

Supporting Information

Synthesis, Structure and Antileishmanial Evaluation of Endoperoxide–Pyrazole Hybrids

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Table of contents

S1.	¹ H, ¹³ C{ ¹ H} NMR, COSY, HSQC, HMBC spectra of the synthesised compounds	S2
S2.	HRMS spectra of the synthesised compounds	S51
S3.	X-ray crystallography	S60

S1. ^1H , $^{13}\text{C}\{^1\text{H}\}$ NMR, COSY, HSQC, HMBC spectra of the synthesised compounds

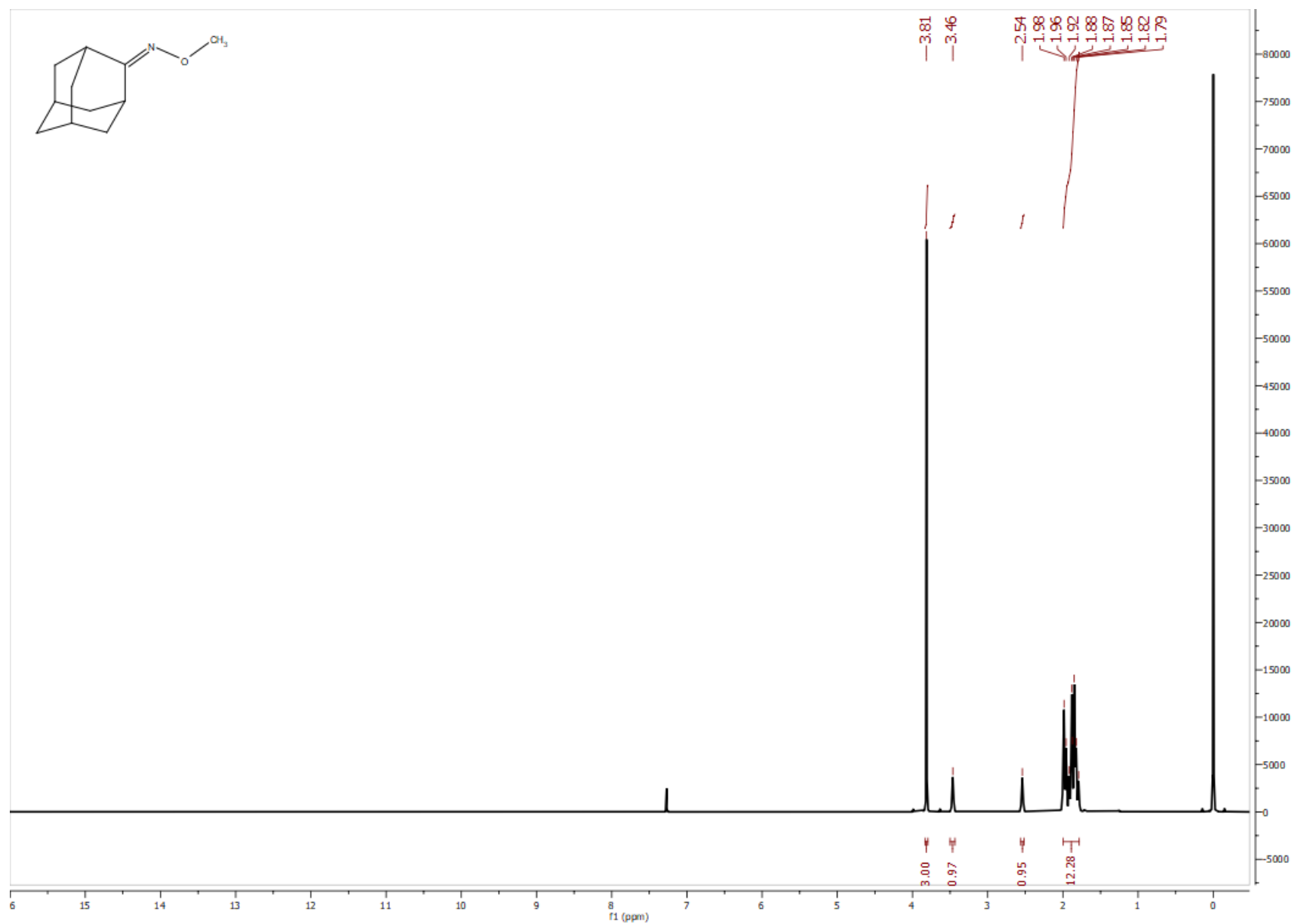


Figure S1. ^1H NMR spectrum (400 MHz) of **1o** in CDCl_3 .

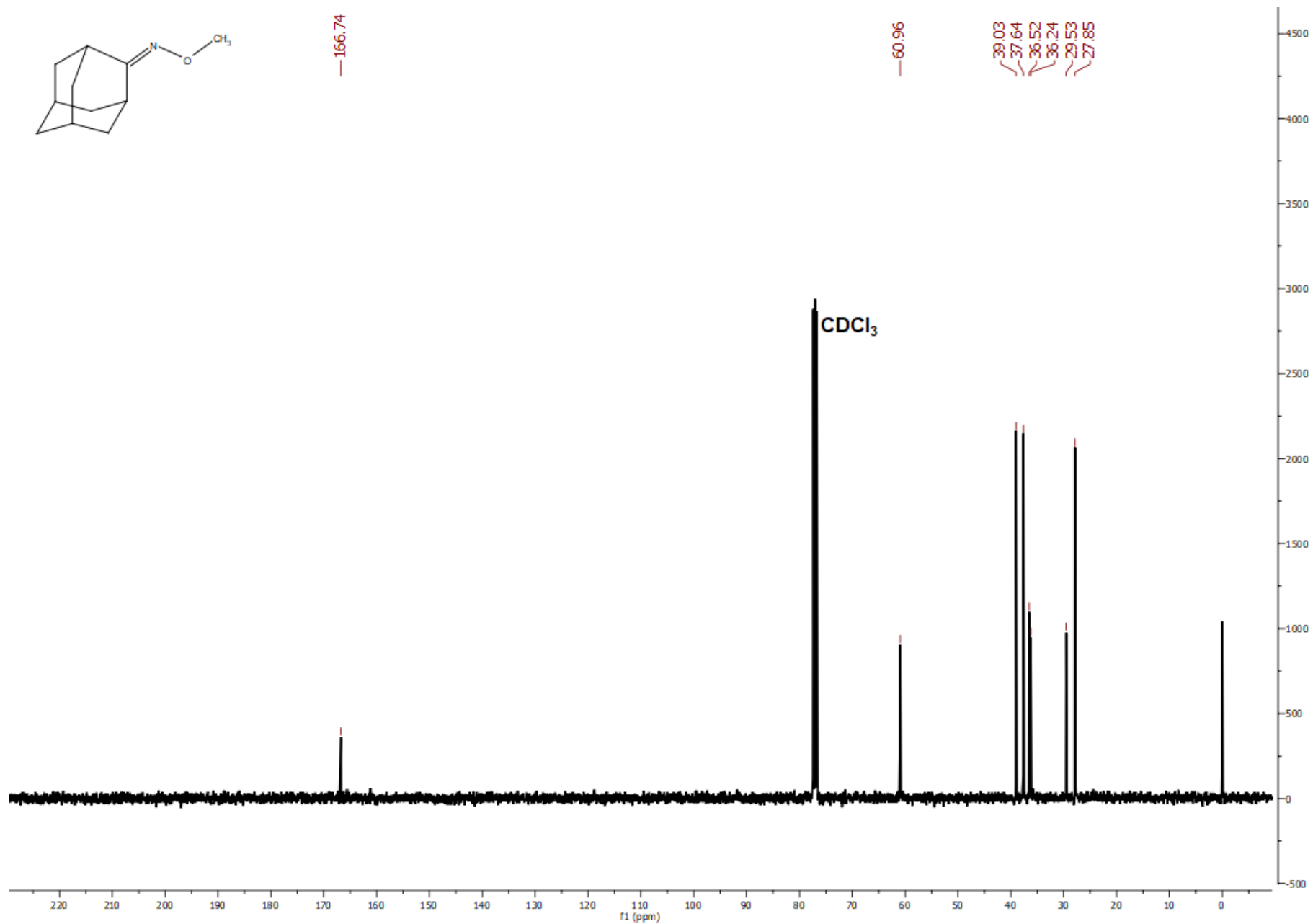


Figure S2. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (100 MHz) of **1o** in CDCl_3 .

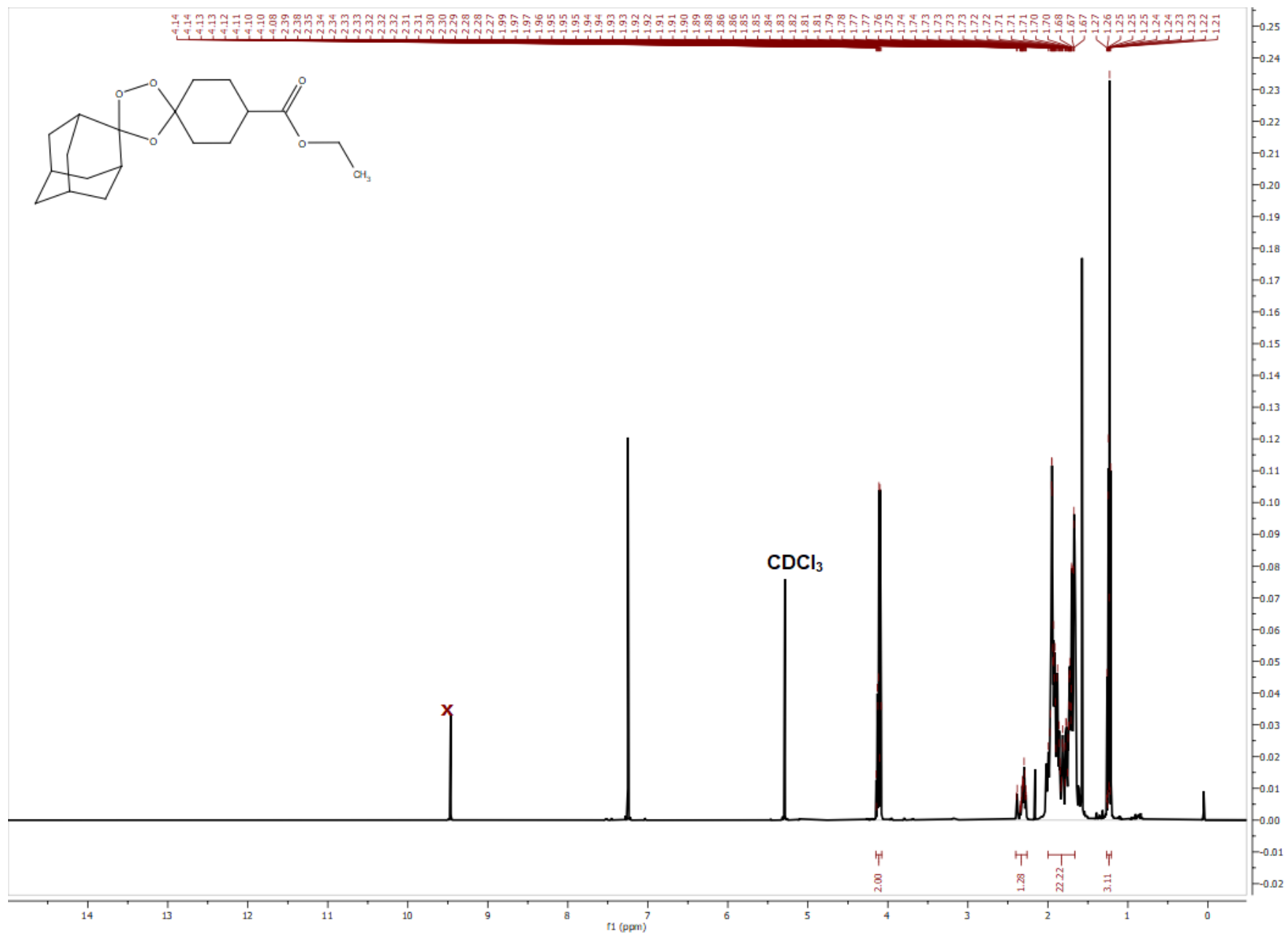


Figure S3. ¹H NMR spectrum (500 MHz) of **2o** in CDCl₃.

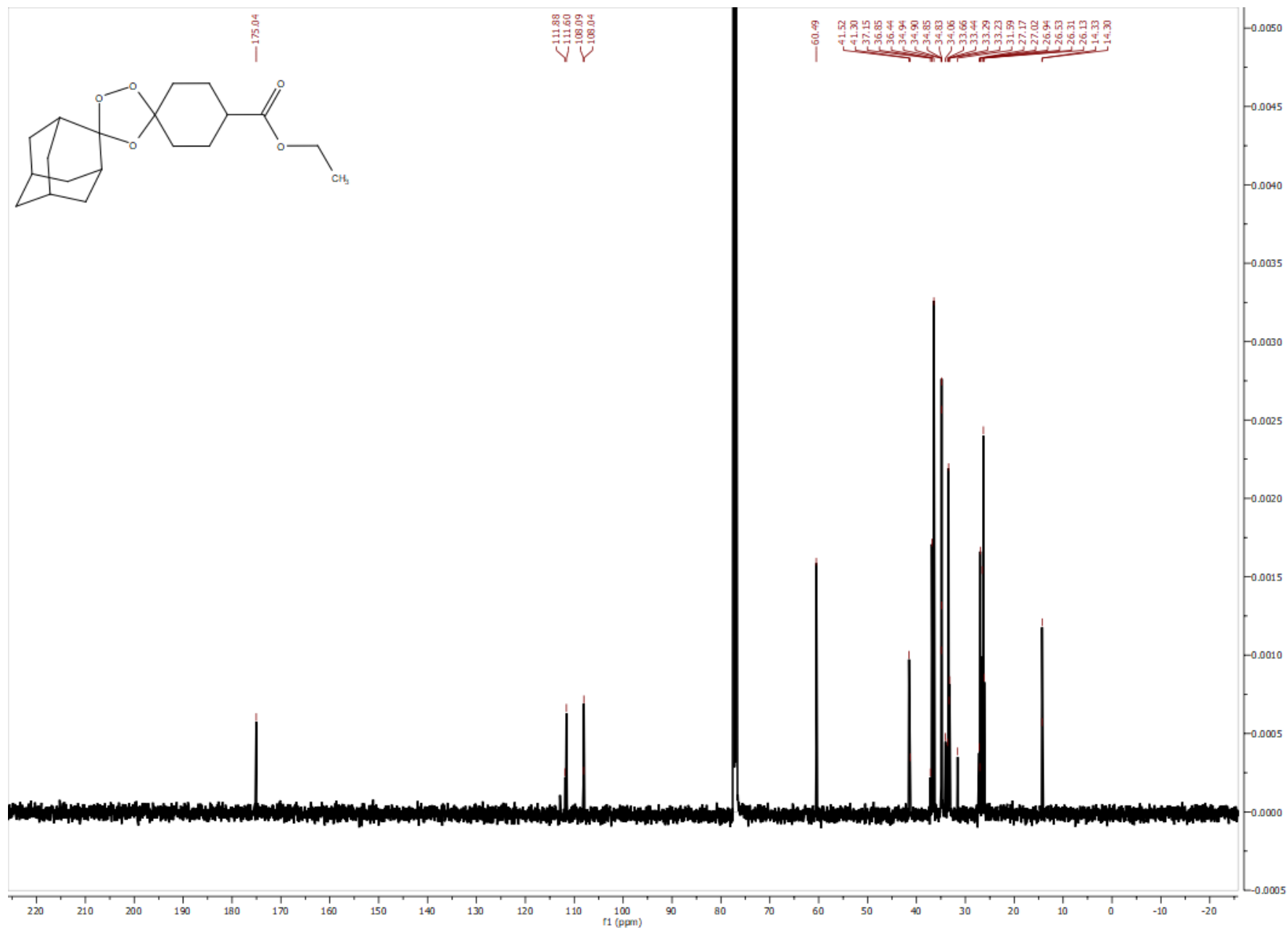


Figure S4. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (126 MHz) of **2o** in CDCl_3 .

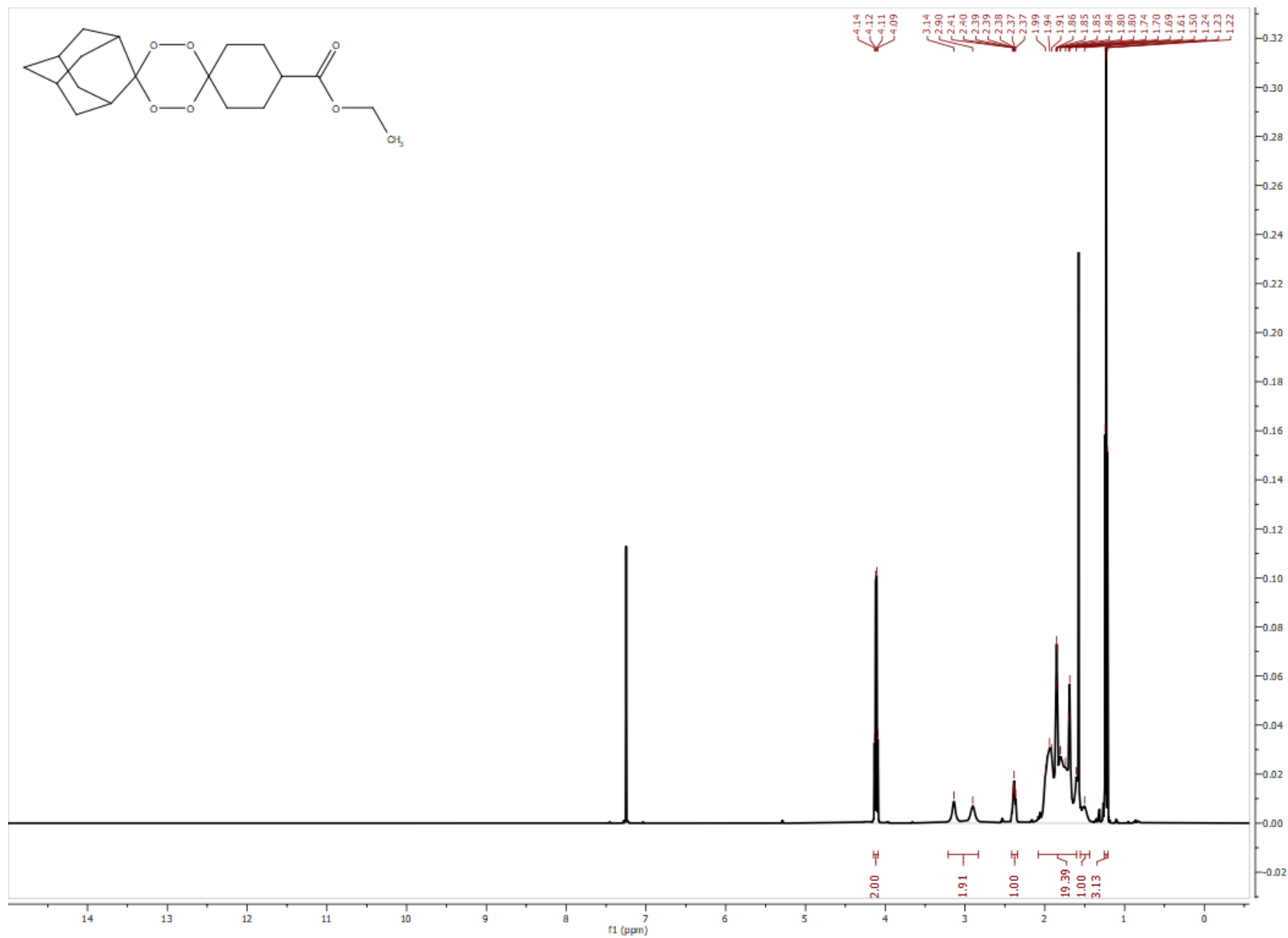


Figure S5. ¹H NMR spectrum (500 MHz) of **2t** in CDCl₃.

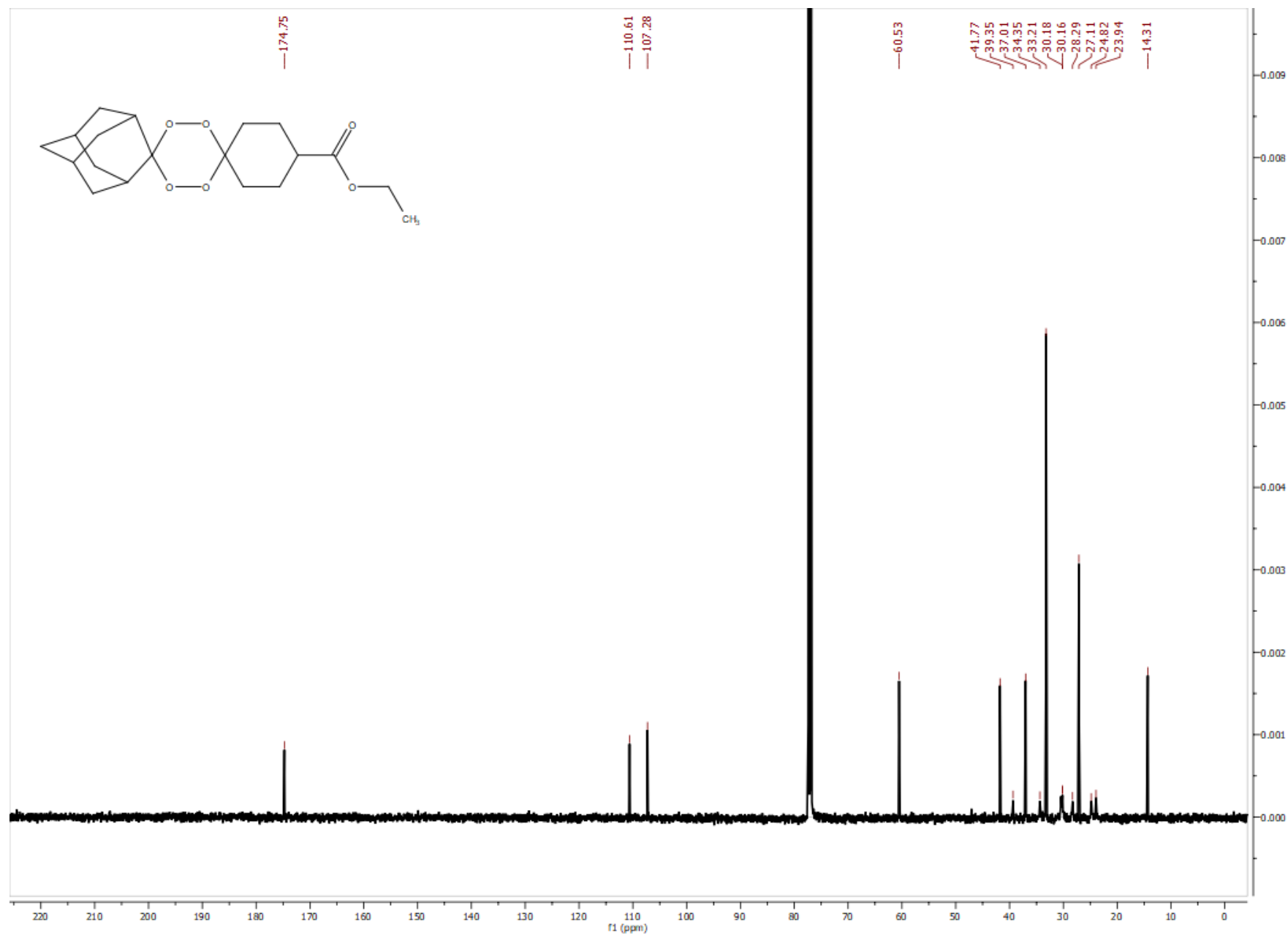


Figure S6. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (126 MHz) of **2t** in CDCl_3 .

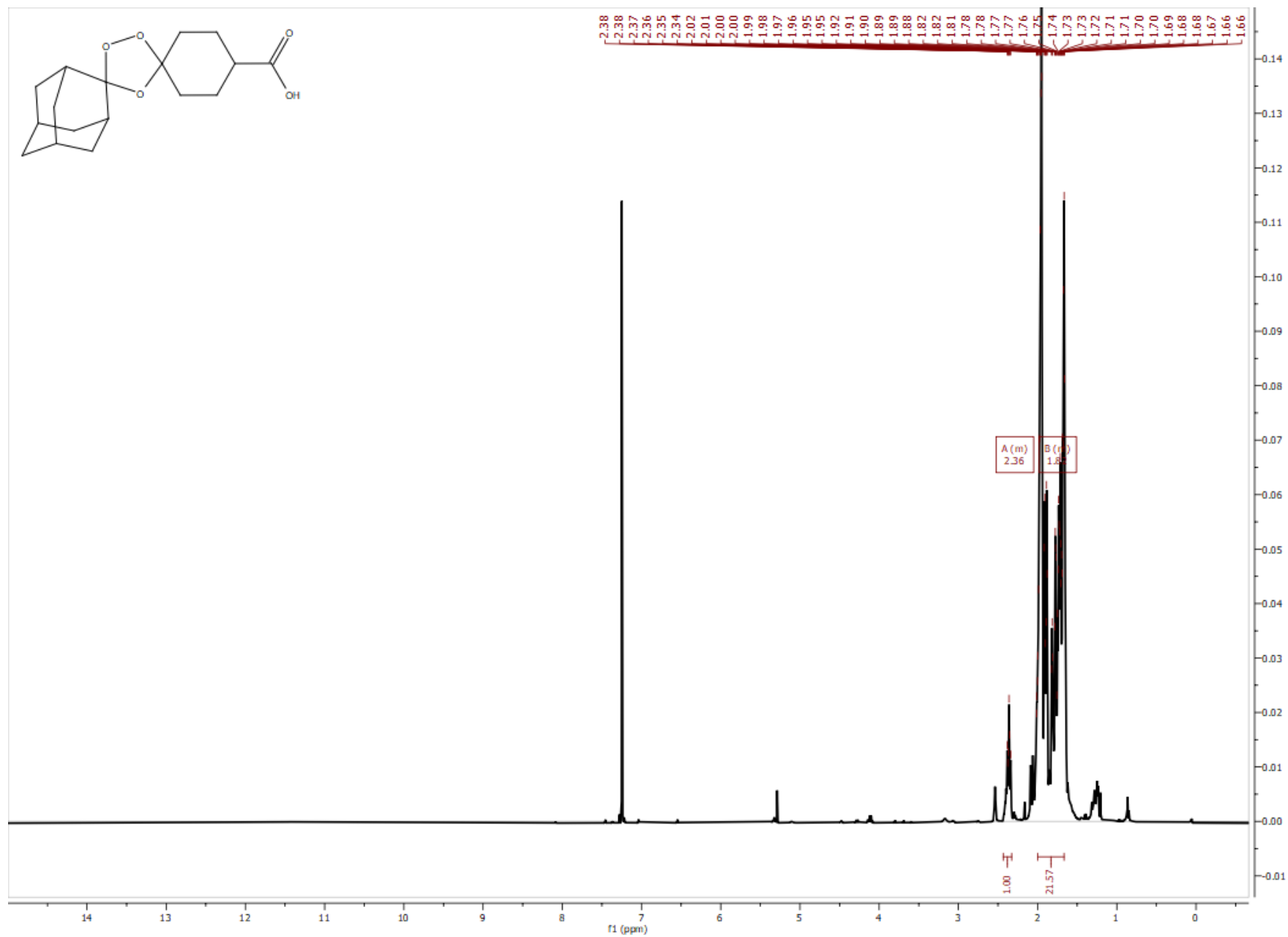


Figure S7. ^1H NMR spectrum (500 MHz) of **3o** in CDCl_3 .

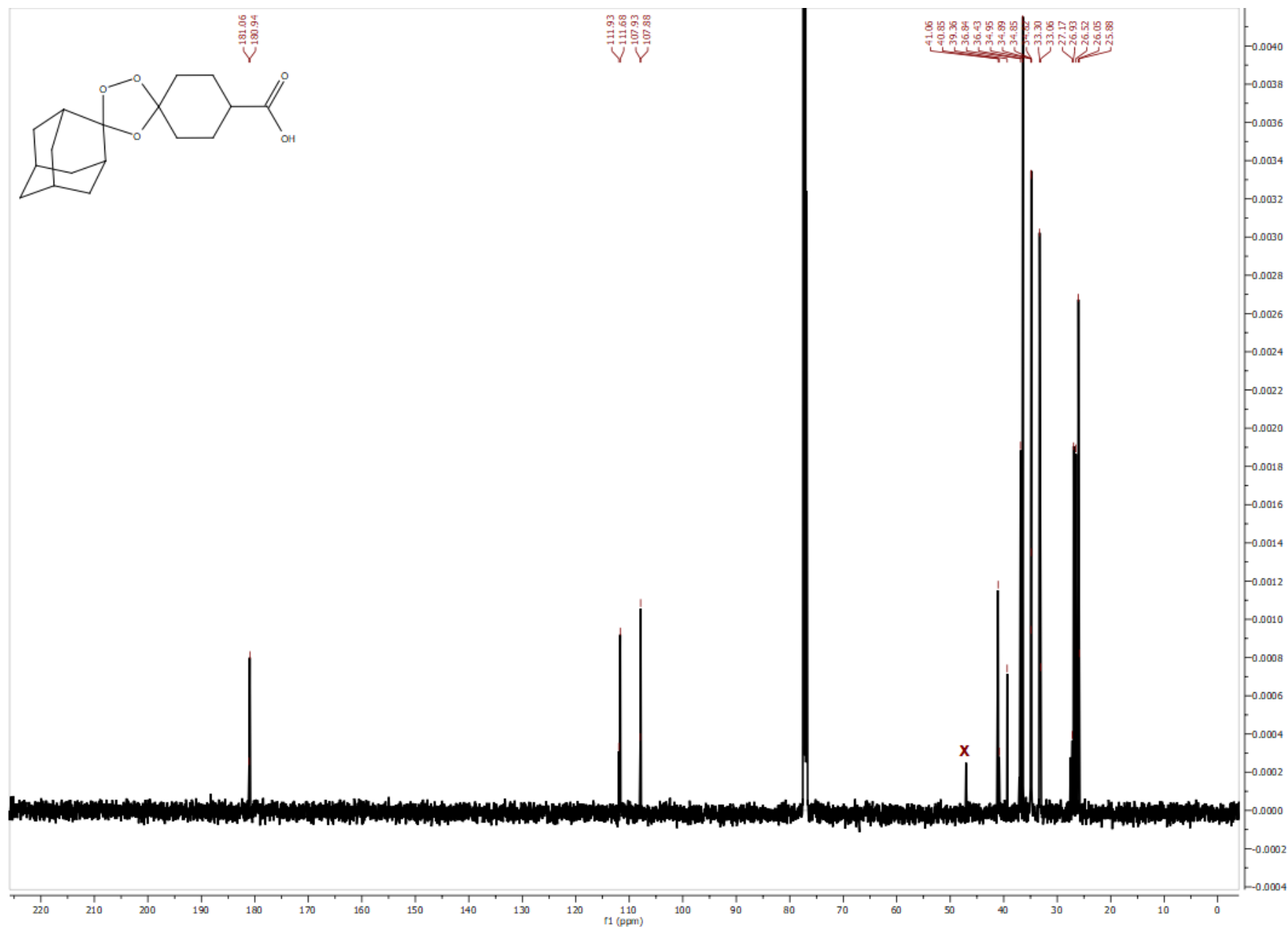


Figure S8. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (126 MHz) of **3o** in CDCl_3 .

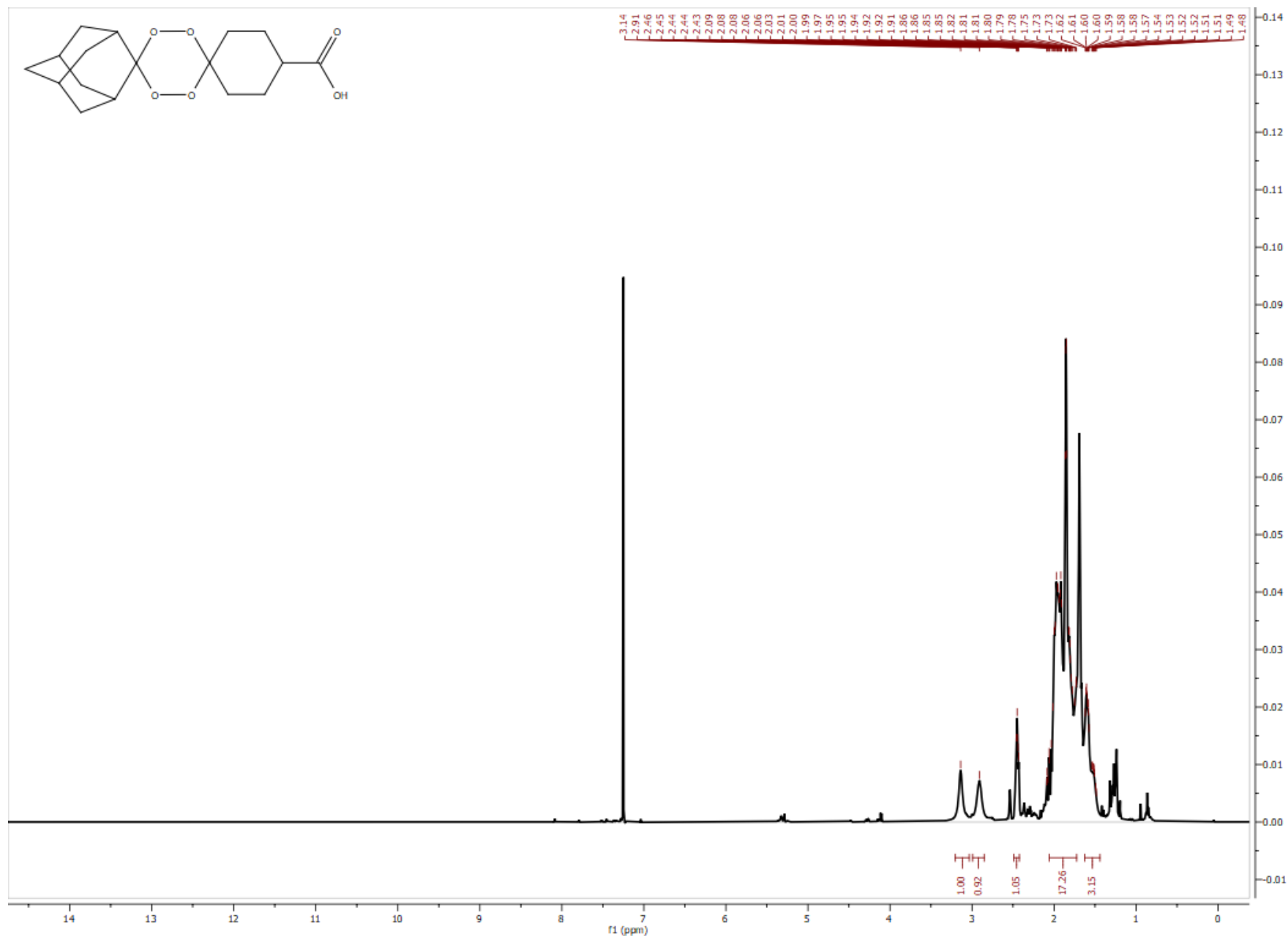


Figure S9. ¹H NMR spectrum (500 MHz) of **3t** in CDCl₃.

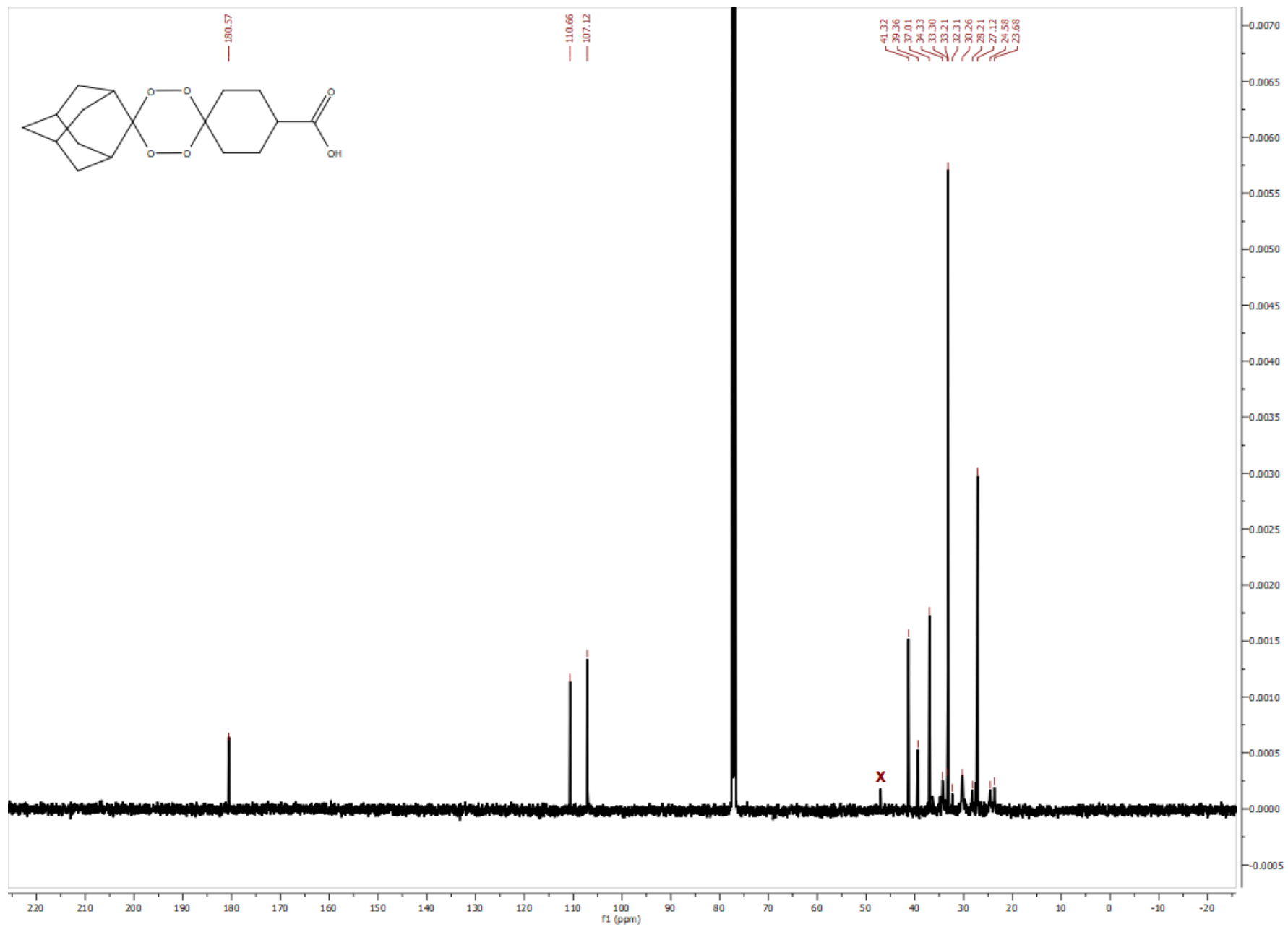


Figure S10. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (126 MHz) of **3t** in CDCl_3 .

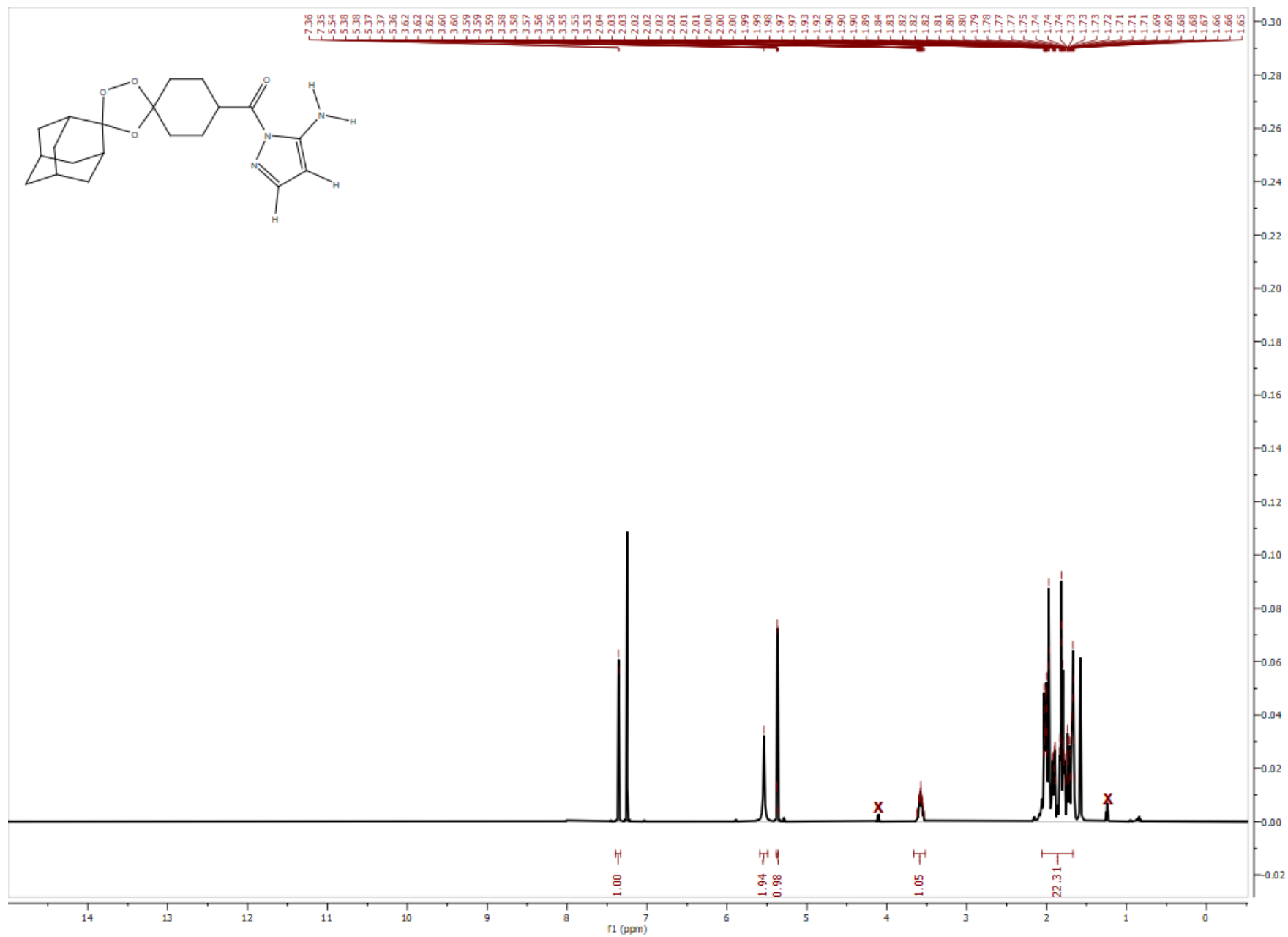


Figure S11. ¹H NMR spectrum (500 MHz) of **OZ1** in CDCl₃.

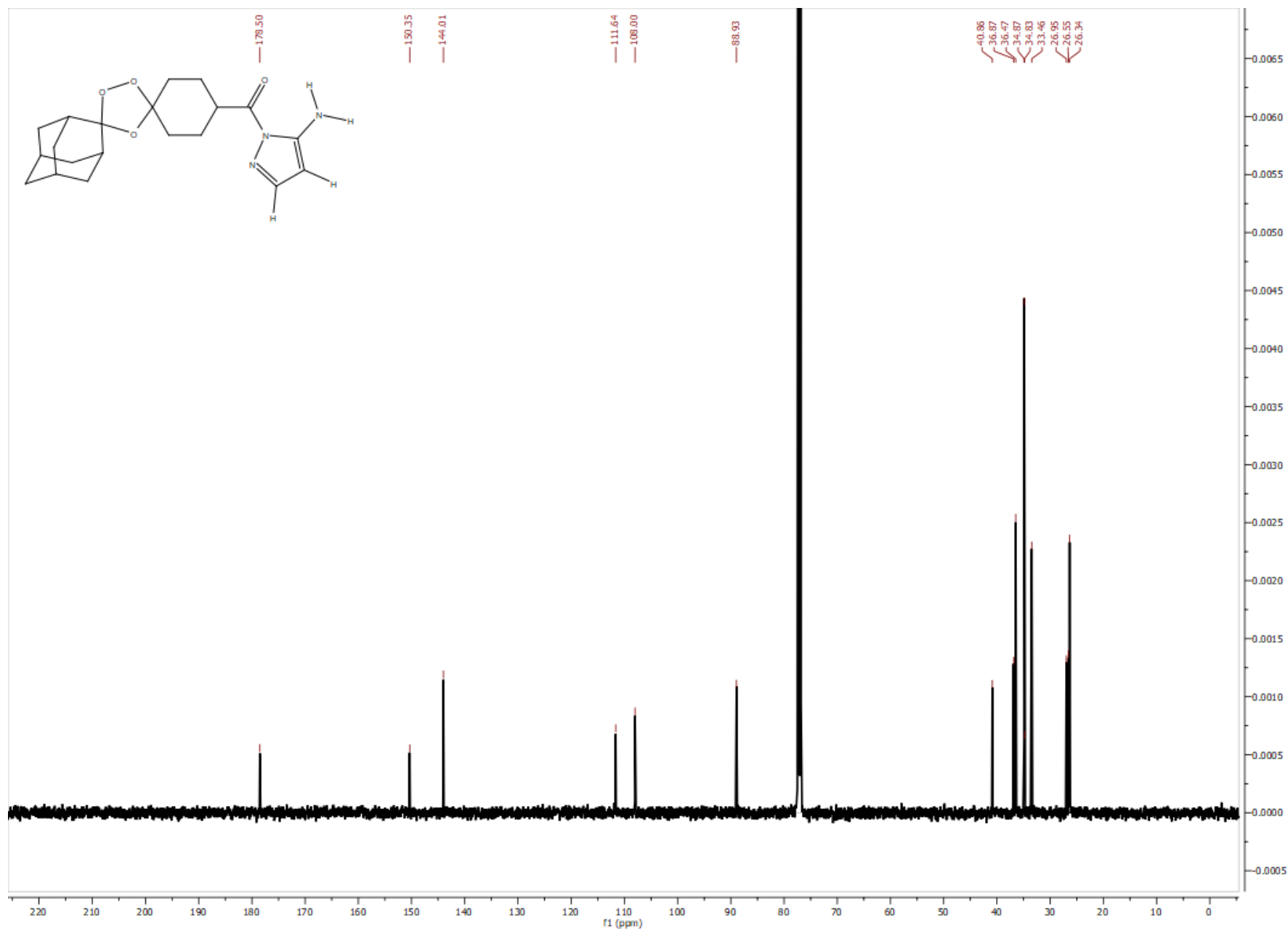


Figure S12. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (126 MHz) of **OZ1** in CDCl_3 .

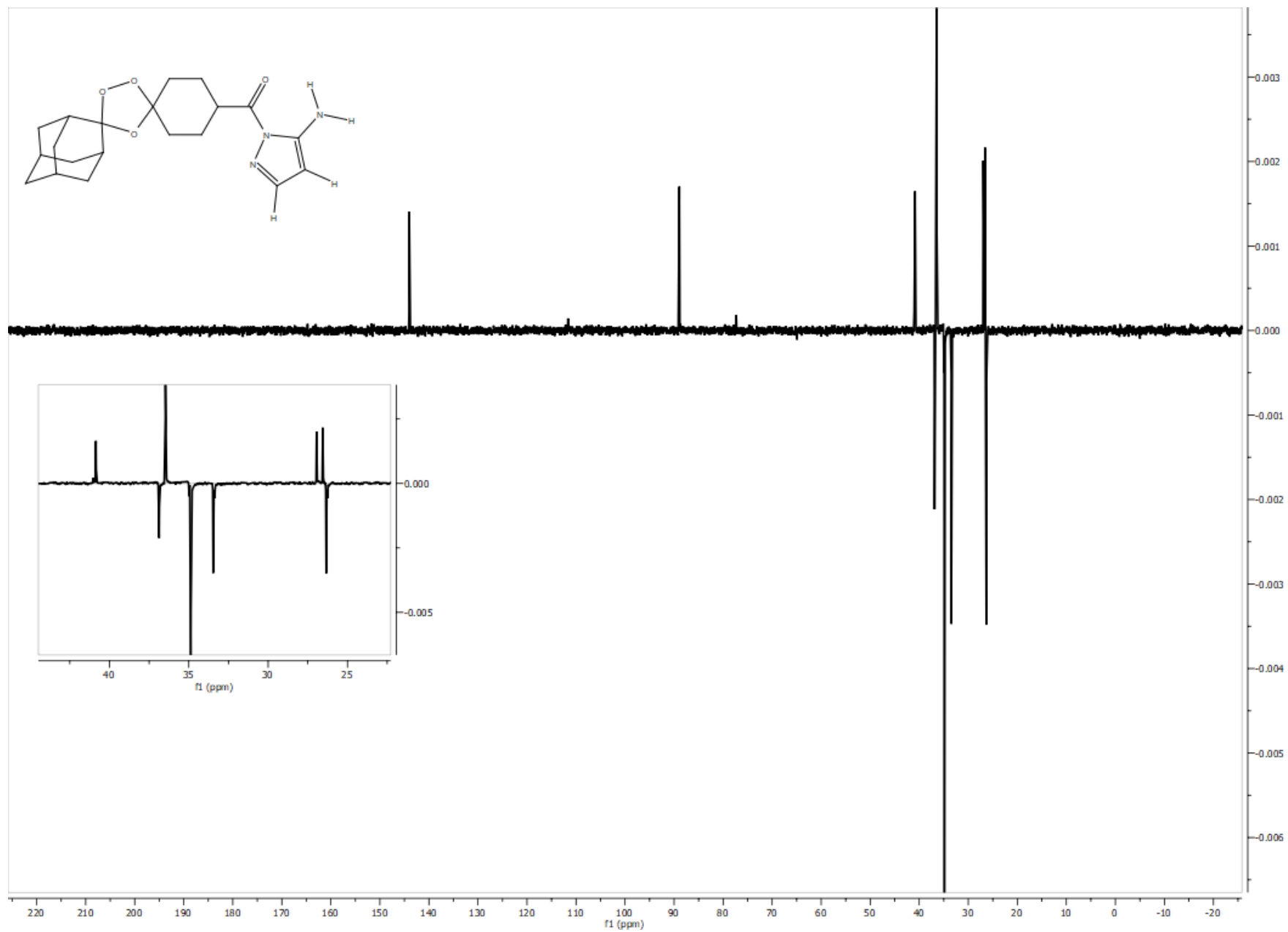


Figure S13. $^{13}\text{C}\{^1\text{H}\}$ DEPT-135 NMR spectrum (126 MHz) of **OZ1** in CDCl_3 .

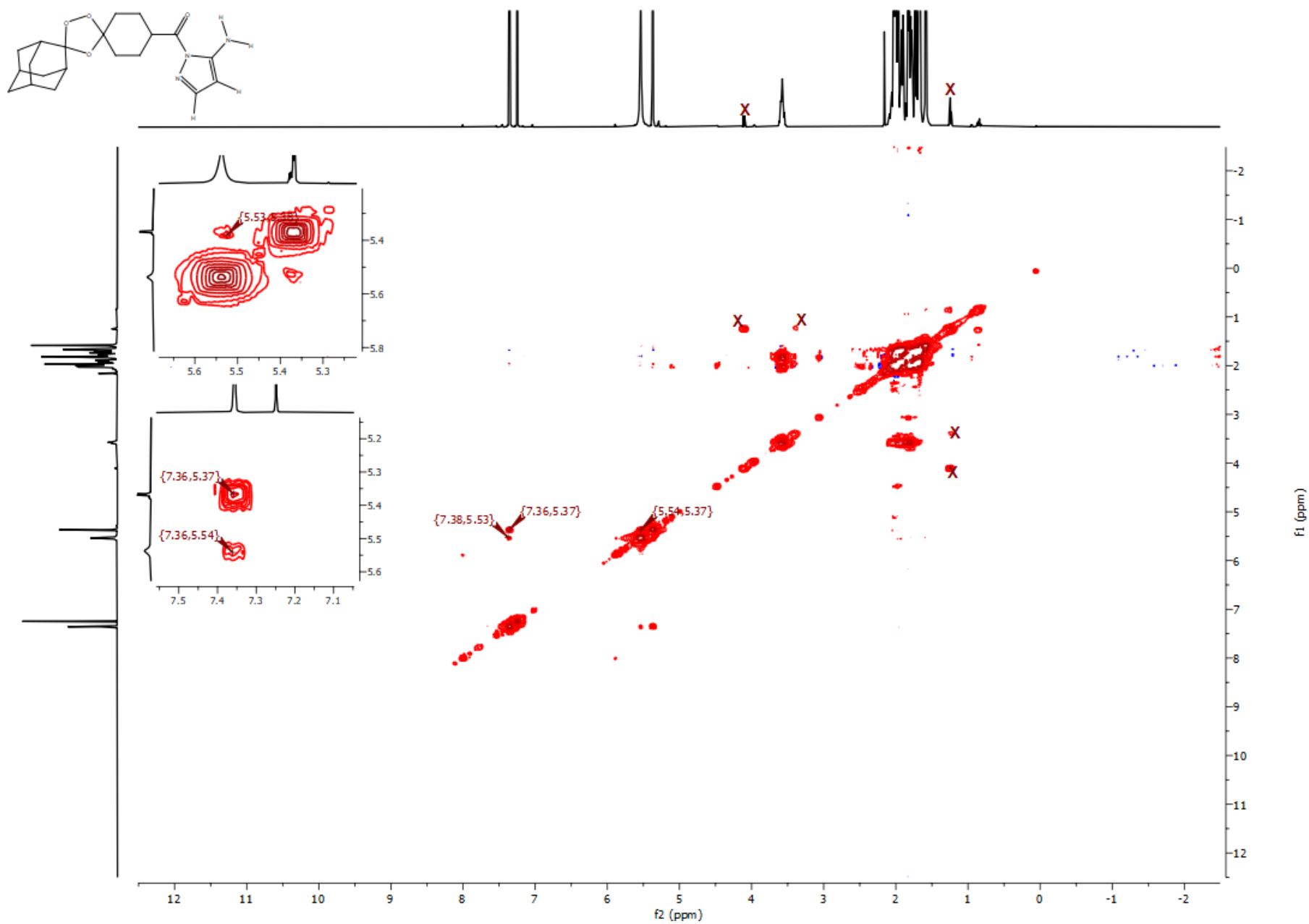


Figure S14. COSY spectrum (500 MHz) of **OZ1** in CDCl₃.

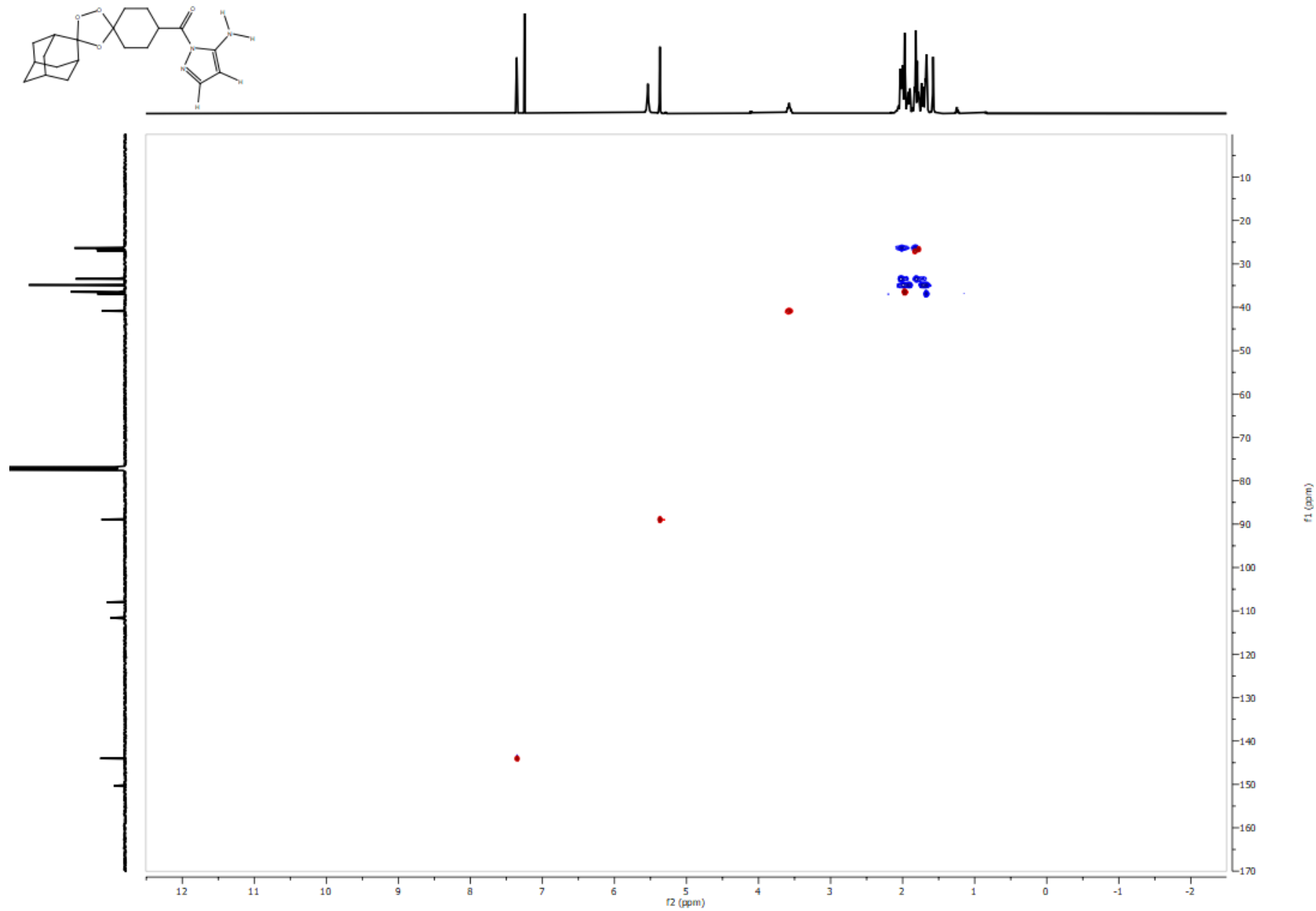


Figure S15. HSQC spectrum (500 MHz) of **OZ1** in CDCl_3 .

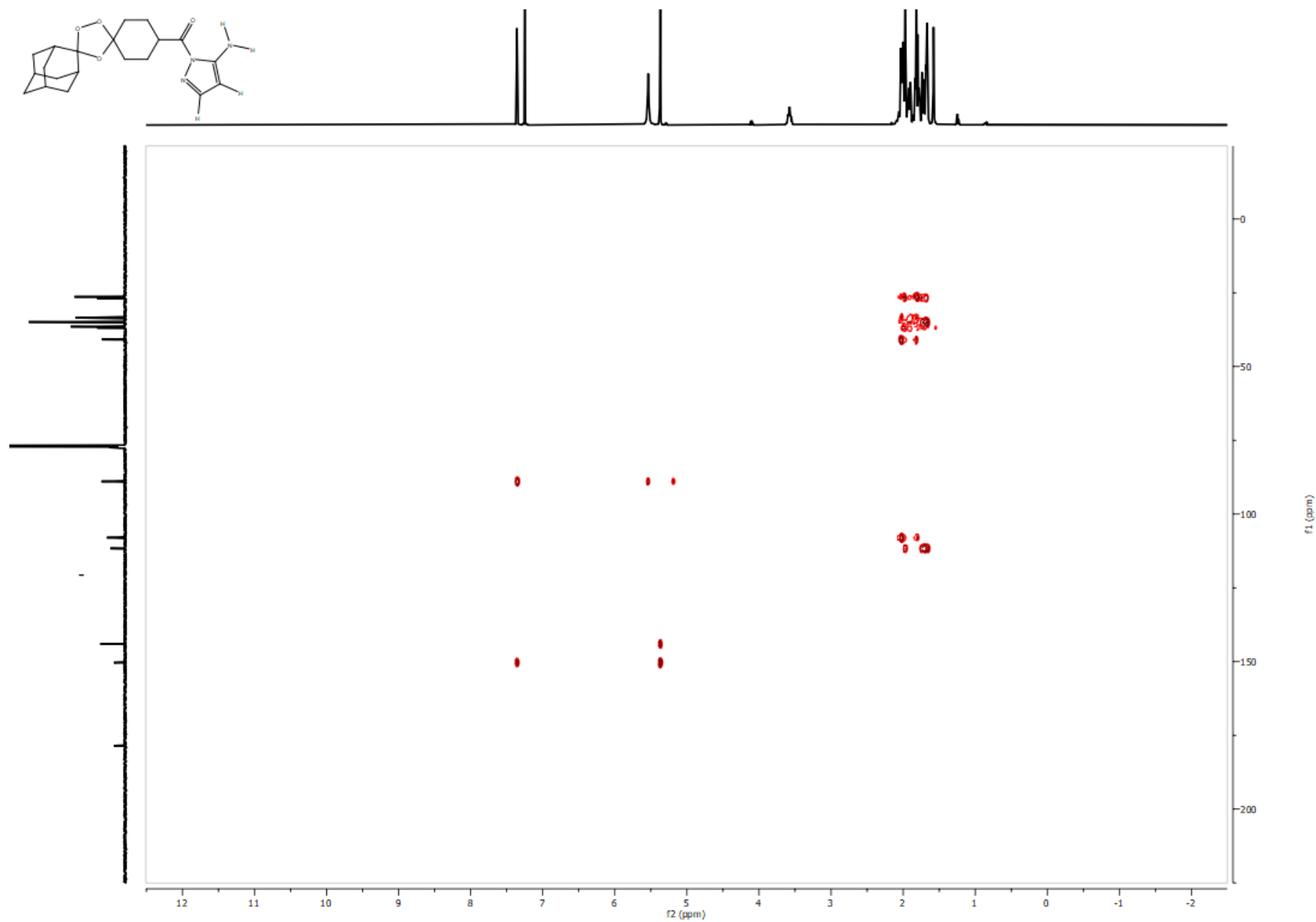


Figure S16. HMBC spectrum (500 MHz) of **OZ1** in CDCl₃.

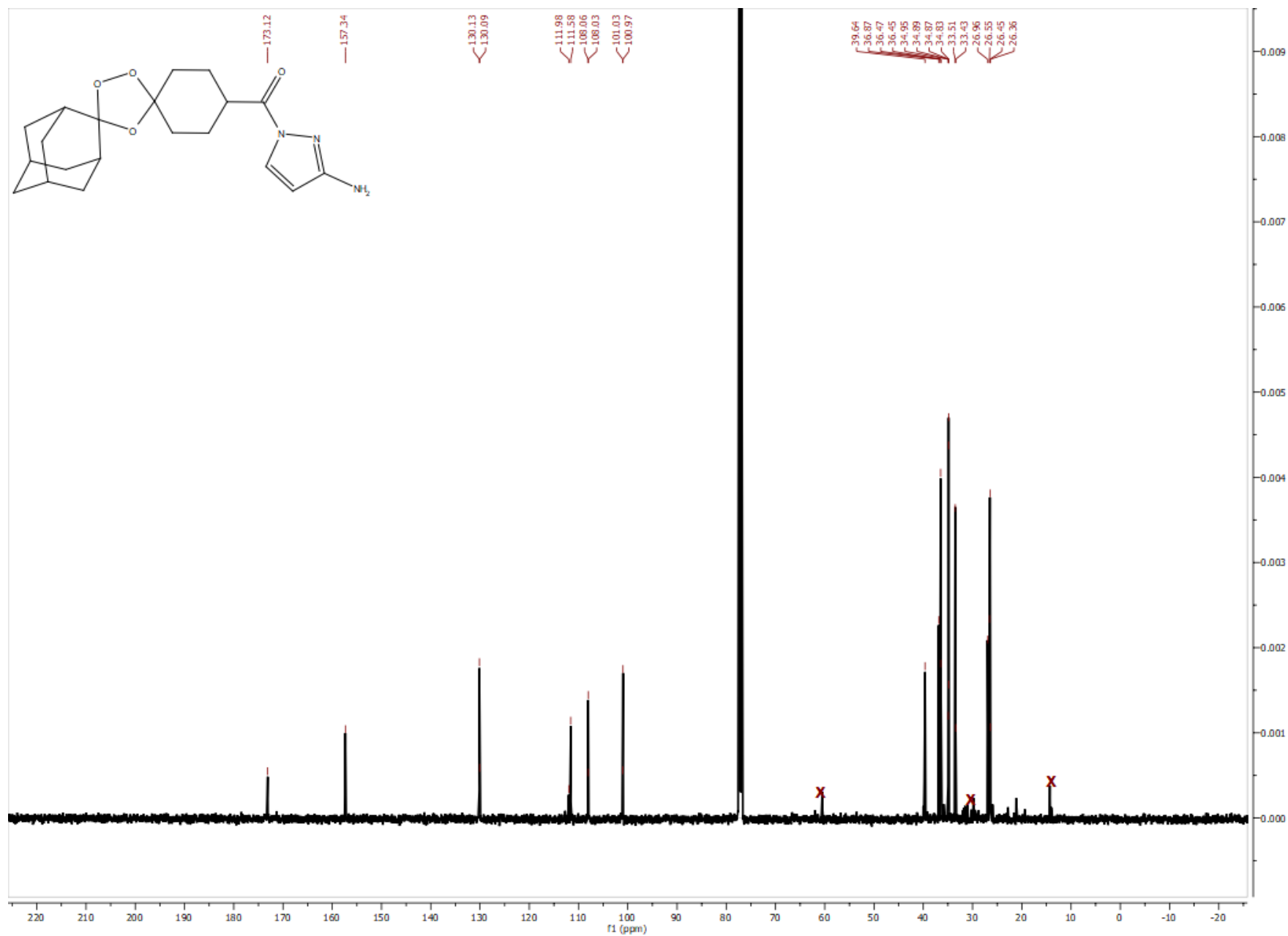


Figure S18. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (126 MHz) of **OZ2** in CDCl_3 .

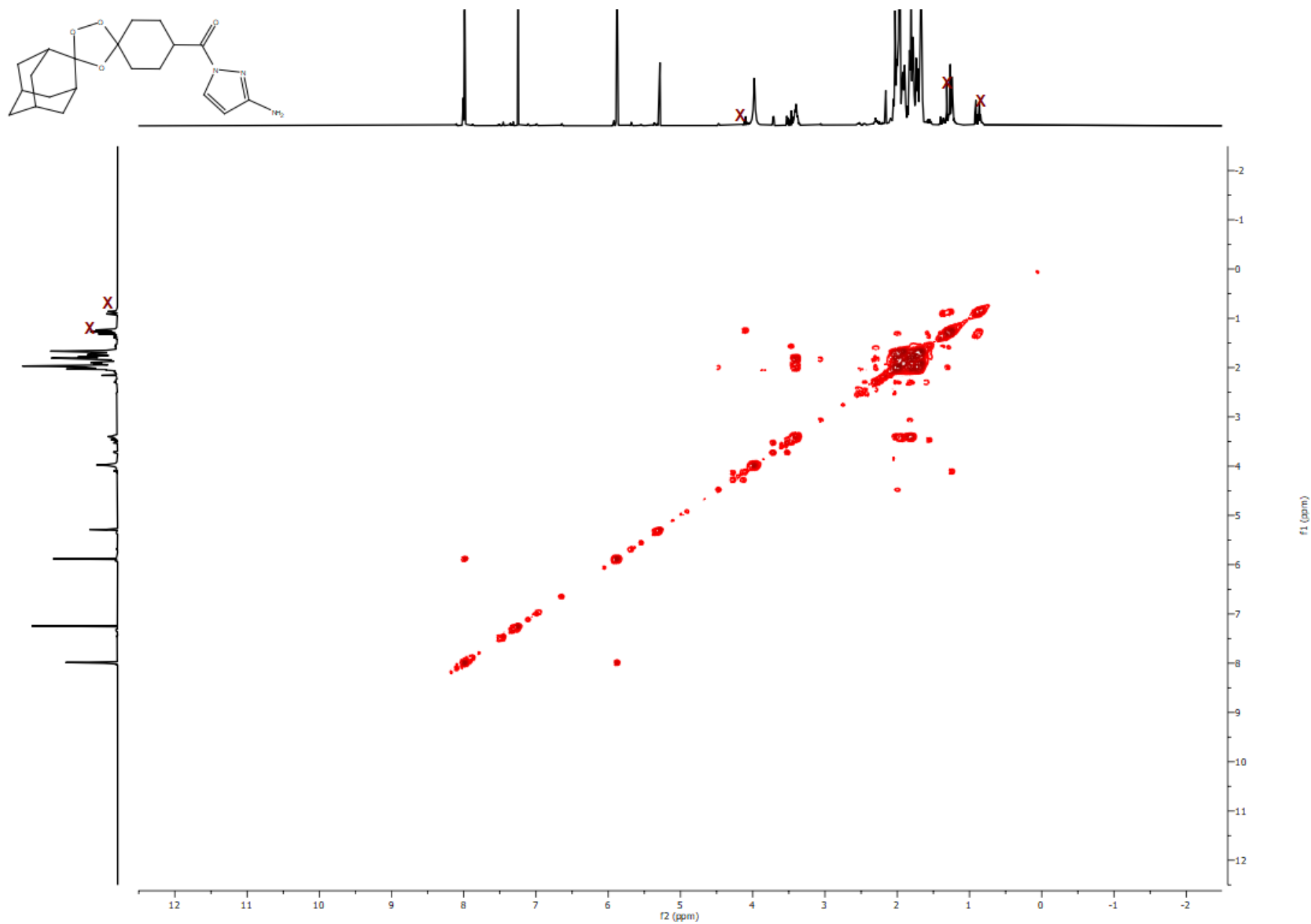


Figure S19. COSY spectrum (500 MHz) of **OZ2** in CDCl_3 .

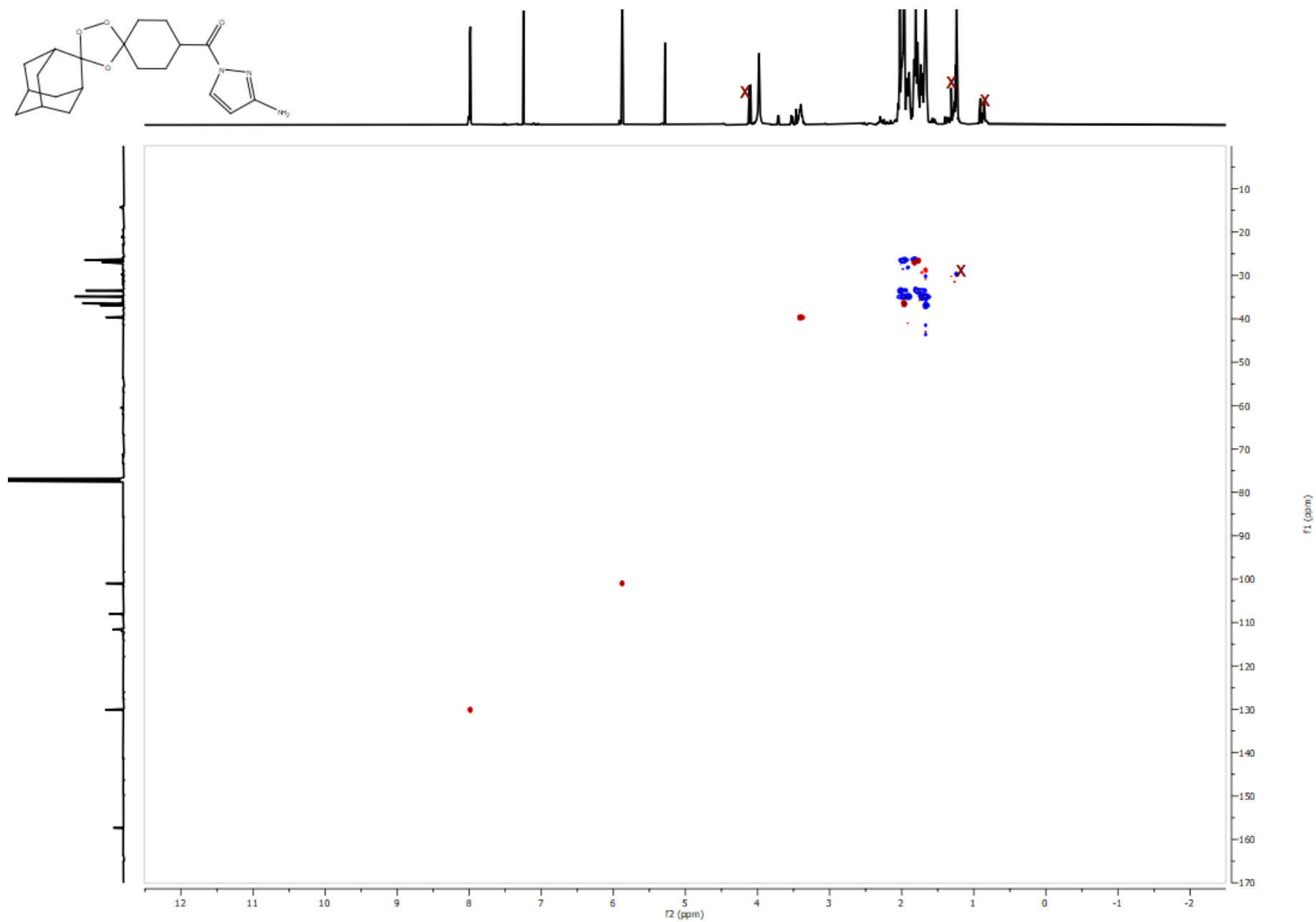


Figure S20. HSQC spectrum (500 MHz) of **OZ2** in CDCl_3 .

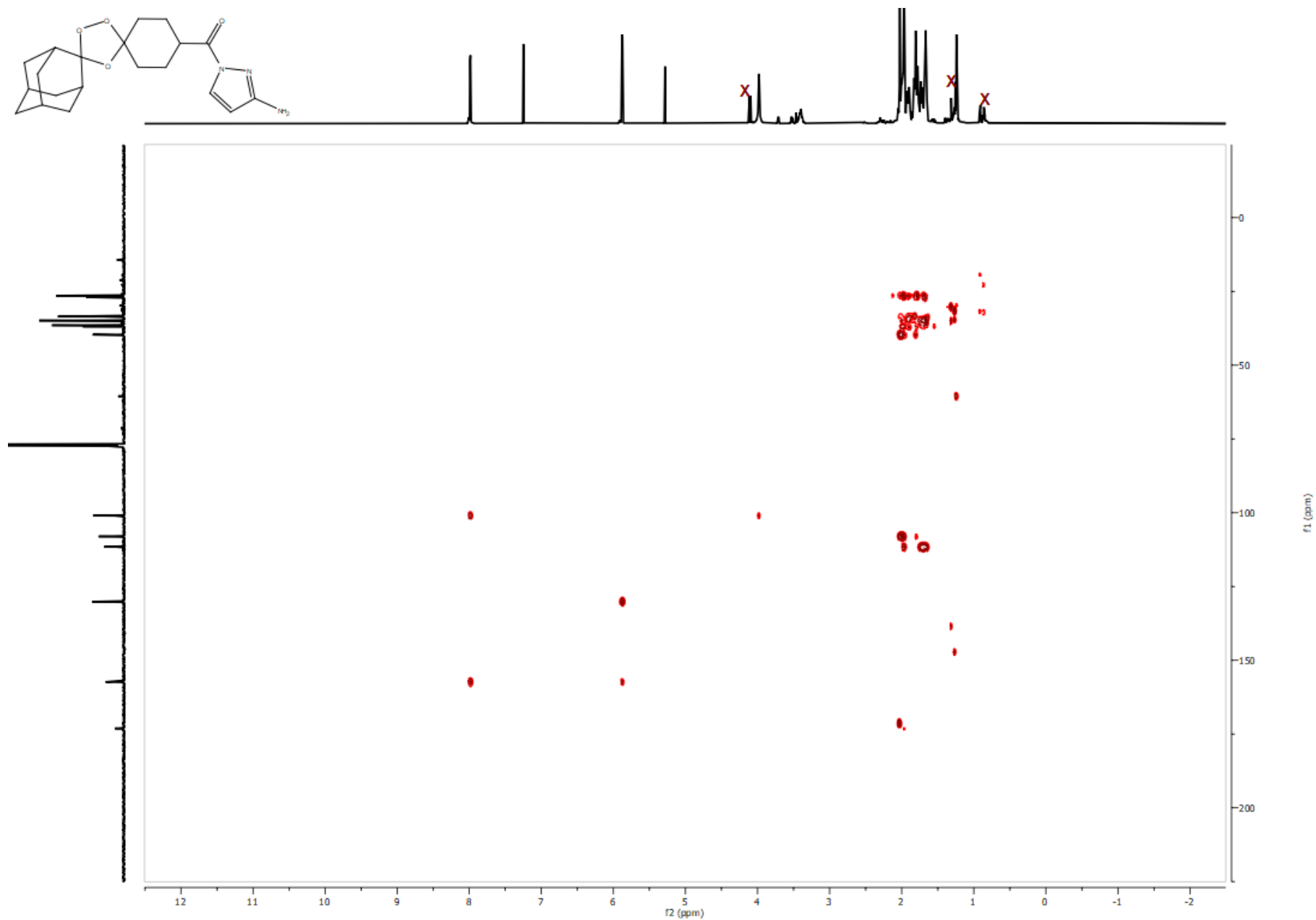


Figure S21. HMBC spectrum (500 MHz) of **OZ2** in CDCl₃.

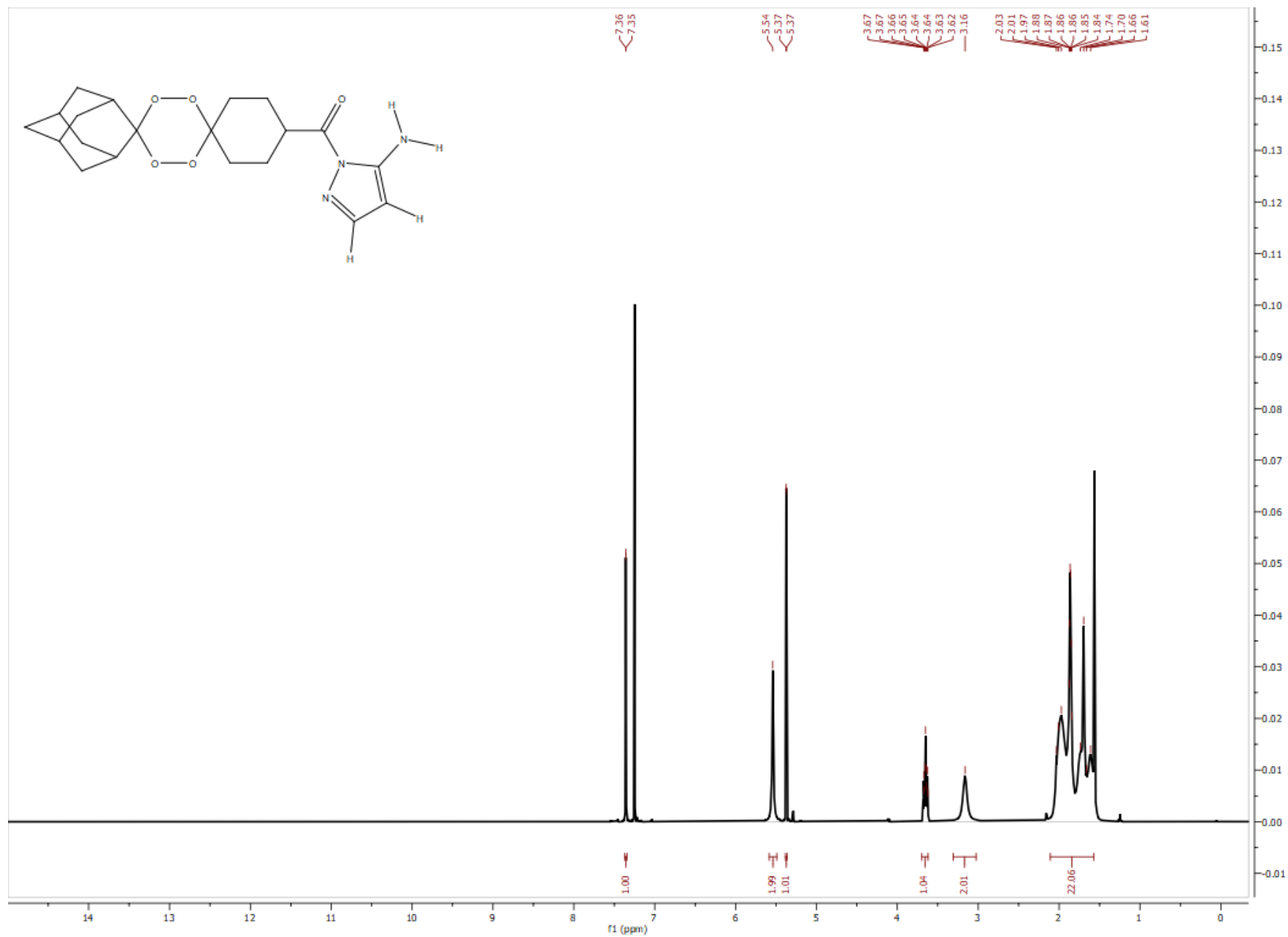


Figure S22. ¹H NMR spectrum (500 MHz) of **T1** in CDCl₃.

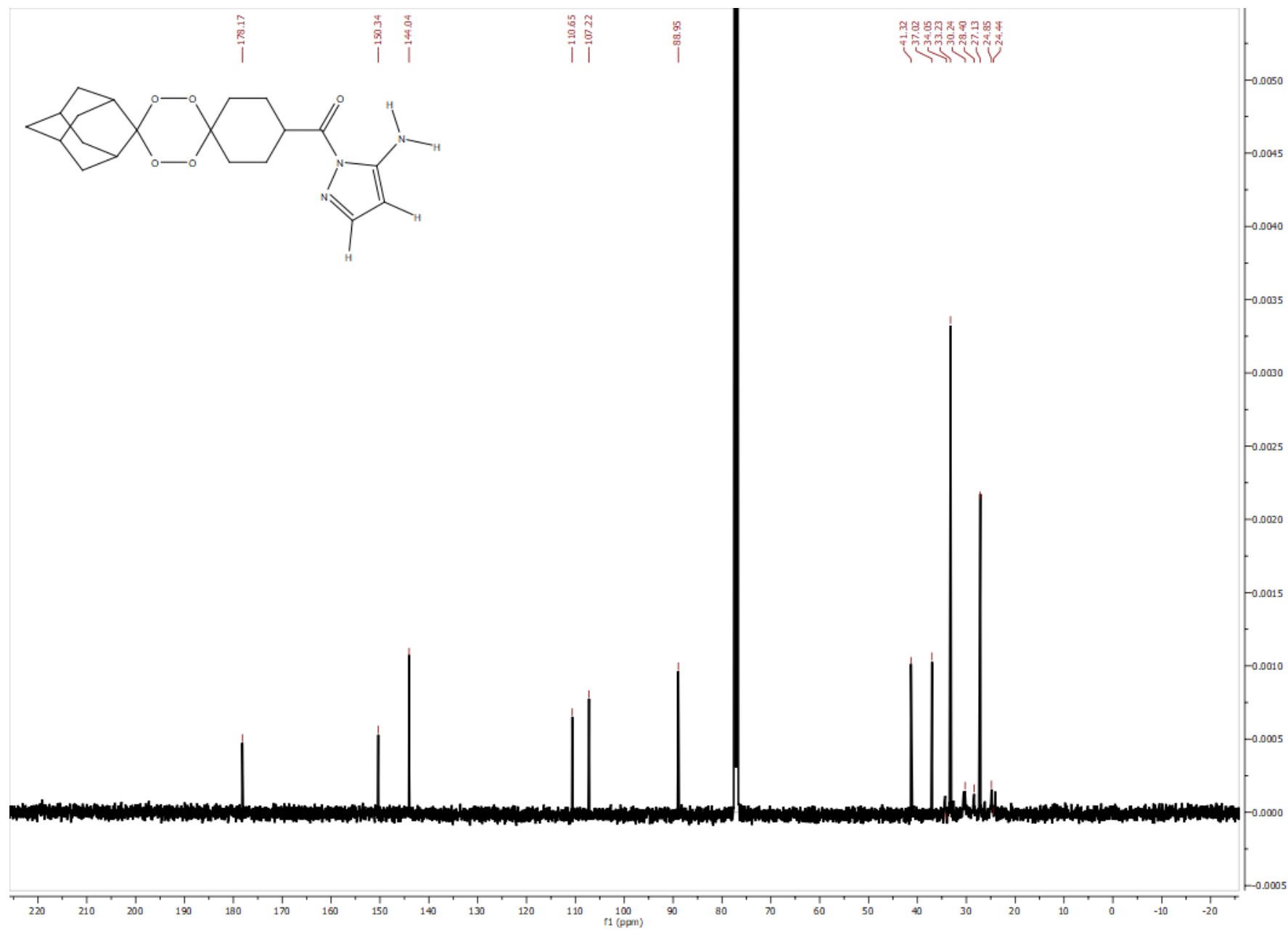


Figure S23. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (126 MHz) of **T1** in CDCl_3 .

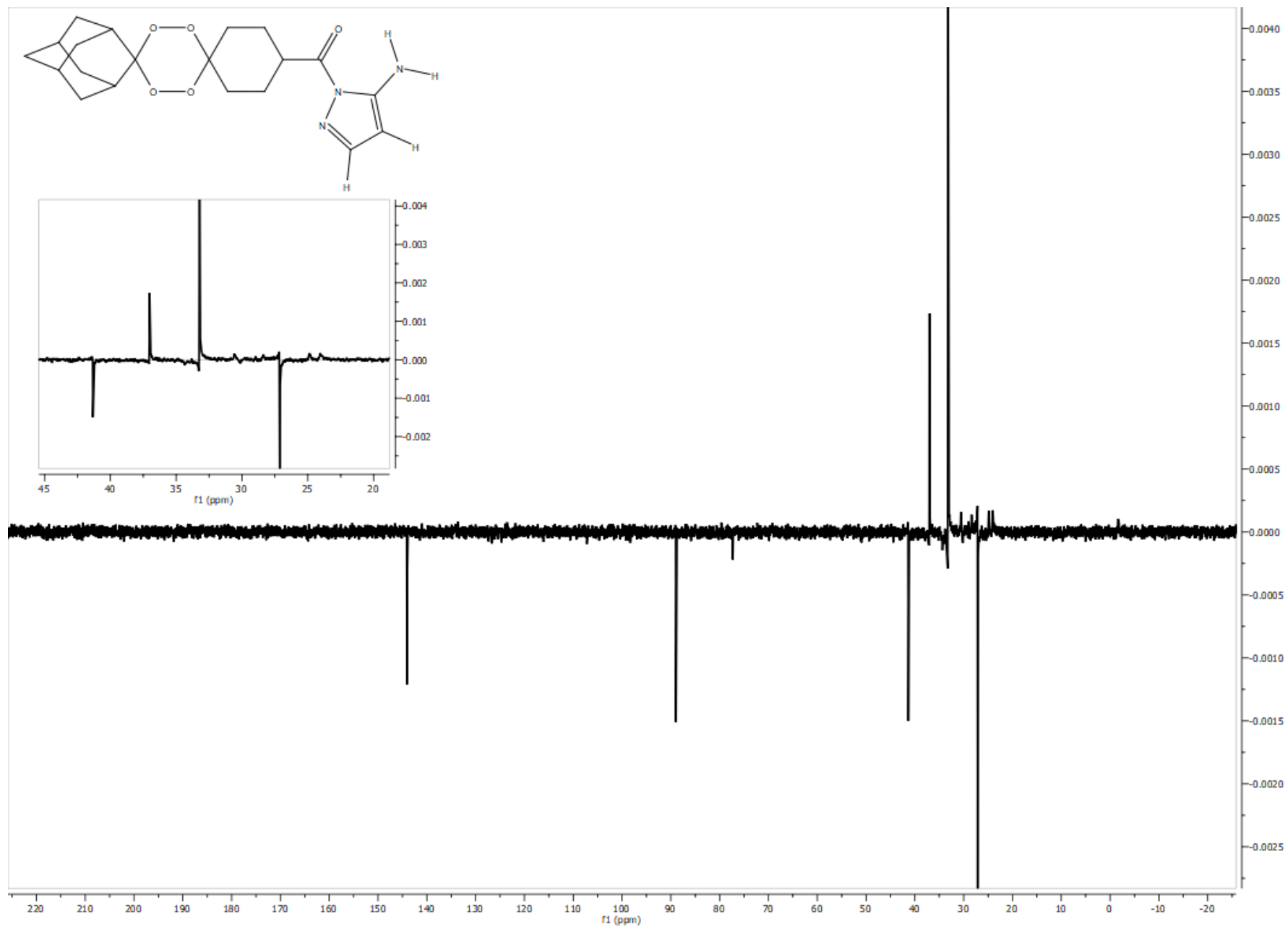


Figure S24. $^{13}\text{C}\{^1\text{H}\}$ DEPT-135 NMR spectrum (126 MHz) of **T1** in CDCl_3 .

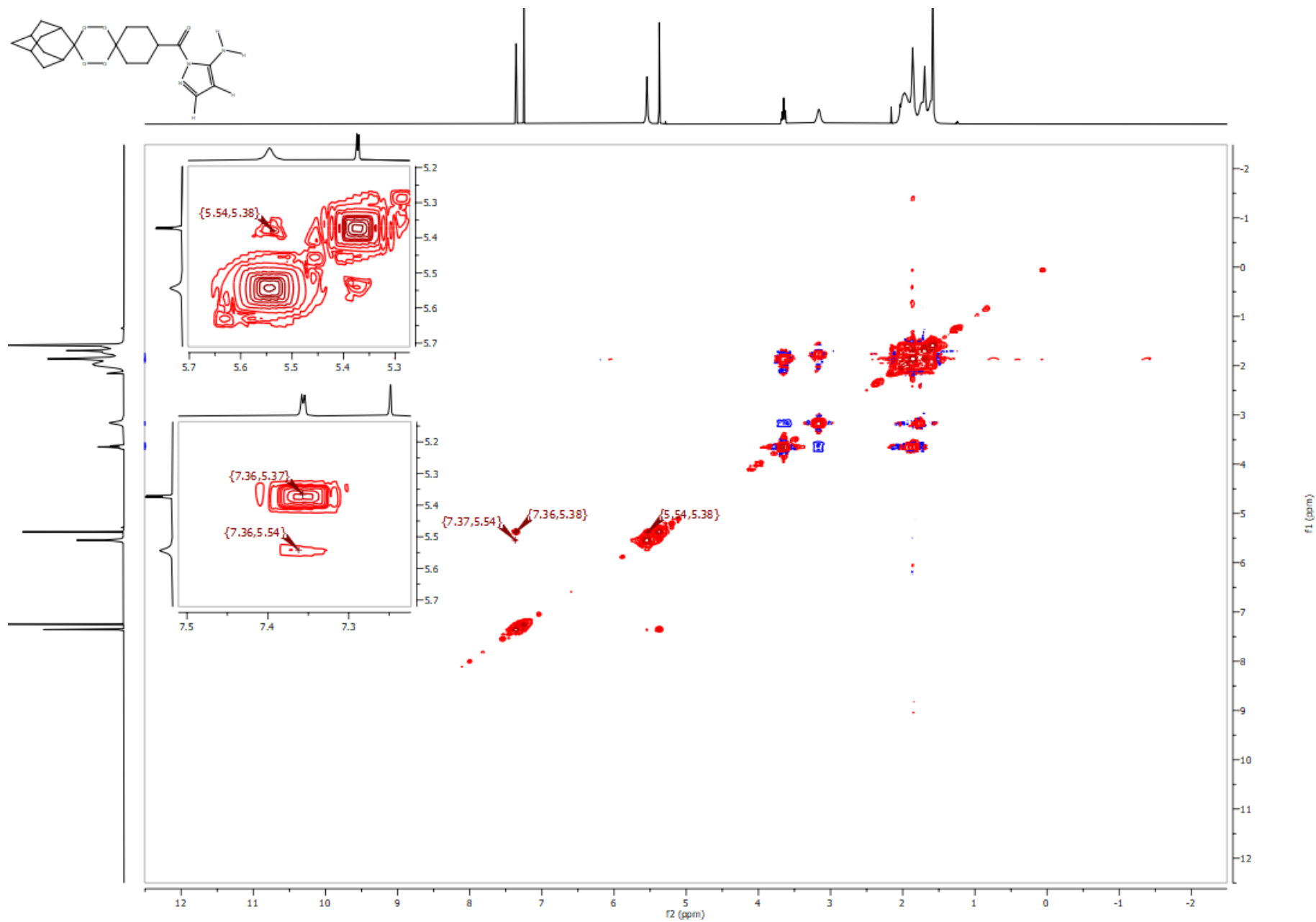


Figure S25. COSY spectrum (500 MHz) of **T1** in CDCl₃.

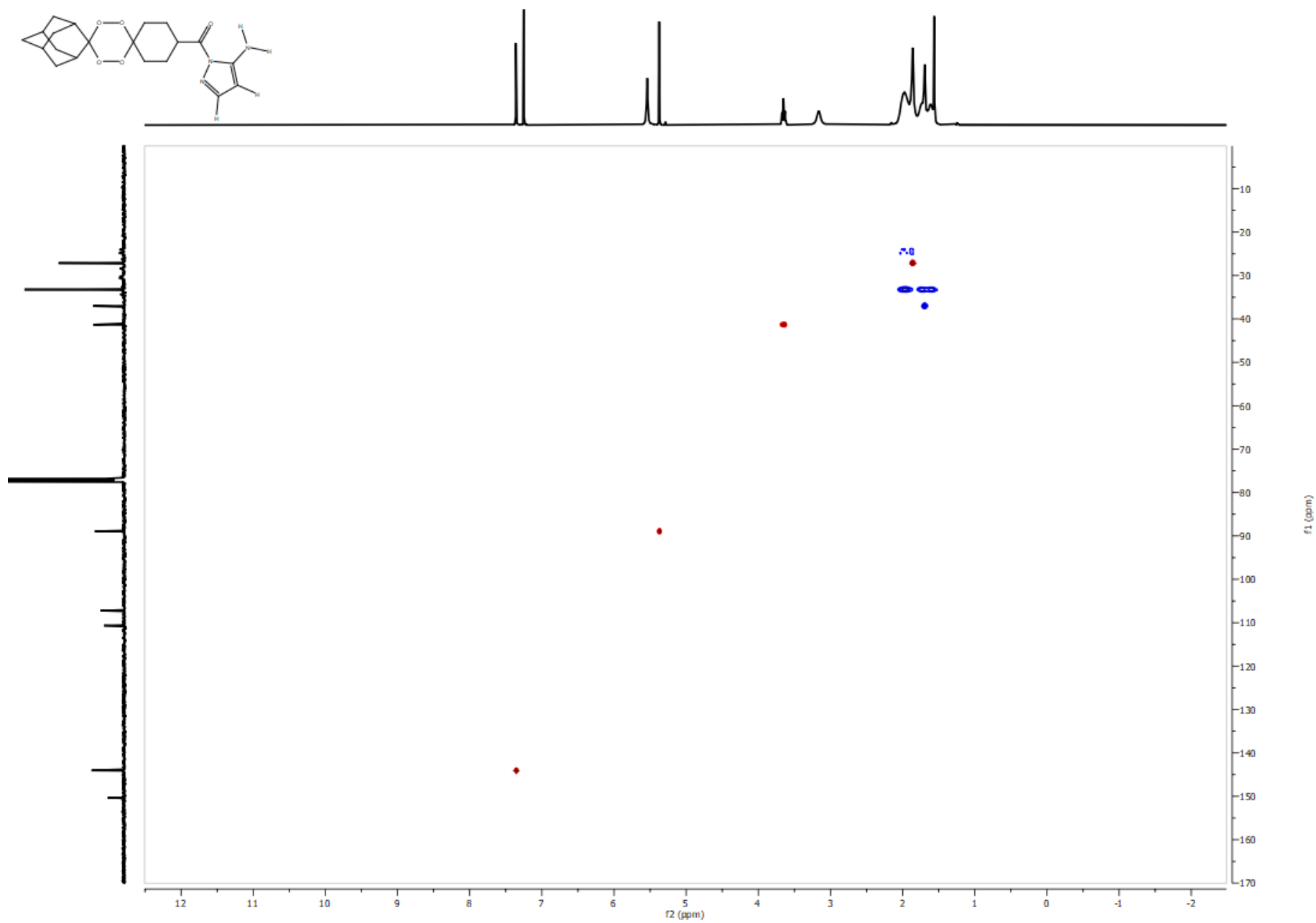


Figure S26. HSQC spectrum (500 MHz) of **T1** in CDCl_3 .

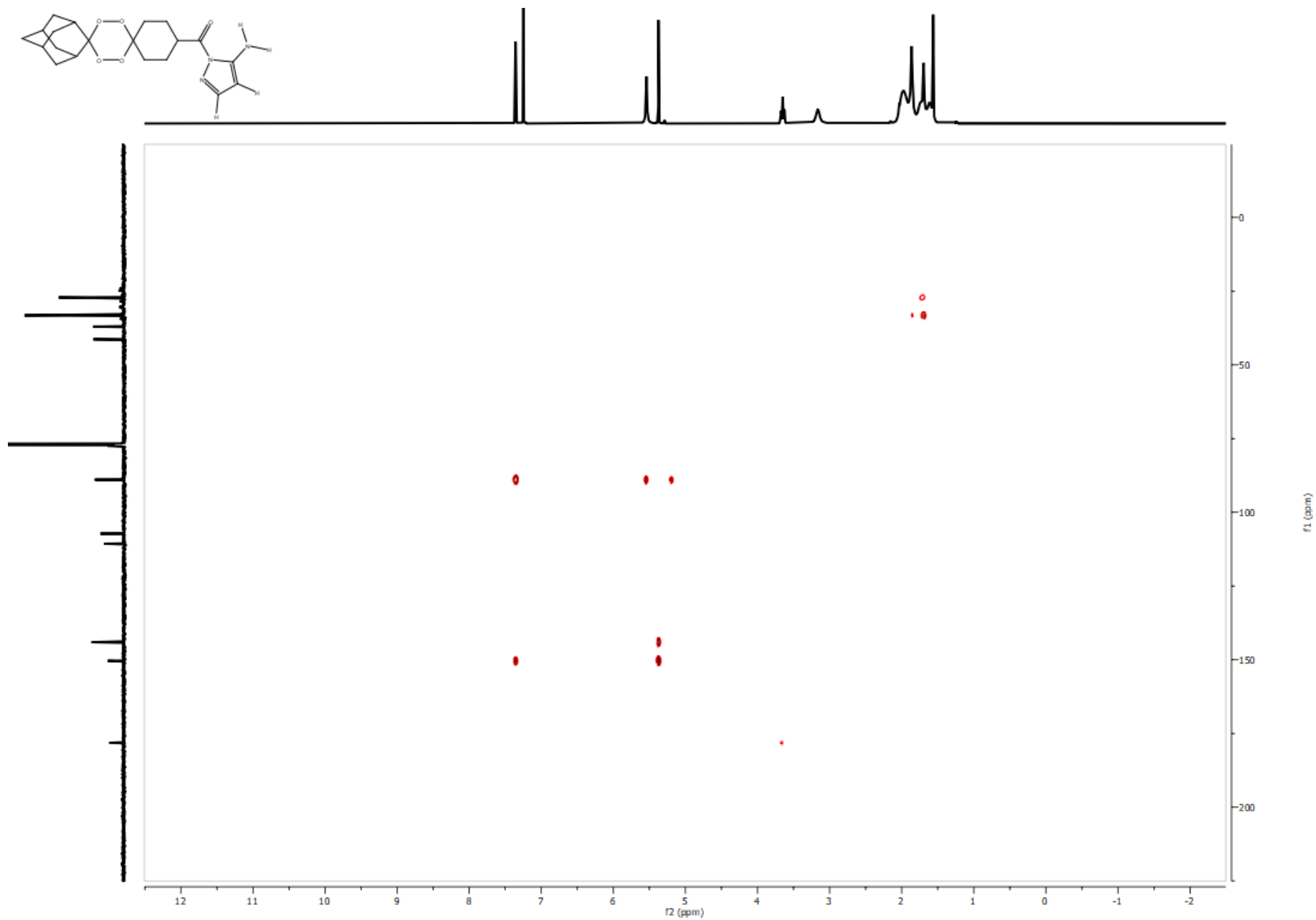


Figure S27. HMBC spectrum (500 MHz) of **T1** in CDCl_3 .

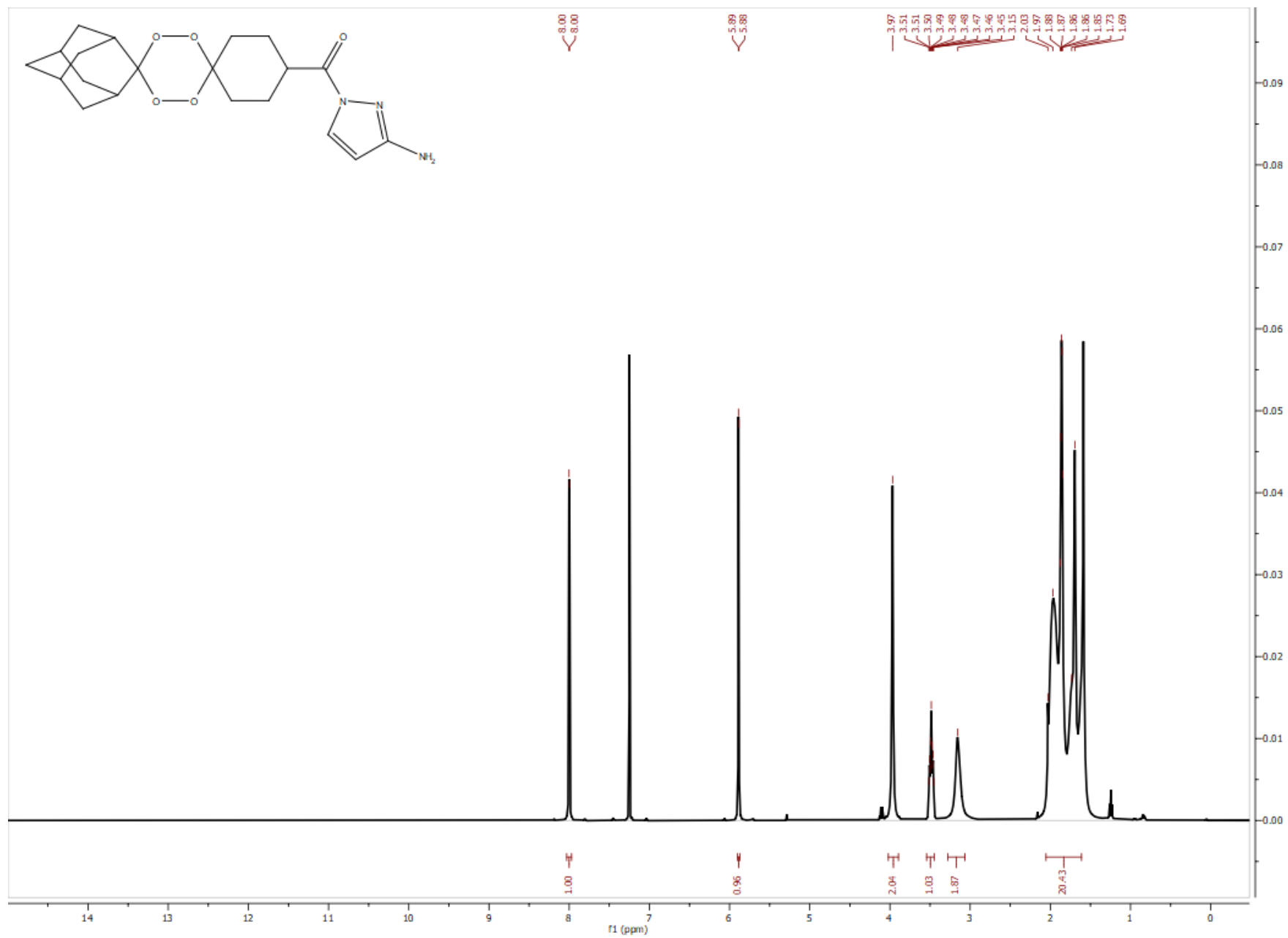


Figure S28. ¹H NMR spectrum (500 MHz) of T2 in CDCl₃.

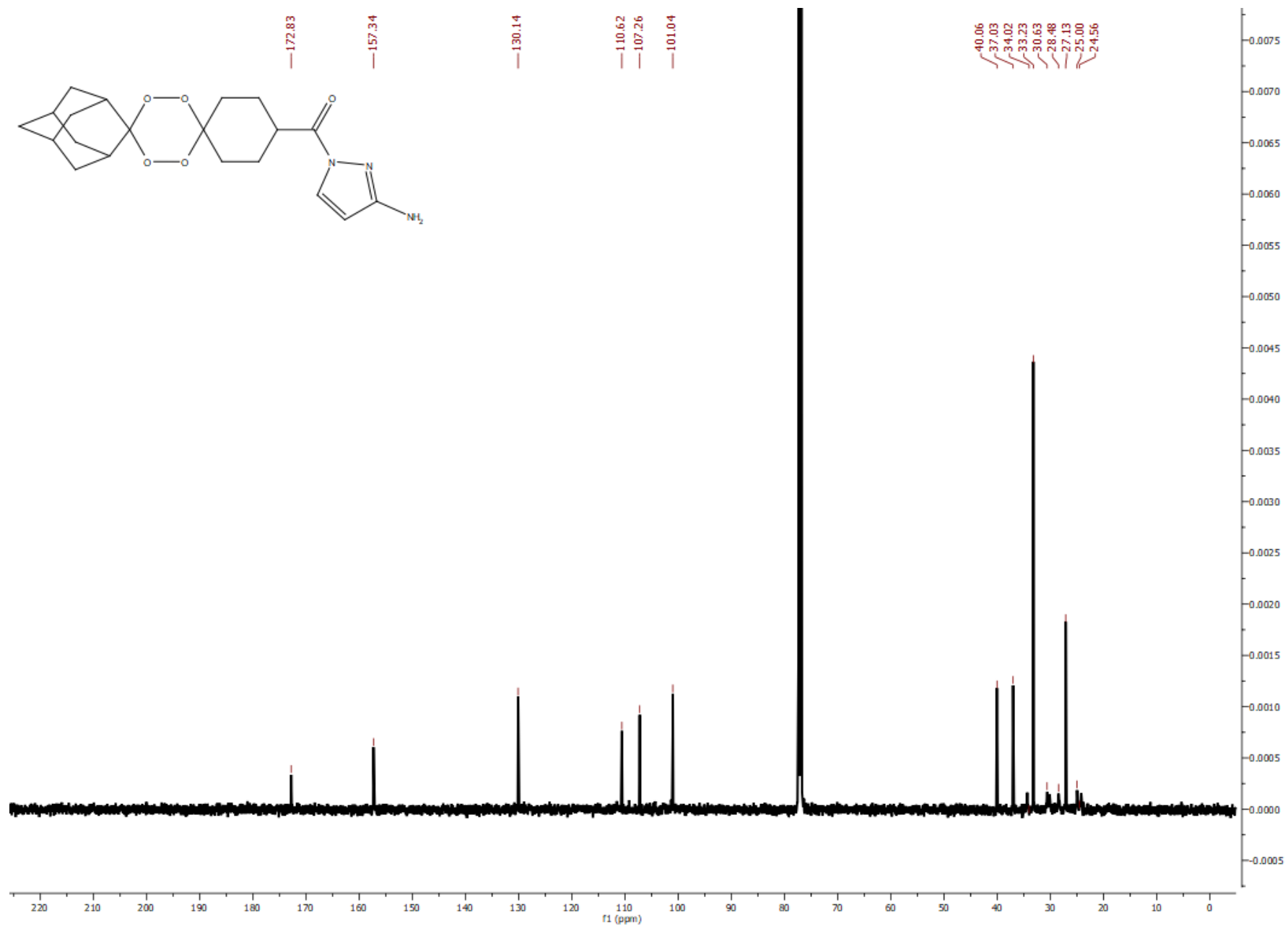


Figure S29. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (126 MHz) of **T2** in CDCl_3 .

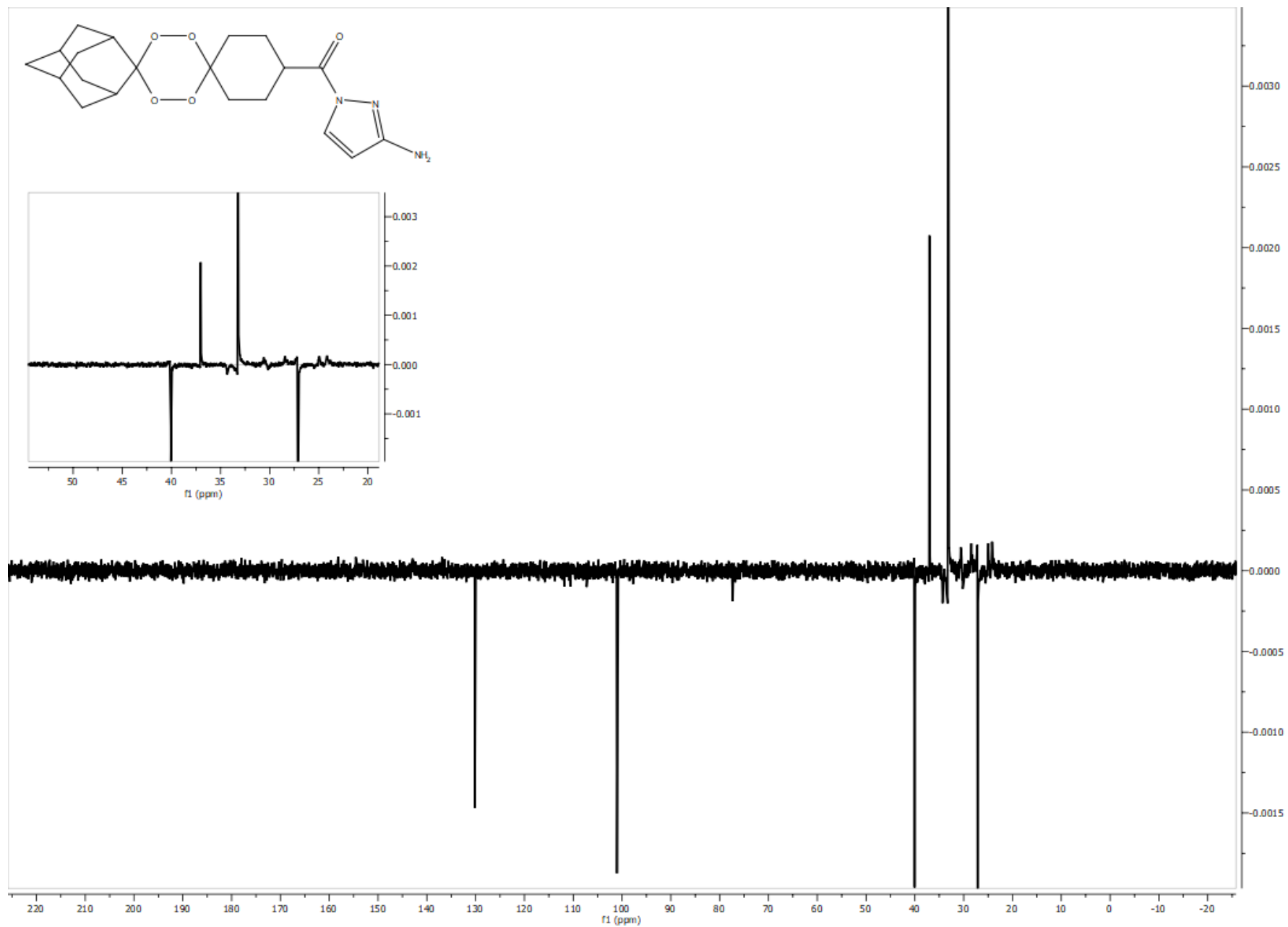


Figure S30. $^{13}\text{C}\{^1\text{H}\}$ DEPT-135 NMR spectrum (126 MHz) of **T2** in CDCl_3 .

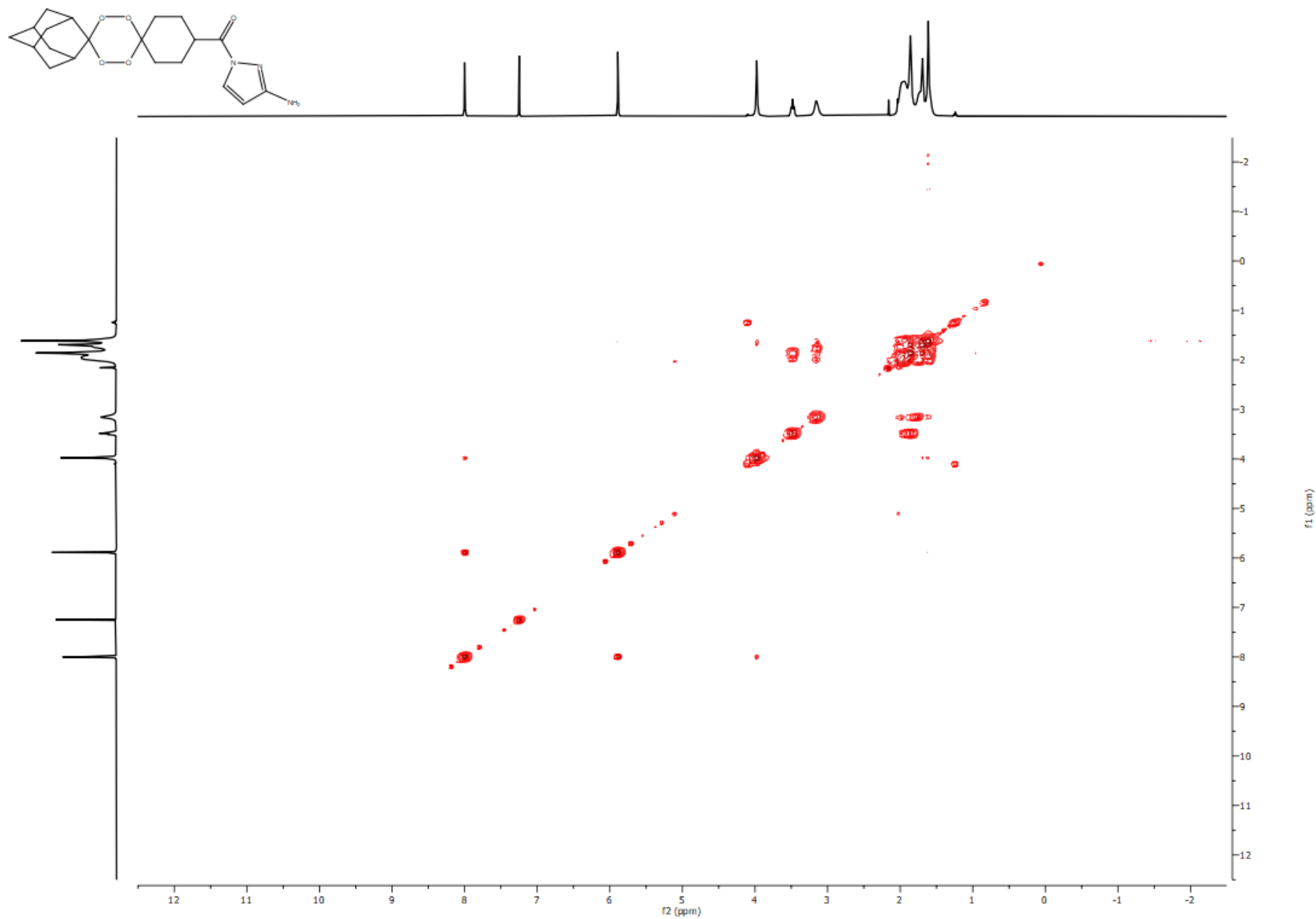


Figure S31. COSY spectrum (500 MHz) of **T2** in CDCl₃.

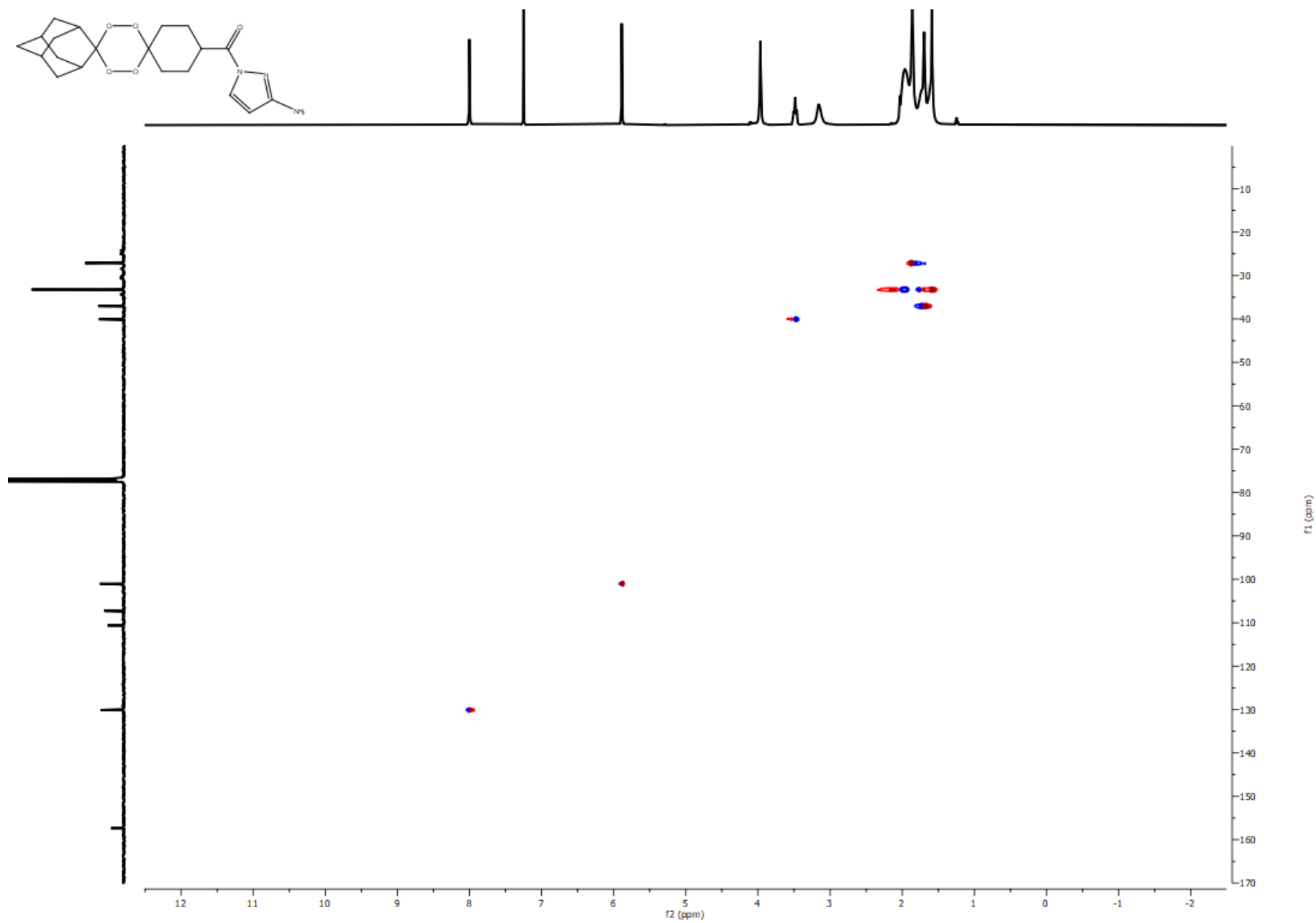


Figure S32. HSQC spectrum (500 MHz) of **T2** in CDCl₃.

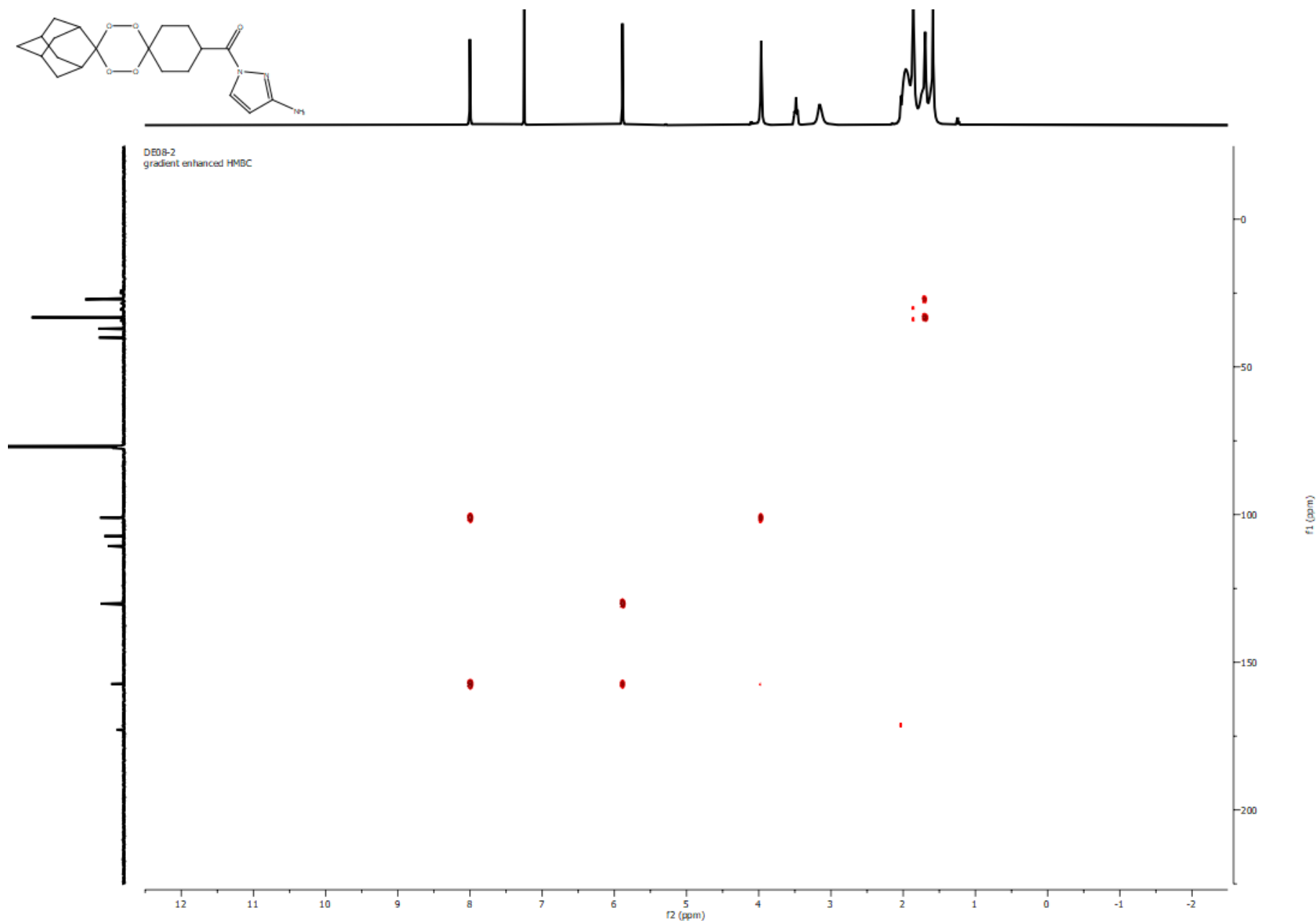


Figure S33. HMBC spectrum (500 MHz) of **T2** in CDCl_3 .

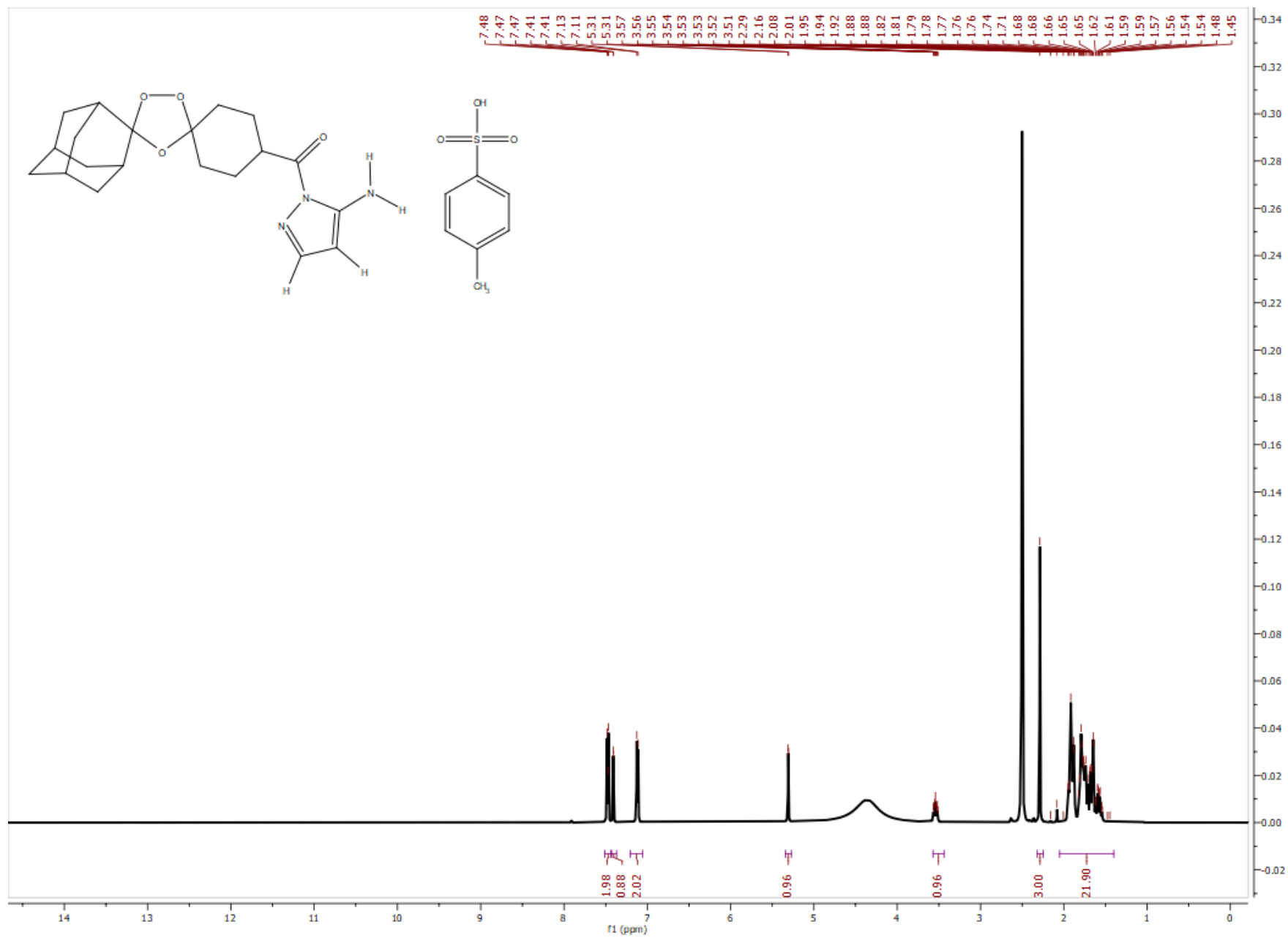


Figure S34. ^1H NMR spectrum (500 MHz) of **OZ1•TsOH** in $\text{DMSO-}d_6$.

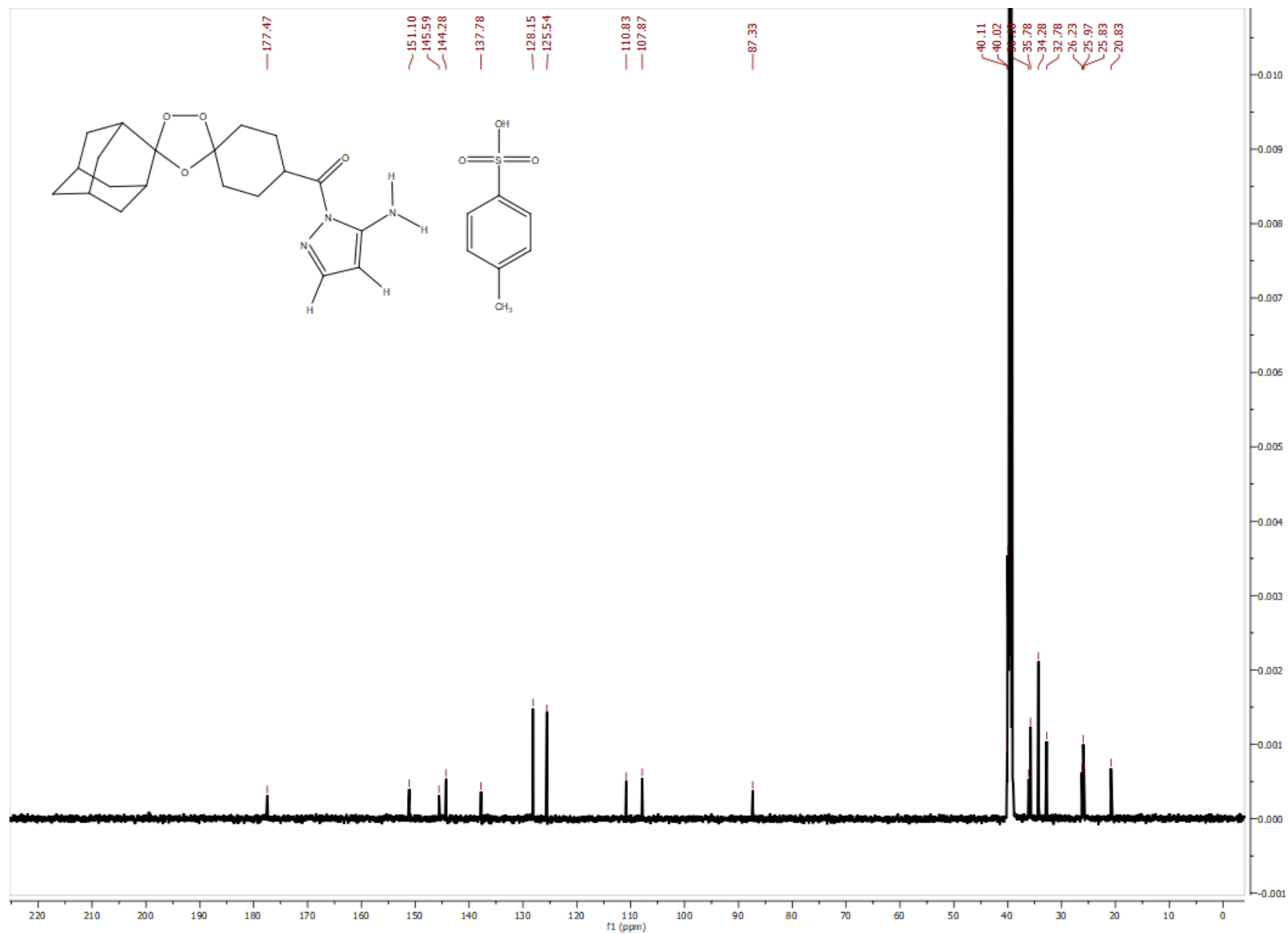


Figure S35. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (126 MHz) of **OZ1•TsOH** in $\text{DMSO-}d_6$.

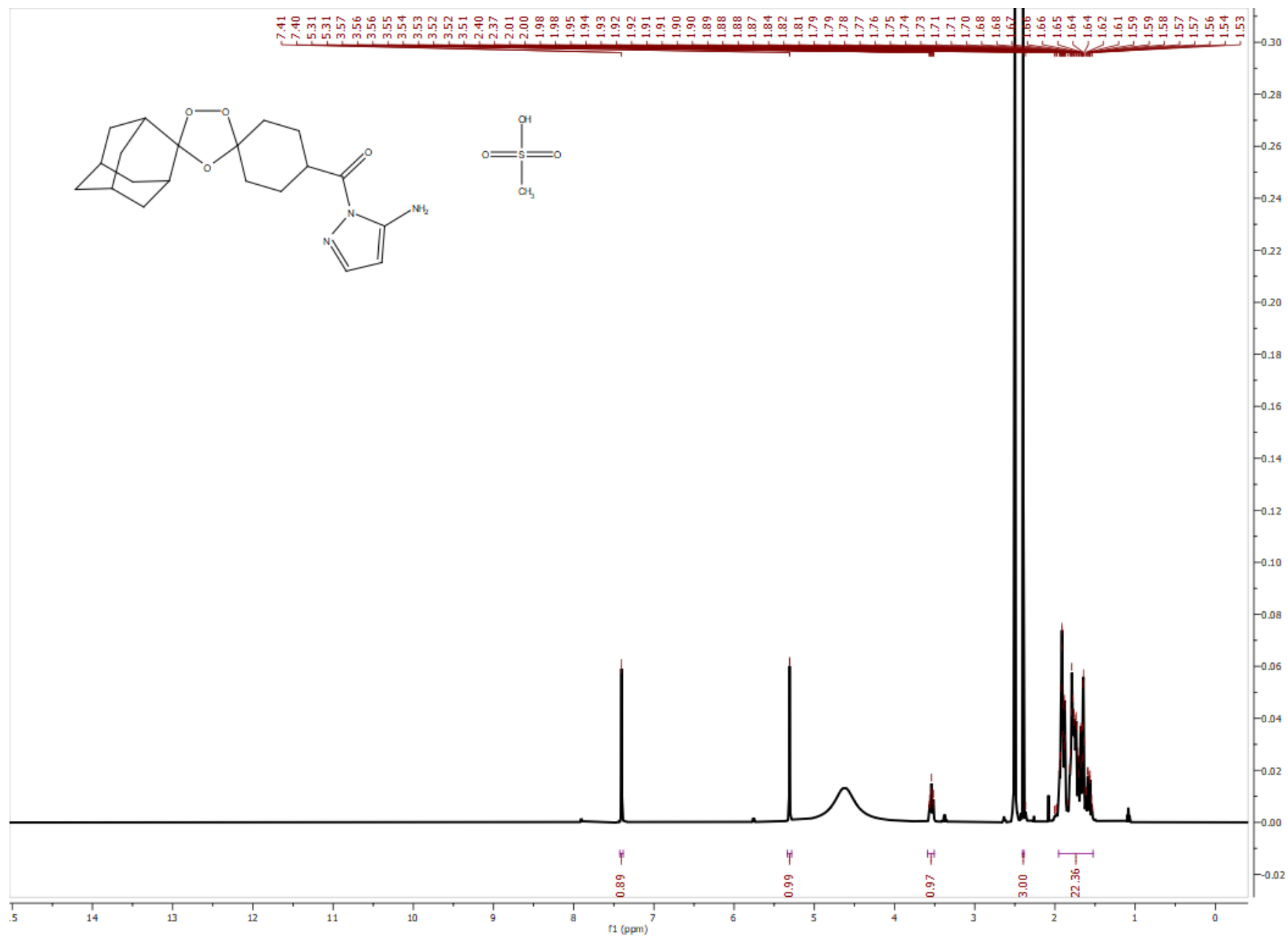


Figure S36. ^1H NMR spectrum (500 MHz) of **OZ1•MsOH** in $\text{DMSO}-d_6$.

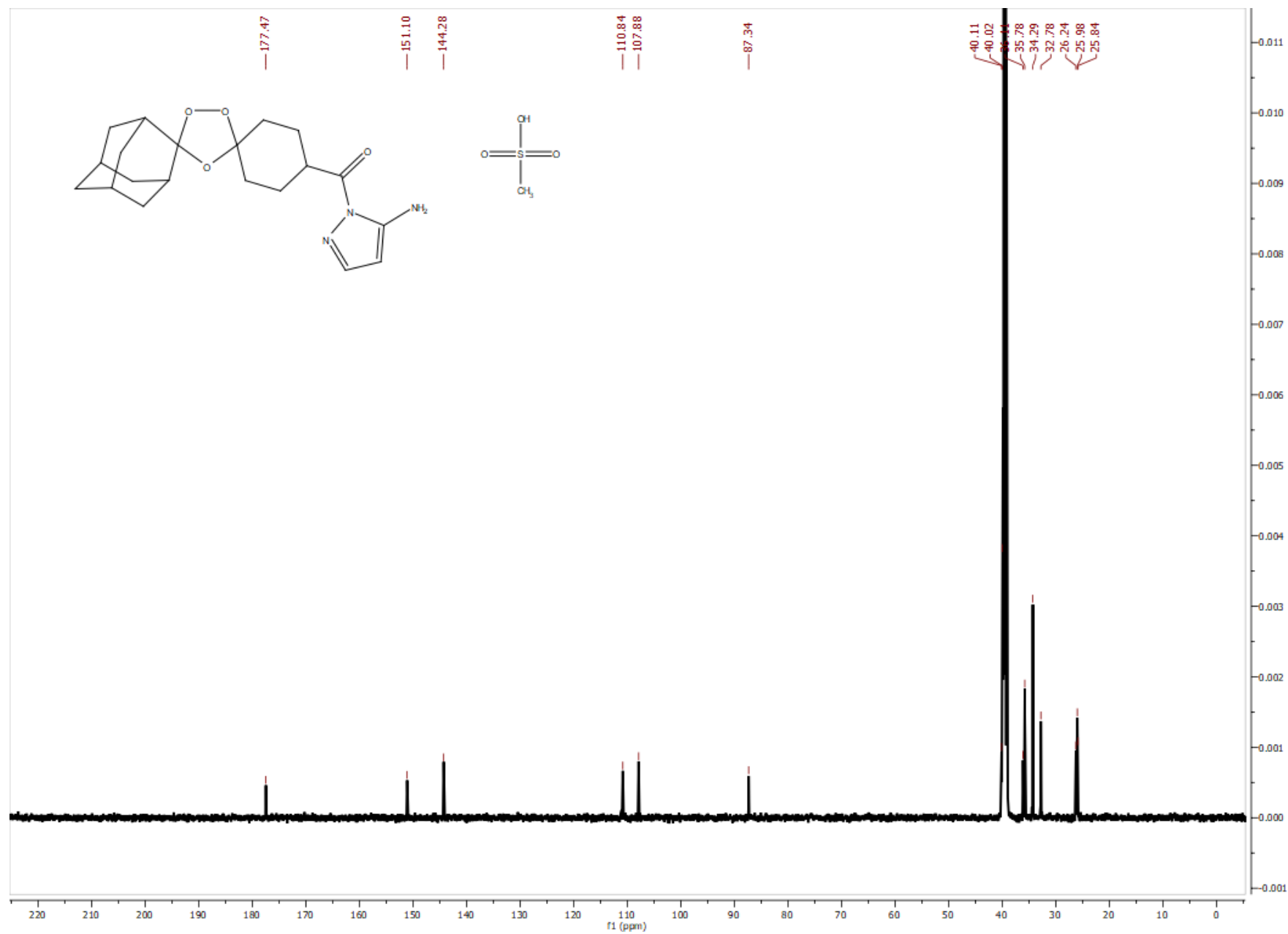


Figure S37. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (126 MHz) of **OZ1•MsOH** in $\text{DMSO-}d_6$.

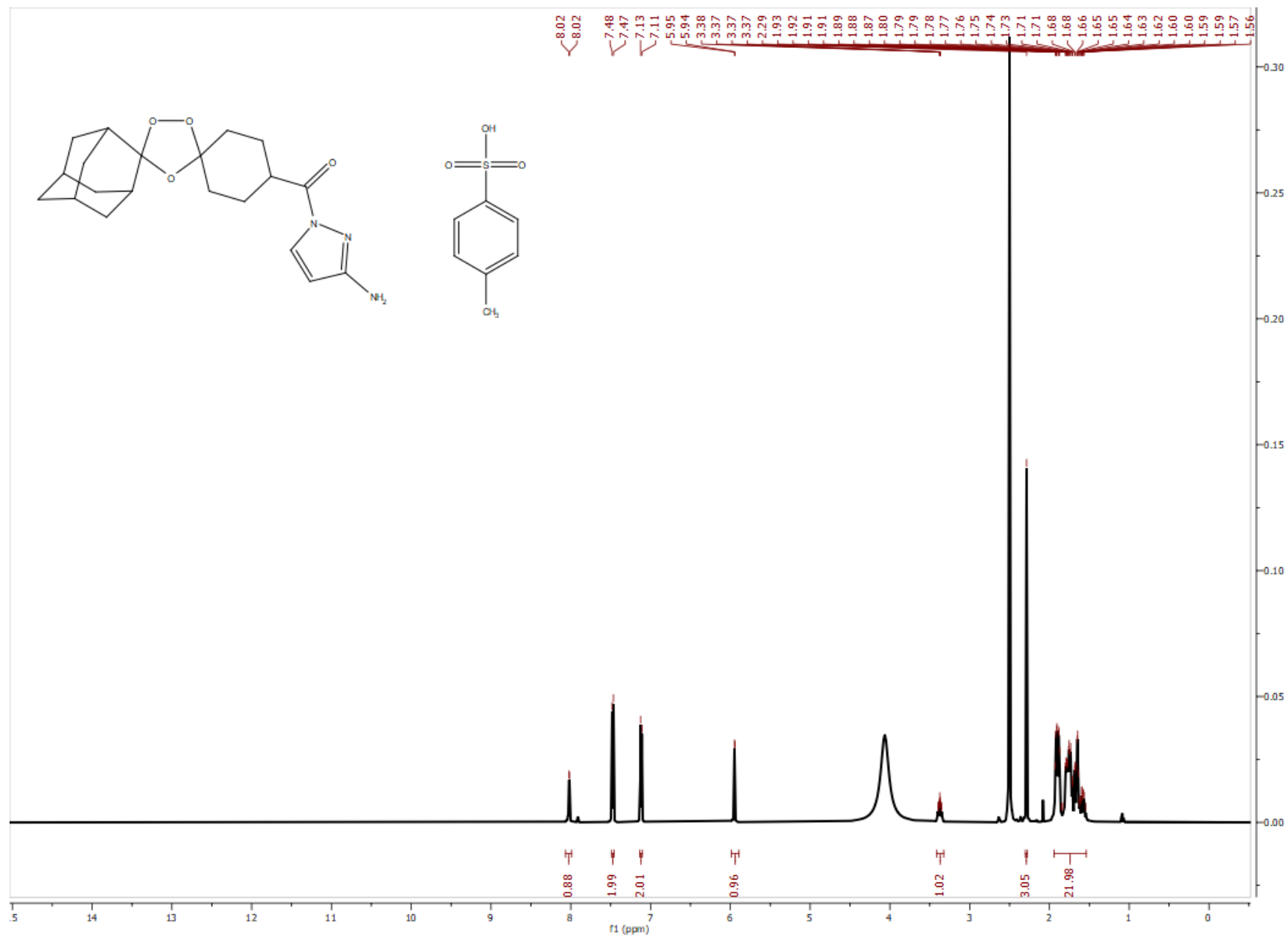


Figure S38. ^1H NMR spectrum (500 MHz) of **OZ2•TsOH** in $\text{DMSO-}d_6$.

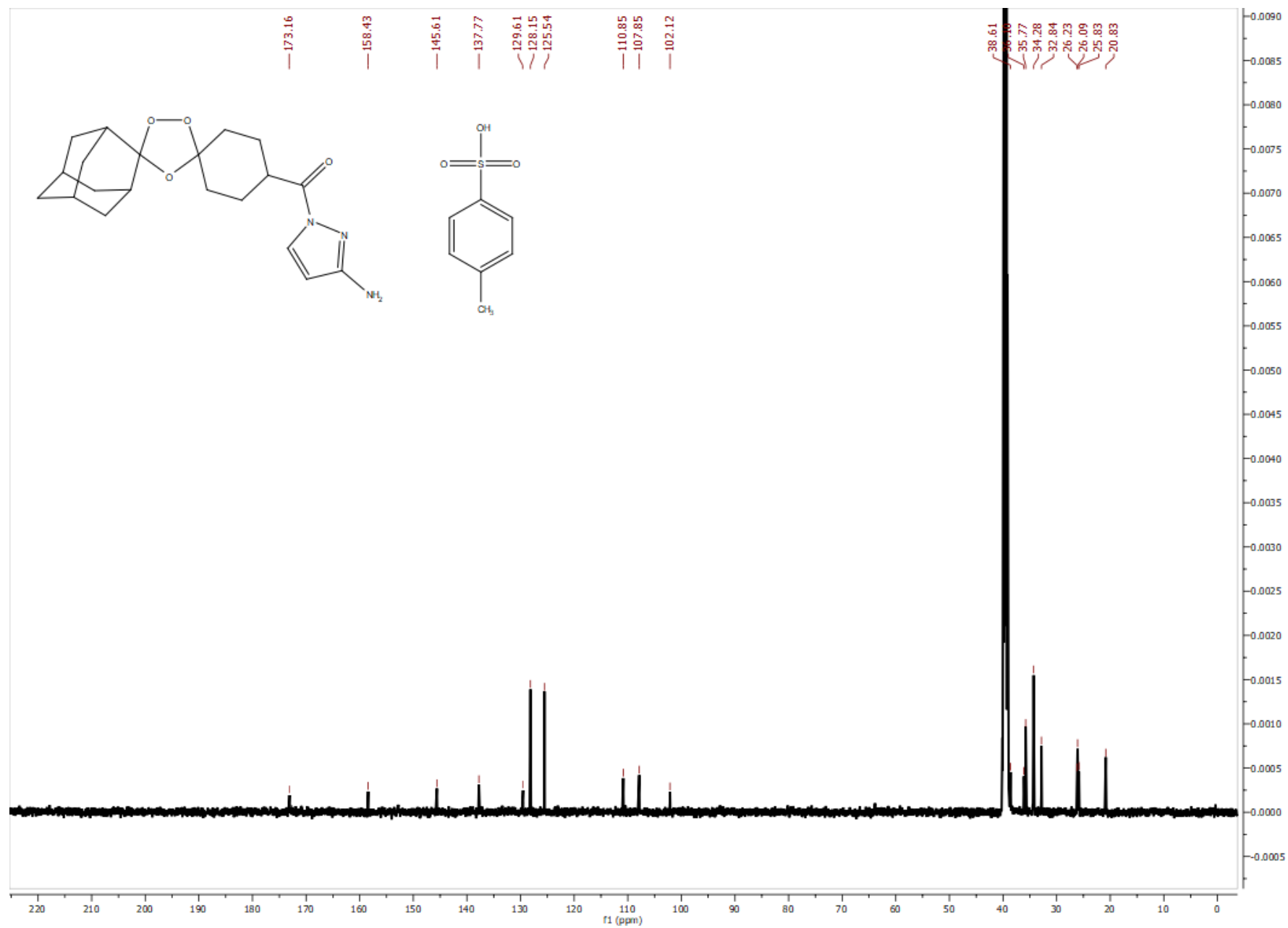


Figure S39. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (126 MHz) of **OZ2•TsOH** in $\text{DMSO-}d_6$.

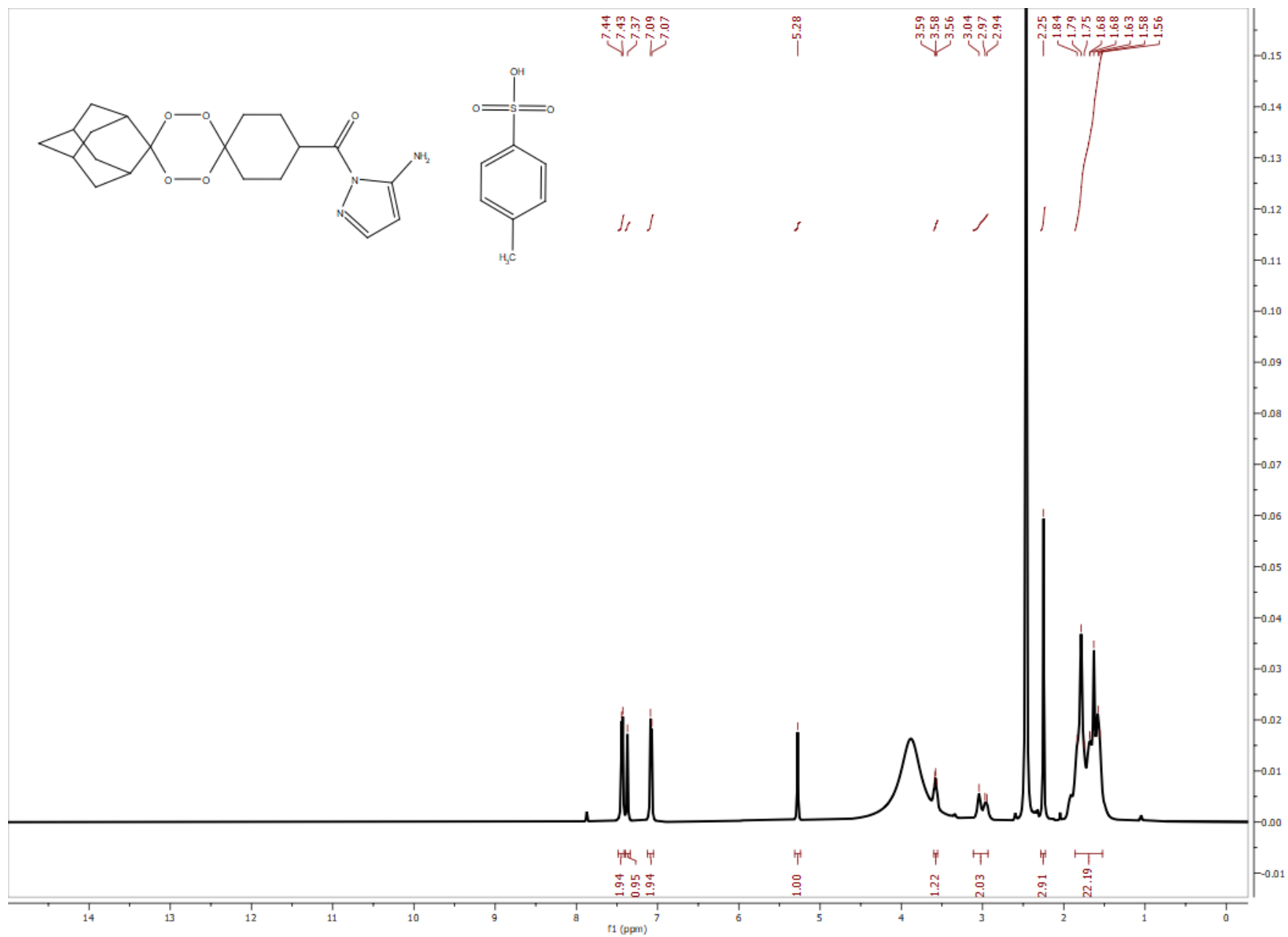


Figure S40. ^1H NMR spectrum (500 MHz) of **T1•TsOH** in $\text{DMSO-}d_6$.

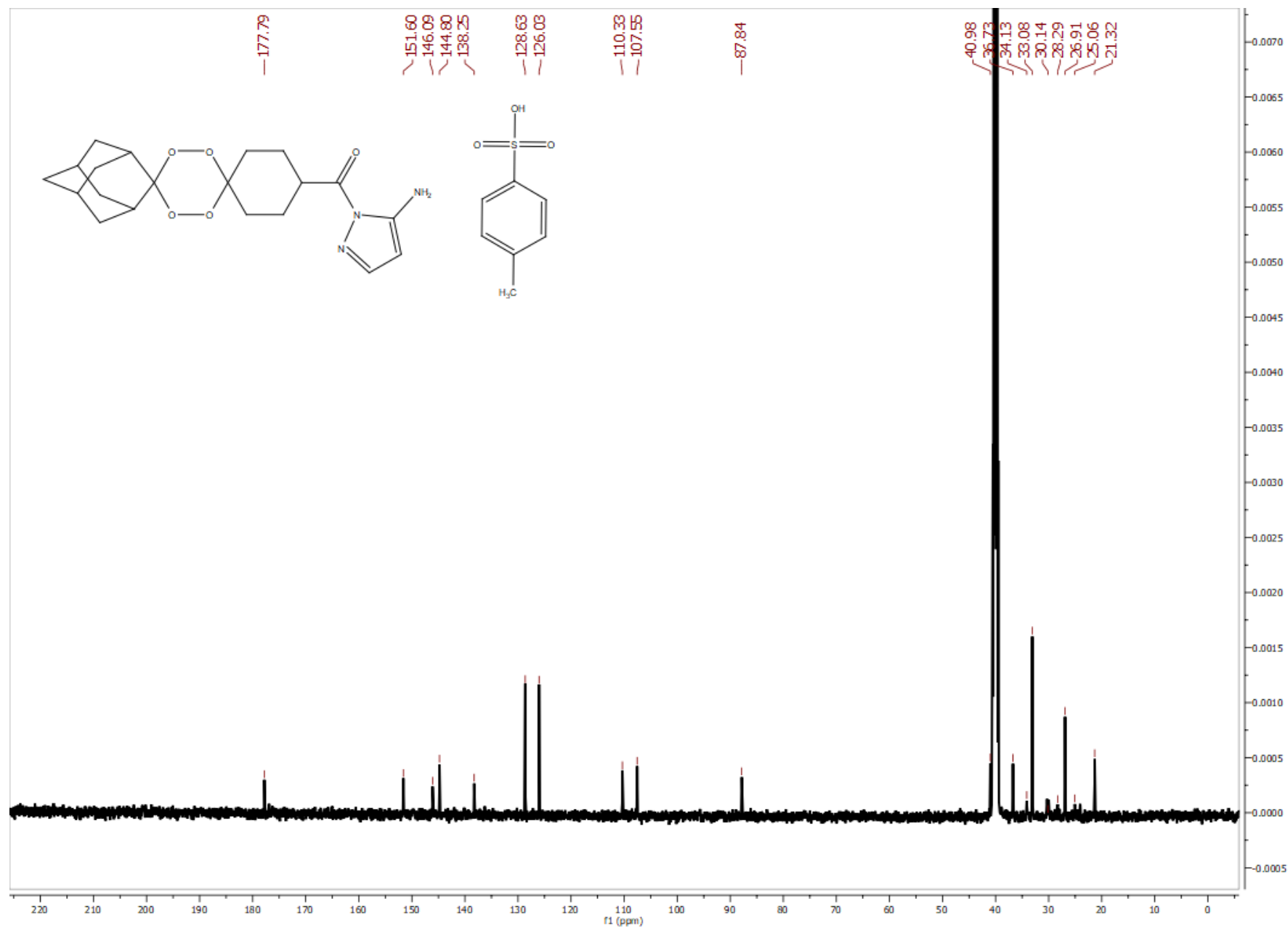


Figure S41. ¹³C{¹H} NMR spectrum (126 MHz) of T1•TsOH in DMSO-*d*₆.

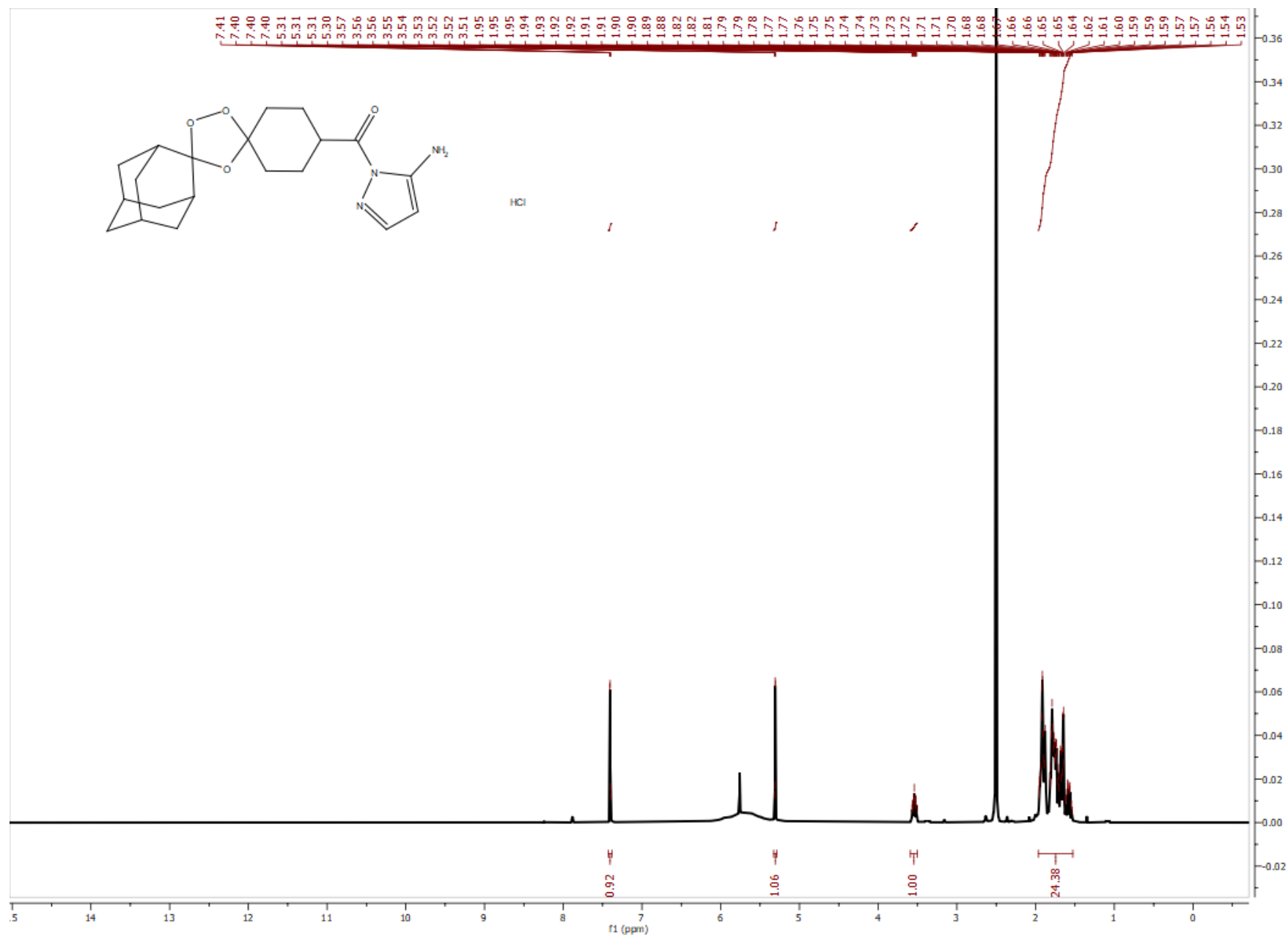


Figure S42. ^1H NMR spectrum (500 MHz) of **OZ1•HCl** in $\text{DMSO}-d_6$.

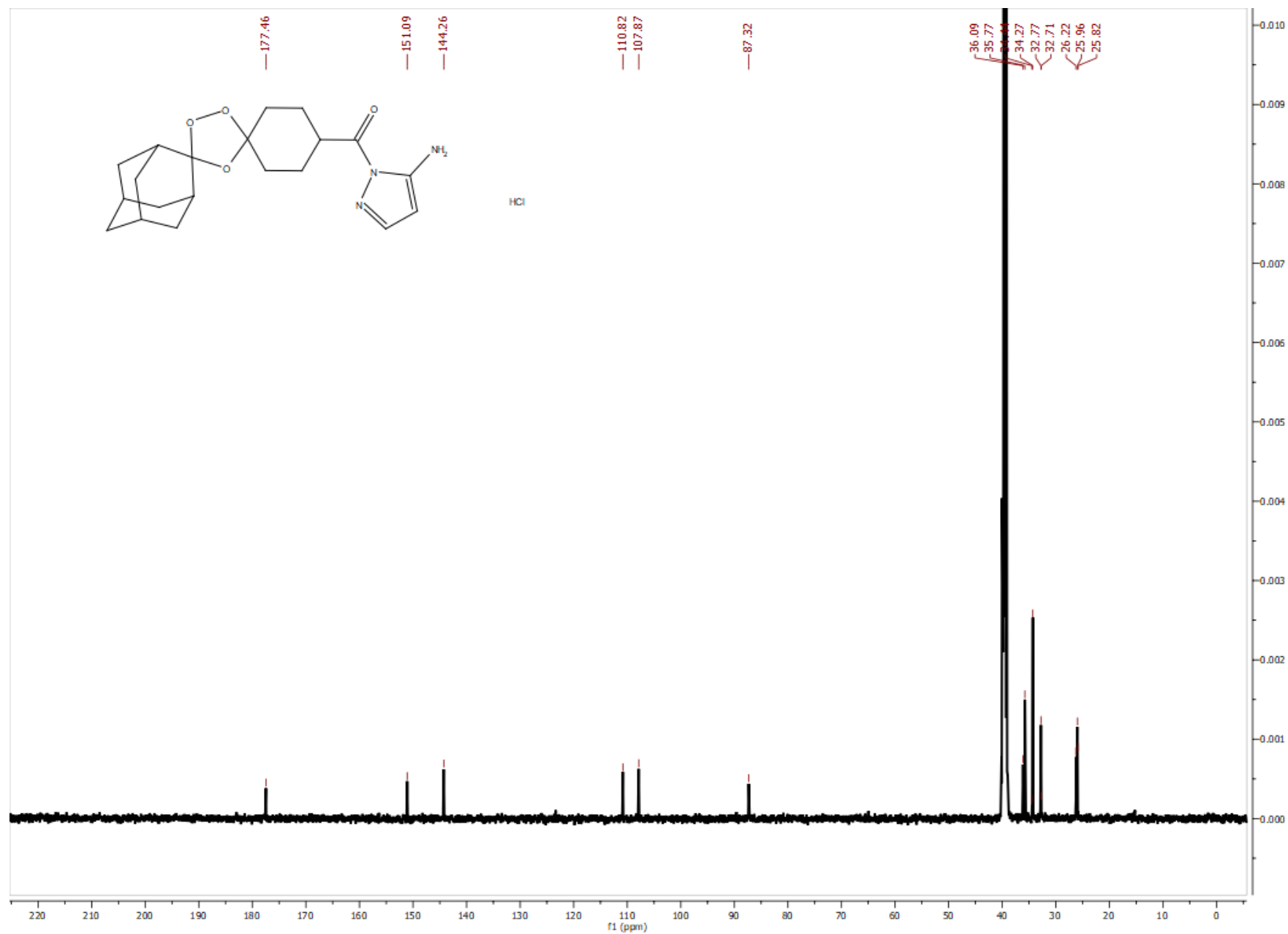


Figure S43. ¹³C{¹H} NMR spectrum (126 MHz) of **OZ1•HCl** in DMSO-*d*₆.

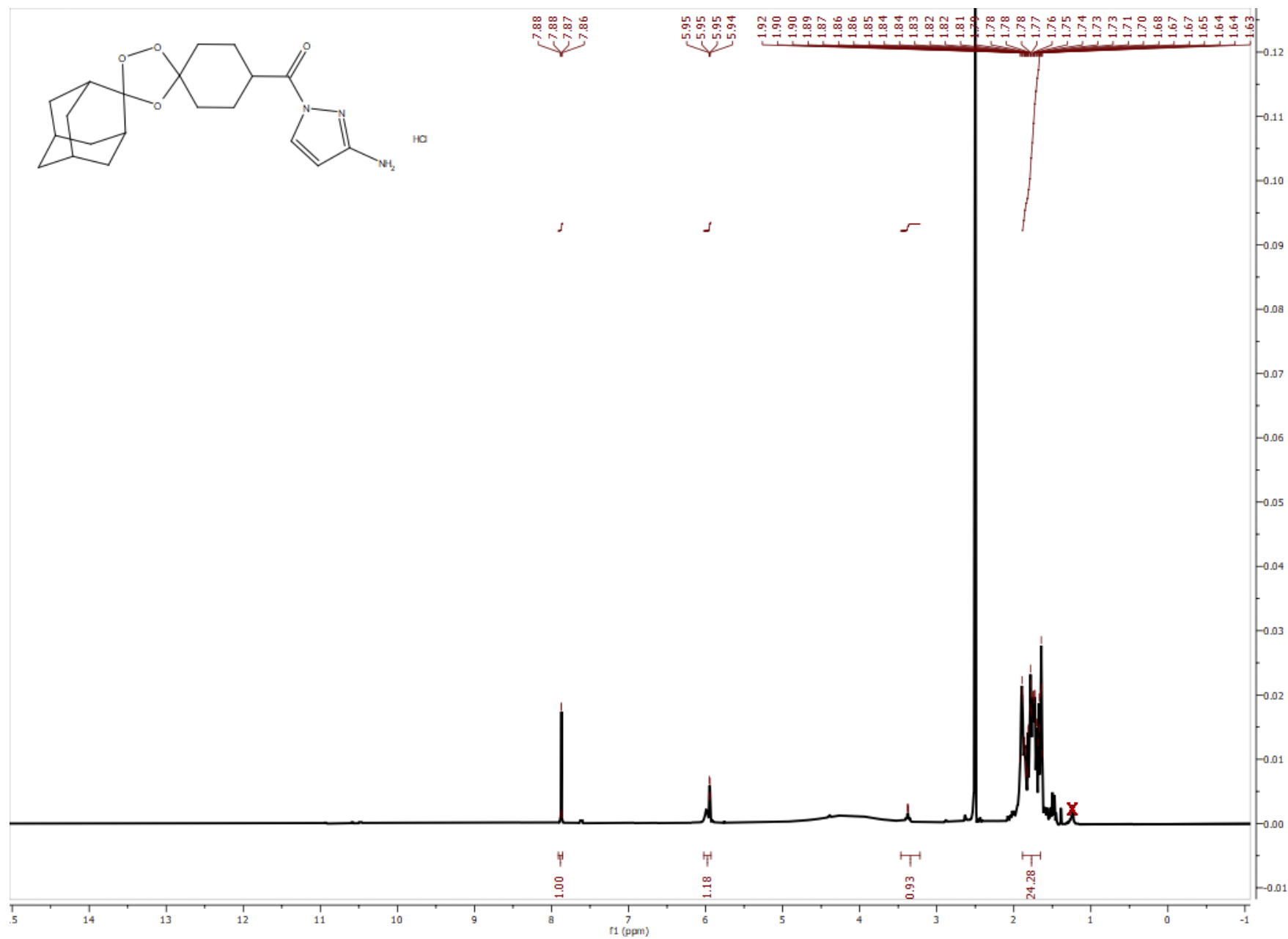
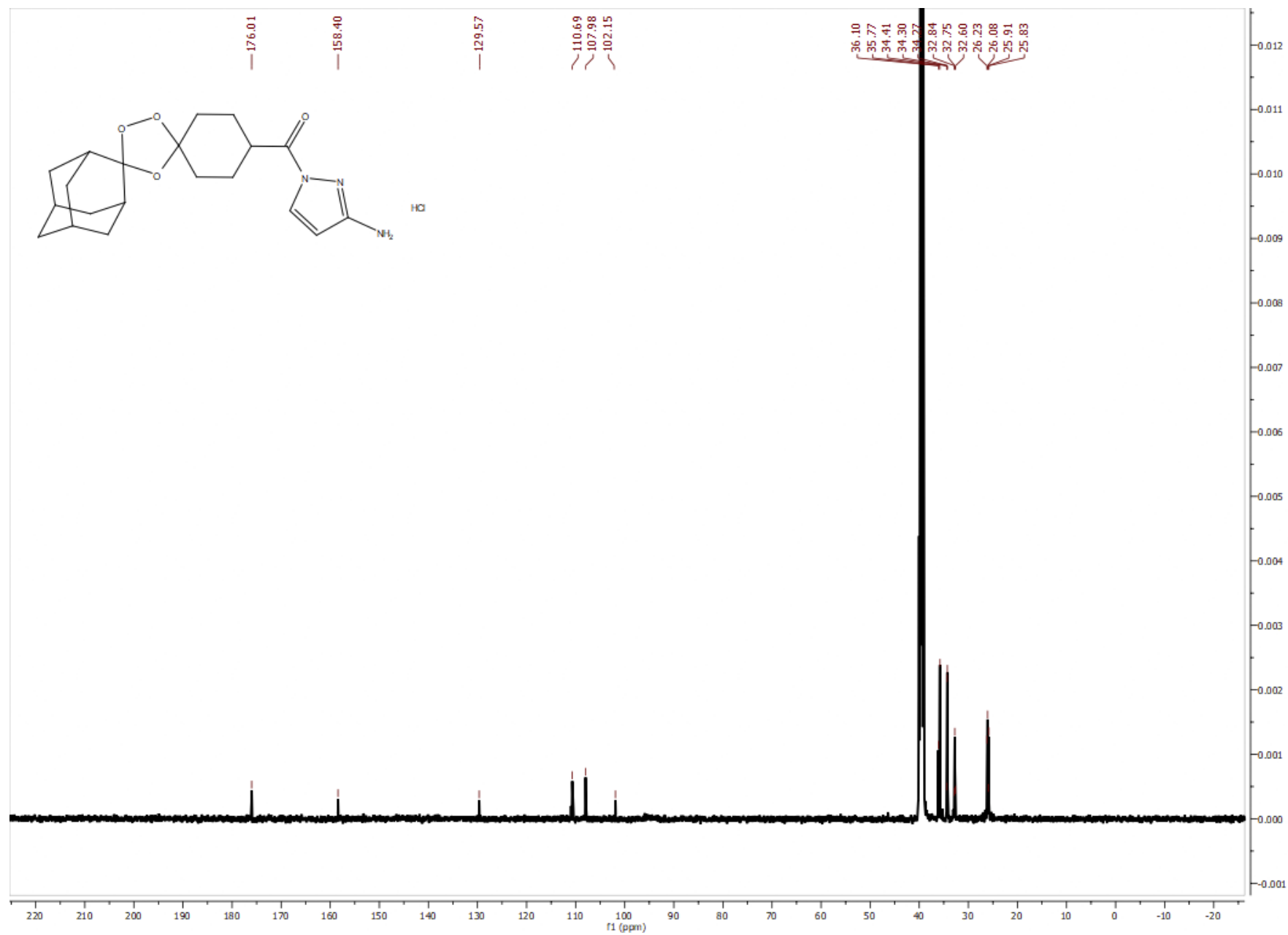


Figure S44. ^1H NMR spectrum (500 MHz) of **OZ2·HCl** in $\text{DMSO-}d_6$.



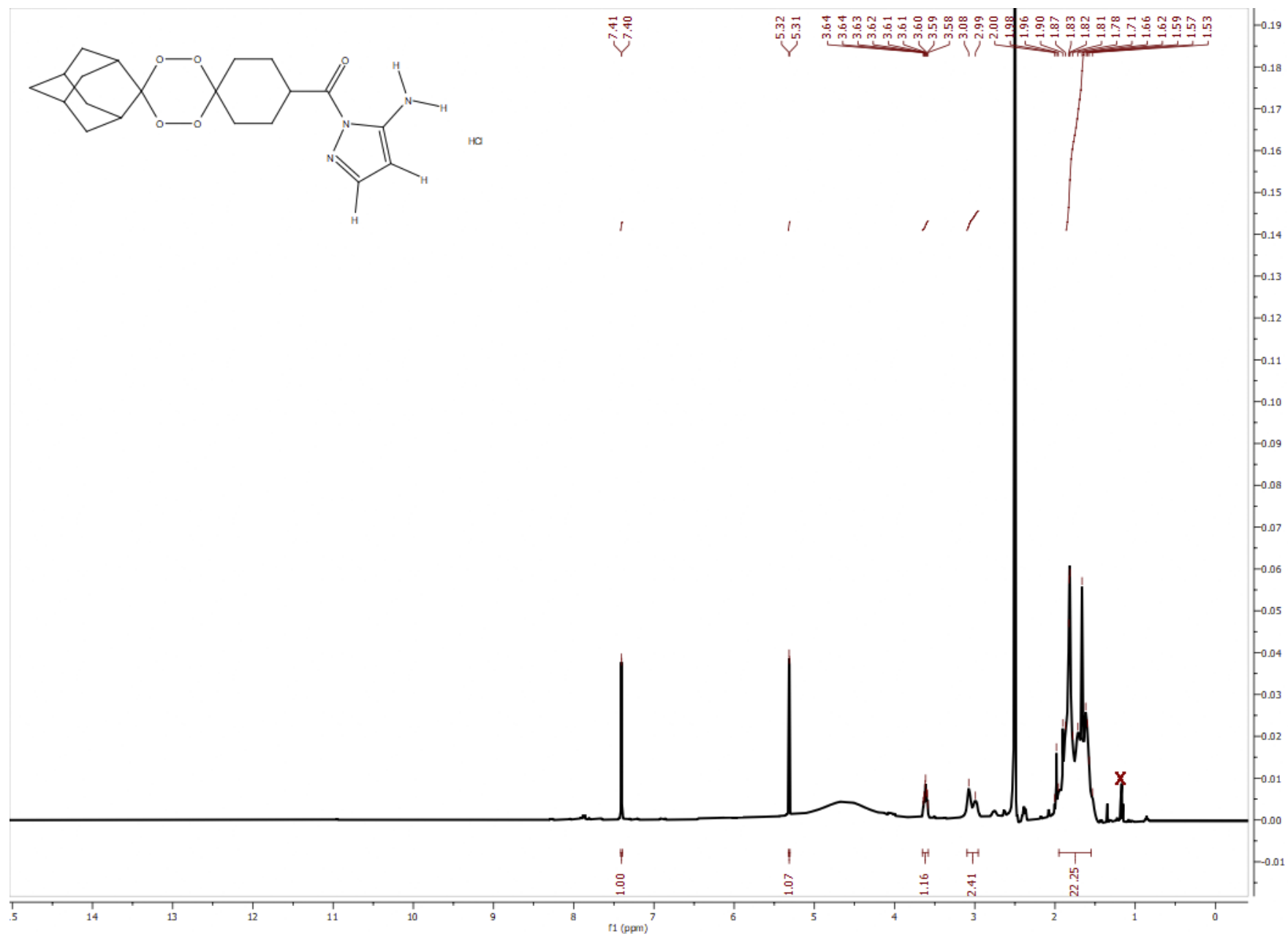


Figure S46. ¹H NMR spectrum (500 MHz) of T1•HCl in DMSO-*d*₆.

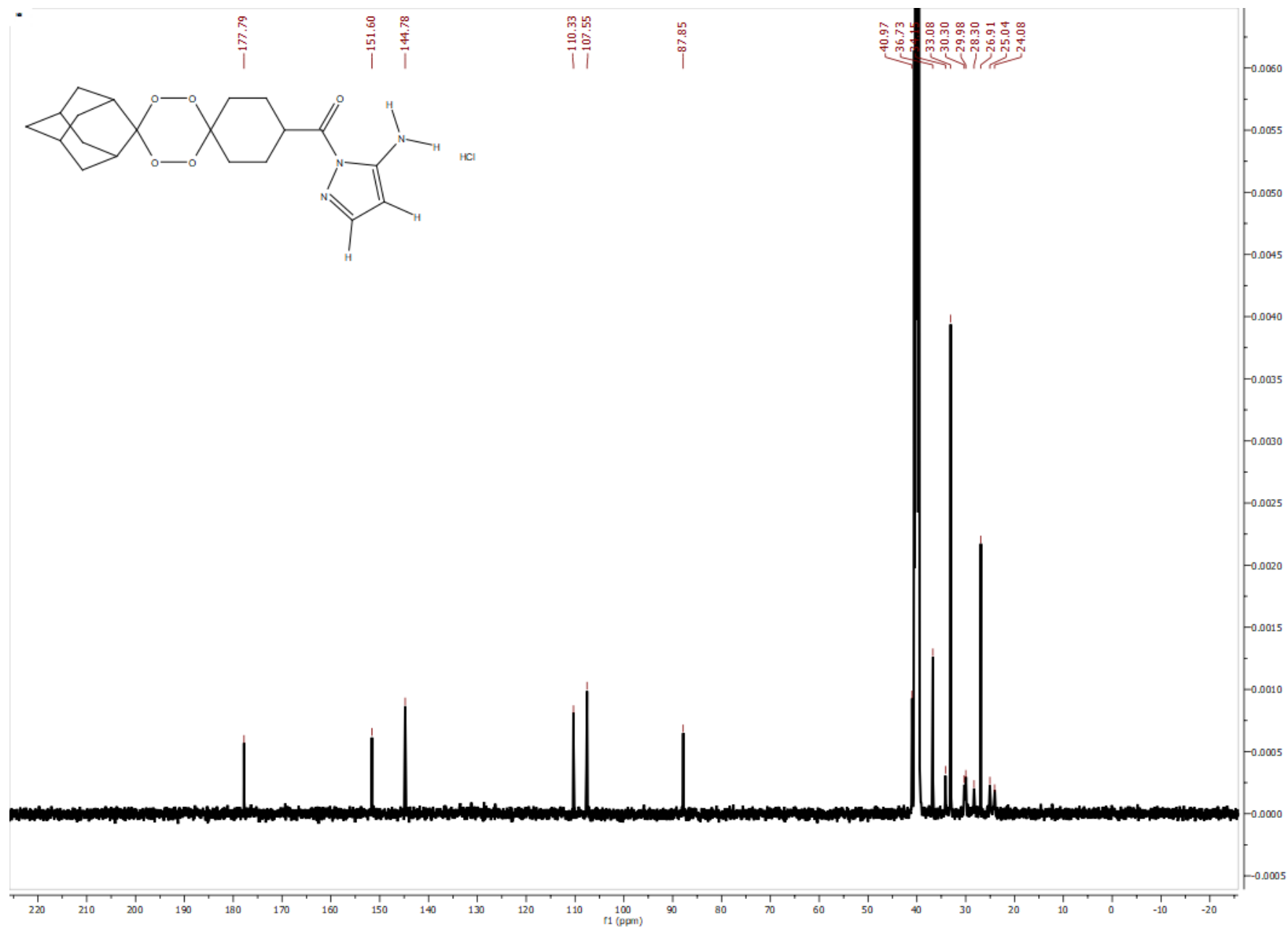


Figure S47. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (126 MHz) of **T1**·HCl in $\text{DMSO-}d_6$.

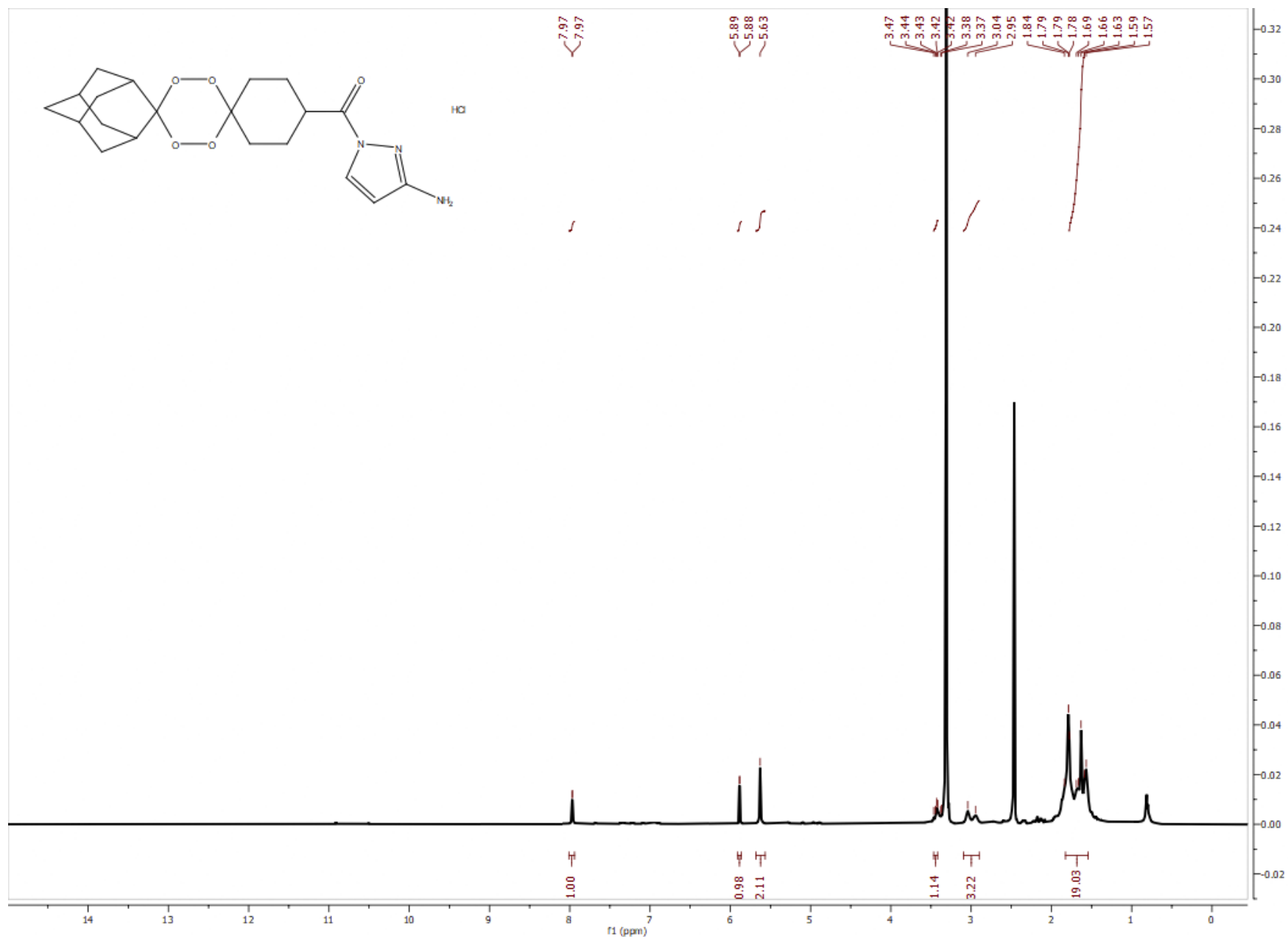


Figure S48. ^1H NMR spectrum (500 MHz) of $\text{T2}\cdot\text{HCl}$ in $\text{DMSO}-d_6$.

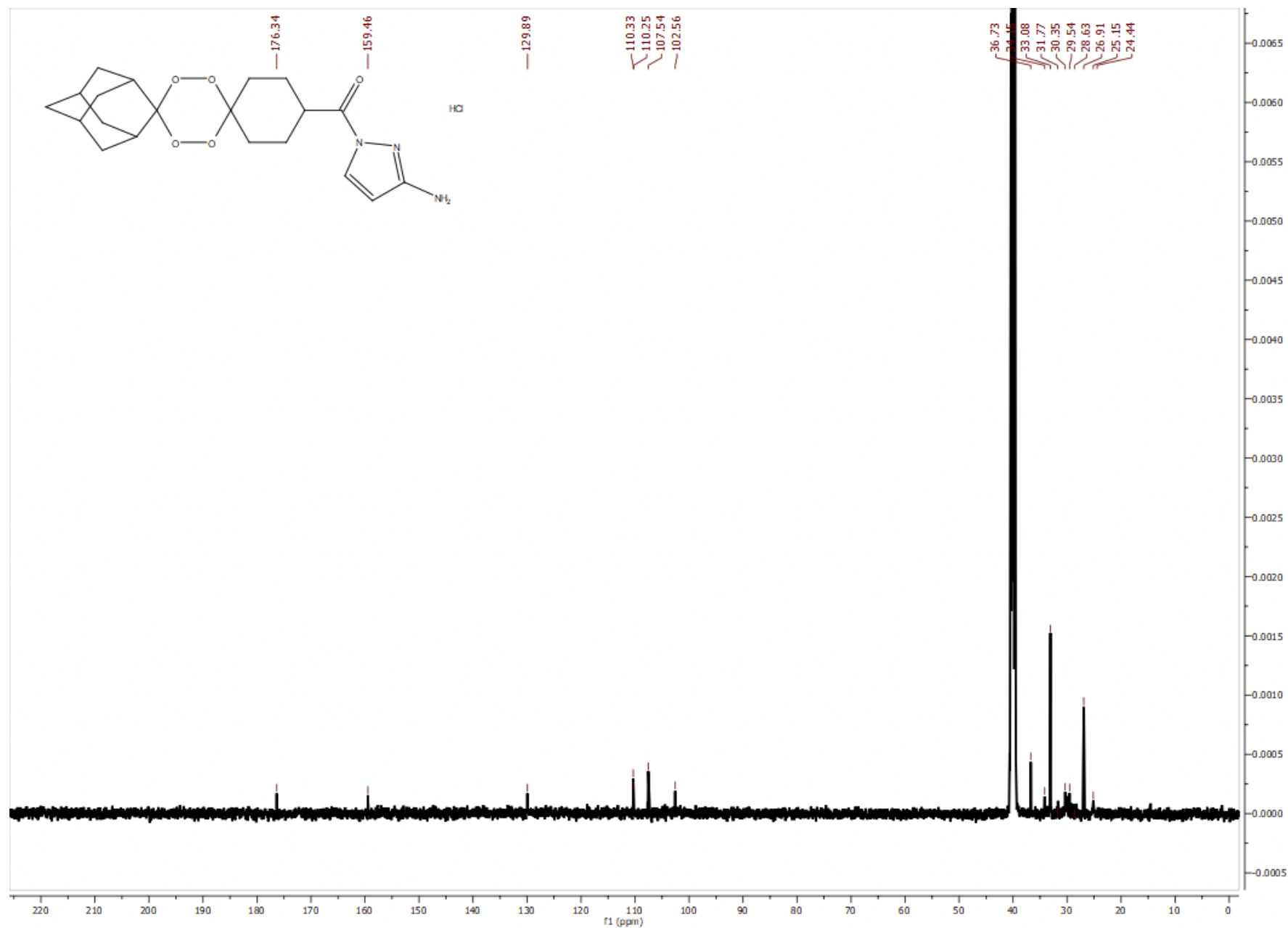
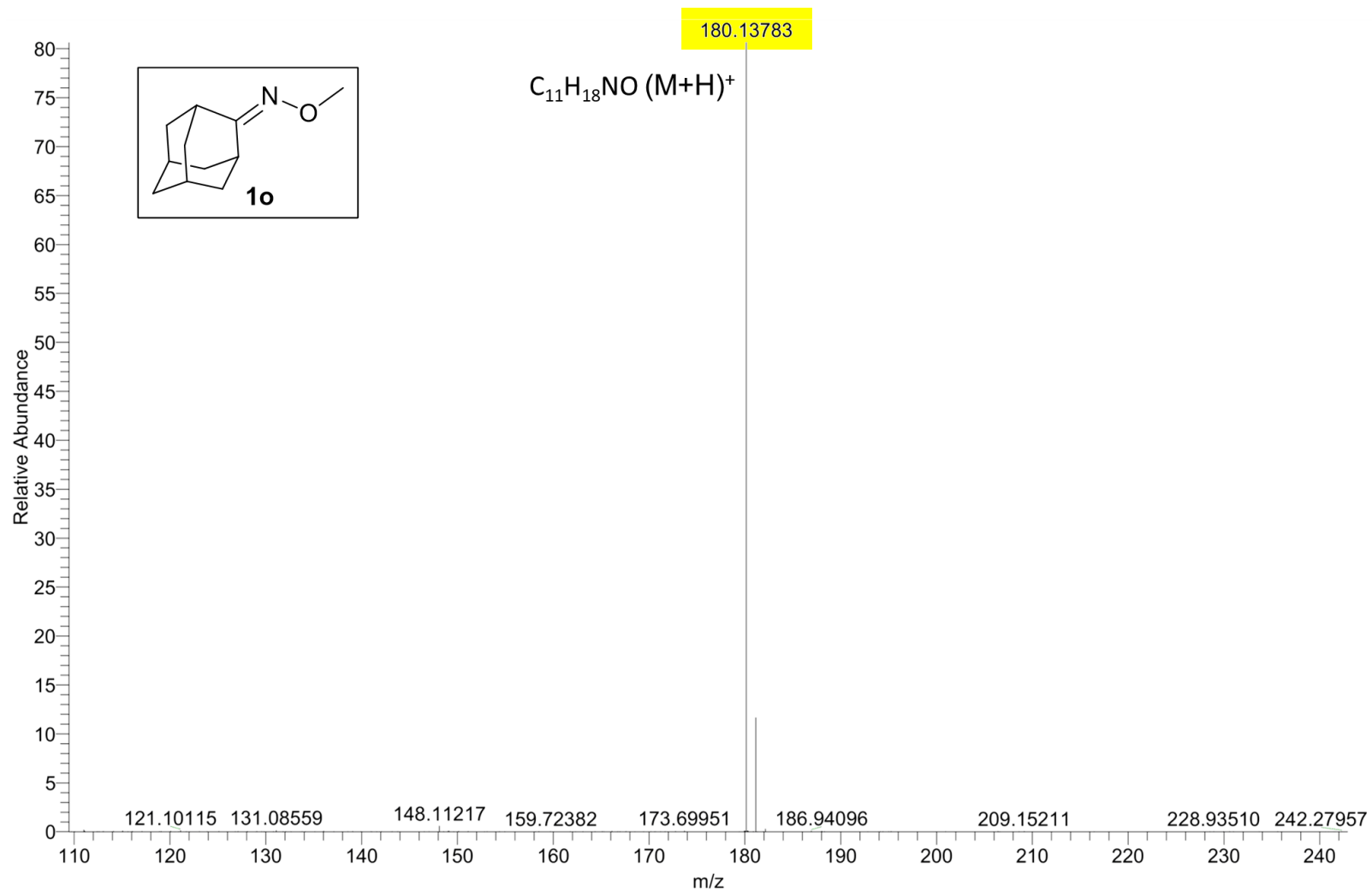


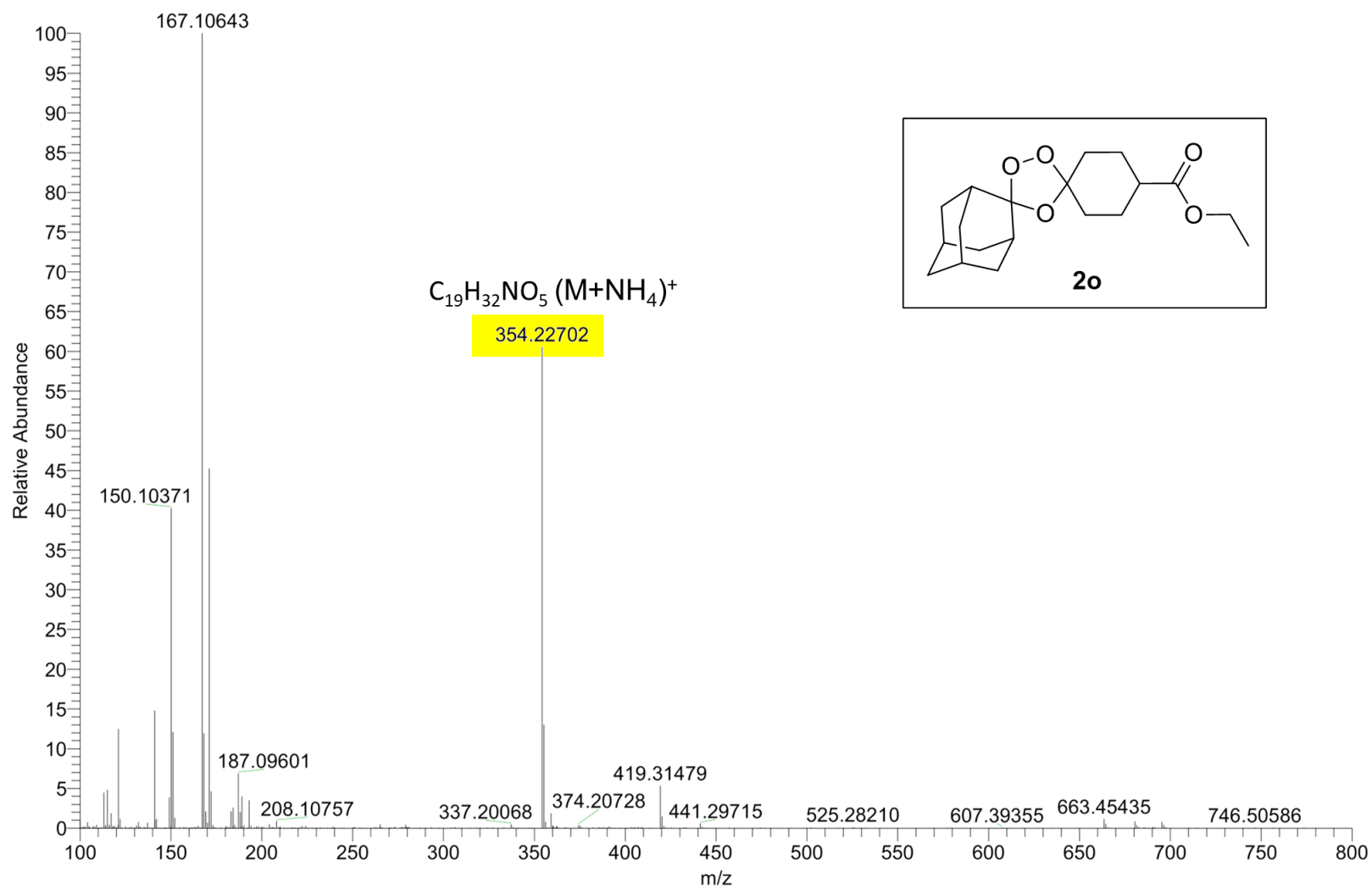
Figure S49. ^1H NMR spectrum (500 MHz) of **T2•HCl** in $\text{DMSO-}d_6$.

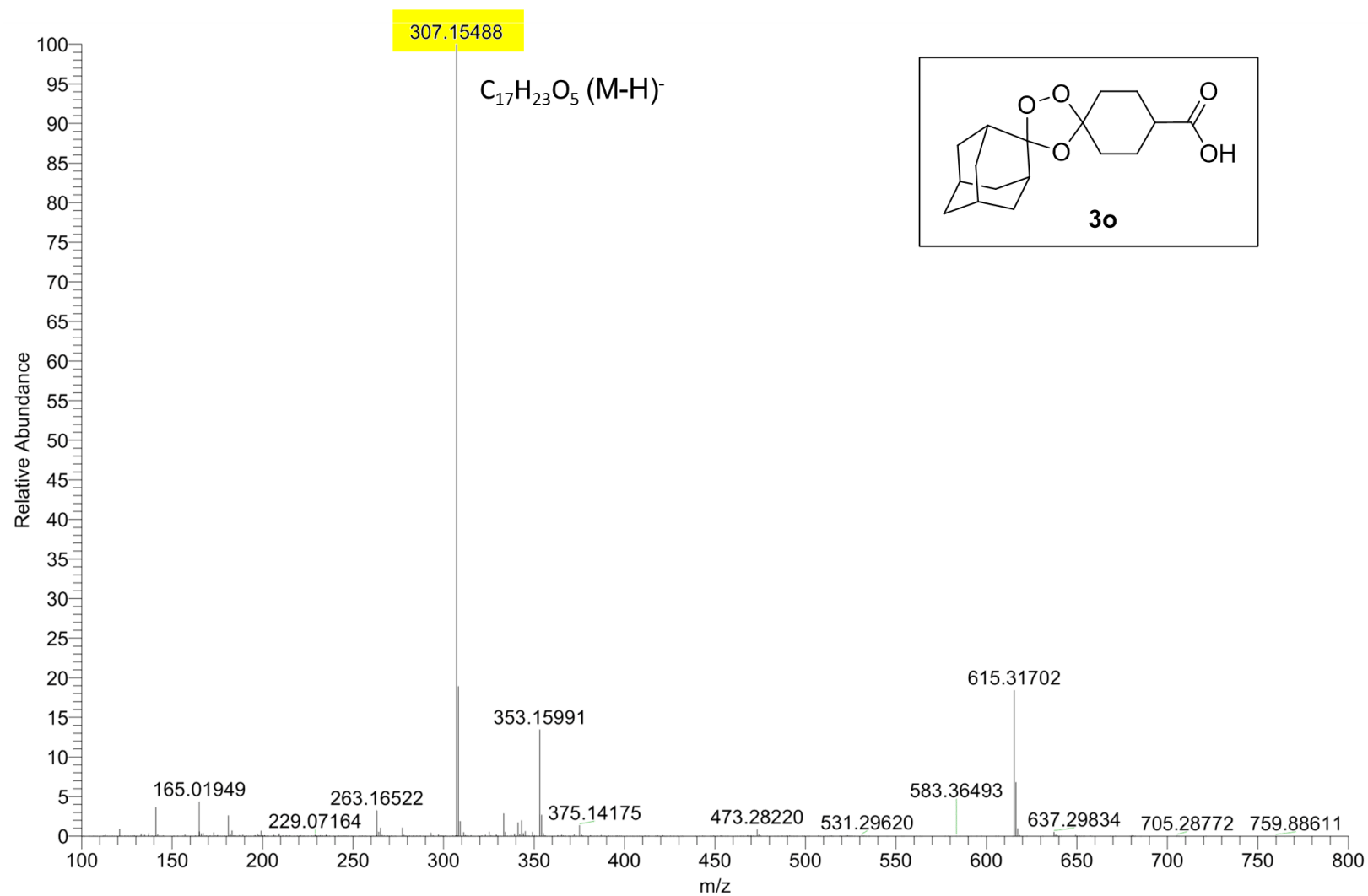
S2. HRMS spectra of the synthesised compounds

Electrospray ionization mass spectrum in positive-ion mode (HRMS-ESI⁺) of **compound 1o**

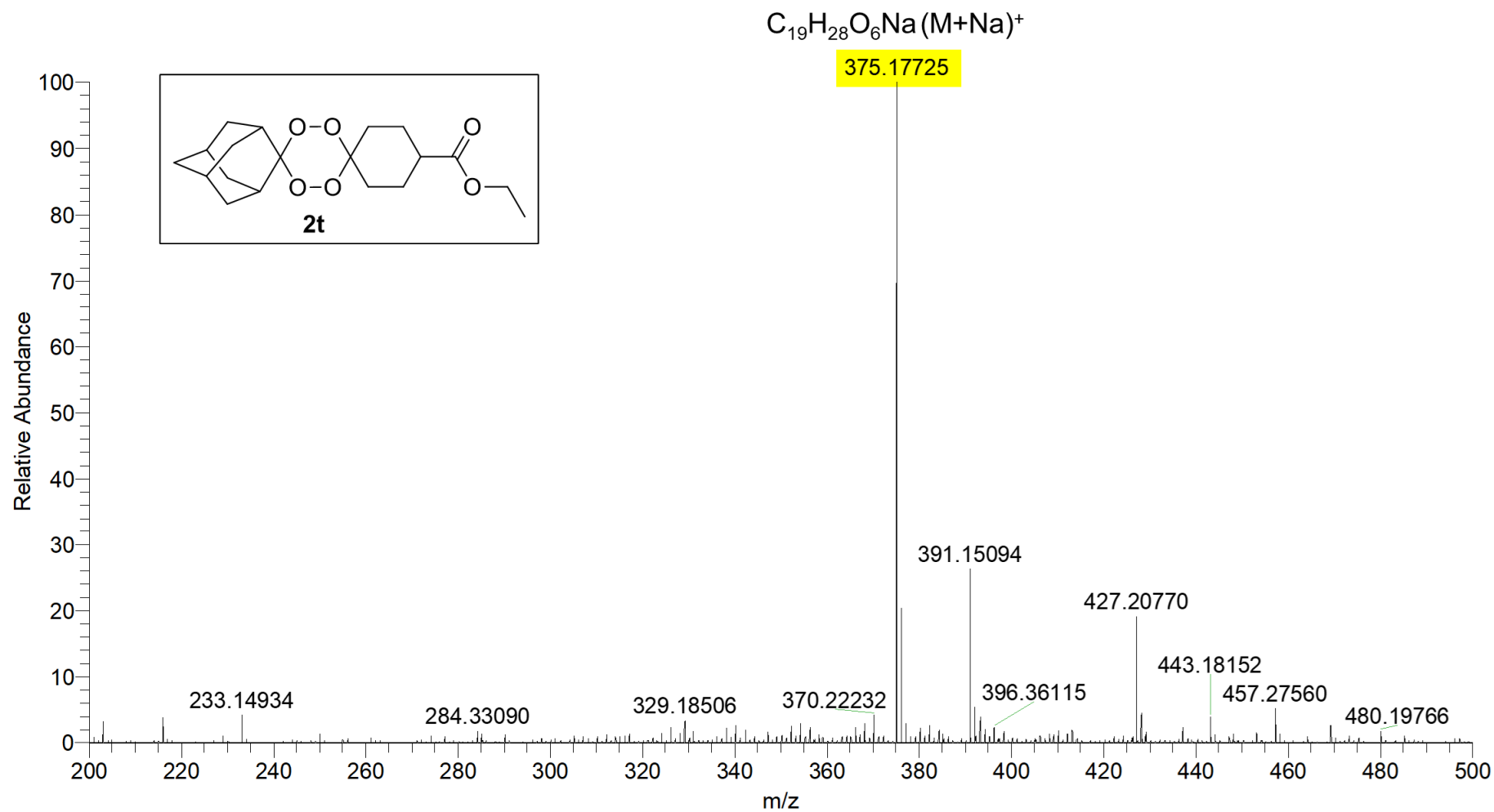


Electrospray ionization mass spectrum in positive-ion mode (HRMS-ESI⁺) of **compound 2o**

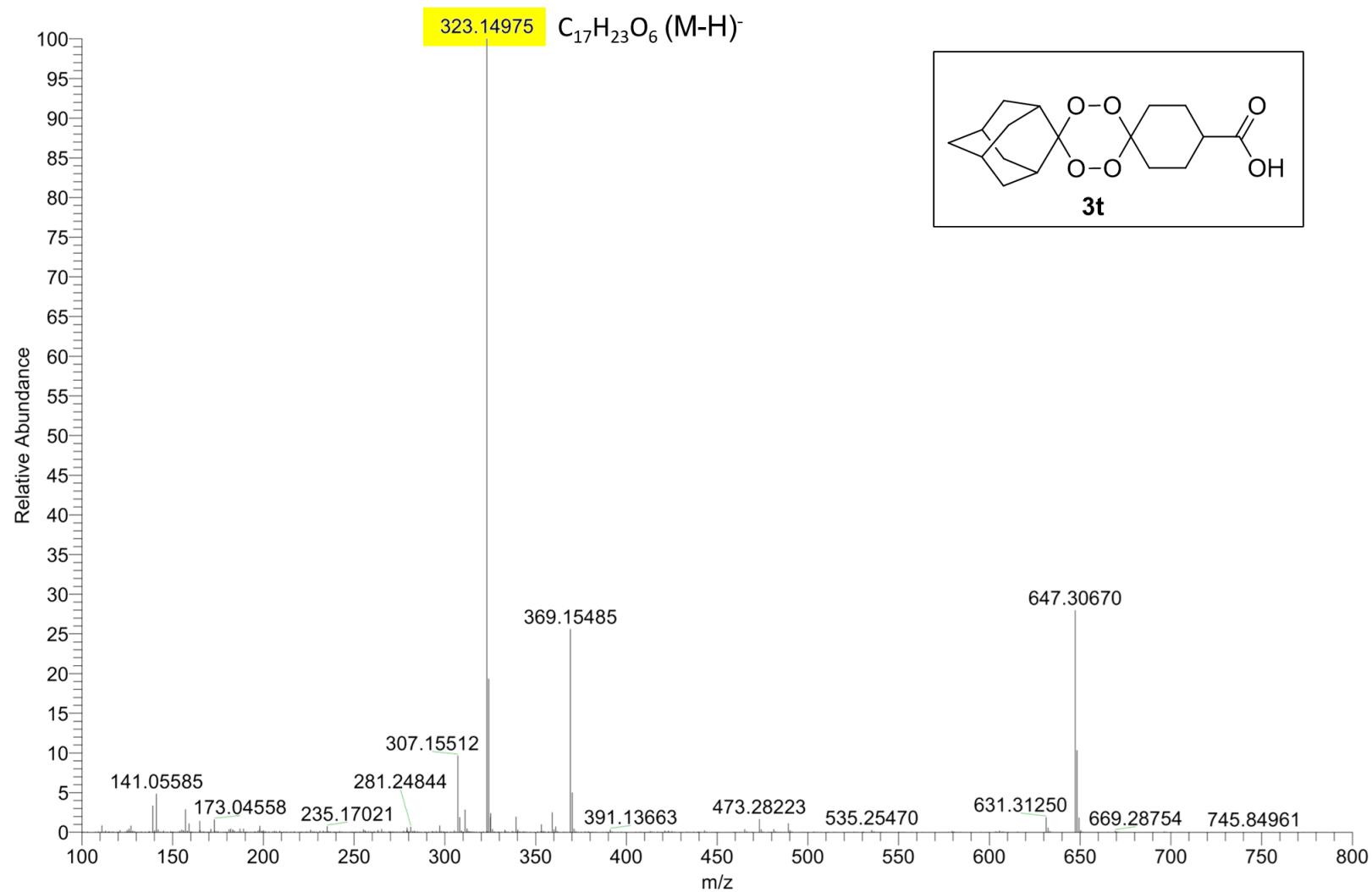


Electrospray ionization mass spectrum in negative-ion mode (HRMS-ESI) of **compound 3o**

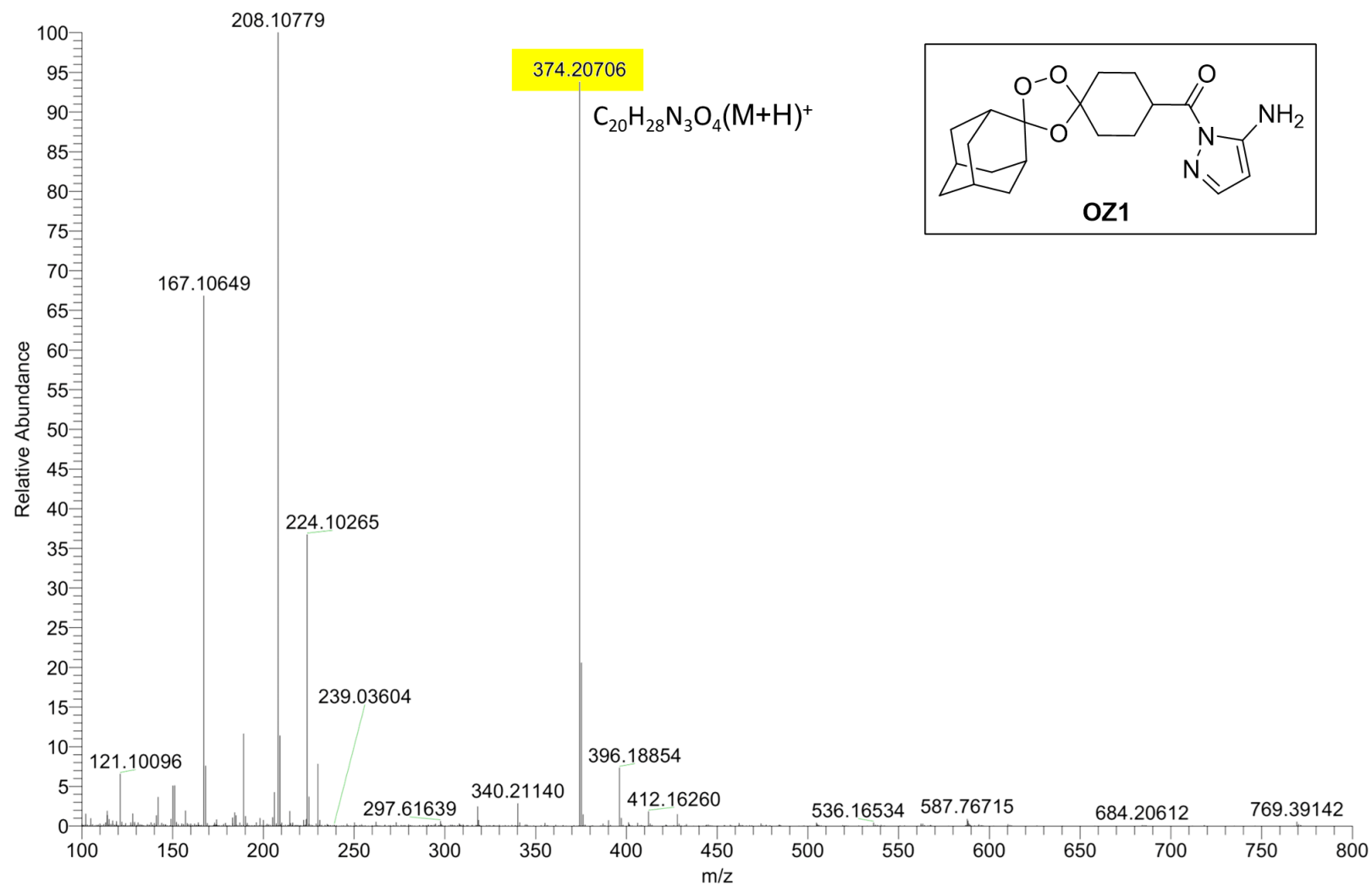
Electrospray ionization mass spectrum in positive-ion mode (HRMS-ESI⁺) of **compound 2t**



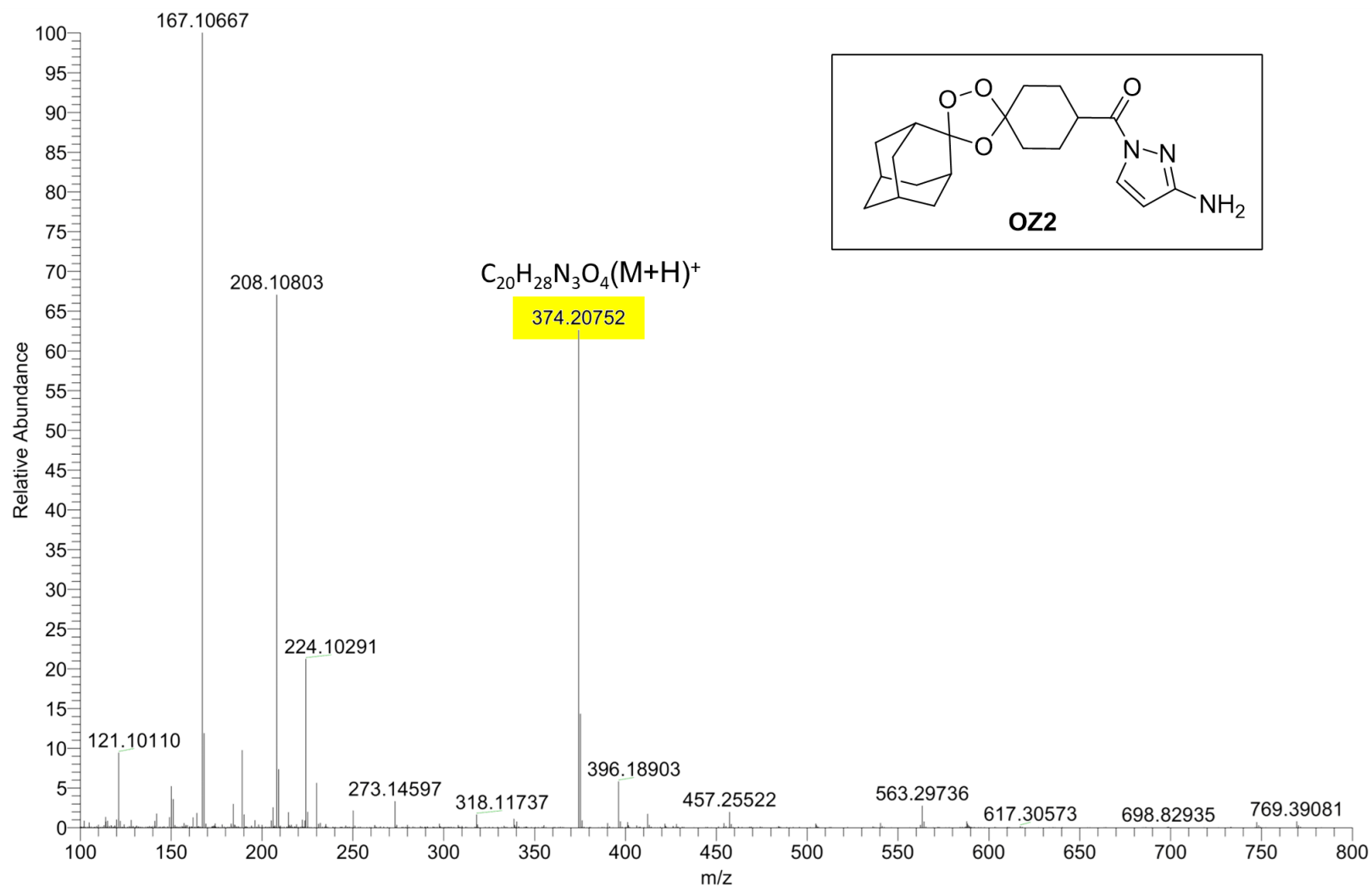
Electrospray ionization mass spectrum in negative-ion mode (HRMS-ESI) of **compound 3t**



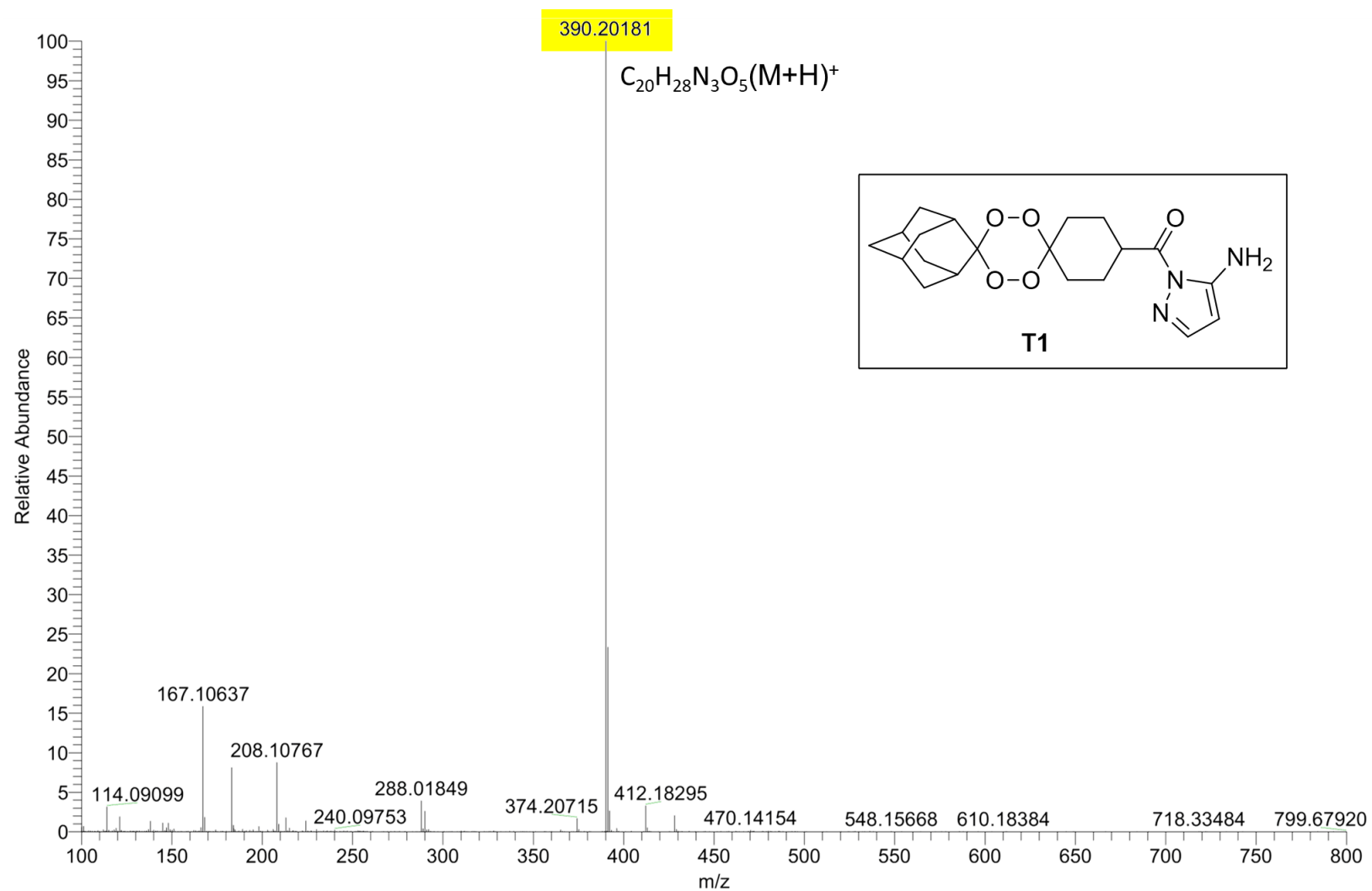
Electrospray ionization mass spectrum in positive-ion mode (HRMS-ESI⁺) of **compound OZ1**



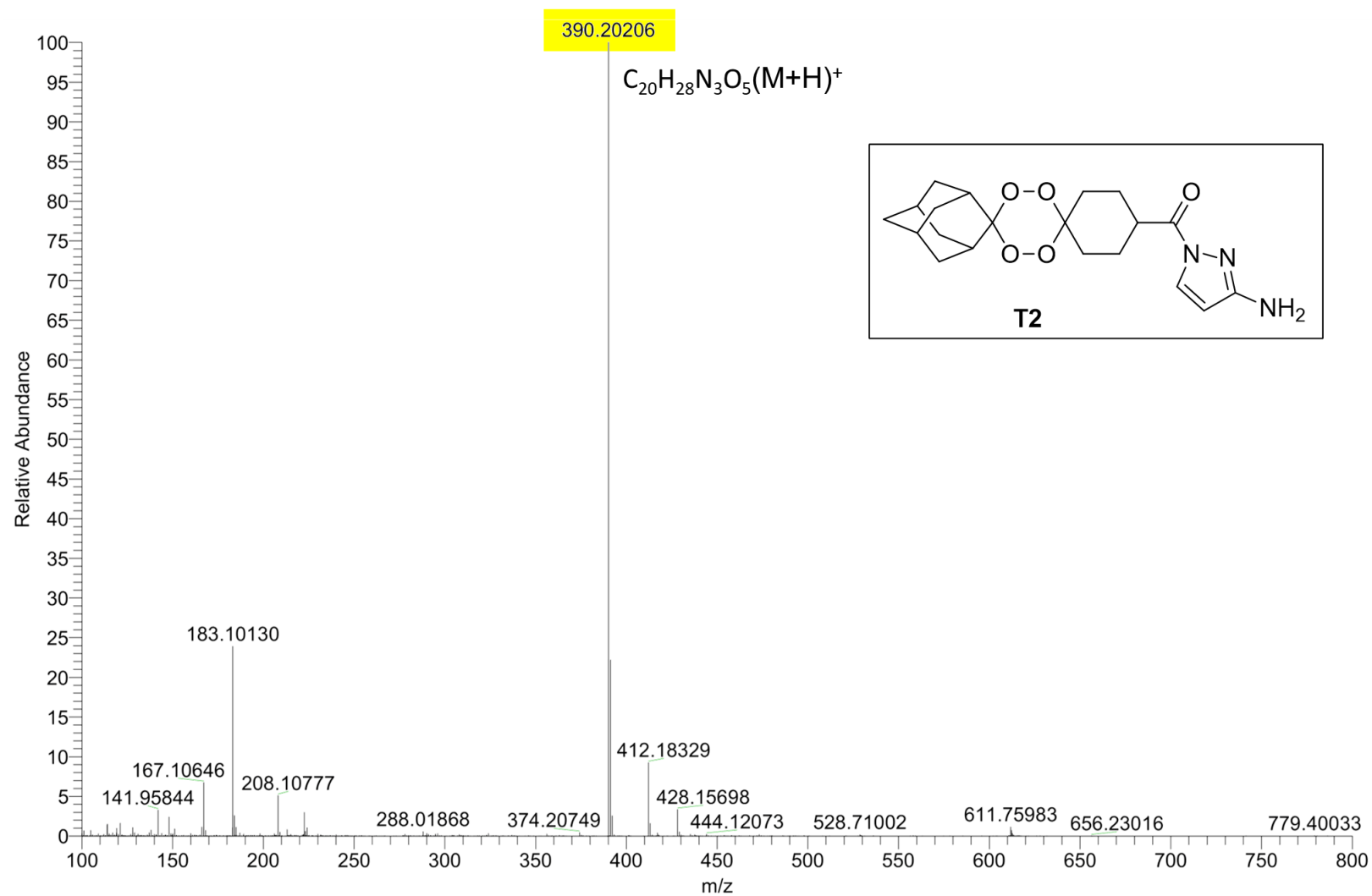
Electrospray ionization mass spectrum in positive-ion mode (HRMS-ESI⁺) of **compound OZ2**



Electrospray ionization mass spectrum in positive-ion mode (HRMS-ESI⁺) of **compound T1**



Electrospray ionization mass spectrum in positive-ion mode (HRMS-ESI⁺) of **compound T2**



S3. X-ray crystallography

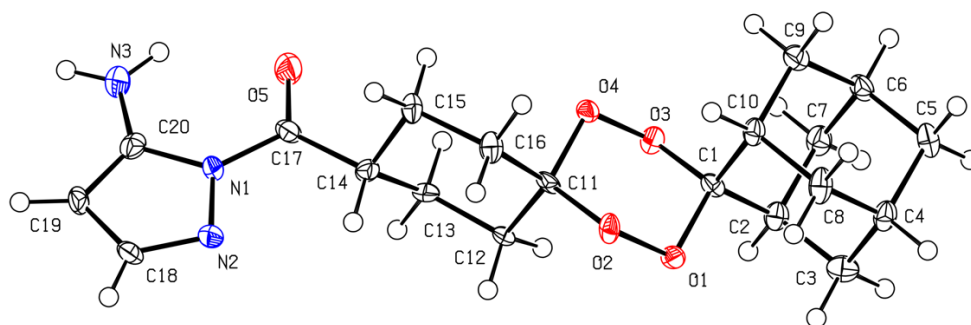


Figure S50. ORTEP drawing of the molecule of (5-amino-1*H*-pyrazol-1-yl) (dispiro[cyclohexane-1,3'-[1,2,4,5]tetraoxane-6',2''-tricyclo[3.3.1.1^{3,7}]decan]-4-yl)-methanone (**T1**). Displacement ellipsoids are drawn at the 50% probability level.

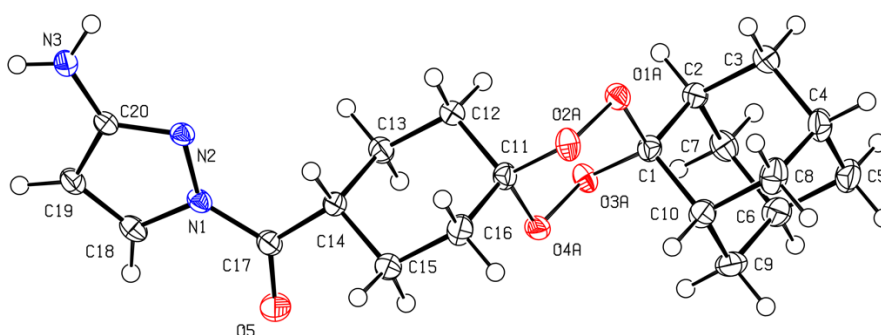


Figure S51. ORTEP drawing of the molecule of (3-amino-1*H*-pyrazol-1-yl) (dispiro[cyclohexane-1,3'-[1,2,4,5]tetraoxane-6',2''-tricyclo[3.3.1.1^{3,7}]decan]-4-yl)-methanone (**T2**). Displacement ellipsoids are drawn at the 50% probability level. The tetraoxane group has minor disorder over two alternate chair conformations; for the sake of clarity, only the major conformation is shown.

CIF files containing supplementary crystallographic data were deposited at the Cambridge Crystallographic Data Centre with references 2151742 (**T1**) and 2151175 (**T2**).