

Supplementary Materials: Eremophilane Sesquiterpenes from a Deep Marine-Derived Fungus, *Aspergillus* sp. SCSIOW2, Cultivated in the Presence of Epigenetic Modifying Agents

Liyan Wang, Mengjie Li, Jianqiang Tang and Xiaofan Li

Table S1. Conformer distribution of 1 in solvated models (methanol) calculation at the B3LYP/aug-cc-PVDZ level.

Conformers	Contribution %
1	26.05
2	19.17
3	19.17
4	14.77
5	6.69
6	5.01
7	4.03
8	2.25
9	2.25
10	0.61

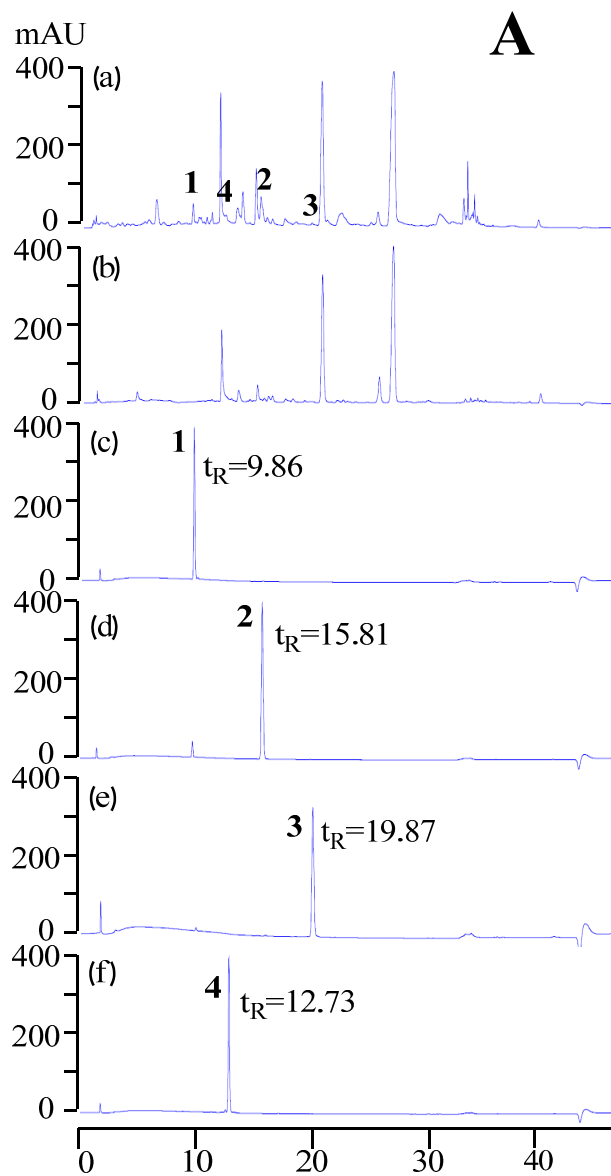


Figure S1. Cont.

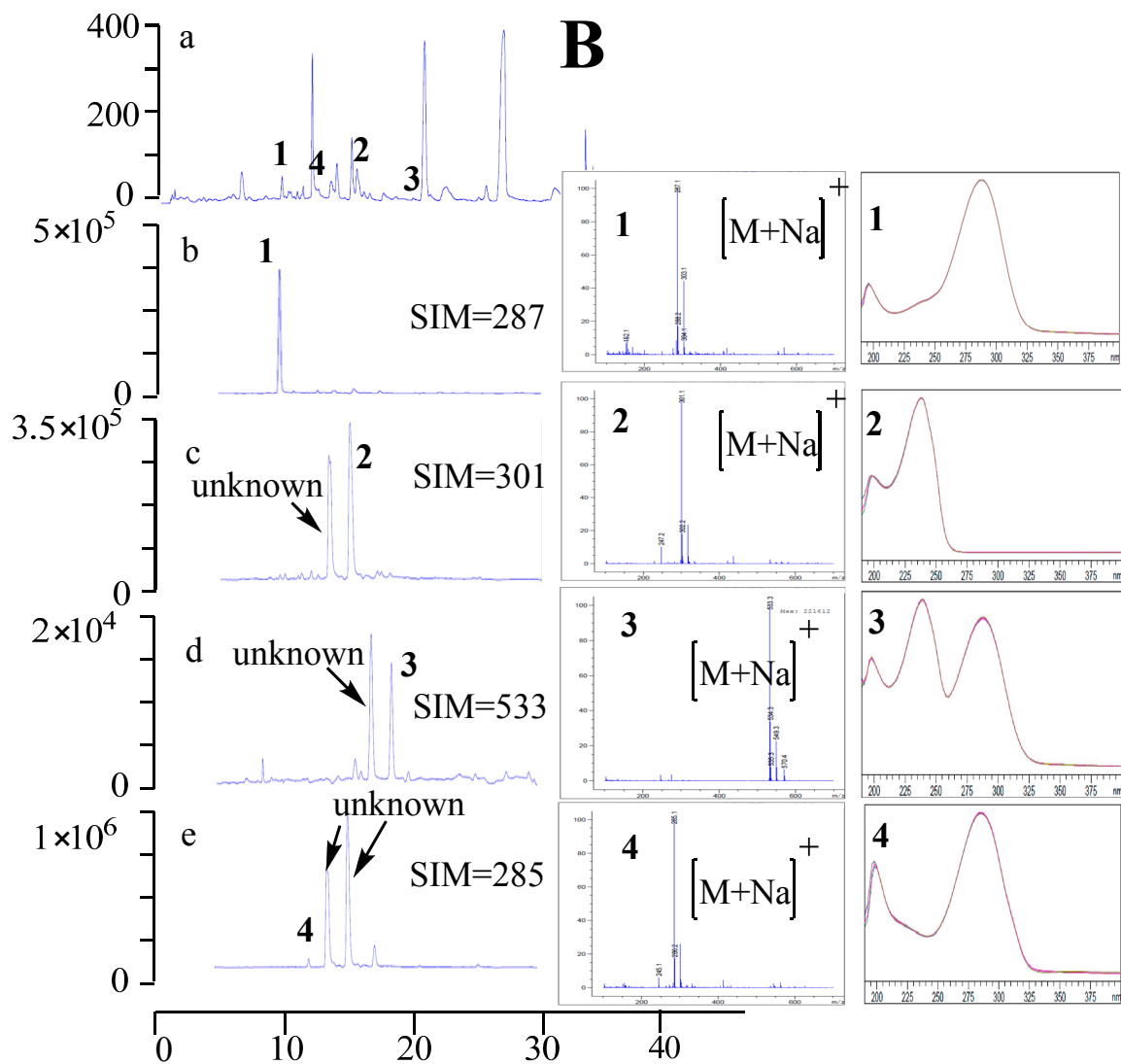


Figure S1. Cont.

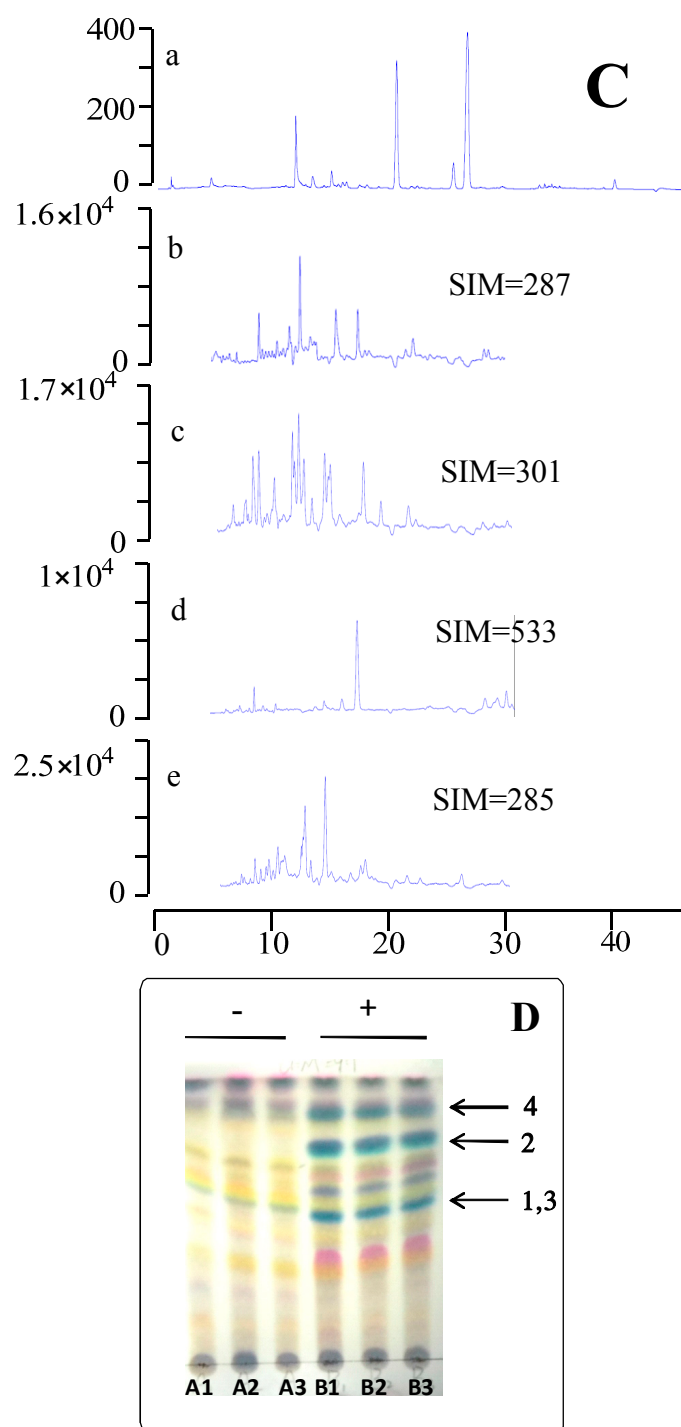


Figure S1. Effects of SBHA and 5-AZA on secondary metabolites (SMs) production by *Aspergillus* sp. SCSiOW2. SMs were extracted from one week cultures with (+) or without (-) 1 mM SBHA and 1 mM 5-AZA. (A) HPLC analyses [(a) = +; (b) = -; (c-f) = standards of 1-4]; Effects of SBHA and 5-AZA on secondary metabolites (SMs) production by *Aspergillus* sp. SCSiOW2. SMs were extracted from one week cultures with (+) or without (-) 1 mM SBHA and 1 mM 5-AZA. (B) LCMS analyses of samples with epigenetic modifiers. (a) = HPLC of +; (b-e) = SIM287, 301, 533, 285; Effects of SBHA and 5-AZA on secondary metabolites (SMs) production by *Aspergillus* sp. SCSiOW2. SMs were extracted from one week cultures with (+) or without (-) 1 mM SBHA and 1mM 5-AZA. (C) LCMS analyses of samples without epigenetic modifiers. (a) = HPLC of -; (b-e) = SIM287, 301, 533, 285; Effects of SBHA and 5-AZA on secondary metabolites (SMs) production by *Aspergillus* sp. SCSiOW2. SMs were extracted from one week cultures with (+) or without (-) 1 mM SBHA and 1mM 5-AZA. (D) TLC analysis.

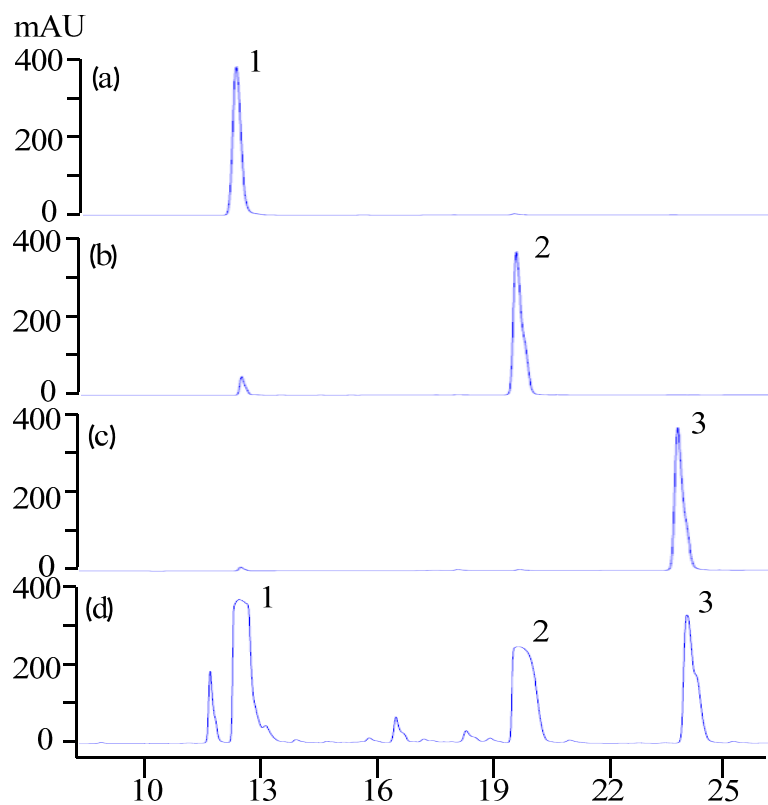


Figure S2. HPLC analysis of **1** (a), **2** (b) and **3** (c), and profile of **1** changed to **2** and **3** after storage for 1 week in MeOH:H₂O (9:1) solution (d); HPLC was performed with a YMC Pack pro ODS C18 column (4.6 × 250 mm I.D. 5 μ) eluted with MeOH-H₂O (0:100–50:50 from 0 to 10 min; 50:50–80:20 from 10 to 20 min; 1.0 mL/min) with detection at 254 nm.

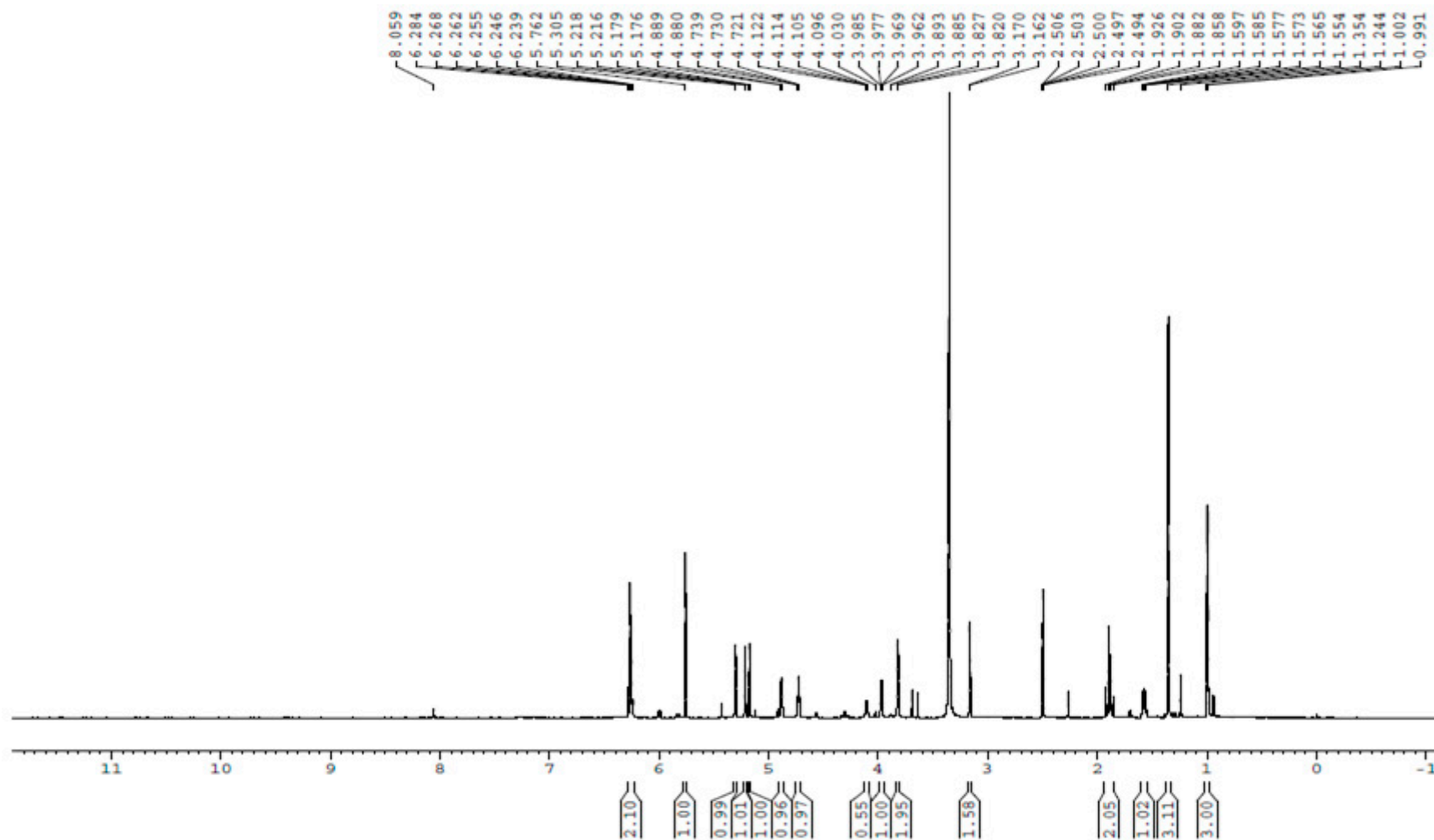


Figure S3. Cont.

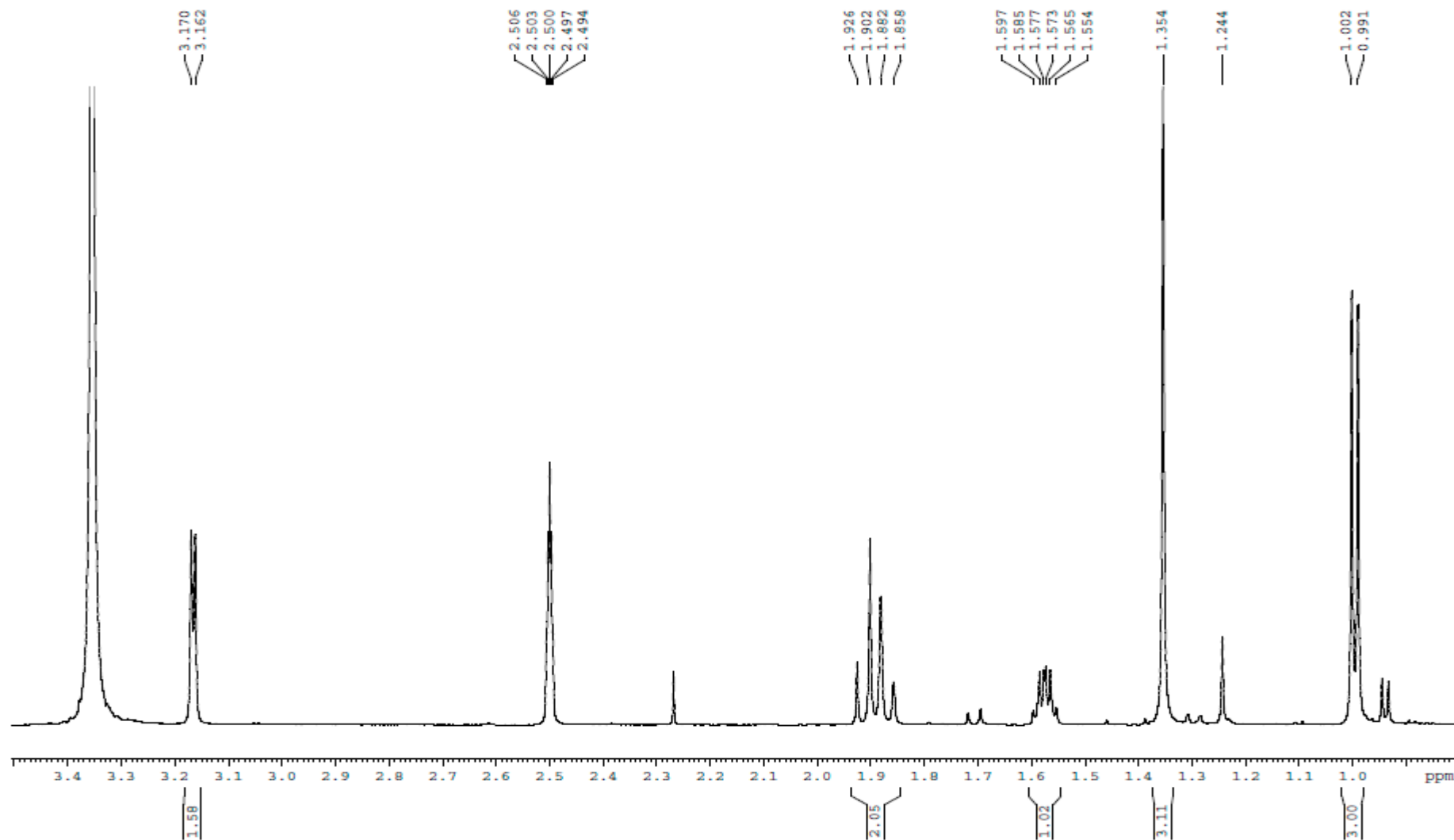


Figure S3. Cont.

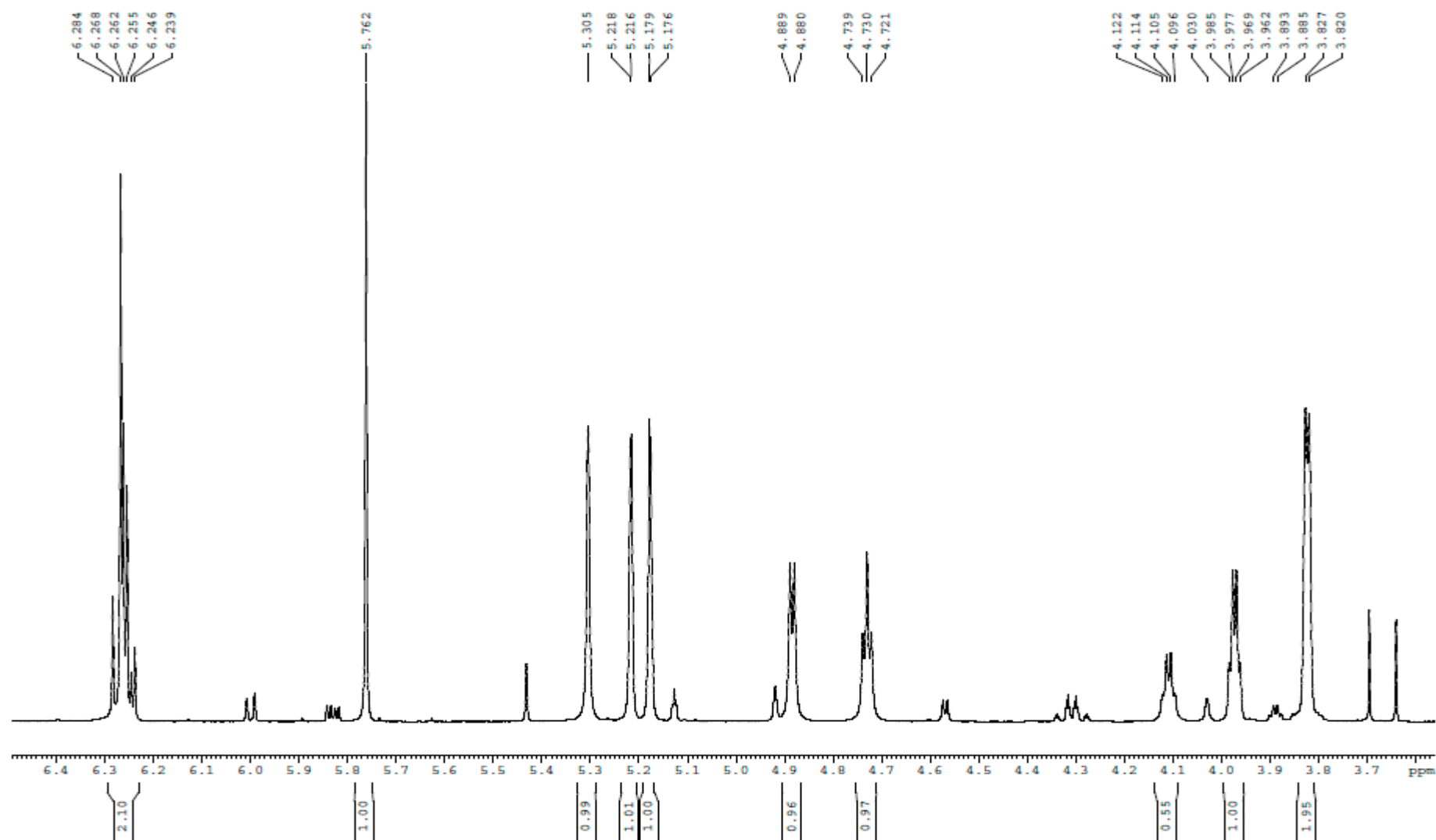


Figure S3. ¹H-NMR spectrum of 1 in DMSO-d₆.

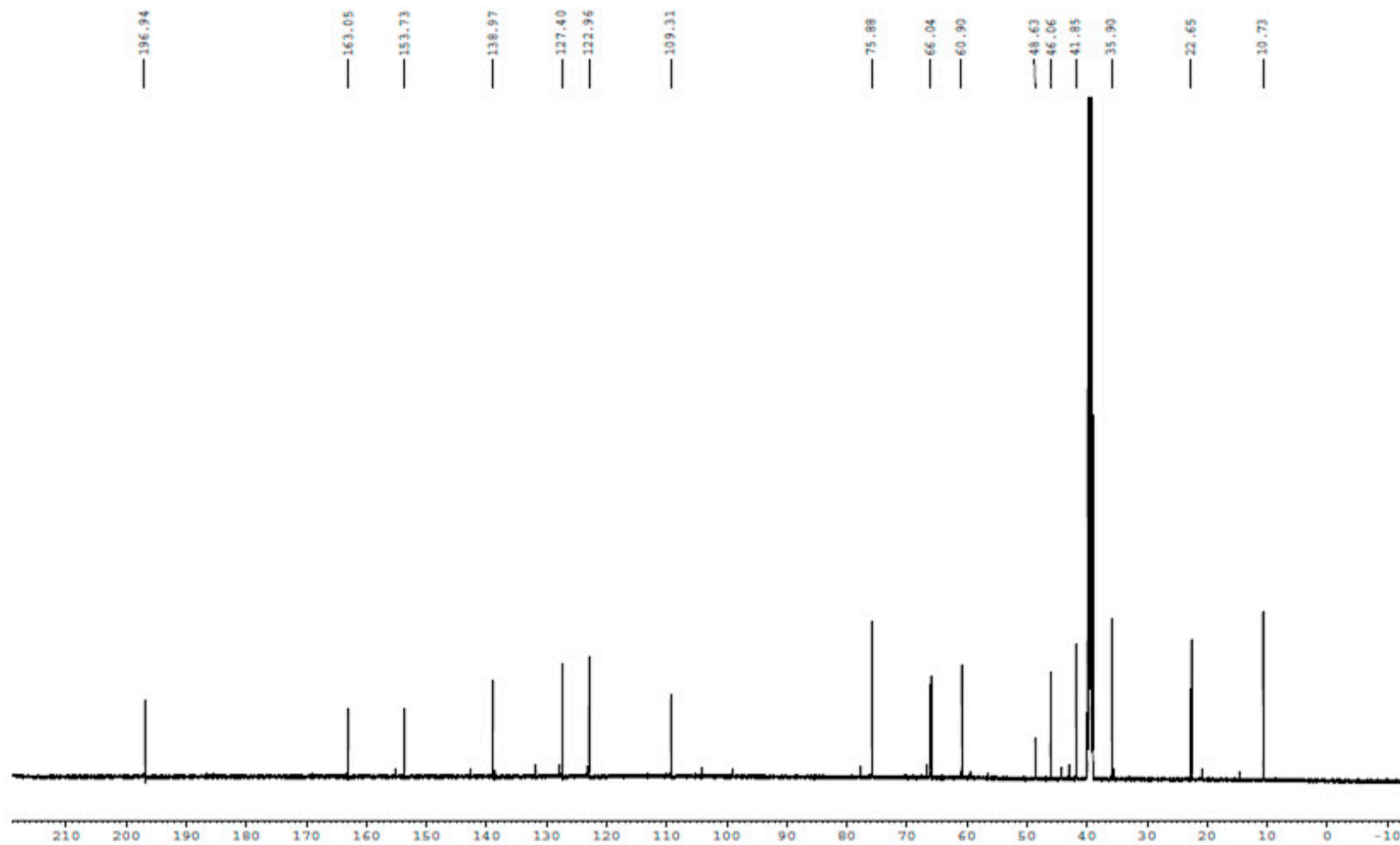


Figure S4. Cont.

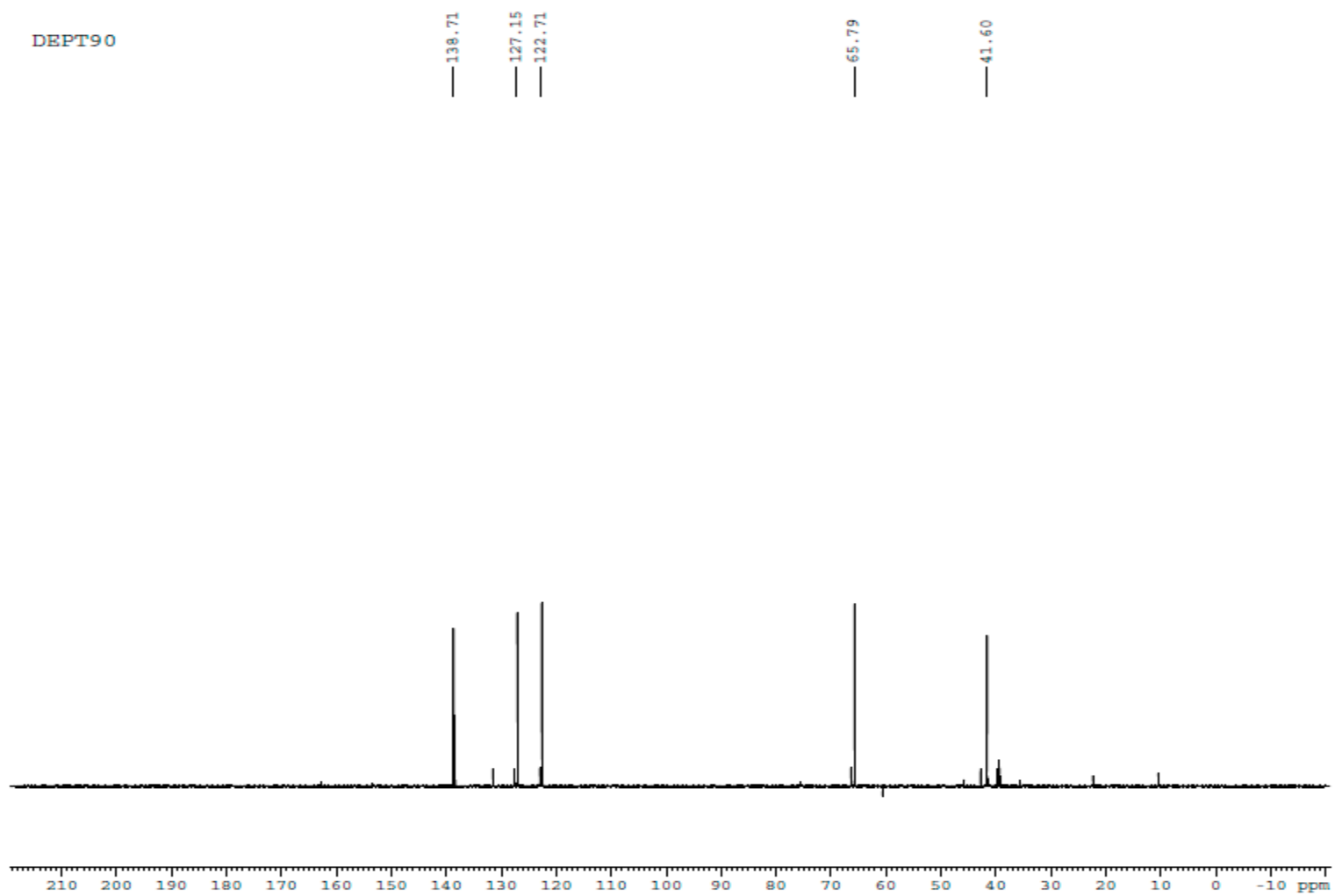


Figure S4. Cont.

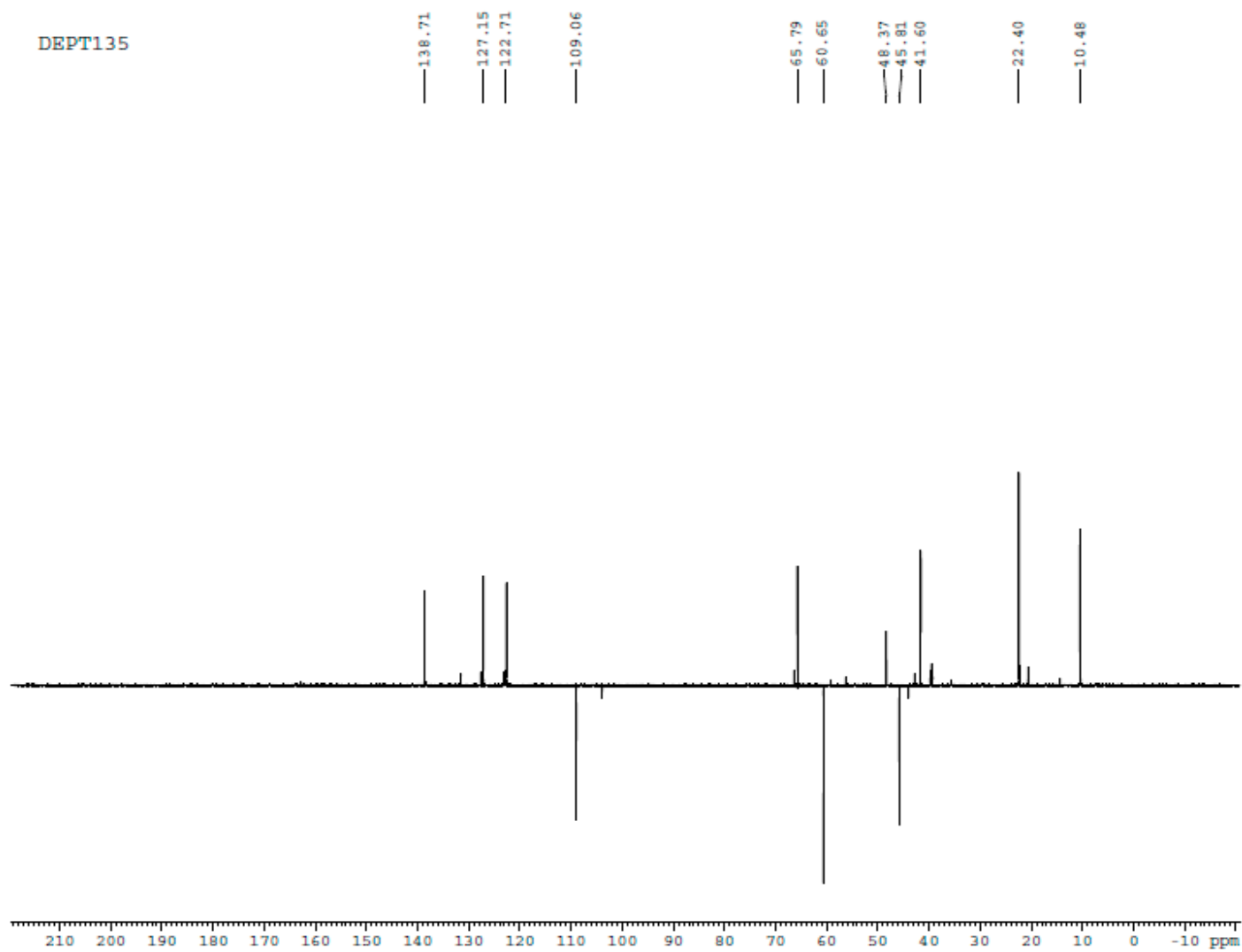


Figure S4. ^{13}C -NMR spectrum and DEPT of 1 in $\text{DMSO-}d_6$.

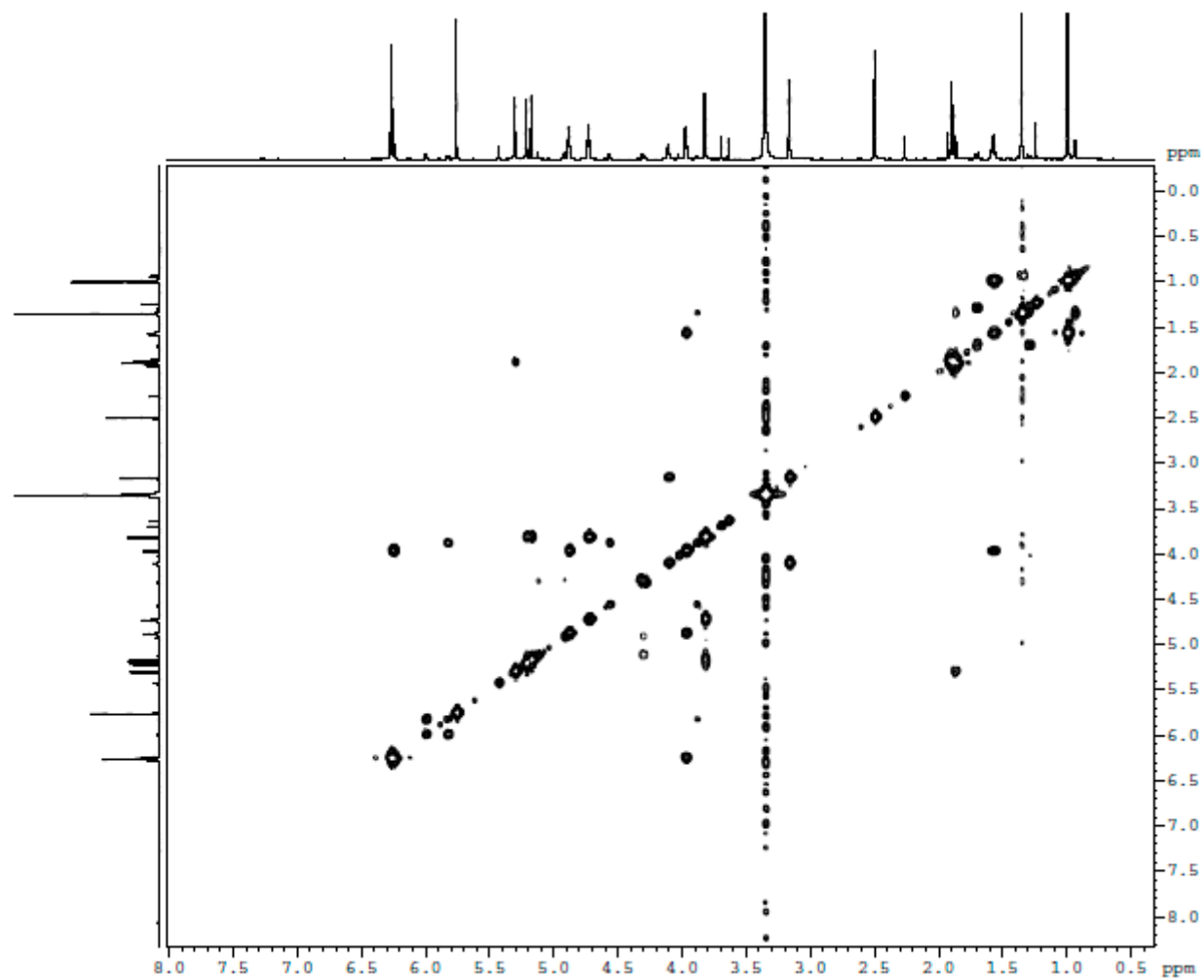


Figure S5. ^1H - ^1H COSY spectrum of 1 in $\text{DMSO-}d_6$.

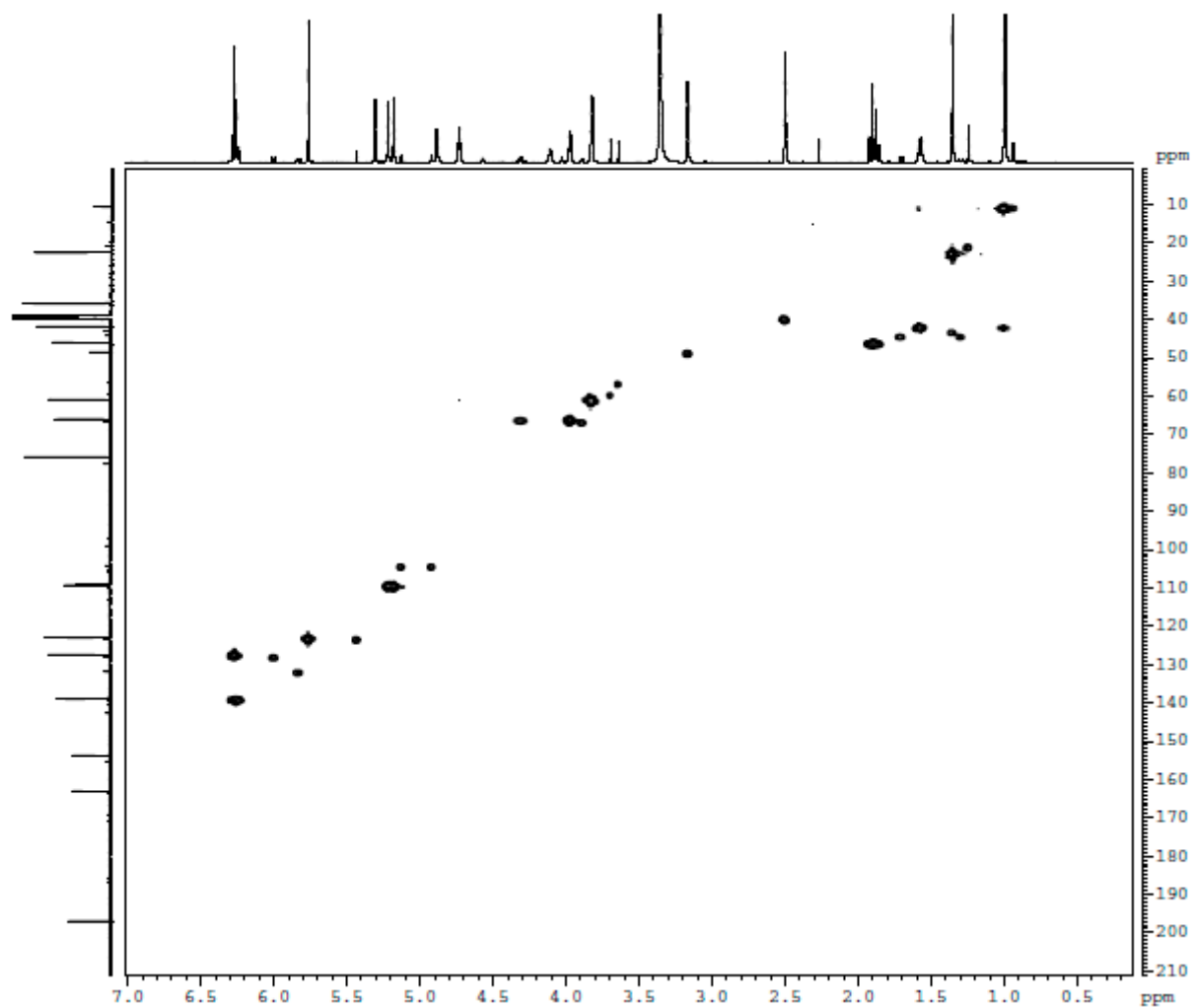


Figure S6. HSQC spectrum of 1 in DMSO-*d*₆.

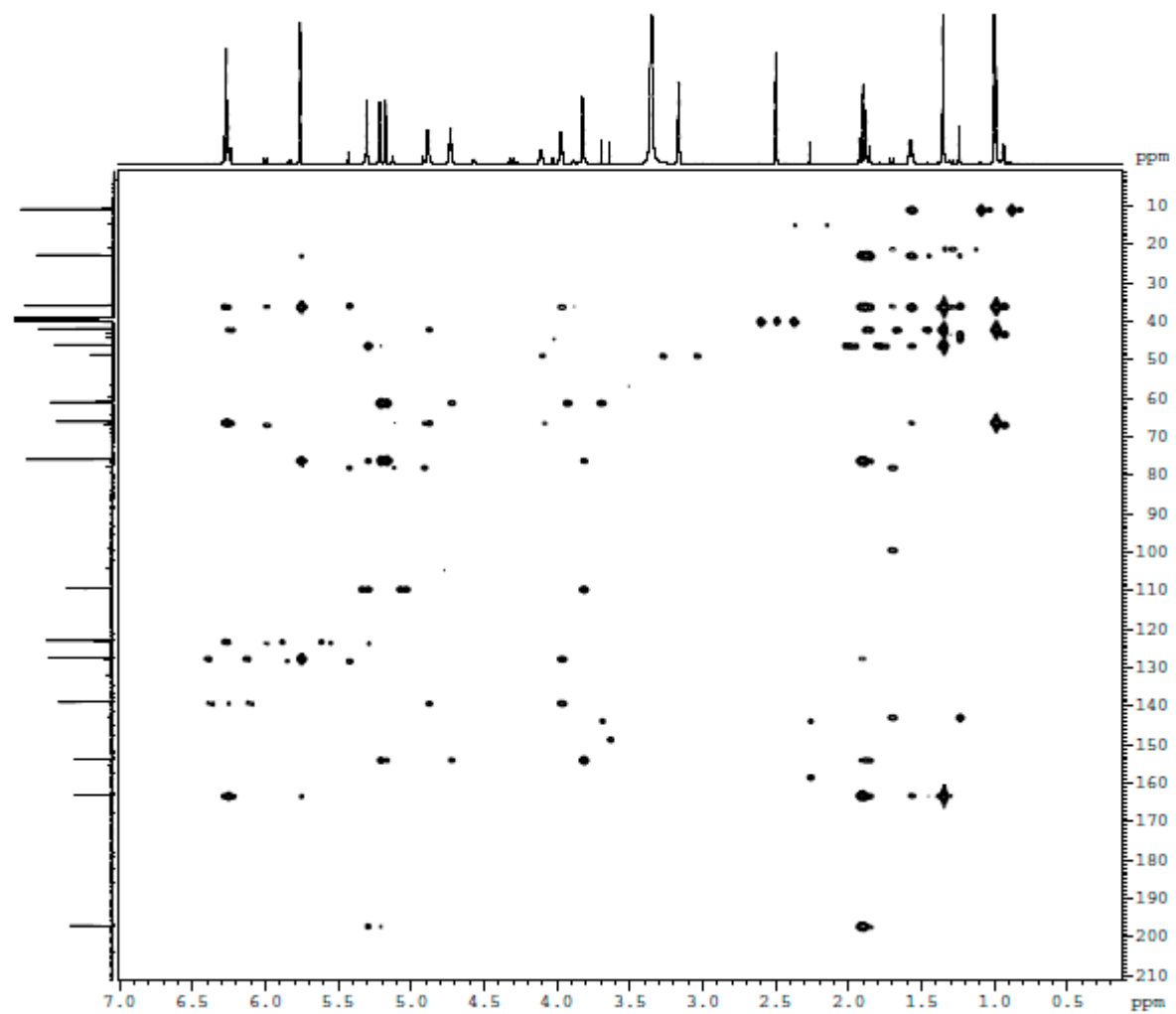


Figure S7. HMBC spectrum of 1 in DMSO-d₆.

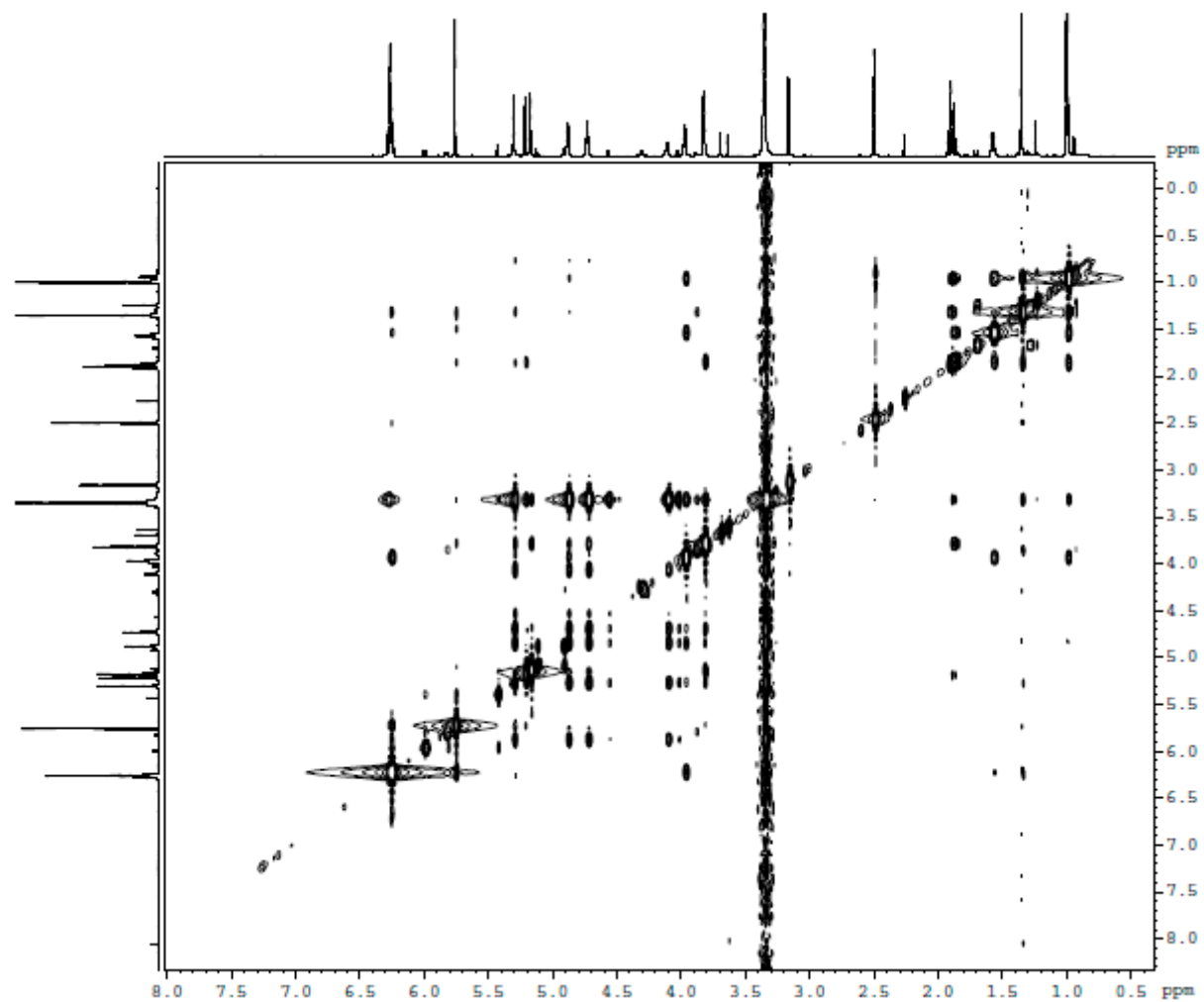


Figure S8. NOESY spectrum of 1 in DMSO-*d*₆.

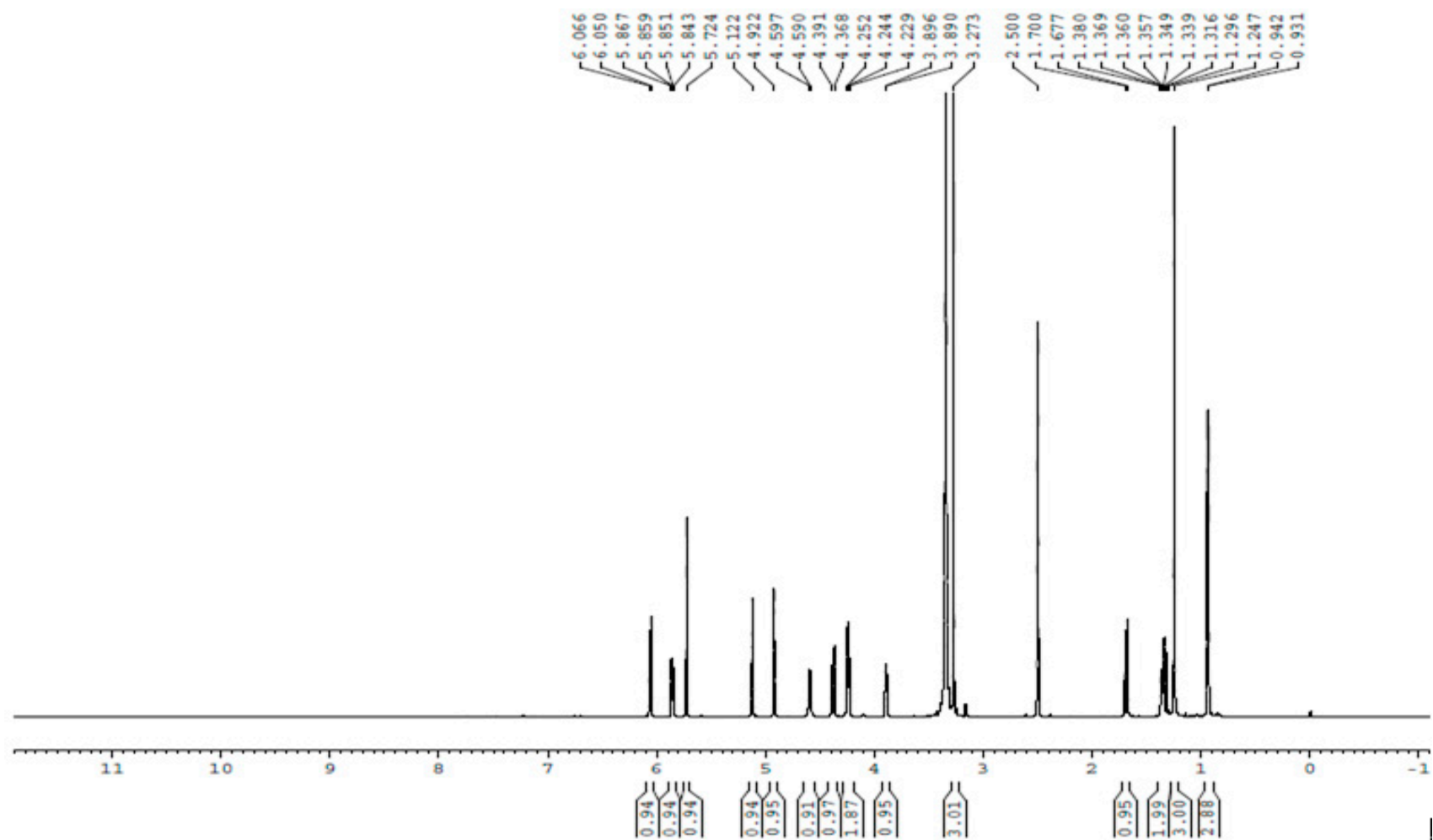


Figure S9. Cont.

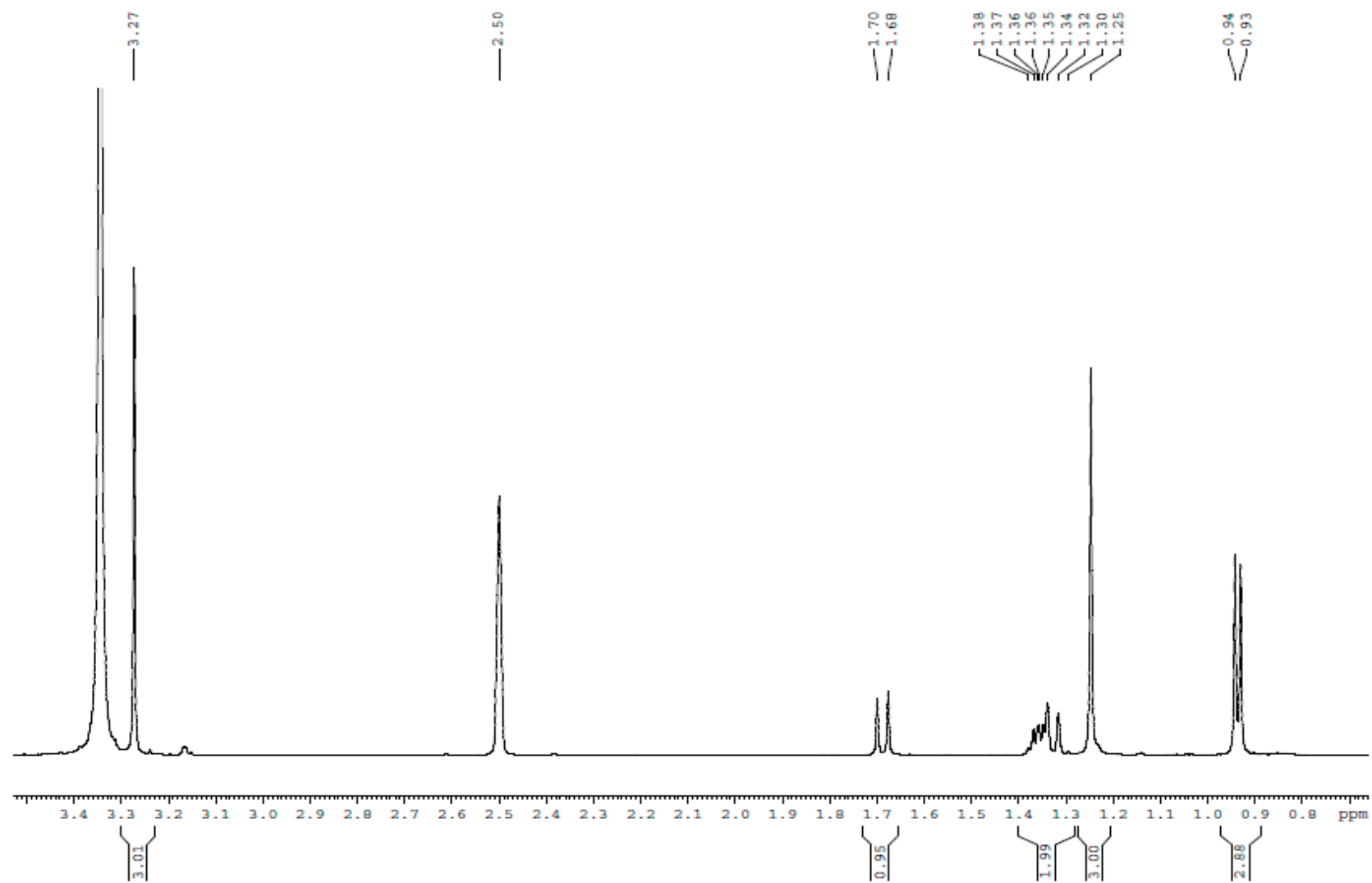


Figure S9. Cont.

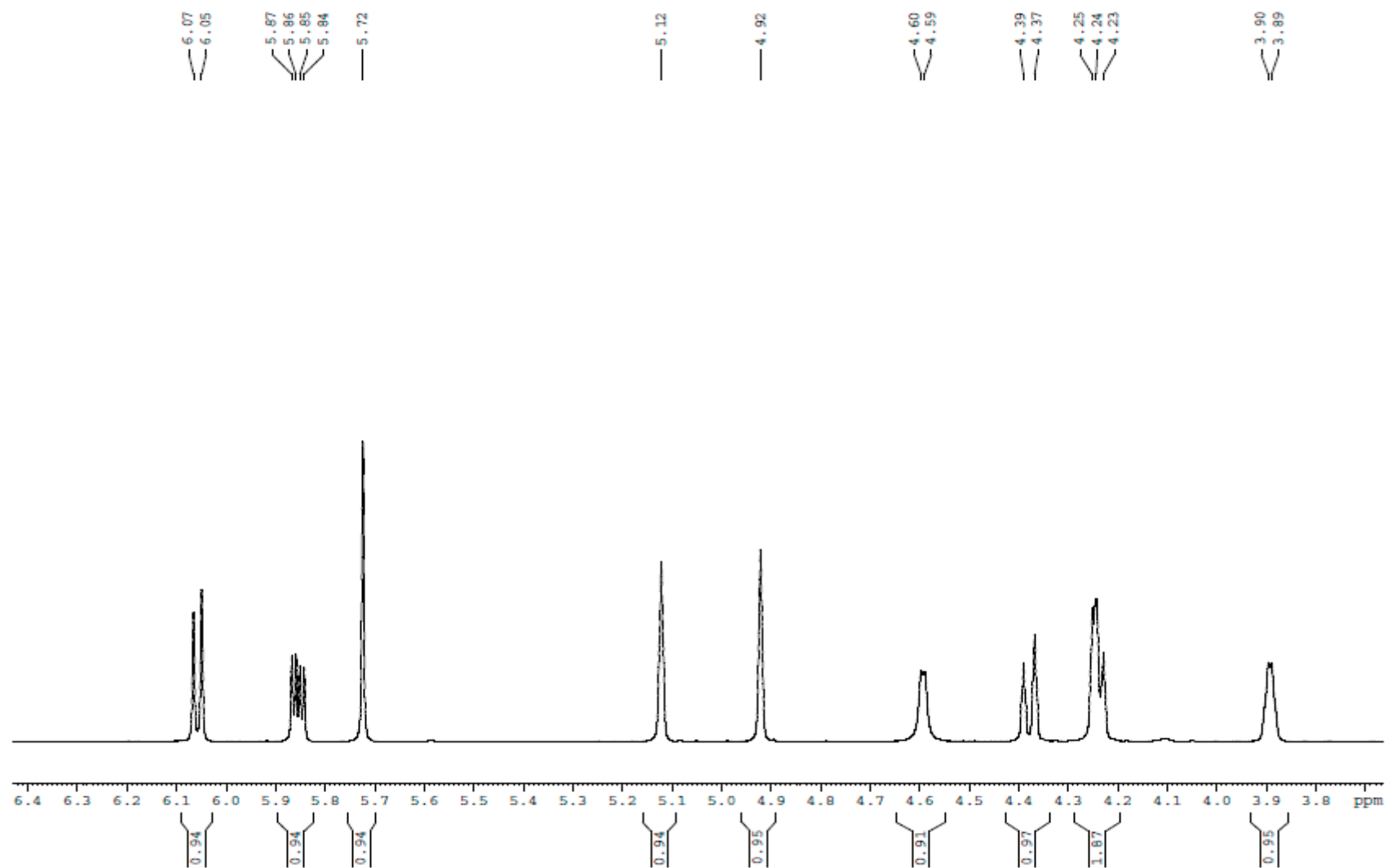


Figure S9. ¹H-NMR spectrum of 2 in DMSO-*d*₆.

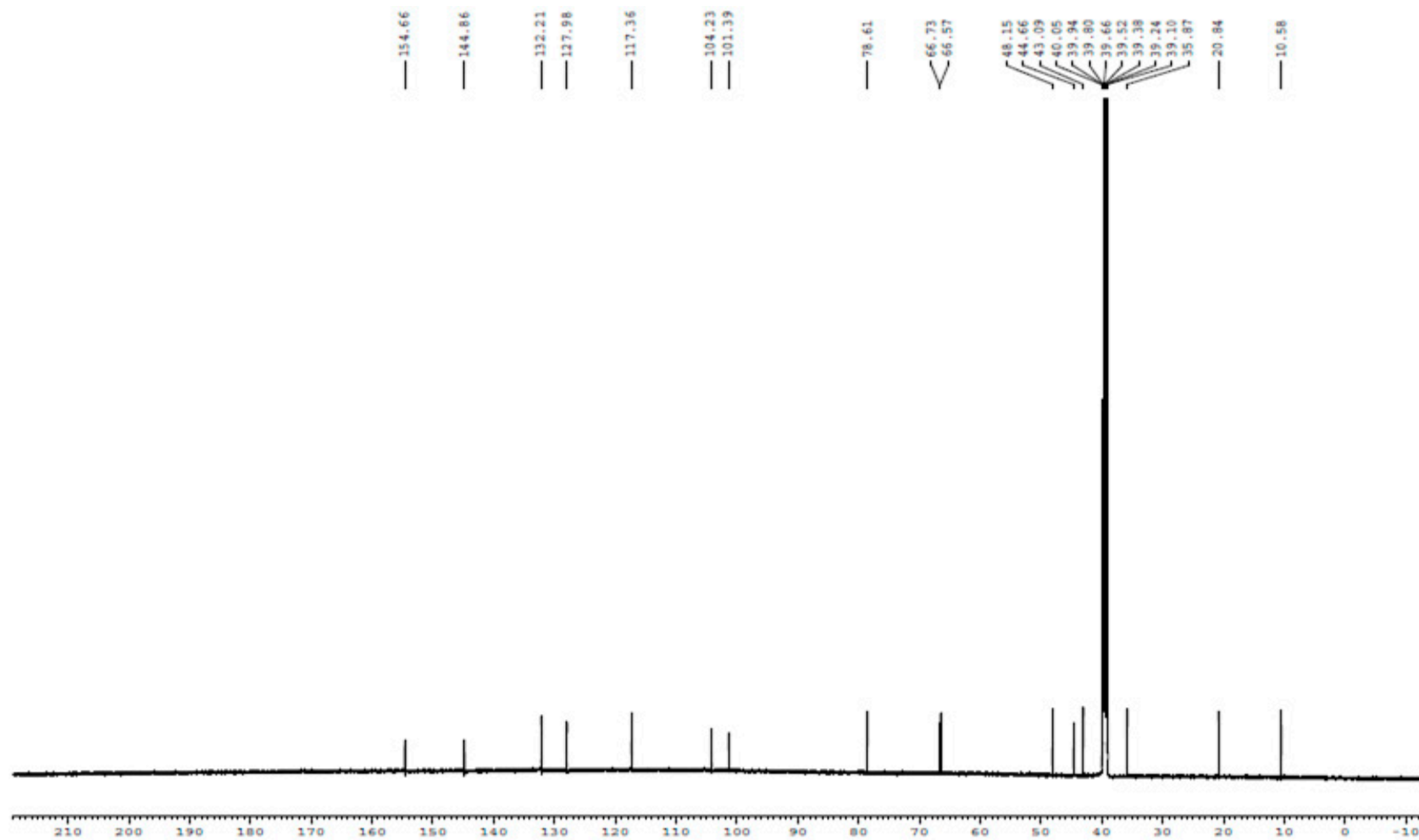


Figure S10. Cont.

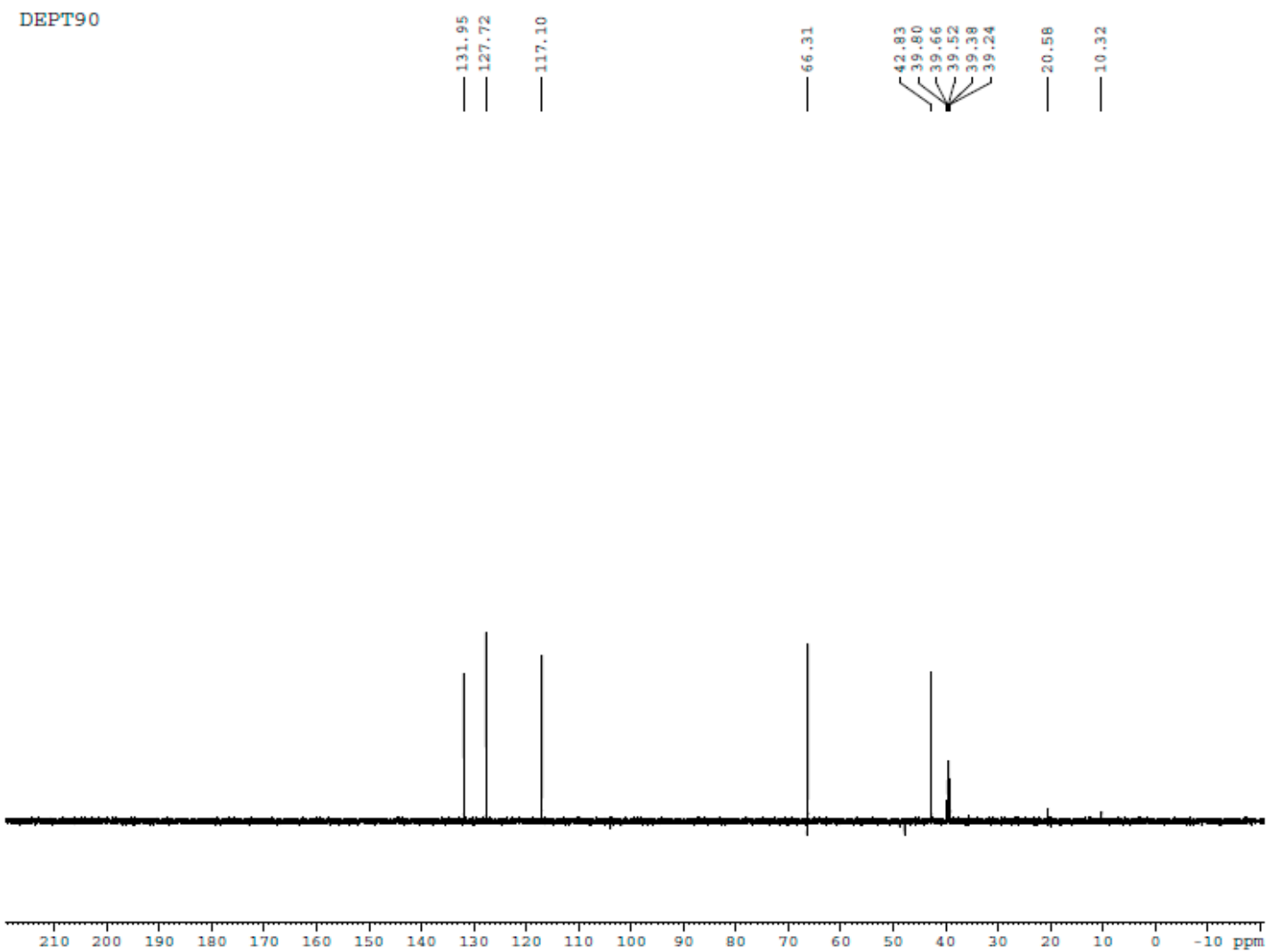


Figure S10. Cont.

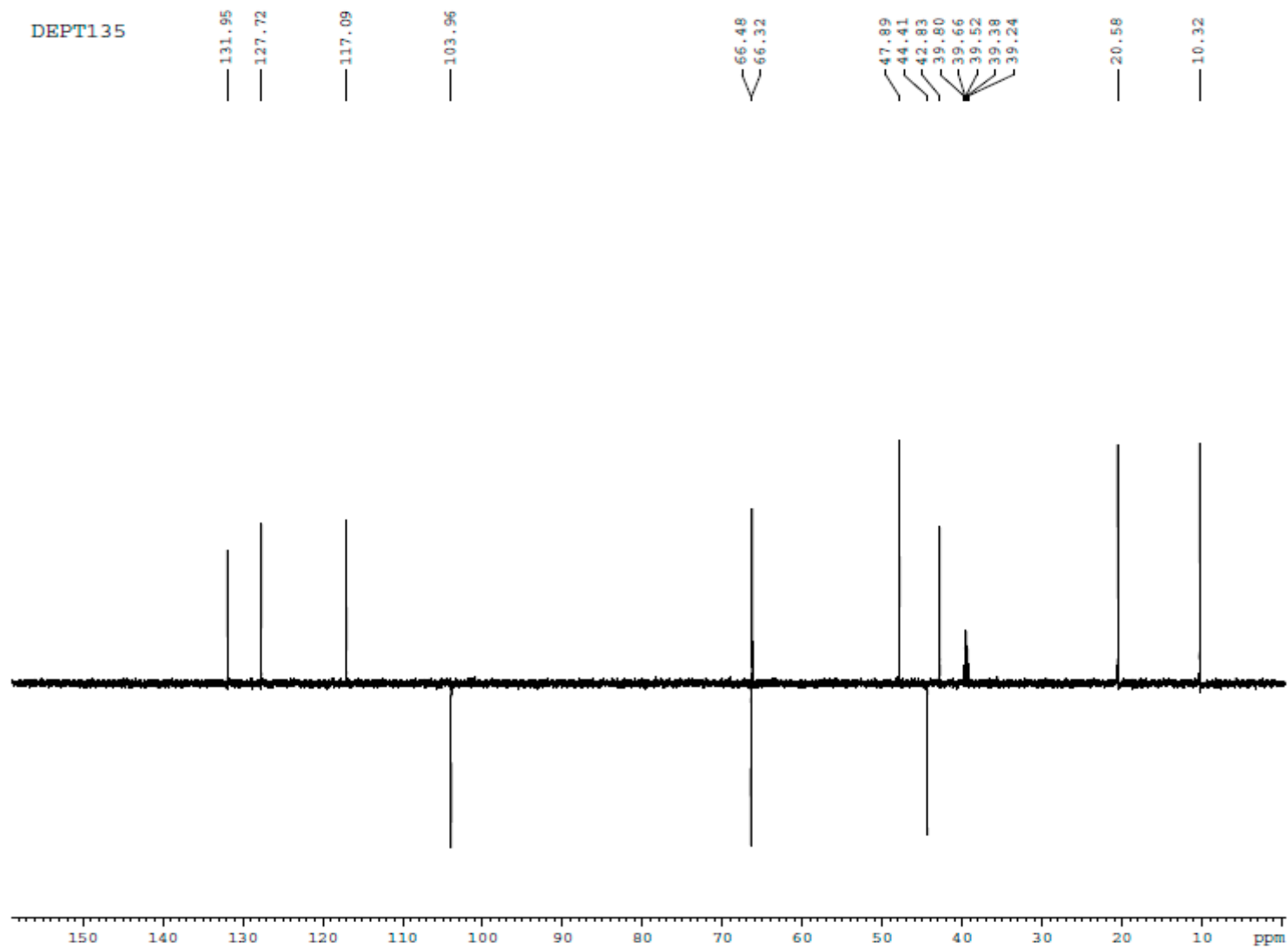


Figure S10. ^{13}C -NMR spectrum and DEPT of **2** in $\text{DMSO-}d_6$.

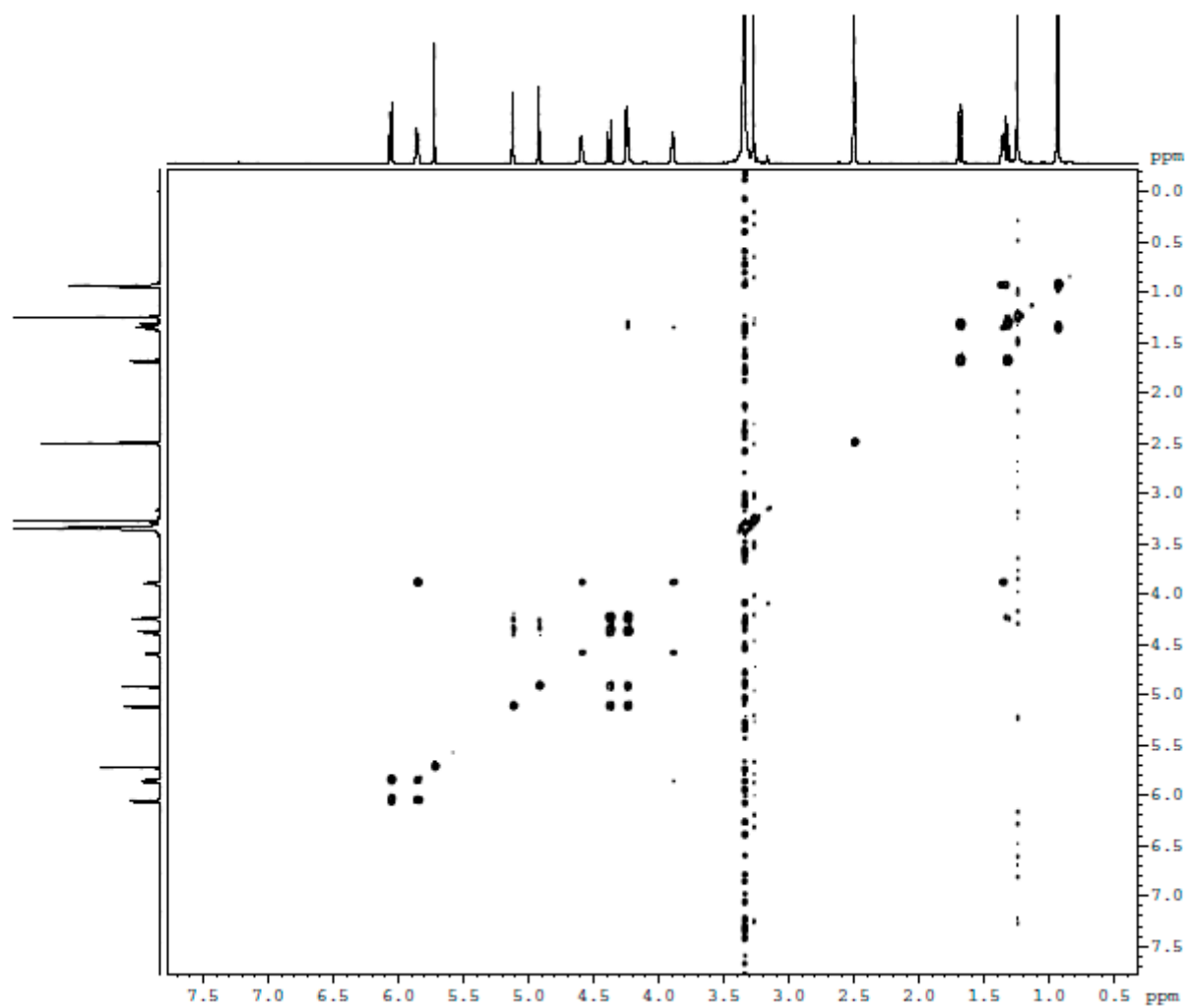


Figure S11. ^1H - ^1H COSY spectrum of 2 in $\text{DMSO-}d_6$.

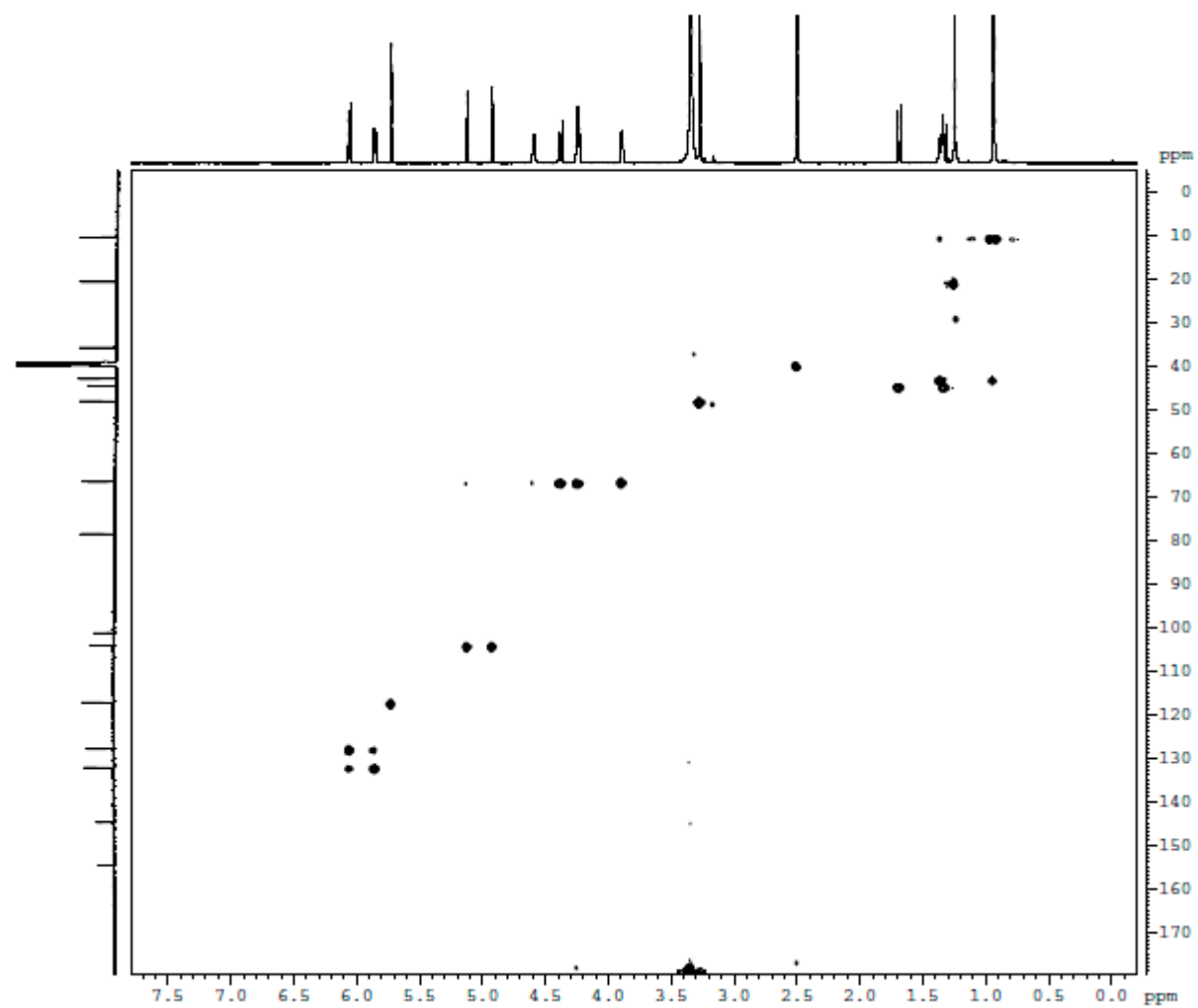
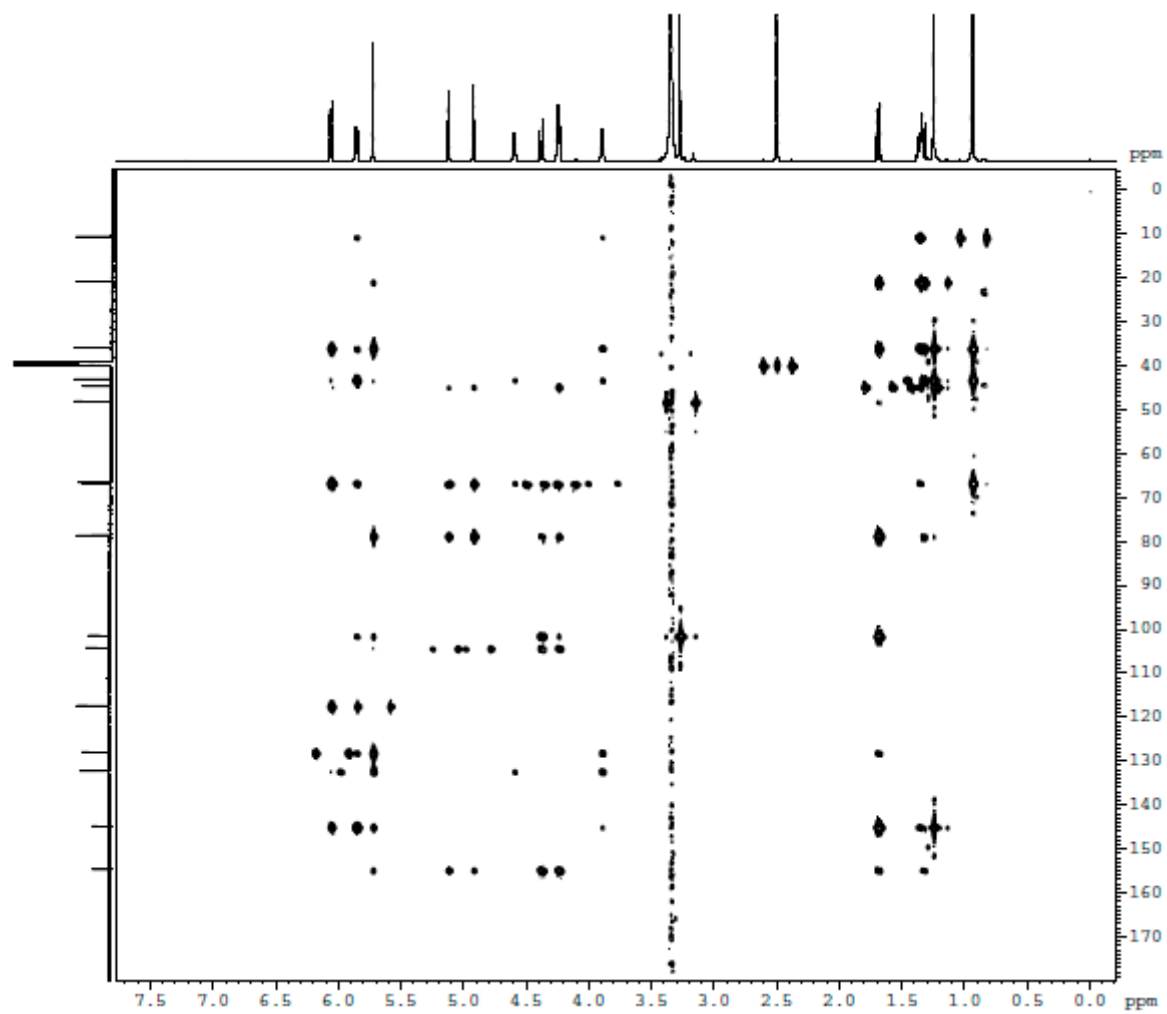


Figure S12. HSQC spectrum of 2 in DMSO-*d*₆.

Figure S13. HMBC spectrum of 2 in DMSO- d_6 .

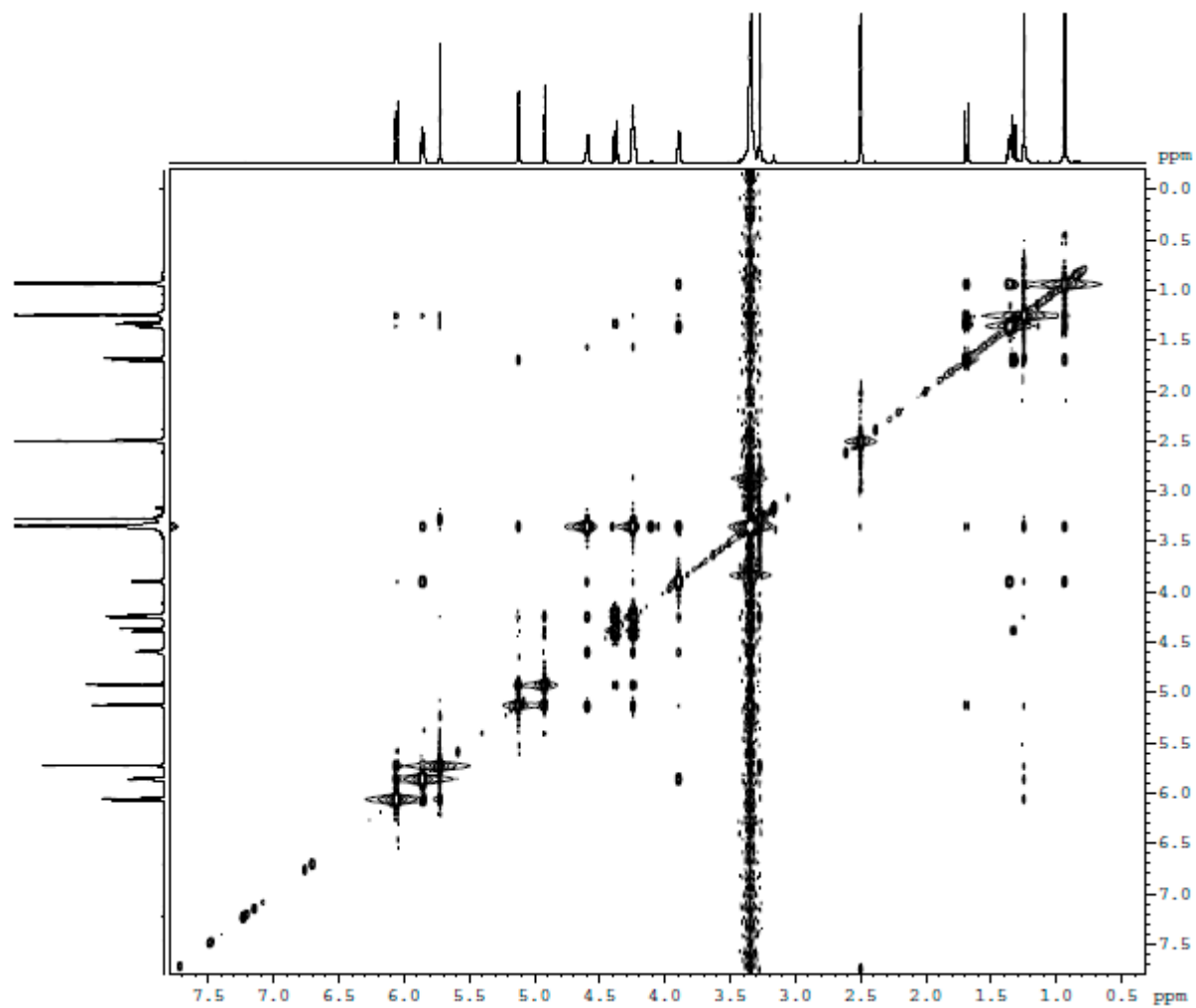


Figure S14. NOESY spectrum of 2 in DMSO-*d*₆.

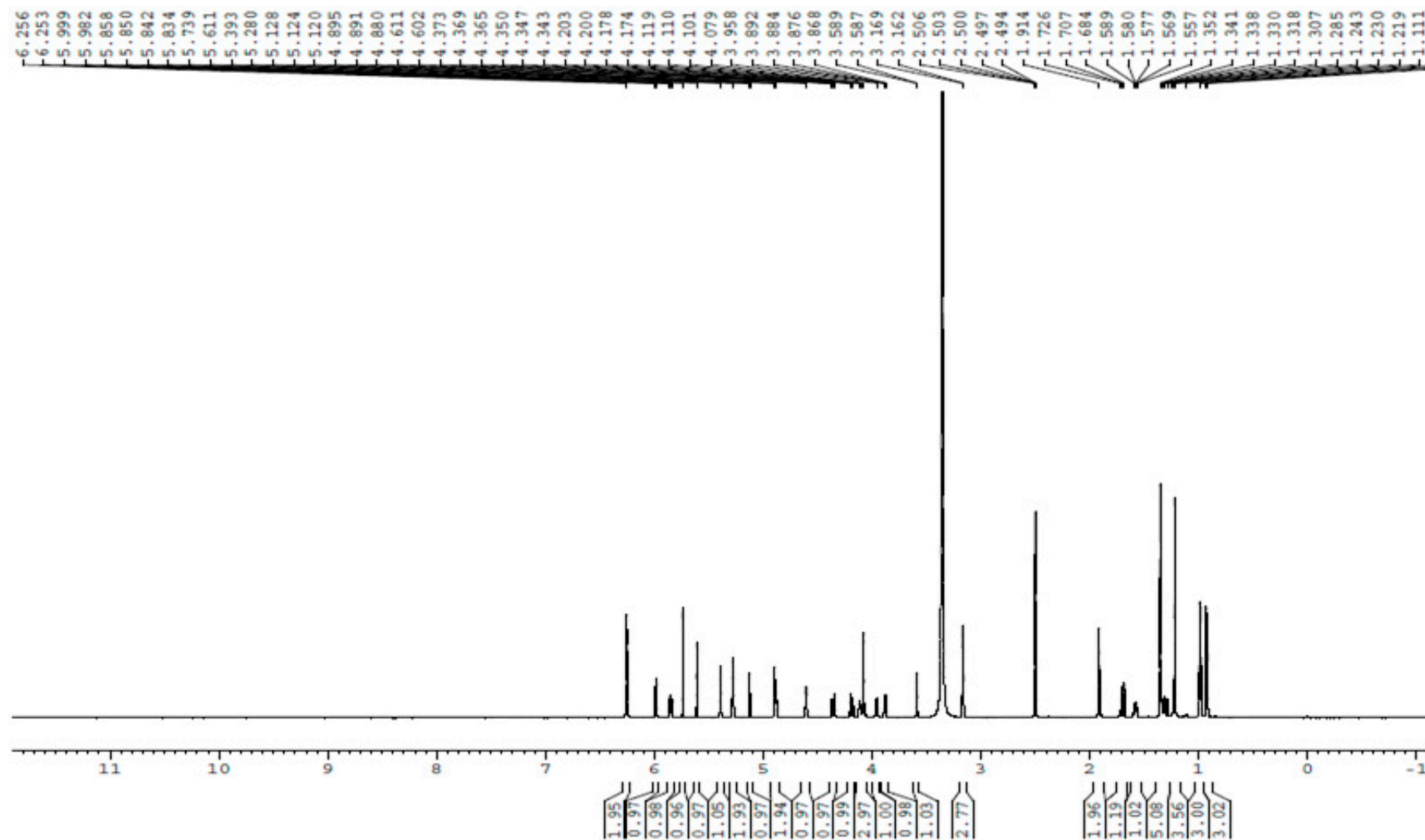


Figure S15. Cont.

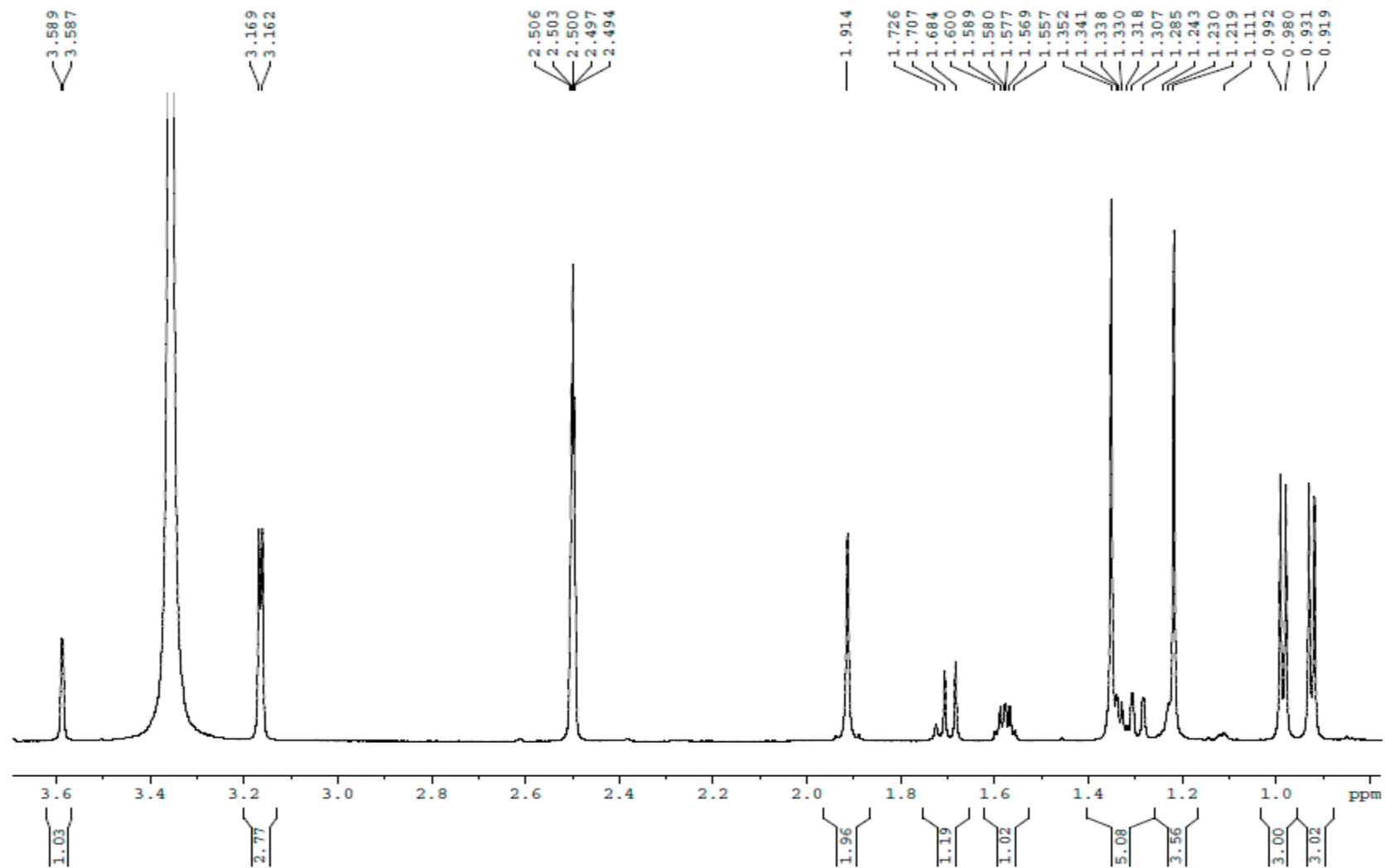
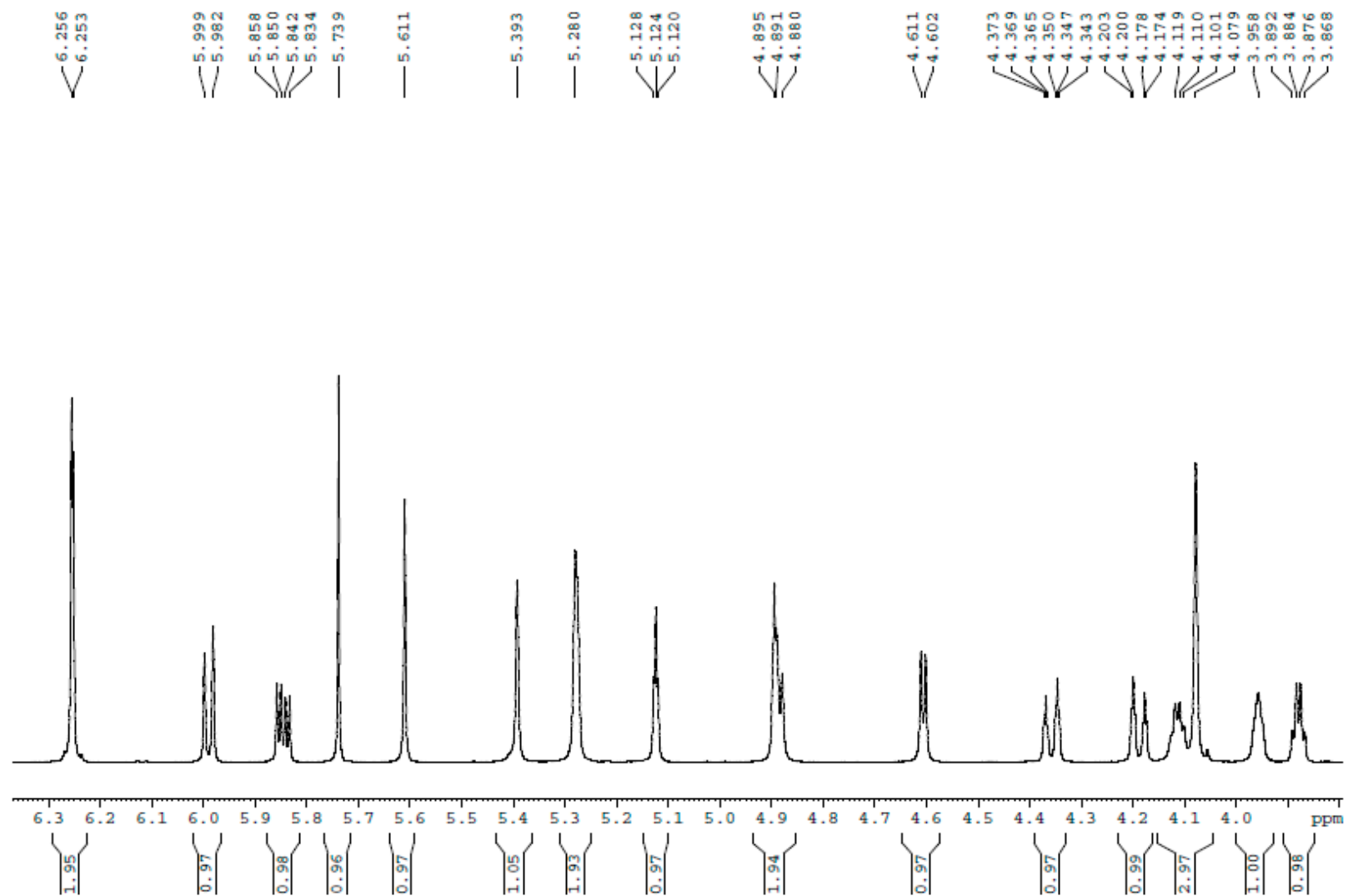


Figure S15. Cont.

Figure S15. ¹H-NMR spectrum of 3 in DMSO-d₆.

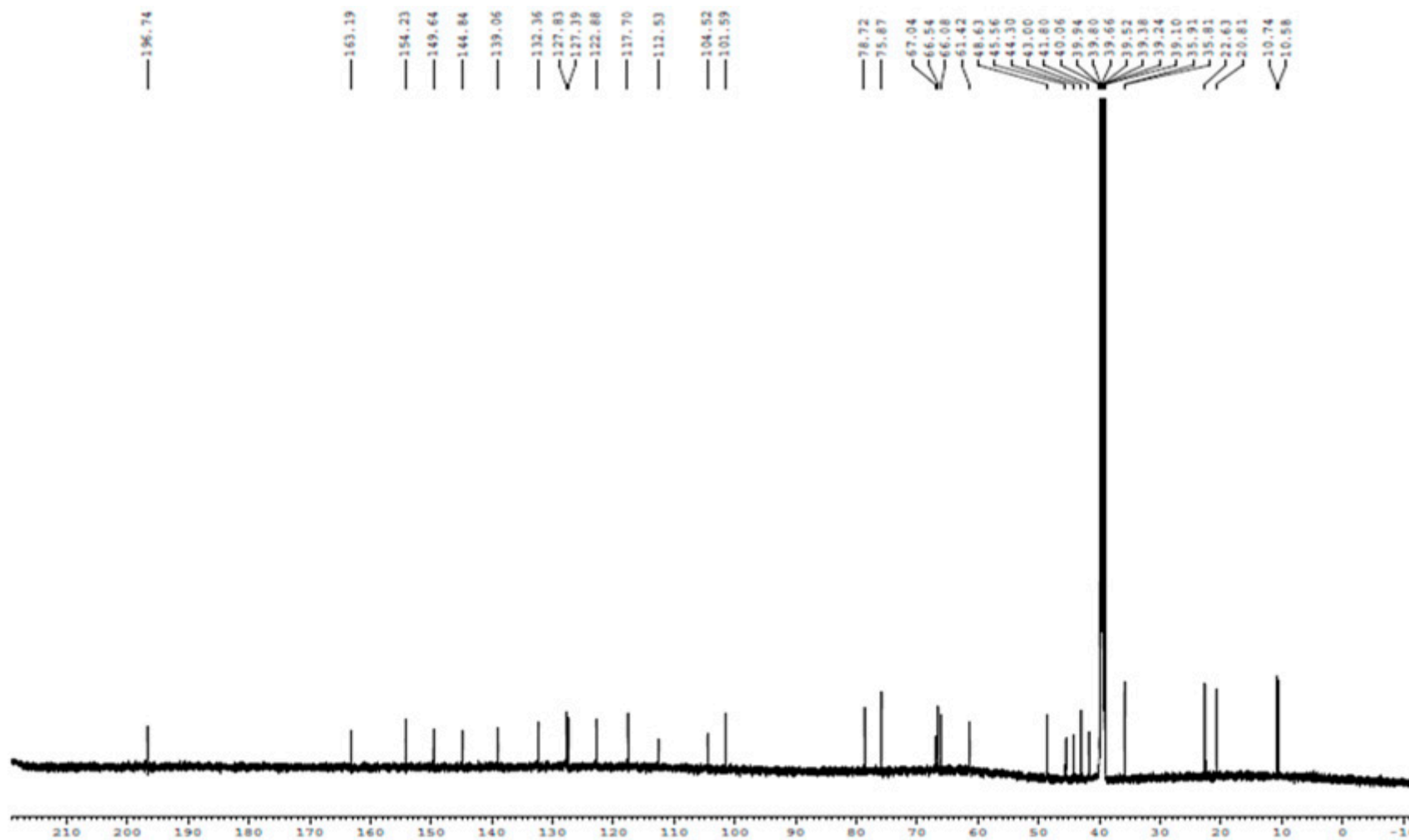


Figure S16. Cont.

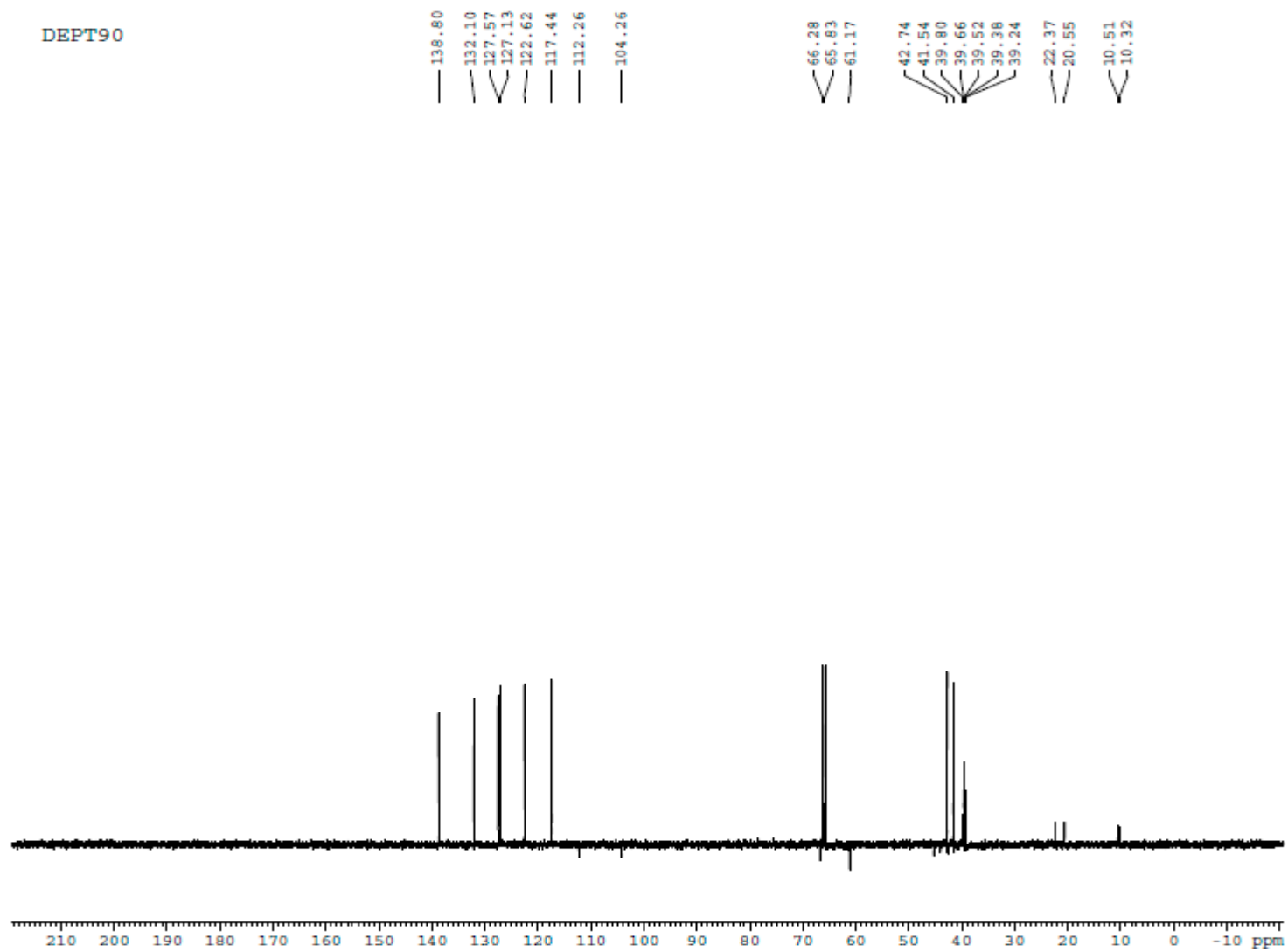
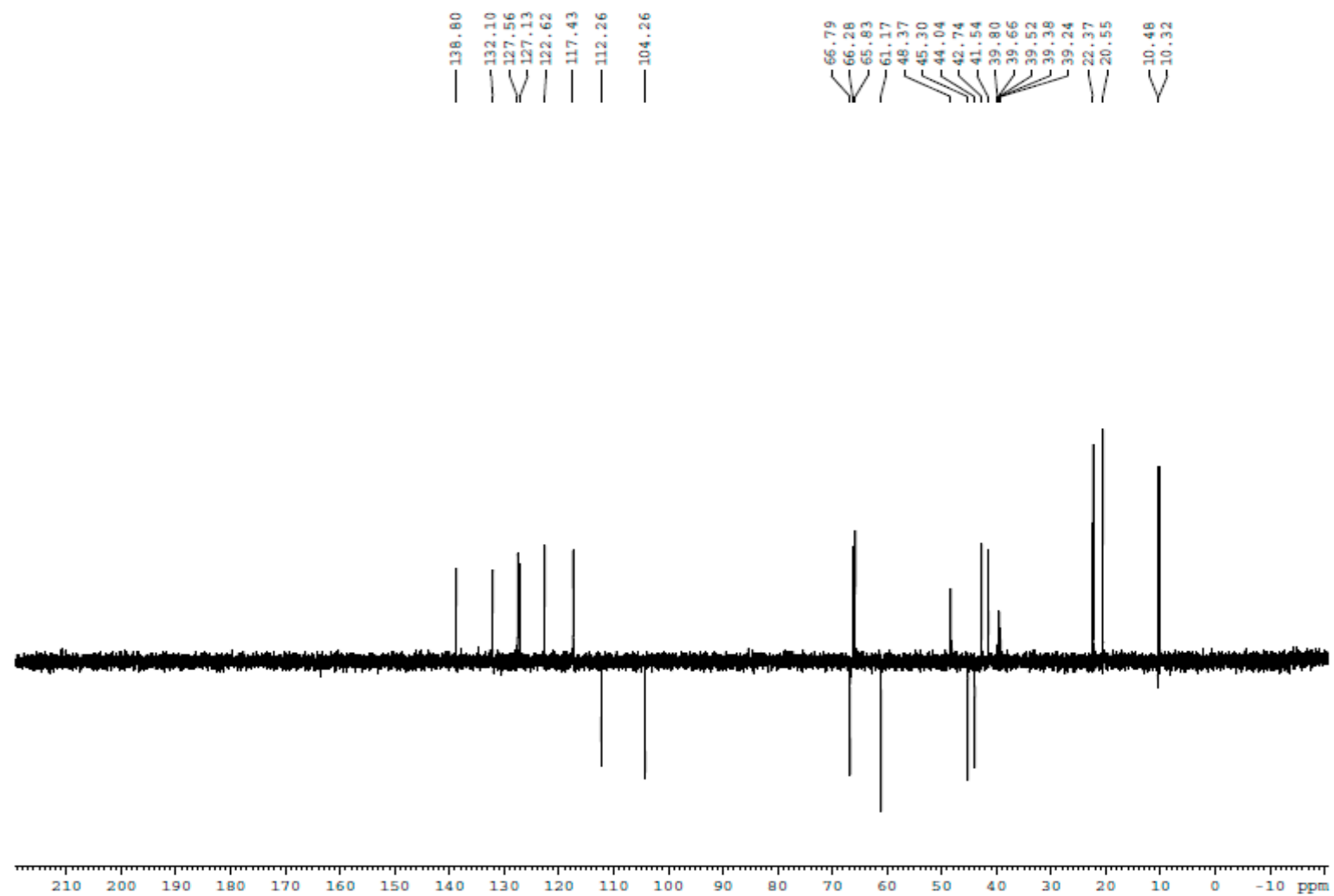


Figure S16. Cont.

DEPT135

Figure S16. ^{13}C -NMR spectrum and DEPT of 3 in $\text{DMSO-}d_6$.

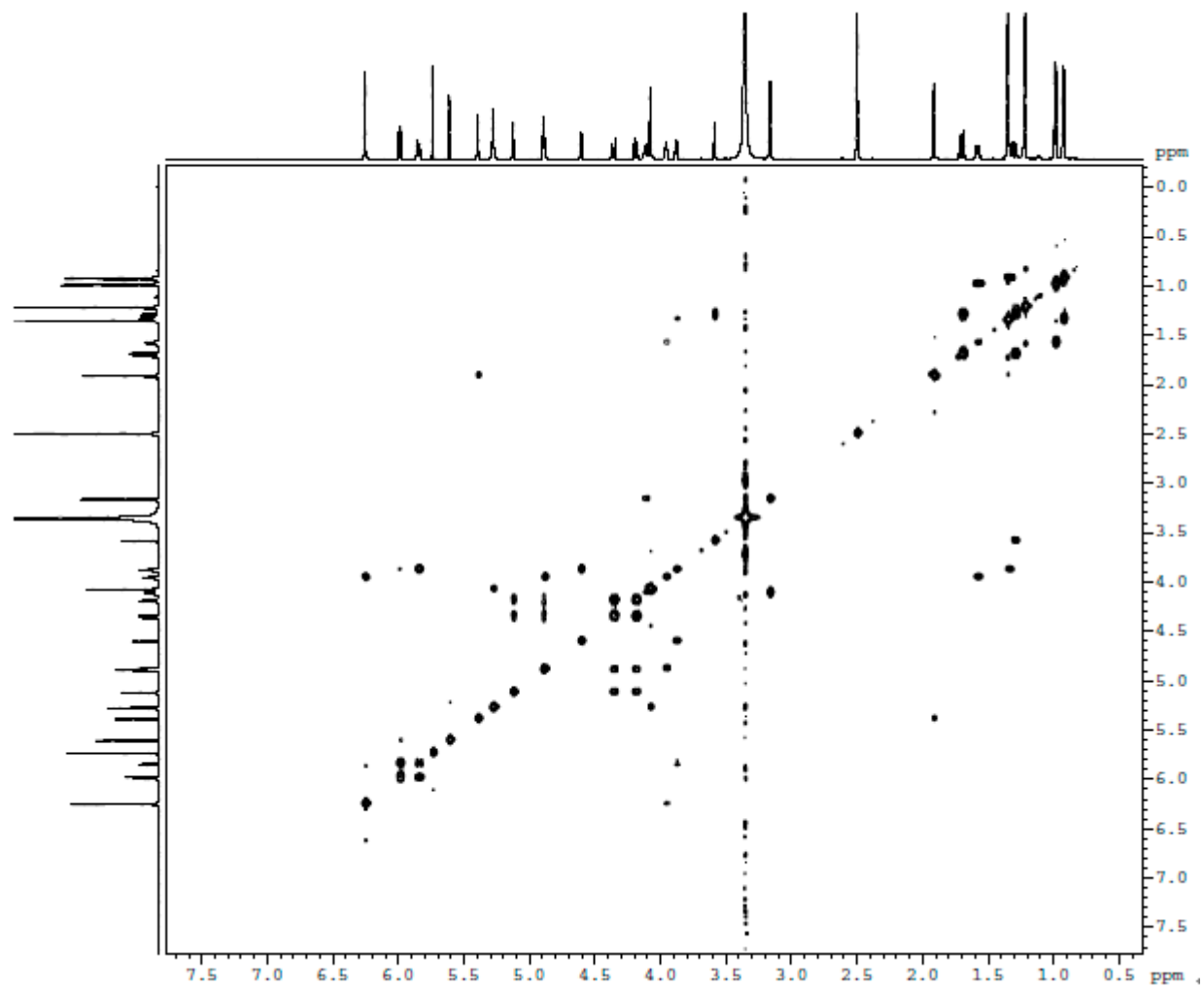


Figure S17. ^1H - ^1H COSY spectrum of 3 in $\text{DMSO-}d_6$.

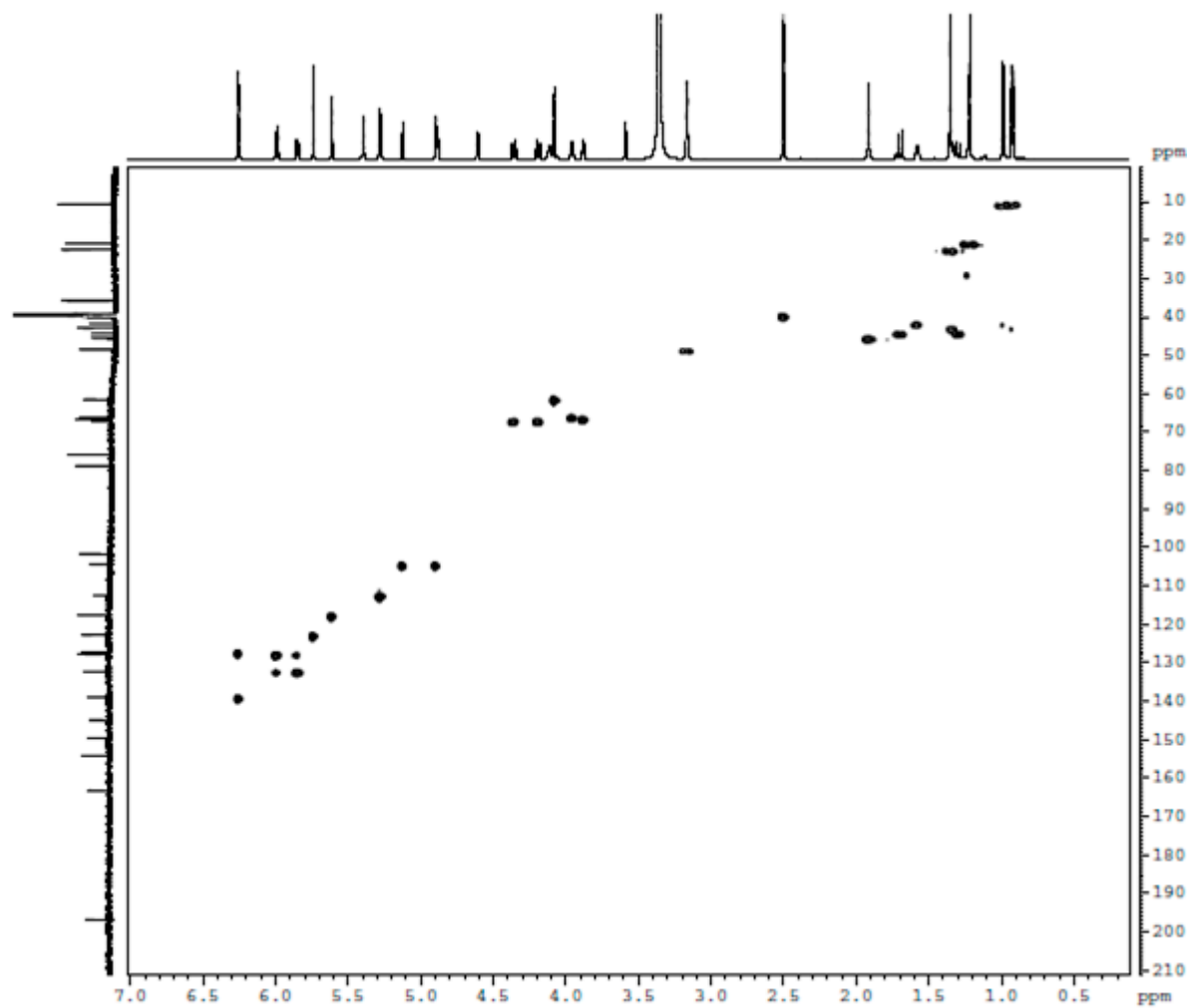
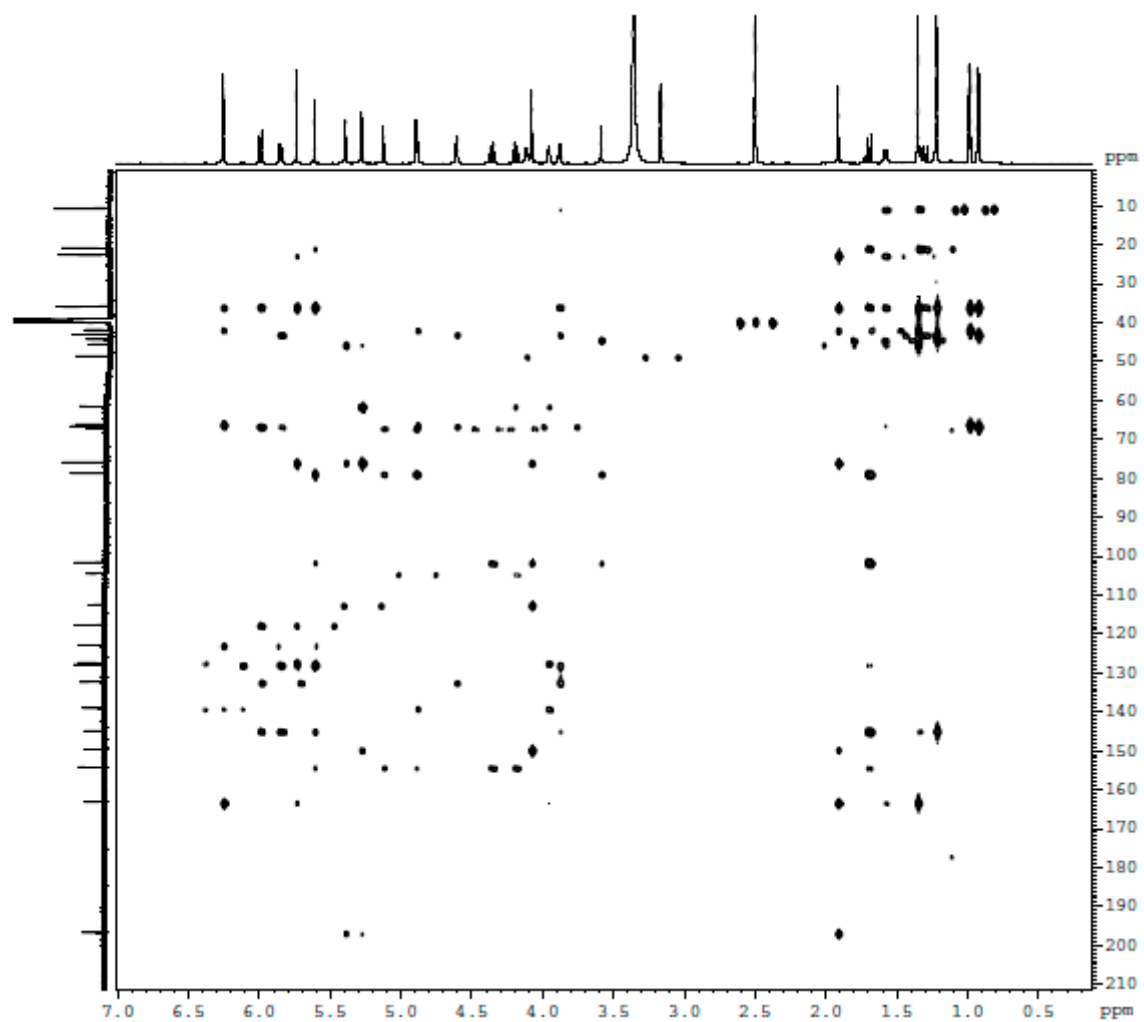


Figure S18. HSQC spectrum of 3 in DMSO-*d*₆.

Figure S19. HMBC spectrum of 3 in DMSO-*d*₆.

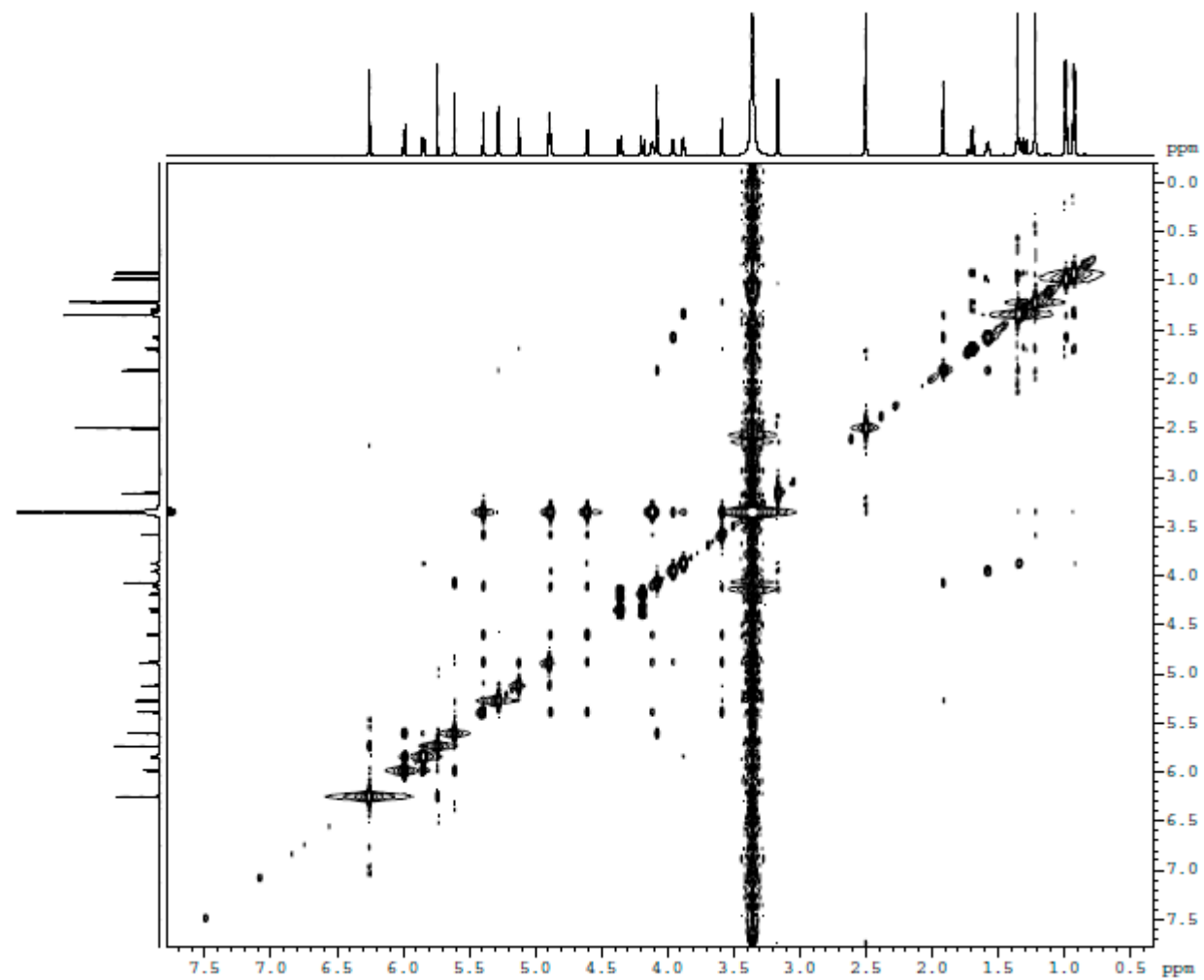


Figure S20. NOESY spectrum of 3 in DMSO-*d*₆.

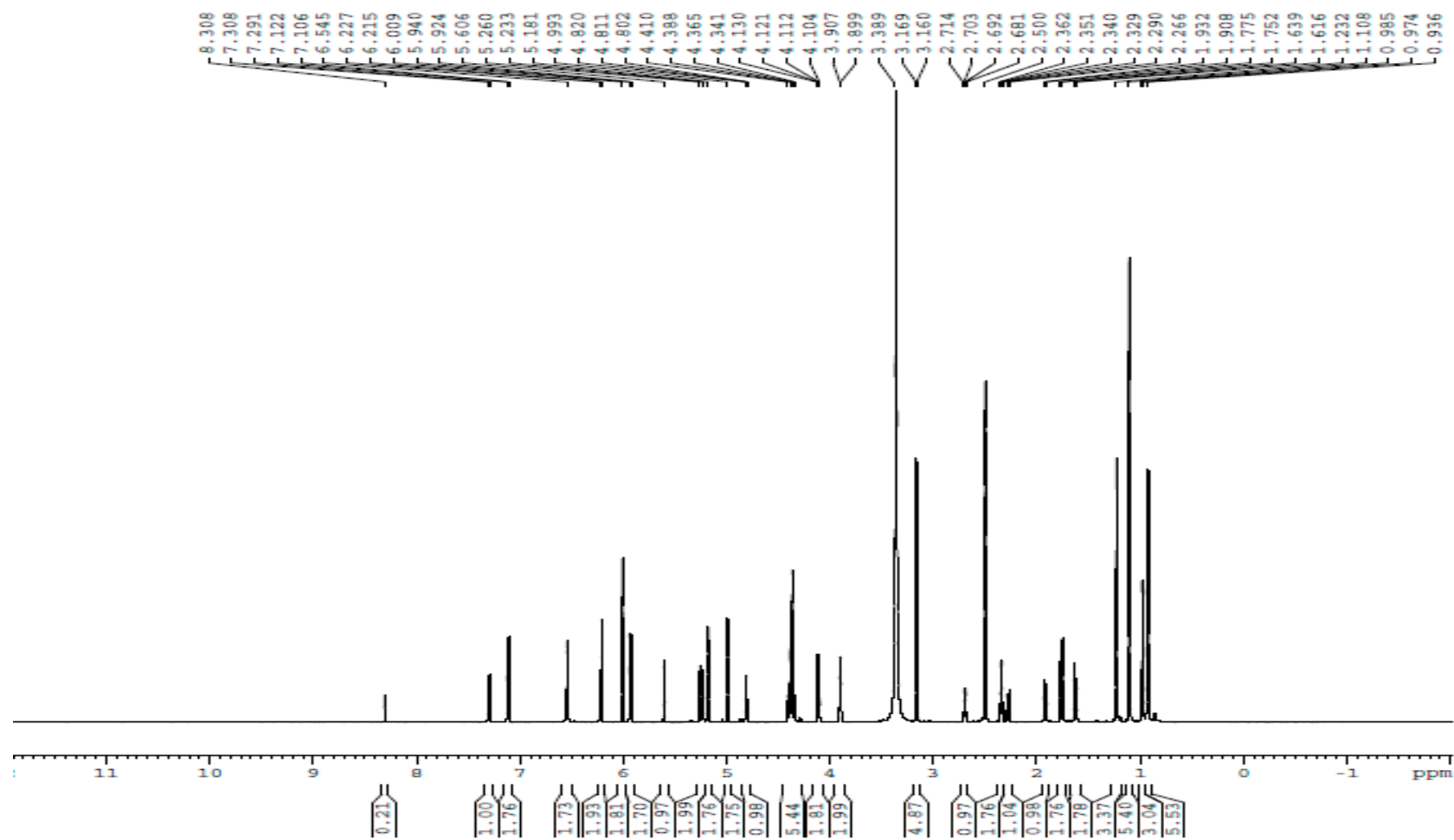


Figure S21. Cont.

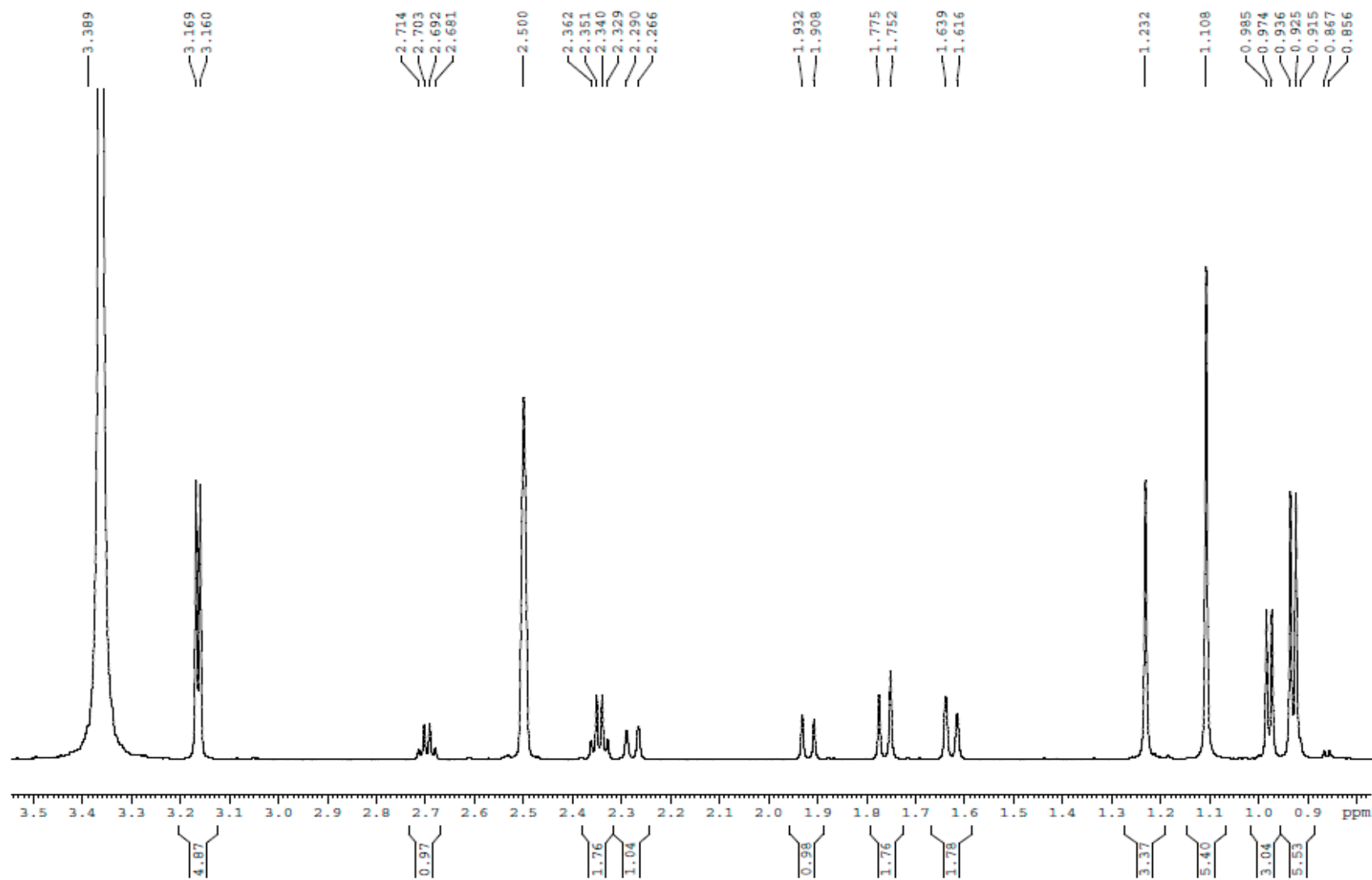
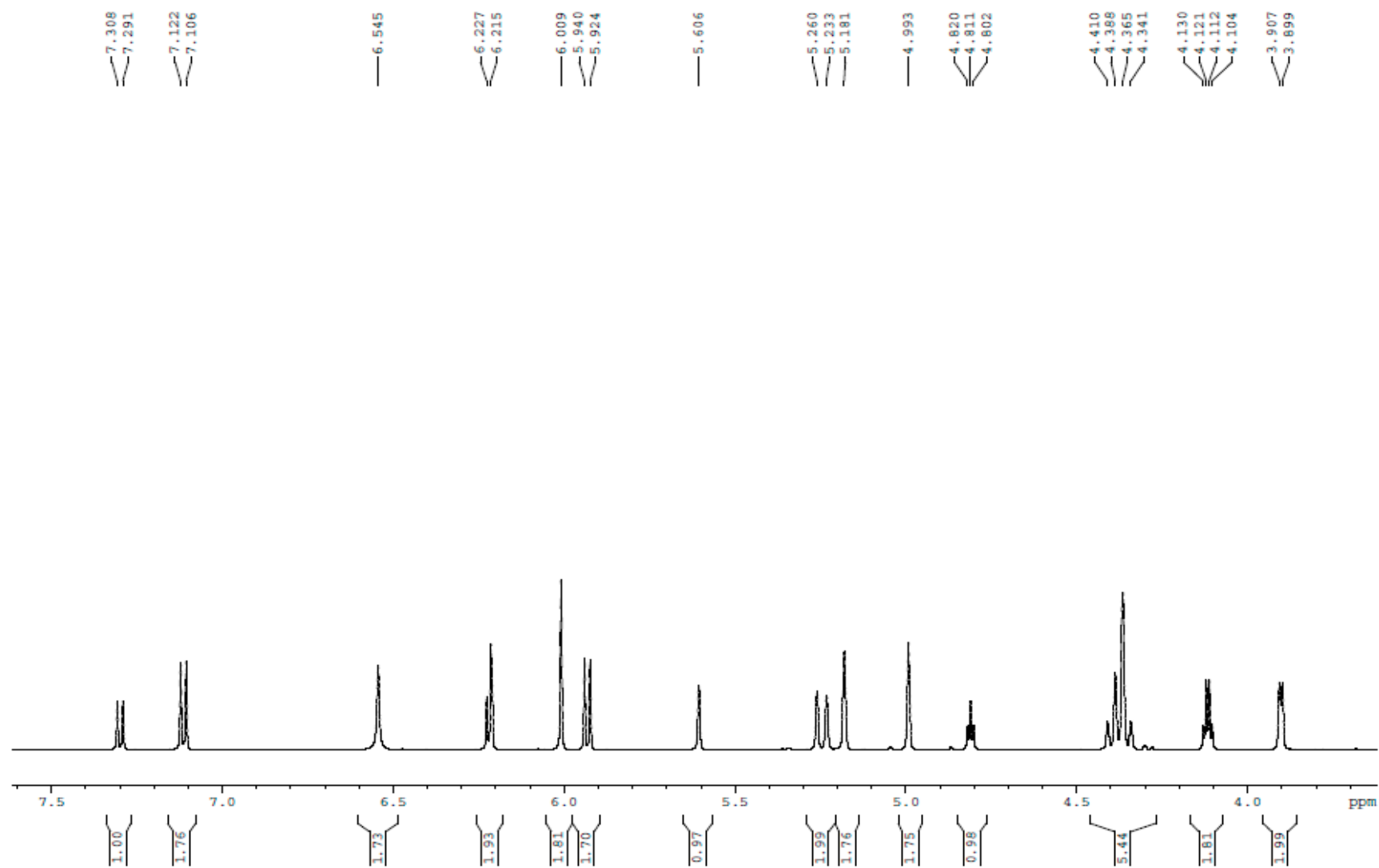


Figure S21. Cont.

Figure S21. $^1\text{H-NMR}$ spectrum of 4 in $\text{DMSO-}d_6$.

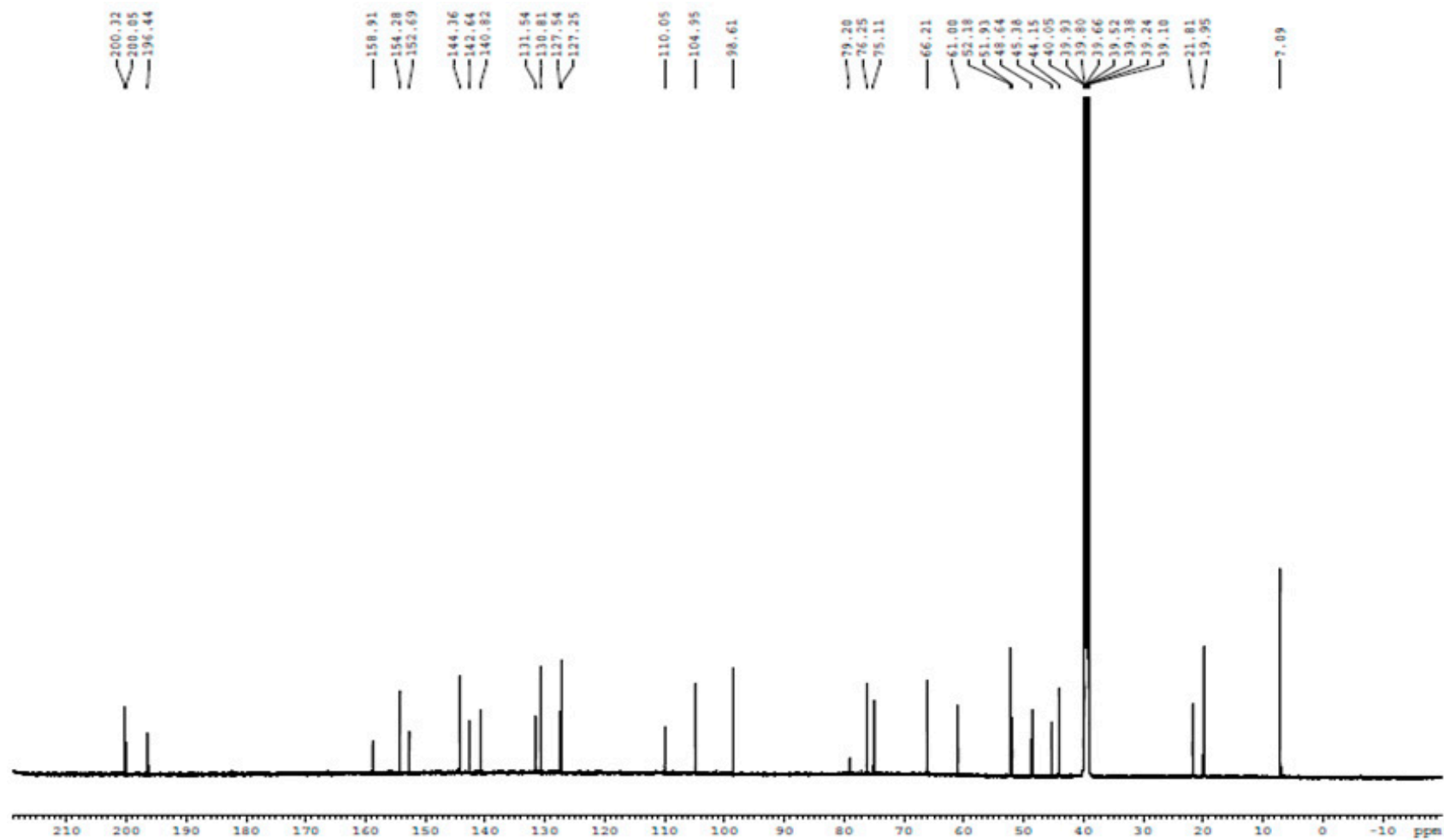


Figure S22. Cont.

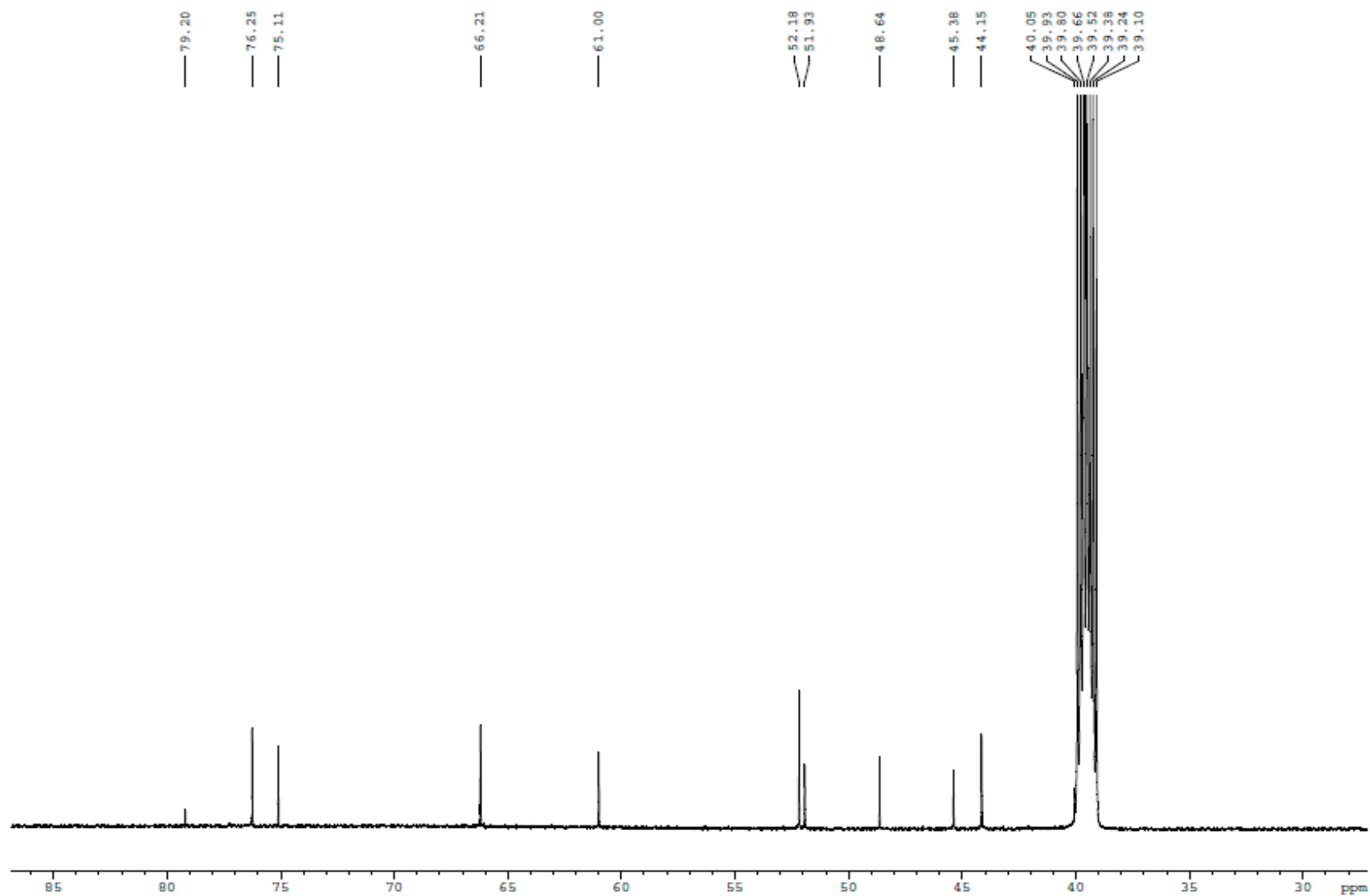


Figure S22. Cont.

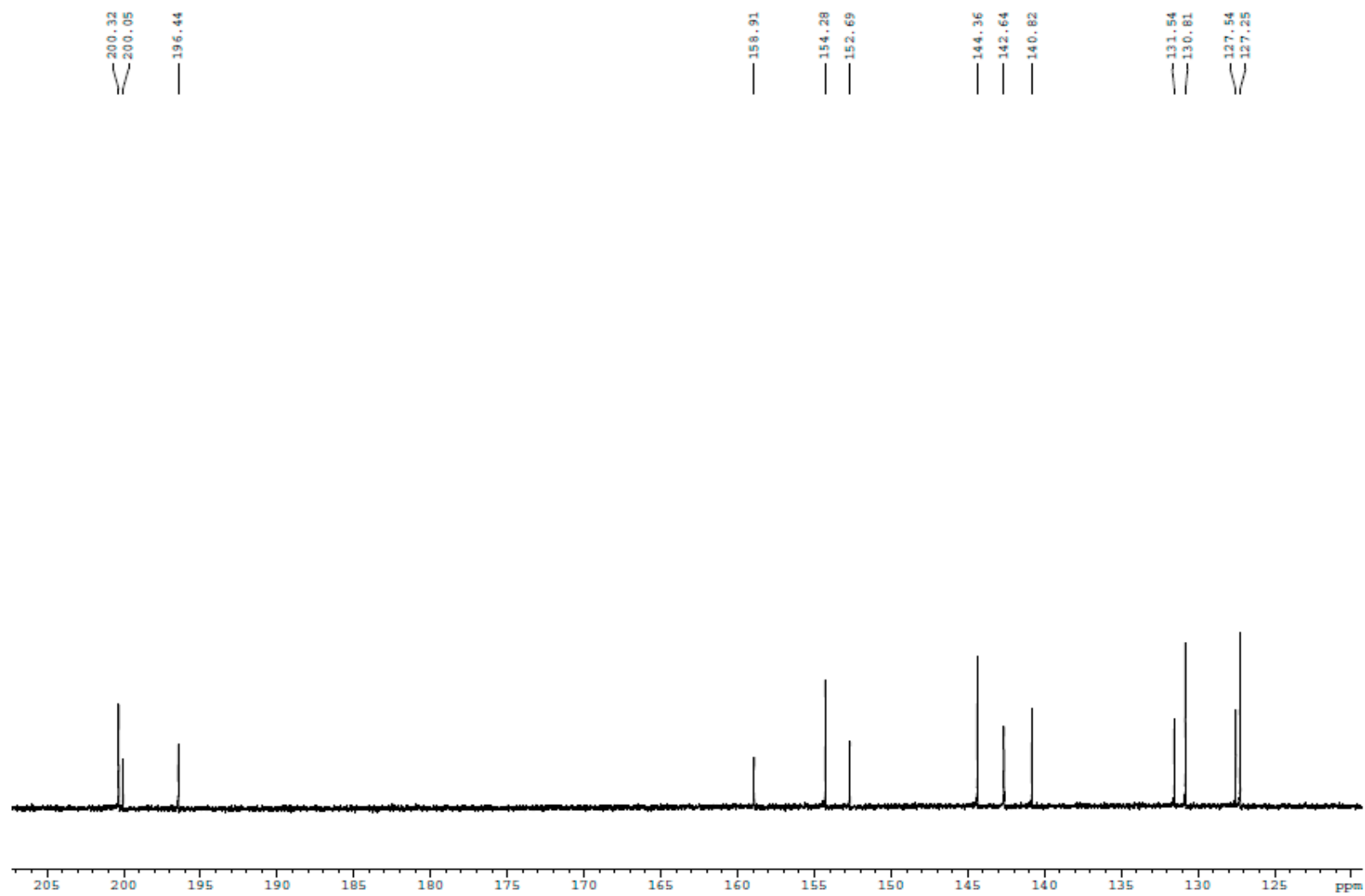


Figure S22. Cont.

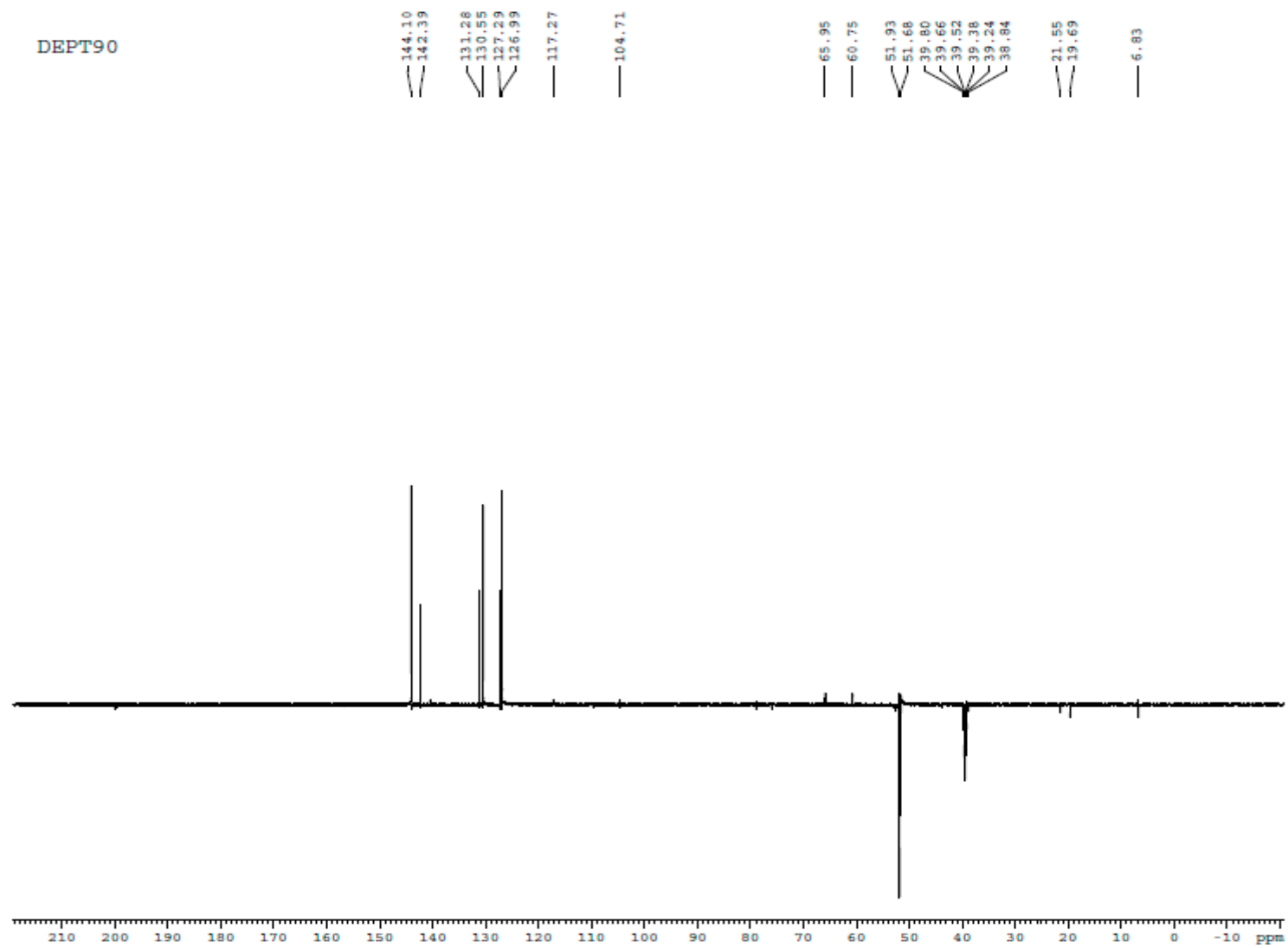


Figure S22. Cont.

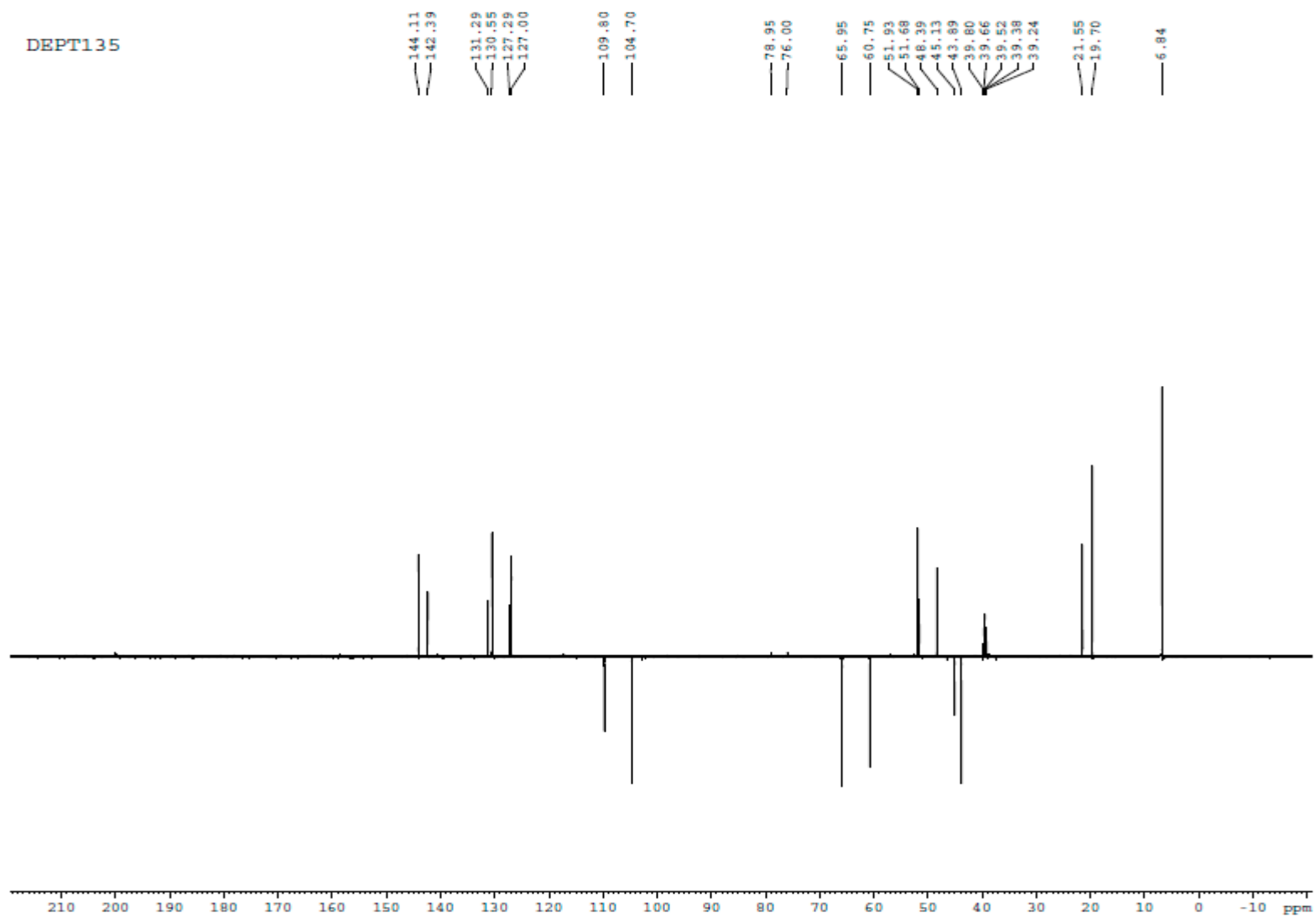


Figure S22. ^{13}C -NMR spectrum and DEPT of 4 in $\text{DMSO-}d_6$.

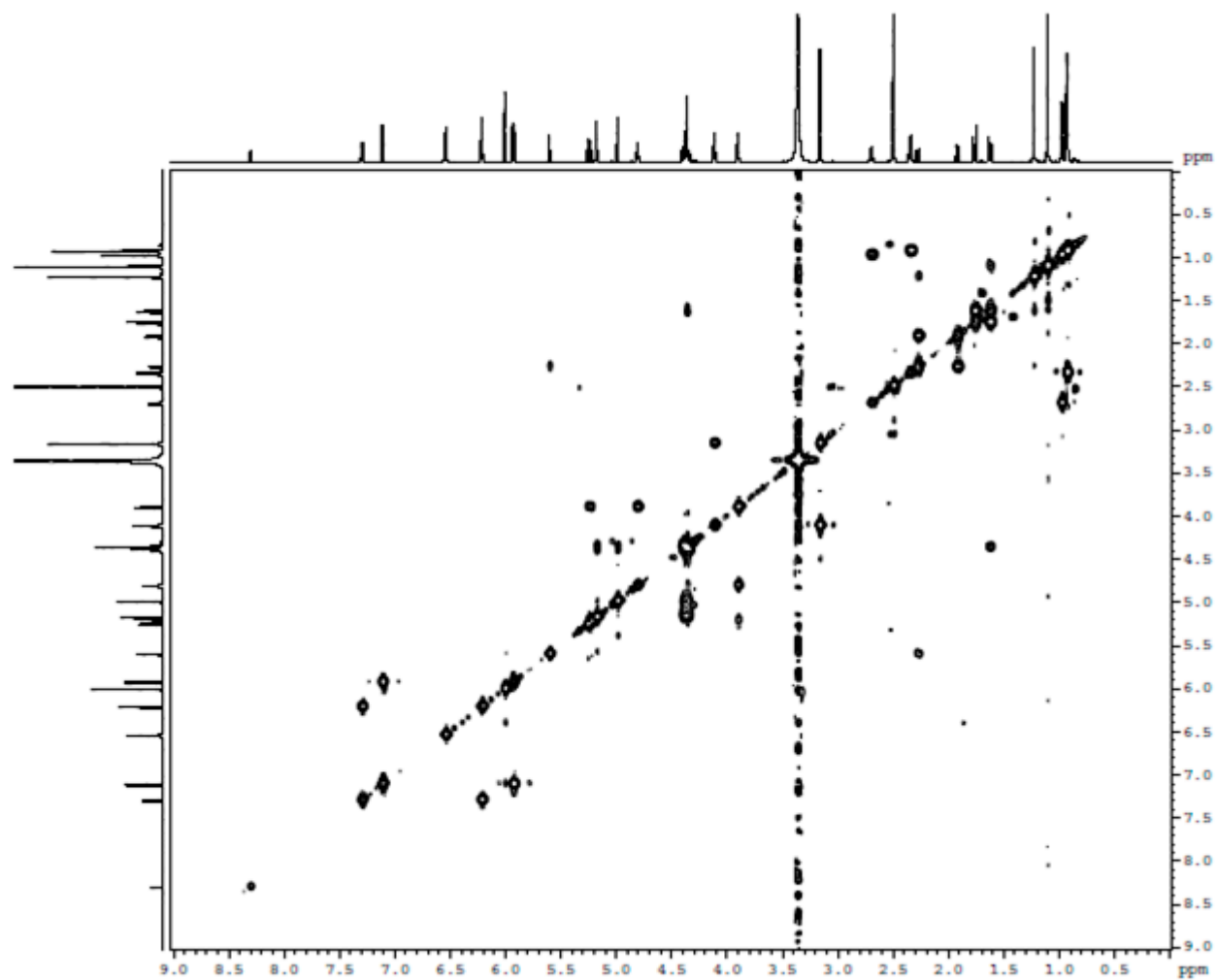


Figure S23. ^1H - ^1H COSY spectrum of 4 in $\text{DMSO-}d_6$.

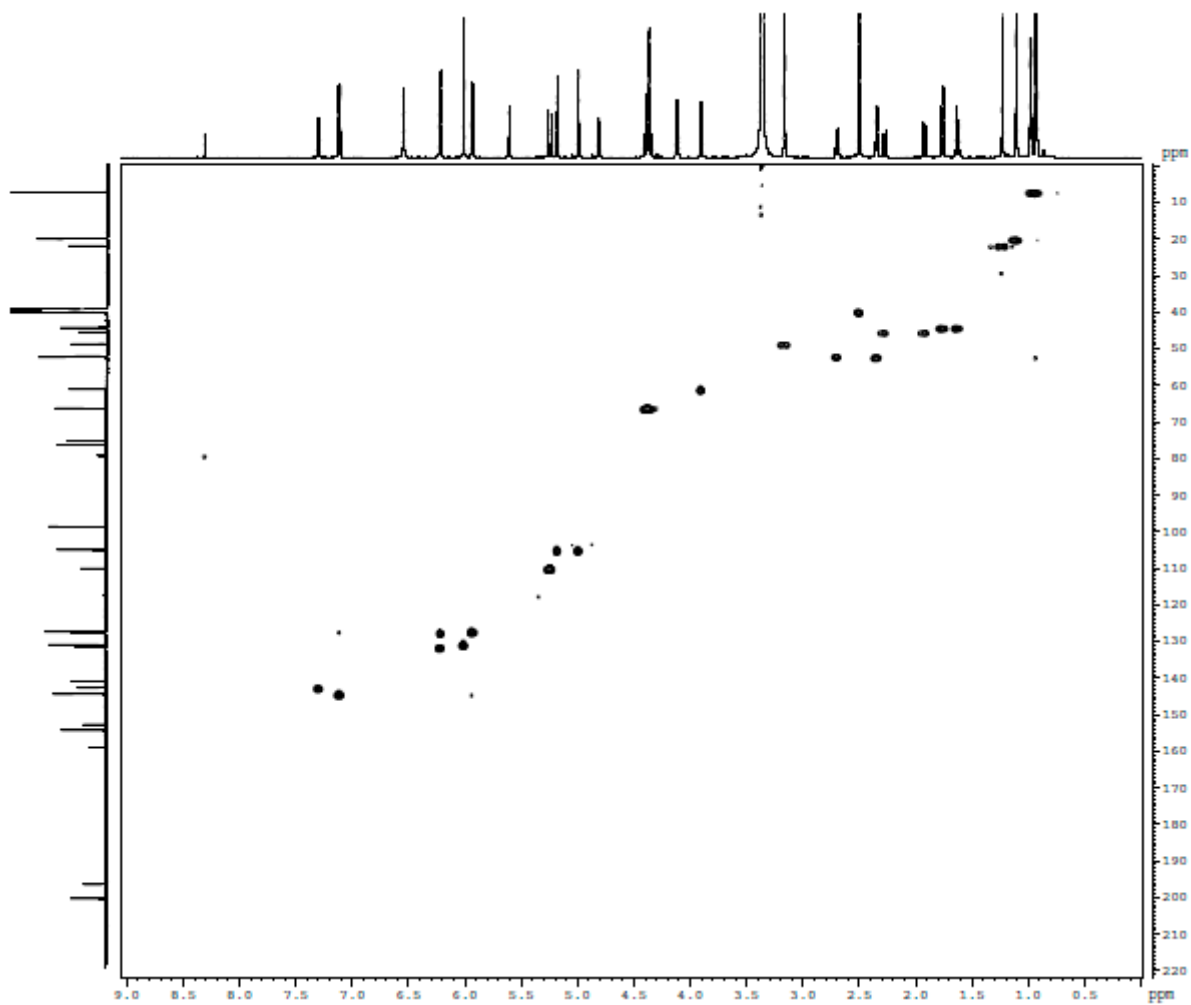
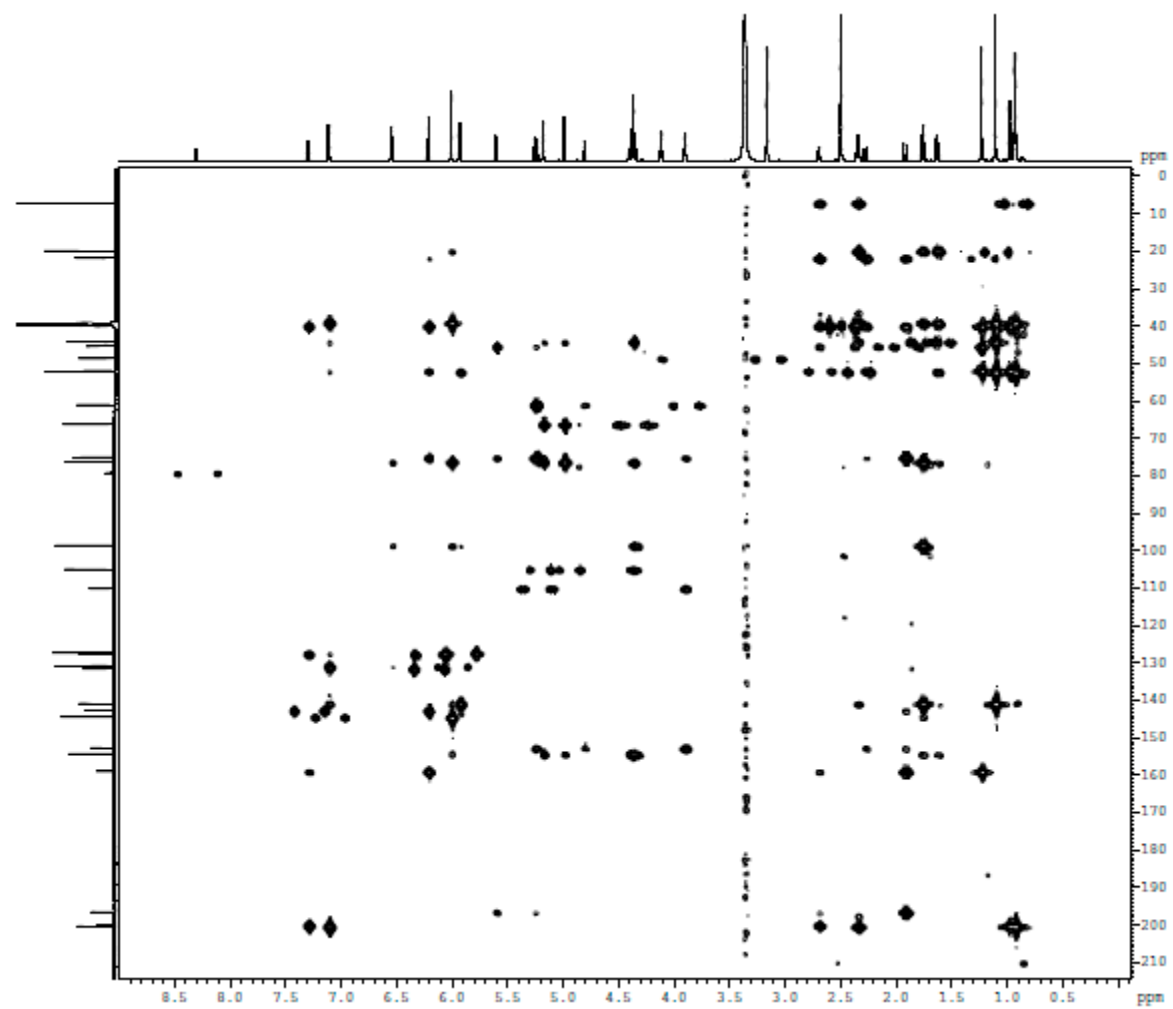


Figure S24. HSQC spectrum of 4 in DMSO- d_6 .

Figure S25. HMBC spectrum of 4 in DMSO-*d*₆.

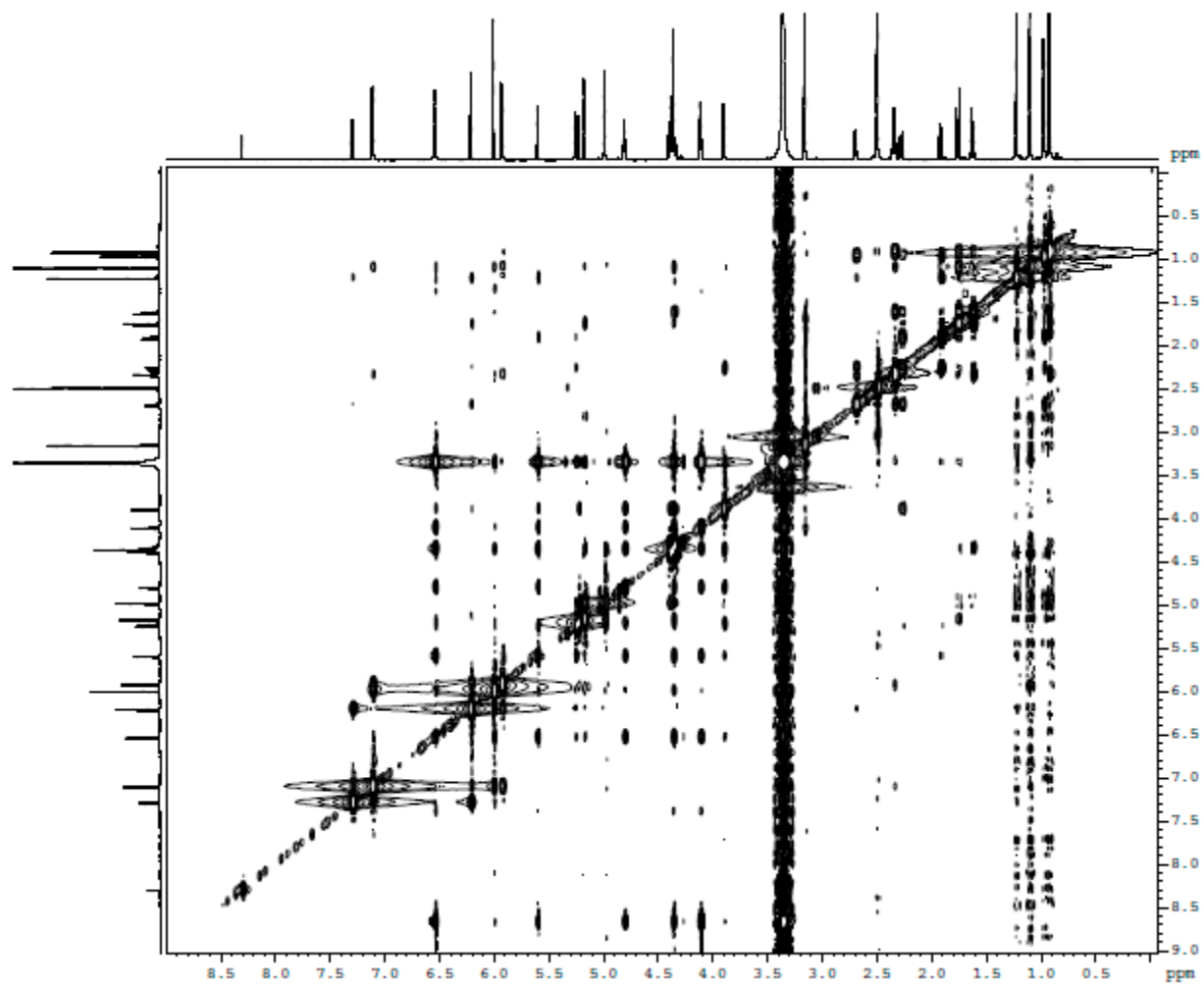


Figure S26. NOESY spectrum of 4 in DMSO-*d*₆.

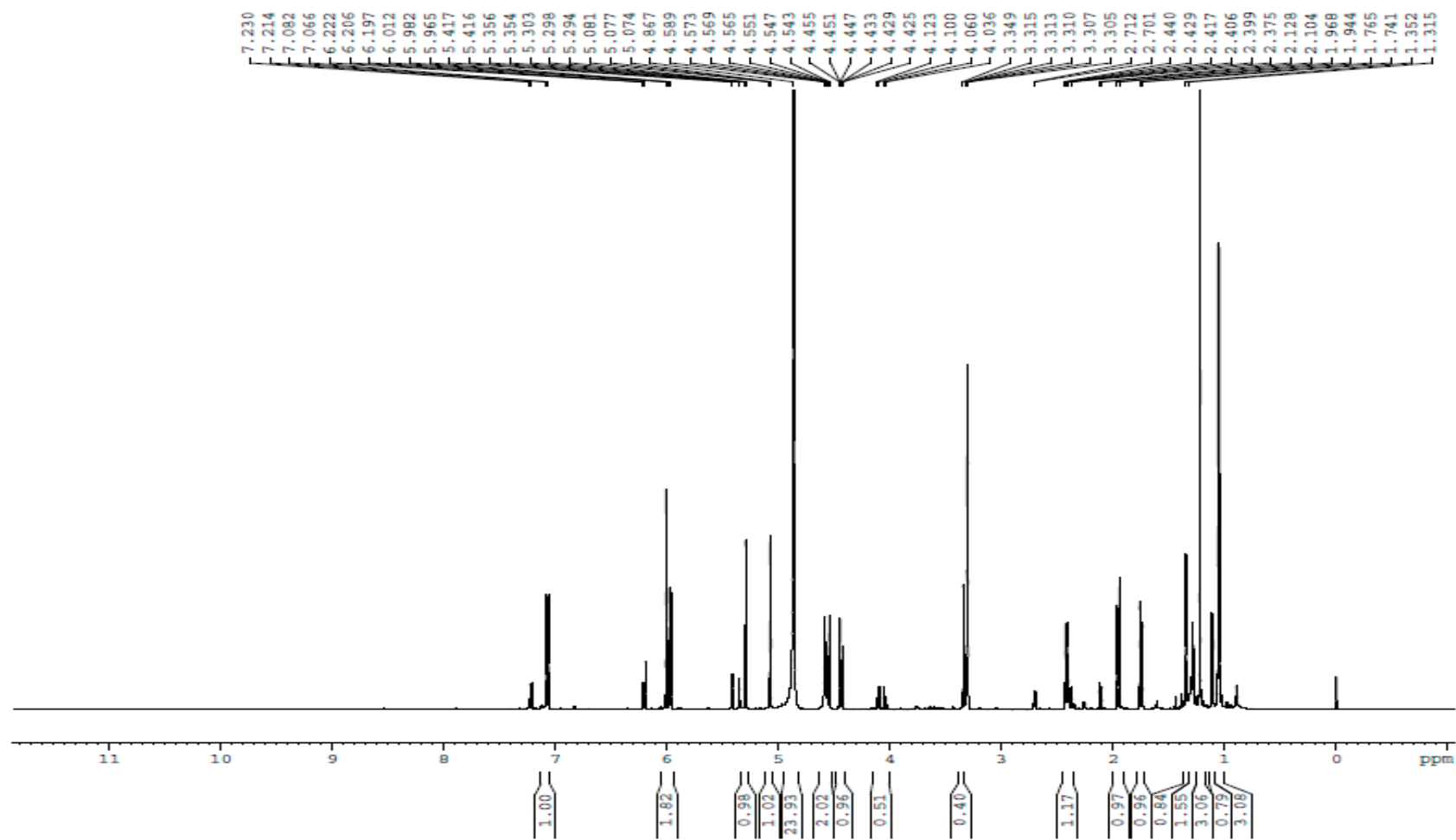


Figure S27. Cont.

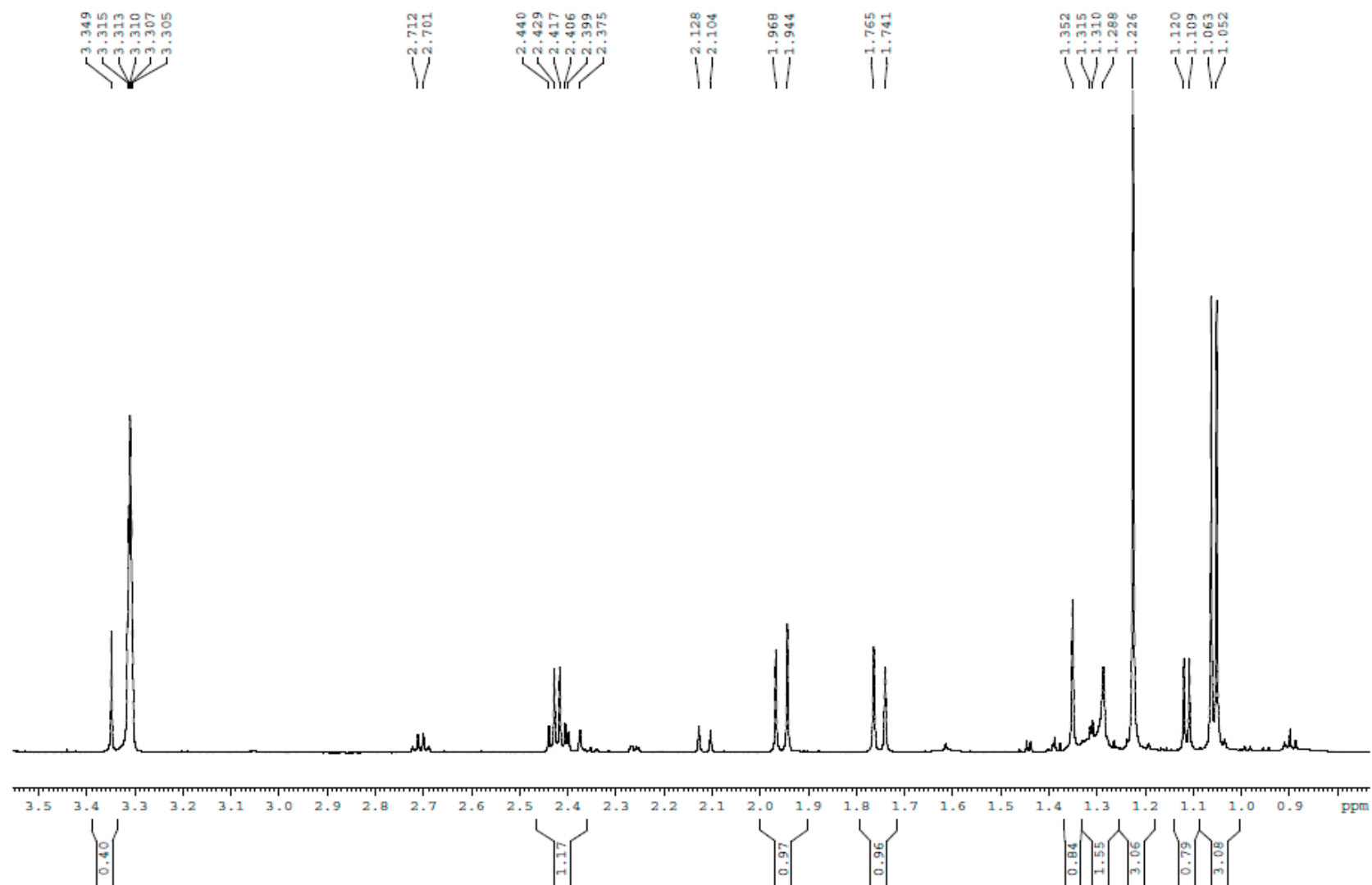
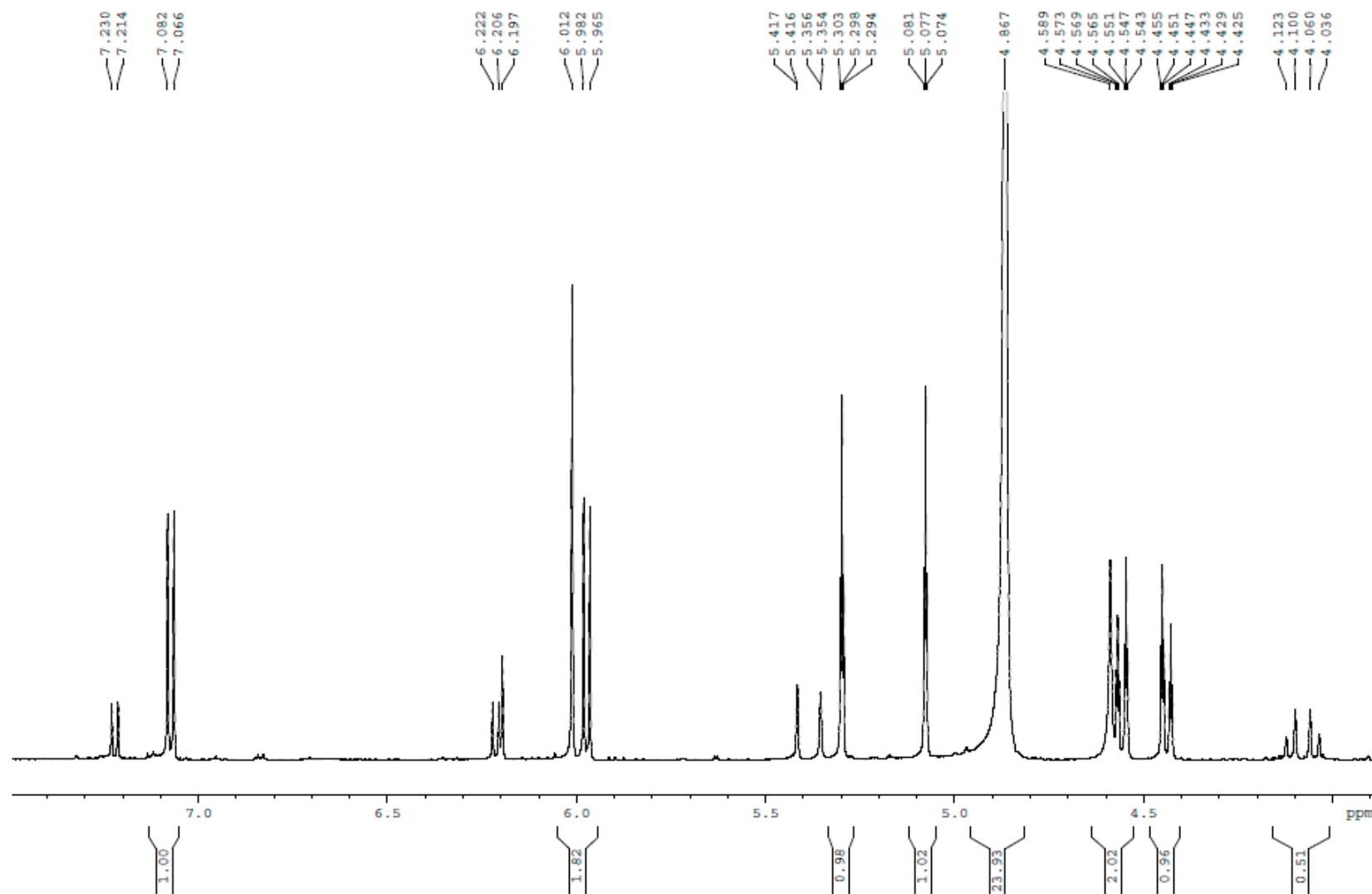


Figure S27. Cont.

Figure S27. ¹H-NMR spectrum of 4 in MEOD-d₄.