The Sponge-Derived Fijianolide Polyketide Class: Further Evaluation of Their Structural and Cytotoxicity Properties

Tyler A. Johnson,[†] Karen Tenney,[†] Robert H. Cichewicz,[†] Brandon I. Morinaka,[†] Kimberly N. White,[†] Taro Amagata,[†] Balanehru Subramanian,[§] Joseph Media,[§] Susan L. Mooberry,[‡] Frederick A. Valeriote[§] and Phillip Crews.[*,†]

[Supporting Information]

Department of Chemistry and Biochemistry and Institute for Marine Sciences, University of California, Santa Cruz, California 95064, Josephine Ford Cancer Center, Henry Ford Health System, Detroit, Michigan 48202, and Southwest Foundation for Biomedical Research, San Antonio, Texas 78245

[Contents]

Figure S25. Gradient LCMS chromatogram of **1** using: 30:70 to 80:20 (50min) in CH_3CN/H_2O.
Figure S26. Gradient LCMS chromatogram of **2** using: 30:70 to 80:20 (50min) in CH_3CN/H_2O.
Figure S27. Gradient LCMS chromatogram of **7** using: 30:70 to 80:20 (50min) in CH_3CN/H_2O.
Figure S28. Gradient LCMS chromatogram of **8** using: 10:90 to 100 (50min) in CH_3CN/H_2O.
Figure S29. Gradient LCMS chromatogram of **9** using: 30:70 to 80:20 (50min) in CH_3CN/H_2O.
Figure S30. Gradient LCMS chromatogram of **10** using: 30:70 to 80:20 (50min) in CH_3CN/H_2O.
Figure S31. Gradient LCMS chromatogram of **11** using: 30:70 to 80:20 (50min) in CH_3CN/H_2O.
Figure S32. Gradient LCMS chromatogram of **12** using: 30:70 to 80:20 (50min) in CH_3CN/H_2O.

Chart S1. Isolation of the fijianolides, latrunculin A and mycothiazole

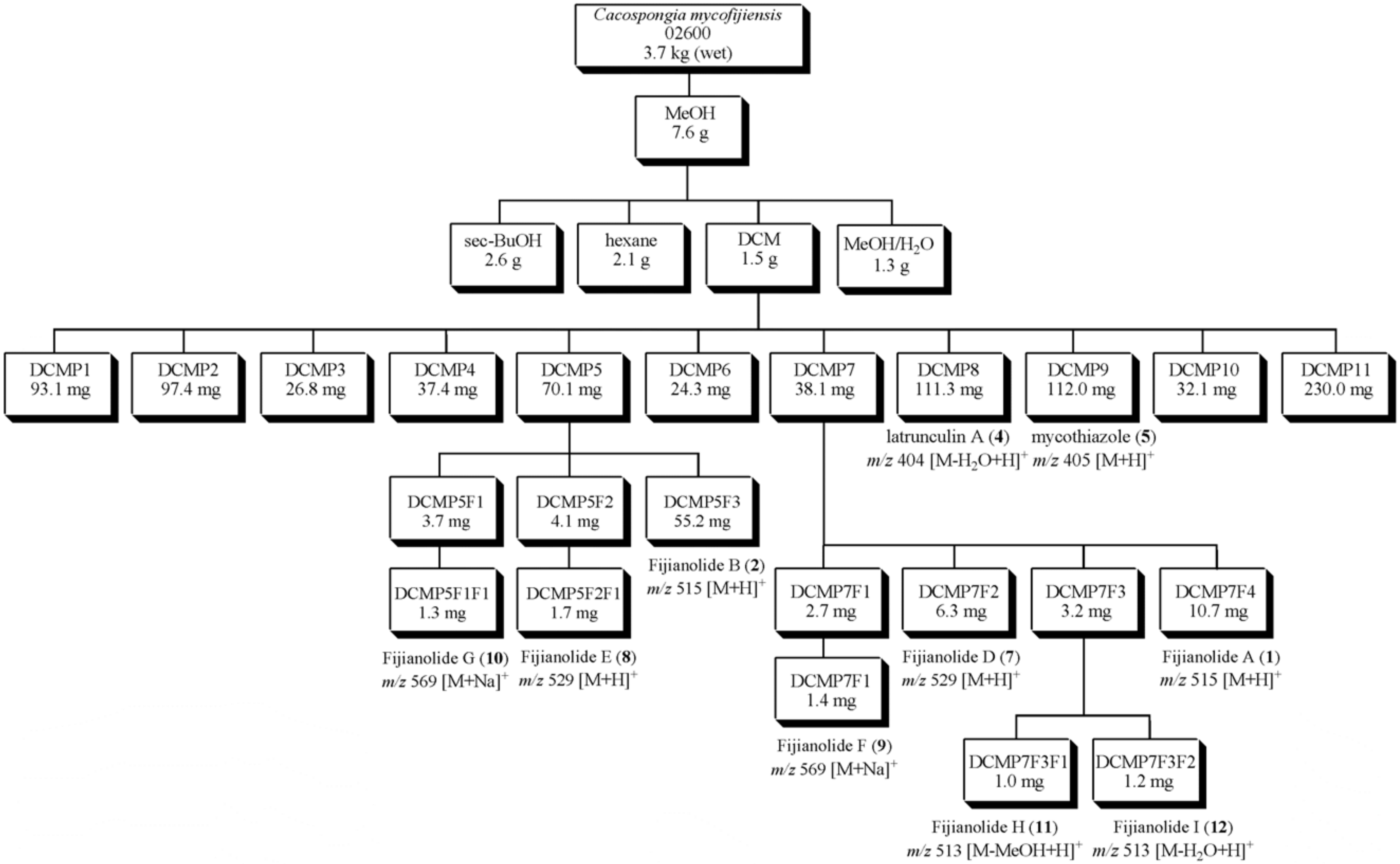
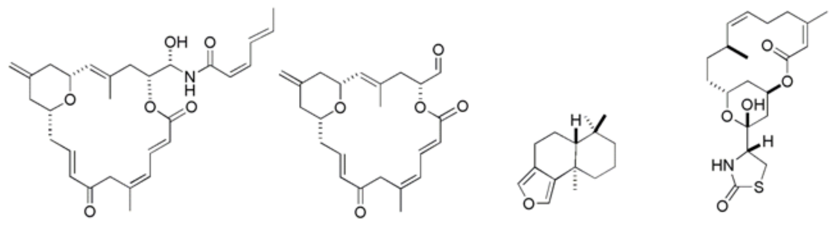


Table S1. Summary of *Cacospongia mycofijiensis* Type Natural Products Studied by Others



Entry number	Taxonomic identification	Collection Site	Major Constituents
1	*unidentifiable* (Bergquist)[a]	American Samoa	**1, 4, s3**
2	*Negombata magnifica*[b, c]	Djibouti	**4, s4**
3	*N. magnifica*[d]	Egypt	**4**
4	*Hyatella* sp. (Bergquist)[e]	Indonesia	**1, 2, 4**
5	*N. magnifica*[d]	Israel	**s4**
6	*Fasciospongia rimosa* (Hooper)[f, g]	Japan	**1, 2, s1, 3, 4**
7	*Cacospongia mycofijiensis*[h]	Marshall Islands	**1, 2, 4**
8	*N. magnifica*[c]	Saudi Arabia	**4**
9	*N. magnifica*[c]	Saudi Arabia	**s4**
10	*Dactylospongia* sp. (Hooper)[i]	Vanuatu	**1, 2, s2, 4, 5**

[a] Gulavita, N. L.; Gunasekera, S. P. and Pomponi, S. A. *J. Nat. Prod.* **1992,** 55, 4, 506-508. [b] Previously known as *Latrunculia magnifica.* [c] Ilan, M. *Biol. Bull.* **1995,** 188: 306-312. [d] Groweiss, A.; Shmeuli, U. Kashman, Y. Marine Toxins of *Latrunculia magnifica*. *J. Org. Chem.* **1983**, 48, 3512-3516. [e] Corley, D. G., Herb, R.; Moore, R. E.; Scheuer, P. J. *J. Org. Chem.* **1988,** 53, 3644-6. [f] Tanaka, J.; Higa, T.; Bernardineli, G.; Jefford, C. *Chemistry. Lett.* **1996,** 255. [g] Tanaka J., Higa, T. *Tetrahedron Lett.* **1996,** 37, 5535-5538. [h] Mooberry, S. L.; Tien, G.; Hernandez, A. H.; Plubrukarn, A.; Davidson, B. *Cancer Research* **1999,** 59, 653-660. [i] Cutignano, A.; Bruno, I.; Bifulco, G.; Casapullo, A.; Debitus, C.; Gomez- Paloma, L.; Riccio, R. *Eur. J. Org. Chem.* **2001**, 775-778.

Table S2. ^{1}H and ^{13}C NMR[a] data of **1** in C_6D_6

	1		
position	δ_H (*J* in HZ)	δ_C	C mult.
1		165.6	C
2	5.80 d (12.0)	123.7	CH
3	5.71 ddd (11.4, 9.6, 6.0)	142.2	CH
4a	3.08 ddd (15.9, 10.8, 4.8)	36.1	CH_2
4b	2.28 m		
5	4.37 dddd (10.2, 7.2, 4.8, 3.0)	73.2	CH
6	5.56 ddt (10.2, 2.4, 1.2)	128.9	CH
7	5.65 m	125.4	CH
8a	1.81 dd (15.0, 9.6)	32.1	CH_2
8b	1.61 m		
9	3.64 tt (12.2, 2.4)	66.7	CH
10a	1.51 ddd (13.8, 9.6, 1.8)	43.0	CH_2
10b	0.93 ddd (13.8, 9.0, 1.8)		
11	1.93 ddd (14.4, 7.8, 6.6)	27.4	CH
12a	2.19 m	46.0	CH_2
12b	2.03 m		
13		146.1	C
14	2.23 dd (15.6, 10.2)	35.8	CH_2
15	4.15 ddd (6.6, 4.2, 1.2)	71.5	CH
16	4.11 dd (4.8, 1.8)	75.5	CH
17	4.47 ddd (10.2, 5.4, 4.8)	78.3	CH
18	2.13 ddd (13.8, 7.8, 1.8)	35.2	CH_2
19	5.70 ddd (3.9, 3.6, 1.2)	77.0	CH
20	4.45 dd (6.0, 5.4)	82.0	CH
21	5.91 ddd (15.6, 6.0, 1.8)	126.0	CH
22	6.06 ddd (15.6, 5.4, 1.8)	134.0	CH
23	3.93 dddd (11.4, 5.4, 4.8, 0.6)	73.5	CH
24a	2.01 m	36.1	CH_2
24b	1.66 dt (16.8, 3.0)		
25		131.3	C
26	5.13 bs	120.5	CH
27a	4.11 brs	65.7	CH_2
27b	4.04 brs		
28	0.85 d (6.6)	20.2	CH_3
29	4.95 s, 4.89 s	113.4	CH_2
30	1.50 s	23.0	CH_3

[a] measured at 500 MHz (^{1}H) and 125 MHz (^{13}C)

`

Table S3. ^{1}H and ^{13}C NMR[a] data of **2** in C_6D_6

	2		
position	δ_H (*J* in HZ)	δ_C	C mult.
1		166.3	C
2	5.72 d (12.0)	120.8	CH
3	6.06 ddd (11.4, 9.6, 3.6)	150.7	CH
4a	3.90 m	34.1	CH_2
4b	2.15 ddd (16.8, 6.6, 3.6)		
5	4.37 m	73.3	CH
6	5.56 dq (10.2, 3.0)	129.3	CH
7	5.65 ddd (9.6, 4.8, 2.4)	125.4	CH
8a	1.79 m	32.1	CH_2
8b	1.71 (17.8, 7.8, 4.2)		
9	3.70 dd (9.0, 3.0)	68.0	CH
10a	1.55 dd (14.4, 8.4)	44.0	CH_2
10b	1.19 ddd (14.4, 4.2, 3.0)		
11	1.75 m	30.0	CH
12a	2.60 dd (13.2, 4.8)	46.0	CH_2
12b	1.80 m		
13		146.1	C
14a	2.15 m	35.8	CH_2
14b	2.14 m		
15	3.95 m	67.6	CH
16	2.76 dd (3.2, 2.8)	60.7	CH
17	2.95 ddd (9.0, 3.6, 2.4)	51.6	CH
18a	2.22 ddd (13.8, 3.0, 1.2)	33.7	CH_2
18b	1.48 ddd (14.4, 8.4, 3.6)		
19	5.15 ddd (9.6, 5.4, 1.8)	72.7	CH
20	4.13 m	73.4	CH
21	5.74 ddd (16.2, 5.4, 1.8)	129.0	CH
22	5.85 ddd (15.6, 4.8, 1.2)	133.7	CH
23	3.88 m	73.4	CH
24a	1.95 m	36.1	CH_2
24b	1.62 m		
25		131.3	C
26	5.13 brs	120.5	CH
27a	4.11 brs	65.8	CH_2
27b	4.04 brs		
28	0.88 d (6.6)	21.1	CH_3
29	4.93 s, 4.89 s	112.6	CH_2
30	1.51 s	23.0	CH_3

[a] measured at 500 MHz (^{1}H) and 125 MHz (^{13}C)

Table S4. ^{1}H and ^{13}C NMR[a] data of **7** in C_6D_6 and $CDCl_3$[b]

	7				
position	δ_H (*J* in HZ)[b]	δ_C	C mult.	COSY	HMBC
1		165.3	C		
2	5.85 d (11.5)	123.5	CH	3	1
3	6.21 ddd (10.5,10.0, 7.0)	142.6	CH	2, 4a	
4a	3.16 ddd (11.0, 11.0,4.5)	35.8	CH_2	3, 5	2, 3, 5, 6
4b	2.51 ddd (11.0, 10.5, 7.0)				
5	4.26 m	73.3	CH	4	
6	5.76 ddd (10.5, 4.5, 3.0)	129.2	CH	7	8
7	5.89 ddd (10.5, 5.0, 2.5)	125.3	CH	6, 8	6, 8
8a	2.00 dd (14.0, 9.0)	32.1	CH_2	7, 9	
8b	1.95 ddd (11.0, 6.0, 2.5)				
9	3.64 m	66.7	CH	8, 10	8
10a	1.51 ddd (13.5, 9.5, 2.0)	42.9	CH_2	9, 11	9, 11, 12
10b	1.15 ddd (14.0, 10.0, 2.5)				
11	1.86 m	27.3	CH	10, 28	
12a	2.11 dd (13.5, 6.5)	45.9	CH_2		
12b	1.95 m				
13		146	C		
14	2.32-2.18 (H14a,b, H18a,18b, H24a,b)*	35.1	CH_2	15	15
15	4.07 ddd (9.5, 2.5, 2.5)	71.4	CH	14, 16	
16	4.11 m	76.1	CH	15, 17	15, 17
17	4.38 ddd (10.5, 5.0, 5.0)	78.4	CH	16, 18	
18	2.32-2.18 (H14a,b, H18a,18b, H24a,b)*	34.2	CH_2	17, 19	19, 20
19	5.59 dd (3.5, 3.5)	76.8	CH	18, 20	
20	4.65 dd (4.5, 4.5)	81.4	CH	19, 21	
21	5.80 ddd (16.0, 5.0, 1.0)	125.5	CH	20, 22	20, 22
22	5.95 ddd (15.5, 6.0, 1.5)	130	CH	21, 23	20, 23
23	4.86 ddd (10.5, 5.5, 5.0)	75.7	CH	22, 24	24, 25
24	2.32-2.18 (H14a,b, H18a,18b, H24a,b)*	36.2	CH_2	23	25, 26
25		155.3	C		
26	5.80 s	117.3	CH		27
27		163.7	C		
28	0.86 d (6.5)	20.1	CH_3	11	10, 11, 12
29	4.90 s	113.6	CH_2		12, 13 14
30	1.97 s	22.2	CH_3		24, 25, 26

[a] measured at 500 MHz (^{1}H) and 125 MHz (^{13}C)
[b] sample run in $CDCl_3$
* can be interchanged

`

Table S5. ^{1}H and ^{13}C NMR[a] data of **8** in C_6D_6

	8		
position	δ_H (*J* in Hz)[b]	δ_C	C mult.
1		166.2	C
2	5.72 d (11.5)	120.6	CH
3	6.11 ddd (11.0,10.5, 2.5)	151.0	CH
4a	3.90 m	34.1	CH_2
4b	2.02 m		
5	3.96 m	73.3	CH
6	5.50 brd (10.5)	129.8	CH
7	5.62 brd (10.5)	125.4	CH
8a	1.79 m	32.1	CH_2
8b	1.67 m		
9	3.70 ddd (8.5, 5.0, 4.0)	68.1	CH
10a	1.50 brd (17.0)	44.0	CH_2
10b	1.20 ddd (16.0, 4.5, 3.5)		
11	1.78 m	30.0	CH
12a	2.60 dd (13.0, 4.5)	46.4	CH_2
12b	1.85 dd (13.0, 10.0)		
13		145.8	C
14	2.12 brs	37.6	CH2
15	3.88 m	67.4	CH
16	2.78 dd (2.0, 2.0)	60.8	CH
17	2.96 brd (10.5)	52.1	CH
18a	2.16 m	34.2	CH2
18b	1.40 m		
19	5.12 ddd (11.0, 6.0, 1.0)	72.4	CH
20	4.13 brd (9.0)	72.5	CH
21	5.68-5.60 m	129.2	CH
22	5.68-5.60 m	130.0	CH
23	4.33 brdd (14.0, 3.0)	75.7	CH
24b	1.60 m	34.4	CH_2
24a	1.25 m		
25		155.2	C
26	5.61 s	117.3	CH
27		163.5	C
28	0.92 d (6.5)	20.1	CH_3
29	4.98 brs, 4.96 brs	112.6	CH_2
30	1.22 s	22.2	CH_3

[a] measured at 500 MHz (^{1}H) and 125 MHz (^{13}C)

Table S6. ^{1}H and ^{13}C NMR[a] data of **9** in C_6D_6 and acetone d_6[b]

	9				
position	δ_H (J in Hz)	δ_C	C mult.	COSY	HMBC[b]
1		165.3	C		
2	5.84 d (11.5)	123.6	CH	3	1
3	5.72 ddd (11.5,10.5, 7.0)	142.2	CH	2, 4a	1
4a	3.05 ddd (14.0, 10.5, 5.0)	35.7	CH_2	3, 5	2, 3, 5
4b	2.15 ddd (14.0, 11.5, 6.5)				
5	4.35 m	73.2	CH	4	
6	5.60 dd (10.0, 2.5)	128.8	CH	7	8
7	5.69 ddd (10.5, 7.5, 2.5)	125.5	CH	6, 8	6, 8
8a	1.84 ddd (12.5, 10.0, 2.5)	32.1	CH_2	7, 9	
8b	1.60 dd (14.0, 2.5)				
9	3.45 dq (10.0, 2.4)	66.7	CH	8, 10	8
10a	1.55 dt (14.0, 9.5)	42.9	CH_2	9, 11	9, 11, 12
10b	0.93 ddd (13.5, 8.5, 2.0)				
11	1.95 m	27.3	CH	10, 28	
12a	2.11 dd (14.0, 7.5)	45.9	CH_2		
12b	2.05 m				
13		146.1	C		
14	2.30 m	35.7	CH_2	15	15
15	4.12 ddd (9.5, 3.5, 2.5)	71.4	CH	14, 16	
16	3.99 dd (5.0, 2.5)	75.7	CH	15, 17	15, 17
17	4.40 ddd (11.5, 6.0, 2.0)	78.3	CH	16, 18	
18	2.15 m	35.3	CH_2	17, 19	19, 20
19	5.47 dt (4.0, 4.0)	76.9	CH	18, 20	
20	4.31 dd (4.0, 3.5)	81.7	CH	19, 21	
21	5.87 dd (13.0, 4.0)	126.2	CH	20, 22	20, 22
22	5.90 dd (14.5, 4.5)	132.5	CH	21	20, 23
23	4.25 dddd (11.4, 3.6, 2.8, 0.6)	64.6	CH	22, 24	
24a	1.50 m	36.1	CH_2	23	25
24b	1.39 dd (14.5, 11.5)				23
25		59.3	C		
26	2.68 d (4.2)	59.5	CH	27	27
27	5.13 dd (12.0, 4.2)	88.5	CH	26, OH	
28	0.86 d (6.5)	20.1	CH_3	11	10, 11, 12
29	4.88 s, 4.87 s	113.5	CH_2		12, 13 14
30	0.95 s	21.7	CH_3		24, 25, 26
OH	3.30 d (12.0)			27	

[a] measured at 500 MHz (^{1}H) and 125 MHz (^{13}C)
[b] sample run in acetone d_6

Table S7. ^{1}H and ^{13}C NMR[a] data of **10** in C_6D_6

	10				
position	δ_H (J in Hz)	δ_C	C mult.	COSY	HMBC
1		166.3	C		
2	5.74 d (12.0)	121.0	CH	3	1
3	5.72 ddd (11.4,10.2, 3.6)	150.2	CH	2, 4a	1
4a	3.92 m	34.1	CH_2	3, 5	2, 3, 5
4b	1.46 m				
5	3.92 m	73.1	CH	4	
6	5.46 brd (10.2)	129.4	CH	7	8
7	5.67 brd (10.2)	125.3	CH	6, 8	6, 8
8a	1.81 m	32.1	CH_2	7, 9	
8b	1.70 m				
9	3.71 m	68.0	CH	8, 10	8
10a	1.54 ddd (16.8, 9.0, 2.4)	43.9	CH_2	9, 11	9, 11, 12
10b	1.20 ddd (14.4, 4.8, 3.0)				
11	1.78 m	29.9	CH	10, 28	
12a	2.61 dd (12.6, 6.0)	46.3	CH_2		
12b	1.90 dd (13.2, 10.2)				
13		145.8	C		
14a	2.16 dd (13.2, 3.6)	35.7	CH_2	15	15
14b	2.15 m				
15	3.96 m	67.5	CH	14, 16	
16	2.78 dd (2.4, 2.4)	60.7	CH	15, 17	15, 17
17	2.94 ddd (9.0, 3.0, 1.2)	52.0	CH	16, 18	
18a	2.05 ddd (10.2, 4.2, 1.2)	33.6	CH_2	17, 19	19, 20
18b	2.02 ddd (10.8, 3.6, 1.2)				
19	5.11 m	72.6	CH	18, 20	
20	4.15 brd (10.2)	73.3	CH	19, 21	
21	5.62 m	129.2	CH	20, 22	20, 22
22	5.62 m	132.5	CH	21	20, 23
23	4.18 m	64.4	CH	22, 24	
24a	1.50 m	36.1	CH_2	23	
24b	1.27 m				23
25		59.3	C		
26	2.68 d (4.2)	59.5	CH	27	27
27	5.13 d (4.2)	88.4	CH	26, OH	
28	0.89 d (6.6)	21.0	CH_3	11	10, 11, 12
29	4.93 s, 4.92 s	112.5	CH_2		12, 13 14
30	0.93 s	21.7	CH_3		24, 26
OH	3.25 d (12.0)			27	

[a] measured at 500 MHz (^{1}H) and 125 MHz (^{13}C)

Table S8. ^{1}H and ^{13}C NMR[a] data of **11** in C_6D_6

	11			
position	δ_H (*J* in Hz)	δ_C	C mult.	COSY
1		165.3	C	
2	5.83 d (12.0)	123.6	CH	3
3	5.72 ddd (11.4,10.8, 7.2)	142.2	CH	2, 4a
4a	3.08 ddd (14.4, 10.2, 4.8)	35.8	CH_2	3, 5
4b	2.16 ddd (15.6, 11.4, 7.0)			3, 5
5	4.37 m	73.2	CH	4, 4'
6	5.50 dt (10.8, 3.6)	128.8	CH	7
7	5.62 ddd (10.2, 6.0, 2.4)	125.4	CH	6, 8
8a	1.78 ddd (16.8, 9.0, 4.2)	32.1	CH_2	9
8b	1.60 m			7
9	3.45 dq (10.2, 1.8)	66.7	CH	8, 8'
10a	1.57 m	42.8	CH_2	9
10b	0.92 ddd (14.4, 9.6, 1.8)			11
11	1.90 m	27.4	CH	10, 28
12a	2.04 m	46.0	CH_2	
12b	2.02 m			
13		146.1	C	
14a	2.25 m	35.7	CH_2	15
14b	2.24 m			
15	4.09 ddd (9.0, 3.6, 2.4)	71.3	CH	14
16	3.97 dd (4.8, 1.8)	75.4	CH	15, 17
17	4.42 ddd (10.8, 3.6, 2.4)	78.2	CH	16, 18
18a	2.06 m	35.1	CH_2	17
18b	2.02 m			19
19	5.48 dd (3.6, 3.6)	76.8	CH	18, 20
20	4.31 dd (4.8,4.8)	81.9	CH	19, 21
21	5.94 dd (15.0, 4.8)	125.8	CH	20, 22
22	6.04 dd (15.6, 4.8)	132.9	CH	21
23	4.50 dddd (12.0, 4.8, 2.4, 1.0)	66.6	CH	22, 24
24a	1.93 dd (15.0, 10.8)	36.1	CH_2	23
24b	1.45 m			
25		136.4	C	
26	5.45 brs	120.8	CH	27, 30
27	4.92 brs	96.8	CH	26, 30
28	0.84 d (6.6)	20.2	CH_3	11
29	4.85 brs, 4.87 brs	113.3	CH_2	14
30	1.43 s	22.5	CH_3	26, 27
OMe	3.34 s	54.9	CH_3	

[a] measured at 500 MHz (^{1}H) and 125 MHz (^{13}C)

Table S9. [1]H and [13]C NMR[a] data of **12** in C_6D_6

	12			
position	δ_H (*J* in Hz)	δ_C	C mult.	COSY
1		165.3	C	
2	5.86 d (12.0)	123.6	CH	3
3	5.73 ddd (12.0,10.5, 7.0)	142.3	CH	2, 4a
4a	3.12 ddd (11.0, 5.0, 1.2)	35.8	CH_2	3, 5
4b	2.12 m			3, 5
5	4.44 m	73.3	CH	4, 4'
6	5.58 ddd (10.5, 3.0, 1.5)	128.9	CH	7
7	5.65 dd (10.5, 5.5)	125.5	CH	6, 8
8a	1.84 ddd (12.5, 9.5, 2.0)	32.1	CH_2	9
8b	1.50 m			7
9	3.48 tt (10.0, 2.5)	66.8	CH	8, 8'
10a	1.55 m	42.8	CH_2	9
10b	0.94 ddd (13.5, 9.0, 2.0)			11
11	1.95 m	27.4	CH	10, 28
12a	2.15 m	46.0	CH_2	
12b	2.05 m			
13		146.1	C	
14a	2.35 m	35.7	CH_2	15
14b	2.34 m			
15	4.14 dt (9.5, 3.0)	71.5	CH	14
16	4.09 dd (9.0, 6.5)	75.6	CH	15, 17
17	4.48 ddd (10.5, 5.5, 5.1)	78.4	CH	16, 18
18a	2.15 m	35.1	CH_2	17
18b	2.02 m			19
19	5.54 dt (4.5, 3.5)	77.0	CH	18, 20
20	4.50 dd (4.5, 3.5)	82.0	CH	19, 21
21	5.97 ddd (16.0, 5.5, 1.0)	126.2	CH	20, 22
22	6.07 ddd (15.5, 5.0, 1.0)	133.4	CH	21
23	4.57 dddd (10.7, 4.5, 2.0, 1.0)	66.6	CH	22, 24
24a	2.15 m	36.1	CH_2	23
24b	1.60 m			23
25		136.3	C	
26	5.41 brs	121.6	CH	27, 30
27	5.35 brs	89.0	CH	26, 30
28	0.87 d (6.0)	20.2	CH_3	11
29	4.92 brs, 4.89 brs	113.5	CH_2	14
30	1.46 s	22.7	CH_3	26, 27

[a] measured at 500 MHz ([1]H) and 125 MHz ([13]C)

Table 10. 1D ^{1}H NMR Difference of NOE Enhancements[a] Observed for Fijianolide G (**10**) at H-23,[b] H-26,[c] H-27[d] and CH_3-30[e] in C_6D_6.

Expt	H irrad	NOE	rel enhanc inten[a]
A	23	21	2.2
		22	2.2
		24a	1.1
B	26	27	1.7
		30	1.9
C	27	26	1

[a] Relative enhanced intensity data based on setting the height of the weakest difference NOE peak as "1". [b] Actual spectrum is shown in Figure S22. [c] Actual spectrum is shown in Figure S23. [d] Actual spectrum is shown in Figure S24.

Table S11. Cytotoxicity in zone units of the fijianolides in the disk diffusion soft agar colony formation assay[a]

Compound	Conc.	Murine tumor cell lines		Human tumor cell lines			
	μg/disk	L1210	C 38	H-116	H-125	CEM	CFU-GM
Fijianolide A	30	150	0	100	50		
Fijianolide B	36		800			>1000	
“	9	500		700	250		550
Fijianolide D	100	0	150	0	0		
Fijianolide E	40	350	400	500	400	550	500
Fijianolide F	60	150	0	50	100		
Fijianolide G	30	150	350	200	200		100
Fijianolide H	40	0	150	0	0		
Fijianolide I	30	0	50	0	0		

[a] measured in zone units: 200 zone units = 6mm. Murine cell lines: L1210 (lymphocytic leukemia), C38 (colon adenocarcinoma), CFU(GM) (colony-forming unit-granulocyte macrophage; normal hematopoietic); Human cell lines: H116 (colon), H125 (lung), CEM (leukemia), CFU(GM) (colony-forming unit-granulocyte macrophage; normal hematopoietic). [b] Significant selectivity is defined by a difference of 250 zone units.

Figure S1. Selected examples of cytotoxic marine-derived polyketides.

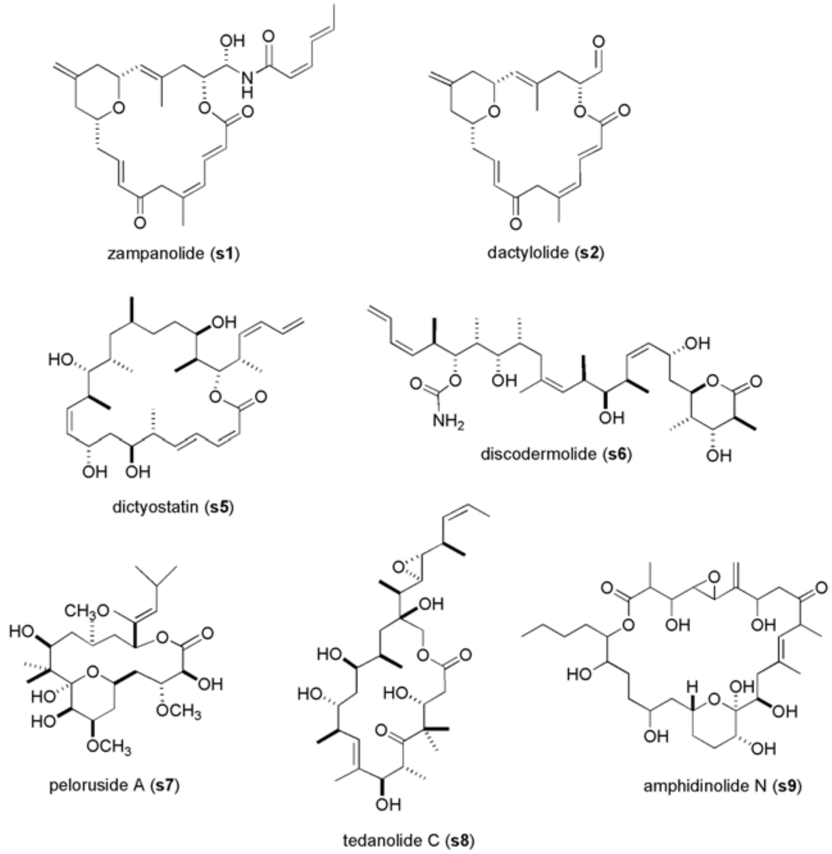


Figure S2. ^{1}H NMR spectrum of fijianolide A (**1**), (500 MHz, C_6D_6)

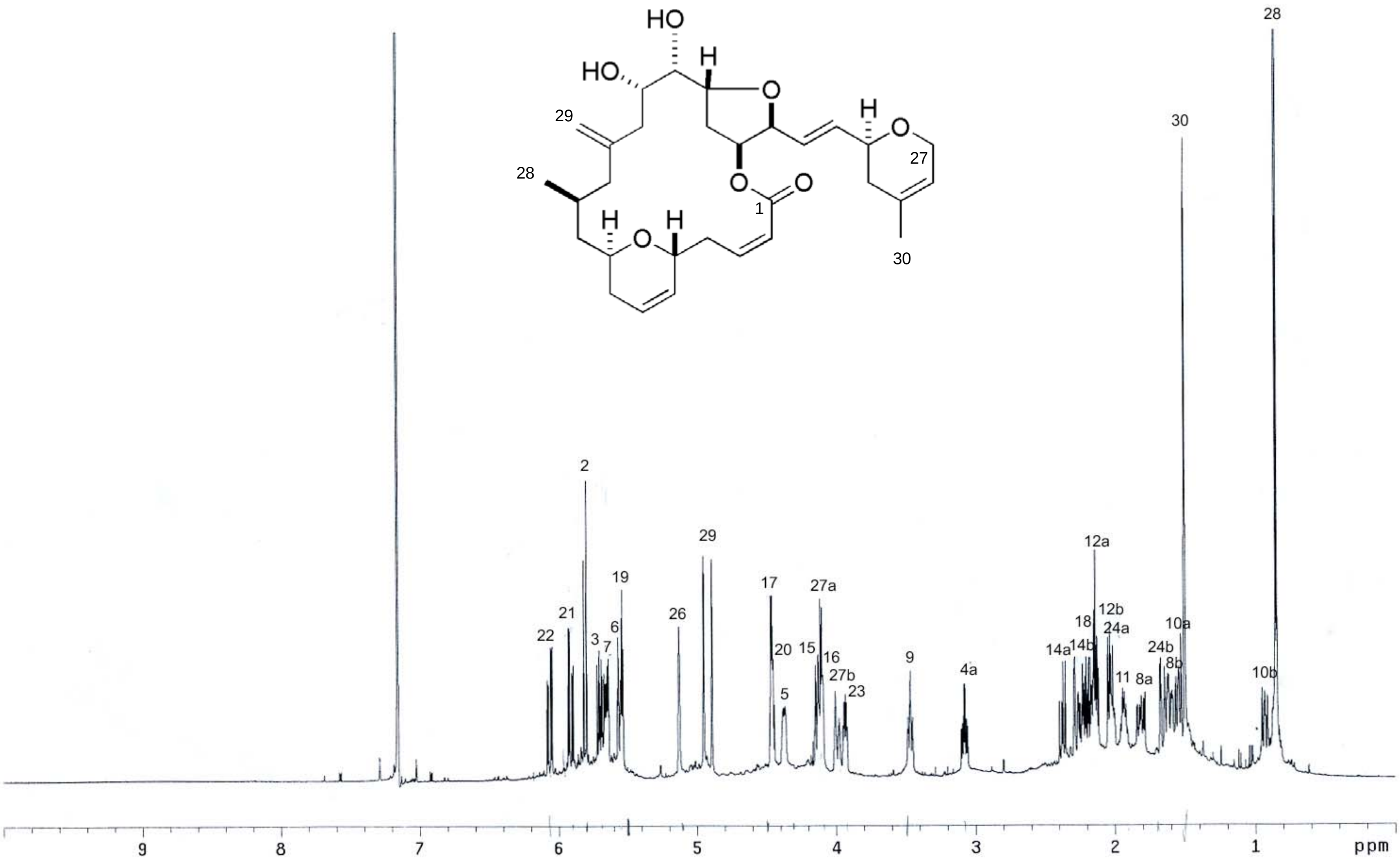


Figure S3. ^{13}C NMR spectrum of fijianolide A (**1**), (125 MHz, C_6D_6)

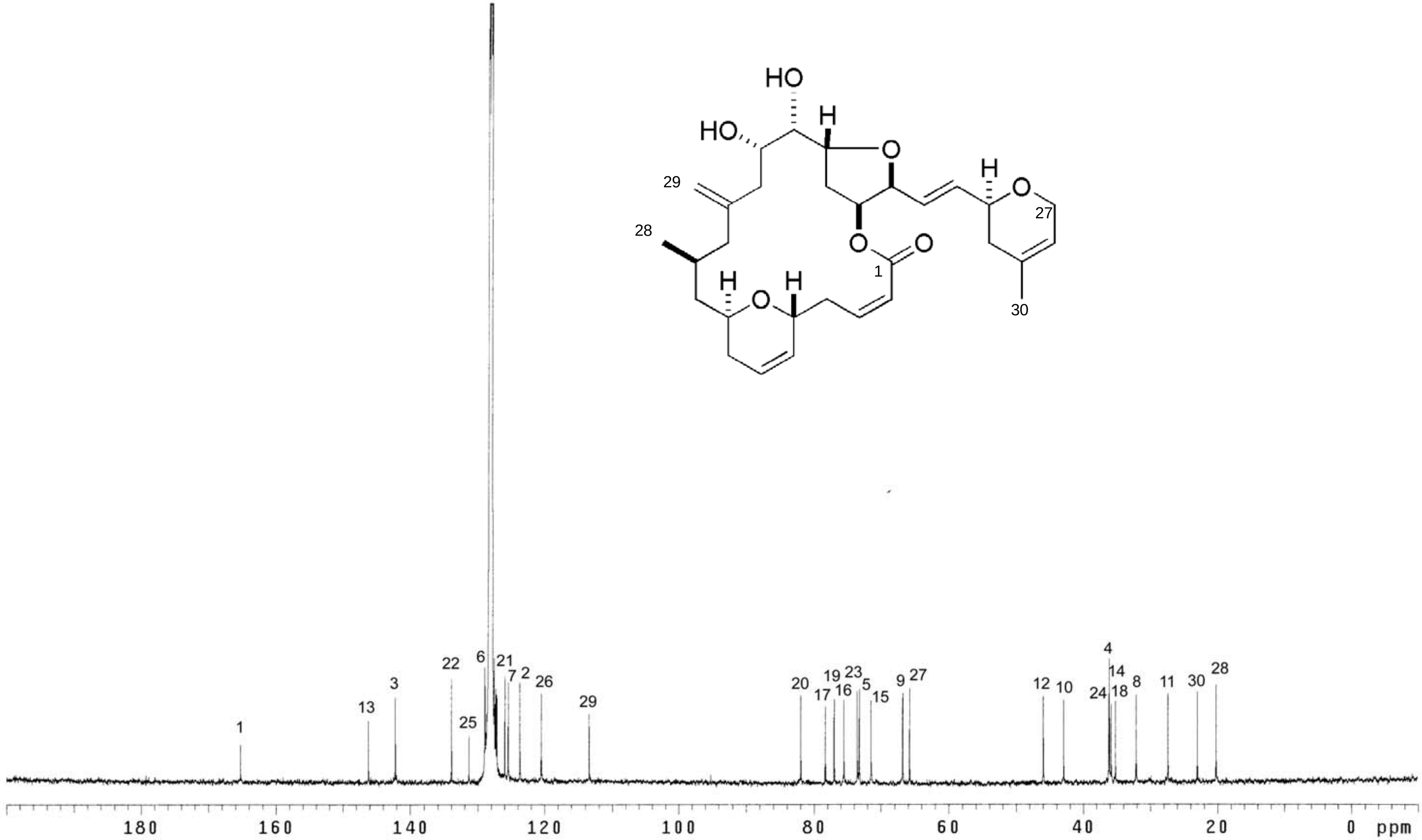


Figure S4. [1]H NMR spectrum of fijianolide B (**2**), (500 MHz, C_6D_6)

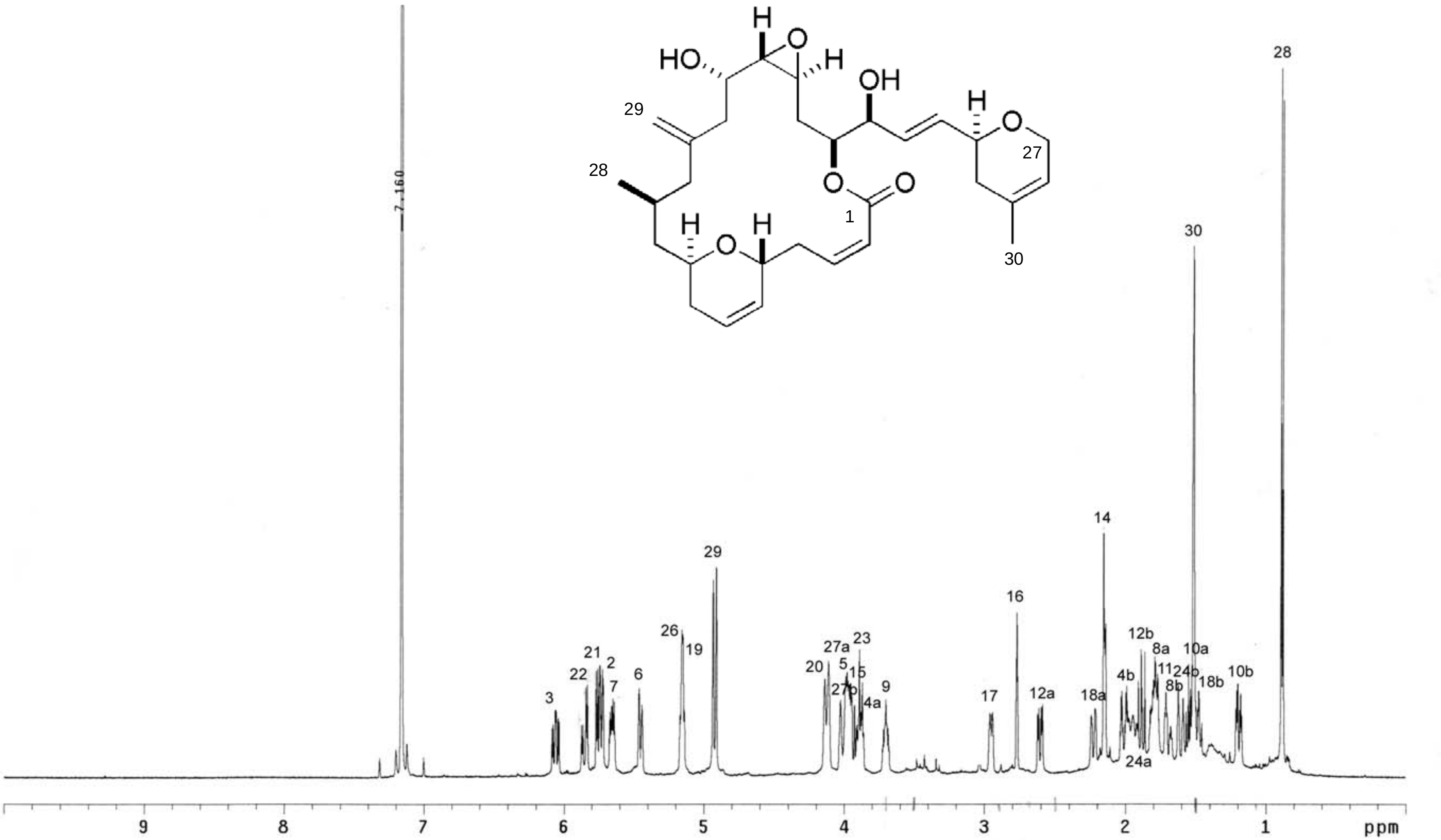


Figure S5. ^{13}C NMR spectrum of fijianolide B (**2**), (125 MHz, C_6D_6)

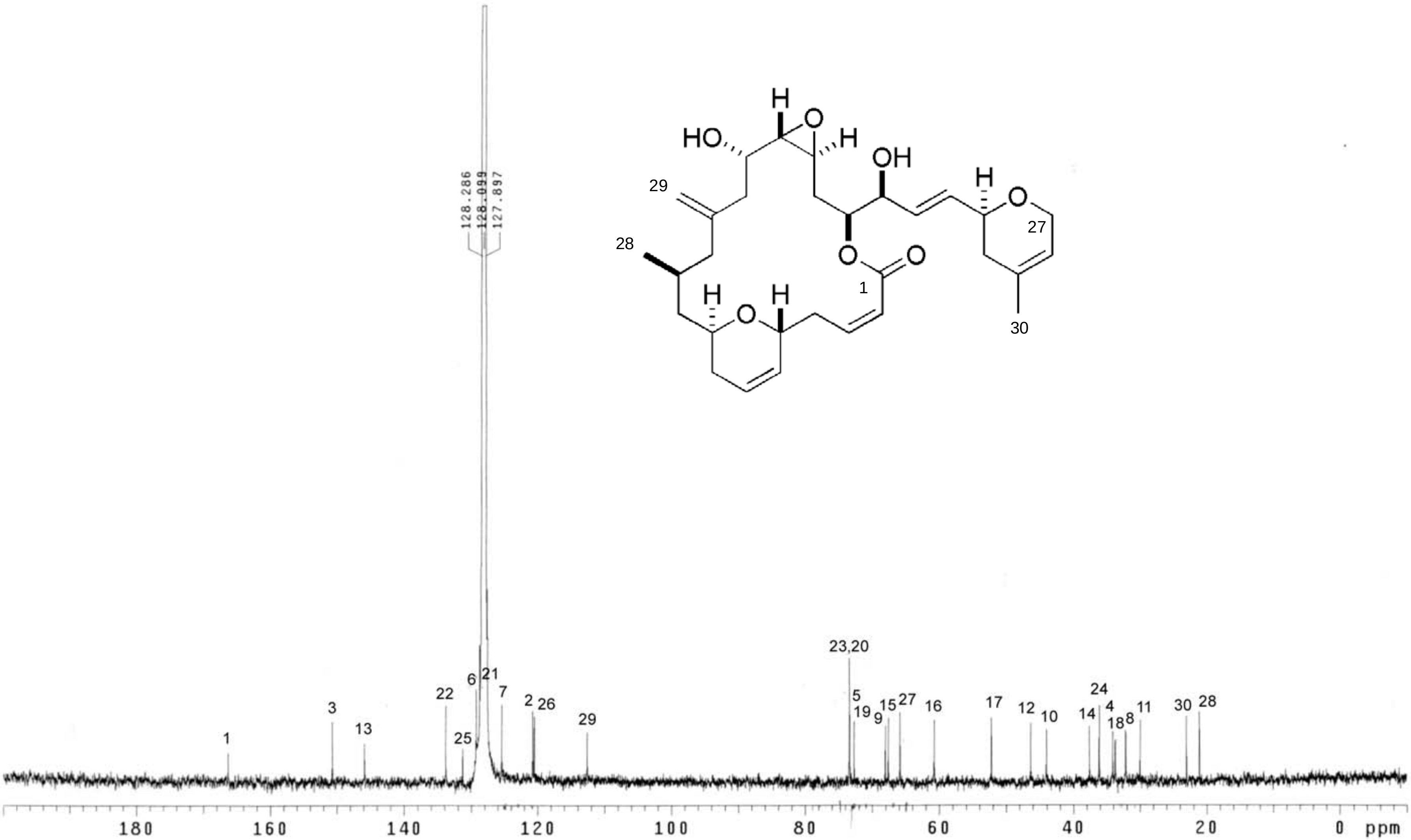


Figure S6. [1]H NMR spectrum of fijianolide D (**7**), (500 MHz, $CDCl_3$)

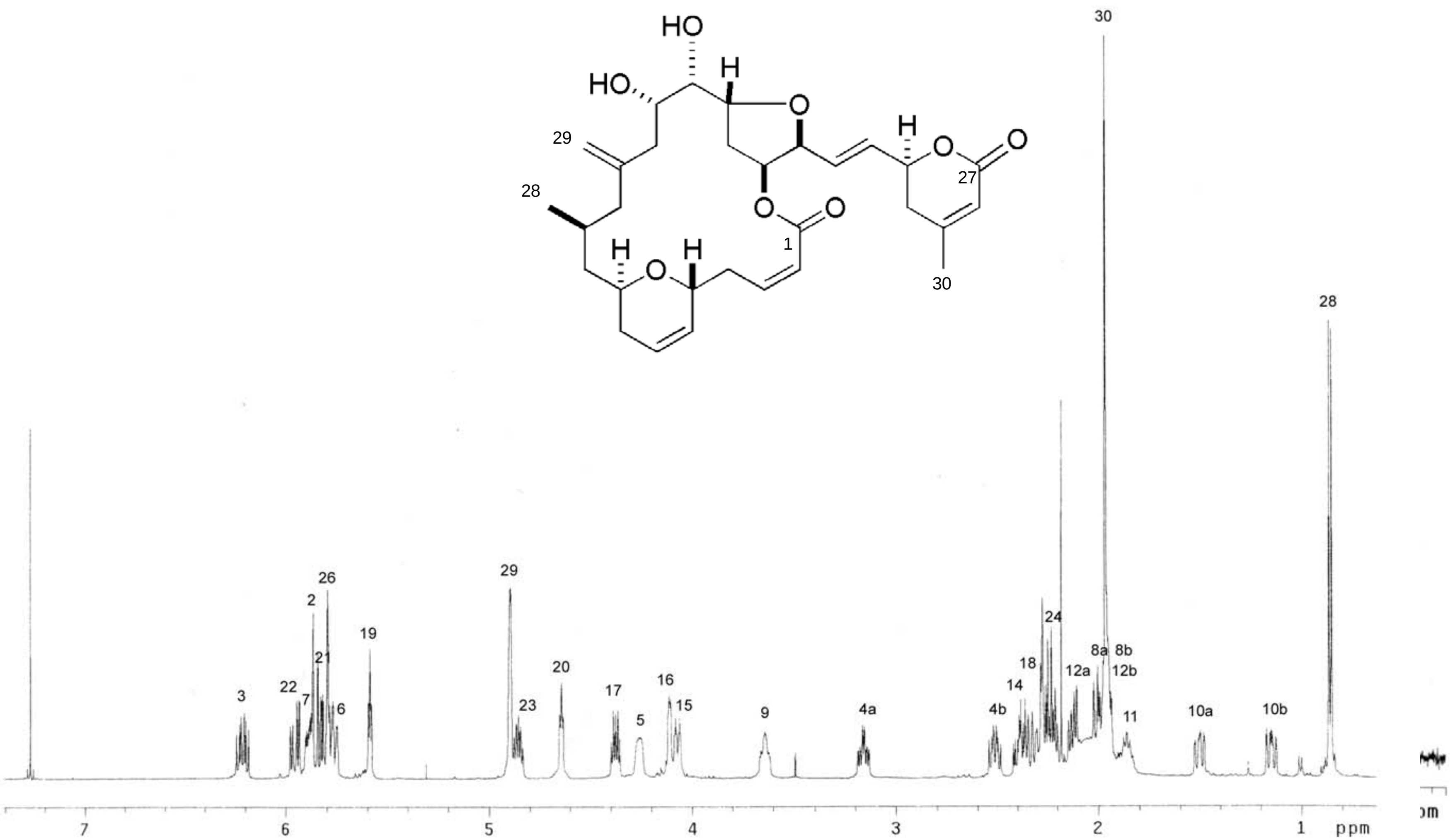


Figure S7. ^{13}C NMR spectrum of fijianolide D (**7**), (125 MHz, C_6D_6)

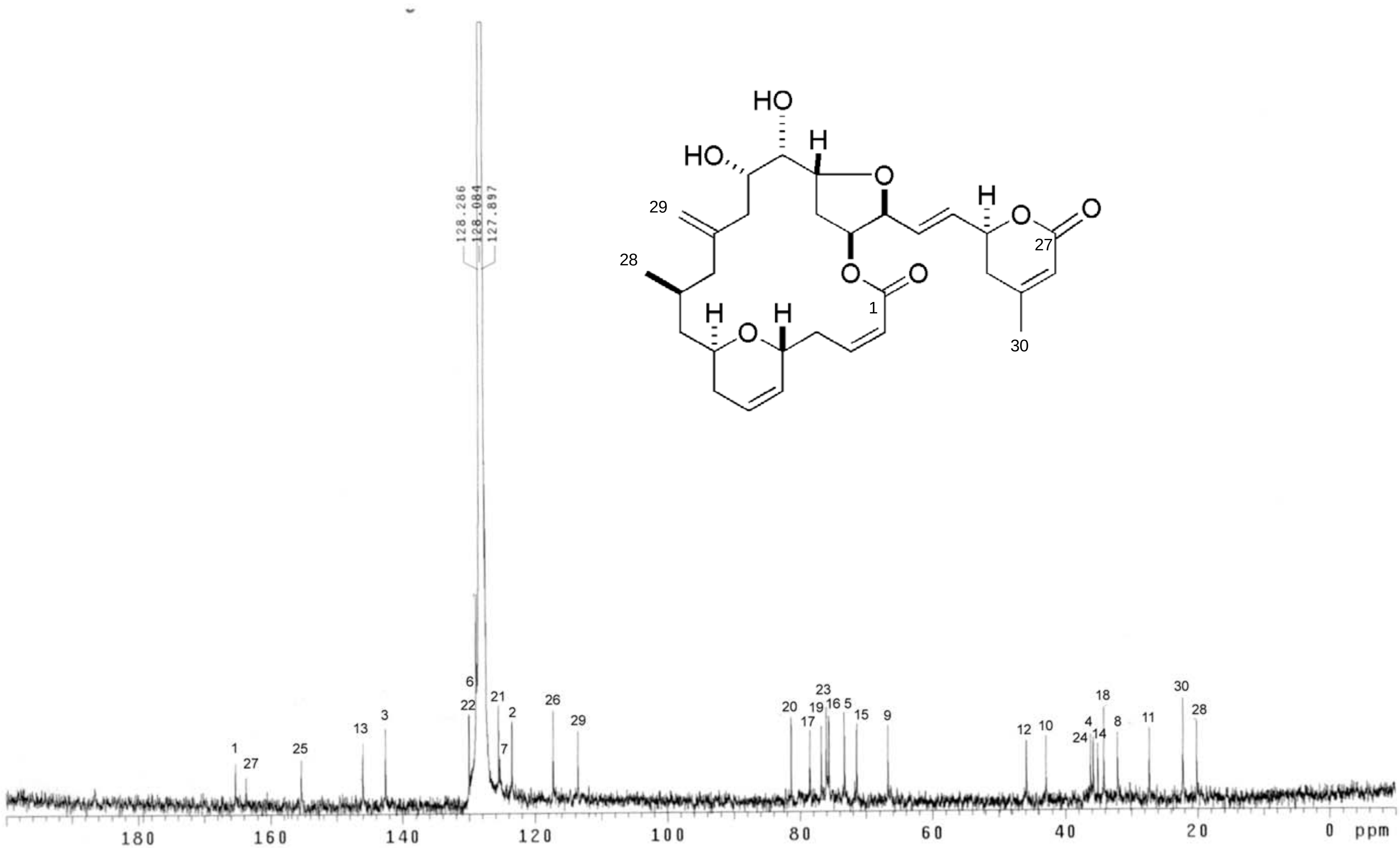


Figure S8. [1]H NMR spectrum of fijianolide E (8), (500 MHz, C_6D_6)

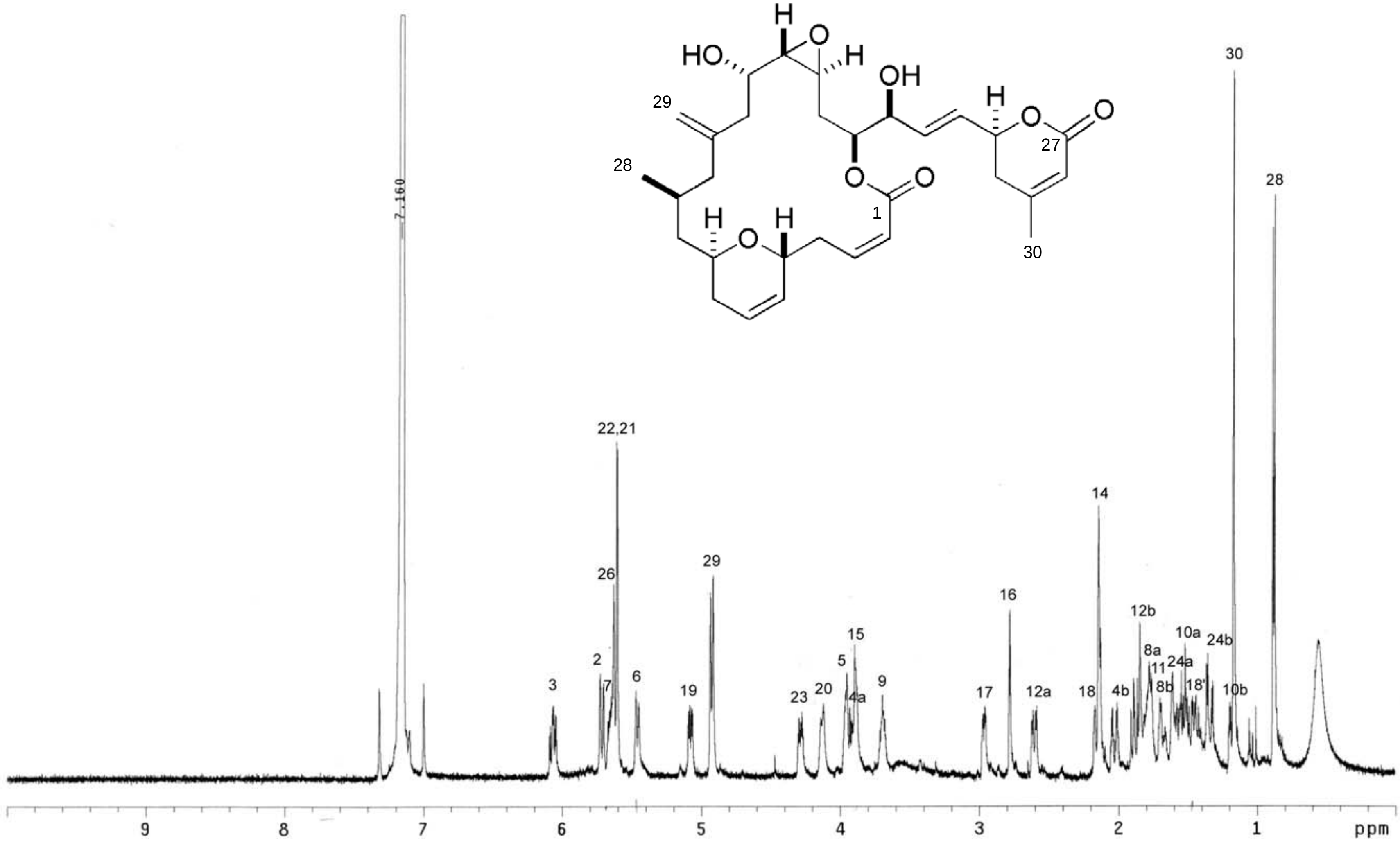


Figure S9. ^{13}C NMR spectrum of fijianolide E (**8**), (125 MHz, C_6D_6)

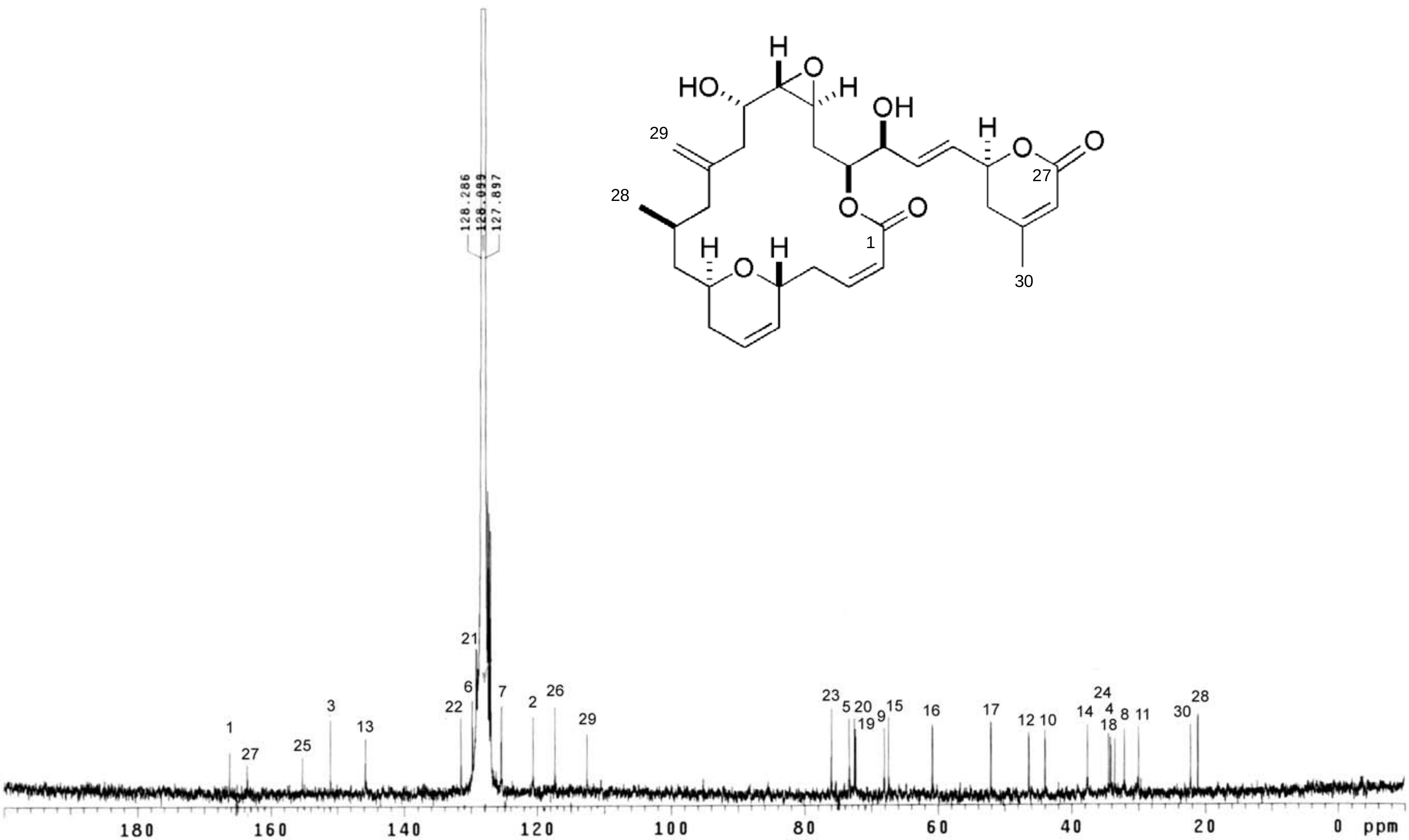


Figure S10. ^{1}H NMR spectrum of fijianolide F (**9**), (500 MHz, C_6D_6)

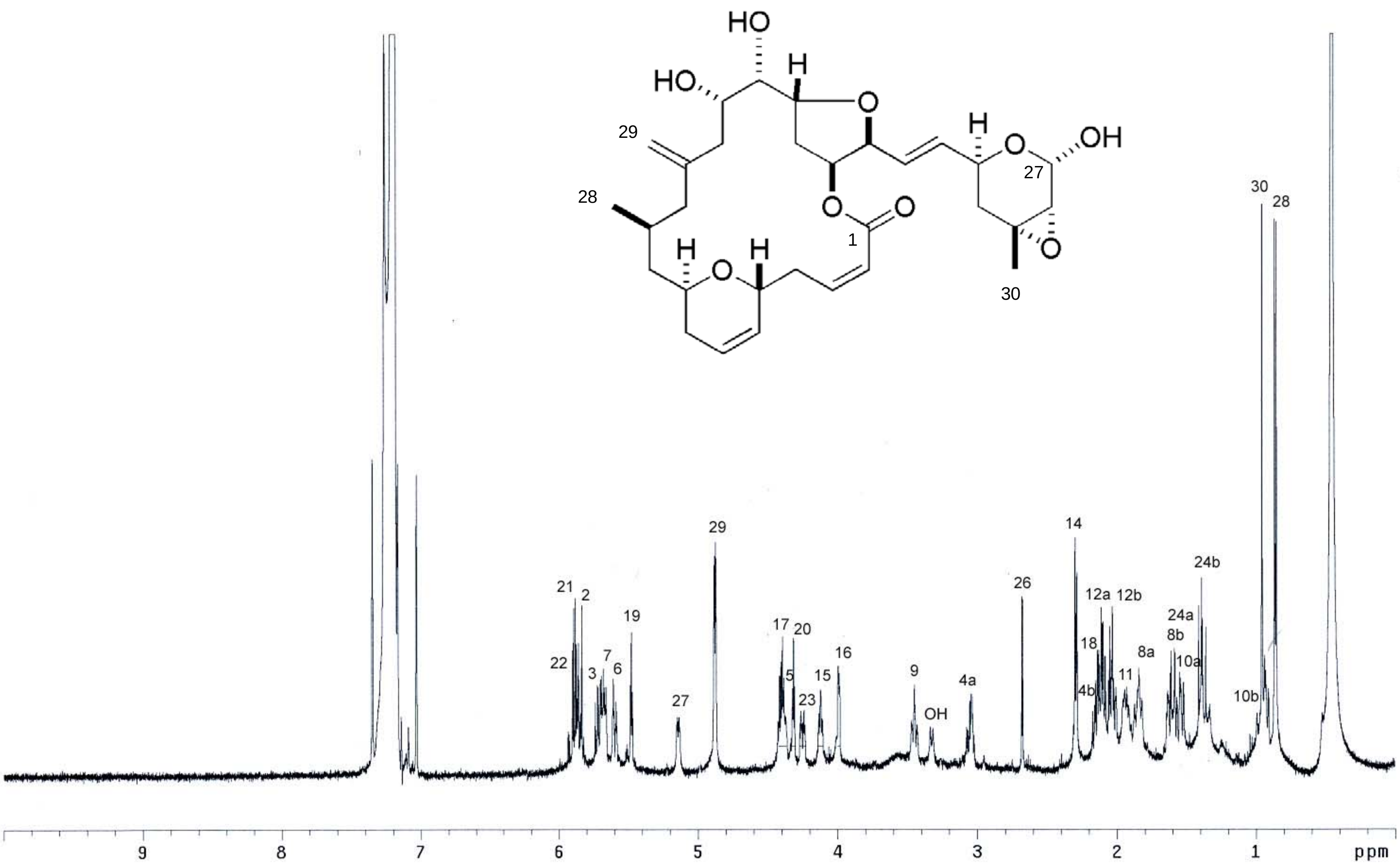


Figure S11. ^{13}C NMR spectrum of fijianolide F (**9**), (125 MHz, C_6D_6)

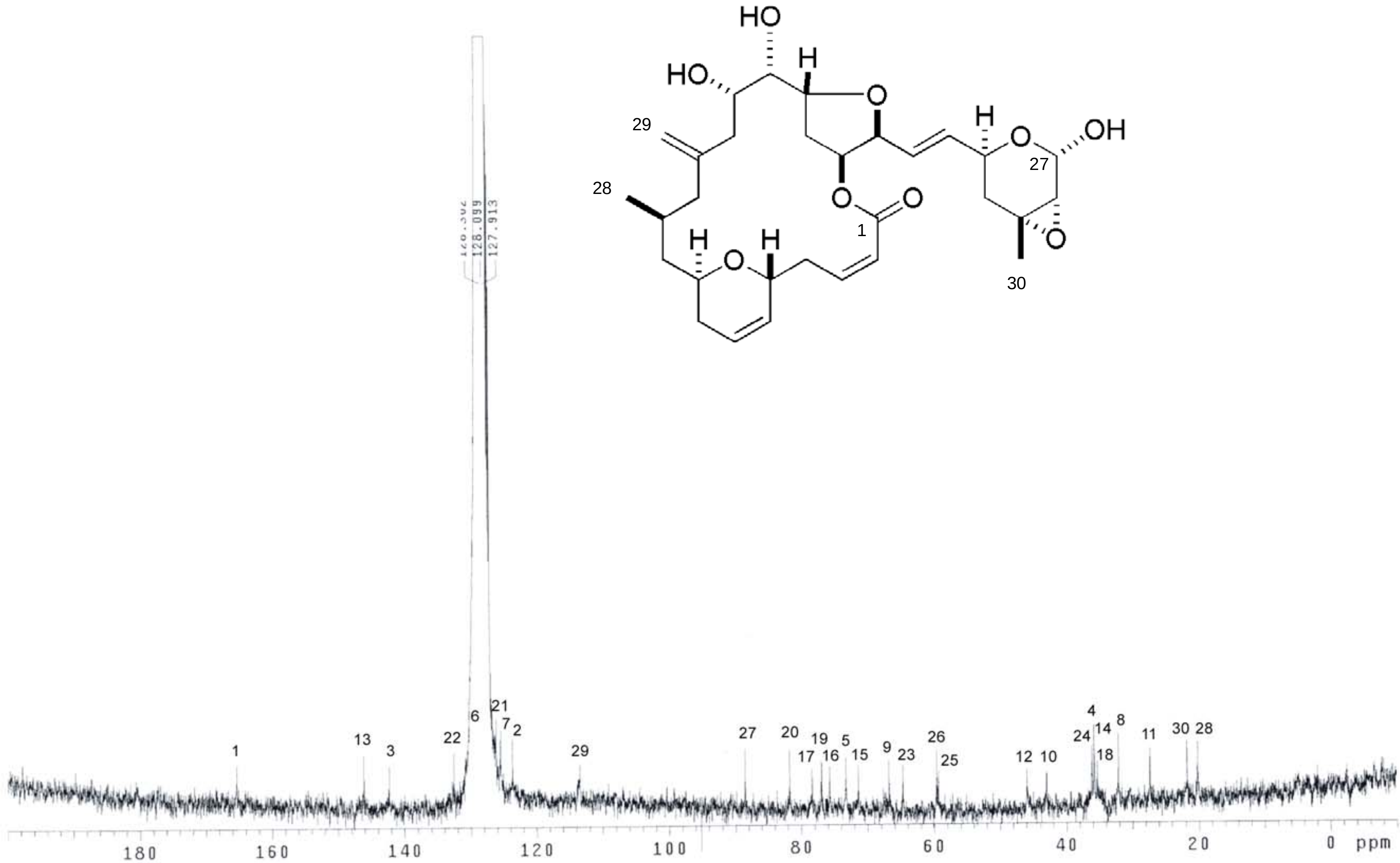


Figure S12. [1]H NMR spectrum of fijianolide G (**10**), (500 MHz, C_6D_6)

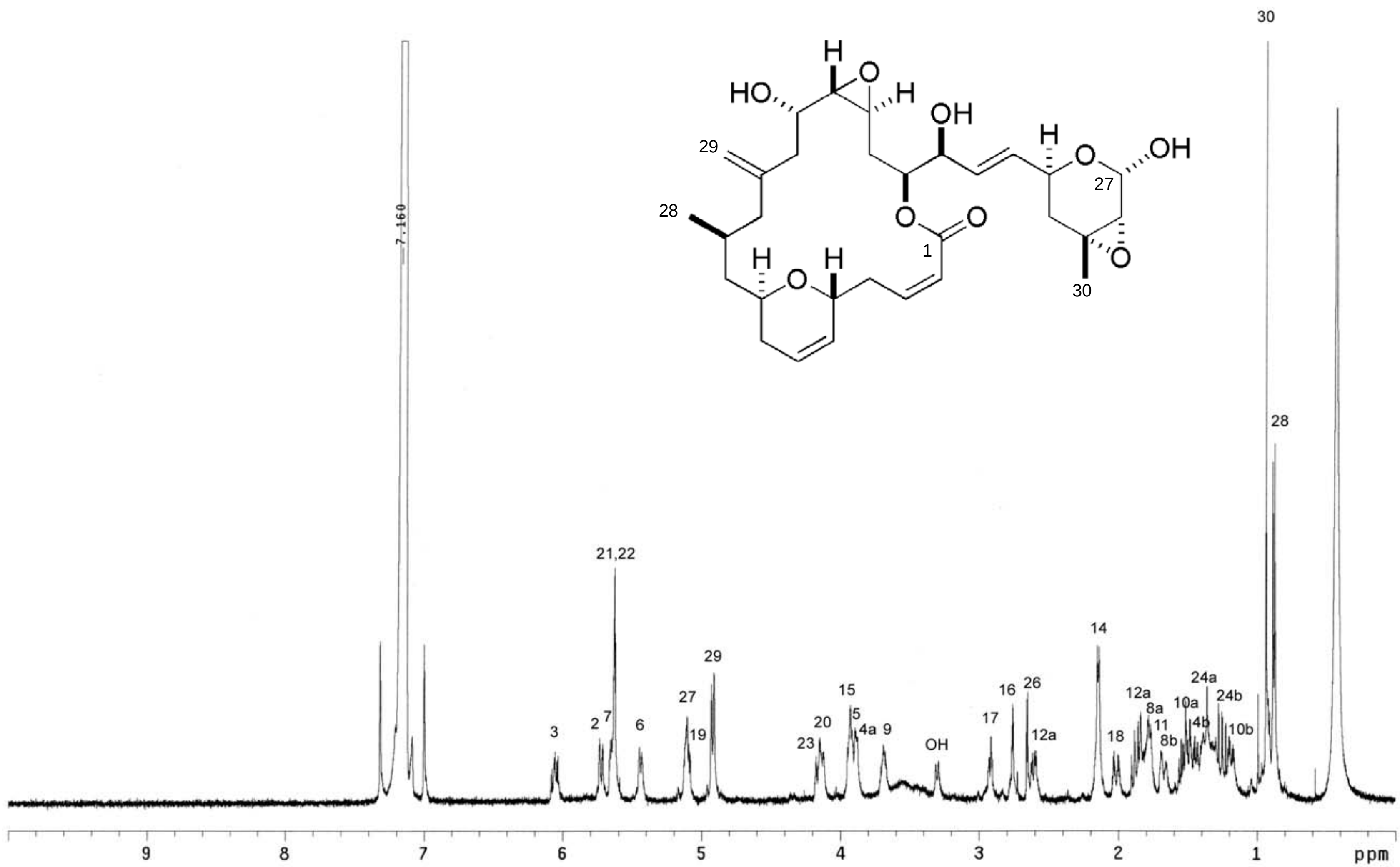


Figure S13. ^{13}C NMR spectrum of fijianolide G (**10**), (125 MHz, C_6D_6)

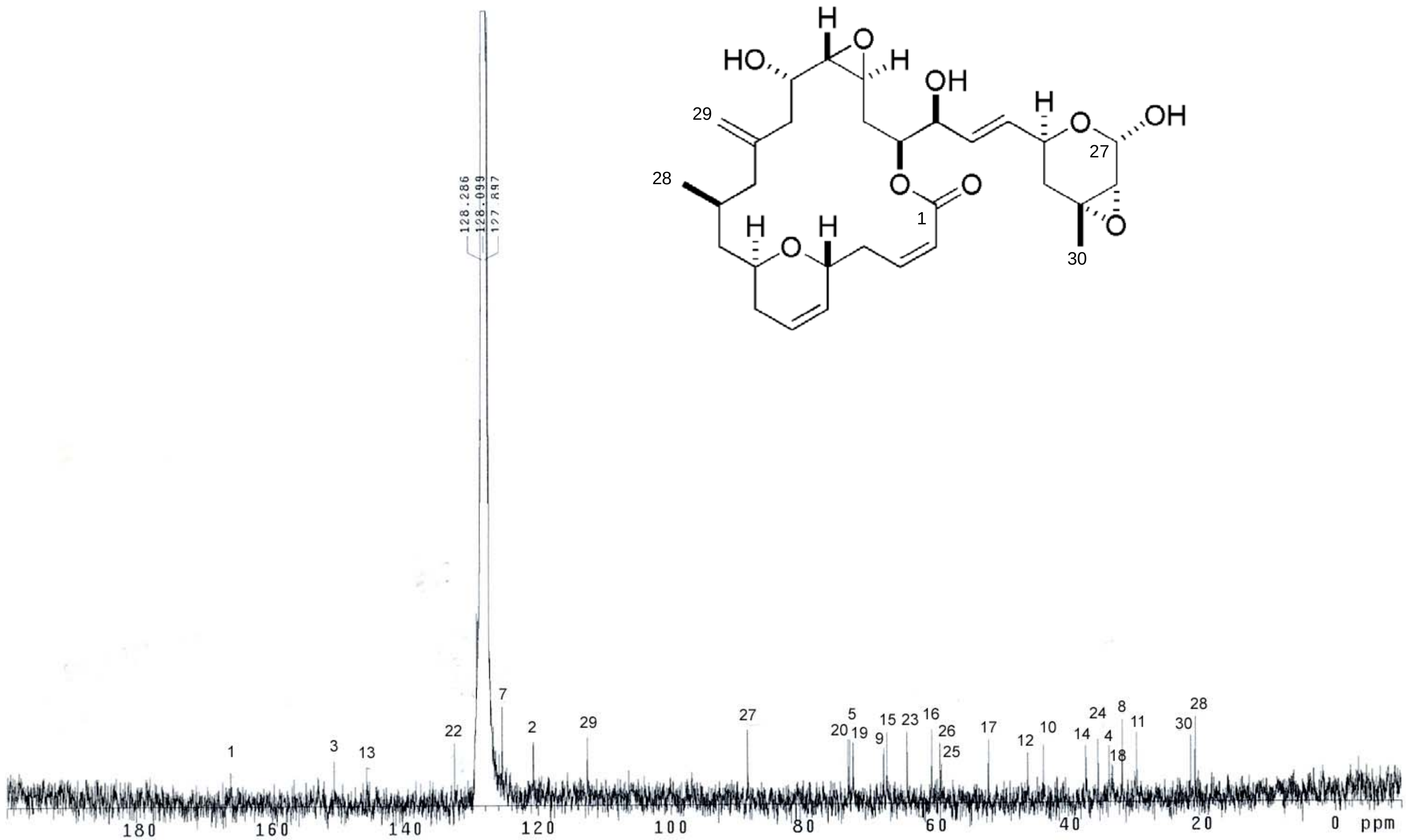


Figure S14. ^{1}H NMR spectrum of fijianolide H (**11**), (500 MHz, C_6D_6)

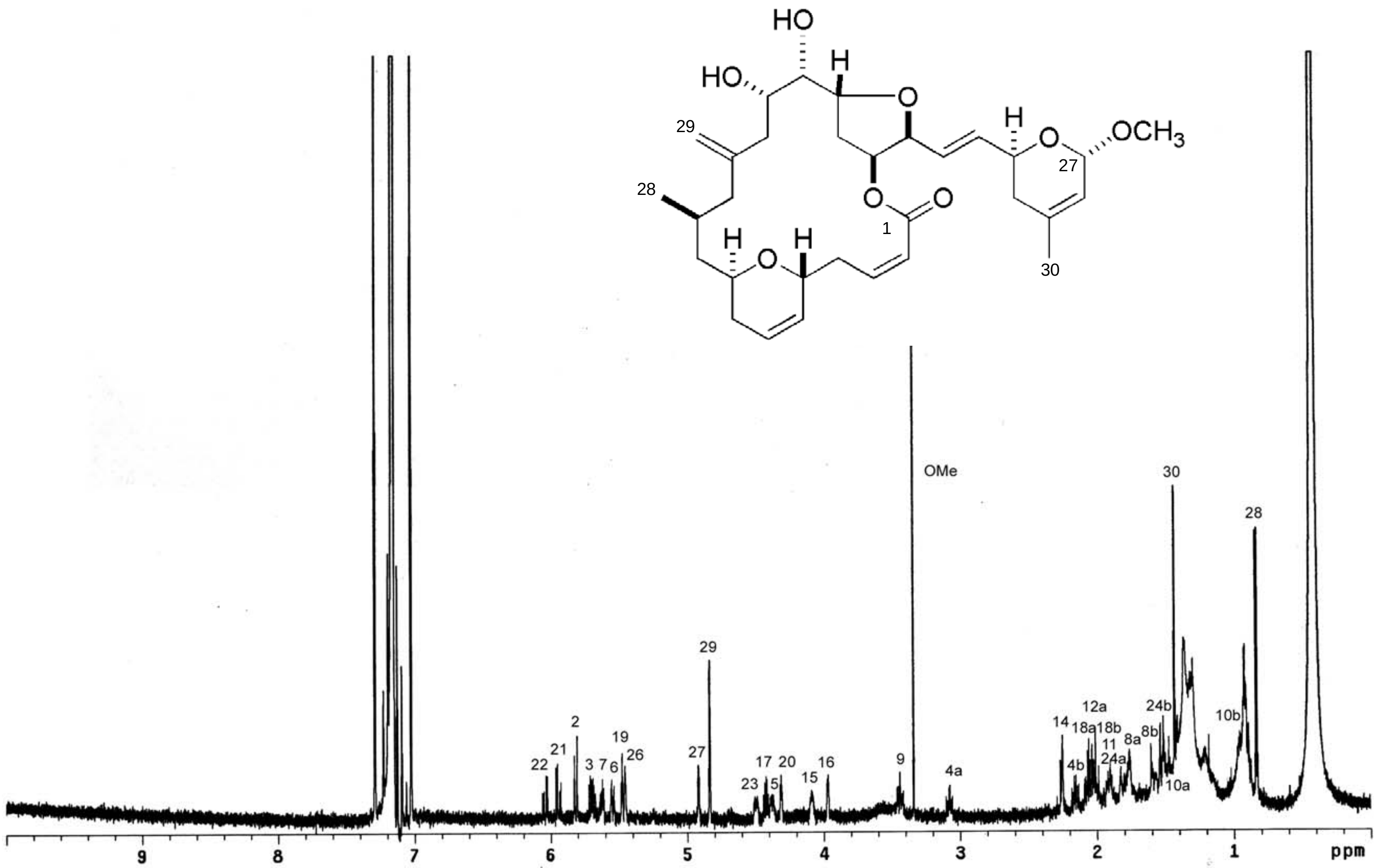


Figure S15. ^{13}C NMR spectrum of fijianolide H (**11**), (125 MHz, C_6D_6)

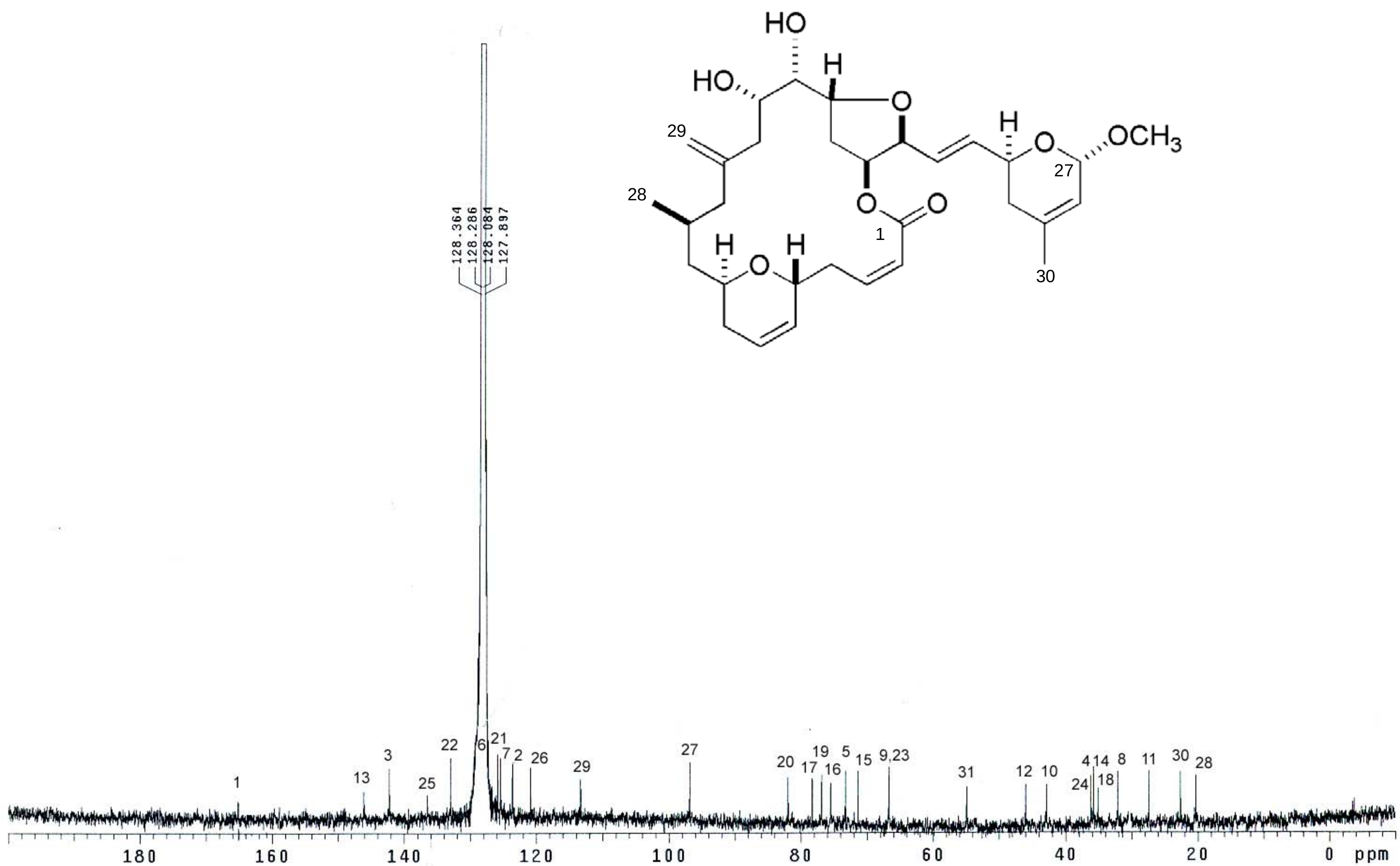


Figure S16. [1]H NMR spectrum of fijianolide I (**12**), (500 MHz, C_6D_6)

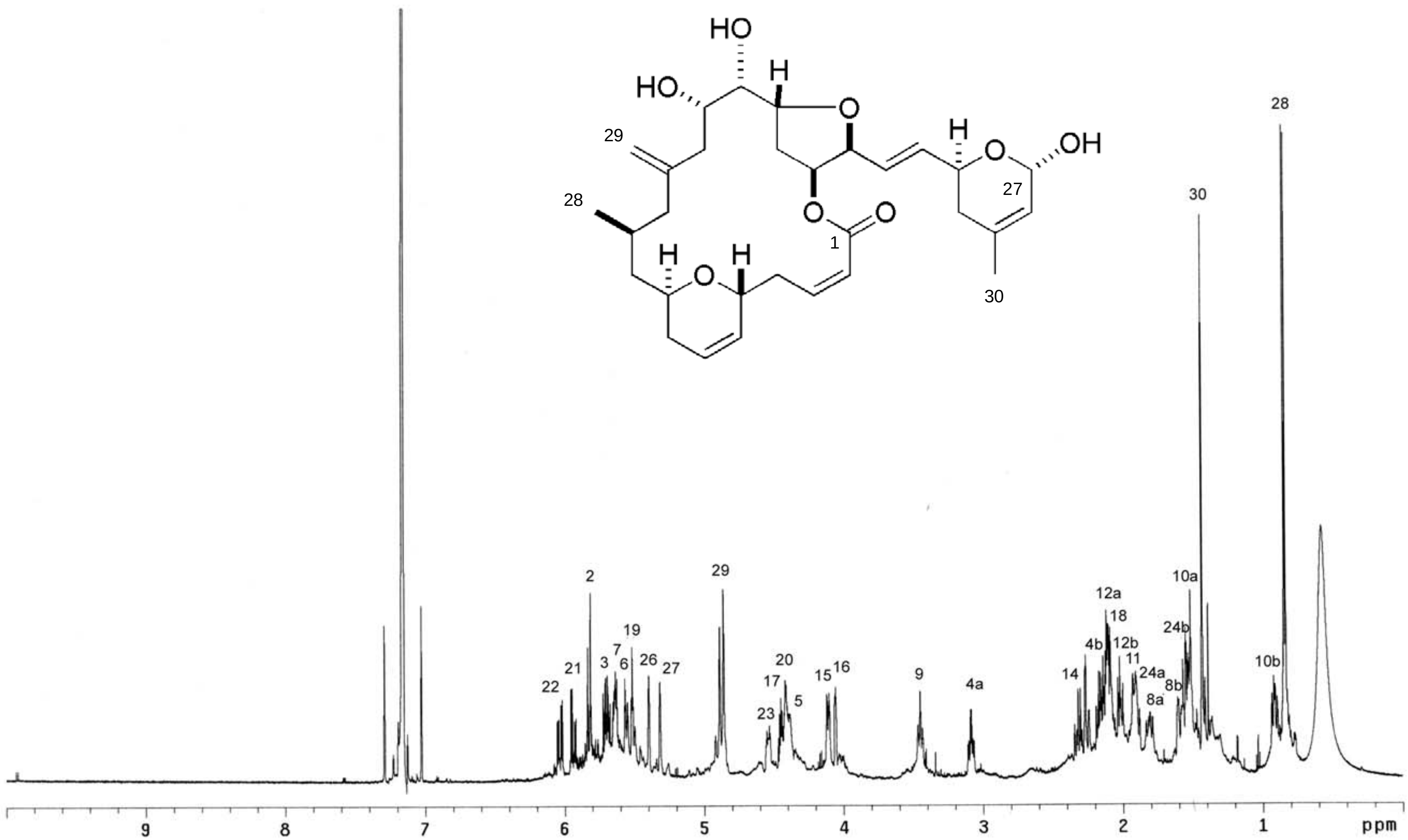


Figure S17. ^{13}C NMR spectrum of fijianolide I (**12**), (125 MHz, C_6D_6)

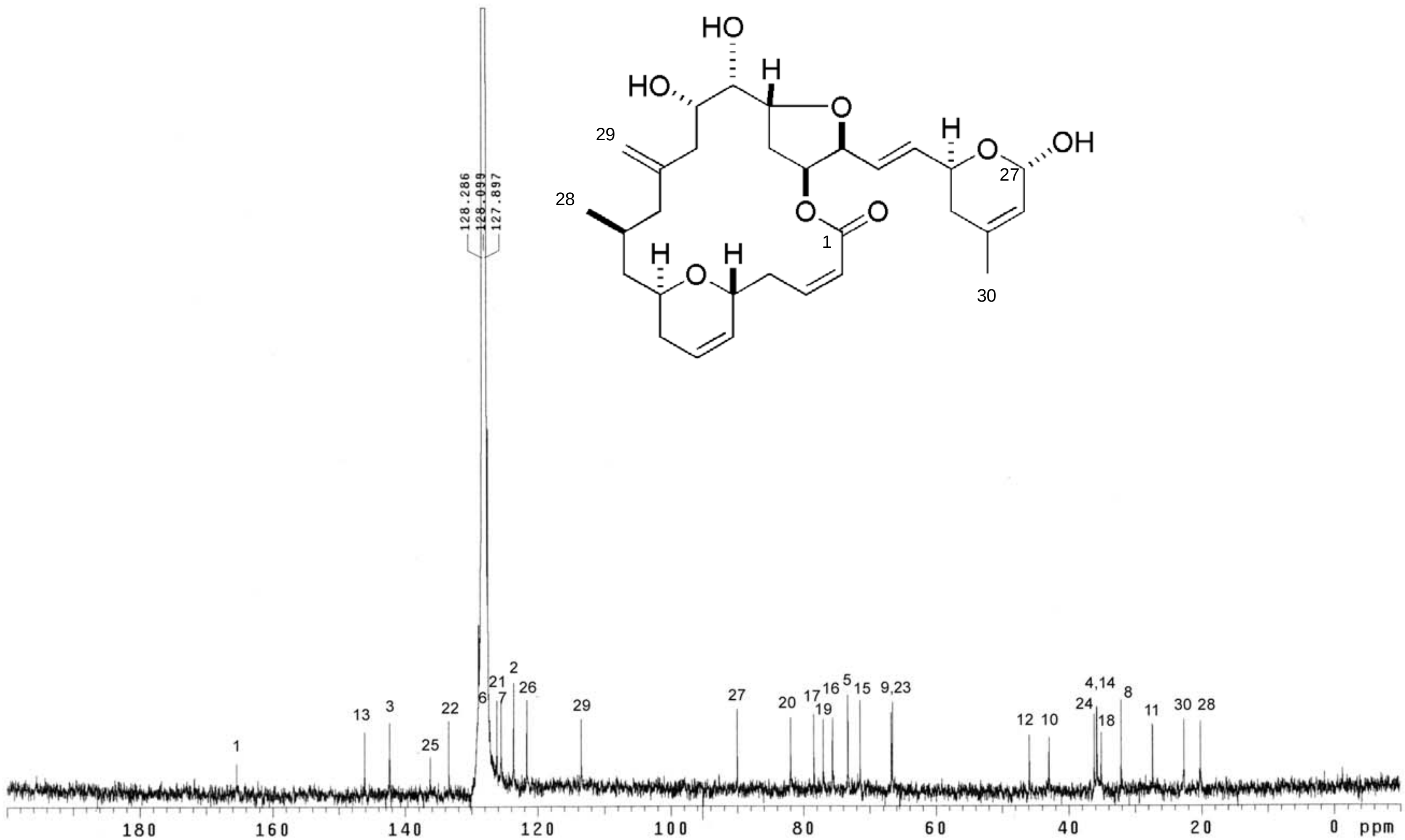


Figure S18. NOE enhancement of H-23 of **9** in benzene-d_6 at 600 MHz.

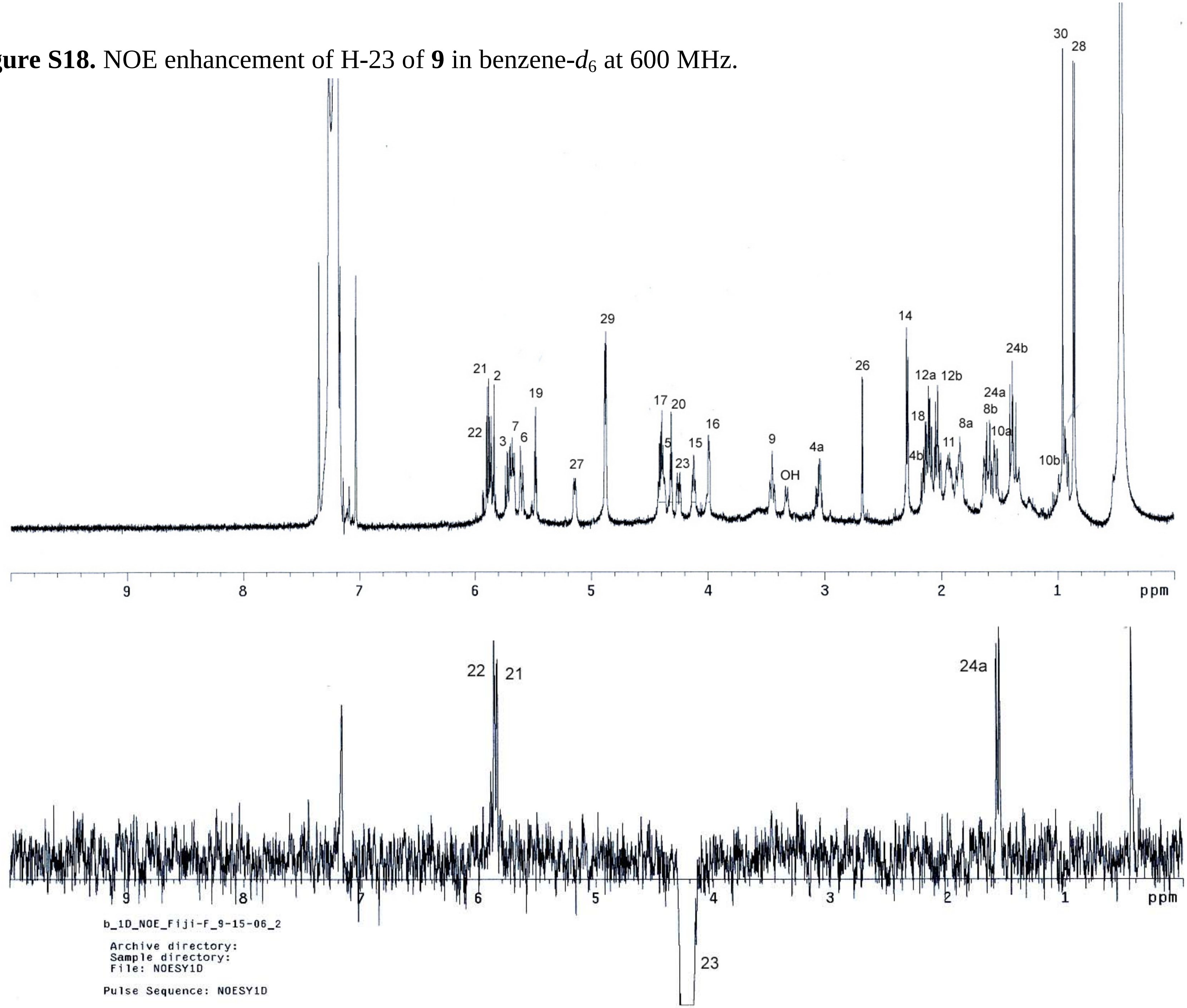


Figure S19. NOE enhancement of H-26 of **9** in benzene-d_6 at 600 MHz.

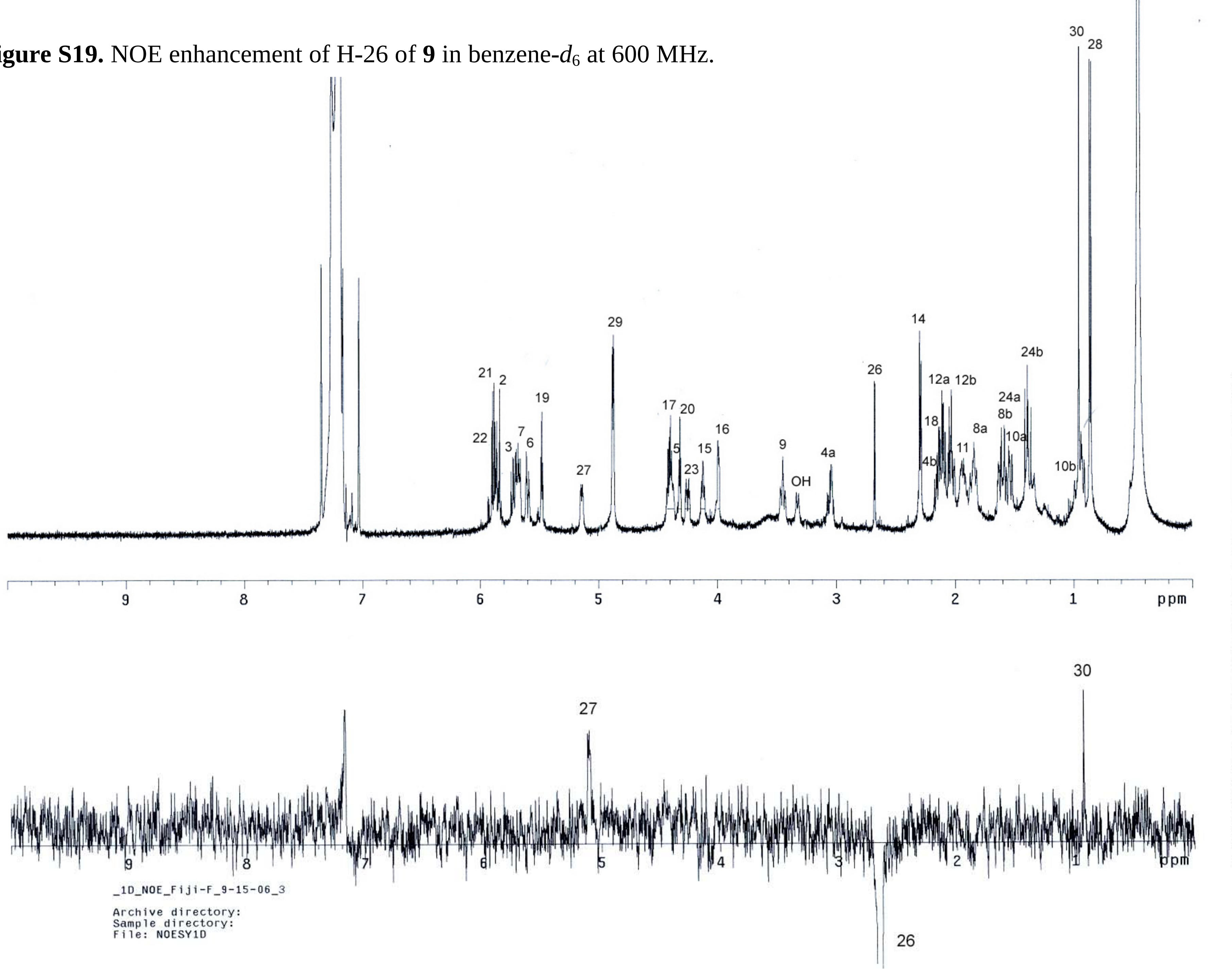


Figure S20. NOE enhancement of H-27 of **9** in benzene-d_6 at 600 MHz.

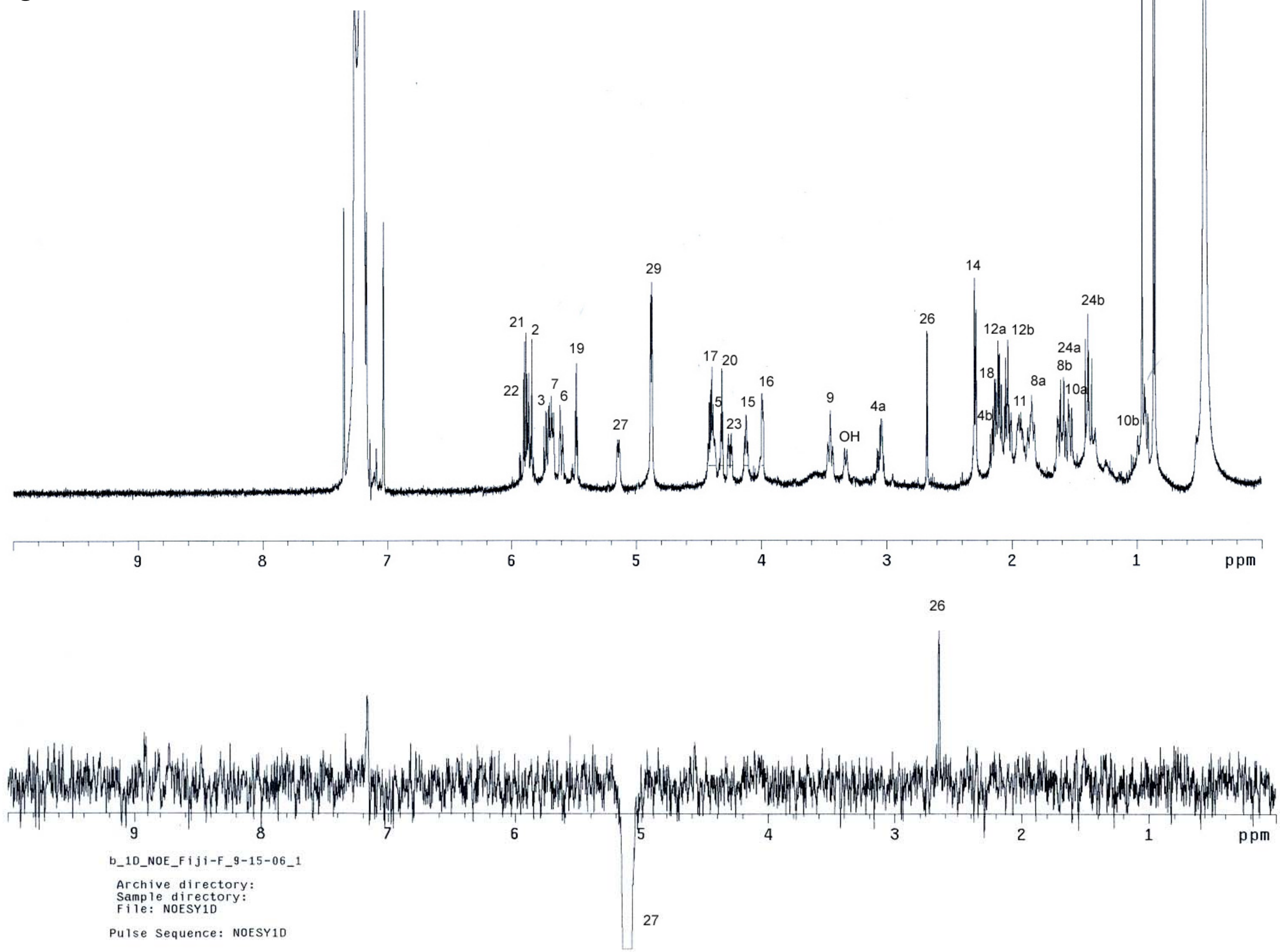


Figure S21. NOE enhancement of CH_3-30 of **9** in benzene-d_6 at 600 MHz.

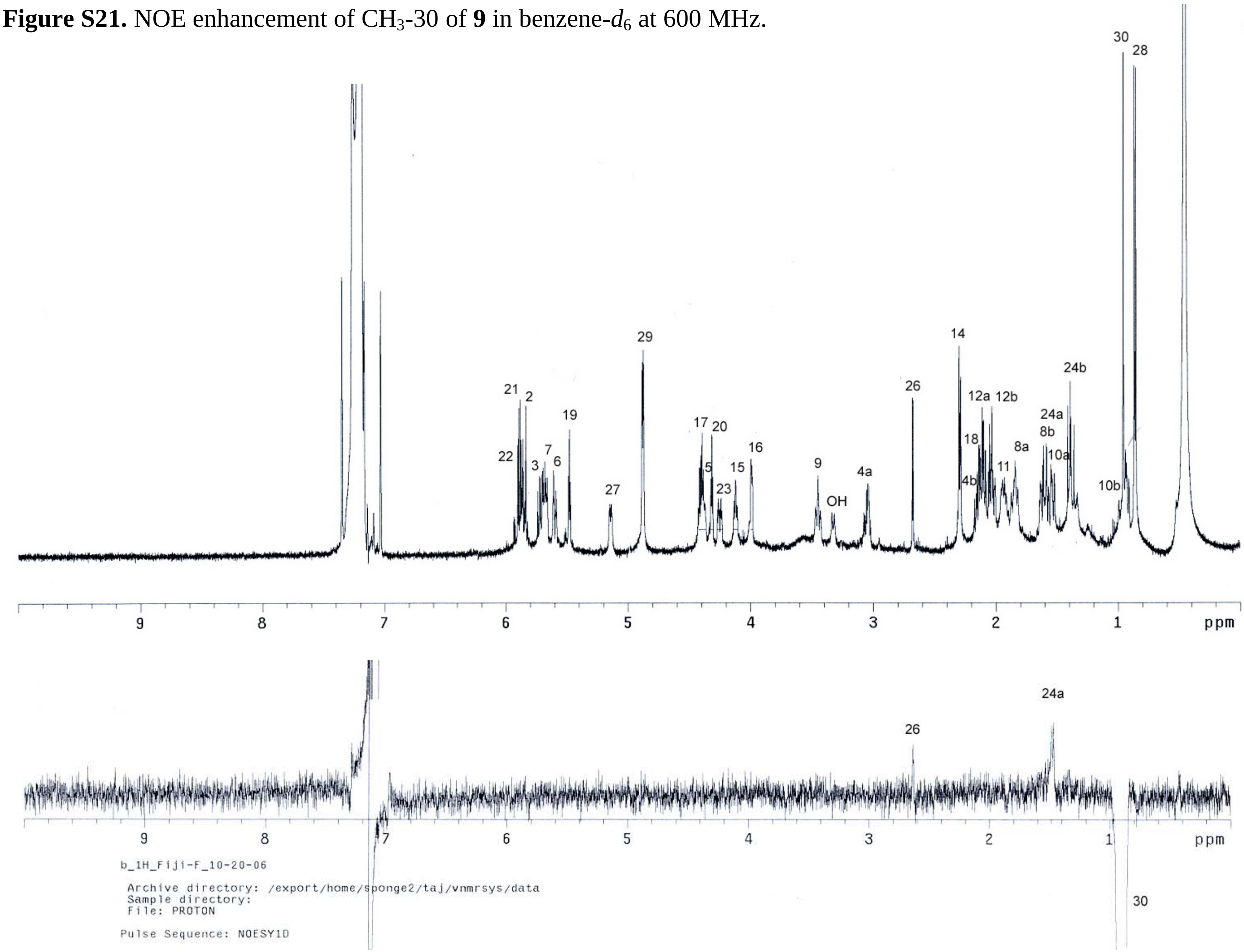


Figure S22. NOE enhancement of H-23 of **10** in benzene-d_6 at 600 MHz.

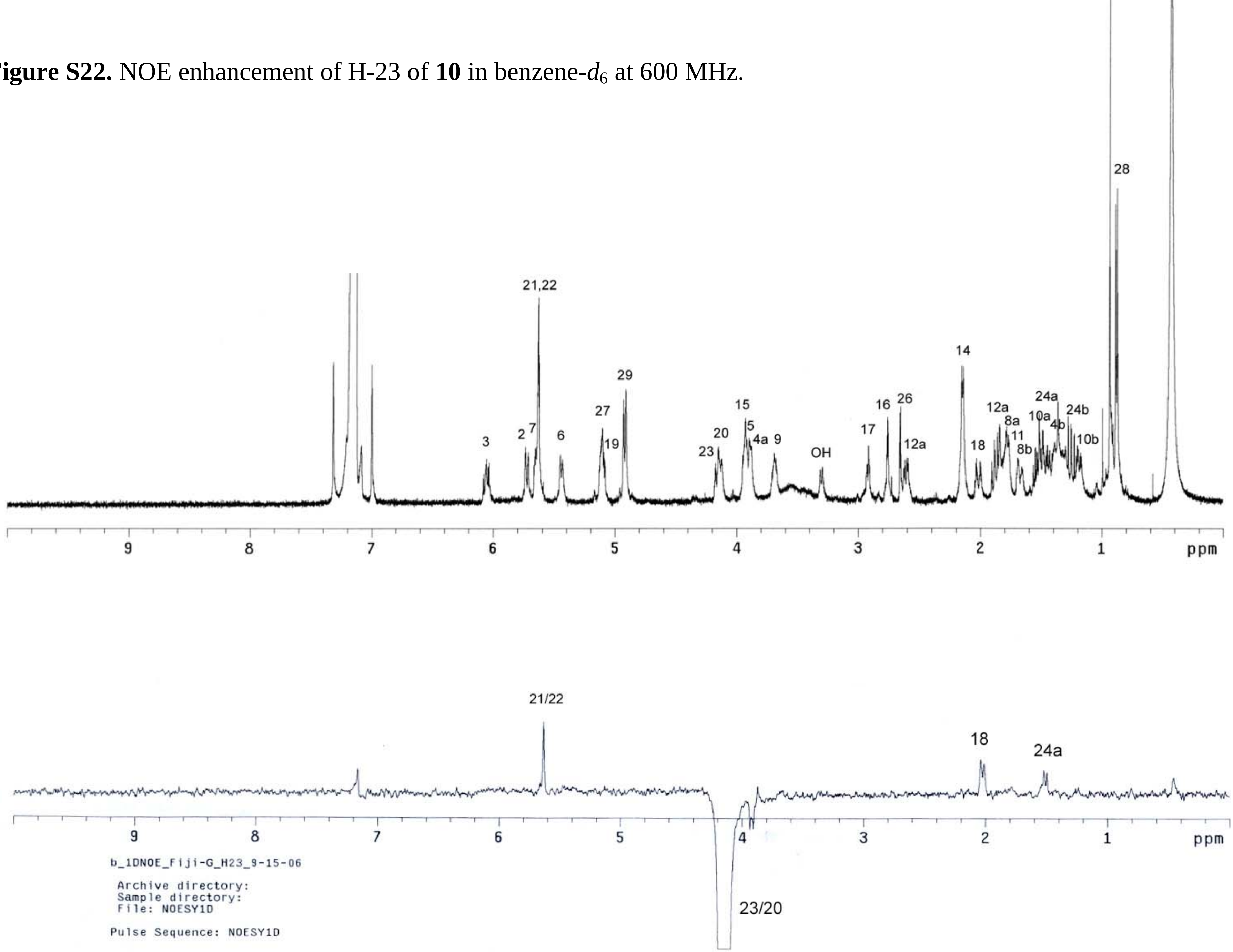


Figure S23. NOE enhancement of H-26 of **10** in benzene-d_6 at 600 MHz.

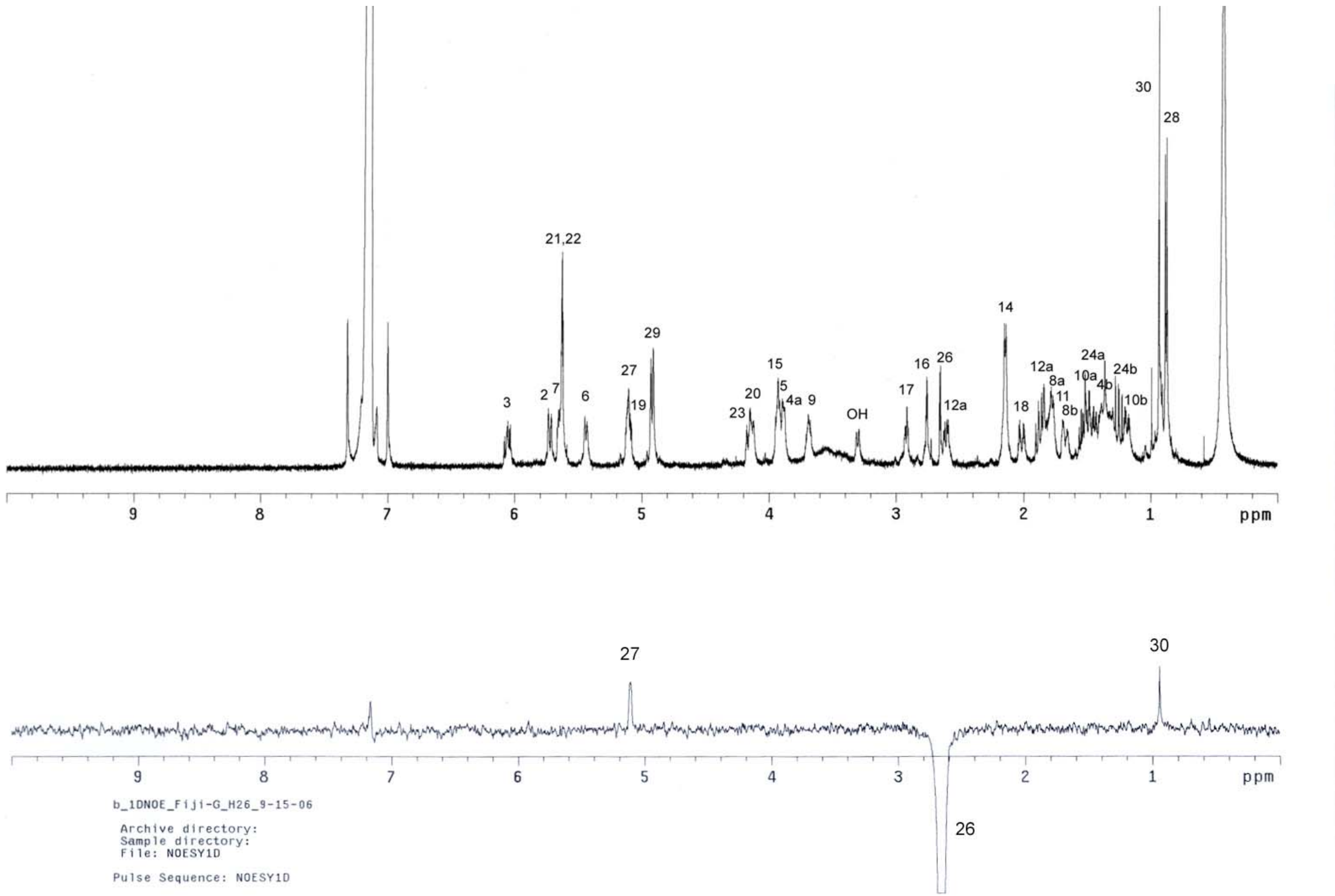


Figure S24. NOE enhancement of H-27 of **10** in benzene-d_6 at 600 MHz.

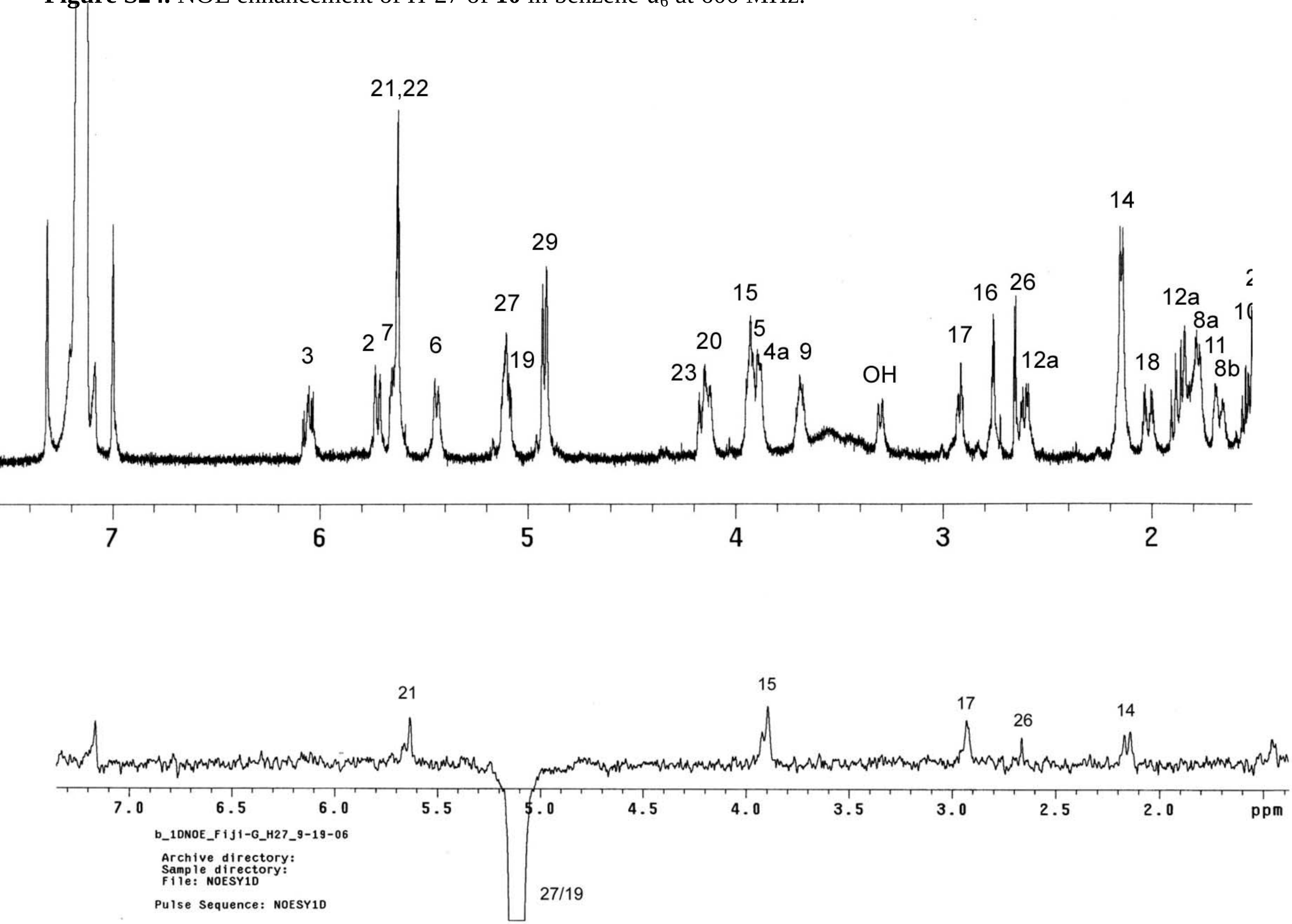


Figure S25. Gradient LCMS chromatogram of **1** using: 30:70 to 80:20 (50min) in CH_3CN/H_2O.

Sample Information

SampleName	02600 FD P7 F4	Date Acquired	10/26/03 11:54:04 AM
Injection	1	Acq Method Set	ELSD_stdgrad_30 70_80 20_ 50min
Injection Volume	15.00 ul	Processing Method	sponge@254
Run Time	60.0 Minutes		
Vial 1			

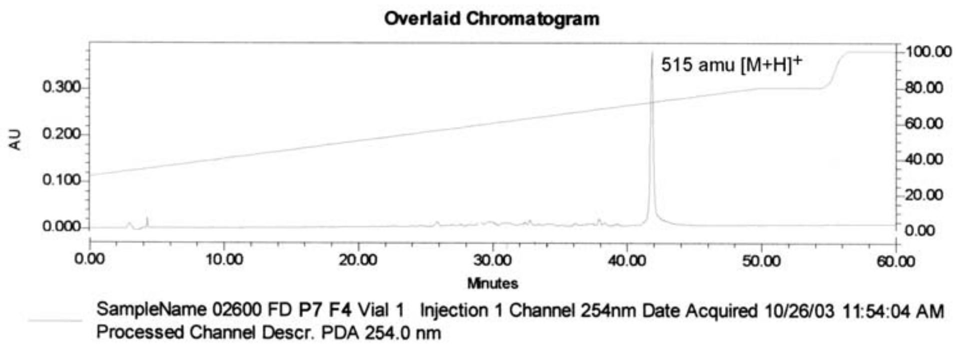


Figure S26. Gradient LCMS chromatogram of **2** using: 30:70 to 80:20 (50min) in CH_3CN/H_2O.

Sample Information

SampleName	02600 FD P5 F3	Date Acquired	10/26/03 7:06:07 AM
Injection	1	Acq Method Set	ELSD_stdgrad_30 70_80 20_50min
Injection Volume	15.00 ul	Processing Method	sponge@254
Run Time	60.0 Minutes		
Vial 15			

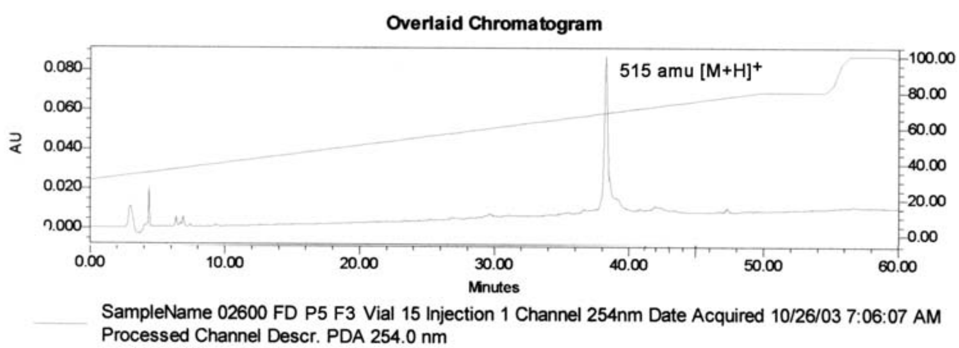


Figure S27. Gradient LCMS chromatogram of **7** using: 30:70 to 80:20 (50min) in CH_3CN/H_2O.

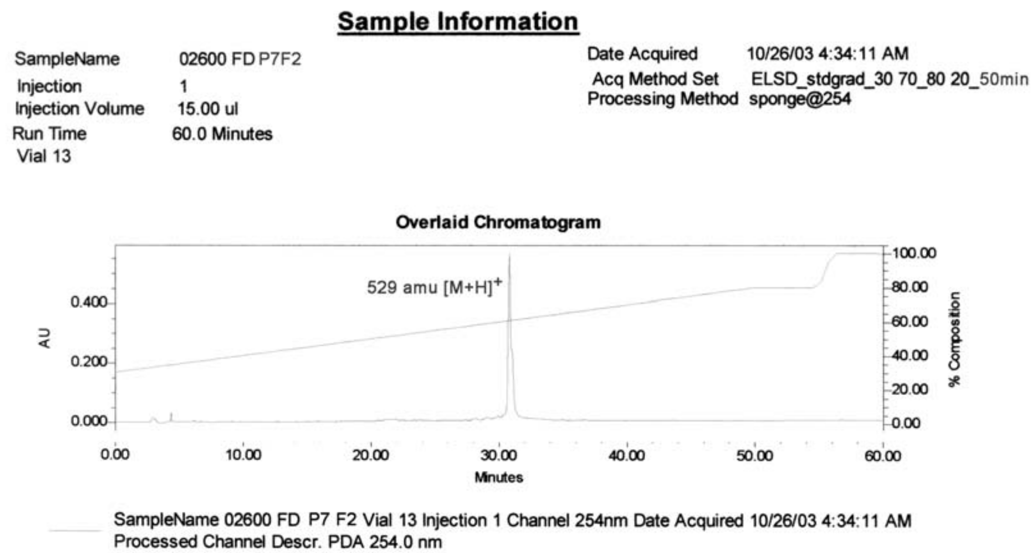


Figure S28. Gradient LCMS chromatogram of **8** using: 10:90 to 100 (50min) in CH_3CN/H_2O.

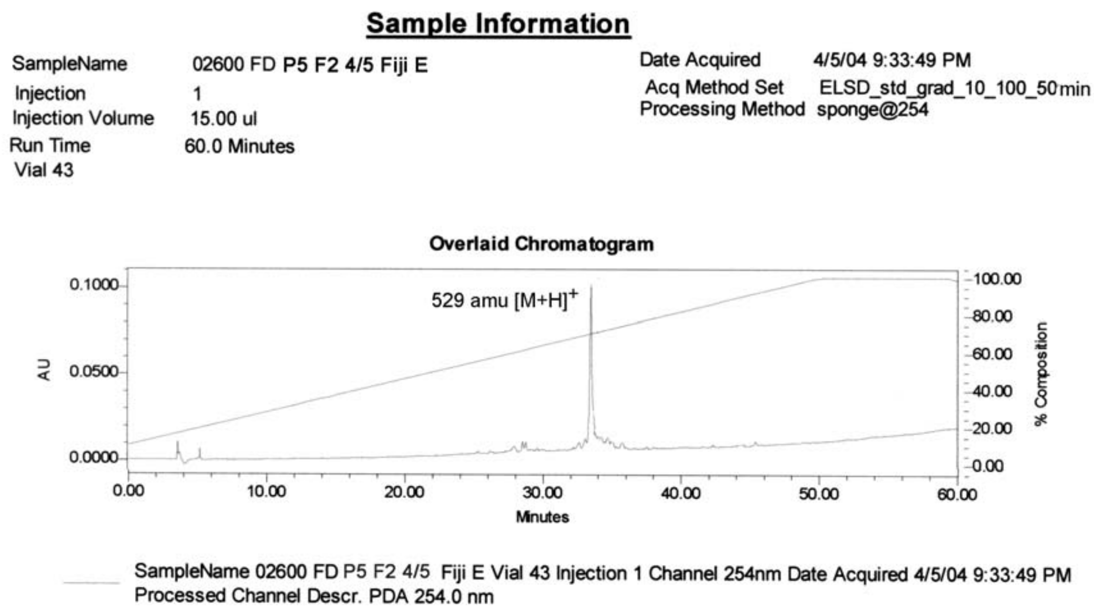


Figure S29. Gradient LCMS chromatogram of **9** using: 30:70 to 80:20 (50min) in CH_3CN/H_2O.

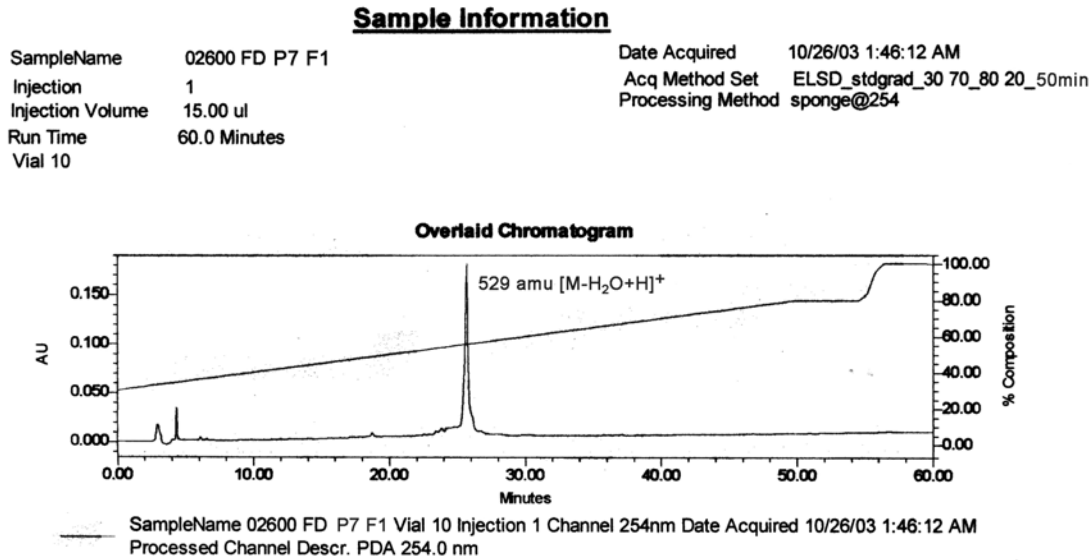


Figure S30. Gradient LCMS chromatogram of **10** using: 30:70 to 80:20 (50min) in CH_3CN/H_2O.

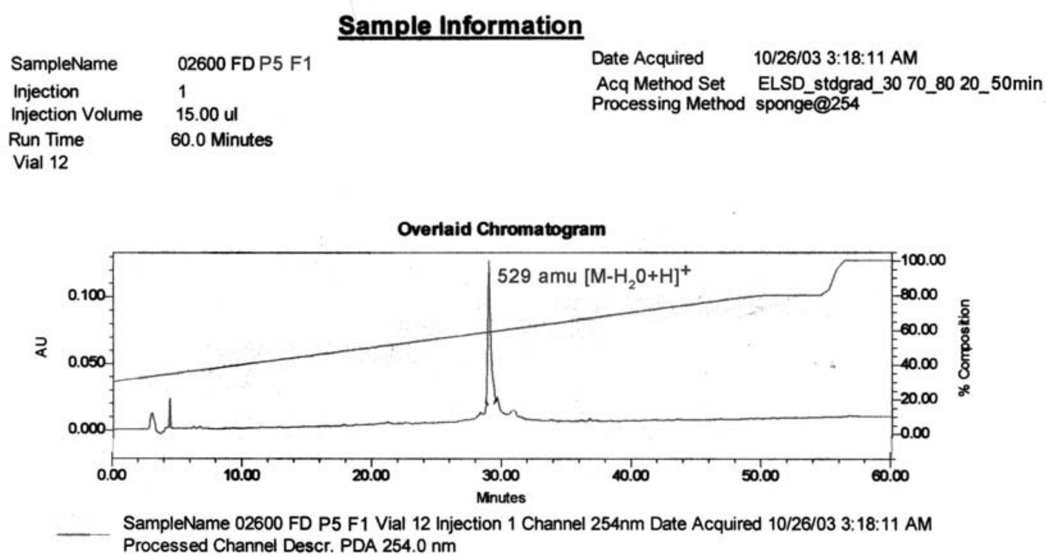


Figure S31. Gradient LCMS chromatogram of **11** using: 30:70 to 80:20 (50min) in CH_3CN/H_2O.

Sample Information

SampleName	02600FDP7F3F1	Date Acquired	10/26/03 8:22:07 AM
Injection	1	Acq Method Set	ELSD_stdgrad_30 70_80 20_50min
Injection Volume	15.00 ul	Processing Method	sponge@254
Run Time	60.0 Minutes		
Vial 16			

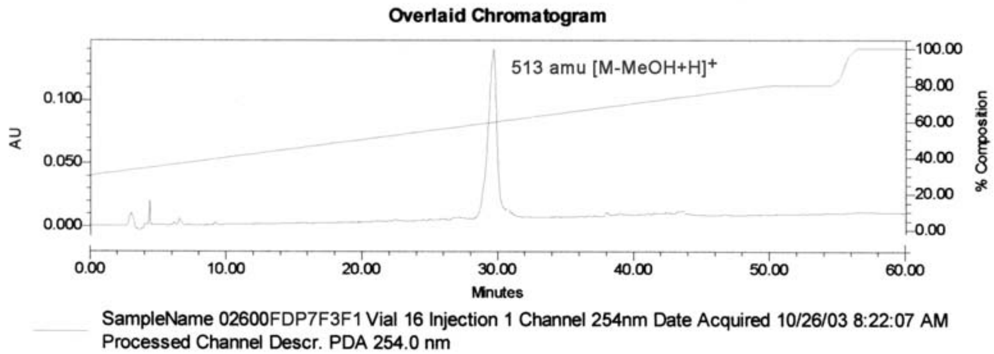


Figure S32. Gradient LCMS chromatogram of **12** using: 30:70 to 80:20 (50min) in CH_3CN/H_2O.

Sample Information

SampleName	02600FDP7F3F2	Date Acquired	10/26/03 10:54:04 AM
Injection	1	Acq Method Set	ELSD_stdgrad_30 70_80 20_50min
Injection Volume	15.00 ul	Processing Method	sponge@254
Run Time	60.0 Minutes		
Vial 18