

Supporting Informations

**Three New Cytotoxic Steroidal Glycosides Isolated from *Conus pulicarius*
Collected in Kosrae, Micronesia**

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Table S1. Complete NMR data of **3** in methanol-*d*₄

position	$\delta^{13}\text{C}$	$\delta^1\text{H}$ (mult, <i>J</i> in Hz)	COSY	HMBC ^c	NOESY
1 α	37.6	1.23 (m)	1 β	2	2 α , 3
1 β		1.88 (m)	1 α		19
2 α	29.7	2.07 (brd, 12.9)	2 β		1 α , 3
2 β		1.65 (m)	2 α		4β, 19
3	79.3	4.21 (dddd, 16.0, 13.0, 4.8, 4.8)	4 α , 4 β		1α, 2α, 4α, 4β
4 α	40.4	2.61 (dd, 13.0, 4.8)	3	2, 3, 5, 6, 10	3, 6
4 β		2.40 (dd, 13.0, 13.0)	3	3, 5, 6	2β, 3, 19
5	148.2				
6	122.0	5.74 (dd, 5.5, 1.5)	7	7, 8	4α, 7, 1'
7	70.1	3.98 (brs)	6	5, 6, 9, 1'	6, 8, 15α, 1'
8	38.5	1.55 (ovl)	14		7, 11β, 18
9	43.0	1.54 (ovl)			12α, 14
10	38.7				
11 α	21.8	1.54 (ovl)	11 β		
11 β		1.21 (ovl)	11 α , 12 β	9	8, 18
12 α	40.0	1.23 (ovl)	12 β		9, 14
12 β		1.93 (m)	11 β , 12 α	13	
13	43.0				
14	49.8	1.72 (m)	8	8, 15	12α, 17
15 α	24.6	1.97 (ovl)	15 β , 16 β	16	
15 β		1.10 (m)	15 α		7, 1'
16 α	29.0	1.98 (ovl)	16 β	13, 17, 20	
16 β		1.44 (m)	15 α , 16 α , 17		
17	53.3	1.57 (ovl)	16 β		14, 20, 22
18	11.9	0.75 (s)		12, 13, 14, 17	8, 11β
19	18.5	1.03 (s)		1, 5, 9, 10	2β, 4β
20	40.1	1.97 (m)	21	21	22
21	13.3	0.76 (d, 6.8)	20	17, 20, 22	
22	80.8	4.12 (brs)		17, 20, 21, 23	17, 20
23	215.0				
24	48.5	2.38 (dd 18.3, 6.8)	25	23, 25, 26, 27	25
		1.96 (ovl)			
25	25.4	2.12 (m)	24, 26, 27	24	24
26	22.9	0.91 (d, 6.8)	25	24, 25, 27	
27	23.0	0.93 (d, 6.8)	25	24, 25, 26	
1'	101.3	4.40 (d, 7.4)	2'	7, 5'	6, 7, 3', 5β
2'	75.2	3.10 (dd, 8.9, 7.4)	1', 3'	1', 3'	4'
3'	77.9	3.31 (ovl)	2', 4'	2', 4', 5'	1', 5β

4'	71.4	3.46 (ddd, 10.0, 9.0, 5.3)	3', 5'	3', 5'	2'
5' α	66.8	3.83 (dd, 11.4, 5.3)	4'	1', 3', 4'	
5' β		3.19 (dd, 11.4, 10.0)	4'	1', 3', 4'	1', 3'

Table S2. Complete NMR data of **4** in methanol-*d*₄

position	$\delta^{13}\text{C}$	$\delta^1\text{H}$ (mult, <i>J</i> in Hz)	COSY	HMBC ^c	NOESY
1 α	37.7	1.22 (m)	1 β , 2 β	2	2 α , 3
1 β		1.86 (m)	1 α		19
2 α	29.7	2.07 (brd, 12.0)	2 β , 1 α		1 α , 3
2 β		1.65(m)	2 α , 3		1 α , 4β , 19
3	79.3	4.20 (dddd, 15.0, 13.1, 5.5, 5.2)	2 β , 4 α , 4 β		1α , 2 α , 4 α
4 α	40.4	2.61 (dd, 13.1, 5.2)	3	2, 3, 5, 6	3, 6
4 β		2.42 (dd, 13.1, 13.1)	3	3, 5	2β , 19
5	148.1				
6	122.1	5.74 (dd, 5.0, 1.3)	7	8	4α , 1'
7	70.1	4.00 (brs)	6, 8	5, 6	15 α , 1'
8	38.7	1.53 (ovl)	7, 14		18
9	43.0	1.54 (ovl)			12α , 14
10	38.4				
11 α	21.8	1.54 (ovl)	11 β		
11 β		1.29 (ovl)	11 α , 12 β	9	12 β , 18
12 α	40.5	1.22 (ovl)	12 β		9 , 14
12 β		1.98 (brd, 12.4)	11 β , 12 α	13	18
13	43.0				
14	49.8	1.68 (m)	8	9	9 , 12α
15 α	24.7	1.95 (ovl)	15 β , 16 β	13, 14	
15 β		1.09 (m)	15 α		7 , 1'
16 α	28.9	1.95 (m)	16 β	20	
16 β		1.25 (ovl)	15 α , 16 α		17, 22
17	53.4	1.56 (ovl)			16 β , 22
18	11.8	0.71 (s)		12, 13, 14, 17	8 , 11β , 12 β
19	18.6	1.02 (s)		1, 5, 9, 10	1 β , 2β , 4β
20	38.9	1.53 (m)	21		
21	12.6	0.91 (d 6.4)	20	17, 20, 22	23
22	78.2	3.31 (ovl)	23		16 β , 17 , 23
23	72.2	3.55 (ddd 10.5, 8.2, 2.6)	22, 24		21, 22
24	43.3	1.14 (ddd 13.6, 10.5, 2.6)	23, 25		
		1.24 (ovl)		23, 25, 26, 27	
25	25.3	1.86 (m)	24, 26, 27	24	
26	21.7	0.92 (d, 6.6)	25	24, 25, 27	
27	24.5	0.94(d, 6.7)	25	24, 25, 26	
1'	101.3	4.40 (d, 7.4)	2'	7	6 , 7 , 3' , 5'β
2'	75.2	3.10 (dd, 8.9, 7.4)	1', 3'	1', 3'	3' , 4'
3'	77.8	3.33 (ovl)	2', 4'	2'	1' , 5'β

4'	71.4	3.46 (ddd, 10.2, 9.4, 5.3)	3', 5'		2'
5' α	66.8	3.83 (dd, 11.4, 5.3)	4'	1', 4'	4'
5' β		3.19 (dd, 11.4, 10.2)	4'	1', 3', 4'	1', 3'

Table S3. Complete NMR data of **5** in methanol-*d*₄

position	$\delta^{13}\text{C}$	$\delta^1\text{H}$ (mult, <i>J</i> in Hz)	COSY	HMBC ^c	NOESY
1 α	37.7	1.22(m)	1 β , 2 β	2	2 β , 3
1 β		1.88 (m)	1 α		19
2 α	29.8	2.07 (brd, 12.4)	2 β , 1 α		1 α , 2 β , 3,
2 β		1.64(m)	2 α , 3		1 α , 19
3	79.3	4.20 (dddd, 16.0, 13.1, 4.5, 4.5)	2 β , 4 α , 4 β		1α , 2 α , 4 α
4 α	40.4	2.61 (dd, 13.1, 4.5)	3	3, 5	3, 6
4 β		2.42 (dd, 13.1, 13.1)	3	2, 3, 5, 6	3, 19
5	148.2				
6	122.1	5.73 (dd, 4.9, 1.3)	7	8	4α , 7, 1'
7	70.2	3.96 (brs)	6, 8	5, 6	6, 1'
8	38.4	1.53 (ovl)	7, 14		18
9	43.0	1.54 (ovl)			14
10	38.7				
11 α	21.8	1.54 (ovl)	11 β		
11 β		1.29 (ovl)	11 α , 12 β	9	18, 19
12 α	40.4	1.21 (ovl)	12 β		
12 β		2.00 (brd, 12.4)	11 β , 12 α	13	18
13	43.3				
14	49.7	1.63 (m)	8	9	9, 17
15 α	24.8	1.92 (ovl)	15 β , 16 β	13, 14	17
15 β		1.05 (m)	15 α		18
16 α	29.6	2.05 (m)	16 β	20	
16 β		1.21 (ovl)	15 α , 16 α		
17	58.2	1.15 (m)			14, 15α
18	11.9	0.70 (s)		12, 13, 14, 17	8, 11β, 12β, 15β
19	18.6	1.02 (s)		1, 5, 9, 10	1 β , 2β, 4β, 11β
20	35.2	1.44 (m)	21		
21	20.0	0.98 (d, 6.4)	20	17, 20, 22	
22	46.3	1.44 (ovl)	23		
		1.54 (ovl)		17, 20, 21, 23	23
23	69.1	3.69 (m)	22, 24		22 24
24	475	1.22 (ovl)	23, 25		23
		1.25 (ovl)		23, 25, 26, 27	
25	25.5	1.84 (m)	24, 26, 27	24	
26	22.0	0.90 (d, 6.7)	25	24, 25, 27	
27	24.3	0.92 (d, 6.7)	25	24, 25, 26	
1'	101.3	4.40 (d, 7.5)	2'	7	6, 7, 3', 5'β
2'	75.2	3.10 (dd, 8.9, 7.5)	1', 3'	1', 3'	3', 4'

3'	77.9	3.32 (ovl)	2', 4'	2'	2', 1'
4'	71.4	3.47 (ddd, 9.9, 8.9, 5.3)	3', 5'		2', 5'
5' α	66.8	3.83 (dd, 11.4, 5.3)	4'	1', 4'	4'
5' β		3.19 (dd, 11.4, 9.9)	4'	1', 3', 4'	1'

Figure S1. ^1H and ^{13}C NMR Spectra (500 MHz and 125 MHz, chloroform-*d*) of **1**

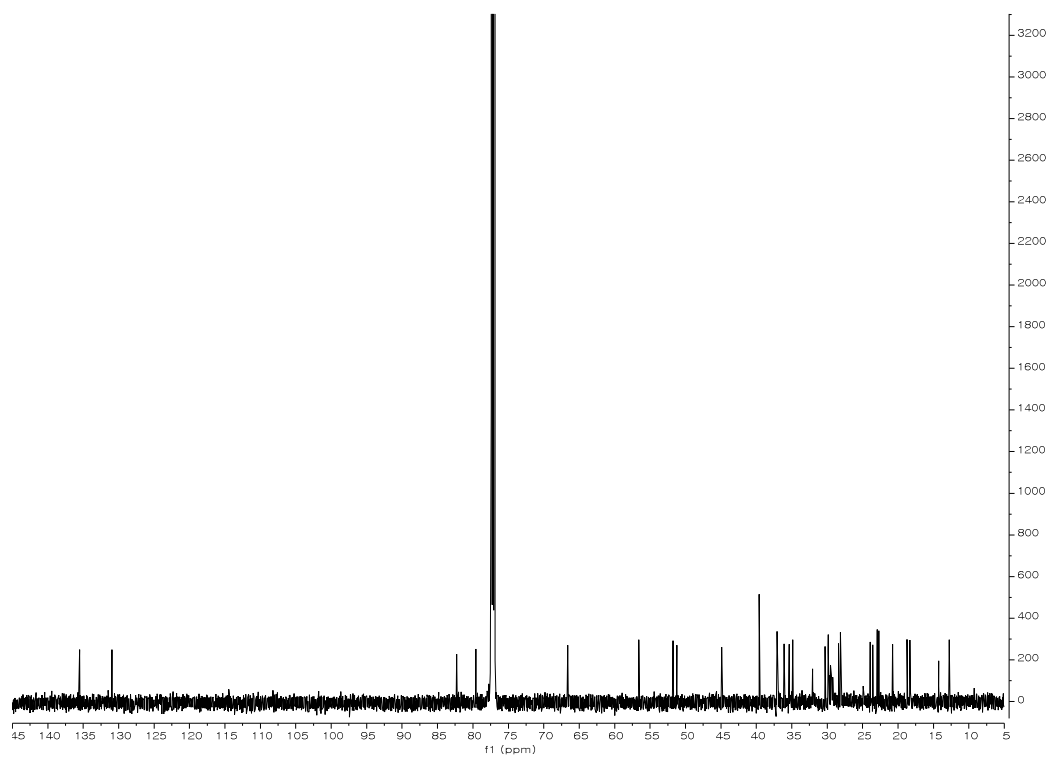
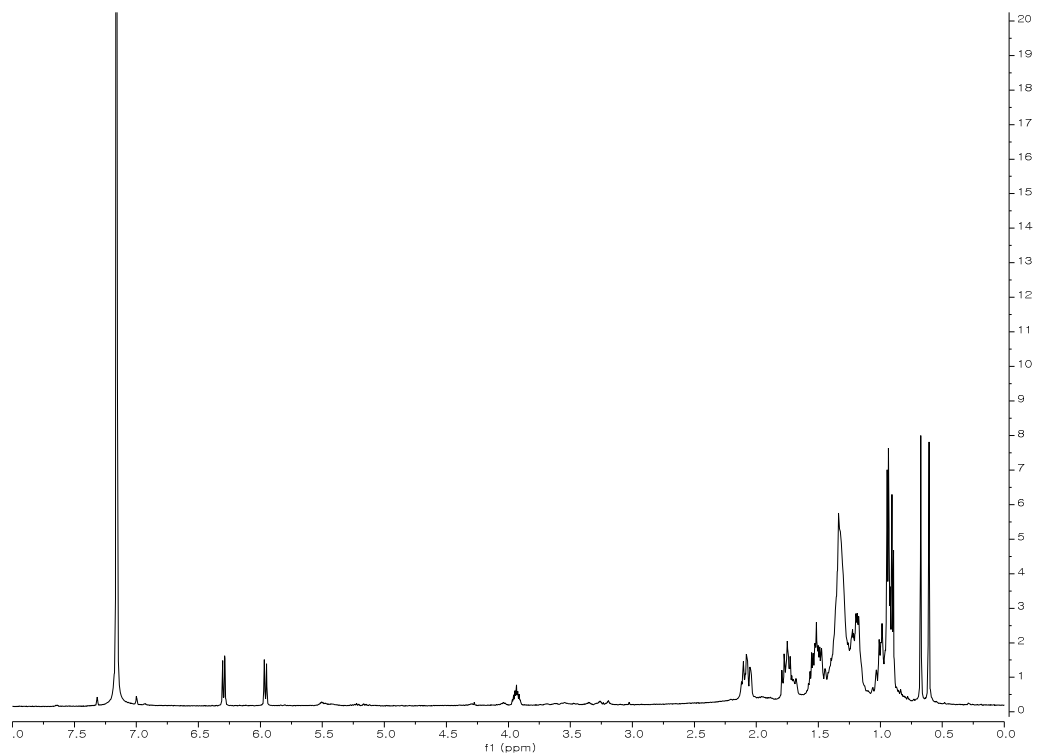


Figure S2. ^1H and ^{13}C NMR Spectra (500 MHz and 125 MHz, methanol- d_4) of **2**

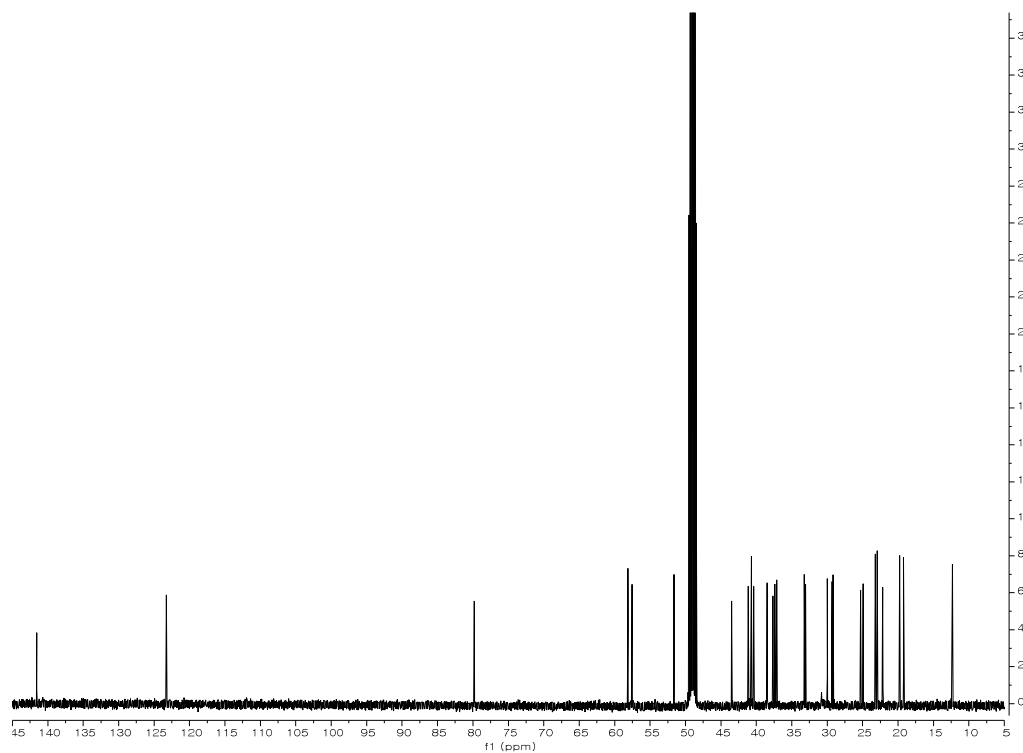
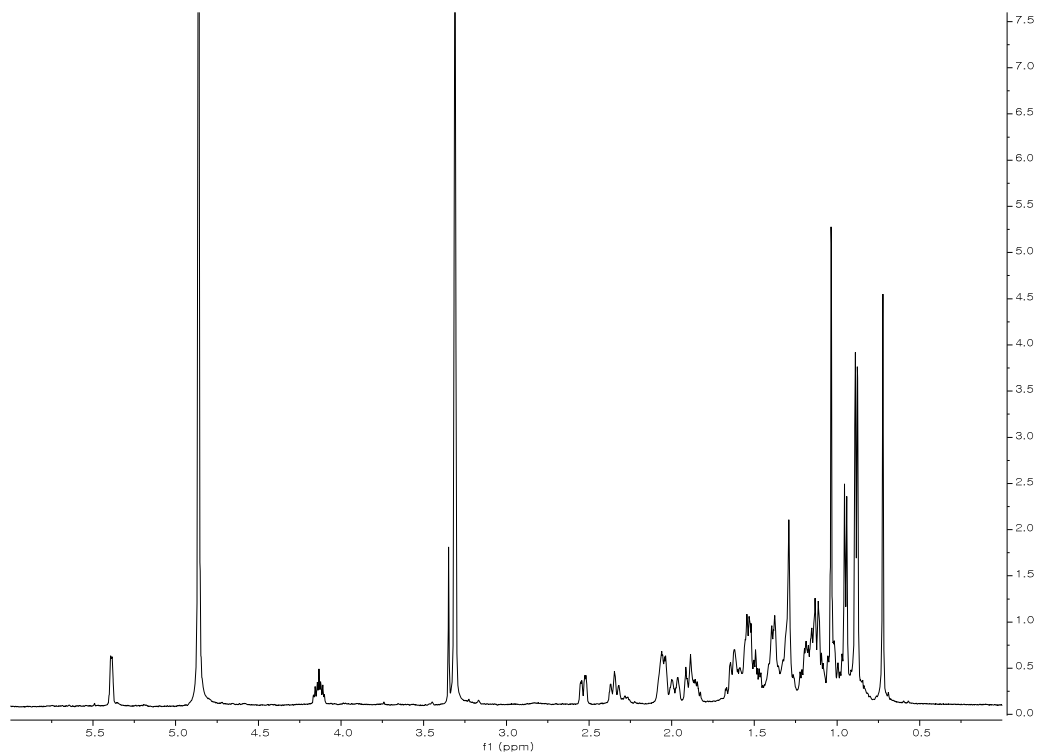


Figure S3. ^1H NMR Spectra (500 MHz, $\text{DMSO-}d_6$) of **2**

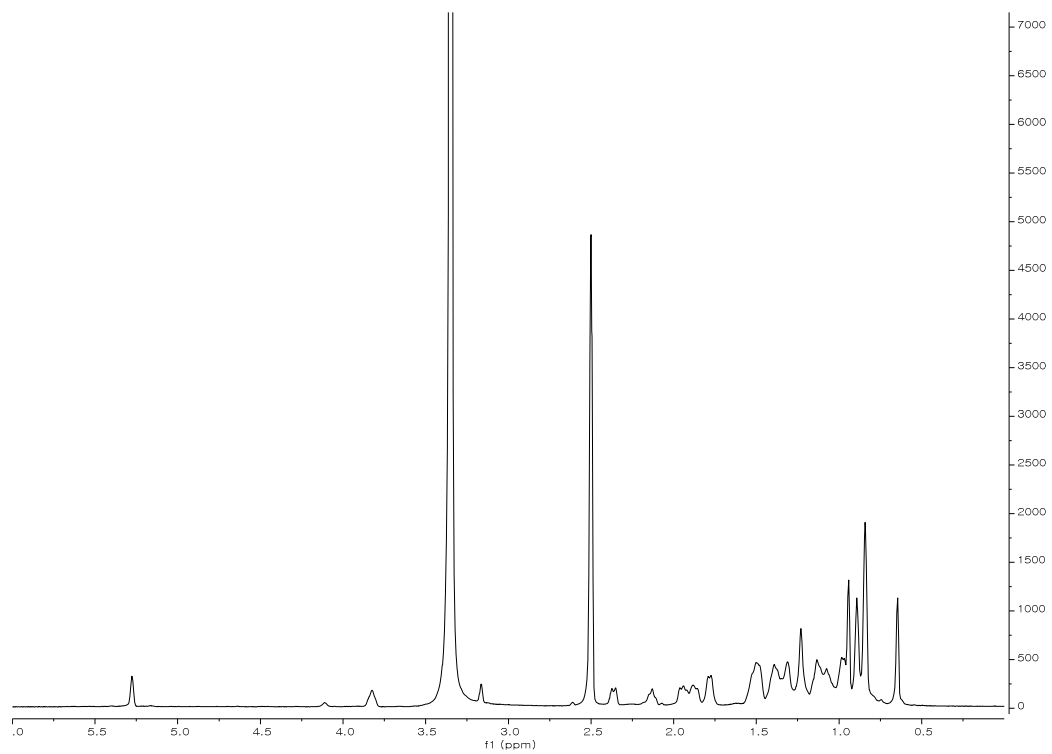


Figure S4. ^1H and ^{13}C NMR Spectra (500 MHz and 125 MHz, methanol- d_4) of **3**

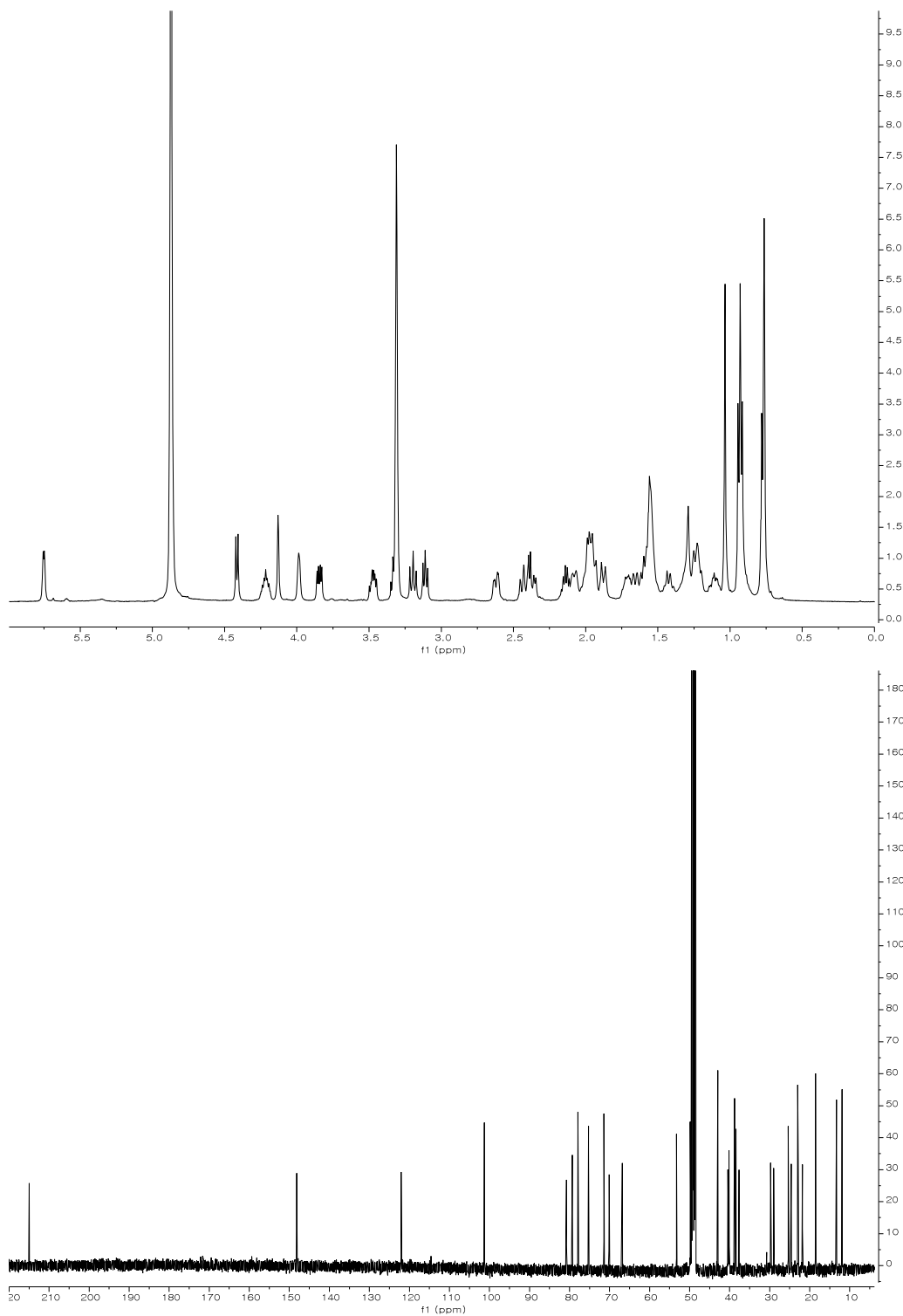


Figure S5. HMBC and HSQC NMR spectra of **3**

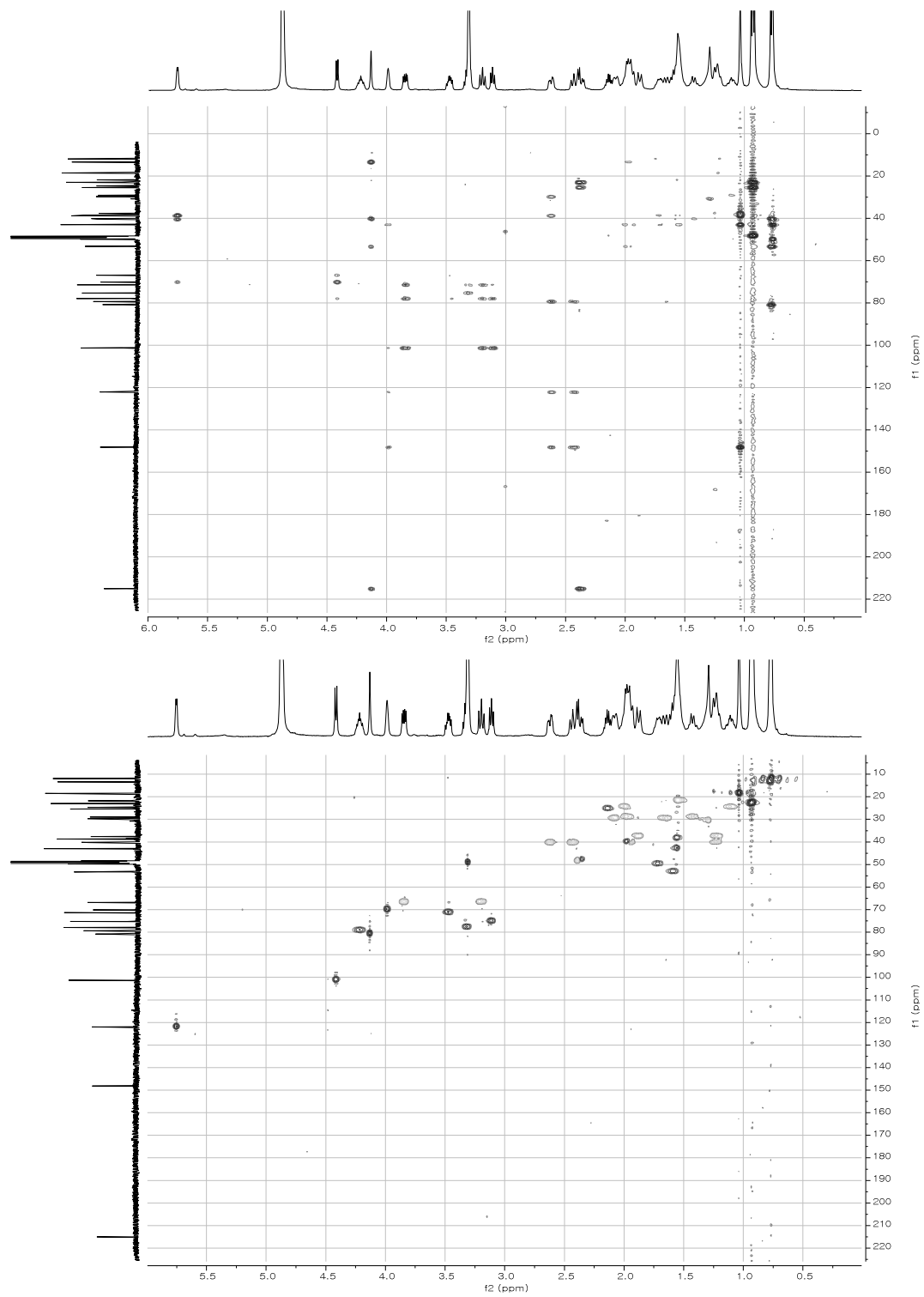


Figure S6. COSY and NOESY NMR spectra of **3**

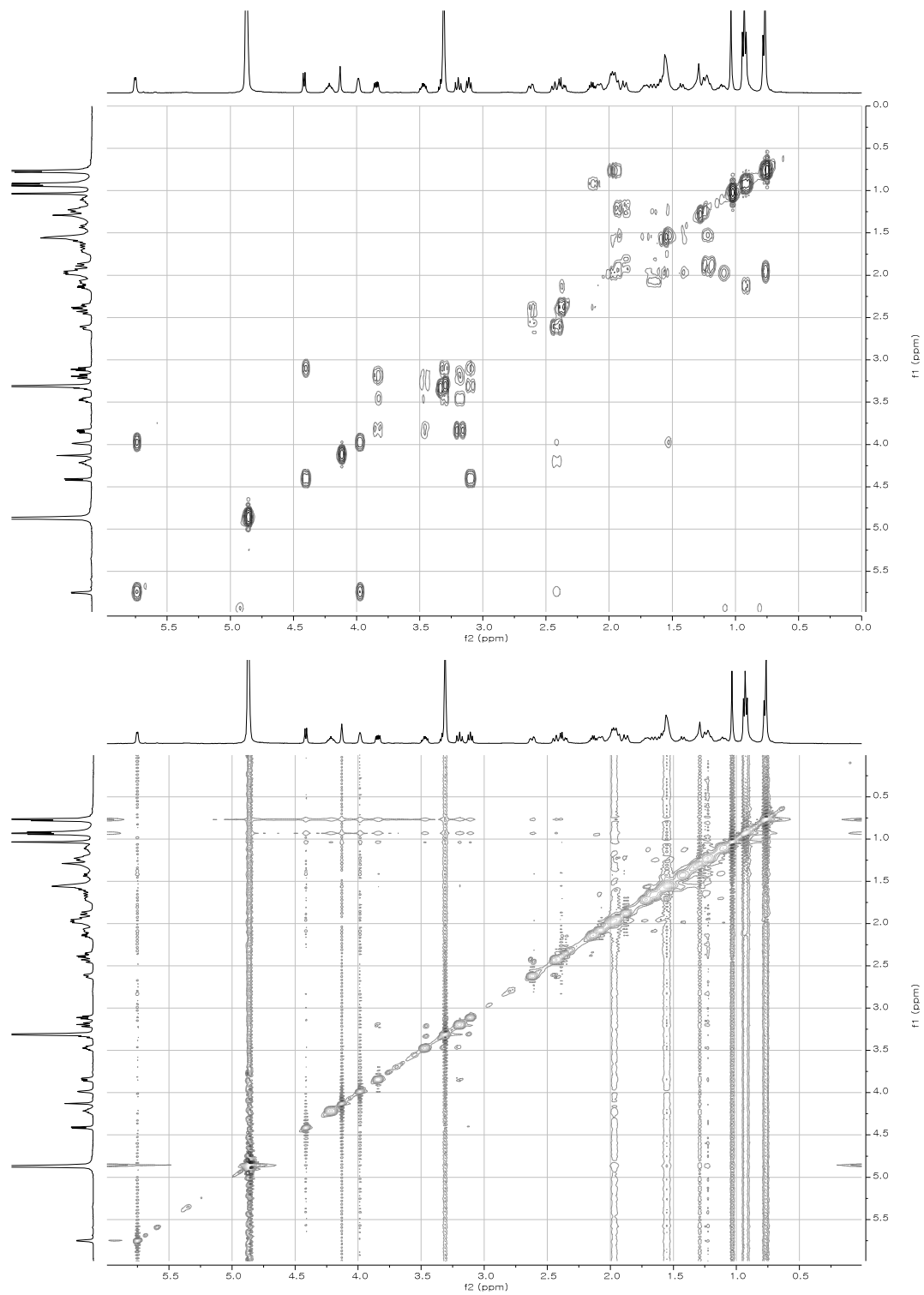


Figure S7. ^1H and ^{13}C NMR Spectra (500 MHz and 125 MHz, methanol- d_4) of **4**

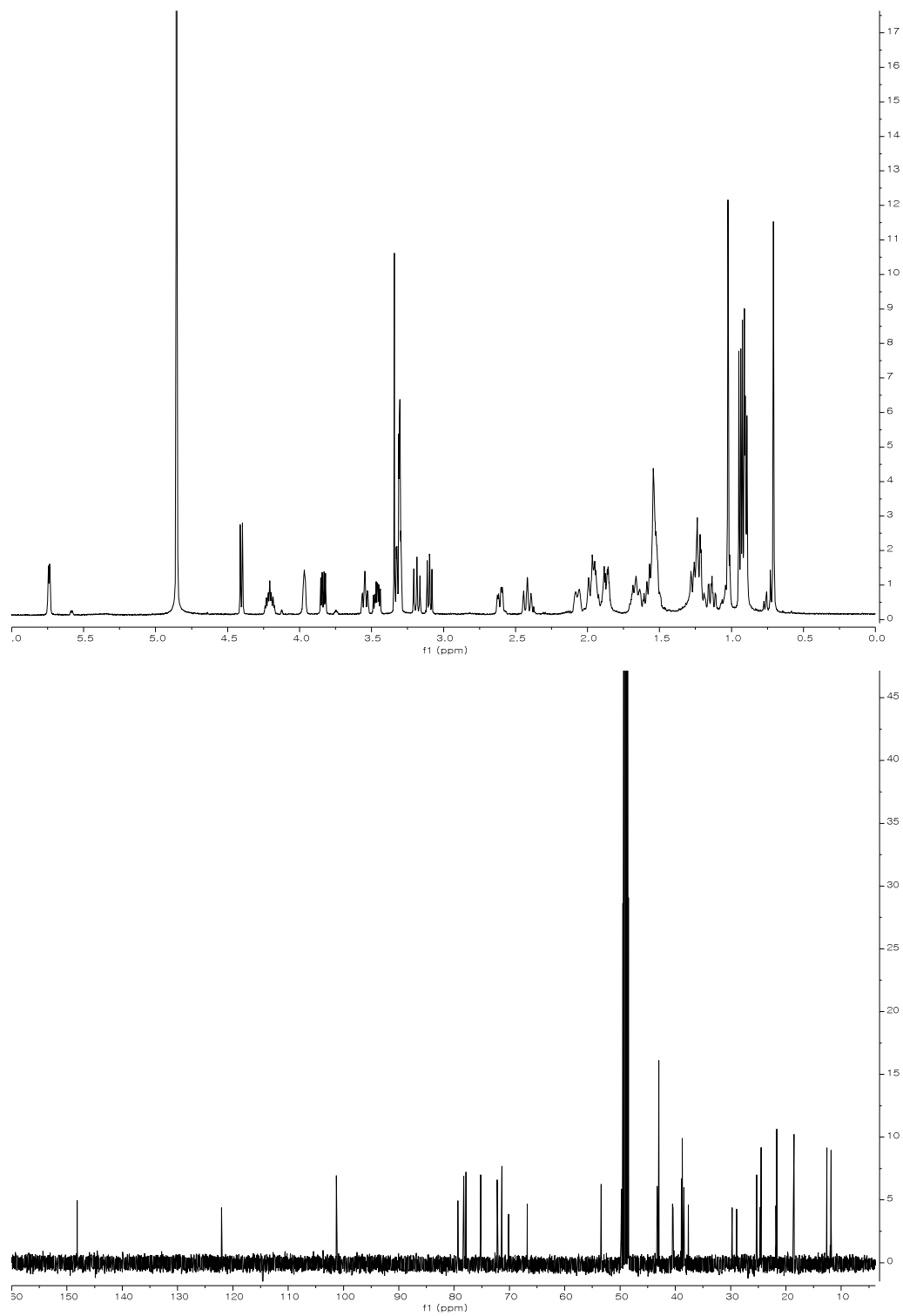


Figure S8. HMBC and HSQC NMR spectra of **4**

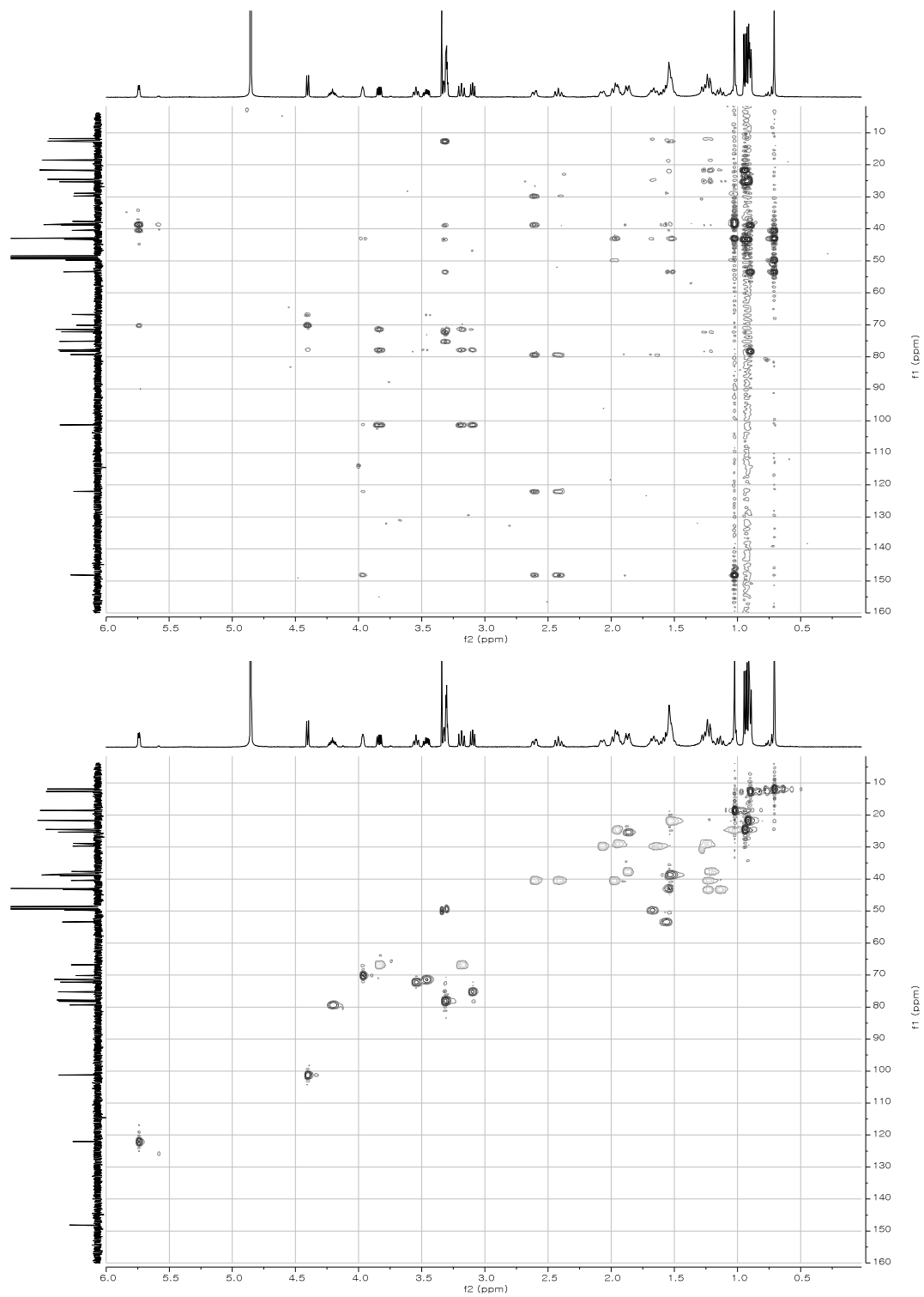


Figure S9. COSY and NOESY NMR spectra of **4**

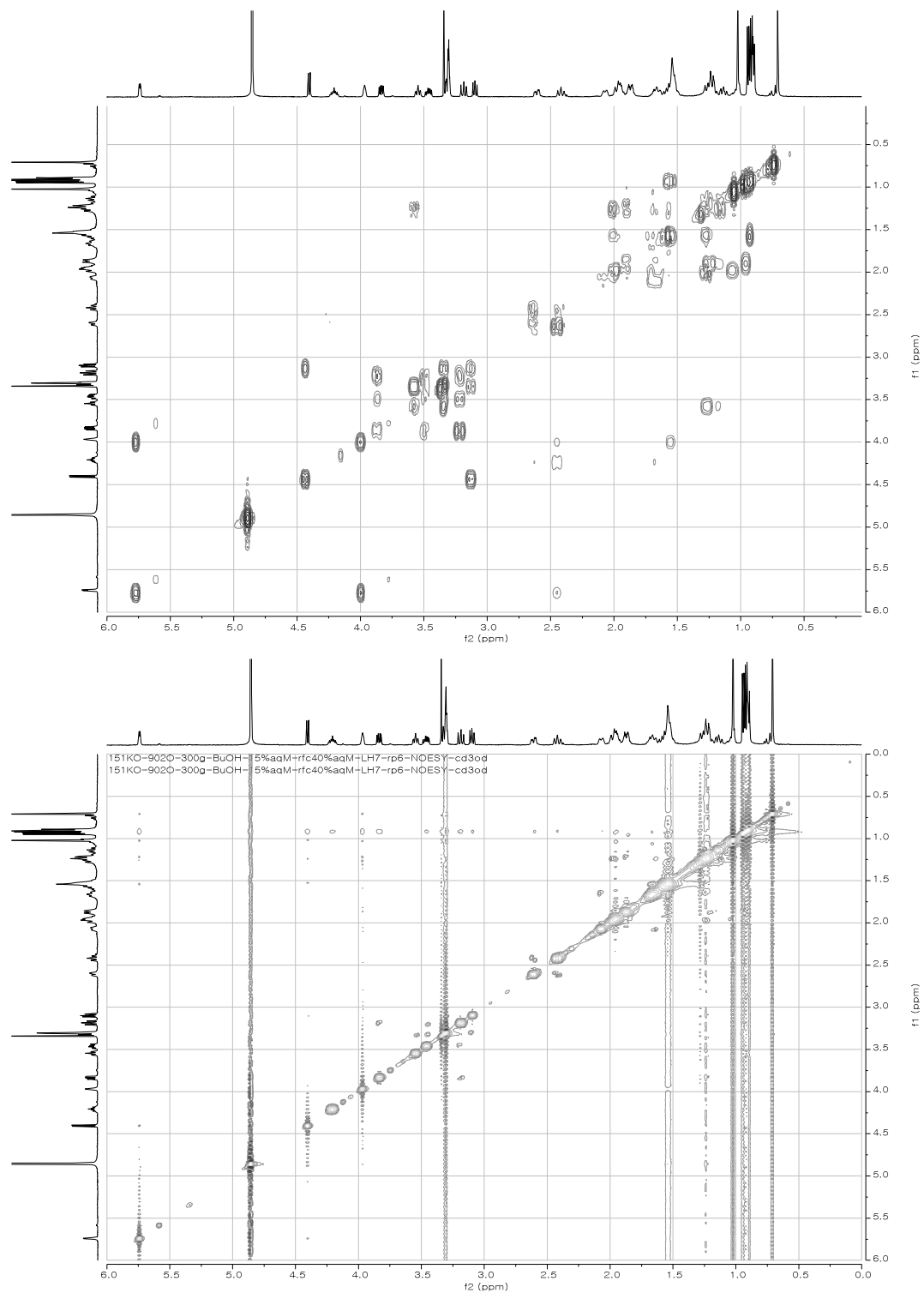


Figure S10. ^1H and ^{13}C NMR Spectra (500 MHz and 125 MHz, methanol- d_4) of **5**

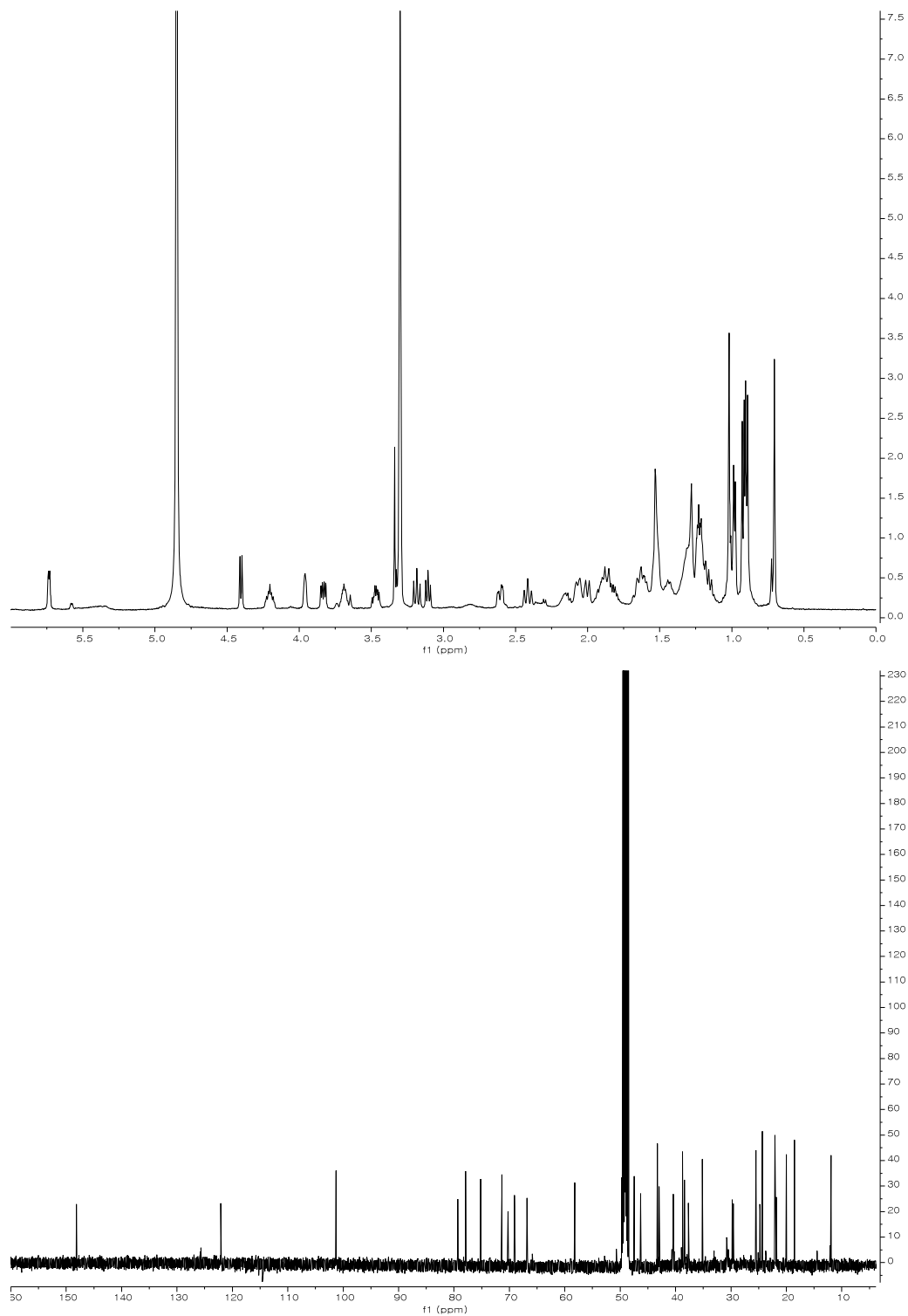


Figure S11. HMBC and HSQC NMR spectra of **5**

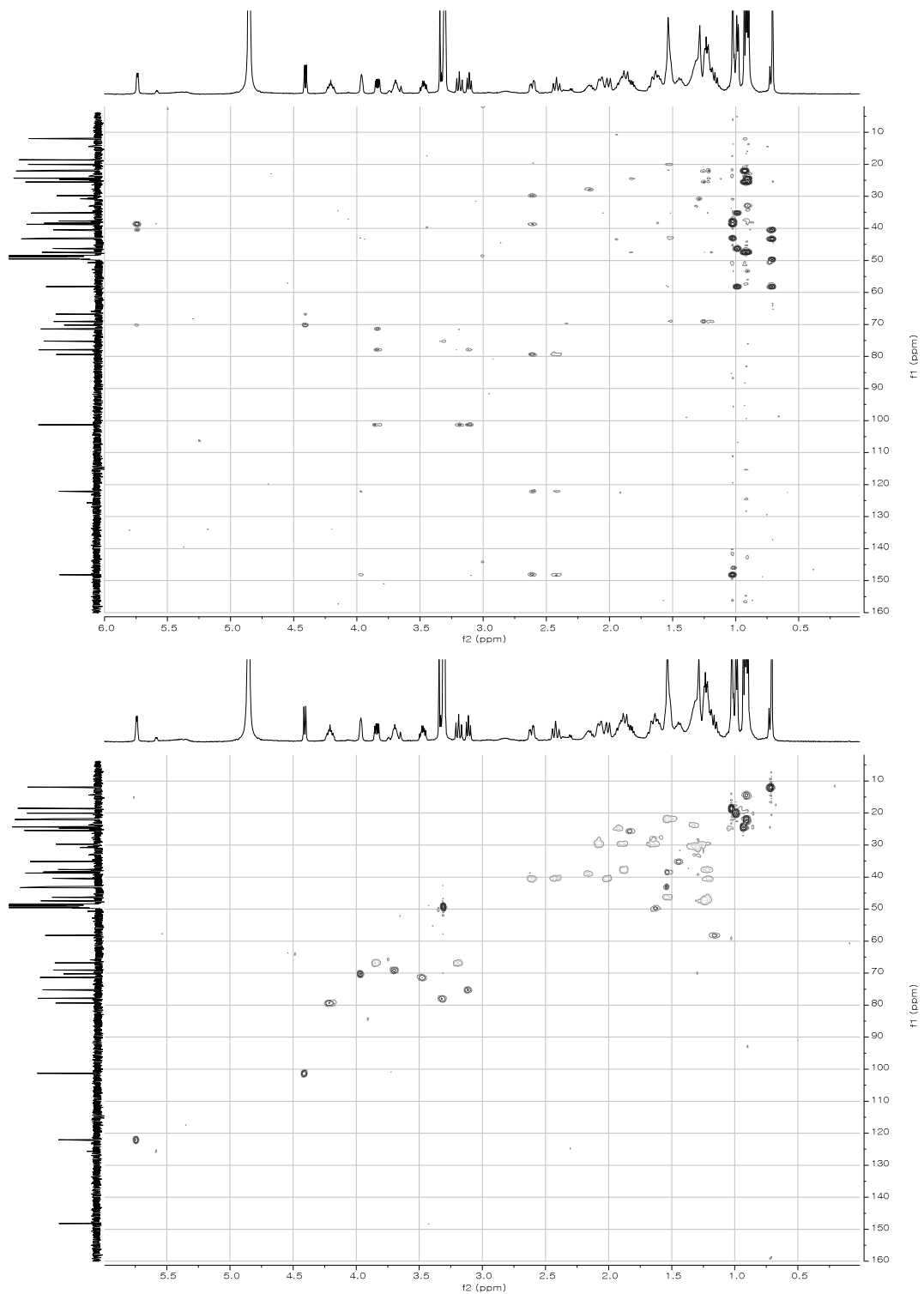


Figure S12. COSY and NOESY NMR spectra of **5**

