Supporting Information

for

Interrogating the Bioactive Pharmacophore of the Latrunculin Chemotype by Investigating the Metabolites of Two Taxonomically Unrelated Sponges

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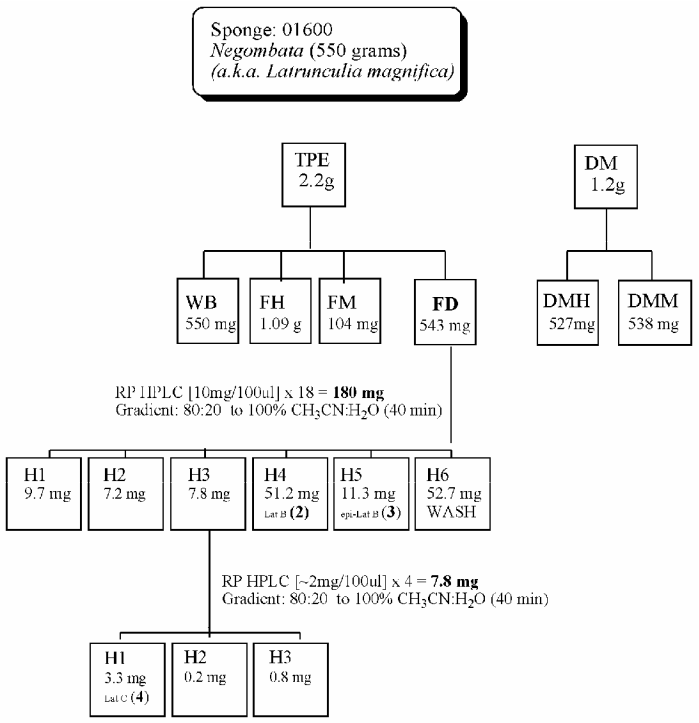
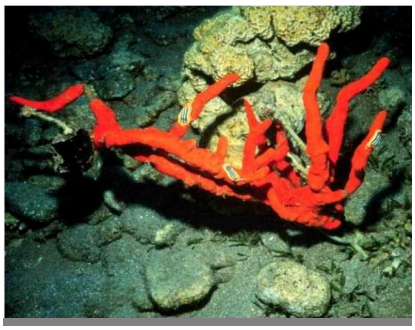
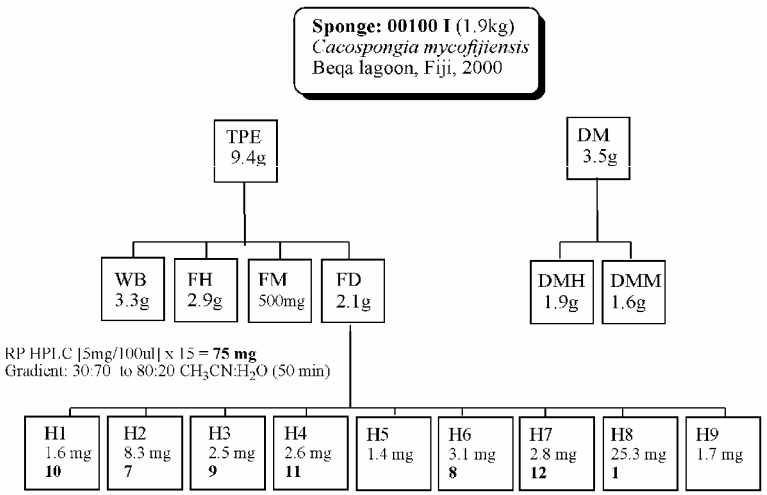
Chart S1. Isolation Scheme and Underwater Photo for the Sponge, *N. magnifica* (coll. # 01600).





N. magnifica
(Red Sea, coll # 01600)

Chart S2. Isolation Scheme and Underwater Photo for the Sponge, *C. mycofijiensis* (coll. # 00100 I and II).



C. mycofijiensis
(Fiji, coll # 00100)

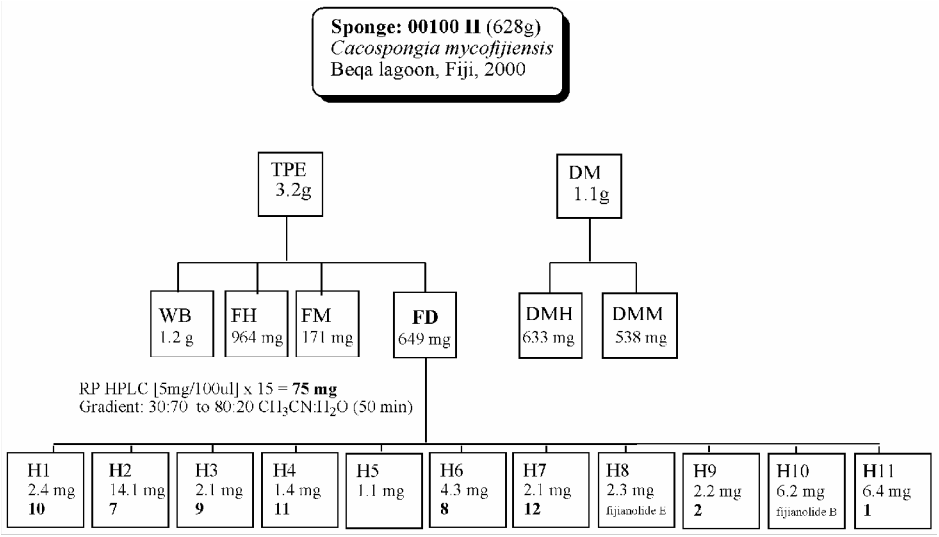
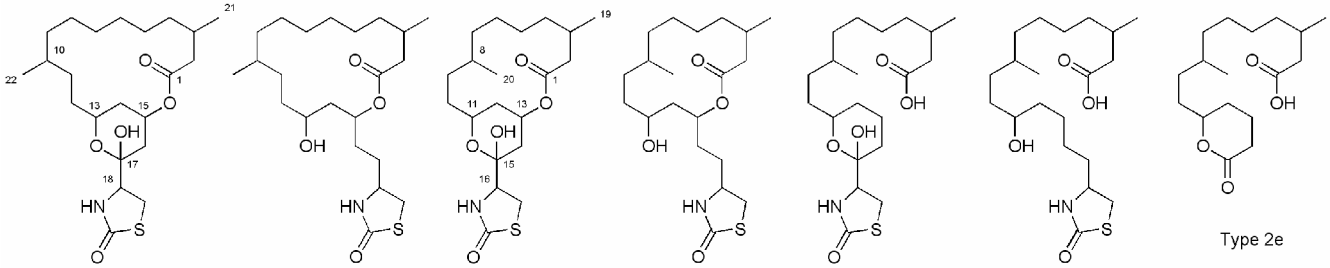


Table S1. Summary of Latrunculin Frameworks and Their Biological Sources



Type 1a Type 1b Type 2a Type 2b Type 2c Type 2d Type 2e

				Type 1		Type 2				
	taxnomic identification	organism*	collection site	1a	1b	2a	2b	2c	2d	2e
Group A	*Negombata magnifica*[a]	S	Dahlak Archipelago[b]	x						
		S	Djibouti[b]	x		x				
		S	Egypt[b]	x						
		S	Egypt[c]			x				
		S	Egypt[d]			x			x	
		S	Israel[b]			x				
		S	Israel[f]			x	x			x
		S	Israel**			x	x			
		S	Tiran Straits[b,d]	x		x			x	
	N. corticata	S	Egypt[g]			x				
	Latrunculia magnifica	S	Israel[h]			x	x			
		S	not specified[i]	x				x		
Group B	*Cacospongia mycofijiensis*	S	Fiji[i,j]	x						
		S	Fiji**	x		x				
		S	Indonesia[m]	x						
		S	Marshall Islands[n]	x						
		S	Papua New Guinea[m]	x						
		S	Solomon Islands[m]	x						
		S	Tonga[m]	x						
		S	Vanuatu[o]	x						
Group C	*Dactylospongia* sp.	S	Vanuatu[p]	x						
	Fasciospongia rimosa	S	Okinawa[q]	x	x					
	Hyattella sp.	S	Indonesia[r]	x						
	unidentifiable	S	American Samoa[s]	x						
Group D	*Chromodoris elizabethina*	N	Guam[t]	x						
		N	Indonesia[r]	x						
		N	Marshall Islands[t]	x						
	C. lochi	N	Fiji[k]	x						
		N	Indonesia[r]	x						
	C. hamiltoni	N	South Africa[u]			x				
		N	South Africa[v]	x		x				
	C. quadricolor[w]	N	Egypt[b]	x						
		N	Israel[p]			x				
		N	Jordan[x]	x		x				
	C. willani	N	Indonesia[r]	x						

* Sponge (S), Nudibranch (N). ** This study. [a] Previously known as *Latrunculia magnifica.* [b] Ilan, M. *Biol. Bull.* **1995** *188*, 306-312. [c] Hoye, T. R.; Ayyad, S. N.; Eklov, B. M.; Hashish, N. E.; Shier, W. T.; ElSayed, K. A.; Hamann, M. T. *J. Am. Chem. Soc.* **2002**, *124*, 7405-7410. [d] El Sayed, K. A.; Youssef, D. T. A.; Marchetti, D. *J. Nat. Prod.* **2006**, *69*, 219-223. [e] Samples posses either **1** or **2** but not both within the same individual. [f] Vilozny, B.; Amagata, T.; Mooberry, S. L.; Crews, P. *J. Nat. Prod.* **2004**, *67*, 1055-1057. [g] Ahmed, S. A.; Odde, S.; Daga, P. R.; Bowling, J. J.; Mesbah, M. K.; Youssef, D. T.; Khalifa, S. I.; Doerksen, R. J.; Hamann, M. T. *Org. Lett.* **2007**, *9*, 4773-4776. [h] Kashman, Y.; Groweiss, A.; Lidor, R.; Blasberger, D.; Carmely, S. *Tetrahedron* **1985,** *41*, 1905-1914. [i] Blasberger, D.; Carmely, S.; Cojocaru, M.; Spector, I.; Shochet, N. R.; Kashman, Y. *Liebigs. Ann. Chem.***1989,** 1171-1181. [j] Previously known as *Spongia mycofijiensis.* [k] Sanders, M. L.; van Soest, R. W. M. In Recent Advances in Sponge Biodiversity Inventory and Documentation; Willenz, P. Ed.; Bull. Inst. R. Sci. Nat. Bel. Biol. 66 (Suppl.): 117-122, 1996. [l] Kakou, Y.; Crews, P. *J. Nat. Prod.* **1987,** *50*, 482-484. [m] Johnson, T. A.; Tenney, K.; Cichewicz, R. H.; Morinaka, B. I.; White, K. N.; Amagata, T.; Subramanian, B.; Media, J.; Mooberry, S. L.; Valeriote, F. A.; Crews, P. *J. Med. Chem.* **2007**, *50*, 3795-3803. [n] Mooberry, S. L.; Tien, G.; Hernandez, A. H.; Plubrukarn, A.; Davidson, B. *Cancer Res.* **1999,** *59*, 653-660. [o] Quinoa, E.; Kakou, Y.; Crews, P. *J. Org. Chem.* **1988**, *53*, 3642-3644. [p] Cutignano, A.; Bruno, I.; Bifulco, G.; Casapullo, A.; Debitus, C.; Gomez-Paloma, L.; Riccio, R. *Eur. J. Org. Chem.* **2001**, 775-778. [q] Jefford, C. W.; Bernardinelli, G.; Tanaka J.; Higa, T. *Tetrahedron Lett.* **1996,** *37*, 159-162. [r] Corley, D. G.; Herb, R.; Moore, R. E.; Scheuer, P. J. *J. Org. Chem.* **1988,** *53*, 3644-3646. [s] Gulavita, N. L.; Gunasekera, S. P.; Pomponi, S. A. *J. Nat. Prod.* **1992** *55*, 506-508. [t] Okuda, R. K.; Scheuer, P. J. *Experientia* **1985,** *41*, 1355-1356. [u] McPail, K.; Davies-Coleman, M. T. *Tetrahedron* **1997**, *53*, 4655-4660. [v] Pika, J.; Faulkner, D. J. *Tetrahedron* **1995**, *51*, 8189-8198. [w] Previously known as *Glossodoris quadricolor.* [z] Mebs, D. *J. Chem Ecol.* **1985**, *11*, 713-716.

Table S2. NMR Data for **1** in $CDCl_3$[a]

position	δ_H (mult, *J* in Hz)	δ_C (mult)
1		165.5 (C)
2	5.69 (d, 1.0)	117.4 (CH)
3		156.6 (C)
4a	2.60 (td, 12.5 8.0)	32.7 (CH_2)
4b	3.00 (td, 12.5 8.0)	
5a	2.25 (m)	30.5 (CH_2)
5b	2.25 (m)	
6	5.75 (td, 15.0, 6.0)	131.9 (CH)
7	6.41 (dd, 15.0, 10.5)	126.1 (CH)
8	5.98 (t, 11.0)	127.3 (CH)
9	5.02 (t, 11.0)	136.6 (CH)
10	2.83 (m)	29.2 (CH)
11a	1.05 (m)	31.5 (CH_2)
11b	1.75 (m)	
12	1.45 (2H, m)	31.0 (CH_2)
13	4.28 (m)	62.3 (CH)
14a	1.49 (m)	34.9 (CH_2)
14b	1.72 (m)	
15	5.41 (m)	68.2 (CH)
16a	1.81 (dd, 14.5, 4.5)	31.7 (CH_2)
16b	2.09 (dt, 15.5, 2.5)	
17		97.3 (C)
18	3.84 (ddd, 9.0, 8.0, 1.0)	61.4 (CH)
19a	3.44 (dd, 11.5, 7.0)	28.7 (CH_2)
19b	3.46 (dd, 11.5, 8.0)	
20		174.9 (C)
21	1.92 (d, 1.0)	24.5 (CH_3)
22	0.98 (d, 6.5)	21.6 (CH_3)
NH	(br. s)	
17-OH	nd[b]	

[a] Measured at 500 MHz (H), 125 MHz (C). [b] Not detected.

Table S3. NMR Data for **2** in $CDCl_3$[a]

position	δ_H (mult, *J* in Hz)	δ_C (mult)
1		165.5 (C)
2	5.69 (d, 1.5)	117.9 (CH)
3		154.8 (C)
4a	1.98 (td, 12.5 4.5)	35.8 (CH_2)
4b	2.67 (td, 12.0 5.0)	
5a	2.20 (m)	26.9 (CH_2)
5b	2.35 (m)	
6	5.26 (td, 11.5, 3.0)	127.5 (CH)
7	5.06 (td, 10.5, 1.0)	135.9 (CH)
8	2.64 (m)	28.9 (CH)
9a	1.12 (m)	31.0 (CH_2)
9b	1.72 (m)	
10	1.37 (2H, m)	31.0 (CH_2)
11	4.25 (td, 11.5, 1.0)	62.5 (CH)
12a	1.40 (m)	35.3 (CH_2)
12b	1.75 (m)	
13	5.45 (br. t, 3.0)	68.7 (CH)
14a	1.93 (m)	31.4 (CH_2)
14b	2.10 (ddd, 14.5, 2.5, 1.5)	
15		97.9 (C)
16	3.84 (ddd, 8.0, 6.5, 1.5)	61.5 (CH)
17a	3.40 (dd, 11.5, 6.5)	28.7 (CH_2)
17b	3.47 (dd, 11.5, 9.0)	
18		175.3 (C)
19	1.91 (d, 1.5)	24.0 (CH_3)
20	0.96 (d, 6.5)	22.2 (CH_3)
NH	5.85 (br. s)	
15-OH	nd[b]	

[a] Measured at 500 MHz (H), 125 MHz (C). [b] Not detected.

Table S4. NMR Data for **3** in $CDCl_3$[a]

position	δ_H (mult, *J* in Hz)	δ_C (mult)
1		165.9 (C)
2	5.64 (d, 0.9)	118.2 (CH)
3		155.6 (C)
4a	1.99 (td, 12.2 4.6)	35.7 (CH_2)
4b	2.81 (ddd, 12.9, 12.5, 4.4)	
5a	2.16 (m)	26.7 (CH_2)
5b	2.40 (ddd, 13.2, 12.5, 4.2)	
6	5.24 (ddd, 11.7, 11.2, 2.9)	127.9 (CH)
7	5.05 (ddd, 11.2, 11.0, 2.0)	135.6 (CH)
8	2.60 (m)	29.1 (CH)
9a	1.14 (ddd, 14.9, 11.5, 4.1)	31.2 (CH_2)
9b	1.66 (m)	
10a	1.37 (m)	31.2 (CH_2)
10b	1.44 (m)	
11	4.35 (m)	62.9 (CH)
12a	1.55 (m)	35.5 (CH_2)
12b	1.73 (m)	
13	5.30 (br. t, 3.0)	67.7 (CH)
14a	1.60 (m)	32.4 (CH_2)
14b	2.19 (m)	
15		96.6 (C)
16	3.86 (ddd, 8.3, 8.3, 1.0)	62.9 (CH)
17a	3.29 (dd, 11.2, 8.4)	29.0 (CH_2)
17b	3.40 (dd, 11.2, 9.0)	
18		175.8 (C)
19	1.93 (d, 0.9)	24.5 (CH_3)
20	0.98 (d, 6.5)	22.3 (CH_3)
NH	5.60 (br. s)	
15-OH	nd[b]	

[a] Measured at 500 MHz (H), 125 MHz (C). [b] Not detected.

Table S5. NMR Data for **4** in $CDCl_3$[a]

position	δ_H (mult, *J* in Hz)	δ_C (mult)	COSY
1		167.4 (C)	
2	5.64 (d, 1.2)	118.2 (CH)	19
3		155.9 (C)	
4a	3.55 (td, 11.4, 8.4)	34.9 (CH_2)	
4b	(m)		
5a	2.07 (m)	26.0 (CH_2)	6
5b	2.35 (m)		
6	5.31 (td, 11.4, 4.2)	128.1 (CH)	5, 7
7	5.03 (td, 11.4, 1.2)	135.9 (CH)	6, 8
8	2.64 (m)	29.0 (CH)	7, 9, 20
9a	1.24[b] (m)	31.8 (CH_2)	8
9b	1.62[b] (m)		
10	1.44 (2H, m)	35.0 (CH_2)	11
11	4.11 (m)	65.7 (CH)	10, 12
12a	1.85 (m)	40.9 (CH_2)	11, 13
12b	2.04 (m)		
13	5.07 (m)	70.5 (CH)	12, 14
14a	1.95 (m)	35.3 (CH_2)	13, 15
14b	2.64 (m)		
15	3.88 (br.t, 3.0)	69.8 (CH)	14
16	3.84 (ddd, 8.3, 8.3, 1.0)	58.5 (CH)	17
17a	3.42 (dd, 11.2, 9.0)	31.2 (CH_2)	16
17b	3.55 (dd, 11.2, 8.4)		
18		175.4 (C)	
19	1.91 (d, 1.2)	24.5 (CH_3)	2
20	0.98 (d, 6.5)	22.0 (CH_3)	8
NH	6.28 (br. s)		
11-OH	nd[c]		
15-OH	nd[c]		

[a] Measured at 500 MHz (H), 125 MHz (C). [b] Observed under H_2O (δ 1.55) and impurity (δ 1.25). [c] Not detected.

Table S6. NMR Data for **7** in Acetone-d_6[a]

position	δ_H (mult, *J* in Hz)	δ_C (mult)	gCOSY	gHMBC	NOESY
1		166.6 (C)			
2	5.54 (q, 1.0)	118.7 (CH)	21		21
3		158.3 (C)			
4a	2.58 (td, 11.6, 5.4)	32.2 (CH_2)	5a, 5b	2, 6	
4b	2.63 (td, 11.6, 5.2)		5a, 5b	2, 6	
5a	1.82 (m)	35.4 (CH_2)	4a, 4b, 6		6
5b	1.88 (m)		4a, 4b, 6		
6	3.36 (dd, 8.9, 4.5, 1.5)	76.6 (CH)	5a, 5b, 7		5a, 8
7	4.34 (d, 9.6)	70.1 (CH)	6, 8	8, 9	
8	5.64 (t, 10.3)	132.3 (CH)	7, 9	6	6, 7, 9, 11a, 22
9	5.05 (td, 10.9, 1.0)	136.5 (CH)	8, 10	7	7, 8
10	2.73 (m)	29.7 (CH)	9, 11a, 22	8, 9	13, 22
11a	1.06 (ddt, 13.7, 11.5, 4.0)	32.0 (CH_2)	10, 11b	9, 13	8
11b	1.89 (m)		11a, 12a, 12b	9, 22	11b, 22
12a	1.45 (2H, m)	32.9 (CH_2)	11a, 13a	11	11a
12b			11a, 13a	13, 14	
13	4.29 (tdd, 11.0, 3.8, 1.9)	62.3 (CH)	12a, 12b, 14a, 14b	17	10
14a	1.59 (ddd, 14.7, 11.6, 3.6)	36.6 (CH_2)	13, 14b, 15	2, 12, 13, 15	14b, 15
14b	1.80 (m)		13, 14a	2	14a, 15
15	5.19 (m)	68.2 (CH)	14a, 16a, 16b	2, 17	14a, 14b, 16a, 16b
16a	1.81 (dd, 14.9, 4.3)	32.0 (CH_2)	15, 16b	15, 17, 18	15, 16b, 18, 19a, 19b, NH
16b	2.25 (dt, 15.0, 2.0)		15, 16a	17	15, 16a, NH
17		97.6 (C)			
18	3.86 (ddd, 8.6, 6.5, 1.2)	63.4 (CH)	19a, 19b, NH		16a, 19a, 19b, NH
19a	3.45 (dd, 11.5, 8.6)	28.9[d] (CH_2)	18	17, 20	16a, 18
19b	3.48 (dd, 11.5, 6.5)		18	17, 20	16a, 18
20		173.9 (C)			
21	1.90 (d, 1.5)	25.4 (CH_3)	2	2, 3, 4	2
22	0.92 (d, 6.5)	23.1 (CH_3)	10	9	8, 10, 11b
NH	7.04 (br. s)		18		16a, 16b, 18
6-OH	4.83 (br. s)				6
7-OH	3.59[b]				
17-OH	nd[b,c] (br. s)				

[a] Measured at 600 MHz (H), 125 MHz (C). [b] Assignments may be switched. [c] Not detected. [d] Assignment from HMQC correlation.

Table S7. NMR Data for **8** in Acetone-d_6[a]

position	δ_H (mult, *J* in Hz)	δ_C (mult)	gCOSY	HMBC (C)	NOESY
1		166.7 (C)			
2	5.55 (q, 1.0)	118.7 (CH)	21	4, 21	21
3		158.5 (C)			
4a	2.54 (td, 11.4, 5.4)	32.5 (CH_2)	4b, 5a, 5b	3	4b
4b	2.66 (td, 11.4, 5.2)		4a, 5a, 5b	3	4a
5a	1.81 (m)	35.9 (CH_2)	4a, 4b, 6	4, 6	
5b	1.86 (m)		4a, 4b, 6	4, 6	
6	3.34 (br. s)	76.5 (CH)	5a, 5b		
7	3.99 (d, 9.8)	79.6 (CH)	8	5, 7-O$\underline{C}H_3$	10, 7-OCH$_3$
8	5.57 (t, 10.3)	129.2 (CH)	7, 9	10	9
9	5.33 (td, 10.9, 1.0)	140.3 (CH)	8	10, 11, 22	8, 22
10	2.81 (m)	29.8[c] (CH)	11a, 22		7, 22
11a	1.10 (ddt, 13.7, 11.4, 3.8)	31.9 (CH_2)	10, 11b, 12a	13	11b
11b	1.93 (m)		11a, 12a, 12b	9, 10	11a
12a	1.47 (2H, m)	32.9 (CH_2)	11a, 11b, 12b, 13	10, 13	
12b			11b, 12a, 13		
13	4.29 (tdd, 11.0, 3.9, 1.9)	62.3 (CH)	12a, 12b, 14a		
14a	1.60 (ddd, 14.8, 11.5, 3.6)	36.6 (CH_2)	13, 14b, 15		14b, 15
14b	1.83 (m)		14a, 15		14a, 15
15	5.21 (m)	68.2 (CH)	14a, 14b, 16b		14a, 14b, 16a, 16b
16a	1.84 (dd, 14.8, 4.3)	32.0 (CH_2)	16b	14, 15	15, 16b
16b	2.26 (dt, 15.0, 2.0)		15, 16a	14, 15	15, 16a, 19a, 19b
17		97.7 (C)			
18	3.86 (ddd, 8.6, 6.5, 1.2)	63.5 (CH)	19a, 19b, NH	16	19a, 19b, NH
19a	3.45 (dd, 11.5, 8.6)	29.0[c] (CH_2)	18, 19b	18	16b, 18
19b	3.48 (dd, 11.5, 6.5)		18, 19a	18	16b, 18
20		174.0 (C)			
21	1.92 (d, 1.5)	25.5 (CH_3)	2	2, 3	2
22	0.97 (d, 6.5)	23.0 (CH_3)	10	9	9, 10
7-OCH$_3$	3.24 (s)	56.5 (CH_3)		7	7
NH	7.05 (br. s)		18		18
6-OH	3.12[b] (br. s)				
17-OH	4.84[b] (br. s)				

[a] Measured at 600 MHz (H), 125 MHz (C). [b] Assignments may be switched. [c] Assignments from HMQC correlations.

Table S8. NMR Data for **9** in Acetone-d_6[a]

position	δ_H (mult, *J* in Hz)	δ_C (mult)	gCOSY	gHMBC
1		166.8 (C)		
2	5.56 (q, 1.2)	118.7 (CH)	21	4, 21
3		158.7 (C)		
4a	2.57 (td, 11.5, 5.3)	31.9 (CH_2)	4b, 5a	2, 3, 5, 6, 21
4b	2.69 (td, 11.5, 5.0)		4a, 5b	2, 3, 5, 6, 21
5a	1.81 (m)	33.2 (CH_2)	4a, 6	6, 7
5b	1.88 (m)		4b	6, 7
6	3.38 (ddd, 9.1, 4.5, 1.5)	76.7 (CH)	5a, 7	4, 5, 8
7	4.37 (d, 9.6)	70.2 (CH)	6, 8	6, 8, 9
8	5.65 (t, 10.3)	132.4 (CH)	7, 9	6, 10
9	5.07 (td, 10.9, 1.0)	136.7 (CH)	8, 10	7, 10, 11, 22
10	2.78 (m)	29.9[c] (CH)	9, 11a, 11b, 22	8, 9
11a	1.07 (ddt, 13.6, 11.5, 4.0)	32.2 (CH_2)	10, 11b, 12a, 12b	
11b	1.96 (m)		10, 11a, 12a, 12b	9
12a	1.47 (2H, m)	35.4 (CH_2)	11a, 11b	11
12b			11a, 11b	
13	4.33 (tdd, 11.3, 3.2, 2.1)	62.6 (CH)		
14a	1.61 (ddd, 14.8, 11.7, 3.6)	36.9 (CH_2)	14b, 15	13
14b	1.82 (m)		14a	15, 16
15	5.16 (m)	68.1 (CH)	14a, 16a, 16b	
16a	1.79 (dd, 14.9, 4.2)	32.6 (CH_2)	15, 16b	17, 18
16b	2.17 (dt, 14.9, 2.0)		15, 16a	14, 15, 17
17		97.4 (C)		
18	3.92 (td, 8.1, 1.2)	64.0 (CH)	19a, 19b, NH	16, 19, 20
19a	3.43 (dd, 11.2, 7.7)	29.4[c] (CH_2)	18	17, 18, 20
19b	3.45 (dd, 11.2, 8.1)		18	17, 18, 20
20		174.2 (C)		
21	1.92 (d, 1.5)	25.5 (CH_3)	2	3
22	0.94 (d, 6.7)	23.2 (CH_3)	10	9, 10, 11
NH	6.58 (br. s)		18	18, 19
6-OH	nd[b]			
7-OH	nd[b]			
17-OH	nd[b]			

[a] Measured at 600 MHz (H), 125 MHz (C). [b] Not detected. [c] Assignments from HMQC correlation.

Table S9. NMR Data for **10** in Acetone-d_6[a]

position	δ_H (mult, *J* in Hz)	δ_C (mult)	gCOSY	HMBC (C)	NOESY
1		166.6 (C)			
2	5.63 (q, 1.0)	118.7 (CH)	21	1, 21	21
3		159.5 (C)			
4a	2.59 (ddd, 13.4, 10.4, 6.3)	27.3 (CH_2)	4b, 5a	2, 3, 5, 21	4b, 7
4b	3.34 (ddd, 13.4, 10.3, 5.2)		4a, 5a, 5b	2, 3, 5, 6, 21	4a, 7
5a	1.84 (m)	30.3[c] (CH_2)	4a, 4b, 5b, 6		6
5b	1.94 (m)		4b, 5a, 6	6, 7	6
6	3.53 (ddd, 8.2, 5.0, 3.1)	73.4 (CH)	5a, 5b, 7		5a, 5b
7	4.26 (t, 8.4)	70.0 (CH)	6, 8, 7-OH	6	4a, 4b, 13
8	5.35 (dd, 11.0, 8.6)	131.4 (CH)	7, 9	9, 10	9
9	5.21 (t, 11.0)	139.2 (CH)	8, 10	8, 22	8
10	2.68 (m)	29.9[c] (CH)	9, 11a, 11b, 22		13, 22
11a	1.13 (m)	32.1 (CH_2)	10, 11b, 12a, 12b		11b
11b	1.55 (m)	31.7	10, 11a	12, 22	11a, 13
12	1.54 (2H, m)	(CH_2)	11a, 11b	10, 11, 13, 14	22
13	4.57 (m)	63.8 (CH)	12a, 12b, 14b	12, 15	7, 10, 11b, 14b
14a	1.52 (ddd, 14.4, 7.8, 2.9)	35.2 (CH_2)	14b, 15		14b, 15
14b	2.04 (m)		13, 14a, 15		13, 14a, 15
15	5.29 (m)	68.3 (CH)	14a, 14b, 16a, 16b		14a, 14b, 16a, 16b
16a	1.88 (dd, 14.6, 4.1)	32.2 (CH_2)	15, 16b	17, 18	15, 16b
16b	2.14 (dt, 14.6, 2.1)		15, 16a	14, 15, 17, 18	15, 16a, 19a, 19b
17		98.1 (C)			
18	3.87 (ddd, 8.9, 6.5, 1.2)	63.5 (CH)	19a, 19b, NH	16, 19	19a, 19b, NH
19a	3.44 (dd, 11.5, 8.9)	29.1[c] (CH_2)	18	17, 18, 20	16b, 18
19b	3.48 (dd, 11.5, 6.3)		18	17, 18, 20	16b, 18
20		173.9[d] (C)			
21	1.92 (d, 1.2)	24.6 (CH_3)	2	2, 3, 4	2
22	0.94 (d, 6.4)	21.4 (CH_3)	10	9, 10, 11	10, 12
NH	6.97 (br. s)		18		18
6-OH	3.22[b]		7		
7-OH	3.75[b]				
17-OH	4.78[b]				

[a] Measured at 600 MHz (H), 125 MHz (C). [b] Assignments may be switched. [c] Assignments from HMQC correlations. [d] Assignment from HMBC correlations.

Table S10. NMR Data for **11** in Acetone-d_6[a]

position	δ_H (mult, *J* in Hz)	δ_C (mult)	gCOSY	gHMBC
1		166.6 (C)		
2	5.59 (q, 1.2)	119.5 (CH)	21	1, 4, 21
3		156.9 (C)		
4a	2.35 (td, 12.0, 5.3)	29.4[d] (CH_2)	4b, 5a, 5b	2, 3, 5, 6, 21
4b	2.96 (td, 12.0, 6.2)		4a, 5a, 5b	2, 3, 5, 21
5a	1.84 (2H, m)	35.6 (CH_2)	4a, 4b, 6	3, 6, 7
5b			4a, 4b, 6	3, 6, 7
6	4.31 (td, 8.4, 4.1)	73.5 (CH)	5a, 5b, 7	8
7	7.03 (dd, 16.3, 8.6)	132.0 (CH)	6, 8	9
8	5.96 (d, 16.1)	149.6 (CH)	7	6, 10
9		205.9[e] (C)		
10	3.69 (m)	36.4 (CH)	11b, 22	9, 12, 22
11a	1.60 (dddd, 13.2, 11.5, 4.8, 3.1	29.4 (CH_2)	11b	
11b	1.82 (m)		11a, 10, 12a	9, 10, 12
12a	1.29 (dddd, 14.2, 12.5, 4.8, 3.4	32.4[d] (CH_2)	11b, 12b	
12b	1.42 (dddd, 14.2, 11.5, 4.3, 3.0)		12a, 13	
13	4.35 (dt, 11.7, 2.8)	63.1 (CH)	12b, 14b	
14a	1.53 (ddd, 14.6, 11.5, 3.4)	36.3 (CH_2)	14b, 15	12
14b	1.65 (ddd, 14.4, 4.8, 2.1)		14a, 13, 15	
15	5.30 (m)	67.9 (CH)	14a, 14b, 16a, 16b	13
16a	1.86 (dd, 15.1, 4.3)	36.5 (CH_2)	15, 16b	17, 18
16b	2.15 (dt, 15.1, 2.2)		15, 16a	14
17		97.7 (C)		
18	3.91 (ddd, 8.8, 6.5, 1.2)	63.6 (CH)		17, 20
19a	3.47 (dd, 11.5, 8.7)	29.0[d] (CH_2)	18, 19b	17, 18, 20
19b	3.51 (dd, 11.5, 6.3)		18, 19a	17, 18, 20
20		174.0 (C)		
21	1.92 (d, 1.5)	25.1 (CH_3)	2	2, 3, 4
22	0.99 (d, 6.9)	19.6 (CH_3)	10	9
NH	7.13 (br.s)			
6-OH	5.12[b]			
17-OH	nd[b,c]			

[a] Measured at 600 MHz (H), 125 MHz (C). [b] Assignments may be switched. [c] Not detected. [d] Assignments from HMQC correlations. [e] Assignment from HMBC correlations.

Table S11. NMR Data for **12** in $CDCl_3$[a]

position	δ_H (mult, *J* in Hz)	δ_C (mult)	gCOSY	gHMBC
1		165.4 (C)		
2	5.69 (q, 1.2)	118.0 (CH)		1, 4, 21
3		156.3 (C)		
4a	2.26 (ddd, 13.2, 8.4, 6.0)	27.7 (CH_2)	4b, 5a, 5b	3, 5, 6, 21
4b	3.29 (ddd, 13.2, 9.0, 7.2)		4a, 5a, 5b	3, 5, 6, 21
5a	2.61 (ddd, 15.6, 9.0, 7.2)	41.0 (CH_2)	4b	3, 4, 6
5b	2.73 (ddd, 14.4, 8.4, 6.0)	207.4 (C)	4b	3, 4, 6
6				
7a	2.96 (ddd, 17.4, 6.6, 1.8)	41.5 (CH_2)	8	6, 8, 9
7b	3.35 (ddd, 17.4, 6.2, 1.1)		8	6, 8, 9
8	5.45 (dddd, 10.8, 9.6, 6.6, 0.6)	119.7 (CH)	7a, 7b	7, 9, 10
9	5.33 (m)	140.0 (CH)	8, 10	7, 8, 10, 22
10	2.40 (m)	29.0 (CH)	9, 11, 22	12, 22
11a	1.16 (dddd, 13.6, 9.5, 5.7, 3.3)	31.0 (CH_2)	10, 11b	
11b	1.66 (m)		11b, 13	
12	1.48 (2H, m)	31.9 (CH_2)	12, 14	10, 11
13	3.88 (tdd, 10.2, 4.2, 2.4)	62.5 (CH)	13	
14a	1.42 (ddd, 15.0, 12.0, 3.0)	34.6 (CH_2)	15	13
14b	2.02 (m)		14, 16	16
15	5.33 (m)	68.4 (CH)	15	16
16a	1.92 (dt, 14.4, 3.6)	31.3 (CH_2)		17
16b				
17		97.3 (C)		
18	2.08 (dt, 14.4, 1.8)	61.5 (CH)	19a, 19b	16, 17, 20
19a	3.82 (ddd, 9.0, 6.0, 1.2)	28.7 (CH_2)	18	17, 18, 20
19b	3.41 (dd, 11.4, 6.0)		18	17, 18, 20
20	3.48 (dd, 11.4, 9.0)	174.9 (C)		
21	1.90 (d, 1.2)	24.7 (CH_3)		2, 3, 4
22	0.94 (d, 6.6)	21.5 (CH_3)	10, 11b	9
NH	5.71 (br. s)			
17-OH	nd[b]			

[a] Measured at 600 MHz (H), 125 MHz (C). [b] Not detected.

Table S12. DFT Calculation Results of the 6*S*,7*S* Isomer for **7**

position	Exp. Shift	Calc. Shift	Abs. Diff.	Corr. Shift	Abs. Diff.
C1	166.6	155.9	10.7	163.7	2.9
C2	118.7	114.7	4.0	119.7	1.0
C3	158.3	153.7	4.6	161.4	3.1
C4	32.2	28.6	3.6	27.8	4.4
C5	35.4	37.0	1.6	36.8	1.4
C6	76.6	76.9	0.3	79.4	2.8
C7	70.1	65.9	4.2	67.6	2.5
C8	132.3	128.2	4.1	134.2	1.9
C9	136.5	127.7	8.8	133.6	2.9
C10	29.3	31.4	2.1	30.8	1.5
C11	32.0	32.4	0.4	31.9	0.1
C12	32.9	33.3	0.4	32.8	0.1
C13	62.3	63.1	0.8	64.6	2.3
C14	36.6	36.3	0.3	36.0	0.6
C15	68.2	67.0	1.2	68.8	0.6
C16	32.0	27.5	4.5	26.6	5.4
C17	97.6	97.9	0.3	101.8	4.2
C18	63.4	63.1	0.3	64.6	1.2
C19	28.9	32.1	3.2	31.5	2.6
C20	173.9	162.7	11.2	171.0	2.9
C21	25.4	26.4	1.0	25.4	0.0
C22	23.1	23.3	0.2	22.1	1.0
% Score/ MAE		77	3.1	96	2.1
TMS		189.63		y=0.9365x+2.5676	

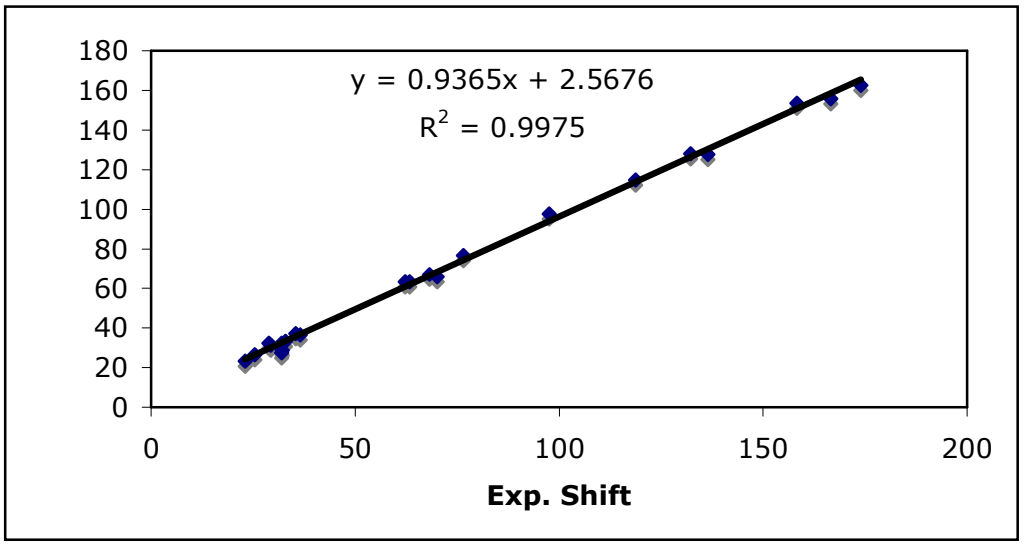


Table S13. DFT Calculation Results of the 6*R*,7*S* Isomer for **7**

position	Exp. Shift	Calc. Shift	Abs. Diff.	Corr. Shift	Abs. Diff.
C1	166.6	155.9	10.7	163.8	2.8
C2	118.7	113.4	5.3	118.4	0.3
C3	158.3	154.9	3.4	162.7	4.4
C4	32.2	25.6	6.6	24.6	7.6
C5	35.4	33.3	2.1	32.8	2.6
C6	76.6	72.8	3.8	75.0	1.6
C7	70.1	68.8	1.3	70.8	0.7
C8	132.3	128.2	4.1	134.2	1.9
C9	136.5	133.1	3.4	139.5	3.0
C10	29.3	31.3	2.0	30.7	1.4
C11	32.0	32.4	0.4	31.9	0.1
C12	32.9	32.3	0.6	31.8	1.1
C13	62.3	63.8	1.5	65.4	3.1
C14	36.6	34.1	2.5	33.7	2.9
C15	68.2	68.3	0.1	70.2	2.0
C16	32.0	28.2	3.8	27.4	4.6
C17	97.6	97.9	0.3	101.9	4.3
C18	63.4	63.4	0.0	65.0	1.6
C19	28.9	32.1	3.2	31.6	2.7
C20	173.9	162.6	11.3	171.0	2.9
C21	25.4	26.7	1.3	25.8	0.4
C22	23.1	23.7	0.6	22.6	0.5
% Score/ MAE		77	3.1	96	2.4
TMS		189.63		y=0.9486x+1.5647	

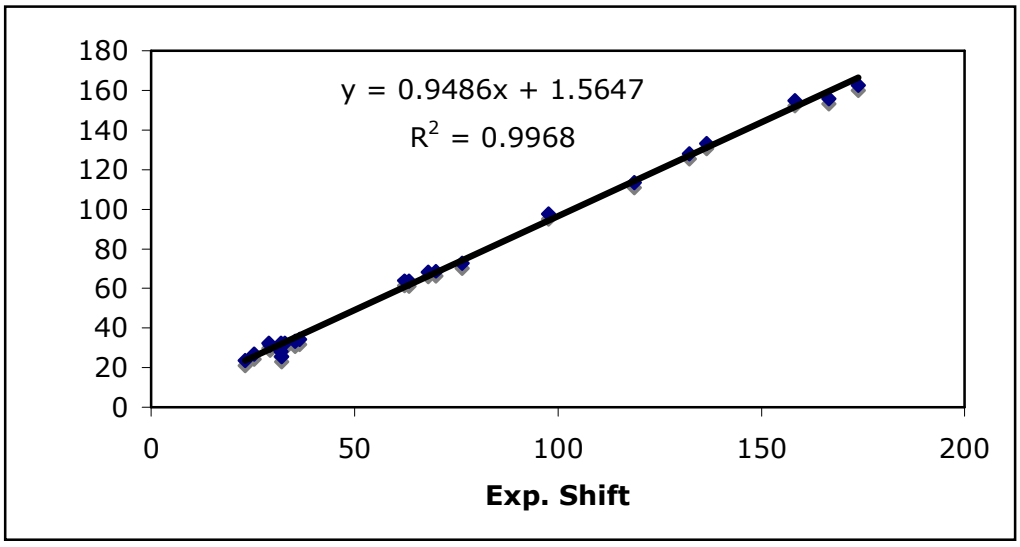


Table S14. DFT Calculation Results of the 6*S*,7*R* Isomer for **7**

position	Exp. Shift	Calc. Shift	Abs. Diff.	Corr. Shift	Abs. Diff.
C1	166.6	156.2	10.4	162.7	3.9
C2	118.7	113.9	4.8	117.5	1.2
C3	158.3	155.6	2.7	162.0	3.7
C4	32.2	30.9	1.3	28.8	3.4
C5	35.4	42.8	7.4	41.5	6.1
C6	76.6	78.8	2.2	80.0	3.4
C7	70.1	77.5	7.4	78.6	8.5
C8	132.3	129.7	2.6	134.4	2.1
C9	136.5	131.2	5.3	136.0	0.5
C10	29.3	30.9	1.6	28.8	0.5
C11	32.0	32.9	0.9	30.9	1.1
C12	32.9	33.5	0.6	31.6	1.3
C13	62.3	63.2	0.9	63.3	1.0
C14	36.6	36.2	0.4	34.5	2.1
C15	68.2	66.6	1.6	67.0	1.2
C16	32.0	27.8	4.2	25.5	6.5
C17	97.6	97.9	0.3	100.4	2.8
C18	63.4	63.1	0.3	63.2	0.2
C19	28.9	32.2	3.3	30.2	1.3
C20	173.9	162.7	11.2	169.6	4.3
C21	25.4	26.9	1.5	24.5	0.9
C22	23.1	24.4	1.3	21.9	1.2
% Score/ MAE		68	3.3	86	2.6
TMS		189.63		y=0.9363x+3.9318	

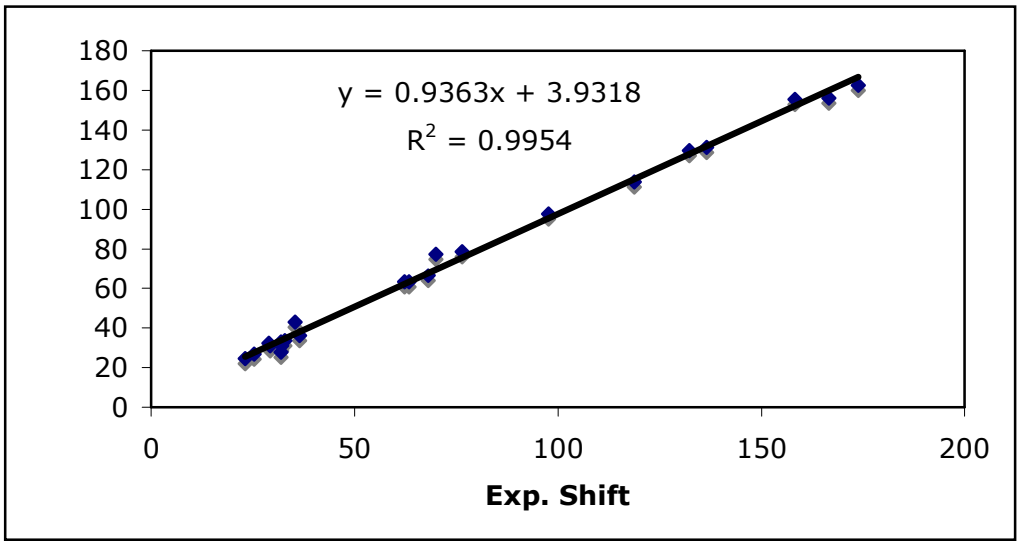


Table S15. DFT Calculation Results of the 6*R*,7*R* Isomer for **7**

position	Exp. Shift	Calc. Shift	Abs. Diff.	Corr. Shift	Abs. Diff.
C1	166.6	156.0	10.6	163.3	3.3
C2	118.7	113.7	5.0	118.2	0.5
C3	158.3	153.8	4.5	160.9	2.6
C4	32.2	27.6	4.6	26.4	5.8
C5	35.4	35.9	0.5	35.2	0.2
C6	76.6	71.4	5.2	73.1	3.5
C7	70.1	81.1	11.0	83.4	13.3
C8	132.3	125.9	6.4	131.2	1.1
C9	136.5	131.0	5.5	136.6	0.1
C10	29.3	30.8	1.5	29.8	0.5
C11	32.0	33.2	1.2	32.4	0.4
C12	32.9	33.0	0.1	32.1	0.8
C13	62.3	63.6	1.3	64.8	2.5
C14	36.6	34.3	2.3	33.5	3.1
C15	68.2	68.3	0.1	69.8	1.6
C16	32.0	28.3	3.7	27.1	4.9
C17	97.6	97.8	0.2	101.2	3.6
C18	63.4	63.0	0.4	64.1	0.7
C19	28.9	32.4	3.5	31.5	2.6
C20	173.9	162.9	11.0	170.6	3.3
C21	25.4	26.2	0.8	24.9	0.5
C22	23.1	23.6	0.5	22.1	1.0
% Score/ MAE		55	3.6	86	2.5
TMS		189.63		y=0.9381x+2.8448	

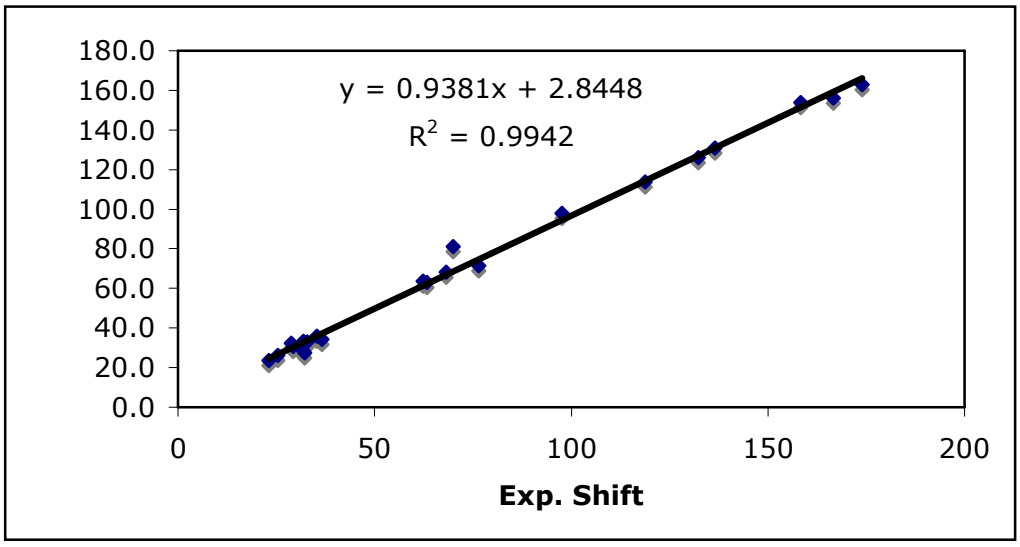


Table S16. DFT Calculation Results of the 6*S*,7*S* Isomer for **10**

position	Exp. Shift	Calc. Shift	Abs. Diff.	Corr. Shift	Abs. Diff.
C1	166.6	155.9	10.7	164.5	2.1
C2	118.7	114.7	4.0	119.9	1.2
C3	159.5	153.7	5.8	162.2	2.7
C4	27.3	28.6	1.3	26.6	0.7
C5	30.5	37.0	6.5	35.7	5.2
C6	73.4	76.9	3.5	78.9	5.5
C7	70.0	65.9	4.1	67.0	3.0
C8	131.4	128.2	3.2	134.5	3.1
C9	139.2	127.7	11.5	134.0	5.2
C10	30.0	31.4	1.4	29.6	0.4
C11	32.1	32.4	0.3	30.7	1.4
C12	31.7	33.3	1.6	31.7	0.0
C13	63.8	63.1	0.7	64.0	0.2
C14	35.2	36.3	1.1	34.9	0.3
C15	68.3	67.0	1.3	68.2	0.1
C16	32.2	27.5	4.7	25.4	6.8
C17	98.0	97.9	0.1	101.7	3.7
C18	63.5	63.1	0.4	64.0	0.5
C19	29.1	32.1	3.0	30.4	1.3
C20	173.9	162.7	11.2	171.9	2.0
C21	24.6	26.4	1.8	24.2	0.4
C22	21.4	23.3	1.9	20.8	0.6
% Score/ MAE		63	3.6	86	2.1
TMS		189.63		y=0.9226x+4.0948	

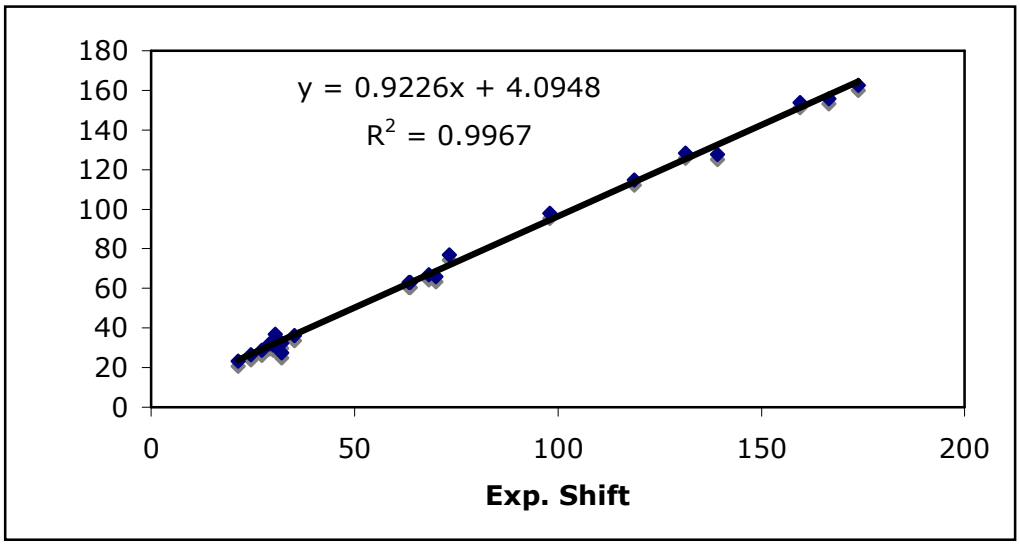


Table S17. DFT Calculation Results of the 6*R*,7*S* Isomer for **10**

position	Exp. Shift	Calc. Shift	Abs. Diff.	Corr. Shift	Abs. Diff.
C1	166.6	155.9	10.7	163.4	3.2
C2	118.7	113.4	5.3	118.0	0.7
C3	159.5	154.9	4.6	162.3	2.8
C4	27.3	25.6	1.7	24.1	3.2
C5	30.5	33.3	2.8	32.3	1.8
C6	73.4	72.8	0.6	74.6	1.2
C7	70.0	68.8	1.2	70.3	0.3
C8	131.4	128.2	3.2	133.8	2.4
C9	139.2	133.1	6.1	139.0	0.2
C10	30.0	31.3	1.3	30.2	0.2
C11	32.1	32.4	0.3	31.4	0.7
C12	31.7	32.3	0.6	31.3	0.4
C13	63.8	63.8	0.0	65.0	1.2
C14	35.2	34.1	1.1	33.2	2.0
C15	68.3	68.3	0.0	69.8	1.5
C16	32.2	28.2	4.0	26.9	5.3
C17	98.0	97.9	0.1	101.4	3.4
C18	63.5	63.4	0.1	64.5	1.0
C19	29.1	32.1	3.0	31.1	2.0
C20	173.9	162.6	11.3	170.6	3.3
C21	24.6	26.7	2.1	25.3	0.7
C22	21.4	23.7	2.3	22.1	0.7
% Score/ MAE		73	2.8	96	1.7
TMS		189.63		y=09355x+3.0388	

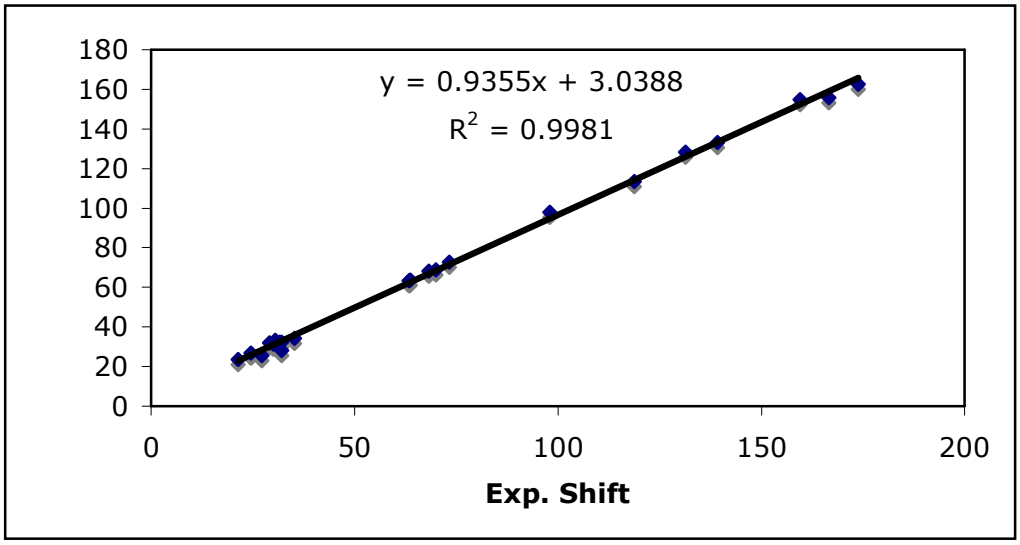


Table S18. DFT Calculation Results of the 6*S*,7*R* Isomer for **10**

position	Exp. Shift	Calc. Shift	Abs. Diff.	Corr. Shift	Abs. Diff.
C1	166.6	156.2	10.4	163.4	3.2
C2	118.7	113.9	4.8	117.6	1.1
C3	159.5	155.6	3.9	162.8	3.3
C4	27.3	30.9	3.6	27.6	0.3
C5	30.5	42.8	12.3	40.5	10.0
C6	73.4	78.8	5.4	79.5	6.1
C7	70.0	77.5	7.5	78.1	8.1
C8	131.4	129.7	1.7	134.7	3.3
C9	139.2	131.2	8.0	136.3	2.9
C10	30.0	30.9	0.9	27.6	2.4
C11	32.1	32.9	0.8	29.7	2.4
C12	31.7	33.5	1.8	30.4	1.3
C13	63.8	63.2	0.6	62.6	1.2
C14	35.2	36.2	1.0	33.3	1.9
C15	68.3	66.6	1.7	66.3	2.0
C16	32.2	27.8	4.4	24.2	8.0
C17	98.0	97.9	0.1	100.2	2.2
C18	63.5	63.1	0.4	62.5	1.0
C19	29.1	32.2	3.1	29.0	0.1
C20	173.9	162.7	11.2	170.5	3.4
C21	24.6	26.9	2.3	23.2	1.4
C22	21.4	24.4	3.0	20.5	0.9
% Score/ MAE		59	4.0	77	3.0
TMS		189.63		y=0.9221x+5.4886	

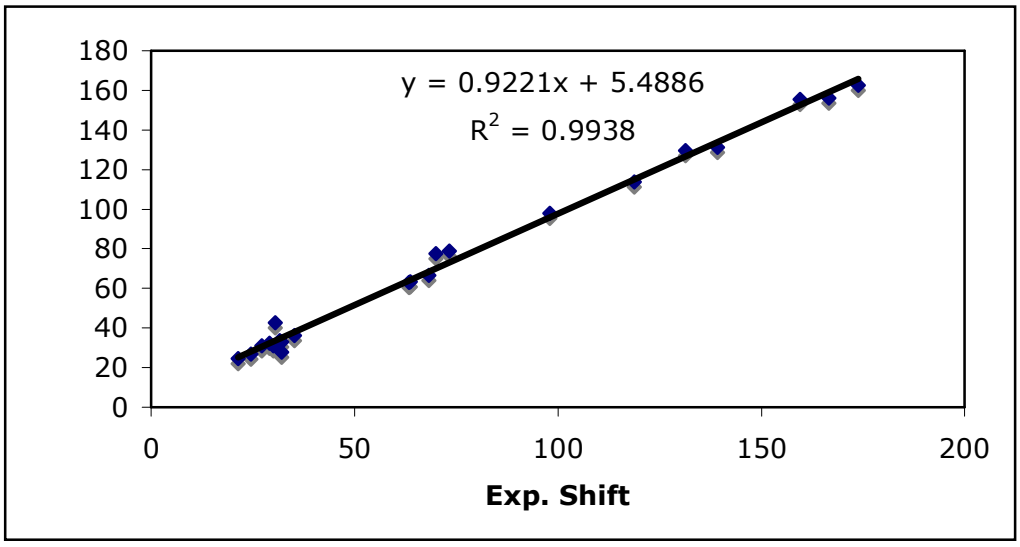


Table S19. DFT Calculation Results of the 6*R*,7*R* Isomer for **10**

position	Exp. Shift	Calc. Shift	Abs. Diff.	Corr. Shift	Abs. Diff.
C1	166.6	156.0	10.6	164.0	2.6
C2	118.7	113.7	5.0	118.3	0.4
C3	159.5	153.8	5.7	161.6	2.1
C4	27.3	27.6	0.3	25.2	2.1
C5	30.5	35.9	5.4	34.1	3.6
C6	73.4	71.4	2.0	72.5	0.9
C7	70.0	81.1	11.1	83.0	13.0
C8	131.4	125.9	5.5	131.4	0.0
C9	139.2	131.0	8.2	137.0	2.2
C10	30.0	30.8	0.8	28.6	1.4
C11	32.1	33.2	1.1	31.2	0.9
C12	31.7	33.0	1.3	31.0	0.7
C13	63.8	63.6	0.2	64.1	0.3
C14	35.2	34.3	0.9	32.4	2.8
C15	68.3	68.3	0.0	69.2	0.9
C16	32.2	28.3	3.9	25.9	6.3
C17	98.0	97.8	0.2	101.1	3.1
C18	63.5	63.0	0.5	63.4	0.1
C19	29.1	32.4	3.3	30.4	1.3
C20	173.9	162.9	11.0	171.4	2.5
C21	24.6	26.2	1.6	23.7	0.9
C22	21.4	23.6	2.2	20.8	0.6
% Score/ MAE		50	3.7	86	2.2
TMS		189.63		y=0.925x+4.3164	

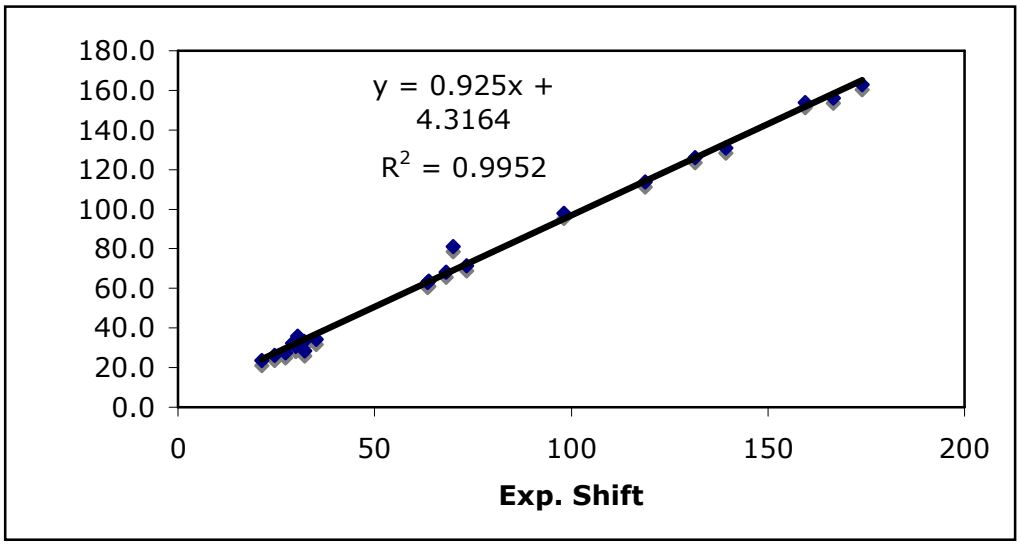


Figure S1. ^{1}H NMR spectrum of **1** in $CDCl_3$ (500 MHz).

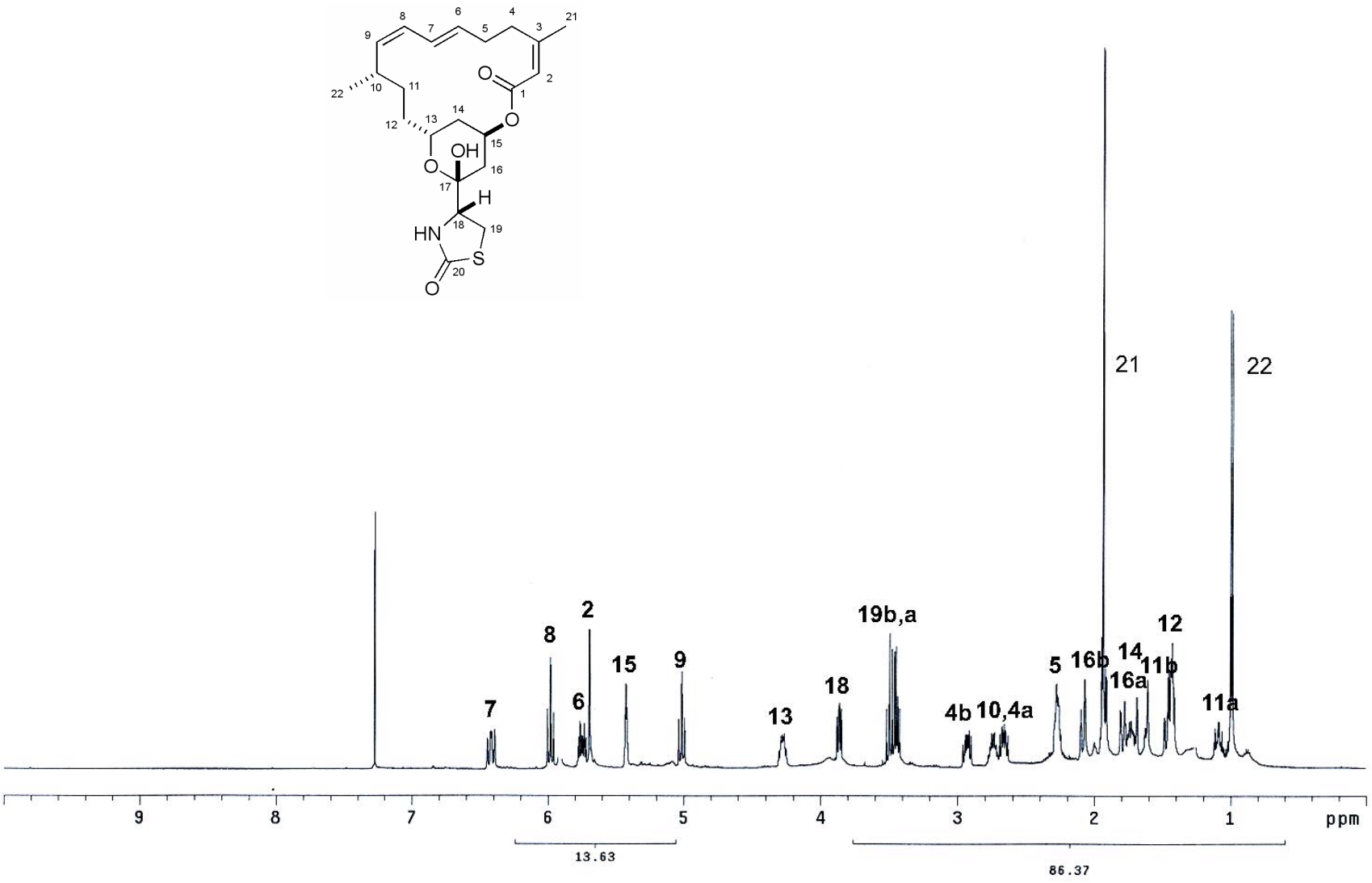


Figure S2. ^{13}C NMR spectrum of **1** in $CDCl_3$ (125 MHz).

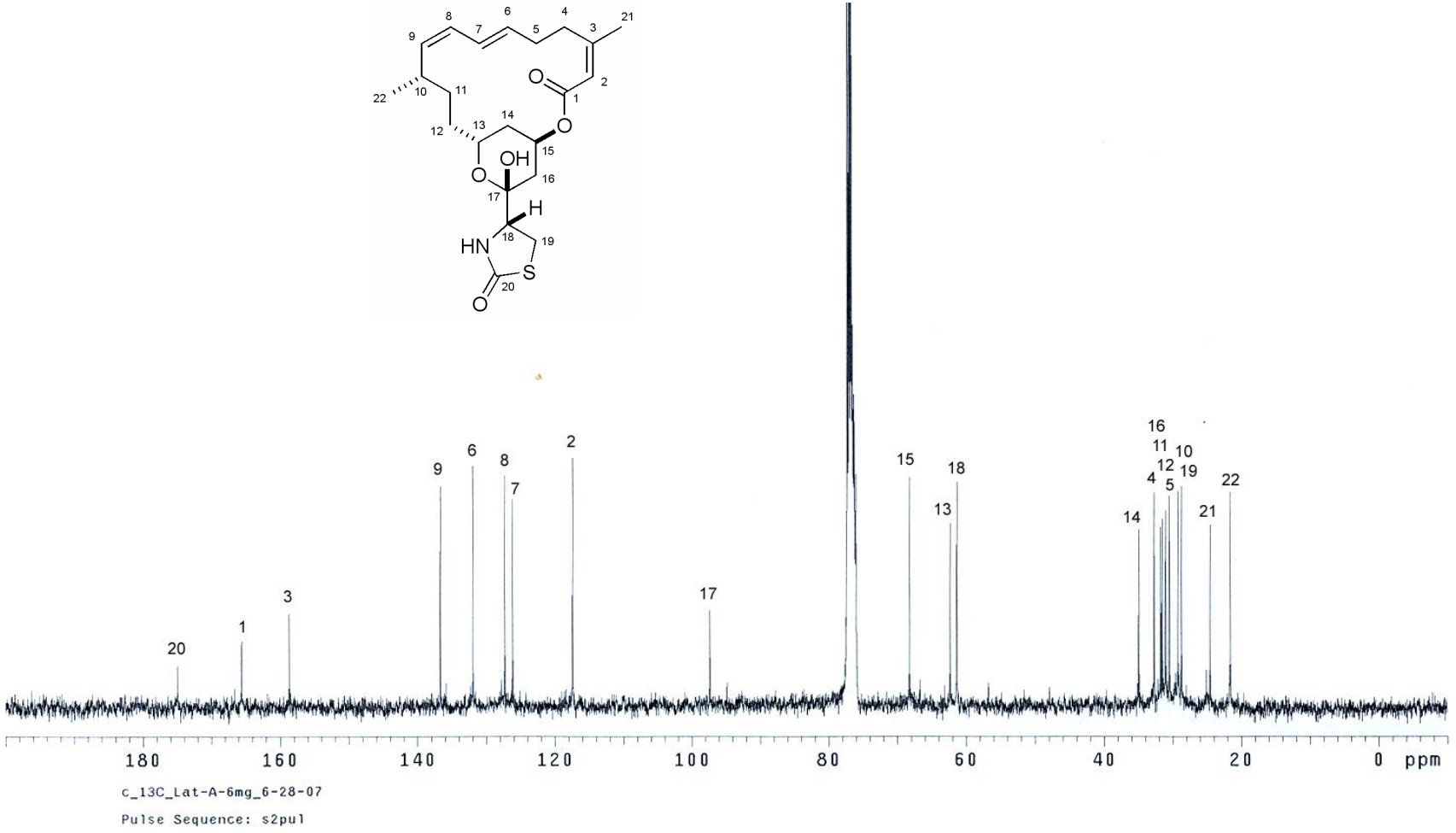


Figure S3. ^{1}H NMR spectrum of **2** in $CDCl_3$ (500 MHz).

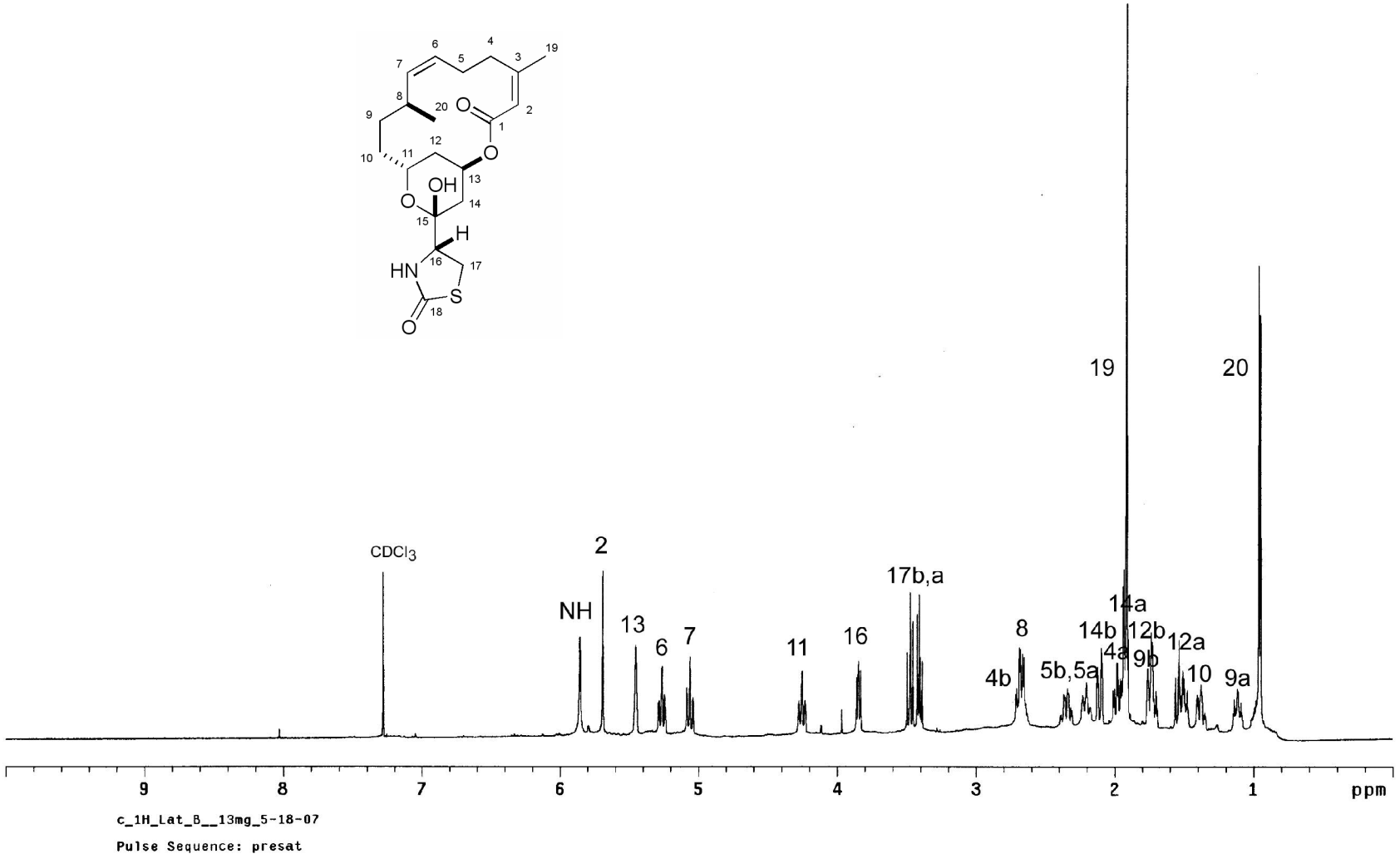


Figure S4. ^{13}C NMR spectrum of **2** in $CDCl_3$ (125 MHz).

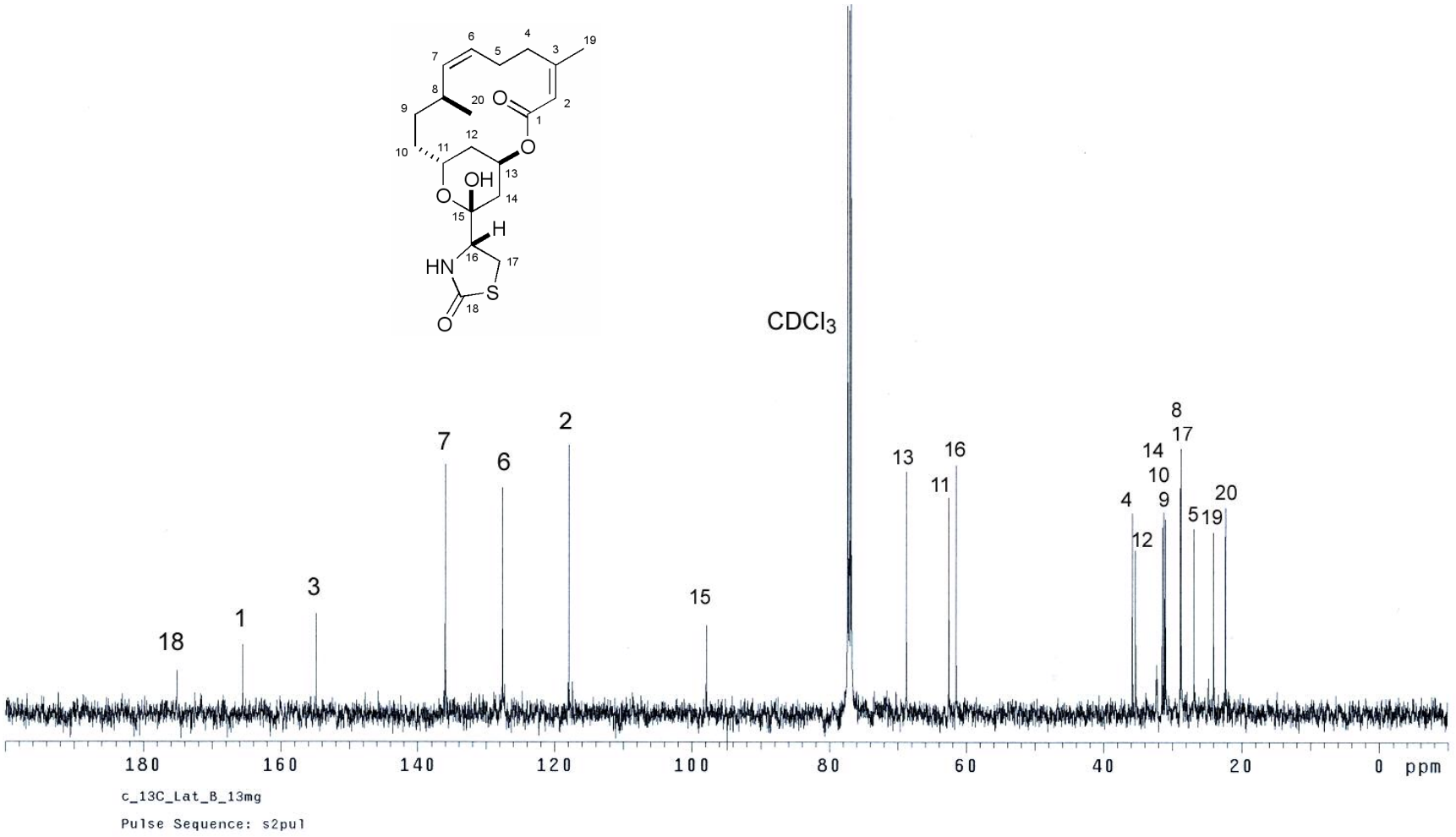


Figure S5. ^{1}H NMR spectrum of **3** in $CDCl_3$ (500 MHz).

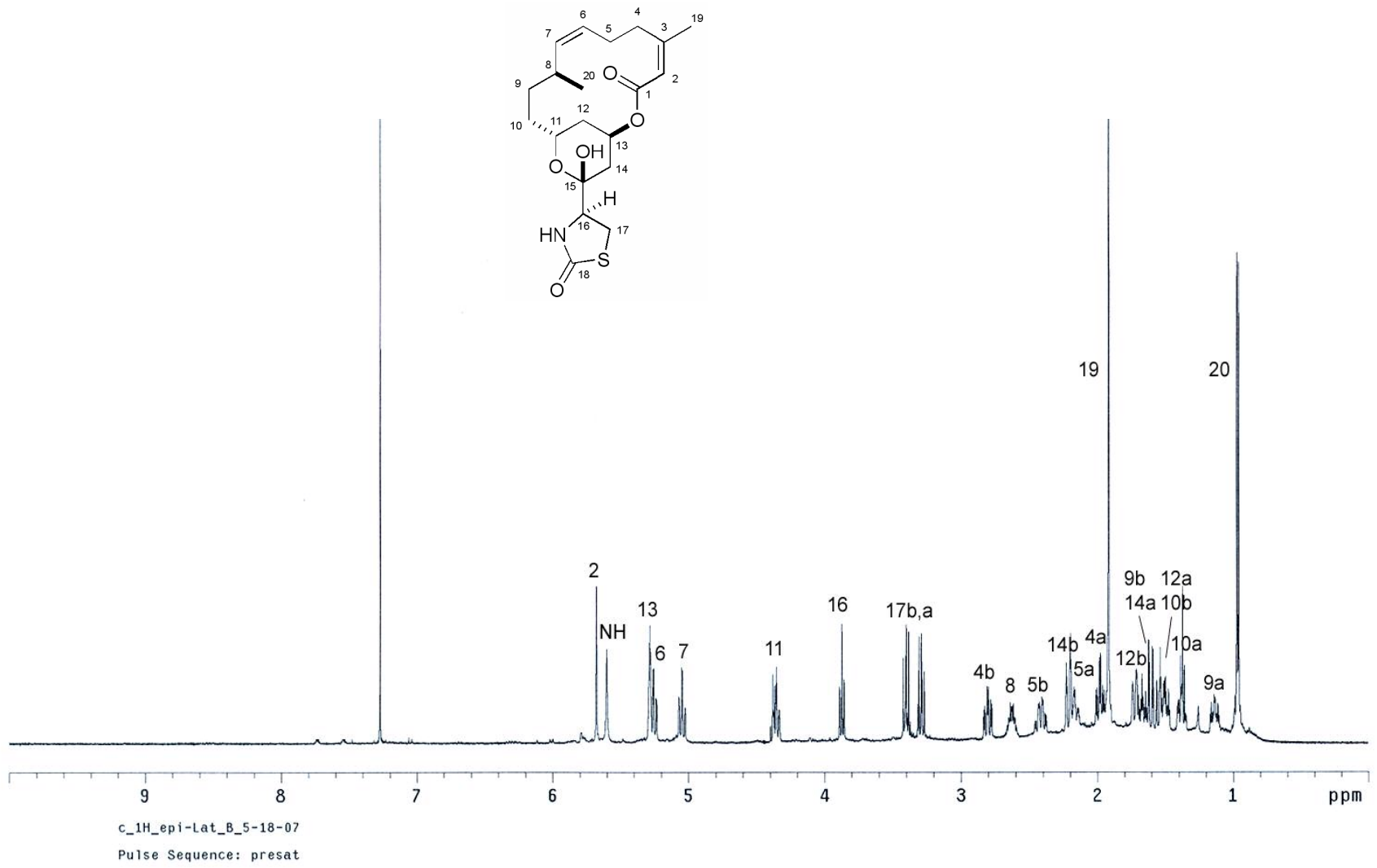


Figure S6. ^{13}C NMR spectrum of **3** in $CDCl_3$ (125 MHz).

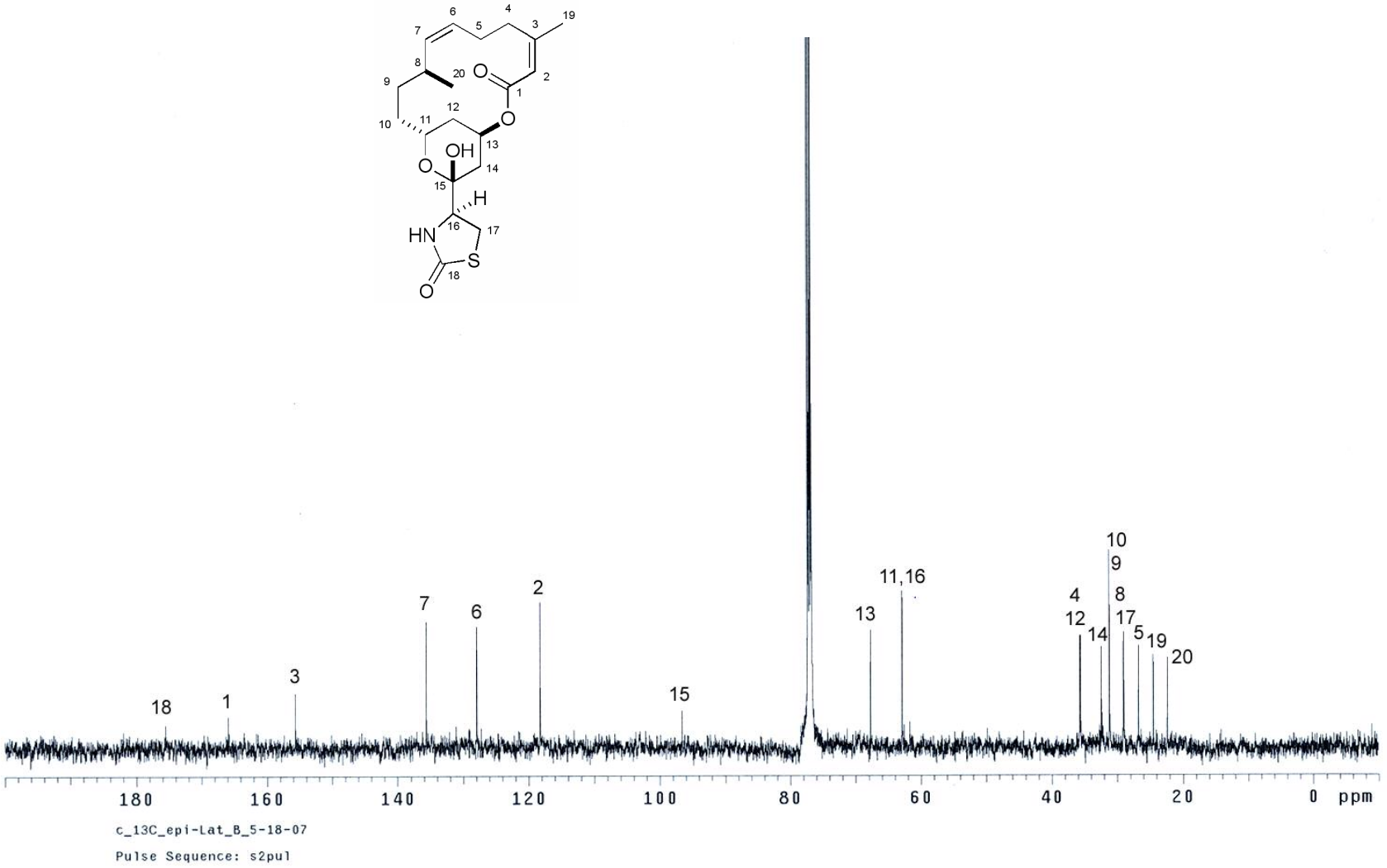


Figure S7. ^{1}H NMR spectrum of **4** in $CDCl_3$ (500 MHz).

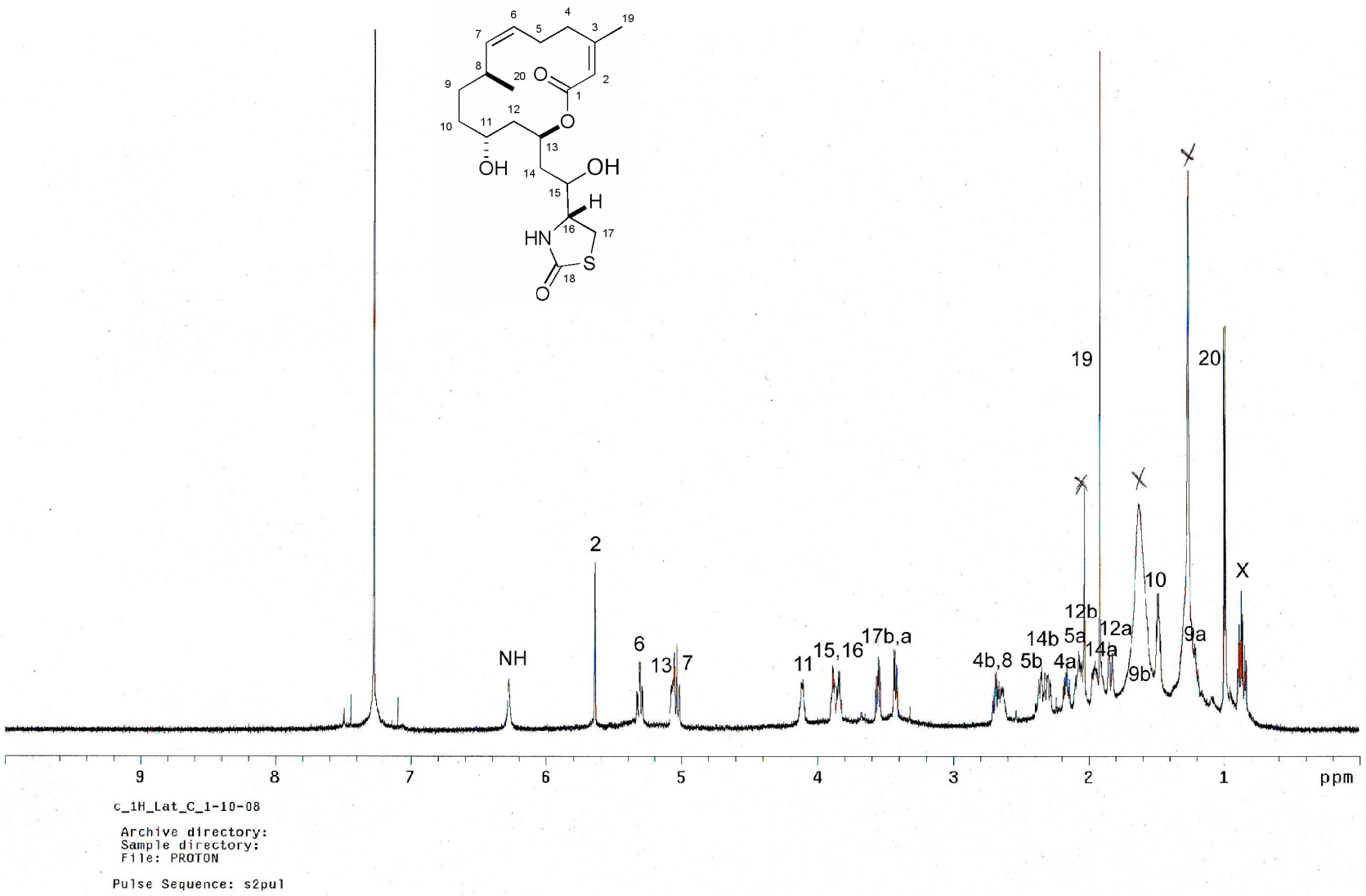


Figure S8. ^{13}C NMR spectrum of **4** in $CDCl_3$ (125 MHz).

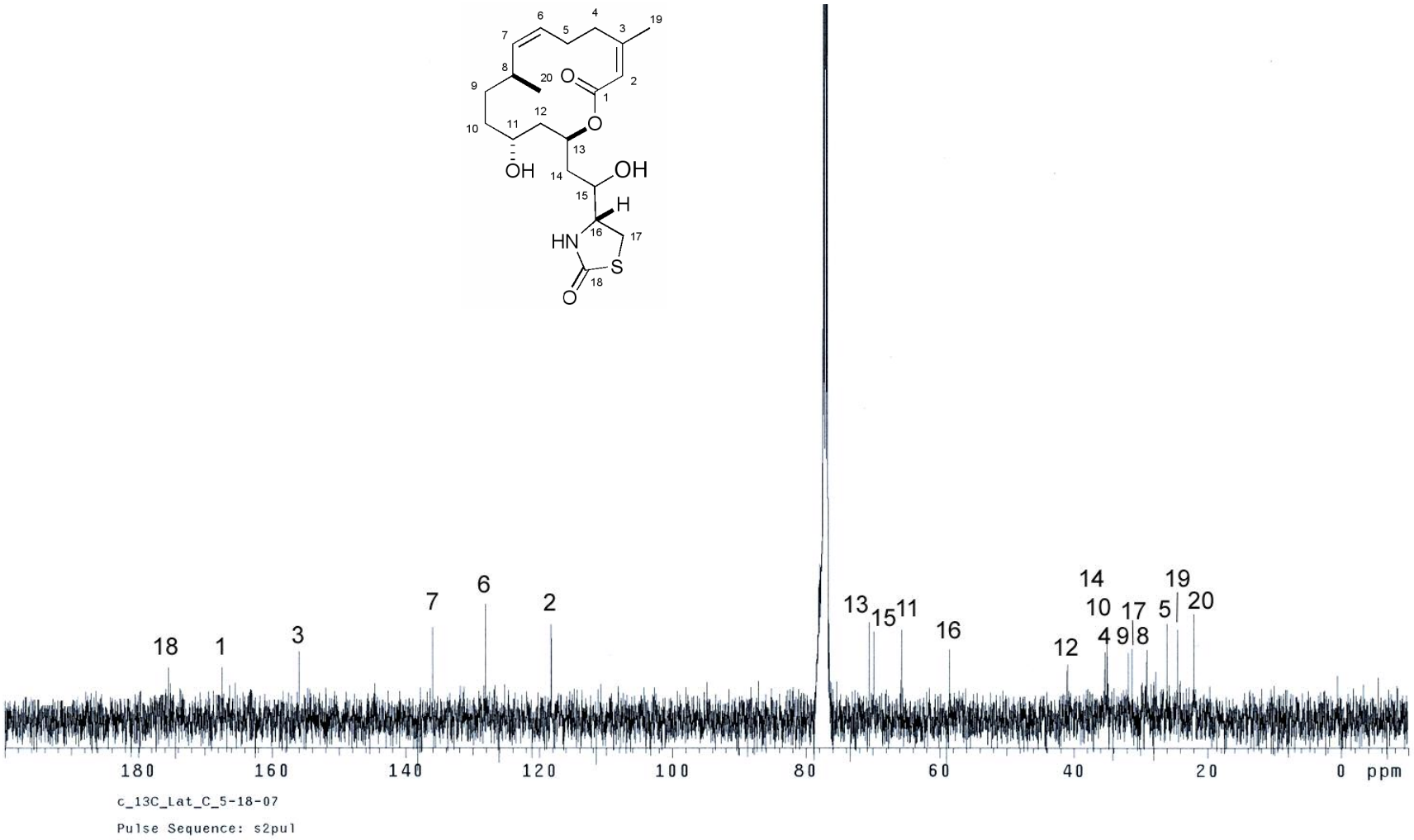


Figure S9. ^{1}H NMR spectrum of **7** in acetone-d_6 (600 MHz).

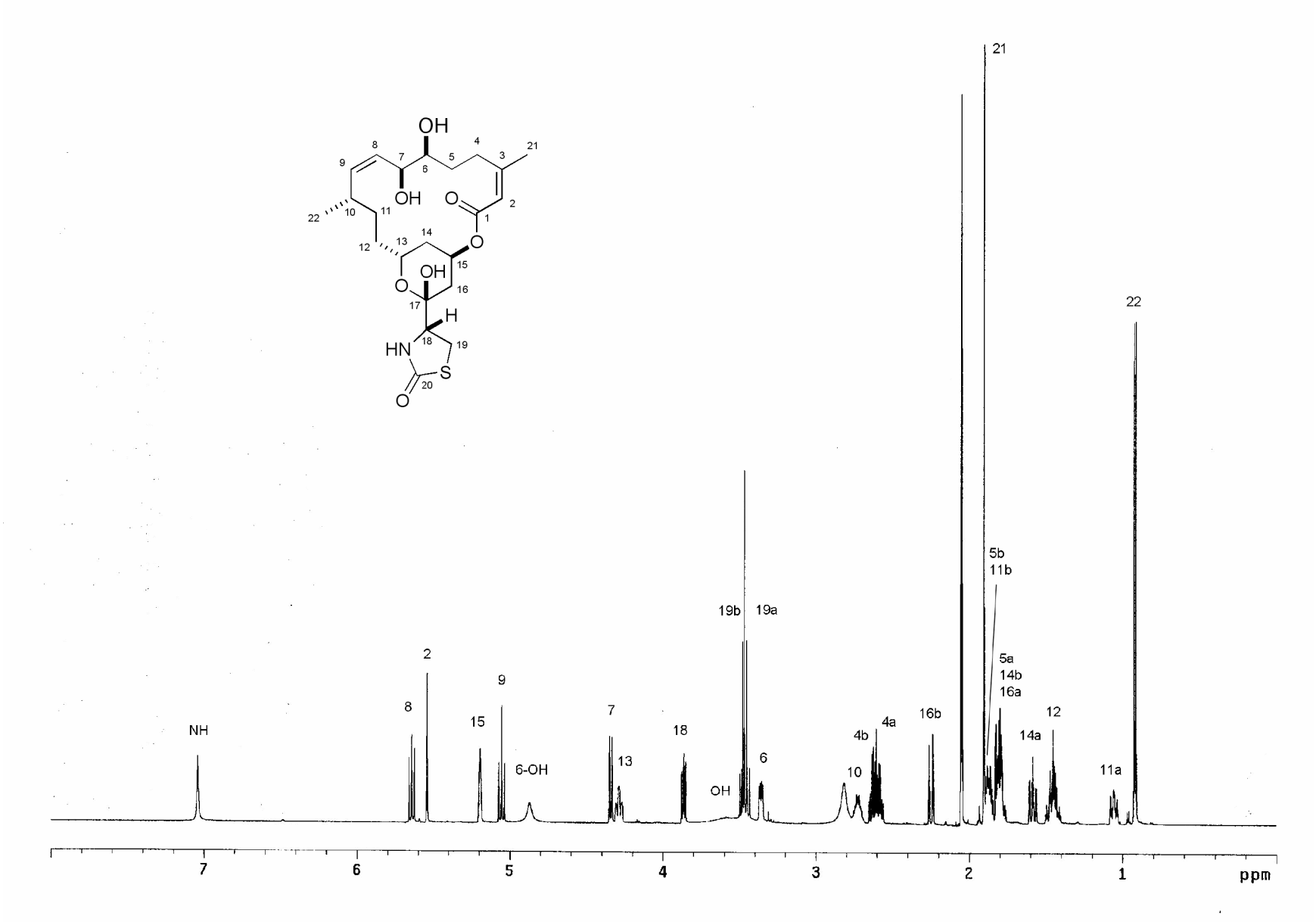


Figure S10. ^{13}C NMR spectrum of **7** in acetone-d_6 (125 MHz).

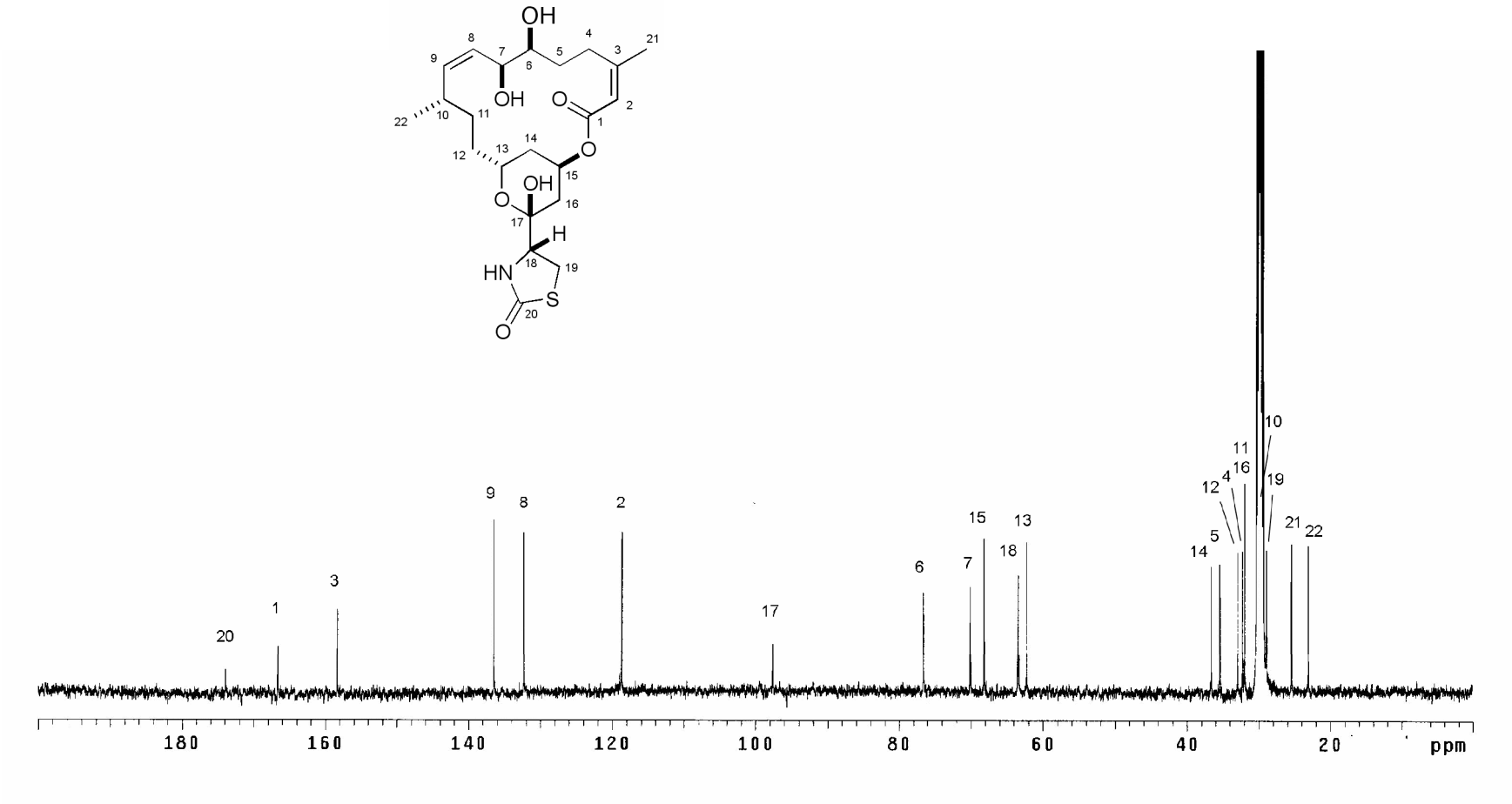


Figure S11. HMQC spectrum of **7** in acetone-d_6 (500 MHz)

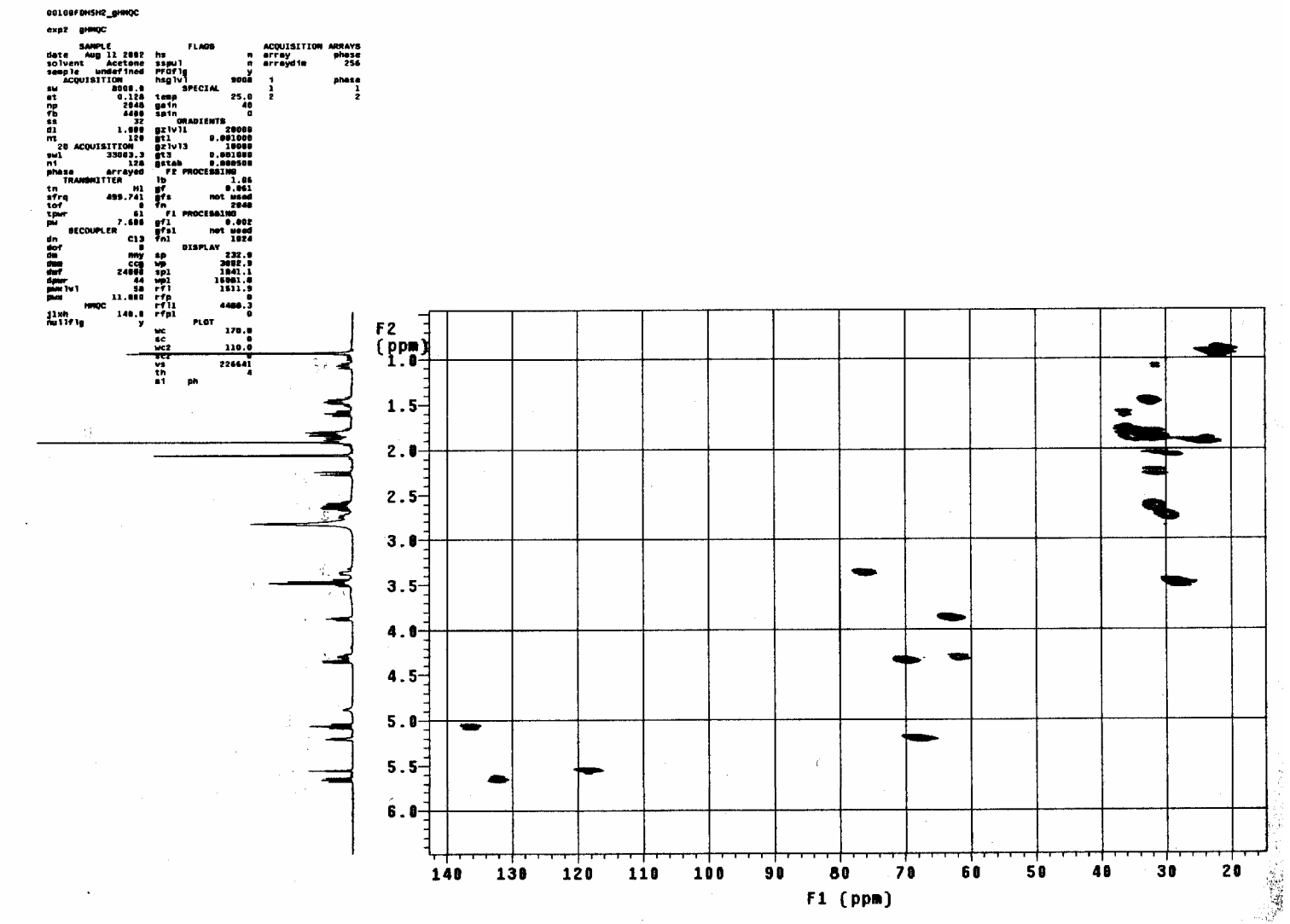


Figure S12. ^{1}H NMR spectrum of **8** in acetone-d_6 (600 MHz).

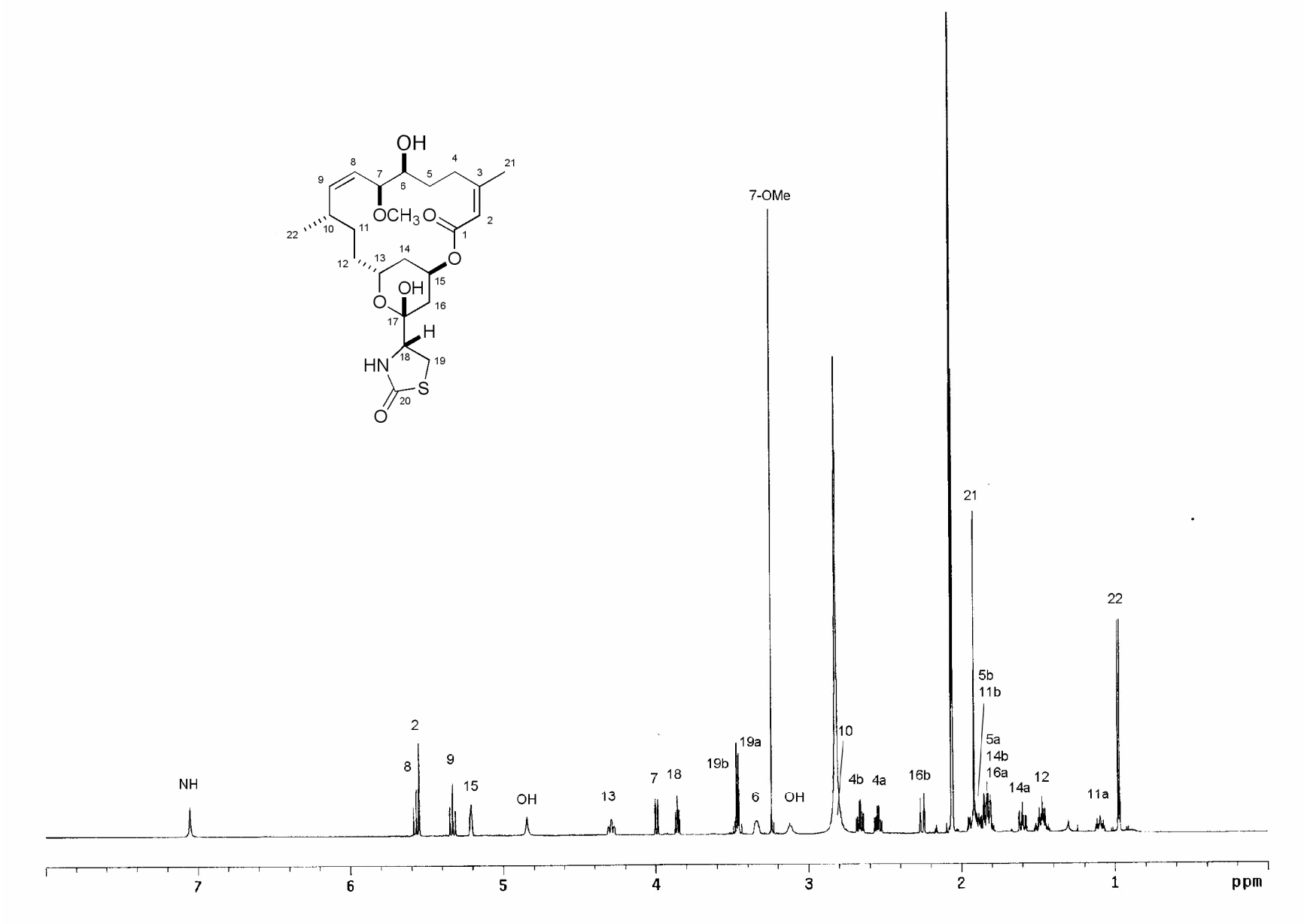


Figure S13. ^{13}C NMR spectrum of **8** in acetone-d_6 (125 MHz).

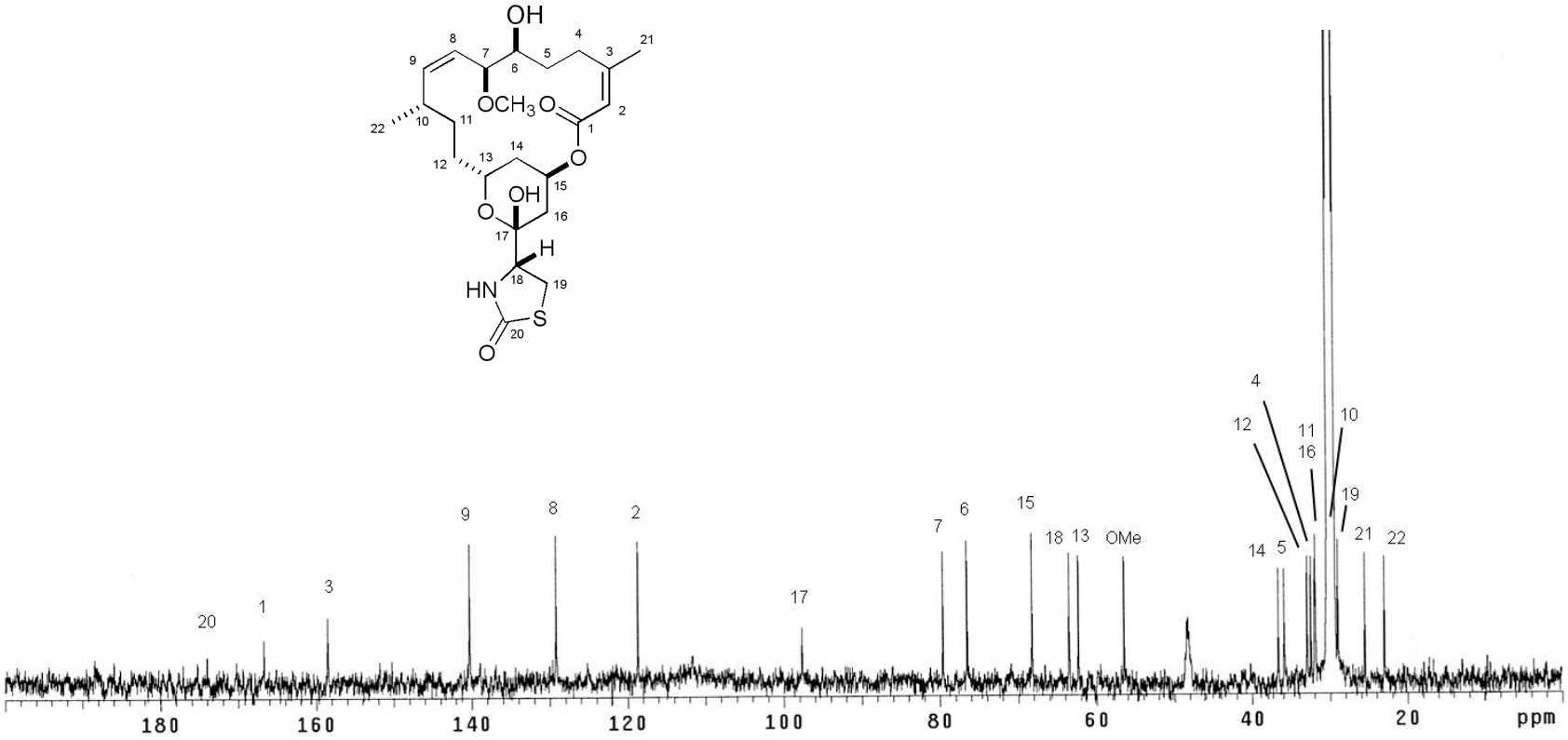


Figure S14. HMQC spectrum of **8** in acetone-d_6 (600 MHz)

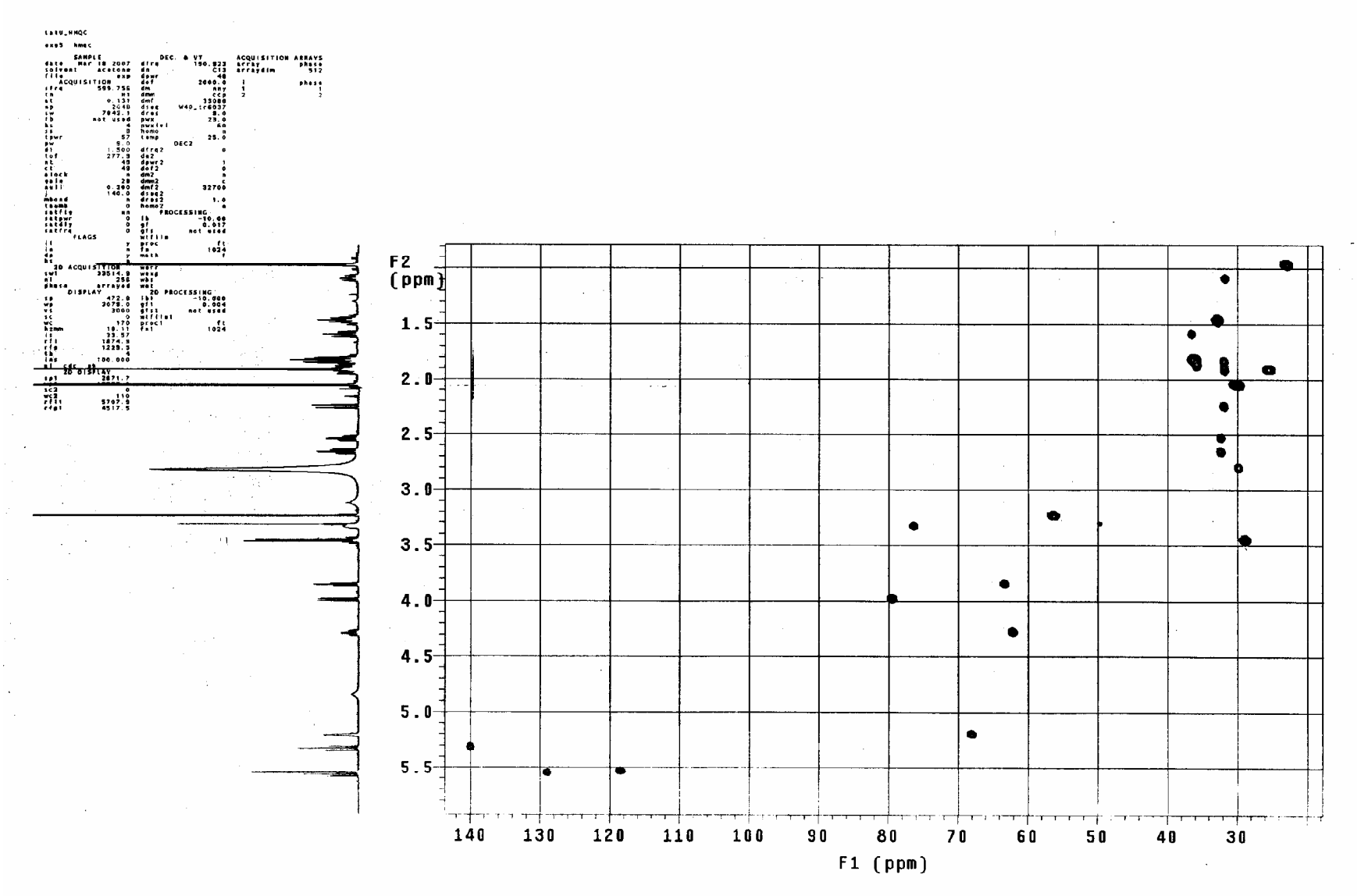


Figure S15. ^{1}H NMR spectrum of **9** in acetone-d_6 (600 MHz).

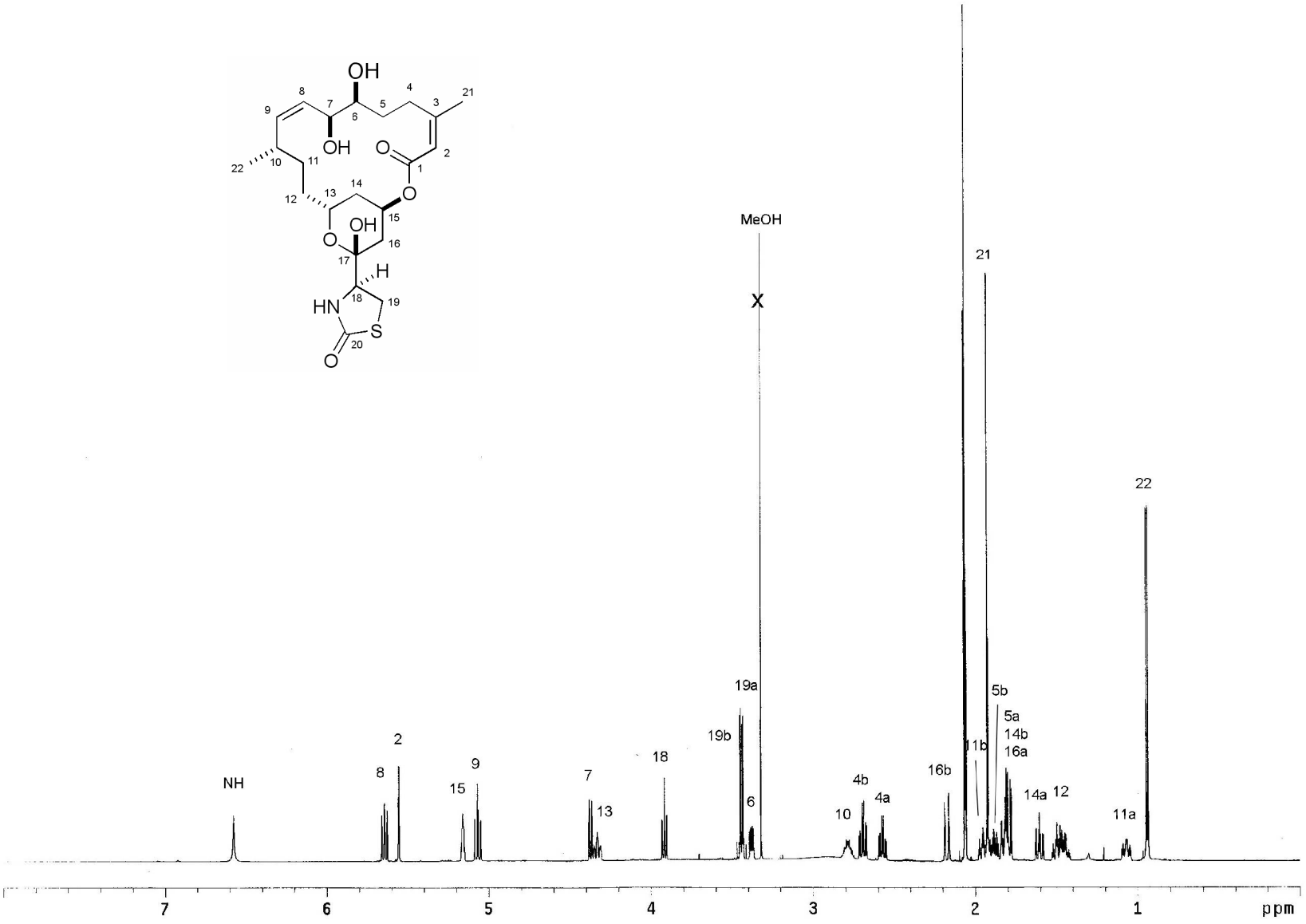


Figure S16. ^{13}C NMR spectrum of **9** in acetone-d_6 (125 MHz).

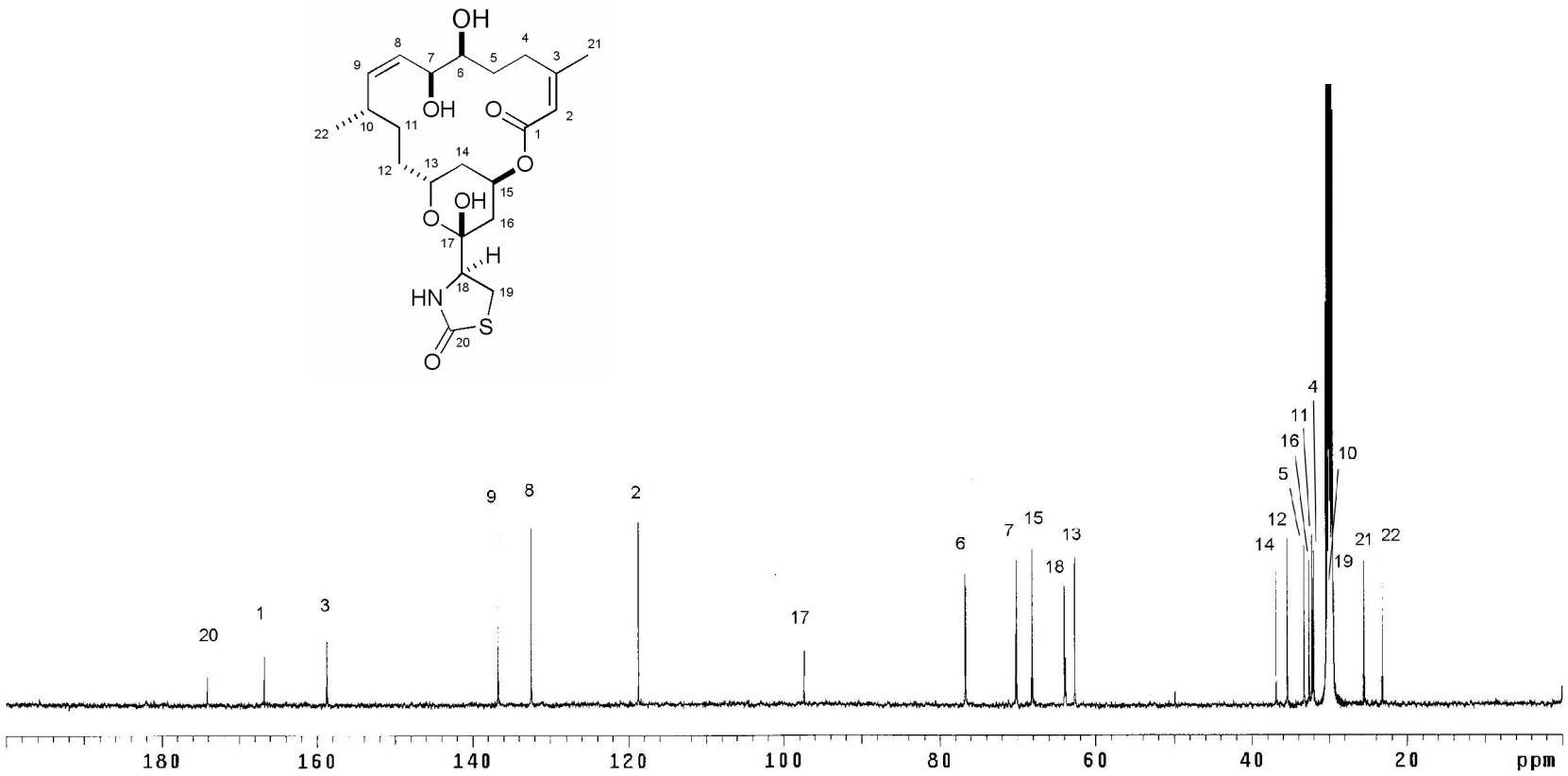


Figure S17. HMQC spectrum of **9** in acetone-d_6 (500 MHz)

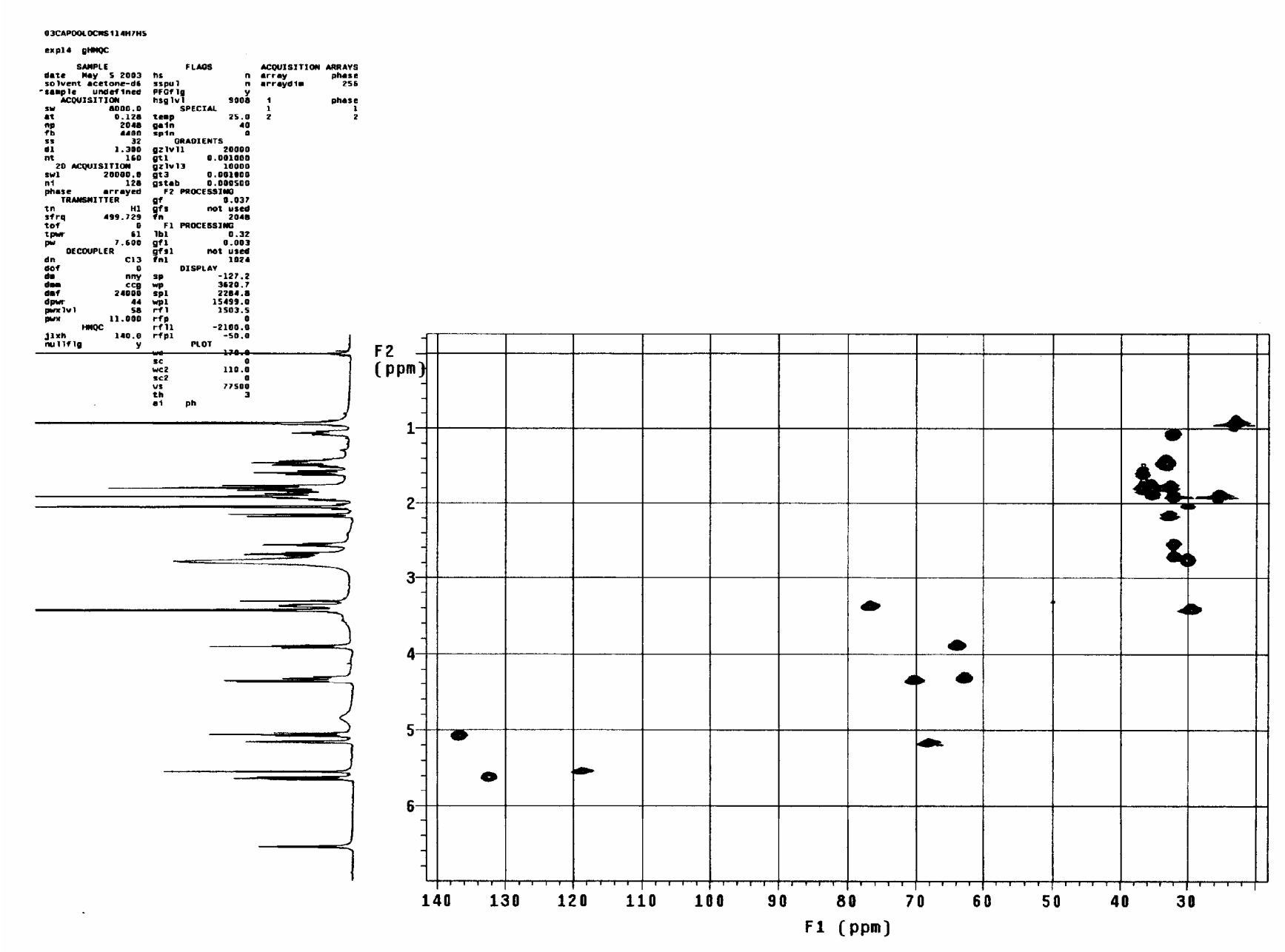


Figure S18. ^{1}H NMR spectrum of **10** in acetone-d_6 (600 MHz).

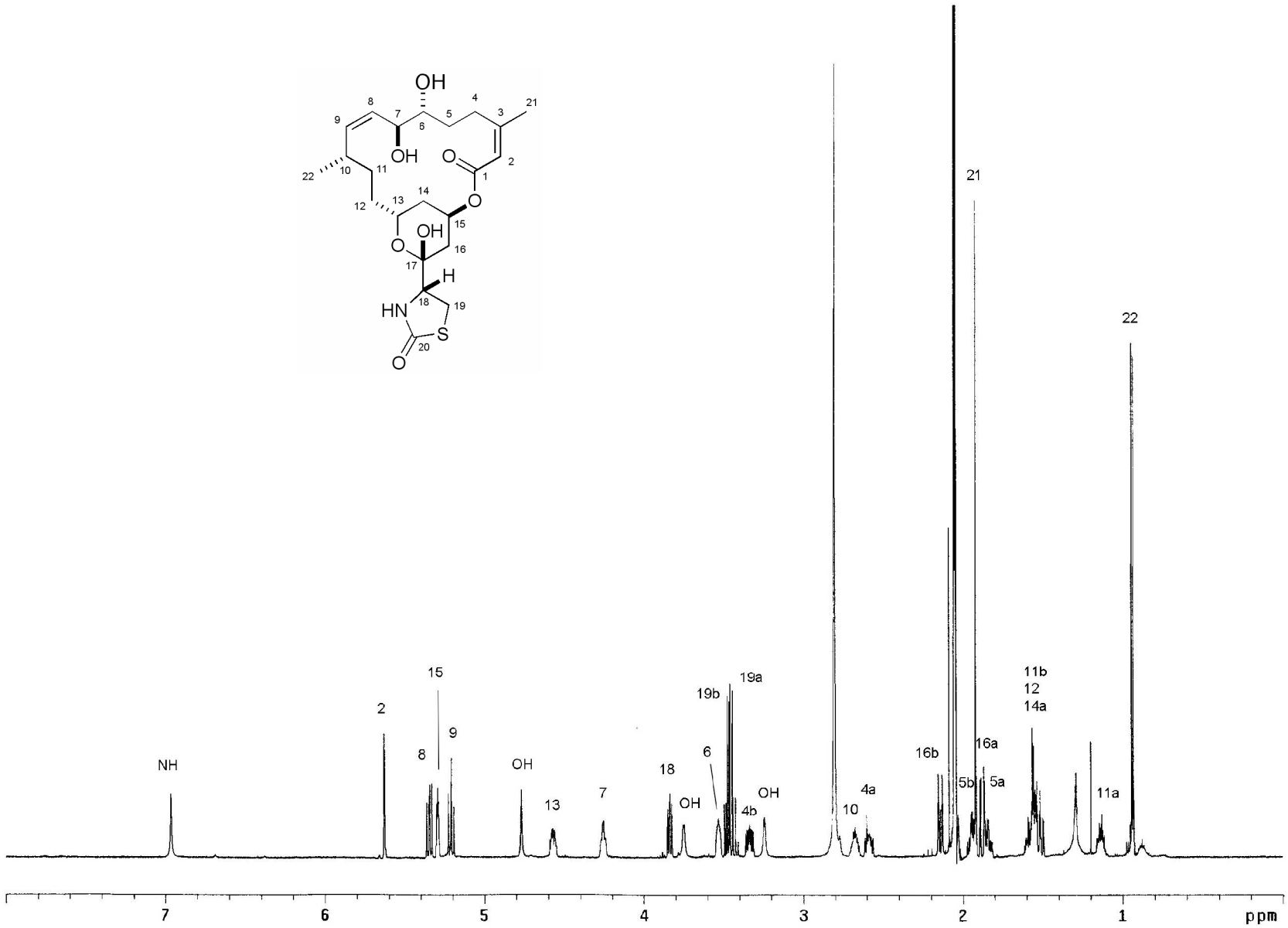


Figure S19. ^{13}C NMR spectrum of **10** in acetone-d_6 (125 MHz).

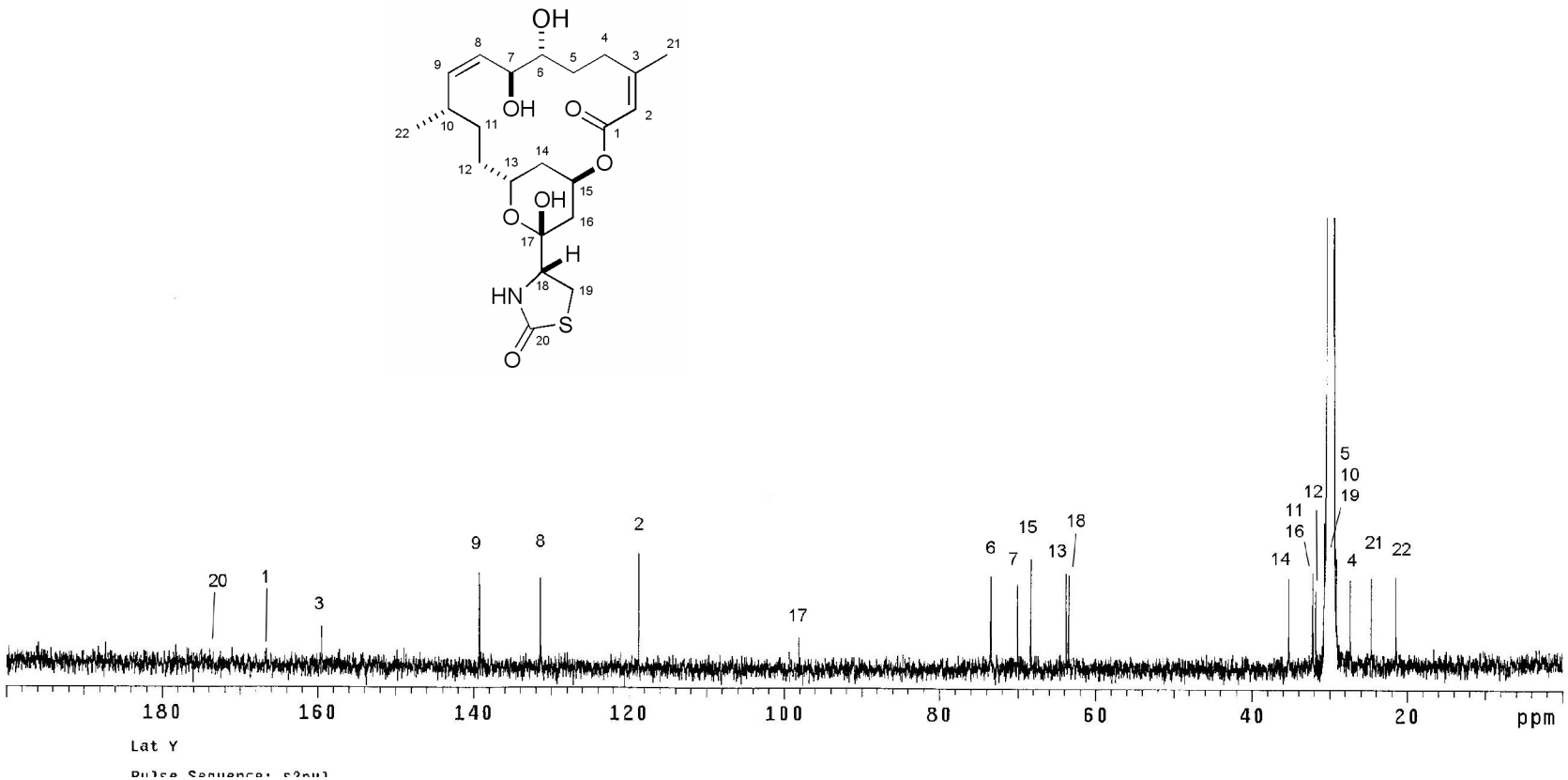


Figure S20. HMQC spectrum of **10** in acetone-d_6 (600 MHz)

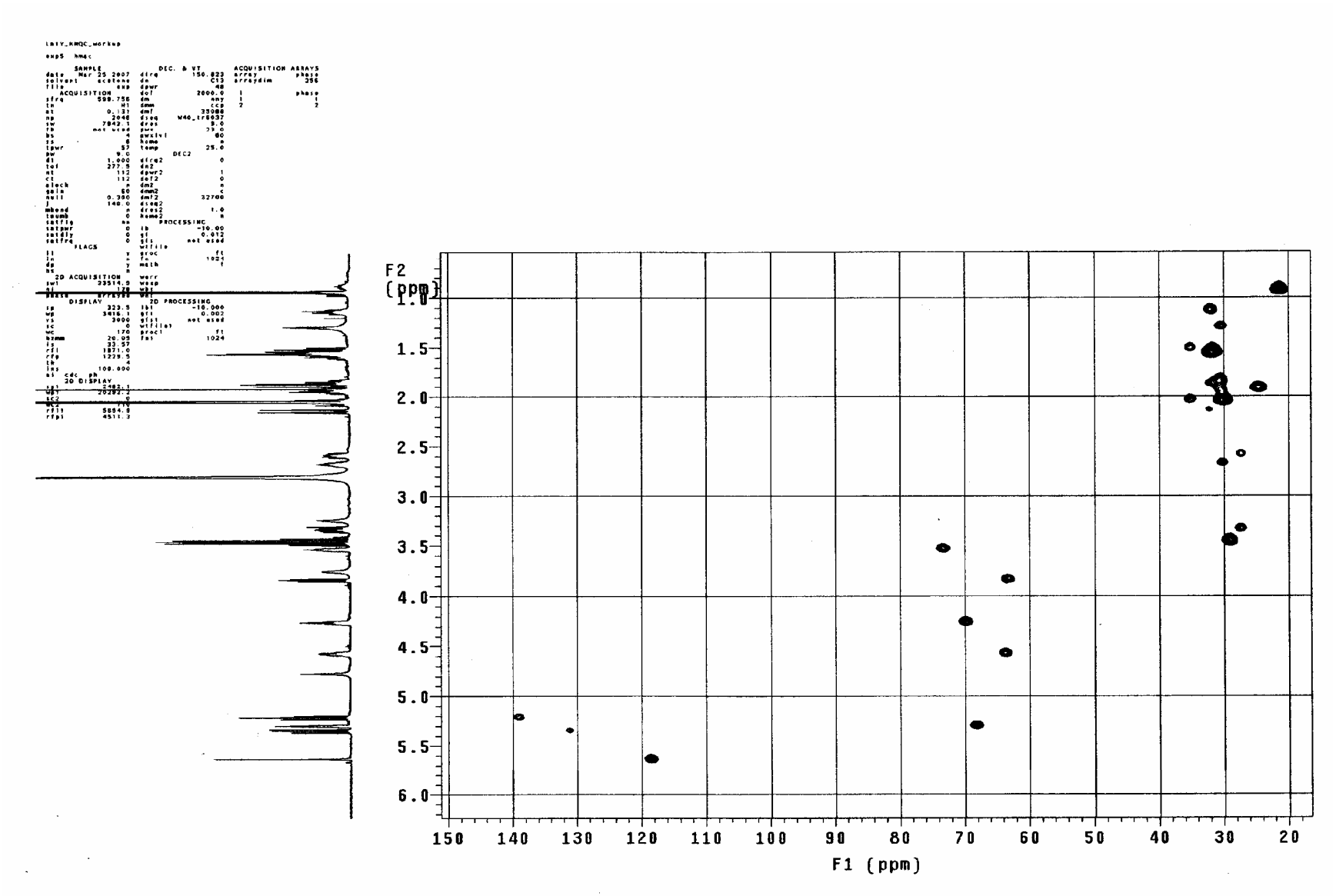


Figure S21. HMBC spectrum of **10** in acetone-d_6 (600 MHz)

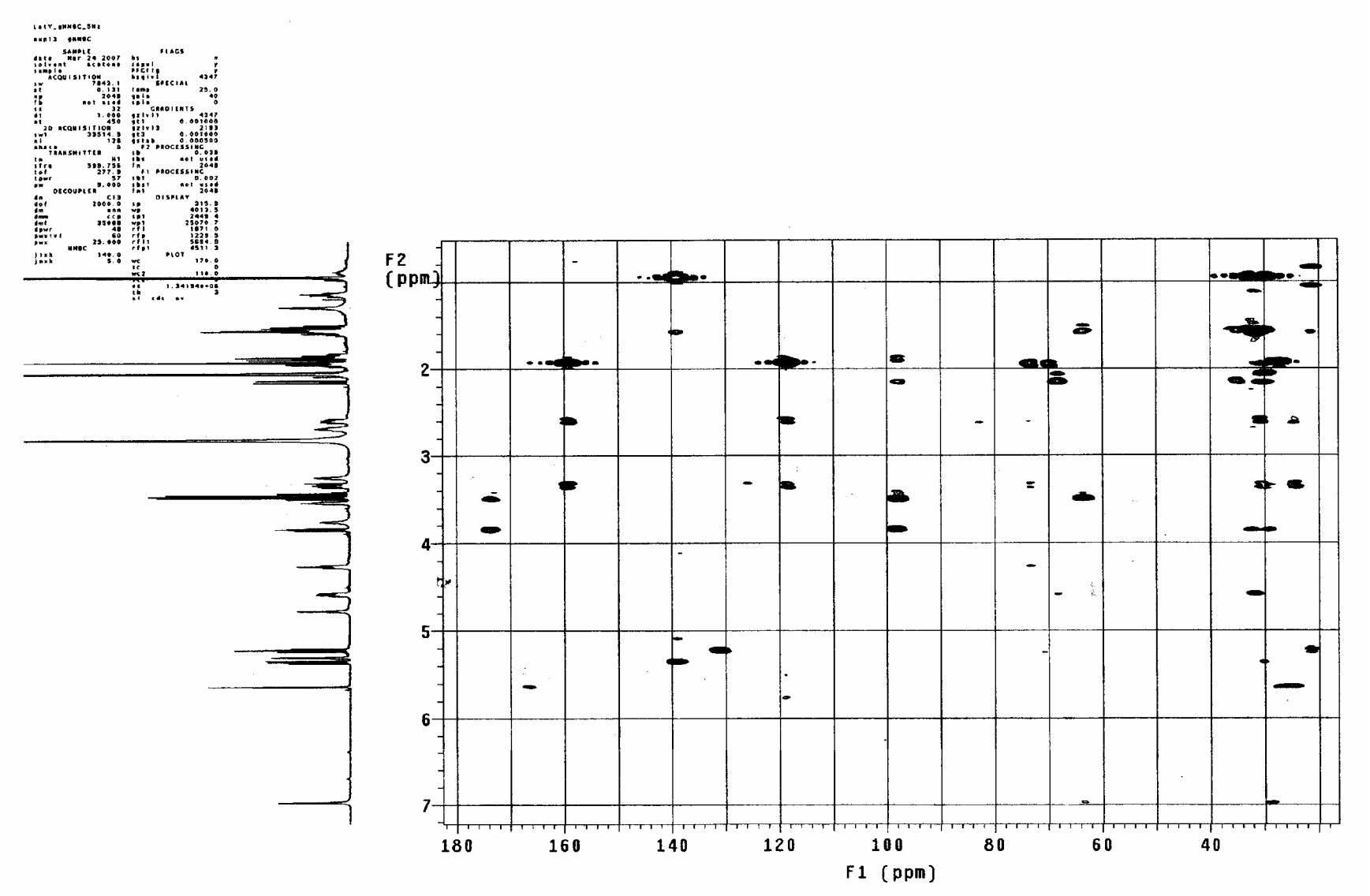


Figure S22. ^{1}H NMR spectrum of **11** in acetone-d_6 (600 MHz).

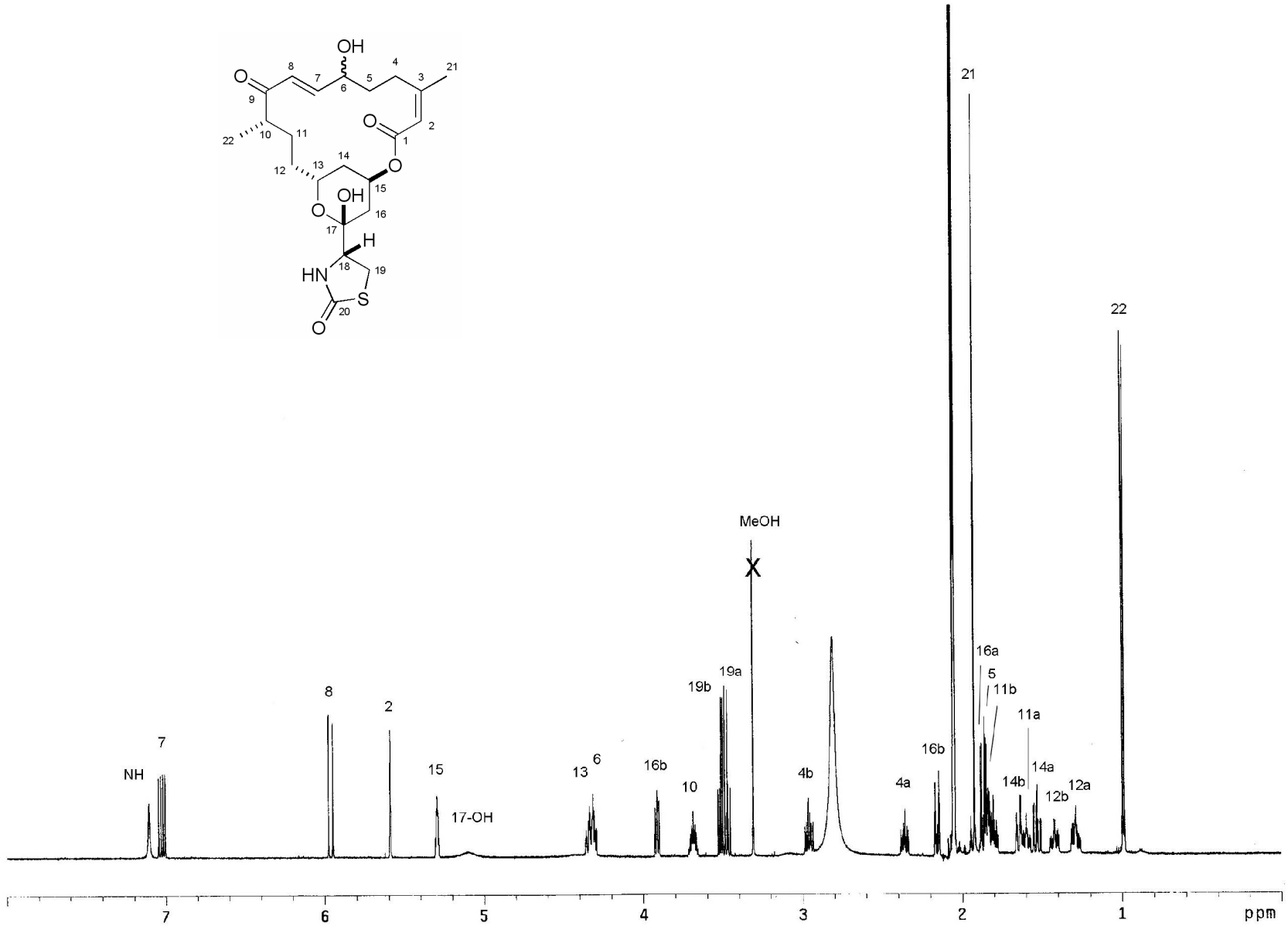


Figure S23. ^{13}C NMR spectrum of **11** in acetone-d_6 (125 MHz).

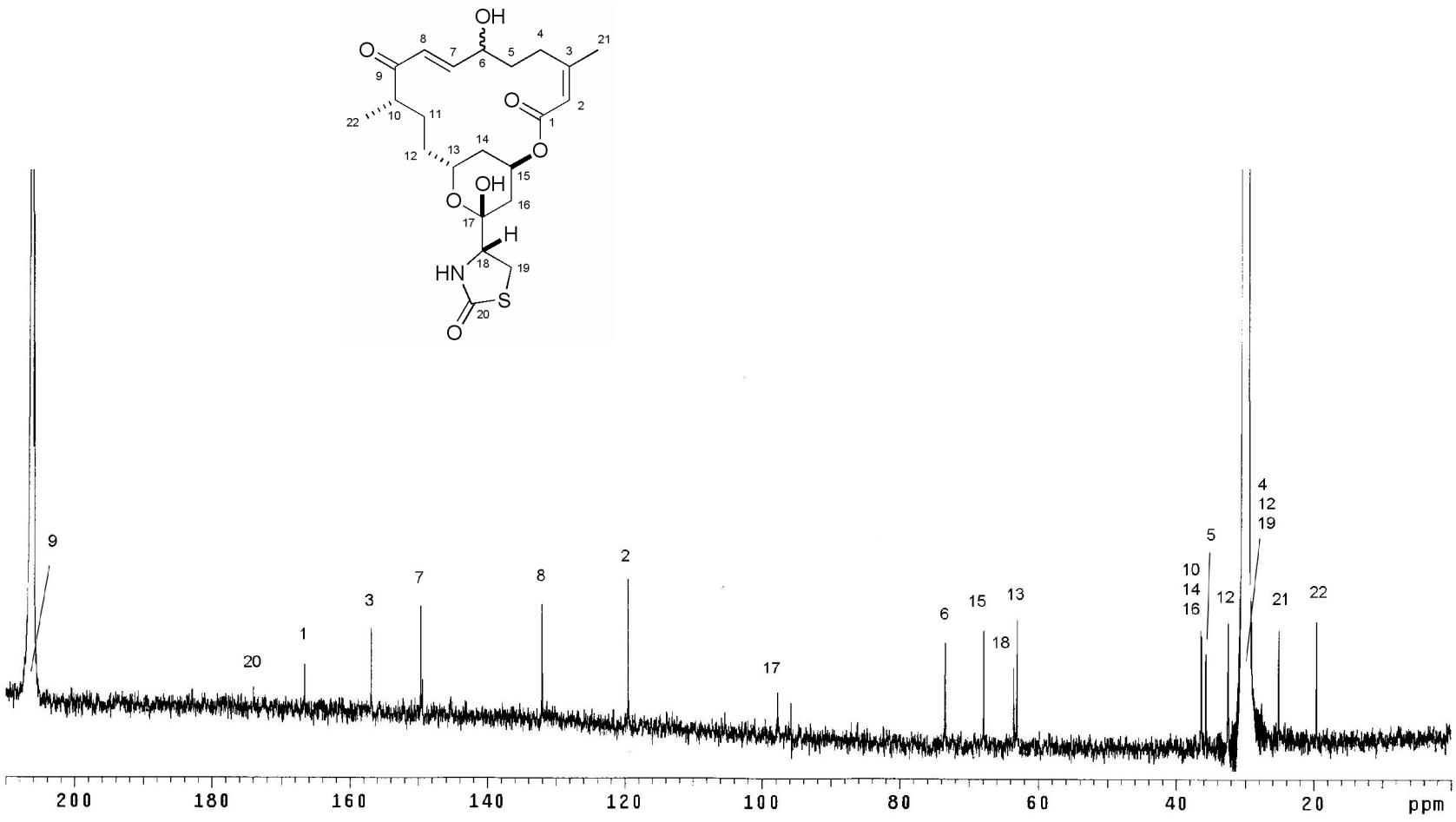


Figure S24. HMQC spectrum of **11** in acetone-d_6 (600 MHz)

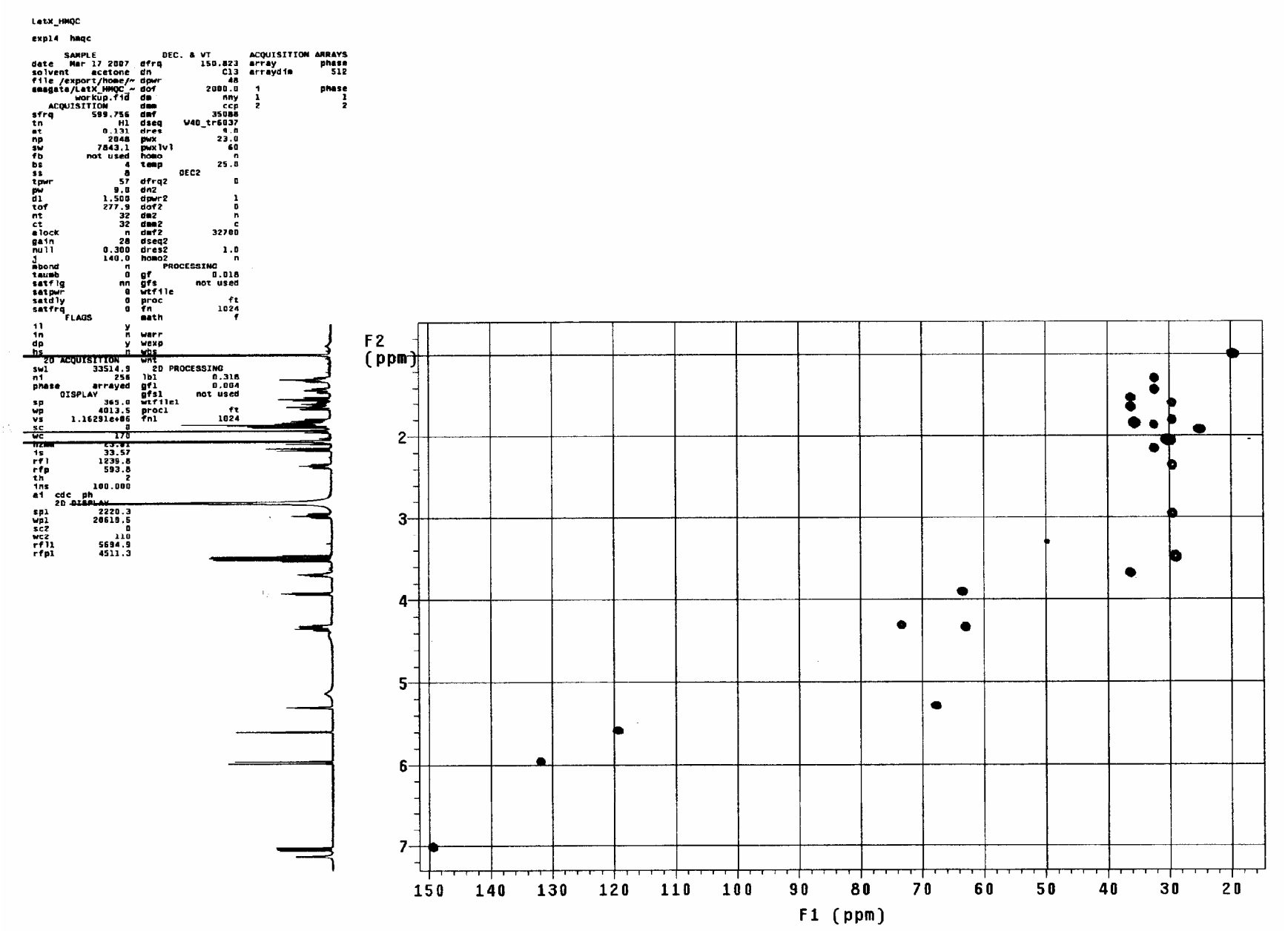


Figure S25. HMBC spectrum of **11** in acetone-d_6 (600 MHz)

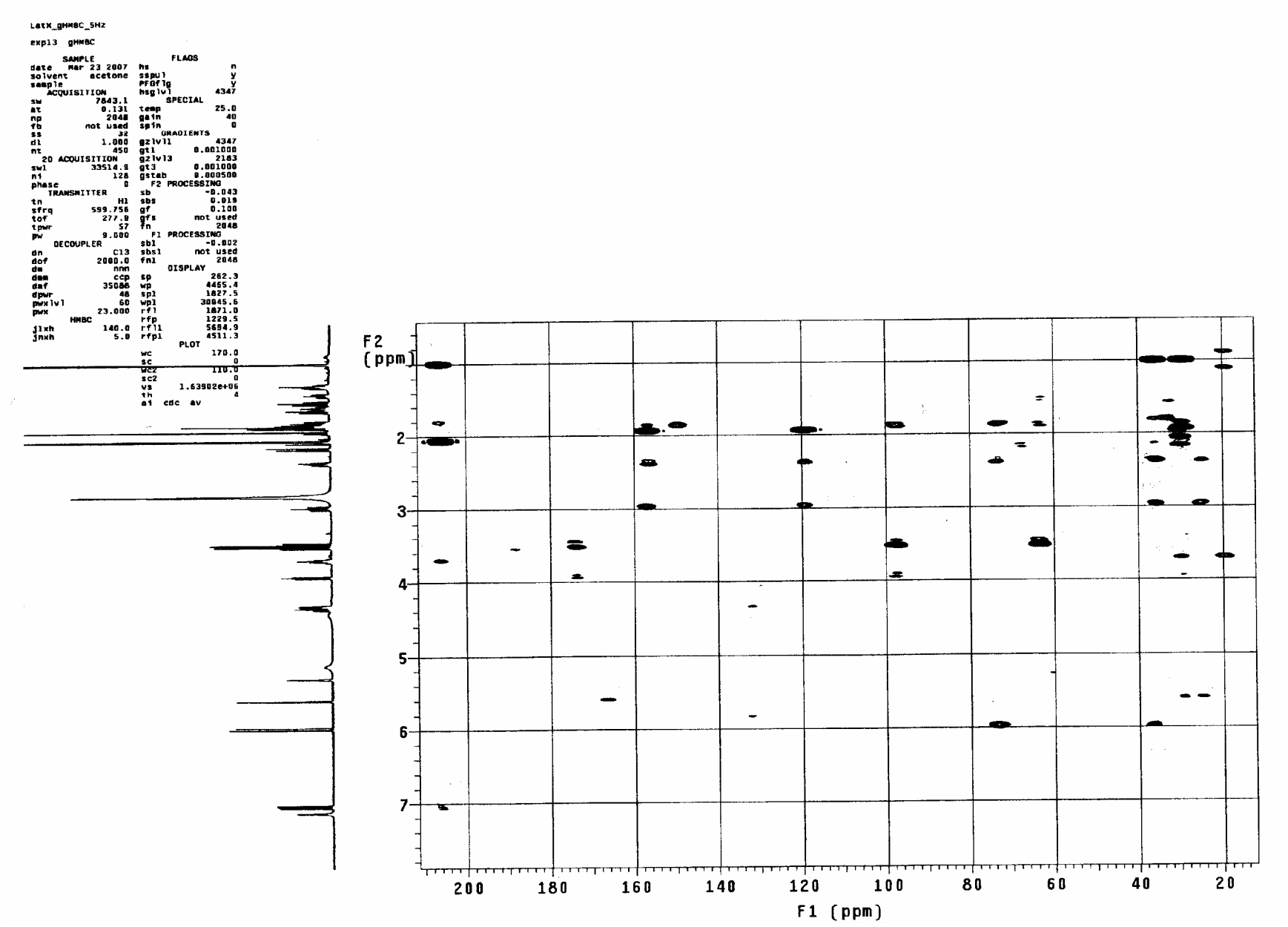


Figure S26. ^{1}H NMR spectrum of **12** in $CDCl_3$ (600 MHz).

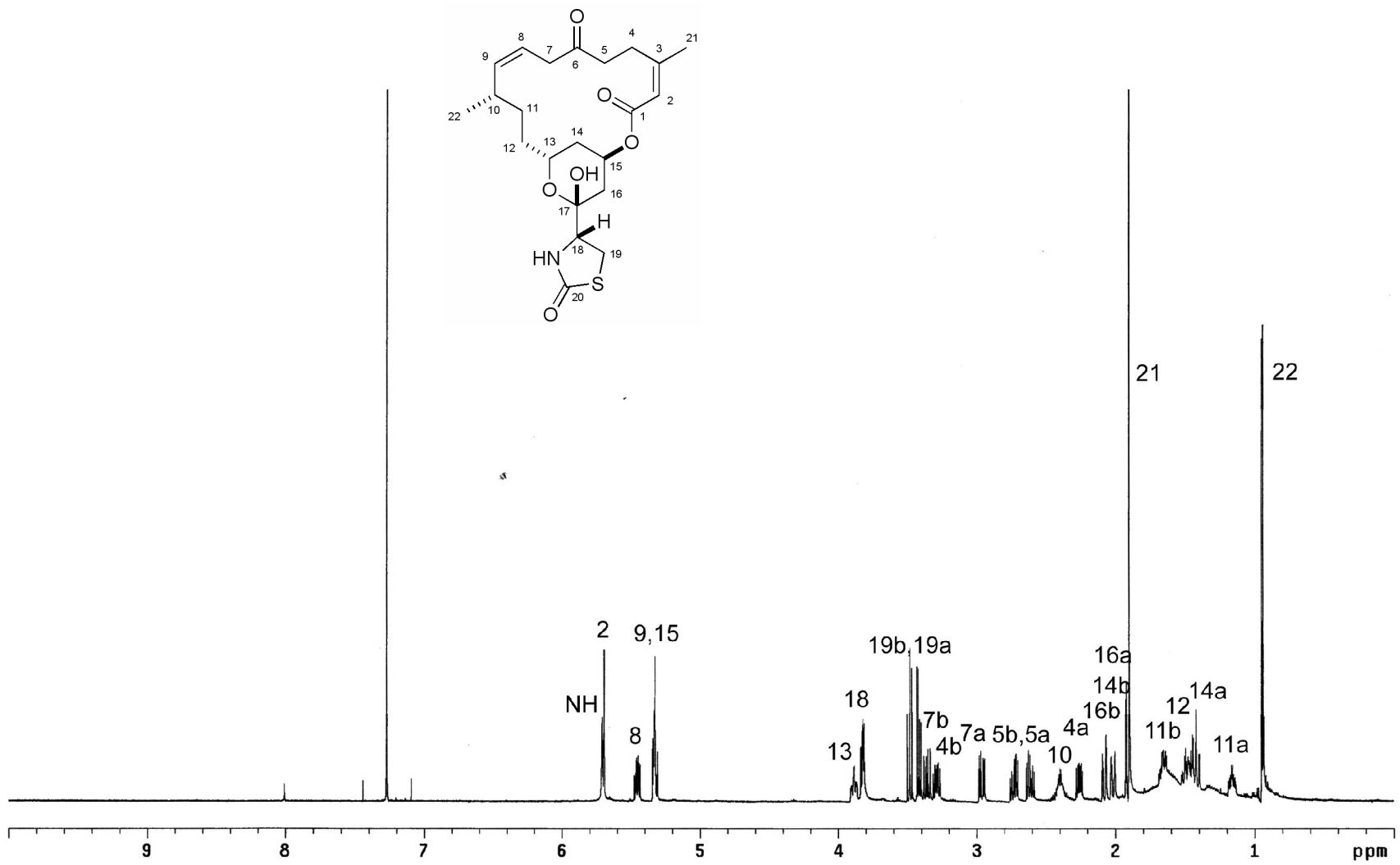


Figure S27. ^{13}C NMR spectrum of **12** in $CDCl_3$ (125 MHz).

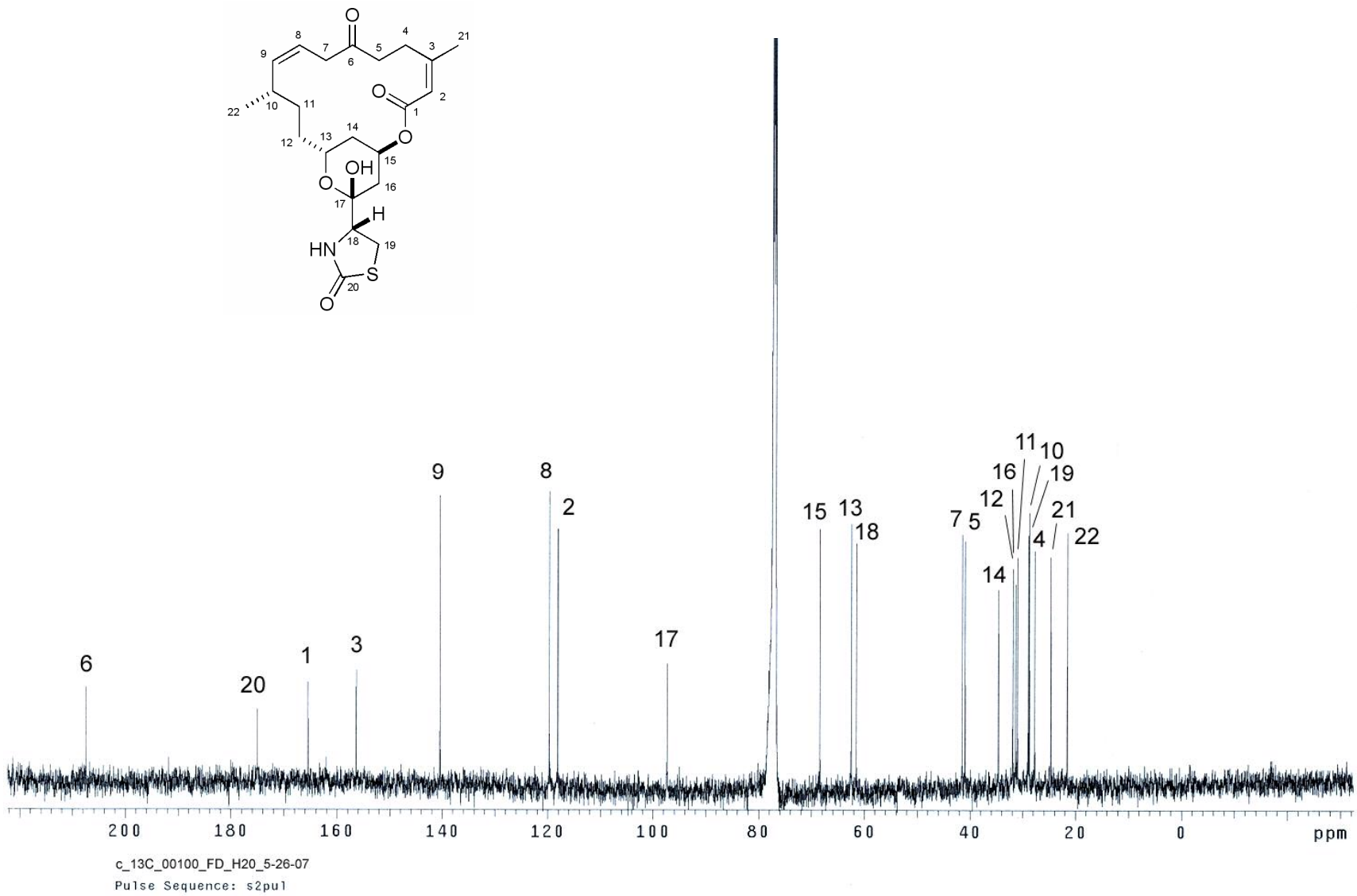
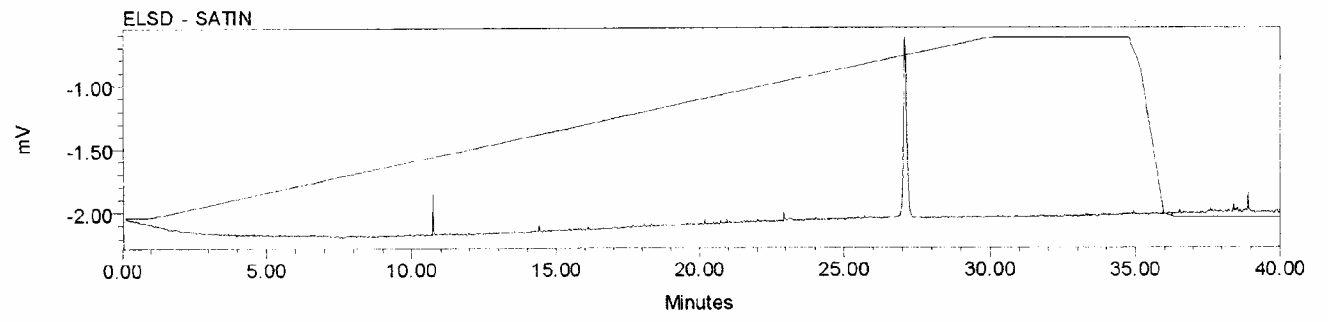


Figure S28. ELSD trace of LCMS chromatogram for **1**.

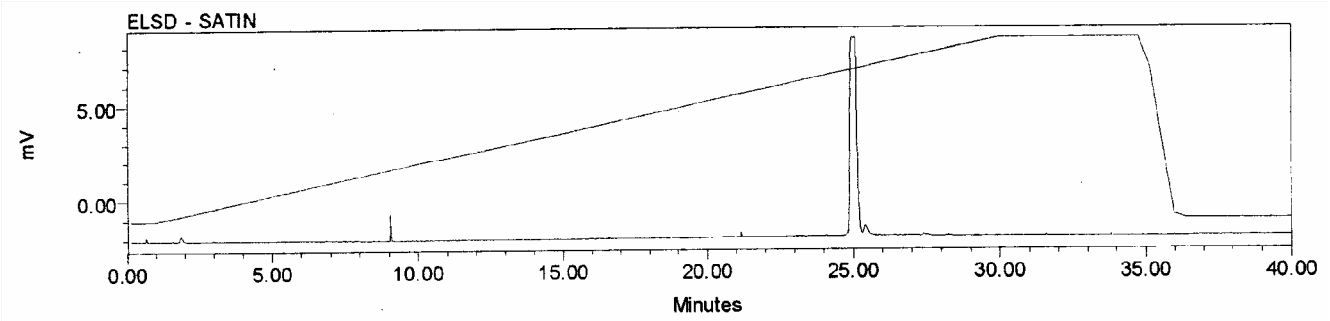
LC condition
Gradient: 1/9 to 1/0 in CH_3CN/H_2O for 30 min
Column: Phenomenex Synergi hydro C_{18} (4μ), 150x4.6 mm



Observed MSs
m/z 444 $[M+Na]^+$
m/z 404 $[M-H_2O+H]^+$
m/z 386 $[M-2H_2O+H]^+$

Figure S29. ELSD trace of LCMS chromatogram for **2**.

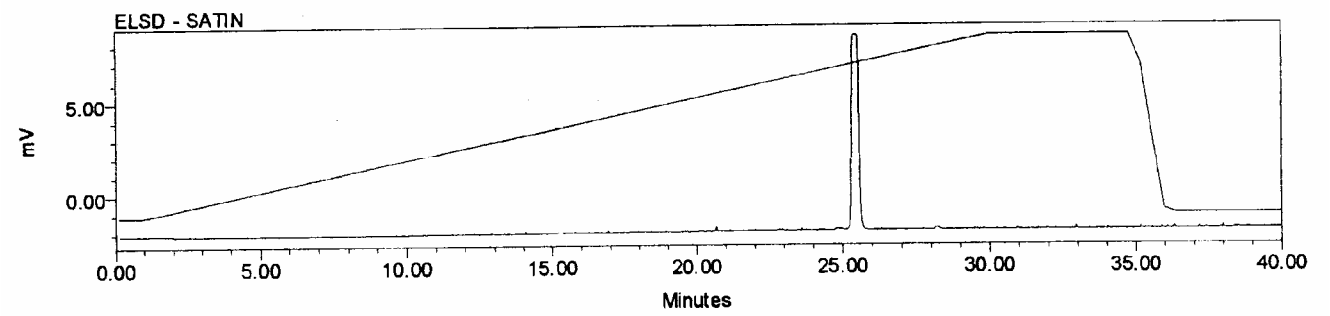
LC condition
Gradient: 1/9 to 1/0 in CH_3CN/H_2O for 30 min
Column: Phenomenex Synergi hydro C_{18} (4μ), 150x4.6 mm



Observed MSs
m/z 418 $[M+Na]^+$
m/z 378 $[M-H_2O+H]^+$
m/z 360 $[M-2H_2O+H]^+$

Figure S30. ELSD trace of LCMS chromatogram for **3**.

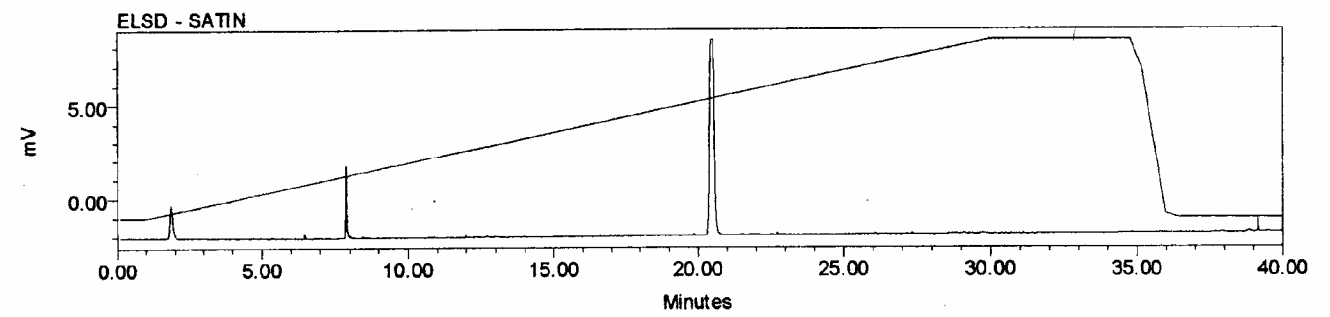
LC condition
Gradient: 1/9 to 1/0 in CH_3CN/H_2O for 30 min
Column: Phenomenex Synergi hydro C_{18} (4μ), 150x4.6 mm



Observed MSs
m/z 418 $[M+Na]^+$
m/z 378 $[M-H_2O+H]^+$
m/z 360 $[M-2H_2O+H]^+$

Figure S31. ELSD trace of LCMS chromatogram for **4**.

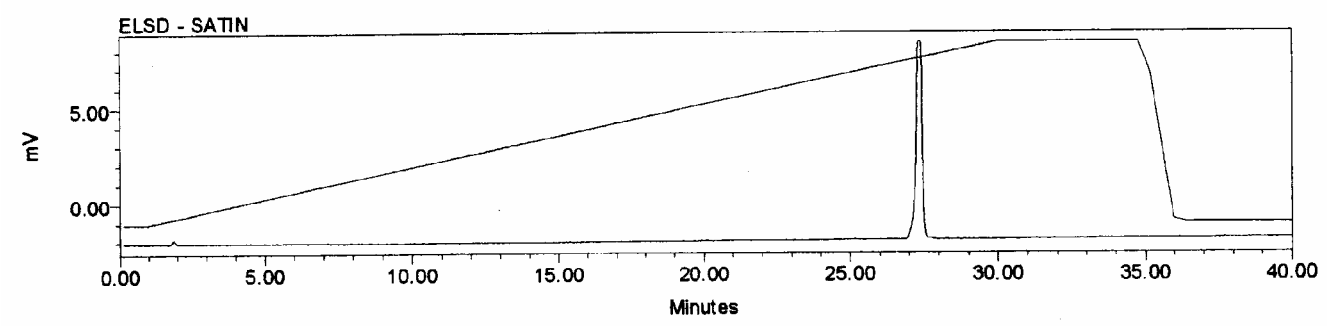
LC condition
Gradient: 1/9 to 1/0 in CH_3CN/H_2O for 30 min
Column: Phenomenex Synergi hydro C_{18} (4μ), 150x4.6 mm



Observed MSs
m/z 420 $[M+Na]^+$
m/z 380 $[M-H_2O+H]^+$
m/z 362 $[M-H_2O+H]^+$

Figure S32. ELSD trace of LCMS chromatogram for **5**.

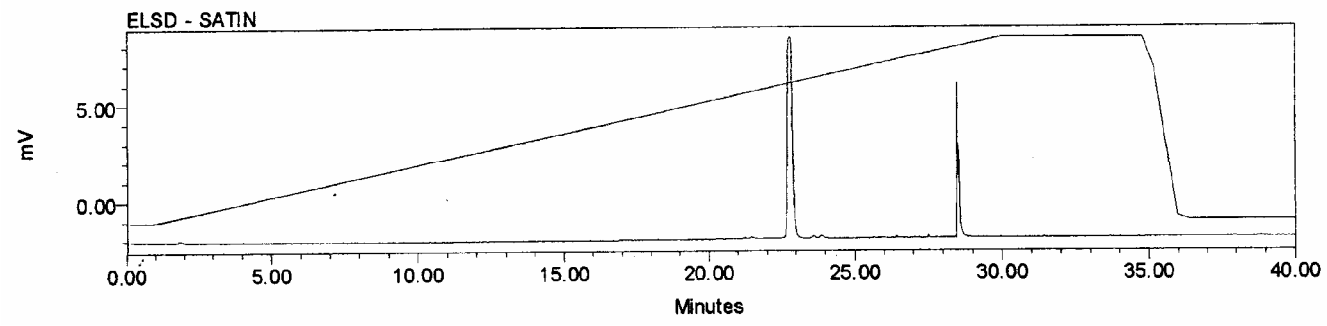
LC condition
Gradient: 1/9 to 1/0 in CH_3CN/H_2O for 30 min
Column: Phenomenex Synergi hydro C_{18} (4μ), 150x4.6 mm



Observed MSs
m/z 434 $[M+Na]^+$
m/z 394 $[M-H_2O+H]^+$
m/z 378 $[M-H_2O+H]^+$

Figure S33. ELSD trace of LCMS chromatogram for **6**.

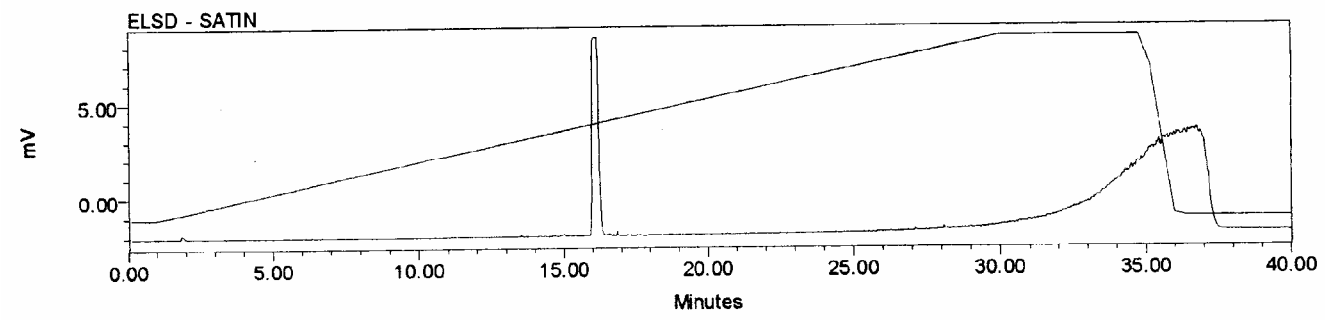
LC condition
Gradient: 1/9 to 1/0 in CH_3CN/H_2O for 30 min
Column: Phenomenex Synergi hydro C_{18} (4μ), 150x4.6 mm



Observed MSs
m/z 315 $[M+Na]^+$
m/z 293 $[M+H]^+$
m/z 275 $[M+Na]^+$

Figure S34. ELSD trace of LCMS chromatogram for **7**.

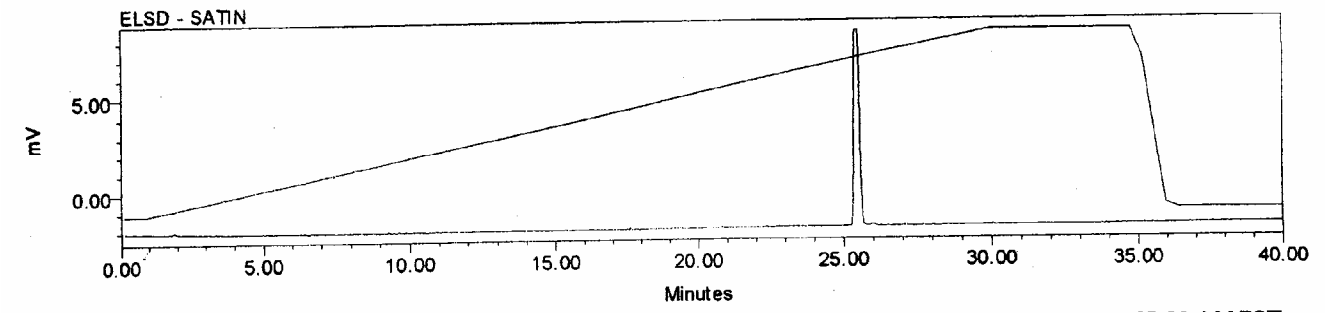
LC condition
Gradient: 1/9 to 1/0 in CH_3CN/H_2O for 30 min
Column: Phenomenex Synergi hydro C_{18} (4μ), 150x4.6 mm



Observed MSs
m/z 478 $[M+Na]^+$
m/z 438 $[M-H_2O+H]^+$
m/z 420 $[M-2H_2O+H]^+$

Figure S35. ELSD trace of LCMS chromatogram for **7a**.

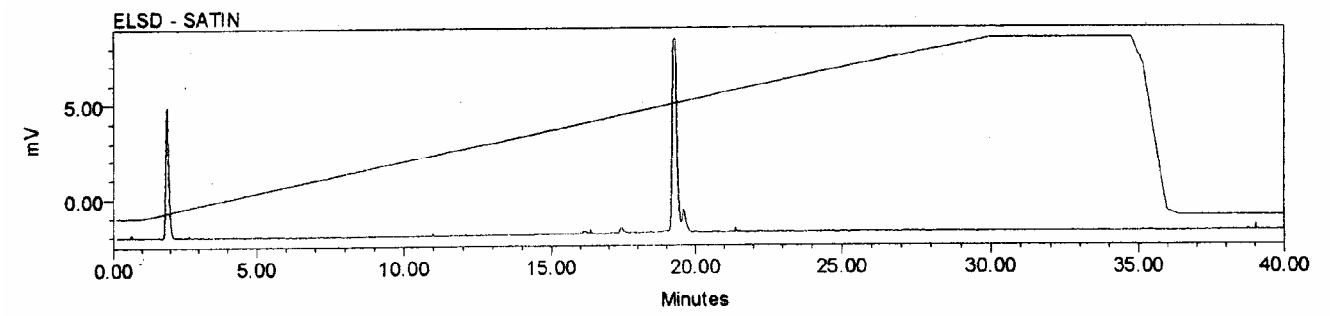
LC condition
Gradient: 1/9 to 1/0 in CH_3CN/H_2O for 30 min
Column: Phenomenex Synergi hydro C_{18} (4μ), 150x4.6 mm



Observed MSs
m/z 518 $[M+Na]^+$
m/z 478 $[M-H_2O+H]^+$
m/z 460 $[M-2H_2O+H]^+$

Figure S36. ELSD trace of LCMS chromatogram for **8**.

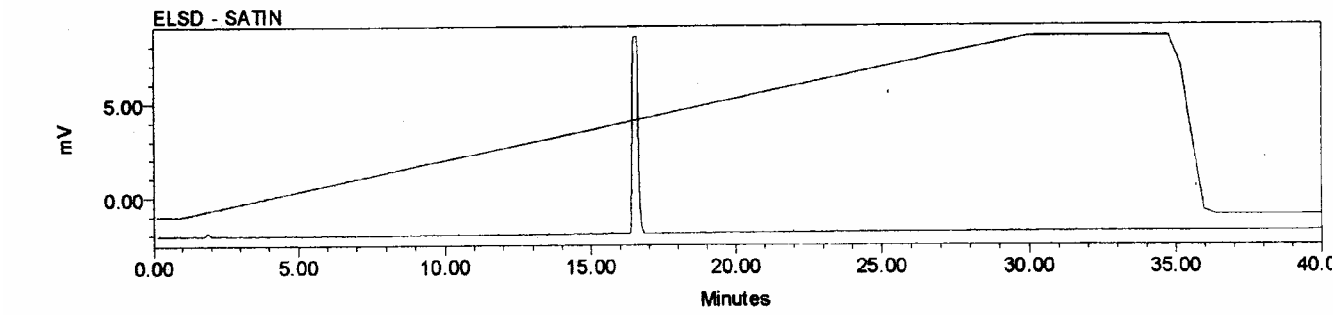
LC condition
Gradient: 1/9 to 1/0 in CH_3CN/H_2O for 30 min
Column: Phenomenex Synergi hydro C_{18} (4μ), 150x4.6 mm



Observed MSs
m/z 492 $[M+Na]^+$
m/z 452 $[M-H_2O+H]^+$
m/z 434 $[M-2H_2O+H]^+$

Figure S37. ELSD trace of LCMS chromatogram for **9**.

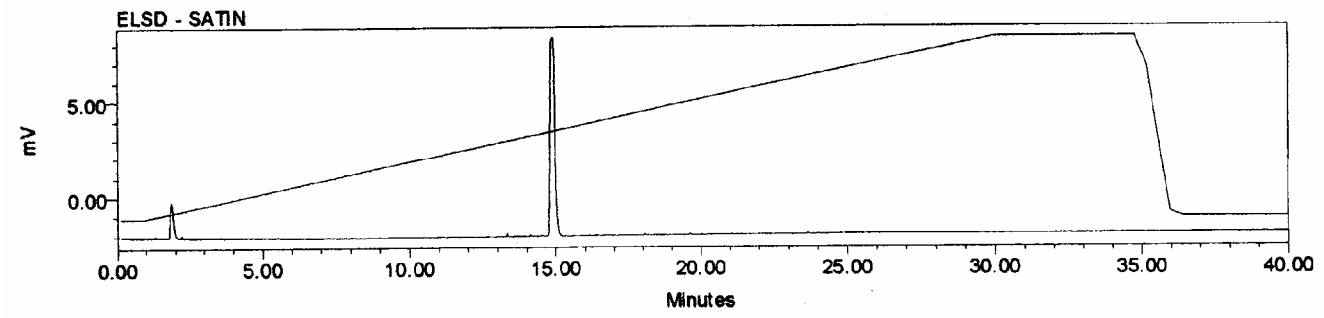
LC condition
Gradient: 1/9 to 1/0 in CH_3CN/H_2O for 30 min
Column: Phenomenex Synergi hydro C_{18} (4μ), 150x4.6 mm



Observed MSs
m/z 478 $[M+Na]^+$
m/z 438 $[M-H_2O+H]^+$
m/z 420 $[M-2H_2O+H]^+$

Figure S38. ELSD trace of LCMS chromatogram for **10**.

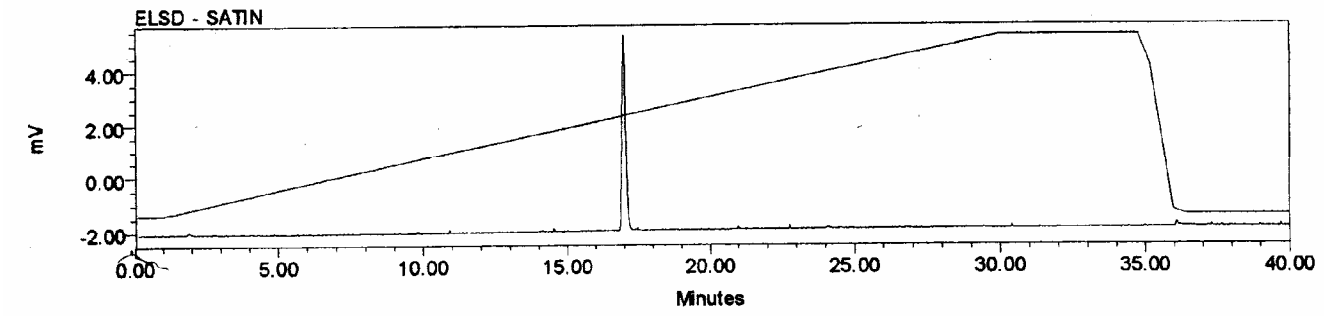
LC condition
Gradient: 1/9 to 1/0 in CH_3CN/H_2O for 30 min
Column: Phenomenex Synergi hydro C_{18} (4μ), 150x4.6 mm



Observed MSs
m/z 478 $[M+Na]^+$
m/z 438 $[M-H_2O+H]^+$
m/z 420 $[M-2H_2O+H]^+$

Figure S39. ELSD trace of LCMS chromatogram for **11**.

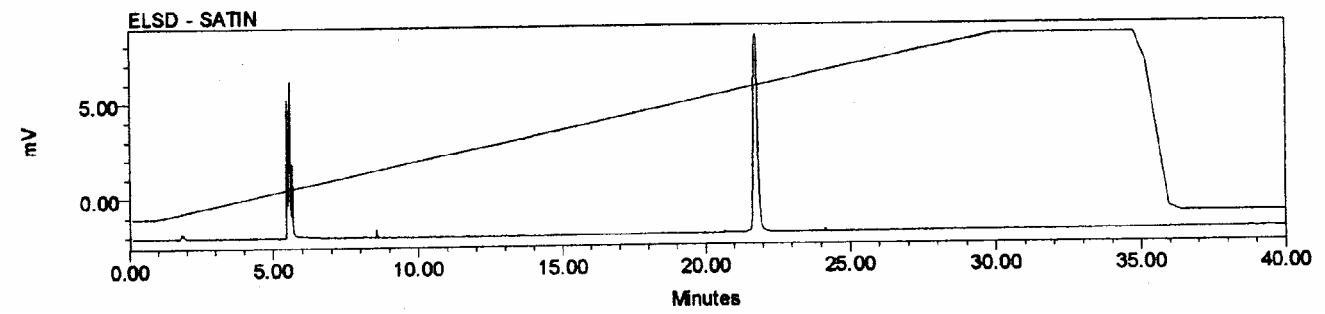
LC condition
Gradient: 1/9 to 1/0 in CH_3CN/H_2O for 30 min
Column: Phenomenex Synergi hydro C_{18} (4μ), 150x4.6 mm



Observed MSs
m/z 476 $[M+Na]^+$
m/z 436 $[M-H_2O+H]^+$
m/z 418 $[M-2H_2O+H]^+$

Figure S40. ELSD trace of LCMS chromatogram for **12**.

LC condition
Gradient: 1/9 to 1/0 in CH_3CN/H_2O for 30 min
Column: Phenomenex Synergi hydro C_{18} (4μ), 150x4.6 mm



Observed MSs
m/z 460 $[M+Na]^+$
m/z 420 $[M-H_2O+H]^+$
m/z 402 $[M-2H_2O+H]^+$