

# Electronic Supplementary Information

## Natural Nitric Oxide (NO) inhibitors from *Aristolochia mollissima*

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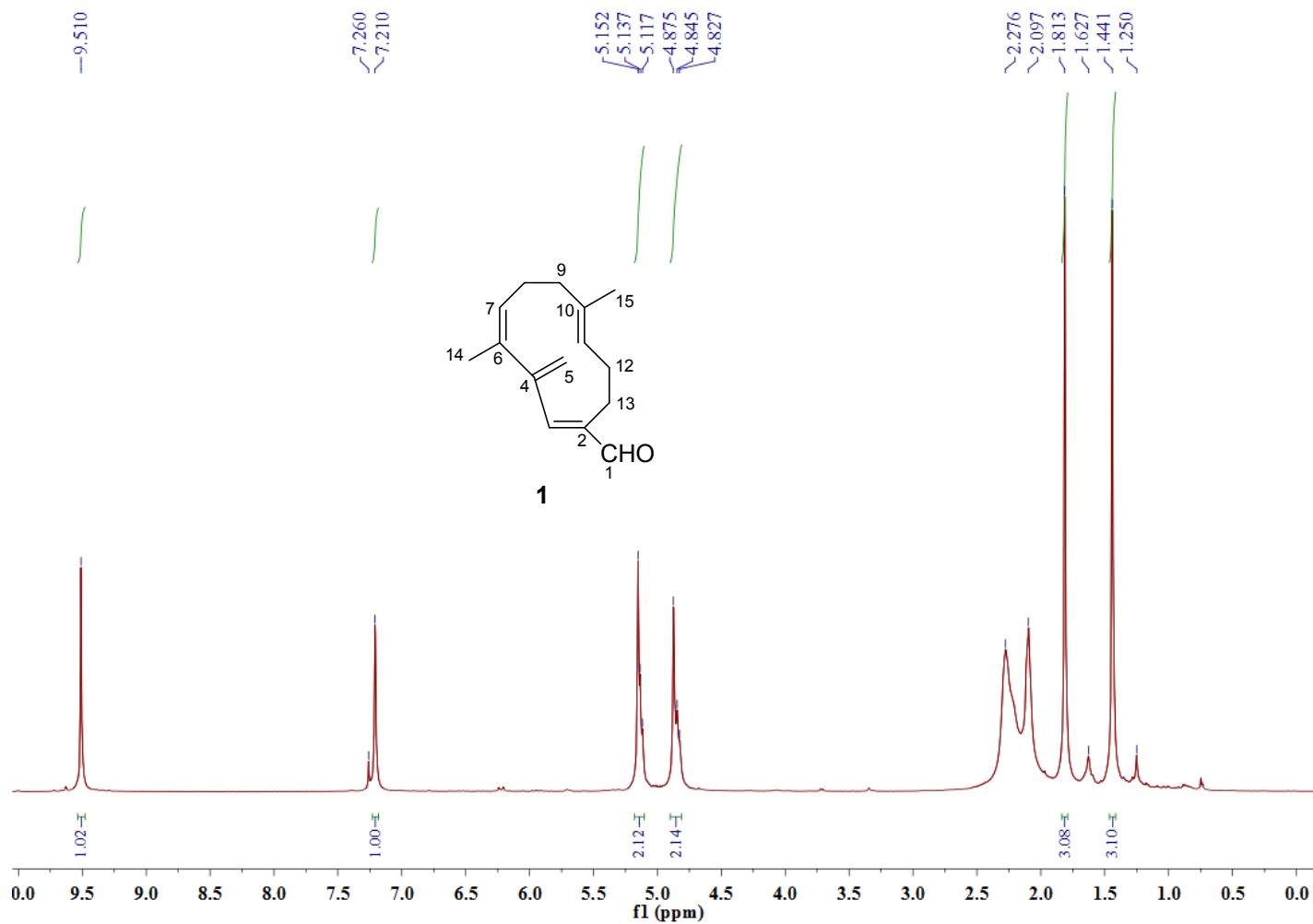
<sup>‡</sup> These authors have contributed equally to this work.

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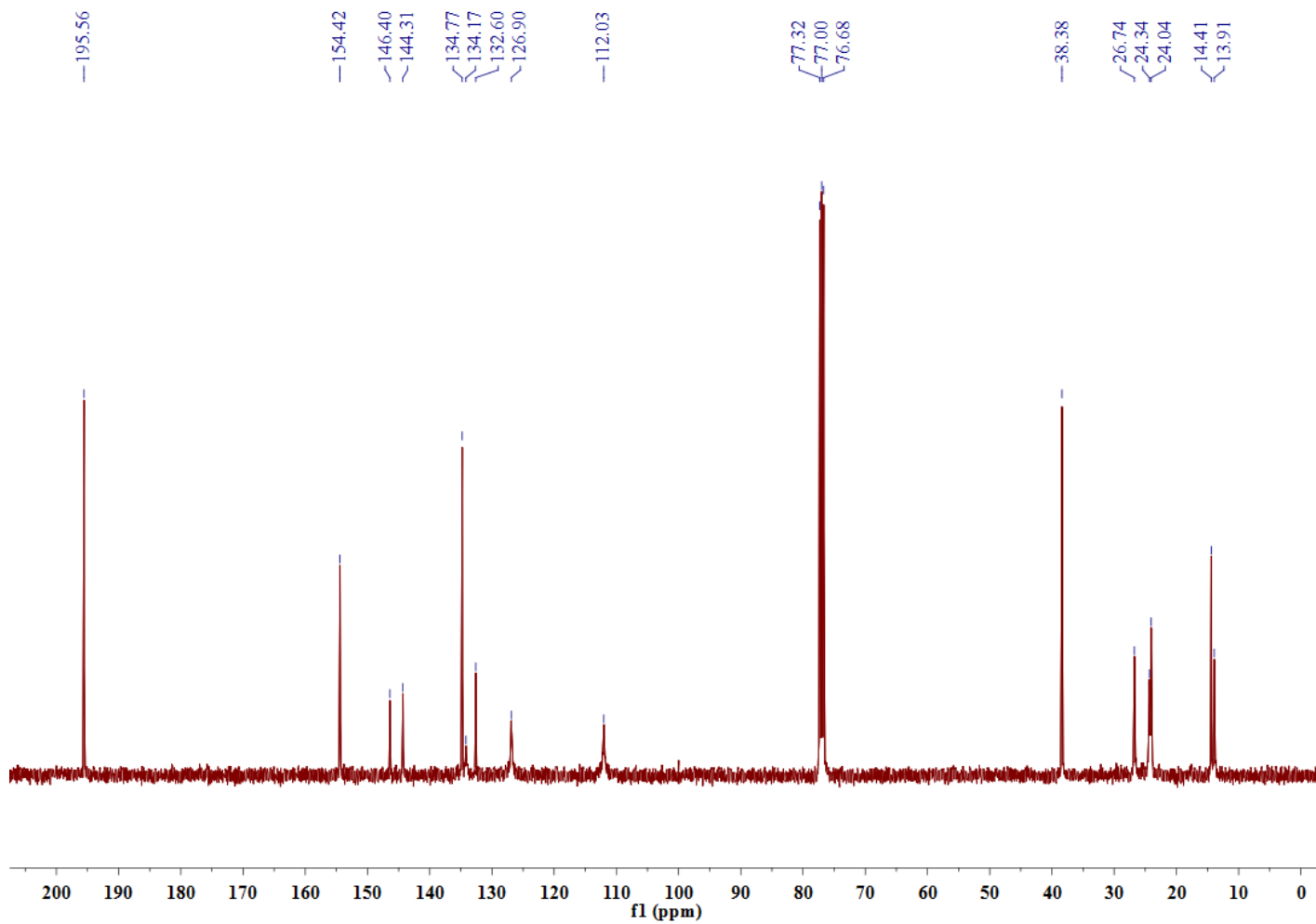
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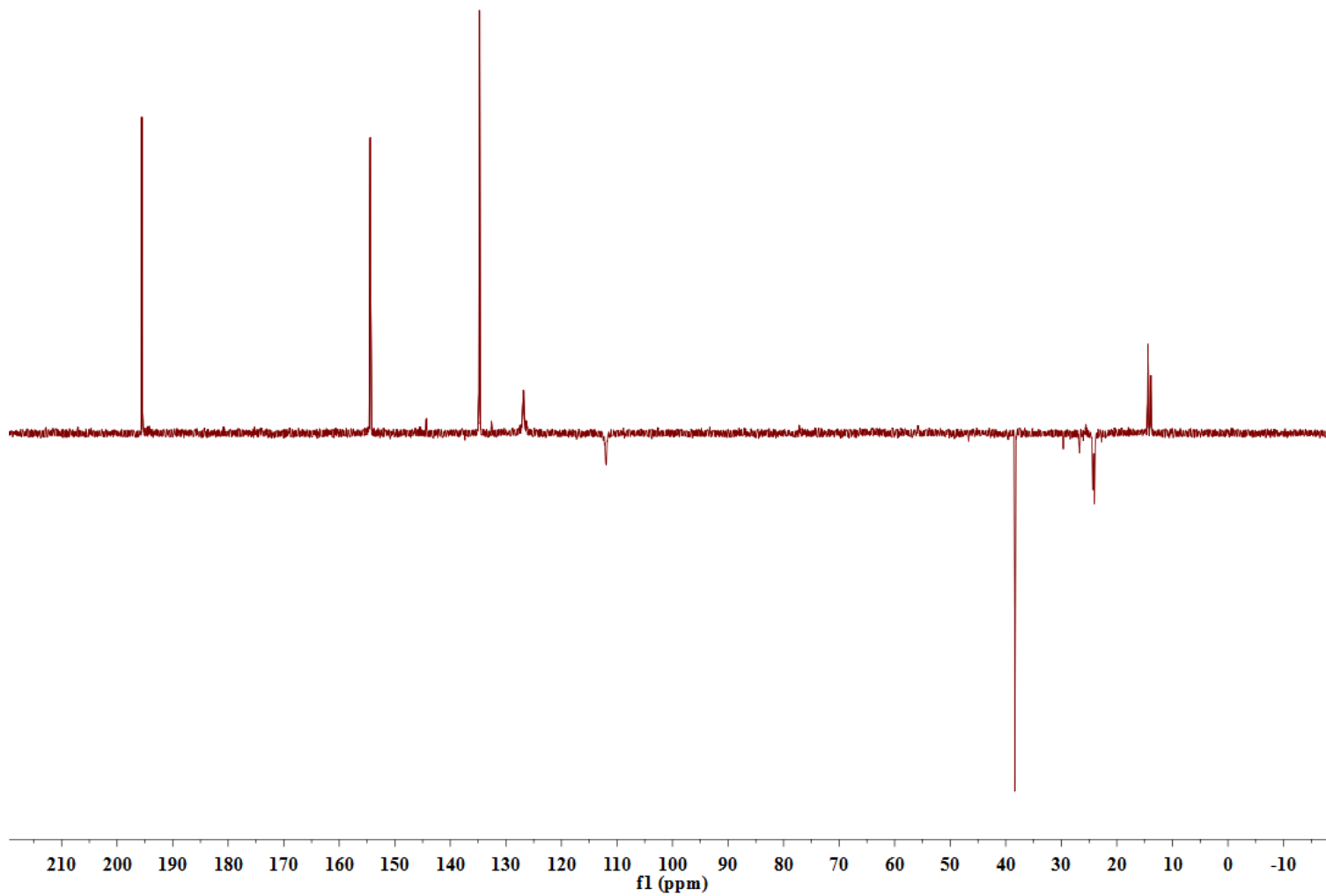
- S51**  $^1\text{H}$  NMR Spectrum of **16** in  $\text{CDCl}_3$
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- S66** Detail information for ECD calculations

S1 <sup>1</sup>H NMR Spectrum of **1** in CDCl<sub>3</sub>

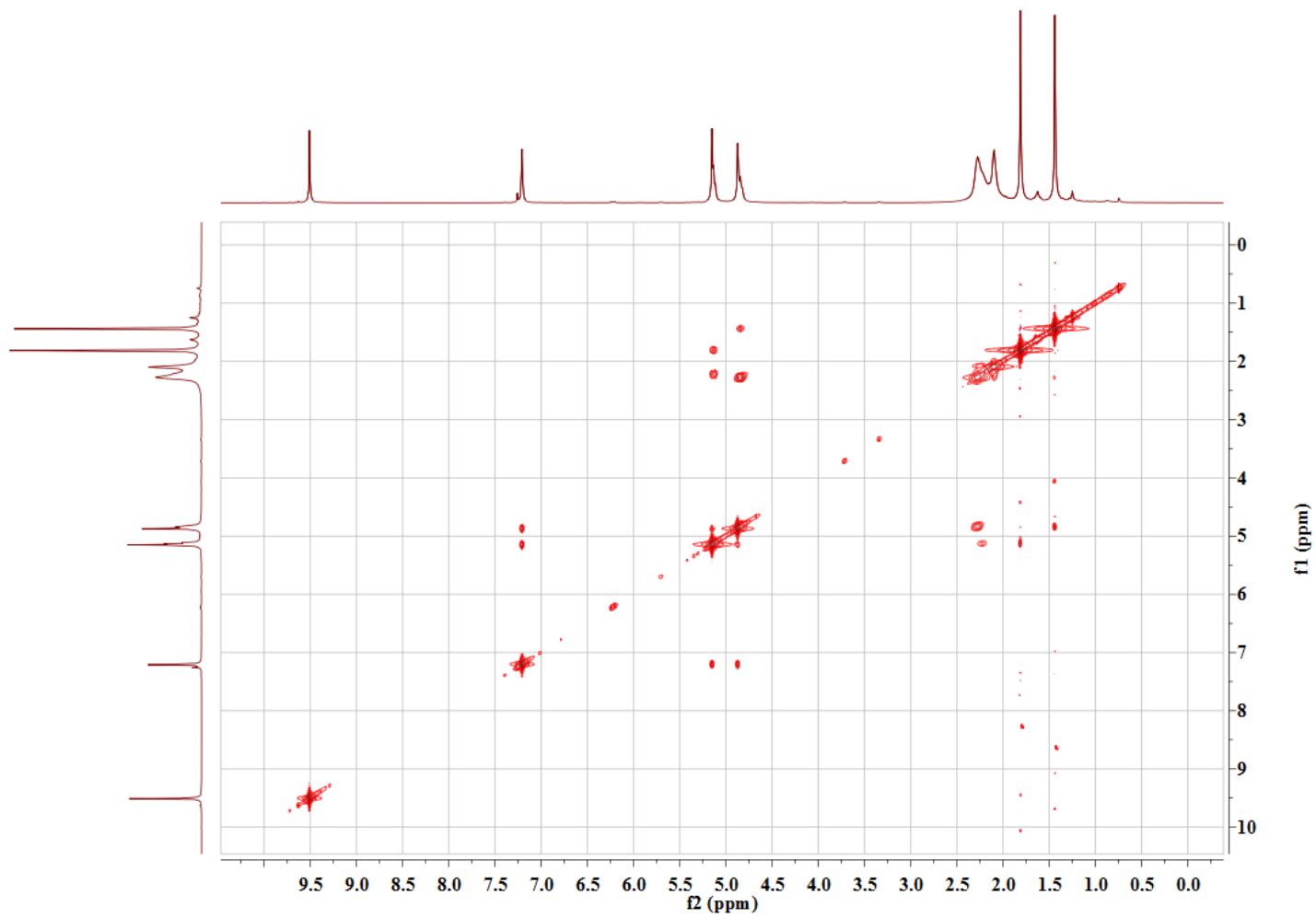


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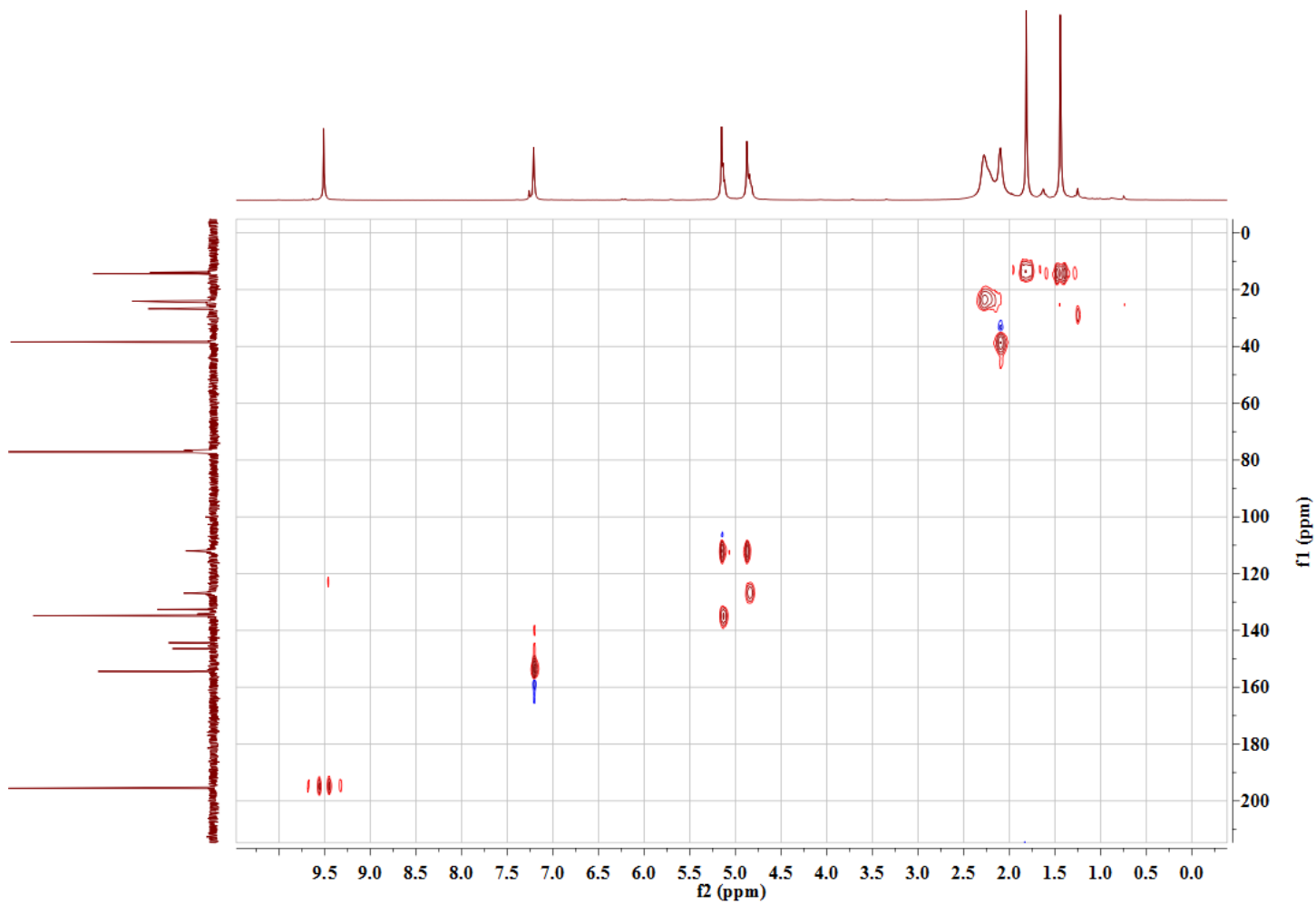


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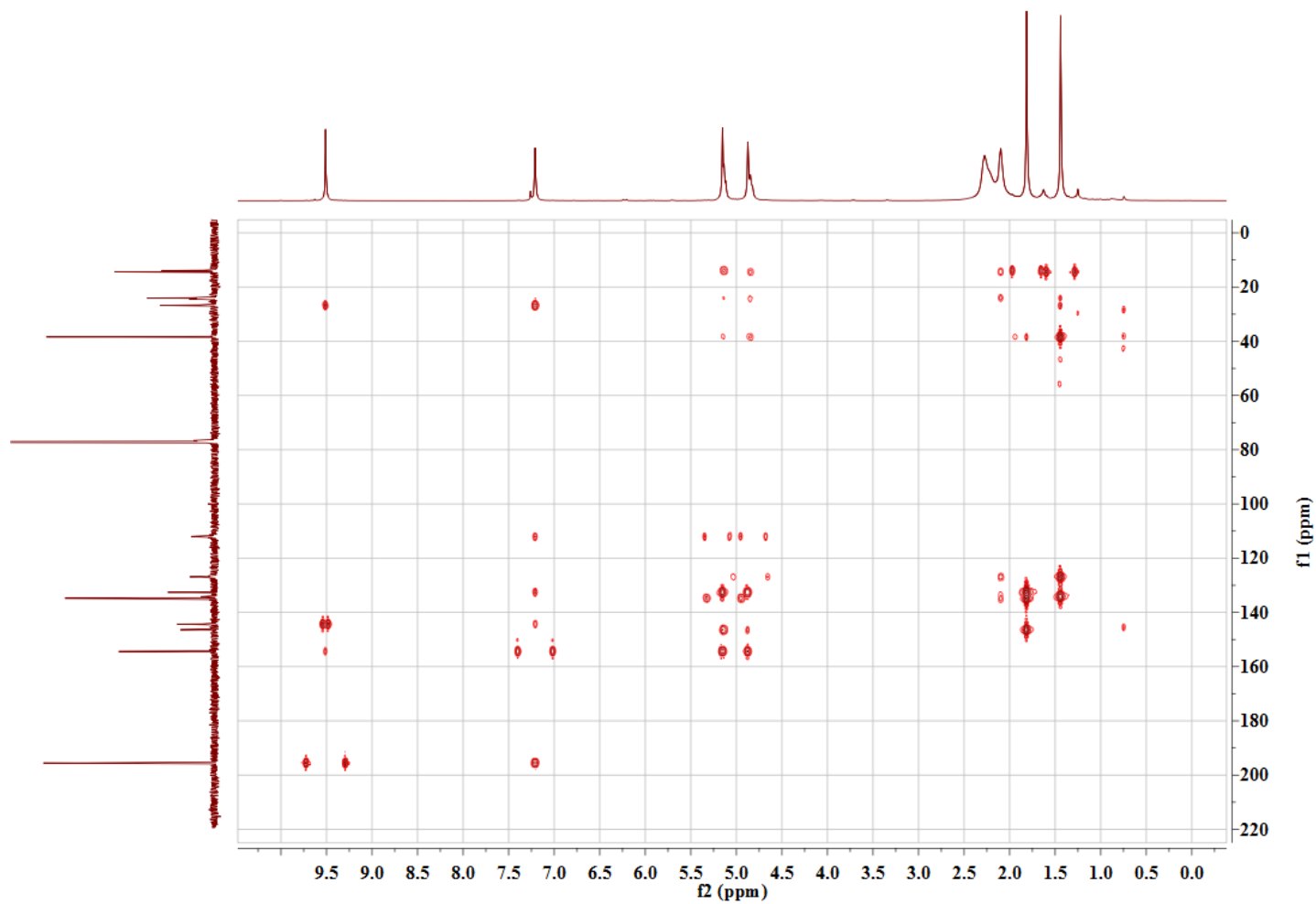




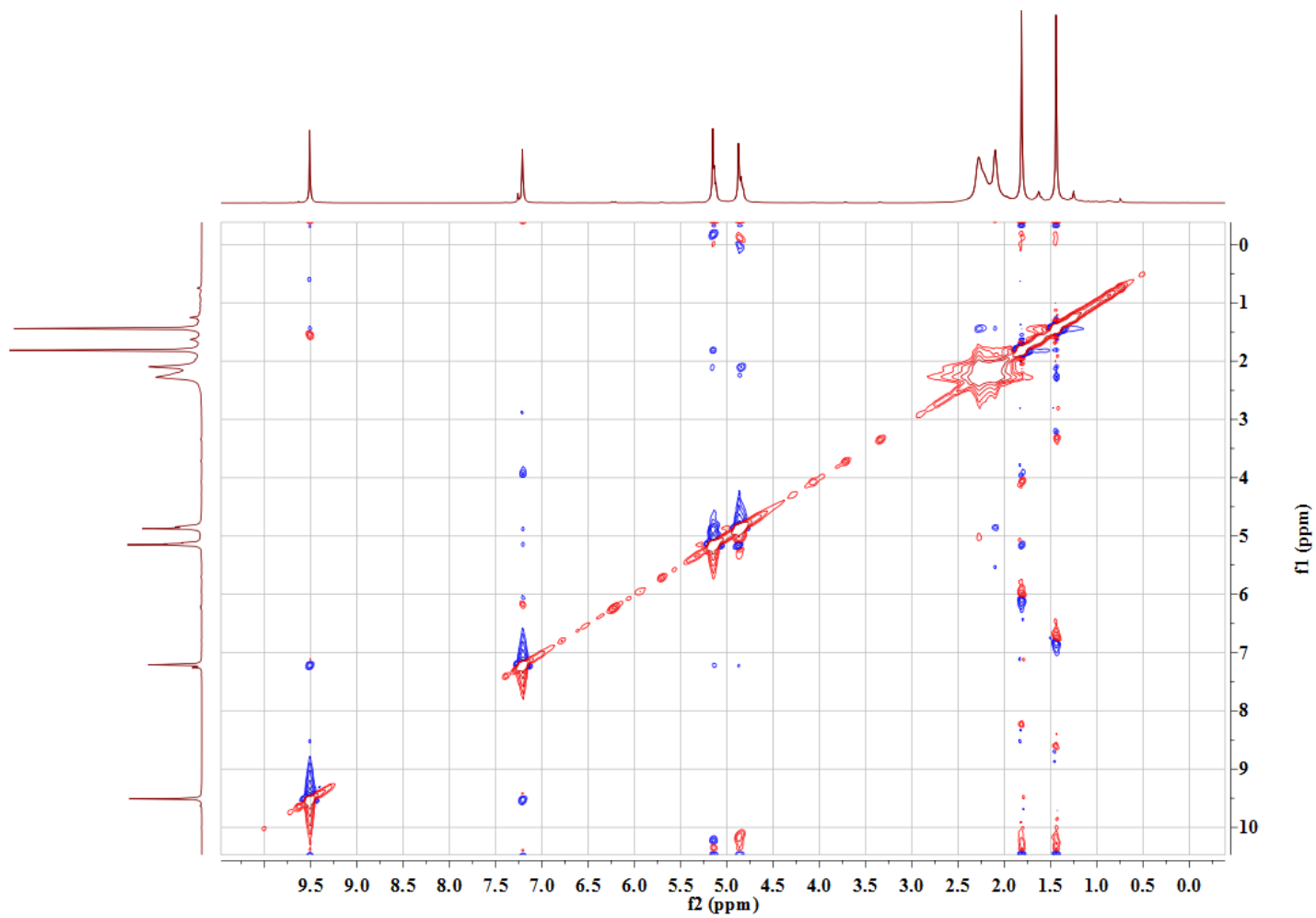
S4 HSQC Spectrum of **1** in CDCl<sub>3</sub>



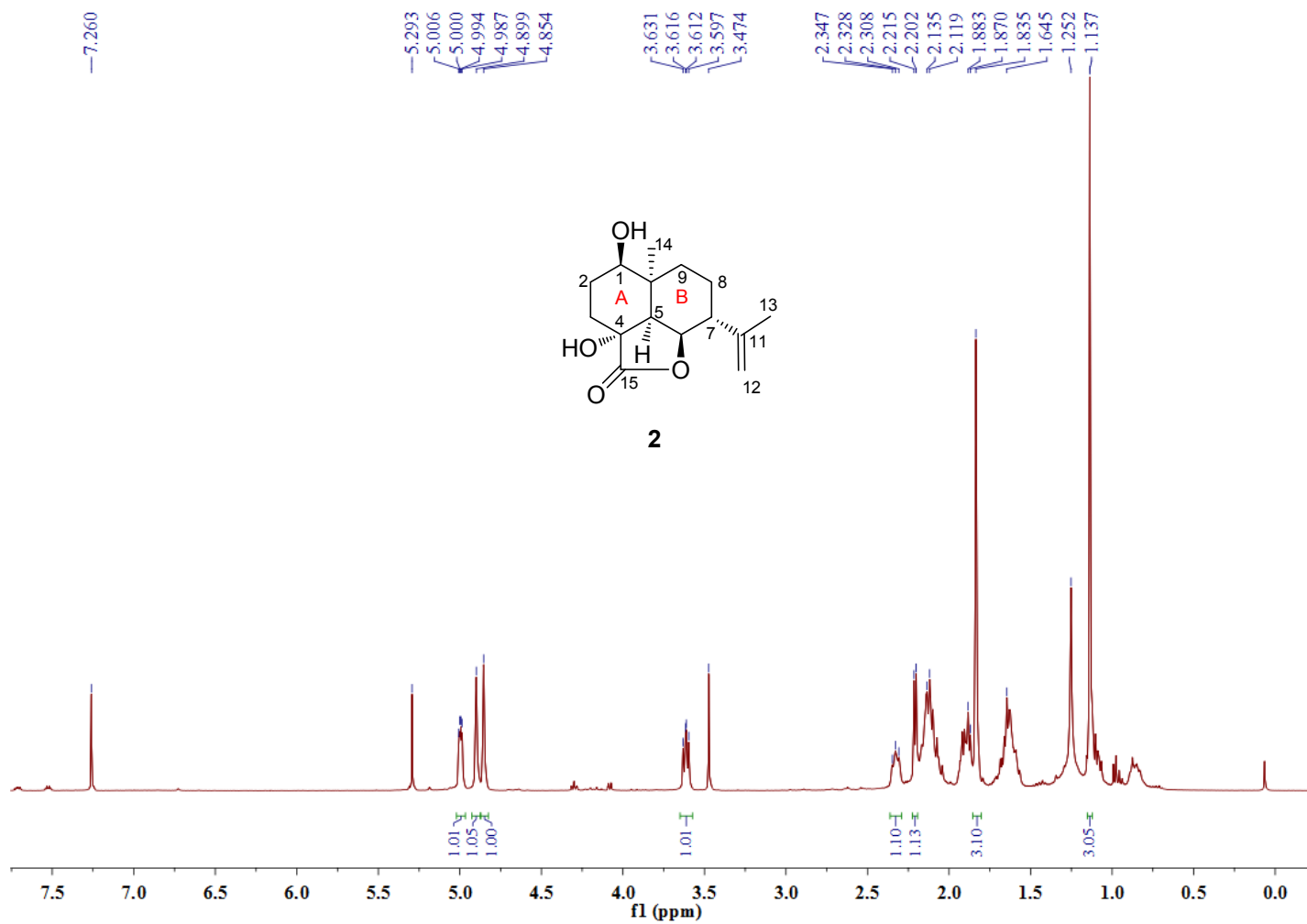
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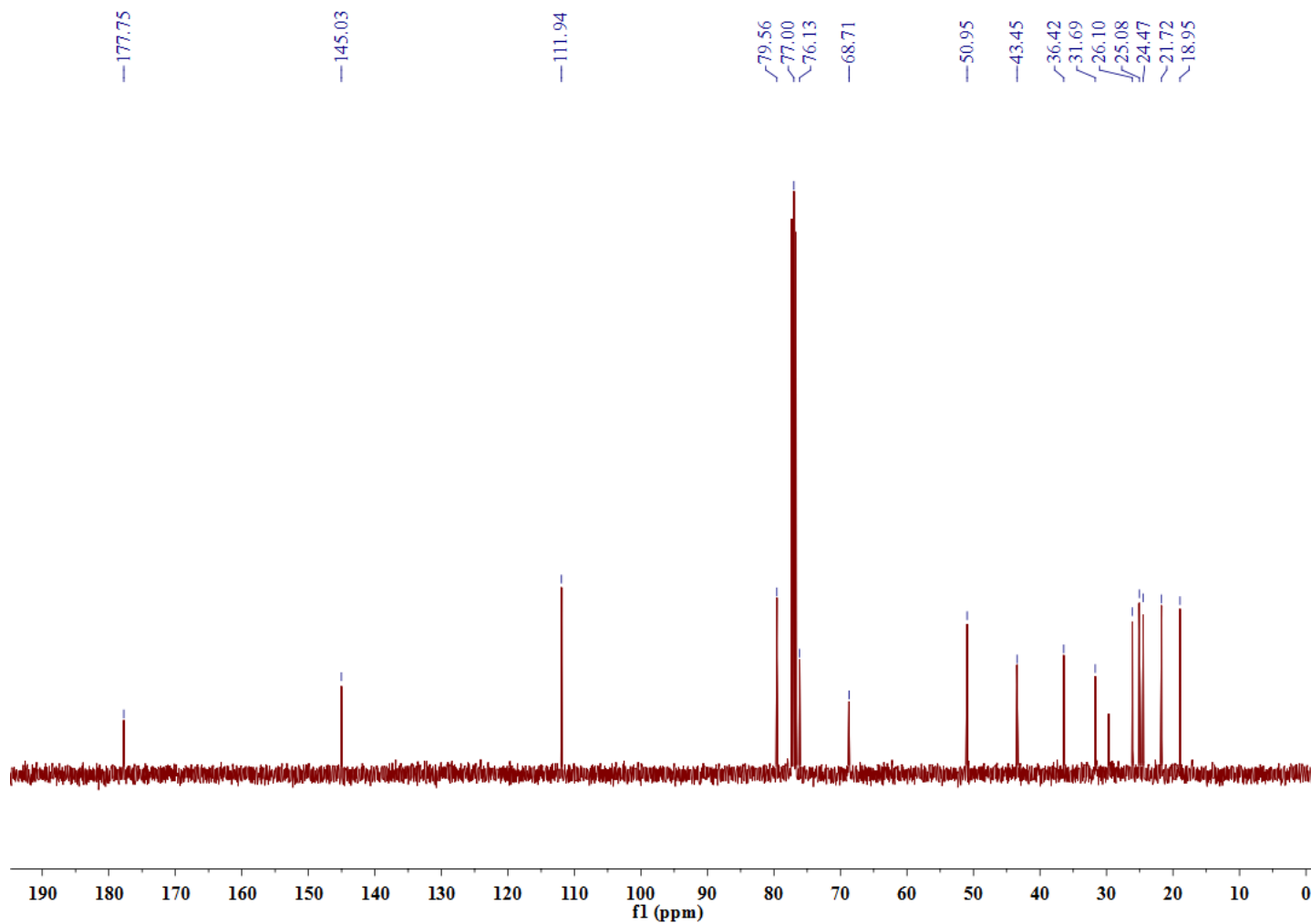
S6 NOESY Spectrum of **1** in CDCl<sub>3</sub>

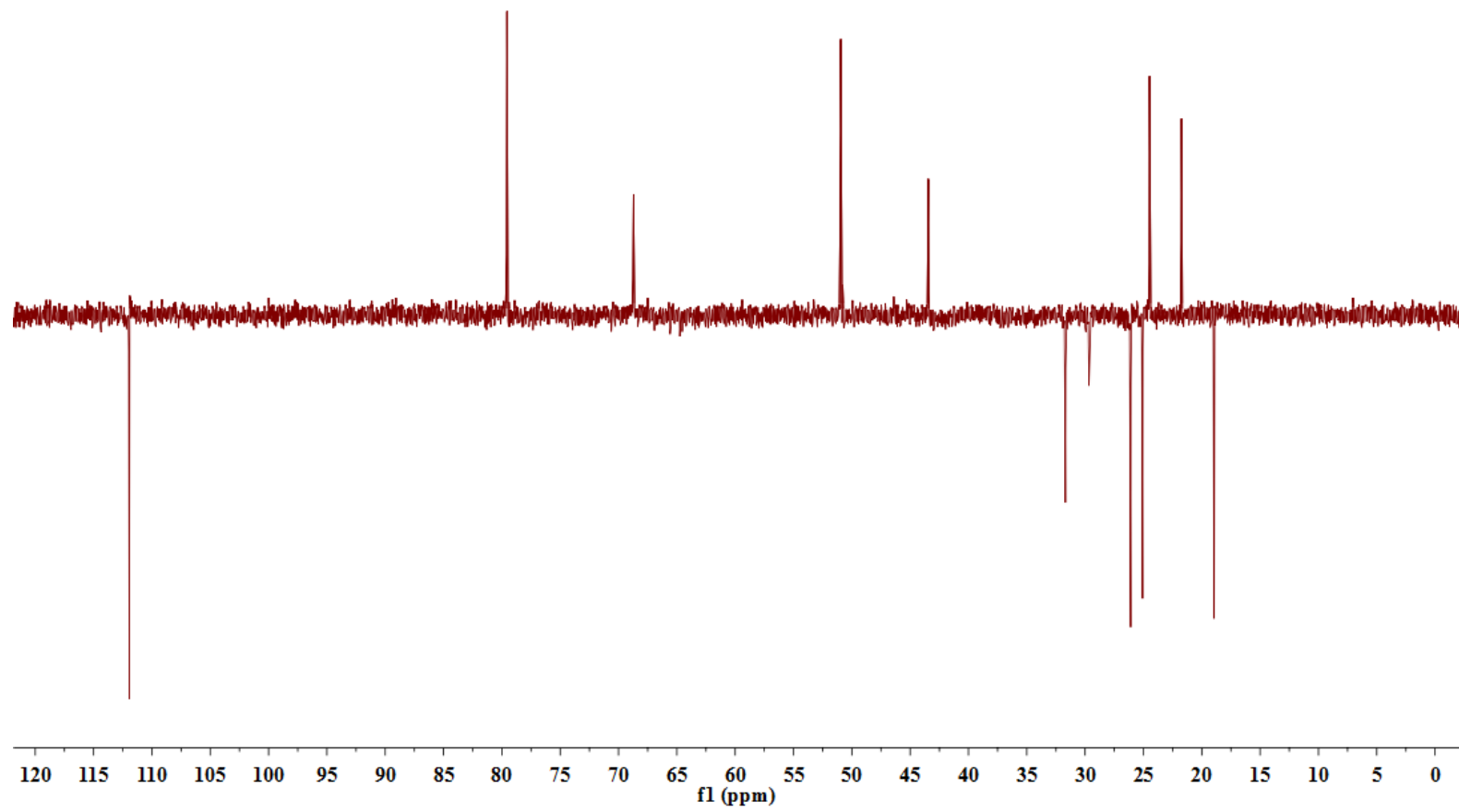


S7  $^1\text{H}$  NMR Spectrum of **2** in  $\text{CDCl}_3$

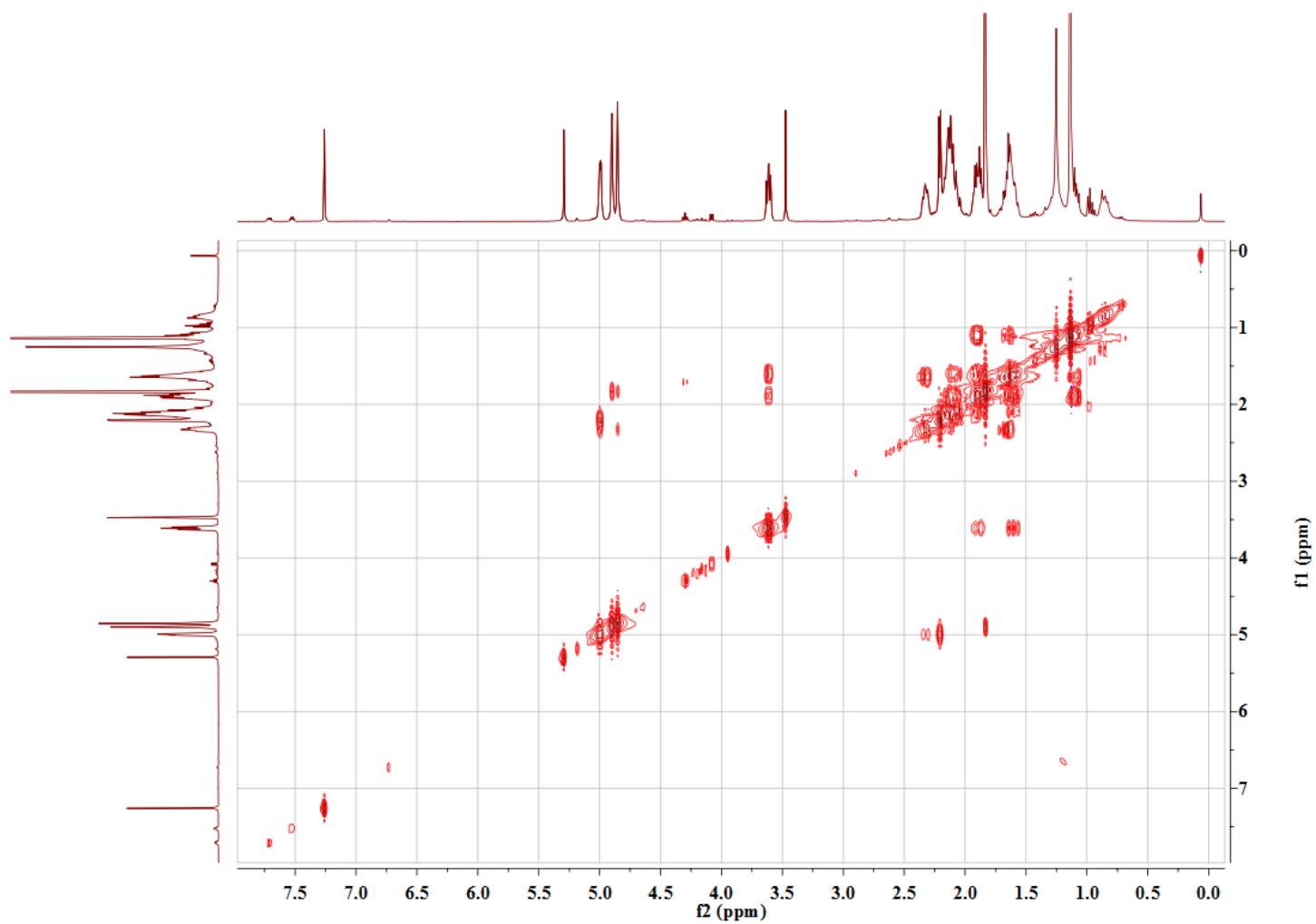


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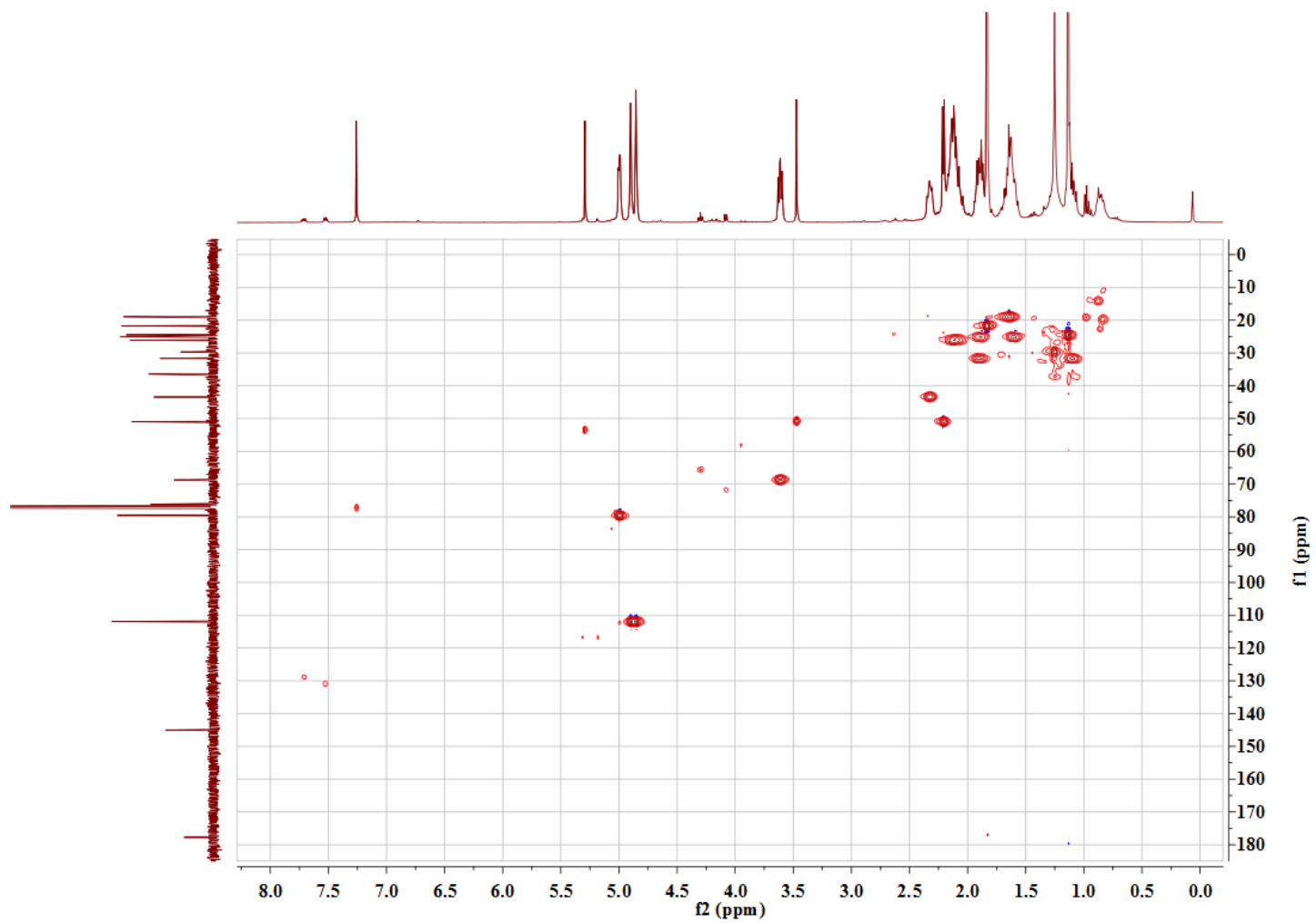




S9  $^1\text{H}$ - $^1\text{H}$  COSY Spectrum of **2** in  $\text{CDCl}_3$

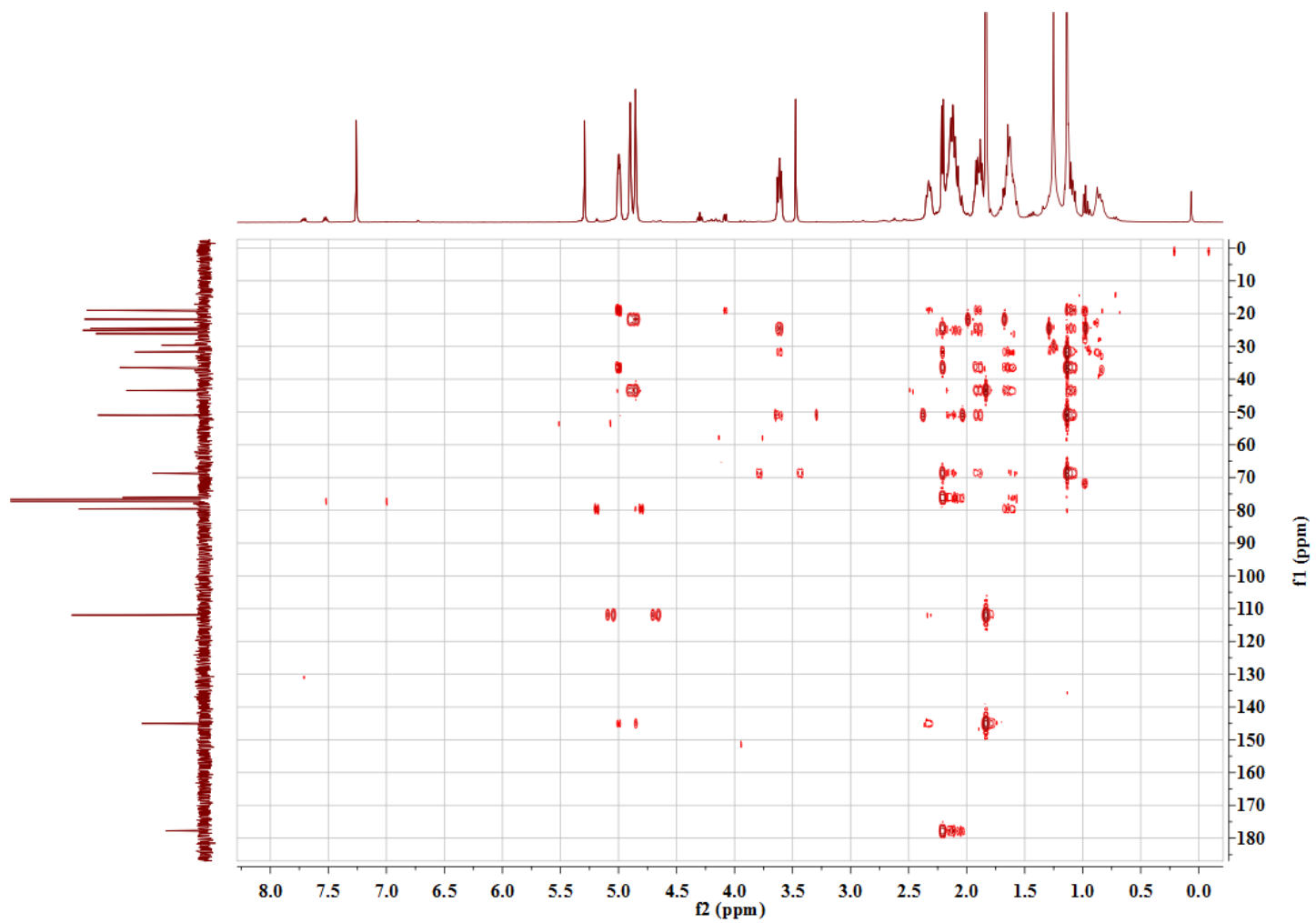


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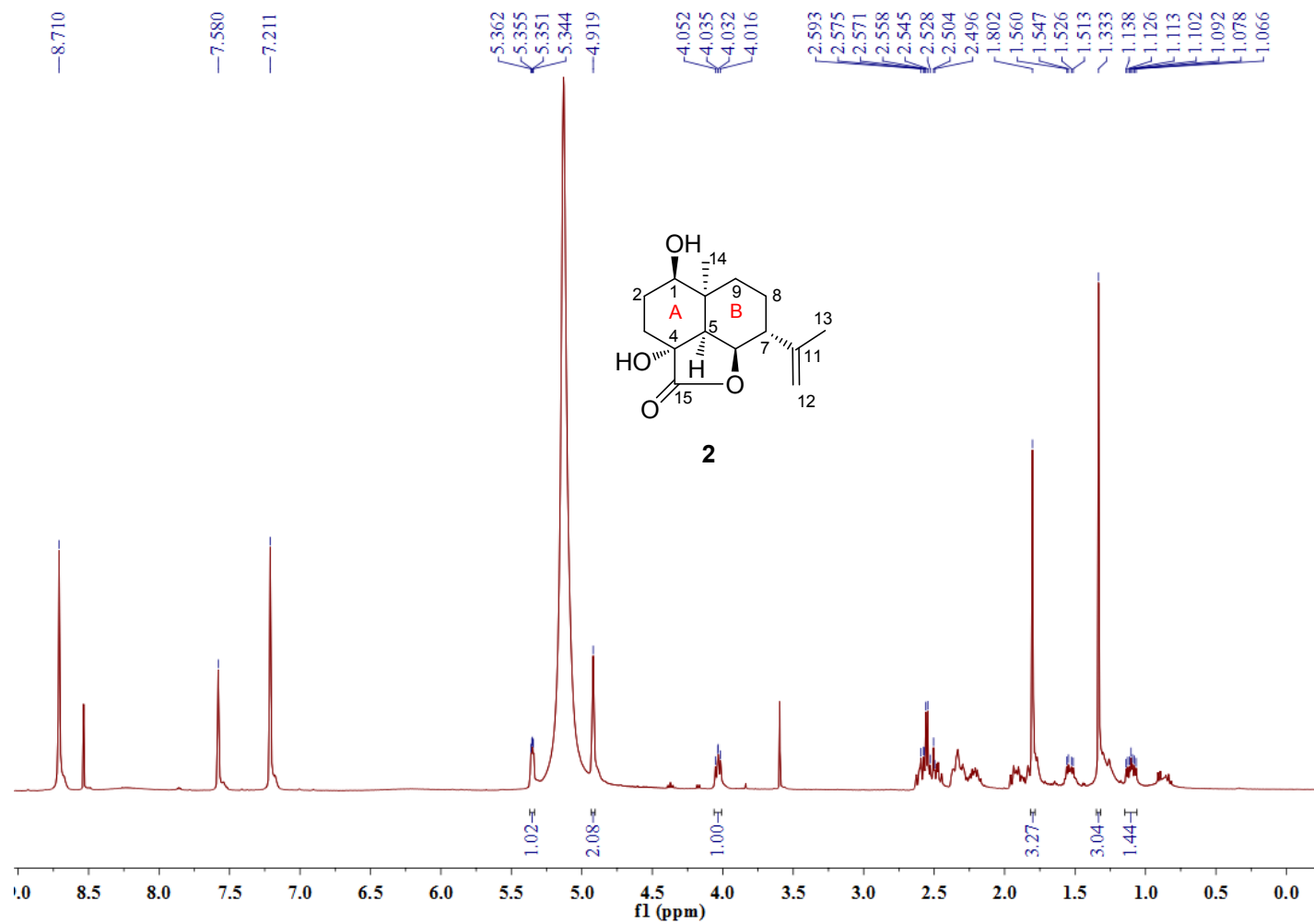




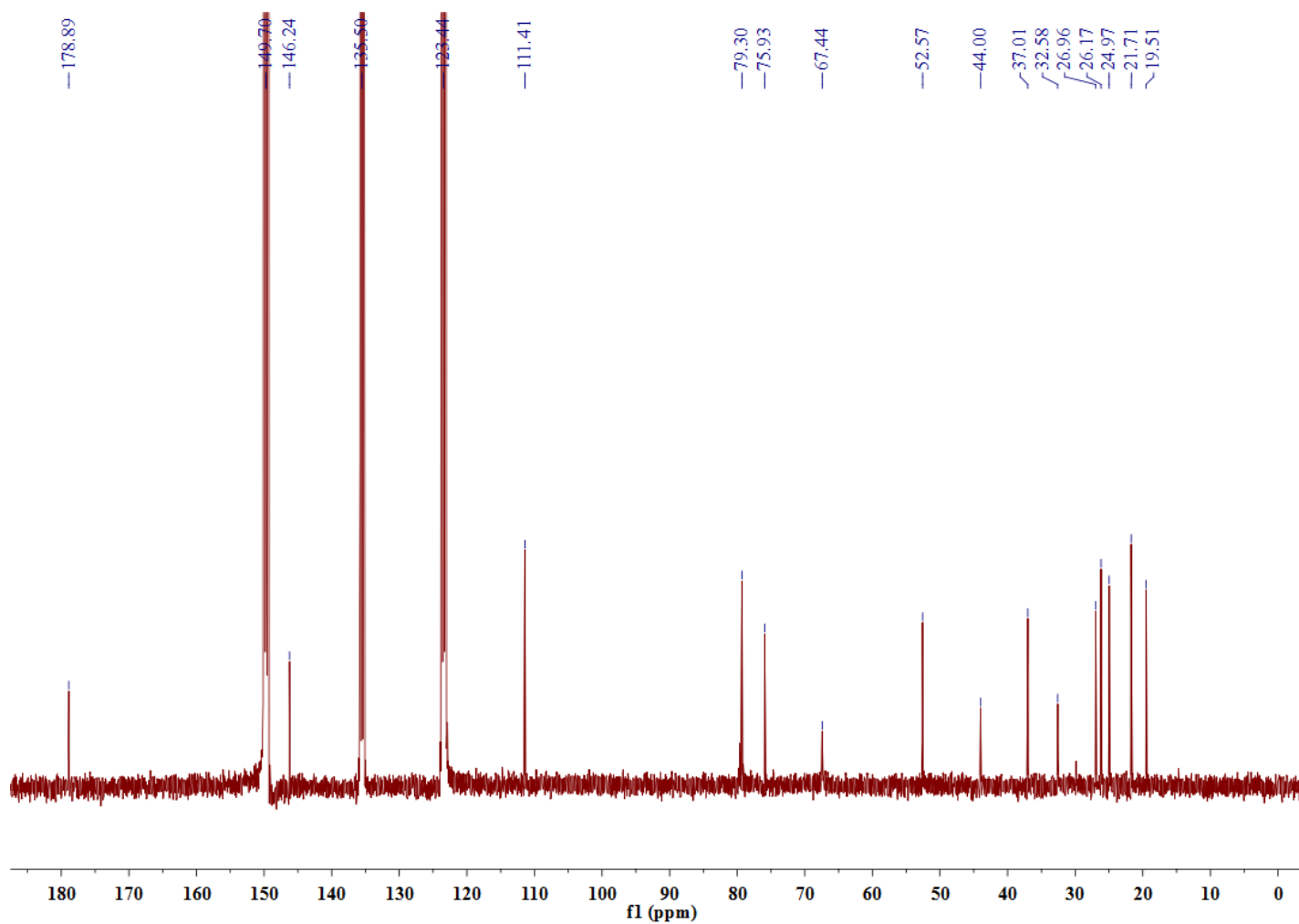
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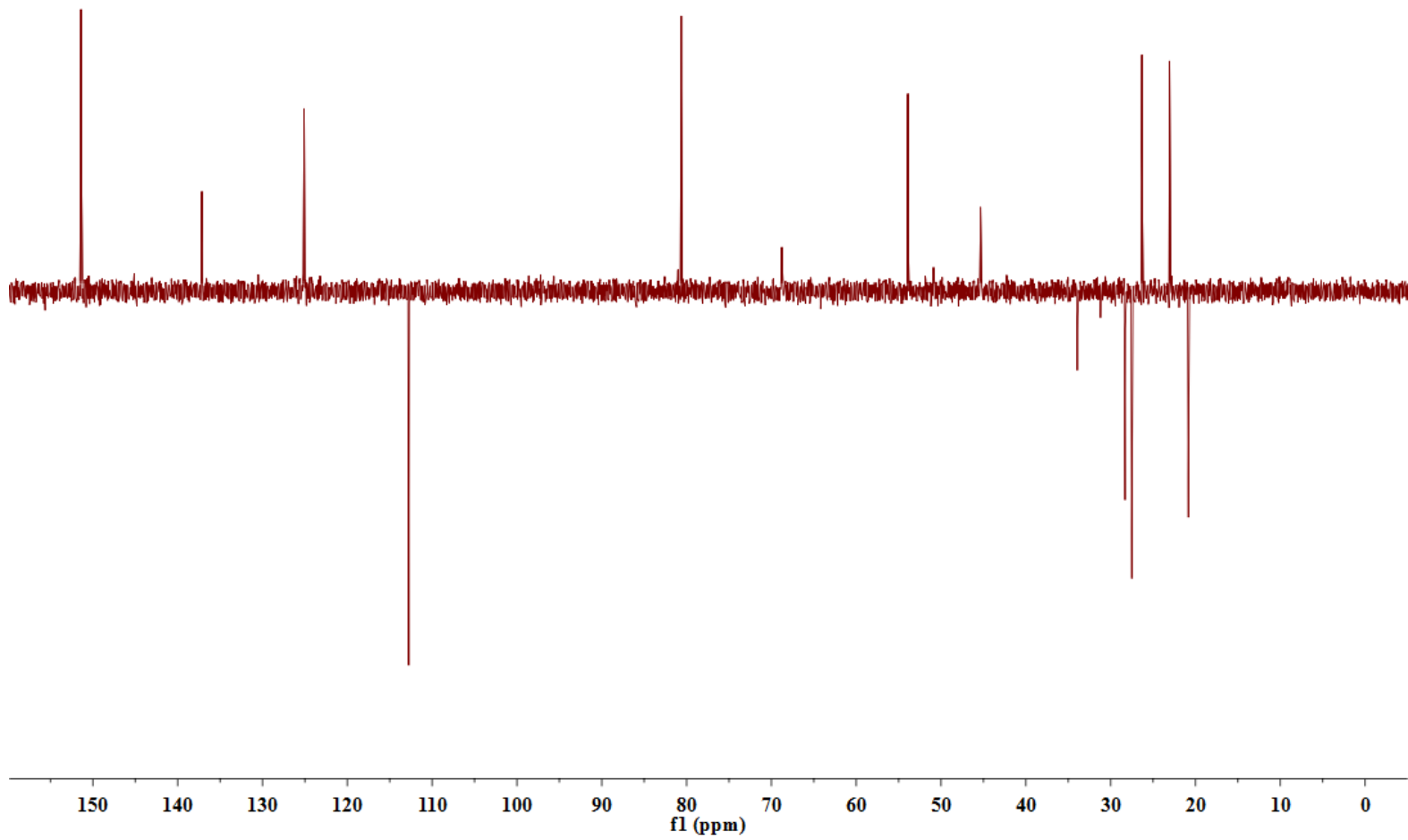


S12  $^1\text{H}$  NMR Spectrum of **2** in  $\text{C}_5\text{D}_5\text{N}$

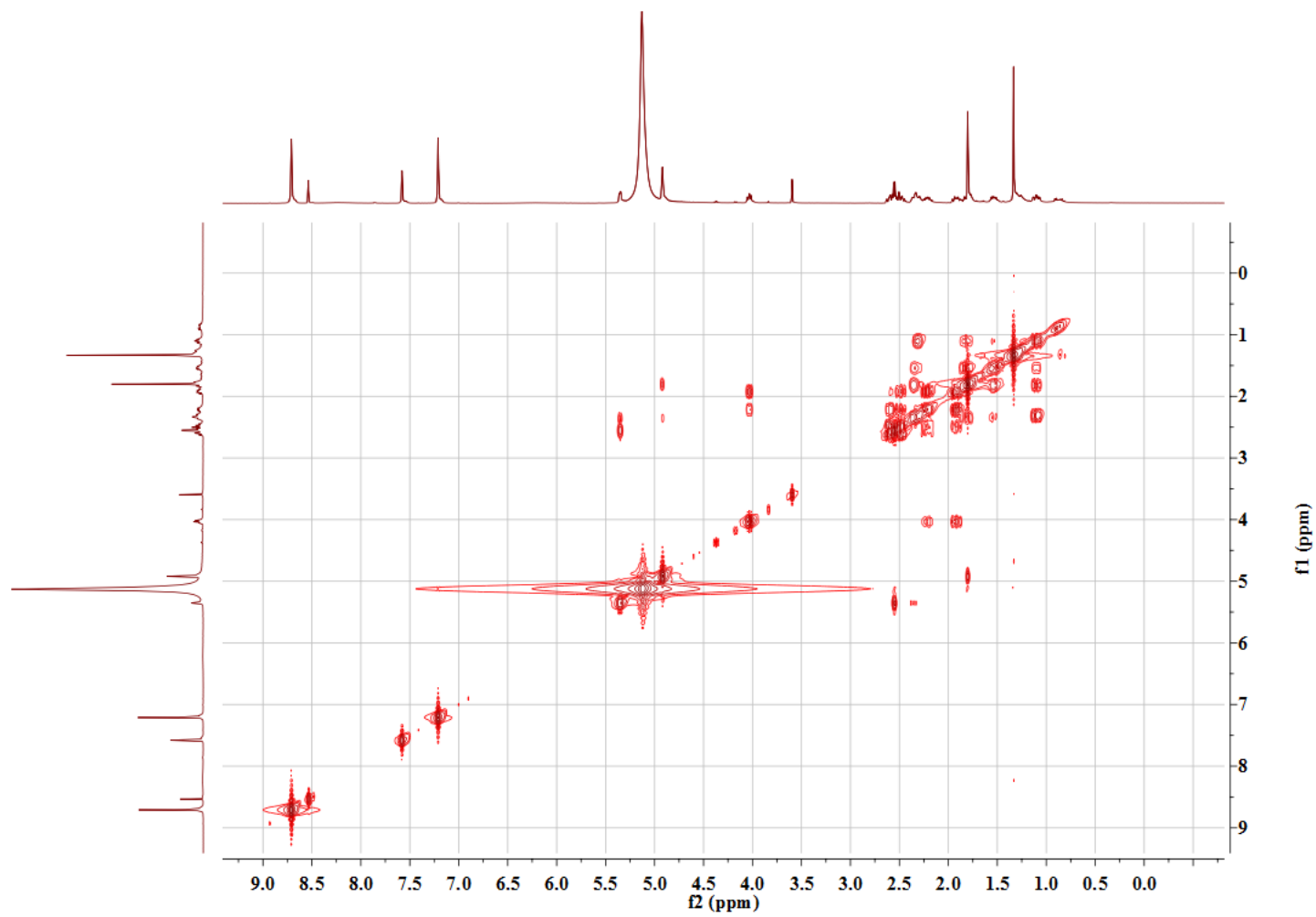


**S13**  $^{13}\text{C}$  NMR Spectra of **2** in  $\text{C}_5\text{D}_5\text{N}$

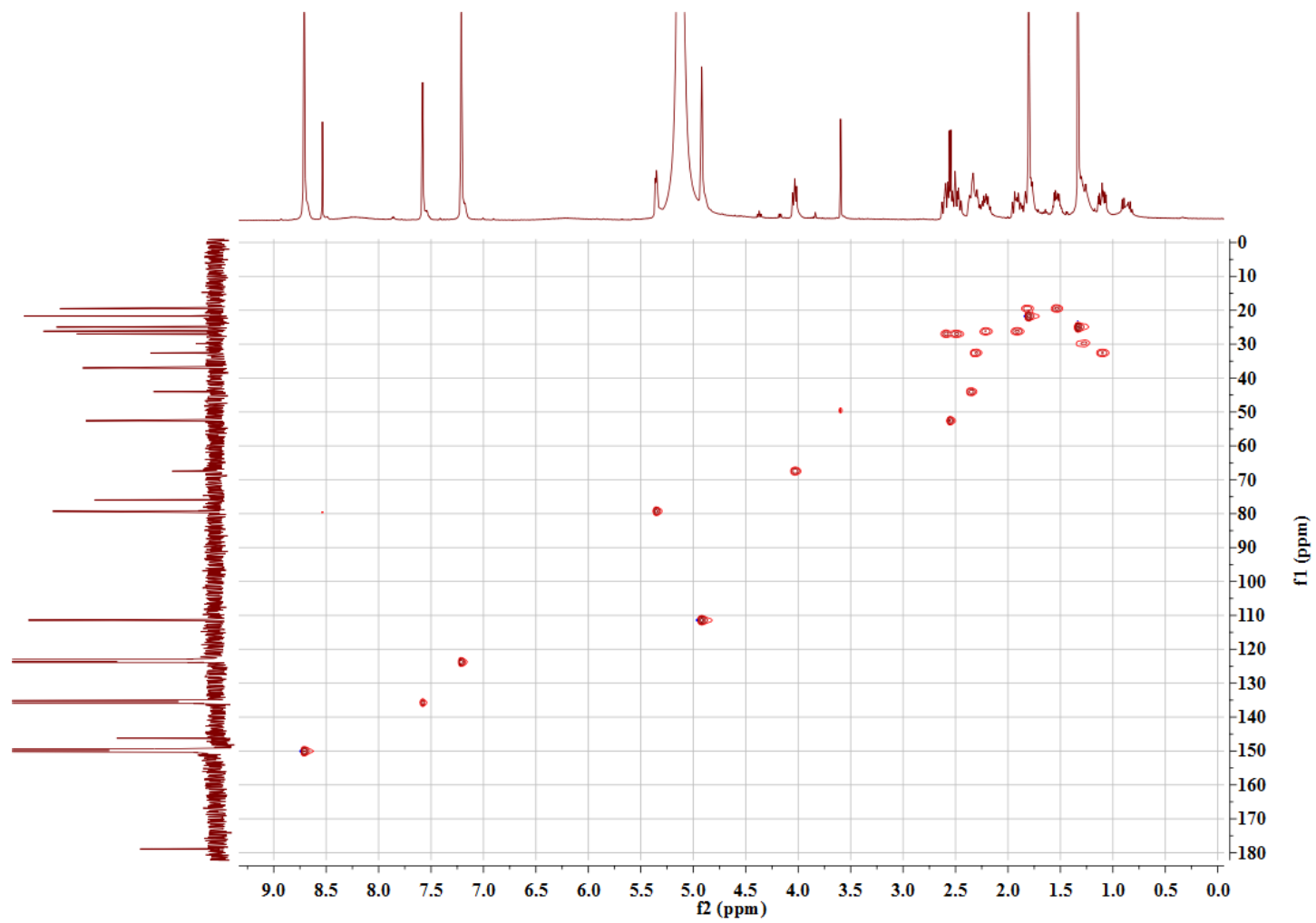




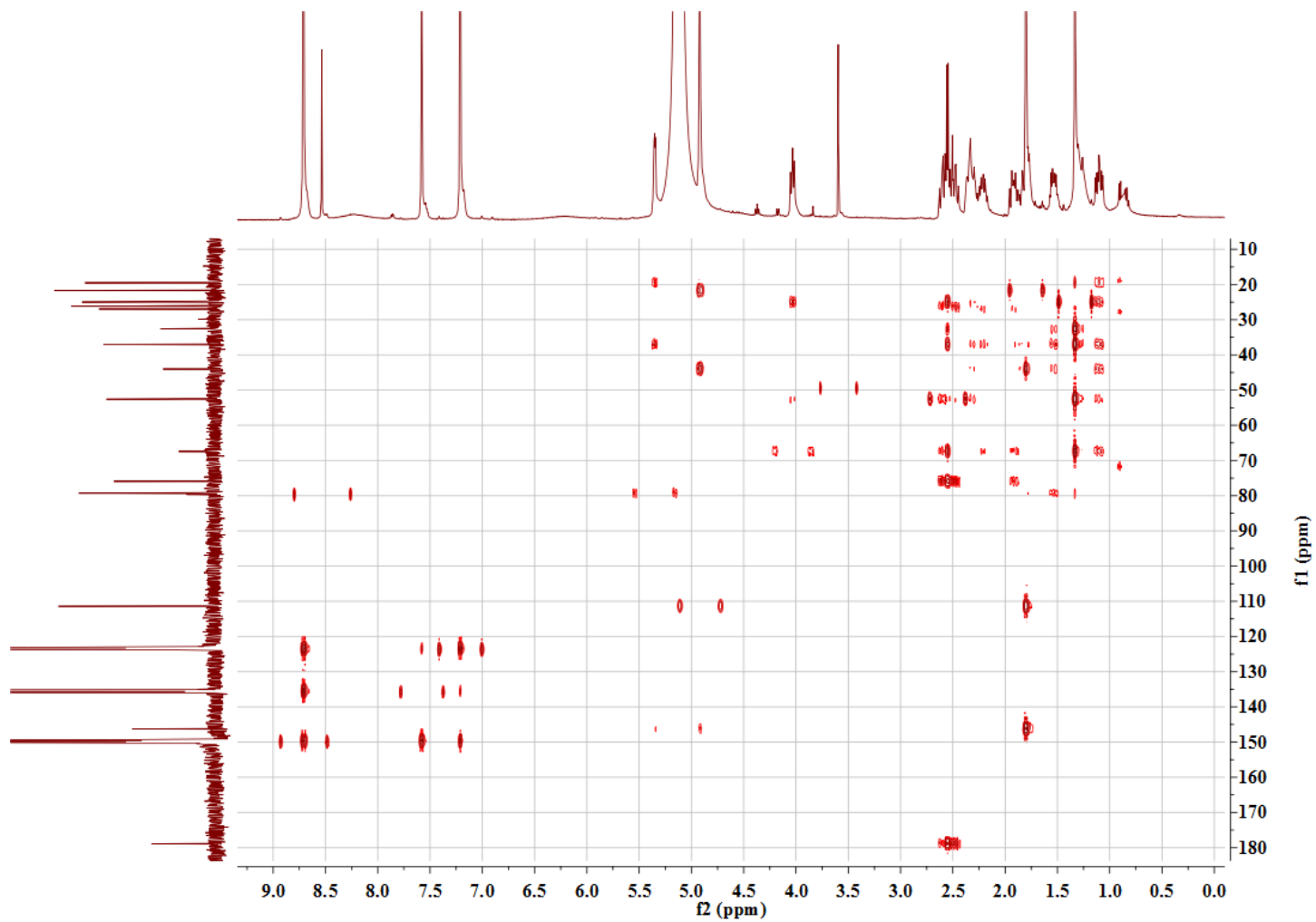
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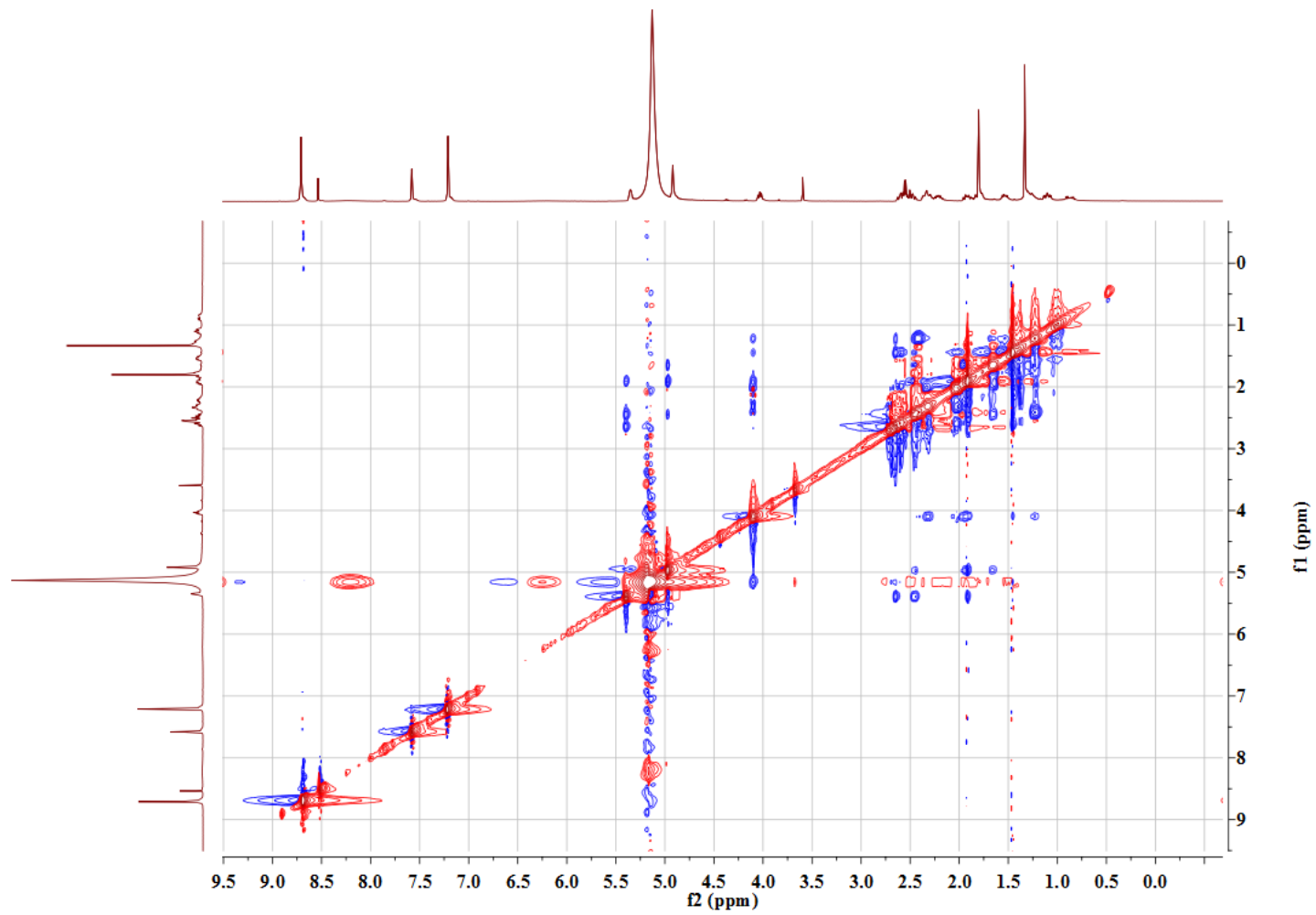
S15 HSQC Spectrum of **2** in C<sub>5</sub>D<sub>5</sub>N



S16 HMBC Spectrum of **2** in C<sub>5</sub>D<sub>5</sub>N

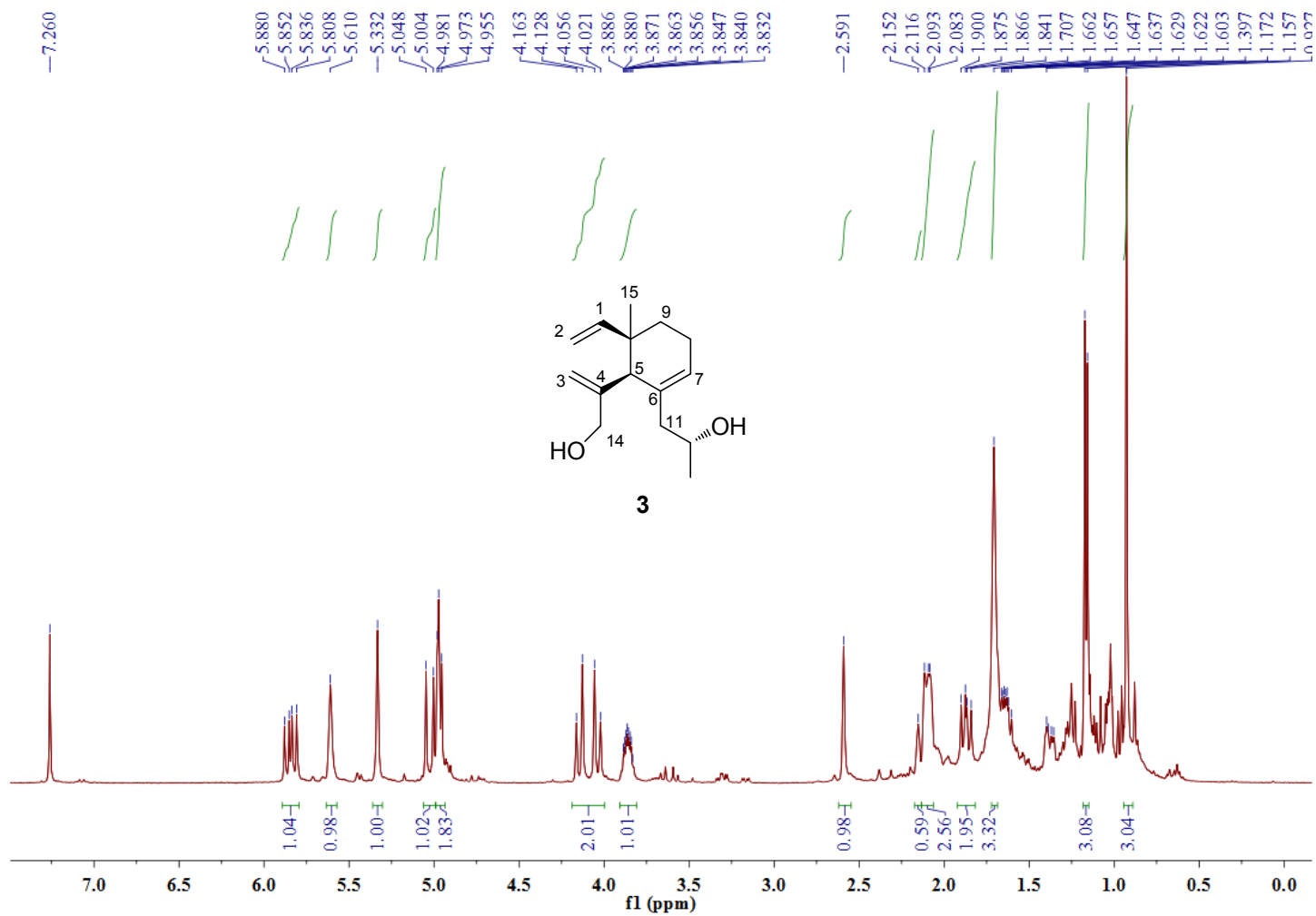


S17 NOESY Spectrum of **2** in C<sub>5</sub>D<sub>5</sub>N

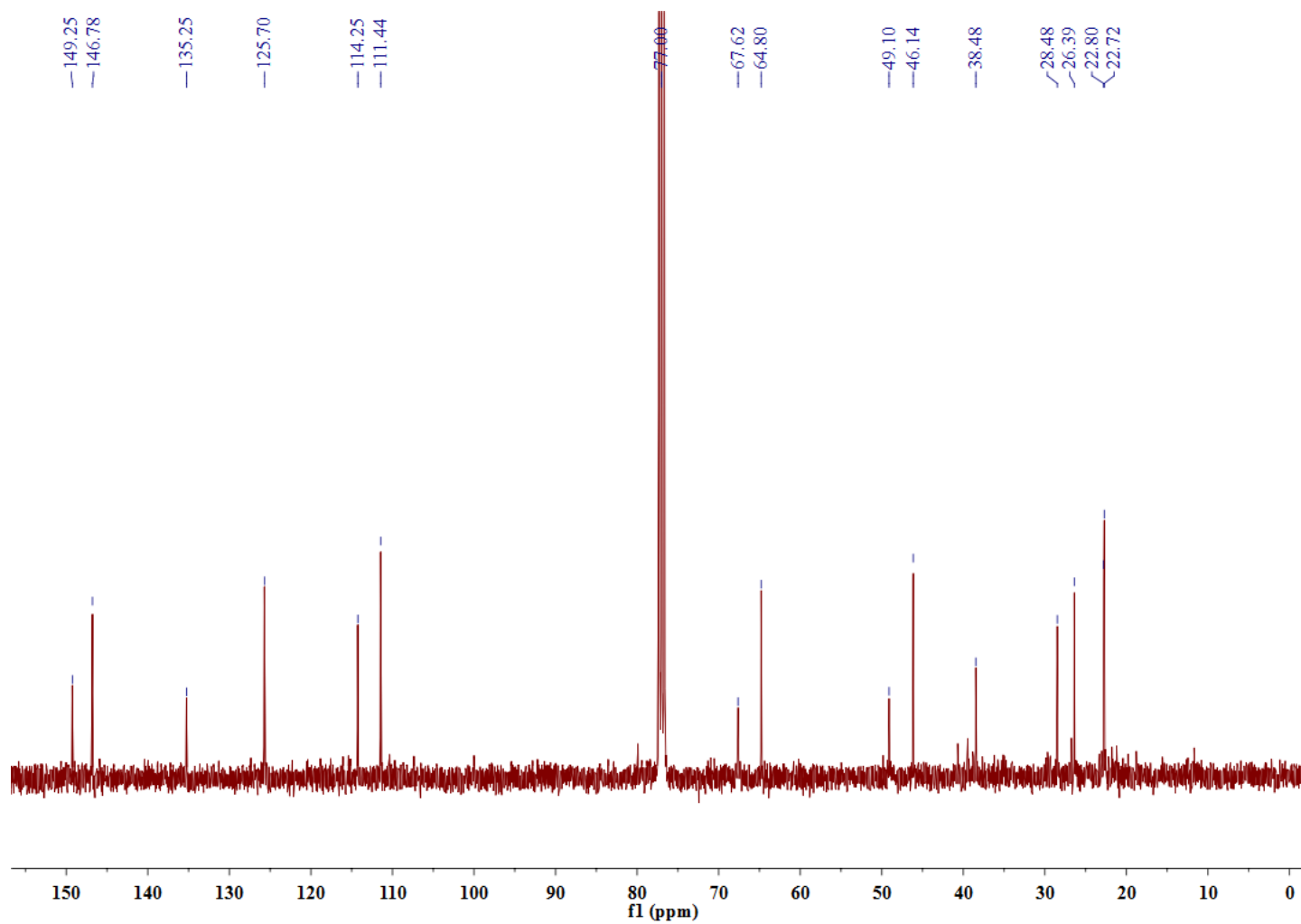


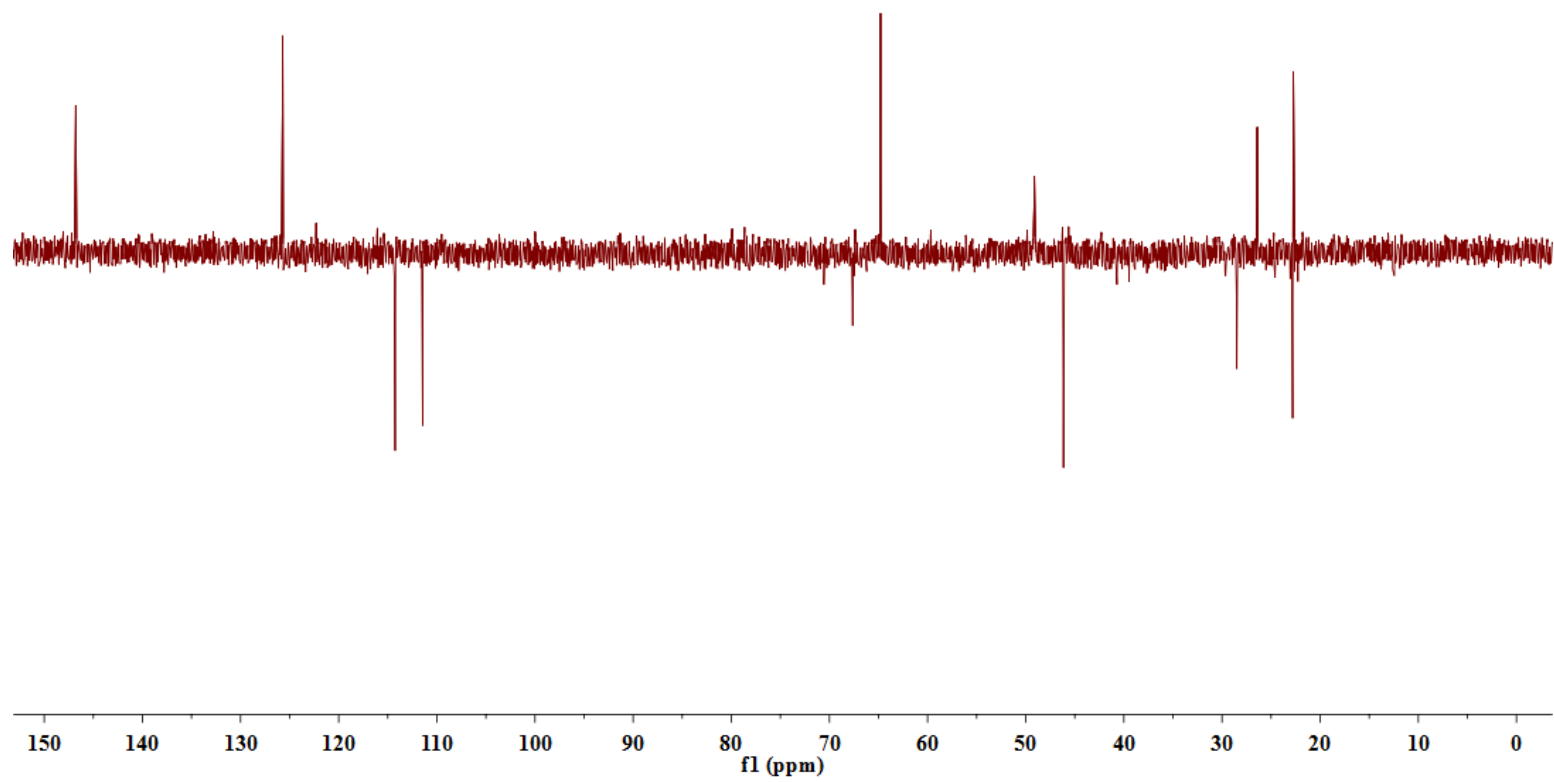


S18 <sup>1</sup>H NMR Spectrum of **3** in CDCl<sub>3</sub>

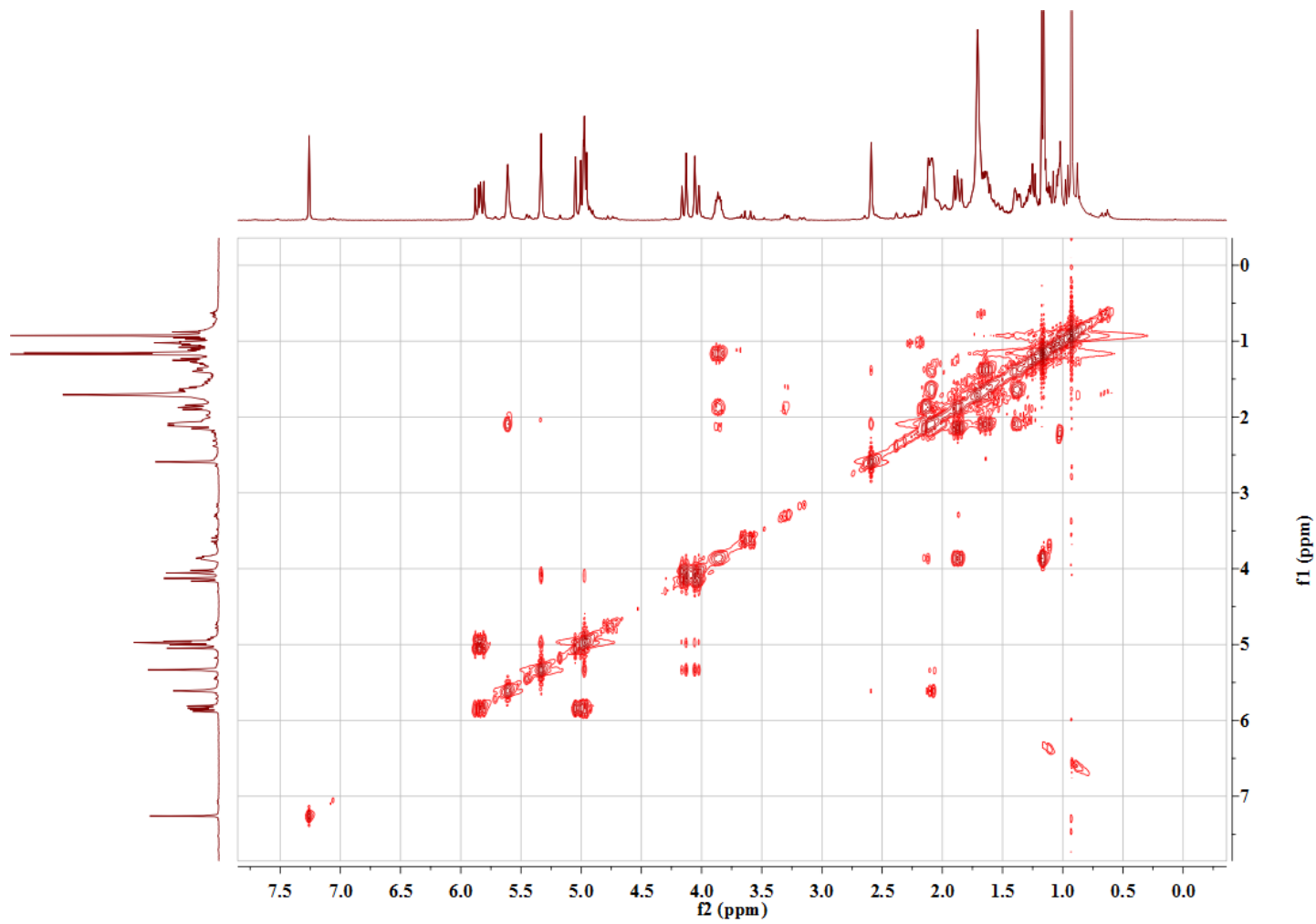


**S19**  $^{13}\text{C}$  NMR Spectra of **3** in  $\text{CDCl}_3$

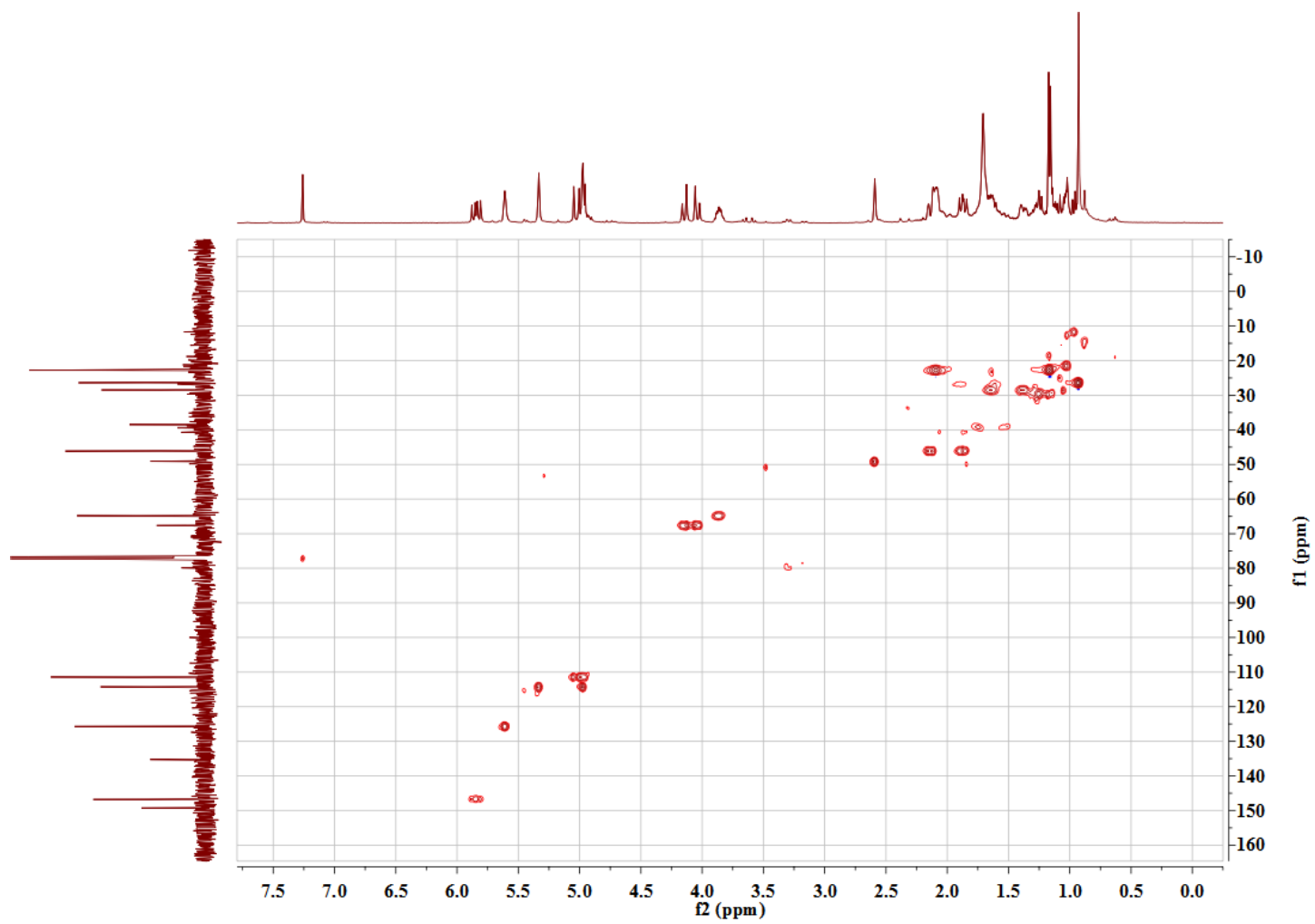




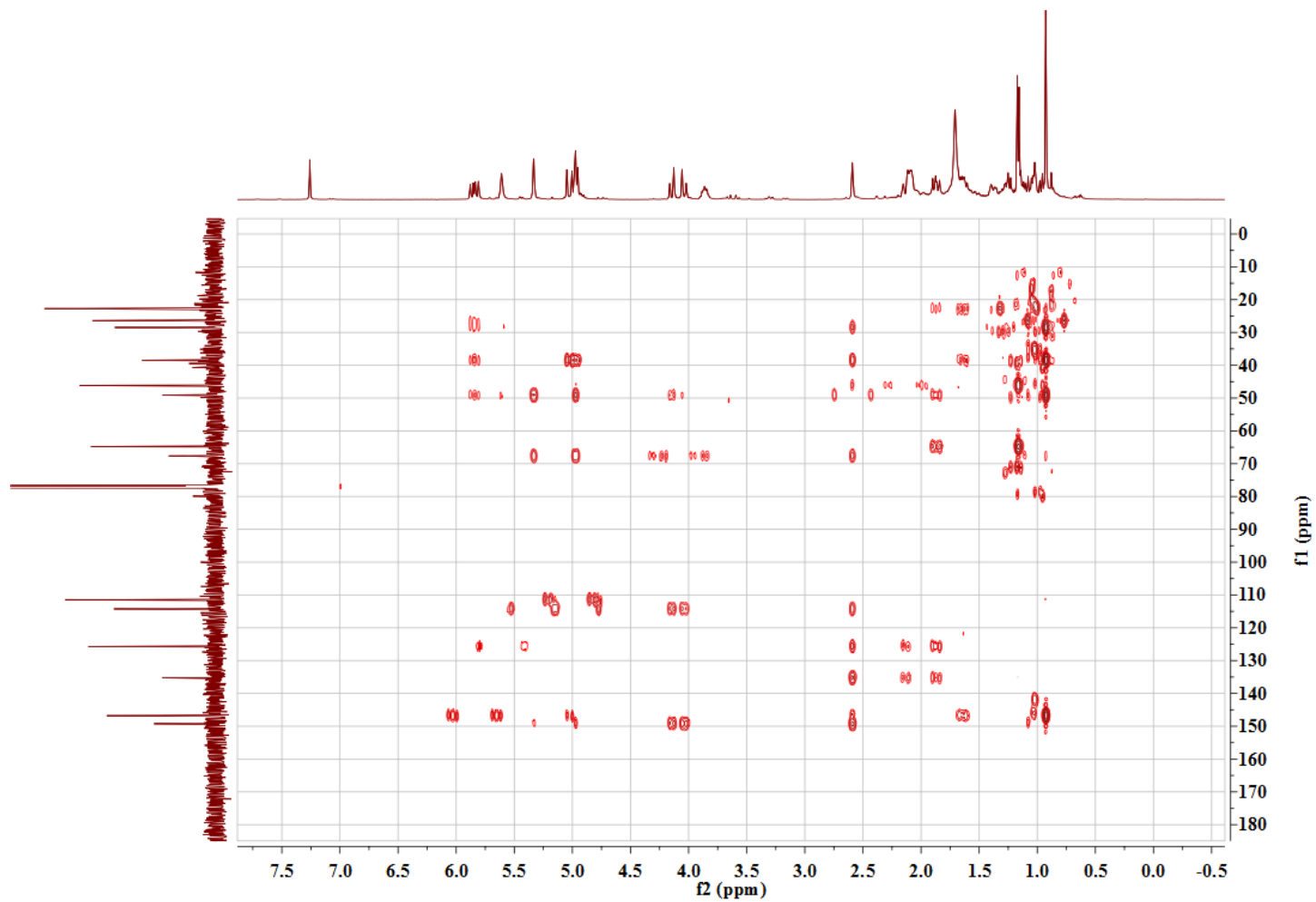
S20  $^1\text{H}$ - $^1\text{H}$  COSY Spectrum of **3** in  $\text{CDCl}_3$



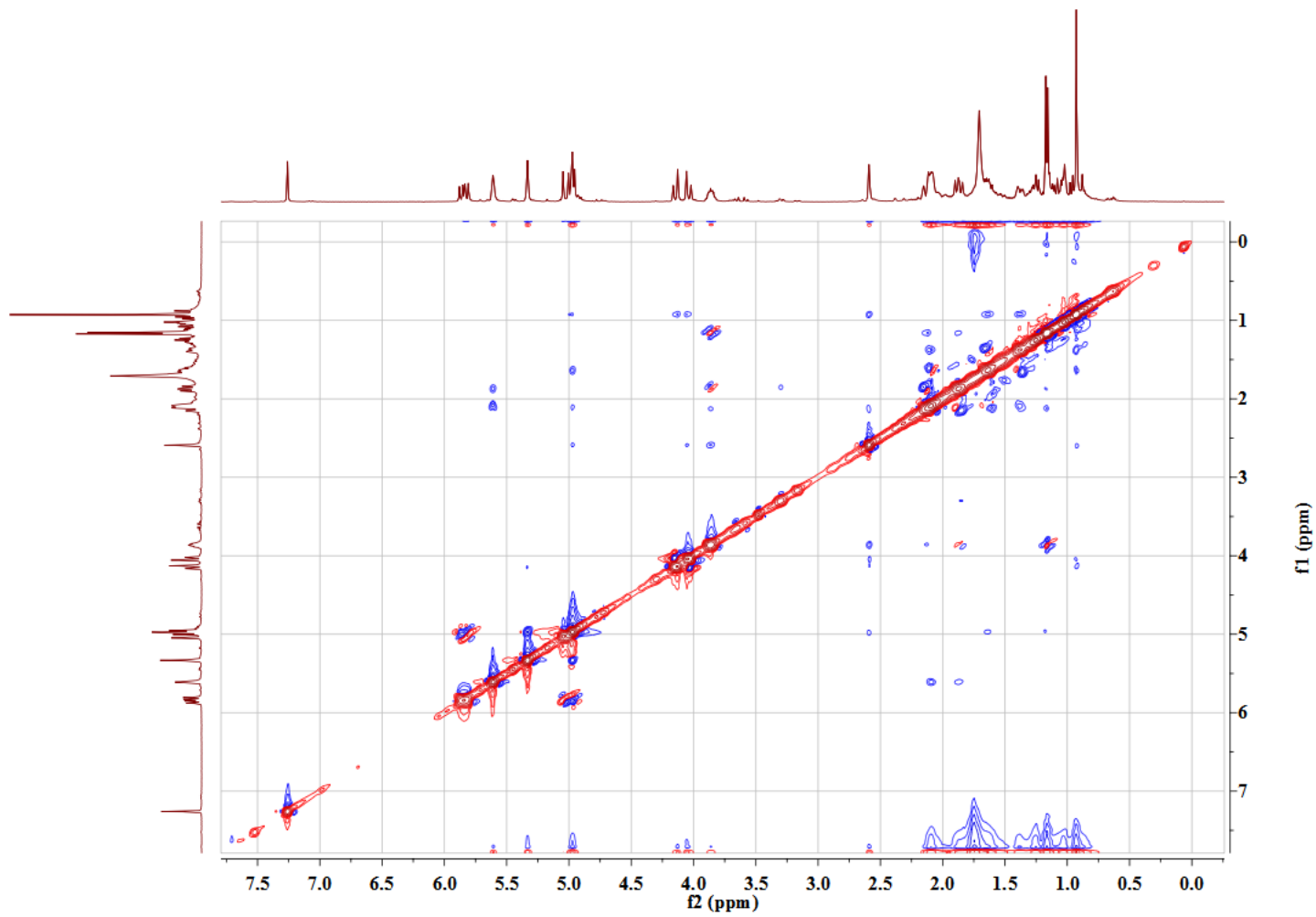
S21 HSQC Spectrum of **3** in CDCl<sub>3</sub>



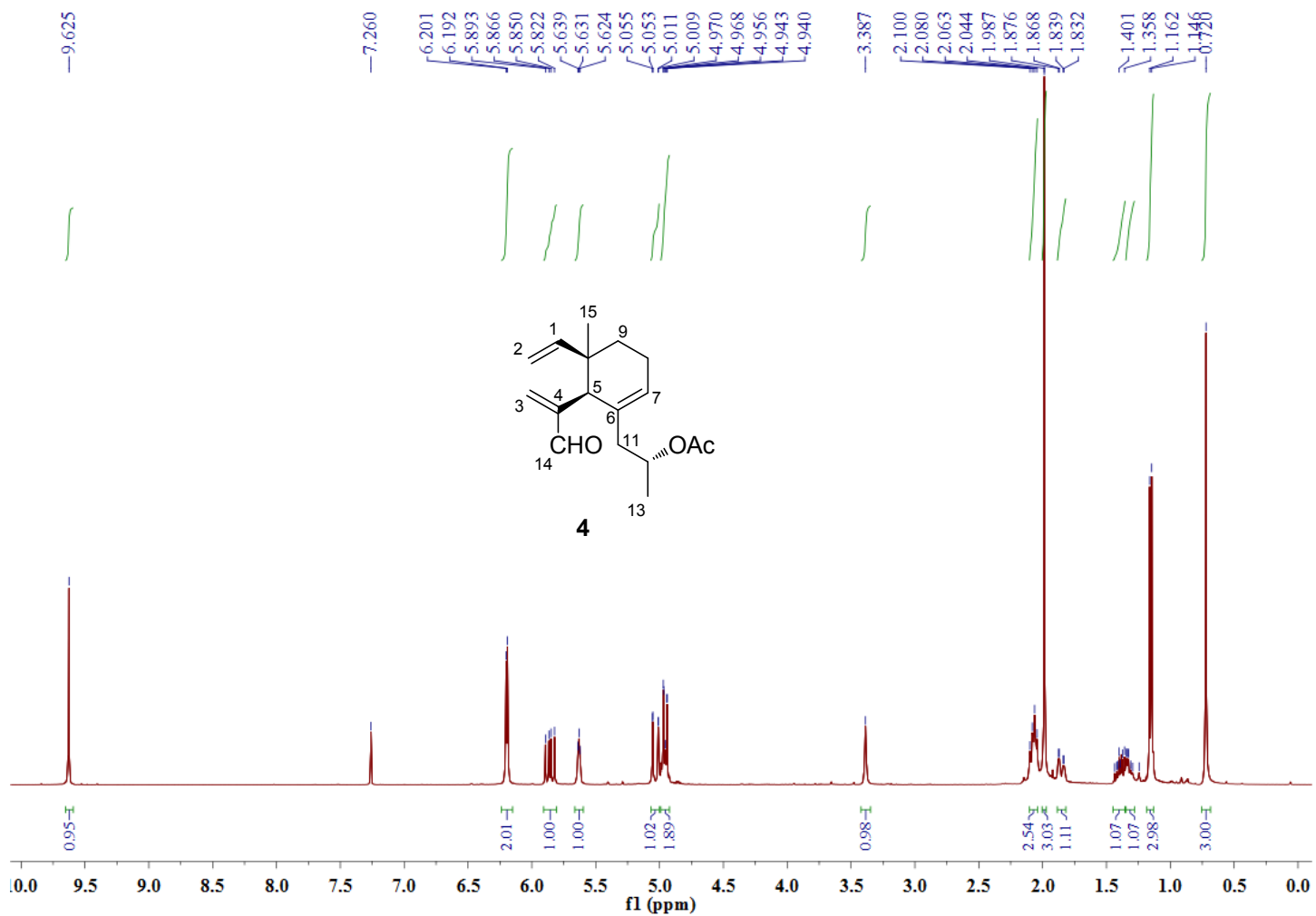
S22 HMBC Spectrum of **3** in CDCl<sub>3</sub>



S23 NOESY Spectrum of **3** in CDCl<sub>3</sub>

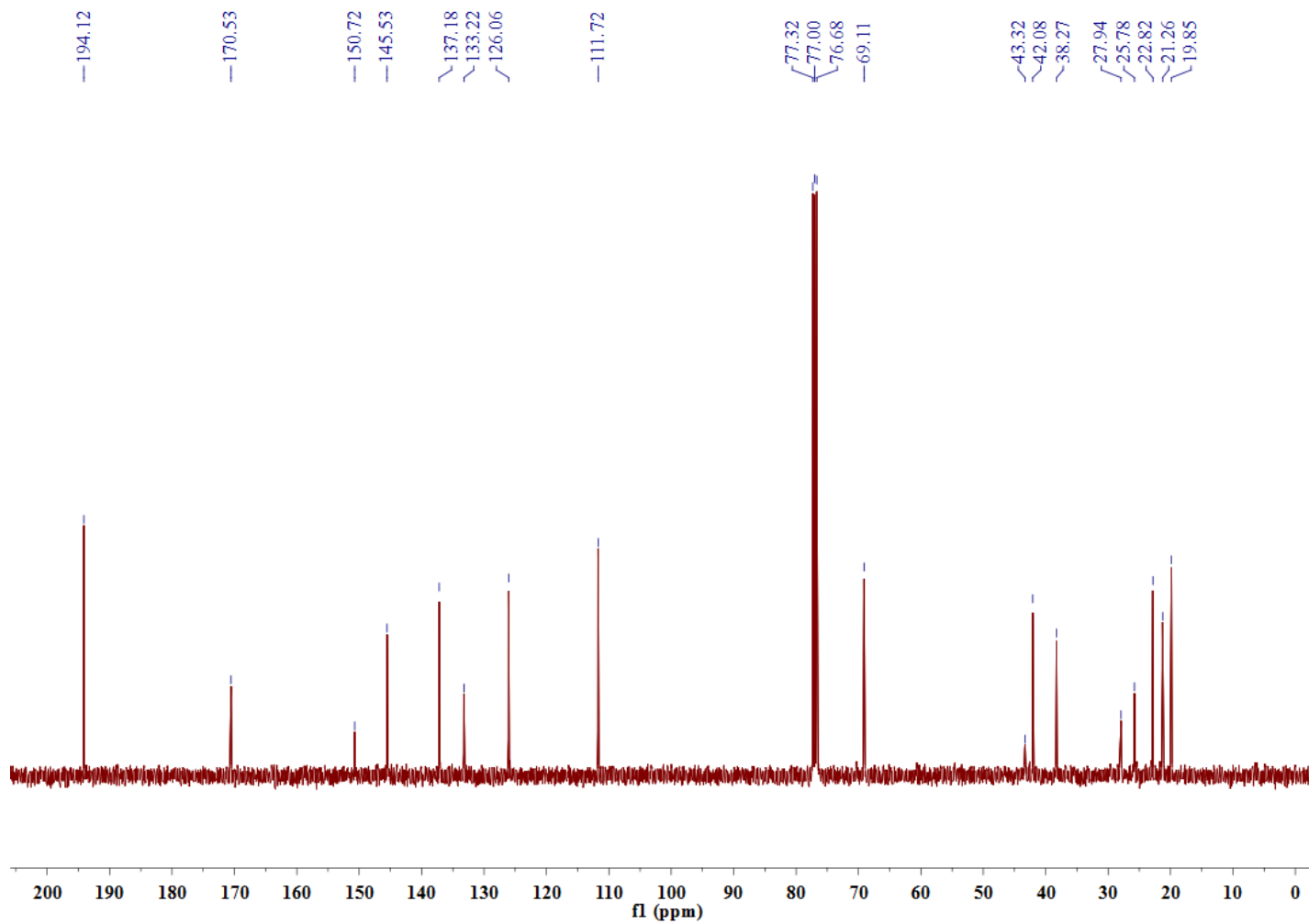


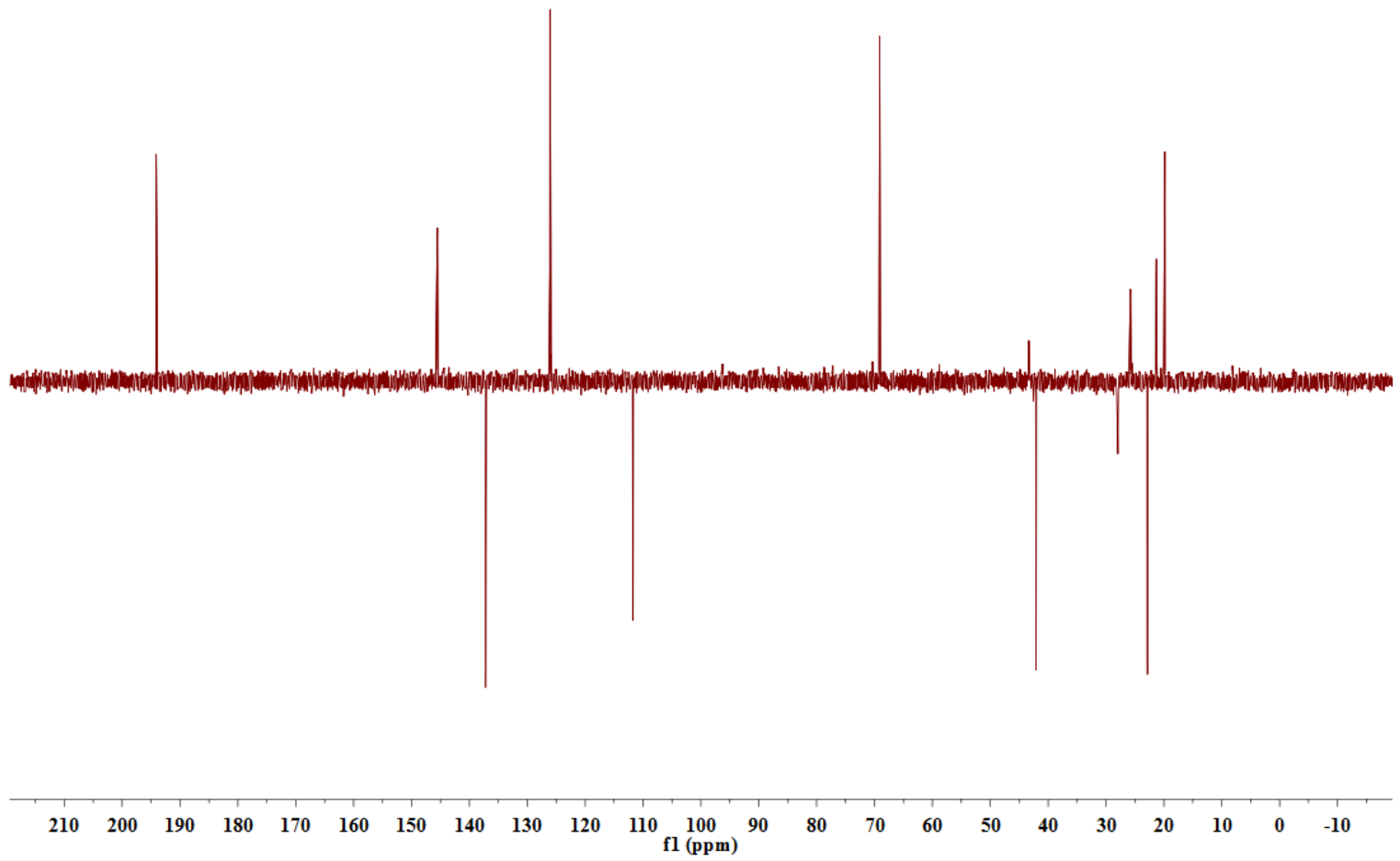
S24 <sup>1</sup>H NMR Spectrum of **4** in CDCl<sub>3</sub>



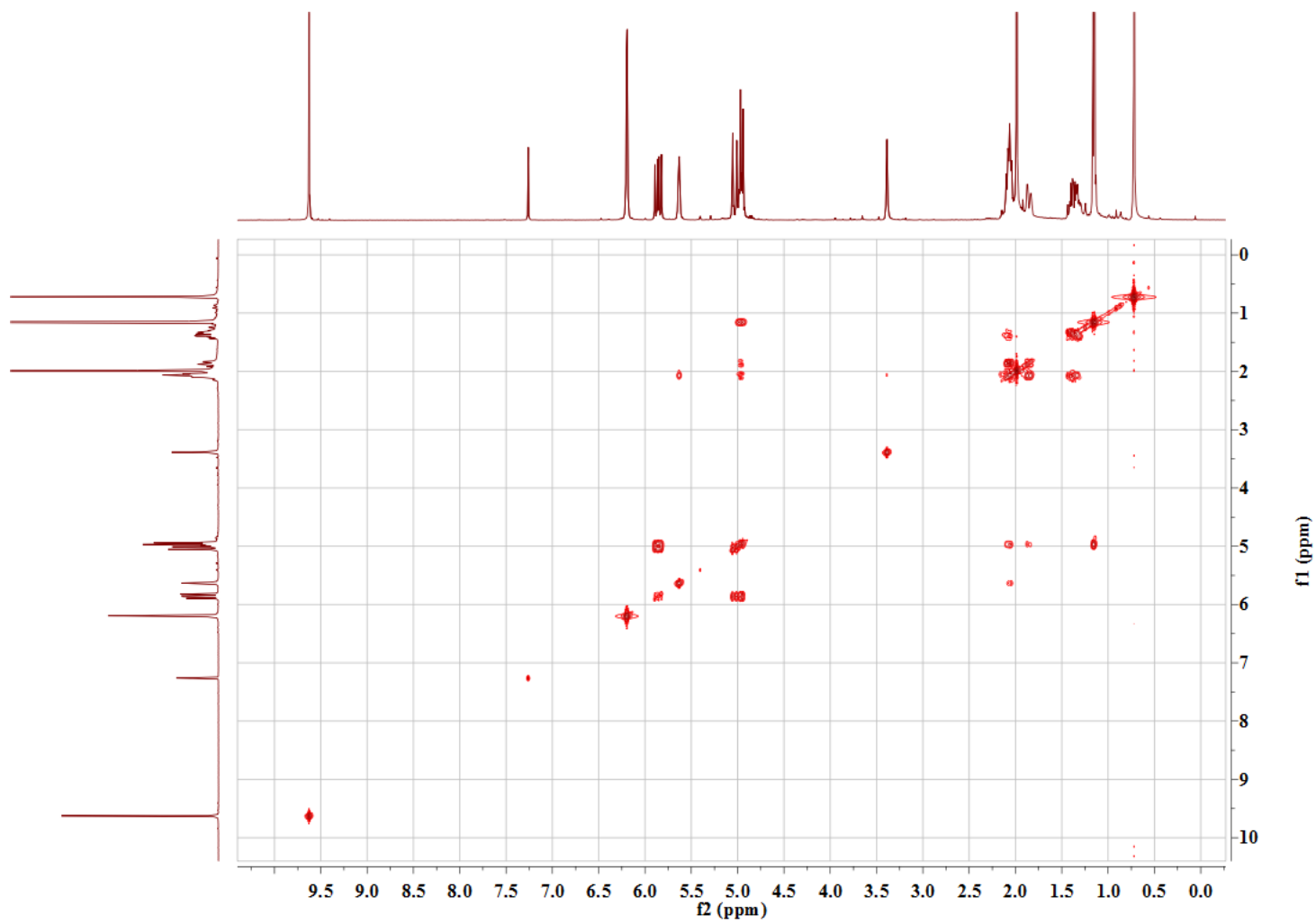


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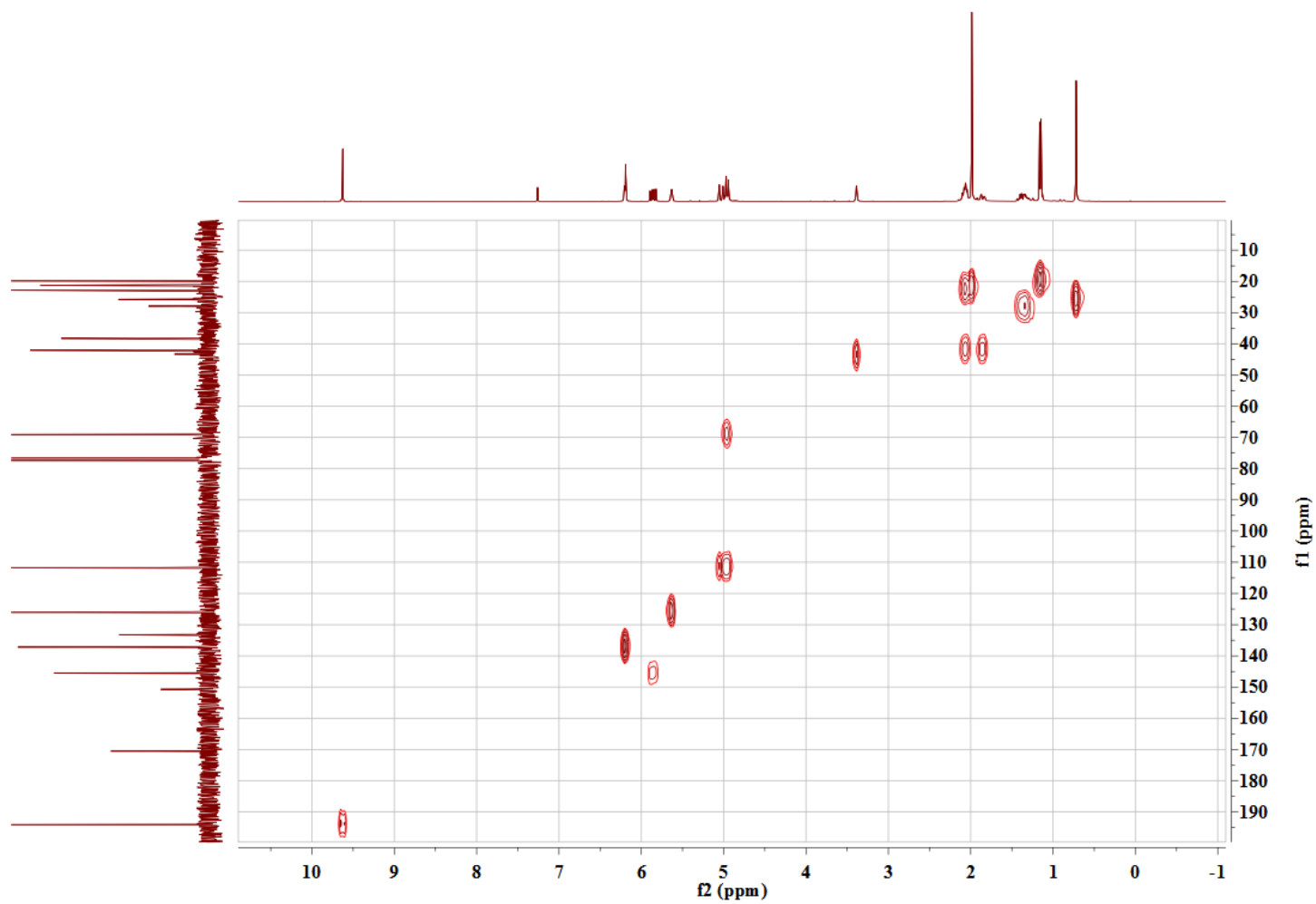




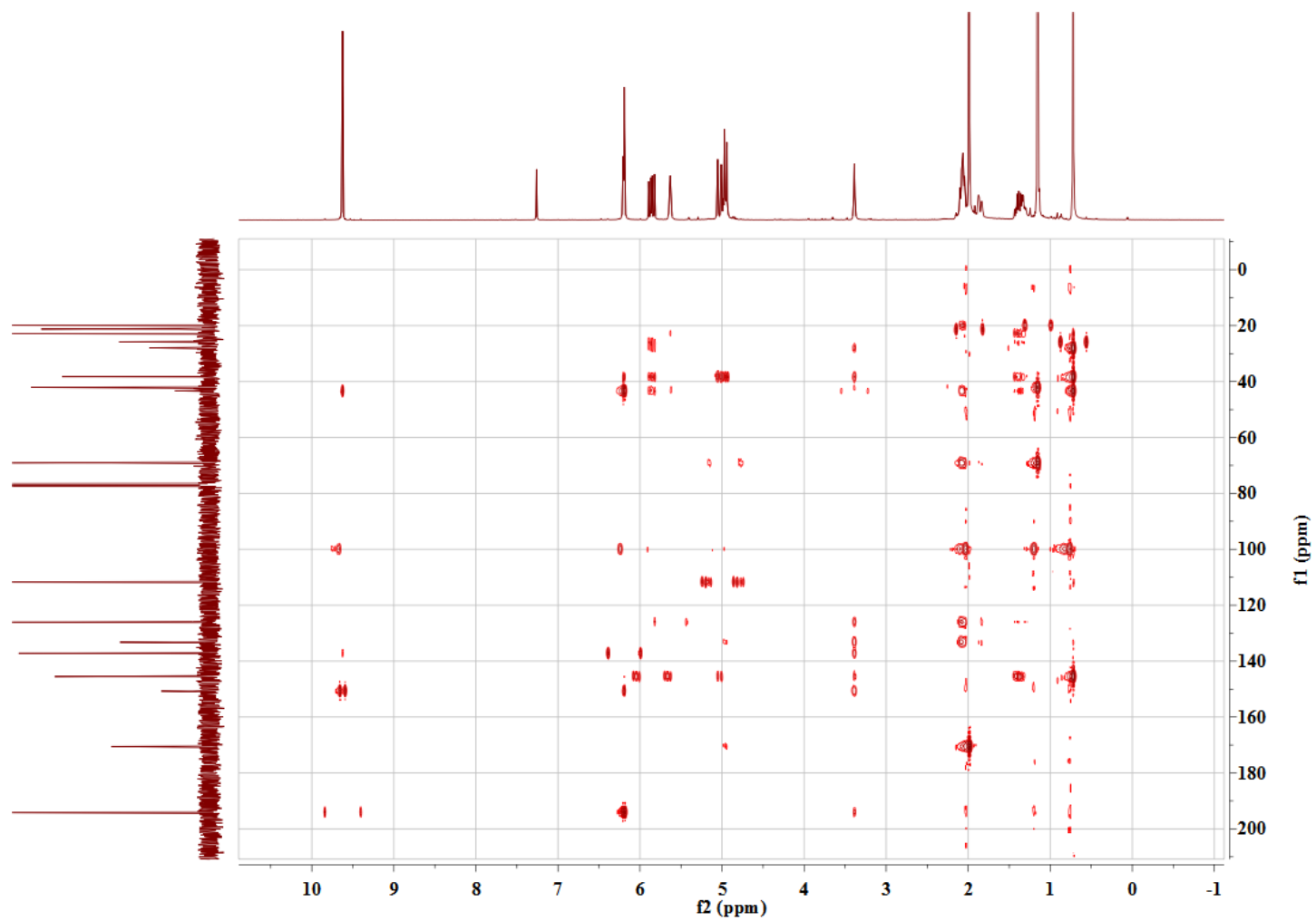
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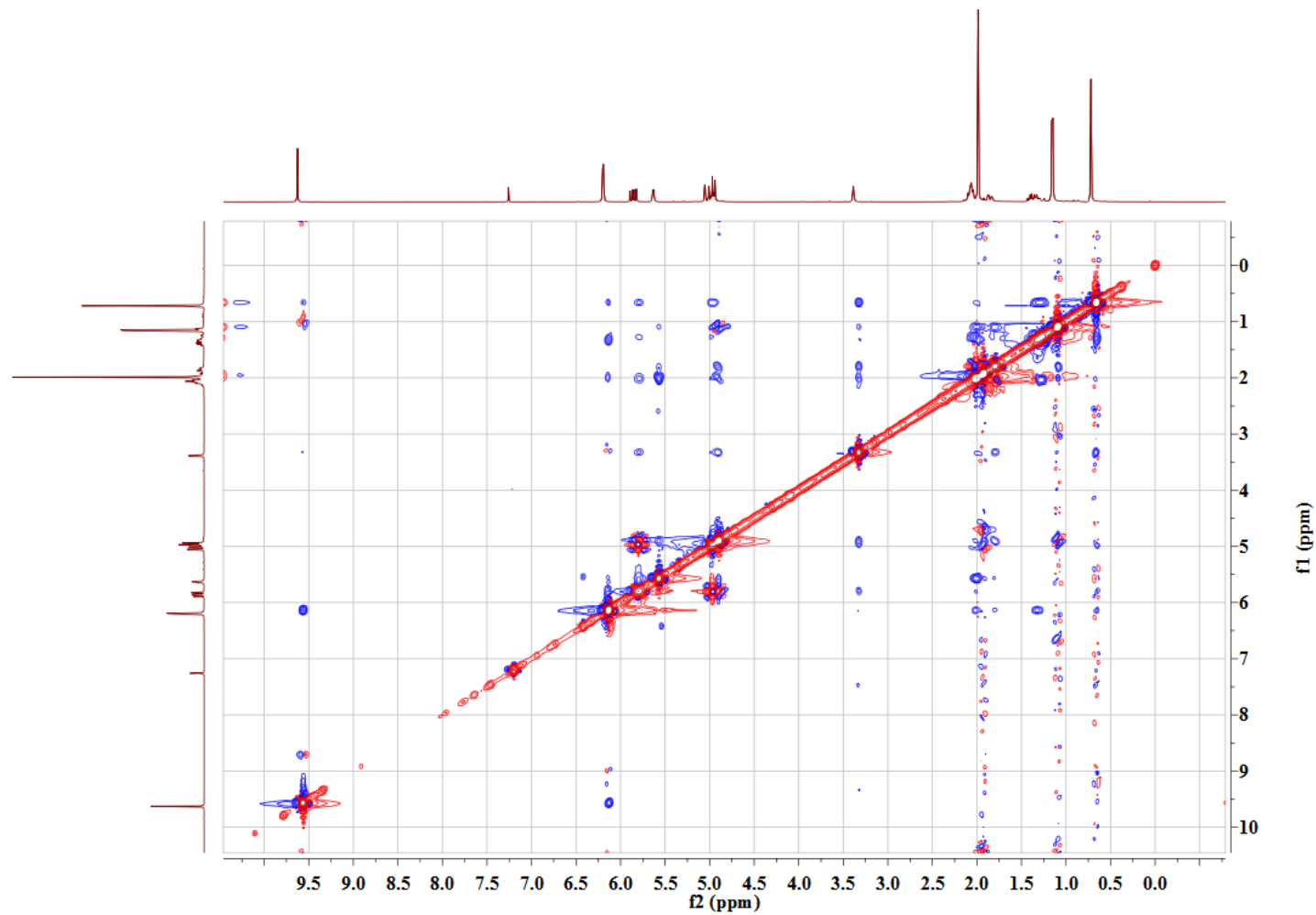
S27 HSQC Spectrum of 4 in CDCl<sub>3</sub>



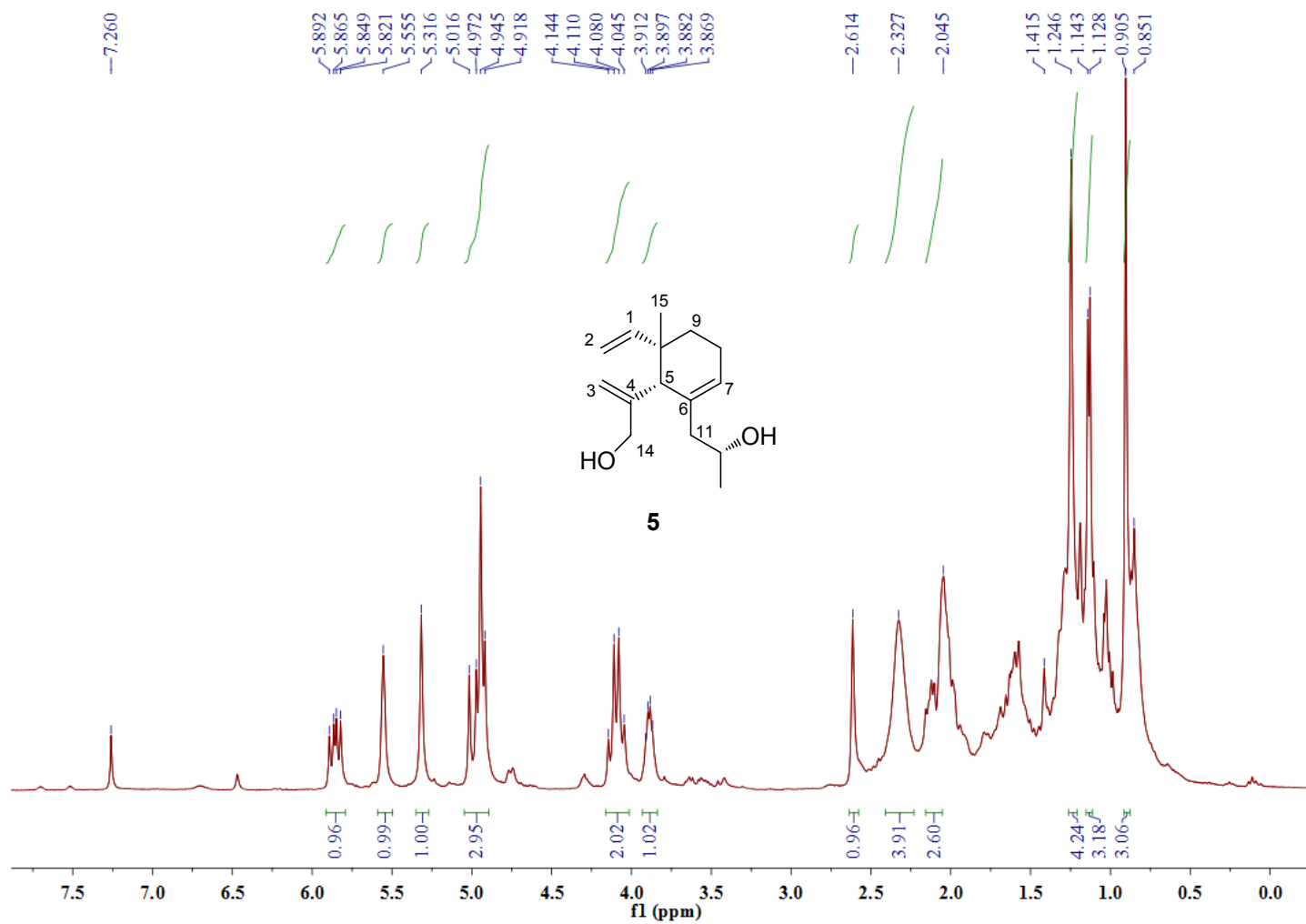
S28 HMBC Spectrum of **4** in CDCl<sub>3</sub>



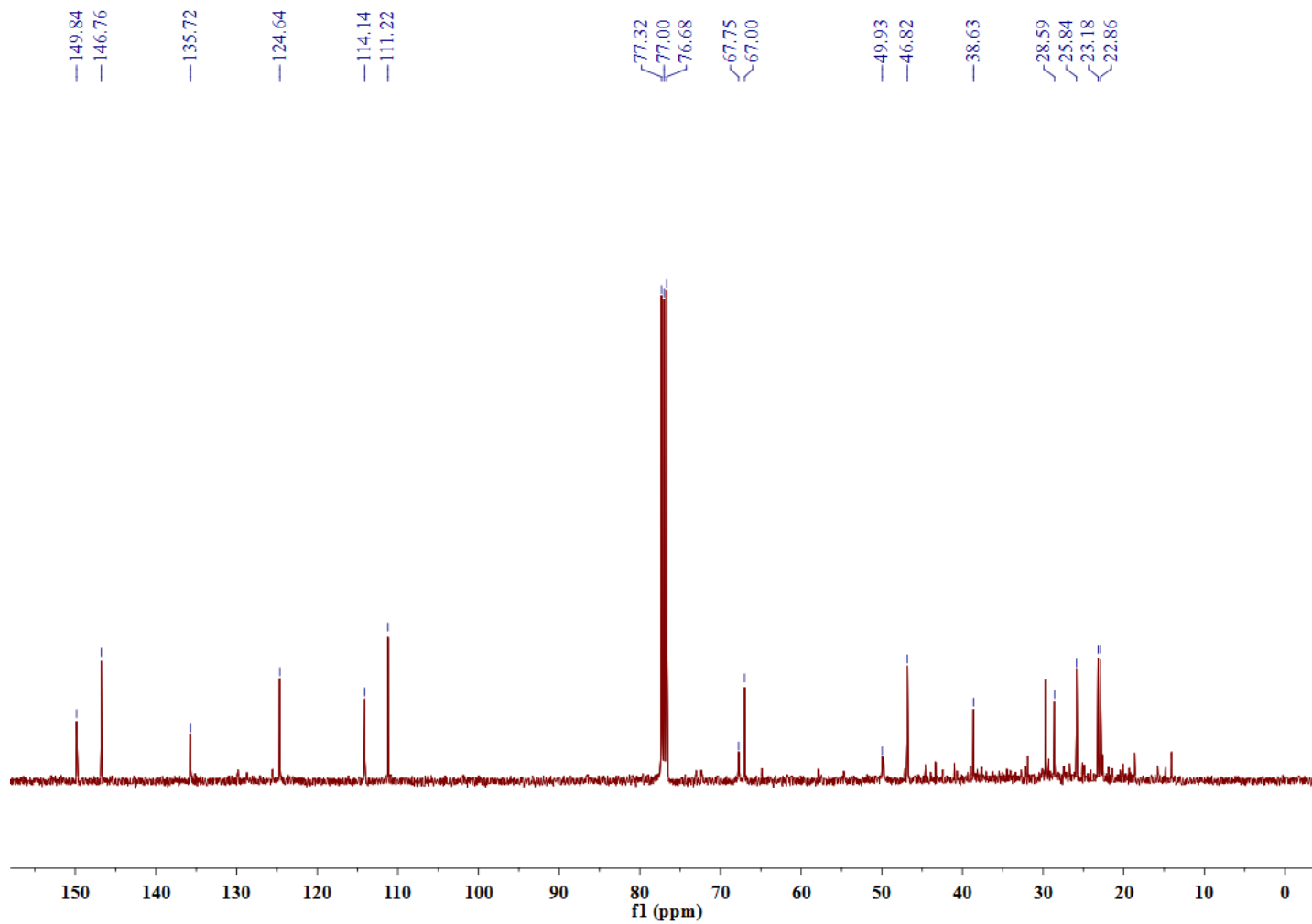
S29 NOESY Spectrum of 4 in CDCl<sub>3</sub>



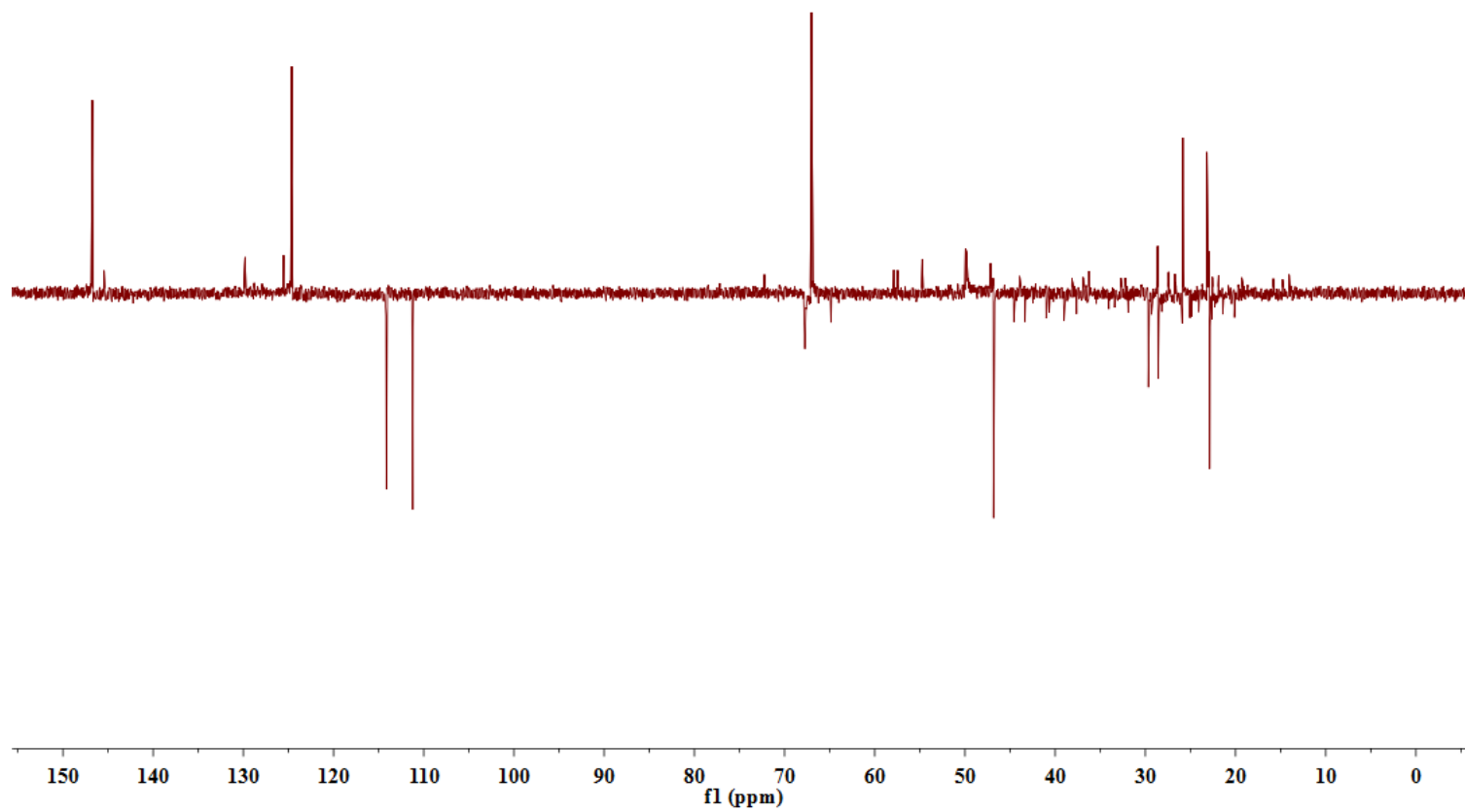
S30  $^1\text{H}$  NMR Spectrum of **5** in  $\text{CDCl}_3$



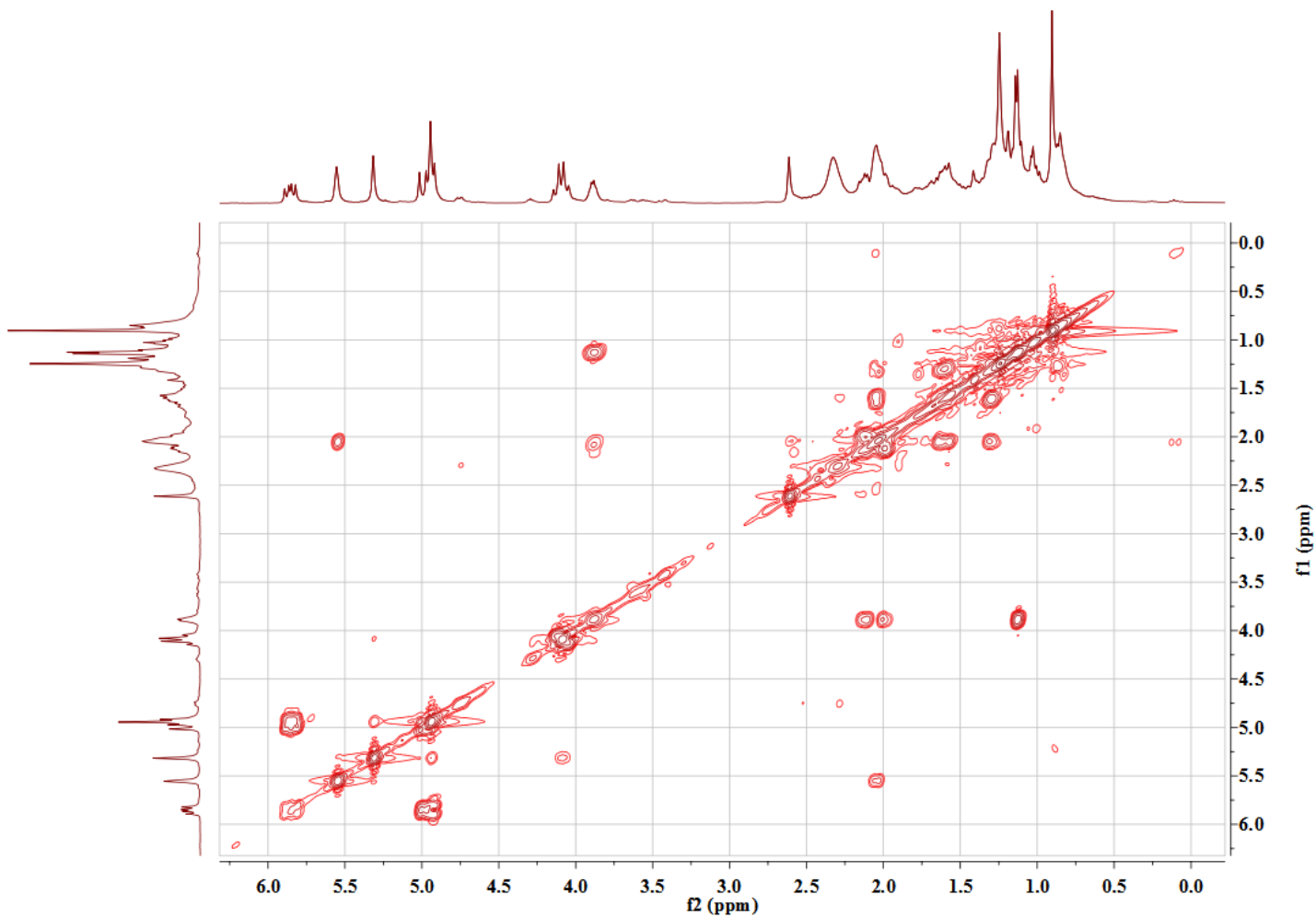
**S31**  $^{13}\text{C}$  NMR Spectra of **5** in  $\text{CDCl}_3$



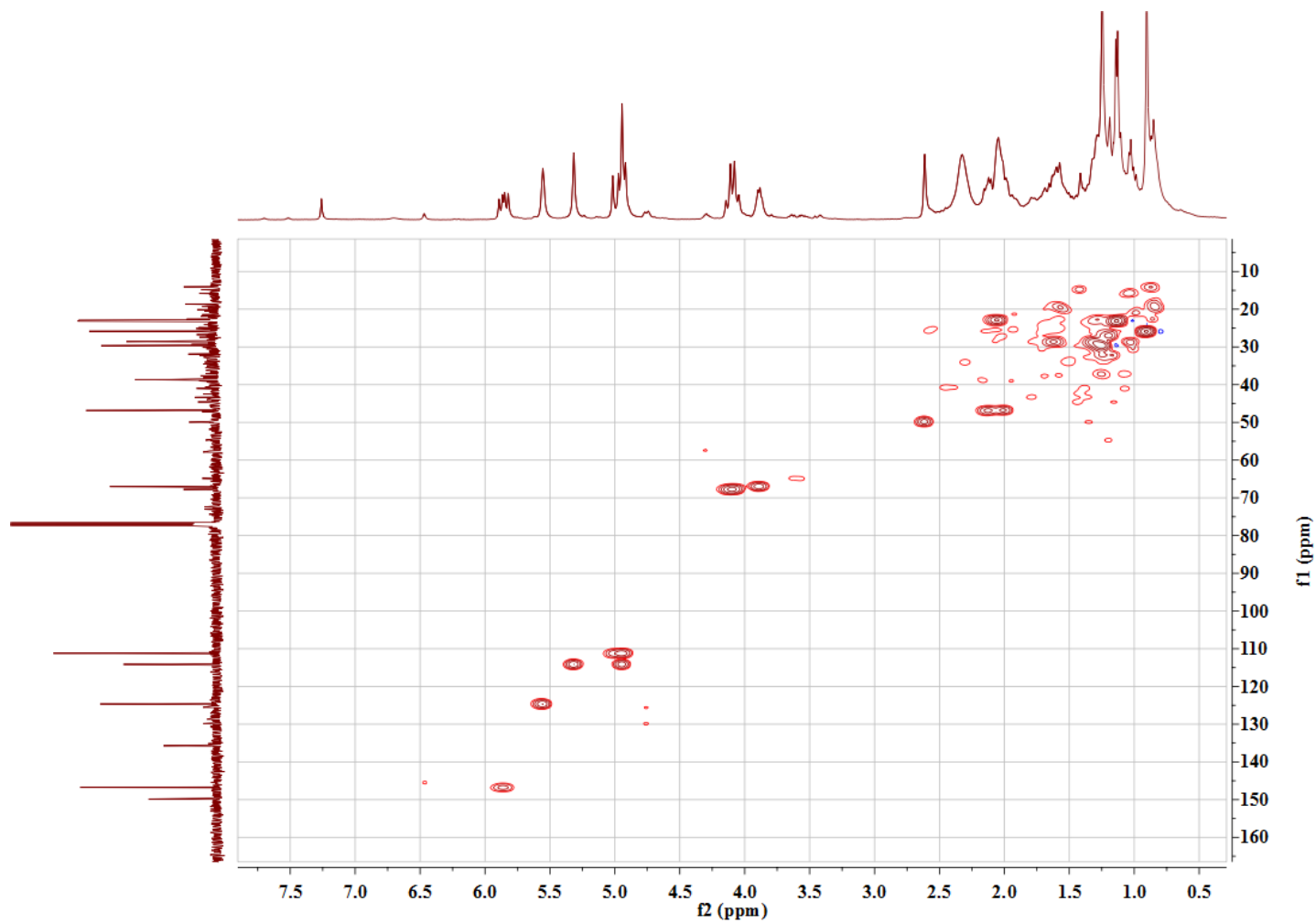




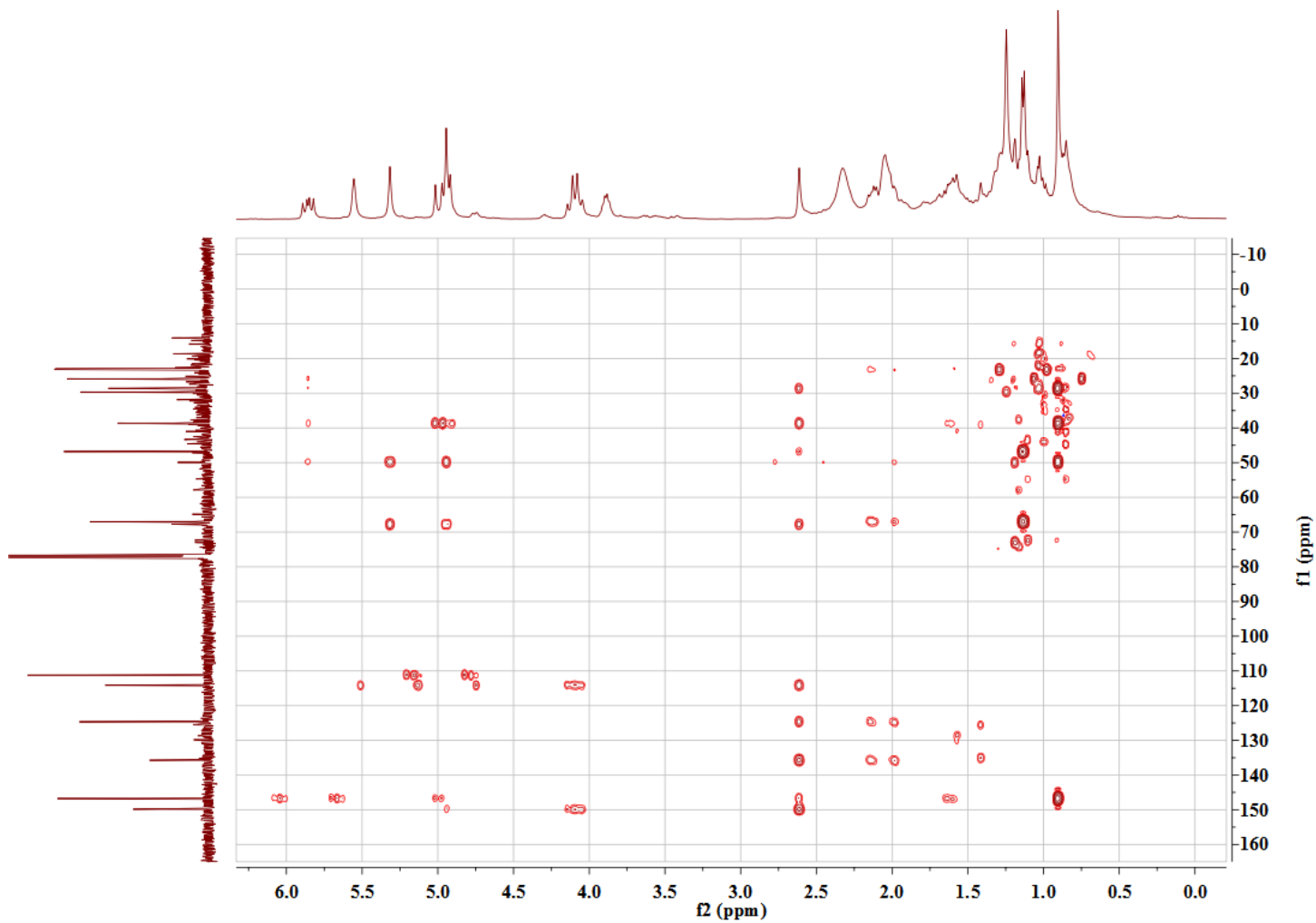
S32  $^1\text{H}$ - $^1\text{H}$  COSY Spectrum of **5** in  $\text{CDCl}_3$



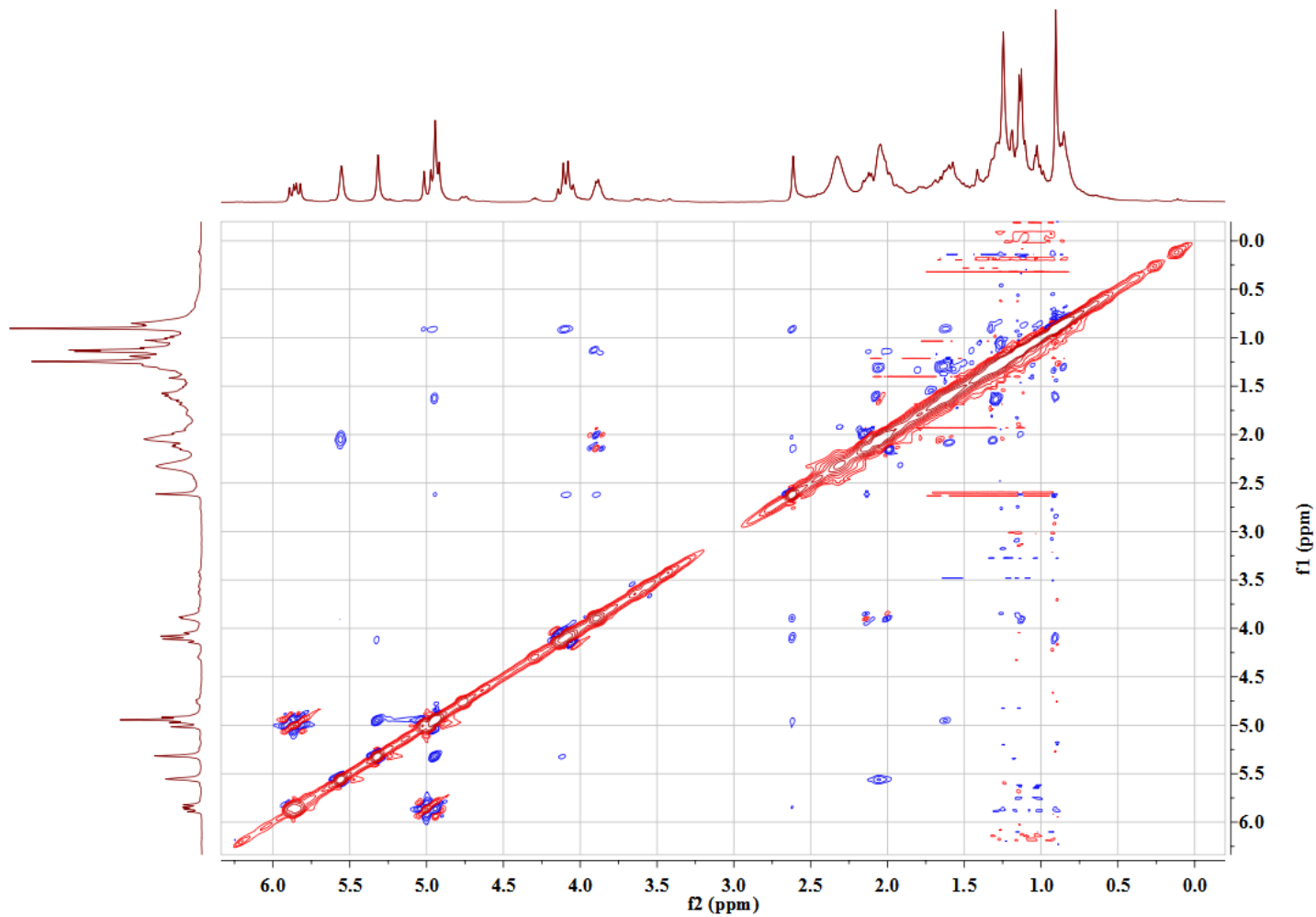
S33 HSQC Spectrum of 5 in CDCl<sub>3</sub>



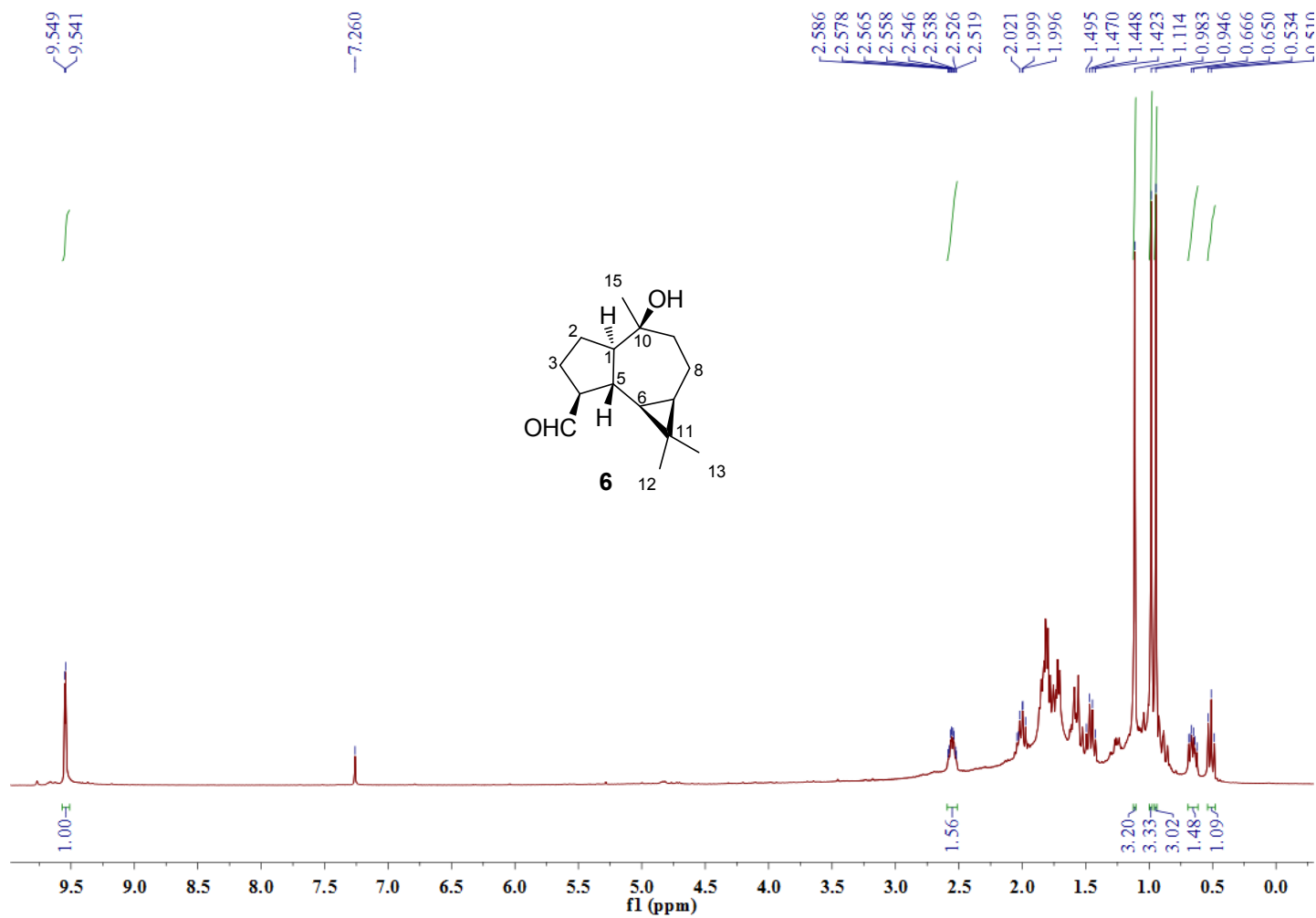
S34 HMBC Spectrum of 5 in CDCl<sub>3</sub>



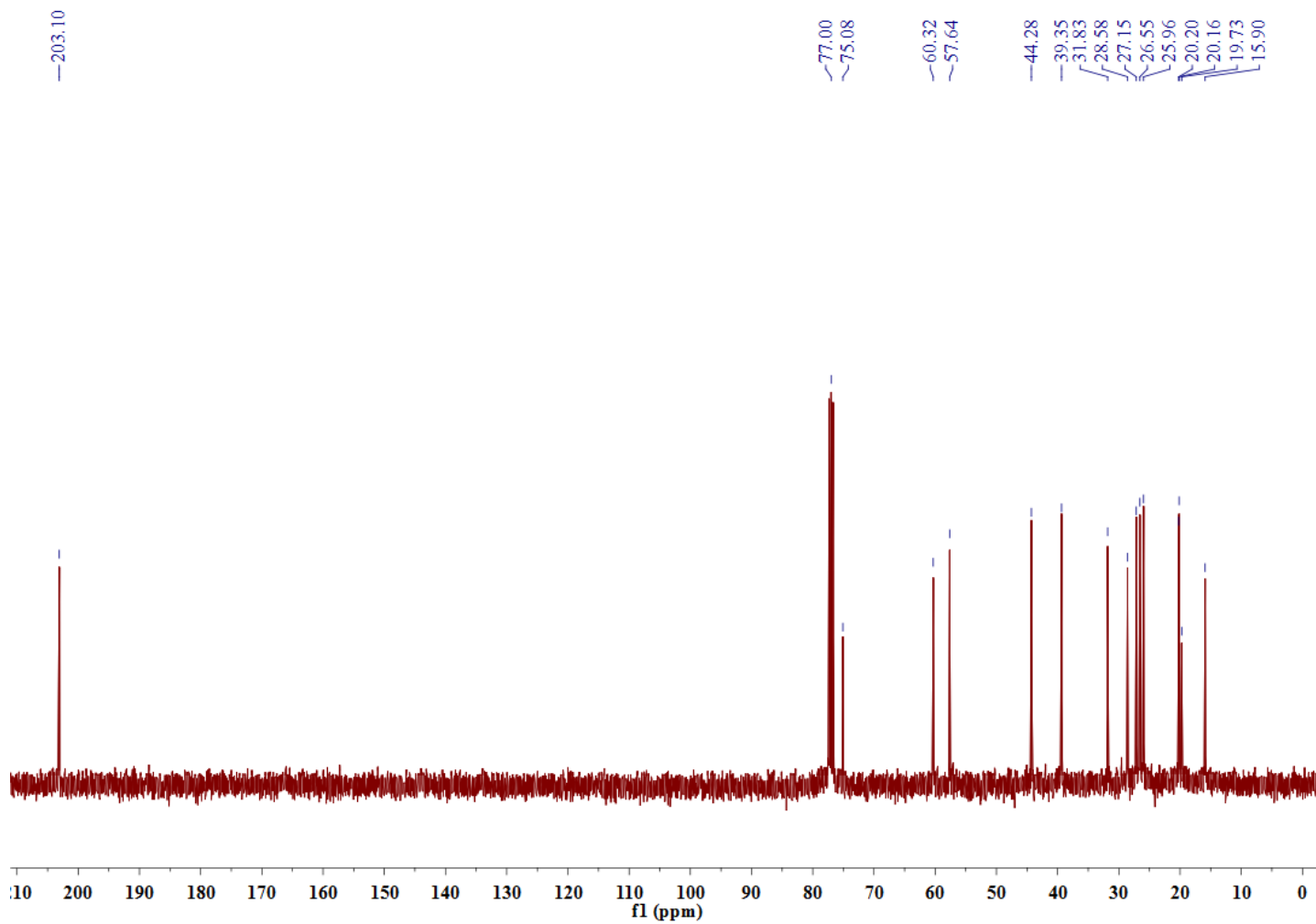
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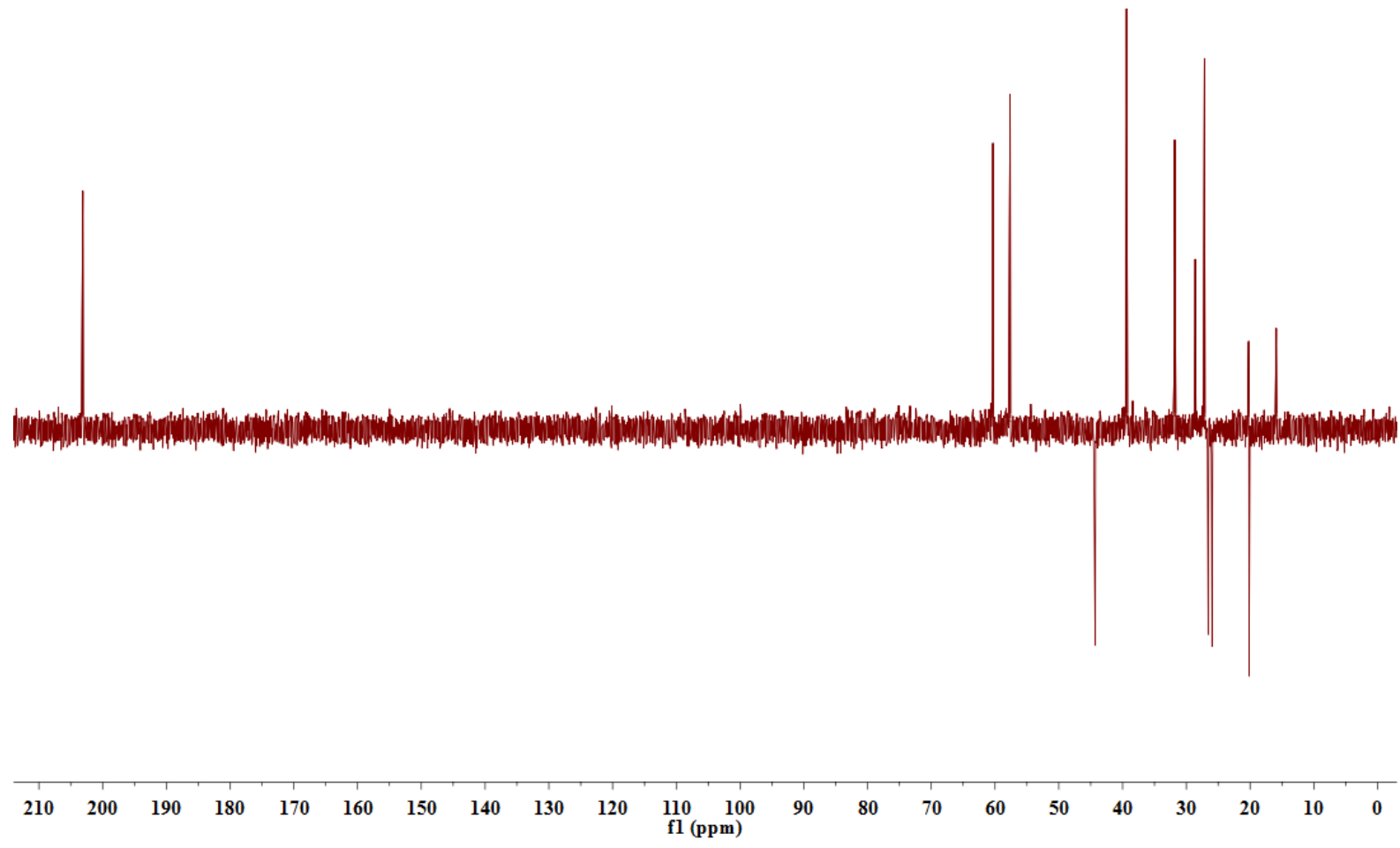


S36  $^1\text{H}$  NMR Spectrum of **6** in  $\text{CDCl}_3$



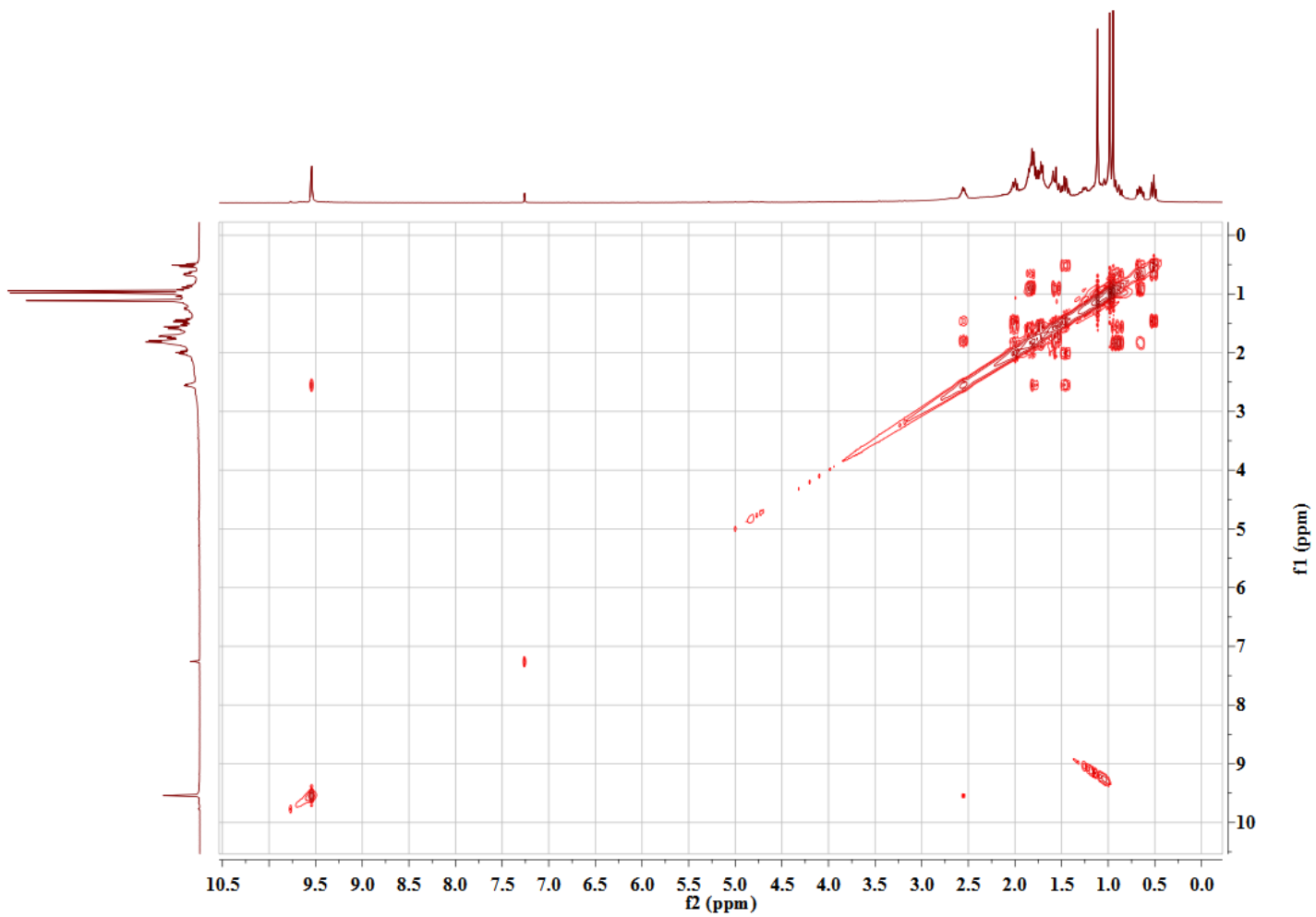
S37  $^{13}\text{C}$  NMR Spectra of **6** in  $\text{CDCl}_3$



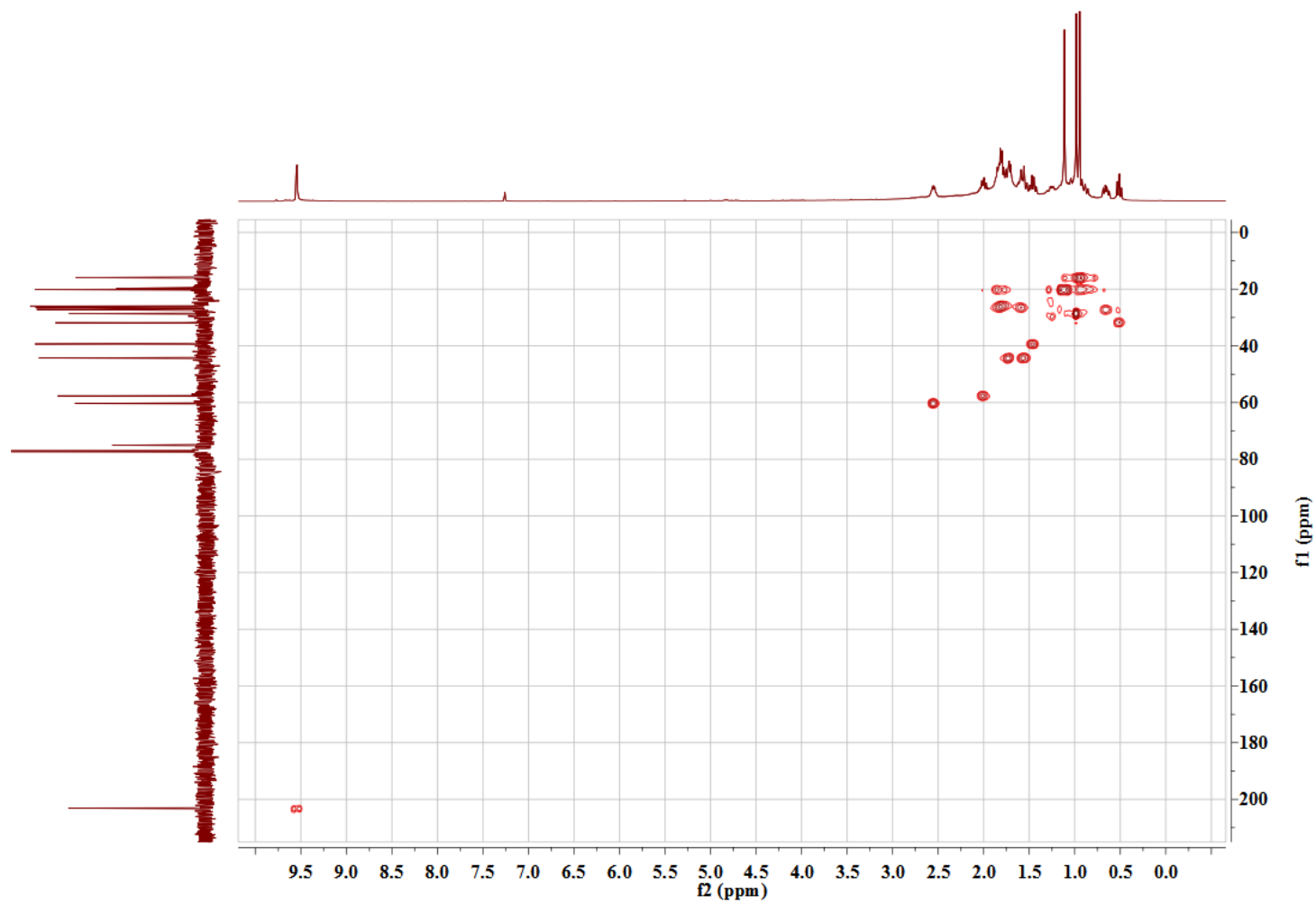




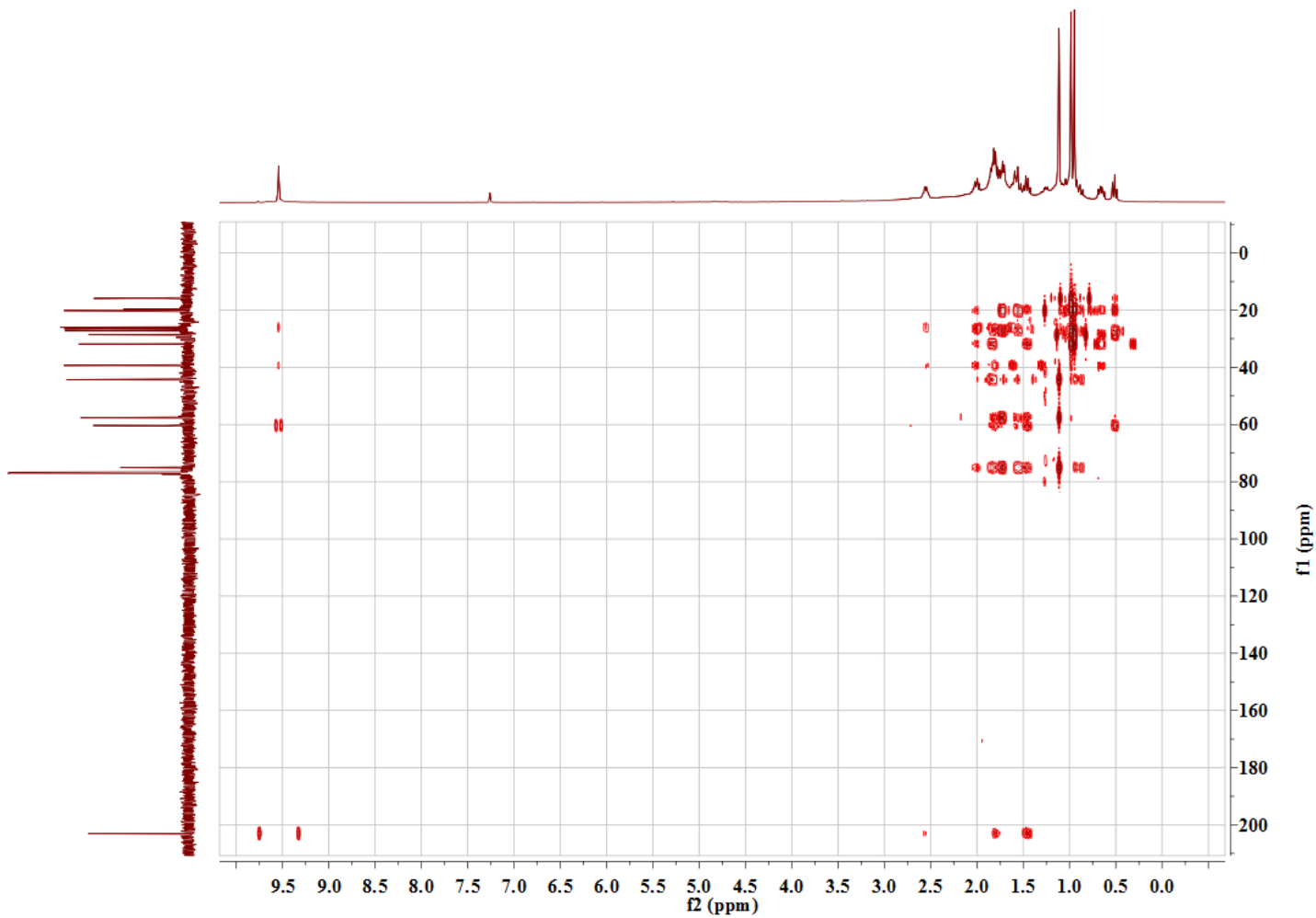
S38  $^1\text{H}$ - $^1\text{H}$  COSY Spectrum of **6** in  $\text{CDCl}_3$



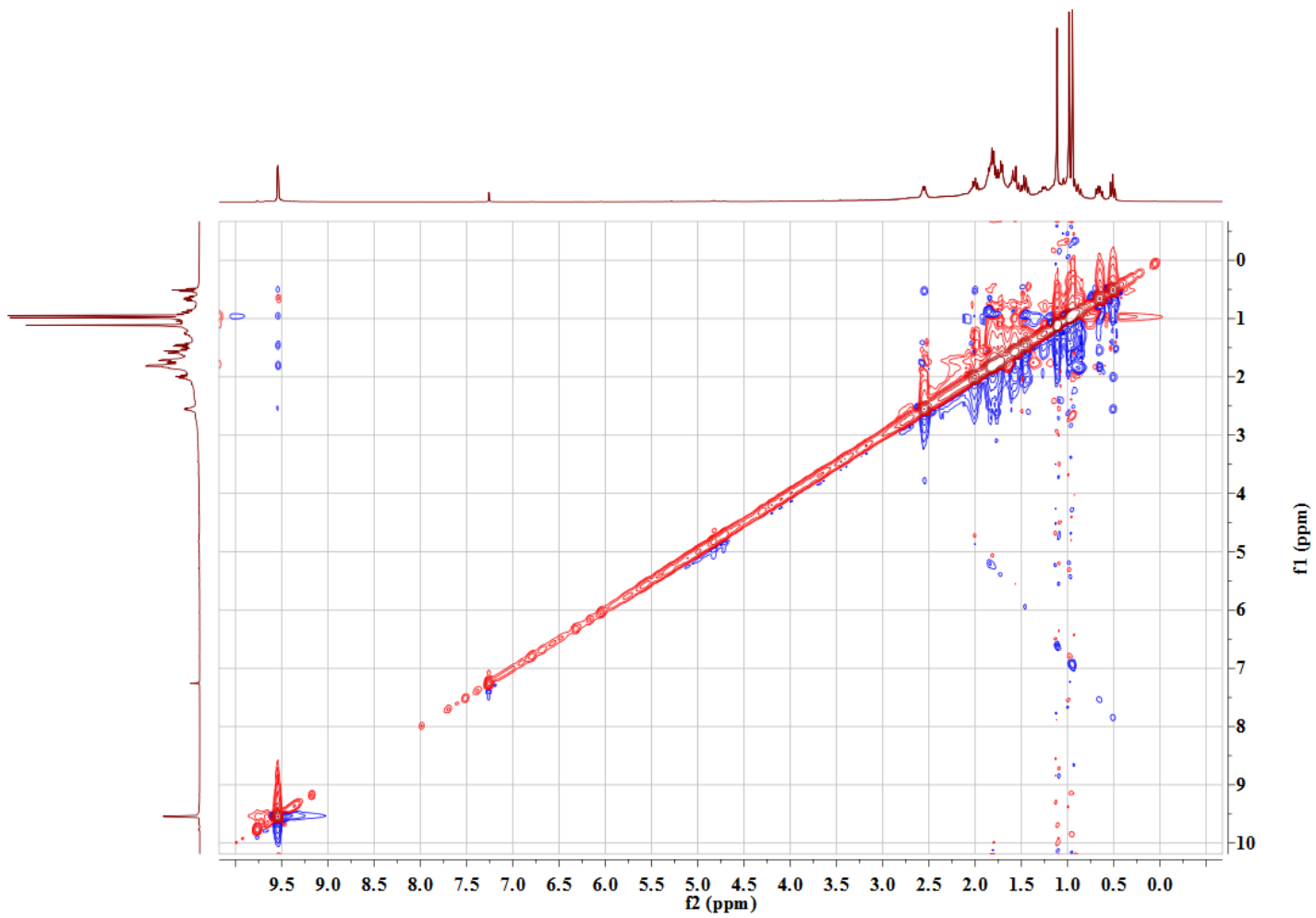
S39 HSQC Spectrum of **6** in CDCl<sub>3</sub>



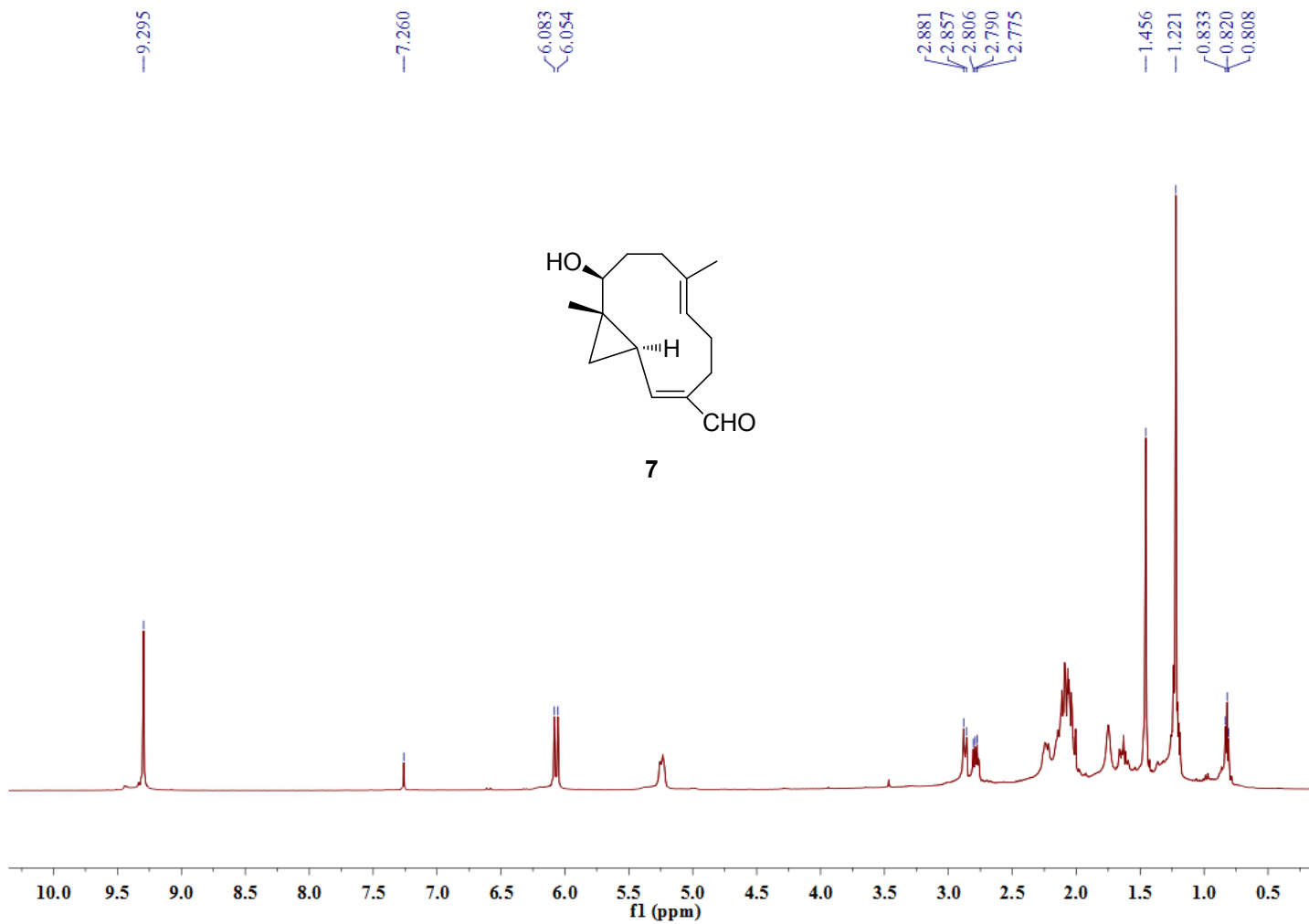
S40 HMBC Spectrum of **6** in CDCl<sub>3</sub>



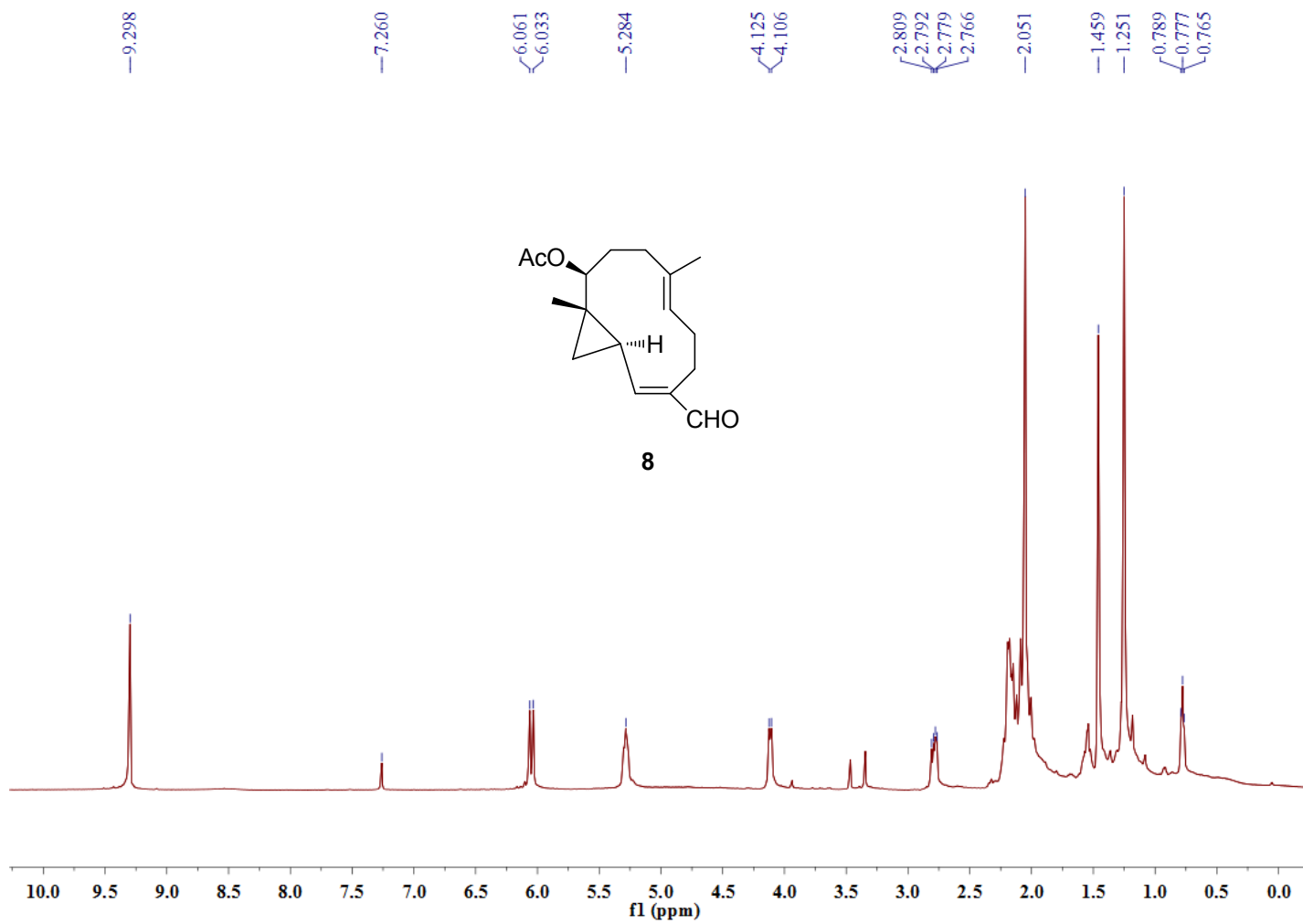
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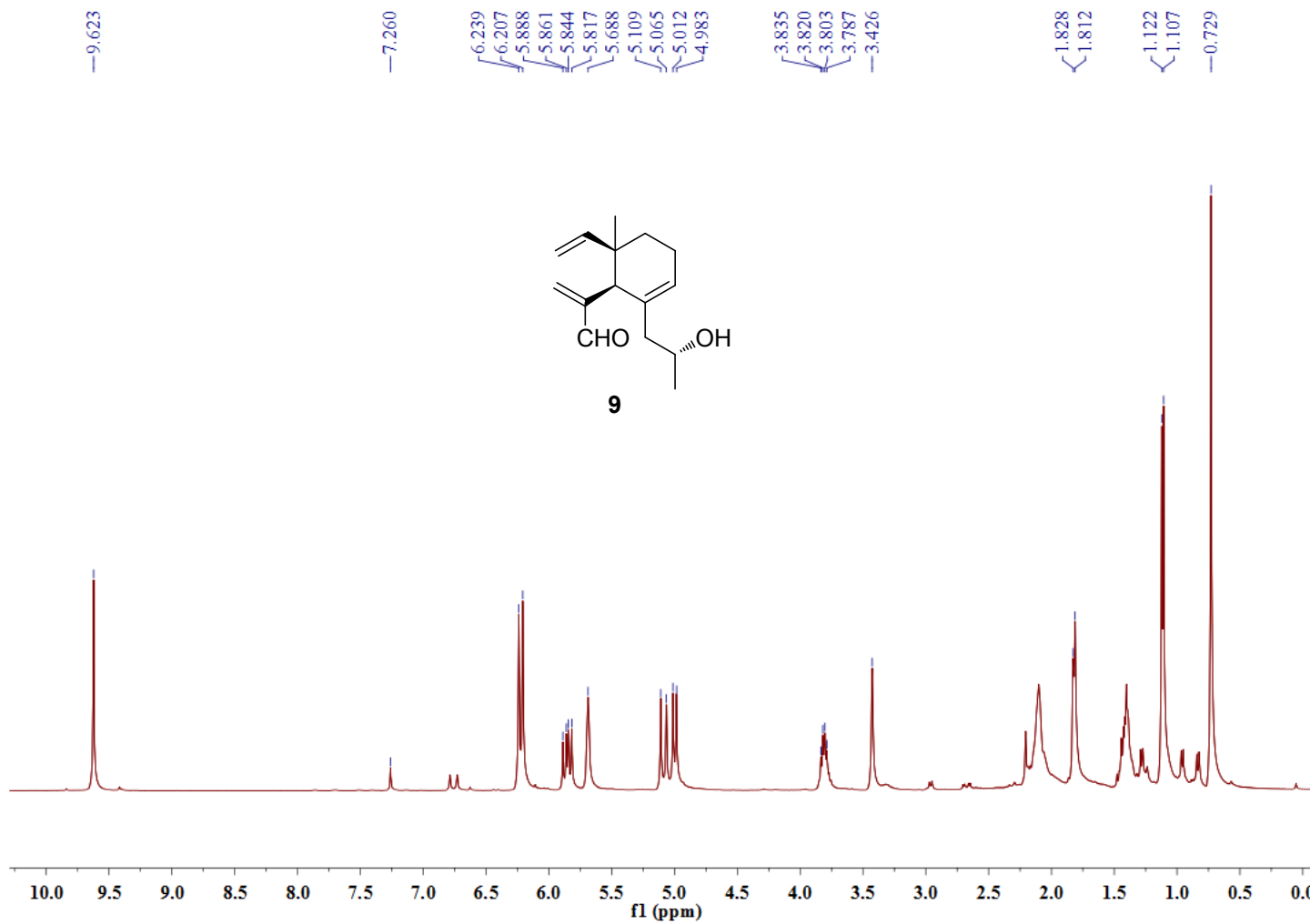
S42 <sup>1</sup>H NMR Spectrum of 7 in CDCl<sub>3</sub>



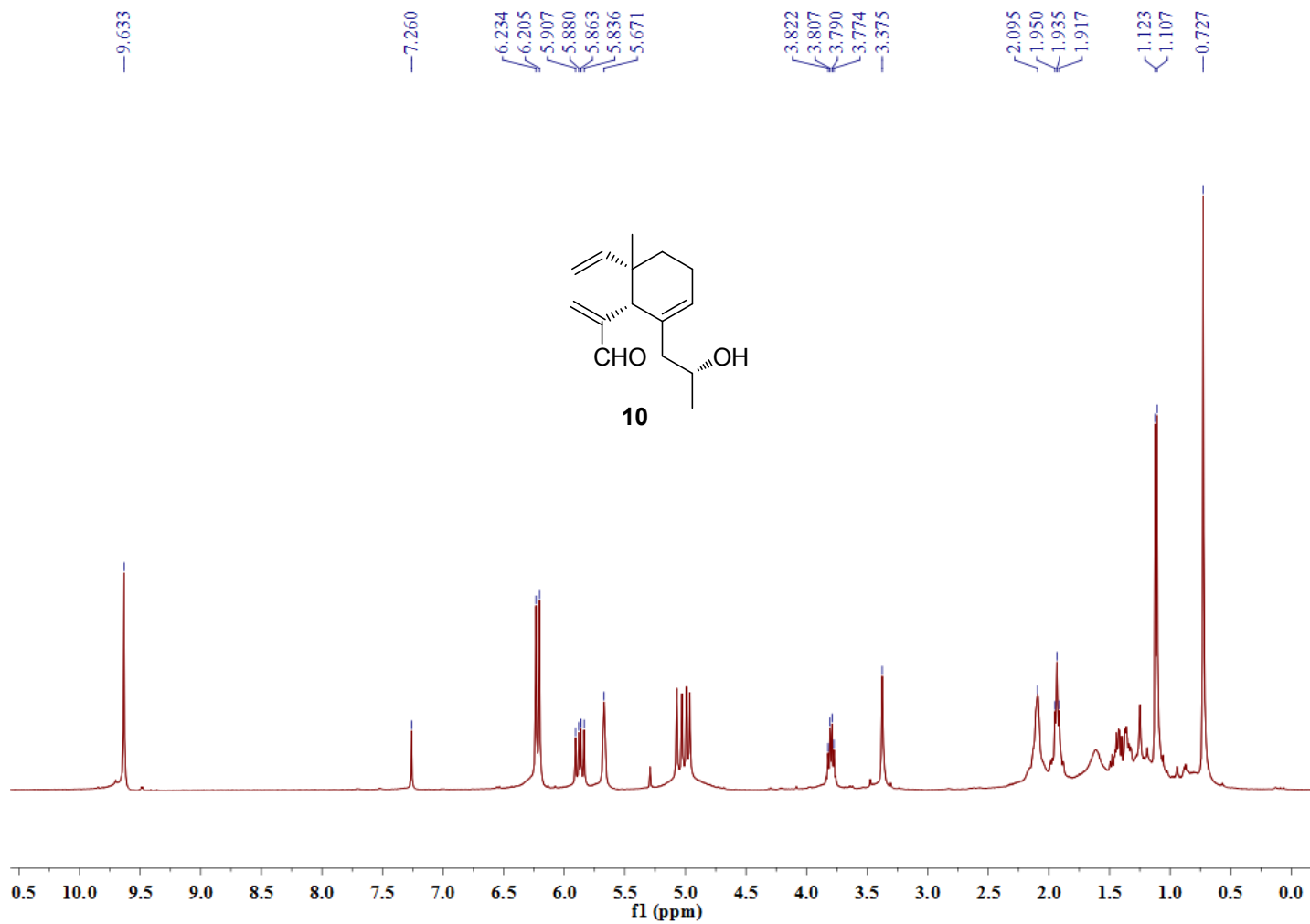
S43 <sup>1</sup>H NMR Spectrum of **8** in CDCl<sub>3</sub>



S44  $^1\text{H}$  NMR Spectrum of **9** in  $\text{CDCl}_3$

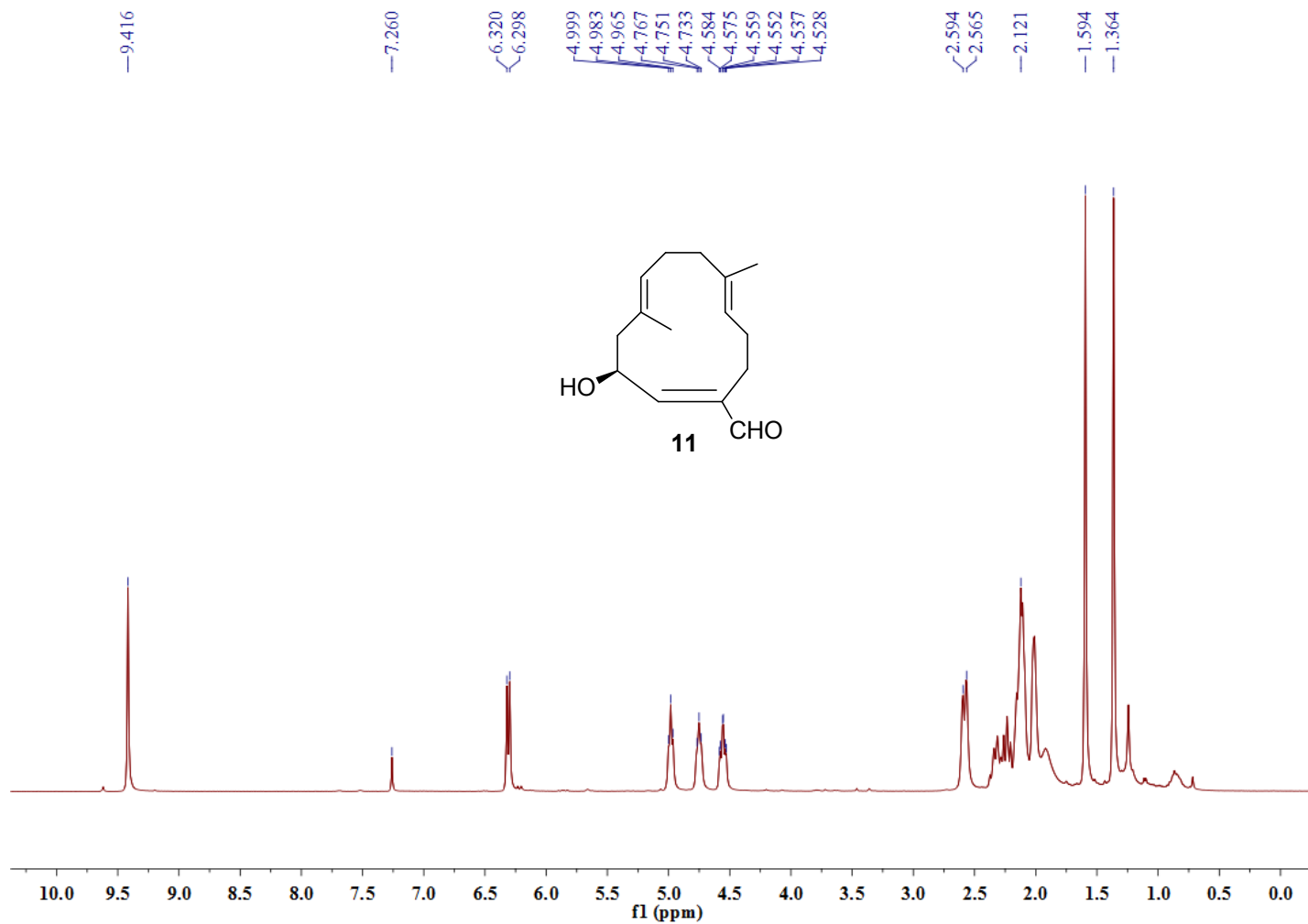


S45  $^1\text{H}$  NMR Spectrum of **10** in  $\text{CDCl}_3$

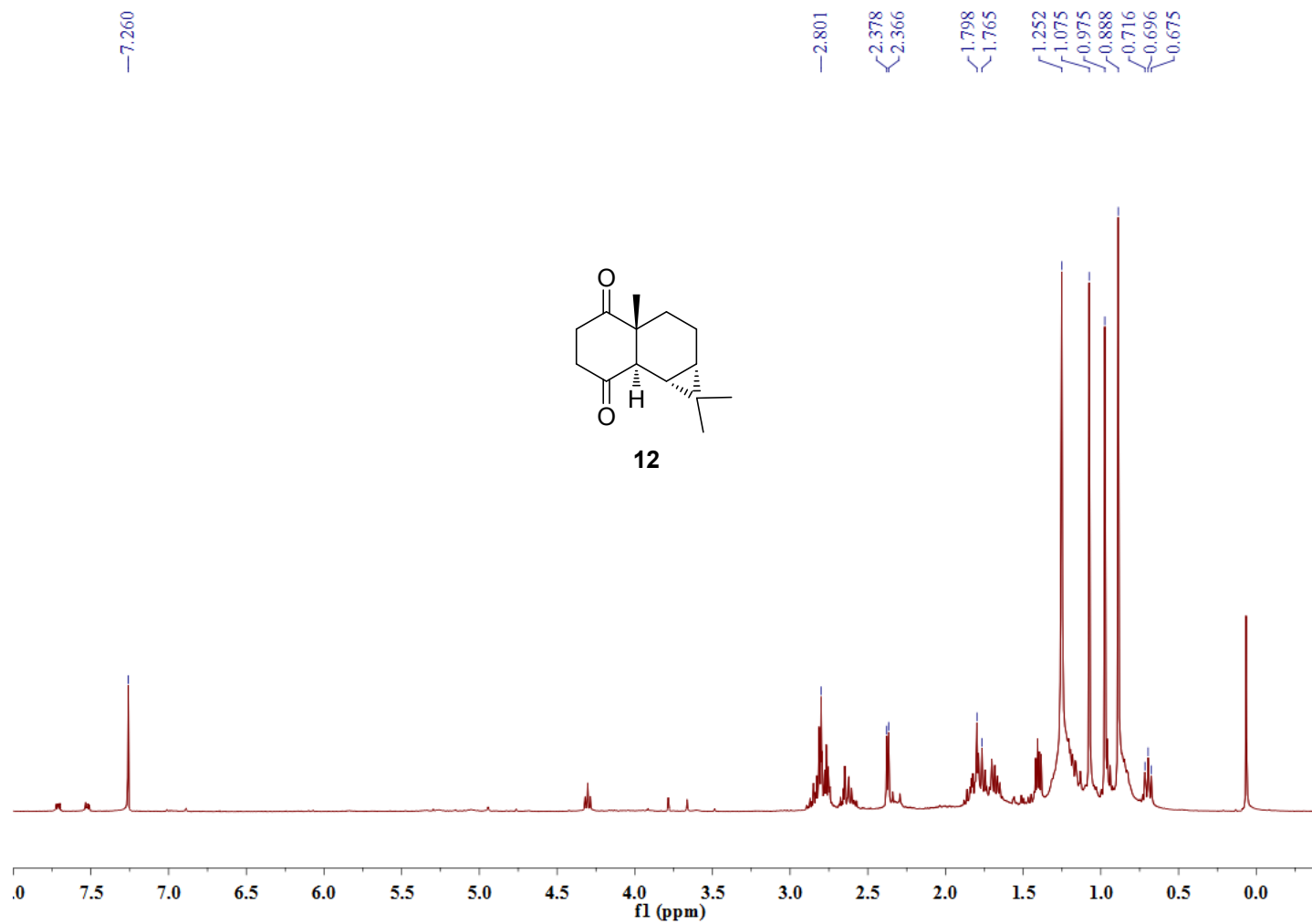




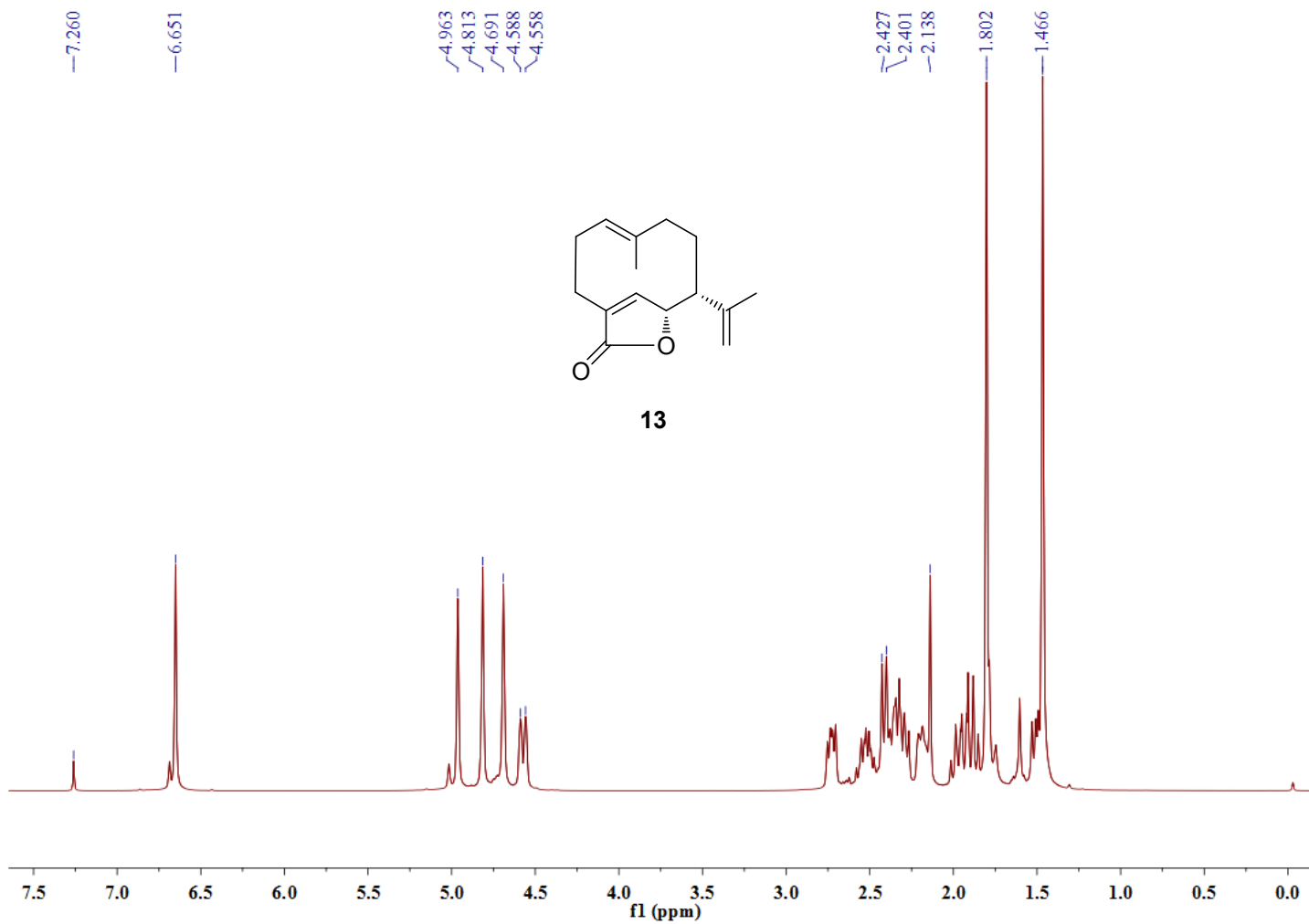
S46  $^1\text{H}$  NMR Spectrum of **11** in  $\text{CDCl}_3$



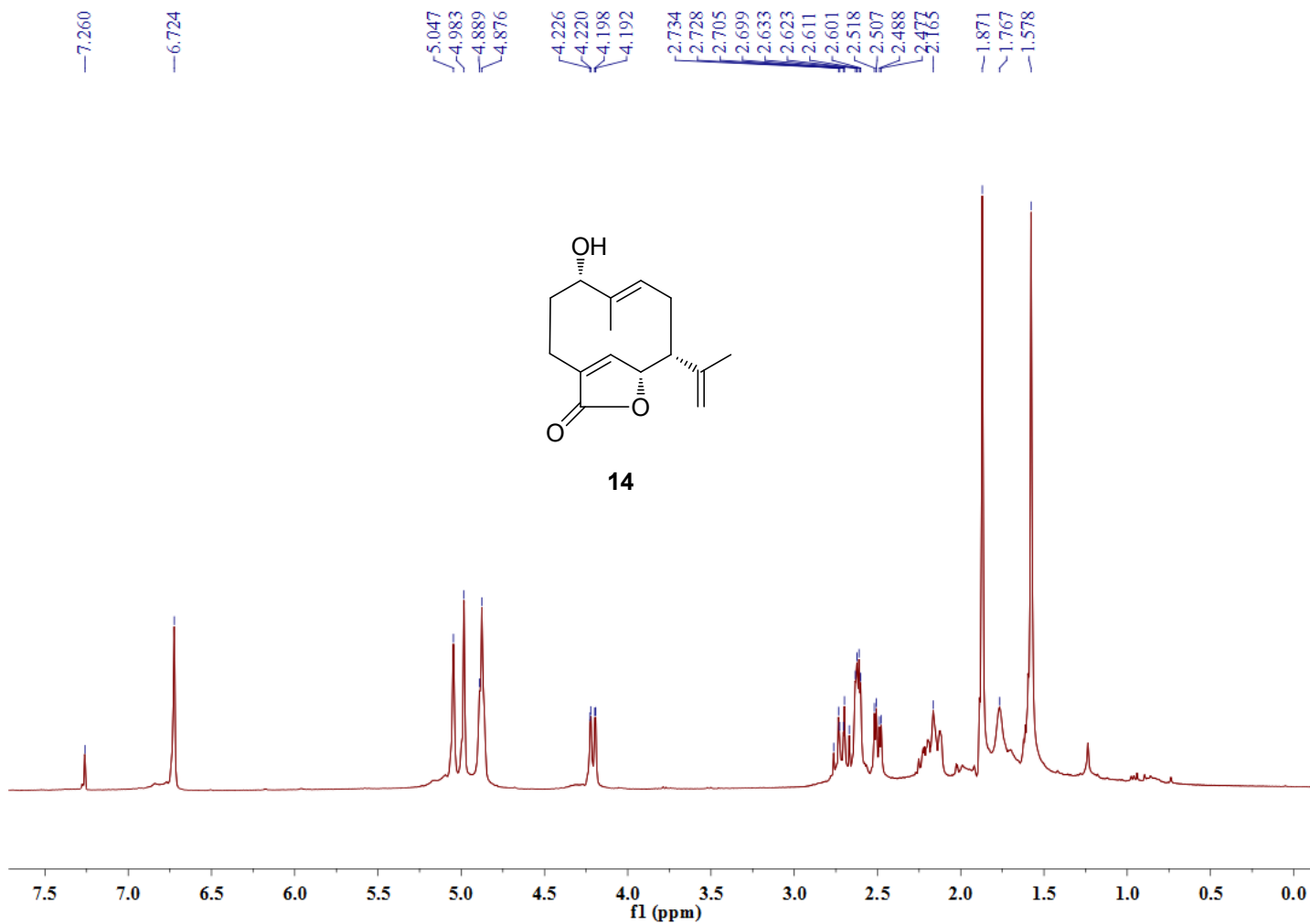
S47  $^1\text{H}$  NMR Spectrum of **12** in  $\text{CDCl}_3$



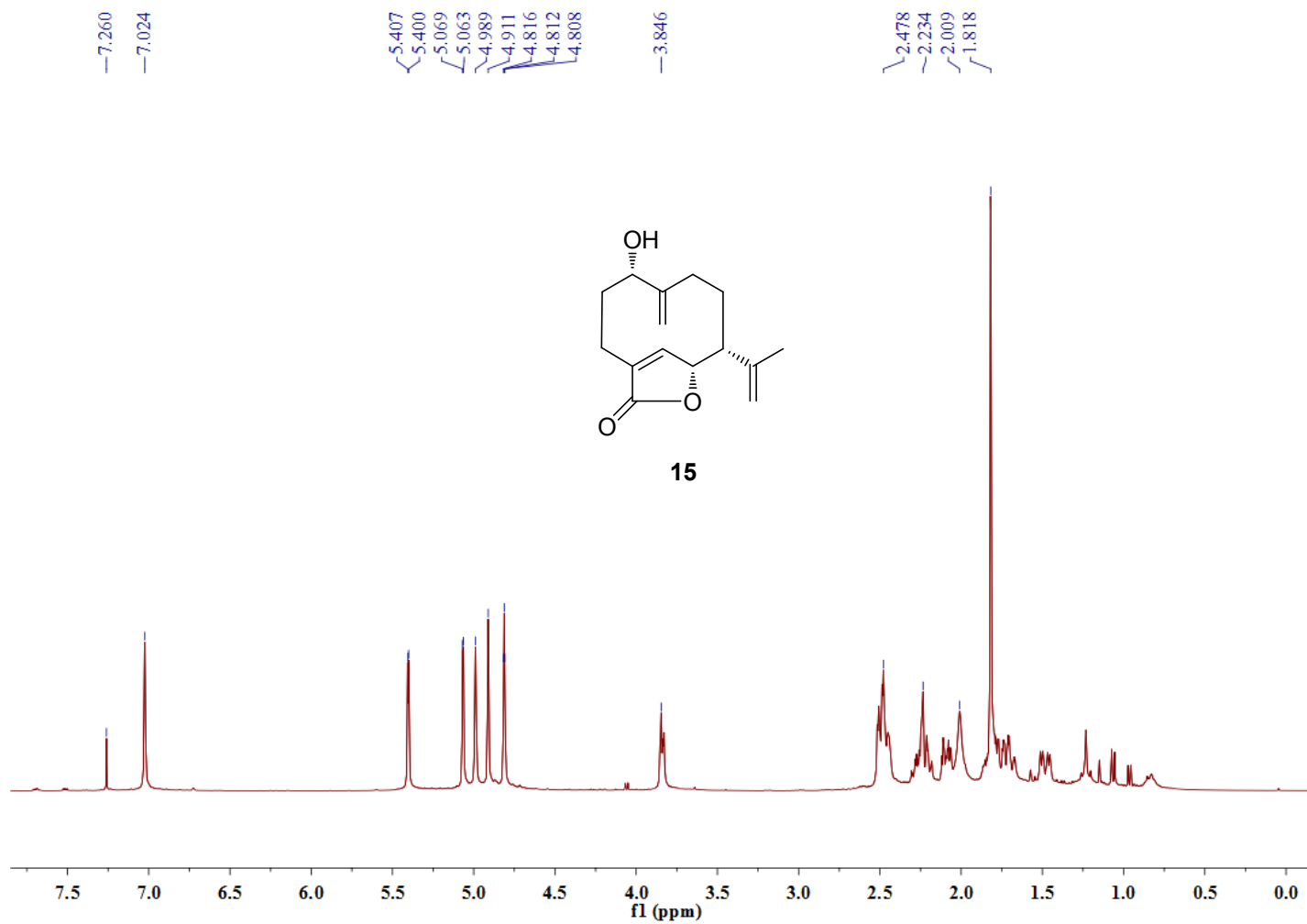
S48  $^1\text{H}$  NMR Spectrum of **13** in  $\text{CDCl}_3$



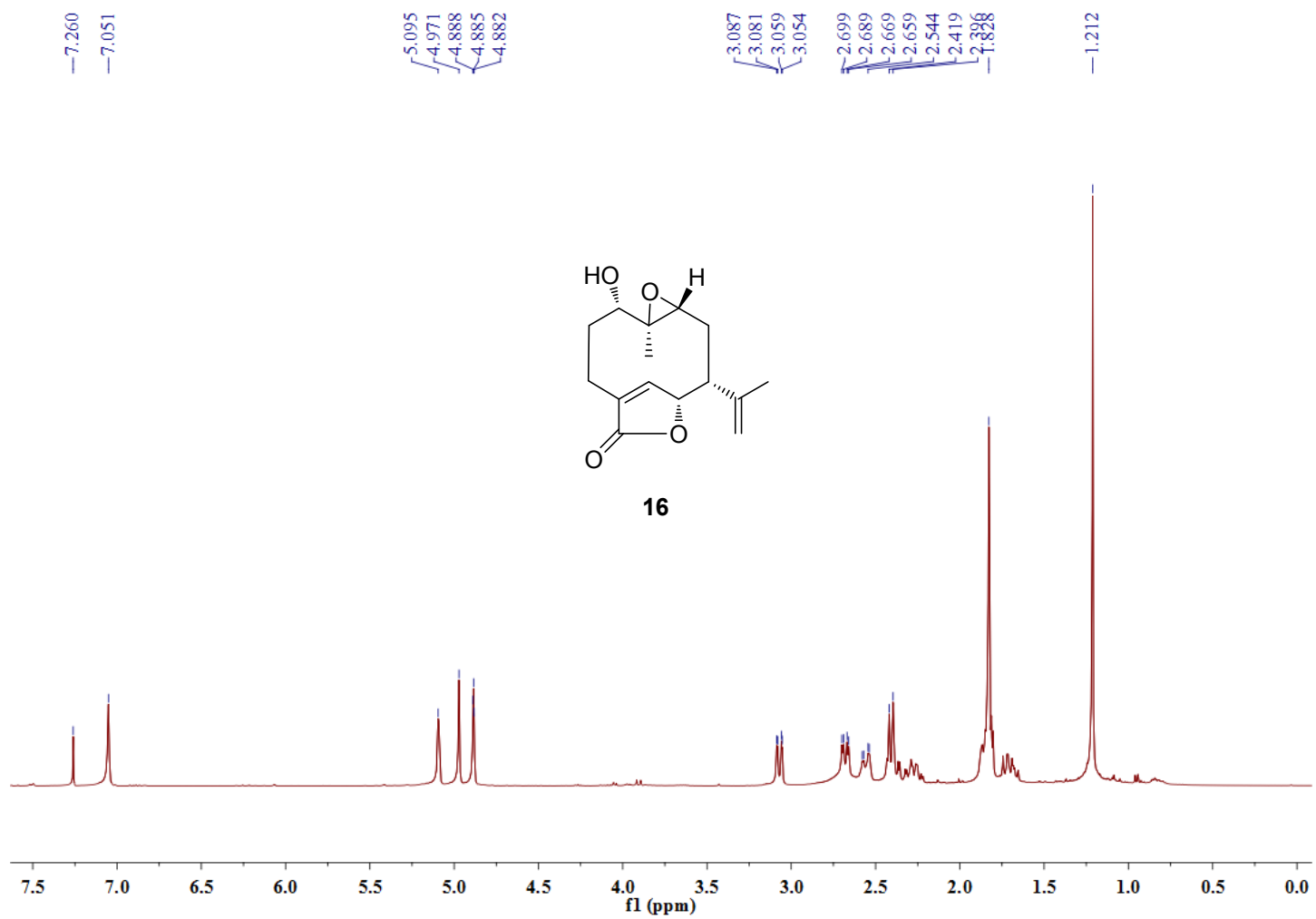
S49 <sup>1</sup>H NMR Spectrum of **14** in CDCl<sub>3</sub>



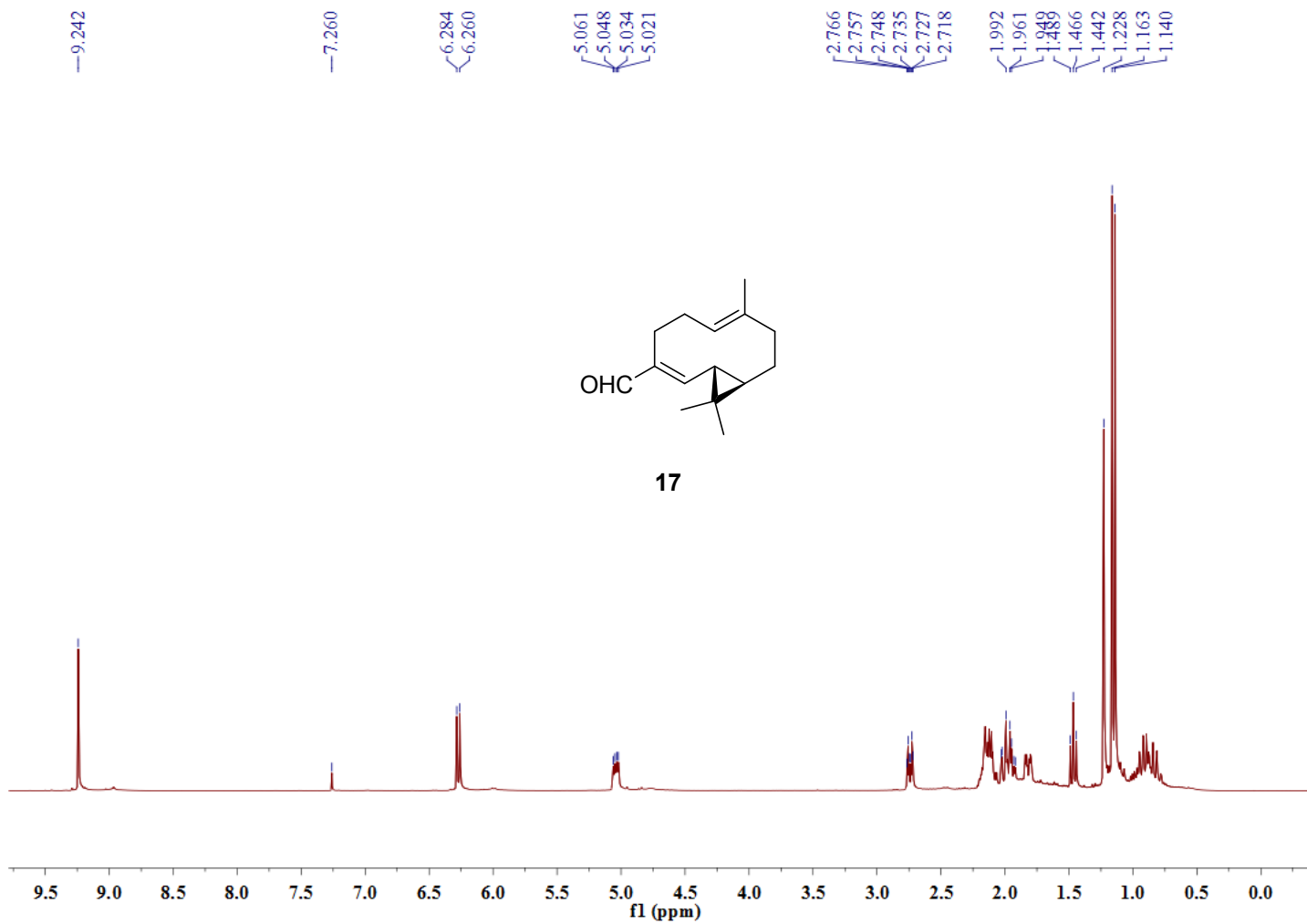
S50 <sup>1</sup>H NMR Spectrum of **15** in CDCl<sub>3</sub>



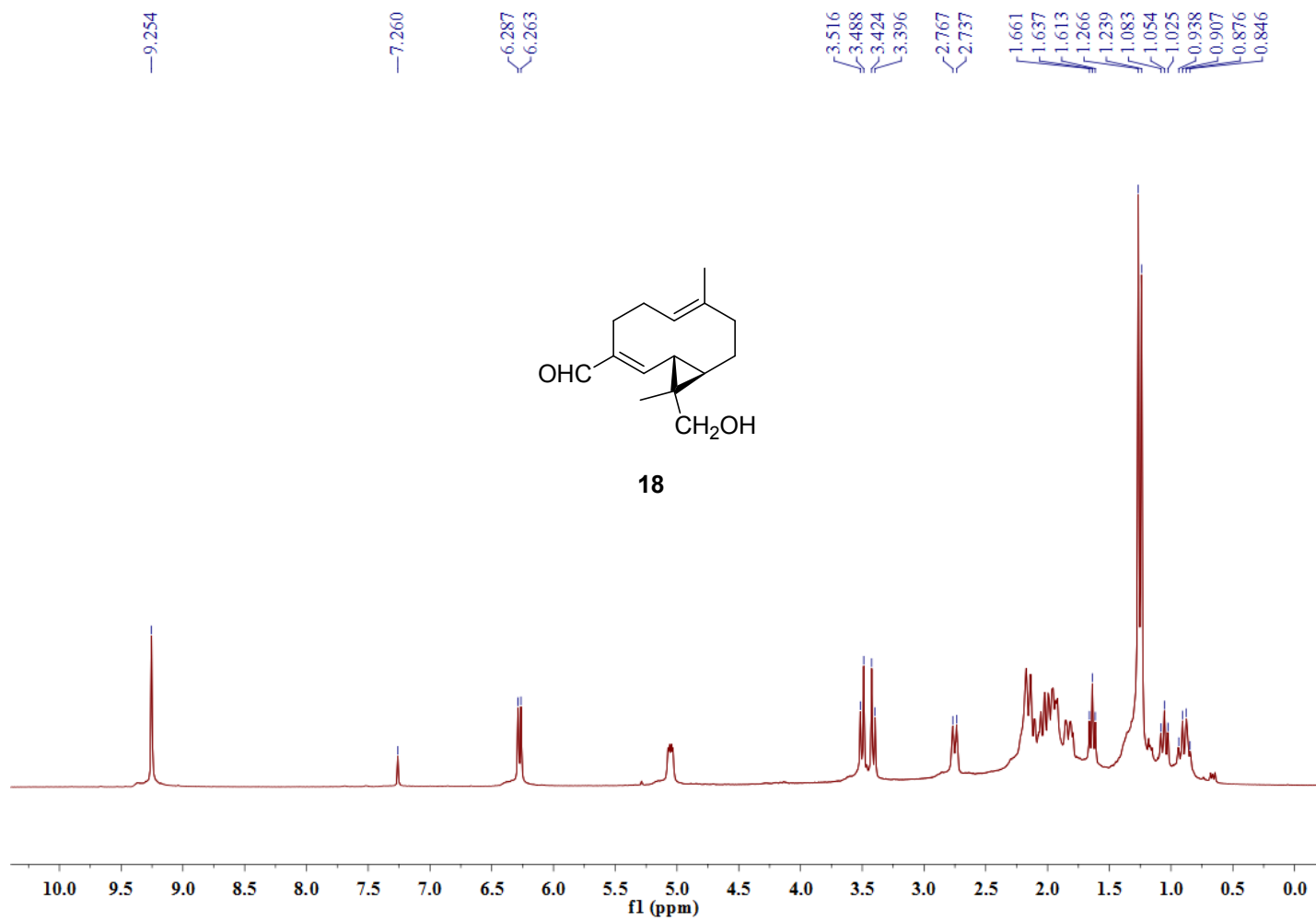
S51  $^1\text{H}$  NMR Spectrum of **16** in  $\text{CDCl}_3$



S52  $^1\text{H}$  NMR Spectrum of **17** in  $\text{CDCl}_3$

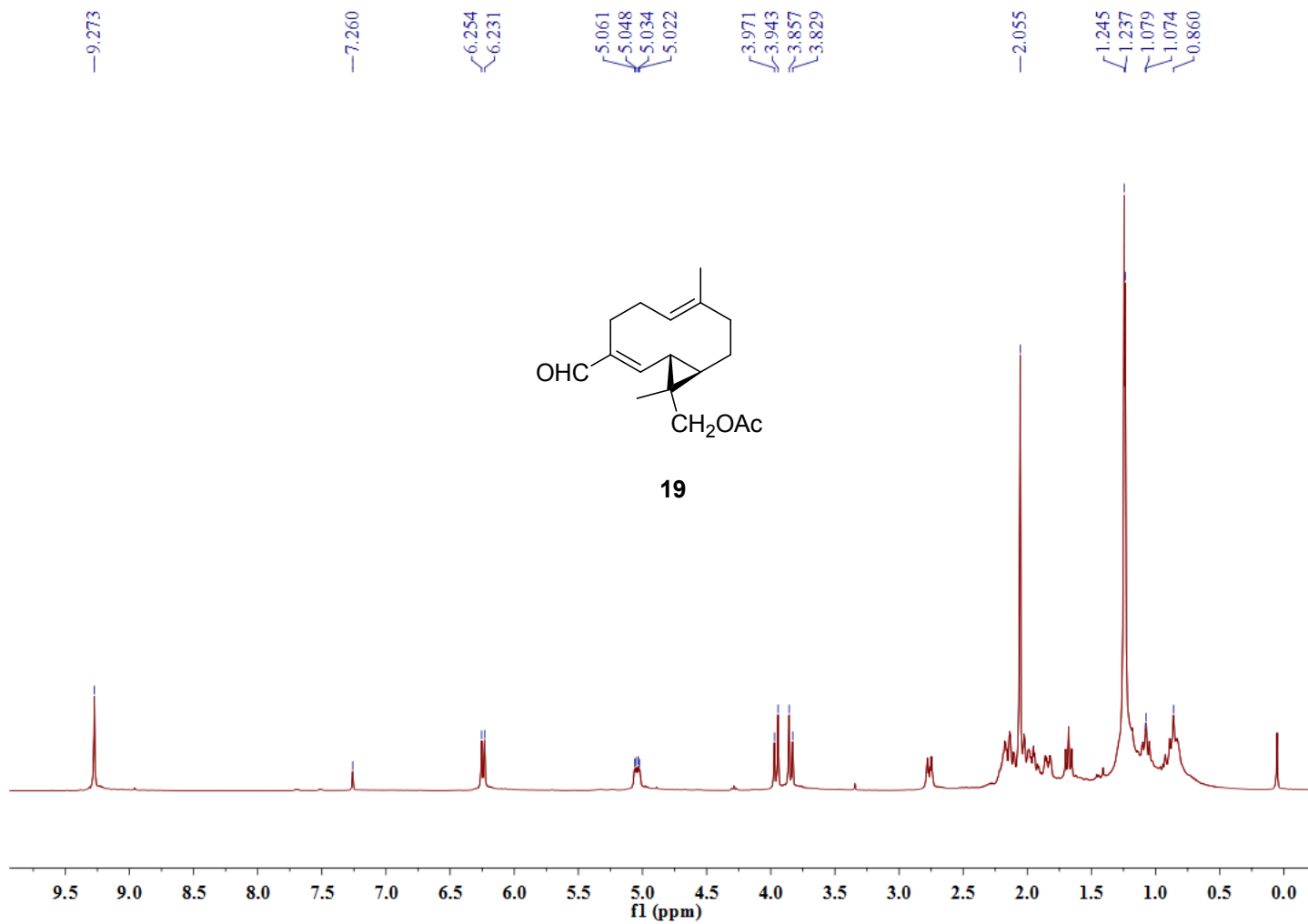


S53 <sup>1</sup>H NMR Spectrum of **18** in CDCl<sub>3</sub>

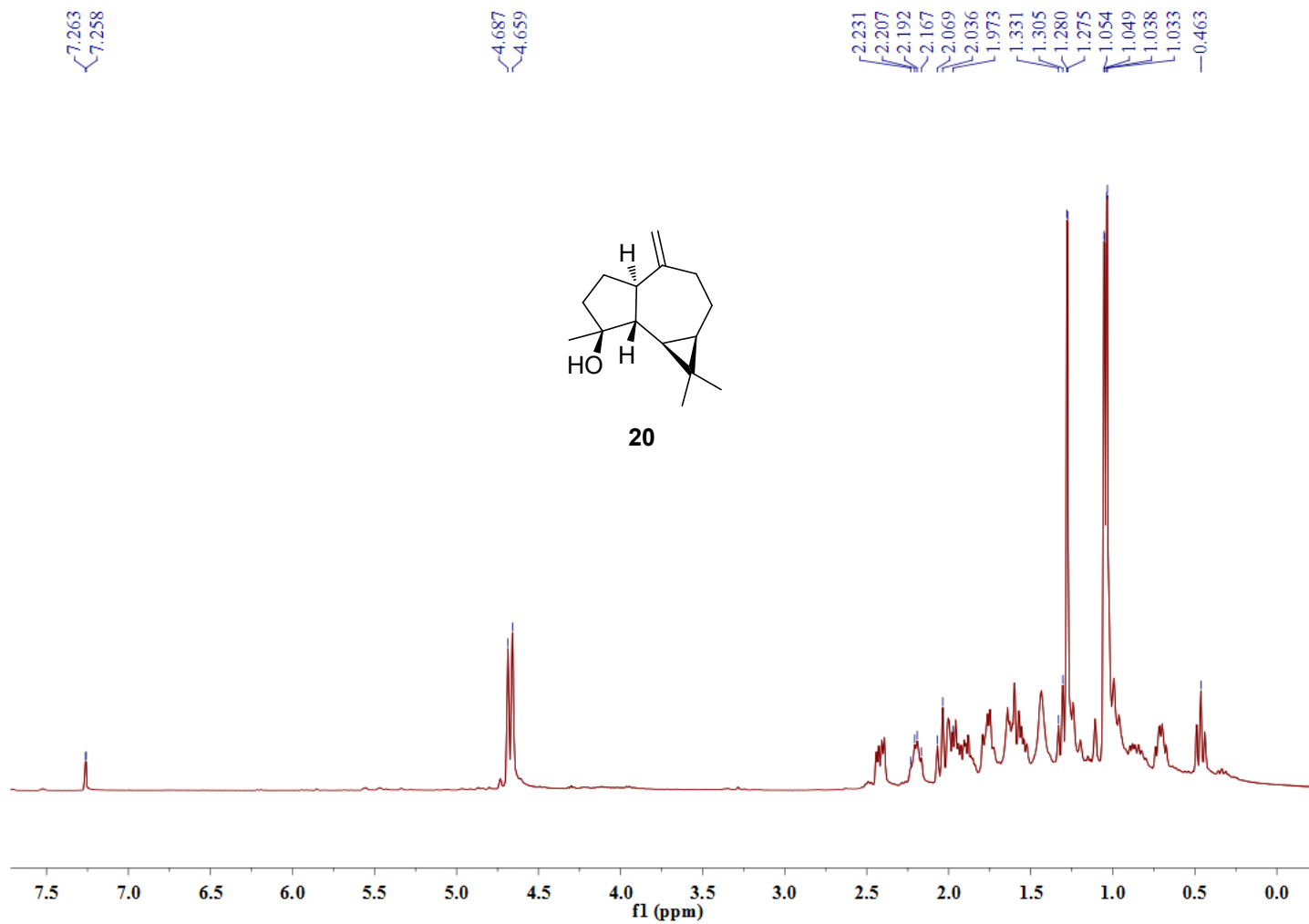




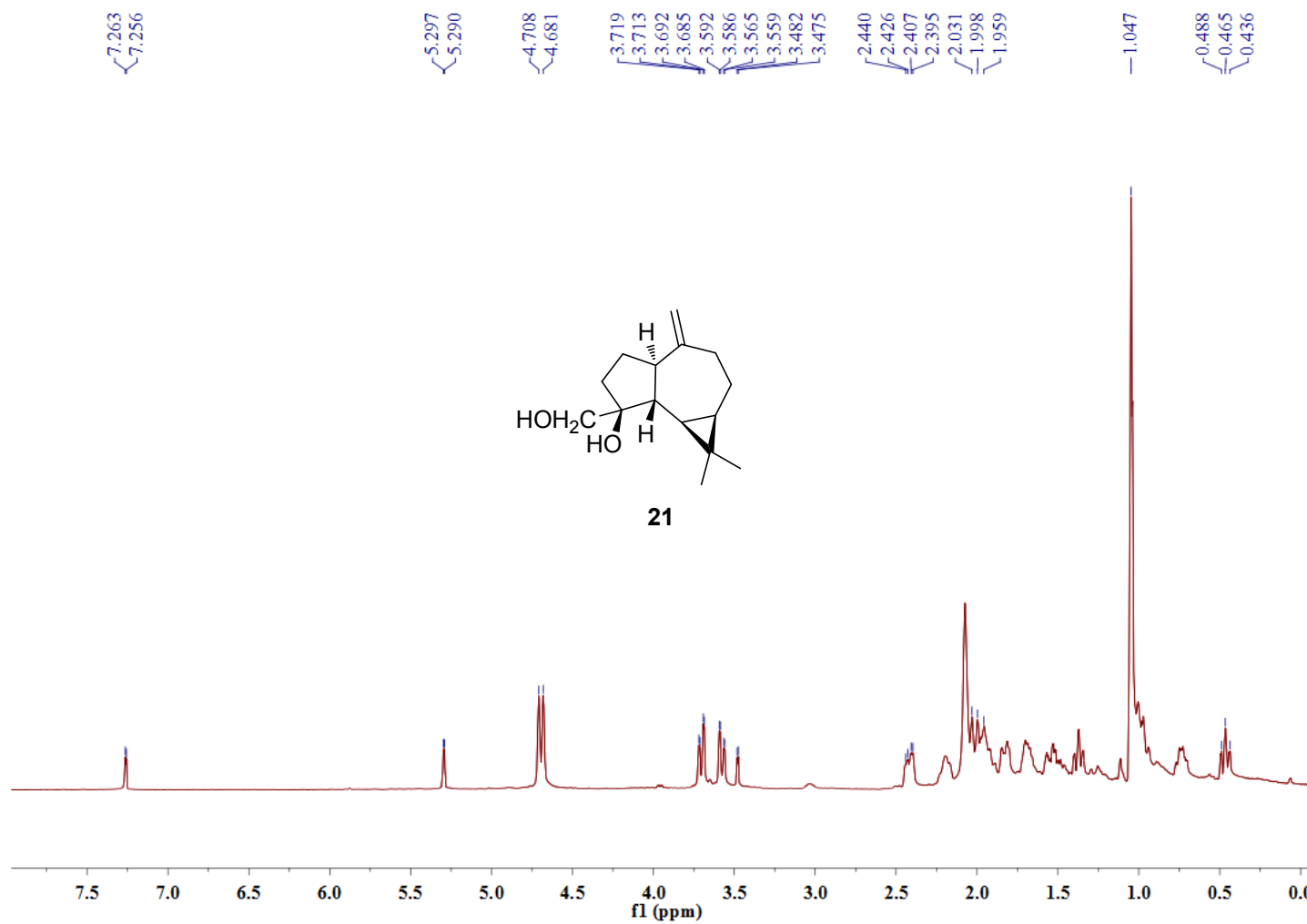
S54  $^1\text{H}$  NMR Spectrum of **19** in  $\text{CDCl}_3$



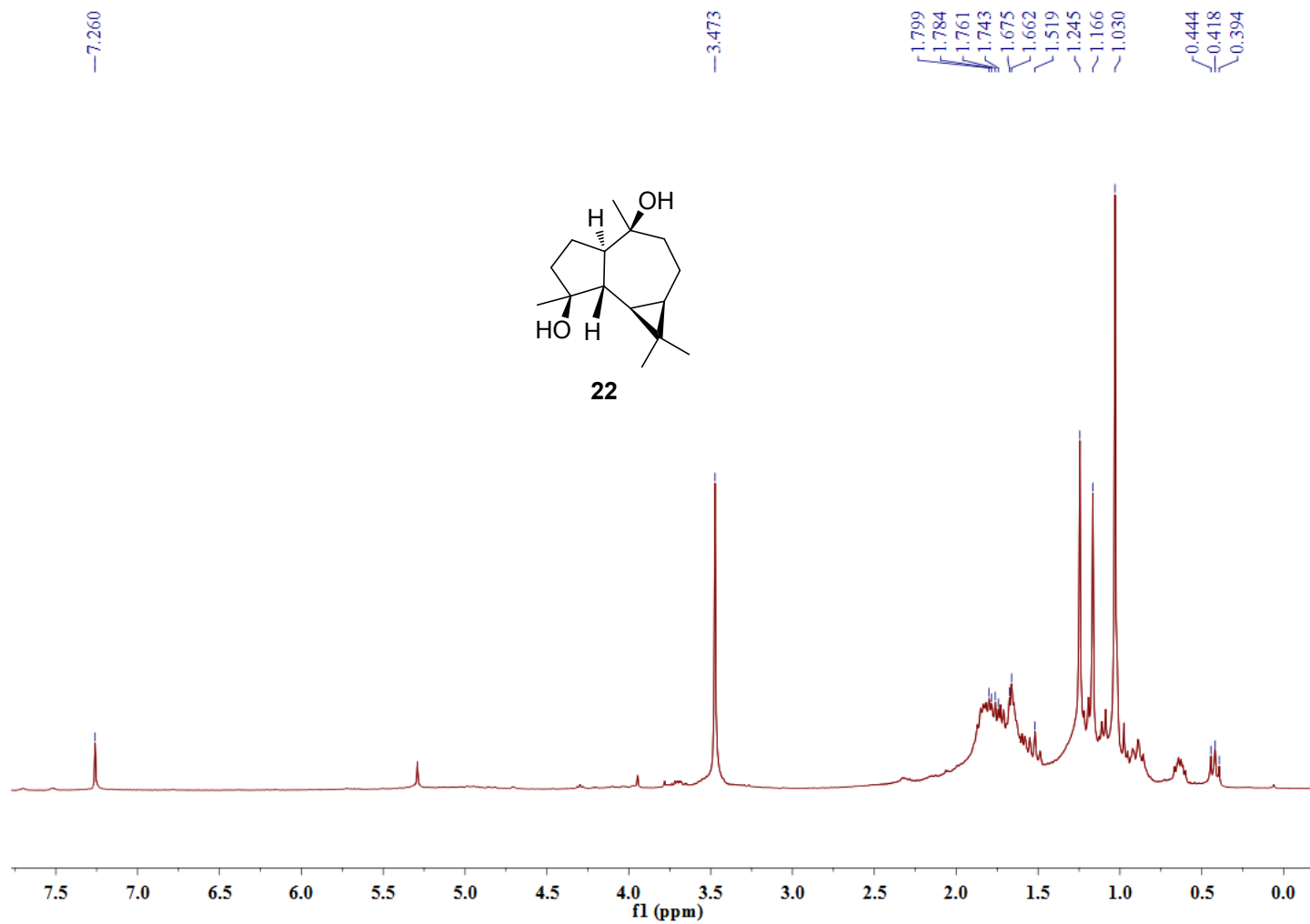
S55  $^1\text{H}$  NMR Spectrum of **20** in  $\text{CDCl}_3$



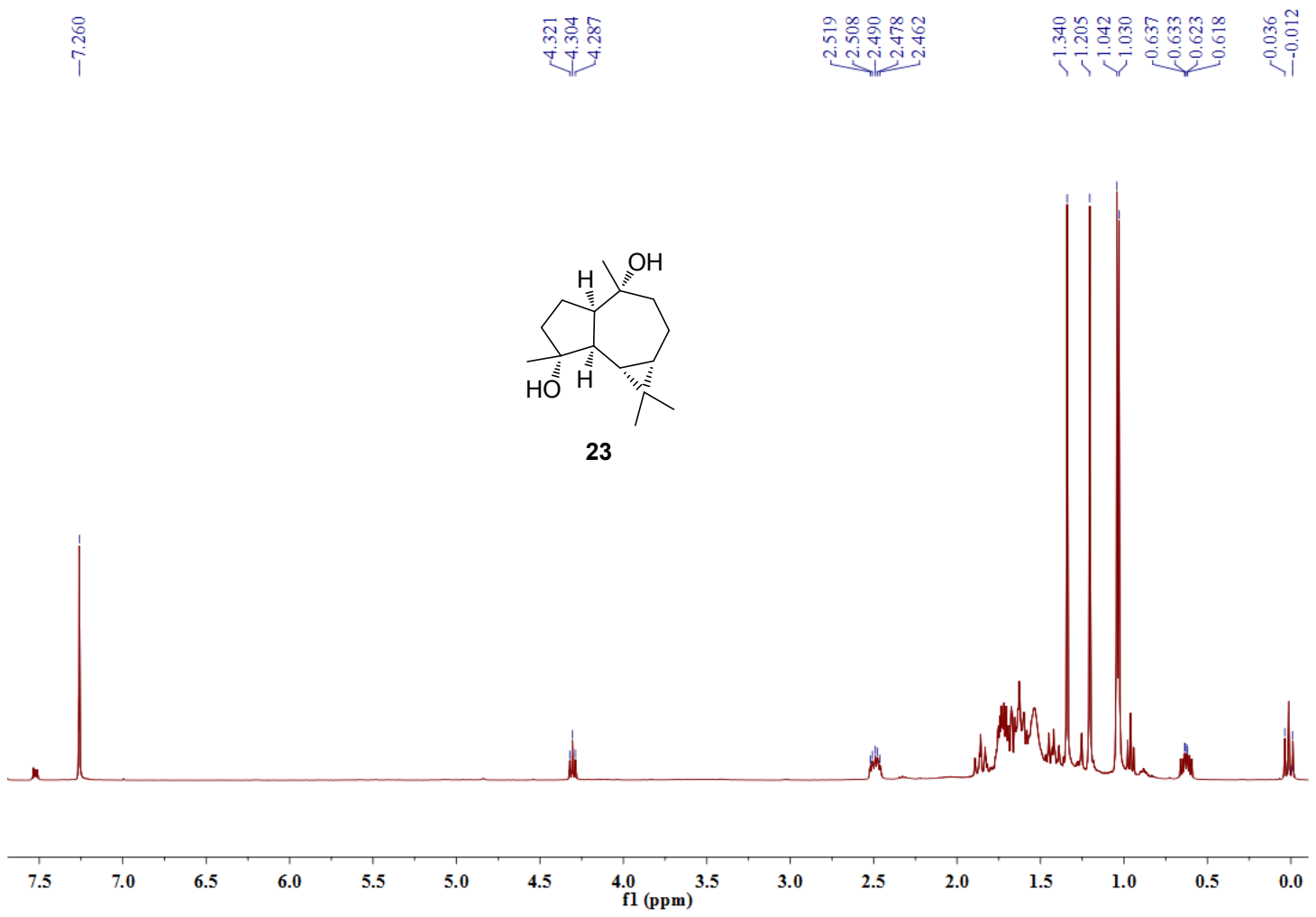
S56 <sup>1</sup>H NMR Spectrum of **21** in CDCl<sub>3</sub>



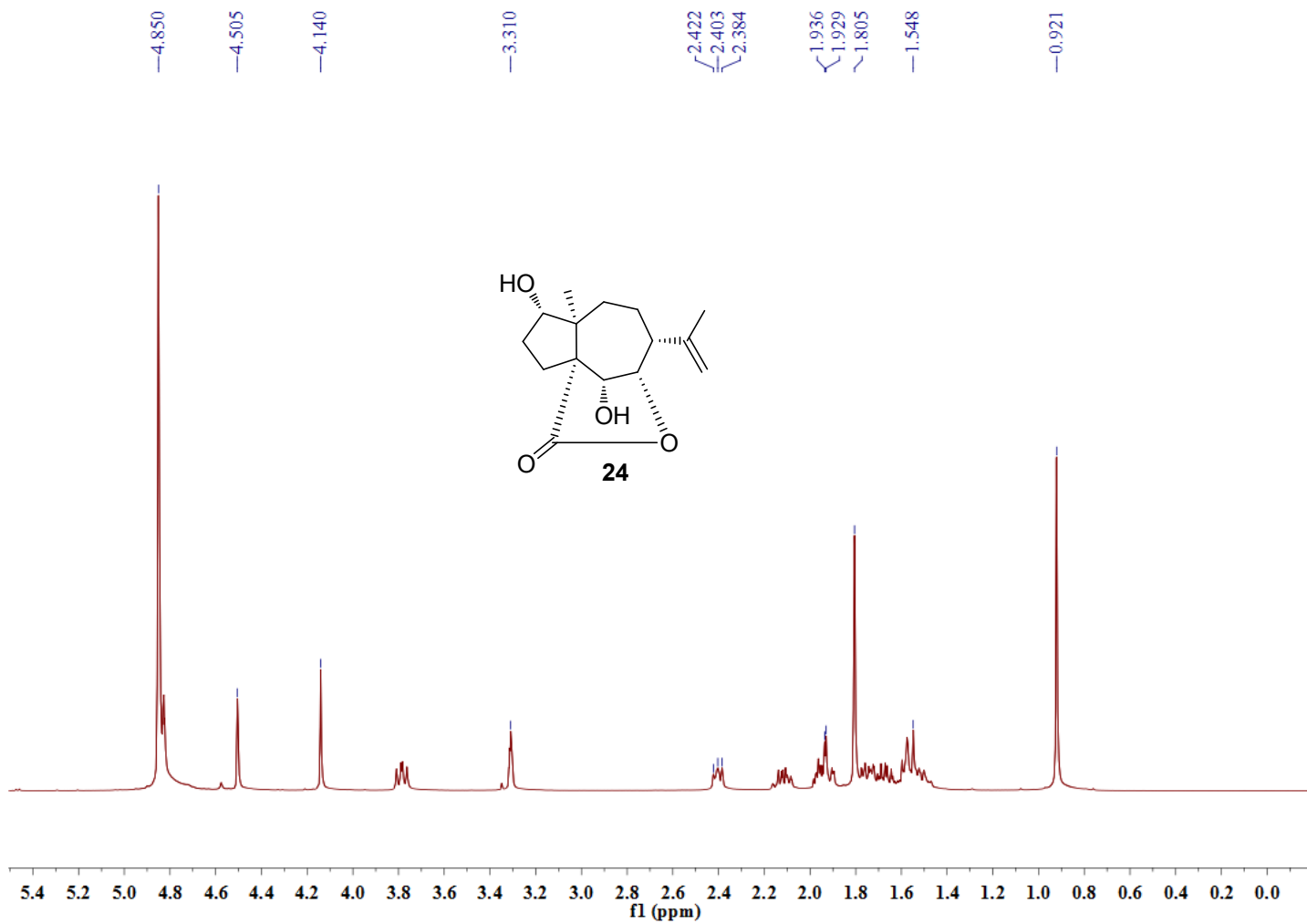
S57 <sup>1</sup>H NMR Spectrum of **22** in CDCl<sub>3</sub>



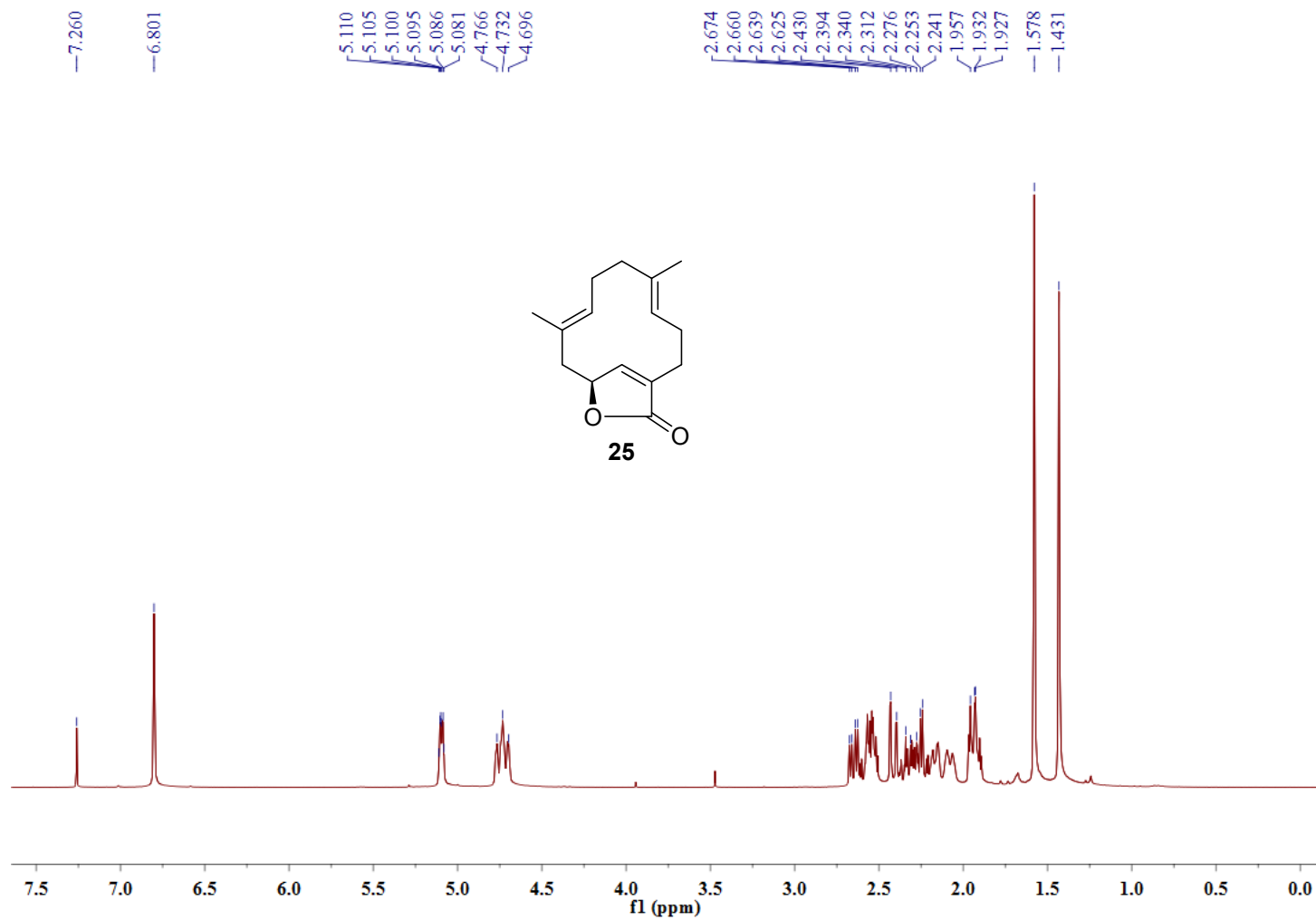
S58  $^1\text{H}$  NMR Spectrum of **23** in  $\text{CDCl}_3$



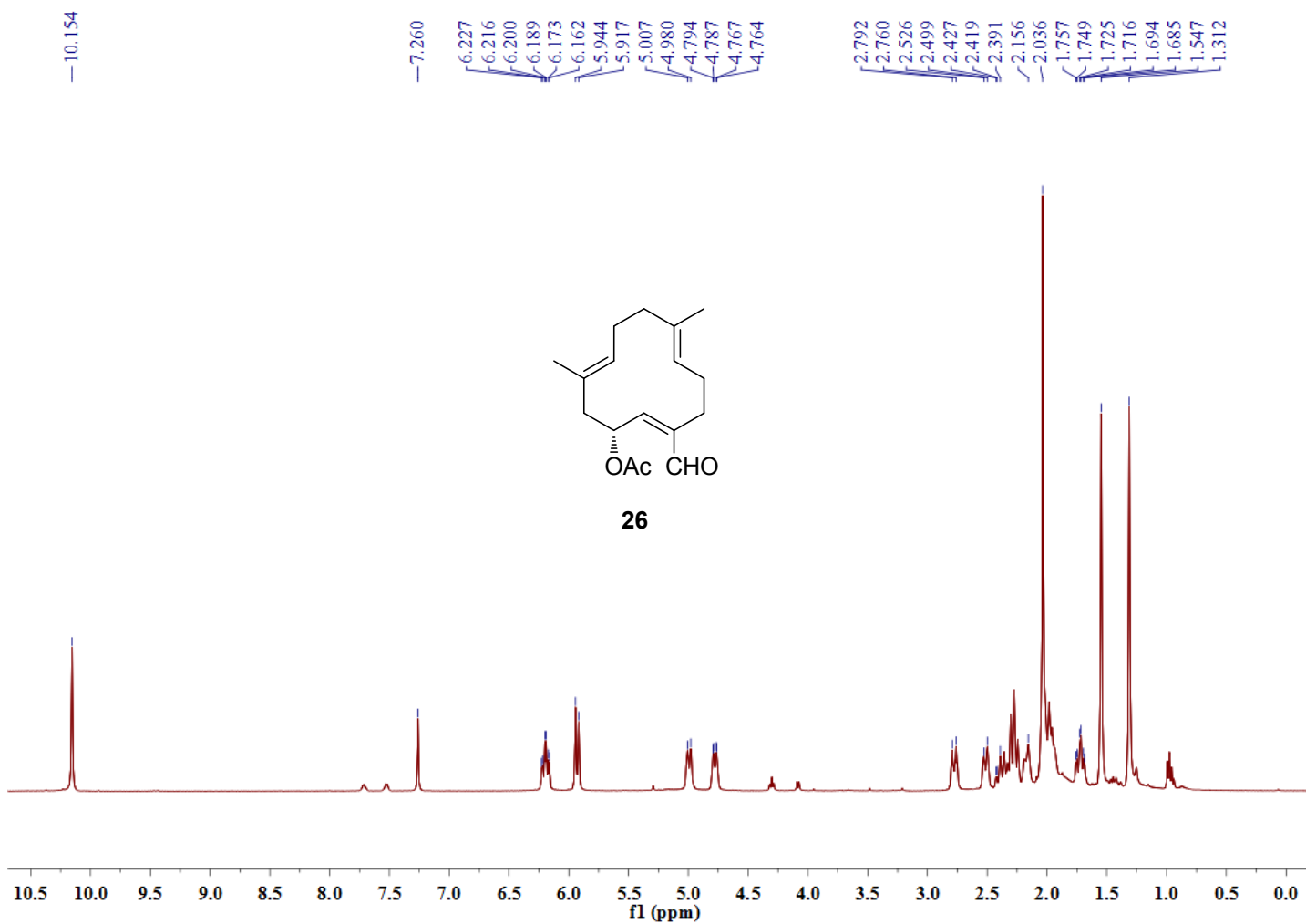
S59  $^1\text{H}$  NMR Spectrum of **24** in  $\text{CDCl}_3$



S60  $^1\text{H}$  NMR Spectrum of **25** in  $\text{CDCl}_3$

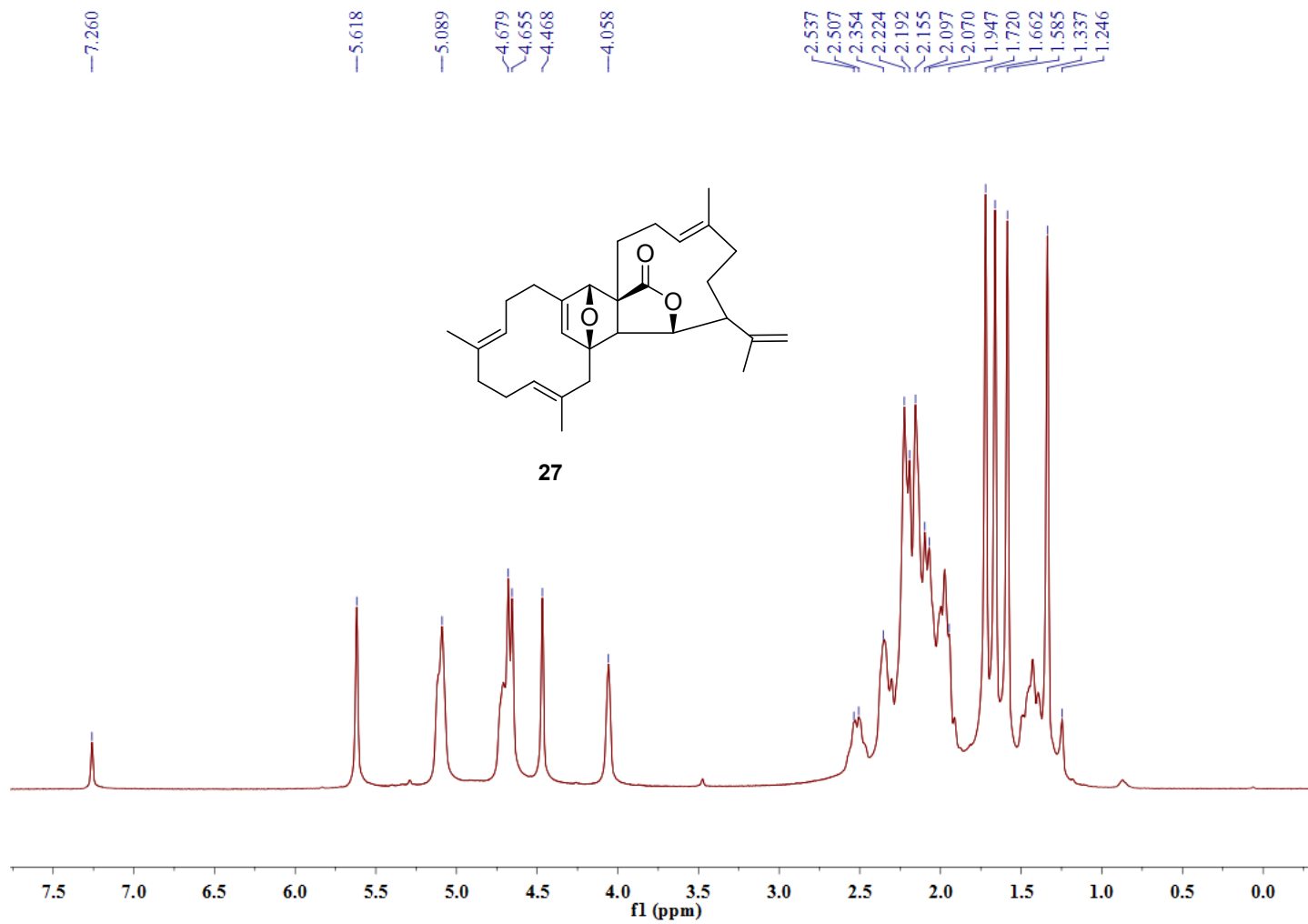


S61 <sup>1</sup>H NMR Spectrum of **26** in CDCl<sub>3</sub>

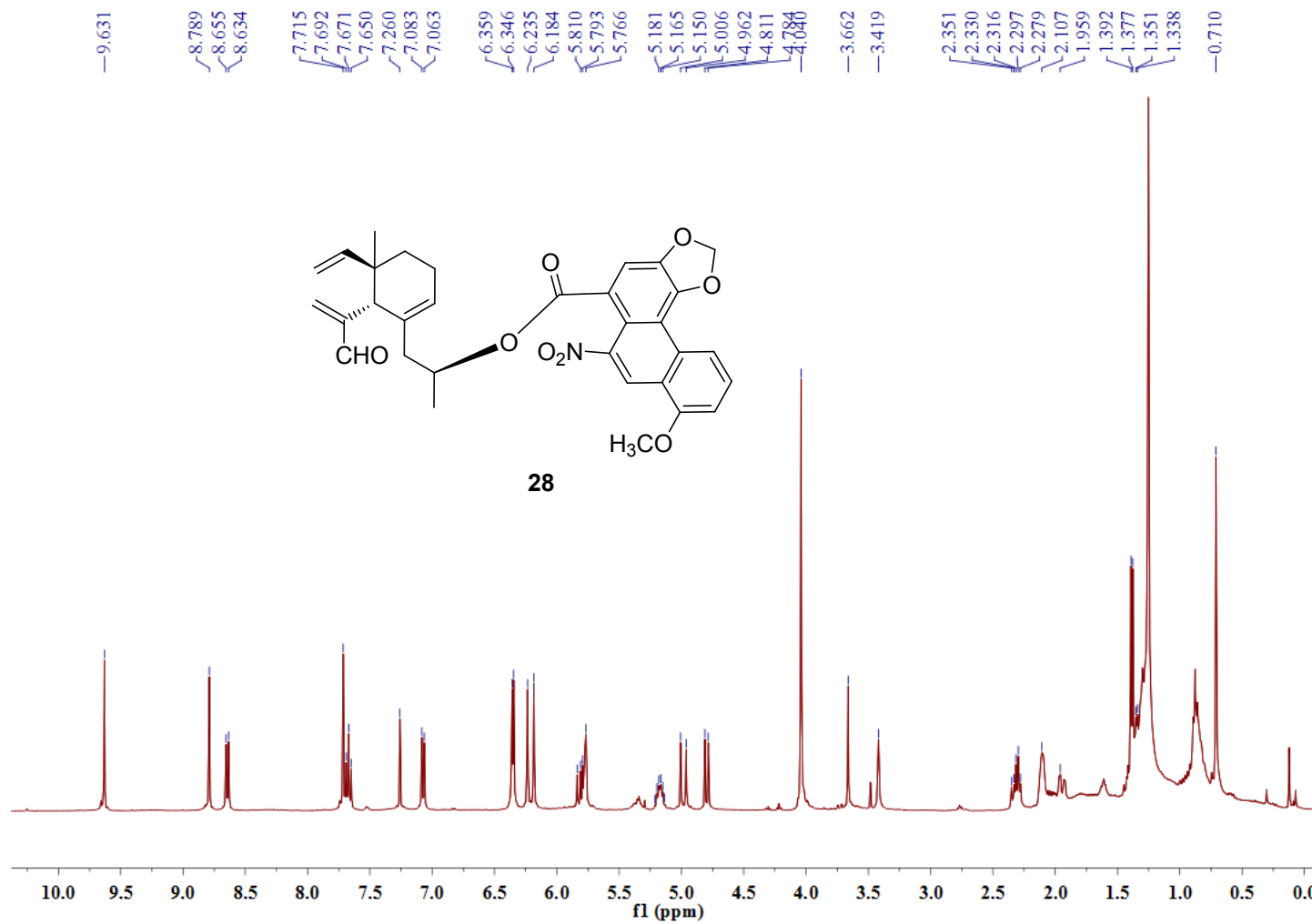




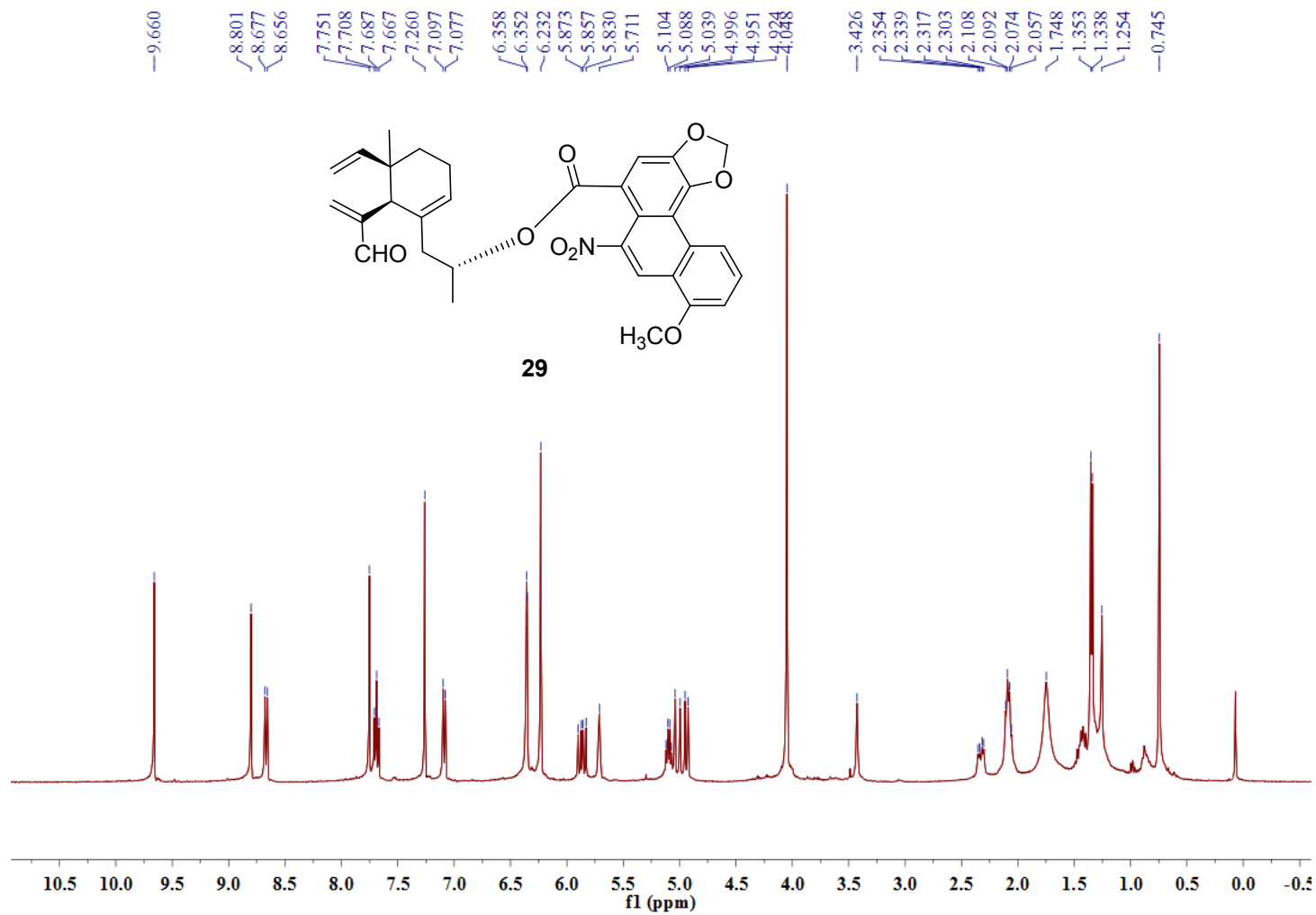
S62  $^1\text{H}$  NMR Spectrum of **27** in  $\text{CDCl}_3$



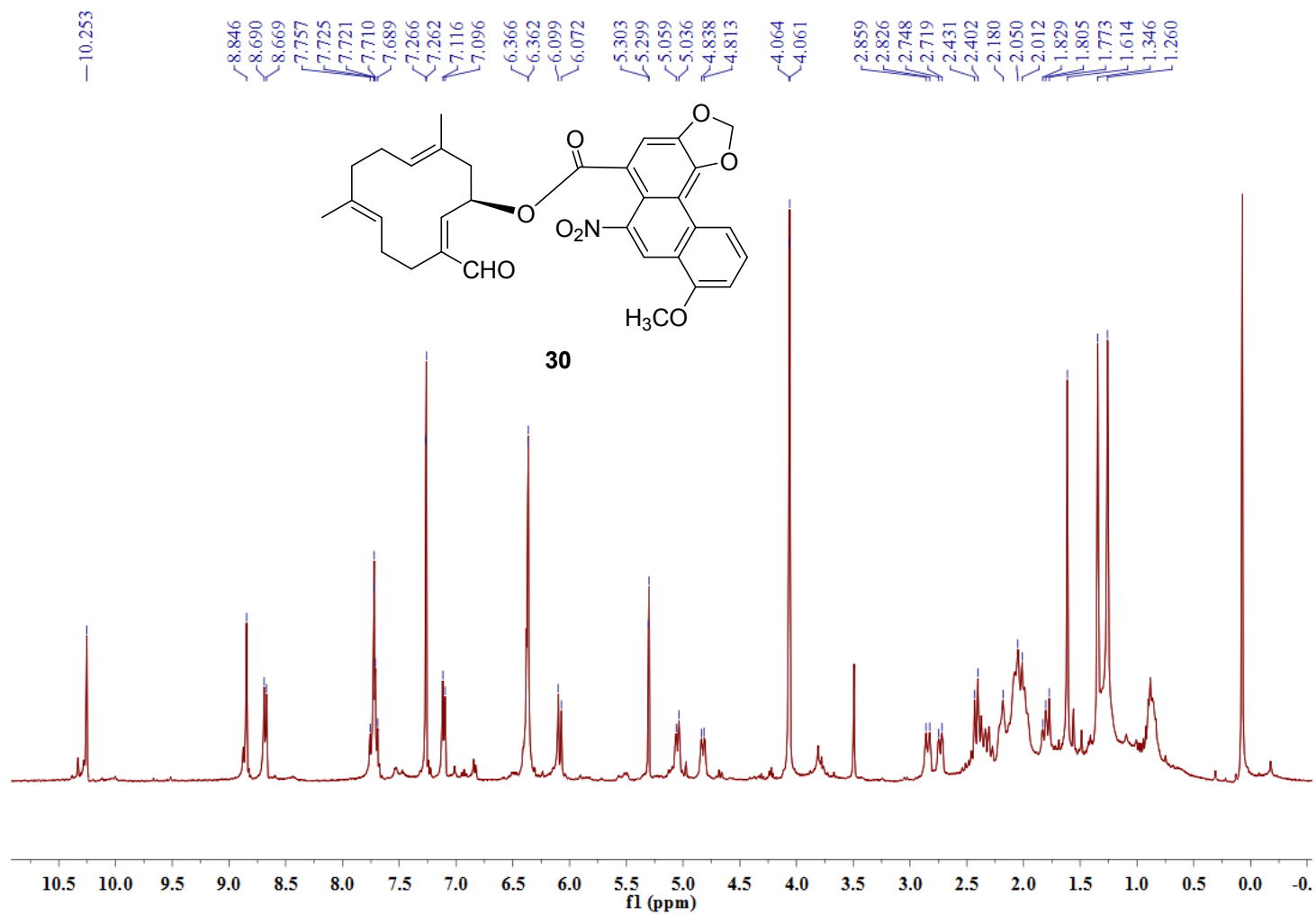
S63 <sup>1</sup>H NMR Spectrum of **28** in CDCl<sub>3</sub>



S64 <sup>1</sup>H NMR Spectrum of **29** in CDCl<sub>3</sub>

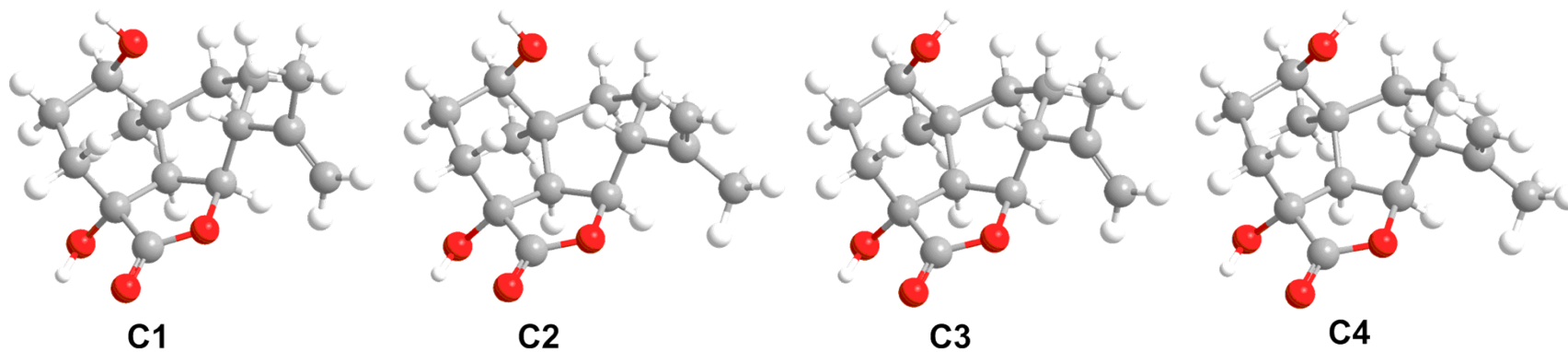


S65 <sup>1</sup>H NMR Spectrum of **30** in CDCl<sub>3</sub>



S66 Detail information for ECD calculation

***Lowest Energy Conformers:***



B3LYP/6-31+G(d) optimized lowest energy 3D conformers of **2**

***Energy Analysis Table:***

Conf.	MMFF energy		Gibbs free energy (298.15 K)		
	rel. E (Kcal/mol)	Boltzmann Distribution	G (Hartree)	$\Delta G$ (Kcal/mol)	Boltzmann Distribution
<b>C1</b>	0.00	0.520	-885.437704	0.957	0.123
<b>C2</b>	0.26	0.333	-885.439229	0.000	0.621
<b>C3</b>	1.10	0.082	-885.436645	1.621	0.040
<b>C4</b>	1.23	0.065	-885.438228	0.628	0.215

**Calculated ECD data:**

No	C1		No	C2		No	C3	
	Excitation energies(eV)	Rotatory Strengths*		Excitation energies(eV)	Rotatory Strengths*		Excitation energies(eV)	Rotatory Strengths*
1	5.5588	3.2774	1	5.5651	0.6142	1	5.5629	1.0376
2	5.6236	-1.7083	2	5.65	3.6988	2	5.6015	-0.5449
3	5.9161	-7.279	3	5.9183	5.737	3	6.0152	9.1321
4	5.9324	12.2887	4	5.9673	-3.4269	4	6.0411	-7.3952
5	6.0889	3.6186	5	6.1444	-4.5373	5	6.1319	-8.0981
	C4							
1	5.5682	0.5574	1					
2	5.6565	4.7385	2					
3	6.0326	-1.1433	3					
4	6.0591	1.2629	4					
5	6.1595	-12.3534	5					

\* R(velocity)  $10^{** -40}$  erg-esu-cm

**Ref. 32.** Gaussian 09, Rev. C. 01. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.