

SUPPORTING INFORMATION

Isolation and Structure Elucidation of Cembranoids from a Dongsha Atoll Soft Coral *Sarcophyton stellatum*

Atallah F. Ahmed^{1,2,†}, **Yi-Wei Chen**^{1,†}, **Chiung-Yao Huang**^{1,†}, **Yen-Ju Tseng**¹, **Chi-Chen Lin**³, **Chang-Feng Dai**⁴, **Yang-Chang Wu**⁵ and **Jyh-Horng Sheu**^{1,5,6,7,*}

¹ Department of Marine Biotechnology and Resources, National Sun Yat-sen University, Kaohsiung 804, Taiwan; afahmed@KSU.EDU.SA (A.F.A.); m985020005@student.nsysu.edu.tw (Y.-W.C.); huangcy@mail.nsysu.edu.tw (C.-Y.H.); d935020003@student.nsysu.edu.tw (Y.-J.T.)

² Department of Pharmacognosy, College of Pharmacy, King Saud University, Riyadh 11451, Saudi Arabia

³ Institute of Biomedical Sciences, National Chung Hsing University, Taichung 402, Taiwan; lincc@dragon.nchu.edu.tw

⁴ Institute of Oceanography, National Taiwan University, Taipei 112, Taiwan; corallab@ntu.edu.tw

⁵ Graduate Institute of Natural Products, Kaohsiung Medical University, Kaohsiung 807, Taiwan; yachwu@kmu.edu.tw

⁶ Frontier Center for Ocean Science and Technology, National Sun Yat-sen University, Kaohsiung 804, Taiwan

⁷ Department of Medical Research, China Medical University Hospital, China Medical University, Taichung 404, Taiwan

* Correspondence: sheu@mail.nsysu.edu.tw; Tel.: +886-7-525-2000 (ext. 5030); Fax: +886-7-525-5020.

[†] These authors contributed equally to this work.

Corresponding author: E-mail: sheu@mail.nsysu.edu.tw; Fax: +886-7-525-5020; Tel: +886-7-525-2000 ext. 5030

List of Supplementary material:

No	Content	page	No	Content	page
Figure S1	^1H NMR spectrum of 1 in CDCl_3	3	Figure S25	COSY spectrum of 3 in CDCl_3	27
Figure S2	^{13}C NMR spectrum of 1 in CDCl_3	4	Figure S26	HMBC spectrum of 3 in CDCl_3	28
Figure S3	DEPT spectra of 1 in CDCl_3	5	Figure S27	NOESY spectrum of 3 in CDCl_3	29
Figure S4	HMQC spectrum of 1 in CDCl_3	6	Figure S28	^1H NMR spectrum of 4 in CDCl_3	30
Figure S5	COSY spectrum of 1 in CDCl_3	7	Figure S29	^{13}C NMR spectrum of 4 in CDCl_3	31
Figure S6	HMBC spectrum of 1 in CDCl_3	8	Figure S30	DEPT spectra of 4 in CDCl_3	32
Figure S7	NOESY spectrum of 1 in CDCl_3	9	Figure S31	HMQC spectrum of 4 in CDCl_3	33
Figure S8	^1H NMR spectrum of 1 in C_6D_6	10	Figure S32	COSY spectrum of 4 in CDCl_3	34
Figure S9	^{13}C NMR spectrum of 1 in C_6D_6	11	Figure S33	HMBC spectrum of 4 in CDCl_3	35
Figure S10	DEPT spectrum of 1 in C_6D_6	12	Figure S34	NOESY spectrum of 4 in CDCl_3	36
Figure S11	COSY spectrum of 1 in C_6D_6	13	Figure S35	^1H NMR spectrum of 5 in CDCl_3	37
Figure S12	HMBC spectrum of 1 in C_6D_6	14	Figure S36	^{13}C NMR spectrum of 5 in CDCl_3	38
Figure S13	NOESY spectrum of 1 in C_6D_6	15	Figure S37	DEPT spectra of 5 in CDCl_3	39
Figure S14	^1H NMR spectrum of 2 in CDCl_3	16	Figure S38	HMQC spectrum of 5 in CDCl_3	40
Figure S15	^{13}C NMR spectrum of 2 in CDCl_3	17	Figure S39	COSY spectrum of 5 in CDCl_3	41
Figure S16	DEPT spectra of 2 in CDCl_3	18	Figure S40	HMBC spectrum of 5 in CDCl_3	42
Figure S17	HMQC spectrum of 2 in CDCl_3	19	Figure S41	NOESY spectrum of 5 in CDCl_3	43
Figure S18	COSY spectrum of 2 in CDCl_3	20	Figure S42	^1H NMR spectrum of 6 in CDCl_3	44
Figure S19	HMBC spectrum of 2 in CDCl_3	21	Figure S43	^{13}C NMR spectrum of 6 in CDCl_3	45
Figure S20	NOESY spectrum of 2 in CDCl_3	22	Figure S44	HMQC spectrum of 6 in CDCl_3	46
Figure S21	^1H NMR spectrum of 3 in CDCl_3	23	Figure S45	COSY spectrum of 6 in CDCl_3	47
Figure S22	^{13}C NMR spectrum of 3 in CDCl_3	24	Figure S46	HMBC spectrum of 6 in CDCl_3	48
Figure S23	DEPT spectra of 3 in CDCl_3	25	Figure S47	NOESY spectrum of 6 in CDCl_3	49
Figure S24	HMQC spectrum of 3 in CDCl_3	26			

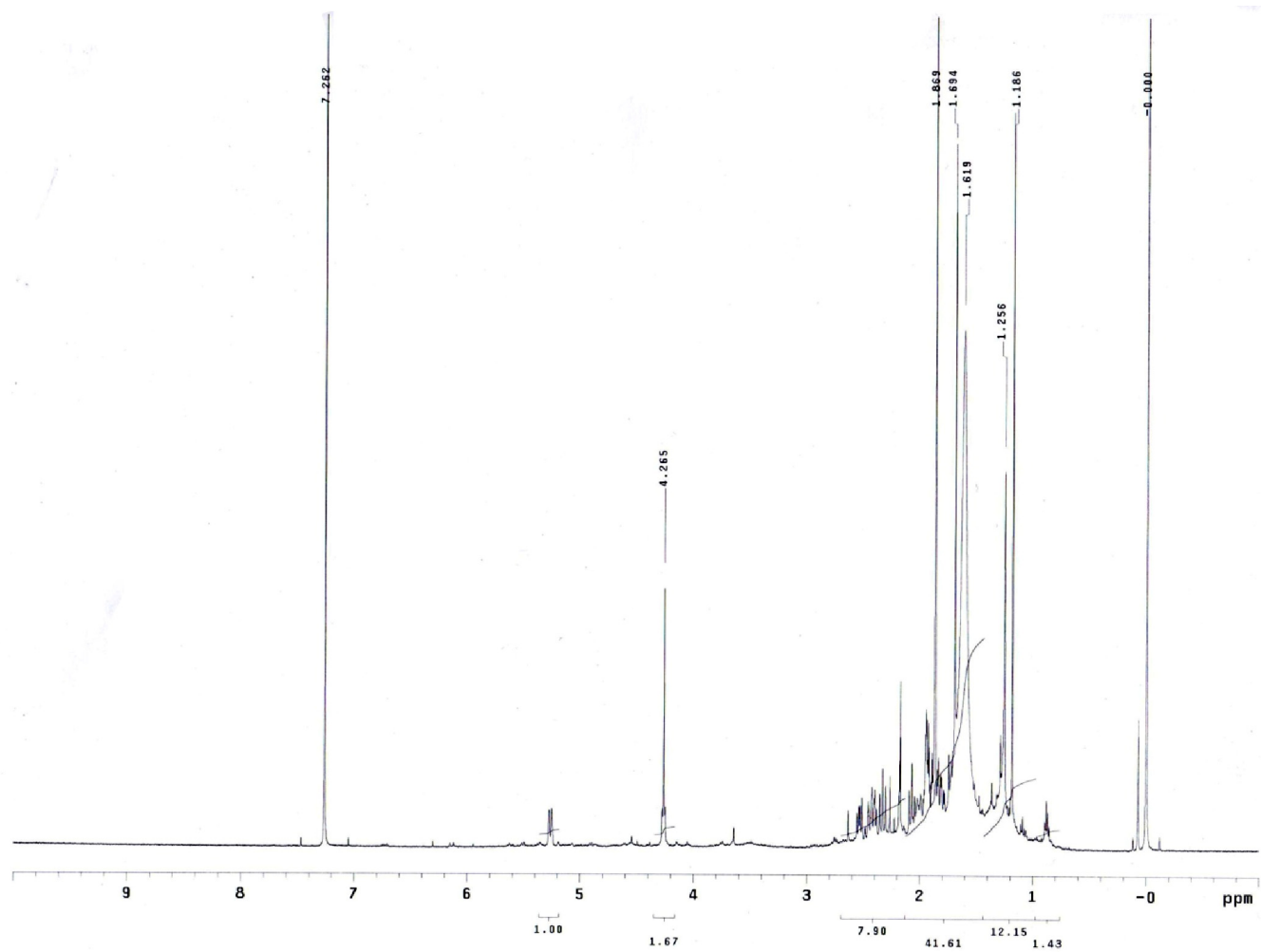


Figure S1. ¹H NMR spectrum of 1 in CDCl₃

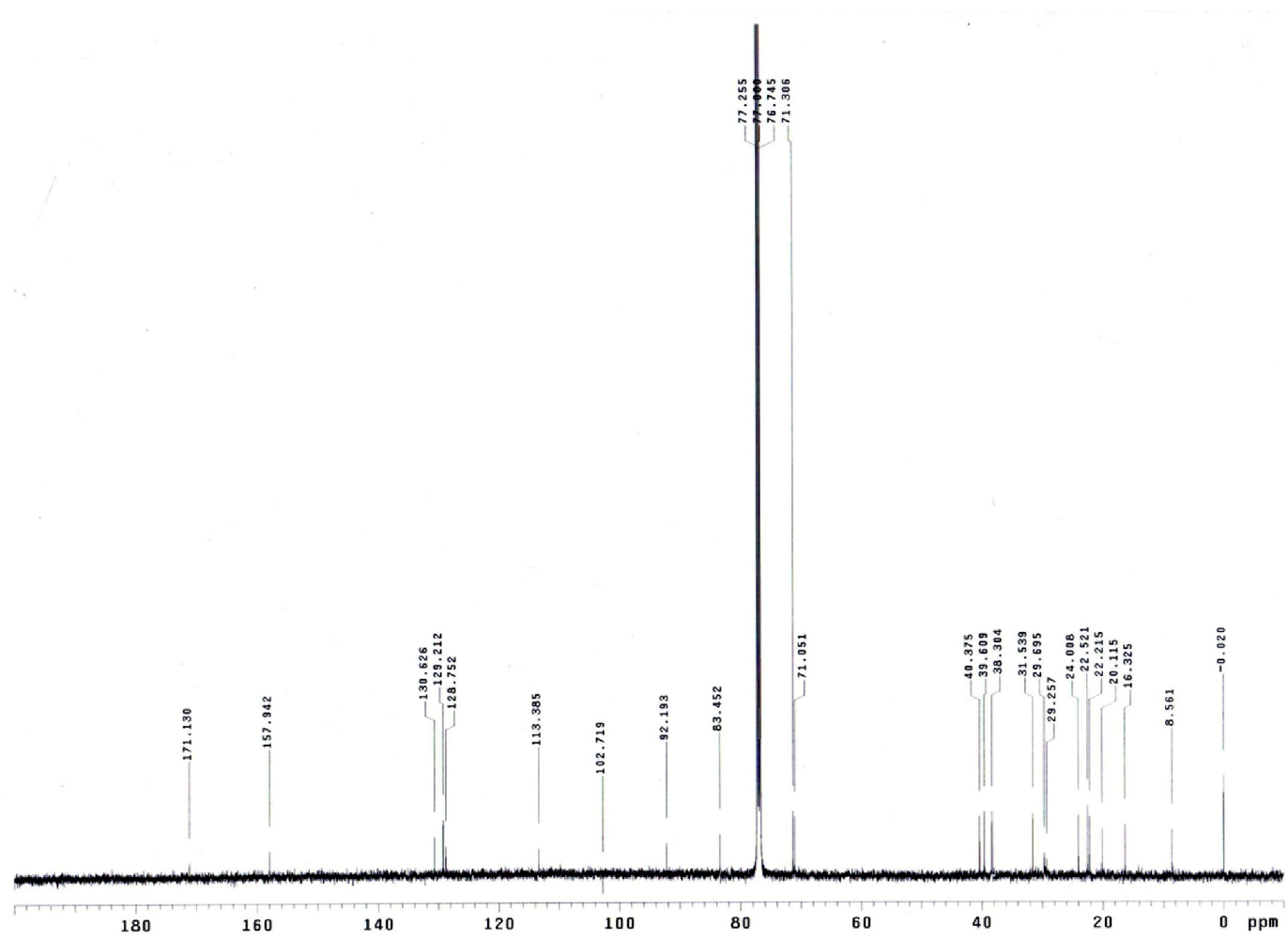


Figure S2. ^{13}C NMR spectrum of 1 in CDCl_3

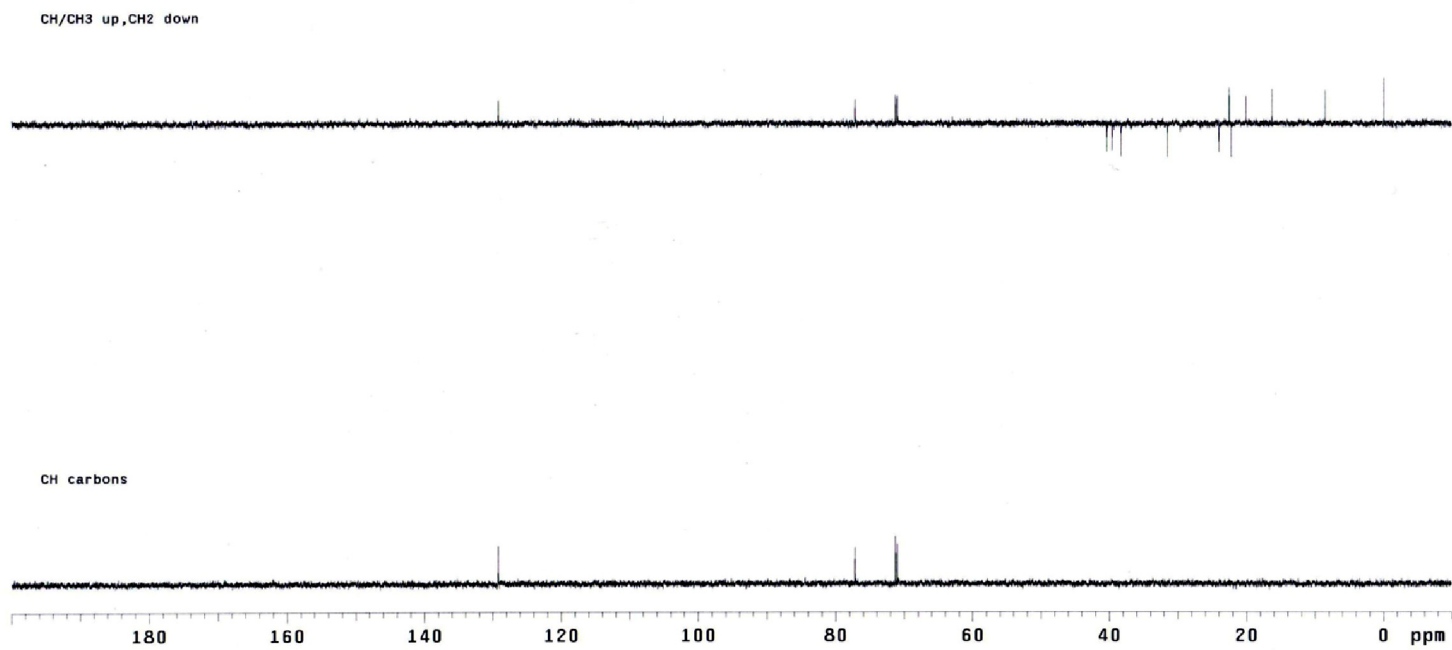


Figure S3. DEPT spectra of **1** in CDCl₃

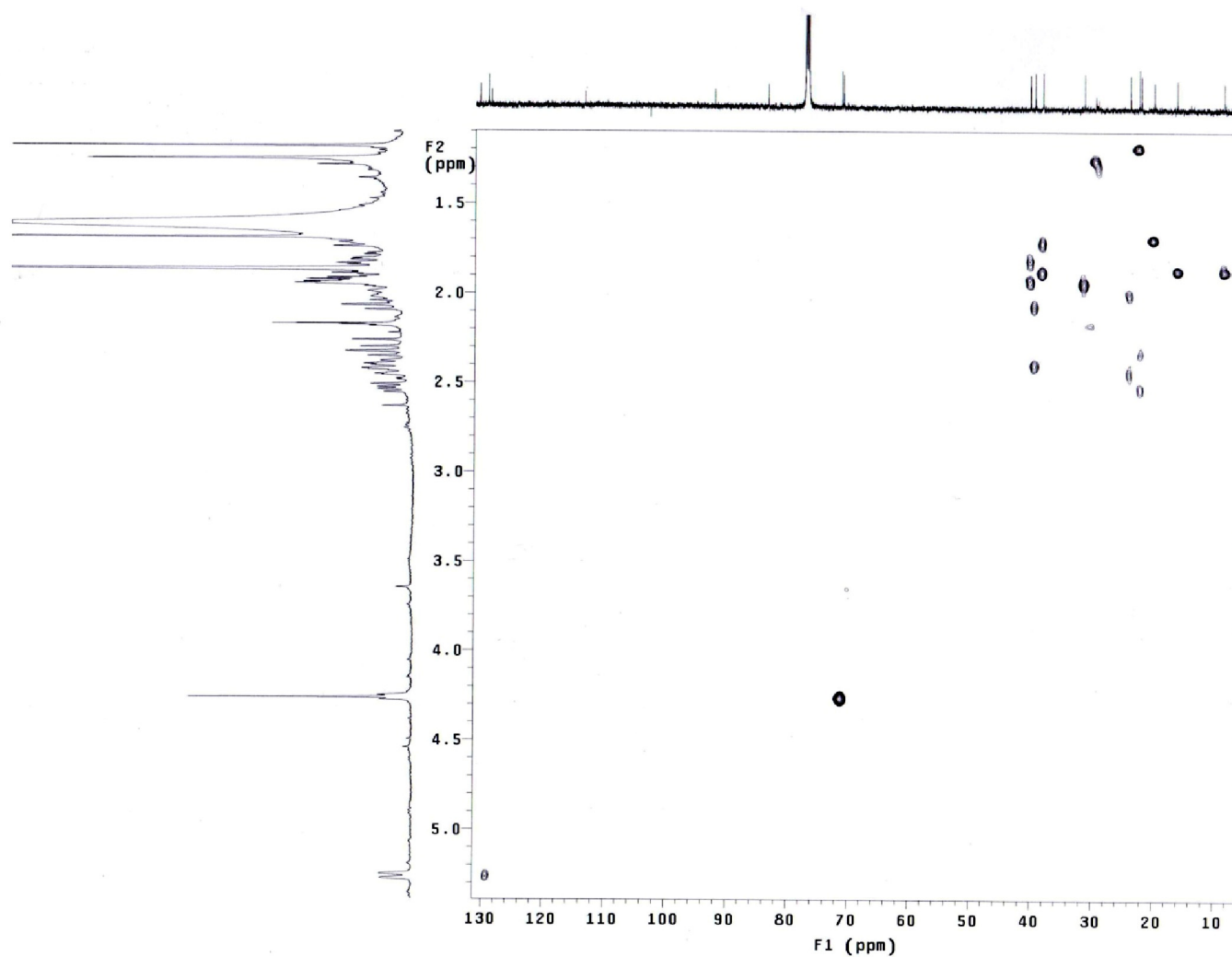


Figure S4. HMQC spectrum of **1** in CDCl₃

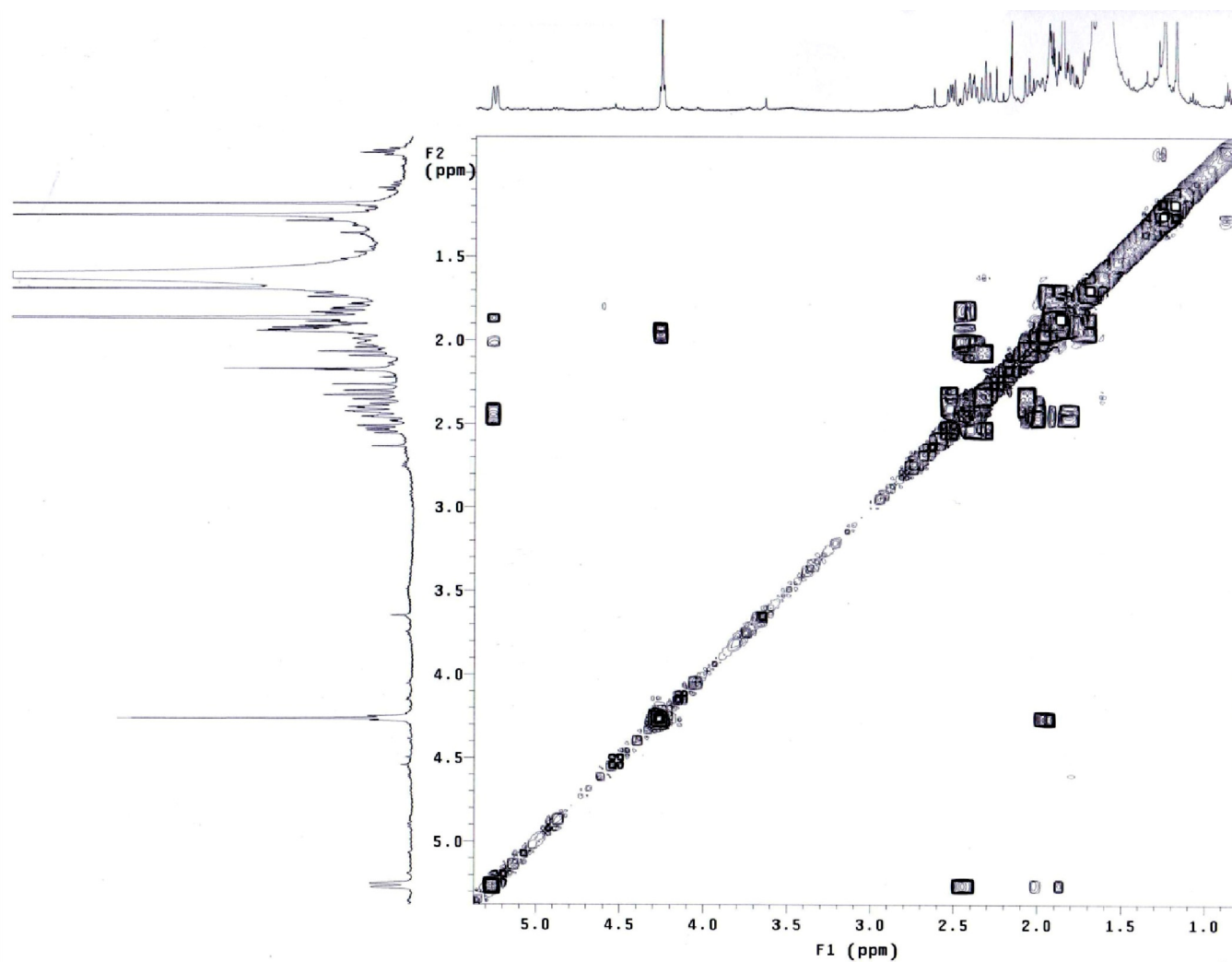


Figure S5. COSY spectrum of **1** in CDCl₃

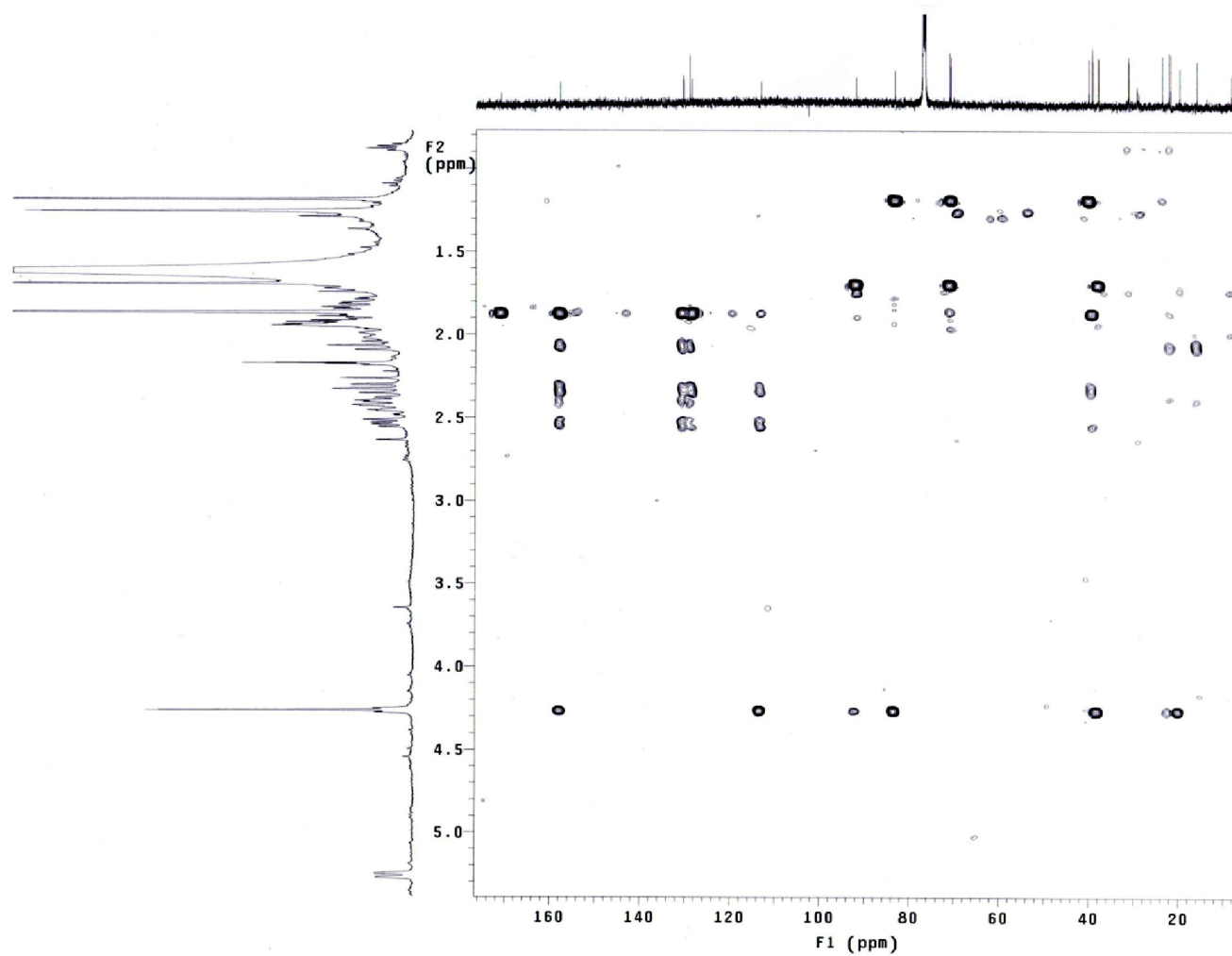


Figure S6. HMBC spectrum of **1** in CDCl₃

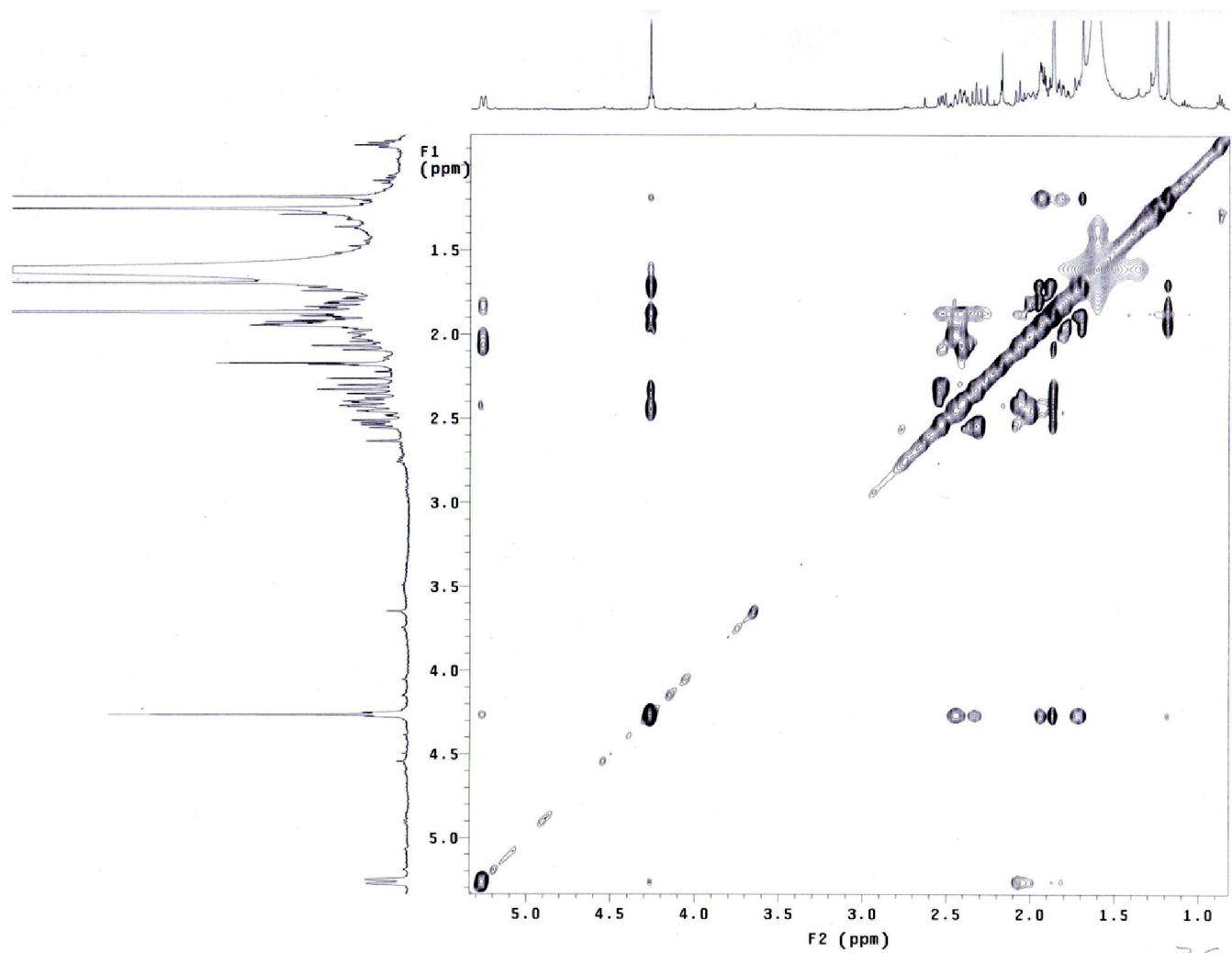


Figure S7. NOESY spectrum of **1** in CDCl₃

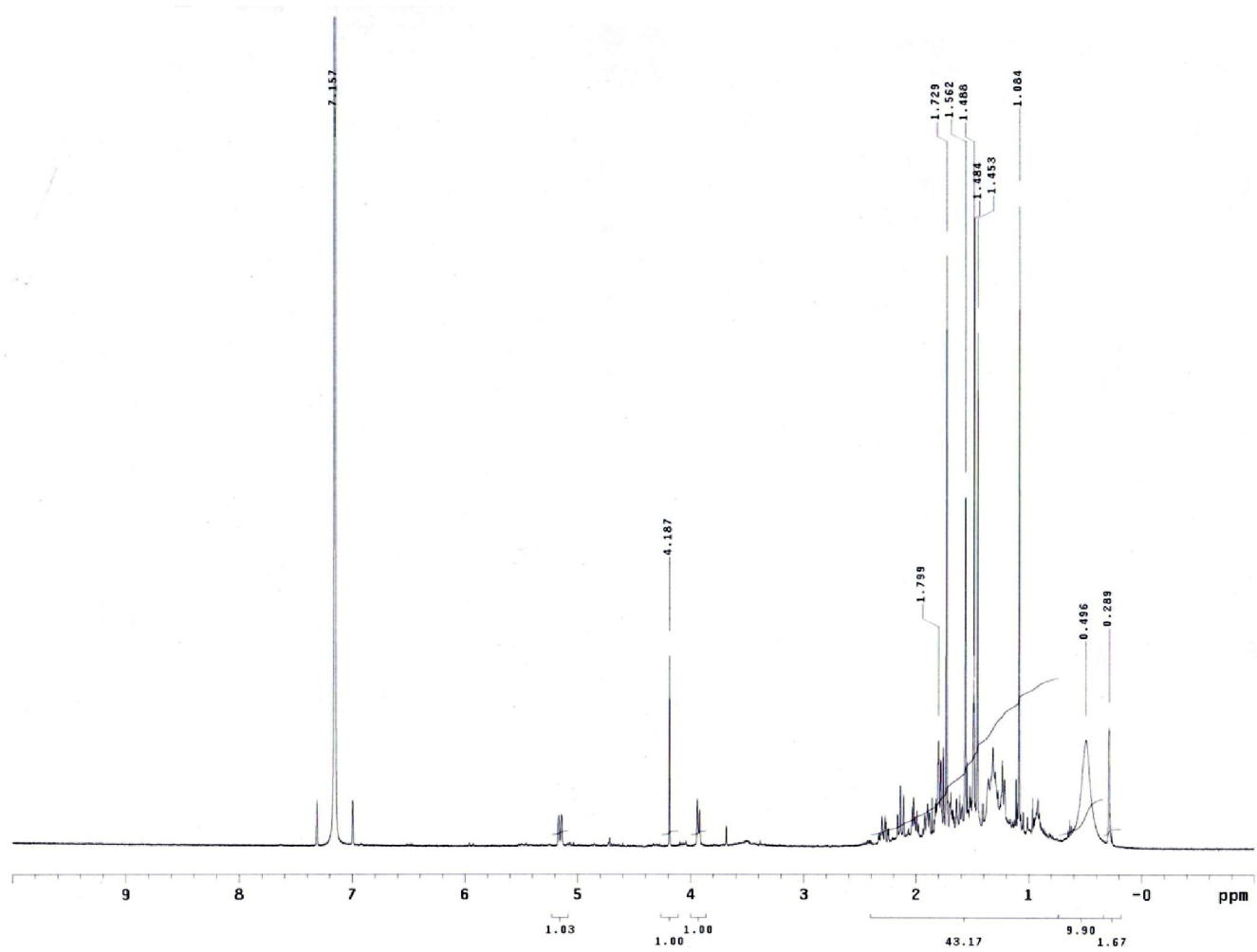


Figure S8. ^1H NMR spectrum of **1** in C_6D_6

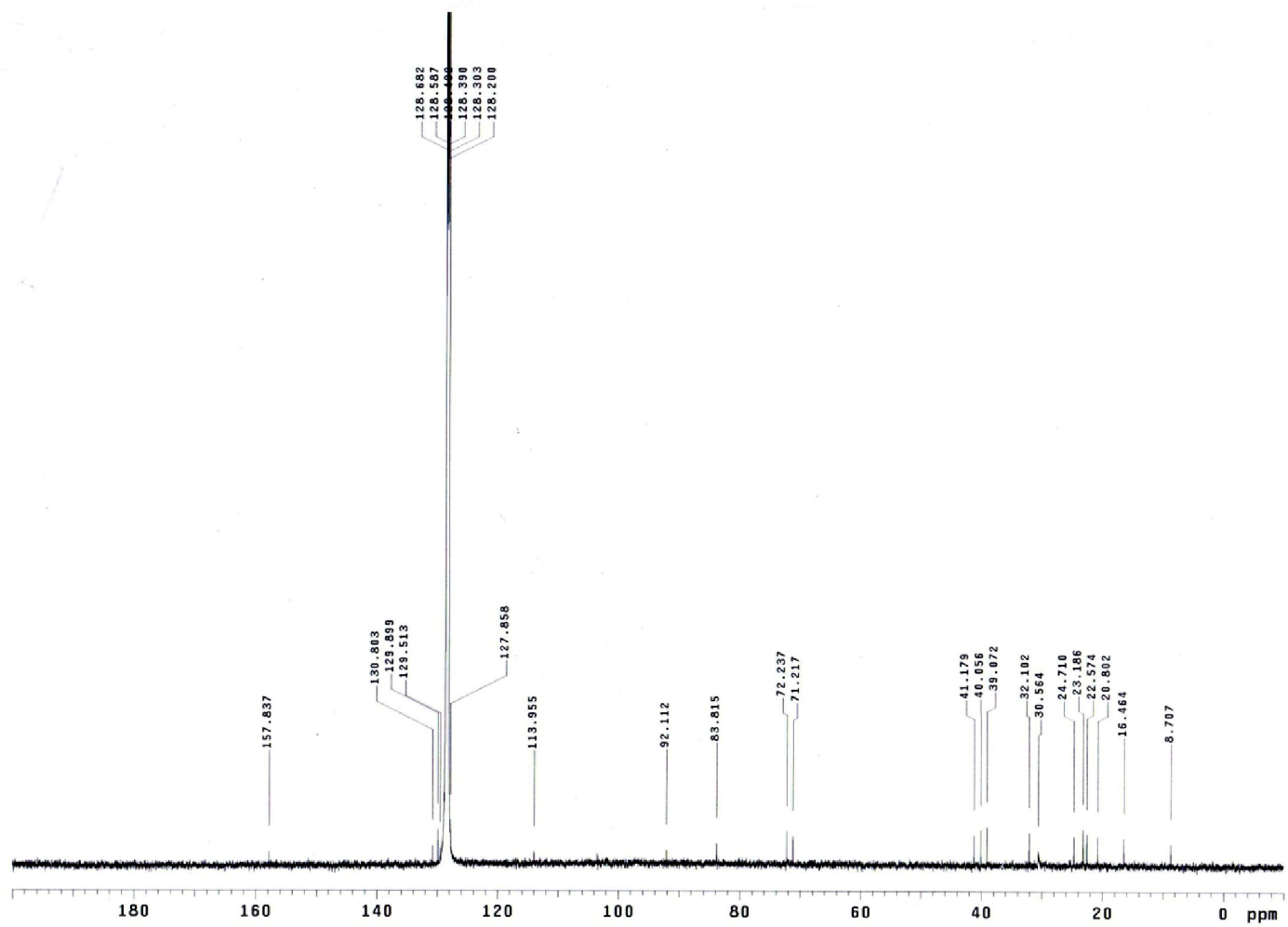


Figure S9. ^{13}C NMR spectrum of 1 in C_6D_6

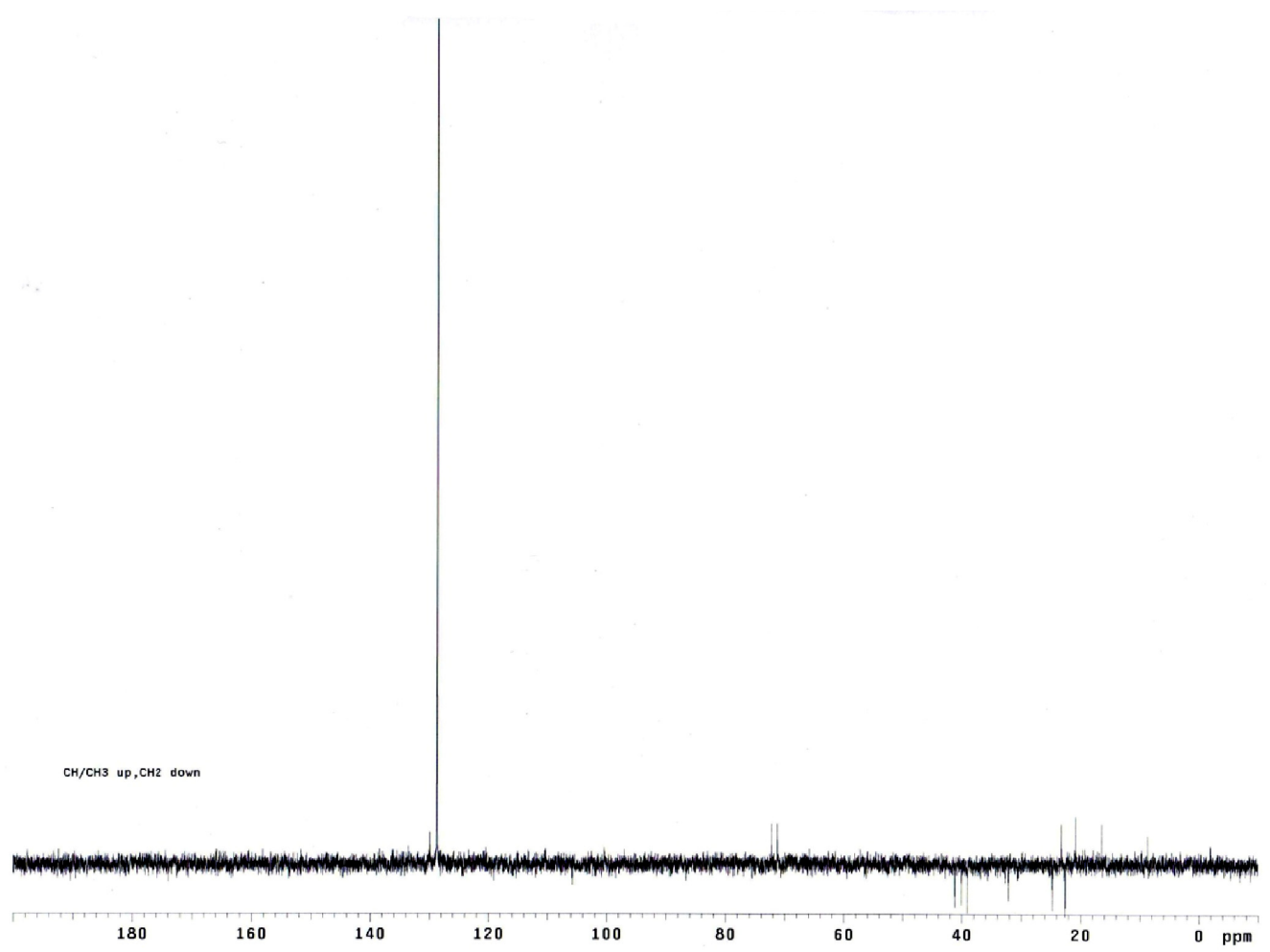


Figure S10. DEPT spectrum of **1** in C₆D₆

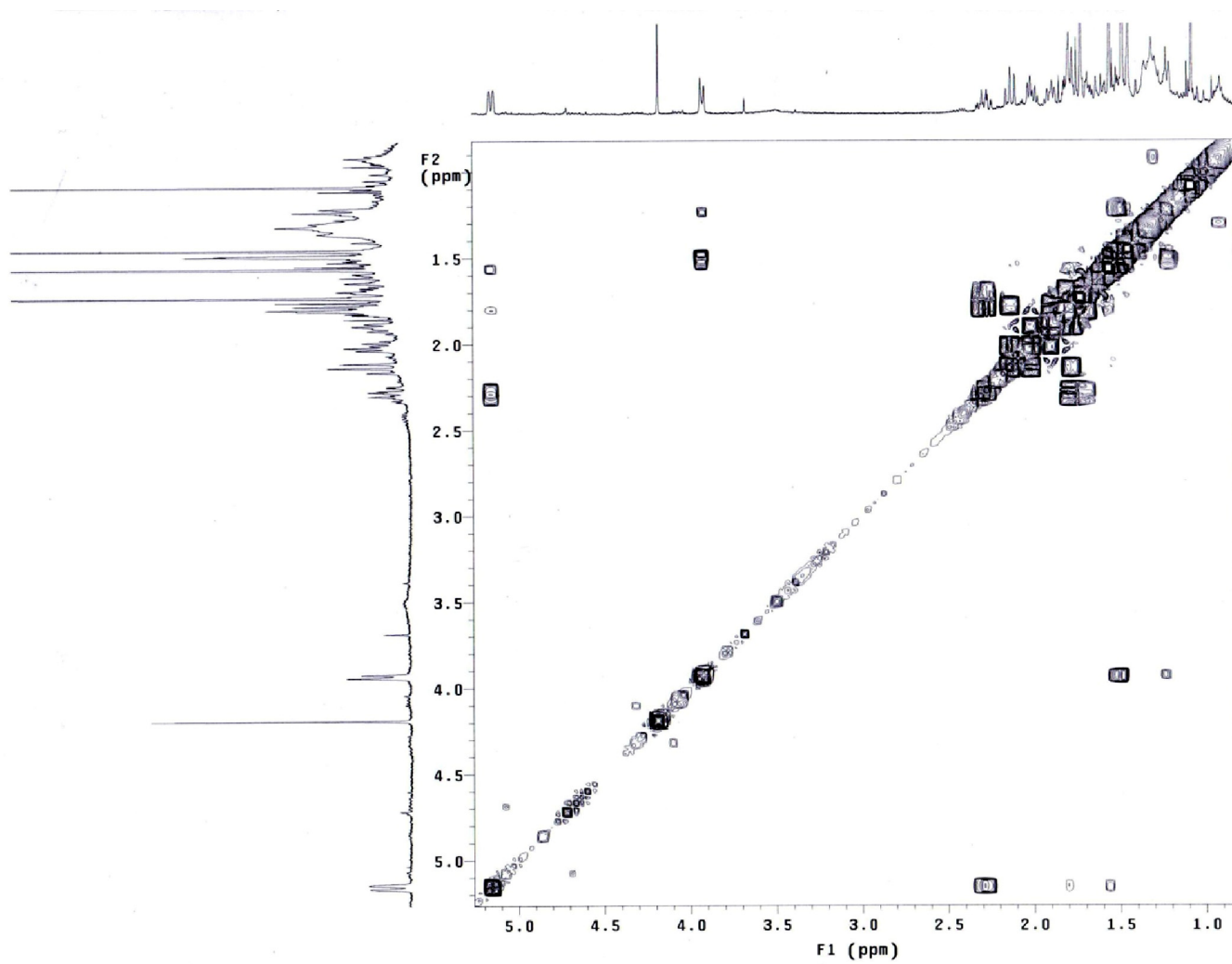


Figure S11. COSY spectrum of **1** in C₆D₆

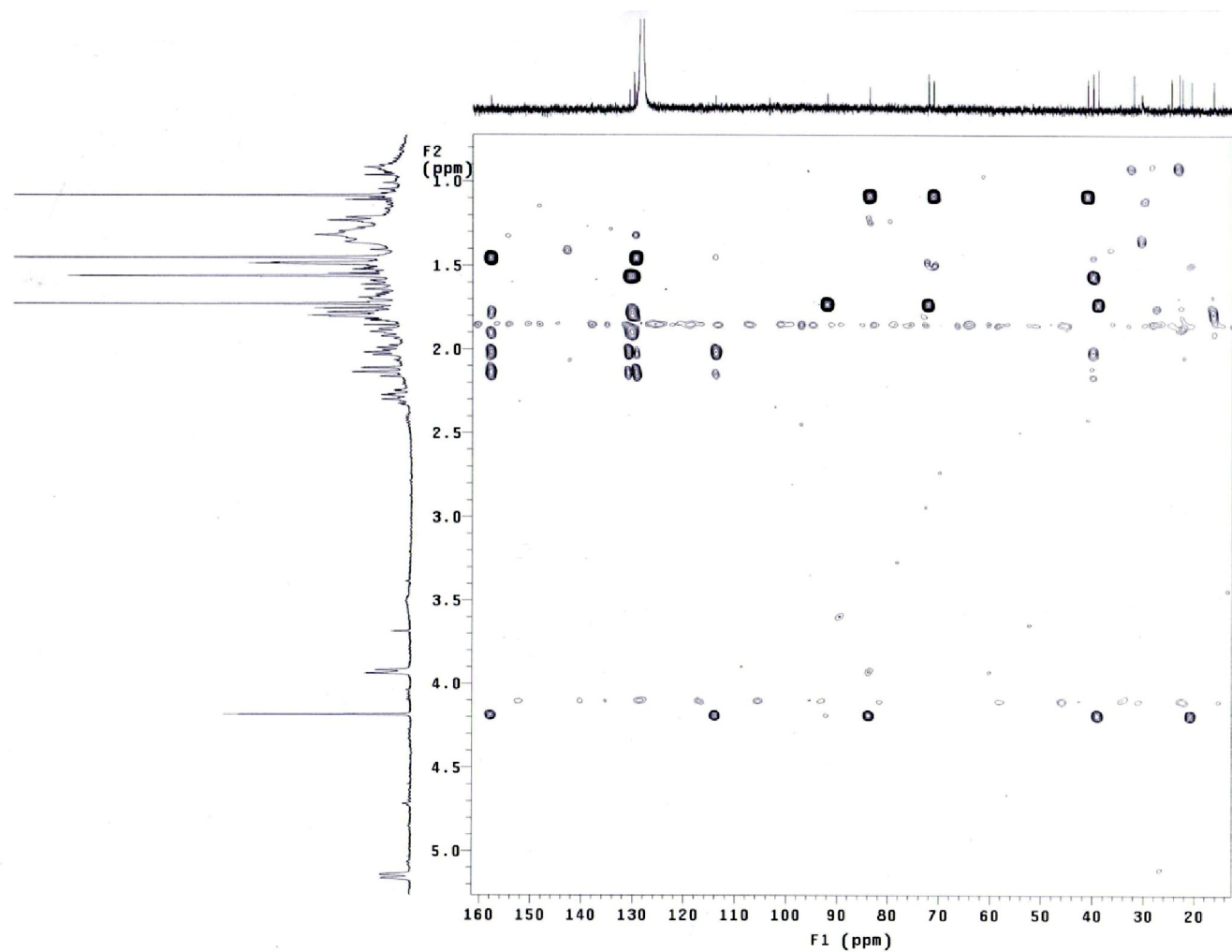


Figure S12. HMBC spectrum of **1** in C_6D_6

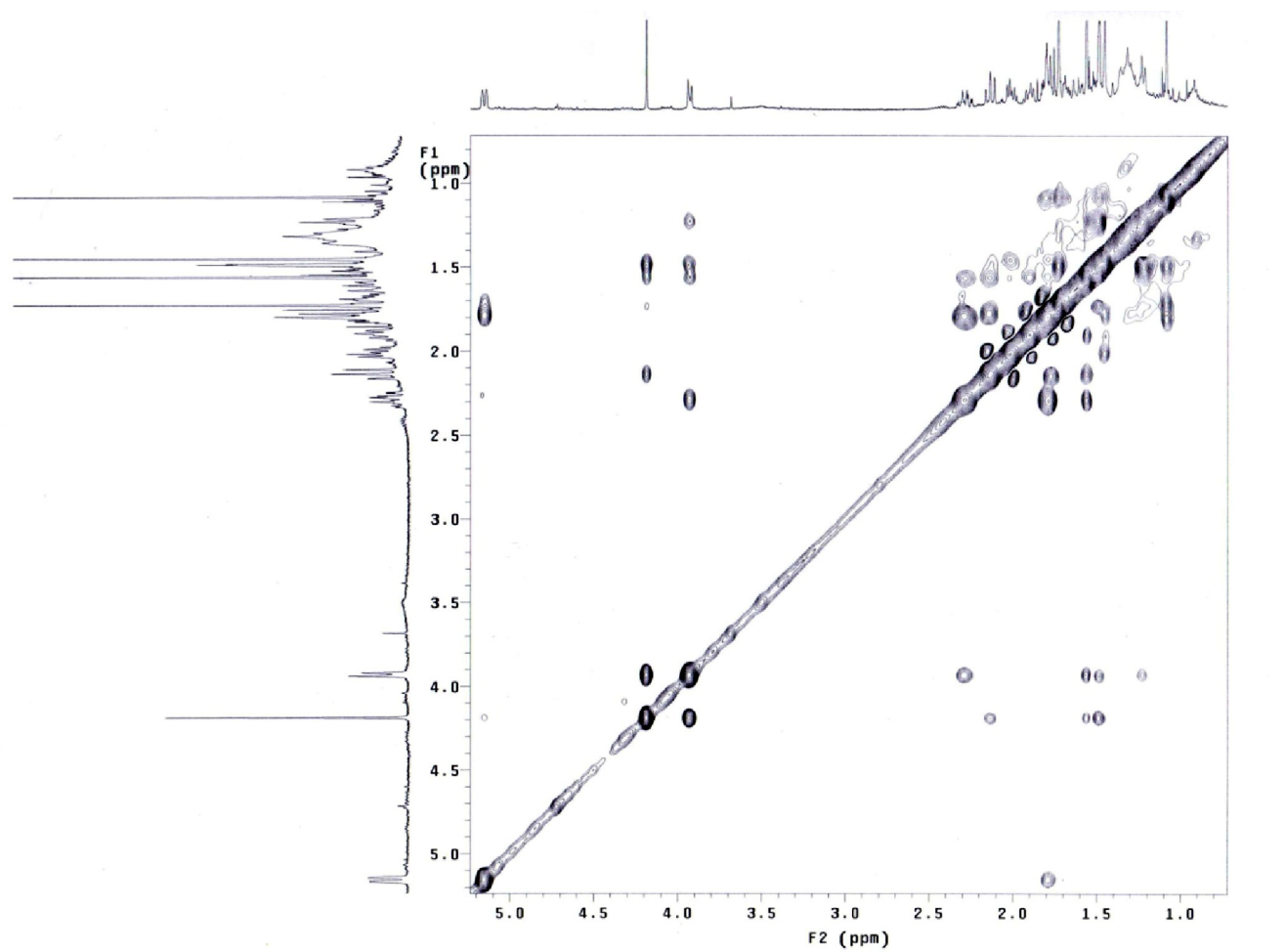


Figure S13. NOESY spectrum of **1** in C_6D_6

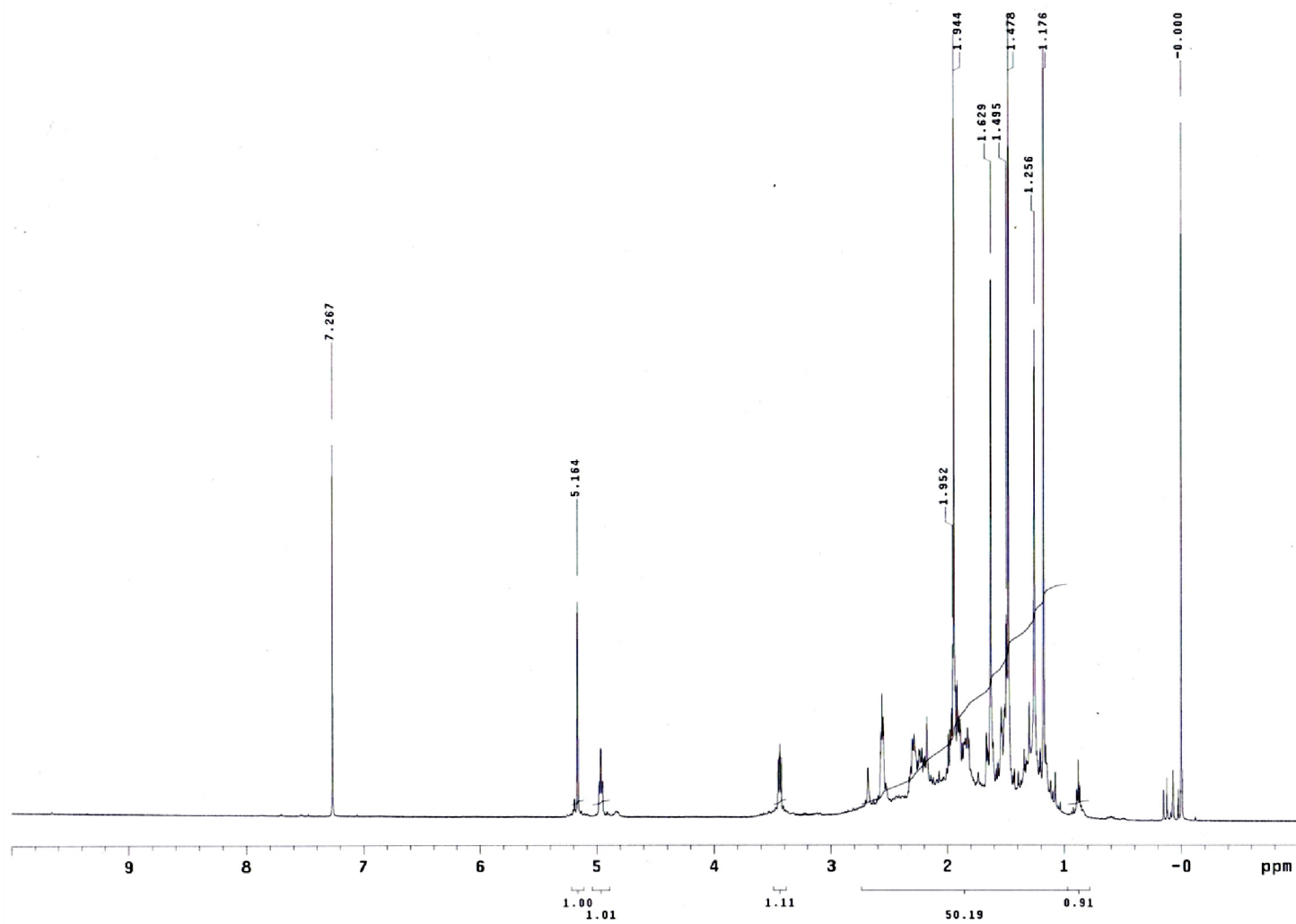


Figure S14. ¹H NMR spectrum of **2** in CDCl₃

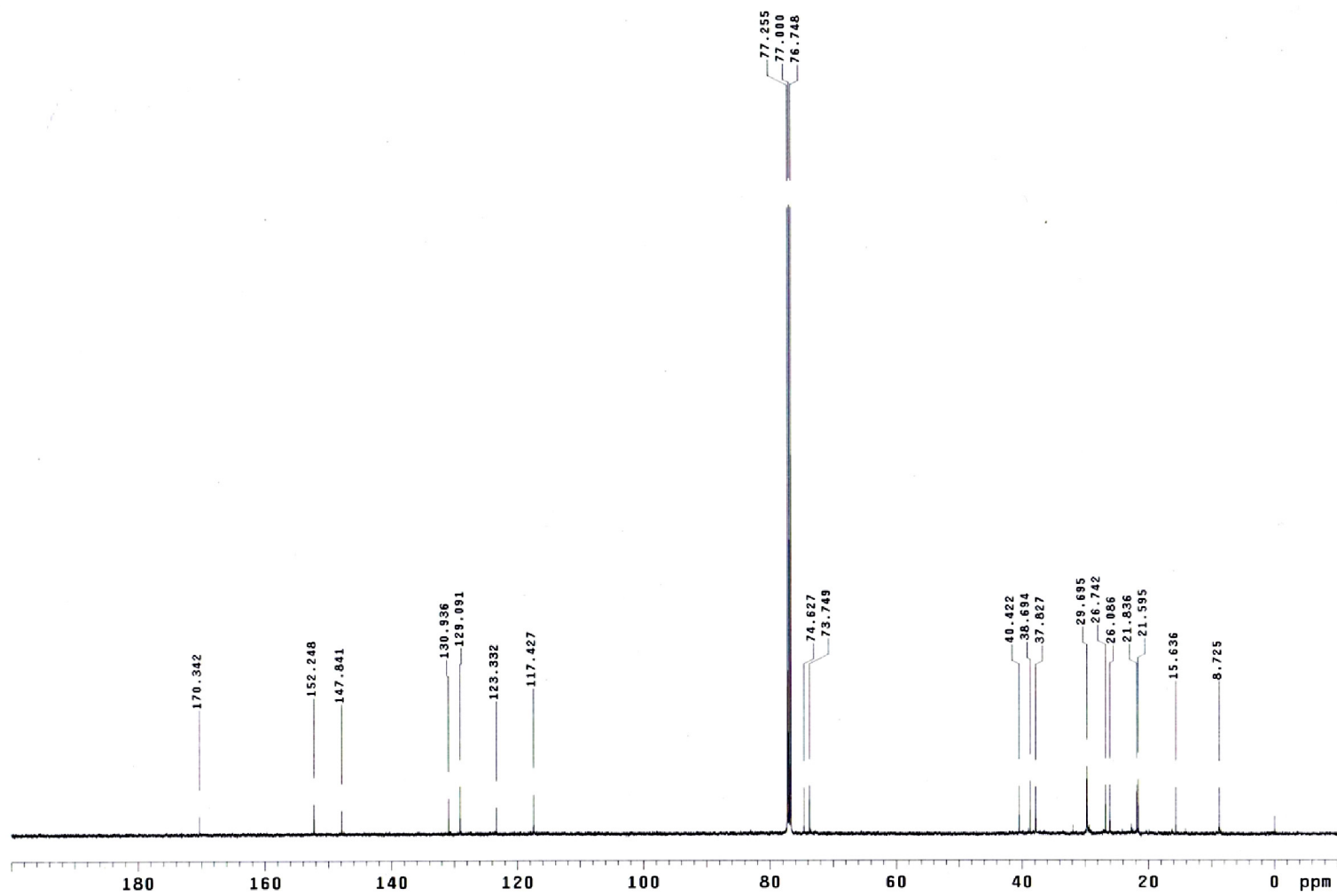


Figure S15. ^{13}C NMR spectrum of **2** in CDCl_3

CH/CH3 up, CH2 down



CH carbons

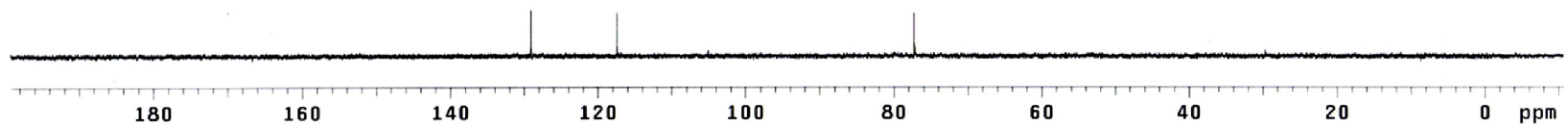


Figure S16. DEPT spectra of **2** in CDCl_3

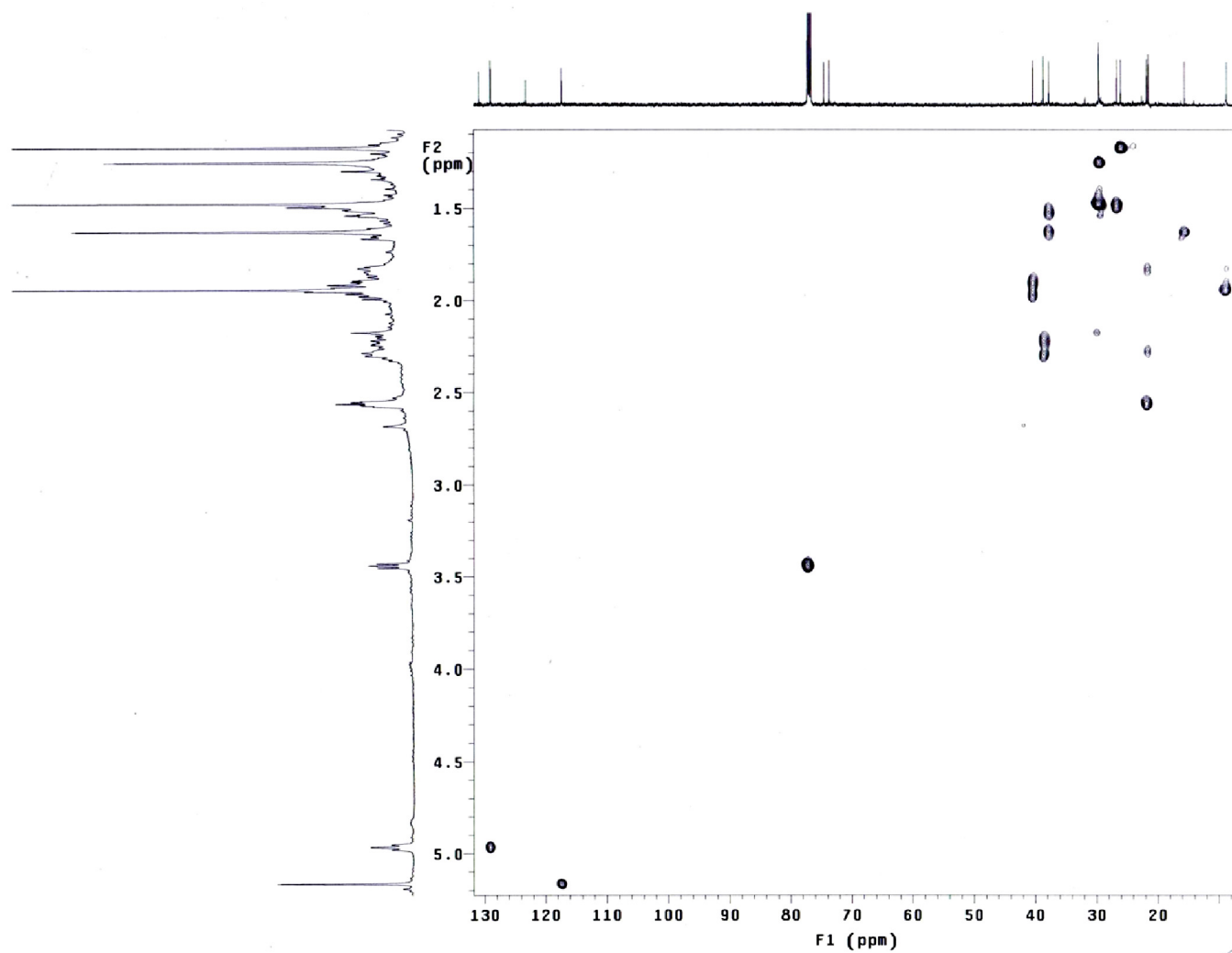


Figure S17. HMQC spectrum of 2 in CDCl₃

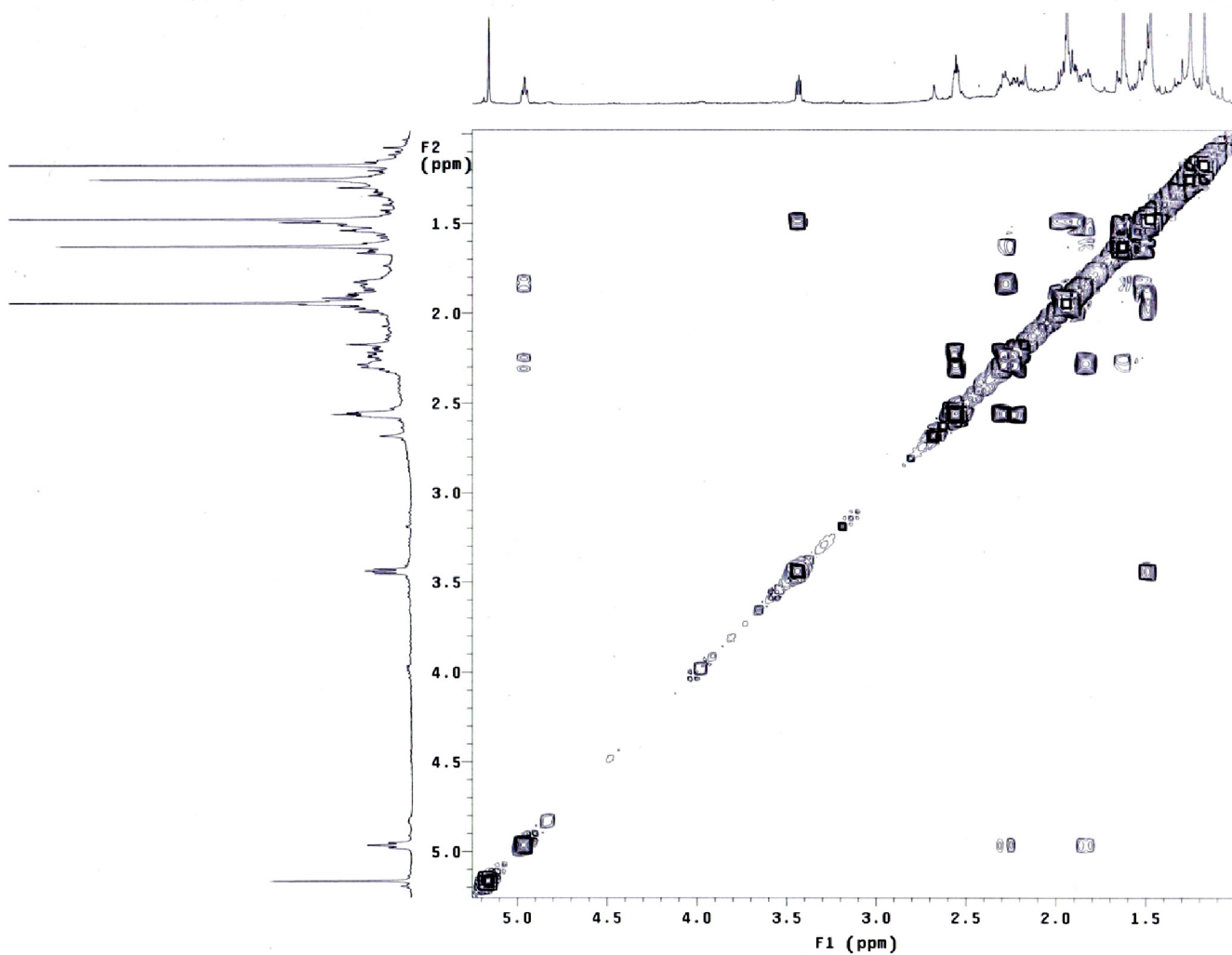


Figure S18. COSY spectrum of **2** in CDCl₃

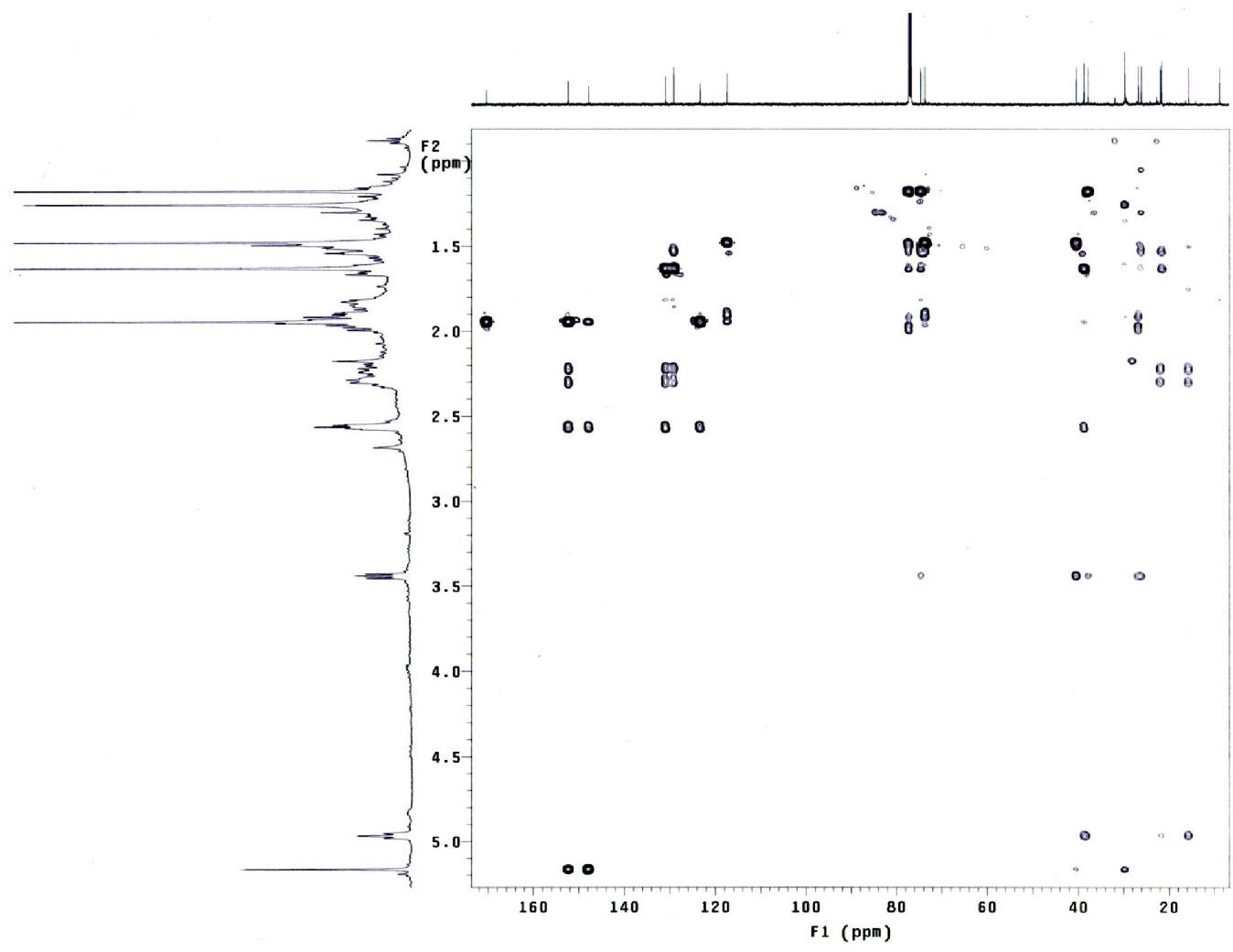


Figure S19. HMBC spectrum of **2** in CDCl₃

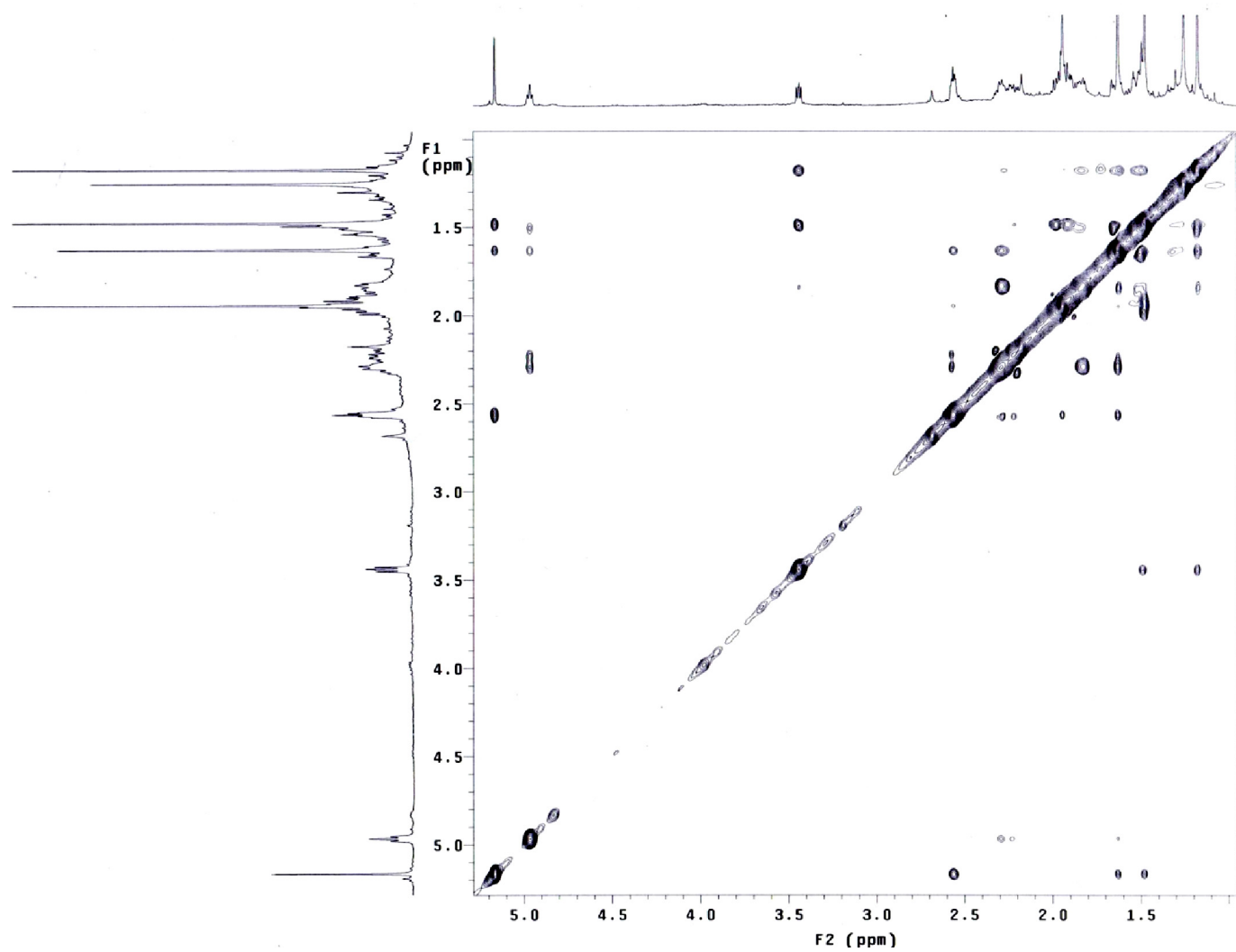


Figure S20. NOESY spectrum of **2** in CDCl₃

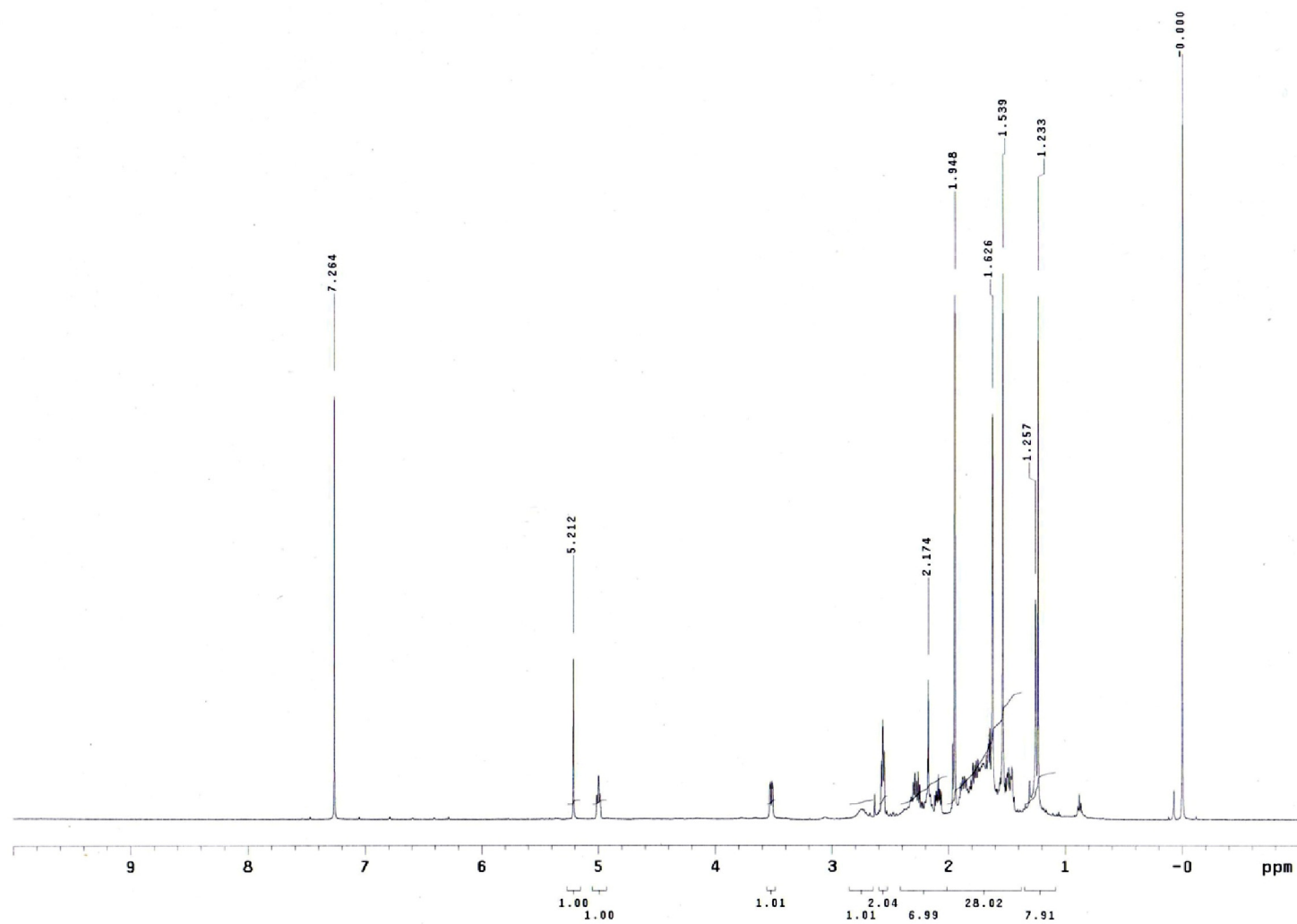


Figure S21. ^1H NMR spectrum of **3** in CDCl_3

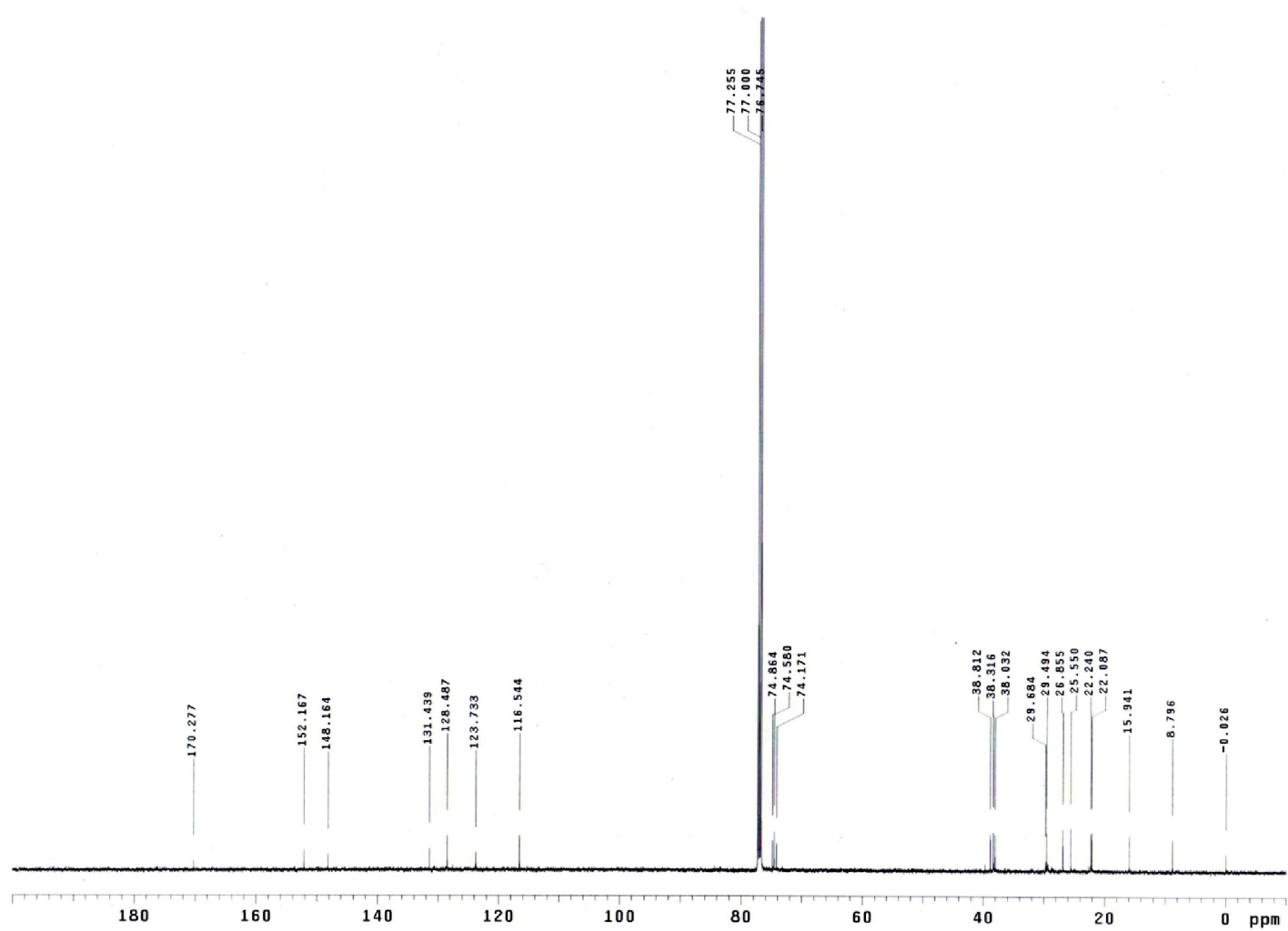


Figure S22. ^{13}C NMR spectrum of **3** in CDCl_3

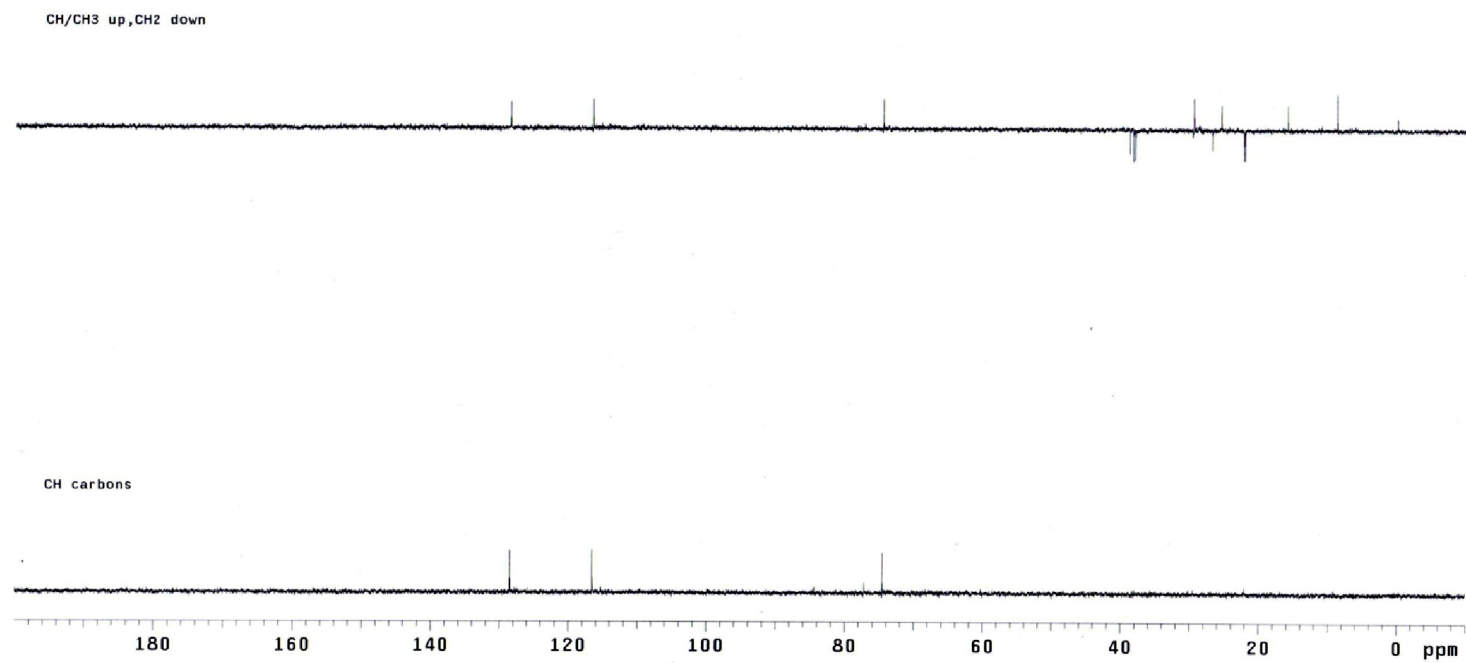


Figure S23. DEPT spectra of **3** in CDCl_3

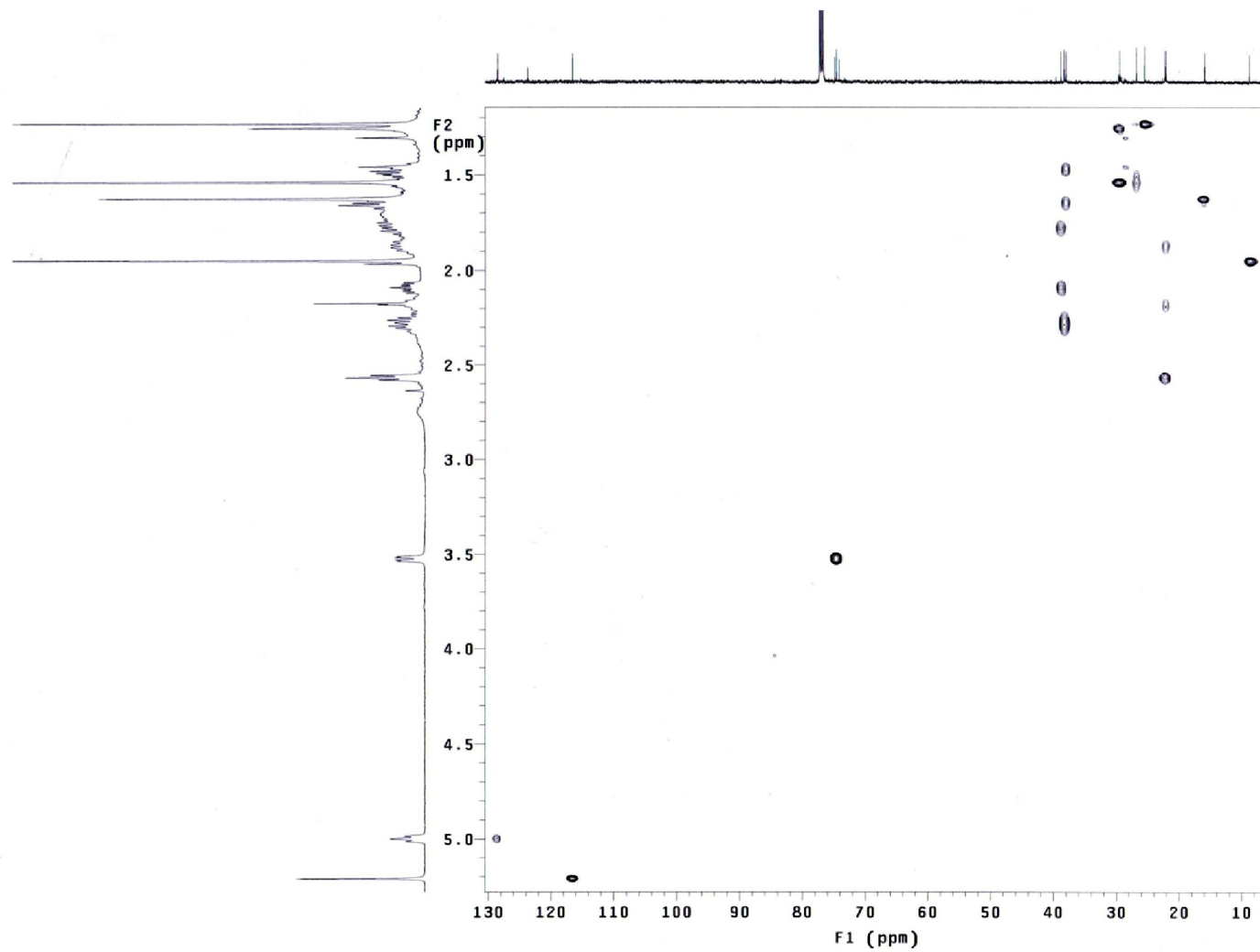


Figure S24. HMQC spectrum of **3** in CDCl₃

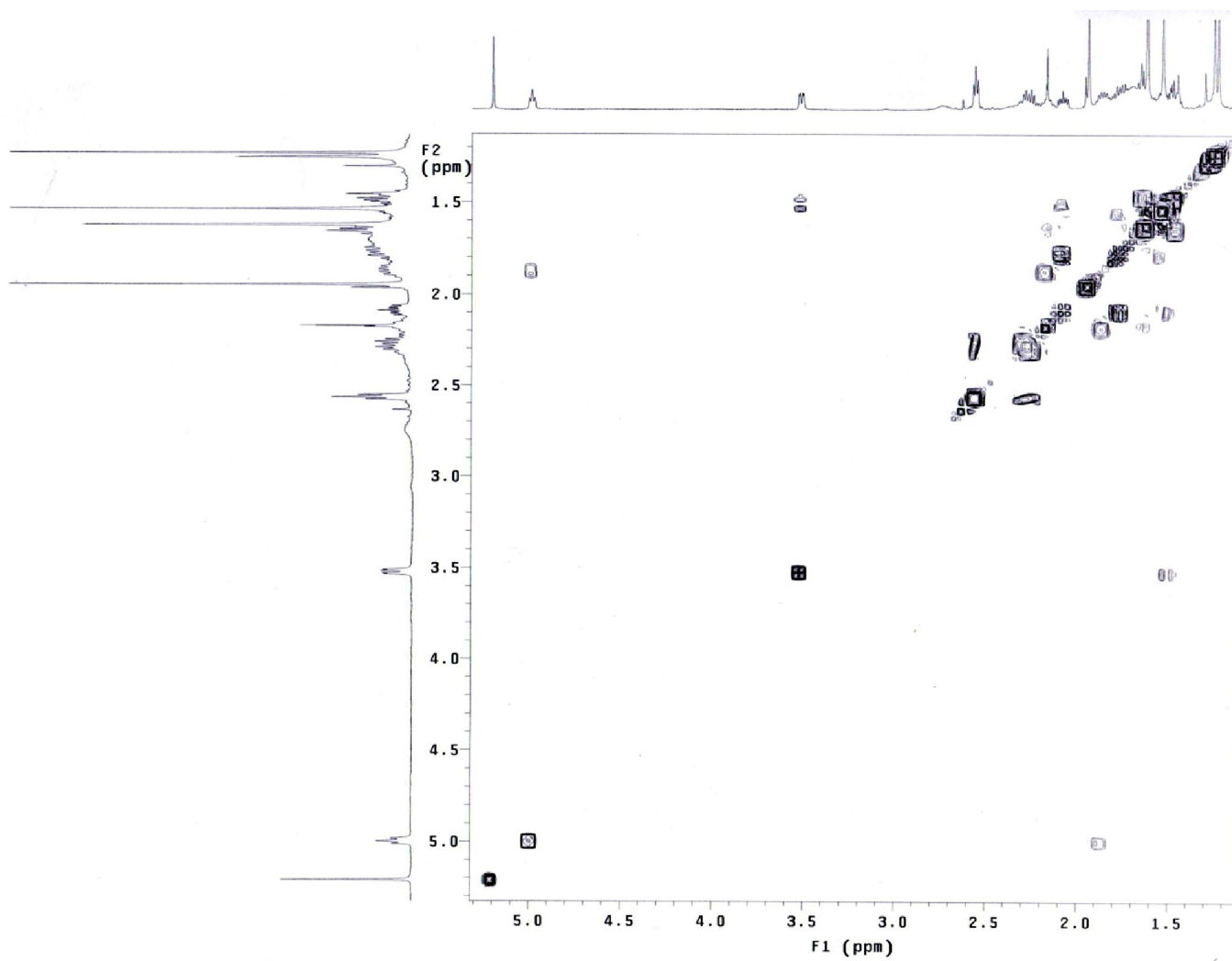


Figure S25. COSY spectrum of **3** in CDCl₃

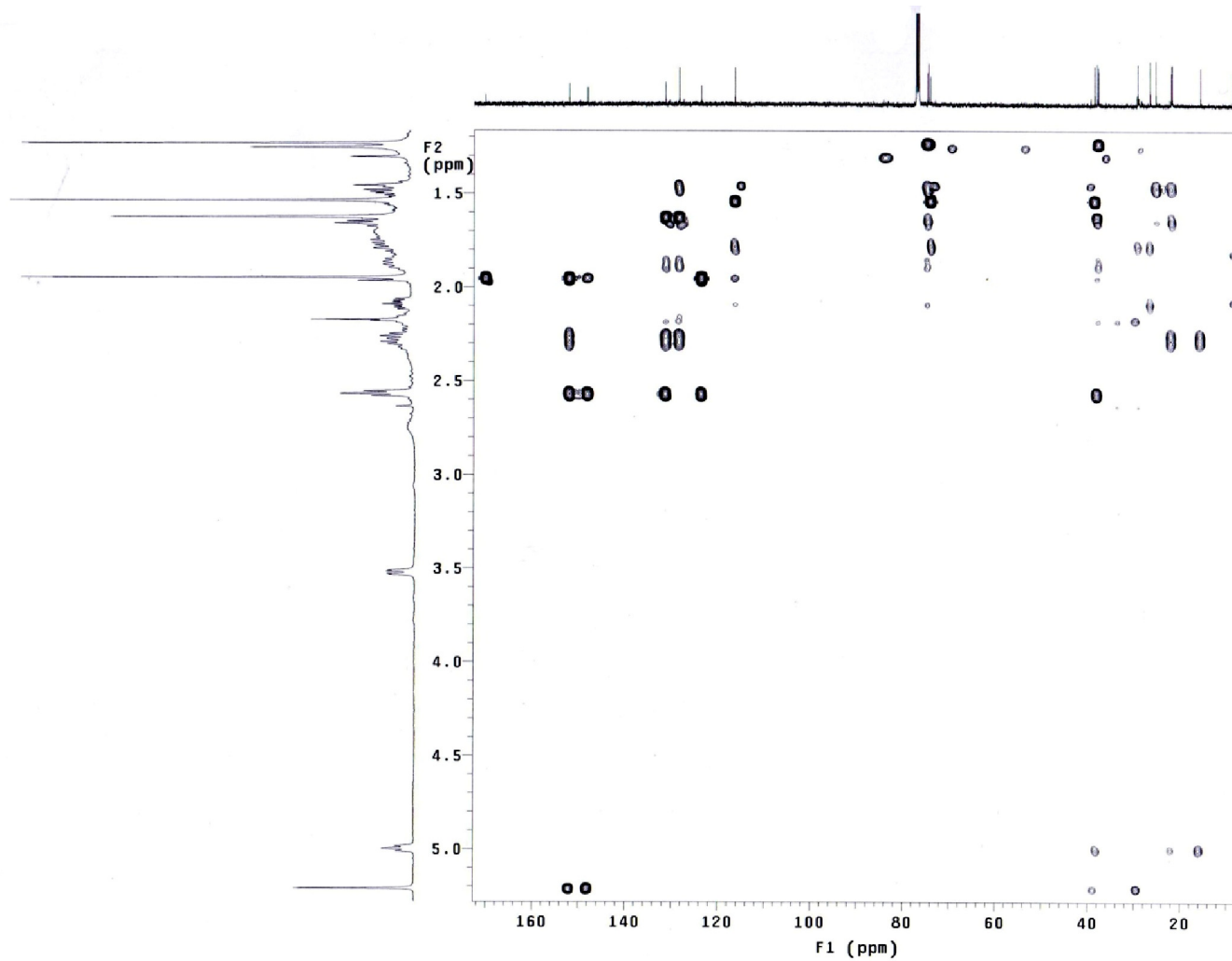


Figure S26. HMBC spectrum of **3** in CDCl₃

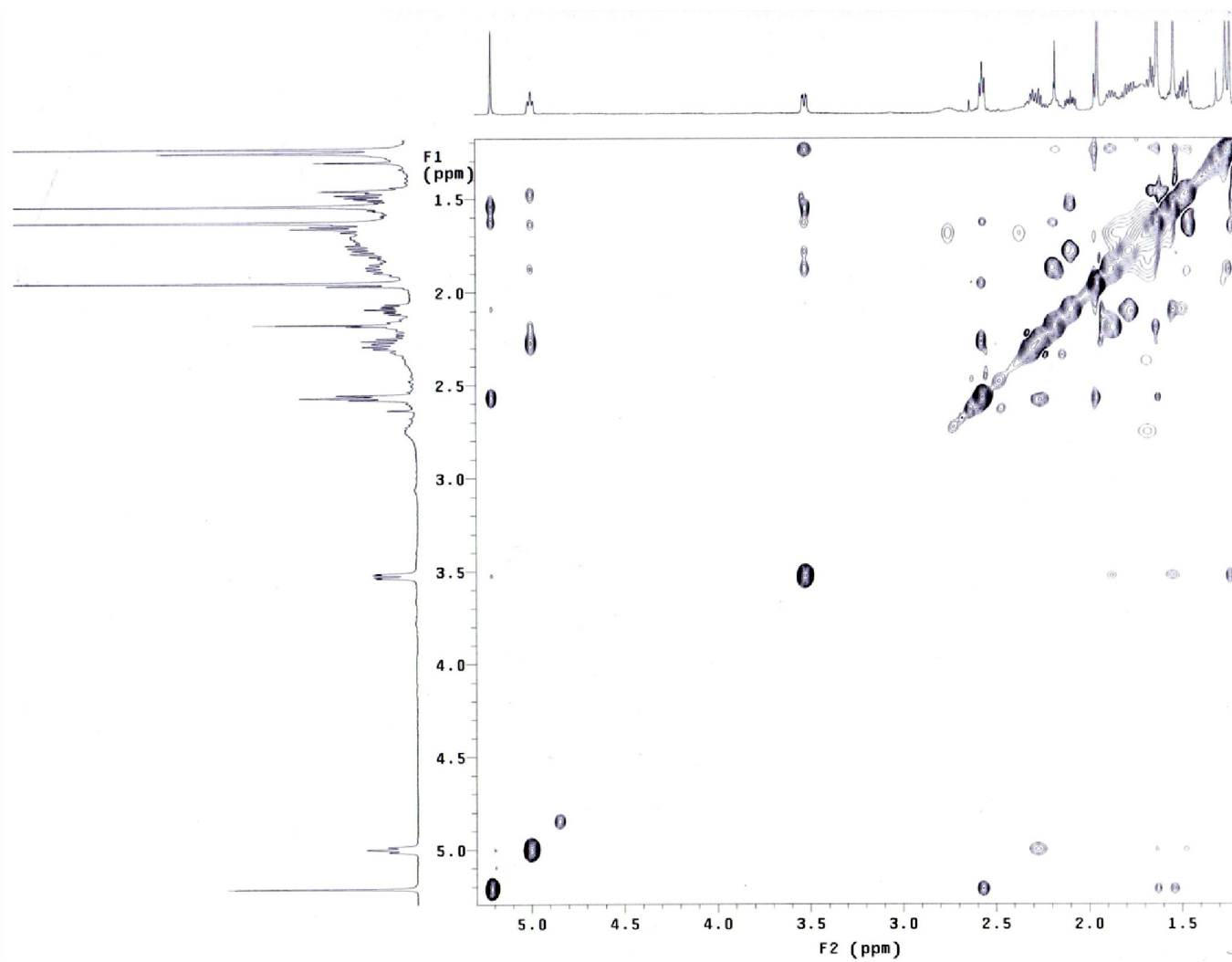


Figure S27. NOESY spectrum of **3** in CDCl₃

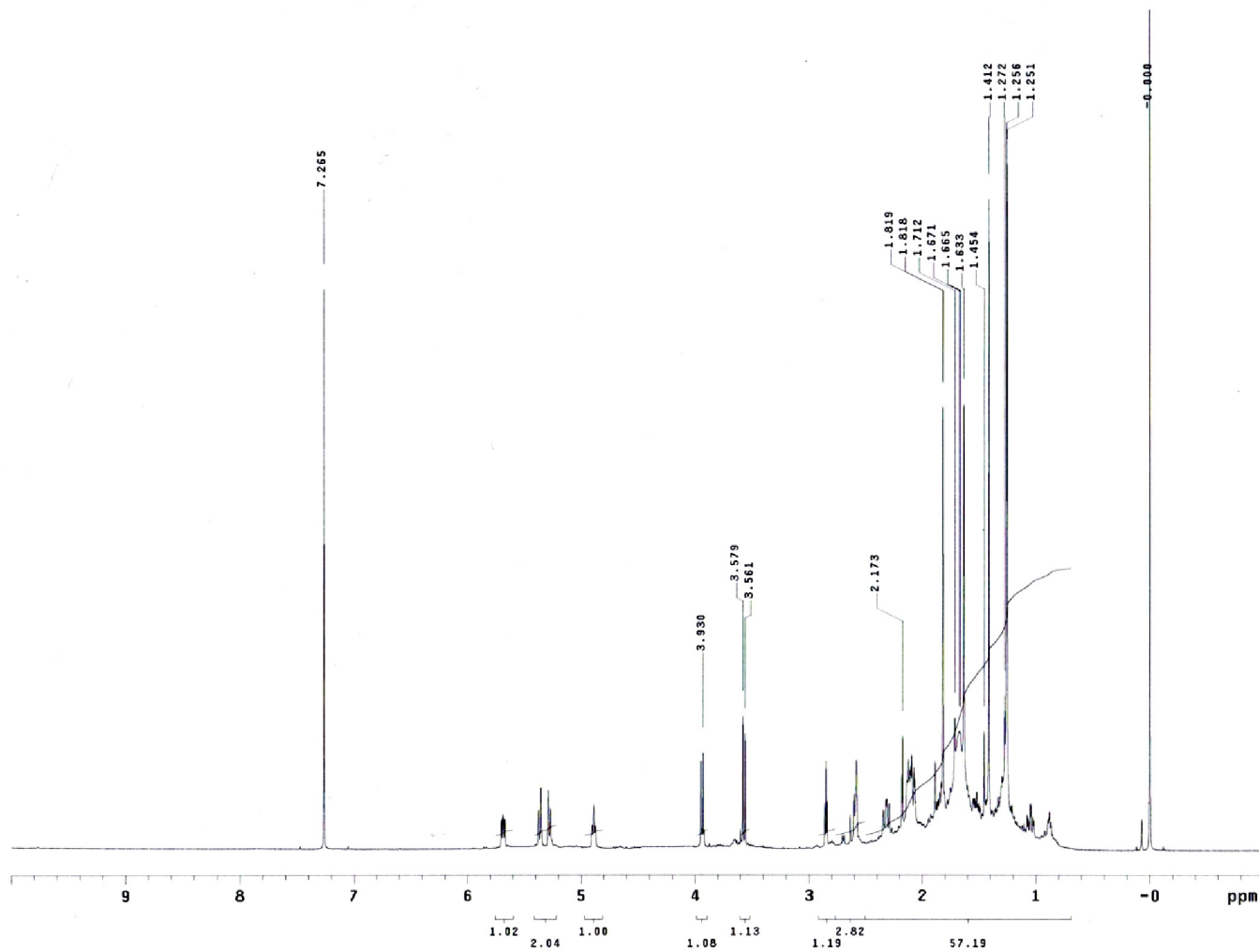


Figure S28. ¹H NMR spectrum of **4** in CDCl₃

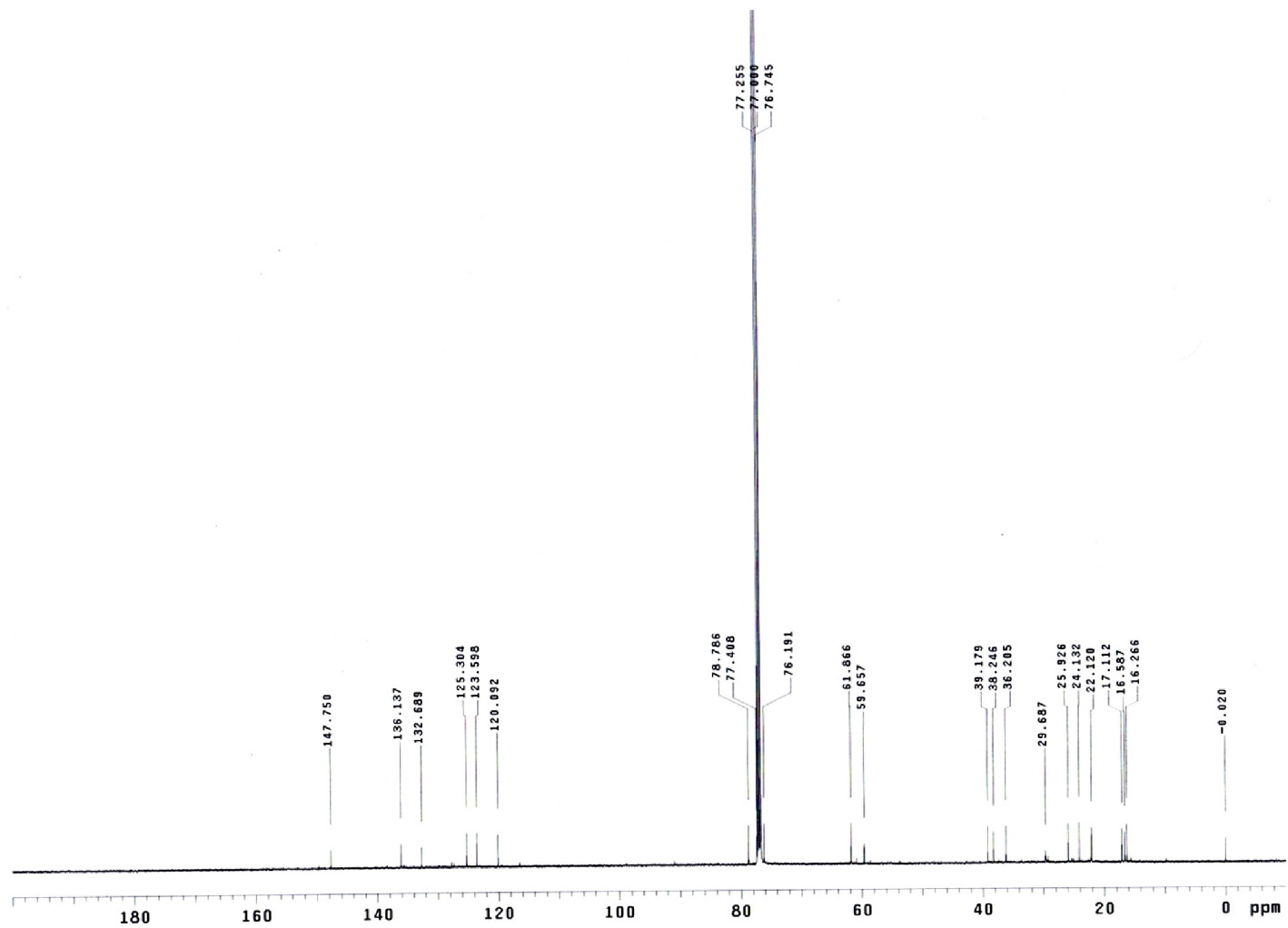


Figure S29. ¹³C NMR spectrum of 4 in CDCl₃

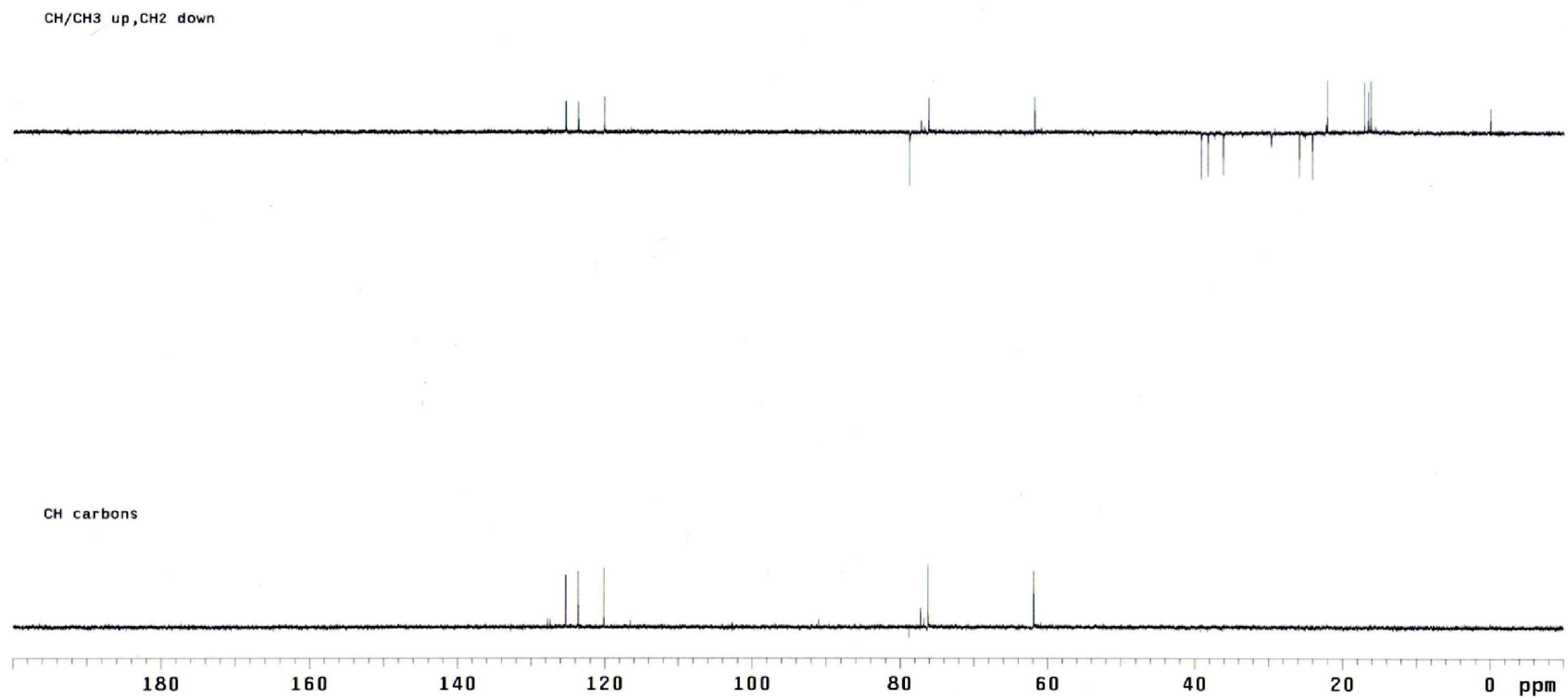


Figure S30. DEPT spectra of **4** in CDCl₃

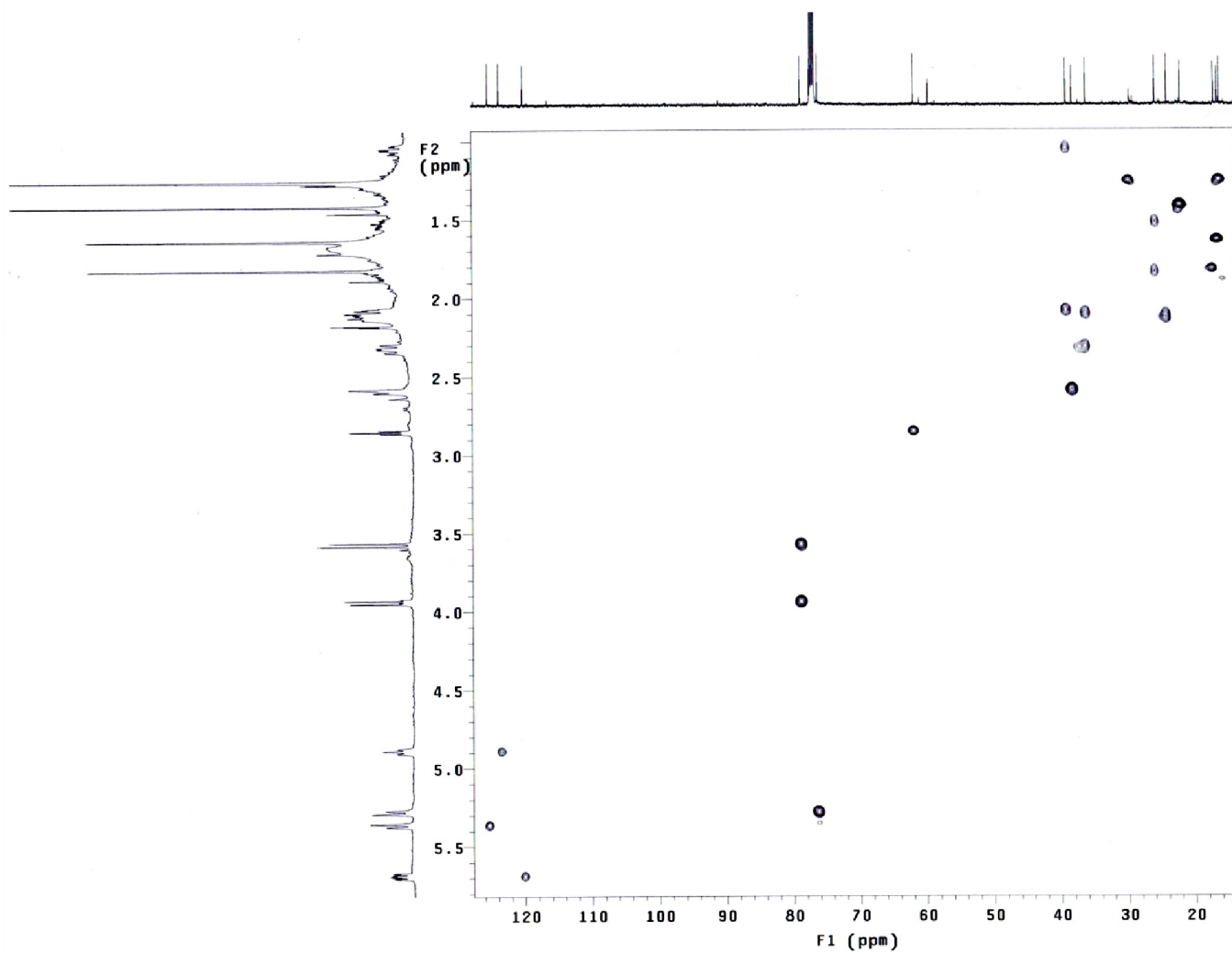


Figure S31. HMQC spectrum of **4** in CDCl₃

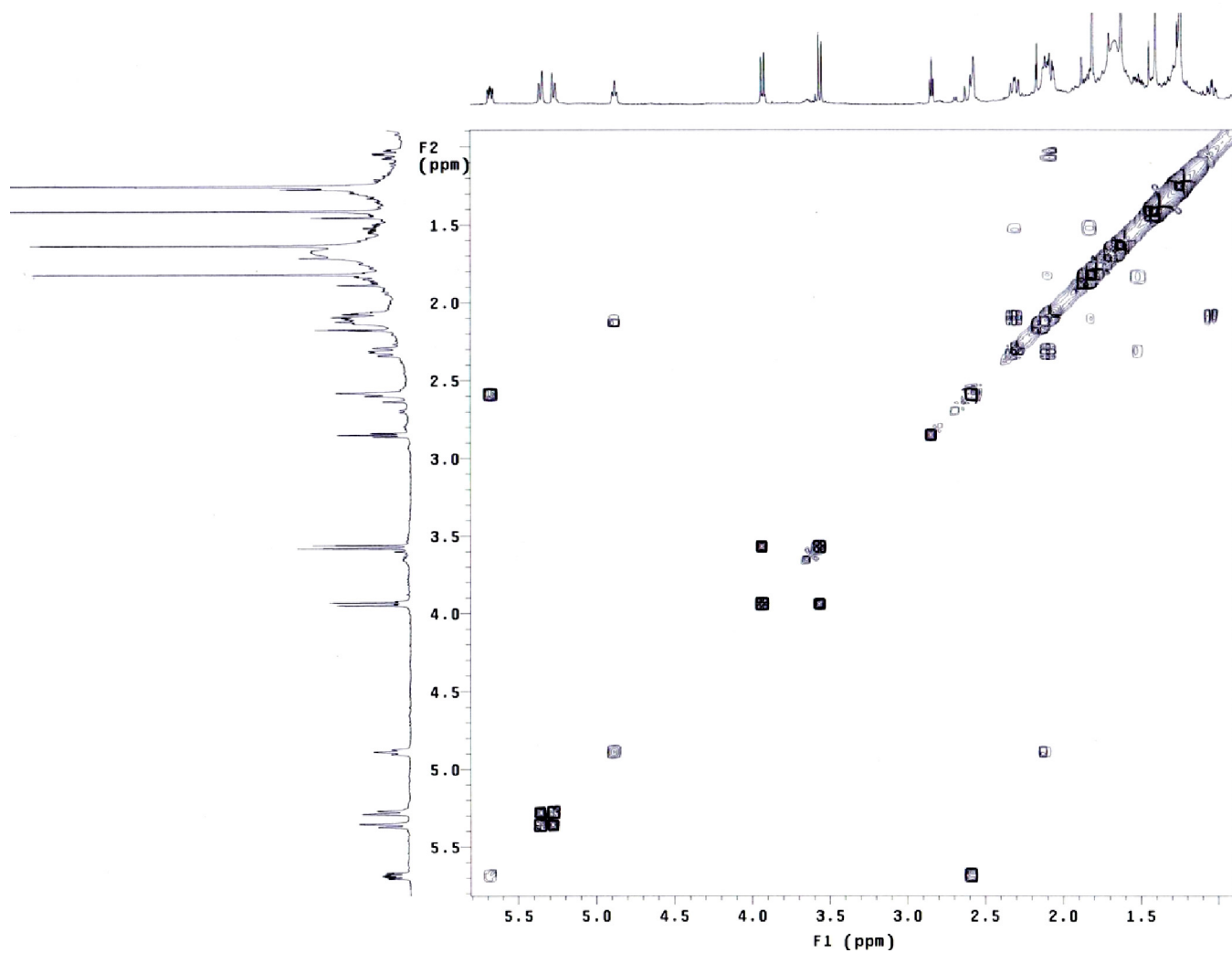


Figure S32. COSY spectrum of 4 in CDCl₃

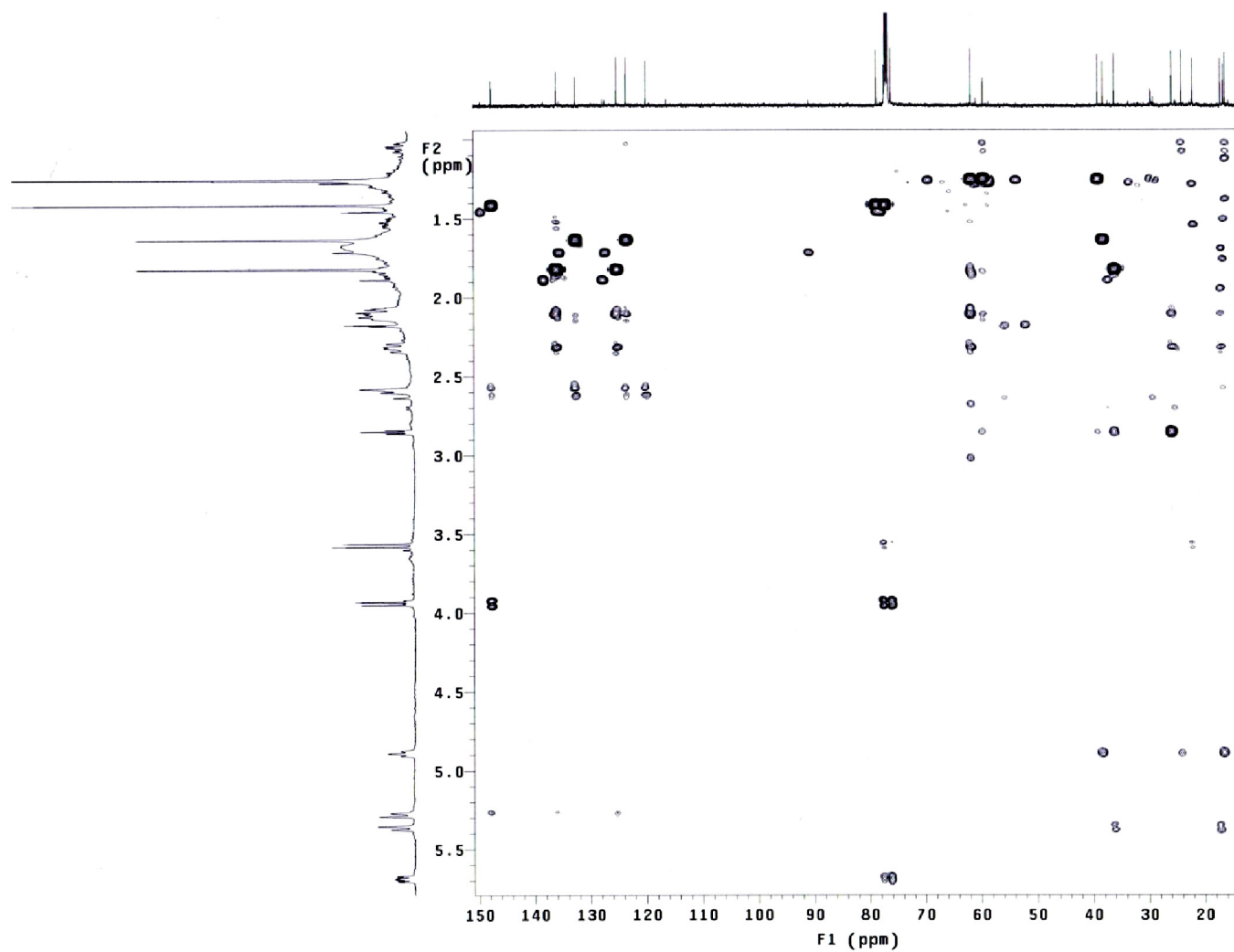


Figure S33. HMBC spectrum of 4 in CDCl₃

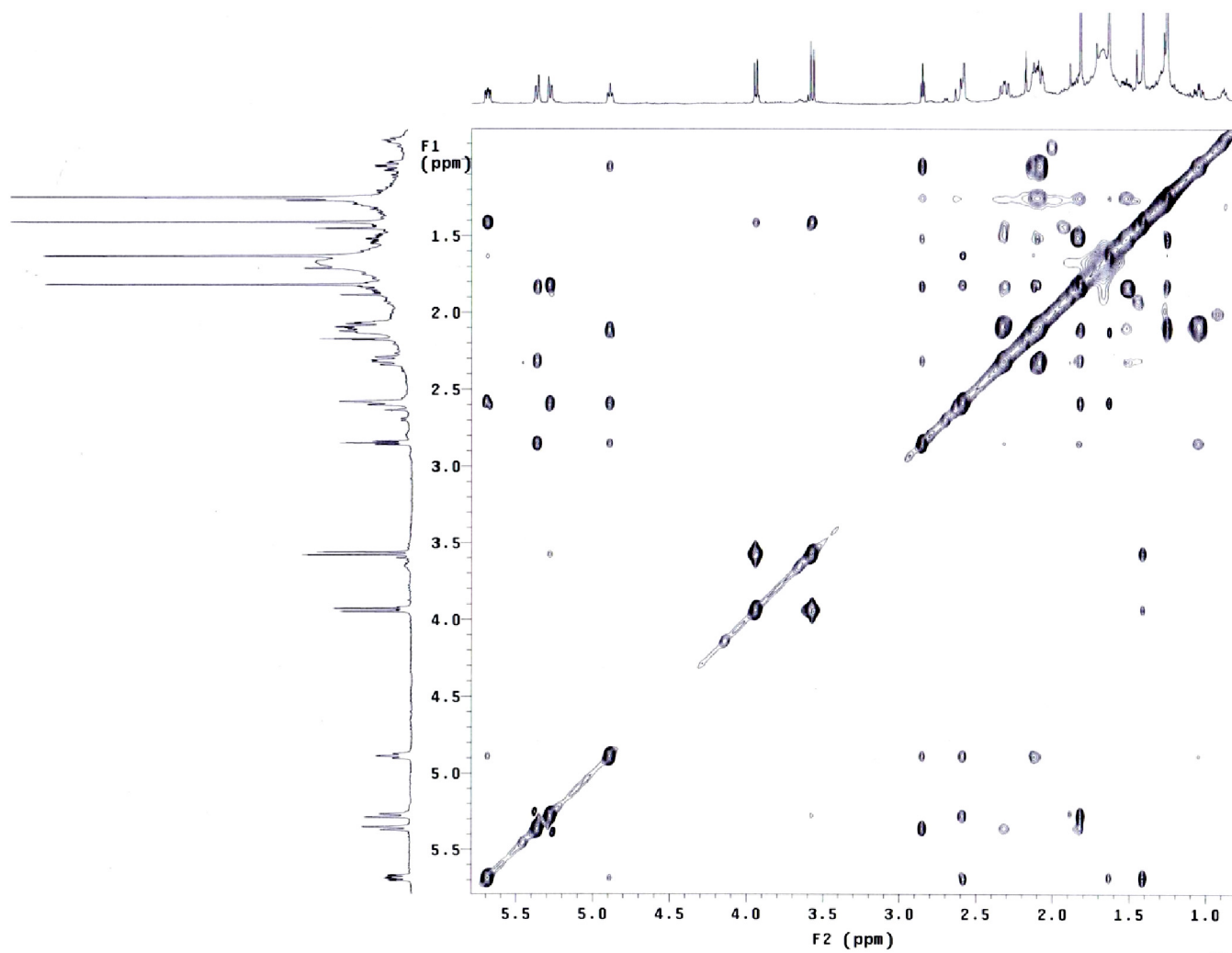


Figure S34. NOESY spectrum of **4** in CDCl₃

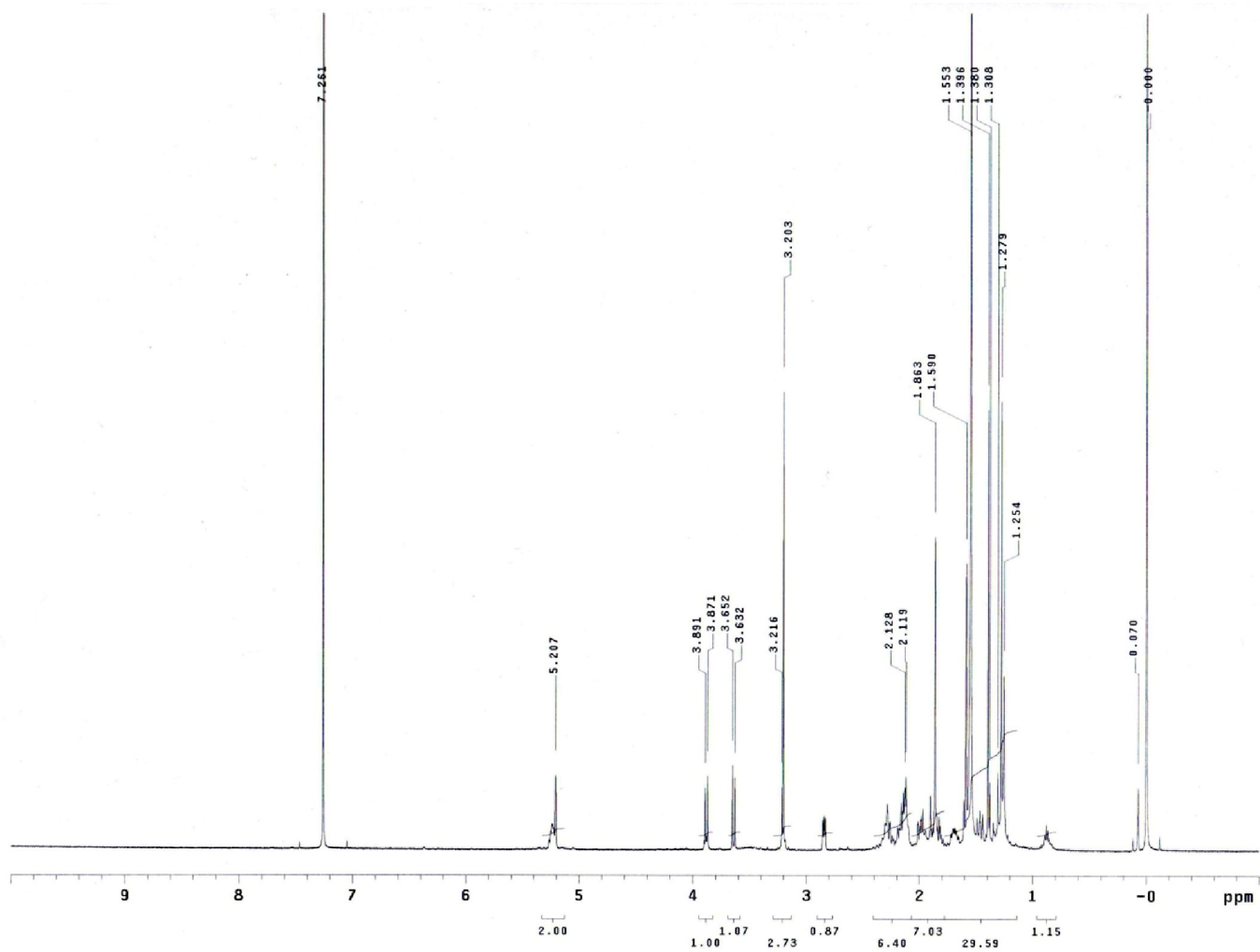


Figure S35. ^1H NMR spectrum of **5** in CDCl_3

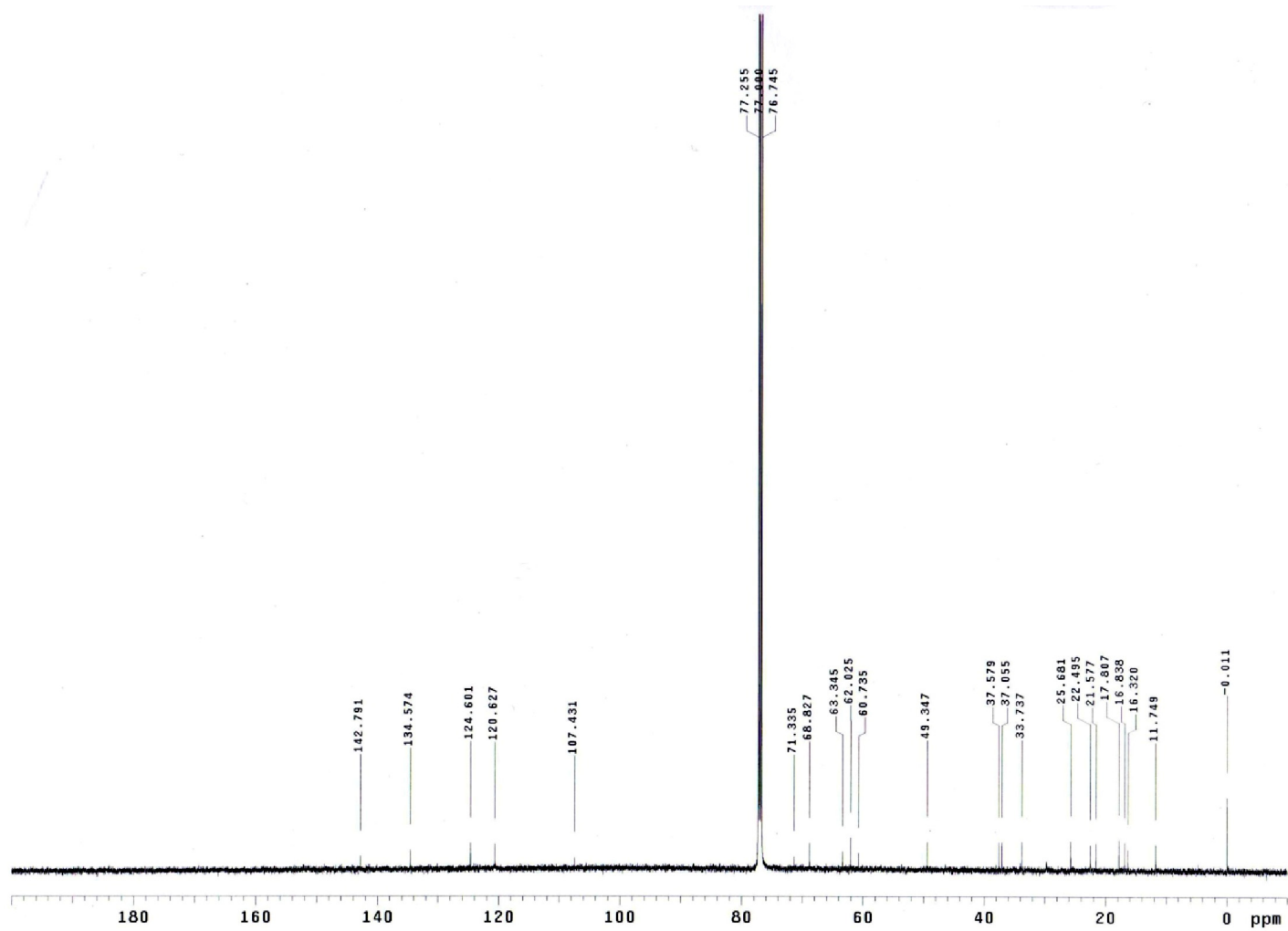


Figure S36. ^{13}C NMR spectrum of **5** in CDCl_3

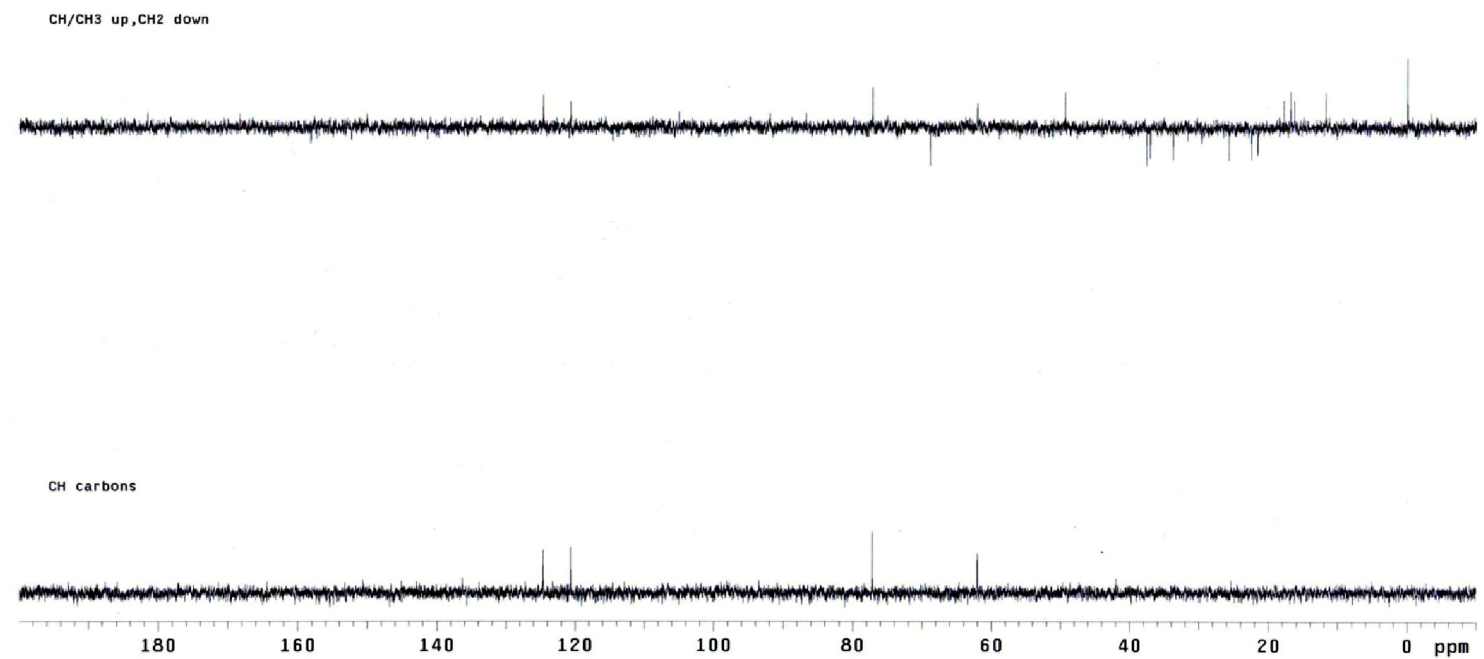


Figure S37. DEPT spectra of 5 in CDCl₃

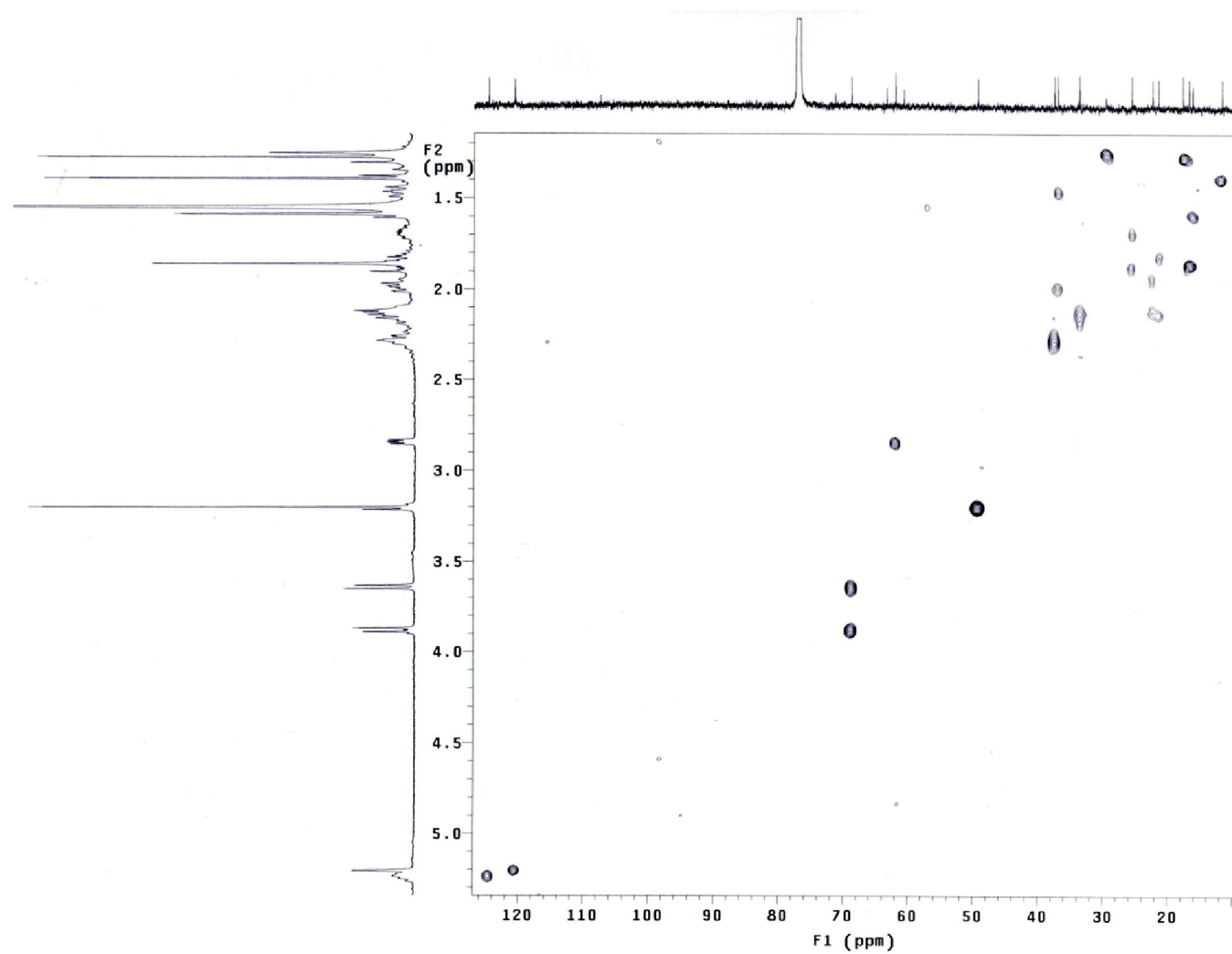


Figure S38. HMQC spectrum of **5** in CDCl₃

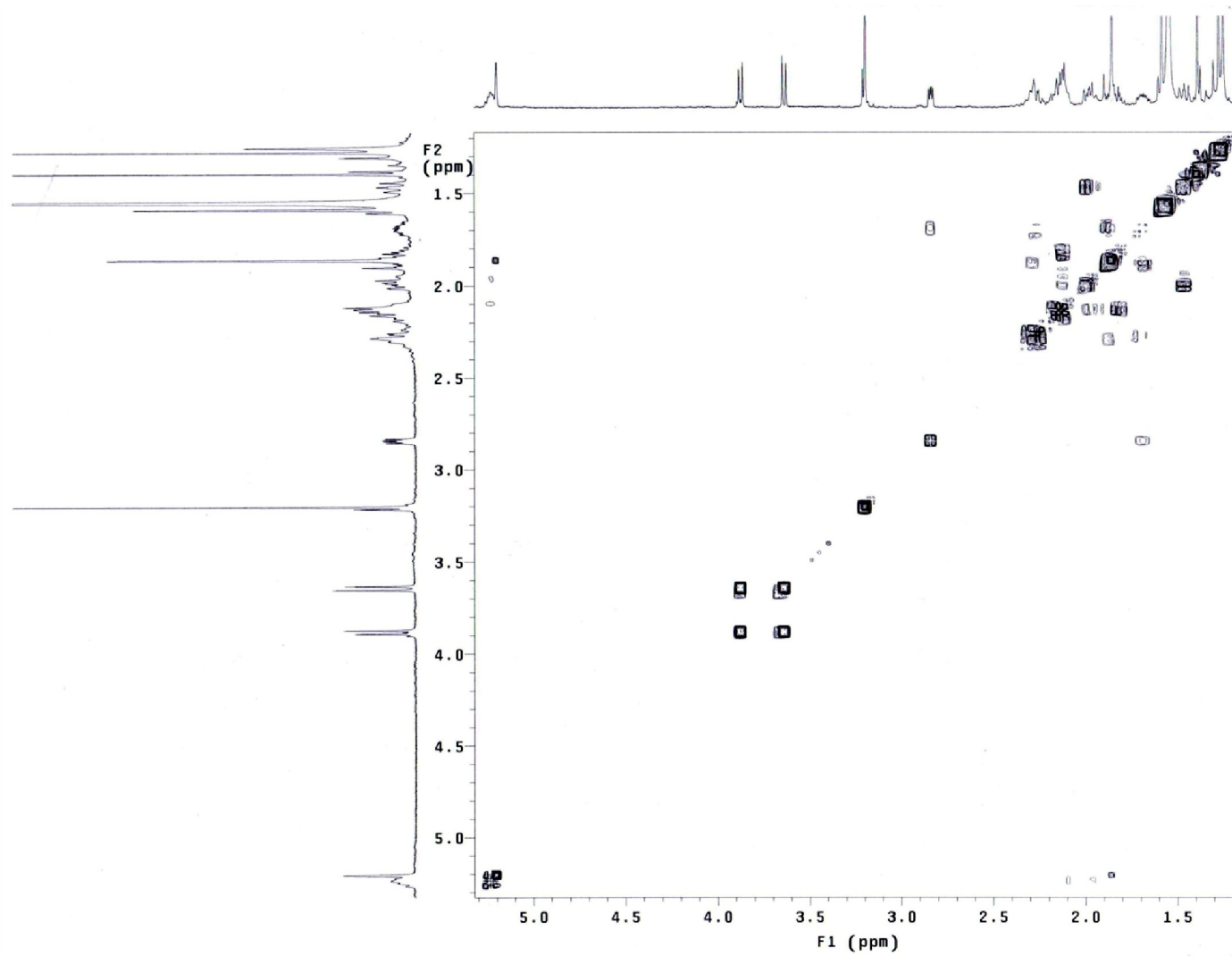


Figure S39. COSY spectrum of **5** in CDCl₃

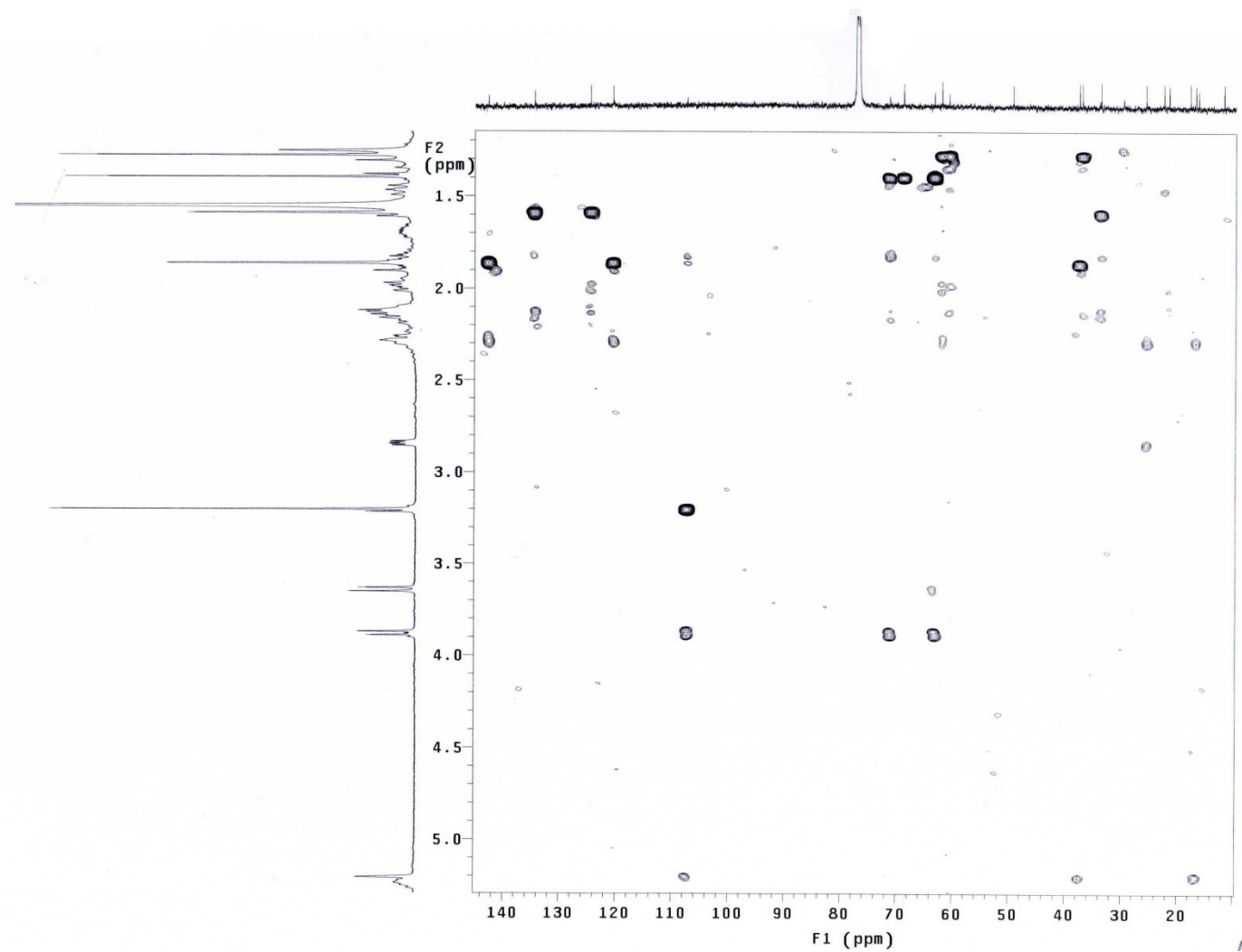


Figure S40. HMBC spectrum of **5** in CDCl₃

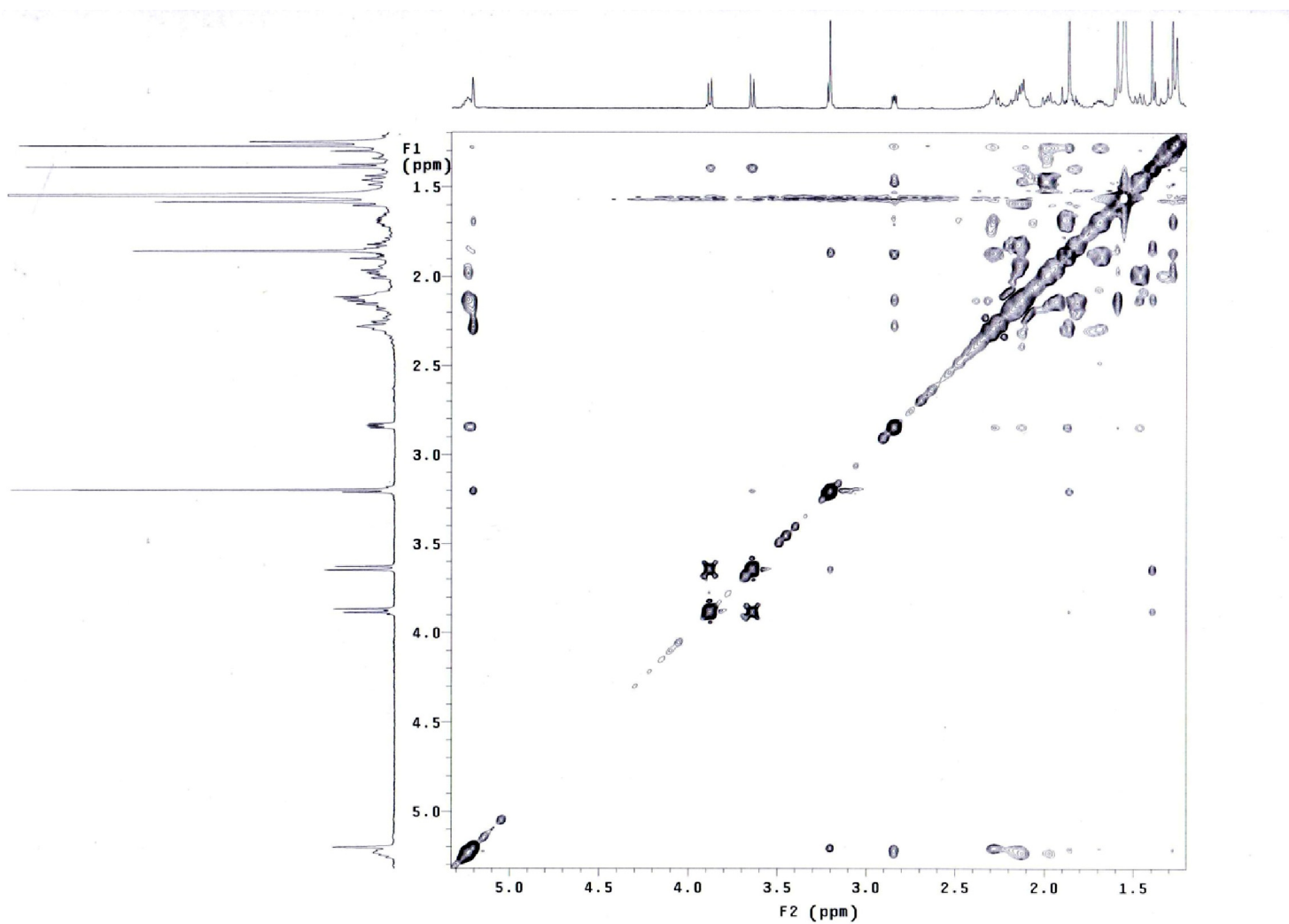


Figure S41. NOESY spectrum of **5** in CDCl₃

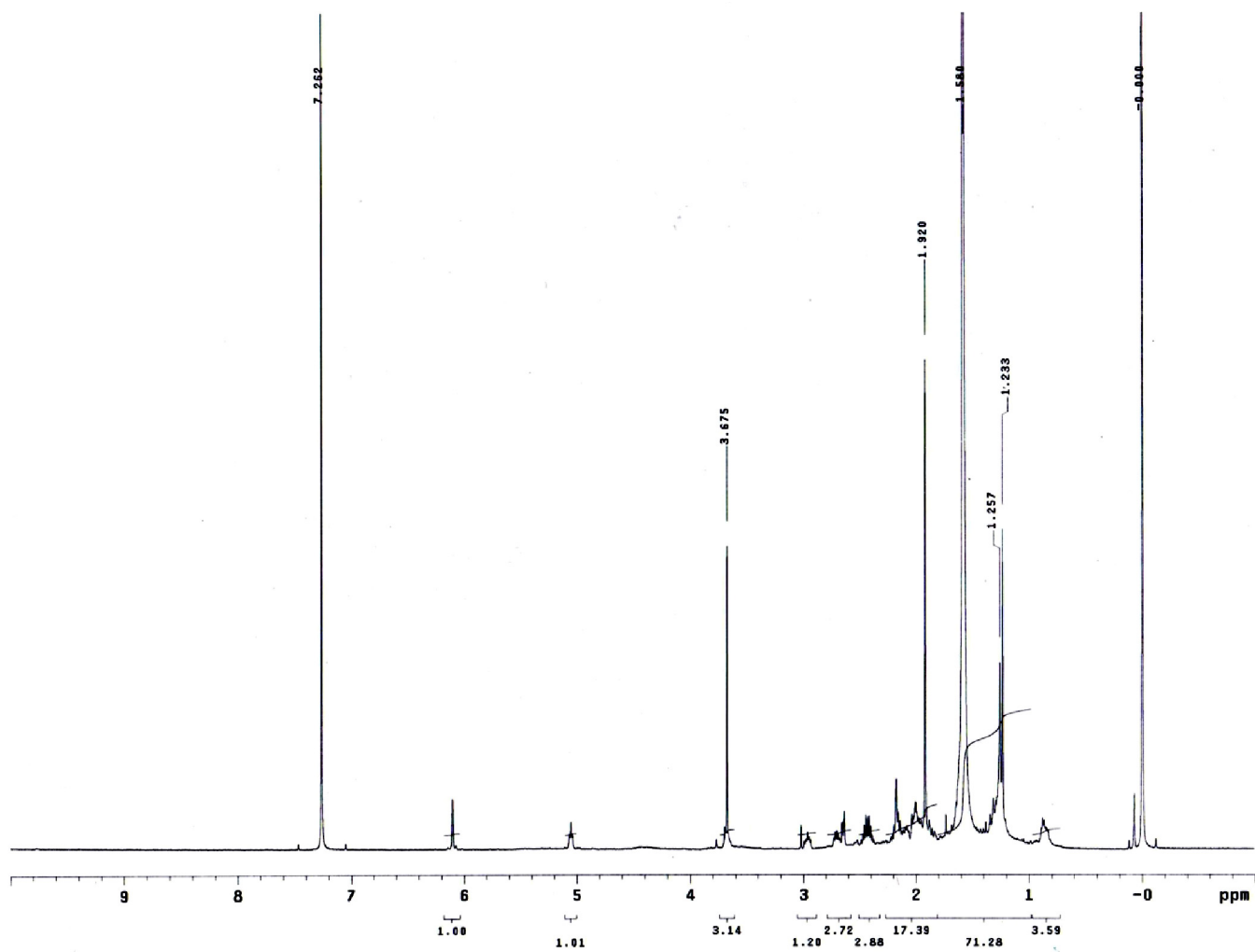


Figure S42. ^1H NMR spectrum of **6** in CDCl_3

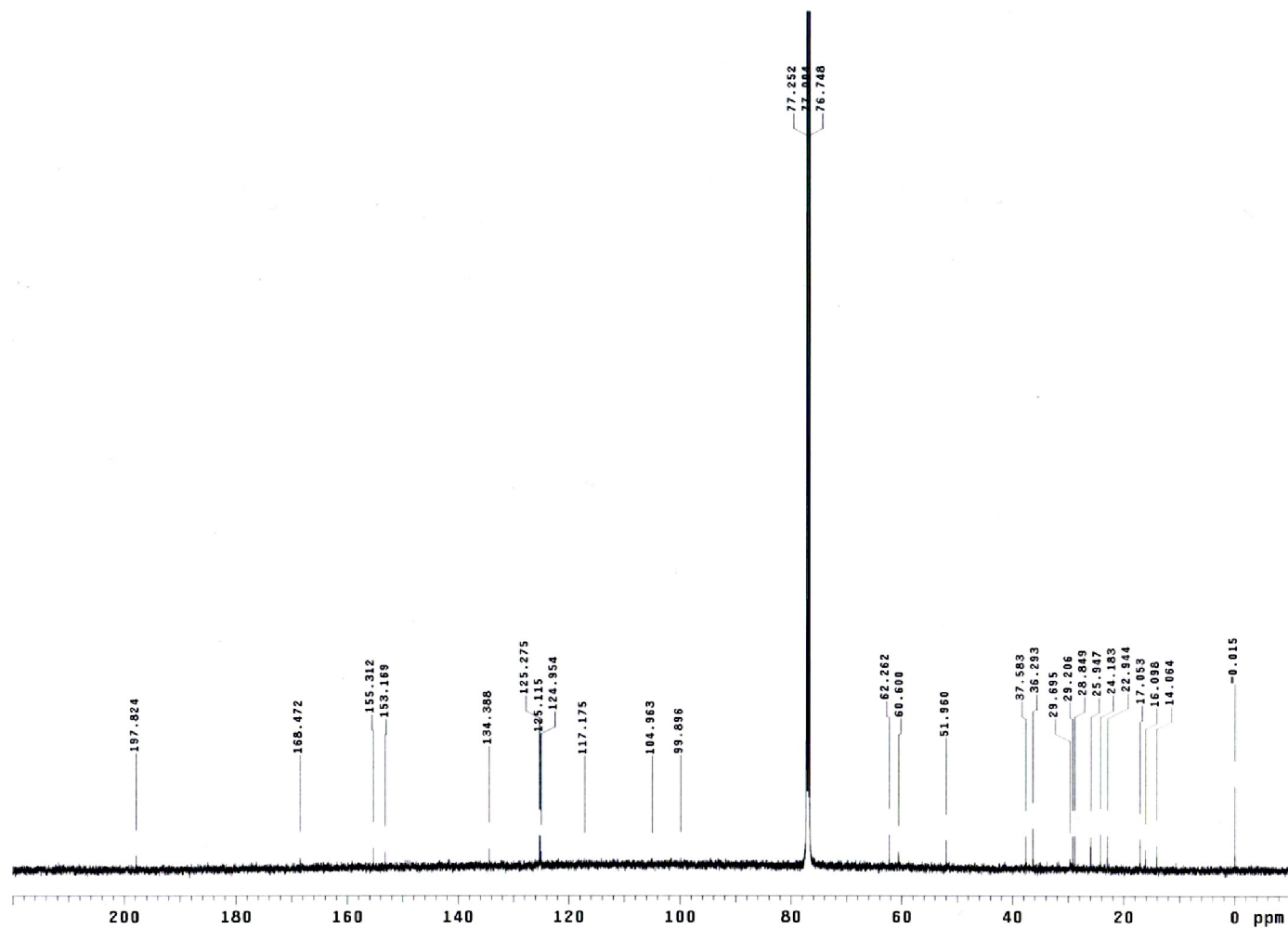


Figure S43. ¹³C NMR spectrum of **6** in CDCl₃

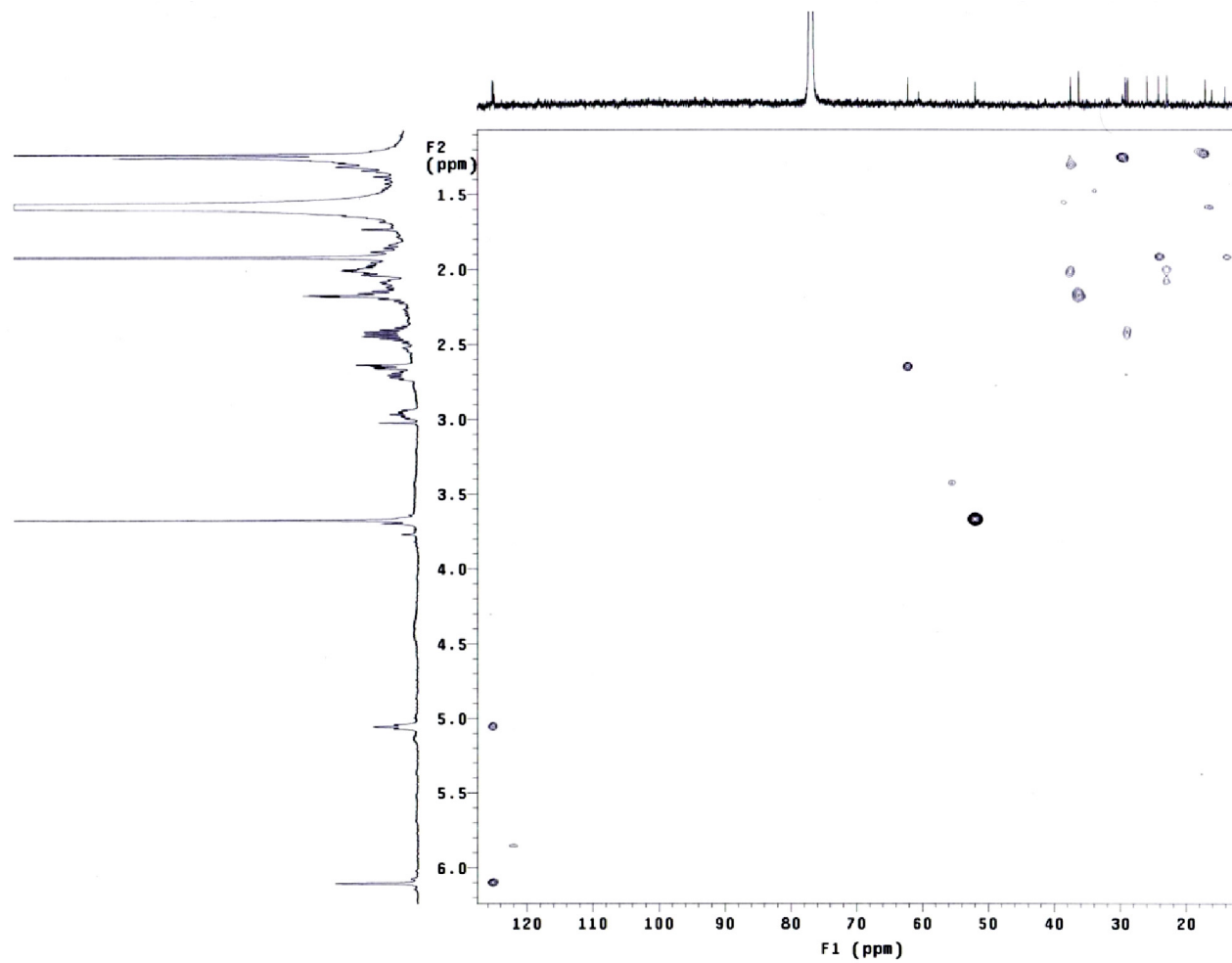


Figure S44. HMQC spectrum of **6** in CDCl_3

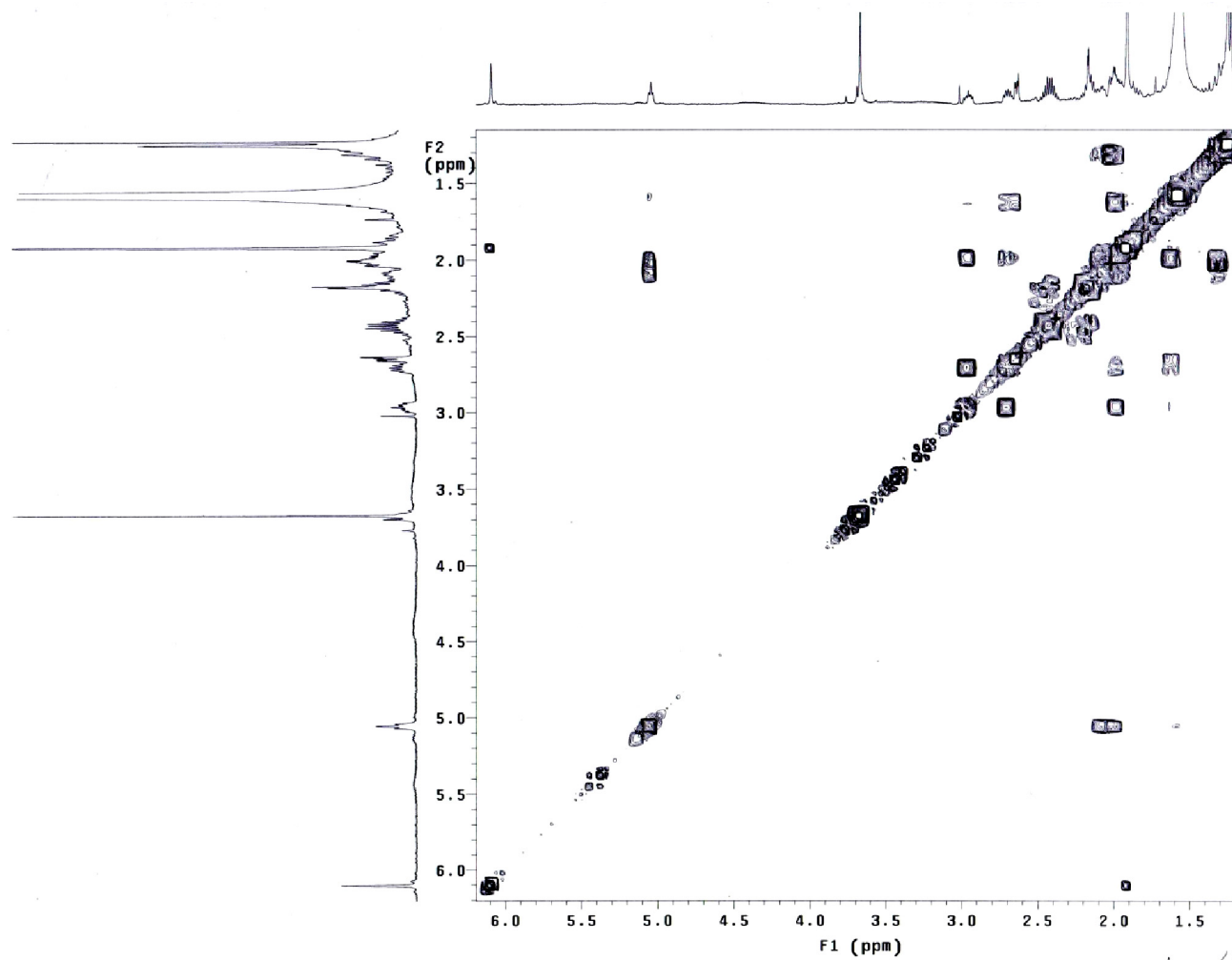


Figure S45. COSY spectrum of **6** in CDCl₃

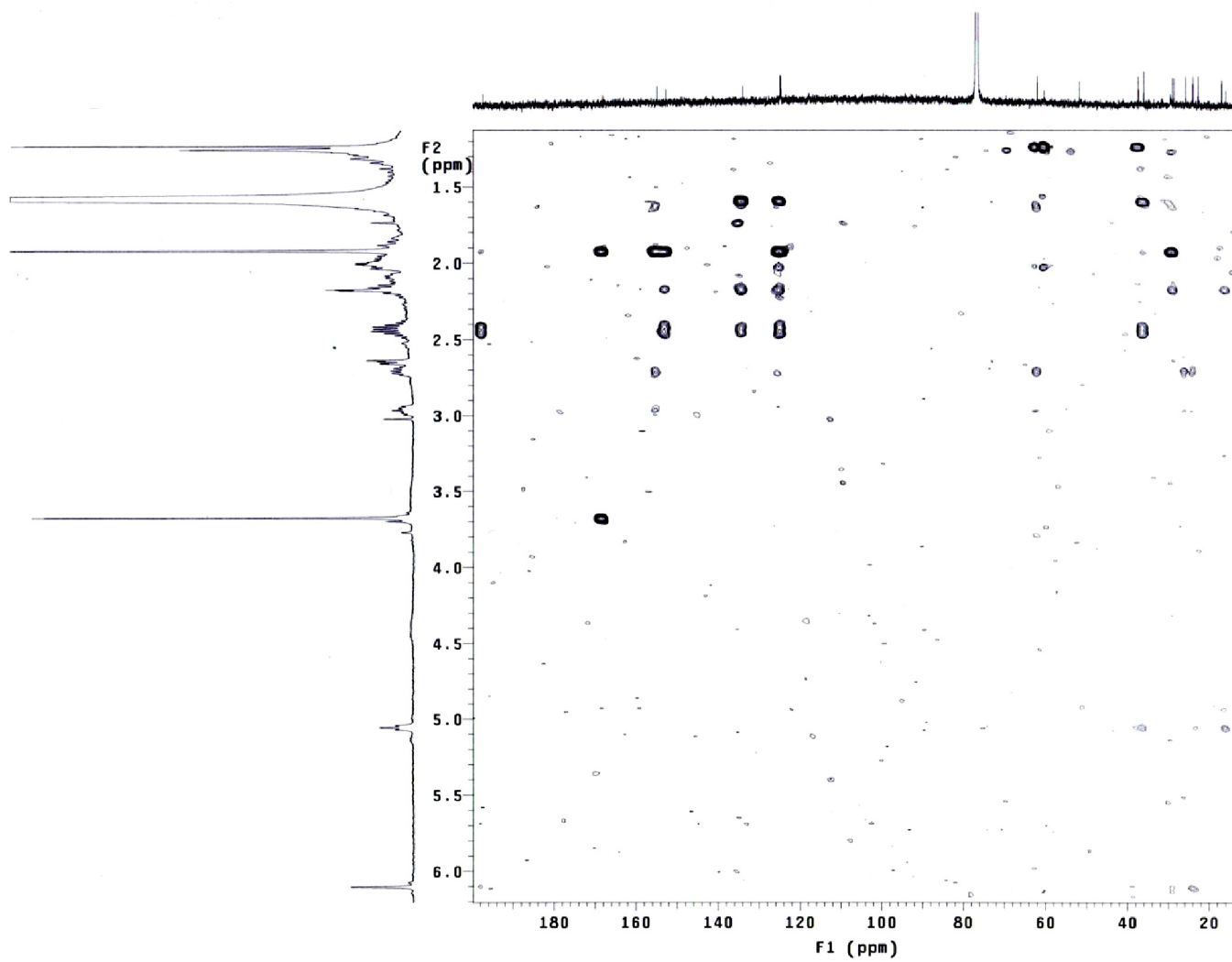


Figure S46. HMBC spectrum of **6** in CDCl₃

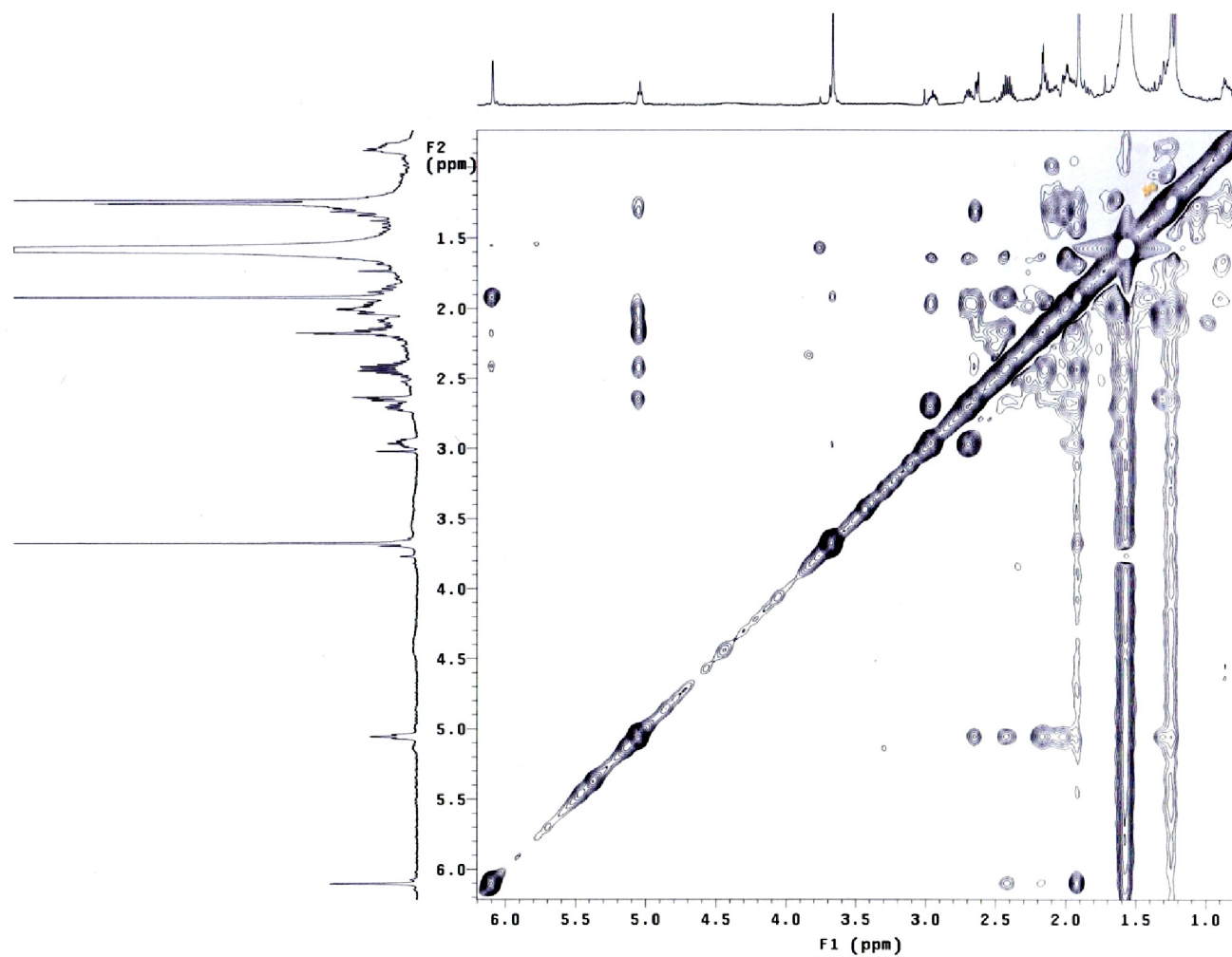


Figure S47. NOESY spectrum of **6** in CDCl₃