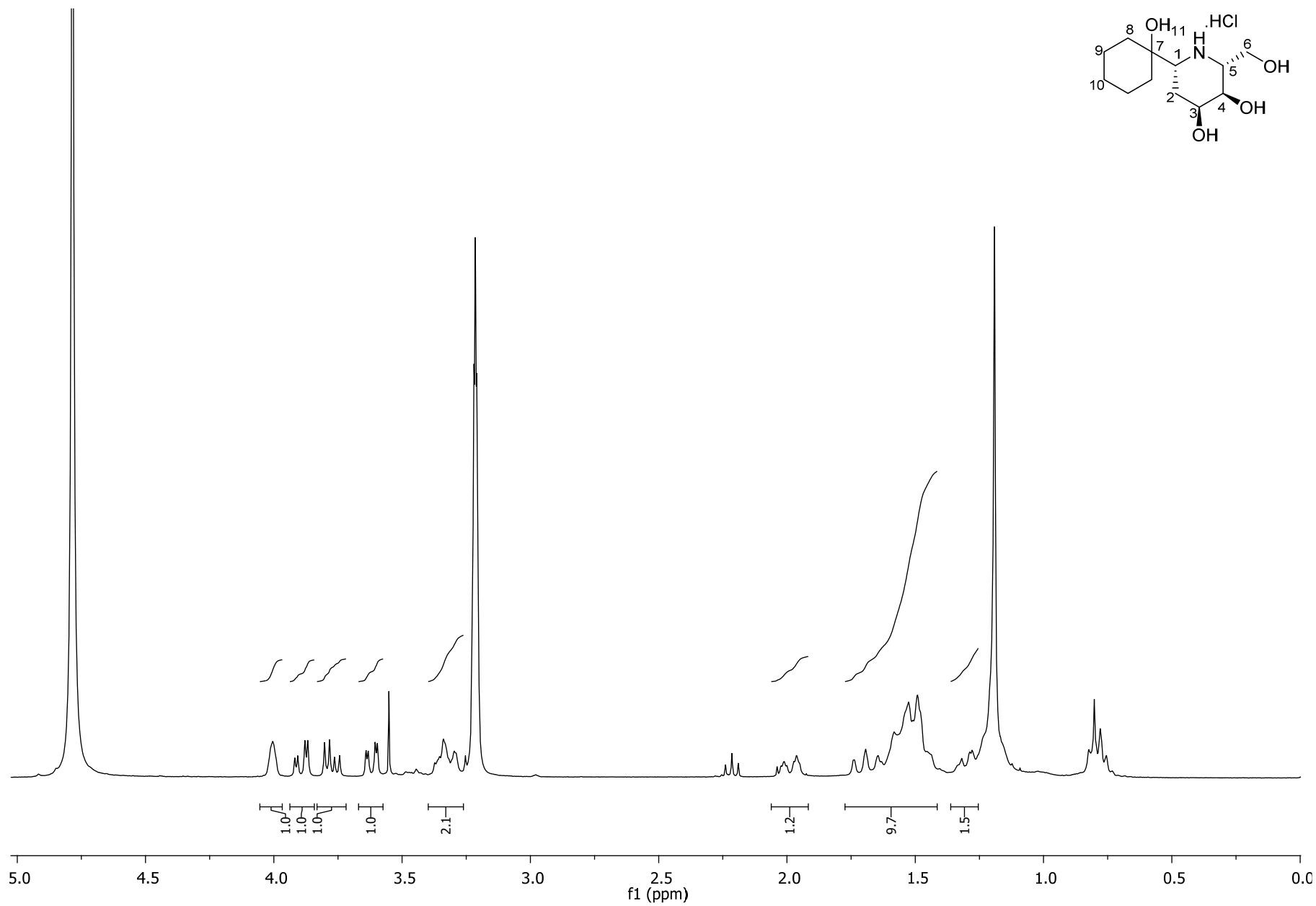
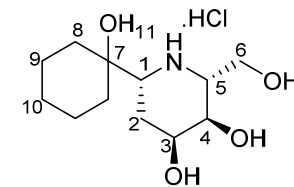
^1H NMR of compound **25** (400 MHz, CD_3OD , 300K)



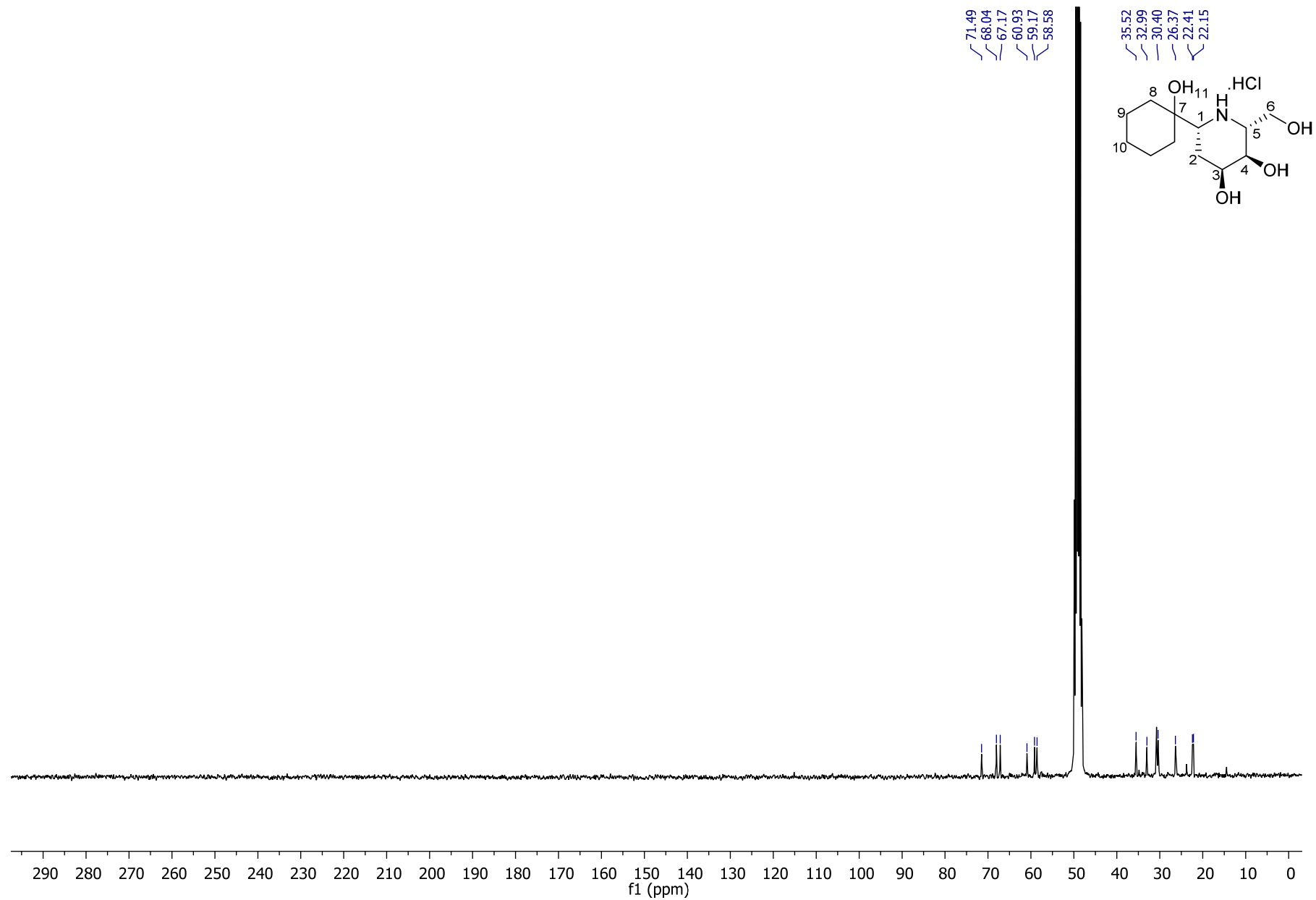
^{13}C NMR of compound **25** (100 MHz, CD_3OD , 300K)



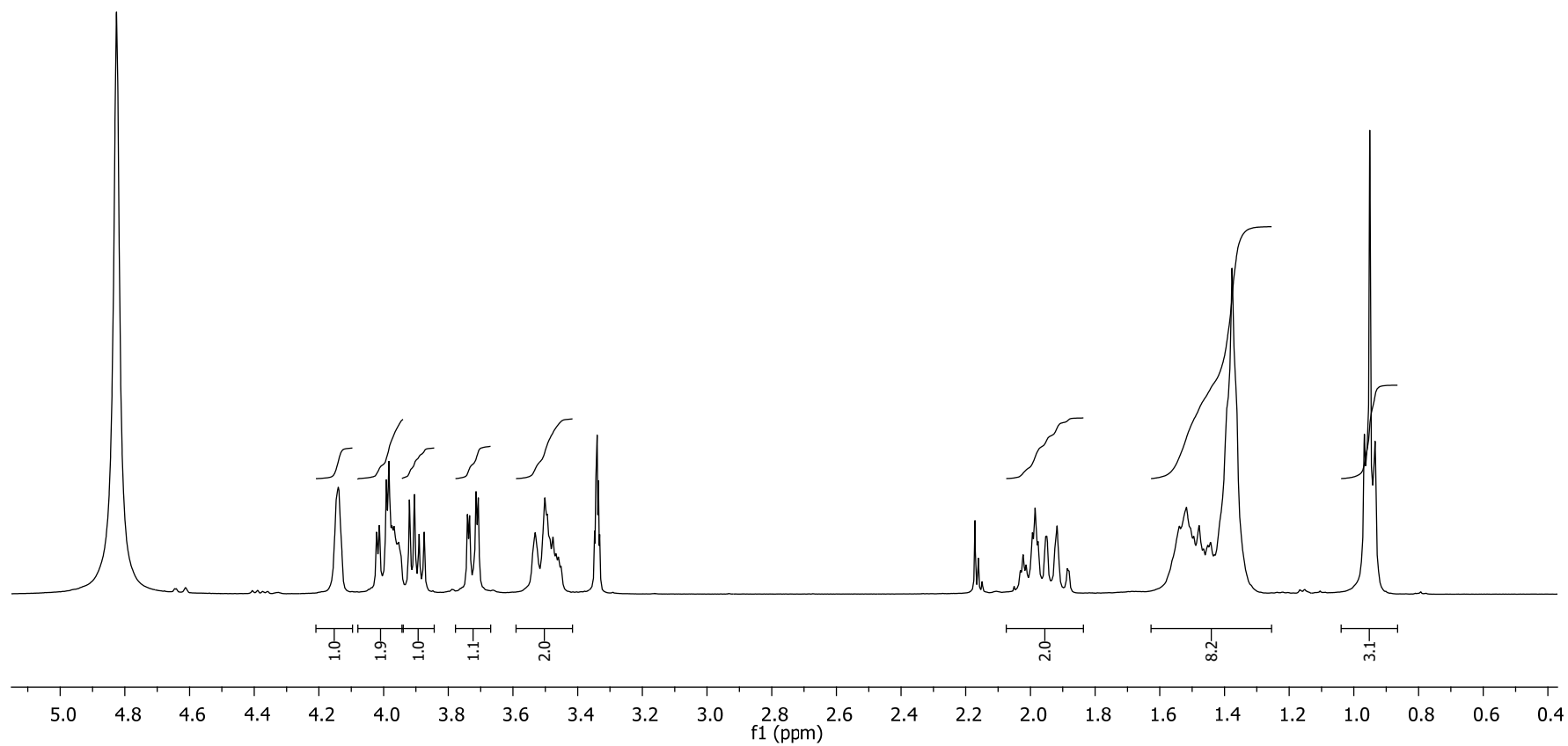
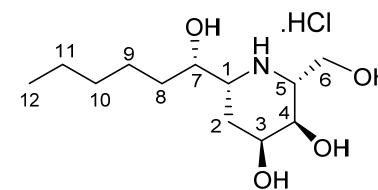
^1H NMR of compound **26** (300 MHz, CD_3OD , 300K)



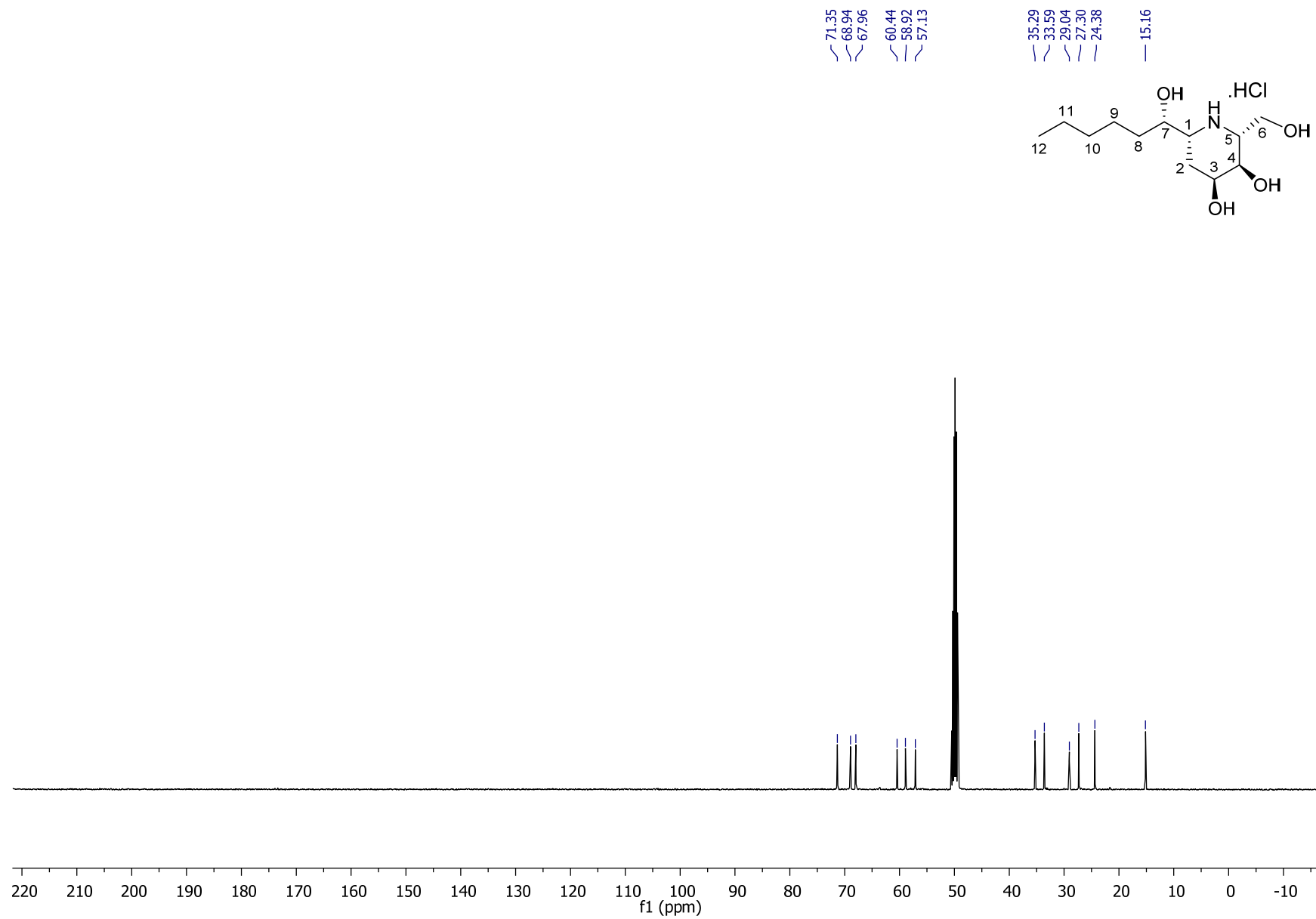
^{13}C NMR of compound **26** (75 MHz, CD_3OD , 300K)



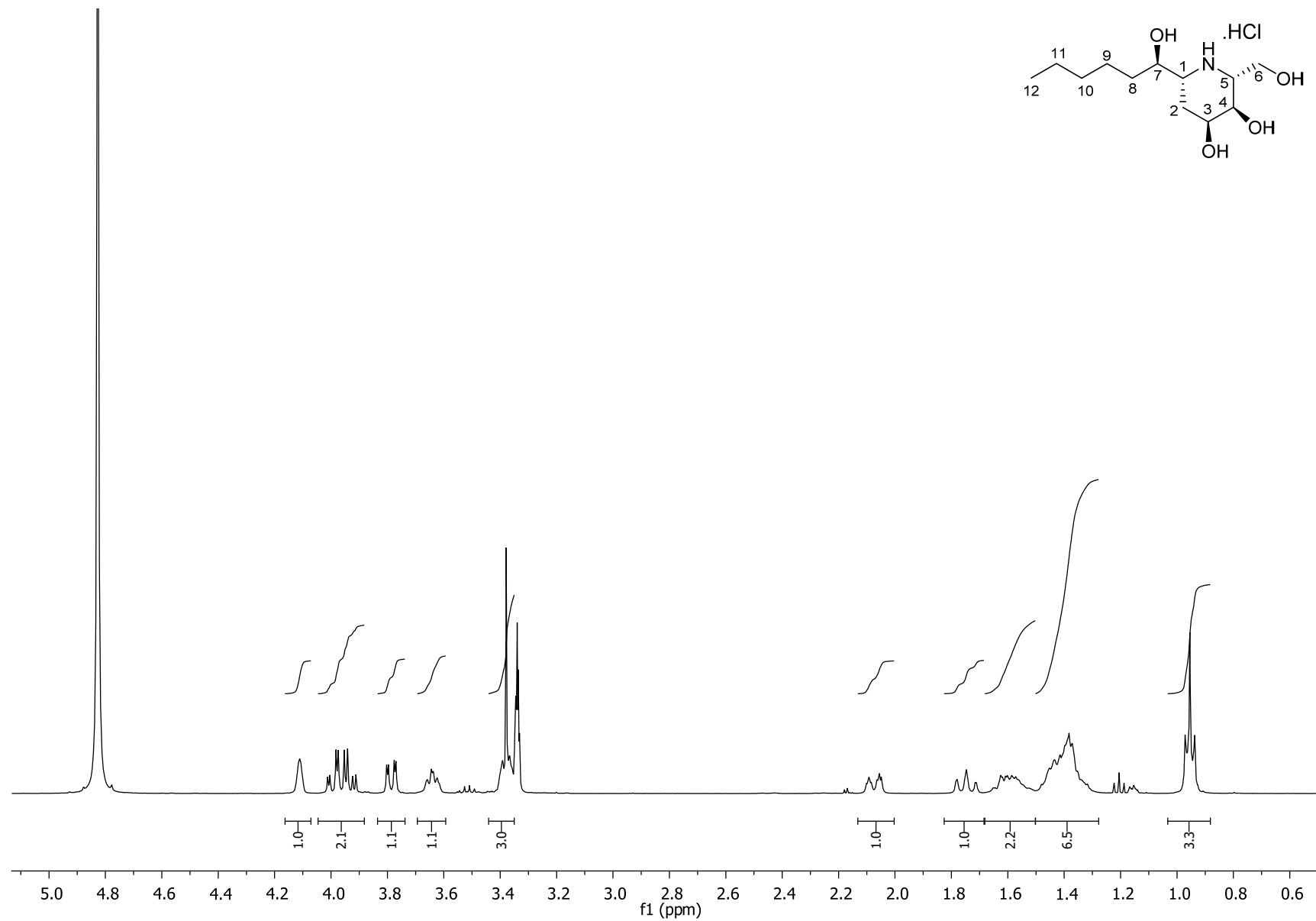
^1H NMR of compound **27** (400MHz, CD_3OD , 300K)



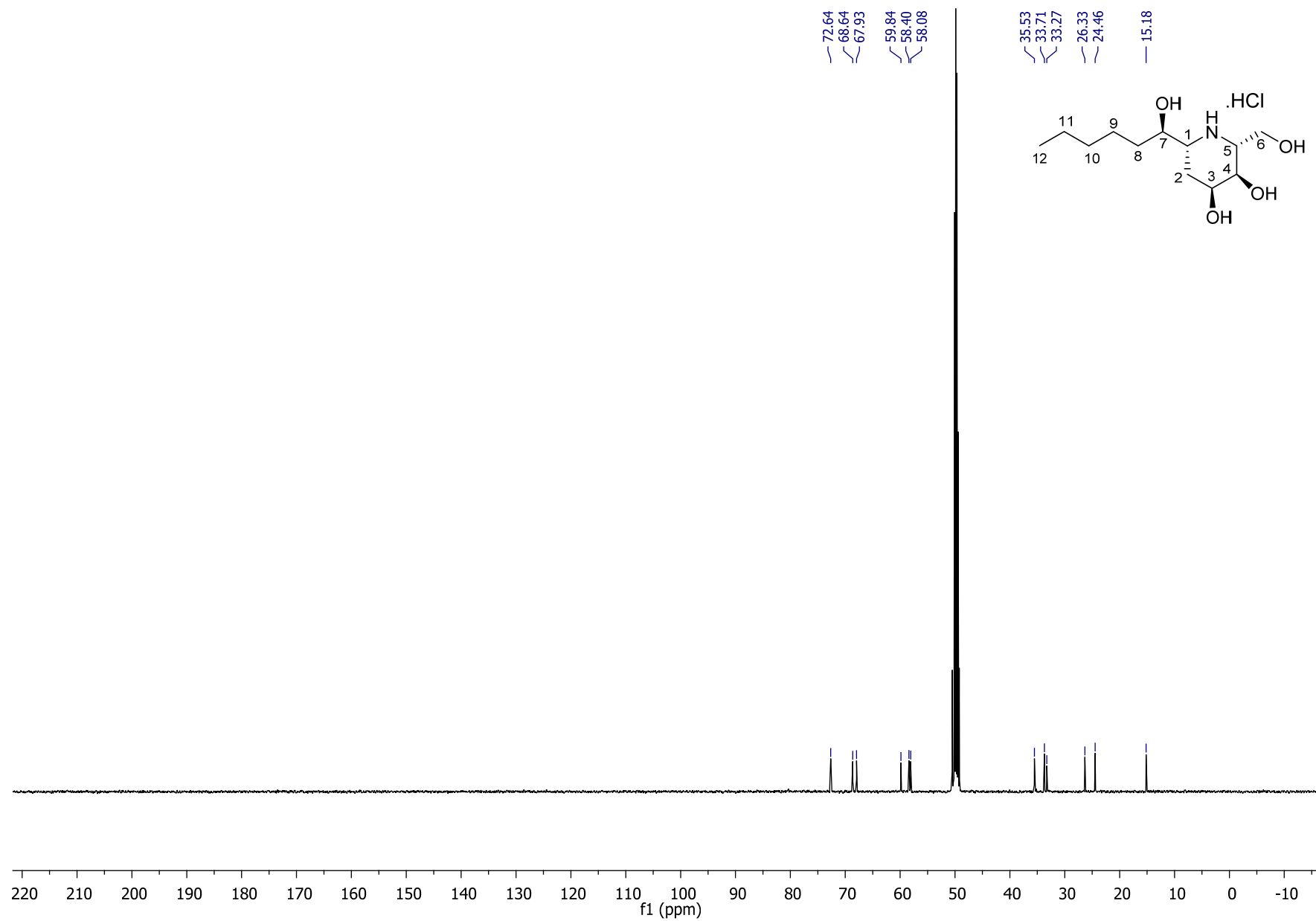
^{13}C NMR of compound **27** (100 MHz, CD_3OD , 300K)



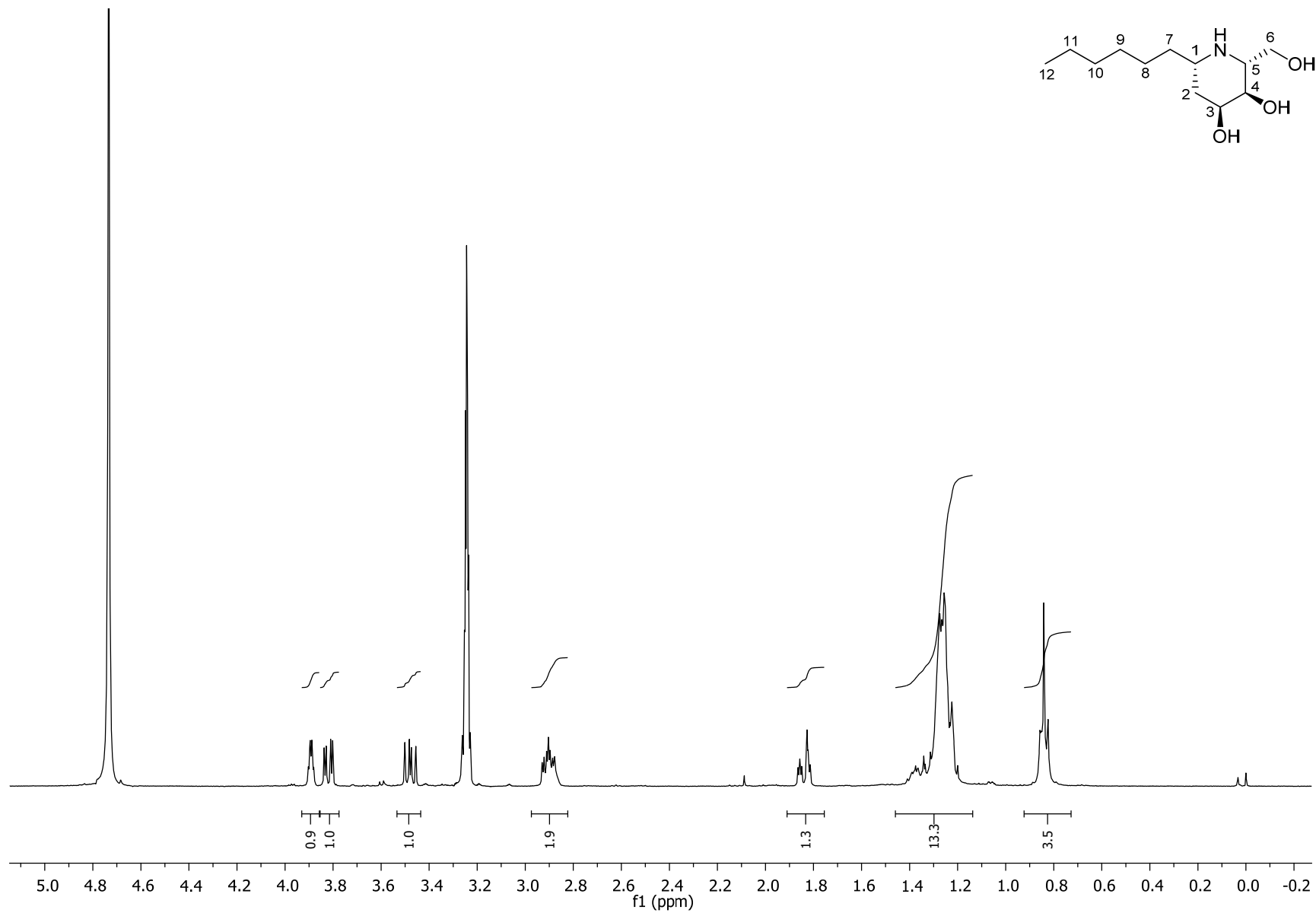
^1H NMR of compound **28** (400MHz, CD_3OD , 300K)



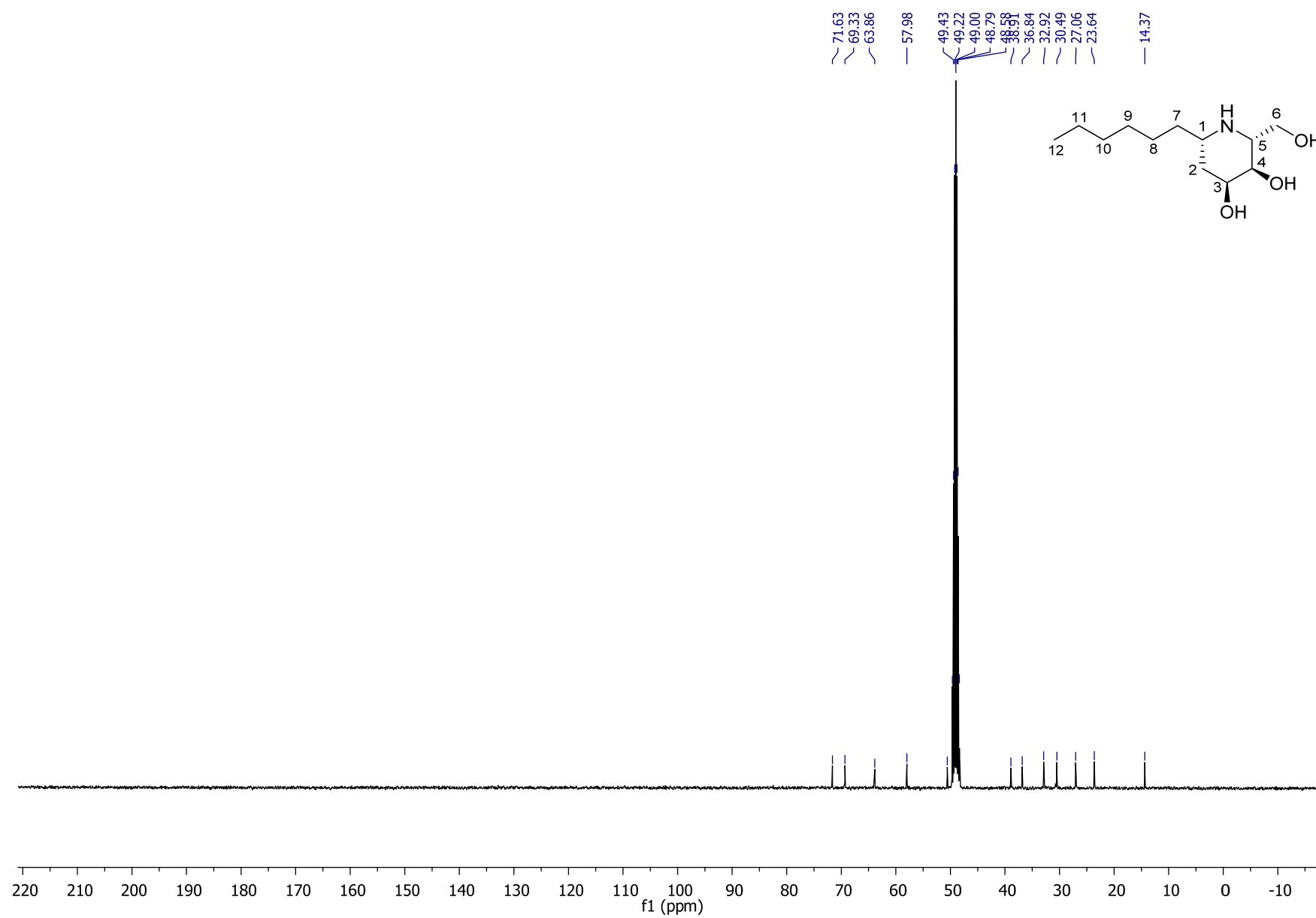
^{13}C NMR of compound **28** (100 MHz, CD_3OD , 300K)



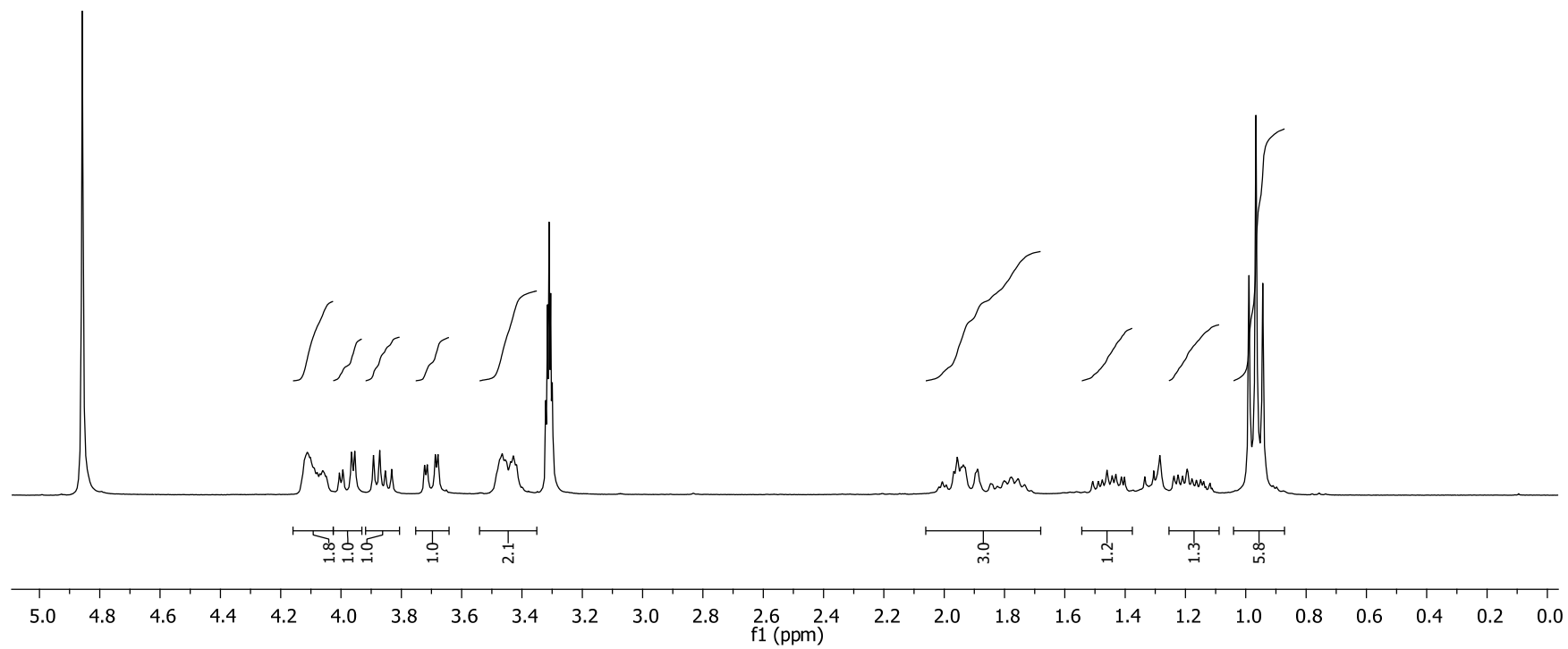
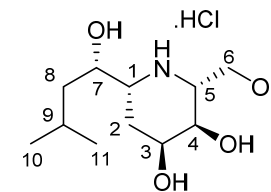
^1H NMR of compound **29** (400 MHz, CD_3OD , 300K)



^{13}C NMR of compound **29** (100 MHz, CD_3OD , 300K)

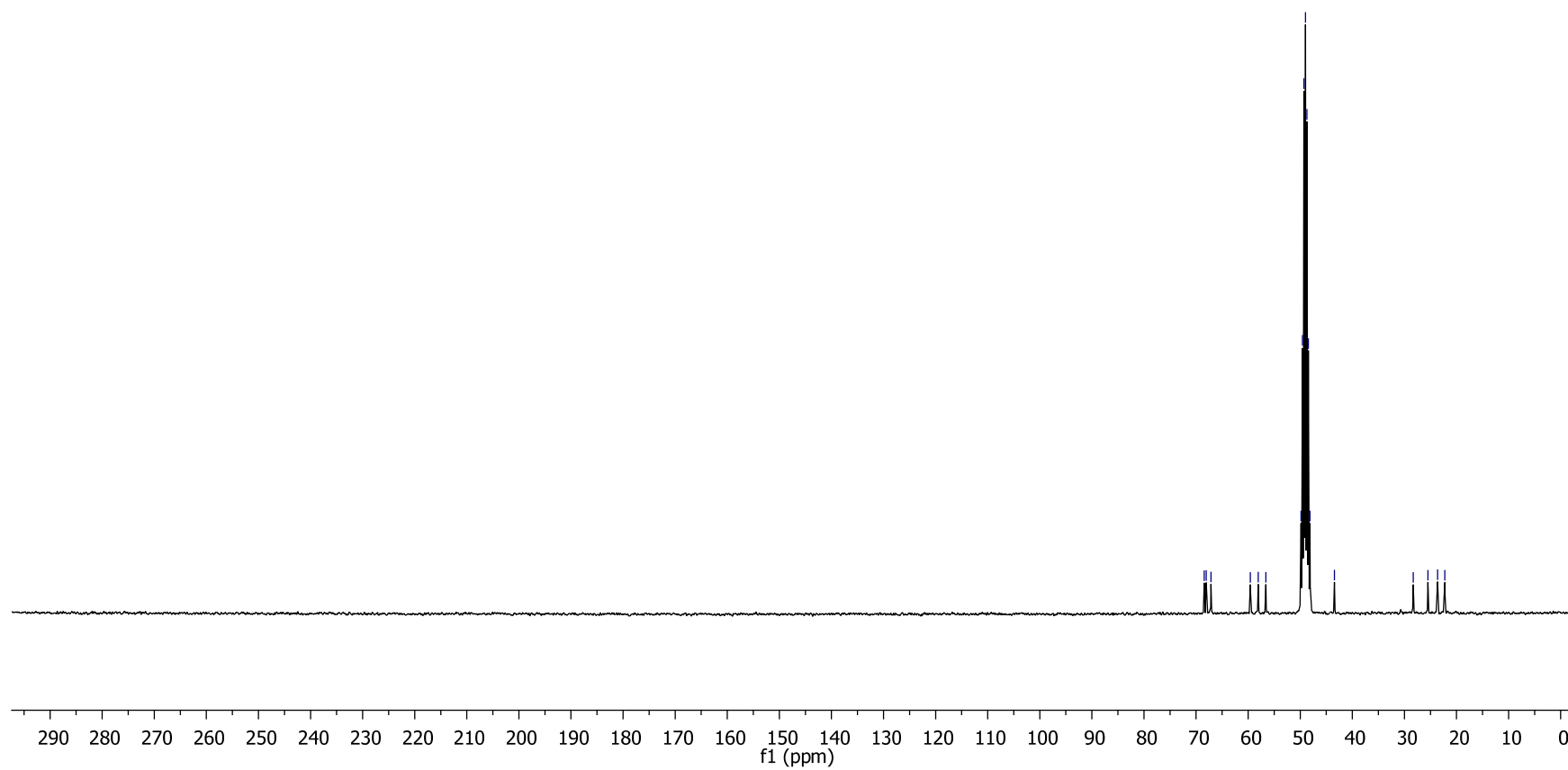
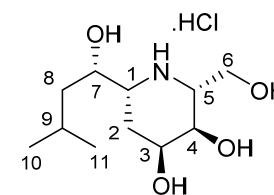


^1H NMR of compound **30** (300 MHz, CD_3OD , 300K)

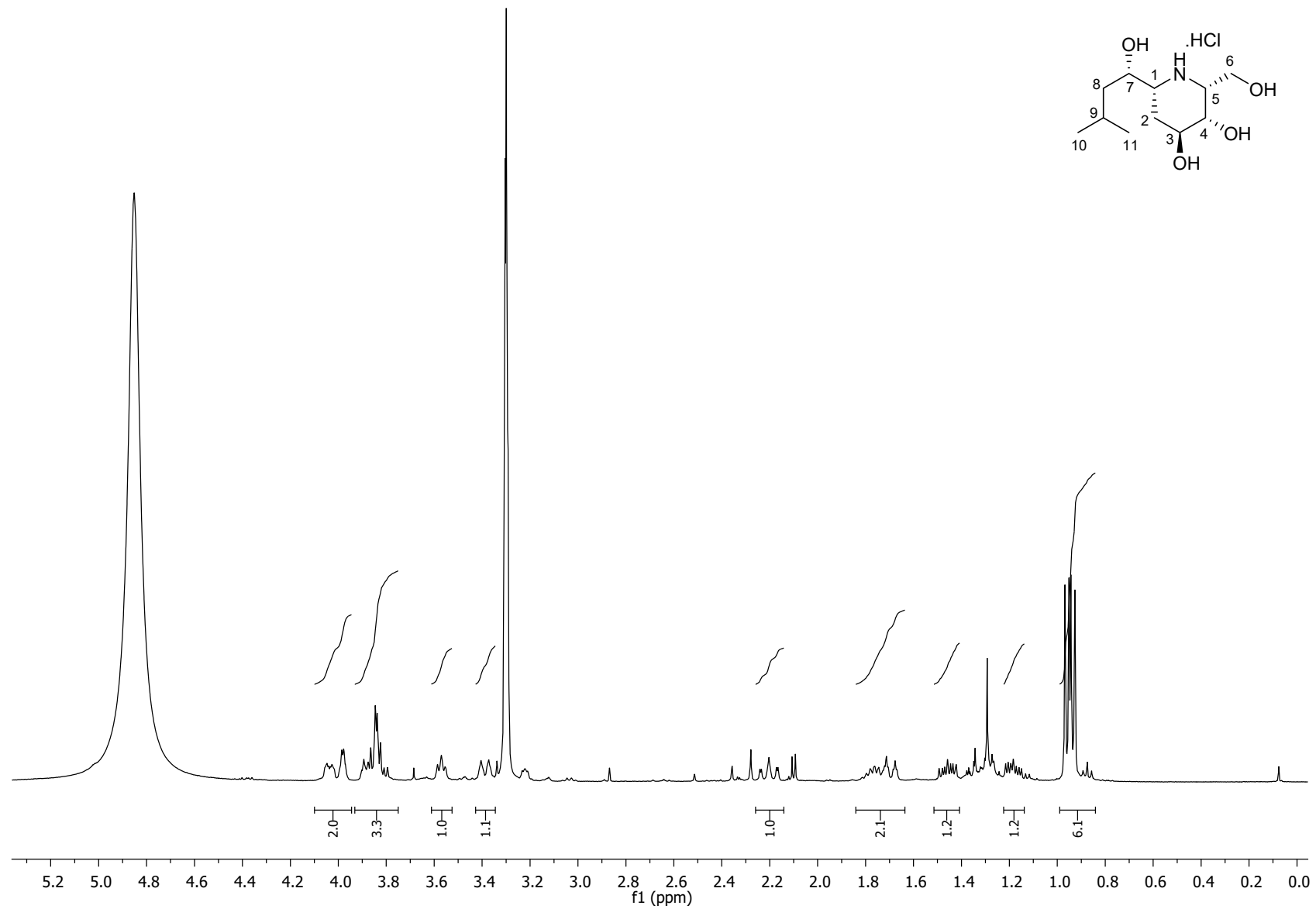


^{13}C NMR of compound **30** (75 MHz, CD_3OD , 300K)

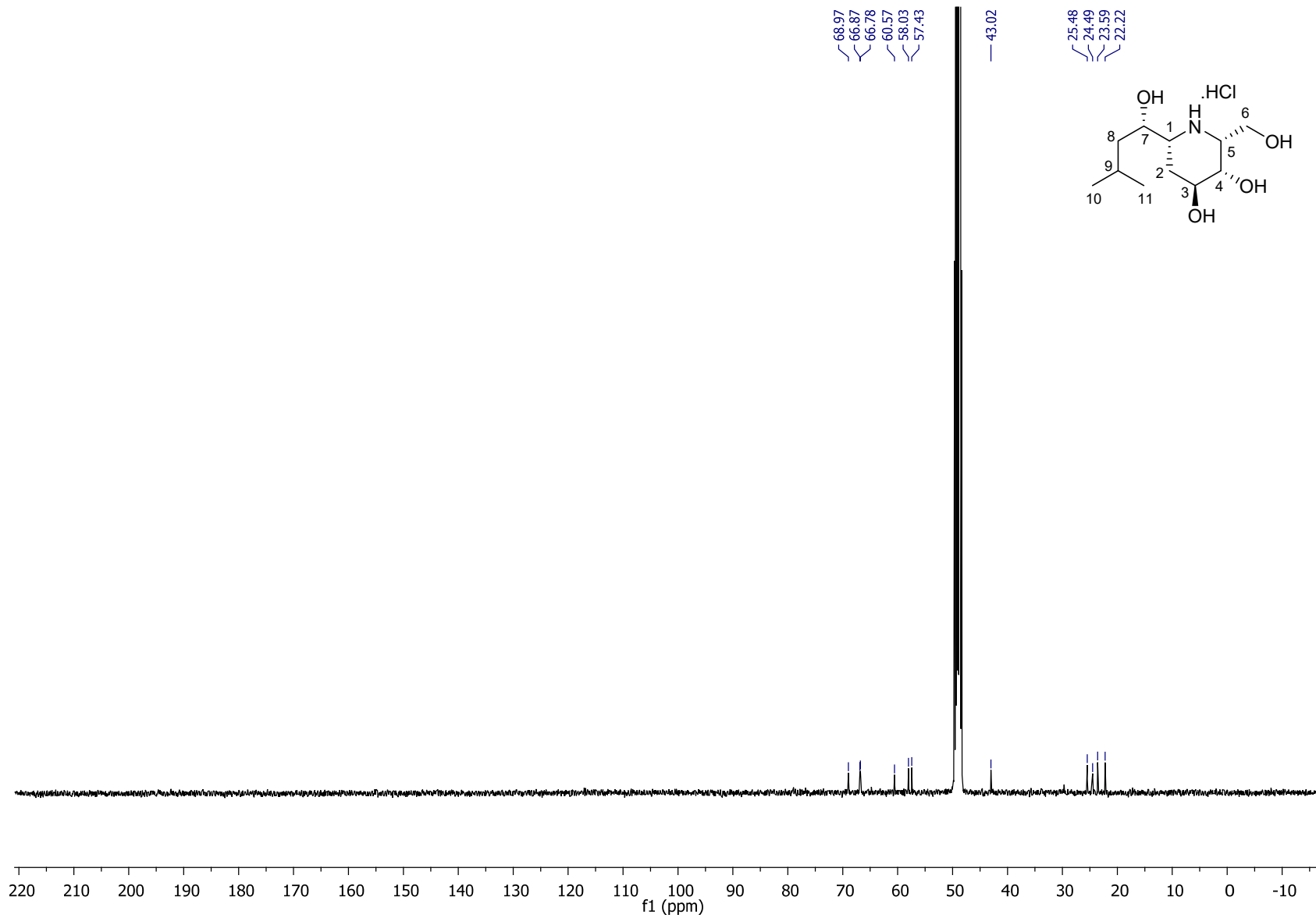
68.44
68.04
67.13
49.85
49.57
49.28
49.00
48.72
48.43
48.15
48.30
25.50
23.64
22.26



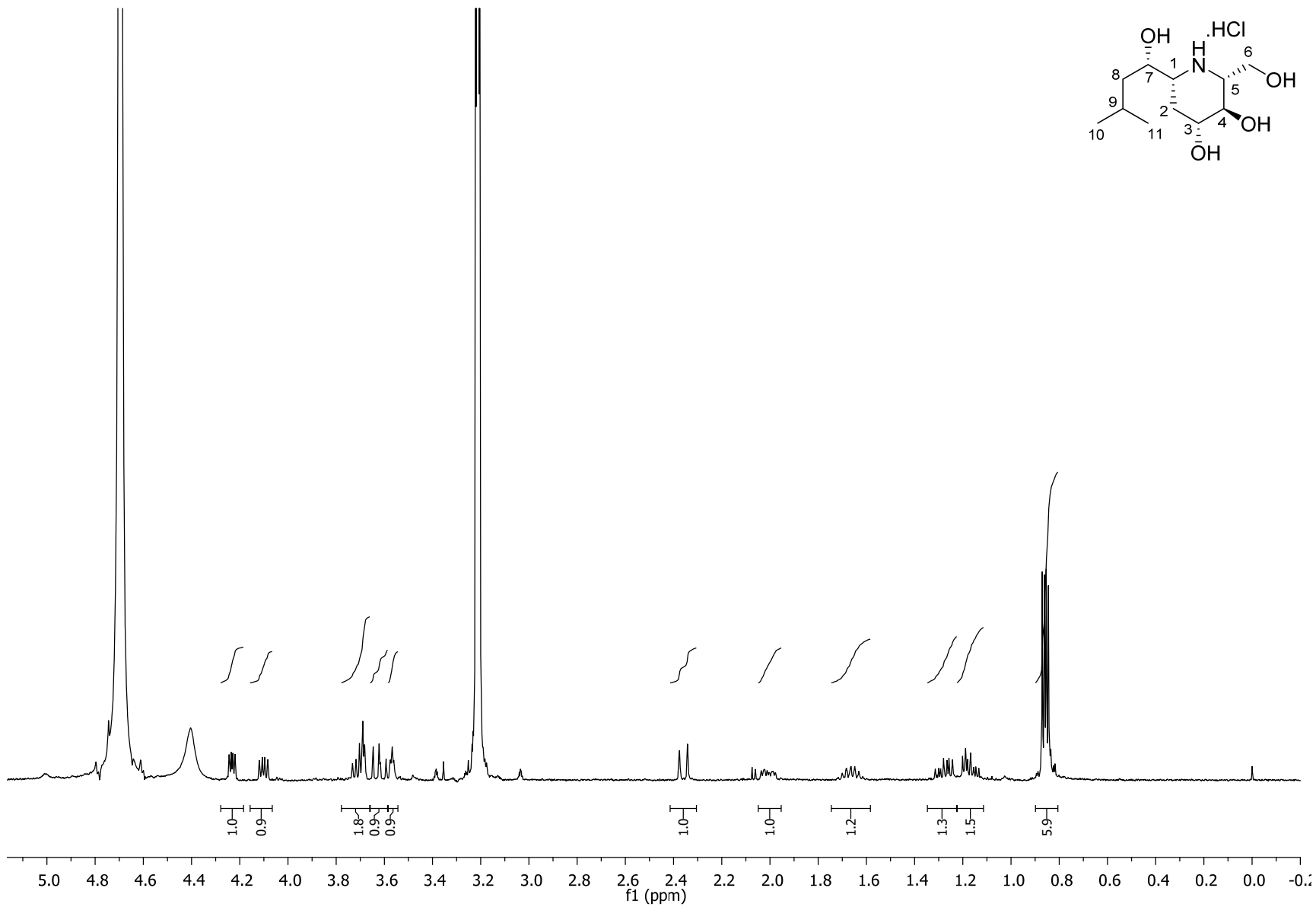
^1H NMR of compound **31** (400 MHz, CD_3OD , 300K)



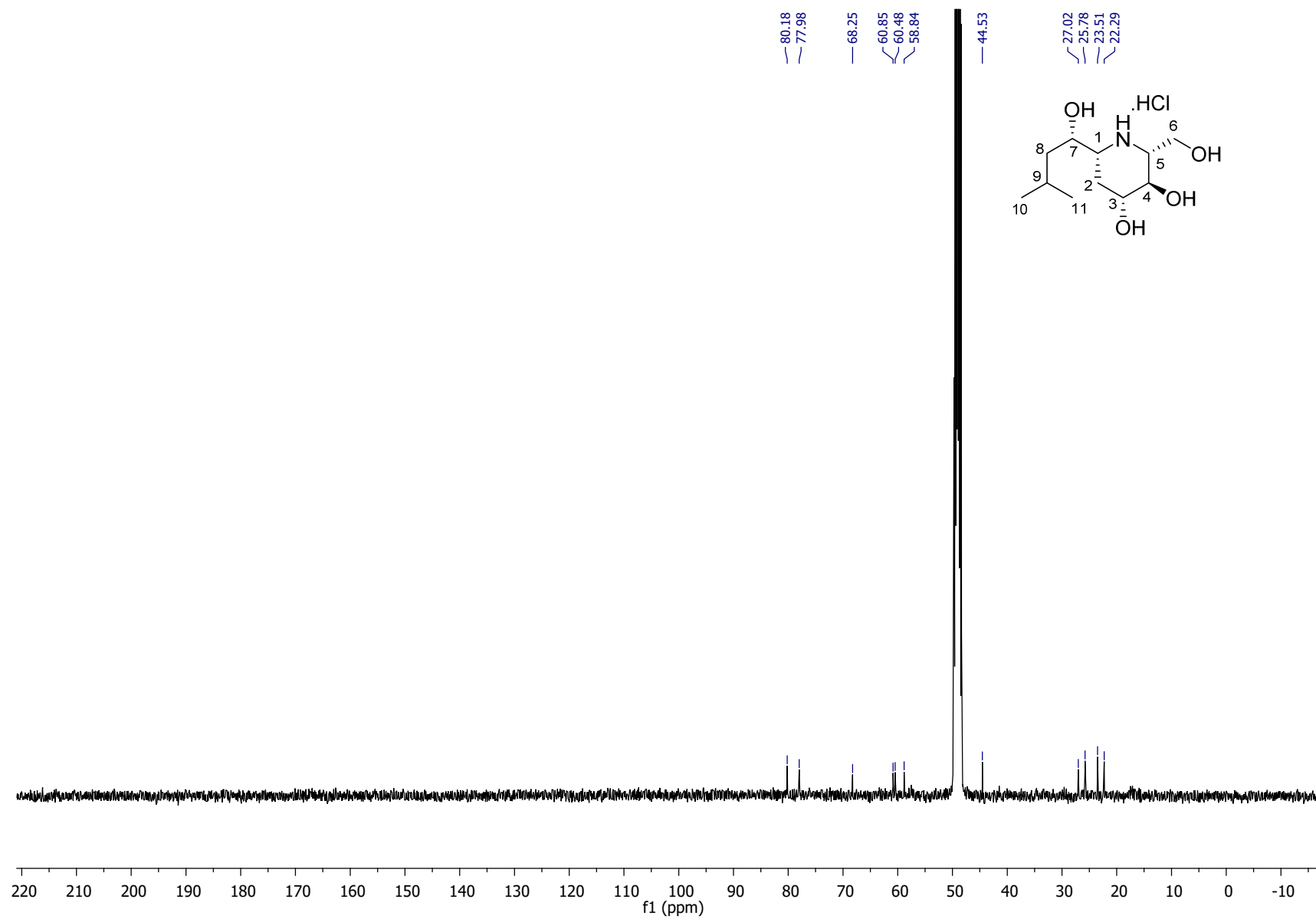
^{13}C NMR of compound **31** (100 MHz, CD_3OD , 300K)



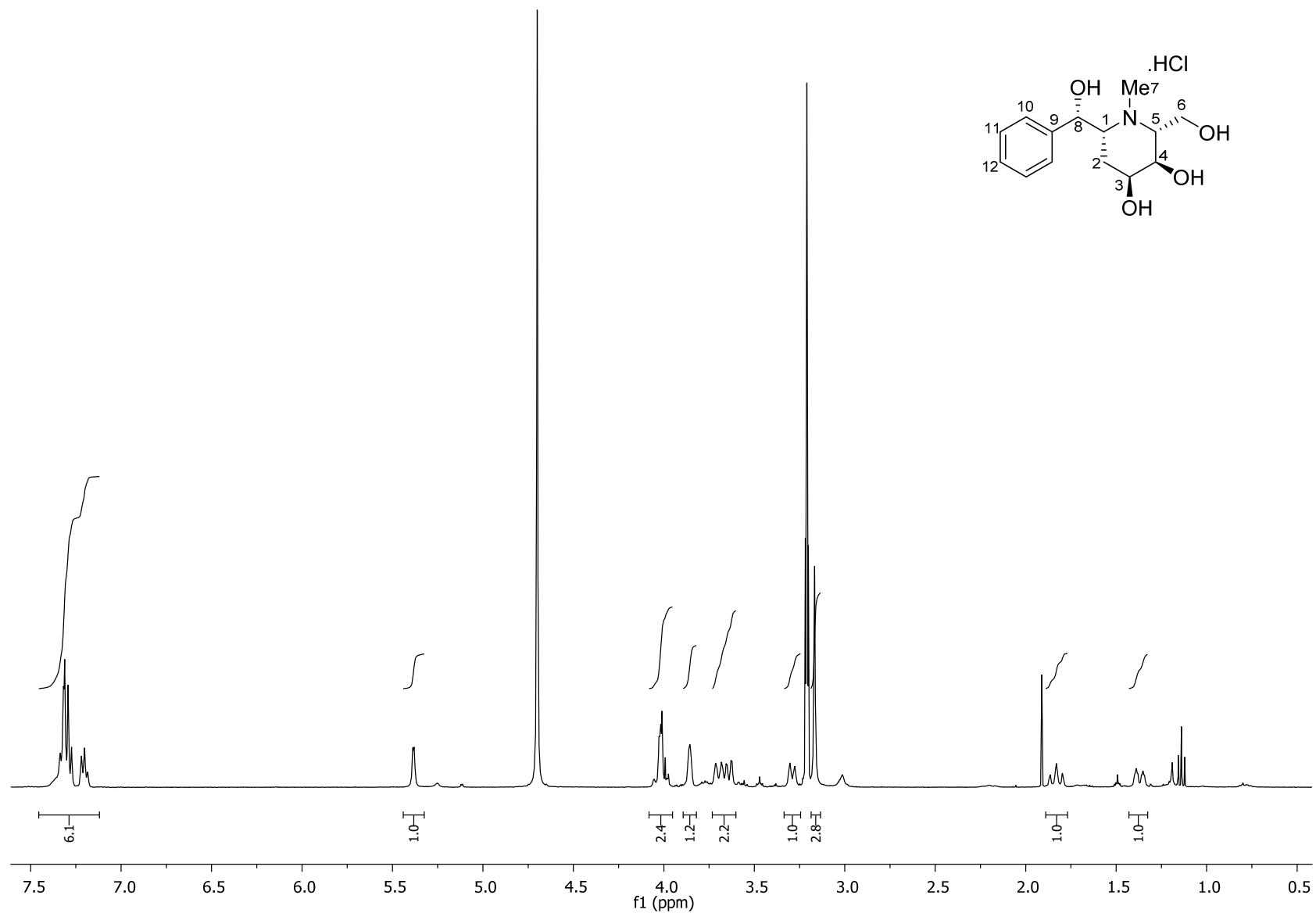
^1H NMR of compound **32** (400 MHz, CD_3OD , 300K)



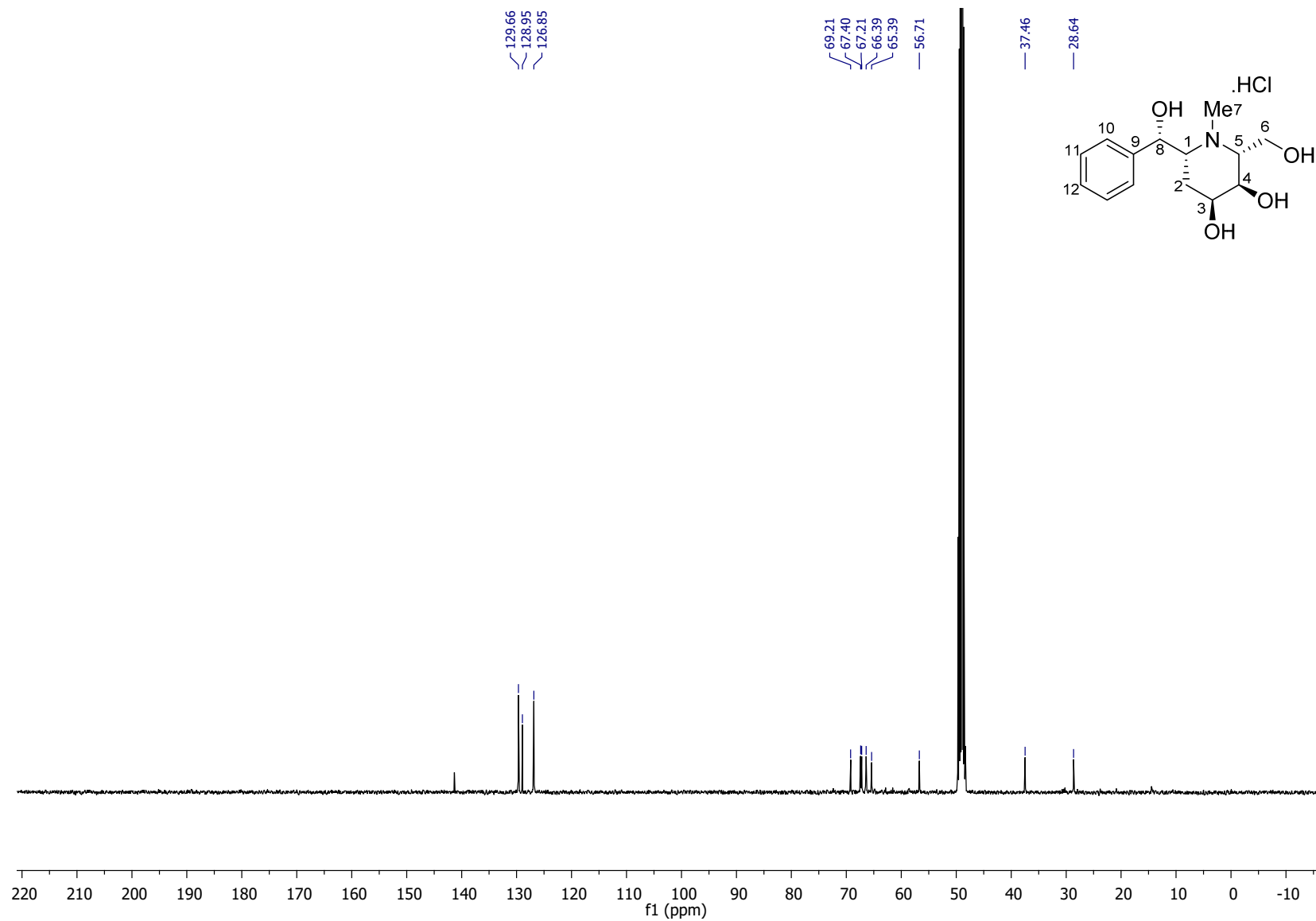
^{13}C NMR of compound **32** (100 MHz, CD_3OD , 300K)



^1H NMR of compound **35** (400 MHz, CD_3OD , 300K)



^{13}C NMR of compound **35** (100 MHz, CD_3OD , 300K)



II- Dixon and Lineweaver-Burk plots for K_i determination

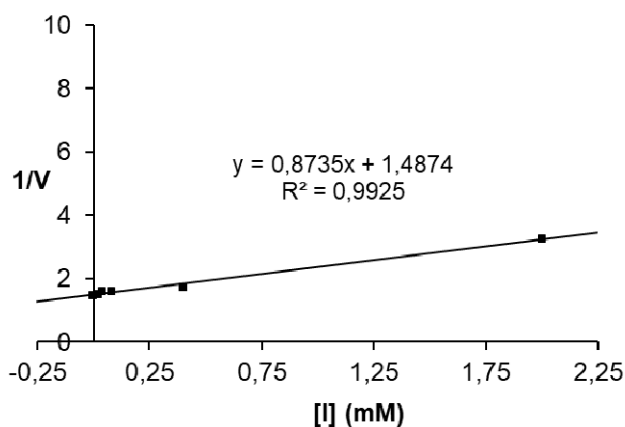


Figure S1. Dixon Plot for K_i determination ($473 \pm 50 \mu\text{M}$) of **23** against *bovine liver* β -galactosidase.

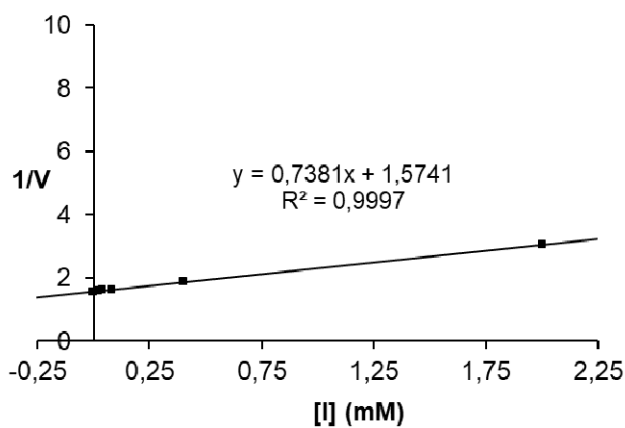


Figure S2. Dixon Plot for K_i determination ($652 \pm 55 \mu\text{M}$) of **24** against *bovine liver* β -galactosidase.

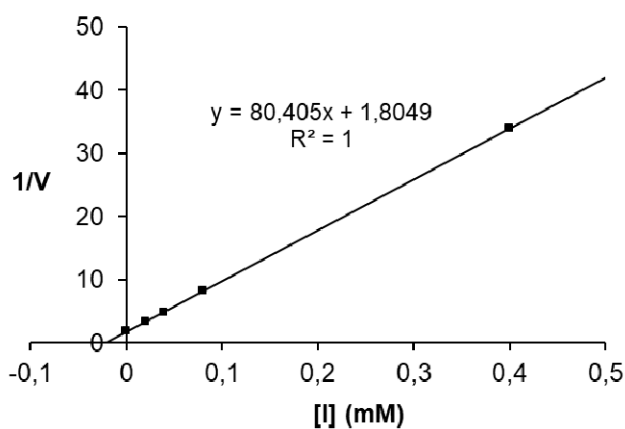


Figure S3. Dixon Plot for K_i determination ($10 \pm 0,2 \mu\text{M}$) of **25** against *bovine liver* β -galactosidase.

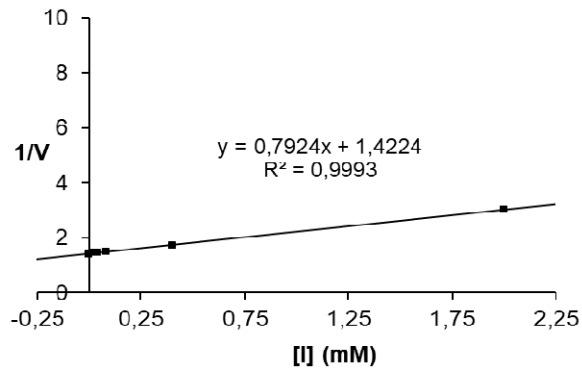


Figure S4. Dixon Plot for K_i determination ($475 \pm 45 \mu\text{M}$) of **33** against bovine liver β -galactosidase.

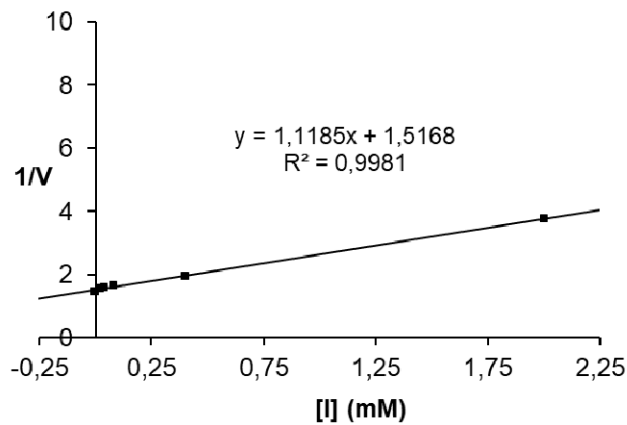


Figure S5. Dixon Plot for K_i determination ($301 \pm 25 \mu\text{M}$) of **26** against bovine liver β -galactosidase.

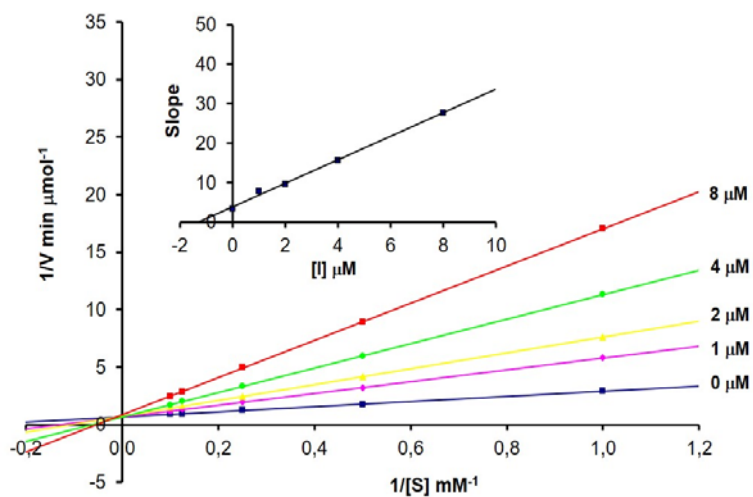


Figure S6. Lineweaver-Burk Plot for K_i determination ($1.3 \pm 0.1 \mu\text{M}$) of **27** against bovine liver β -galactosidase/ β -glucosidase.

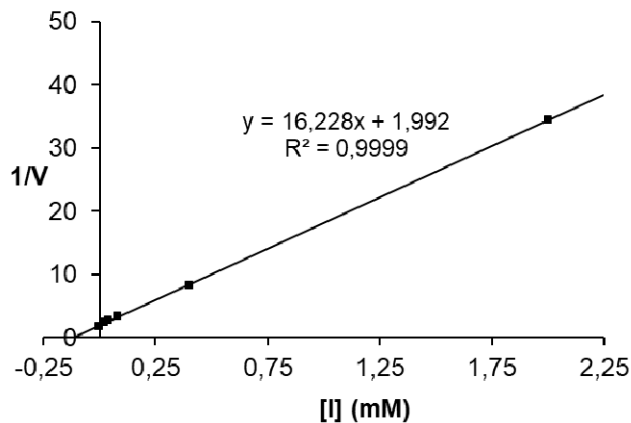


Figure S7. Dixon Plot for K_i determination ($42 \pm 4 \mu\text{M}$) of **28** against *bovine liver* β -galactosidase/ β -glucosidase.

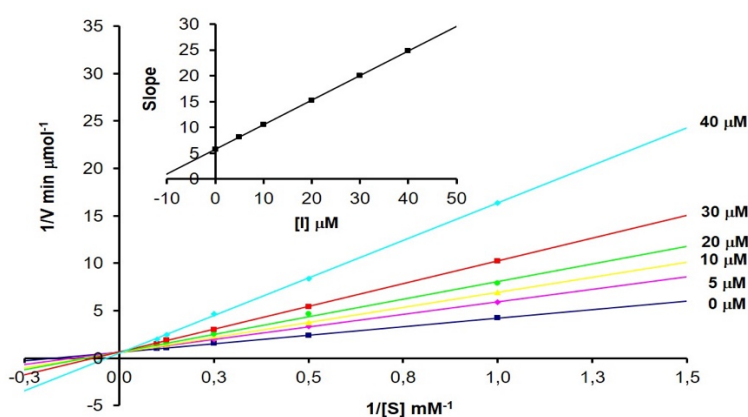


Figure S8. Lineweaver-Burk Plot for K_i determination ($12.1 \pm 2 \mu\text{M}$) of **29** against *bovine liver* β -galactosidase/ β -glucosidase.

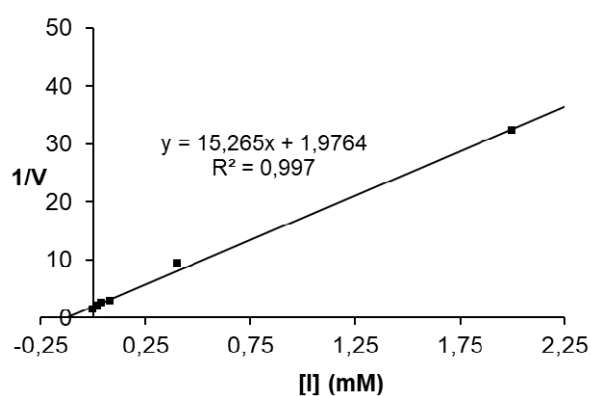


Figure S9. Dixon Plot for K_i determination ($58 \pm 6 \mu\text{M}$) of **30** against *bovine liver* β -galactosidase.

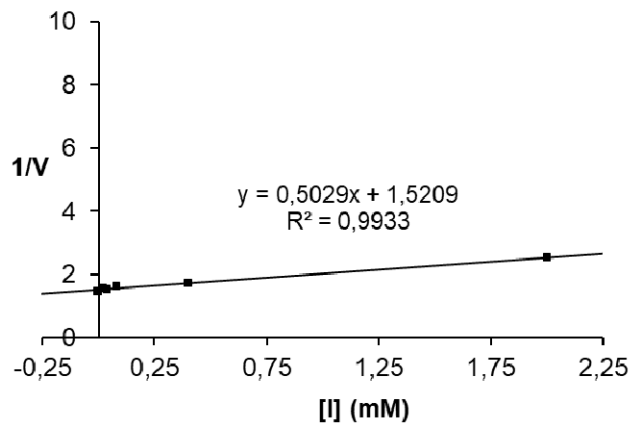


Figure S10. Dixon Plot for K_i determination ($594 \pm 60 \mu\text{M}$) of **34** against *bovine liver* β -galactosidase.

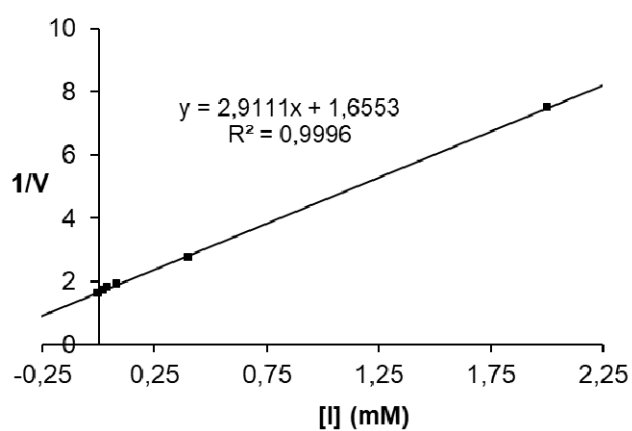


Figure S11. Dixon Plot for K_i determination ($195 \pm 20 \mu\text{M}$) of **35** against *bovine liver* β -galactosidase.

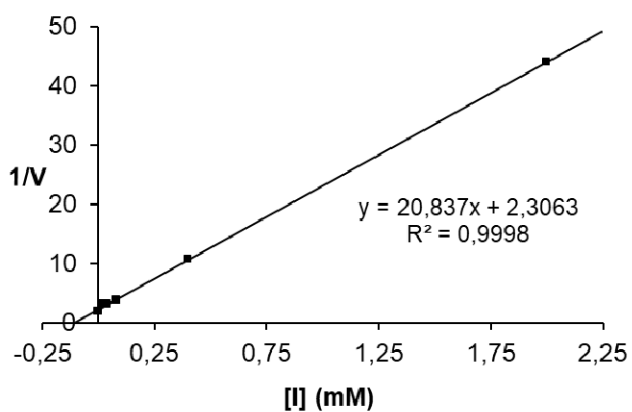


Figure S12. Dixon Plot for K_i determination ($46 \pm 3 \mu\text{M}$) of **24** against *almonds* β -glucosidase.

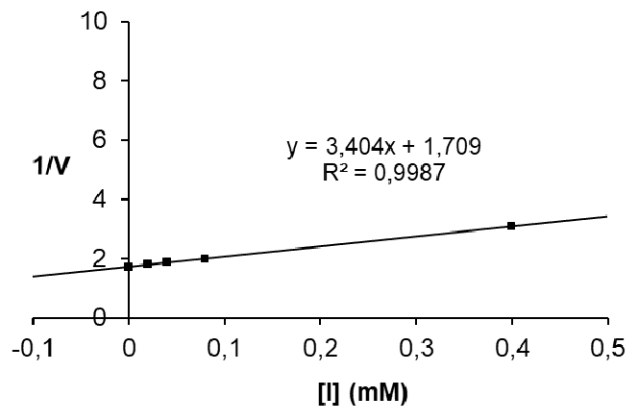


Figure S13. Dixon Plot for K_i determination ($252 \pm 20 \mu\text{M}$) of **25** against *almonds* β -glucosidase.

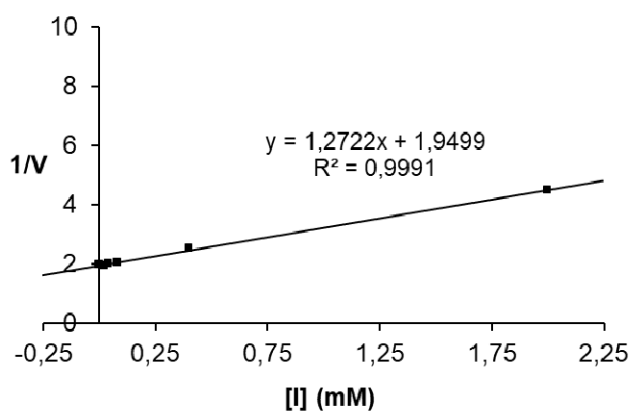


Figure S14. Dixon Plot for K_i determination ($693 \pm 65 \mu\text{M}$) of **26** against *almonds* β -glucosidase.

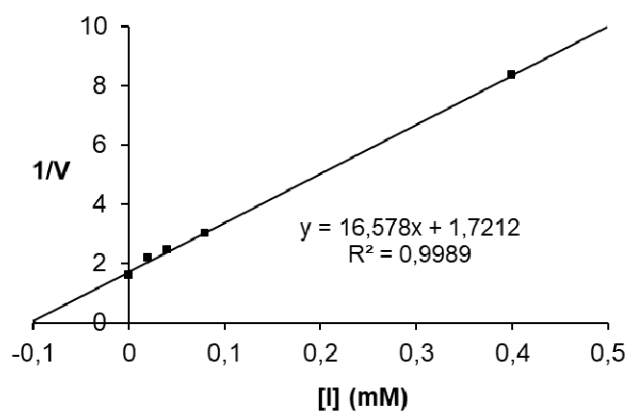


Figure S15. Dixon Plot for K_i determination ($36 \pm 4 \mu\text{M}$) of **27** against *almonds* β -glucosidase.

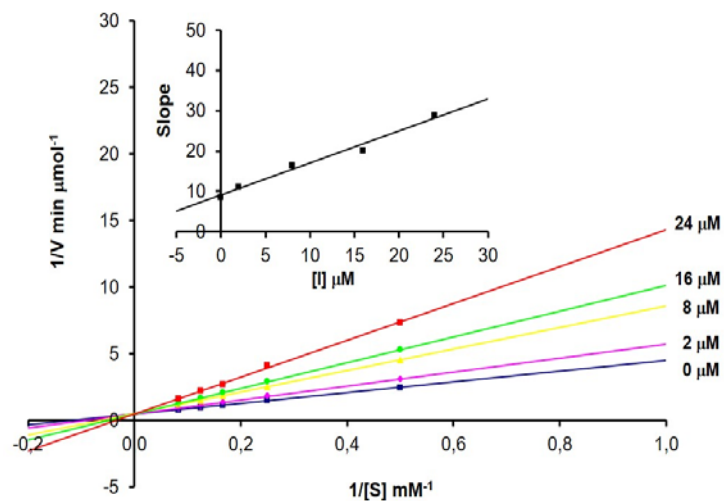


Figure S16. Lineweaver-Burk Plot for K_i determination ($11.4 \pm 2 \mu\text{M}$) of **28** against *almonds* β -glucosidase.

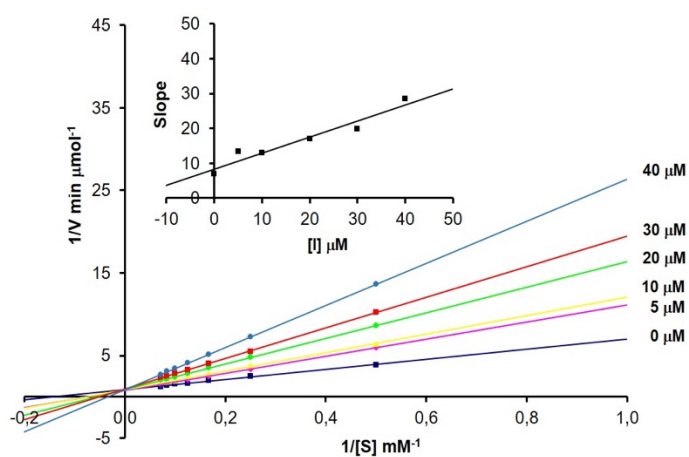


Figure S17. Lineweaver-Burk Plot for K_i determination ($18 \pm 2 \mu\text{M}$) of **29** against *almonds* β -glucosidase.

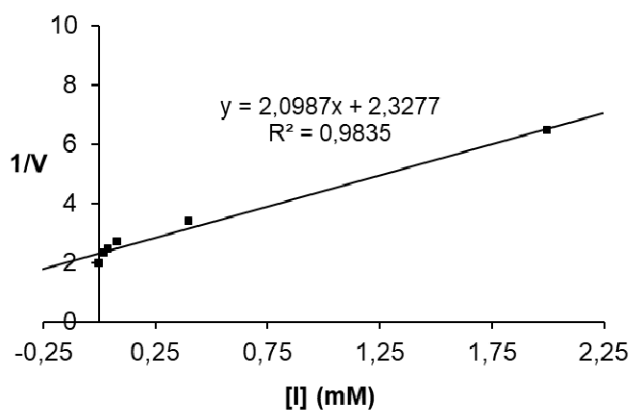


Figure S18. Dixon Plot for K_i determination ($436 \pm 41 \mu\text{M}$) of **30** against *almonds* β -glucosidase.

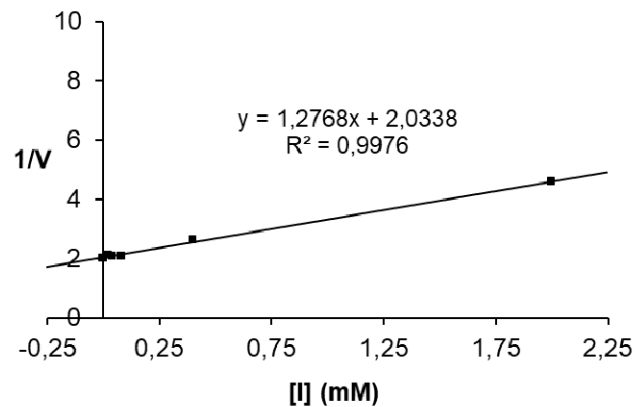


Figure S19. Dixon Plot for K_i determination ($537 \pm 50 \mu\text{M}$) of **34** against *almonds* β -glucosidase.

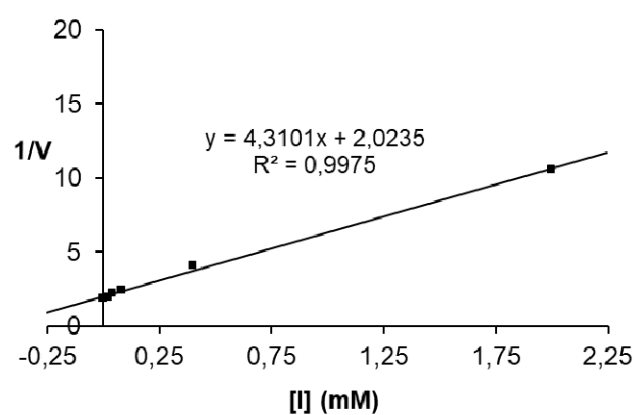


Figure S20. Dixon Plot for K_i determination ($140 \pm 11 \mu\text{M}$) of **35** against *almonds* β -glucosidase.

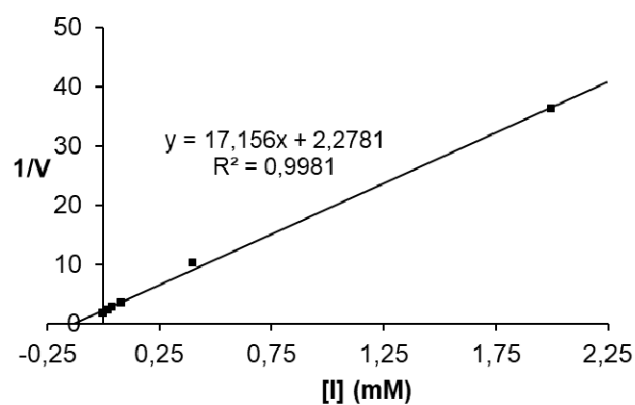


Figure S21. Dixon Plot for K_i determination ($33 \pm 3 \mu\text{M}$) of **23** against *green coffee beans* α -galactosidase.

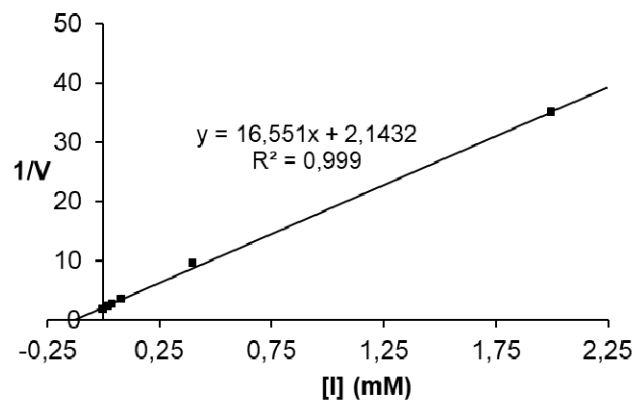


Figure S22. Dixon Plot for K_i determination ($36 \pm 5 \mu\text{M}$) of **24** against green coffee beans α -galactosidase.

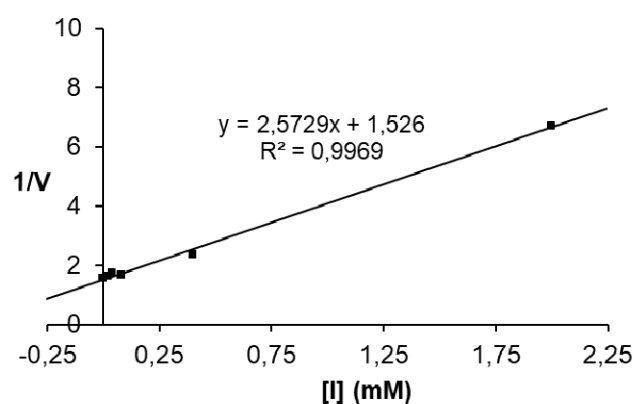


Figure S23. Dixon Plot for K_i determination ($313 \pm 28 \mu\text{M}$) of **25** against green coffee beans α -galactosidase.

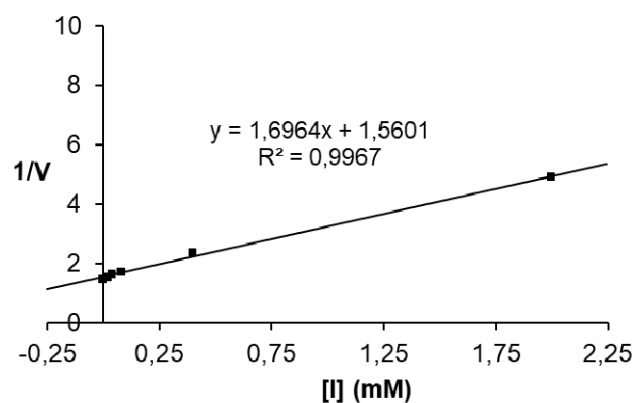


Figure S24. Dixon Plot for K_i determination ($223 \pm 20 \mu\text{M}$) of **33** against green coffee beans α -galactosidase.

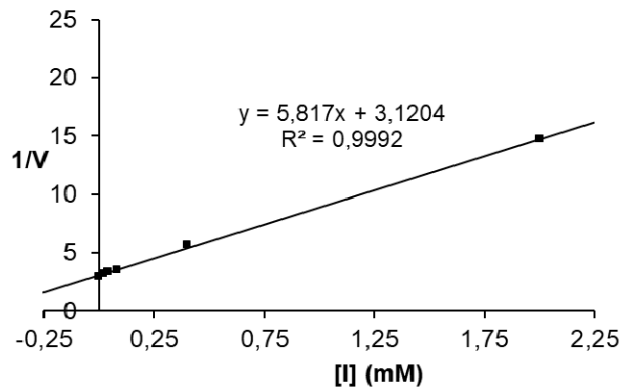


Figure S25. Dixon Plot for K_i determination ($153 \pm 12 \mu\text{M}$) of **24** against *Aspergillus niger* amyloglucosidase.

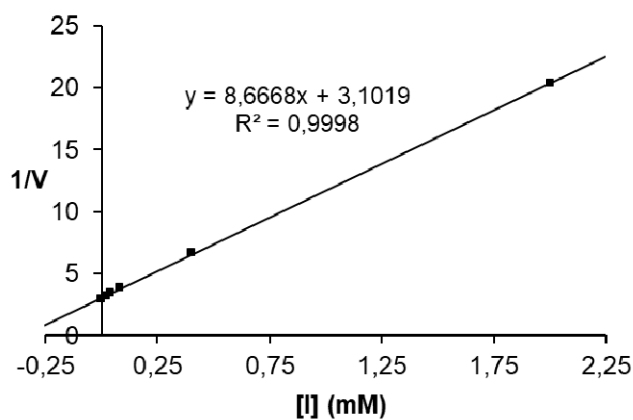


Figure S26. Dixon Plot for K_i determination ($116 \pm 10 \mu\text{M}$) of **26** against *Aspergillus niger* amyloglucosidase.

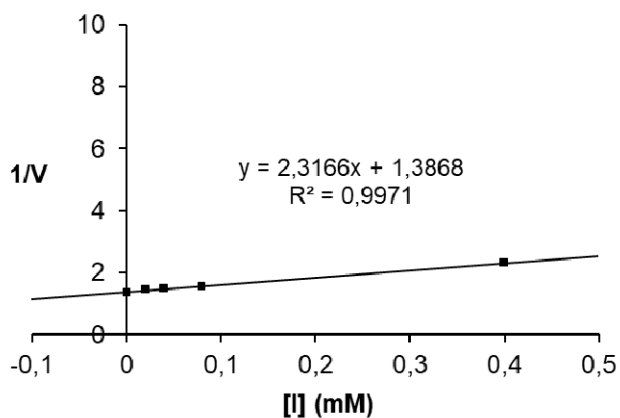


Figure S27. Dixon Plot for K_i determination ($463 \pm 40 \mu\text{M}$) of **27** against *Aspergillus niger* amyloglucosidase.

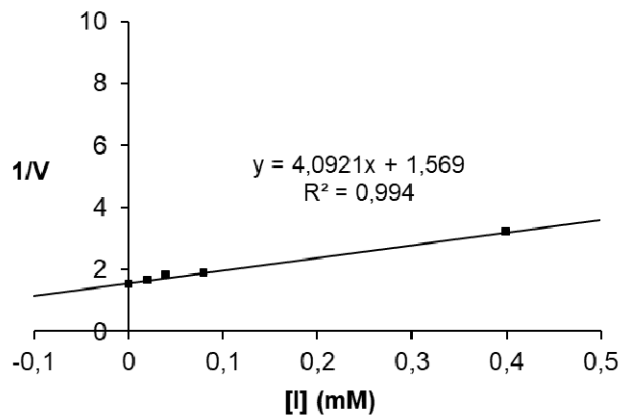


Figure S28. Dixon Plot for K_i determination ($169 \pm 15 \mu\text{M}$) of **28** against *Aspergillus niger* amyloglucosidase.

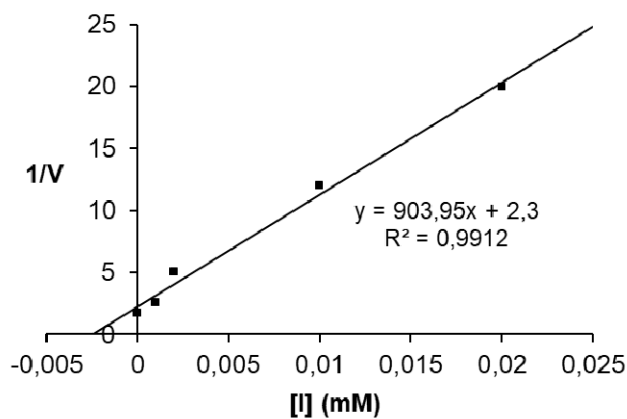


Figure S29. Dixon Plot for K_i determination ($1.4 \pm 0.1 \mu\text{M}$) of **34** against *Aspergillus niger* amyloglucosidase.

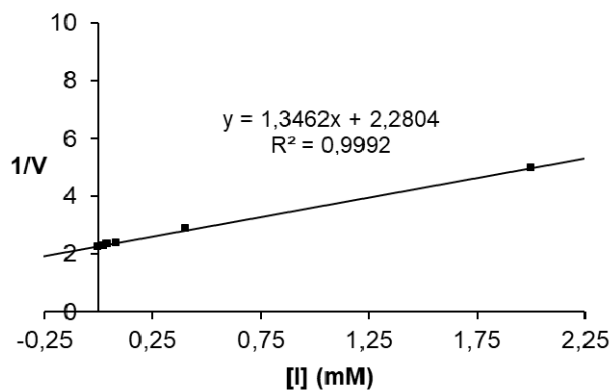


Figure S30. Dixon Plot for K_i determination ($550 \pm 45 \mu\text{M}$) of **35** against *Aspergillus niger* amyloglucosidase.

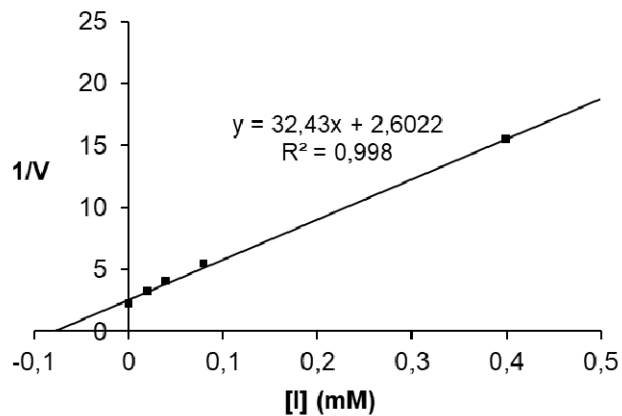


Figure S31. Dixon Plot for K_i determination ($22.8 \pm 1.9 \mu\text{M}$) of **32** against *Aspergillus niger* amyloglucosidase.

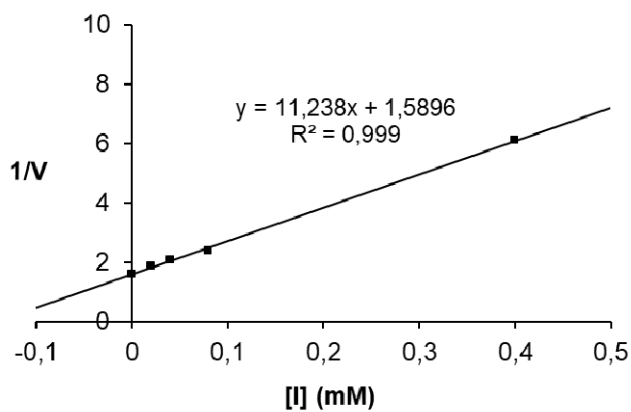


Figure S32. Dixon Plot for K_i determination ($115 \pm 10 \mu\text{M}$) of **25** against *Penicillium decumbes* naringinase.

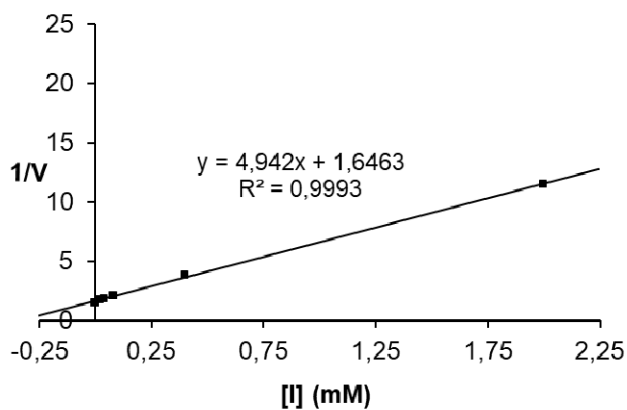


Figure S33. Dixon Plot for K_i determination ($76 \pm 5 \mu\text{M}$) of **26** against *Penicillium decumbes* naringinase.

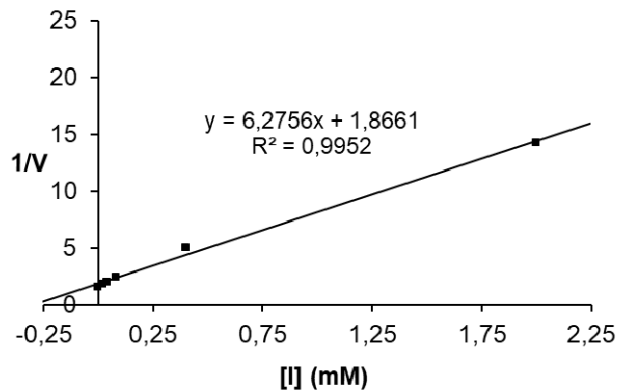


Figure S34. Dixon Plot for K_i determination ($131 \pm 11 \mu\text{M}$) of **27** against *Penicilium decumbes* naringinase.

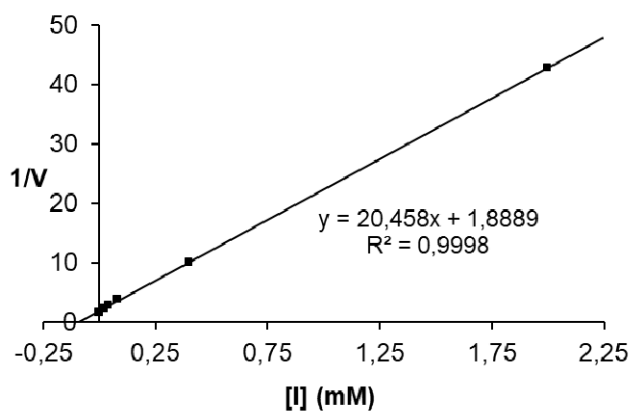


Figure S35. Dixon Plot for K_i determination ($45 \pm 3 \mu\text{M}$) of **28** against *Penicilium decumbes* naringinase.

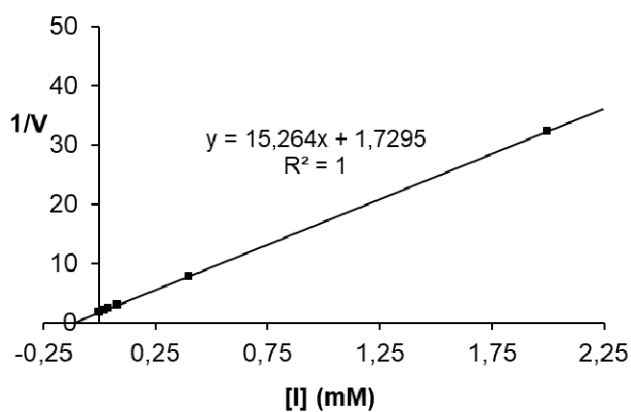


Figure S36. Dixon Plot for K_i determination ($50 \pm 4 \mu\text{M}$) of **29** against *Penicilium decumbes* naringinase.

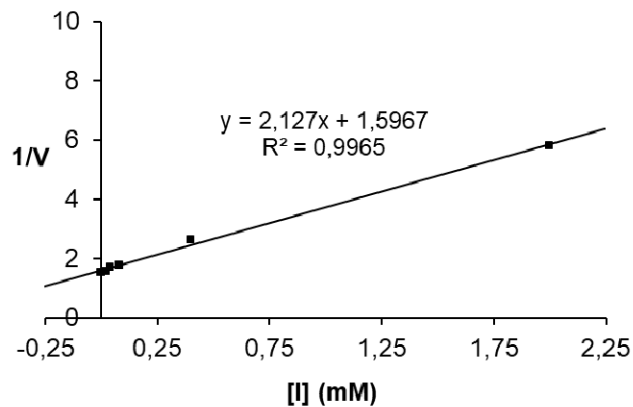


Figure S37. Dixon Plot for K_i determination ($224 \pm 20 \mu\text{M}$) of **30** against *Penicillium decumbes* naringinase.

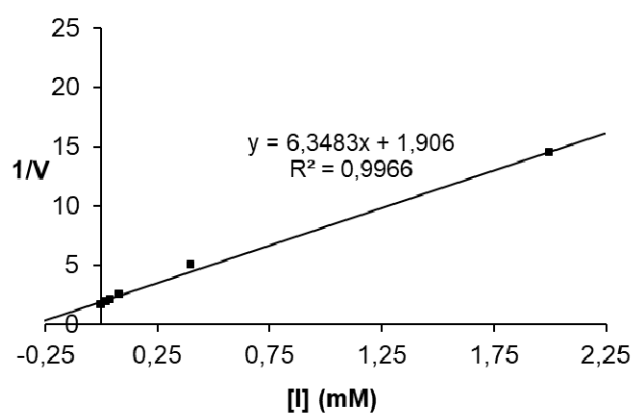


Figure S38. Dixon Plot for K_i determination ($67 \pm 5 \mu\text{M}$) of **34** against *Penicillium decumbes* naringinase.

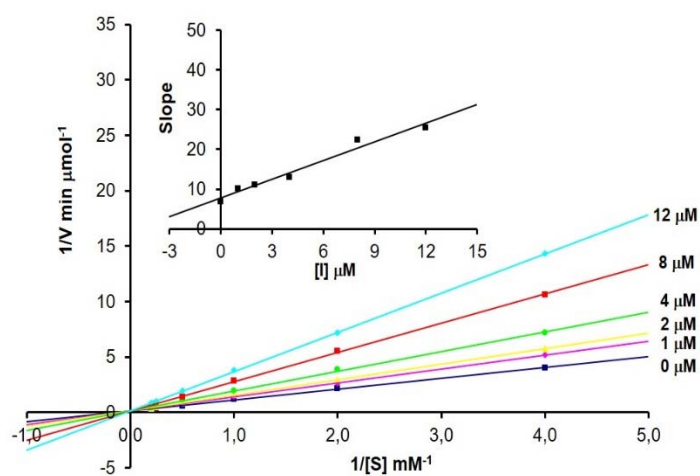


Figure S39. Lineweaver-Burk Plot for K_i determination ($4.9 \pm 0.5 \mu\text{M}$) of **35** against *Penicillium decumbes* naringinase.

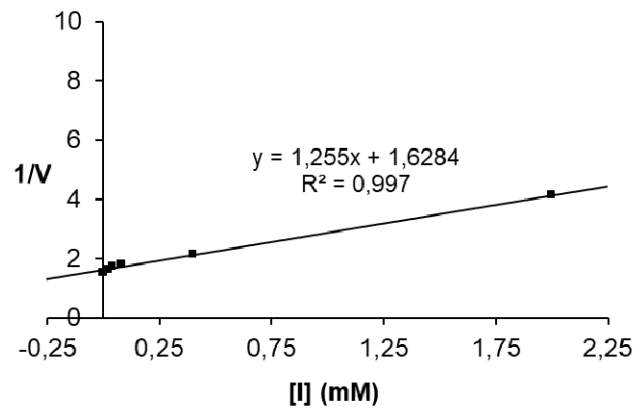


Figure S40. Dixon Plot for K_i determination ($272 \pm 25 \mu\text{M}$) of **32** against *Penicilium decumbes* naringinase.