



Supporting Information

for

Chemical constituents of *Chaenomeles sinensis* twigs and their biological activity

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Beilstein J. Org. Chem. **2020**, *16*, 3078–3085. doi:10.3762/bjoc.16.257

1D and 2D NMR, HRMS, and ECD spectra of compound 1, ^1H and ^{13}C NMR spectra of 1a, and ^1H NMR spectra of 1s and 1r

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Figure S1. The HRMS–FAB spectrum of **1**

140925_MGBC15_002-c1 #155-160 RT: 3.11-3.21 AV: 6 SB: 15 0.02-0.31 NL: 9.30E4
T: + c FAB Full ms [319.50-470.50]

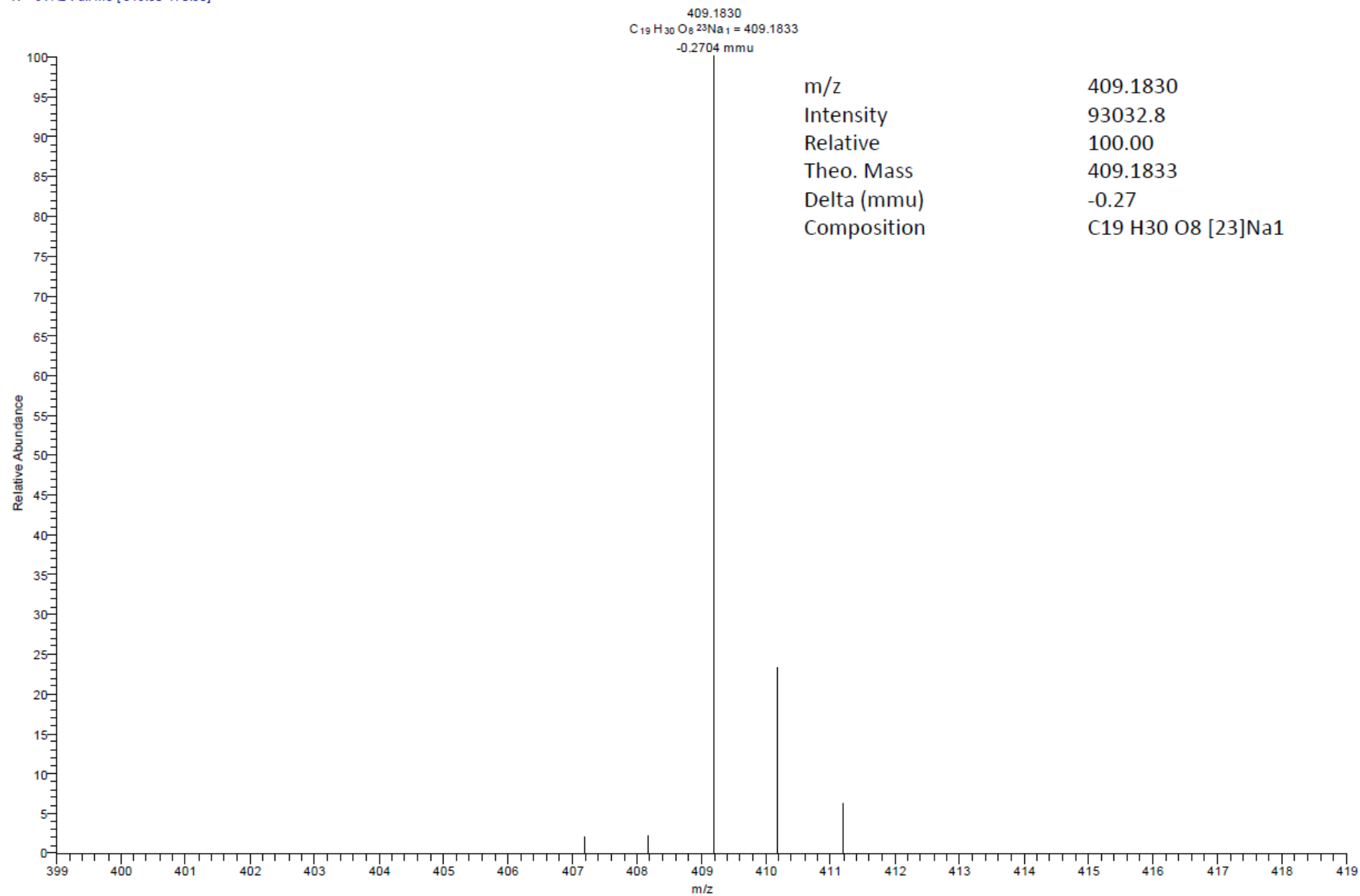


Figure S2. The ^1H NMR spectrum of **1** in methanol- d_4

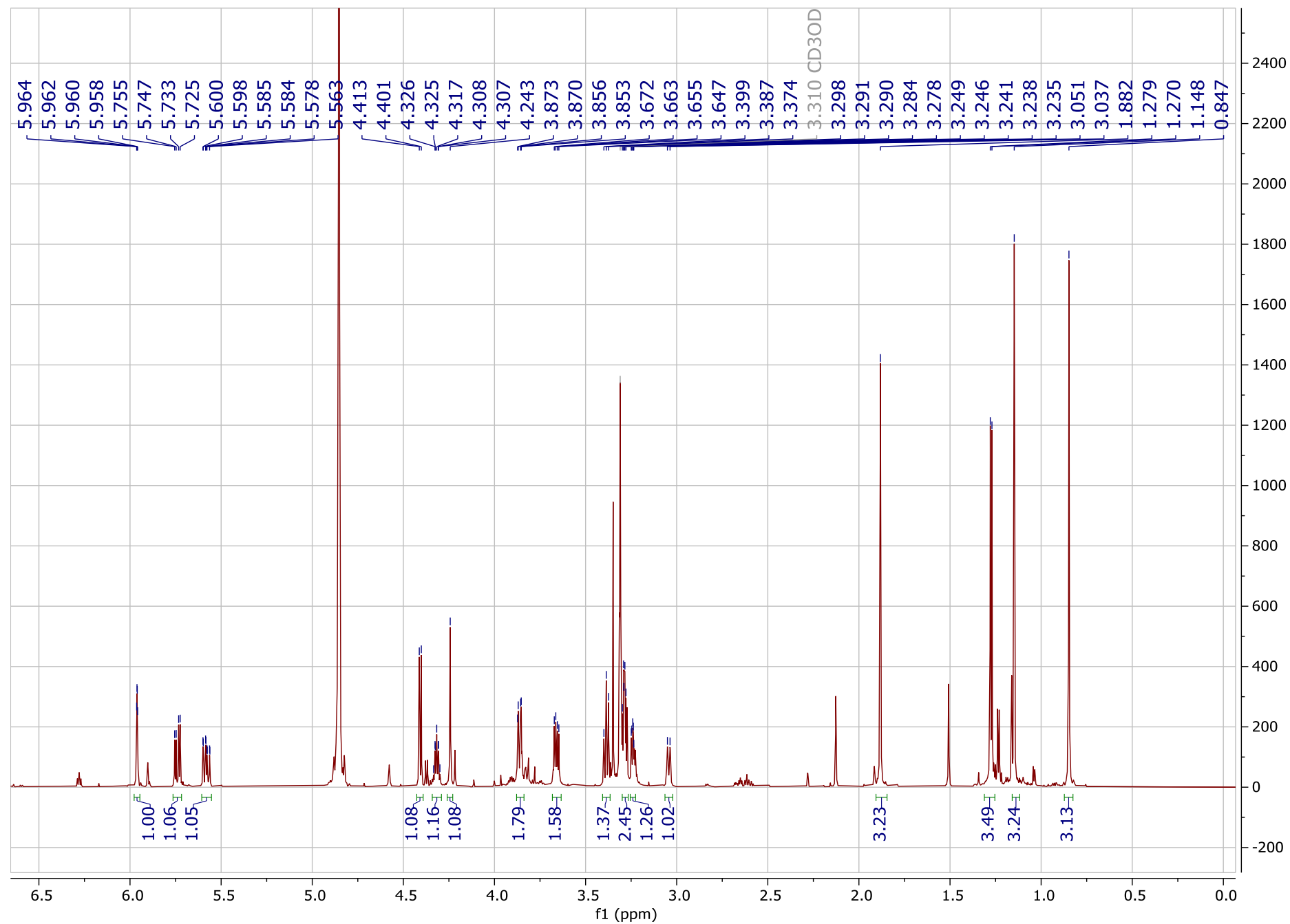


Figure S3. The ^{13}C NMR spectrum of **1** in methanol- d_4

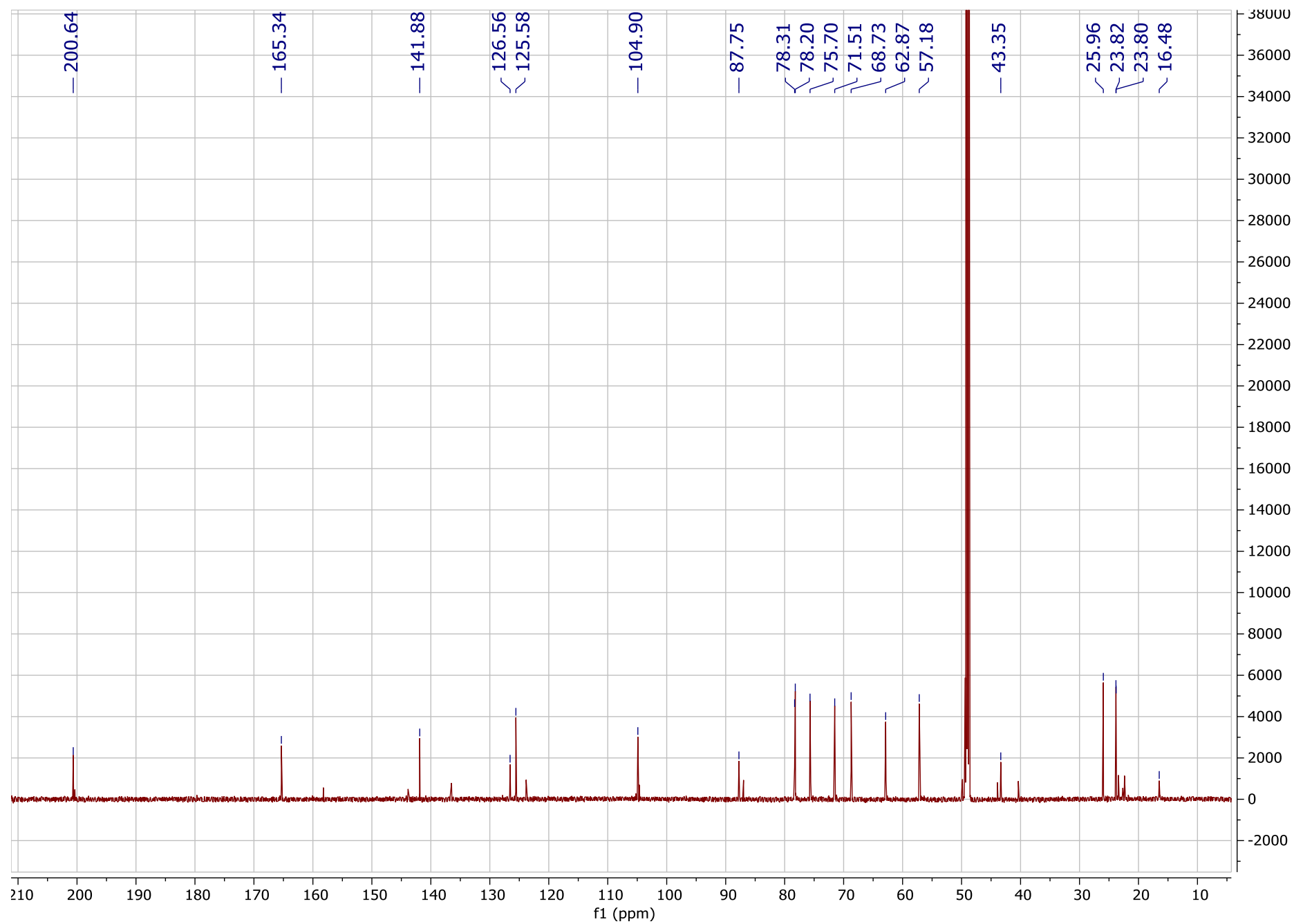


Figure S4. The COSY spectrum of **1** in methanol- d_4

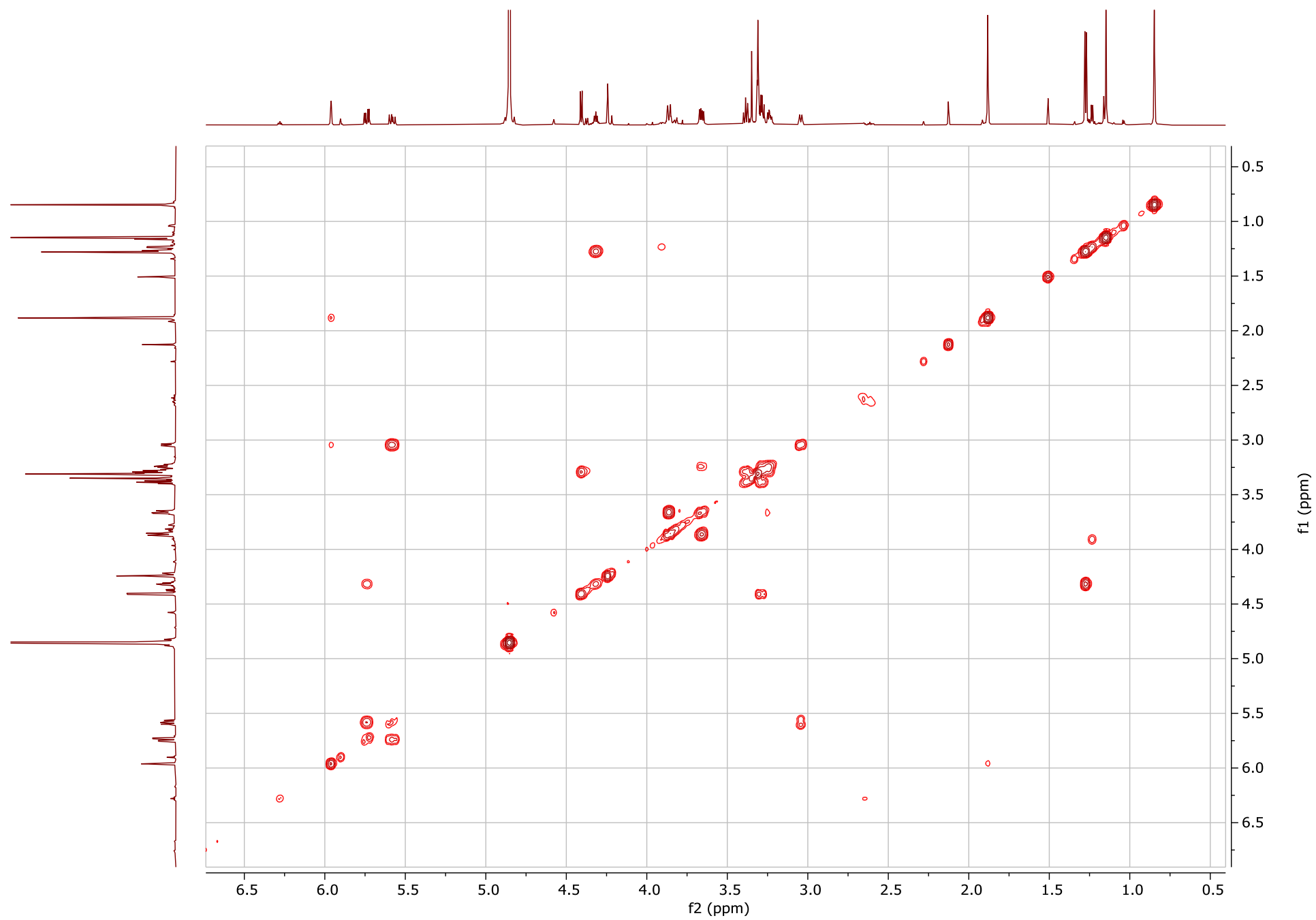


Figure S5. The HSQC spectrum of **1** in methanol- d_4

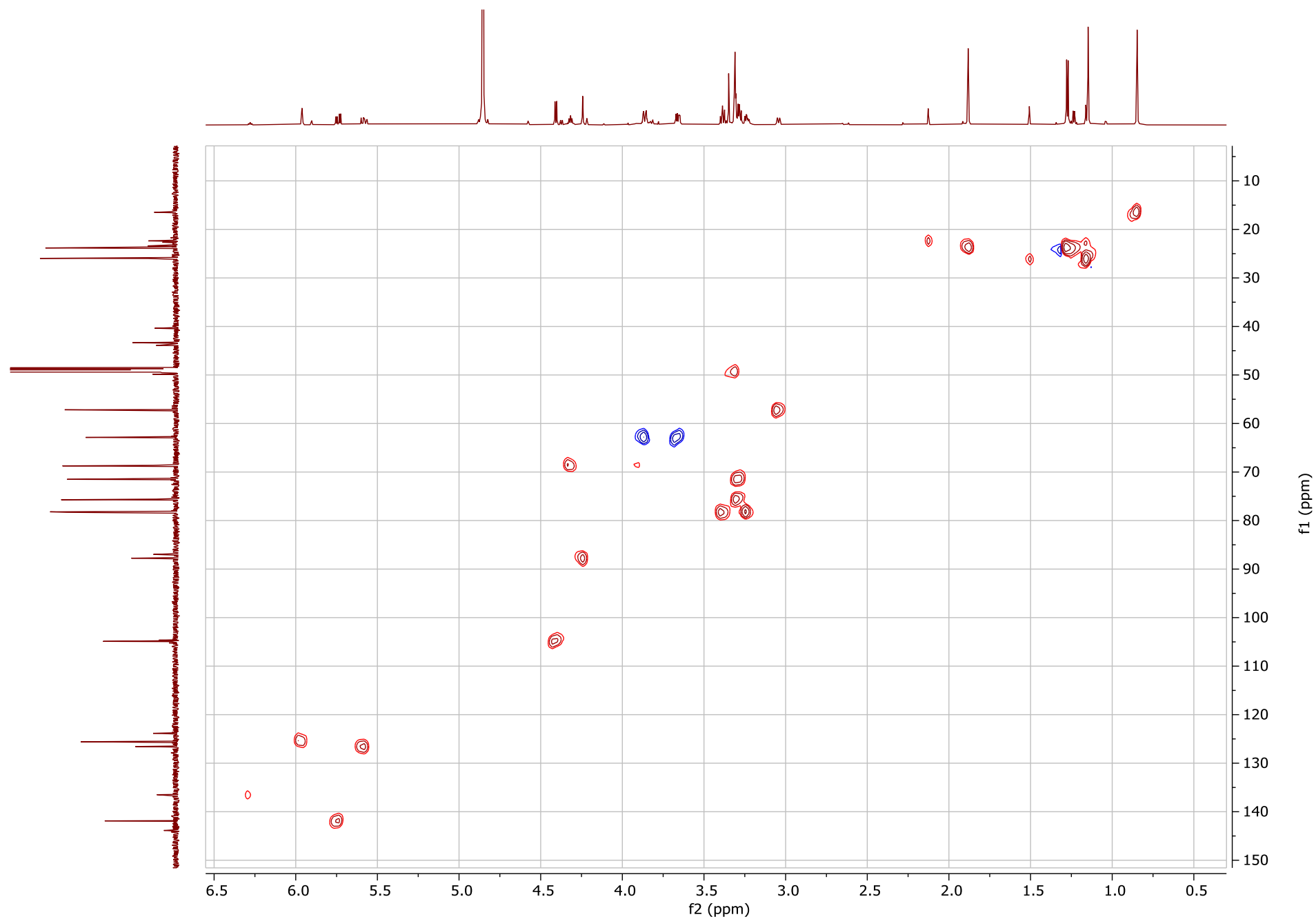


Figure S6. The HMBC spectrum of **1** in methanol- d_4

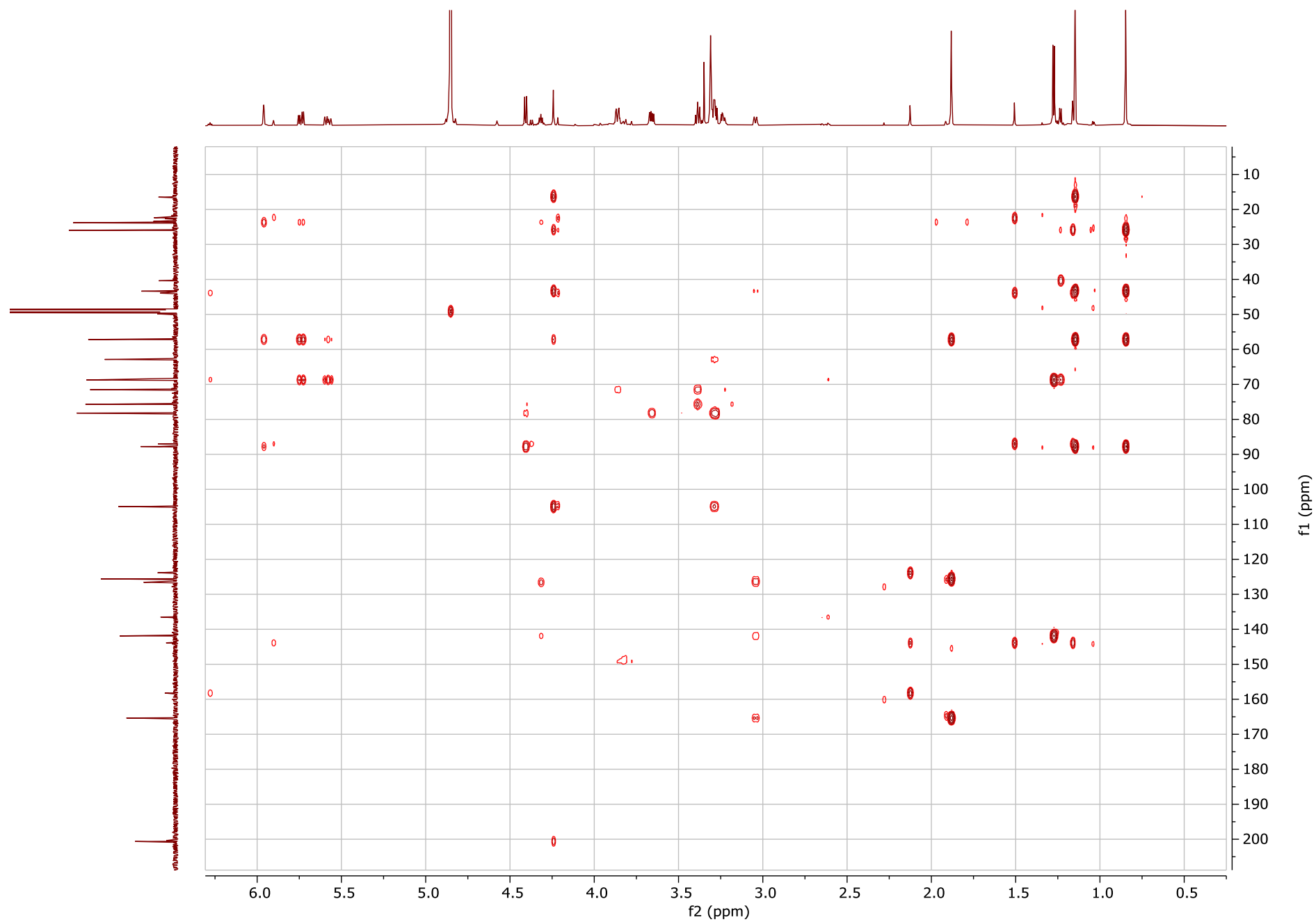


Figure S7. The NOESY spectrum of **1** in methanol- d_4

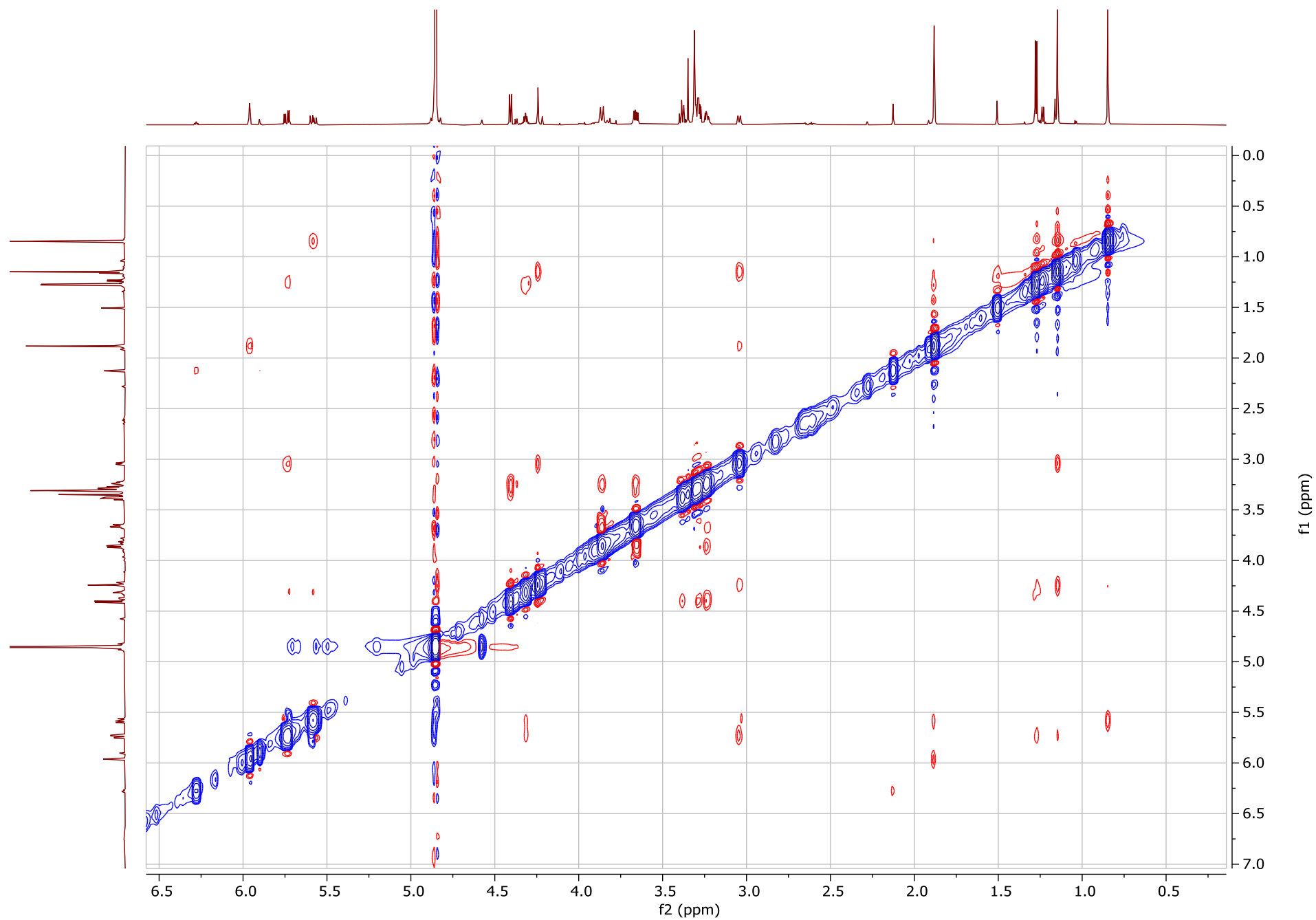


Figure S8. The ECD spectrum of **1** in methanol

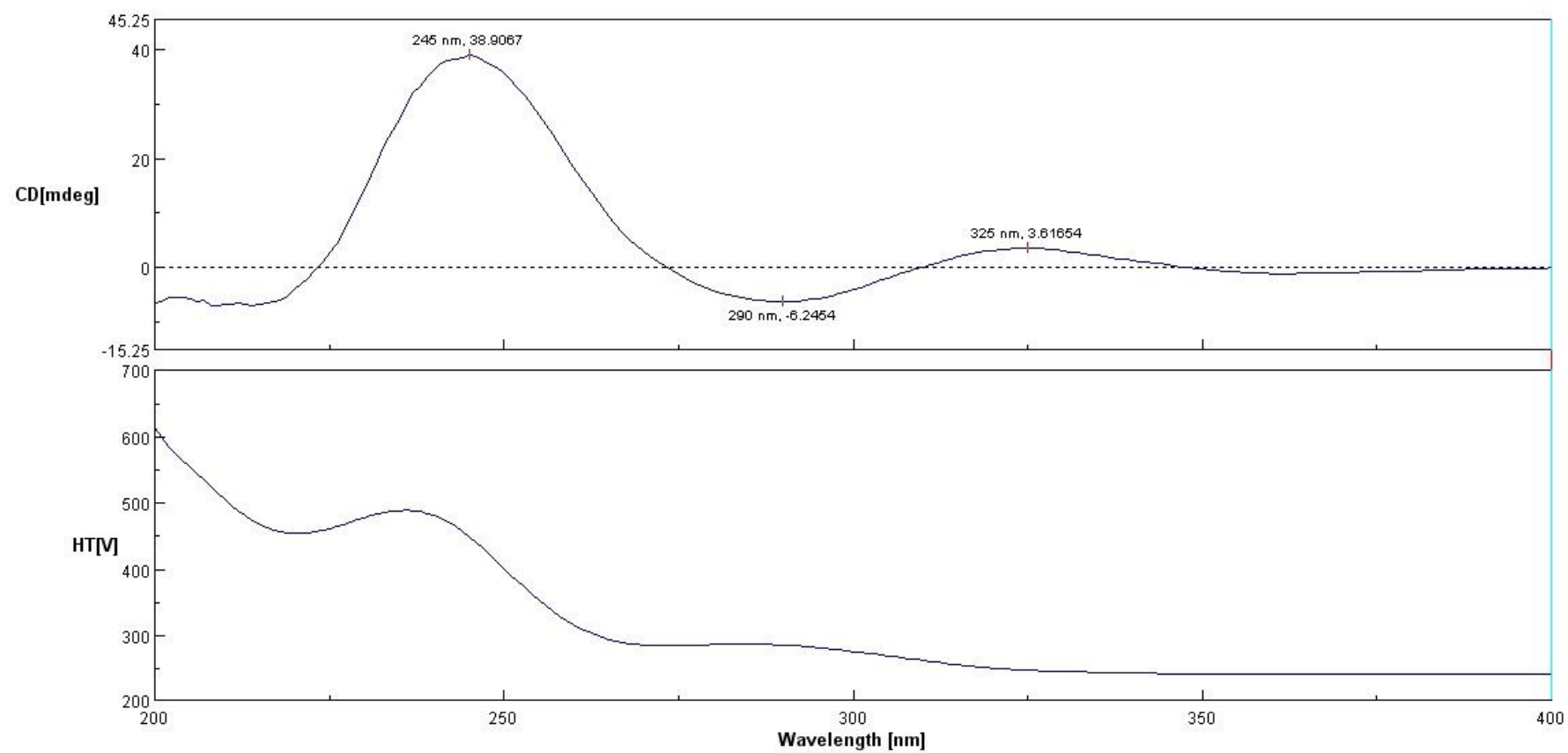


Figure S9. The ^1H NMR spectrum of **1a** in methanol- d_4

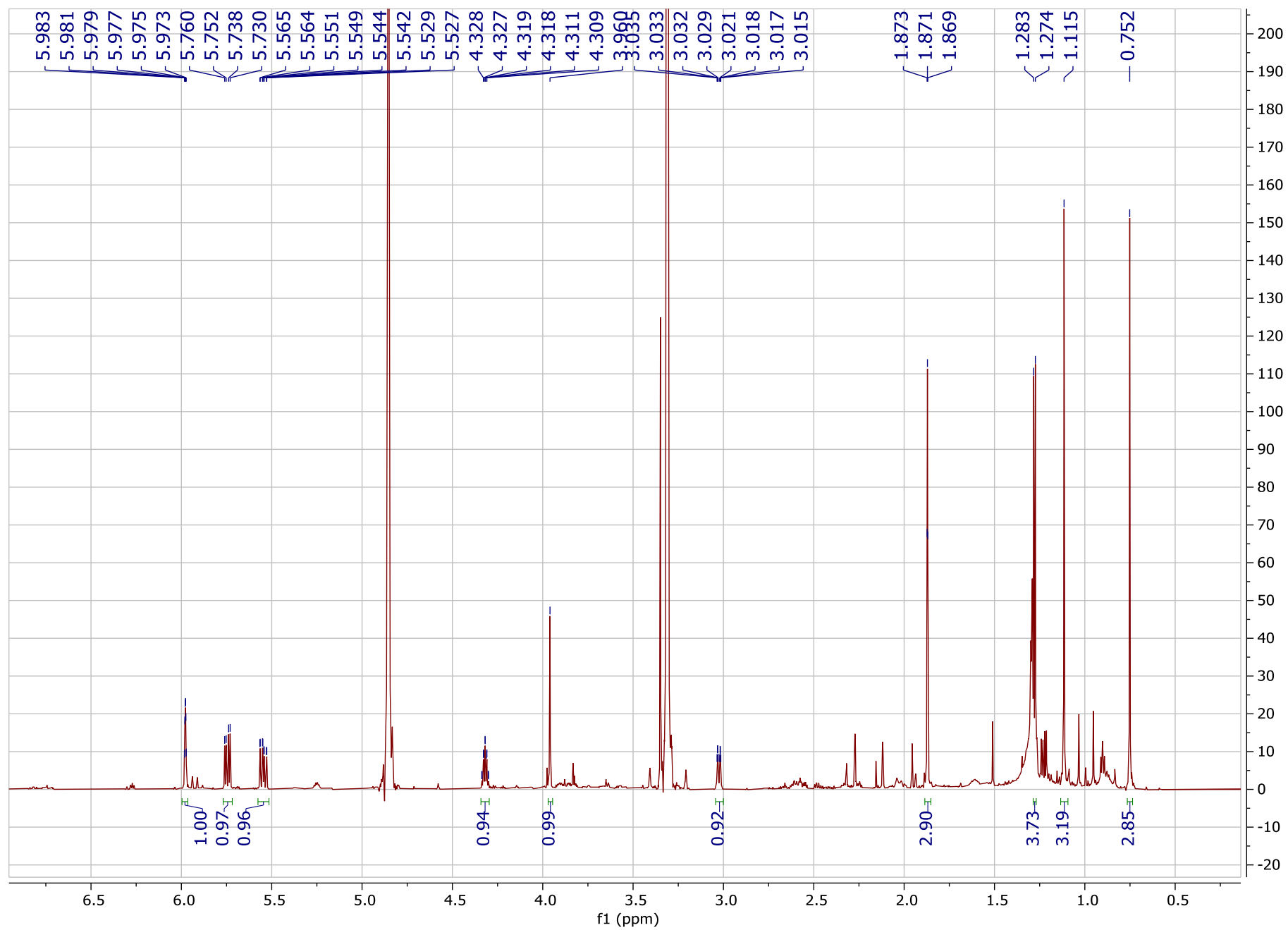


Figure S10. The ^{13}C NMR spectrum of **1a** in methanol- d_4

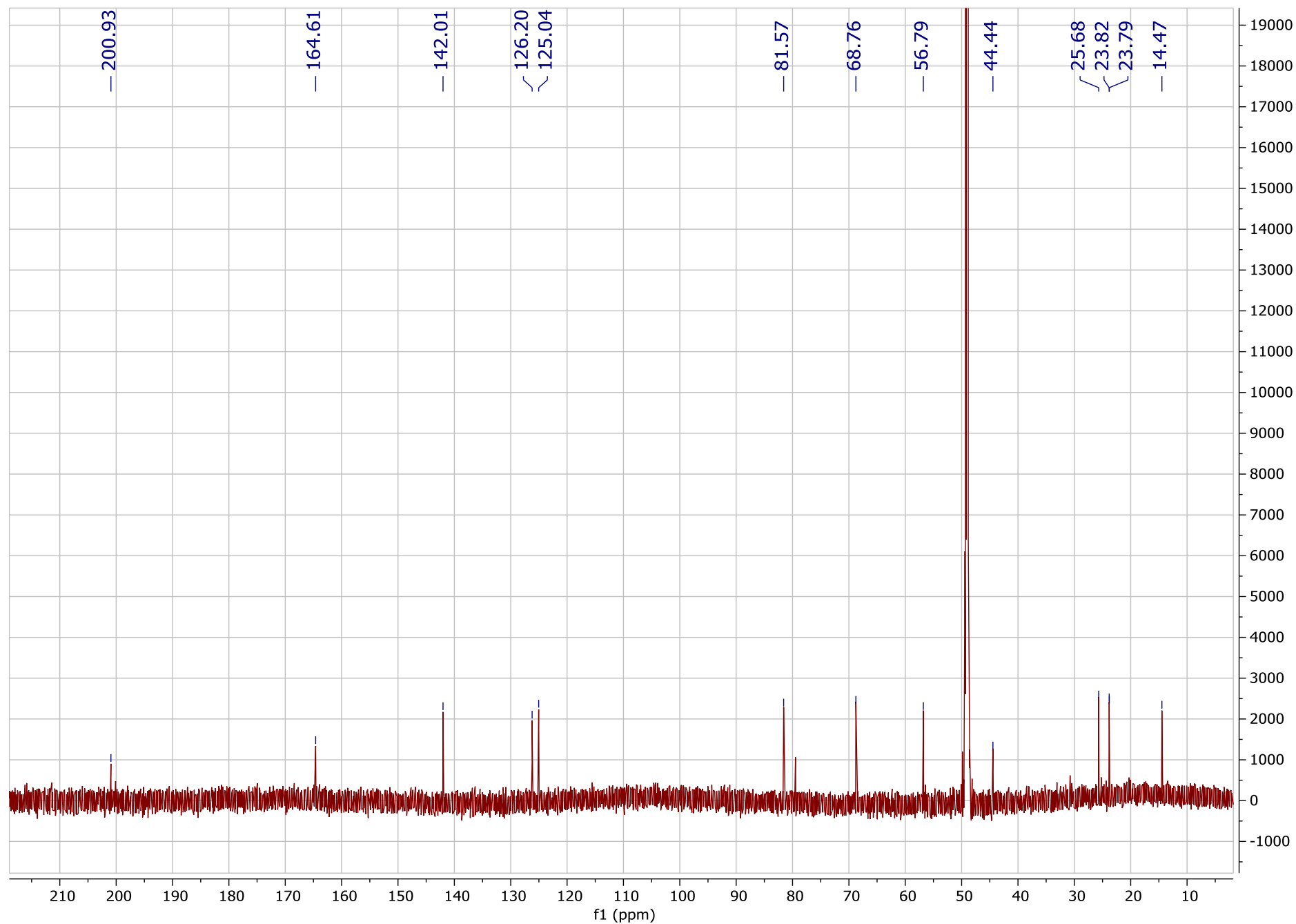


Figure S11. The ^1H NMR spectrum of **1s** in pyridine- d_5

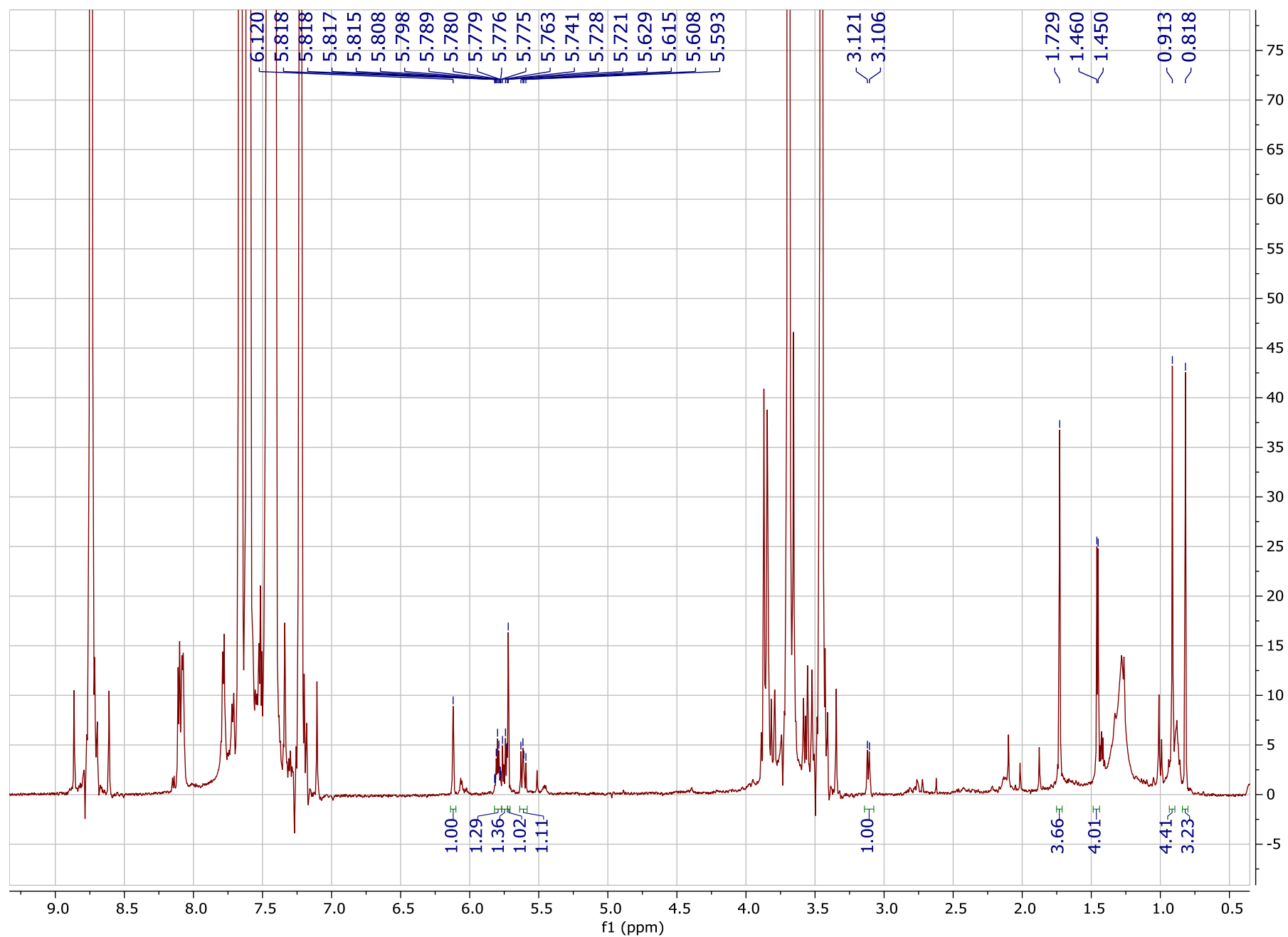


Figure S12. The ^1H NMR spectrum of **1r** in pyridine- d_5

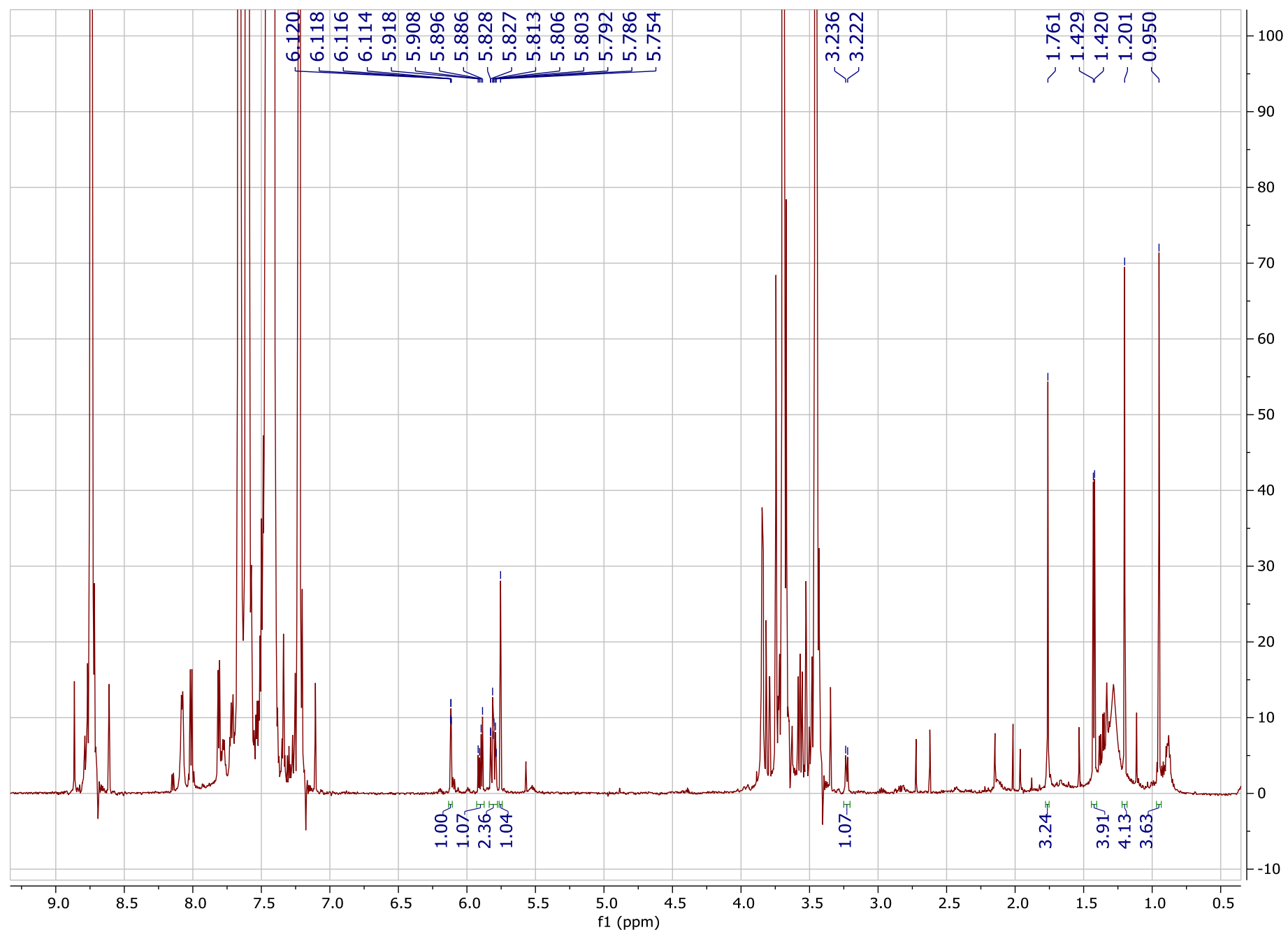


Table S1. ^1H [ppm, mult., (J in Hz)] of two Mosher esters **1s** and **1r** and the $\Delta\delta_{\text{S-R}}$ values in pyridine- d_5

Position	1s	1r	$\Delta\delta_{\text{S-R}}$
2	5.721, s	5.754, s	−0.033
4	6.120, m	6.116, m	+0.004
6	3.114, brd (10.5)	3.228, brd (10.0)	−0.114
7	5.611, dd (15.1, 10.3)	5.805, overlap	−0.194
8	5.747, overlap	5.902, dd (15.2, 7.3)	−0.155
9	5.798, m	5.813, m	−0.015
10	1.455, d (6.4)	1.425, d (6.4)	+0.030
11	0.913, s	1.201, s	−0.288
12	0.818, s	0.950, s	−0.132
13	1.729, s	1.761, s	−0.032

Figure S13. The ^1H NMR spectrum of **2** in methanol- d_4

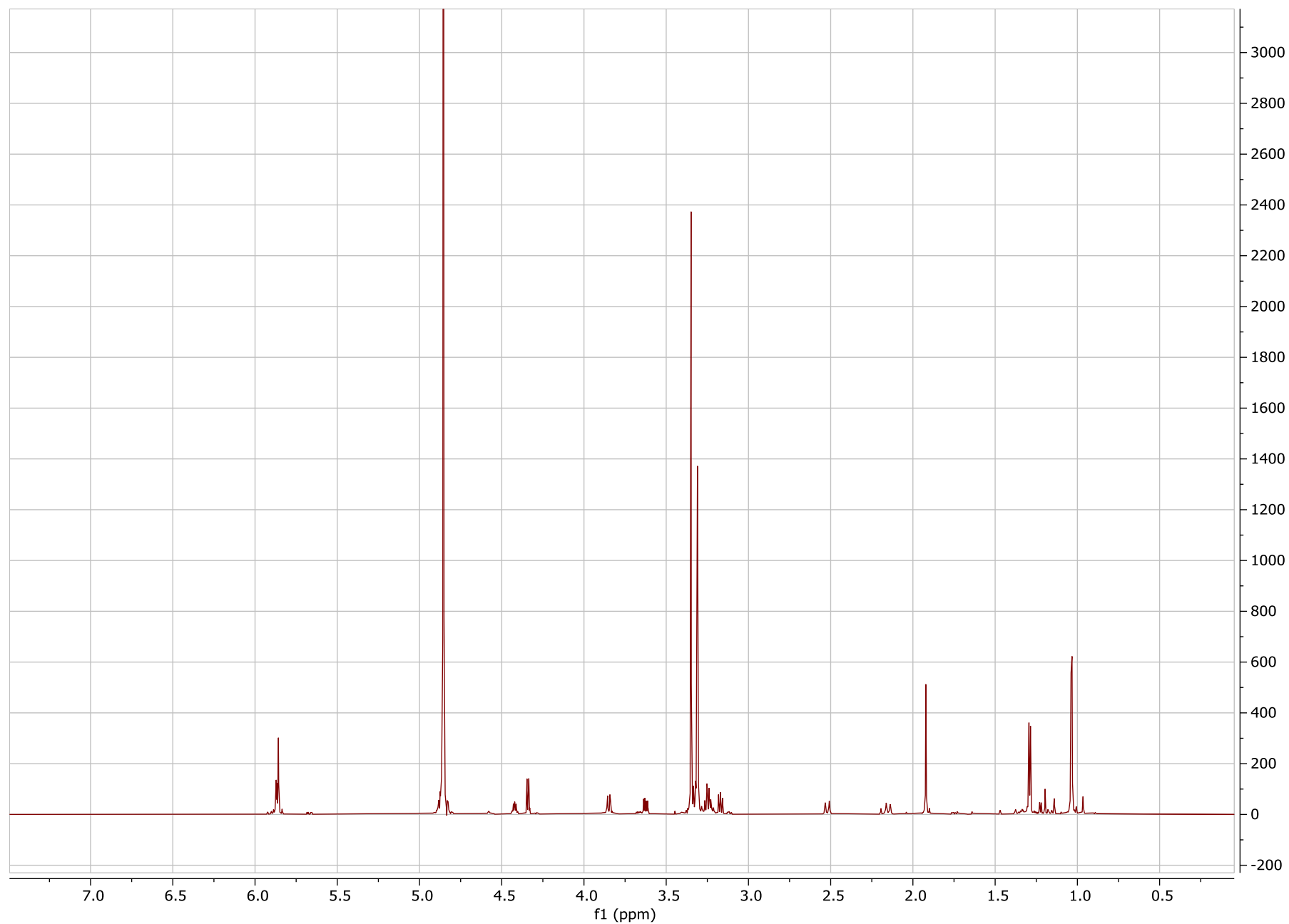


Figure S14. The ^1H NMR spectrum of **3** in methanol- d_4

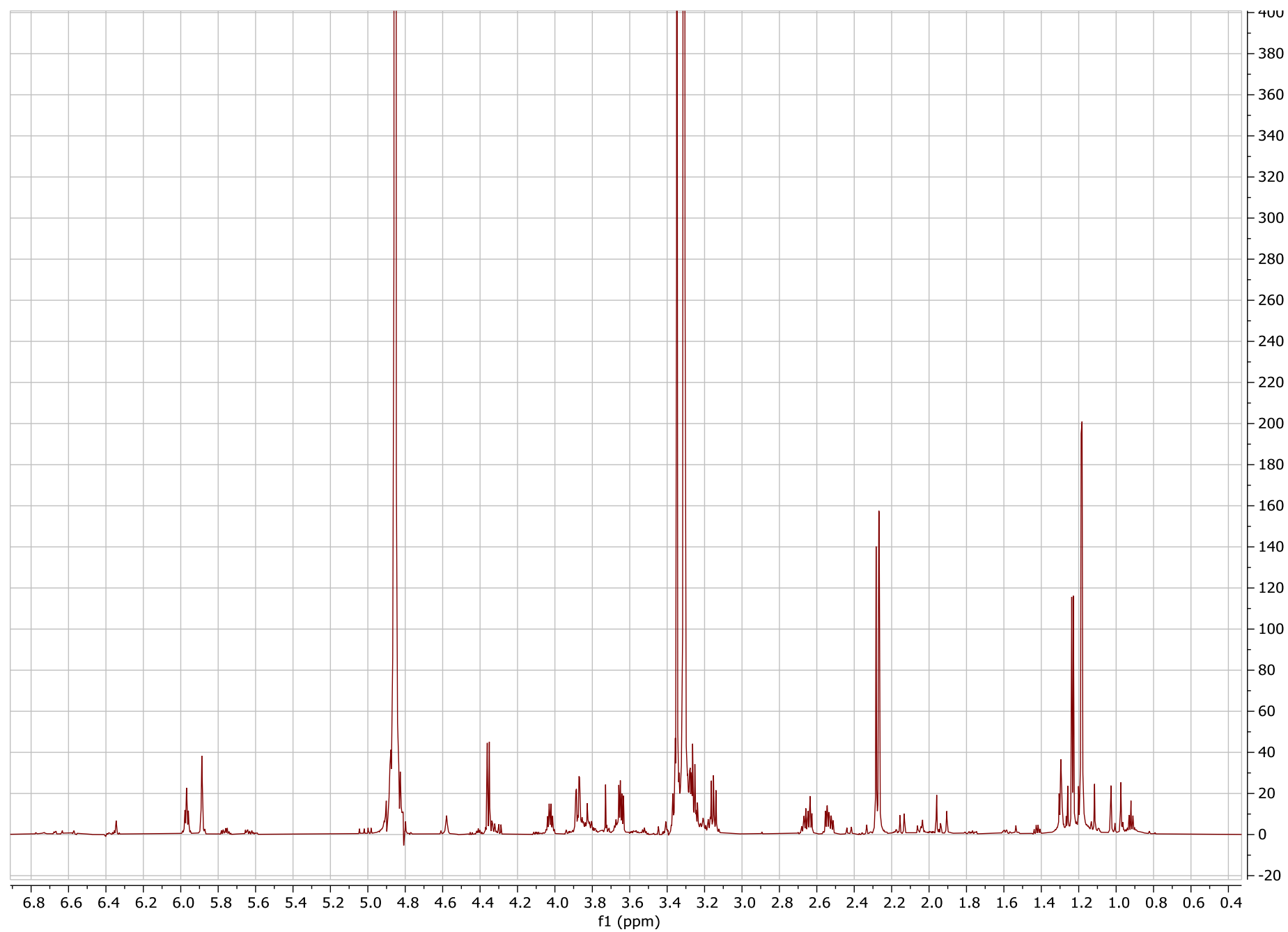


Figure S15. The ^{13}C NMR spectrum of **3** in methanol- d_4

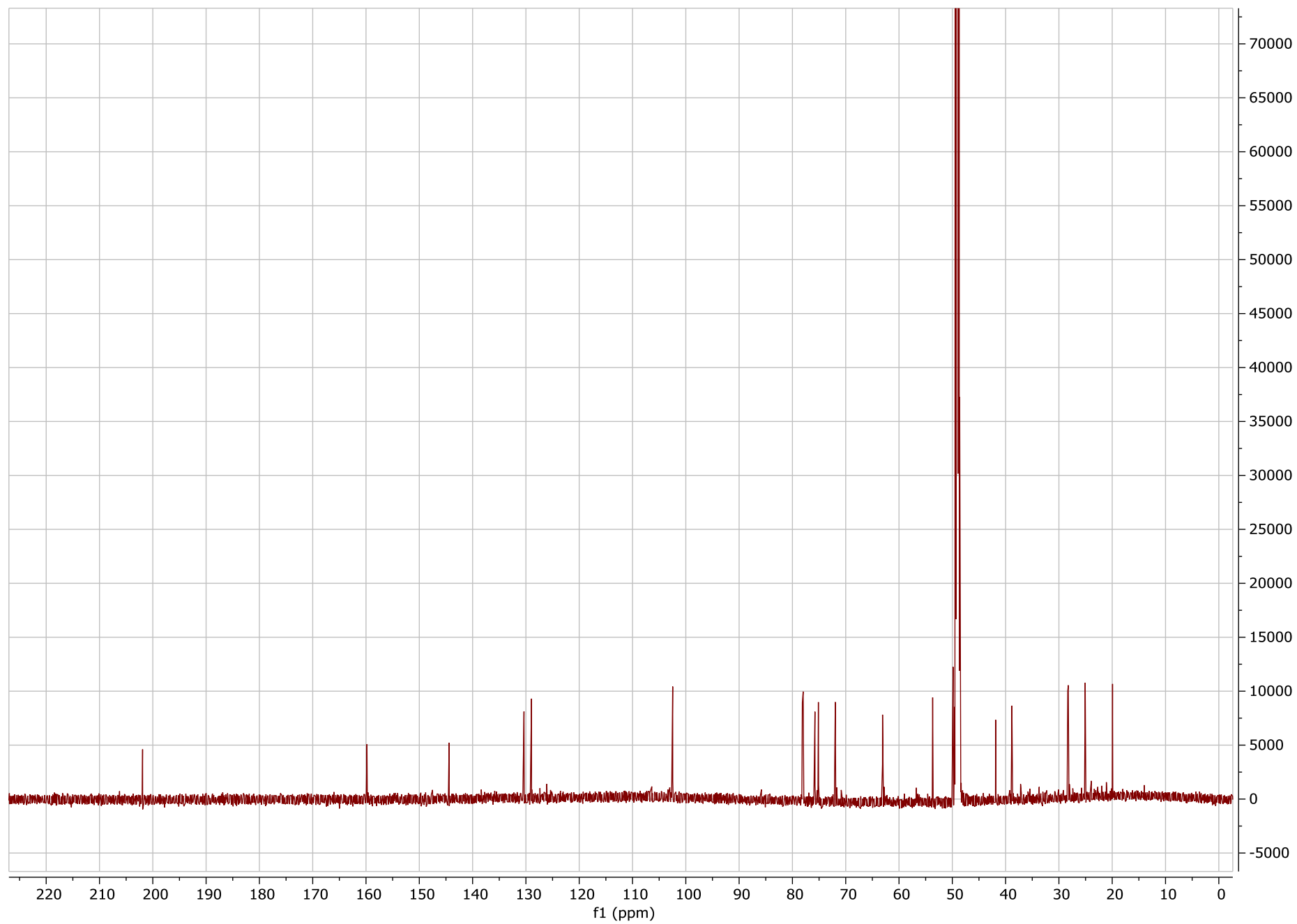


Figure S16. The ^1H NMR spectrum of **4** in methanol- d_4

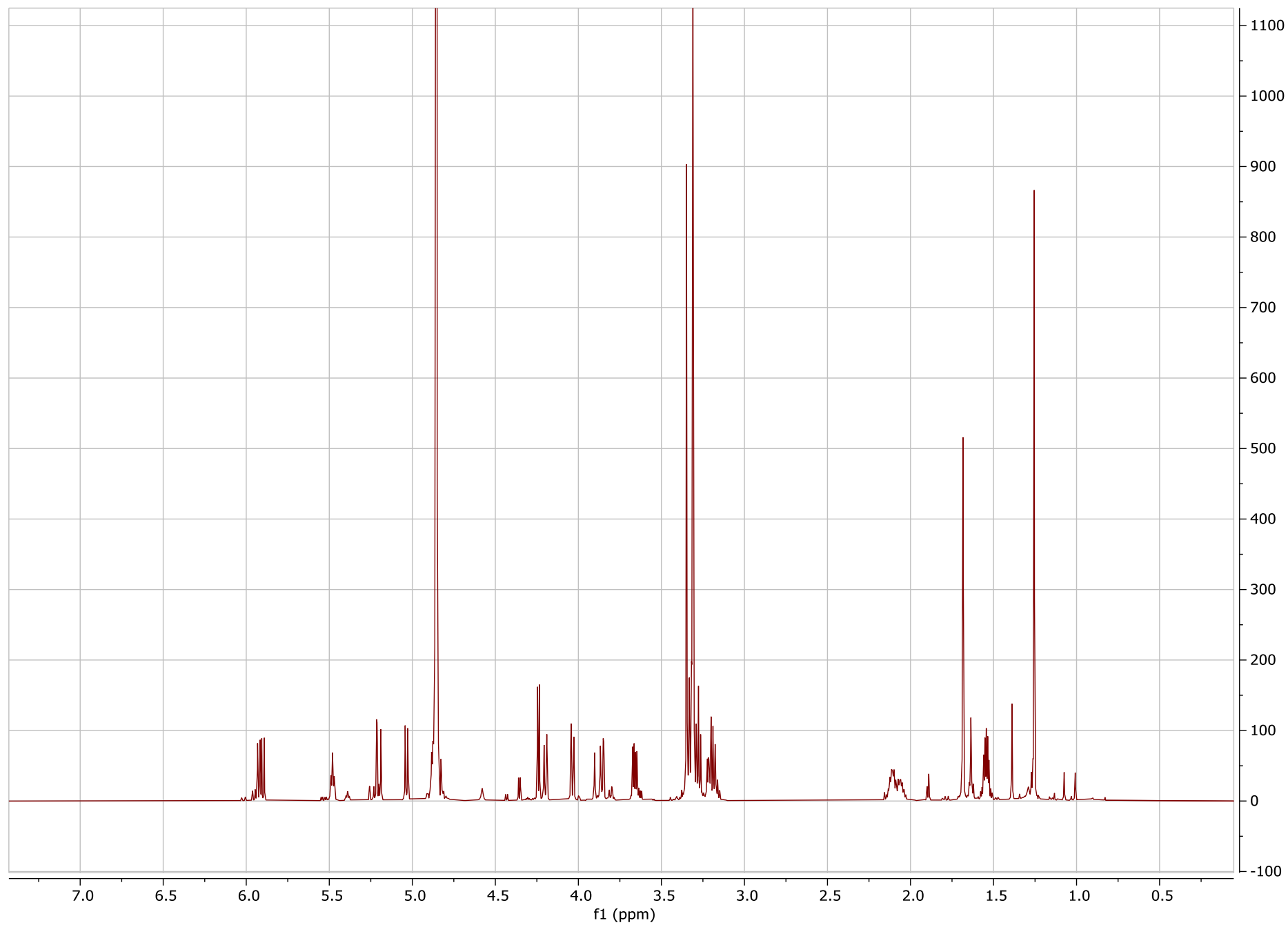


Figure S17. The ^{13}C NMR spectrum of **4** in methanol- d_4

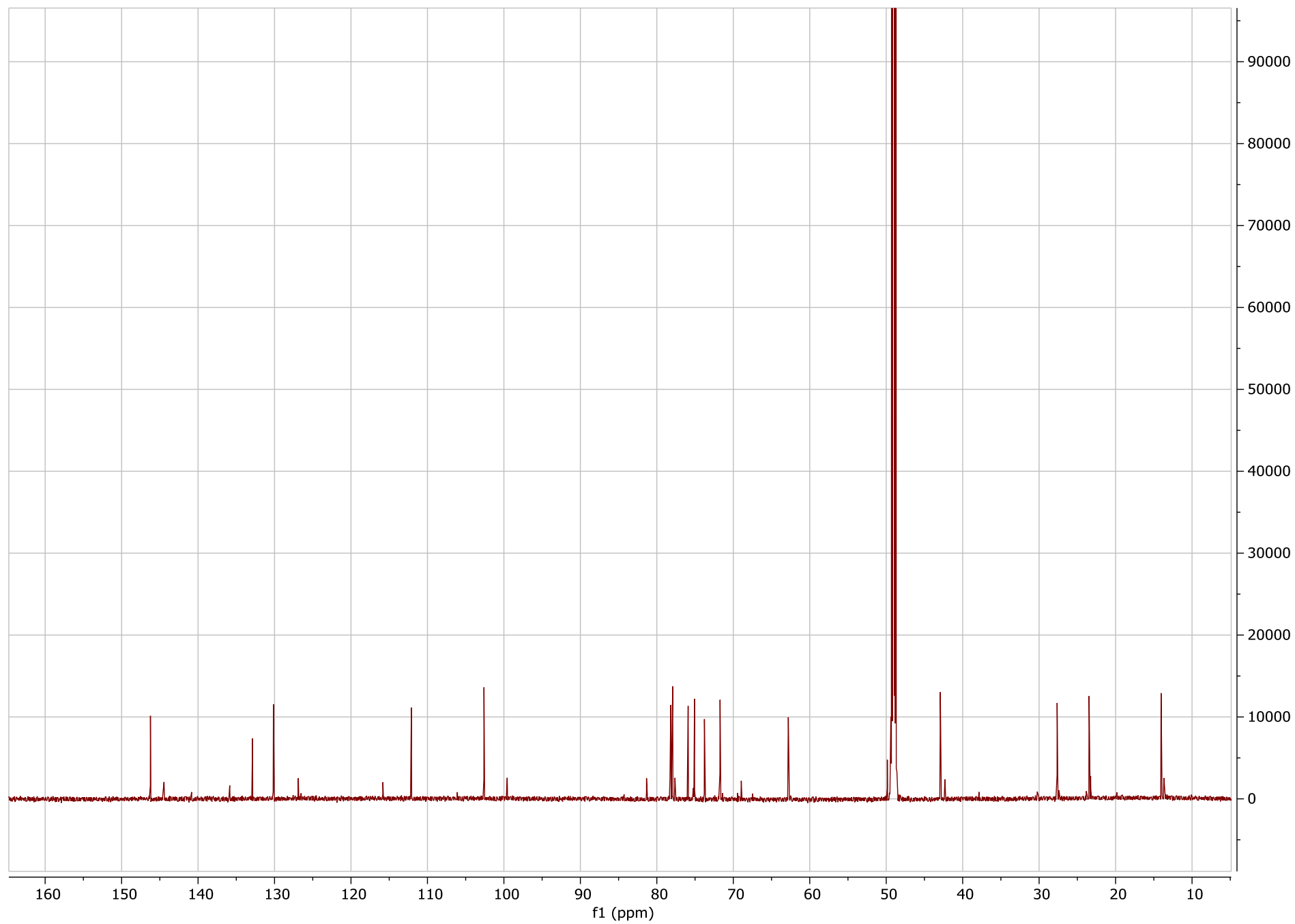


Figure S18. The ^1H NMR spectrum of **5** in methanol- d_4

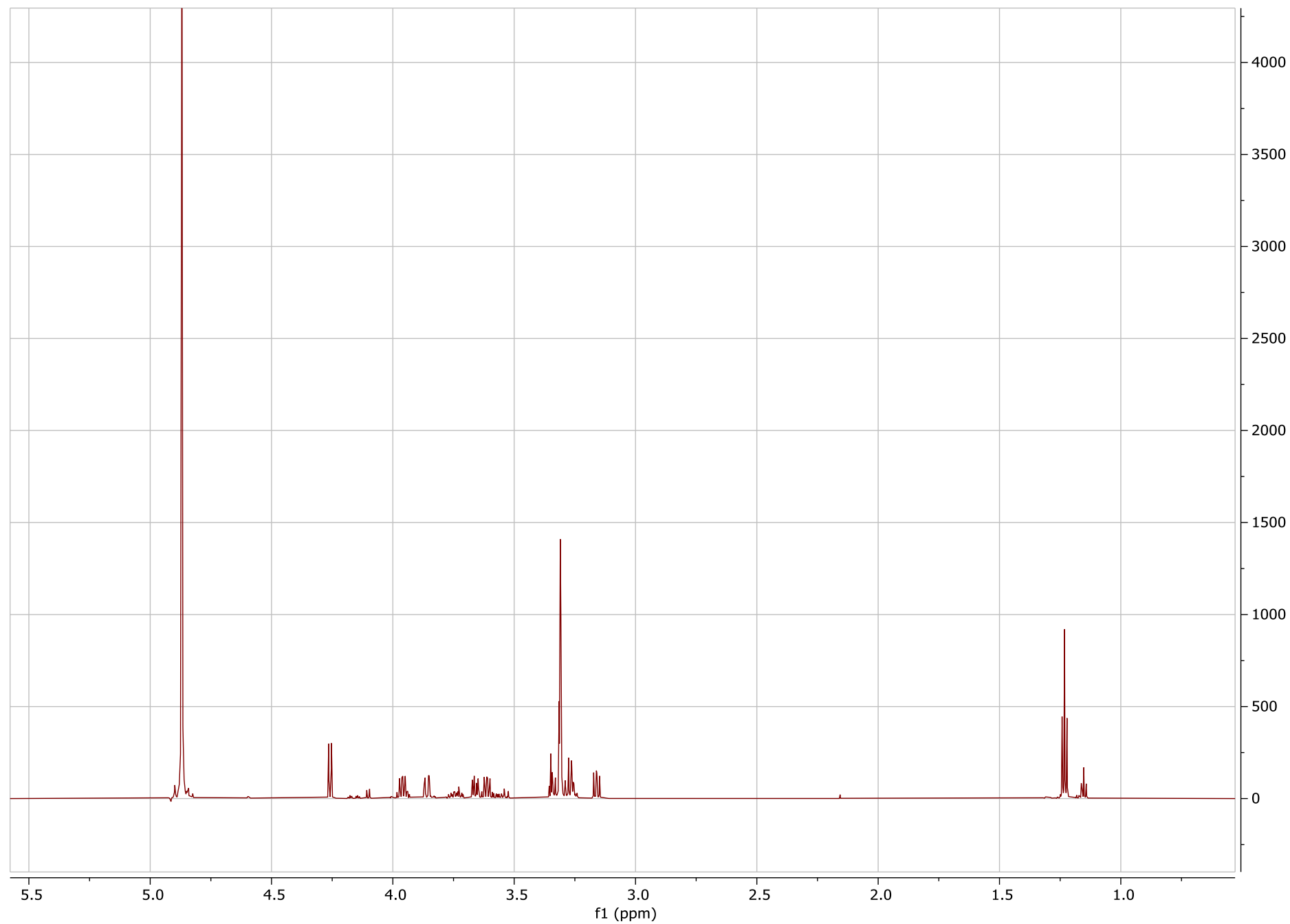


Figure S19. The ^{13}C NMR spectrum of **5** in methanol- d_4

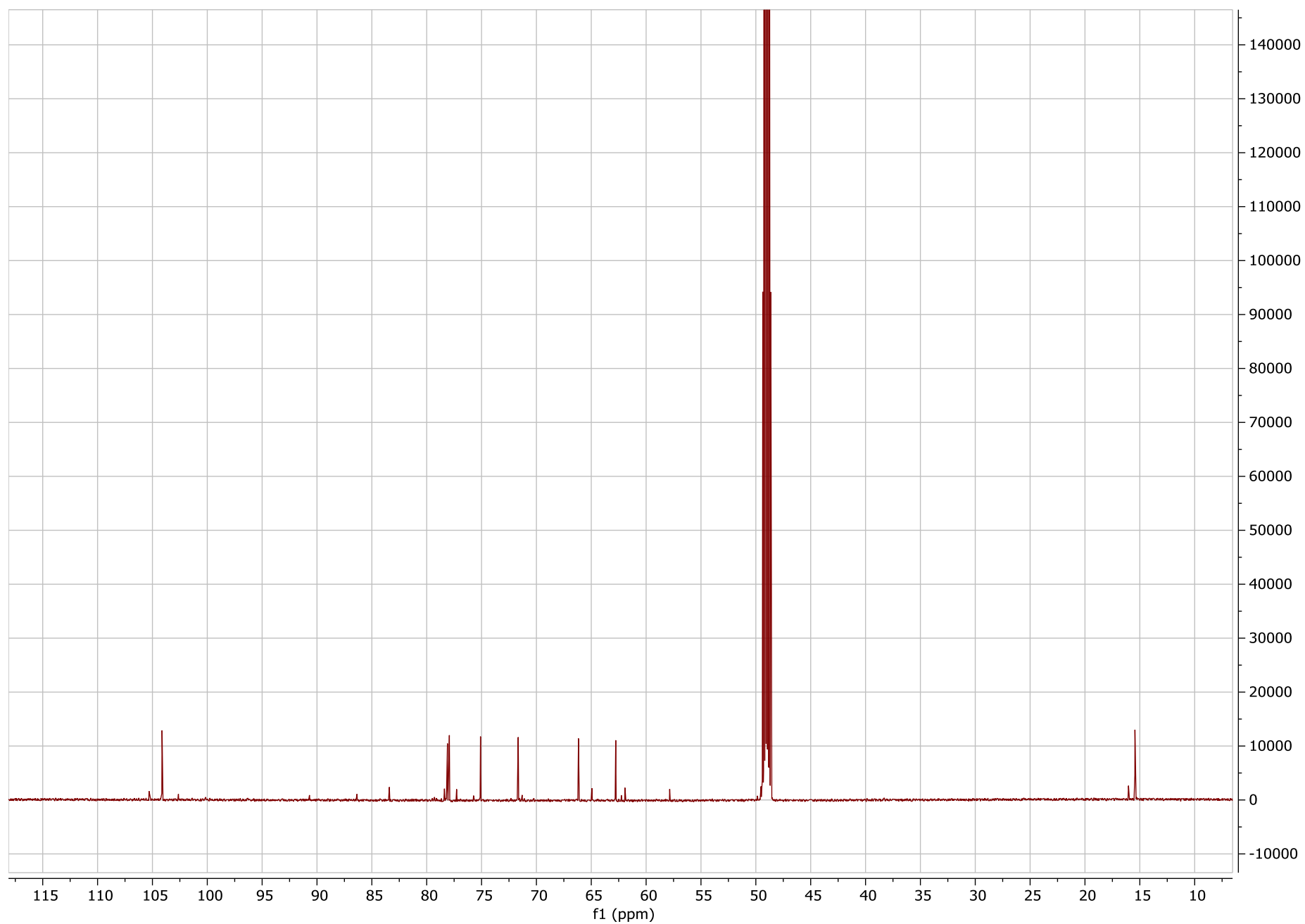


Figure S20. The ^1H NMR spectrum of **6** in methanol- d_4

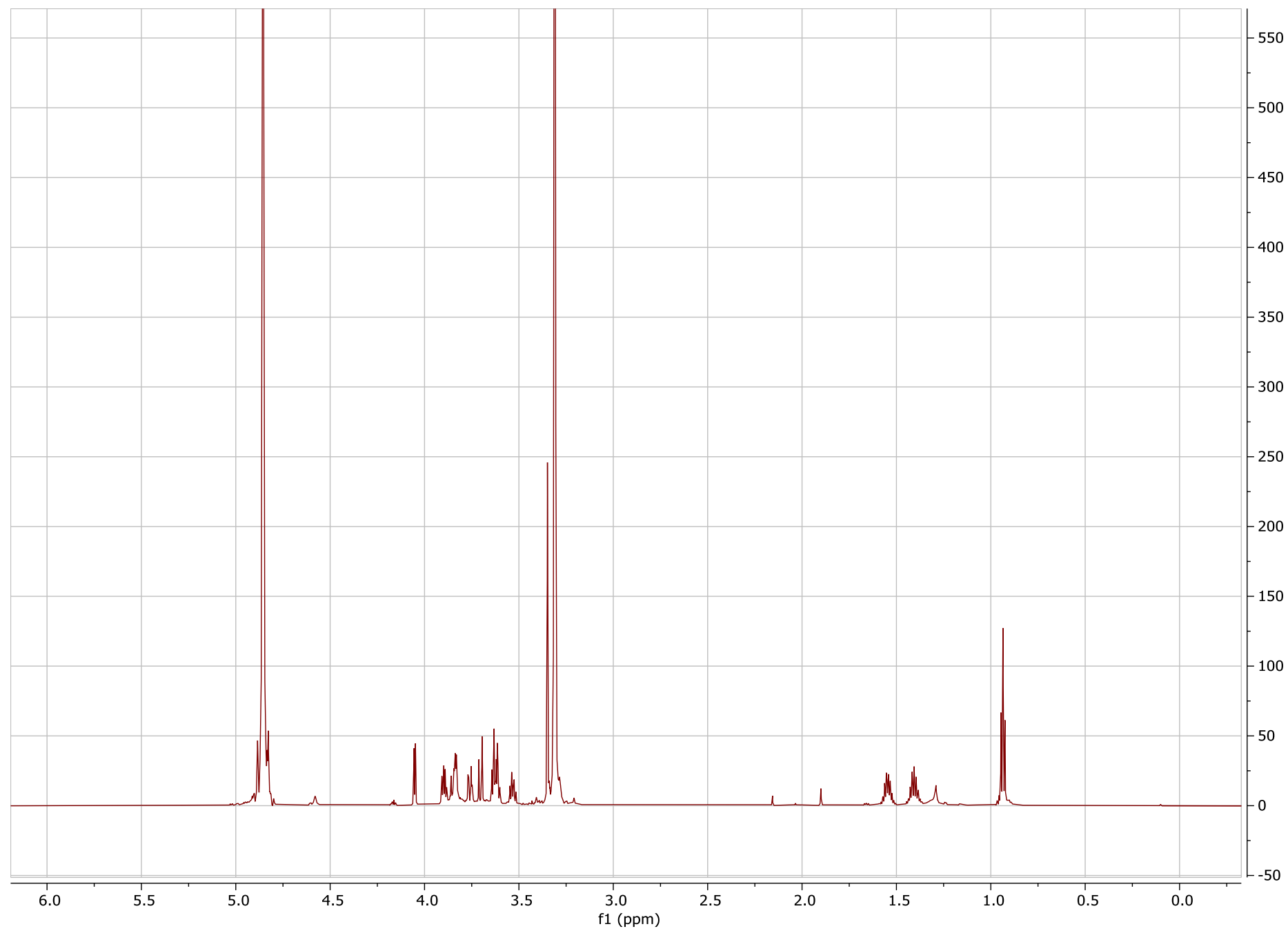


Figure S21. The ^{13}C NMR spectrum of **6** in methanol- d_4

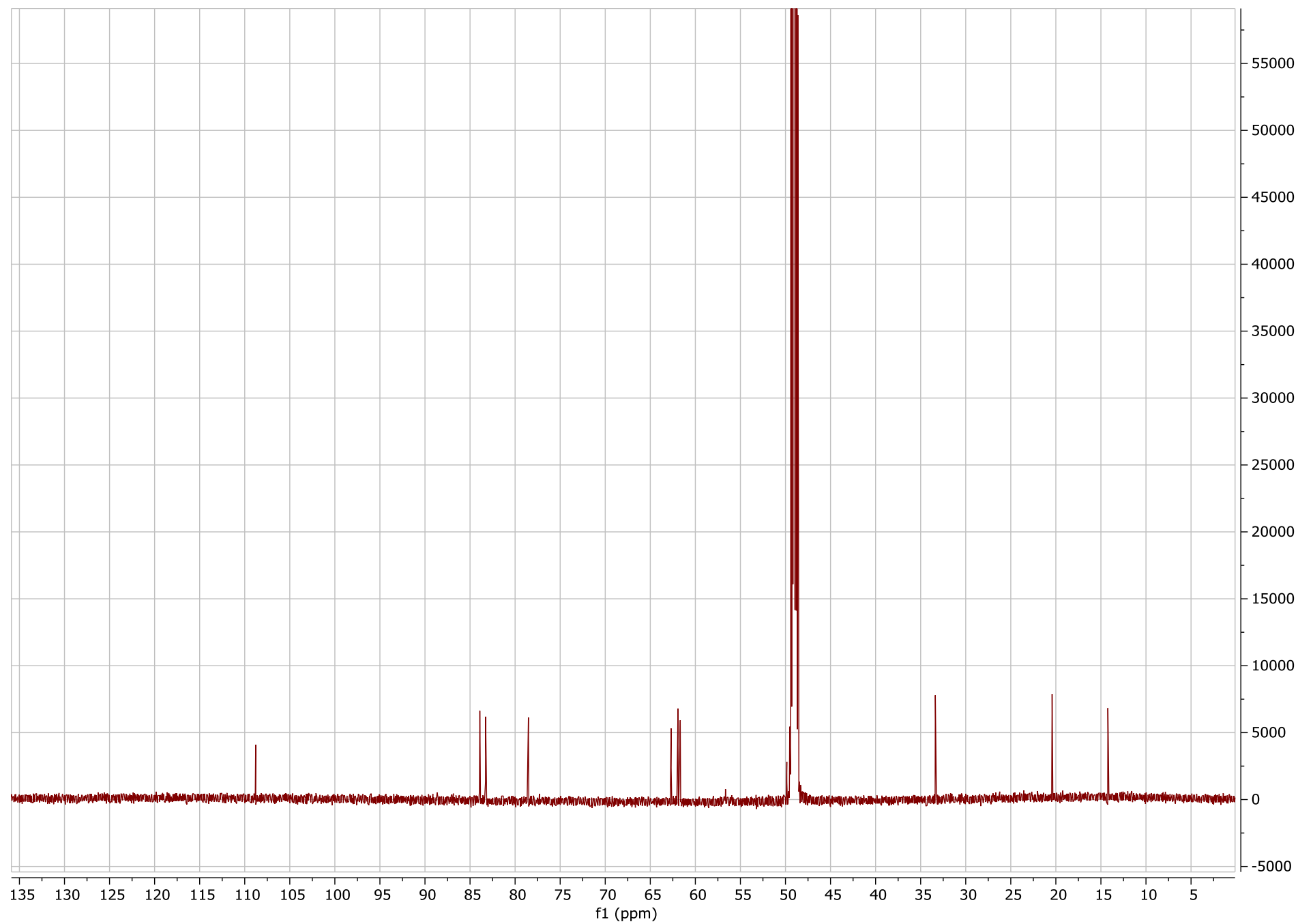


Figure S22. The ^1H NMR spectrum of **7** in methanol- d_4

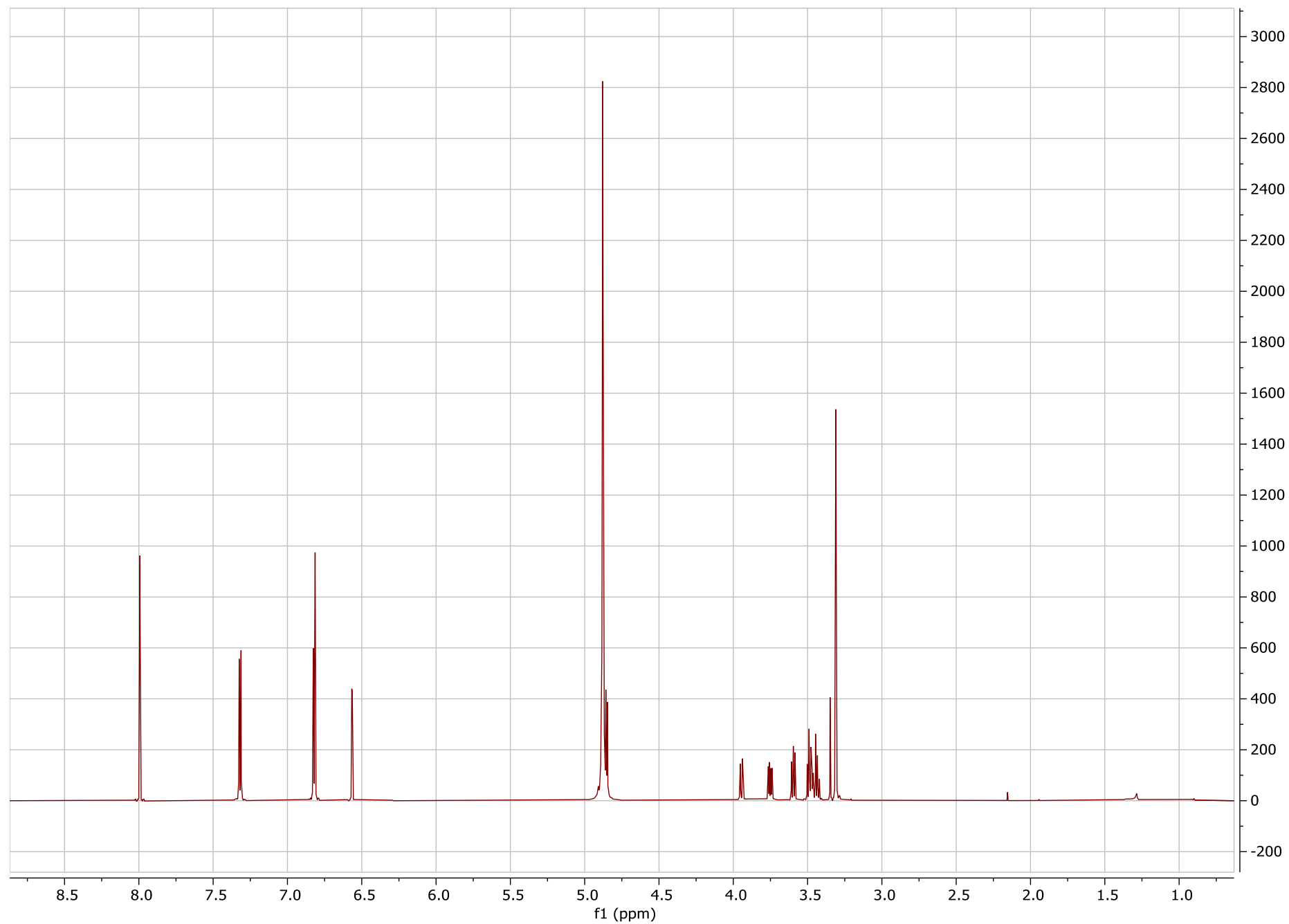


Figure S23. The ^{13}C NMR spectrum of **7** in methanol- d_4

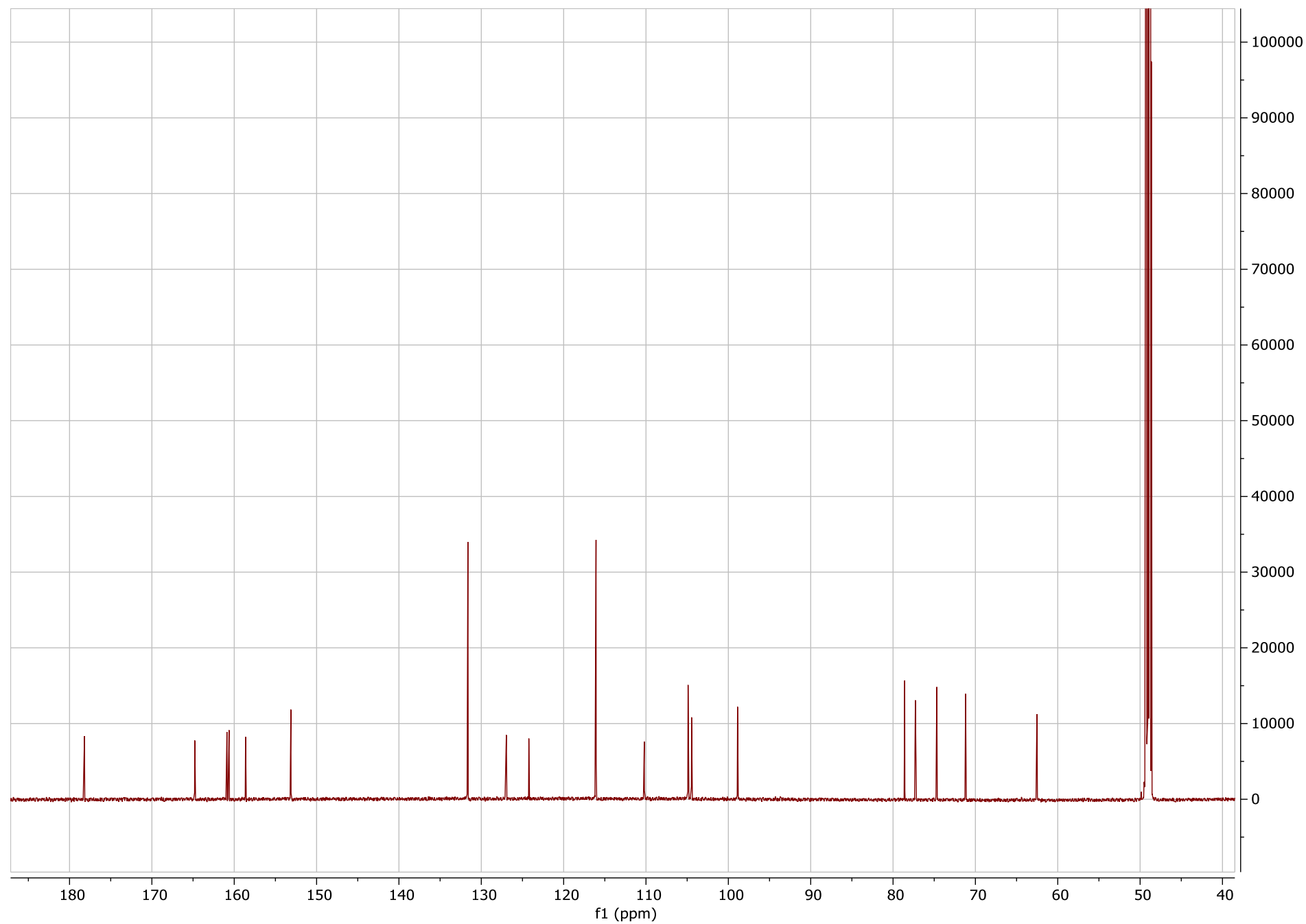


Figure S24. The ^1H NMR spectrum of **8** in methanol- d_4 + chloroform- d

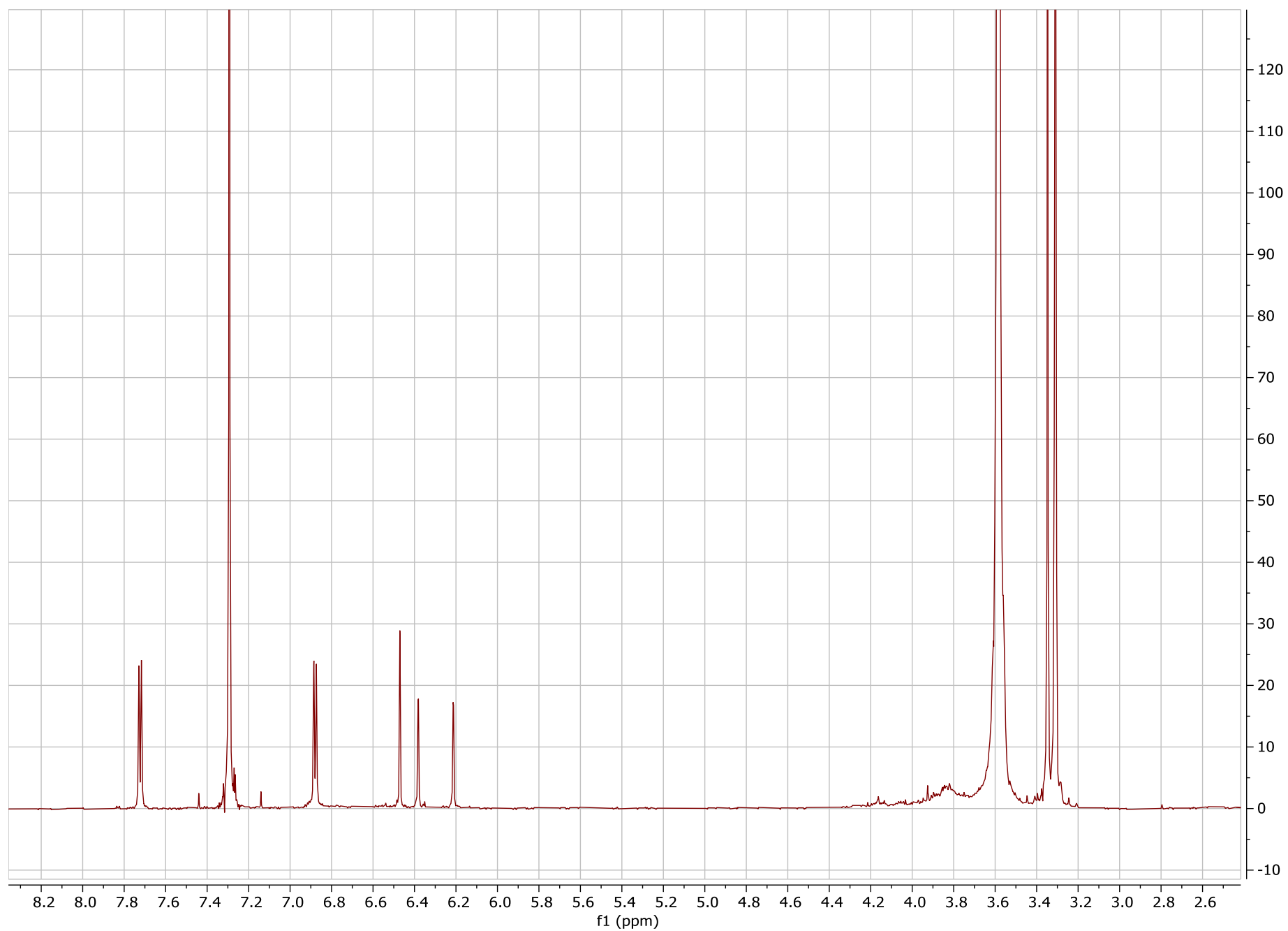


Figure S25. The ^{13}C NMR spectrum of **8** in methanol- d_4 + chloroform- d

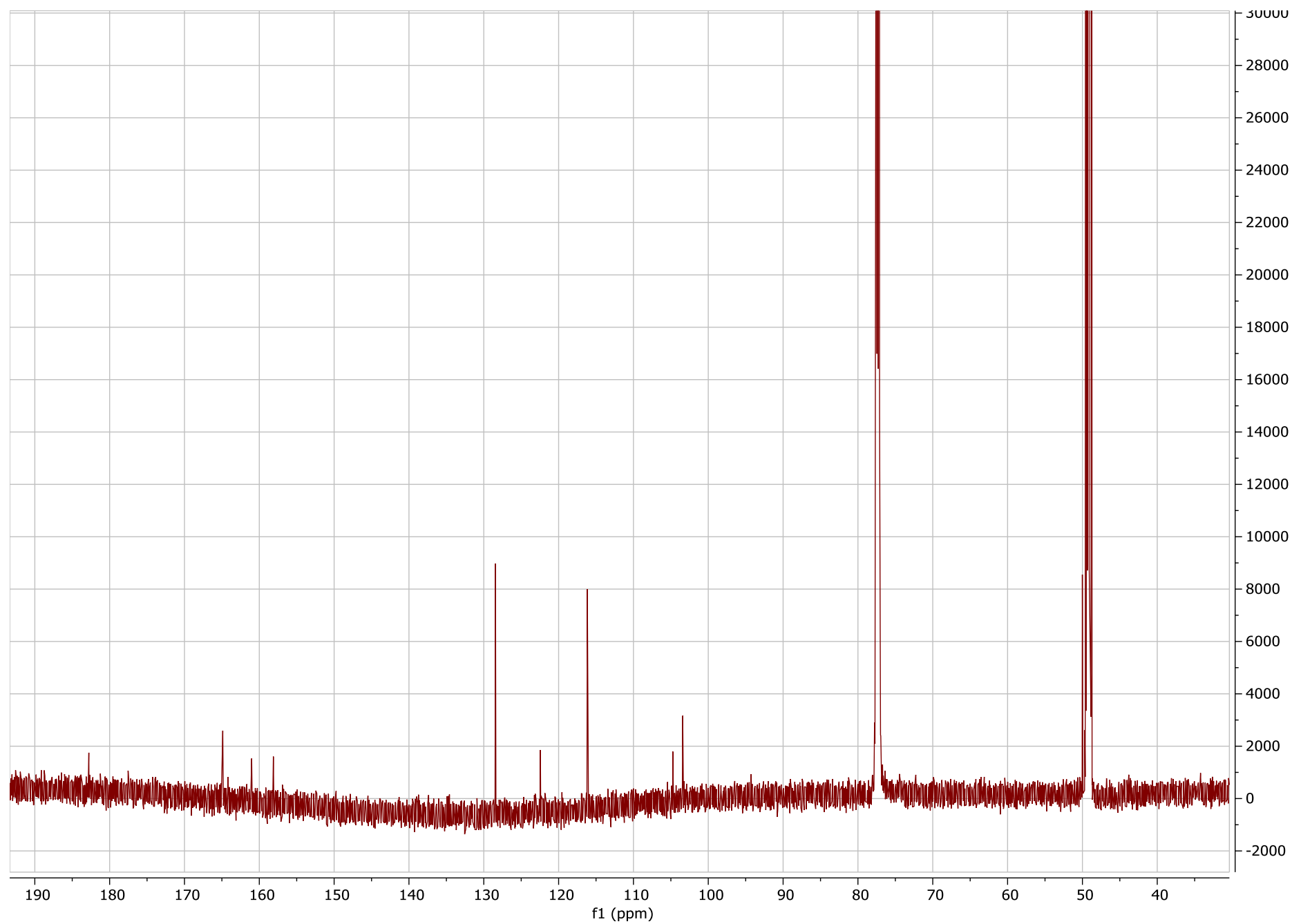


Figure S26. The ^1H NMR spectrum of **9** in methanol- d_4

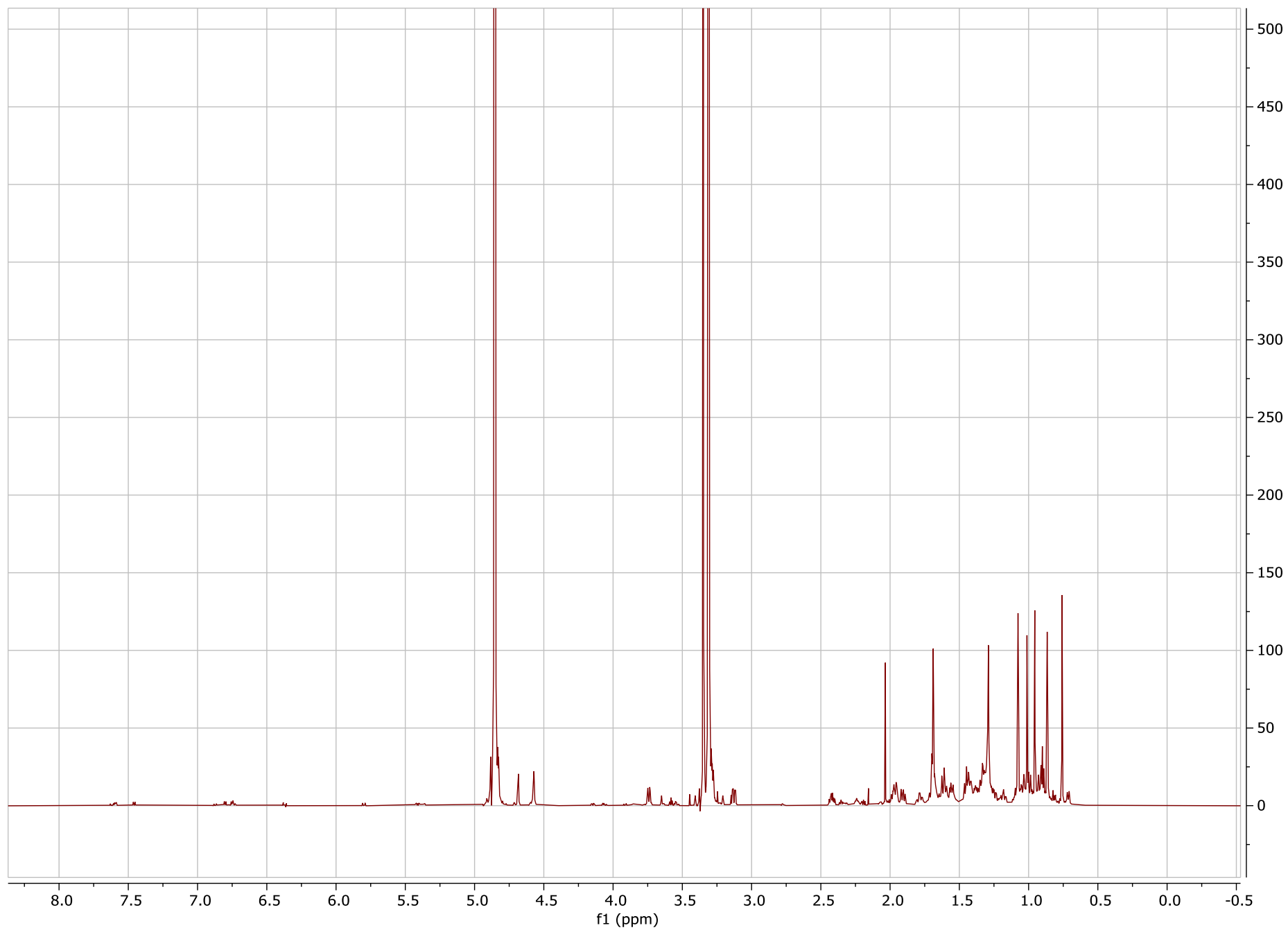


Figure S27. The ^{13}C NMR spectrum of **9** in methanol- d_4

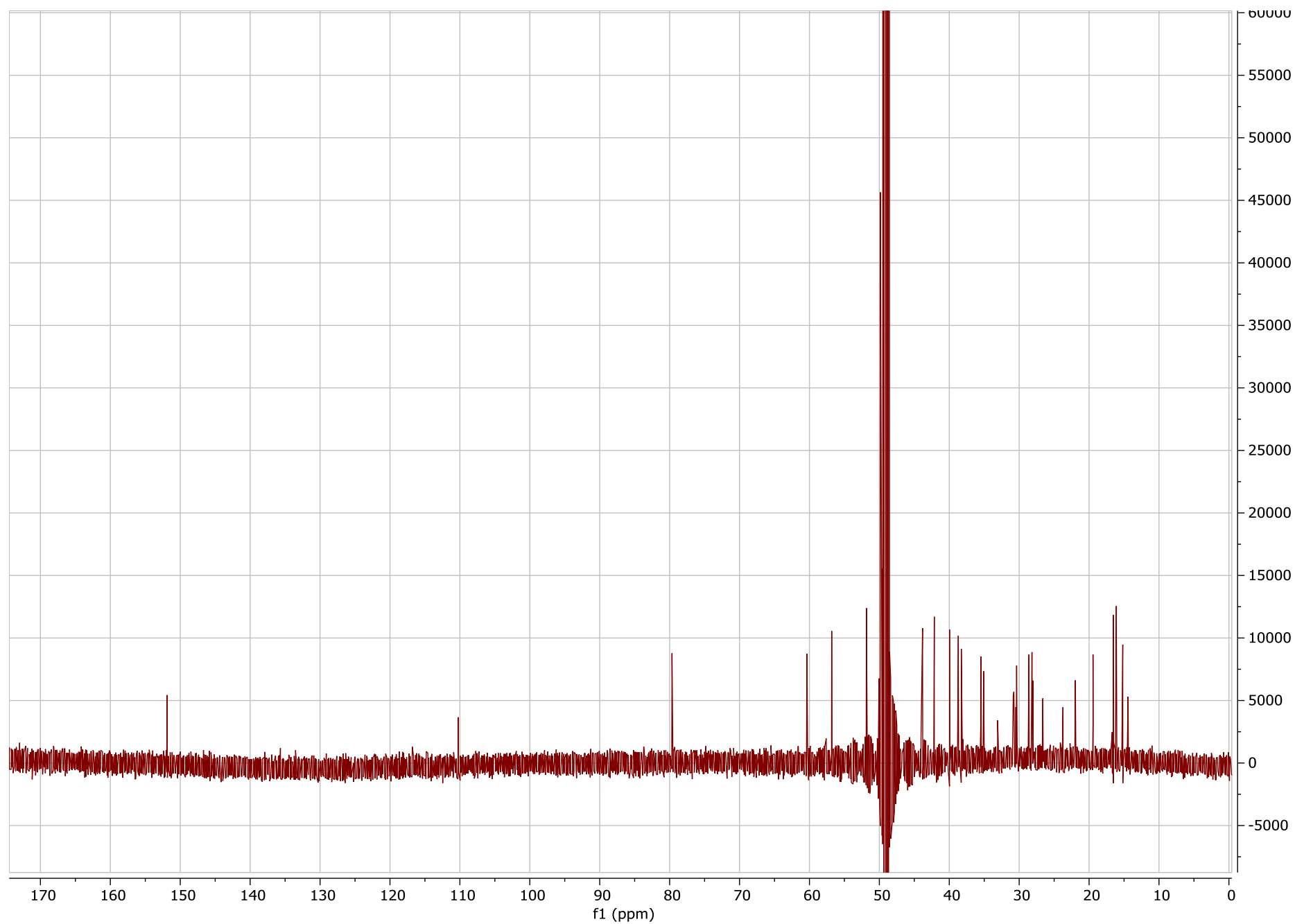


Figure S28. The ^1H NMR spectrum of **10** in methanol- d_4 + chloroform- d

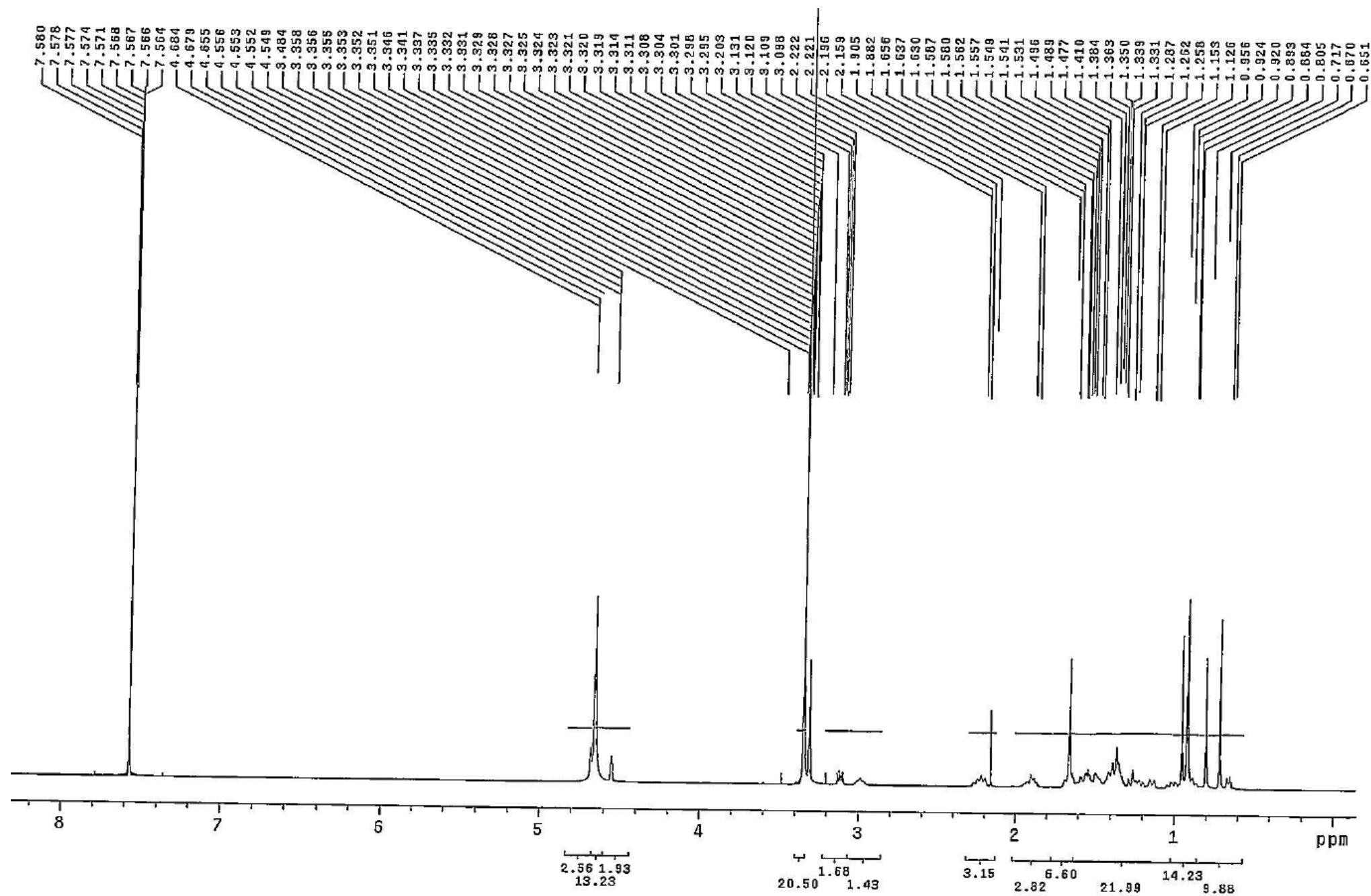


Figure S29. The ^{13}C NMR spectrum of **10** in methanol- d_4 + chloroform- d

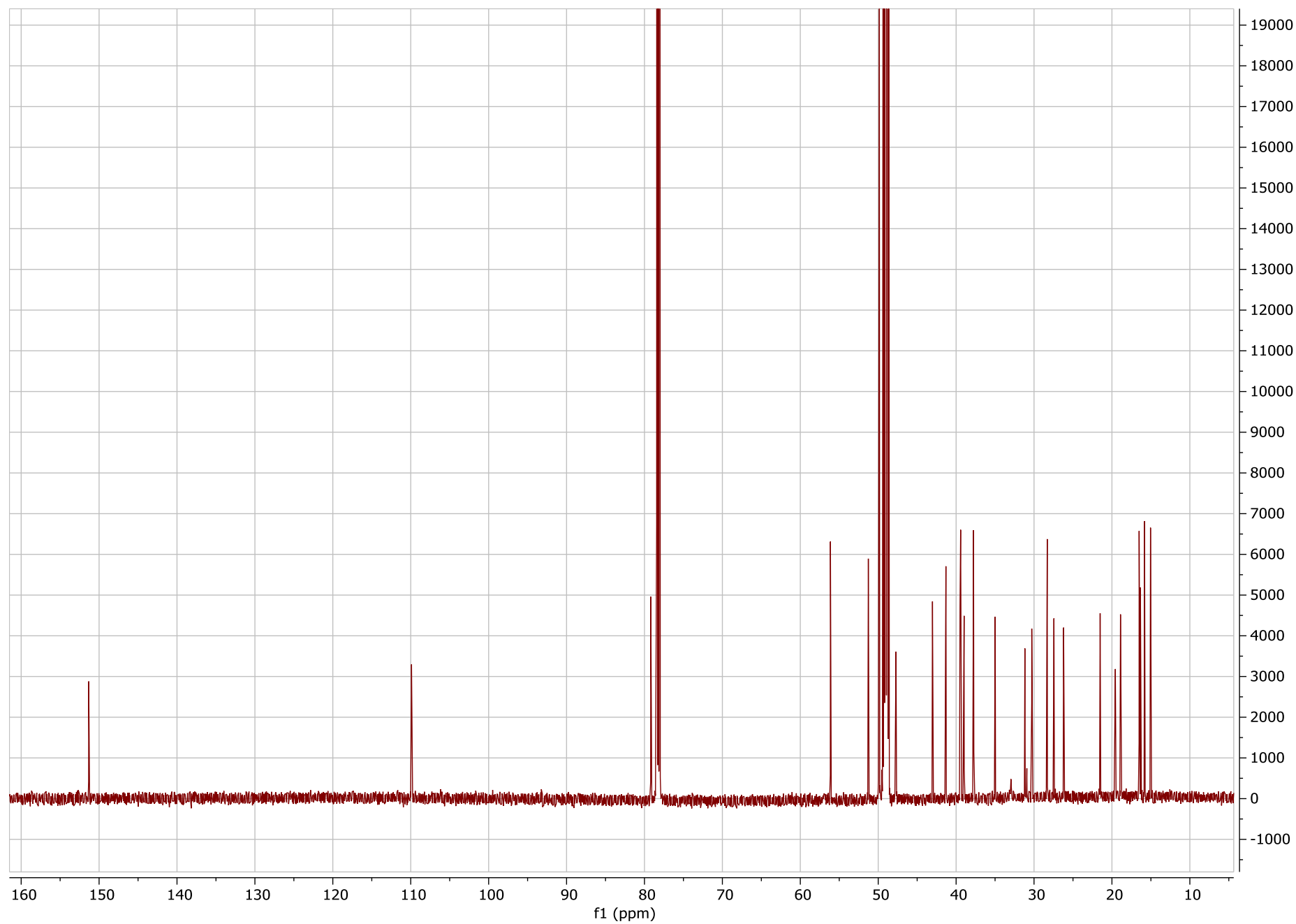


Figure S30. The ^1H NMR spectrum of **11** in chloroform-*d*

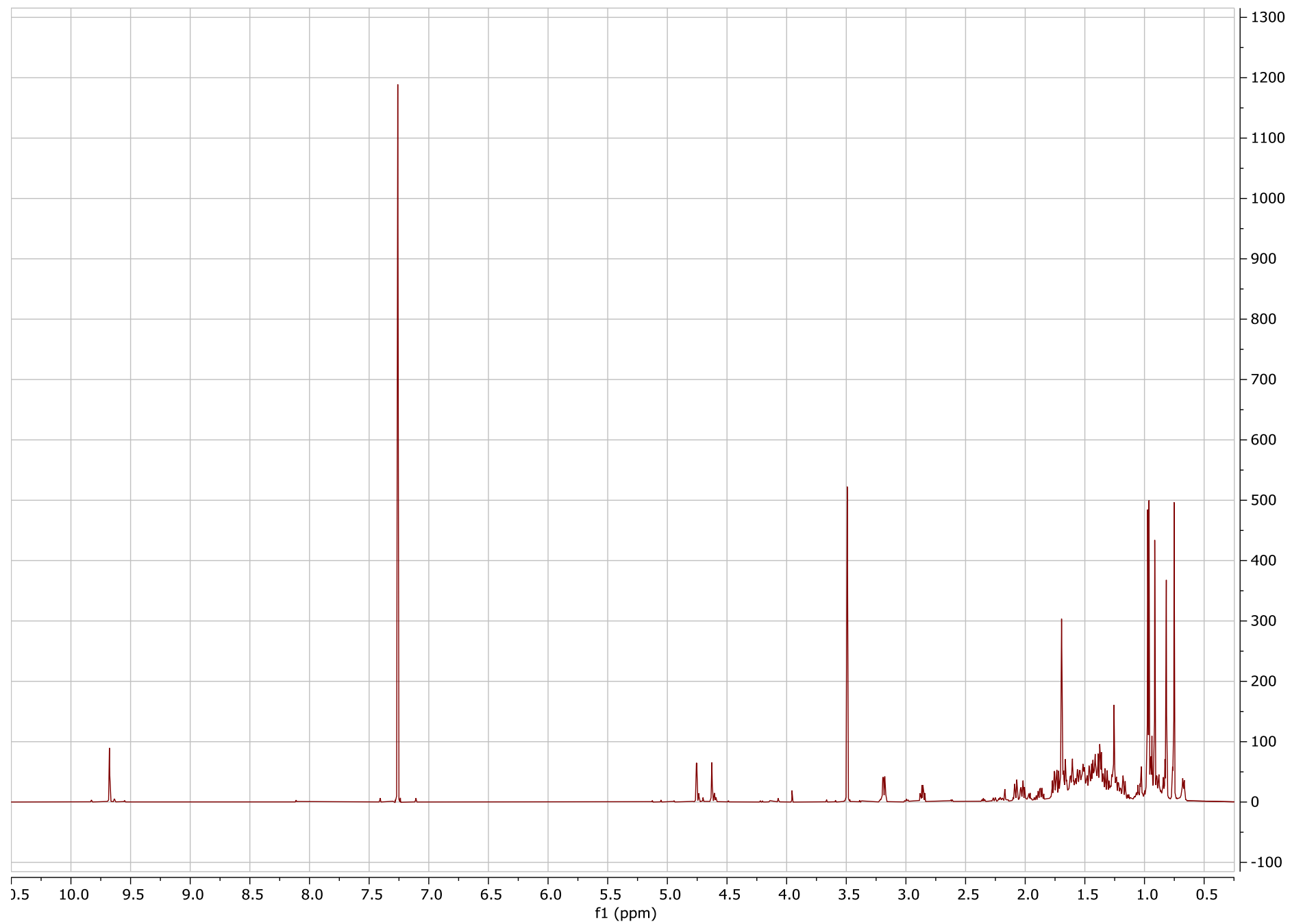


Figure S31. The ^1H NMR spectrum of **12** in pyridine- d_5

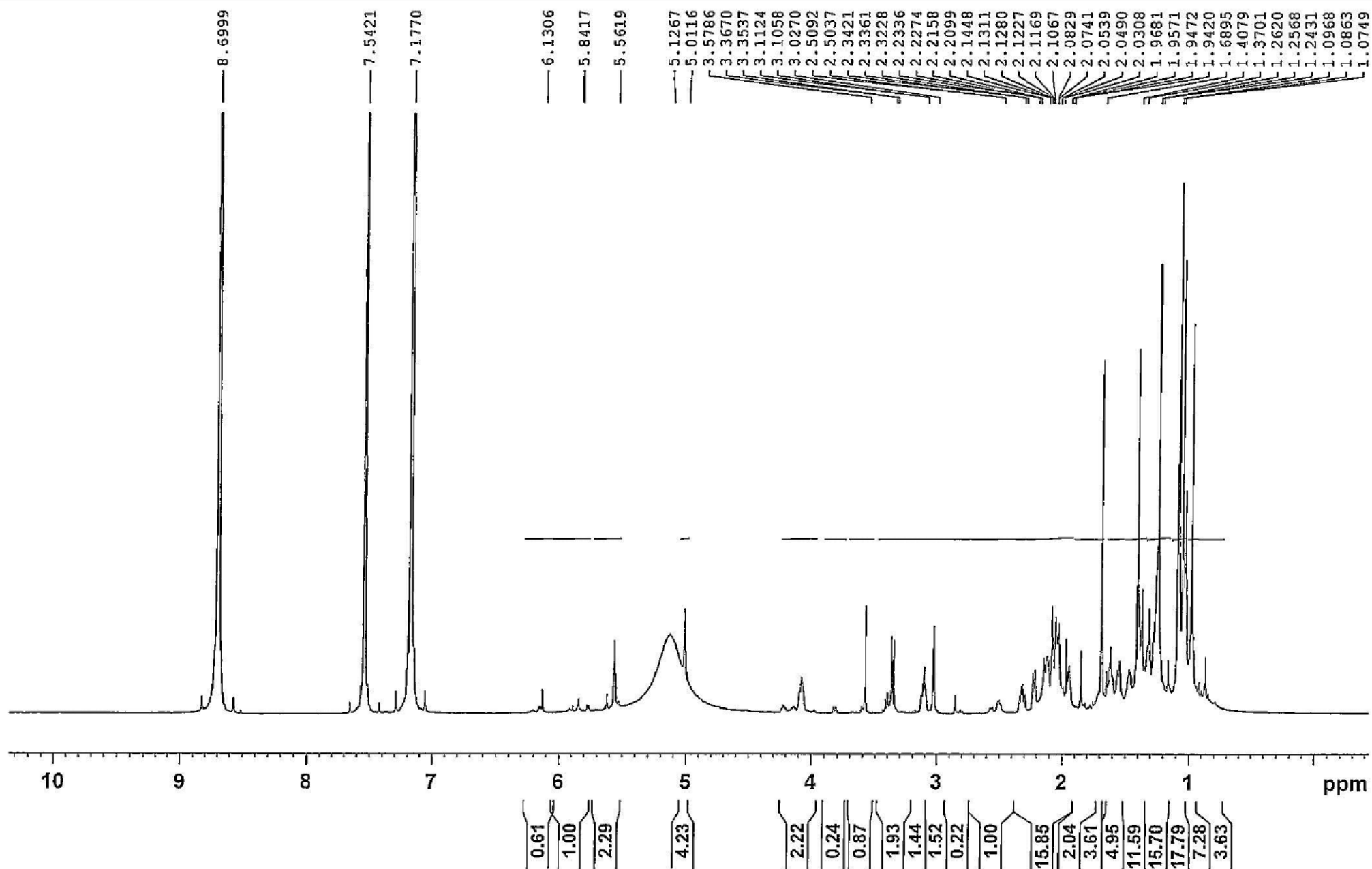


Figure S32. The ^{13}C NMR spectrum of **12** in pyridine- d_5

