

Supplementary Materials

**Cytotoxic Furan- and Pyrrole-Containing Scalarane Sesterterpenoids
Isolated from the Sponge *Scalarispongia* sp.**

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Table S1. Complete NMR data of **3** in CDCl₃

Figure S1. ¹H and ¹³C NMR Spectra (500 MHz and 125 MHz, CDCl₃) of **3**

Figure S2. HMBC and HSQC NMR spectra of **3**

Figure S3. COSY and NOESY NMR spectra of **3**

Table S2. Complete NMR data of **4** in CDCl₃

Figure S4. ¹H and ¹³C NMR Spectra (500 MHz and 125 MHz, CDCl₃) of **4**

Figure S5. HMBC and HSQC NMR spectra of **4**

Figure S6. COSY and NOESY NMR spectra of **4**

Table S3. Complete NMR data of **5** in CDCl₃

Figure S7. ¹H and ¹³C NMR Spectra (500 MHz and 125 MHz, CDCl₃) of **5**

Figure S8. HMBC and HSQC NMR spectra of **5**

Figure S9. COSY and NOESY NMR spectra of **5**

Figure S10. ¹H and ¹³C NMR Spectra (500 MHz and 125 MHz, CDCl₃) of **1**

Figure S11. ¹H and ¹³C NMR Spectra (500 MHz and 125 MHz, CDCl₃) of **2**

Figure S12. ¹H and ¹³C NMR Spectra (500 MHz and 125 MHz, CDCl₃) of **6**

Figure S13. ¹H and NMR Spectra (500 MHz, CDCl₃) of the crude extract obtained by the treatment of the mixture of **1** and **2** with silica and methanol

Table S1. Complete NMR data of **3** in CDCl₃

Position	δ_C , type	δ_H (<i>J</i> in Hz)	HMBC	COSY
1	39.9 CH ₂	0.62 ,br dd (14.0, 14.0) 1.58, m		1.58 0.62
2	18.7 CH ₂	1.38, m 1.61, m		1.61,0.62 1.38
3	42.1 CH ₂	1.13, m 1.36, m		1.36 1.13
4	33.5 C			
5	56.8 CH	0.83, m	37.2, 39.9	
6	18.2 CH ₂	1.31, m 1.57, m		1.57 1.06,1.31
7	41.2 CH ₂	1.06, br dd (13.5,10.5) 1.78, m	37.7, 53.1, 56.8	1.06,1.31 1.57,1.78,
8	37.7 C			
9	53.1 CH	1.31, m	21.9	1.81, 1.92
10	37.2 C			
11	21.9 CH ₂	1.81, m 1.92, m	41.7	1.31, 1.92, 5.48 1.31, 1.81, 5.48
12	73.0 CH	5.48, br s	172.7	1.81, 1.92
13	41.7 C			
14	50.9 CH	2.34, br d (13.5)	34.9, 37.7, 41.7, 194.6	2.47, 2.57
15	34.9 CH ₂	2.47, dd (17.5,13.5) 2.57, br d (17.5)	41.7, 50.9, 120.2, 194.6 41.7, 50.9, 194.6	2.34, 2.57 2.34, 2.47
16	194.6 C			
17	120.2 C			
18	172.7 C			
19	142.9 CH	7.26, br s	106.5, 120.2, 172.7	6.59
20	106.5 CH	6.59, br s	120.2, 142.9, 172.7	7.26
21	33.5 CH ₃	0.85, s	33.5, 42.1, 56.8	
22	21.5 CH ₃	0.81, s	33.5, 42.1, 56.8	
23	16.3 CH ₃	0.85, s	53.1, 56.8	
24	17.0 CH ₃	0.99, s	37.7, 41.2, 50.9, 53.1	
25	20.4 CH ₃	1.32, s	41.7, 50.9, 73.0, 172.7	
12OAc	172.7 C			
	21.4 CH ₃	1.88, s	170.2	

Figure S3. ^1H and ^{13}C NMR Spectra (500 MHz and 125 MHz, CDCl_3) of **3**

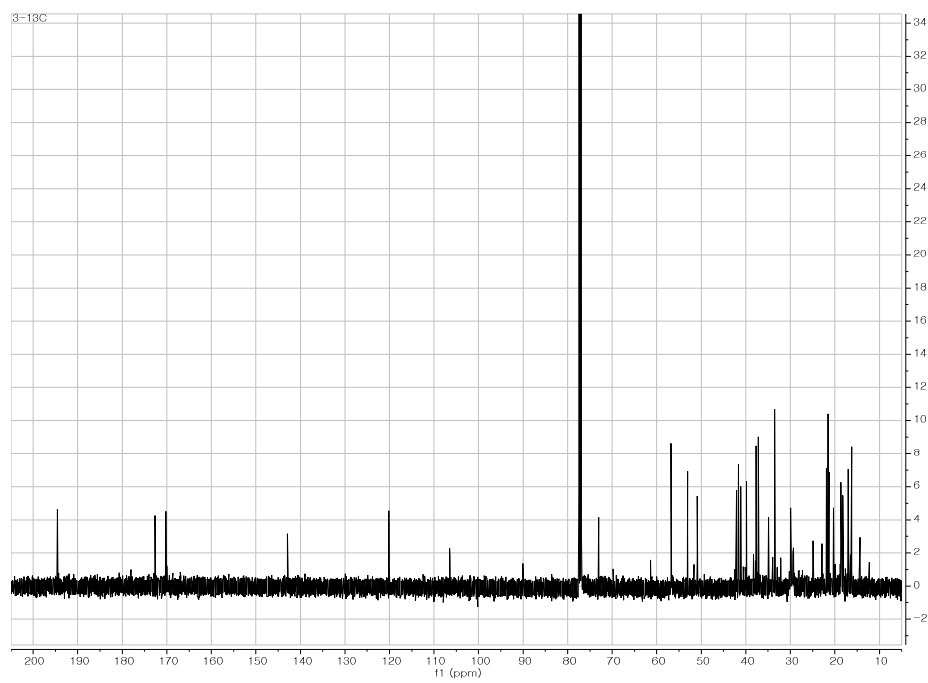
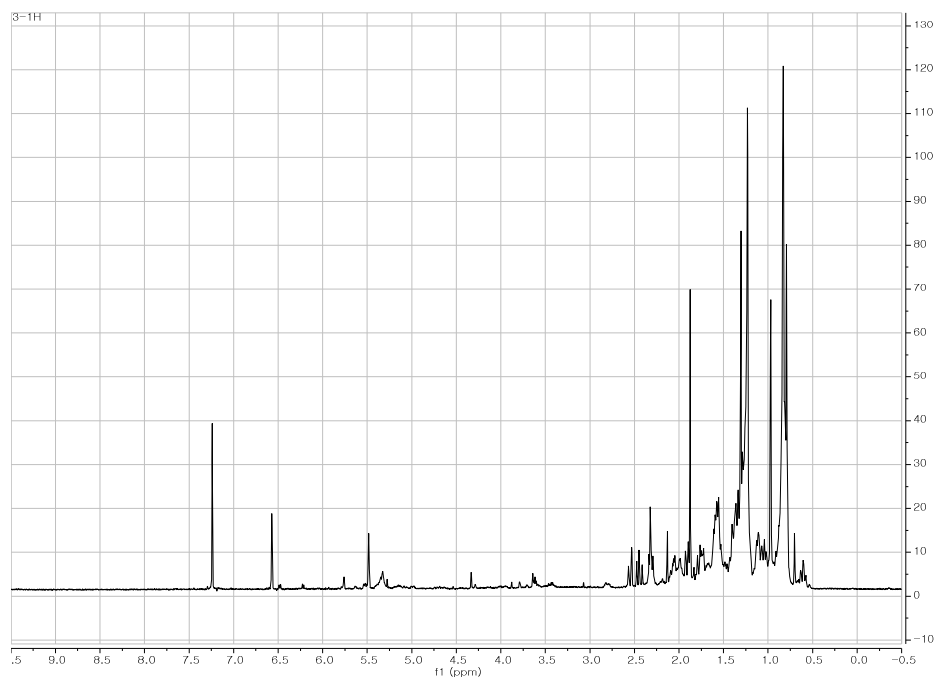


Figure S2. HMBC and HSQC NMR spectra of **3**

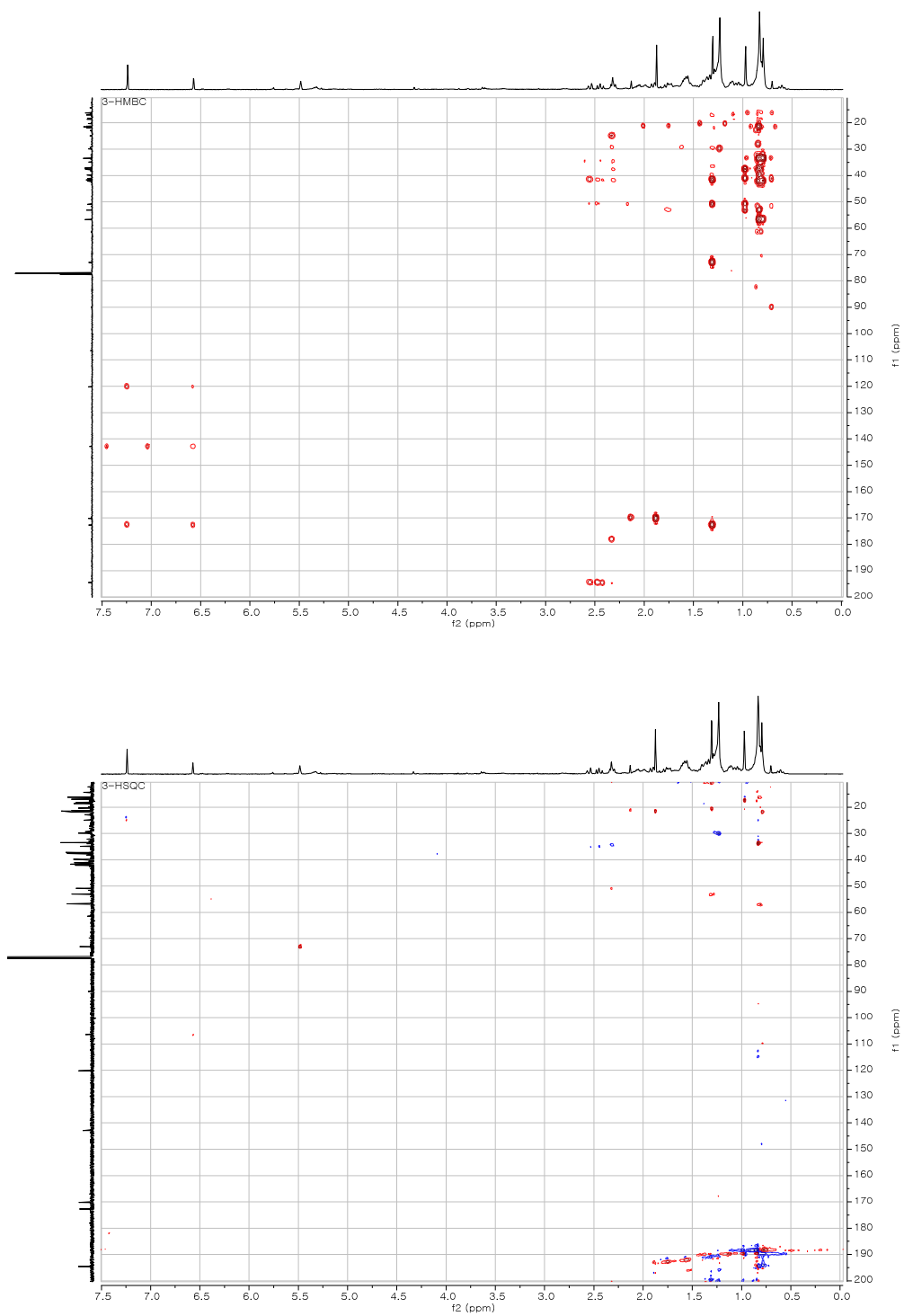


Figure S3. COSY and NOESY NMR spectra of **3**

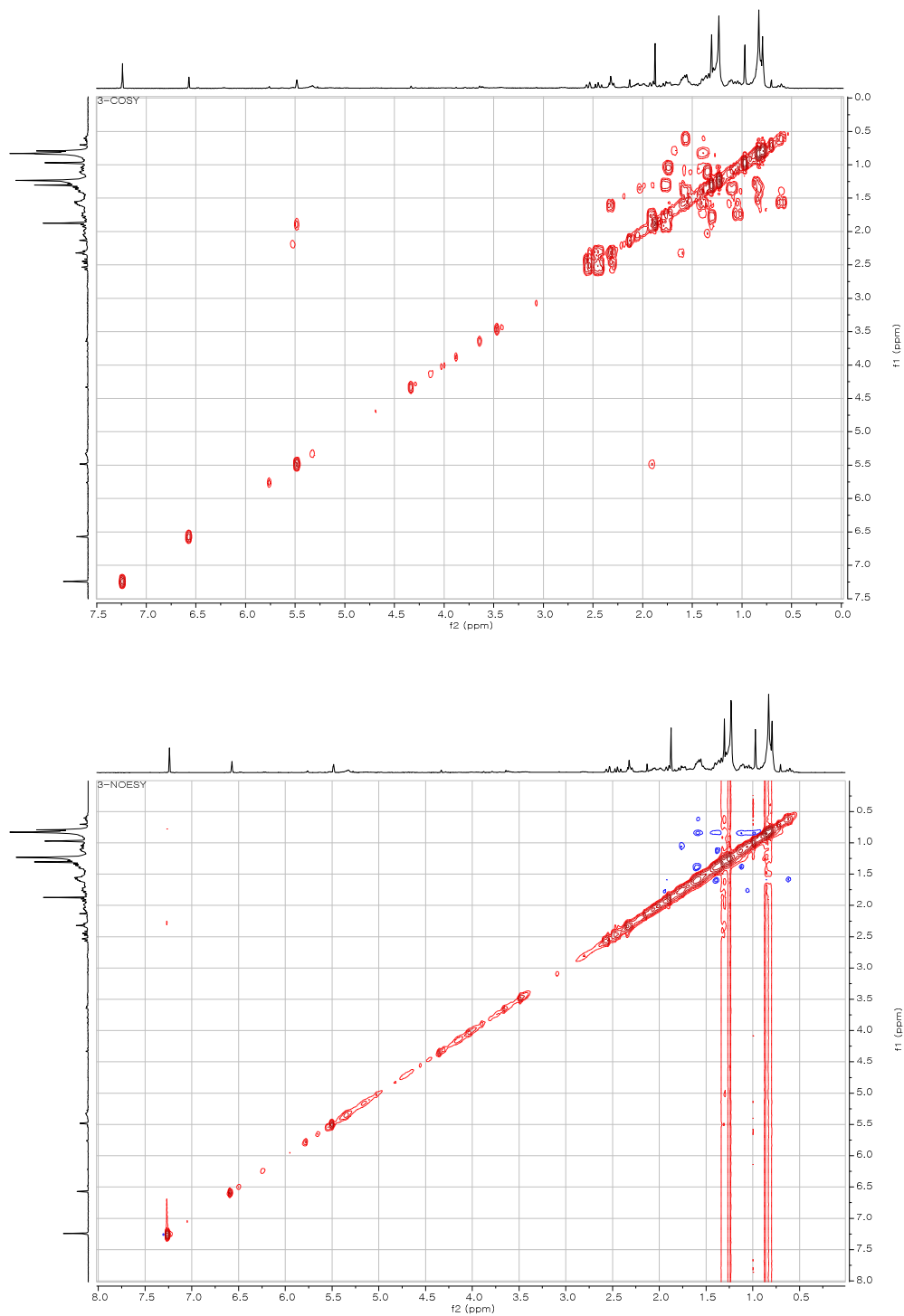


Table S2. Complete NMR data of **4** in CDCl₃

Position	δ_C , type	δ_H (<i>J</i> in Hz)	HMBC	COSY
1	39.9:CH ₂	0.63, ddd (14.5, 14.5, 4.5) 1.58, m	37.2, 42.2	1.39, 1.58 0.63
2	18.3:CH ₂	1.39, m 1.56, m	37.2, 39.9	0.63, 1.56 1.39
3	42.2:CH ₂	1.12, ddd (13.0, 13.0, 4.0) 1.35, m	33.5	1.35 1.12
4	33.5:C			
5	56.7:CH	0.83, m		1.40
6	18.7:CH ₂	1.40, m 1.58, m	56.7 37.2, 38.0, 56.7	0.83 1.77
7	41.4:CH ₂	1.04, ddd (11.5, 11.5, 3.5) 1.77, m	17.1 38.0, 52.7, 56.7	1.77 1.58, 1.84
8	38.0:C			
9	52.7:CH	1.38, m	22.6, 51.6	1.81
10	37.2:C			
11	22.6:CH ₂	1.63, m 1.81, m	38.0, 52.7, 74.8	1.38, 5.45
12	74.8:CH	5.45, br s	52.7, 171.2	1.81
13	39.5:C			
14	51.6:CH	2.19, dd (7.3, 10.0)	17.1, 25.2, 35.4, 38.0, 39.5, 41.4, 52.7, 135.5, 196.8	2.48, 2.49
15	35.4:CH ₂	2.48, br d (7.3) 2.49, br d (10.0)	39.5, 51.6, 121.1, 196.8 39.5, 51.6, 121.1, 196.8	2.19 2.19
16	196.8:C			
17	121.1:C			
18	135.5:C			
19	119.5:CH	7.30, br s	111.2, 121.1, 135.5	6.32
20	111.2:CH	6.32, br s	119.5, 121.1, 135.5	7.30
21	33.5:CH ₃	0.84, s	21.6, 33.5, 42.2, 56.7	
22	21.6:CH ₃	0.81, s	33.5, 42.2, 56.7	
23	16.4:CH ₃	0.84, s	37.2, 39.9, 52.7	
24	17.1:CH ₃	0.98, s	38.0, 41.4, 51.6	
25	25.2:CH ₃	1.27, s	39.5, 51.6, 74.8, 135.5	
12OAc	171.2:C			
	21.5:CH ₃	1.91, s	171.2	

Figure S4. ^1H and ^{13}C NMR Spectra (500 MHz and 125 MHz, CDCl_3) of **4**

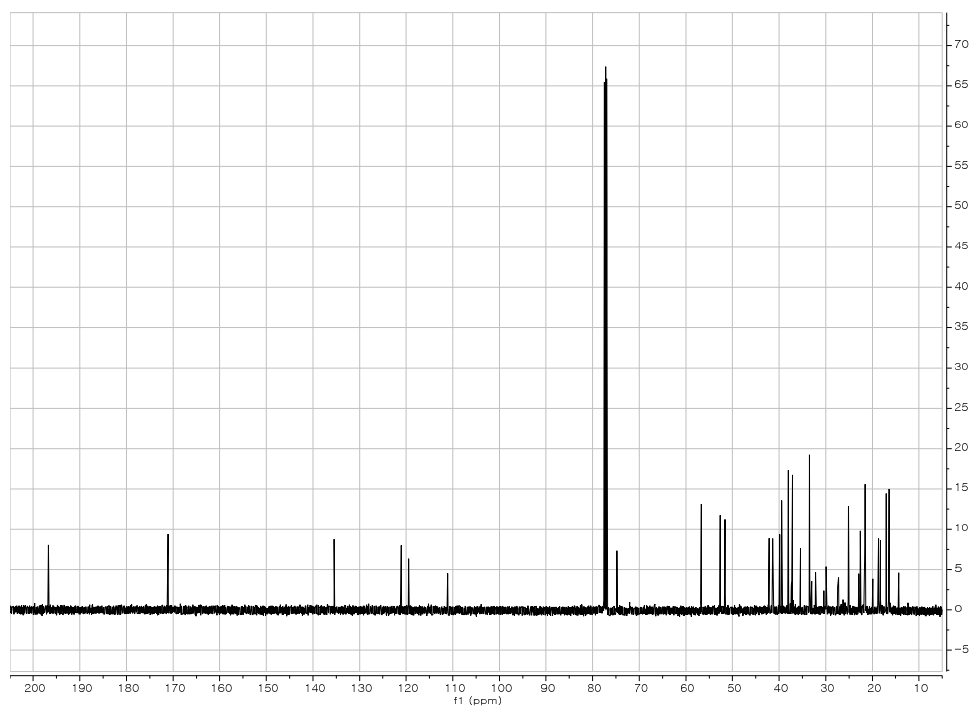
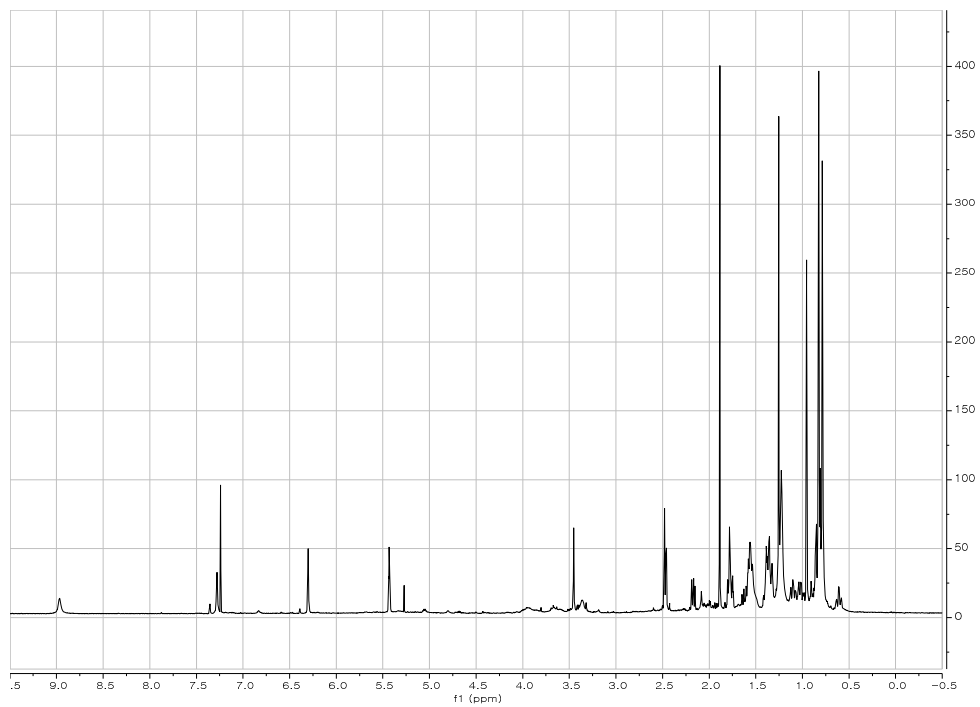


Figure S5. HMBC and HSQC NMR spectra of **4**

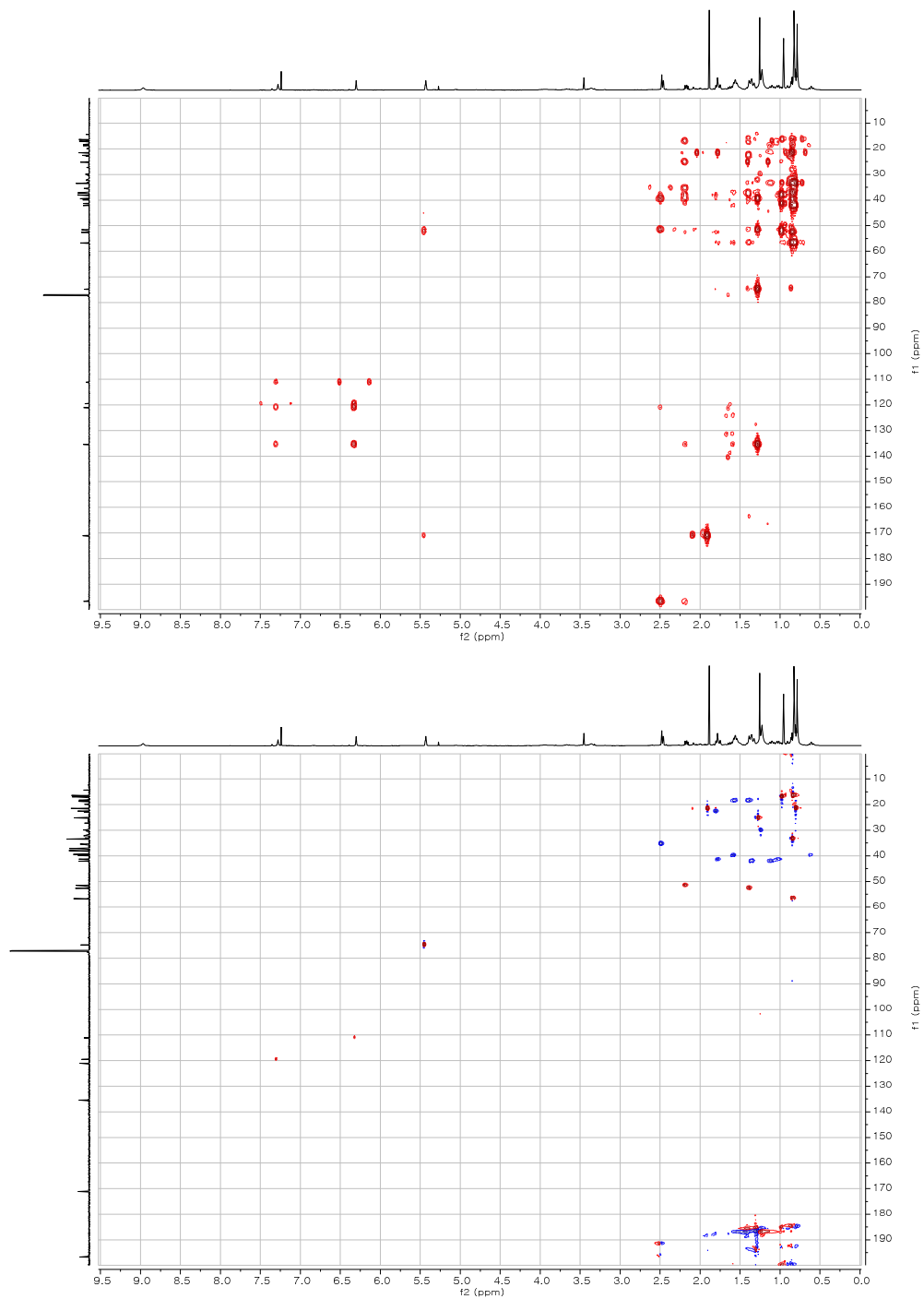


Figure S6. COSY and NOESY NMR spectra of **4**

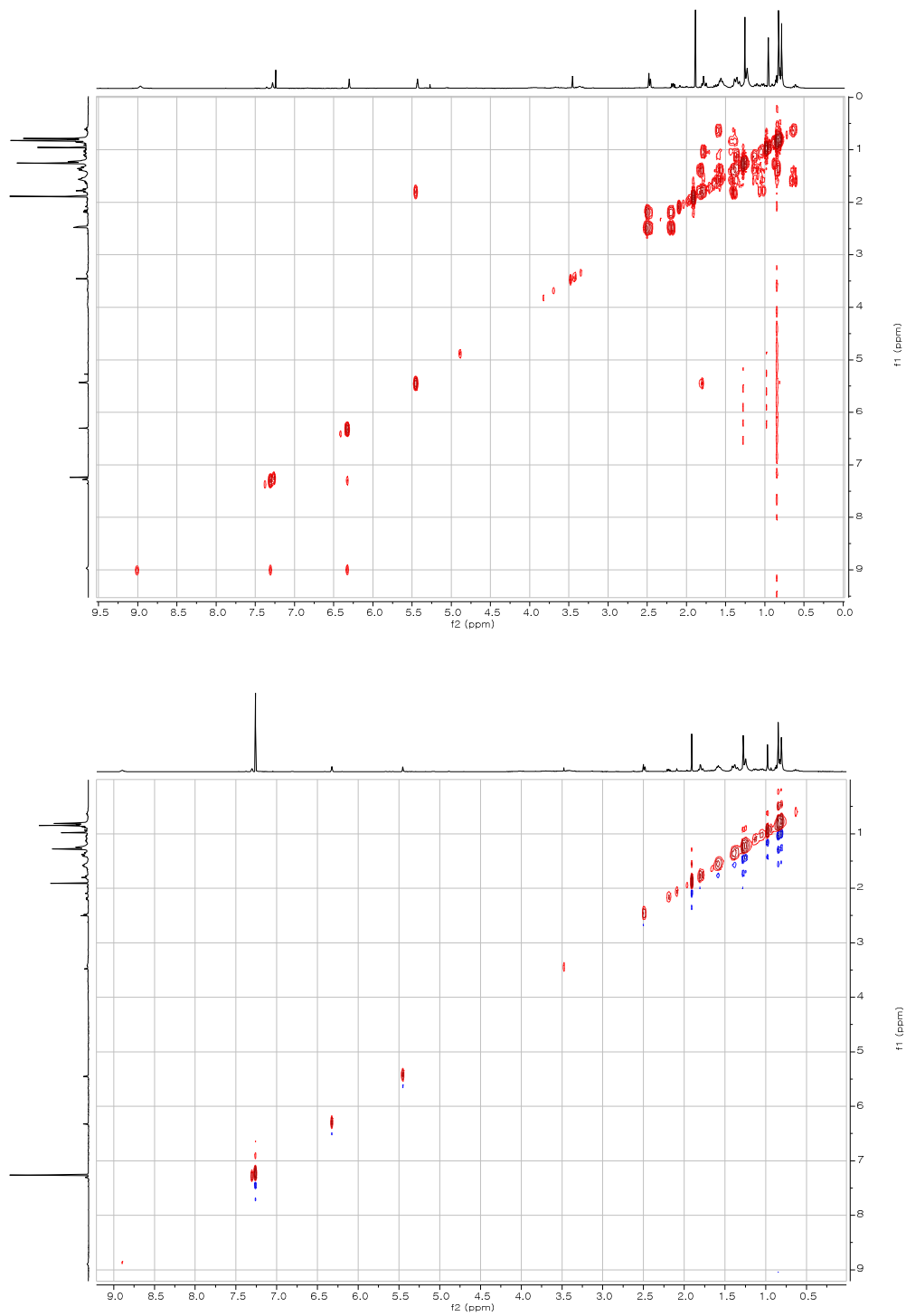


Table S3. Complete NMR data of **5** in CDCl₃

Position	δ_C , type	δ_H (<i>J</i> in Hz)	HMBC	COSY
1	39.9 CH ₂	0.62, ddd (13.0, 13.0, 3.0) 1.57, m	42.2, 56.5	1.40, 1.60 1.60
2	18.7 CH ₂	1.40, m 1.60, m		0.62, 1.11, 1.60 0.62, 1.11, 1.40
3	42.2 CH ₂	1.11, br dd (12.5, 5.0) 1.35, m	21.5 39.9, 56.5	1.35, 1.40, 1.60, 1.11
4	33.5 C			
5	56.5 CH	0.90, m	33.5	1.44
6	18.3 CH ₂	1.44, m 1.60, m	41.4	0.90, 1.11, 1.60 1.44, 1.82
7	41.4 CH ₂	1.11, m 1.82, m	17.6, 37.2	1.44, 1.82 1.11, 1.60
8	37.2 C			
9	53.2 CH	1.35, m	37.2, 45.9, 56.5	1.74
10	37.2 C			
11	22.0 CH ₂	1.74, br d (14.0) 1.82, m	37.2, 53.2 53.2	1.35, 1.82, 5.42 1.74, 5.42
12	73.6 CH	5.42, br s	45.9, 53.2	1.74, 1.82
13	41.2 C			
14	45.9 CH	2.14, br d (13.0)	17.6, 21.0, 23.8, 37.2 41.2, 71.8, 158.9	1.59
15	23.8 CH ₂	1.59, m 2.07, br d (15.0)	45.9 41.2, 71.8, 116.4	2.07, 2.14, 4.18 1.59, 4.18
16	71.8 C	4.18, d (3.5)	45.9, 116.4, 158.9	1.59, 2.07
17	116.4 C			
18	158.9 C			
19	141.0 CH	7.19, br s	110.2, 116.4, 158.9	6.28
20	110.2 CH	6.28, br s	116.4, 141.0, 158.9	7.19
21	33.5 CH ₃	0.85, s	21.5, 33.5, 42.2, 56.5	
22	21.5 CH ₃	0.81, s	33.5, 42.2	
23	16.2 CH ₃	0.83, s	37.2, 39.9, 53.2	
24	17.6 CH ₃	0.93, s	37.2, 41.4, 45.9, 53.2	
25	21.0 CH ₃	1.18, s	41.2, 45.9, 73.6, 158.9	
12OAc	170.8 C			
	21.6 CH ₃	1.86, s	170.8	
16OMe	56.6 CH ₃	3.40, s	71.8	

Figure S7. ^1H and ^{13}C NMR Spectra (500 MHz and 125 MHz, CDCl_3) of **5**

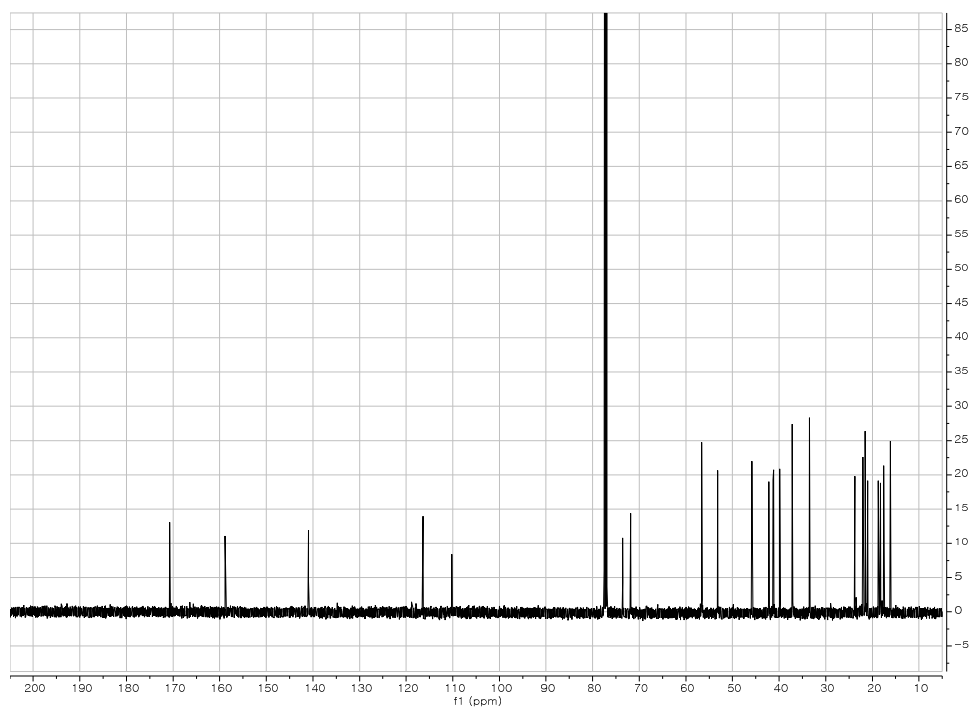
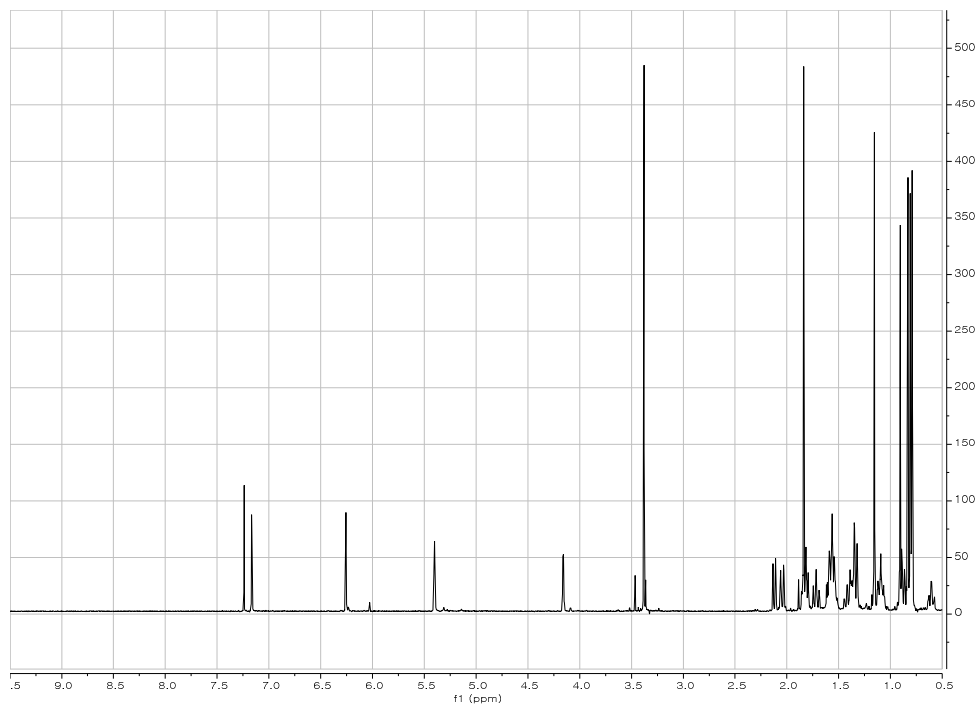


Figure S8. HMBC and HSQC NMR spectra of **5**

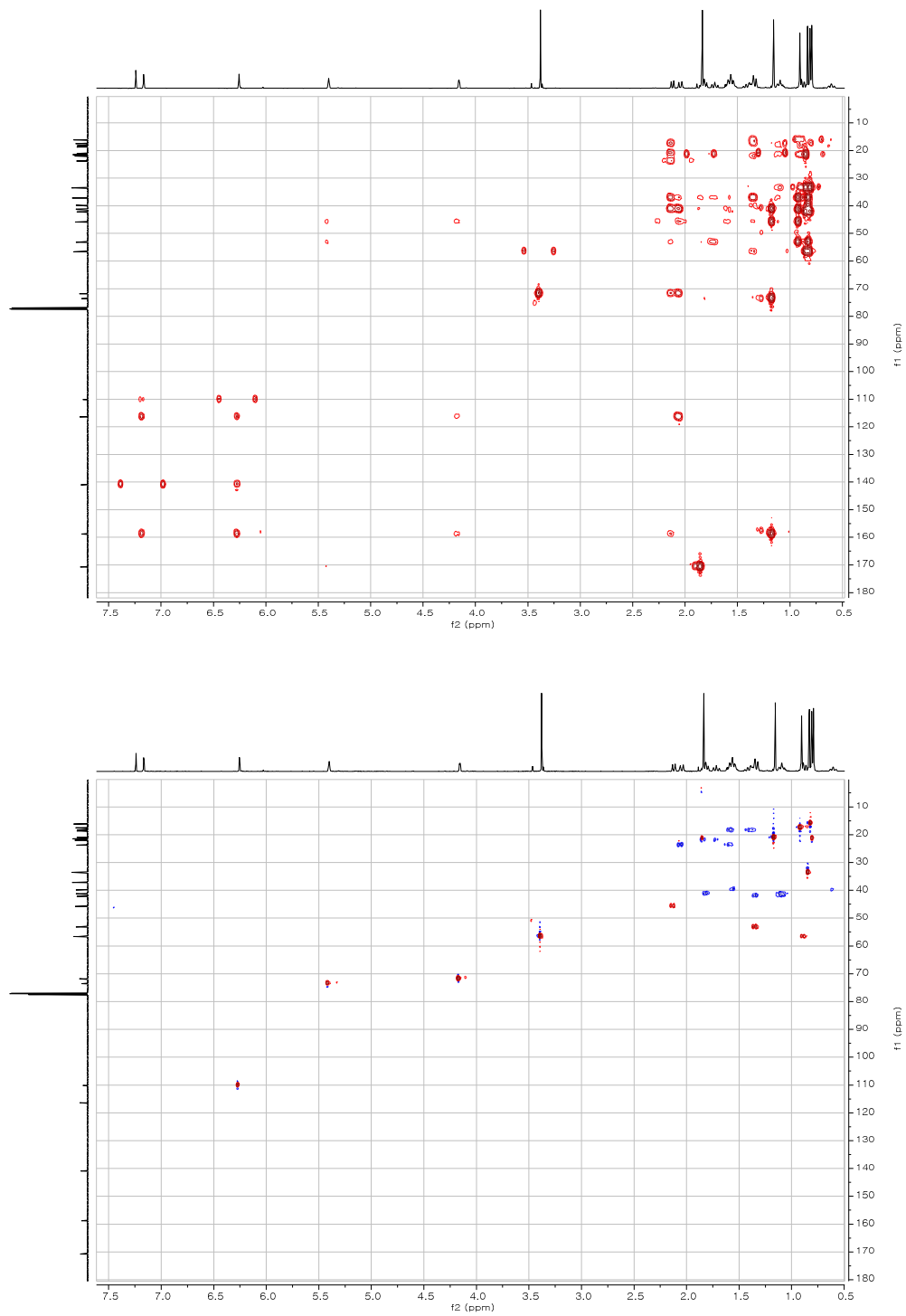


Figure S9. COSY and NOESY NMR spectra of **5**

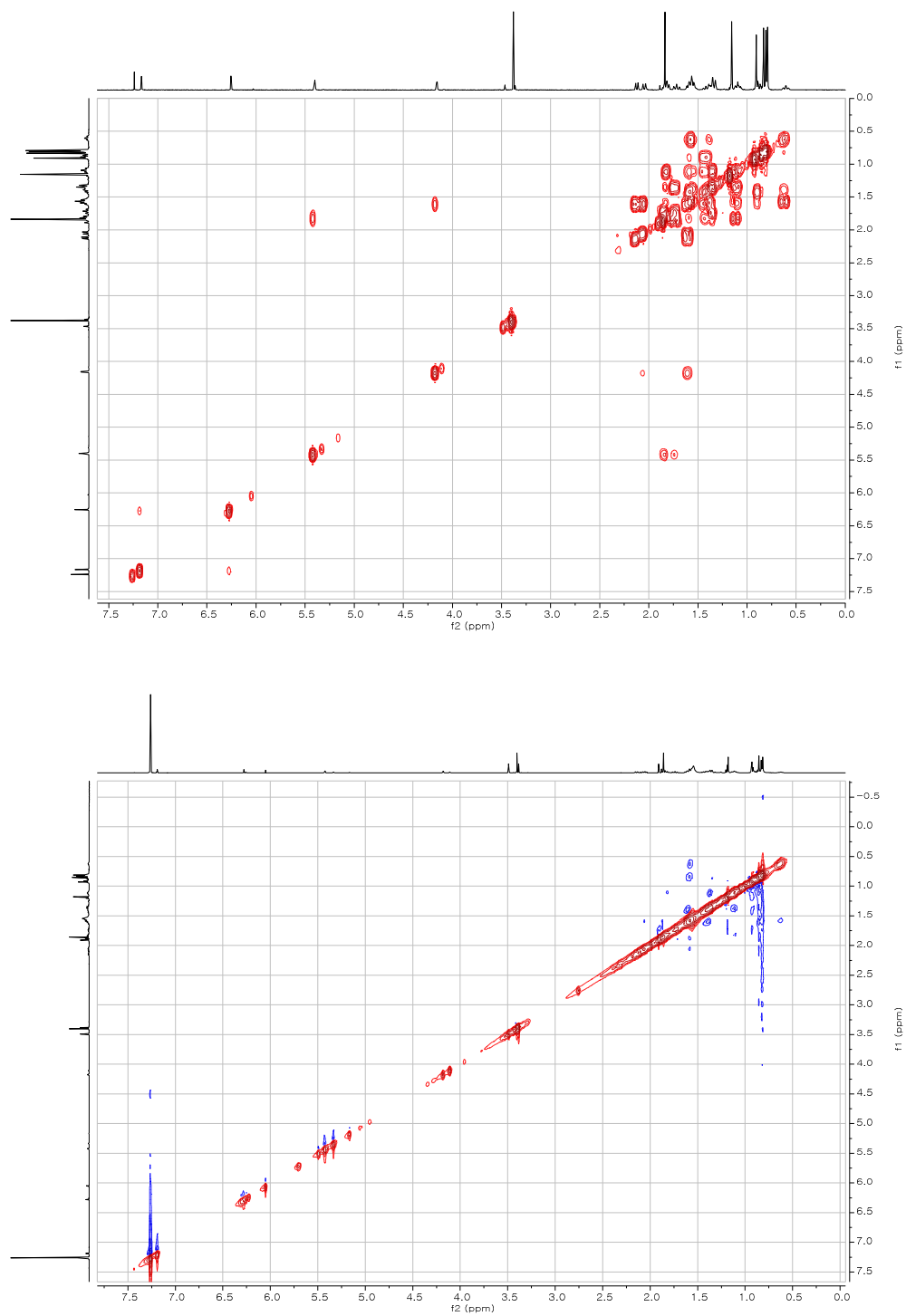


Figure S10. ^1H and ^{13}C NMR Spectra (500 MHz and 125 MHz, CDCl_3) of **1**

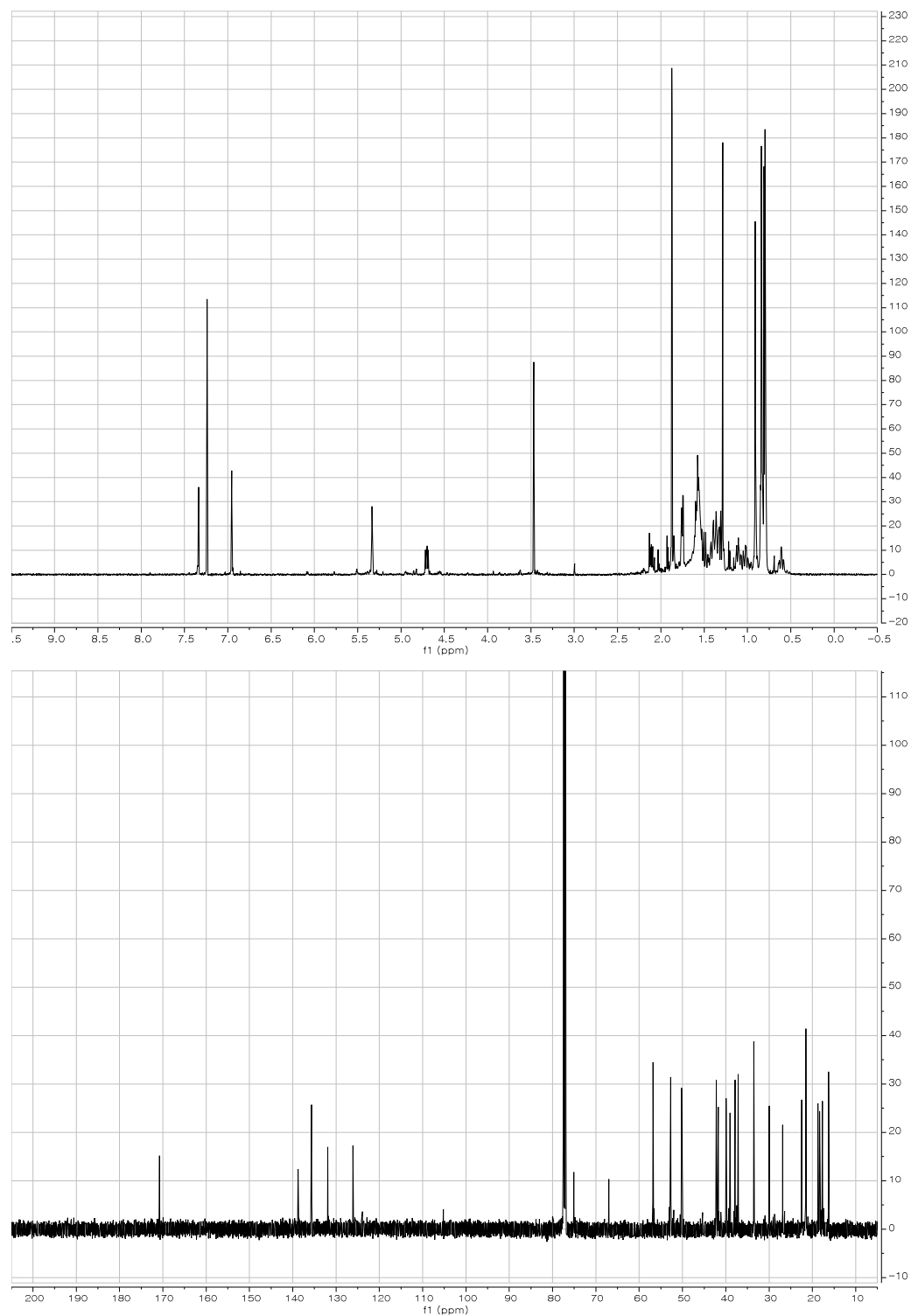


Figure S11. ^1H and ^{13}C NMR Spectra (500 MHz and 125 MHz, CDCl_3) of **2**

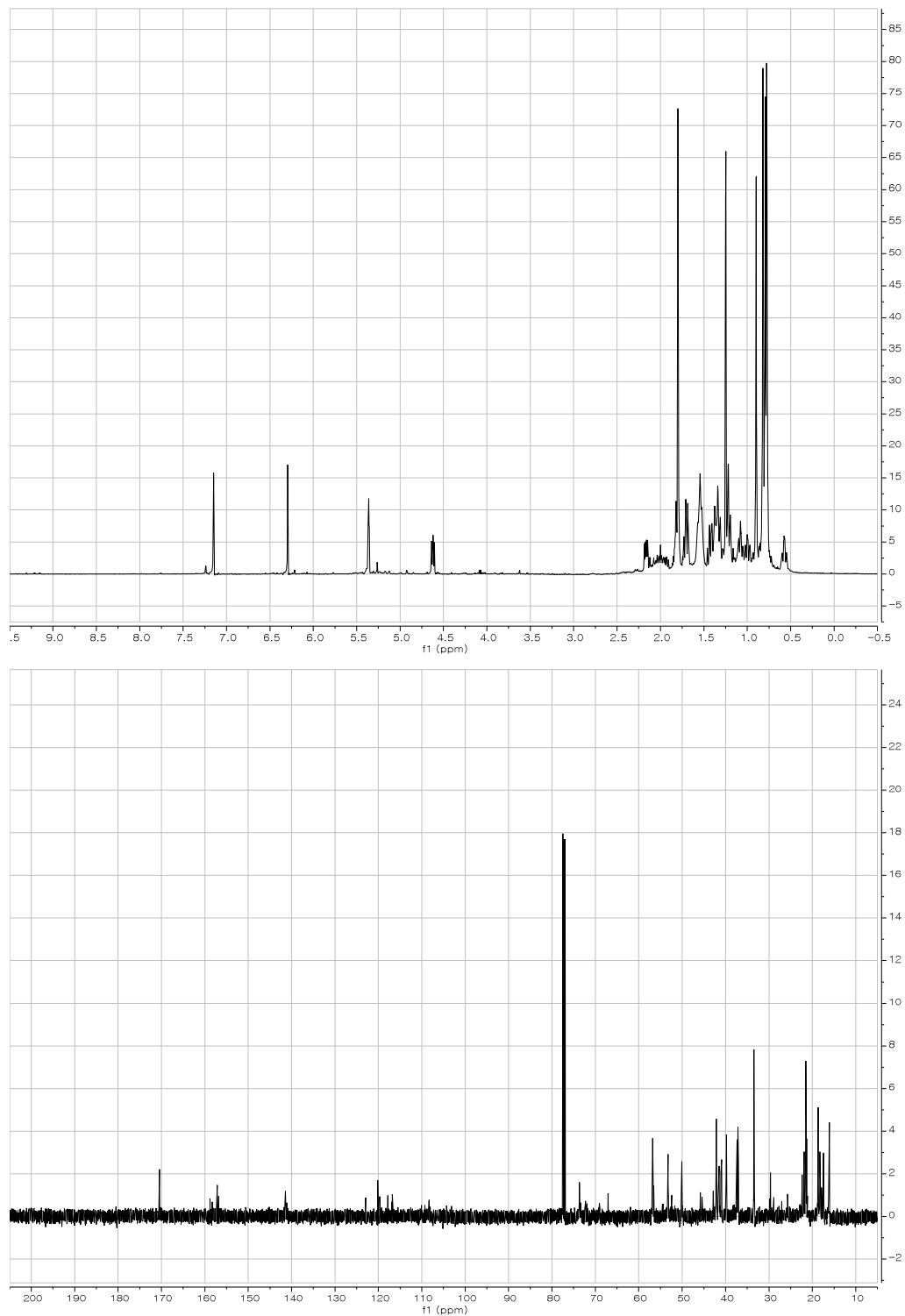


Figure S12. ^1H and ^{13}C NMR Spectra (500 MHz and 125 MHz, CDCl_3) of **6**

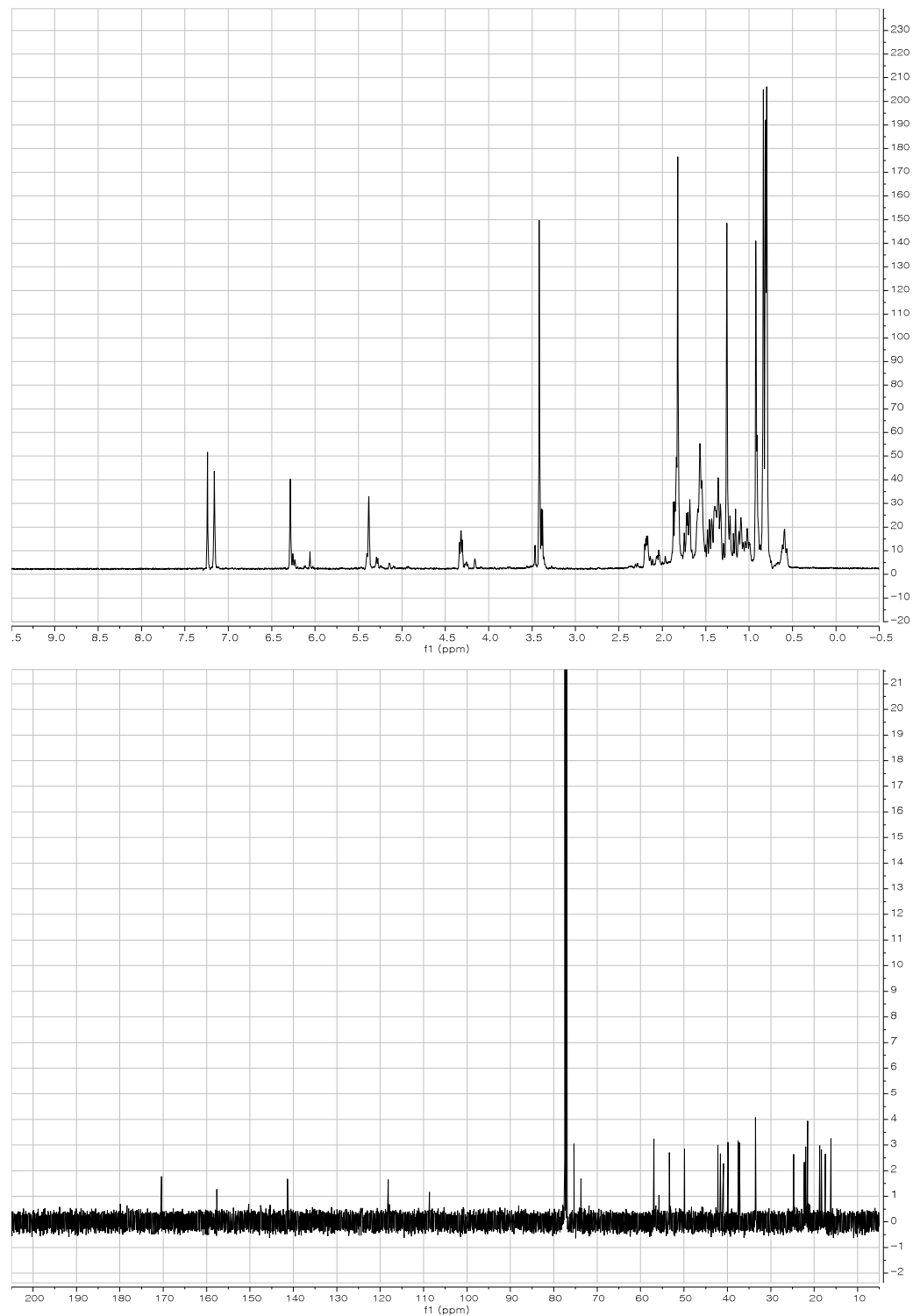
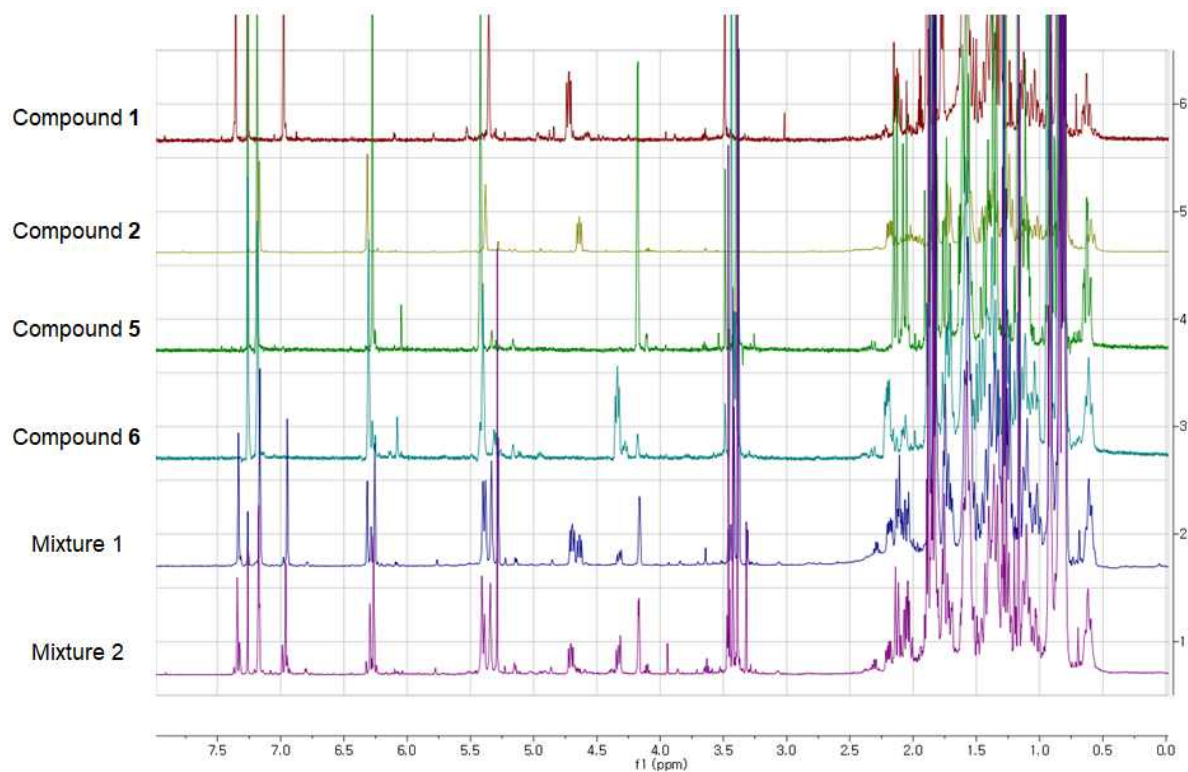


Figure S13. The comparison of ^1H and NMR Spectra (500 MHz, CDCl_3)



Mixture 1 : The fraction obtained by silica HPLC (methanol/dichloromethane) of the mixture of **1** and **2**

Mixture 2: The crude material obtained by the treatment of the mixture of **1** and **2** with silica and methanol for 60 min