

Supplementary Materials

Cytotoxic Furanoditerpenes from the Sponge *Spongia tubulifera* Collected in the Mexican Caribbean

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Table S1. NMR data of **1** in CDCl₃ (125 MHz for ¹³C and 500 MHz for ¹H).

no.	δ_C type	δ_H , mult. (<i>J</i> in Hz)	COSY	HMBC	NOESY
1	53.3, CH	2.67, d (12.1)- 2.13, d (12.1)		2, 3, 5, 10, 20	3, 9, 11, 20
2	211.1, C				
3	83.1, CH	3.90, d (1.5)	OH	2, 4, 18, 19	1, 5, 18
4	45.7, C				
5	55.0, C	1.62, m	6	1, 18, 19	3
6	18.6, CH ₂	1.66, m-1.80, m	5, 7		18
7	40.7, CH ₂	1.68, m-2.20, m	6		17
8	34.7, C				
9	56.1, CH	1.50, m	11		1
10	43.8, C				
11	18.9, CH ₂	1.67, m	9, 12		1
12	20.7, CH ₂	2.49, m-2.82, m	11	13	
13	119.4, C				
14	136.8, C				
15	135.3, CH	7.12, s		13, 16	
16	137.1, CH	7.07, s		13, 14	
17	26.0, CH ₃	1.23, s		7, 8, 14	7, 20
18	29.4, CH ₃	1.21, s		3, 4, 5, 19	6, 19
19	16.5, CH ₃	0.73, s		3, 4, 5, 18	18
20	17.3, CH ₃	0.88, s		1, 9, 10	1, 17
OH		3.48, d (1.5)	3		

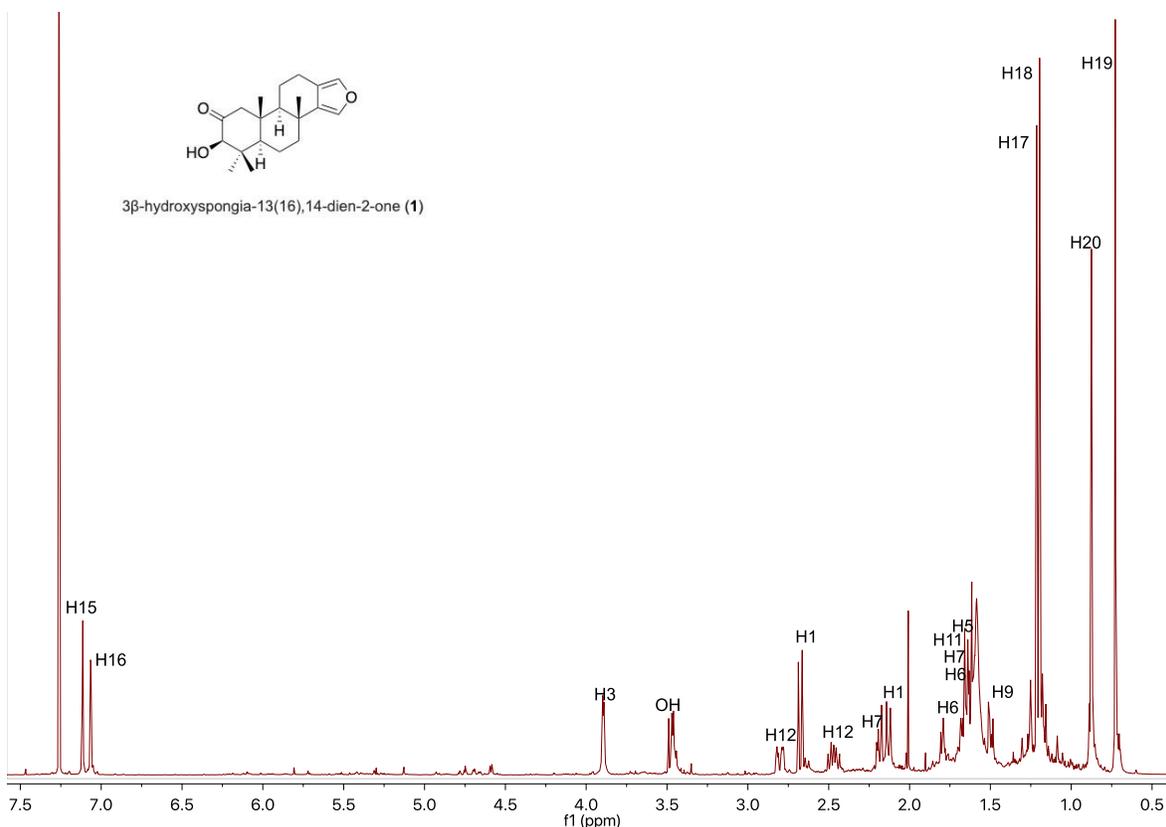


Figure S1. ^1H NMR spectrum of **1** (500 MHz, CDCl_3).

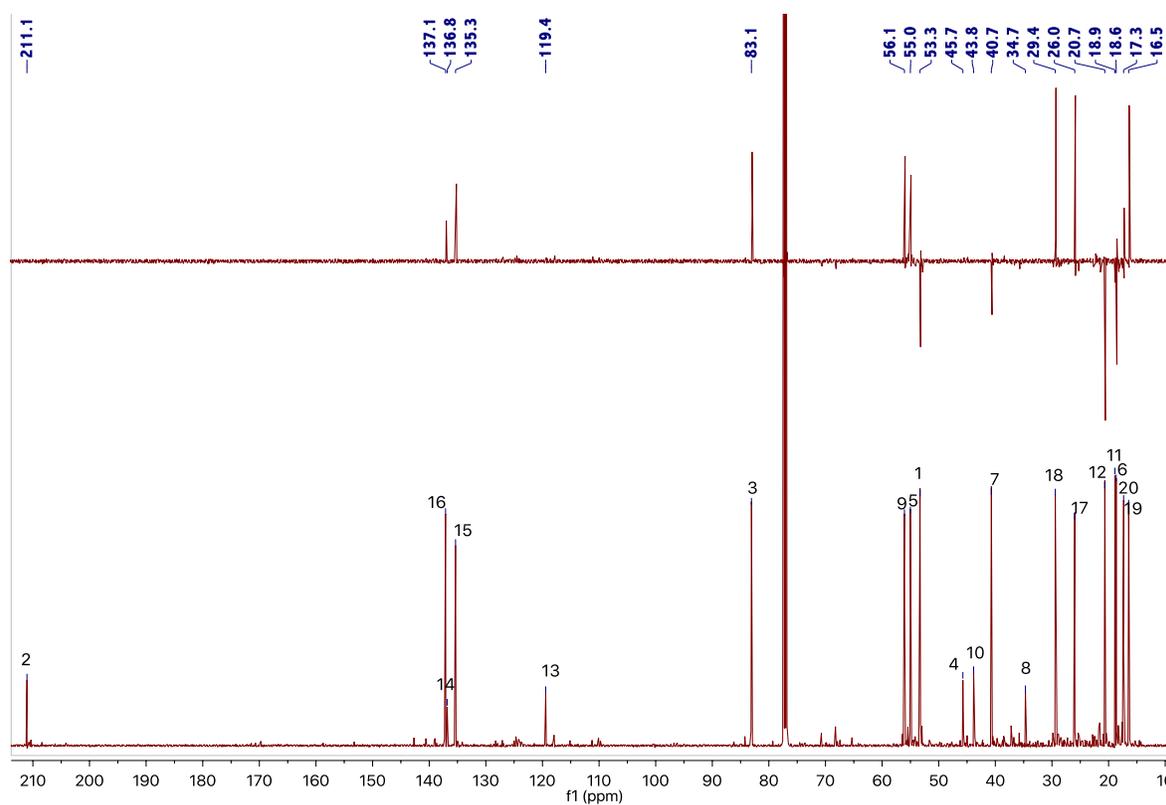


Figure S2. ^{13}C NMR and DEPT-135 spectrum of **1** (125 MHz, CDCl_3).

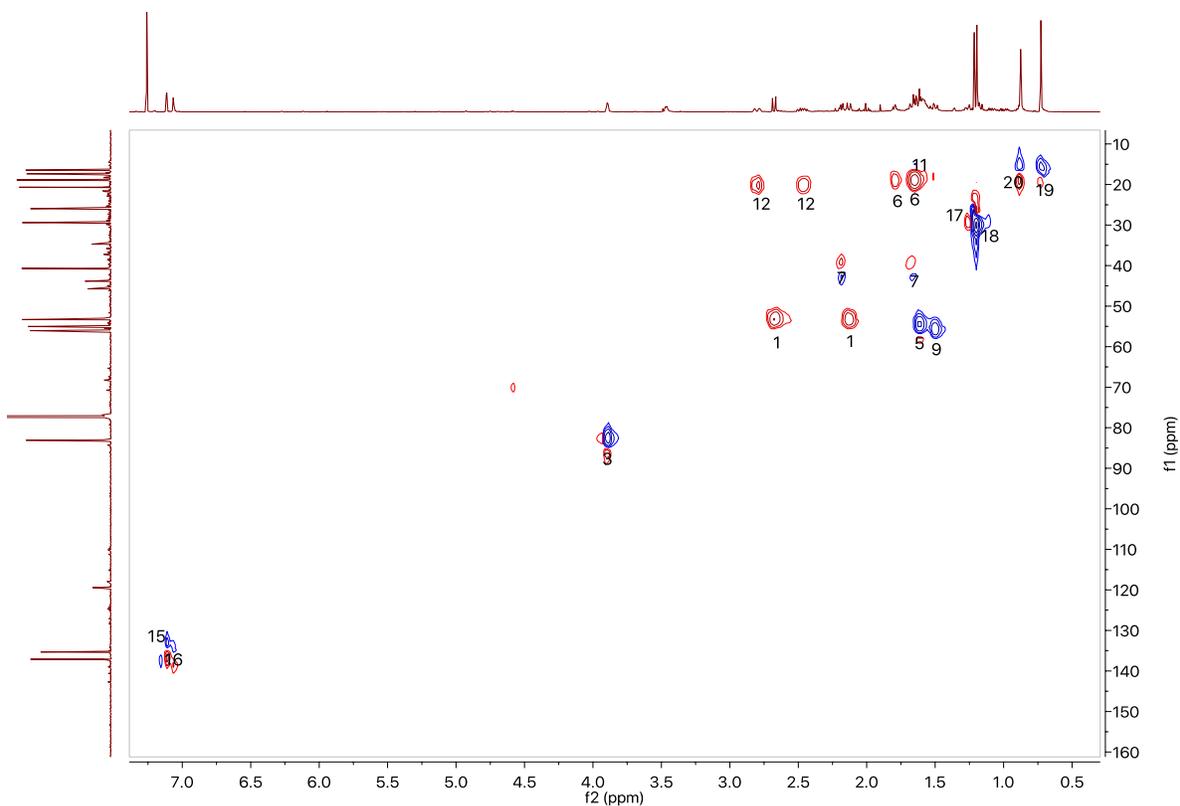


Figure S3. HSQC spectrum of **1** (500 MHz, CDCl_3). CH_2 : blue cross-peaks and CH or CH_3 : red cross-peaks.

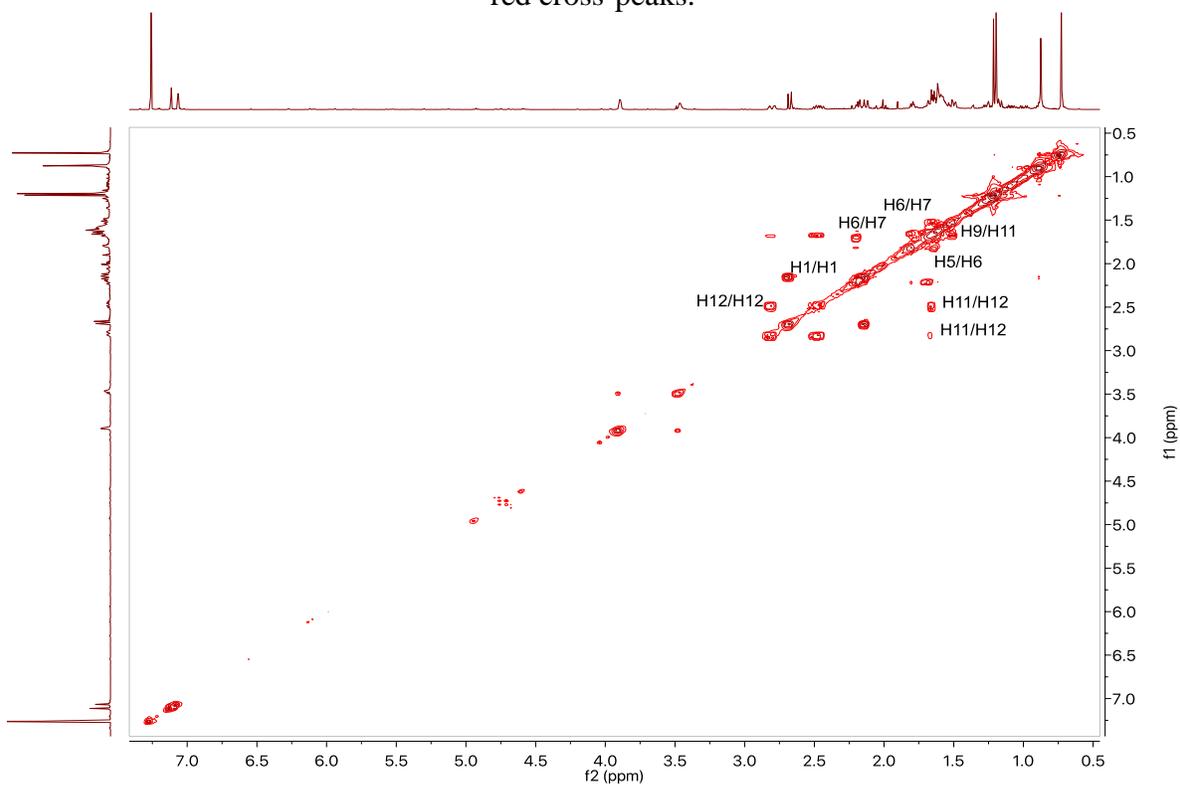


Figure S4. COSY spectrum of **1** (500 MHz, CDCl_3).

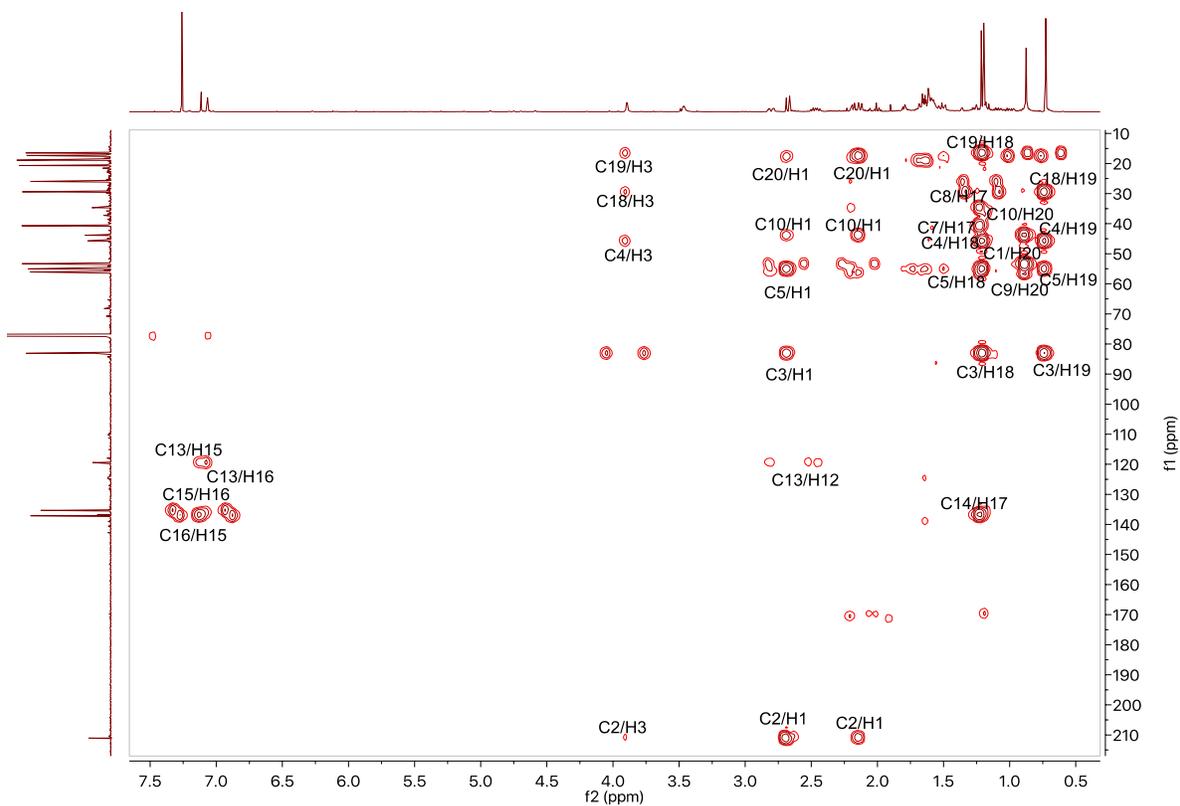


Figure S5. HMBC spectrum of **1** (500 MHz, CDCl₃).

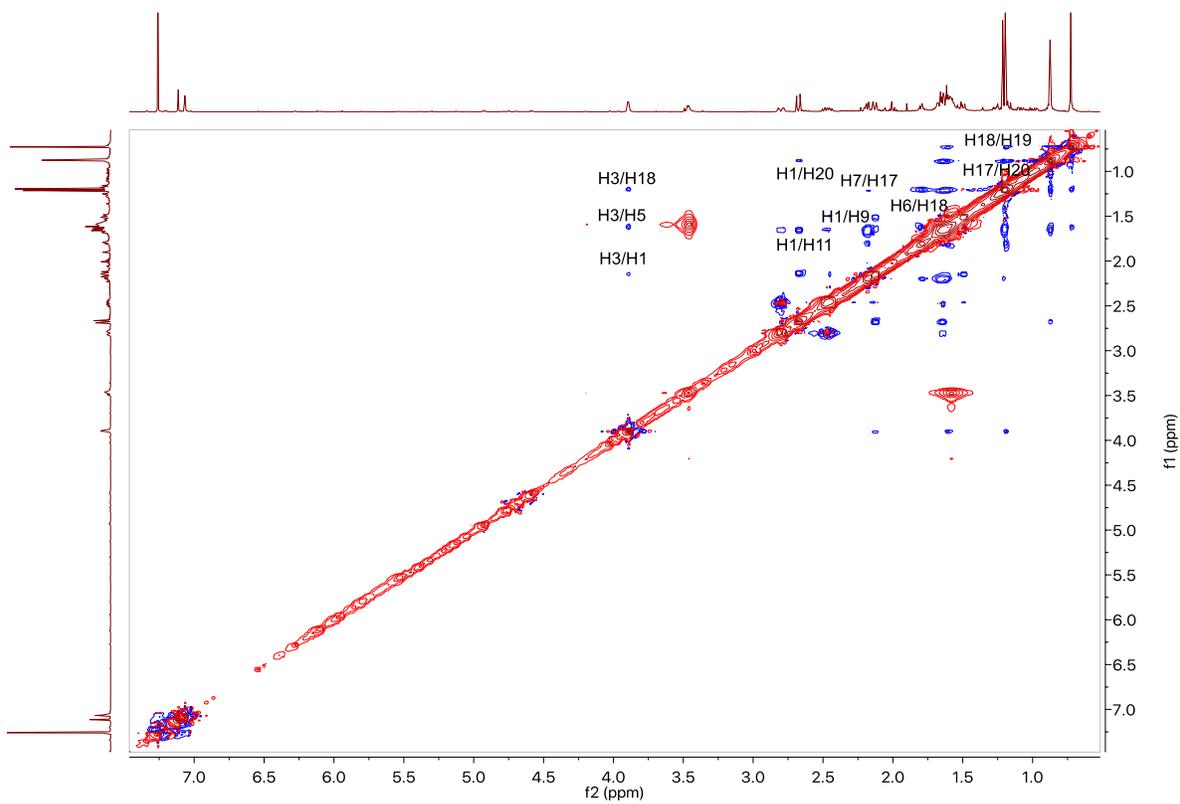


Figure S6. NOESY spectrum of **1** (500 MHz, CDCl₃).

2019_12961_jisthc7h3_el_hr_01-av0 #1 RT: 2.69 AV: 1 NL: 6.84E5
T: [297.22-326.29]

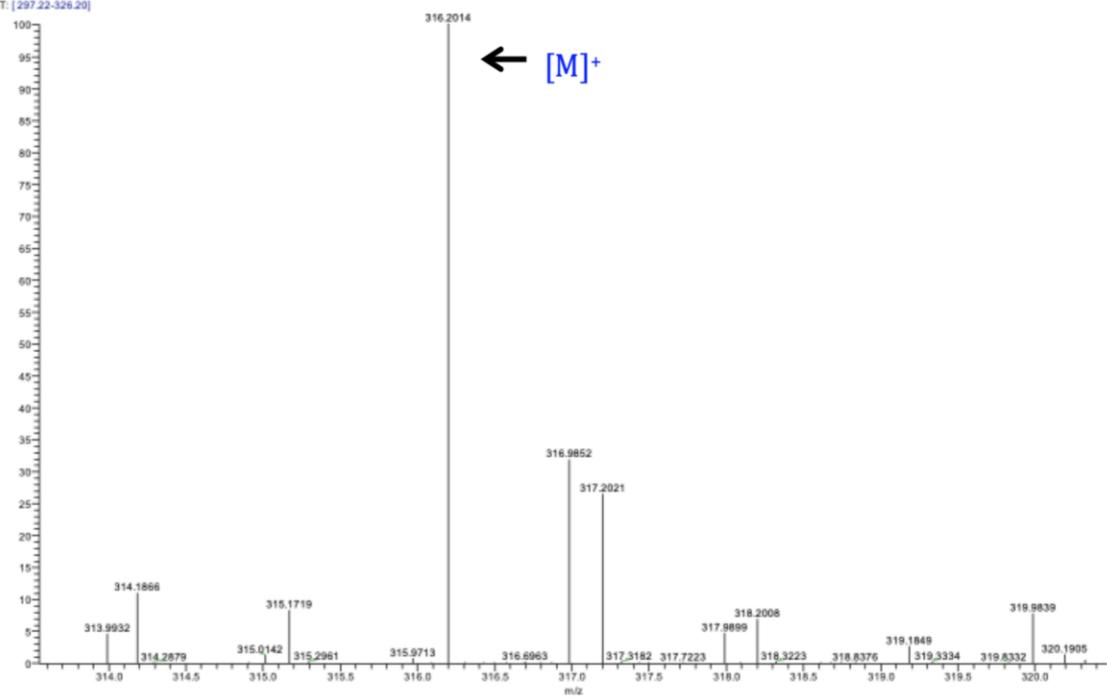


Figure S7. HREIMS of 1.

Table S2. NMR data of **2** in CDCl₃ (125 MHz for ¹³C and 500 MHz for ¹H).

no.	δ _C type	δ _H , mult. (<i>J</i> in Hz)	COSY	HMBC	NOESY
1	128.3, CH	6.54, s		2, 3, 5, 9	9, 11, 20
2	144.3, C				
3	201.2, C				
4	44.3, C				
5	54.5, C	1.80, m	6		
6	19.1, CH ₂	1.67, m	5, 7		
7	40.4, CH ₂	1.66, m-2.18, m	6		15
8	34.9, C				
9	51.7, CH	1.48, dd (11.8, 1.7)	11	5, 9	1
10	38.8, C				
11	18.8, CH ₂	1.91, dt (7.0, 1.7)	9, 12	13	1
12	20.7, CH ₂	2.51, dddd(16.2, 12.2, 7.0, 1.7) 2.83, ddt (16.2, 6.3, 1.5)	11	9, 13	16
13	119.5, C				
14	137.3, C				
15	135.0, CH	7.09, s		13, 16	7, 17
16	137.2, CH	7.06, s		13, 15	12
17	26.7, CH ₃	1.28, s		7, 8, 9, 14	15
18	20.6, CH ₃	1.16, s		3, 4, 5, 19	
19	27.3, CH ₃	1.23, s		3, 4, 5, 18	
20	21.7, CH ₃	1.22, s		1, 9, 10	1
OH		5.93, s		1, 2	

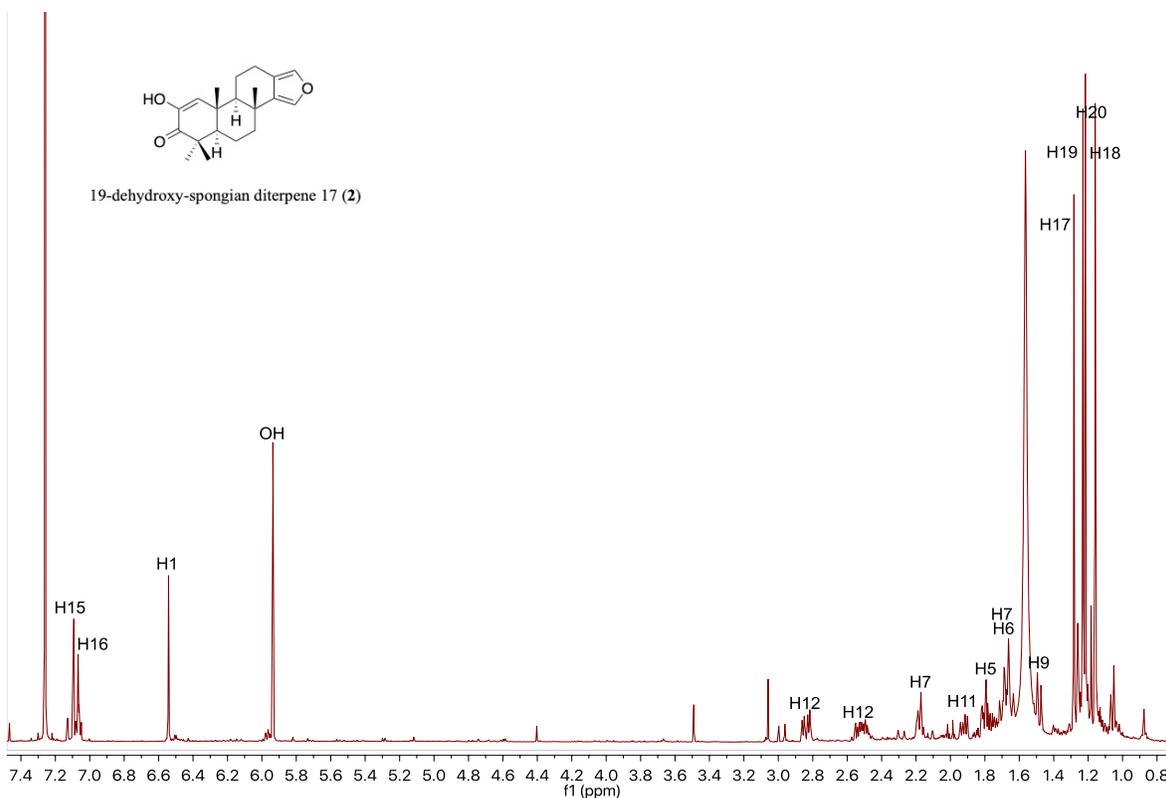


Figure S8. ^1H NMR spectrum of **2** (500 MHz, CDCl_3).

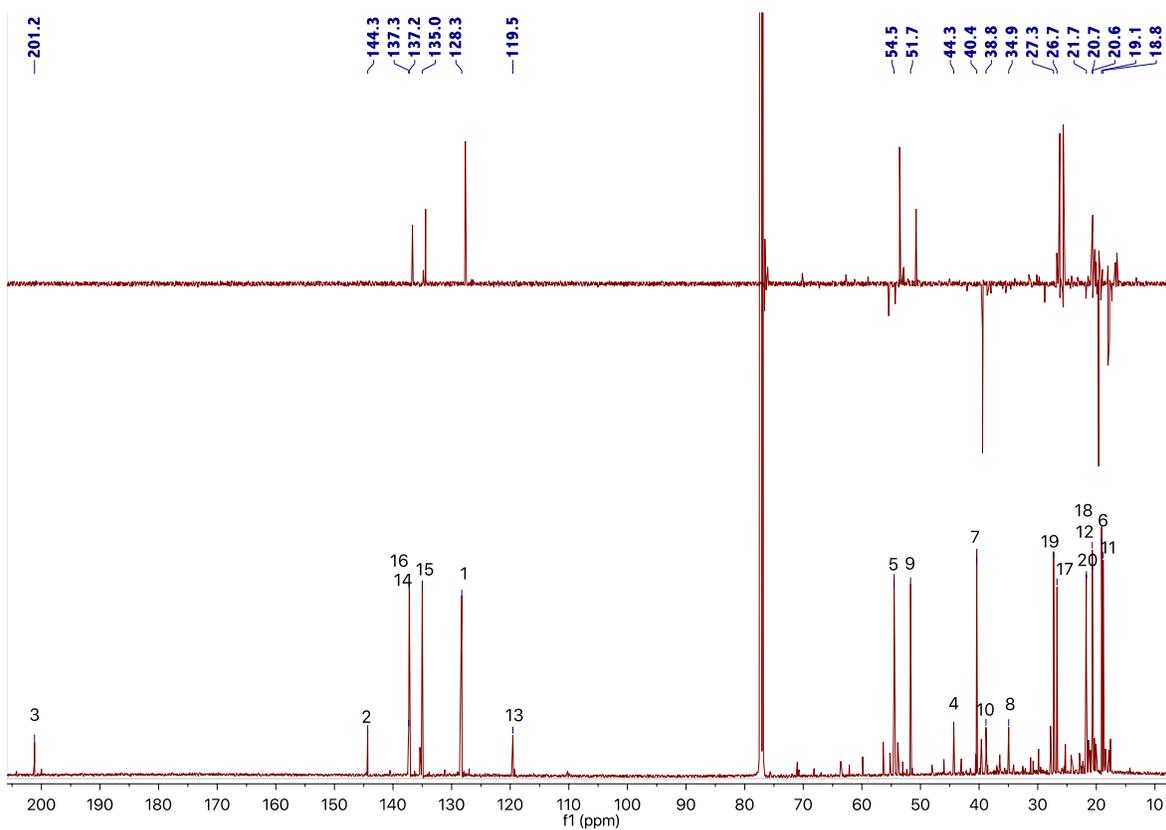


Figure S9. ^{13}C NMR and DEPT-135 spectrum of **2** (125 MHz, CDCl_3).

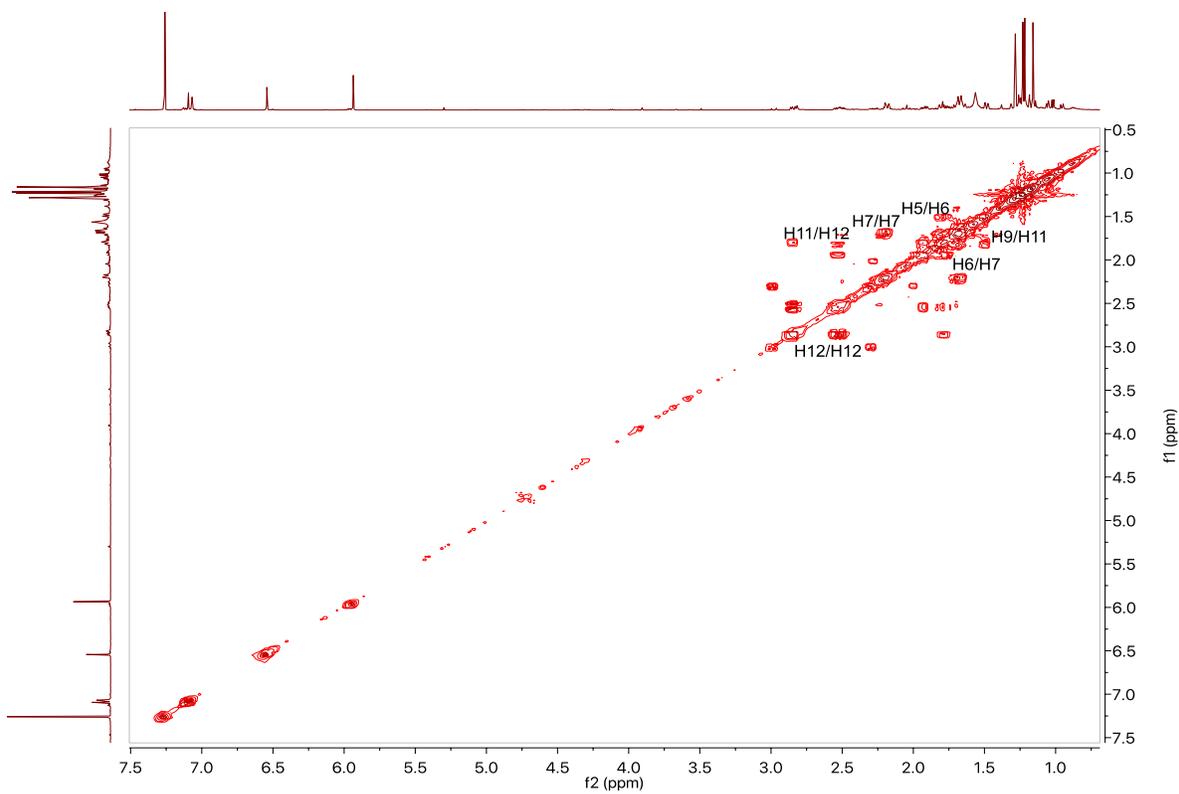


Figure S10. COSY spectrum of **2** (500 MHz, CDCl₃).

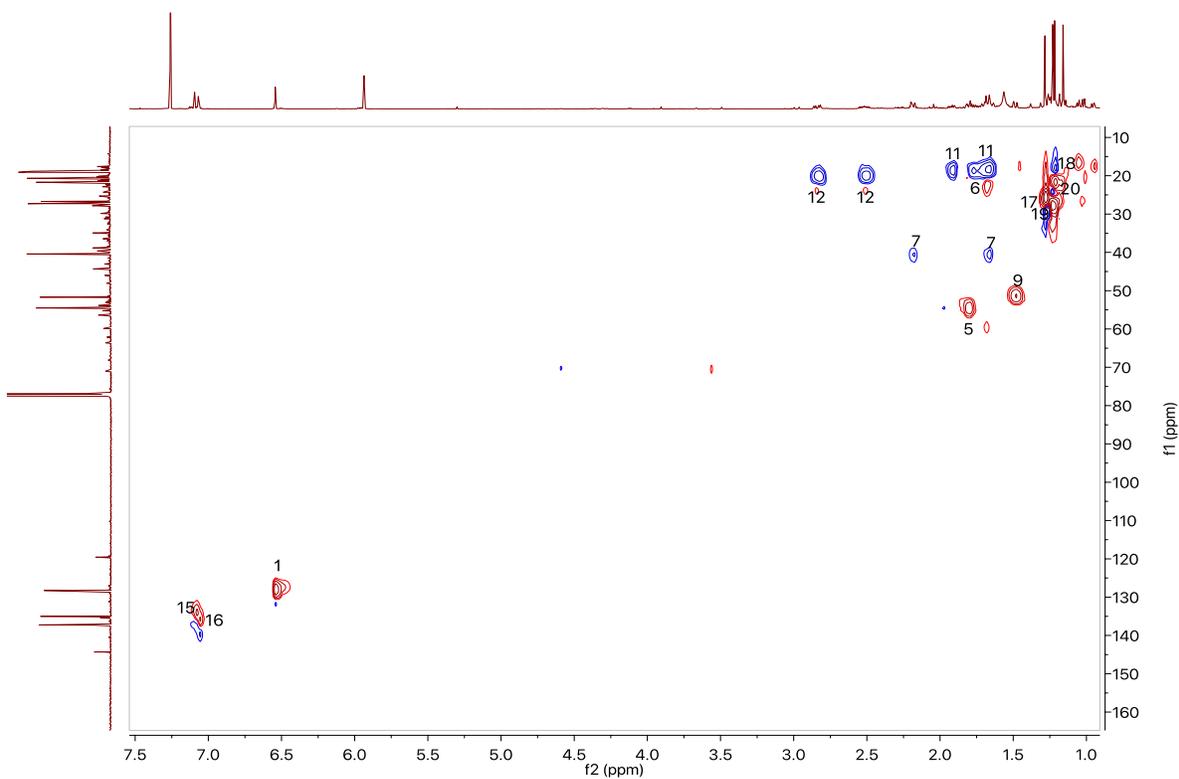


Figure S11. HSQC spectrum of **2** (500 MHz, CDCl₃). CH₂: blue cross-peaks and CH or CH₃: red cross-peaks.

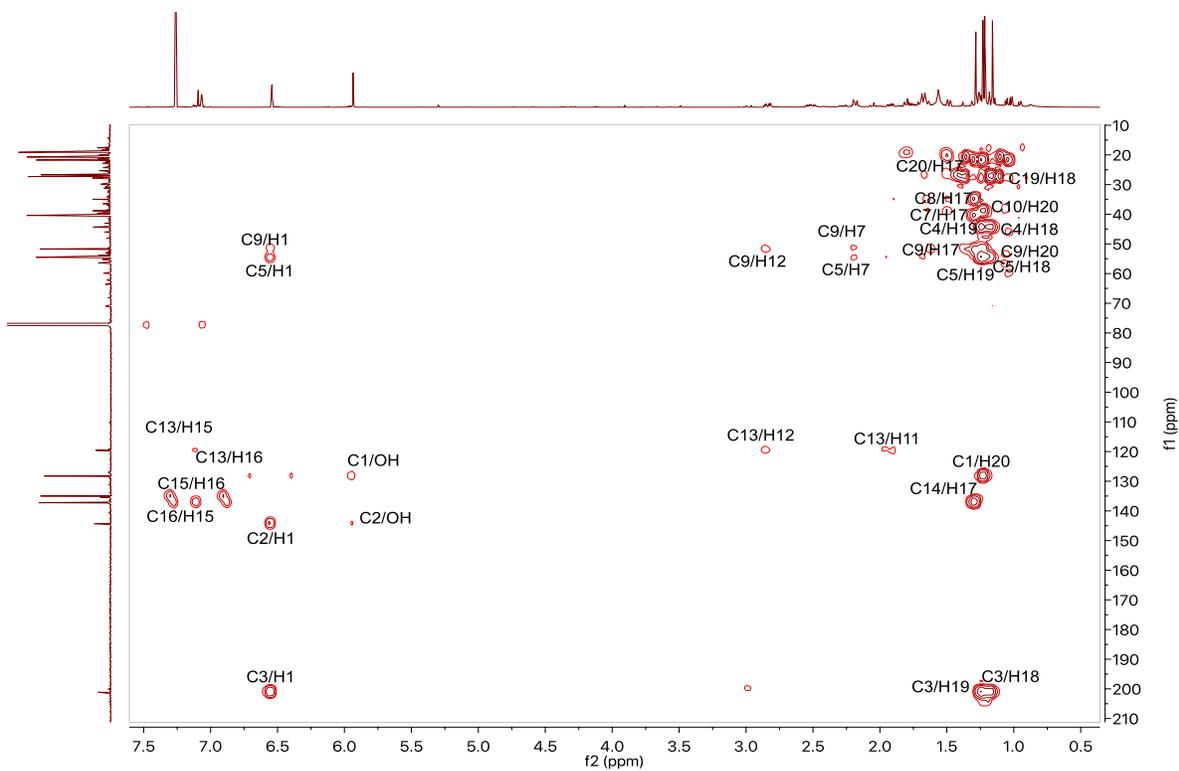


Figure S12. HMBC spectrum of **2** (500 MHz, CDCl_3).

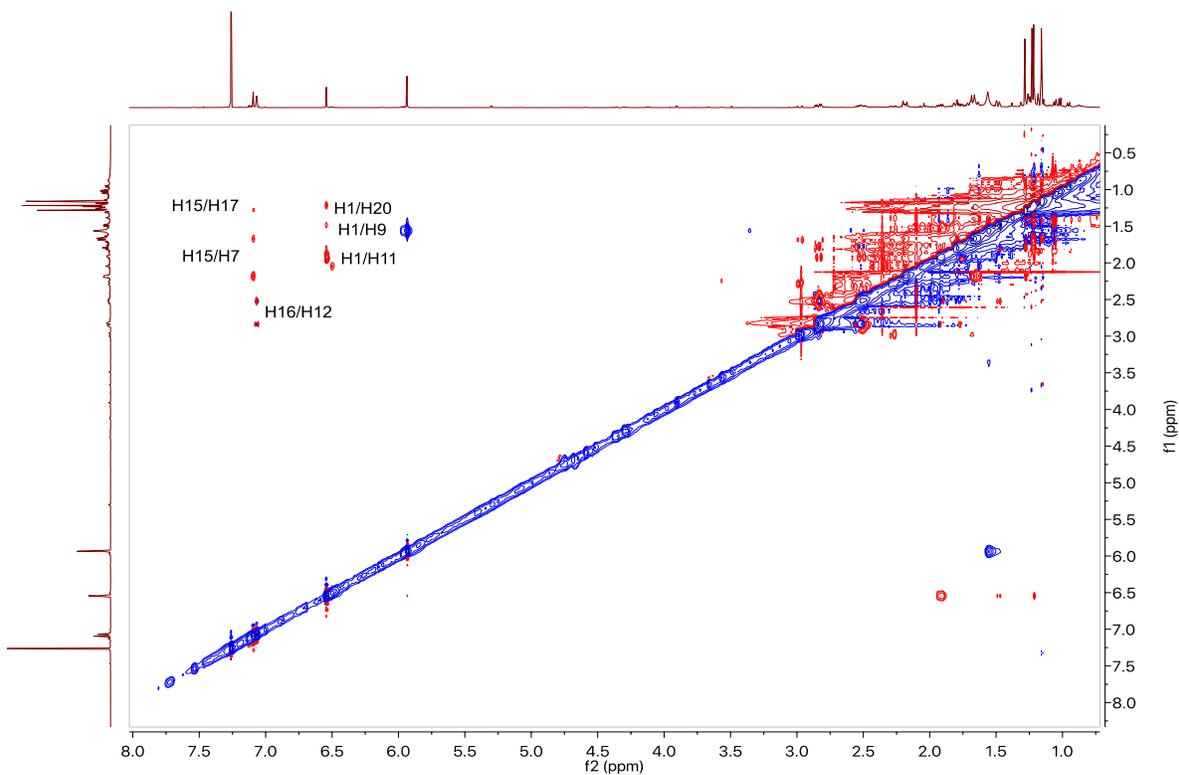


Figure S13. NOESY spectrum of **2** (500 MHz, CDCl_3).

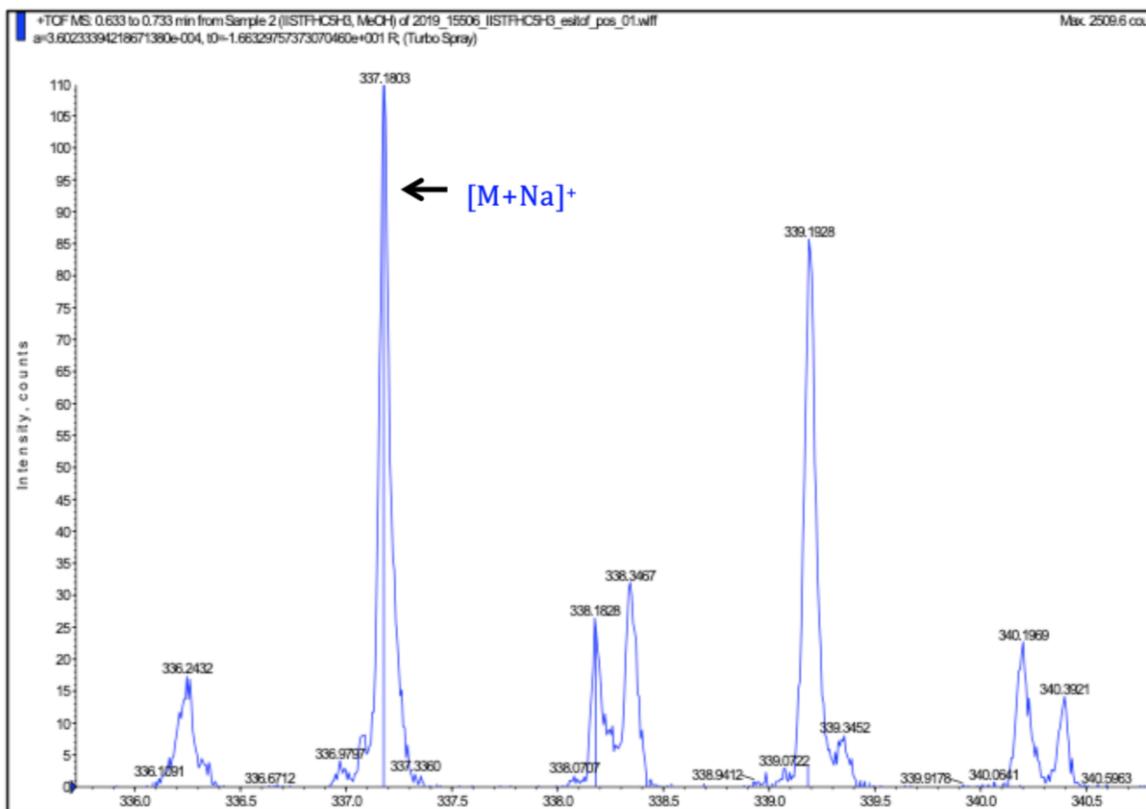


Figure S14. (+)-HRESIMS of **2**.

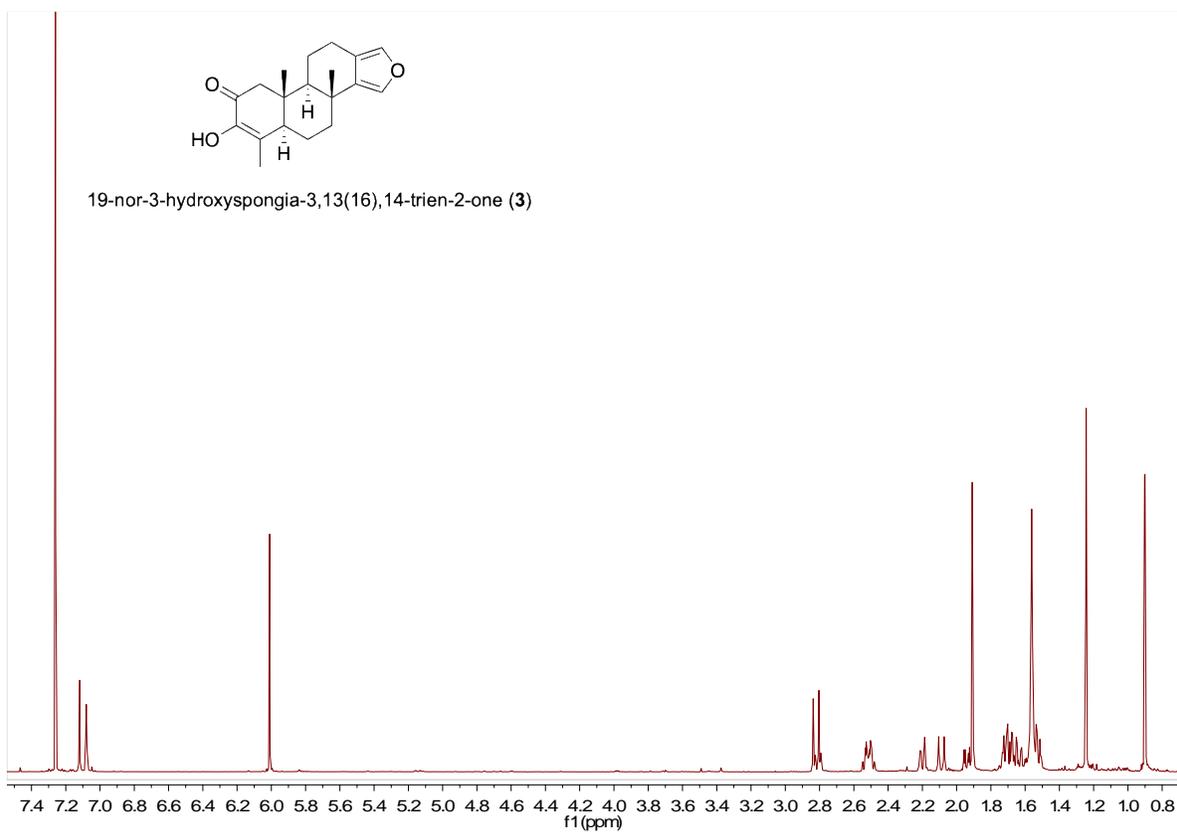


Figure S15. ¹H NMR spectrum of **3** (500 MHz, CDCl₃).

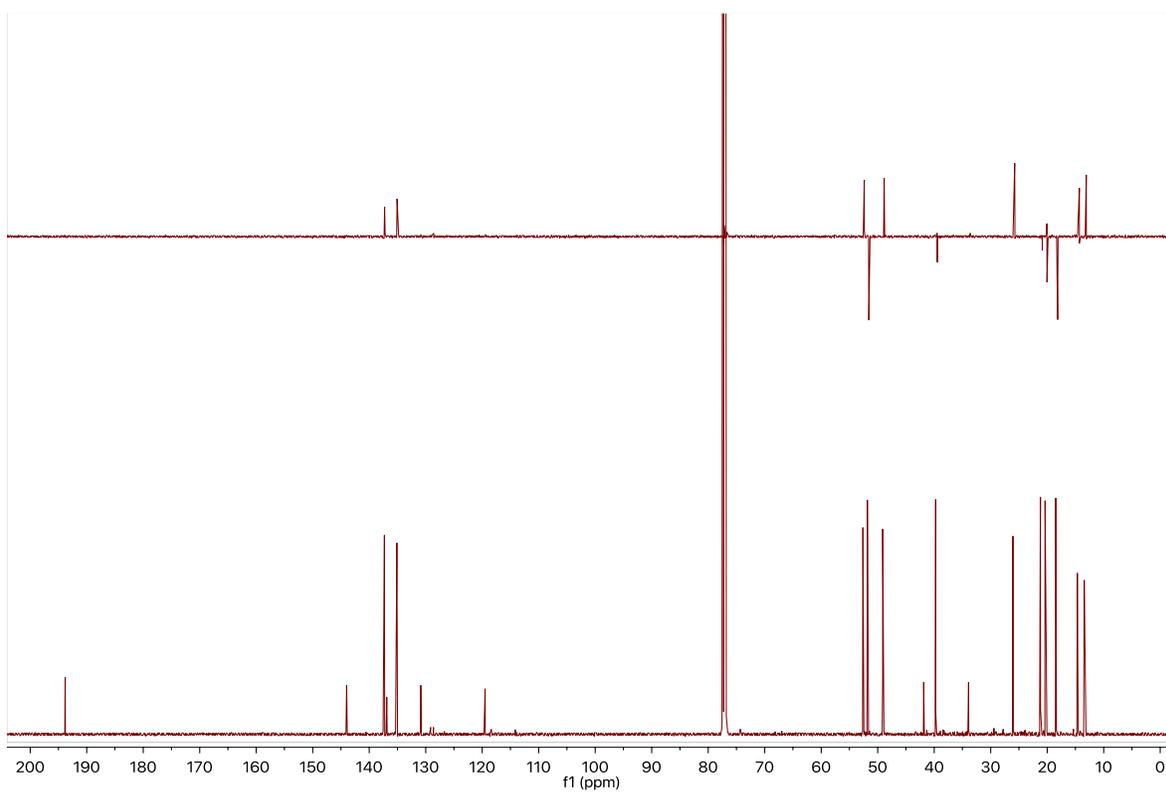


Figure S16. ¹³C NMR and DEPT-135 spectra of **3** (125 MHz, CDCl₃)

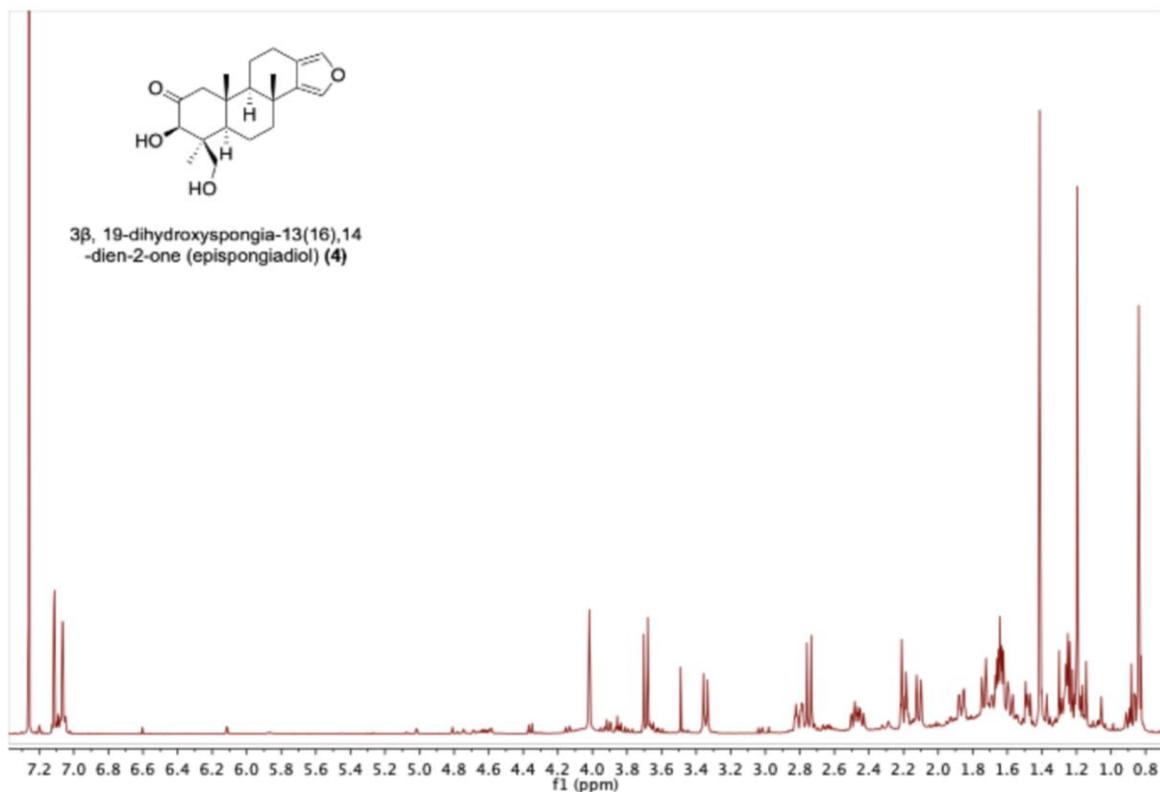


Figure S17. ¹H NMR spectrum of **4** (500 MHz, CDCl₃).

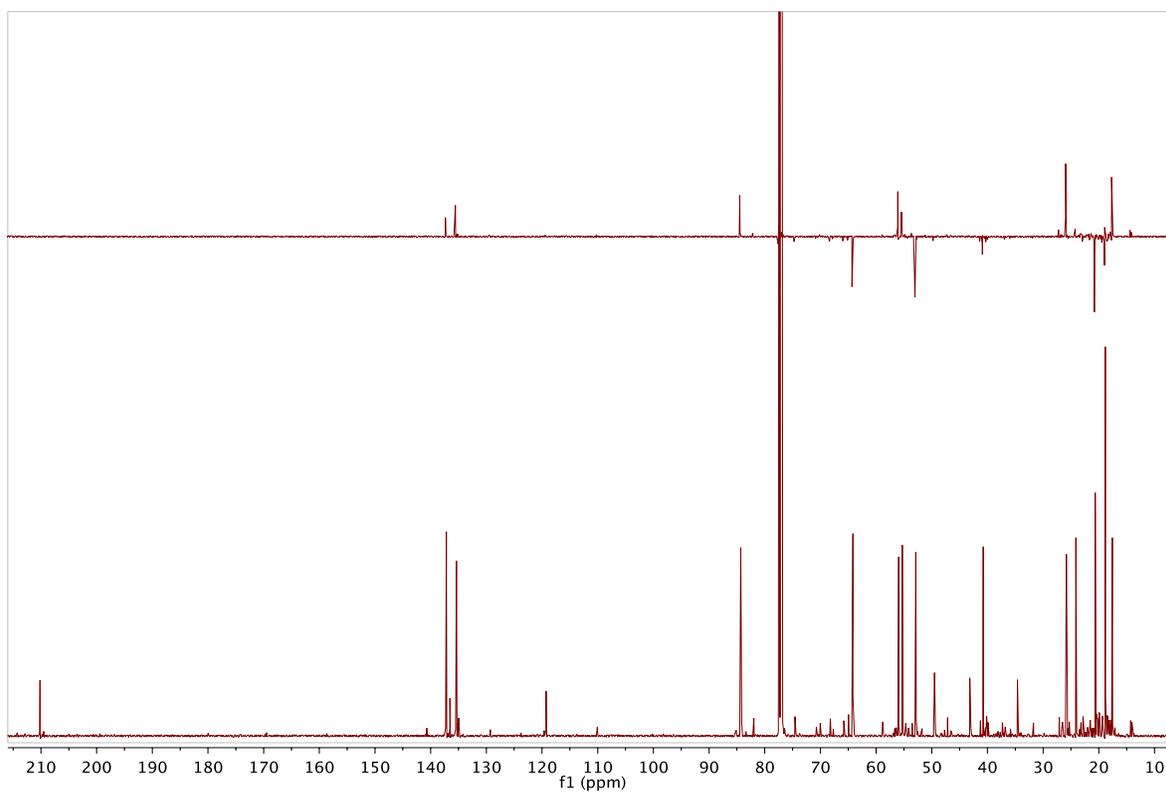


Figure S18. ¹³C NMR and DEPT-135 spectra of **4** (125 MHz, CDCl₃).

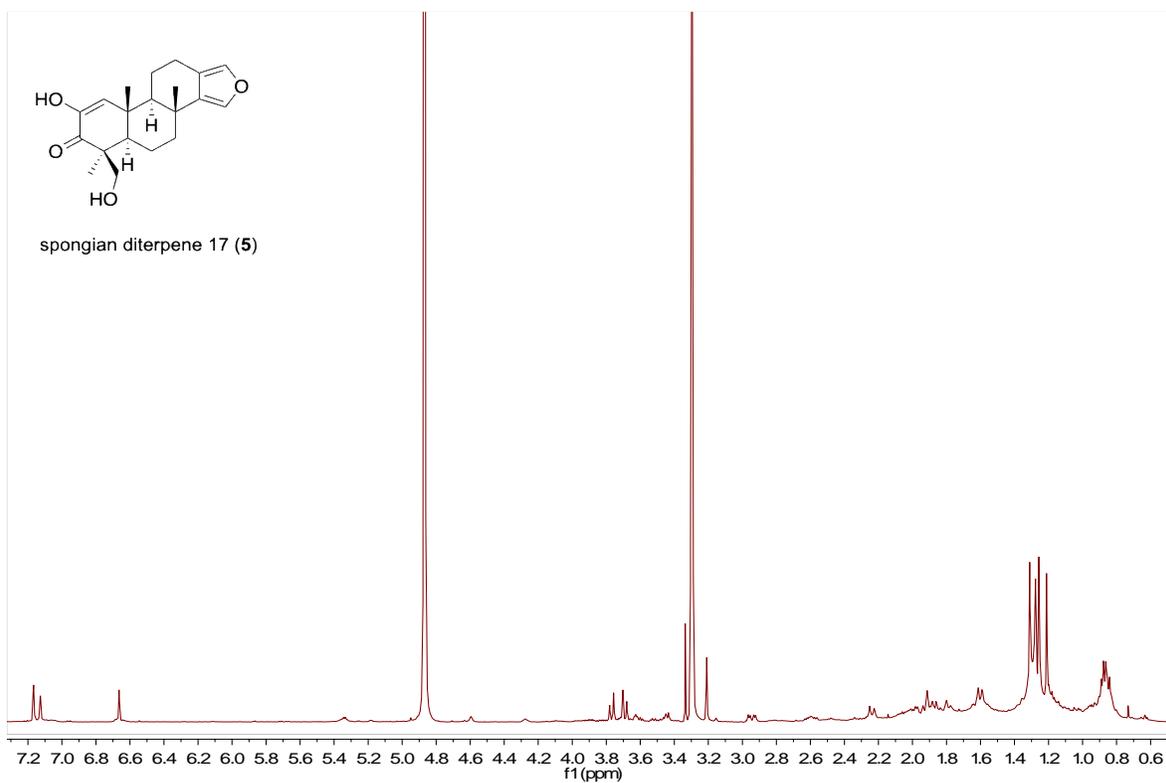


Figure S19. ¹H NMR spectrum of **5** (500 MHz, CH₃OH).

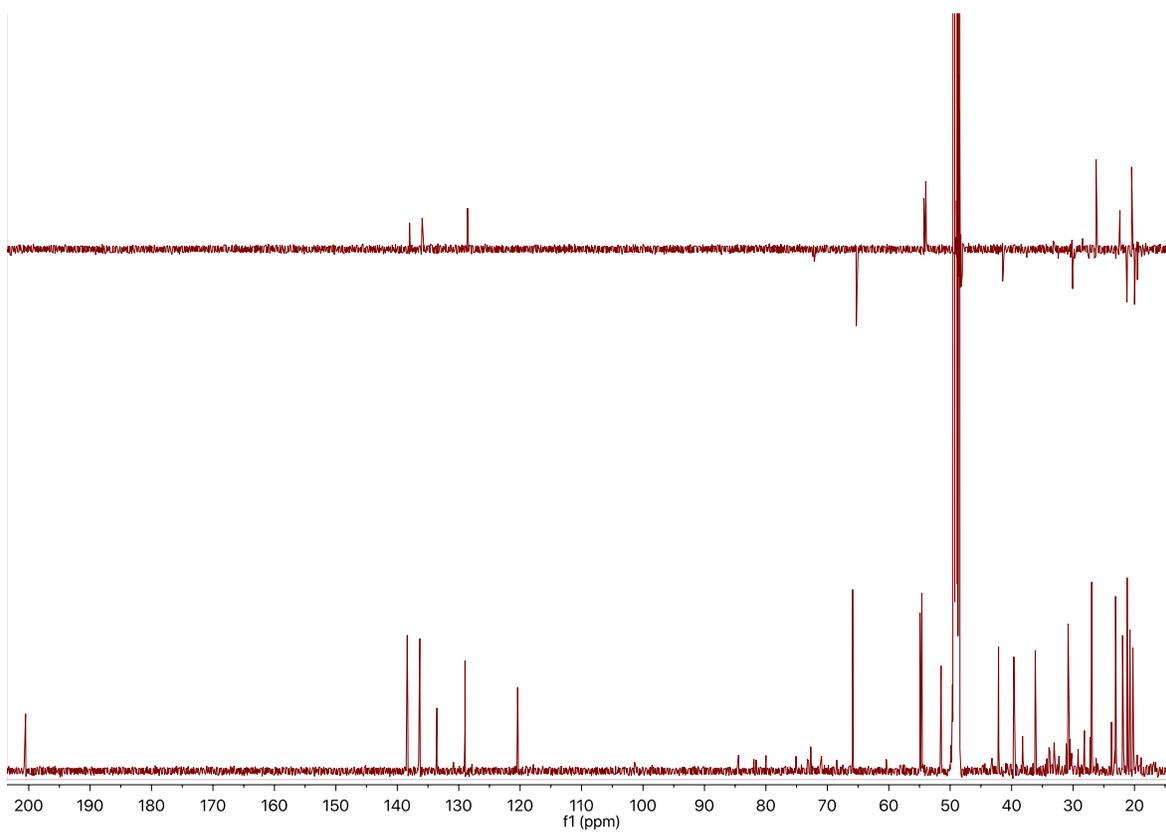


Figure S20. ¹³C NMR and DEPT-135 spectra of **5** (125 MHz, CH₃OH).

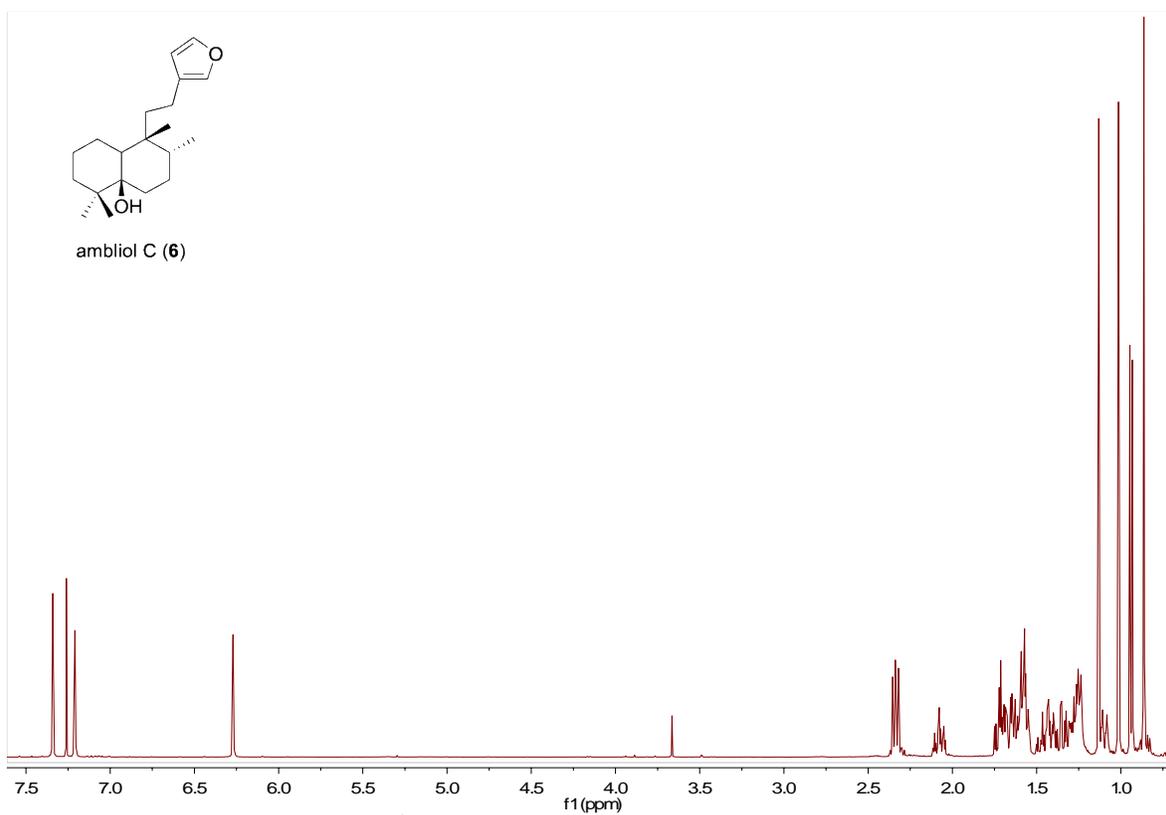


Figure S21. ¹H NMR spectrum of **6** (500 MHz, CDCl₃).

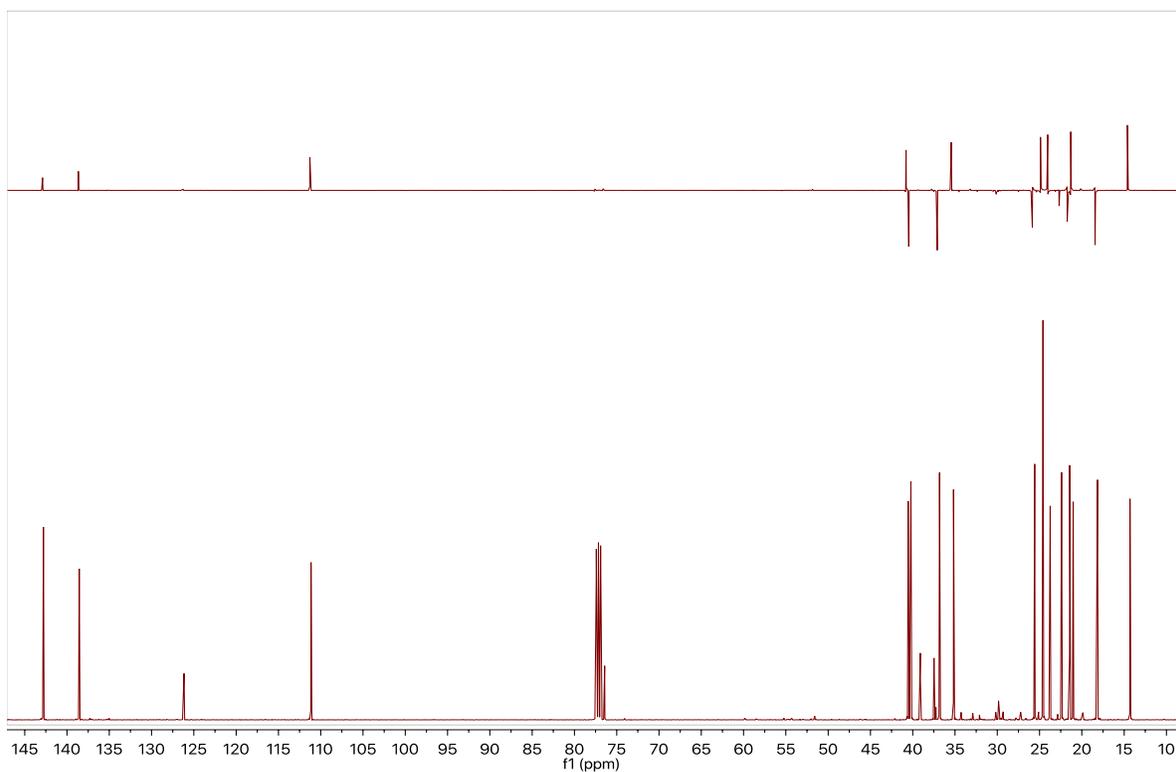


Figure S22. ¹³C NMR and DEPT-135 spectra of **6** (125 MHz, CDCl₃).

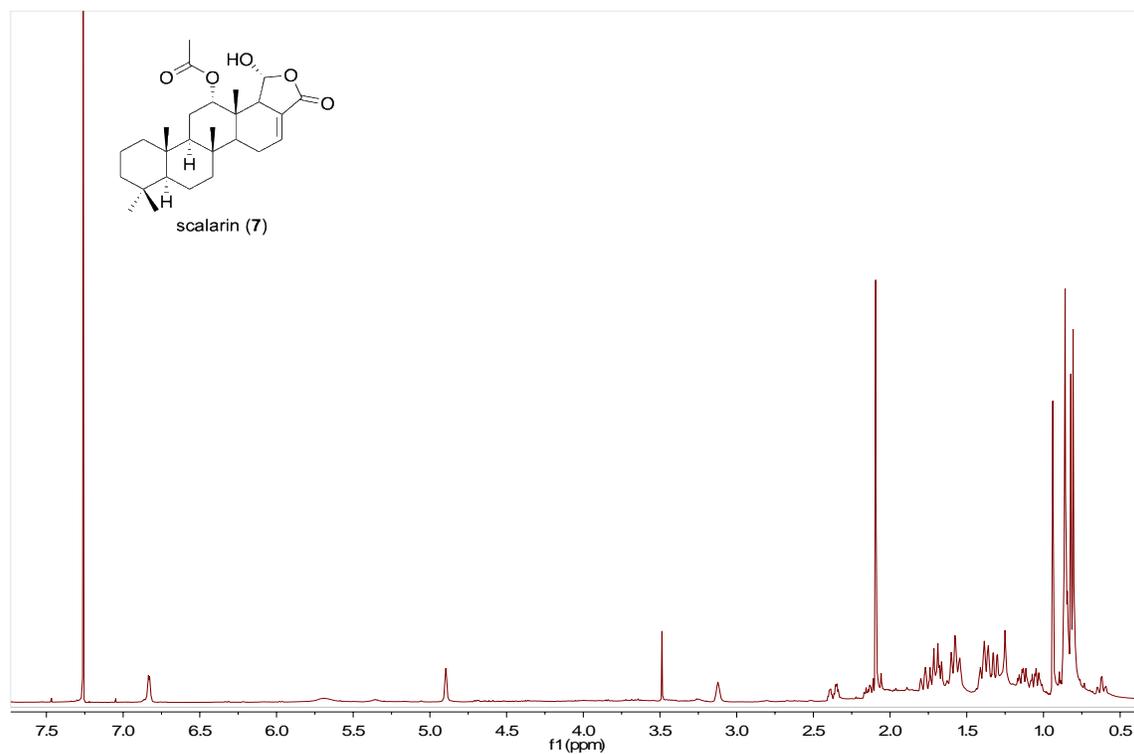


Figure S23. ¹H NMR spectrum of **7** (500 MHz, CDCl₃).

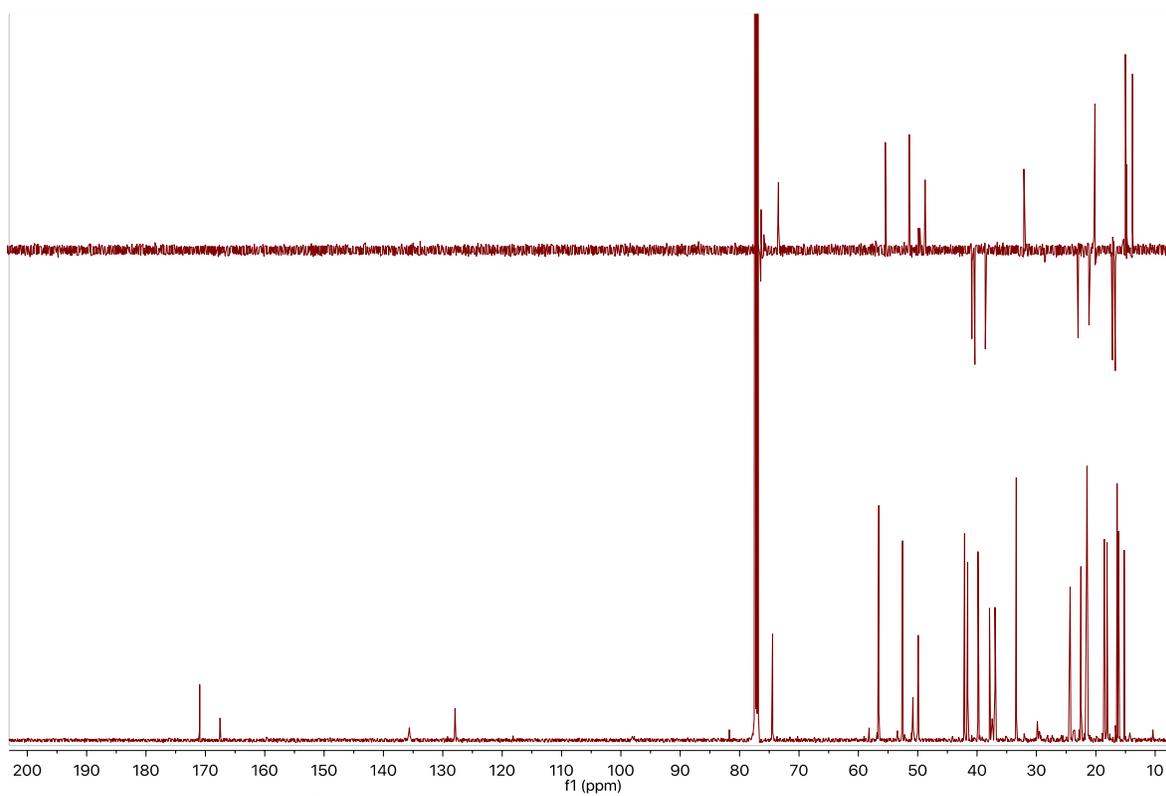


Figure S24. ¹³C NMR and DEPT-135 spectra of **7** (125 MHz, CDCl₃).