SUPPORTING INFORMATION

for

Additional Scalarane Sesterterpenes from the Sponge *Phyllospongia papyracea*

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TABLE OF CONTENTS

Figure S1. Underwater photo of *Phyllospongia papyracea* (Page 3)

Figure S2. Isolation scheme for pure compounds (Page 4)

Figure S3. ^{1}H NMR spectra of **1** (Page 5)

Figure S4. ^{13}C NMR spectra of **1** (Page 6)

Figure S5. ^{1}H NMR spectra of **2** (Page 7)

Figure S6. ^{13}C NMR spectra of **2** (Page 8)

Figure S7. ^{1}H NMR spectra of **3** (page 9)

Figure S8. ^{13}C NMR spectra of **3** (Page 10)

Figure S9. ^{1}H NMR spectra of **4** (Page 11)

Figure S10. ^{13}C NMR spectra of **4** (Page 12)

Figure S11. ^{1}H NMR spectra of **5** (Page 13)

Figure S12. ^{13}C NMR spectra of **5** (Page 14)

Figure S13. ^{1}H NMR spectra of **6** (Page 15)

Figure S14. ^{13}C NMR spectra of **6** (Page 16)

Figure S15. ^{1}H NMR spectra of **7** (Page 17)

Figure S16. ^{13}C NMR spectra of **7** (Page 18)

Table S1. NMR data for **1** (Page 19)

Table S2. NMR data for **2** (Page 20)

Table S3. NMR data for **3** (Page 21)

Table S4. NMR data for **4** (Page 22)

Table S5. NMR data for **5** (Page 23)

Table S6. NMR data for **6** (Page 24)

Table S7. NMR data for **7** (Page 25)

Figure S1. Underwater photo of *Phyllospongia papyracea.*

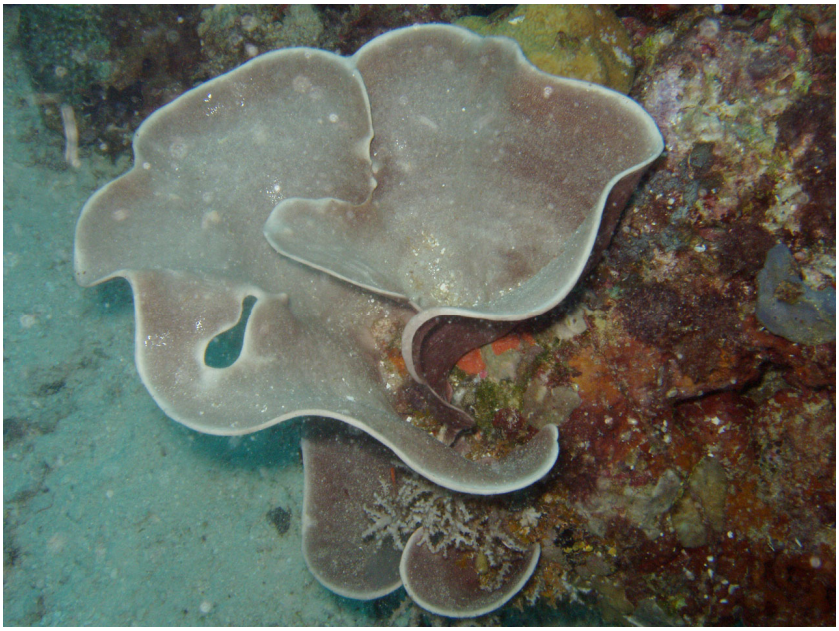

Figure S2. Isolation scheme for pure compounds.

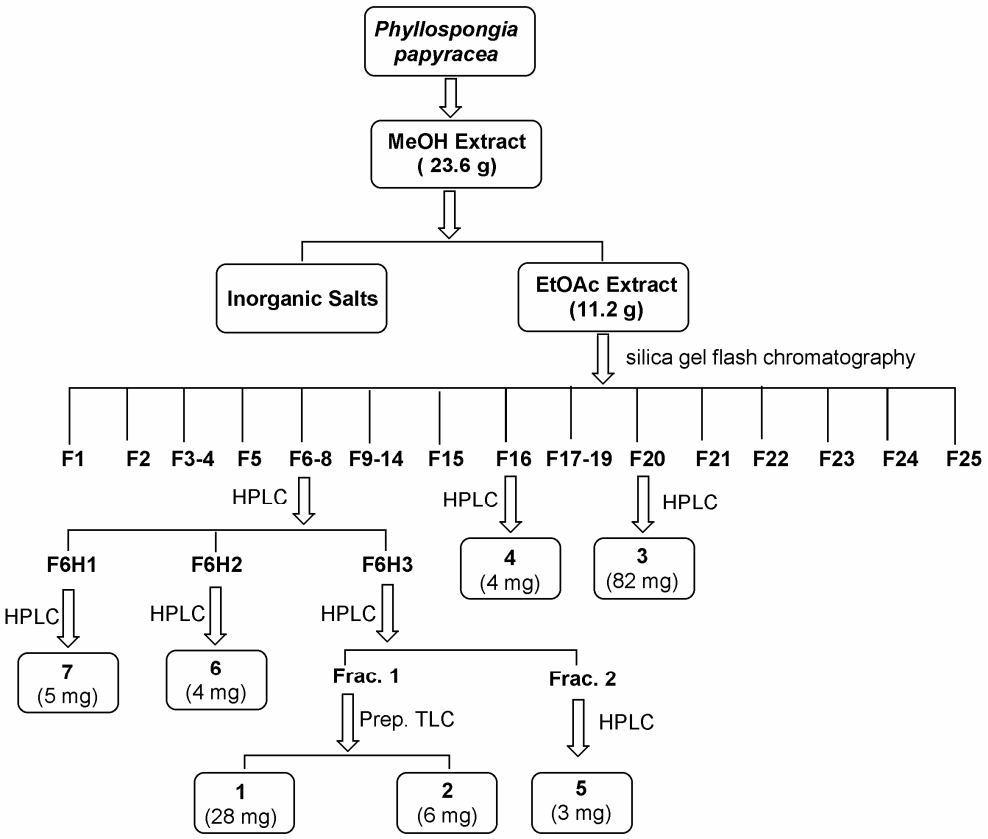

Figure S3. ^{1}H NMR spectrum of **1**.

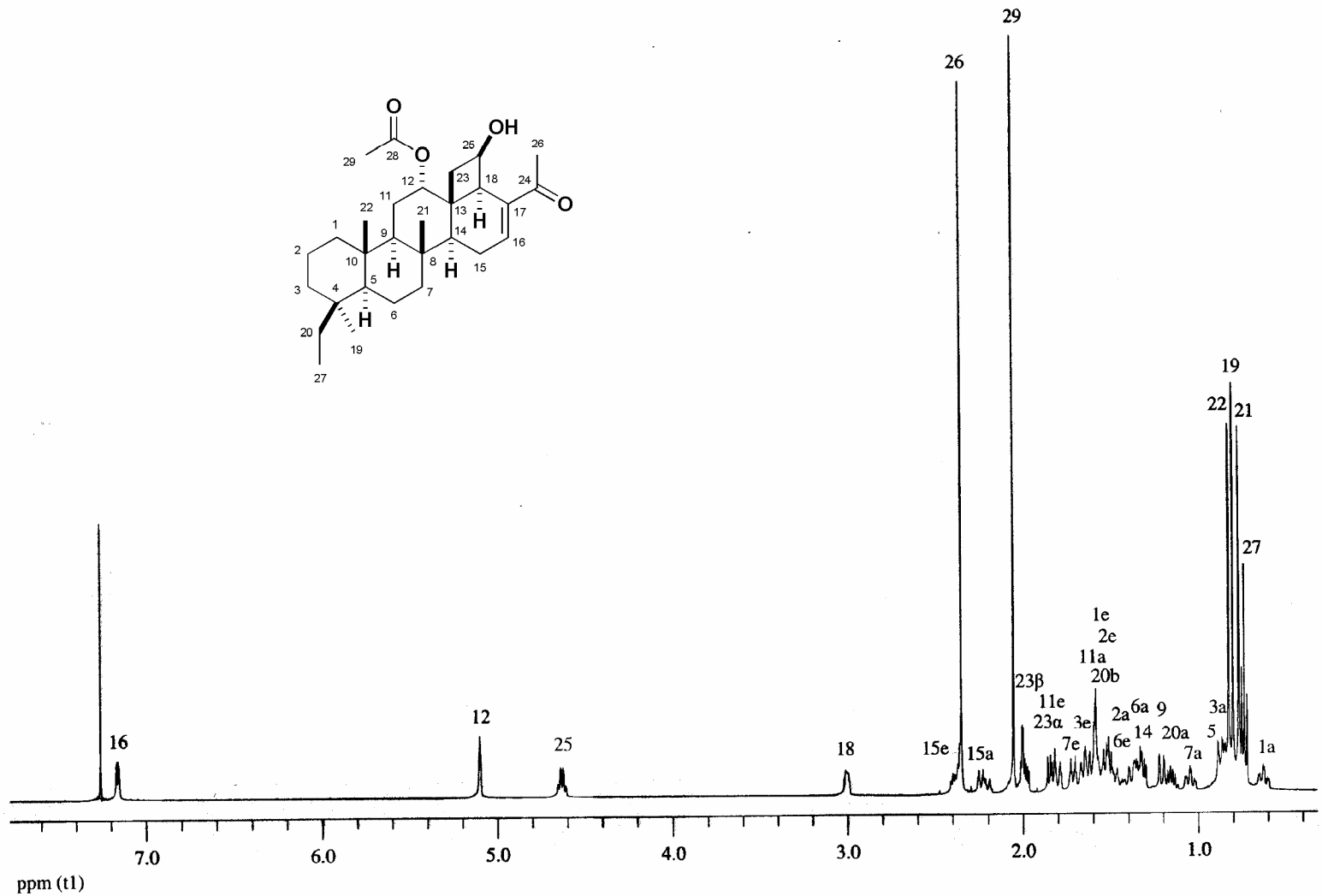

Figure S4. ^{13}C NMR spectrum of **1**.

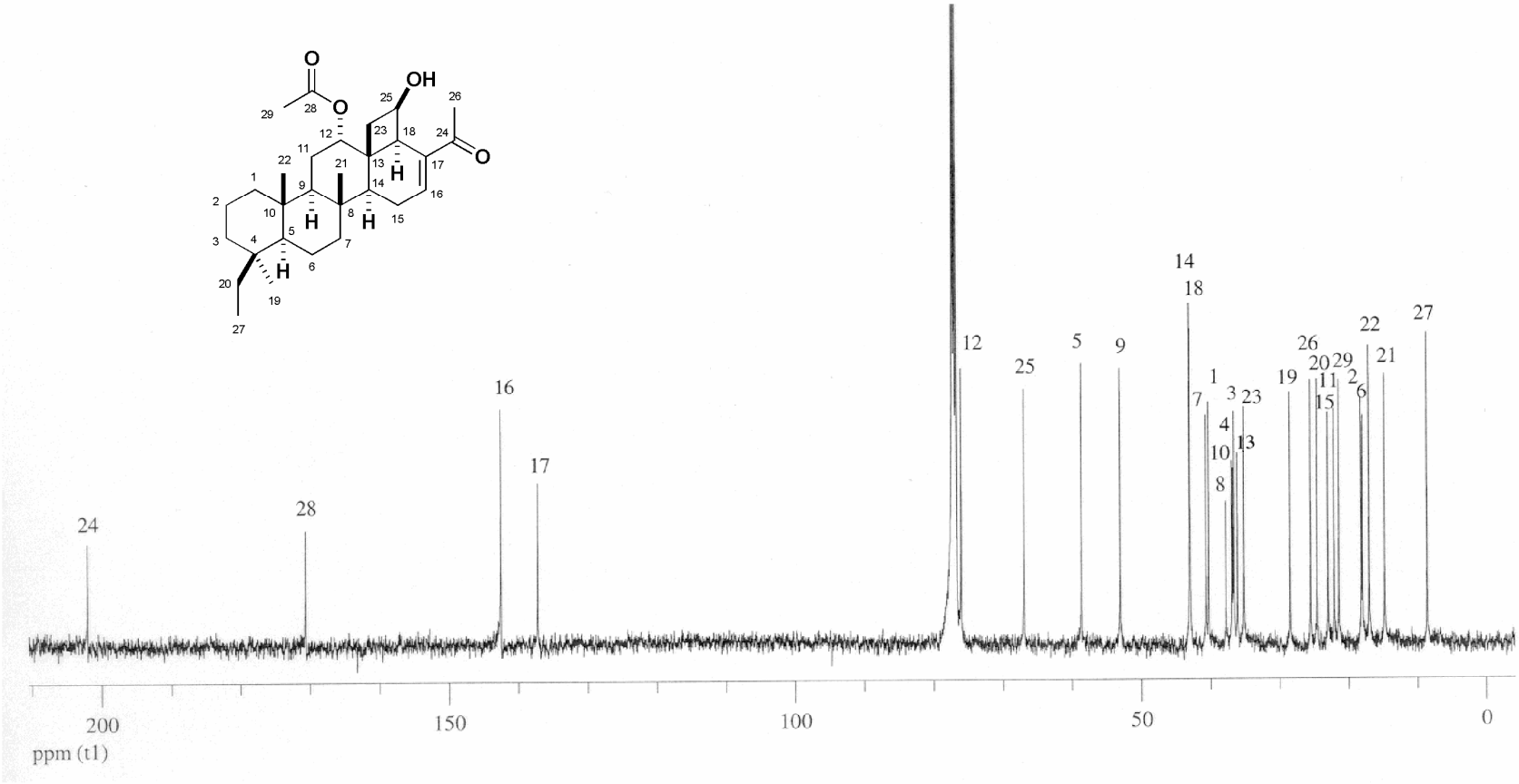

Figure S5. ^{1}H NMR spectrum of **2**.

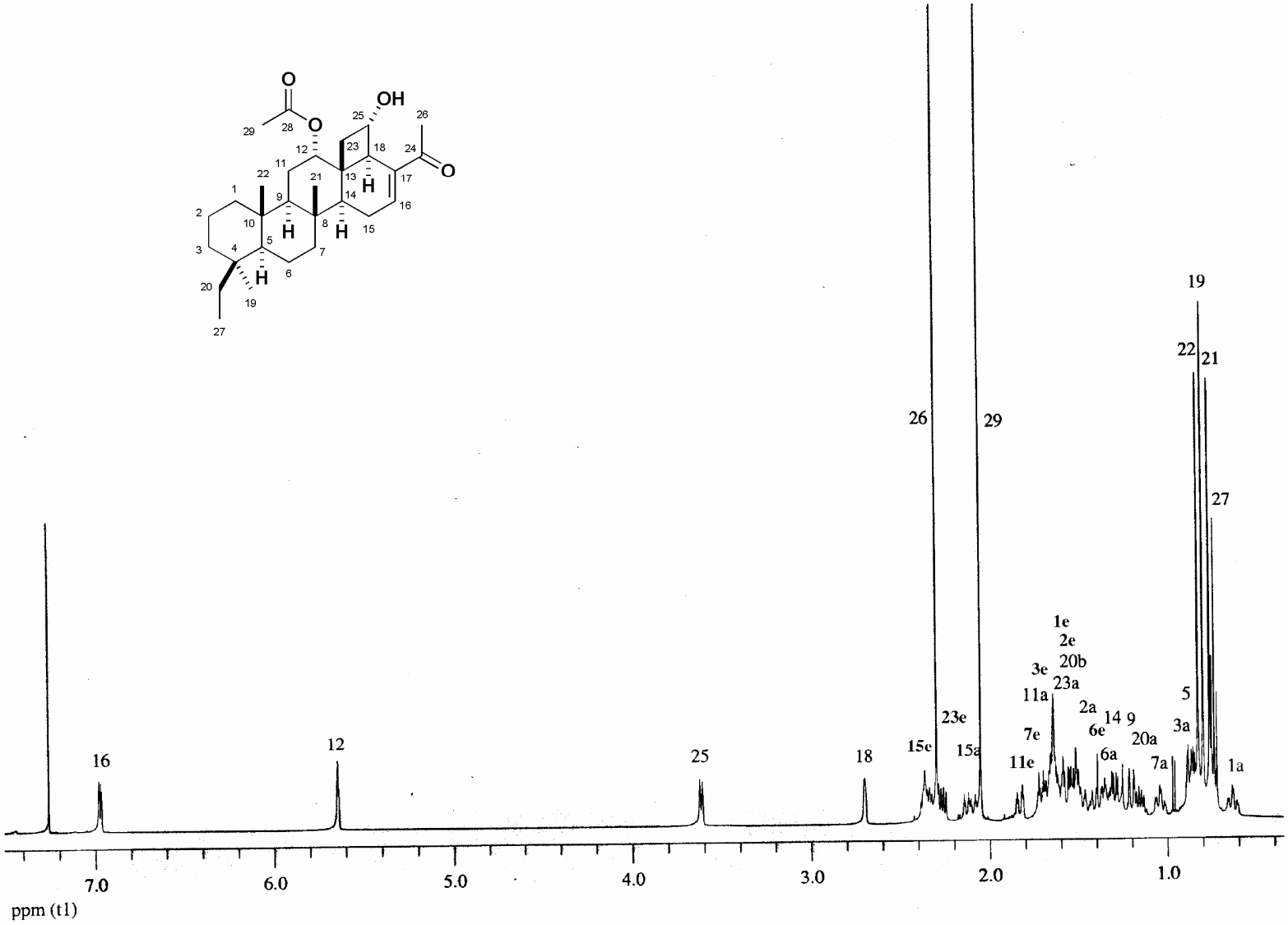

Figure S6. ^{13}C NMR spectrum of **2**.

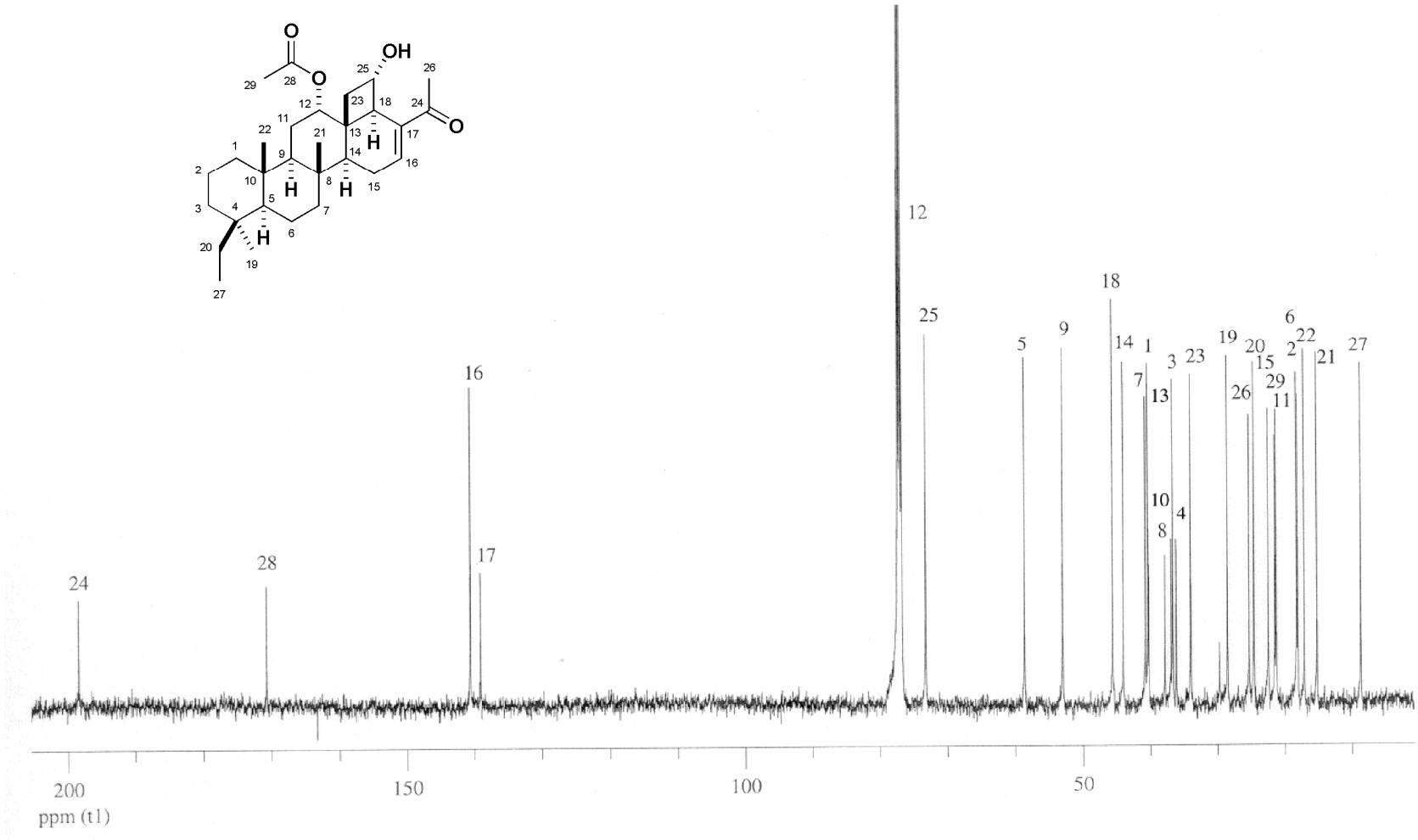

Figure S7. ^{1}H NMR spectrum of **3**.

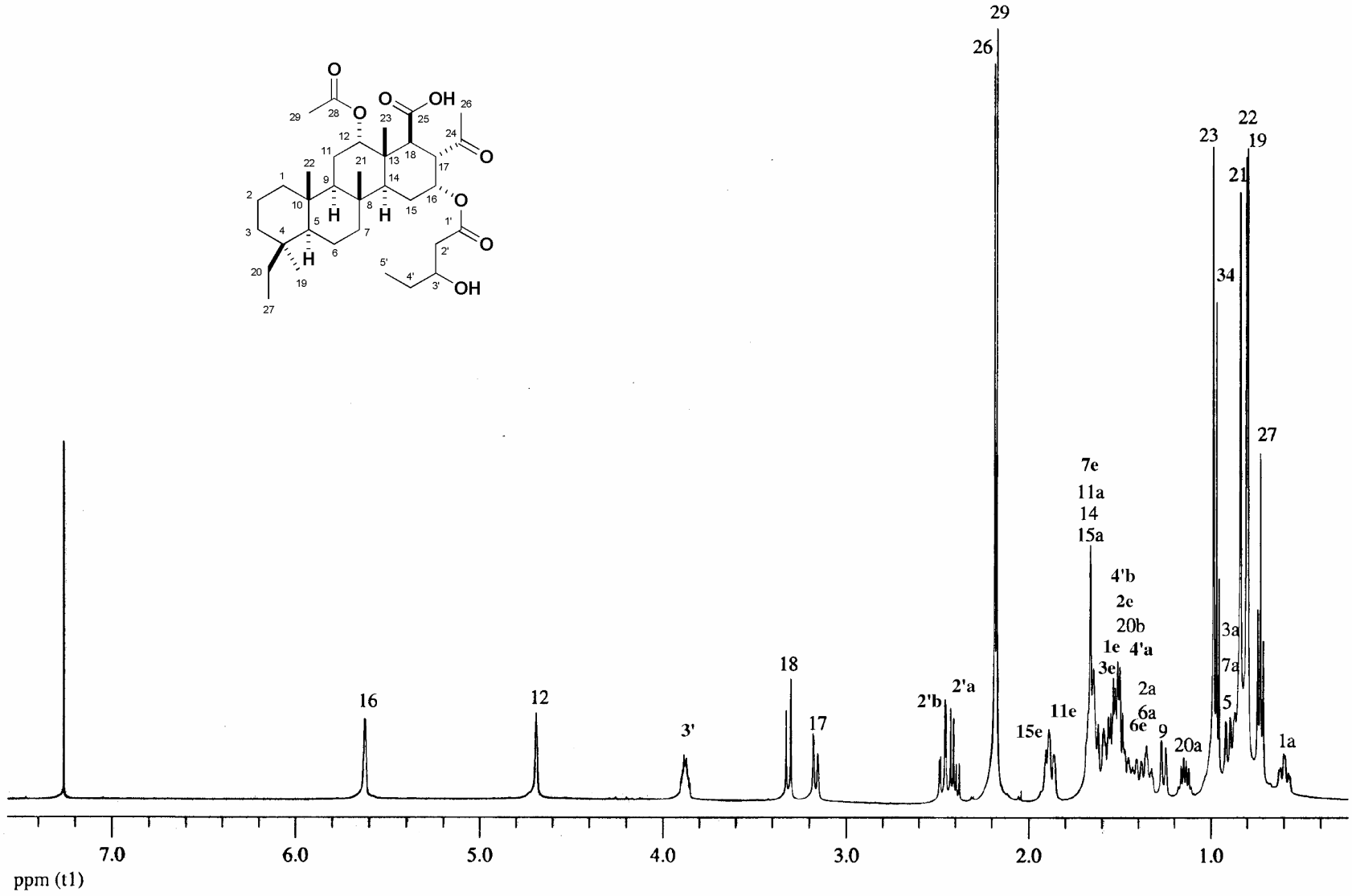

Table S8. ^{13}C NMR spectrum of **3**.

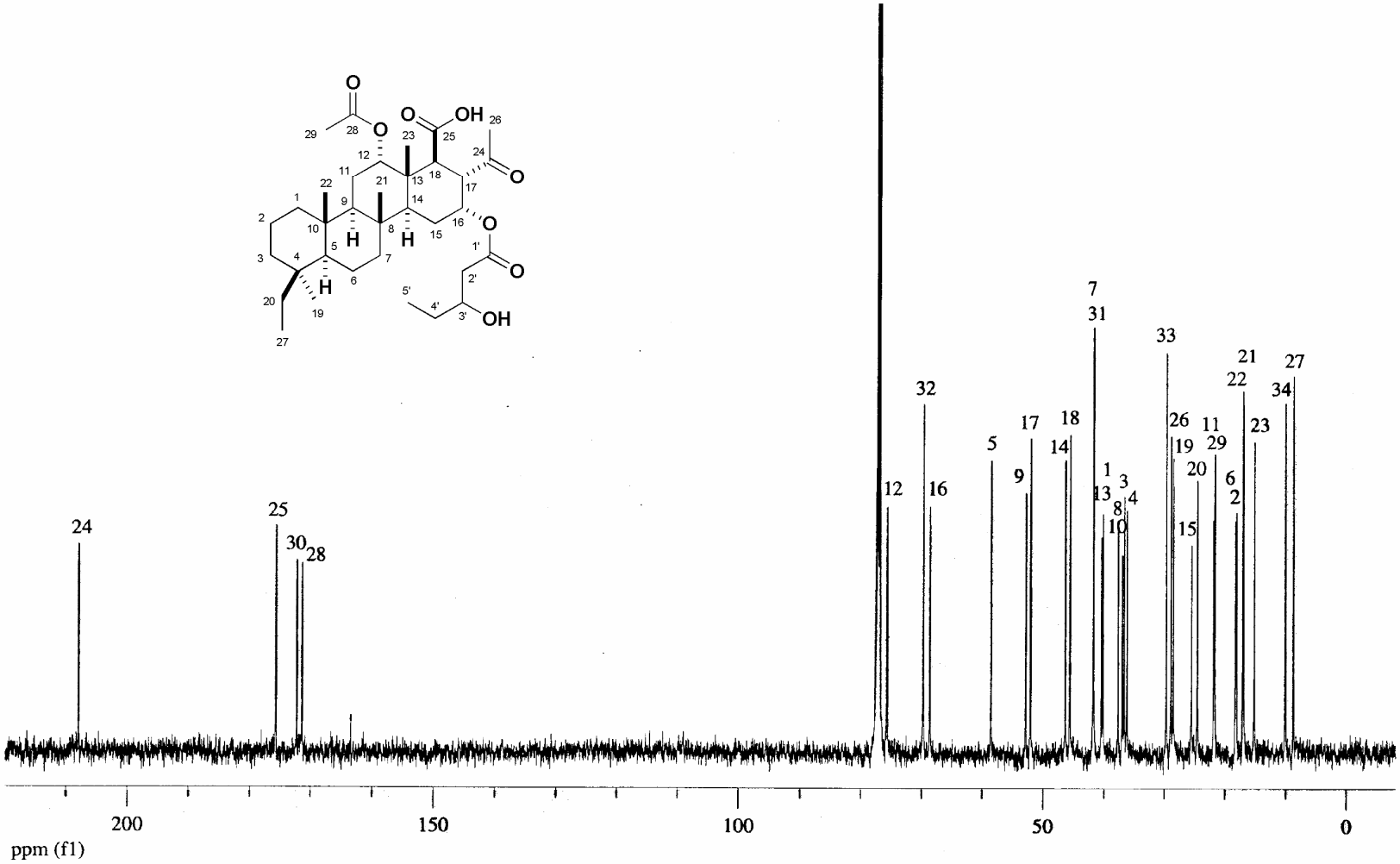

Figure S9. ^{1}H NMR spectrum of **4**.

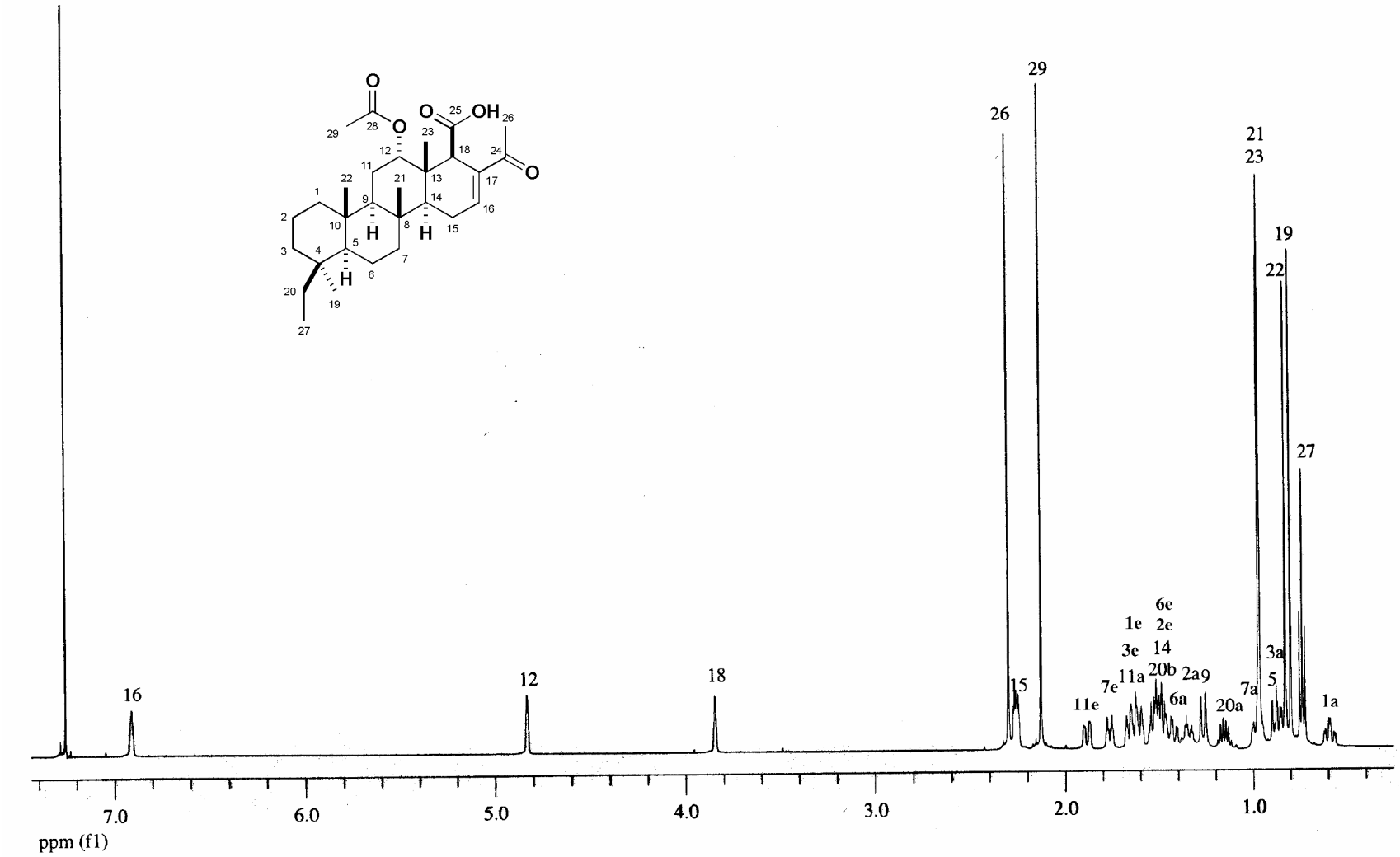

Figure S10. ^{13}C NMR spectrum of **4**.

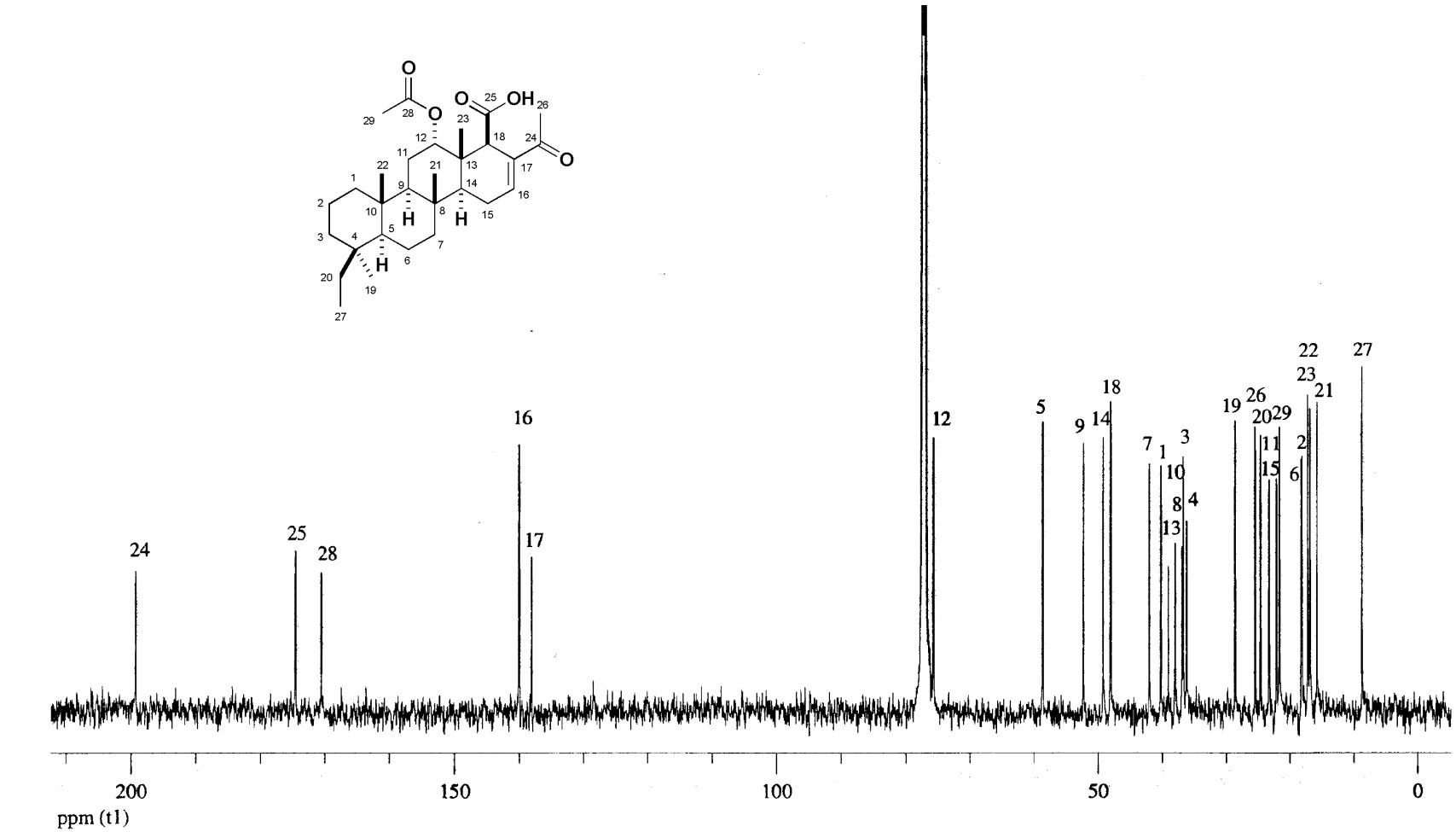

Figure S11. ^{1}H NMR spectrum of **5**.

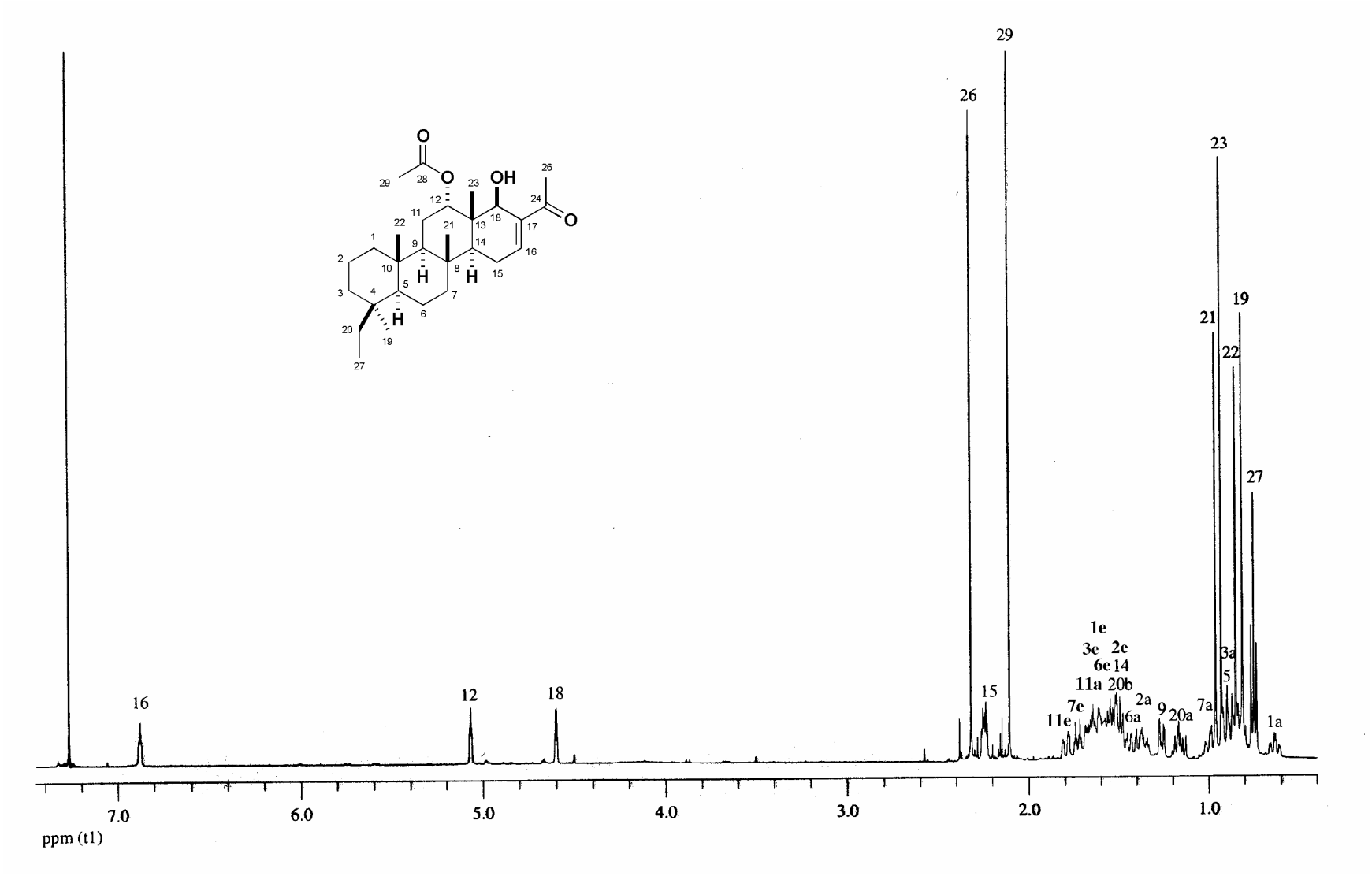

Figure S12. ^{13}C NMR spectrum of **5**.

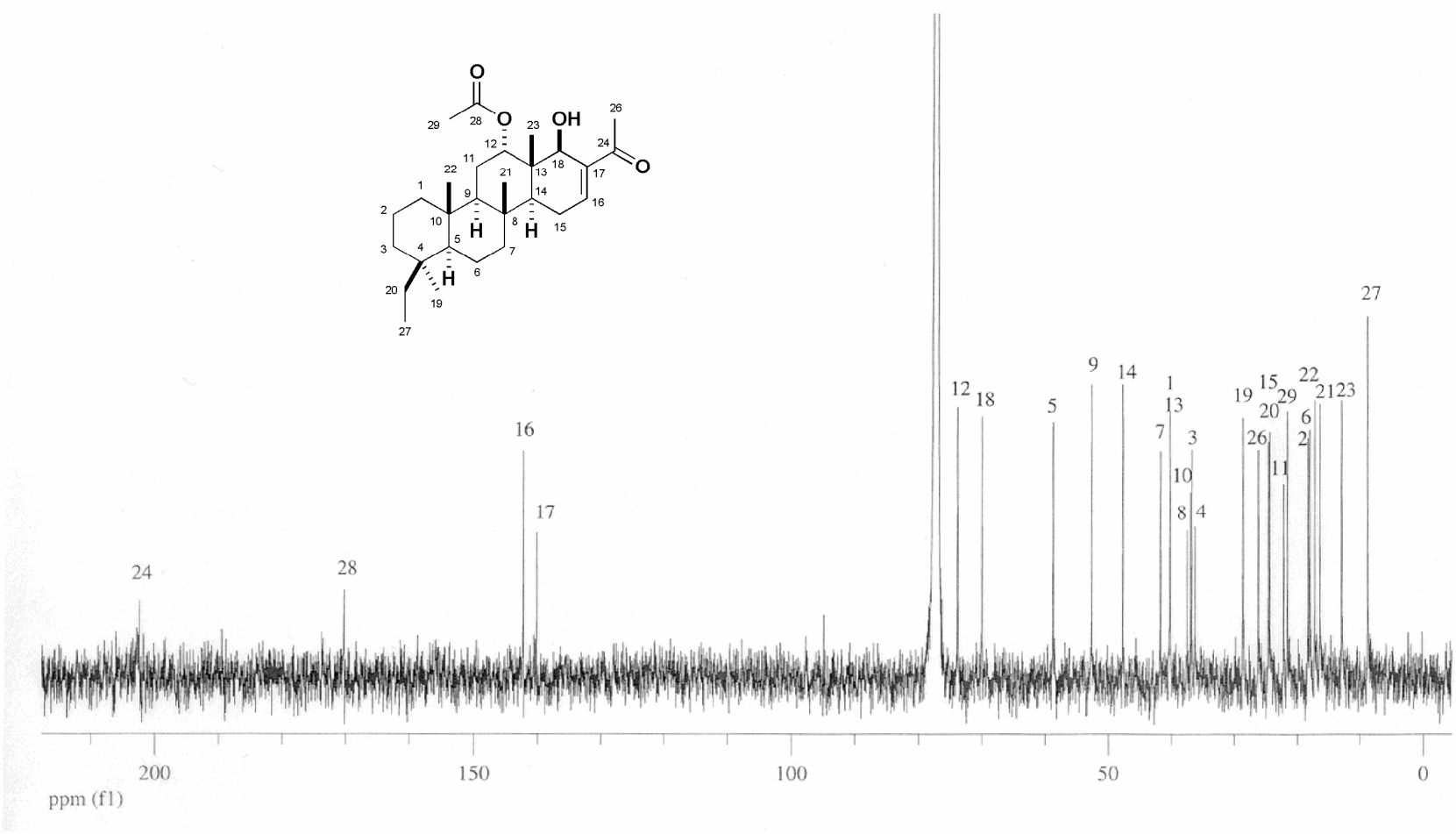

Figure S9. ^{1}H NMR spectrum of **6**.

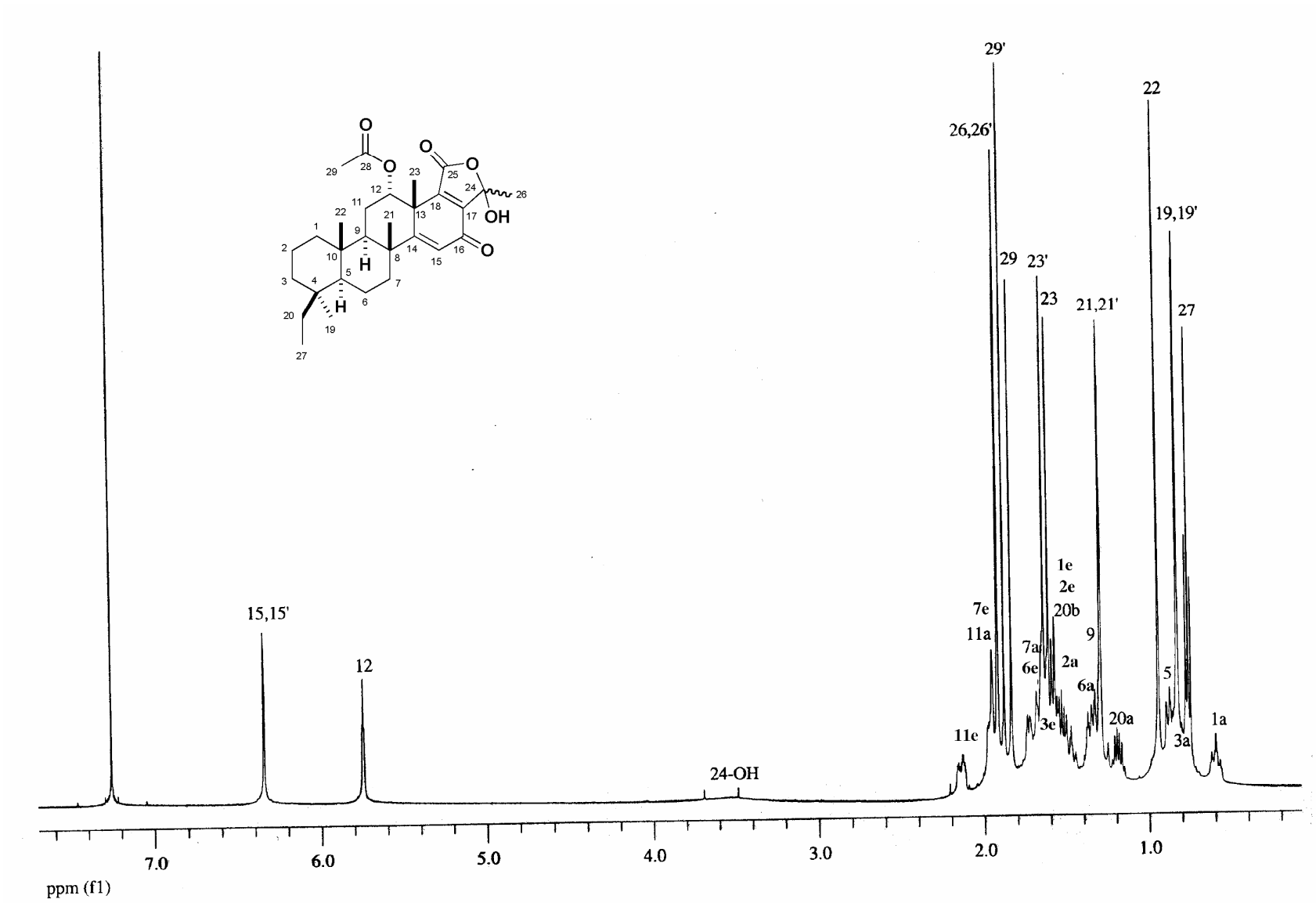

Figure S10. ^{13}C NMR spectrum of **6**.

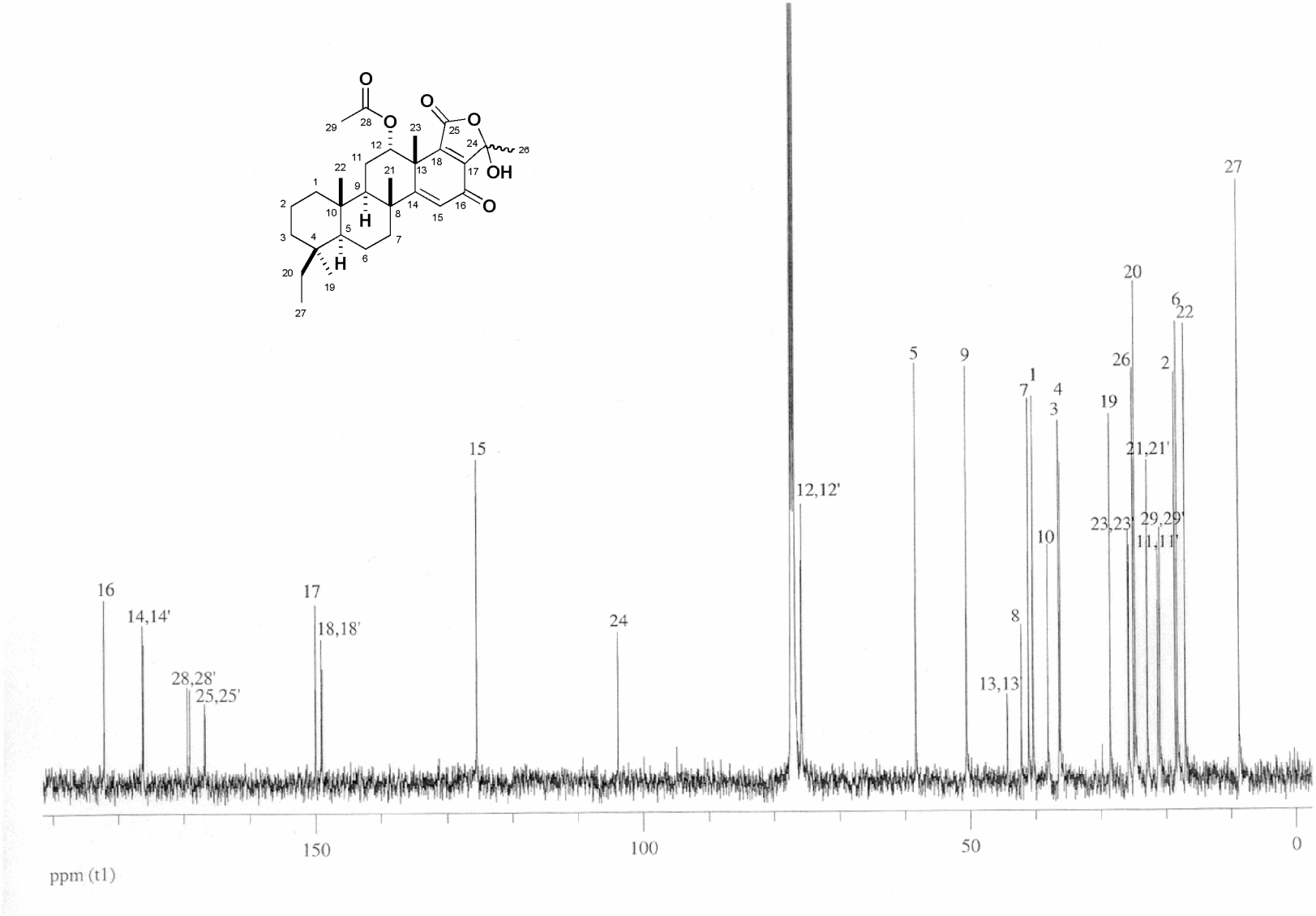

Figure S15. ^{1}H NMR spectrum of **7**.

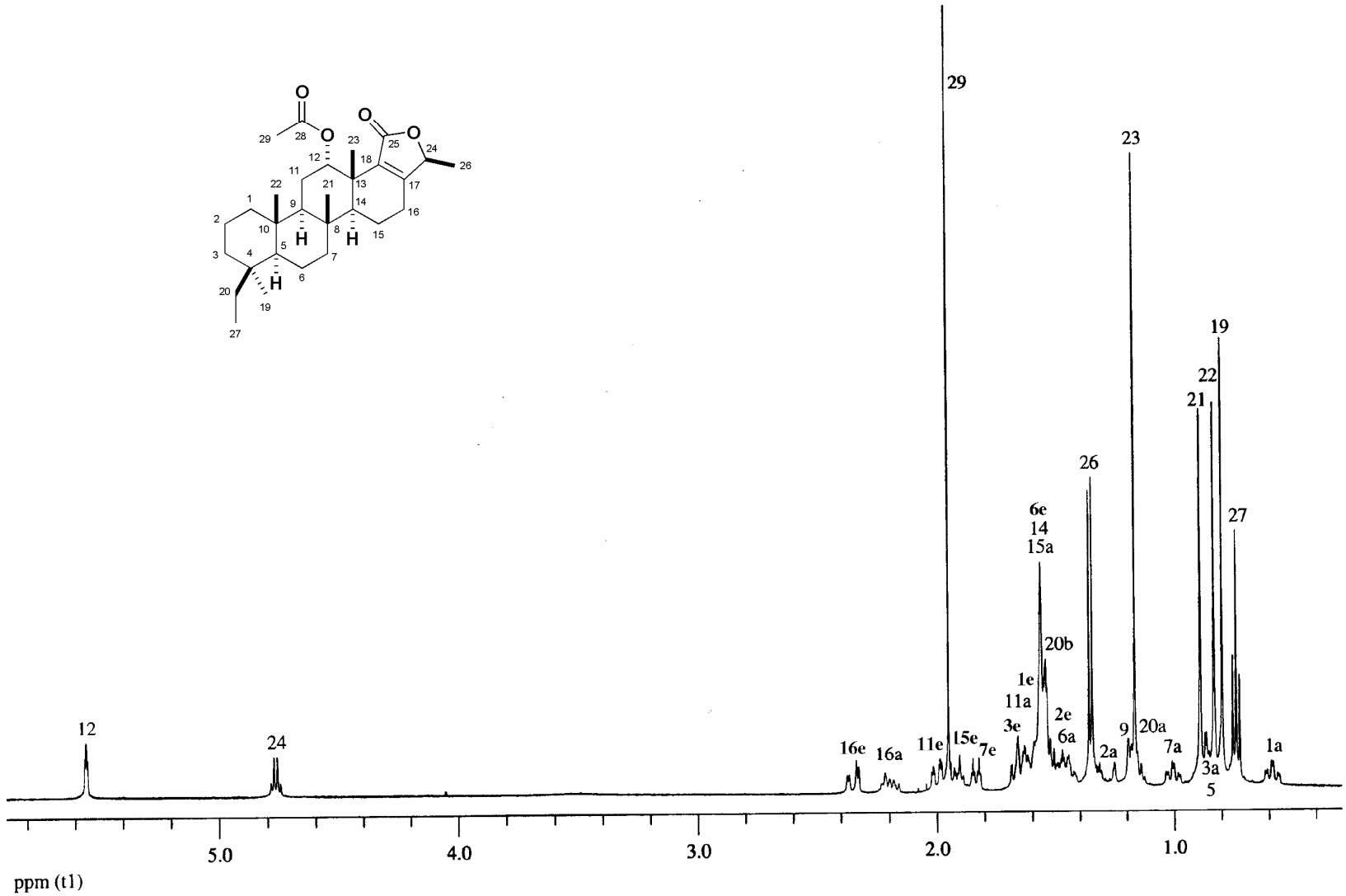

Figure S16. ^{13}C NMR spectrum of **7**.

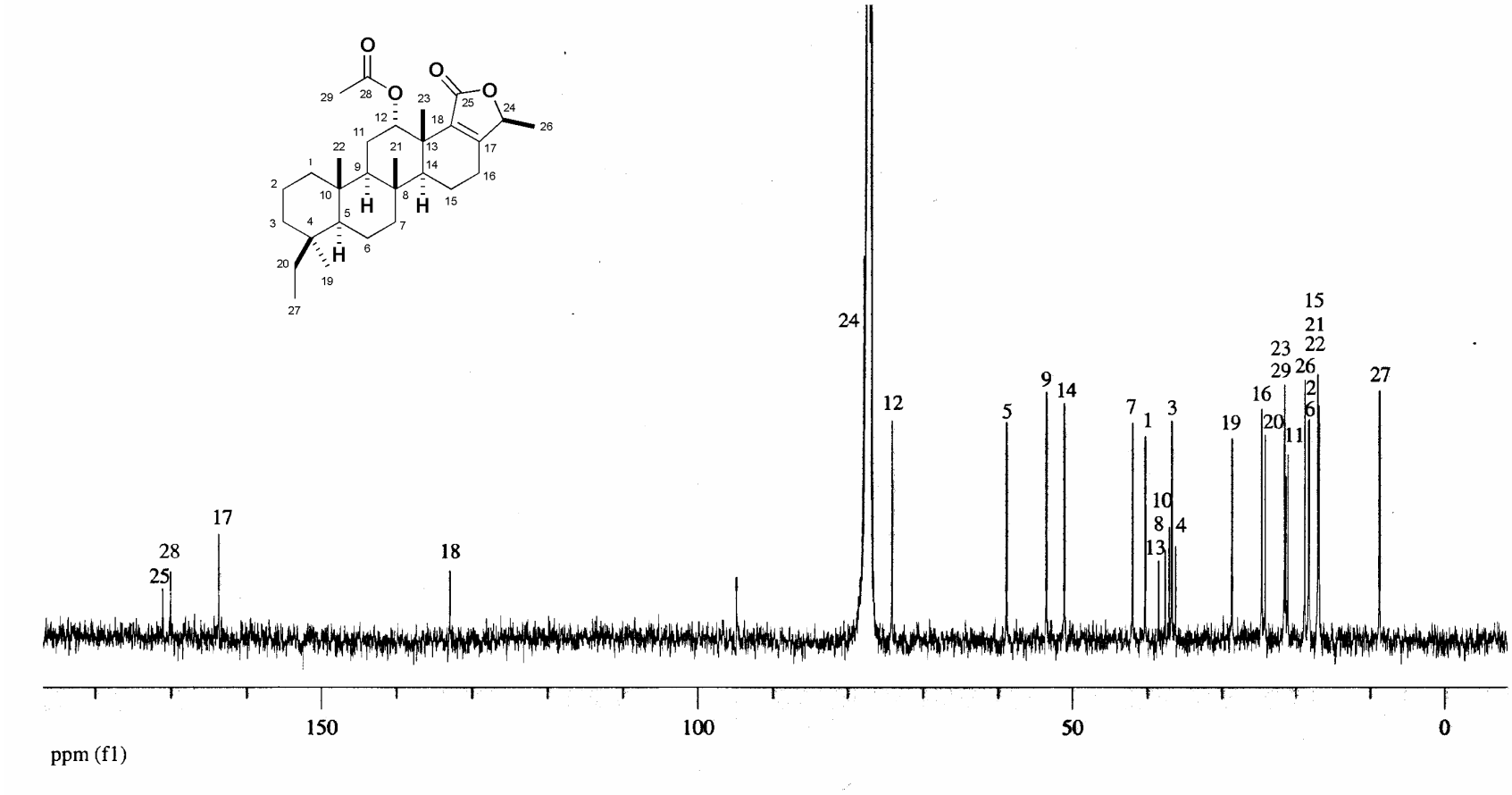

Table S1. NMR Data for **1** in $CDCl_3$

position	δ_H (mult, *J* in Hz)	δ_C (mult)	gCOSY	gHMBC (C)	ROESY
1ax	0.64 (td, 12.5, 4.0)	40.4 (CH_2)	1eq, 2ax, 2eq	2, 3	3ax, 5, 9
1eq	1.58 (m)		1ax, 2ax, 2eq	2	
2ax	1.40 (m)	18.3 (CH_2)	1ax, 1eq, 2eq, 3ax, 3eq	1, 3	
2eq	1.52 (m)		1eq, 1eq, 2eq, 3ax, 3eq	1, 3	
3ax	0.87 (ddd, 12.5, 12.0, 2.0)	36.7 (CH_2)	2ax, 2eq, 3eq	1, 2, 4, 5, 19	1ax
3eq	1.67 (dt, 12.5, 2.5)		2ax, 2eq, 3ax	1, 2, 4, 5, 19, 20	
4		36.2 (C)			
5	0.89 (dd, 12.0, 2.0)	58.7 (CH)		4, 6, 19	1ax
6ax	1.36 (m)	18.1 (CH_2)	5, 6eq, 7ax, 7eq	7	
6eq	1.42 (m)		6ax, 7ax, 7eq	7	
7ax	1.06 (td, 12.5, 4.0)	40.8 (CH_2)	6ax, 6eq, 7eq	5, 6	
7eq	1.73 (dt, 12.5, 3.0)		6ax, 6eq, 7ax	5, 6	15eq
8		37.9 (C)			
9	1.23 (dd, 13.0, 2.0)	53.1 (CH)	11ax, 11eq	11, 12, 14, 21, 22	1ax
10		37.0 (C)			
11ax	1.60 (m)	22.2 (CH_2)	9, 11eq, 12	9	12
11eq	1.82 (ddd, 15.0, 3.0, 2.5)		9, 11ax, 12	9	12
12	5.12 (dd, 2.5, 2.0)	76.2 (CH)	11ax, 11eq	9, 28	11ax, 11eq, 18, 23a, 25
13		36.9 (C)			
14	1.33 (dd, 11.5, 5.0)	43.2 (CH)	15ax	13, 15, 21	
15ax	2.24 (ddt, 19.0, 11.5, 2.5)	23.1 (CH_2)	14, 15eq, 16	13, 14, 16, 17	16, 23b
15eq	2.41 (dt, 19.0, 5.5)		15ax	13, 14, 16, 17	7eq, 16
16	7.18 (dd, 7.0, 2.0)	142.6 (CH)	15ax, 18	14, 15, 18, 24	15ax, 15eq
17		137.3 (C)			
18	3.02 (d, 8.0)	43.1 (CH)	16, 23α, 23β, 25	12, 23, 24, 25	12, 23a, 25
19	0.82 (s)	28.6 (CH_3)		4, 20	
20a	1.19 (dq, 15.0, 7.5)	24.7 (CH_2)	27	3, 4, 19, 27	
20b	1.53 (m)		27	3, 4, 19, 27	
21	0.78 (s)	14.9 (CH_3)		8, 9, 14	
22	0.84 (s)	17.1 (CH_3)		1, 9, 10	
23α	1.86 (dd, 12.0, 8.0)	35.3 (CH_2)	18, 23β, 25	12, 18, 25	12, 18, 25
23β	2.00 (m)		18, 23α, 25	12, 18, 25	15ax,
24		202.1 (C)			
25	4.65 (qd, 8.0, 3.0)	67.0 (CH)	18, 23α, 23β	17, 18, 23	12, 18, 23a
26	2.37 (s)	25.6 (CH_3)		24	
27	0.75 (t, 7.5)	8.7 (CH_3)	20a, 20b	20	
28		170.8 (C)			
29	2.07 (s)	21.5 (CH_3)		28	

Table S2. NMR Data for **2**

position	δ_H (mult, J in Hz)	δ_C (mult)	gCOSY	gHMBC (C)	ROESY
1ax	0.65 (td, 12.5, 3.5)	40.4 (CH_2)	1eq, 2ax, 2eq	2, 3, 22	3ax, 5, 9
1eq	1.60 (m)		1ax, 2ax, 2eq	2, 3	11eq
2ax	1.38 (m)	18.3 (CH_2)	1ax, 1eq, 2eq, 3ax, 3eq	1, 3	
2eq	1.54 (m)		1ax, 1eq, 2ax, 3ax, 3eq	1, 3	
3ax	0.86 (m)	36.7 (CH_2)	2ax, 2eq, 3eq	1, 2, 4, 5, 19, 20	1ax
3eq	1.65 (m)		2ax, 2eq, 3ax	1, 2, 4, 5, 19, 20	
4		36.2 (C)			
5	0.88 (dd, 12.0, 2.0)	58.8 (CH)	6ax, 6eq	4, 6, 10, 19, 22	1ax
6ax	1.33 (m)	18.1 (CH_2)	5, 6eq, 7ax, 7eq	5, 7	
6eq	1.49 (dt, 13.5, 3.5)		5, 6ax, 7ax, 7eq	5, 7	
7ax	1.05 (td, 12.5, 4.0)	40.8 (CH_2)	6ax, 6eq, 7eq	5, 6, 8	
7eq	1.73 (dt, 13.5, 3.5)		6ax, 6eq, 7ax	5, 6, 8	15eq
8		37.9 (C)			
9	1.22 (dd, 13.5, 2.0)	53.1 (CH)	11ax, 11eq	10, 11, 12, 21, 22	1ax
10		37.0 (C)			
11ax	1.66 (m)	21.3 (CH_2)	9, 11eq, 12	9, 12	
11eq	1.85 (dt, 15.0, 3.0)		9, 11ax, 12	9, 12	1eq
12	5.66 (t, 3.0)	76.9 (CH)	11ax, 11eq	9, 28	18, 23α
13		40.3 (C)			
14	1.31 (dd, 12.0, 4.5)	44.1 (CH)	15ax, 15eq	8, 13, 15, 21	
15ax	2.13 (ddt, 19.0, 12.5, 2.0)	22.5 (CH_2)	14, 15eq, 16	13, 14, 16, 17	16, 23β
15eq	2.37 (ddd, 19.0, 6.5, 5.0)		14, 15ax, 16, 18	13, 14, 16, 17	7eq, 16
16	6.99 (dd, 7.0, 2.0)	140.7 (CH)	15ax, 15eq, 18	14, 15, 18, 24	15ax, 15eq
17		139.2 (C)			
18	2.72 (br. s)	45.7 (CH)	16, 23α, 25	12, 23, 25	12
19	0.81 (s)	28.6 (CH_3)		4, 20	
20a	1.16 (dq, 15.0, 7.5)	24.7 (CH_2)	27	3, 4, 19	
20b	1.55 (dq, 15.0, 7.5)			3, 4, 19	
21	0.78 (s)	15.3 (CH_3)		8, 9, 14	
22	0.84 (s)	17.2 (CH_3)		1, 9, 10	
23α	1.58 (m)	34.0 (CH_2)	18, 23β, 25	18, 25	12
23β	2.28 (m)		23α, 25	12, 14, 18, 25	15ax, 25
24		198.5 (C)			
25	3.63 (d, 7.0)	73.4 (CH)	18, 23α, 23β	17, 18, 23	23β
26	2.31 (s)	25.4 (CH_3)		17, 24	
27	0.75 (t, 7.5)	8.7 (CH_3)	20a	20	
28		170.9 (C)			
29	2.07 (s)	21.6 (CH_3)		28	

Table S3. NMR Data for **3**

position	δ_H (mult, *J* in Hz)	δ_C (mult)	gCOSY	gHMBC (C)	ROESY
1ax	0.61 (td, 13.0, 3.5)	40.2 (CH_2)	1eq, 2ax, 2eq,	3	3ax, 5
1eq	1.61 (m)		1ax, 2ax, 2eq	3	
2ax	1.37 (m)	18.3 (CH_2)	1ax, 1eq, 2eq, 3ax, 3eq	3	
2eq	1.48 (m)		1ax, 1eq, 2ax, 3ax, 3eq	3	
3ax	0.86 (m)	36.7 (CH_2)	2ax, 2eq, 3eq	1, 2, 5, 19	1ax
3eq	1.63 (m)		2ax, 2eq, 3ax	2, 5, 19	
4		36.2 (C)			
5	0.92 (dd, 13.0, 2.0)	58.5 (CH)	6ax, 6eq	3, 6, 10, 19, 20, 22	1ax
6ax	1.42 (m)	18.1 (CH_2)	5, 6eq, 7ax, 7eq	5, 7	
6eq	1.55 (m)		5, 6ax, 7ax, 7eq	5, 7	
7ax	0.88 (m)	41.7 (CH_2)	6ax, 6eq, 7eq	5, 6, 8, 14, 21	
7eq	1.69 (m)		6ax, 6eq, 7ax	6, 8, 21	
8		37.7 (C)			
9	1.28 (d, 13.0)	52.8 (CH)	11ax, 11eq	1, 5, 10, 11, 21	11eq
10		37.0 (C)			
11ax	1.68 (m)	21.9 (CH_2)	9, 11eq, 12	9, 13	12, 22
11eq	1.89 (m)		9, 11ax, 12	9, 13	9, 12
12	4.71 (br. s)	75.7 (CH)	11ax, 11eq	9, 14, 23, 28	11ax, 11eq, 18, 23, 29
13		40.4 (C)			
14	1.68 (m)	46.4 (CH)		13, 15, 16, 23	18
15ax	1.67 (m)	25.5 (CH_2)	15eq, 16	13, 14, 16	16, 17
15eq	1.92 (m)		15ax, 16	13, 14, 16	16
16	5.64 (br. s)	68.6 (CH)	15ax, 15eq, 17	18	15ax, 15eq, 17, 26
17	3.18 (dd, 12.0, 3.0)	52.0 (CH)	16	18, 24, 25	15ax, 16, 23, 26
18	3.33 (d, 12.0)	45.6 (CH)		12, 14, 16, 17, 23, 24, 25, 1'	12, 14, 26
19	0.81 (s)	28.5 (CH_3)		2, 3, 4, 5, 20	
20a	1.15 (dq, 15.0, 7.5)	24.6 (CH_2)	20b, 27	3, 4, 19, 27	
20b	1.55 (m)		20a, 27	3, 4, 19, 27	
21	0.85 (s)	17.0 (CH_3)		7, 8, 14	
22	0.82 (s)	17.1 (CH_3)		1, 9	11ax
23	1.00 (s)	15.2 (CH_3)		12, 13, 18	12, 17
24		207.9 (C)			
25		175.6 (C)			
26	2.20 (s)	28.9 (CH_3)		17, 24	16, 17, 18
27	0.74 (t, 7.5)	8.7 (CH_3)	20a, 20b	20	
28		171.3 (C)			
29	2.17 (s)	21.7 (CH_3)		28	12
1'		172.2 (C)			
2'a	2.42 (dd, 15.0, 9.0)	41.7 (CH_2)	2'b, 3	1', 3', 4'	3'
2'b	2.48 (dd, 15.0, 3.5)		2'a, 3	1', 3', 4'	3'
3'	3.89 (m)	69.7 (CH)	2'a, 2'b, 4'a, 4'b		2'a, 2'b, 5'
4'a	1.48 (m)	29.7 (CH_2)	3', 4'b, 5	3'	
4'b	1.52 (m)		3', 4'a, 5	3', 5'	
5'	0.99 (t, 7.5)	10.1 (CH_3)	4'	4'	3'

Table S4. NMR Data for **4**

position	δ_H (mult, J in Hz)	δ_C (mult)	gCOSY	gHMBC (C)	ROESY
1ax	0.60 (td, 12.5, 3.5)	40.2 (CH_2)	1eq, 2ax, 2eq	2, 9	2eq, 3ax, 5, 9
1eq	1.61 (m)		1ax, 2eax, 2eq, 3ax, 3eq	2	2ax
2ax	1.33 (m)	18.3 (CH_2)	1ax, 1eq, 2eq, 3ax, 3eq	1, 3	1eq, 20a, 27
2eq	1.45 (m)		2ax, 2eq, 3eq	1, 3	1ax
3ax	0.89 ((td, 13.5, 3.5)	36.7 (CH_2)	2ax, 2eq, 3ax	20	1ax
3eq	1.64 (m)			20	
4		36.2 (C)			
5	0.90 (dd, 12.5, 2.0)	58.6 (CH)		3, 7, 9	1ax
6ax	1.42 (m)	18.1 (CH_2)	5, 6eq, 7ax, 7eq	7	
6eq	1.56 (m)		5, 6ax, 7ax, 7eq	7	7eq
7ax	0.98 (m)	42.0 (CH_2)	6ax, 6eq, 7eq	5	
7eq	1.78 (m)		6ax, 6eq, 7ax	5	6eq, 15eq
8		38.0 (C)			1ax, 11eq
9	1.28 (br. d, 12.0)	52.3 (CH)	11ax, 11eq	1, 10, 11, 12, 14, 22	
10		36.9 (C)			
11ax	1.64 (m)	22.1 (CH_2)	9, 11eq, 12	8, 12, 13	21, 22
11eq	1.89 (br.d, 14.5)		9, 11ax, 12	8, 12, 13	9, 12
12	4.85 (t, 2.0)	75.7 (CH)	11ax, 11eq	9	11eq, 18, 23
13		39.0 (C)			
14	1.50 (m)	49.2 (CH)	15ax, 15eq	13, 15, 18, 21	15ax, 15eq, 18
15	2.27 (2H, m)	23.3 (CH_2)	14, 16, 18	8, 16, 17	7eq, 14, 16, 18, 21, 23
16	6.93 (td, 3.5, 2.5)	140.0 (CH)	15, 18		15, 18
17		138.0 (C)			
18	3.86 (q, 2.5)	48.1 (CH)	15, 16, 23	13, 17, 25	12, 14, 15, 16
19	0.81 (s)	28.6 (CH_3)		4, 5, 20	
20a	1.16 (dq, 14.5, 7.5)	24.6 (CH_2)	27	4, 19, 27	2ax, 27
20b	1.53 (dq, 14.5, 7.5)		27	4, 19, 27	27
21	0.98 (s)	15.8 (CH_3)		7, 9, 14	11ax, 15ax
22	0.84 (s)	16.9 (CH_3)		9, 10	11ax
23	0.97 (s)	17.2 (CH_3)	18	12, 13, 14	12, 15ax
24		199.3 (C)			
25		174.5 (C)			
26	2.31 (s)	25.5 (CH_3)		24	
27	0.75 (t, 7.5)	8.8 (CH_3)	20a, 20b	3, 20	20a, 20b
28		170.5 (C)			
29	2.14 (s)	21.6 (CH_3)		28	

Table S5. NMR Data for **5**

position	δ_H (mult, J in Hz)	δ_C (mult)	gCOSY	gHMBC (C)	ROESY
1ax	0.63 (td, 12.5, 4.0)	40.2 (CH_2)	1eq, 2ax, 2eq		
1eq	1.61 (m)		1ax, 2ax, 2eq		11eq
2ax	1.36 (m)	18.3 (CH_2)	1ax, 1eq, 2eq, 3ax, 3eq	3, 4	
2eq	1.52 (m)		1ax, 1eq, 2ax, 3ax, 3eq	3, 4	
3ax	0.88 (m)	36.8 (CH_2)	2ax, 2eq, 3eq	1, 2, 19, 20	
3eq	1.66 (m)		2ax, 2eq, 3ax	1, 2, 19, 20	
4		36.2 (C)			
5	0.91 (dd, 12.5, 2.0)	58.7 (CH)	6ax, 6eq	6	
6ax	1.43 (td, 13.5, 3.0)	18.0 (CH_2)	5, 6eq, 7ax, 7eq	7	
6eq	1.58 (m)		5, 6eq, 7ax, 7ax	7	19
7ax	0.99 (td, 12.5, 2.0)	41.7 (CH_2)	6ax, 6eq, 7eq	8	
7eq	1.73 (dt, 12.5, 3.0)		6ax, 6eq, 7ax	8	15, 21
8		37.5 (C)			
9	1.26 (dd, 13.0, 1.5)	52.6 (CH)	11ax, 11eq	11, 12, 22	11eq
10		37.0 (C)			
11ax	1.65 (m)	22.2 (CH_2)	9, 11eq, 12	9, 12, 13	
11eq	1.80 (ddd, 15.0, 3.0, 2.5)		9, 11ax, 12	1, 8, 9, 12, 13	1eq, 9, 12
12	5.07 (t, 3.0)	73.8 (CH)	11ax, 11eq	9, 14	11eq
13		40.1 (C)			
14	1.50 (m)	47.7 (CH)	15, 16	8, 13, 15, 18, 21, 23	18
15	2.25 (2H, m)	24.4 (CH_2)	14, 16	16	7eq, 16
16	6.88 (td, 4.0, 1.5)	142.2 (CH)	14, 18		15, 26
17		140.1 (C)			
18	4.60 (dd, 4.0, 2.5)	70.0 (CH)	16	13, 17	14
19	0.81 (s)	28.6 (CH_3)		5, 20	6eq
20a	1.16 (dq, 15.0, 7.5)	24.6 (CH_2)	27	27	27
20b	1.52 (dq, 15.0, 7.5)		27	27	27
21	0.96 (s)	16.4 (CH_3)		6, 7, 8, 9, 14	7eq
22	0.85 (s)	17.2 (CH_3)		1, 9, 10	
23	0.93 (s)	12.9 (CH_3)		12, 13, 18	
24		202.3 (C)			
26	2.32 (s)	26.2 (CH_3)		16, 24	
27	0.75 (s)	8.8 (CH_3)	20a, 20b	4, 20	20a, 20b
28		170.2 (C)			
29	2.11 (s)	21.6 (CH_3)		28	
18-OH	4.15 (br. s)				

Table S6. NMR Data for **6**

position	δ_H (mult, J in Hz)	δ_C (mult)	gCOSY	gHMBC (C)	ROESY
1ax	0.61 (td, 13.0, 4.0)	40.4 (CH_2)	1eq, 2ax, 2eq		2eq, 9
1eq	1.64 (m)		1ax, 2ax, 2eq		
2ax	1.37 (m)	18.6 (CH_2)	1ax, 1eq, 2eq, 3ax, 3eq	1, 4	
2eq	1.49 (m)		1ax, 1eq, 2eq, 3ax, 3eq	1, 4	1eq
3ax	0.84 (m)	36.5 (CH_2)	2ax, 2eq, 3eq	2, 5, 19, 20	19
3eq	1.67 (m)		2ax, 2eq, 3ax	2, 5, 19, 20	27
4		36.2 (C)			
5	0.90 (dd, 12.0, 2.0)	58.4 (CH)	6ax, 6eq	4, 6, 7, 10	6eq, 9
6ax	1.58 (m)	18.2 (CH_2)	5, 6eq, 7ax, 7eq	5, 8, 10	
6eq	1.72 (m)		5, 6ax, 7ax, 7eq	5, 8, 10	5, 7eq
7ax	1.60 (m)	41.1 (CH_2)	6ax, 6eq, 7eq	5, 6, 9	
7eq	1.98 (m)		6ax, 6eq, 7ax	5, 6, 9	6eq, 15, 21
8		42.2 (C)			
9	1.32 (m)	50.6 (CH)	11ax, 11eq	8, 11, 12, 21, 22	1ax, 5, 11eq
10		38.2 (C)		10	
11ax	1.98 (m)	21.3[f] (CH_2)	9, 11eq, 12	8, 9, 13	12, 21, 22
11eq	2.15[a] (dt, 15.0, 3.0)	21.2[f]	9, 11ax, 12	8, 9, 13	
	2.17[a] (dt, 15.0, 3.0)				
12	5.76 (t, 3.0)	75.9[g] (CH)	11ax, 11eq	9, 13, 14	11ax, 11eq
		75.8[g]			
13		44.3[h] (C)			
		44.2[h]			
14		176.3 (C)			
		176.1			
15	6.360[b] (s)	125.5 (CH)		13, 17, 24	7eq
	6.364[b] (s)				
16		182.2 (C)			
17		150.0 (C)			
18		149.1[i] (C)			
		149.0[i]			
19	0.839[c] (s)	28.6 (CH_3)		4, 5	3ax
	0.841[c] (s)				
20a	1.20 (dq, 15.0, 7.5)	24.7 (CH_2)	20b, 27	3, 4, 19, 27	27
20b	1.55 (dq, 15.0, 7.5)		20a, 27	19, 27	27
21	1.306[d] (s)	22.9[j] (CH_3)		8, 9, 13, 14	7eq, 11ax
	1.310[d] (s)	22.8[j]			
22	0.95 (s)	17.0 (CH_3)		5, 9, 10	11ax
23	1.62 (s)	25.8[k] (CH_3)		12, 13, 14, 18	
	1.65 (s)	25.7[k]			
24		103.8 (C)			
25		166.8[l] (C)			
		166.7[l]			
26	1.85 (s)	25.0 (CH_3)		17, 24	
	1.93 (s)				
27	0.77 (t, 7.5)	8.8 (CH_3)	20a, 20b	4, 20	3eq, 20a, 20b
28		169.5[m] (C)			
		169.1[m]			
29	1.86[e] (s)	21.0[i] (CH_3)		28	
	1.93[e] (s)	20.9[i]			
24-OH	3.60 (br.s)				

[a-m] Values in same superscripts indicate the isomer signals.

Table S7. NMR Data for **7**

position	δ_H (mult, J in Hz)	δ_C (mult)	gCOSY	gHMBC (C)	ROESY
1ax	0.60 (td, 13.0, 3.5)	40.2 (CH_2)	1eq, 2ax, 2eq	22	2eq, 3ax, 5, 9
1eq	1.60 (dt, 13.0, 3.5)		1ax, 2, ax, 2eq	22	
2ax	1.36 (m)	18.3 (CH_2)	1ax, 1eq, 2eq, 3ax, 3eq	1, 3, 4	
2eq	1.49 (m)		1ax, 1eq, 2ax, 3ax, 3eq	1, 3, 4	1ax
3ax	0.86 (m)	36.7 (CH_2)	2ax, 2, eq, 3eq	1, 2, 4	1ax, 19
3eq	1.68 (m)		2ax, 2eq, 3ax	1, 2, 4	
4		36.2 (C)			
5	0.88 (m)	58.9 (CH)			1ax
6ax	1.45 (m)	18.2 (CH_2)	6eq, 7ax, 7eq	7	
6eq	1.57 (m)		6ax, 7ax, 7eq	7	
7ax	1.01 (td, 12.5, 4.0)	41.9 (CH_2)	6ax, 6eq, 7eq	6	
7eq	1.85 (dt, 12.5, 3.0)		6ax, 6eq, 7ax	6	
8		37.6 (C)			
9	1.20 (dd, 13.0, 2.5)	53.5 (CH)	11ax, 11eq	11	1ax
10		37.1 (C)			
11ax	1.67 (ddd, 15.0, 13.0, 2.5)	21.1 (CH_2)	9, 11eq, 12	9, 12, 13	12, 23
11eq	2.02 (dt, 15.0, 2.5)		9, 11ax, 12	9, 12, 13	
12	5.57 (t, 2.5)	74.1 (CH)	11ax, 11eq	11	11ax, 23
13		38.5 (C)			
14	1.56 (m)	51.1 (CH)	15ax, 15eq	16, 17, 21, 23	
15ax	1.56 (m)	17.0 (CH_2)	14, 15eq, 16ax, 16eq	14, 17	16eq
15eq	1.94 (dt, 11.0, 7.5)		14, 15ax, 16ax, 16eq	14, 17	16eq
16ax	2.24 (m)	24.6 (CH_2)	15ax, 15eq, 16eq	14, 15, 18	
16eq	2.34 (dd, 19.5, 4.5)		15ax, 15eq, 16ax	14, 15, 18	15ax, 15eq
17		163.7 (C)			
18		132.9 (C)			
19	0.81 (s)	28.6 (CH_3)		4, 5, 20	3ax
20a	1.16 (dq, 15.0, 7.5)	24.1 (CH_2)	27	3, 4, 27	
20b	1.53 (dq, 15.0, 7.5)		27	3, 4, 27	
21	0.90 (s)	17.1 (CH_3)		7, 8, 9, 14	23
22	0.84 (s)	16.9 (CH_3)		1, 9, 10	
23	1.18 (s)	21.5 (CH_3)		12, 13, 14, 18	11ax, 12, 21
24	4.78 (q, 6.5)	77.8 (CH)	26	17	
25		171.1 (C)			
26	1.37 (d, 6.5)	18.8 (CH_3)	24	17, 24	
27	0.75 (t, 7.5)	8.8 (CH_3)	20a, 20b	20	
28		170.0 (C)			
29	1.96 (s)	21.4 (CH_3)		28	