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Supplementary Information

Chemical constituents of the soft corals *Sinularia vanderlandi* and *Sinularia gravis* from the coast of Madagascar

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Content

Table S1. NMR spectroscopic data of vanderlandin (**1**) recorded at 600 MHz (^{1}H) and 150 MHz (^{13}C) in $CDCl_3$

Position	δ_H (*J* in Hz)	δ_C [a]	COSY [b]	NOESY [b]	HMBC [b,c]
1		89.10, C			2α, 2β, 3α, 3β, 5, 9α, 9β, 14
2α	1.85 ddd (13.7, 8.8, 3.7)	34.57, CH_2	2β, 3α, 3β	2β, 3α	3α, 3β, 15
2β	1.97 ddd (13.7, 8.9, 7.6)		2α, 3α, 3β	2α	
3α	1.78 dt (13.4, 8.0)	34.46, CH_2	2α, 2β, 3β	2α, 3β, 15	2α, 2β, 15
3β	2.07 ddd (13.4, 7.5, 3.7)		2α, 2β, 3α	3α	
4		90.27, C			2α, 2β, 3β, 5, 15
5	6.12 s	124.33, CH		3α, 11, 12, 13, 15	8α, 11
6		148.05, C			2α, 2β, 3α, 3β, 5, 15
7		83.46, C			5, 8α, 8β, 9α, 9β, 11, 12, 13
8α	1.89 ddd (14.7, 11.9, 4.9)	30.61, CH_2	8β, 9α, 9β	8β, 9α, 9β, 12, 13	5, 9α, 9β, 10, 11
8β	1.70 dddd (14.5, 5.3, 3.8, 0.6)		8α, 9α, 9β	8α, 9α, 9β, 12, 13	
9α	1.50 ddd (14.1, 11.9, 5.7)	27.91, CH_2	8α, 8β, 9β	8α, 8β, 9β, 10	8α, 8β, 14
9β	1.41 dddd (14.1, 5.0, 3.7, 2.9)		8α, 8β, 9α	8α, 8β, 9α, 10, 14	
10	1.90–1.96 m	38.50, CH	14	9α, 9β, 14	2β, 5, 8α, 8β, 9α, 9β, 14
11	1.88 sept (6.9)	35.52, CH	12, 13	5, 12, 13	5, 8β, 12, 13
12, 13	0.97 d (7.2), 0.99 d (6.8)	17.03, CH_3	11	5, 8α, 8β, 11	11, 12, 13
14	1.06 d (7.2)	13.40, CH_3	10	9β, 10	9α, 9β, 10
15	1.54 s	19.84, CH_3		3α, 5	3α
OH	7.38 s				

[a] Number of attached protons determined by the DEPT experiment. [b] Only selected signals are shown. [c] HMBC correlations are from carbon atoms (position) to protons.

Table S2. NMR spectroscopic data of gravilin (**3**) recorded at 600 MHz (^{1}H) and 150 MHz (^{13}C) in $CDCl_3$

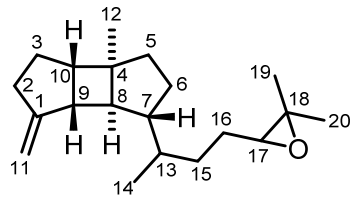
Position	δ_H (*J* in Hz)	δ_C [a]	COSY [b]	NOESY [b]	HMBC [b,c]
1		157.33, C			
2α	2.48–2.56 m	33.75, CH_2	2β, 3α, 3β, 11a, 11b	2β, 3α, 3β, 8, 12	3α, 3β, 9, 10, 11a, 11b
2β	2.28 dd (15.1, 7.9)		2α, 3β, 11a, 11b	2α, 3α, 3β, 11a	
3α	1.80 dd (13.3, 7.9)	27.22, CH_2	2α, 3β, 11b	2α, 2β, 3β, 10, 12	2α, 2β, 9, 10
3β	1.58 m [d]		2α, 2β, 3α, 10	2α, 2β, 3α	
4		43.14, C			3α, 3β, 5, 6β, 8, 10, 12
5	1.52 m [d]	42.19, CH_2		6α, 9, 10, 12	6α, 6β, 7, 8, 10, 12
6α	1.51 m [d]	29.93, CH_2	6β	5, 6β, 12, 13, 14	5, 7, 8, 15b
6β	1.86–1.92 m		6α, 7	6α, 3β/7, 9, 10, 14	
7	1.62 m [d]	55.22, CH	6β, 8, 13	6β, 9, 13, 14	6α, 6β, 9, 13, 14, 15a, 15b
8	1.54 m [d]	55.29, CH	7, 9	2α, 10, 12, 13	9, 10, 12
9	2.42 dd (6.9, 3.9)	48.04, CH	8, 10, 11a, 11b	5, 6β, 7, 11b	2α, 3α, 3β, 10, 11a, 11b
10	2.32 t (7.5)	45.77, CH	3β, 9	3α, 5/8, 6β	2β, 3α, 3β, 5, 8, 9, 12
11a	4.70 s	103.76, CH_2	2α, 2β, 9	2β	
11b	4.73 s		2α, 2β, 3α, 9	9	
12	0.97 s	21.55, CH_3		2α, 3α, 5/6α/8	3β, 5, 6α, 6β
13	1.10–1.15 m	36.38, CH	7, 14	6α, 7, 8, 14, 15a	6α, 6β, 7, 14, 15a, 15b, 16a, 16b
14	0.85 d (6.8)	17.87, CH_3	13	6α, 6β, 7, 13, 15a, 15b, 16a, 16b	13, 15a, 15b
15a	1.49 m [d]	32.10, CH_2	15b, 16a, 16b	13, 14, 15b, 16a, 16b, 17	14, 17, 16a, 16b
15b	1.18–1.22 m		15a, 16a	14, 15a, 16a, 16b, 17	
16a	1.63 m [d]	26.43, CH_2	15a, 15b, 16b, 17	14, 15a, 15b, 16b, 17	15a, 15b, 17
16b	1.31–1.37 m		15a, 16a, 17	14, 15a, 15b, 16a, 17	
17	2.66 t (6.4)	64.70, CH	16a, 16b	15a, 15b, 16a, 16b, 19	15a, 15b, 16a, 16b, 19, 20
18		58.31, C			16a, 16b, 17, 19, 20
19	1.29 s	24.91, CH_3		17	17, 20
20	1.24 s	18.69, CH_3			19

[a] Number of attached protons determined by the DEPT experiment. [b] Only selected signals are shown. [c] HMBC correlations are from carbon atoms (position) to protons.
[d] Chemical shift derived from the HSQC spectrum.

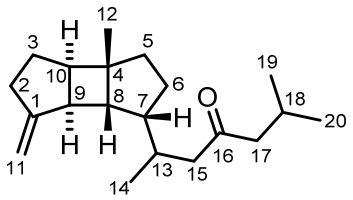
Table S3. Comparison of NMR spectroscopic data of gravilin (**3**), lobophytumin F,[1] and leptoclalin A[2]

Position	**gravilin (3)** δ_H (*J* in Hz) (600 MHz, $CDCl_3$)	**lobophytumin F** [1] δ_H (*J* in Hz) (300 MHz, $CDCl_3$)	**leptoclalin A** [2] δ_H (*J* in Hz) (500 MHz, $CDCl_3$)	**gravilin (3)** δ_C (150 MHz, $CDCl_3$)	**lobophytumin F** [1] δ_C (100 MHz, $CDCl_3$)	**leptoclalin A** [2] δ_C (125 MHz, $CDCl_3$)
1				157.33	157.3	157.5
2α	2.48–2.56 m	2.27 m	2.54 m; 2.28 m	33.75	33.7	33.7
2β	2.28 dd (15.1, 7.9)	2.53 m				
3α	1.80 dd (13.3, 7.9)	1.55 m	1.81 m; 1.59 m	27.22	27.2	27.2
3β	1.58 m [a]	1.92 m				
4				43.14	43.2	43.1
5	1.52 m [a]	1.57 m	1.50 m	42.19	42.0	42.0
6α	1.51 m [a]	1.82 m	1.89 m; 1.55 m	29.93	29.8	29.7
6β	1.86–1.92 m	1.60 m				
7	1.62 m [a]	1.63 m	1.62 m	55.22	55.2	54.5
8	1.54 m [a]	1.46 m	1.62 m	55.29	55.2	55.0
9	2.42 dd (6.9, 3.9)	2.44 m	2.35 m	48.04	48.0	47.8
10	2.32 t (7.5)	2.32 m	2.32 m	45.77	45.7	45.7
11a	4.70 s	4.69 br s	4.74 s; 4.70 s	103.76	103.8	103.7
11b	4.73 s	4.73 br s				
12	0.97 s	0.99 s	1.00 s	21.55	21.4	21.6
13	1.10–1.15 m	1.74 m	1.20 m	36.38	32.3	36.3
14	0.85 d (6.8)	0.84 d (6.4)	0.83 d (6.5)	17.87	18.7	17.8
15a	1.49 m [a]	2.43 dd (15.3, 2.7)	2.15 ddd (13.5, 3.5, 3.5); 1.74 m	32.10	49.8	38.2
15b	1.18–1.22 m	2.12 m				
16a	1.63 m [a]		5.58 m	26.43	211.1	125.8
16b	1.31–1.37 m					
17	2.66 t (6.4)	2.24 d (6.6)	5.58 m	64.70	52.4	139.2
18				58.31	24.5	70.7
19	1.29 s	0.89 d (6.5)	1.31 s	24.91	22.5	29.9
20	1.24 s	0.90 d (6.5)	1.31 s	18.69	22.6	29.8

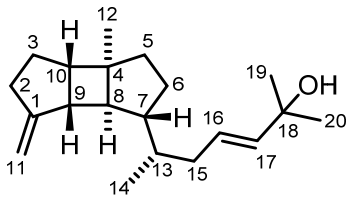
[a] Chemical shift derived from the HSQC spectrum.



gravilin (**3**)



lobophytumin F



leptoclalin A

Table S4. NMR spectroscopic data for 1-*O*-arachidonoyl-3-*O*-stearylglycerol (**4**) recorded at 600 MHz (^{1}H) and 150 MHz (^{13}C) in $CDCl_3$

Position	δ_H (*J* in Hz)	δ_C [a]	NOESY [b]	HMBC [b,c]
1a	4.16 dd (11.7, 4.1)	65.50, CH_2	2, 3a, 3b, OH	2, 3a, 3b, OH
1b	4.11 dd (11.7, 6.4)		2, 3a, 3b, OH	
2	3.96–4.01 m	68.87, CH	1a, 1b, 3a, 3b, 2'', OH	1a, 1b, 3a, 3b, OH
3a	3.48 dd (9.8, 4.5)	71.37, CH_2	1a, 1b, 2, 3b, OH	1a, 1b, 2, 1'', OH
3b	3.41 dd (9.8, 6.4)		1a,1b, 2, 3a, OH	
1′		173.68, C		1a, 1b, 2′, 3′
2′	2.35 t (7.5)	33.53, CH_2	3′, 4′, 5′	3′, 4′
3′	1.71 quint (7.5)	24.75, CH_2	2′, 4′, 5′	2′, 4′
4′	2.11 q (7.3)	26.53, CH_2	2′, 3′, 7′	2′, 3′, 5′
5′	5.29–5.42 m	128.59, CH	2′, 3′	3′, 4′, 7′
6′, 8′, 9′, 11′, 12′	5.29–5.42 m	127.86, 128.13, 128.25, 128.86, 128.93, CH		
7′, 13′	2.80 q (5.6)	25.61–25.63, CH_2	7′/4′, 13′/16′	
10′	2.83 t (6.0)			
14′	5.29–5.42 m	127.53, CH		13′,16′
15′	5.29–5.42 m	130.50, CH		13′, 16′, 17′
16′	2.04 q (7.2)	27.22, CH_2	13′, 17′	14′, 17′
17′	1.32–1.37 m	29.32, CH_2	16′	16′
18′	1.26–1.32 m	31.52, CH_2		16′, 17′, 19′, 20′
19′	1.26–1.32 m	22.57, CH_2		17′, 18′, 20′
20′	0.88 t (6.8)	14.07, CH_3		
1''	3.42–3.46 m	71.78, CH_2	2''	3a, 3b, 2'', 3''
2''	1.53–1.58 m	29.58–29.66, CH_2	2, 1''	1''
3''	1.26–1.32 m	26.08, CH_2		1'', 2'', 4''
4''	1.26–1.32 m	29.47, CH_2		2''
5''–15''	1.24 br s	29.58–29.66, CH_2		
16''	1.24 br s	31.92, CH_2		18''
17''	1.26–1.32 m	22.69, CH_2		18''
18''	0.87 t (7.2)	14.11, CH_3		
OH	2.45 d (4.5)		1a, 1b, 2, 3a, 3b	

[a] Number of attached protons determined by the DEPT experiment. [b] Only selected signals are shown. [c] HMBC correlations are from carbon atoms (position) to protons.

Table S5. NMR data of compound **5** recorded at 600 MHz (^{1}H) and 150 MHz (^{13}C) in $CDCl_3$

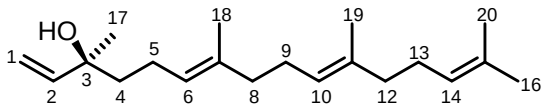
Position	δ_H (*J* in Hz)	δ_C [a]	NOESY [b]	HMBC [b,c]
1	1.74 s	25.72, CH_3	3	3, 17
2		135.39 or 135.23, C		1, 4, 17
3	5.30 br t (7.2)	116.09, CH	1, 4	1, 4, 17
4	3.12 d (6.8)	41.00, CH_2	3, 6, 8, 17, 18	3
5		213.13, C		1, 4, 6, 7b, 17, 18
6	2.48–2.58 m	45.64, CH	4, 7b, 8, 18	7a, 7b, 8, 18
7a	1.57–1.61 m	32.52, CH_2	7b, 9, 18	6, 8, 9, 18
7b	1.27–1.30 m		6, 7a, 9, 18	
8	1.30–1.34 m	25.45, CH_2	4, 6, 9, 18	6, 7b, 9
9	1.93 t (7.1)	39.55, CH_2	7a, 7b, 8	7a, 7b, 8, 11
10		135.23 or 135.39, C		8, 9, 12, 19
11	5.07–5.14 m	124.45, CH	12, 13	9, 12, 13
12	2.02–2.07 m	22.65, CH_2	11, 19, 20	11
13	1.57–1.61 m	42.05, CH_2	11, 20	11, 12, 15, 20, 21
14		73.45, C		12, 13, 15, 16, 20, 21, 22
15, 21	5.90 dd (17.3, 10.9)	145.00, CH	20	13, 16, 20, 22
16a, 22a	5.20 d (17.3)	111.70, CH_2	20	20
16b, 22b	5.05 d (10.9)			
17	1.61 s	18.07, CH_3	4	1, 3
18	1.05 d (6.8)	16.44, CH_3	4, 6, 7a, 7b, 8	6, 7a, 7b
19	1.56 s	15.84, CH_3	12	9, 11, 12
20	1.27 s	27.88, CH_3	12, 13, 15, 16a, 21, 22a	15, 21

[a] Number of attached protons determined by the DEPT experiment. [b] Only selected signals are shown. [c] HMBC correlations are from carbon atoms (position) to protons.

Table S6. ^{13}C NMR spectroscopic data of (+)-(3*S*,6*E*,10*E*)-geranyllinalool (**6**)

Position	**from *S. gravis*** δ_C [a]	**(±)-(6*E*,10*E*)-geranyllinalool** (from Sigma Aldrich) [c], ref. [3] δ_C [b]
1	111.67	111.68
2	145.05	145.06
3	73.49	73.49
4	42.06	42.07
5	22.71	22.72
6	124.19	124.21
7	135.61	135.58
8	39.69	39.72
9	26.55	26.56
10	124.09	124.11
11	135.05	135.04
12	39.71	39.70
13	26.75	26.75
14	124.38	124.39
15	131.27	131.25
16	25.69	25.71
17	27.90	27.88
18	16.03	16.04
19	16.00	16.01
20	17.69	17.69

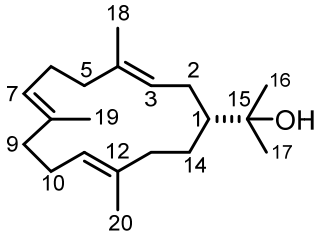
[a] Spectrum recorded at 150 MHz in $CDCl_3$. [b] Spectrum recorded at 50 MHz in $CDCl_3$. [c] (±)-(6*E*,10*E*)-geranyllinalool after separation from other *E*,*Z*-isomers by chromatography on silica gel.



6

Table S7. ^{13}C NMR spectroscopic data of (–)-(*R*)-nephthenol (**7**)

Position	from *Sinularia gravis* δ_C (150 MHz, $CDCl_3$)	from *Litophyton arboreum*[4] δ_C (125 MHz, $CDCl_3$)
1	48.45	48.5
2	28.44	28.5
3	125.94	125.9
4	133.37	134.4
5	38.82	38.8
6	24.65	24.7
7	125.76	125.8
8	133.06	133.0
9	39.40	39.4
10	24.00	24.0
11	124.98	125.0
12	134.04	134.0
13	37.70	37.7
14	28.27	28.3
15	73.97	73.9
16	27.65	27.7
17	27.50	27.5
18	15.56	15.6
19	15.30	15.3
20	15.56	15.6



7

Table S8. ^{1}H and ^{13}C NMR spectroscopic data of 11,12-epoxysarcophytol A (**8**)

Position	from *Sinularia gravis* (600 MHz, $CDCl_3$) δ_H (*J* in Hz)	from *Sinularia gibberosa* [5] (500 MHz, $CDCl_3$) δ_H (*J* in Hz)	from *Sinularia gravis* δ_C (150 MHz, $CDCl_3$)	from *Sinularia gibberosa* [5] δ_C (75 MHz, $CDCl_3$)
1			148.45	148.5
2	5.98 d (10.9)	5.99 d (10.5)	118.32	118.4
3	5.75 br dd (10.5, 1.7)	5.76 d (10.5)	119.52	119.6
4			136.78	136.8
5a	2.22–2.28 m	2.18 m	38.33	38.4
5b	2.13–2.19 m			
6	2.22–2.28 m	2.22 m	25.96	25.0
7	5.10 br t (6.4)	5.11 br dd (5.5, 5.5)	126.90	127.0
8			133.64	133.7
9a	2.22–2.28 m	2.26 m	36.45	36.5
9b	2.04–2.09 m	2.09 m		
10a	1.82–1.89 m	1.86 dddd (13.5, 13.5, 7.5, 3.5)	24.12	24.2
10b	1.45–1.52 m	1.50 dddd (13.5, 13.5, 6.0, 3.5)		
11	3.18 t (6.4)	3.19 dd (7.0, 7.0)	58.60	58.7
12			59.98	60.0
13a	1.97 dd (15.4, 4.5)	1.98 dd (10.5, 5.0)	42.15	42.2
13b	2.10 dd (15.4, 7.5)	2.11 dd (10.5, 7.0)		
14	4.72 br t (6.0)	4.73 dd (7.0, 5.0)	65.76	65.8
15	2.66 sept (6.8)	2.67 sept (6.5)	27.63	27.7
16	1.06 d (6.8)	1.07 d (6.5)	24.22	24.3
17	1.08 d (6.8)	1.09 d (6.5)	23.79	23.9
18	1.73 d (0.8)	1.74 s	17.26	17.3
19	1.58 d (0.8)	1.59 s	15.02	15.1
20	1.29 s	1.30 s	19.44	19.5
OH	2.21 br s			

Table S9. Comparison of the ^{13}C NMR data, melting points, and optical rotation values of isodecaryiol (**9**) and decaryiol (**10**)

Position	^{13}C NMR		
	9	**10**	**10**
	from *S. gravis* δ_C (150 MHz, $CDCl_3$)	**from *S. decaryi*** [6] δ_C (22.6 MHz)	**from *Nephthea* sp.** [7] δ_C (150 MHz, $CDCl_3$)
1	39.97	40.0	39.9
2	28.93	29.0	28.8
3	70.40	70.4	70.3
4	76.79	77.0	76.8
5	38.06	38.2	37.9
6	23.76	23.8	23.6
7	127.70	127.9	127.7
8	132.59	133.0	132.1
9	39.30	36.5	39.2
10	25.27	25.3	25.1
11	128.08	128.6	128.0
12	133.02	132.6	132.6
13	36.42	39.4	36.3
14	25.19	25.3	25.2
15	75.26	75.2	75.1
16	29.61	22.3	29.5
17	22.25	29.7	22.2
18	24.22	24.3	24.2
19	14.82	15.2	14.8
20	15.20	14.8	15.0
mp [° C]	94.0–94.5	126–128.5	oil
$[\alpha]_D$ (T [° C])	+14.0 (20, *c* 0.1, MeOH)	+69 (24, *c* 1.3, $CHCl_3$)	+27.2 (20, *c* 0.01)

Table S10. Comparison of the ^{1}H NMR data of isodecaryiol (**9**) and decaryiol (**10**)

Position	^{1}H NMR		
	9	**10**	**10**
	from *Sinularia gravis* δ_H (600 MHz, $CDCl_3$)	**from *Sarcophyton decaryi*** [6] δ_H (270 MHz)	**from *Nephthea* sp.**[7] δ_H (600 MHz, $CDCl_3$)
1	1.58 tt (11.6, 1.9)	1.60 ddt (11.5, 3.0, 2.0)	
2α 2β	1.23–1.32 m 1.72 ddd (12.5, 5.4, 2.0)	1.28 dt (12.3, 11.5) 1.72 ddd (12.3, 5.7, 2.0)	
3	4.20 dt (11.7, 5.9)	4.20 dd (12.3, 5.7)	4.20 dd (11.7, 5.6)
4	–	–	–
5a 5b	1.81 ddd (14.5, 11.2, 3.3) 1.53 ddd (14.4, 6.0, 3.3)	1.80 ddd (14.4, 10.5, 3.0) 1.50 ddd (14.4, 10.0, 3.8)	
6a 6b	2.62 dddd (15.2, 11.4, 9.9, 3.6) 1.88 dddd (15.4, 7.6, 3.9, 1.9)	2.62 dddd (15.7, 10.0, 10.5, 3.8) 2.25 dddd (15.7, 10.0, 3.8, 3.0)	2.62 br 1.88 s
7	5.24 br d (9.4)	5.26 br dd (3.8, 10.0)	
8	–	–	–
9a 9b	2.22–2.29 m 2.16 ddd (14.0, 11.7, 3.8)	1.95 m	2.20 br 2.17 s
10a 10b	2.48 dtd (15.0, 11.4, 3.6) 1.99–2.03 m	2.49 ddt (15.7, 11.4, 3.8) 2.20 m	
11	4.88 br d (11.6)	4.89 br dd (11.4, 4.0)	
12	–	–	–
13a+13b	2.03 br dd (8.9, 3.7)	2.03 dd (8.0, 3.8)	
14a 14b	1.28–1.34 m 0.89 ddt (13.3, 11.6, 3.6)	1.30 ddt (12.3, 8.0, 3.0) 0.89 ddt (12.3, 11.5, 3.8)	
15	–	–	–
16	1.10 s		
17	1.12 s		
18	1.15 s		
19	1.56 s		
20	1.55 s		
OH	1.27 (br s)		

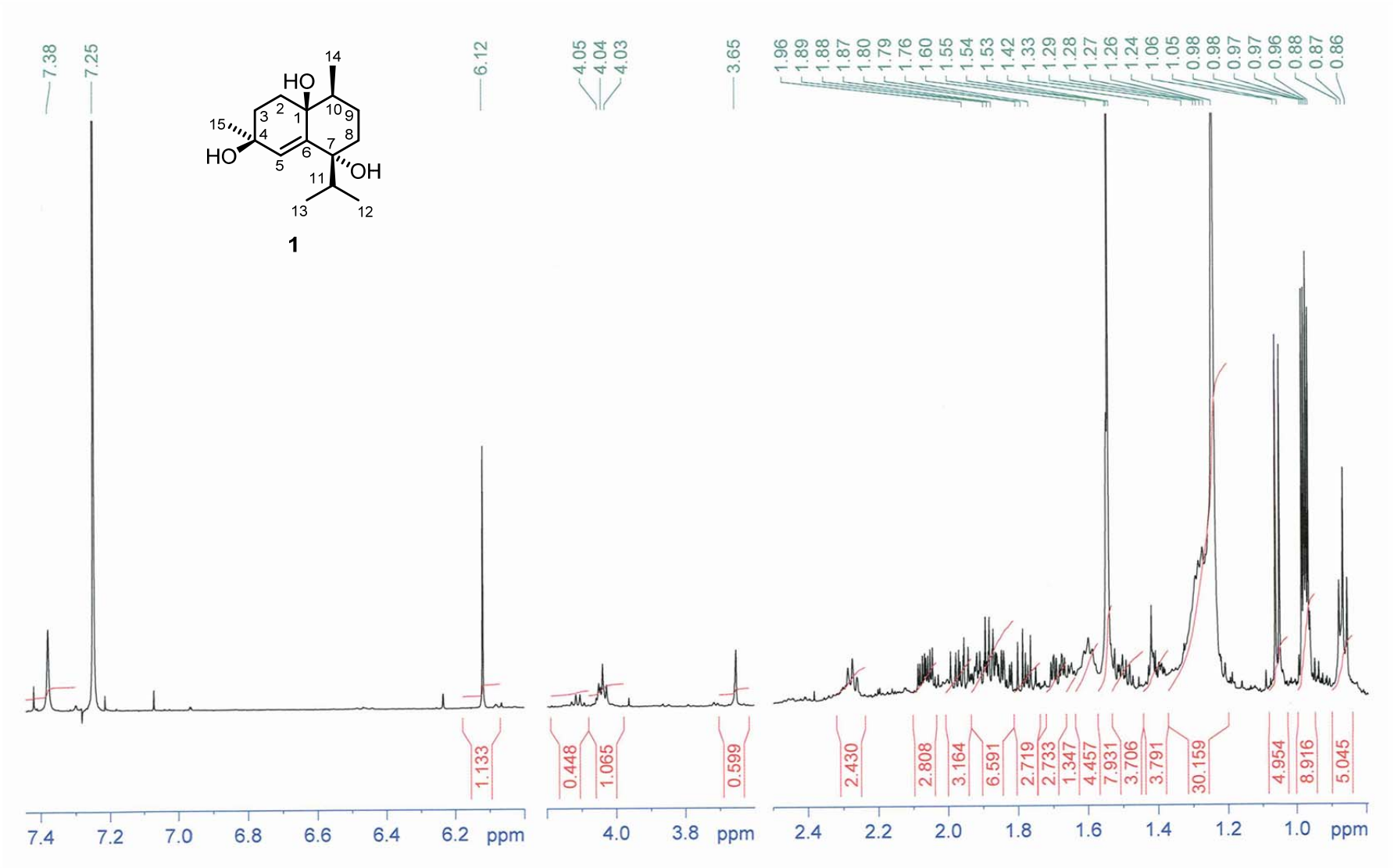


Fig. S1. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of vanderlandin (**1**).

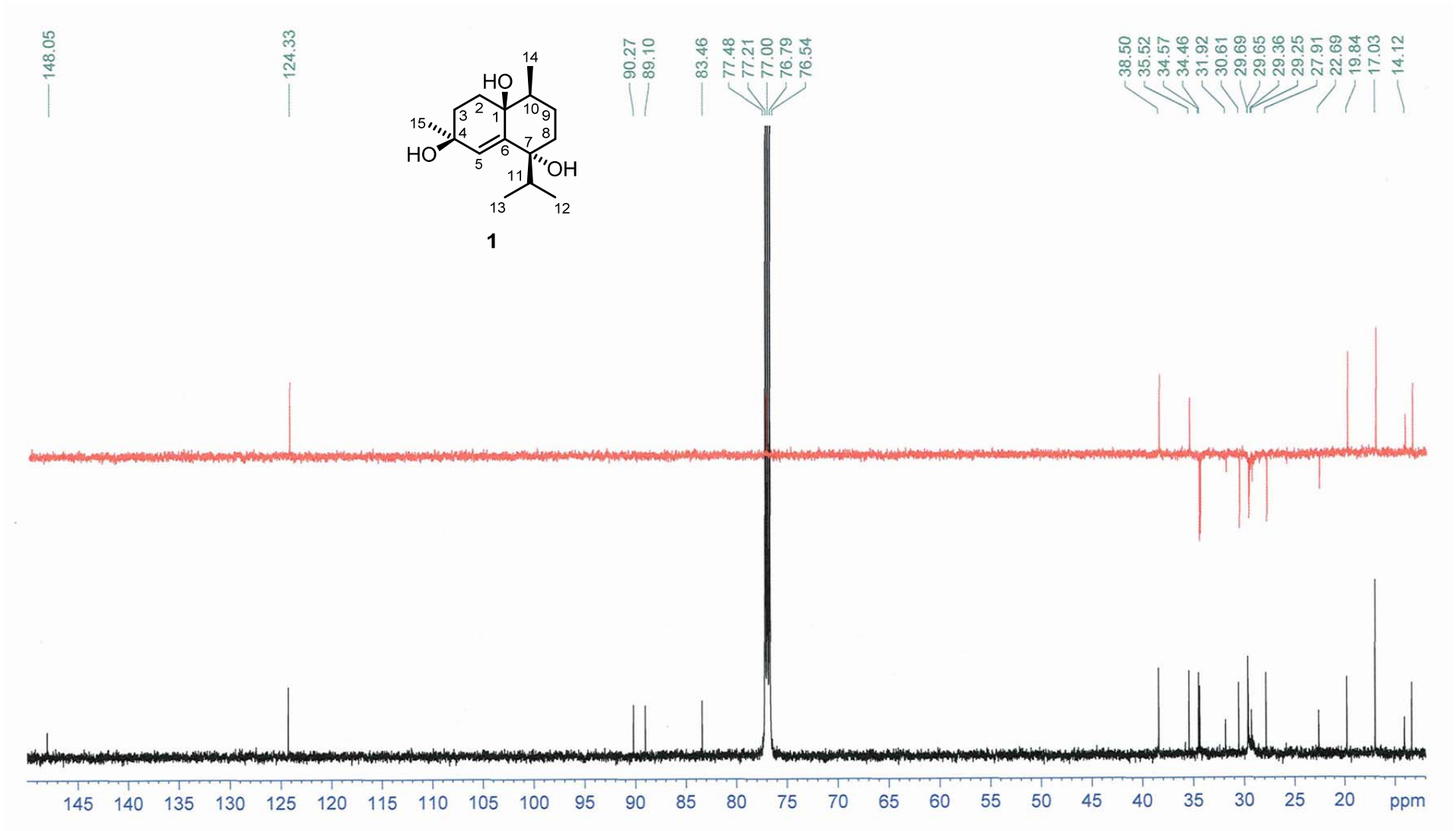


Fig. S2. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of vanderlandin (**1**).

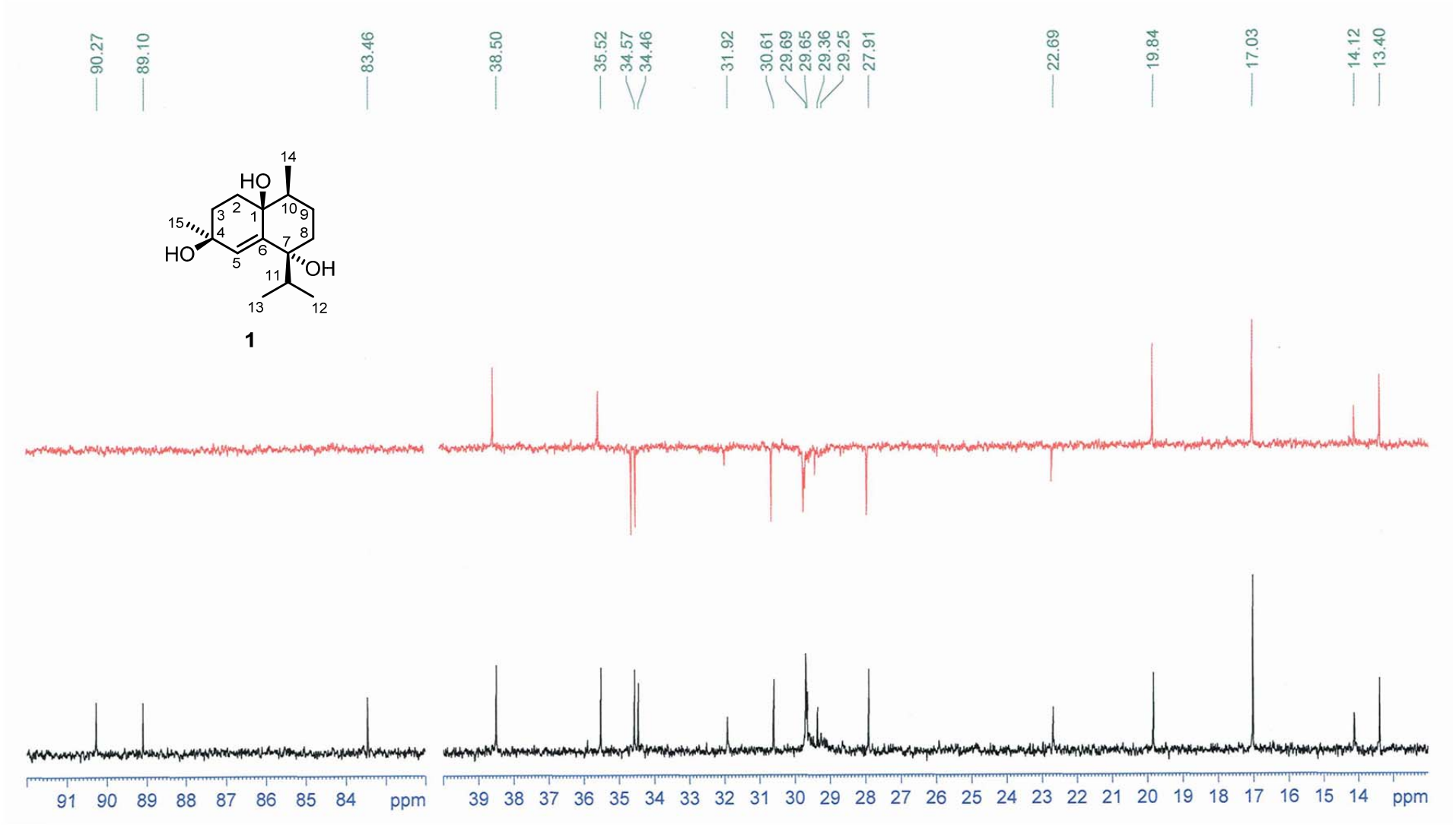
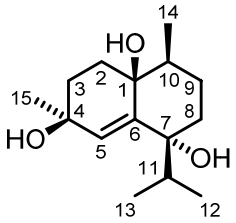


Fig. S3. Details of the ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of vanderlandin (**1**).



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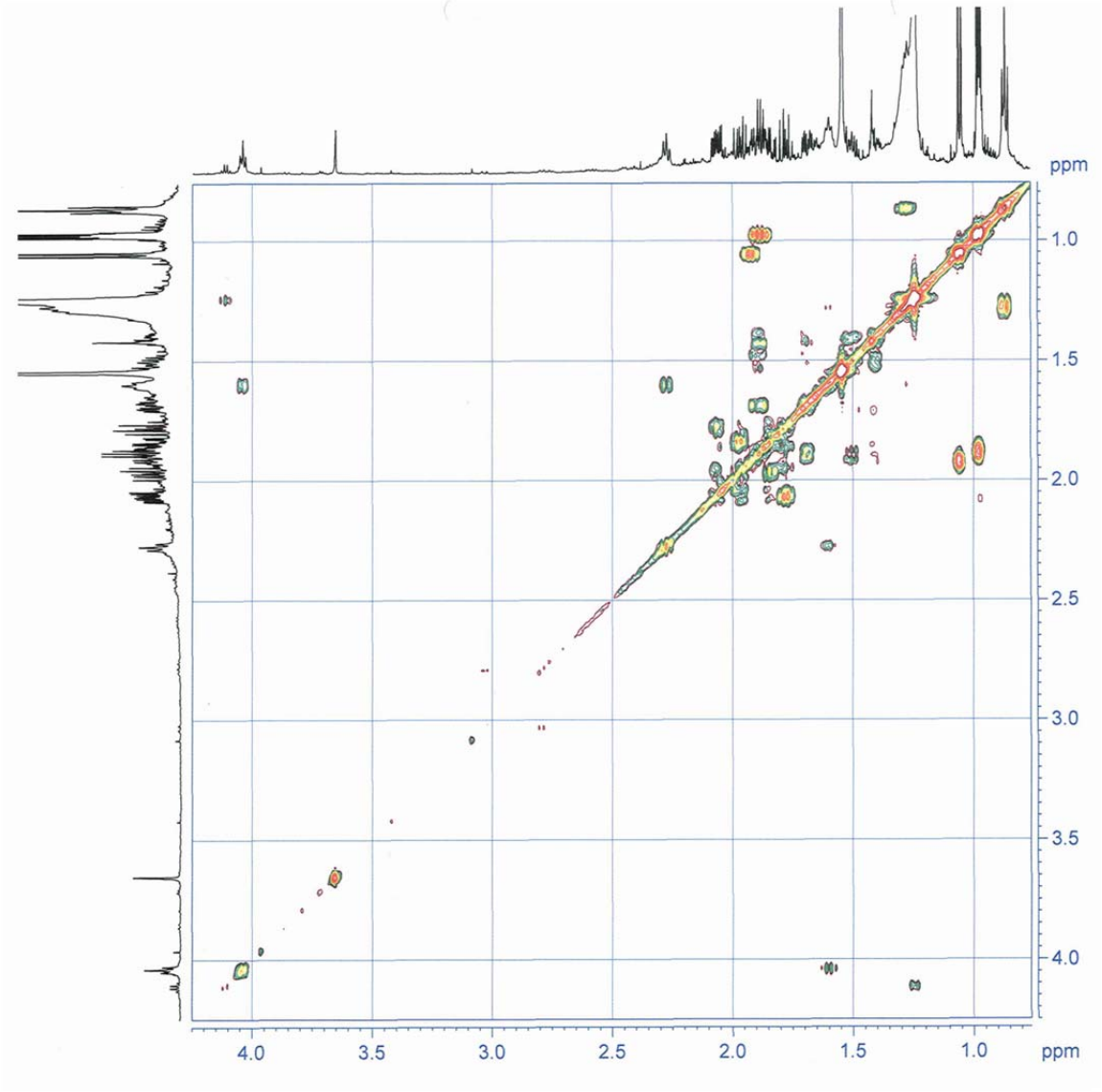


Fig. S4. COSY spectrum of vanderlandin (**1**).

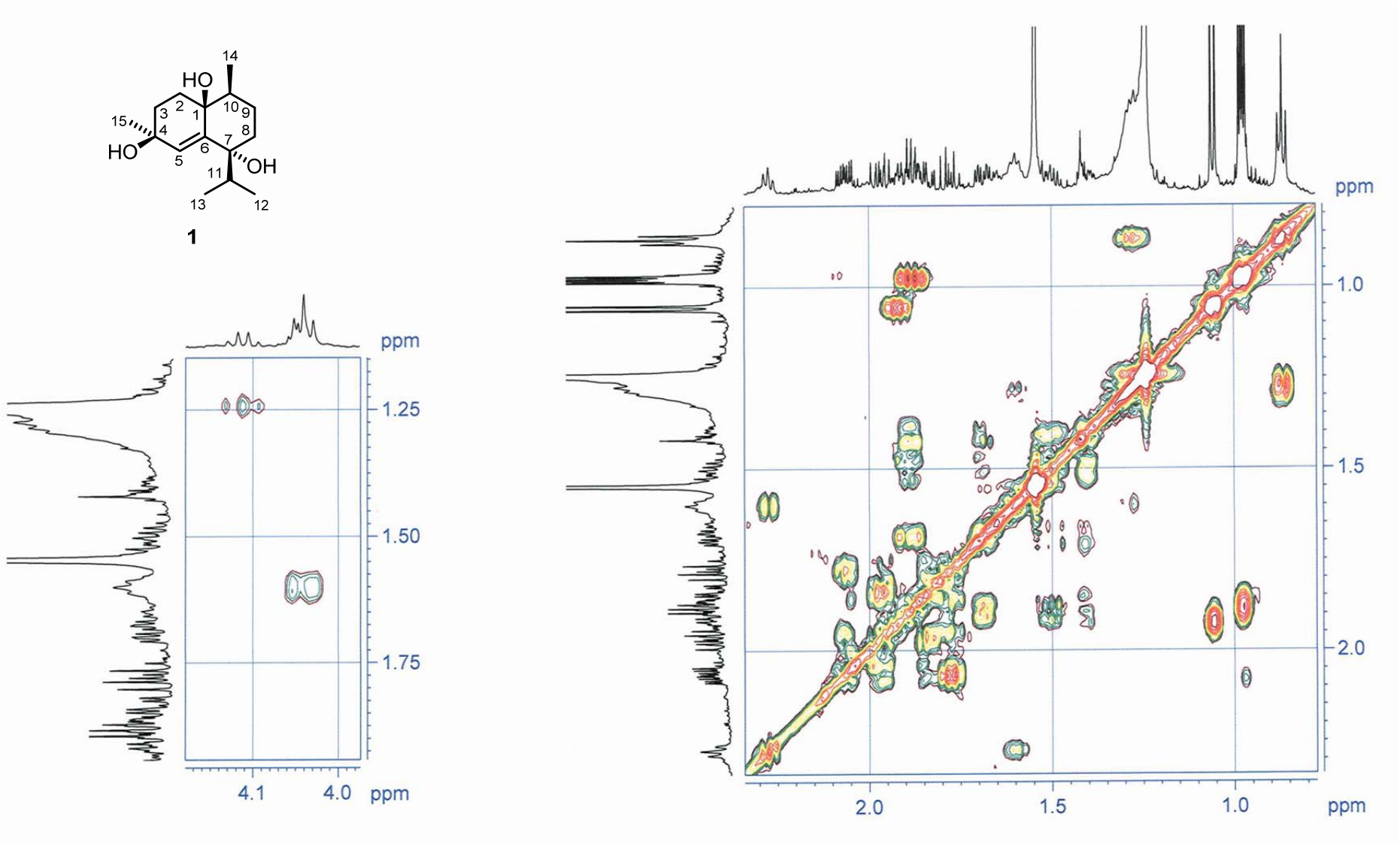
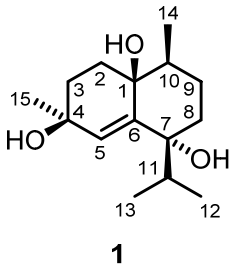


Fig. S5. Details of the COSY spectrum of vanderlandin (**1**).



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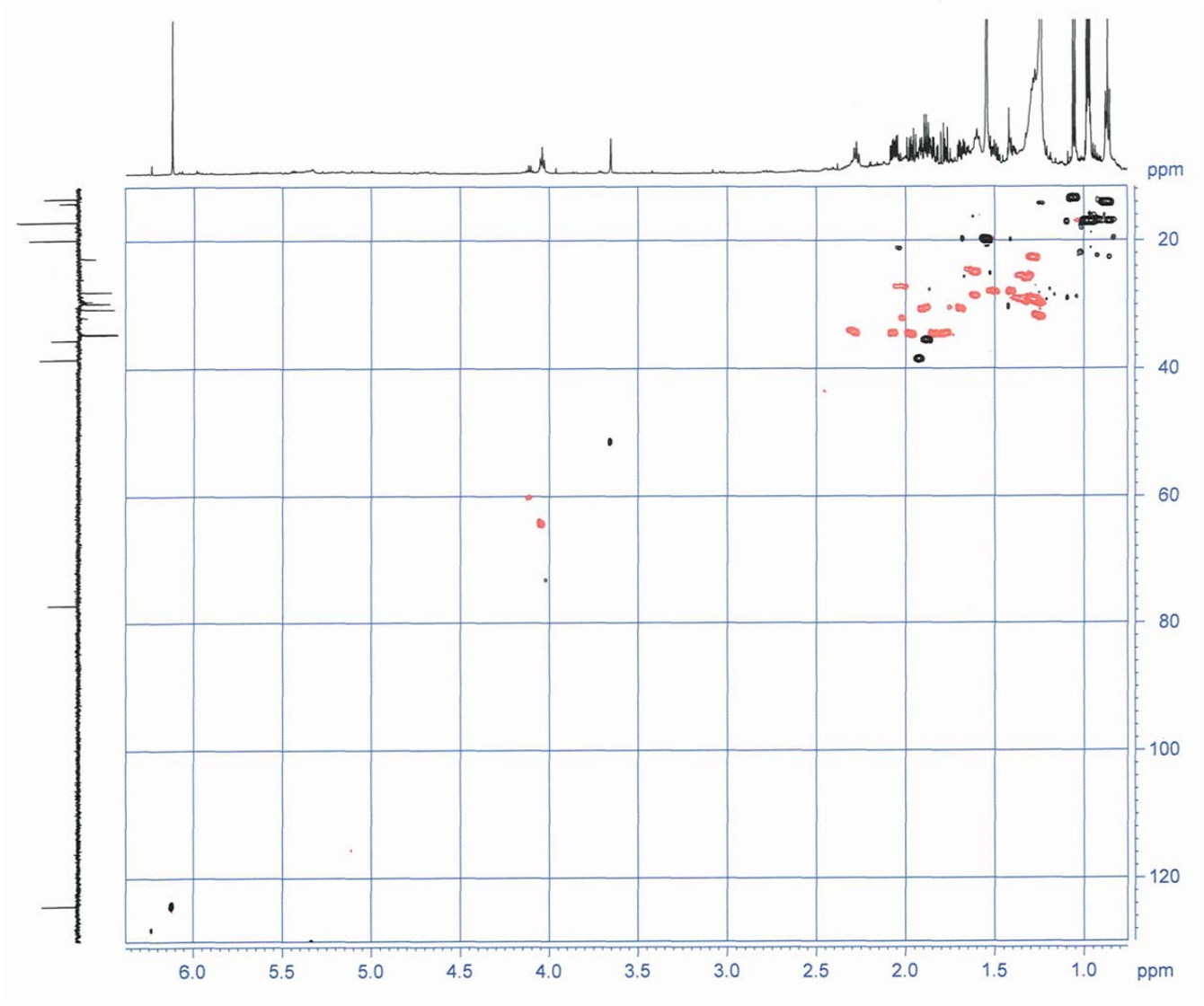


Fig. S6. HSQC spectrum of vanderlandin (**1**).

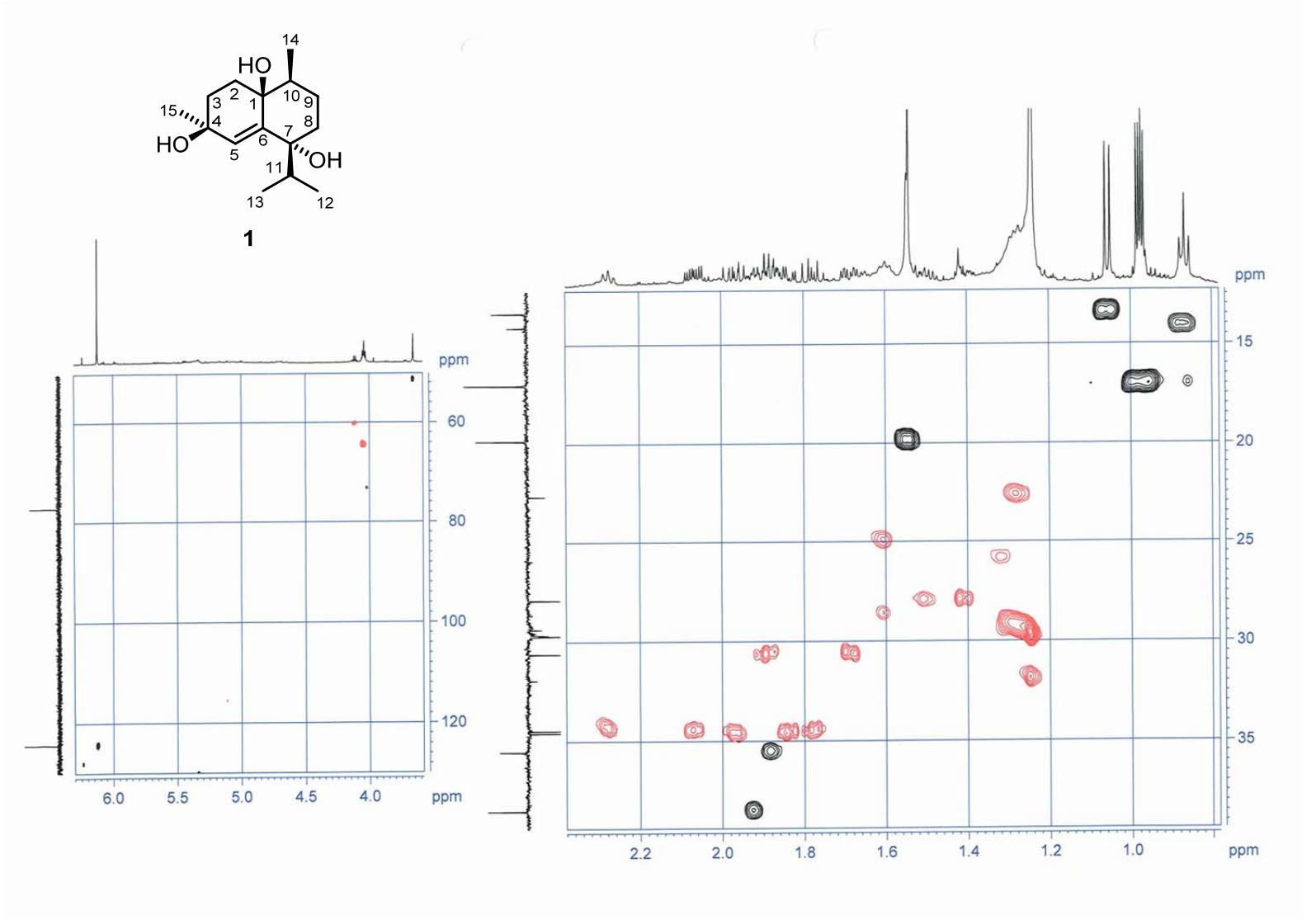


Fig. S7. Details of the HSQC spectrum of vanderlandin (**1**).

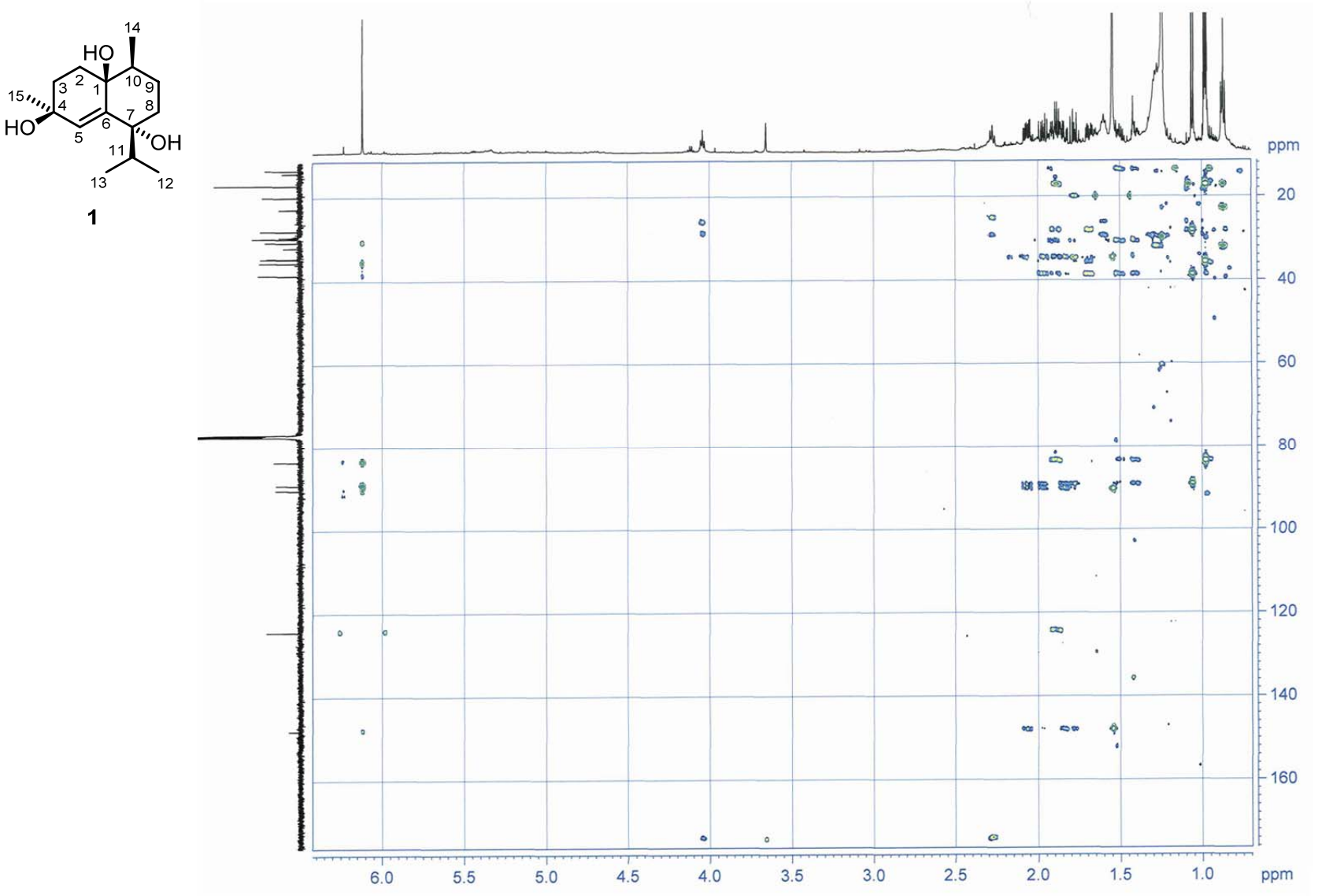
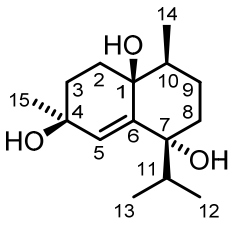


Fig. S8. HMBC spectrum of vanderlandin (**1**).



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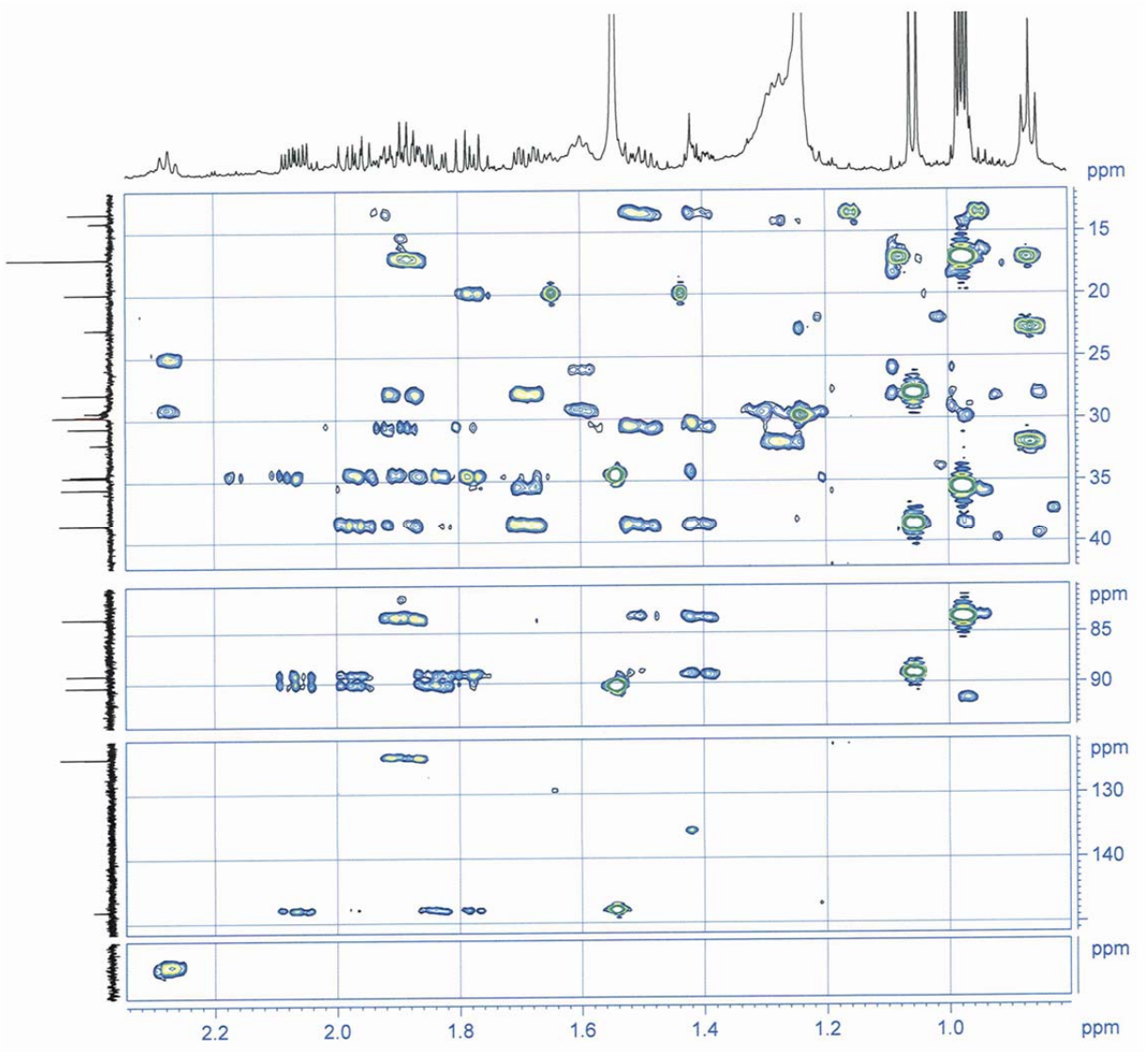
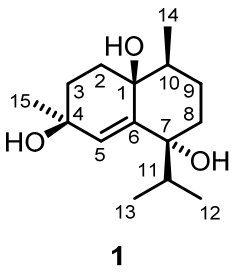


Fig. S9. Details of the HMBC spectrum of vanderlandin (**1**).



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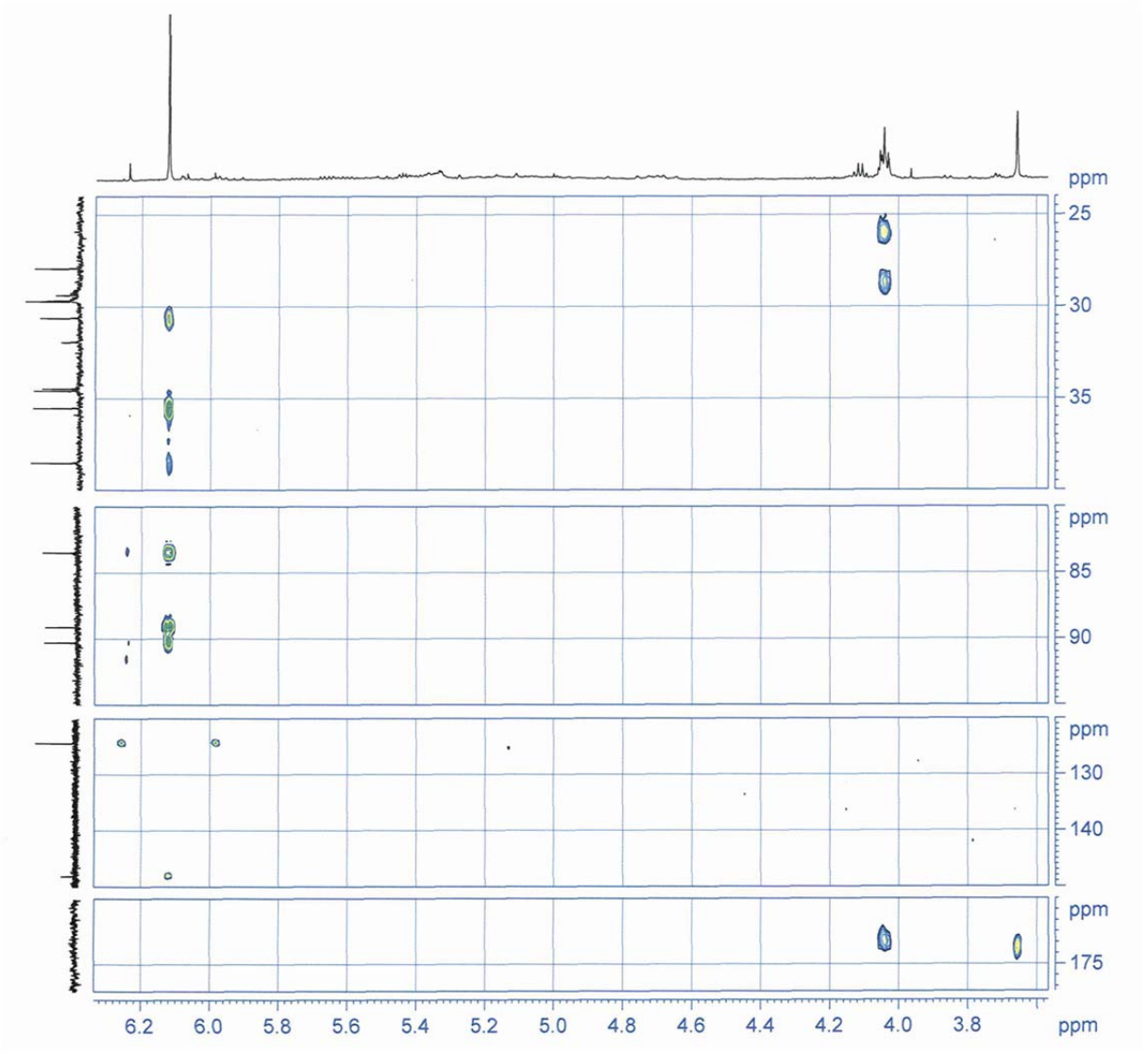
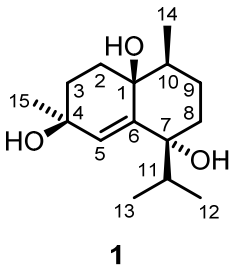


Fig. S10. Details of the HMBC spectrum of vanderlandin (**1**).



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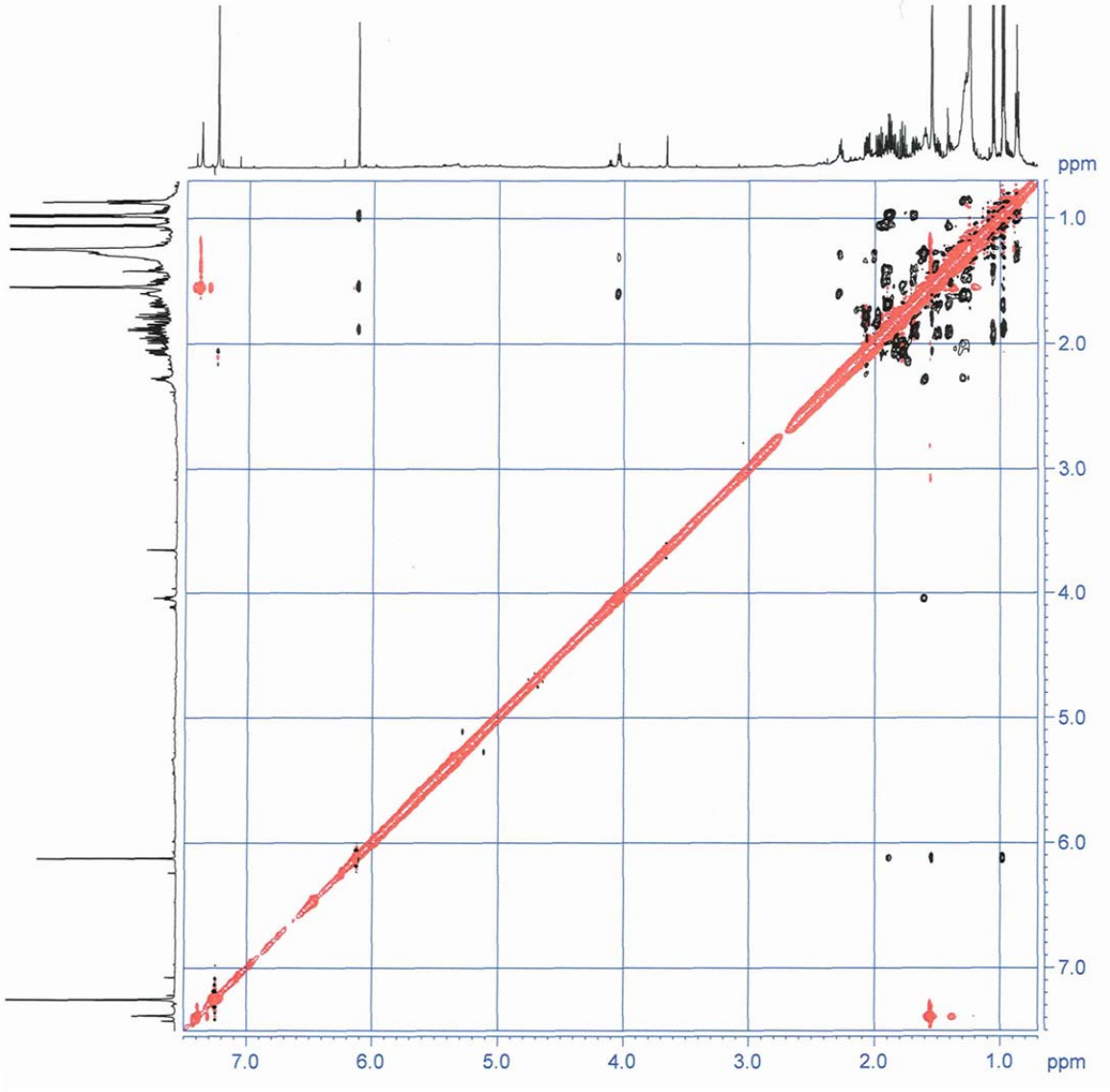


Fig. S11. NOESY spectrum of vanderlandin (**1**).

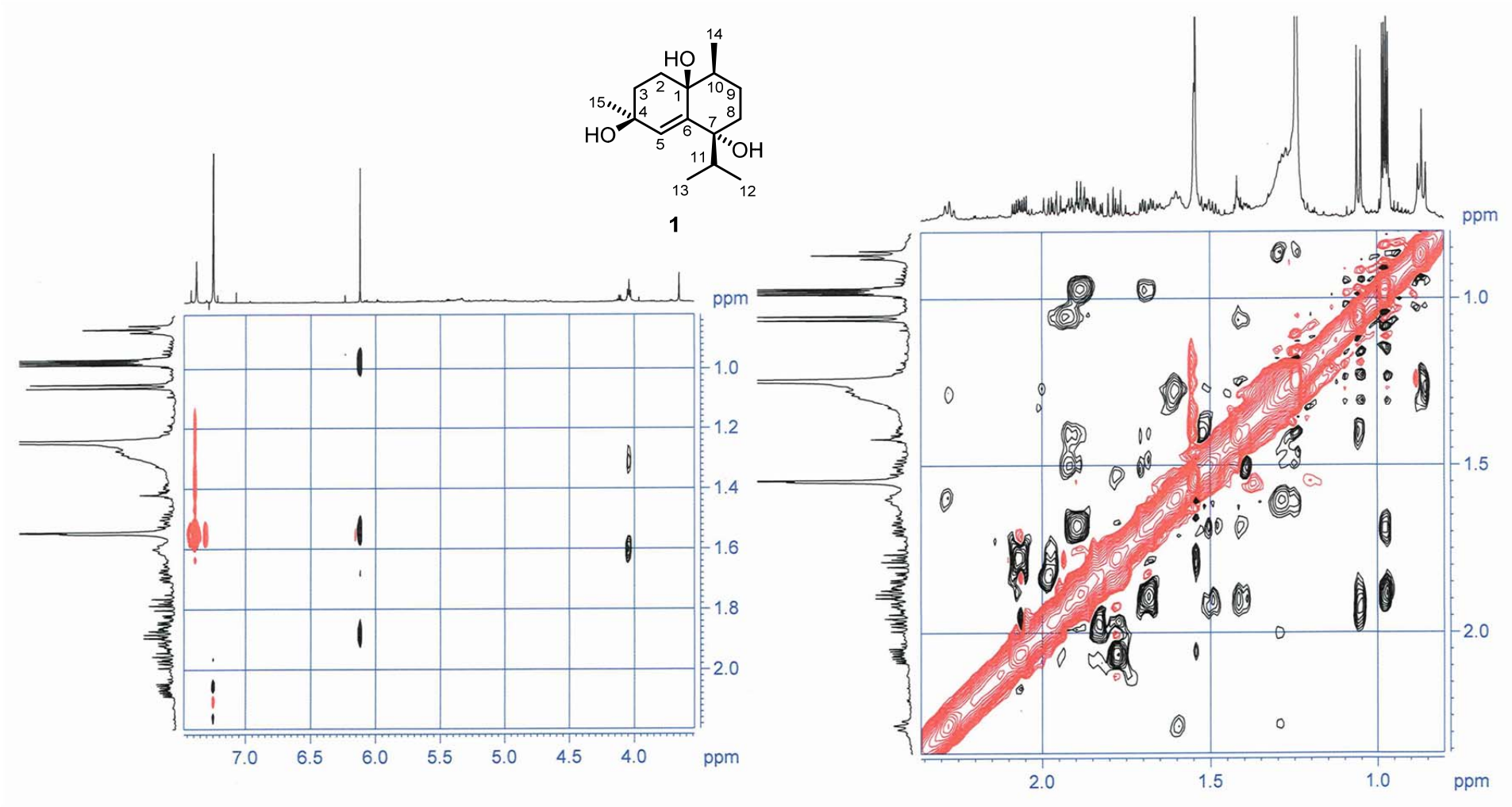


Fig. S12. Details of the NOESY spectrum of vanderlandin (**1**).

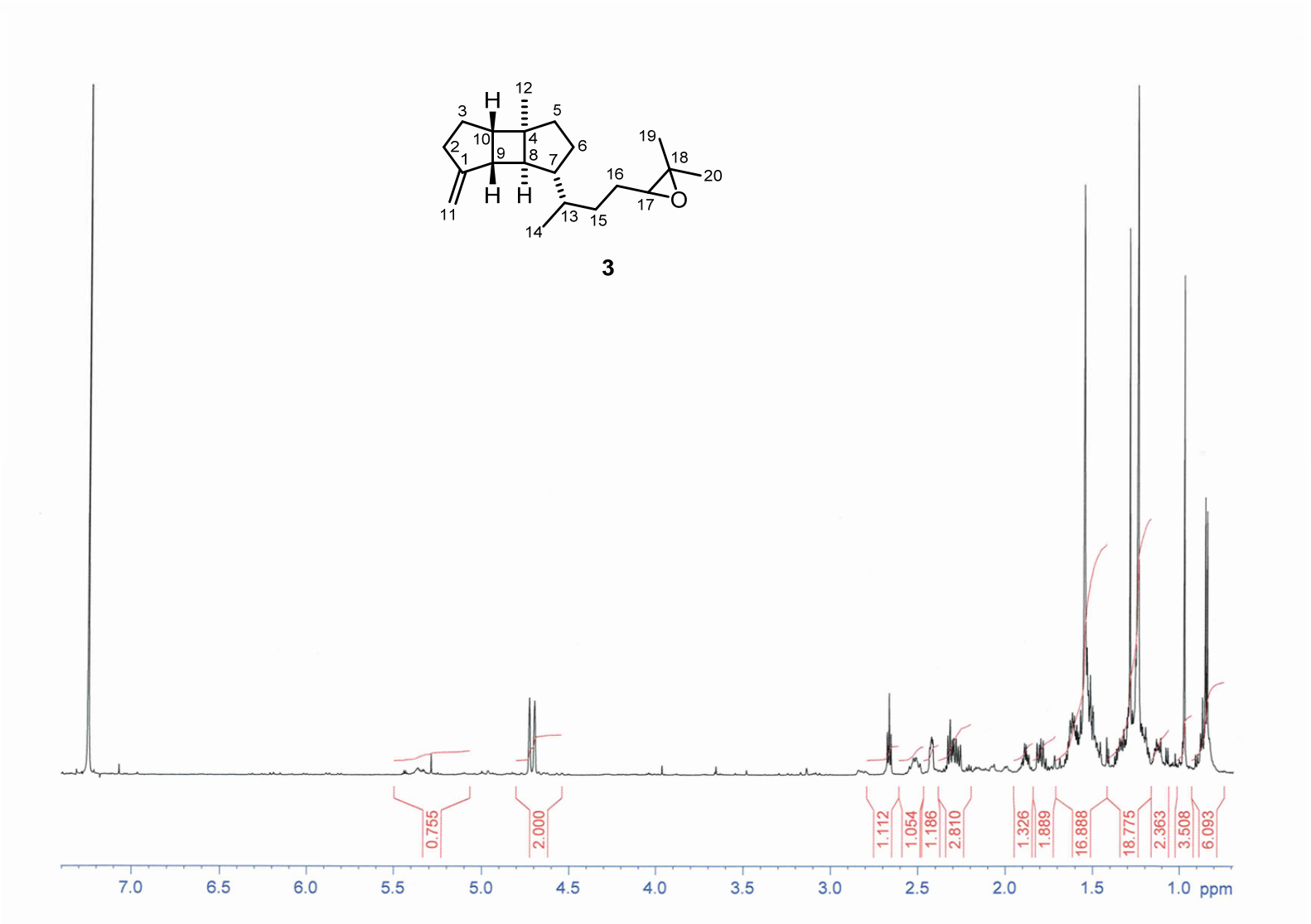
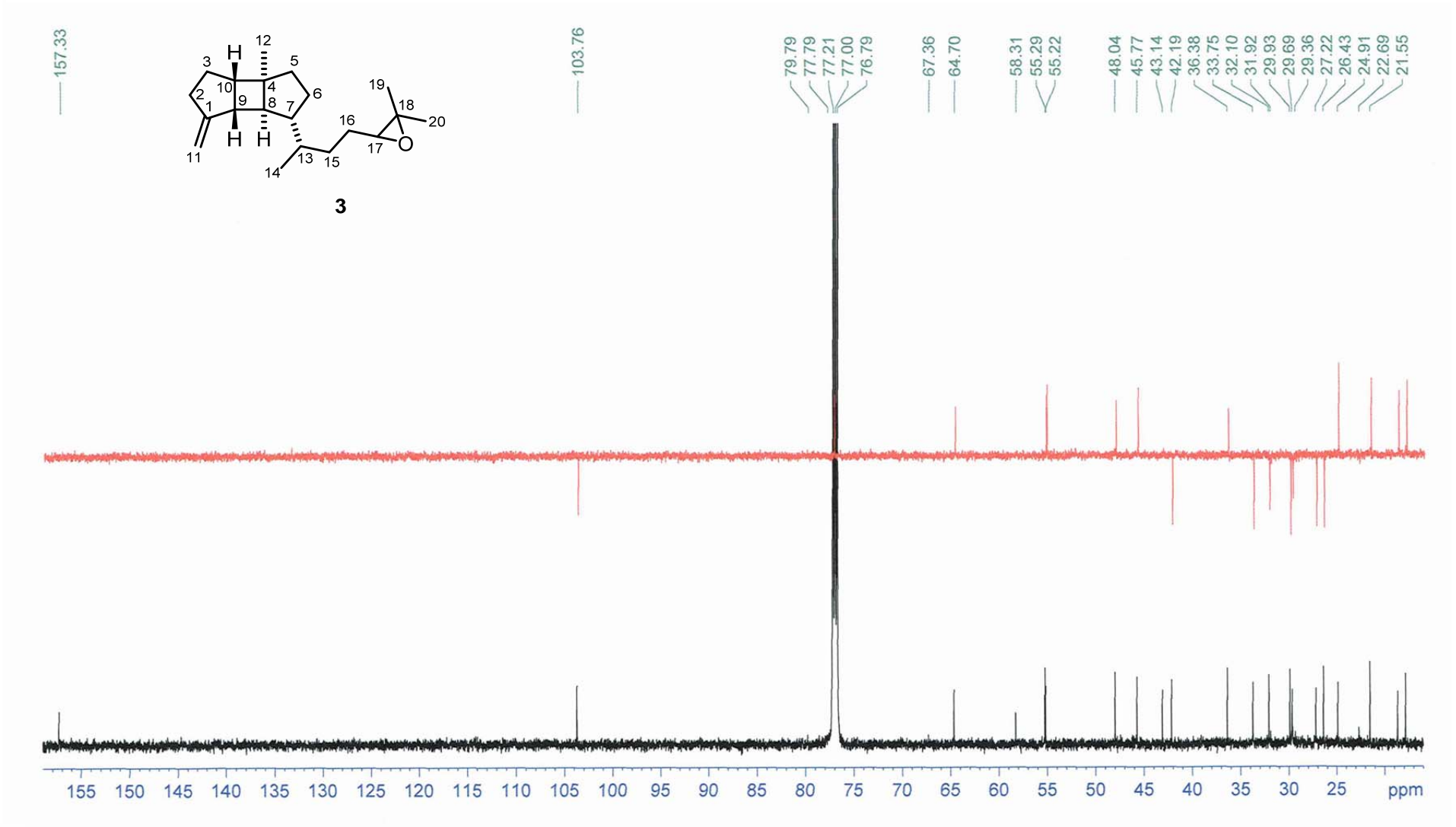


Fig. S13. ^{1}H NMR (600 MHz, $CDCl_3$) of gravilin (**3**).



3

Fig. S14. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of gravilin (**3**).

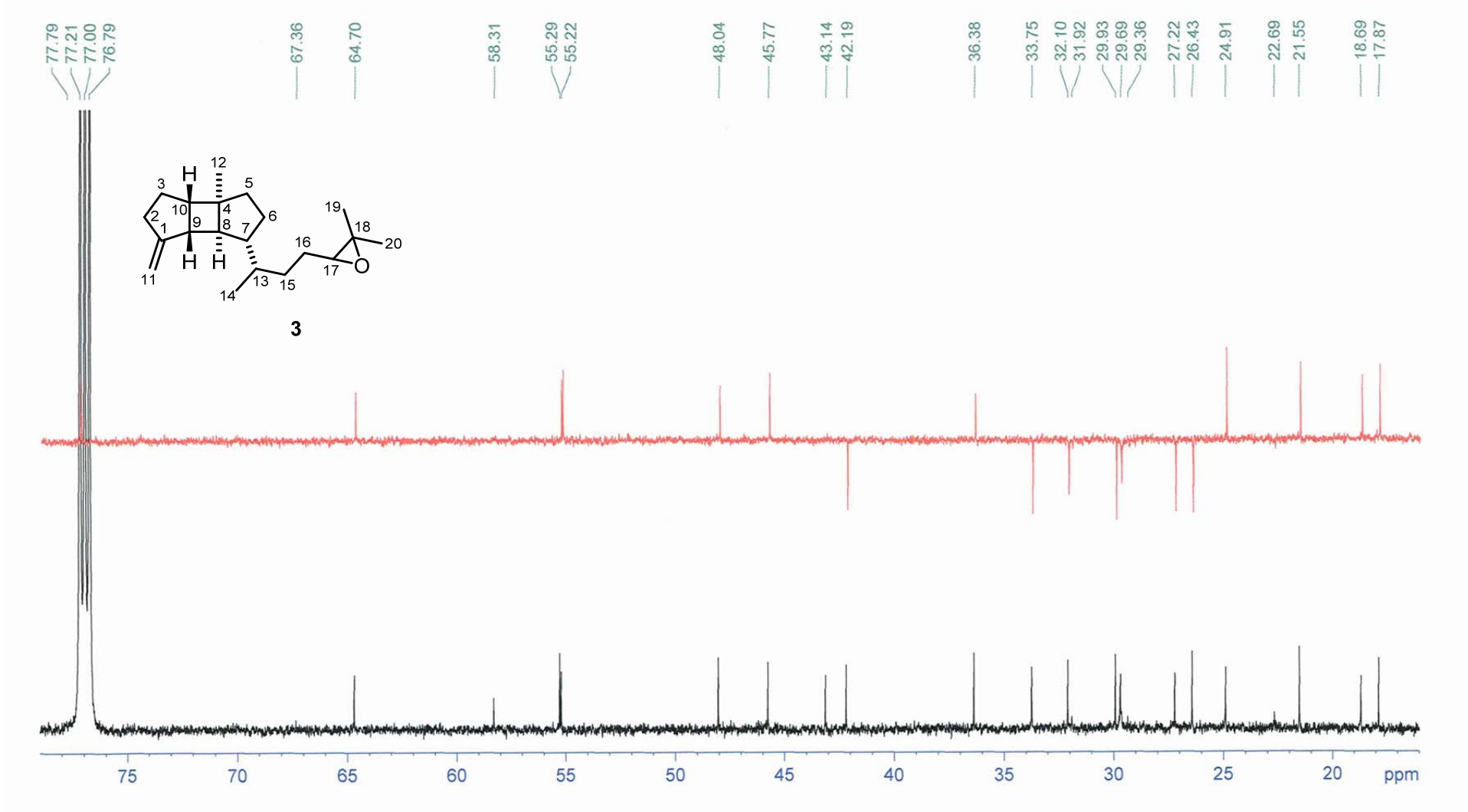
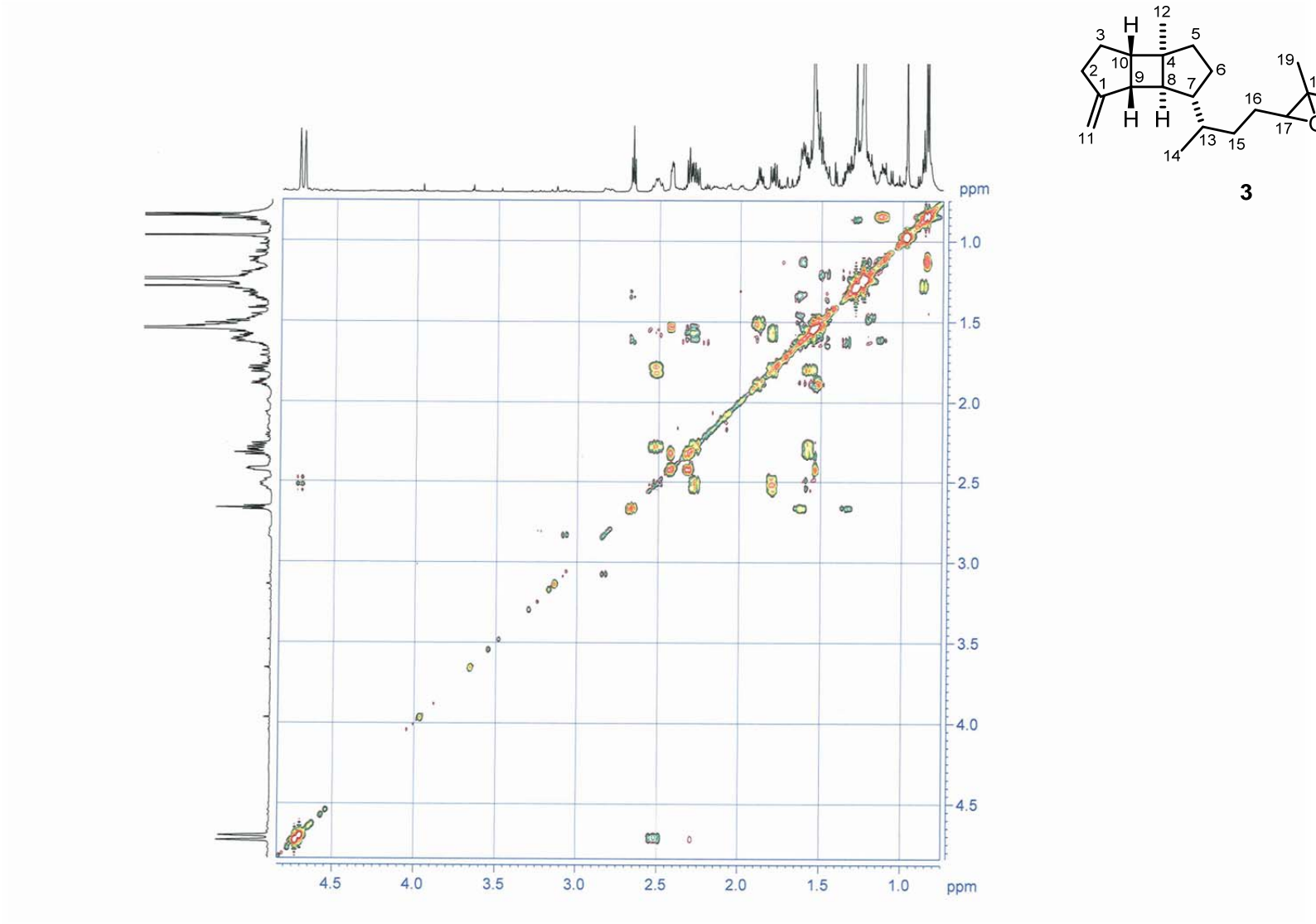


Fig. S15. Details of the ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of gravilin (**3**).



3

Fig. S16. COSY spectrum of gravilin (**3**).

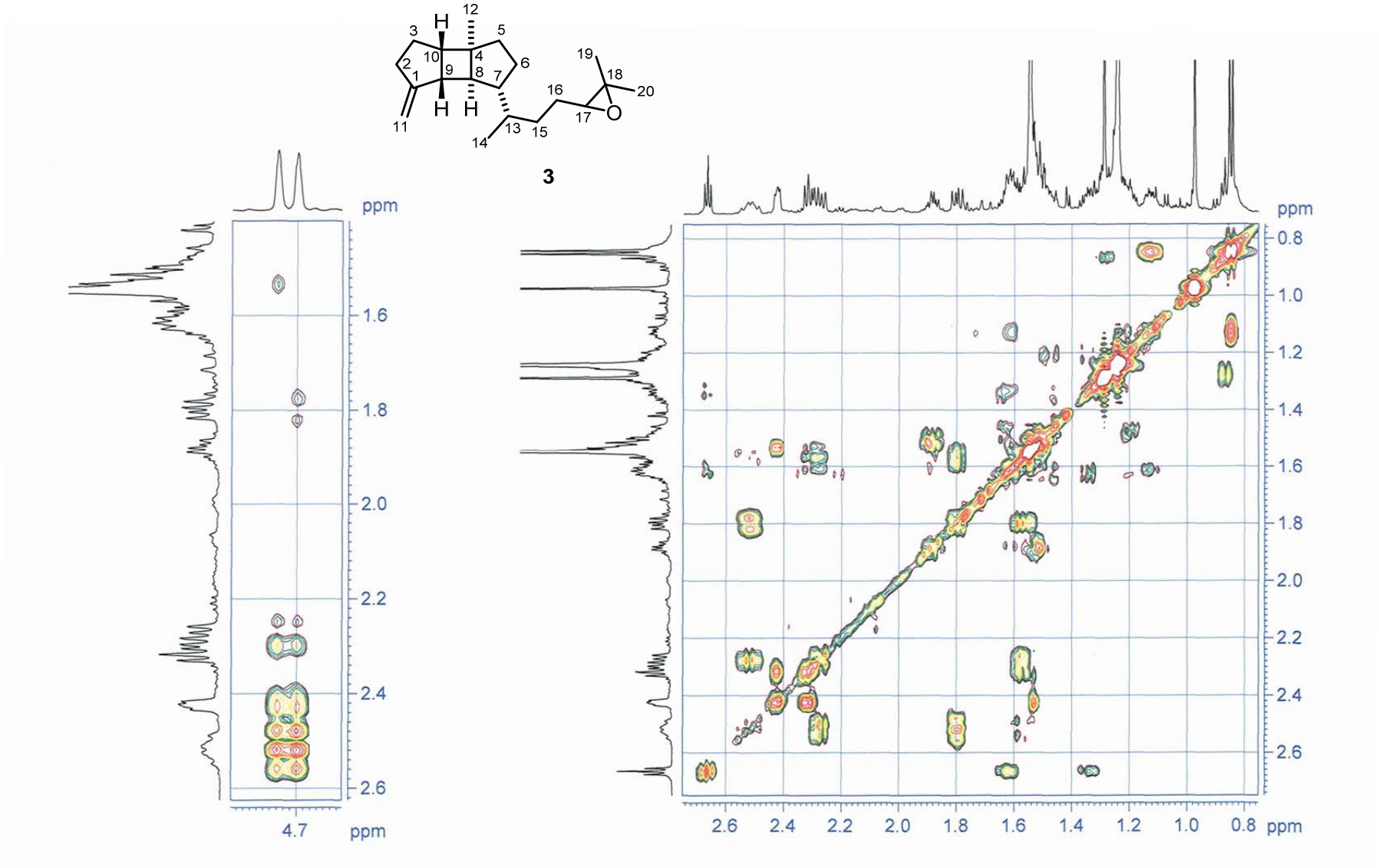


Fig. S17. Details of the COSY spectrum of gravilin (**3**).

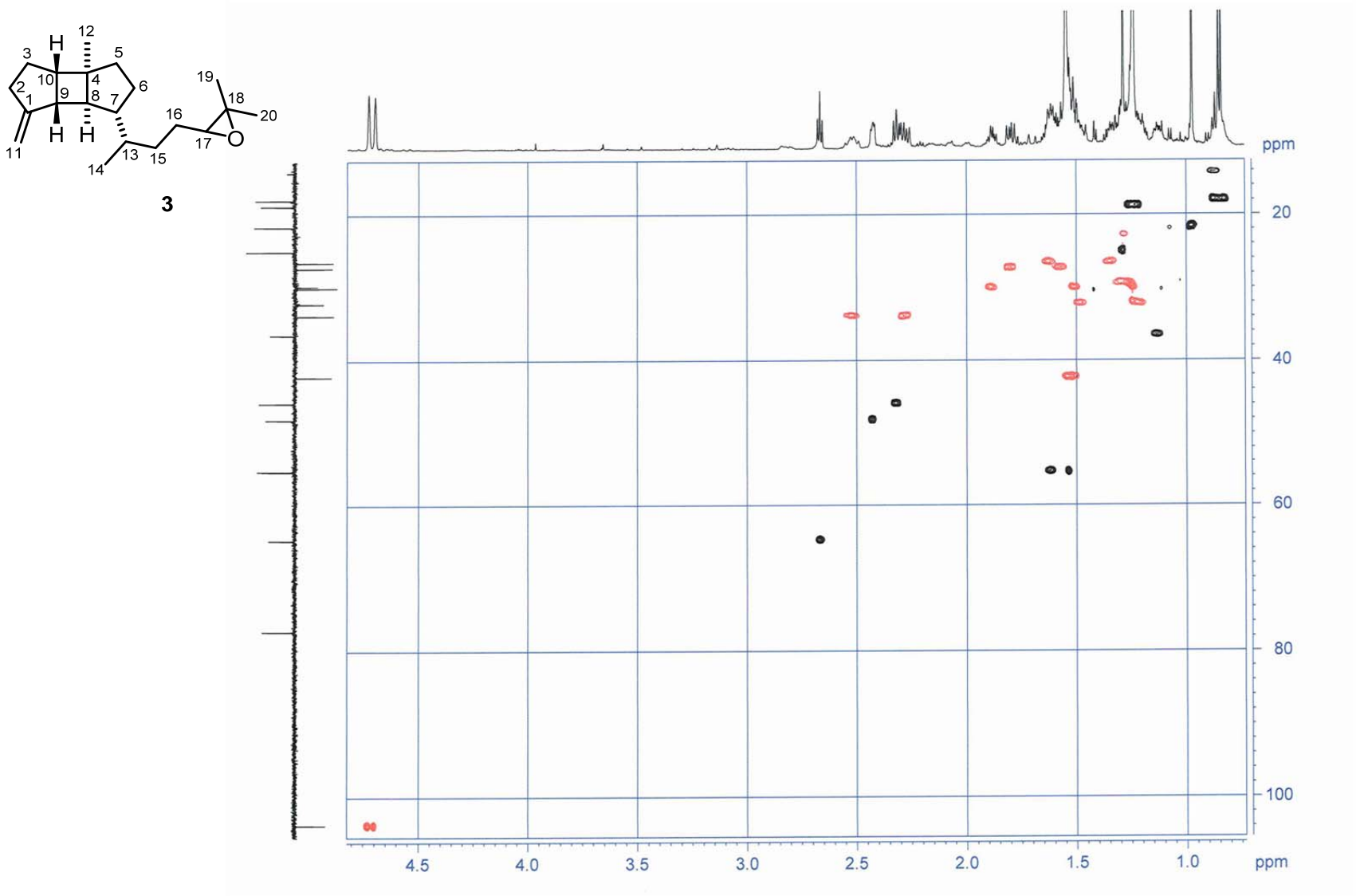


Fig. S18. HSQC spectrum of gravilin (**3**).

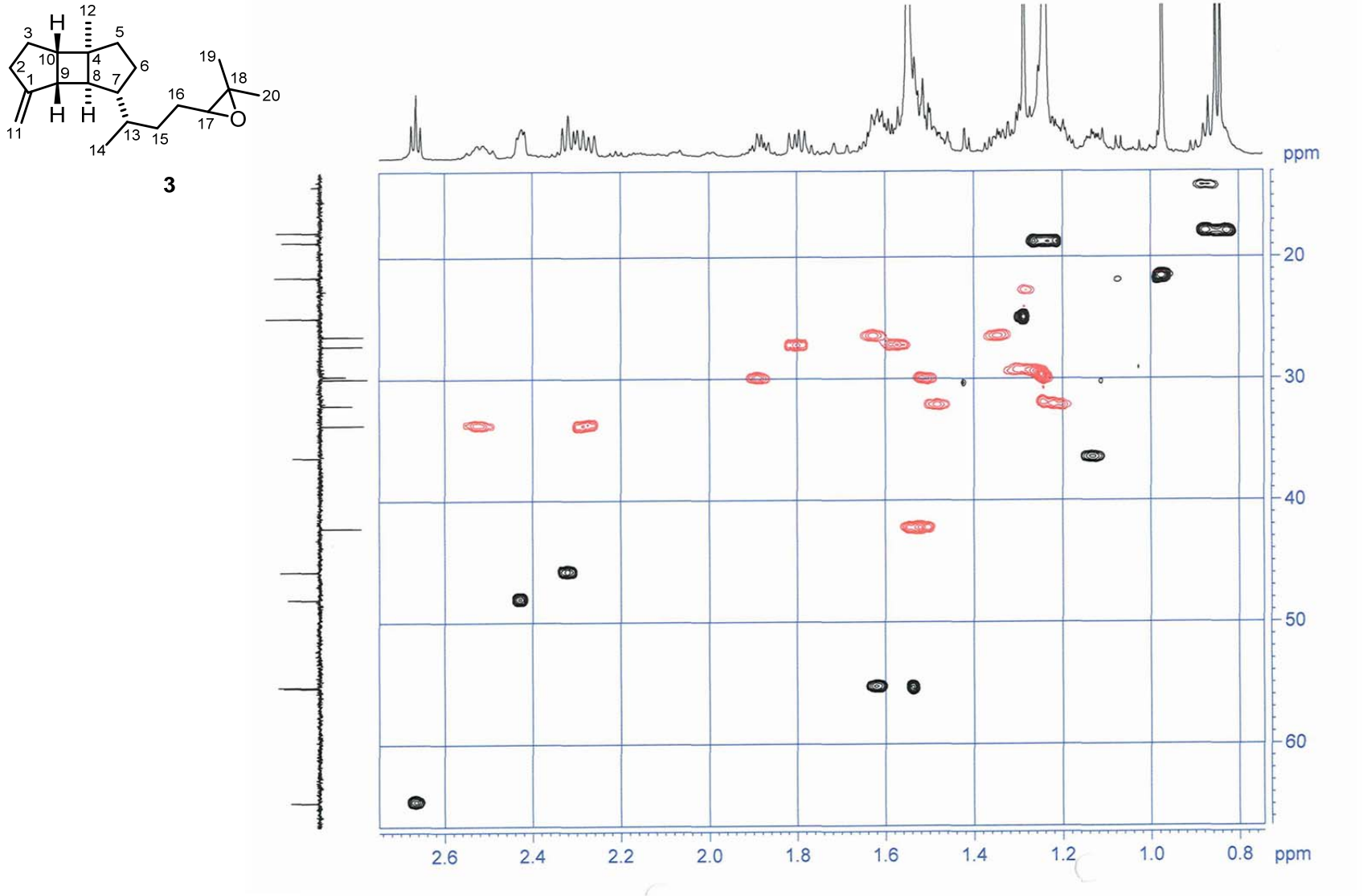


Fig. S19. Details of the HSQC spectrum of gravilin (**3**).

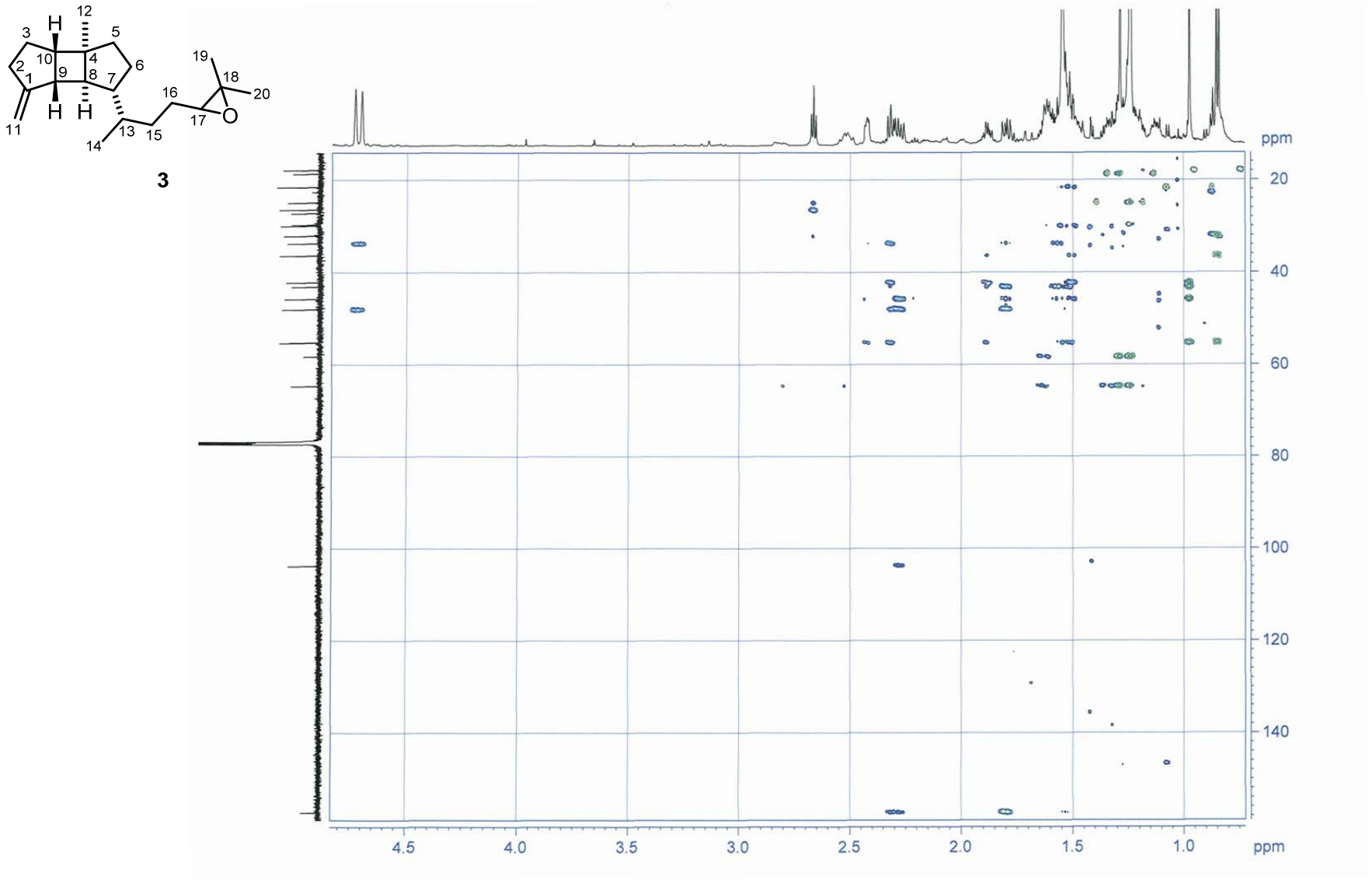


Fig. S20. HMBC spectrum of gravilin (**3**).

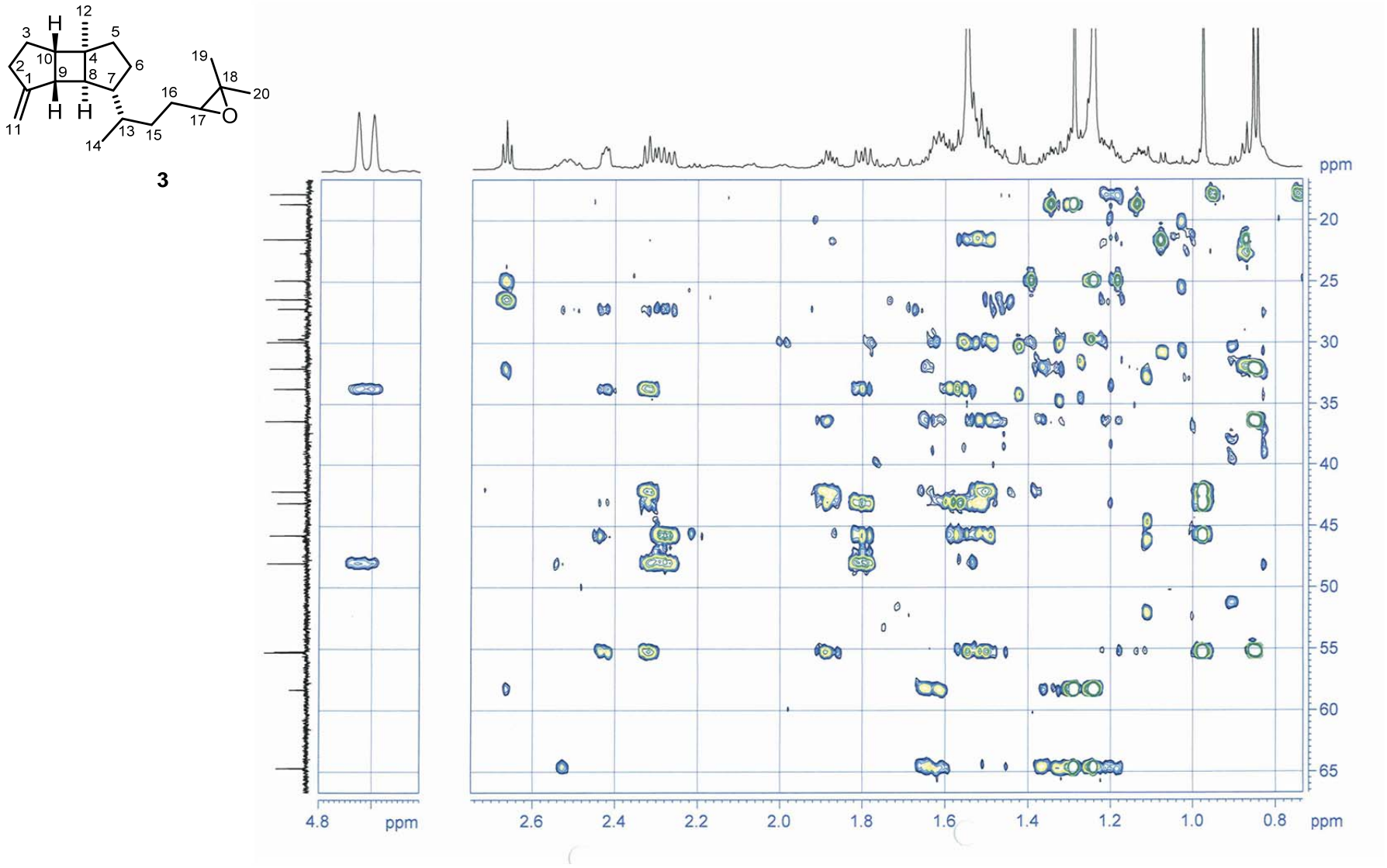


Fig. S21. Details of the HMBC spectrum of gravilin (**3**).

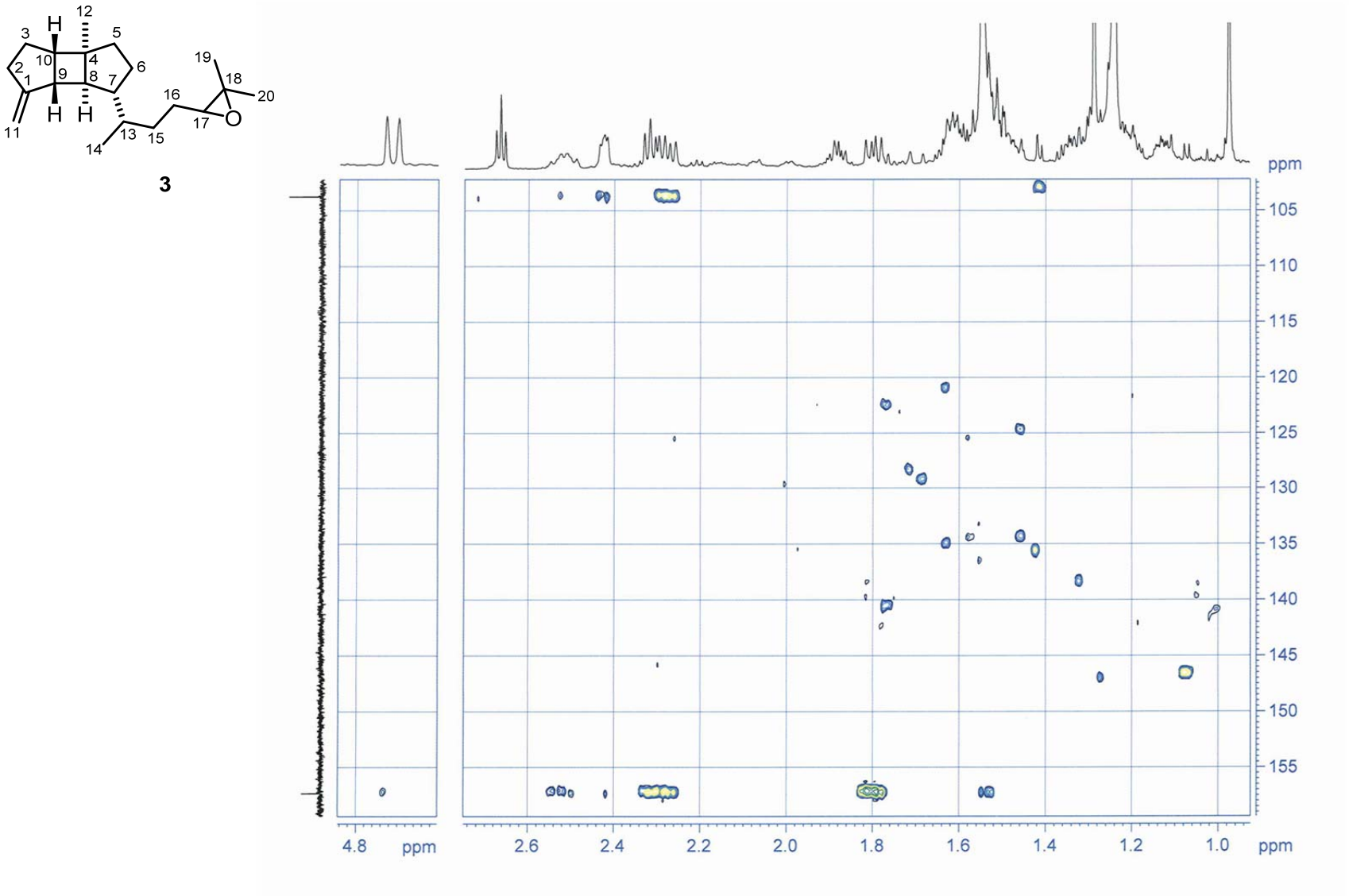
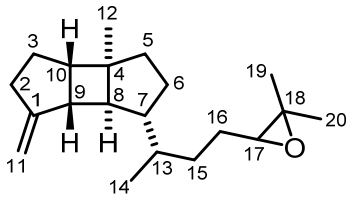


Fig. S22. Details of the HMBC spectrum of gravilin (**3**).



3

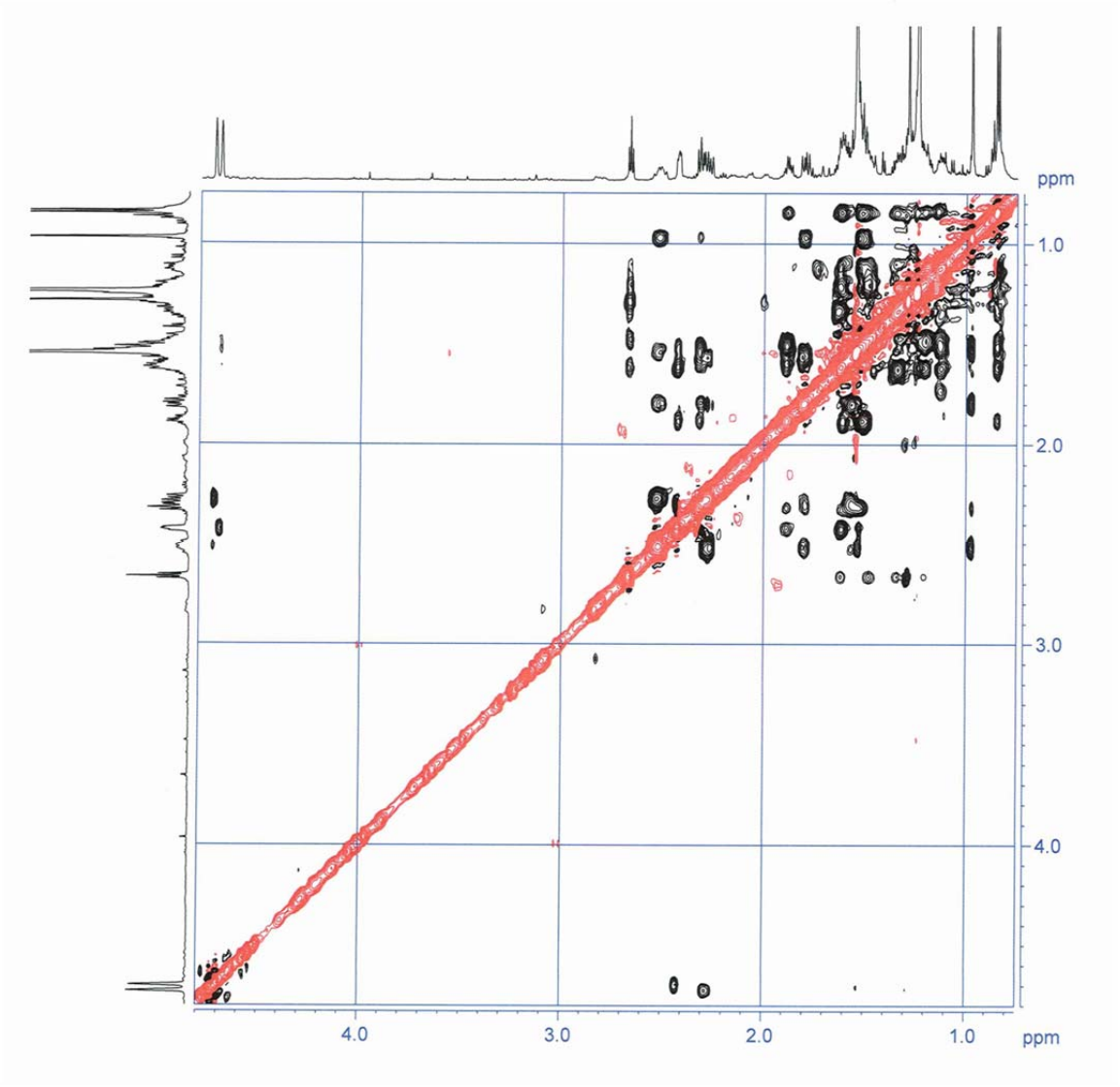


Fig. S23. NOESY spectrum of gravilin (**3**).

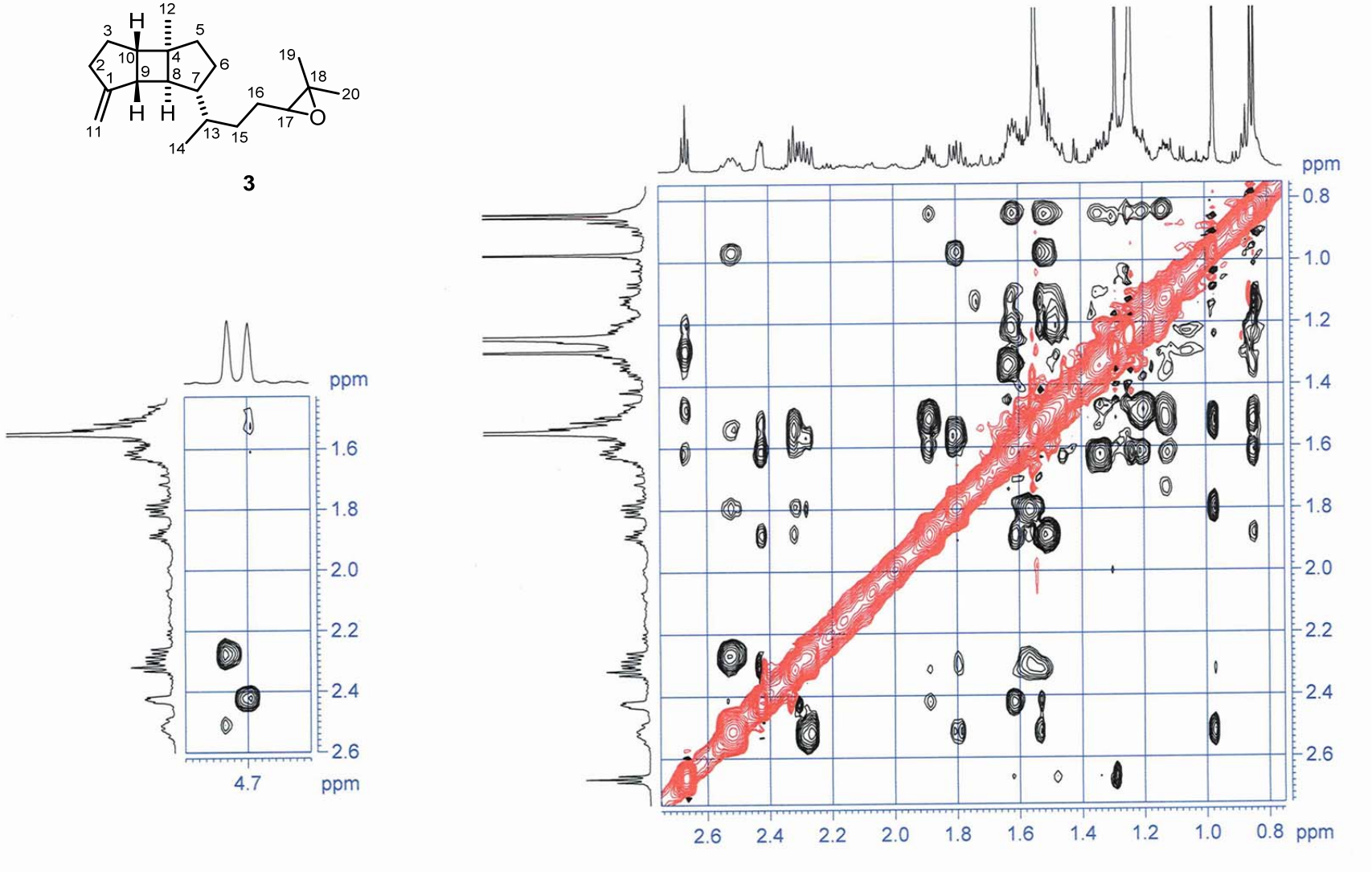


Fig. S24. Details of the NOESY spectrum of gravilin (**3**).

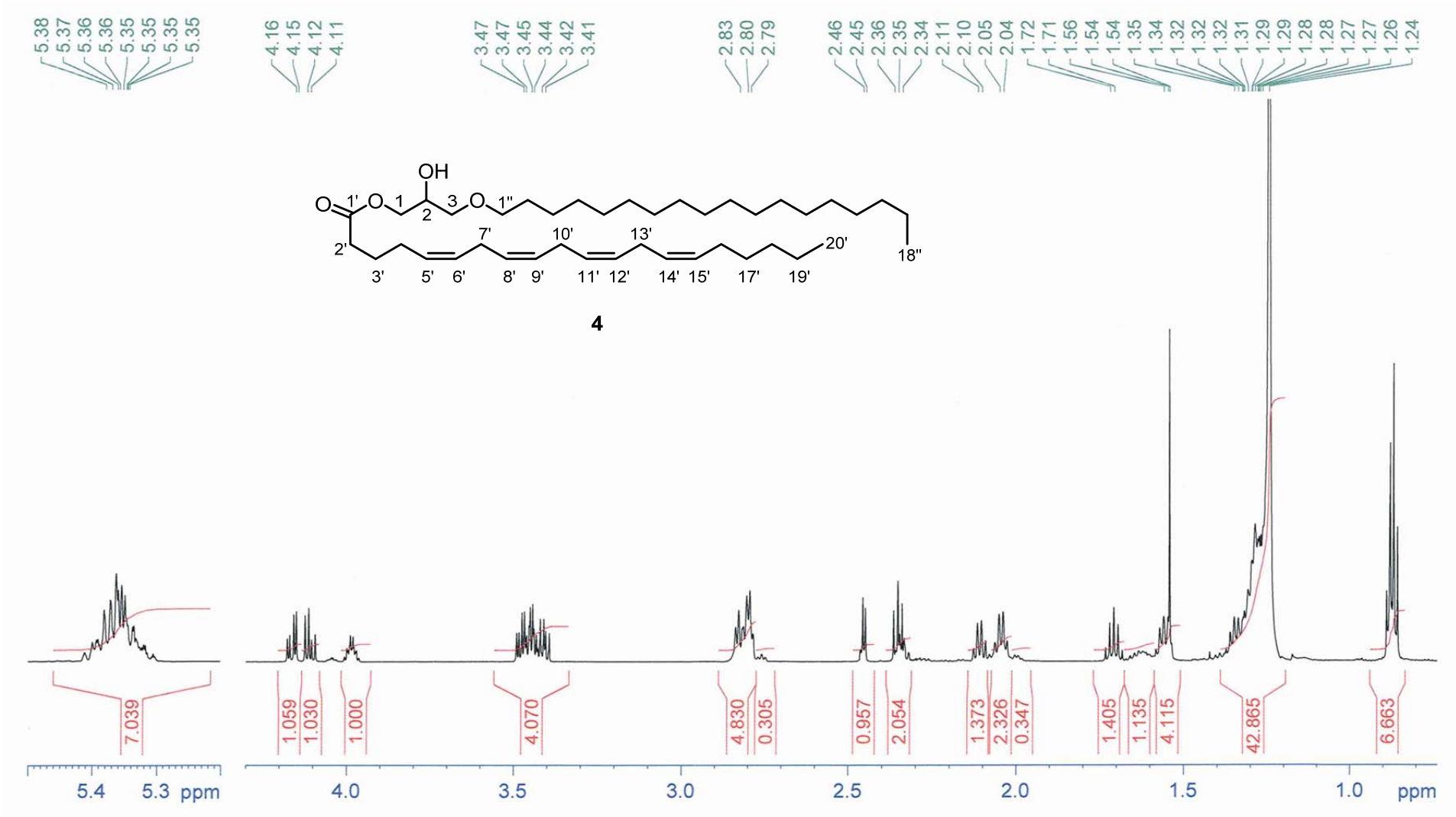


Fig. S25. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of monoalkylmonoacylglycerol **4**.

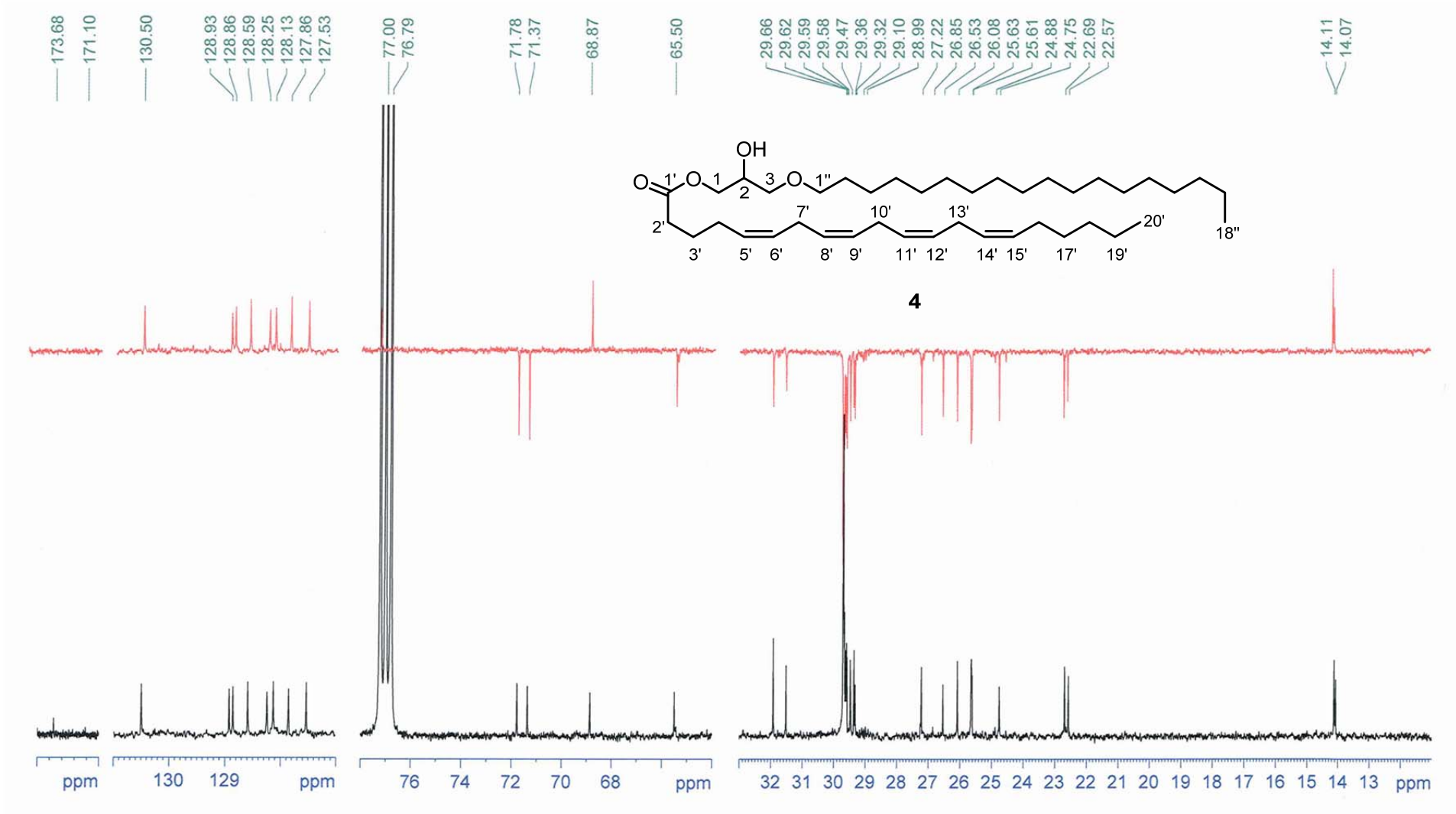
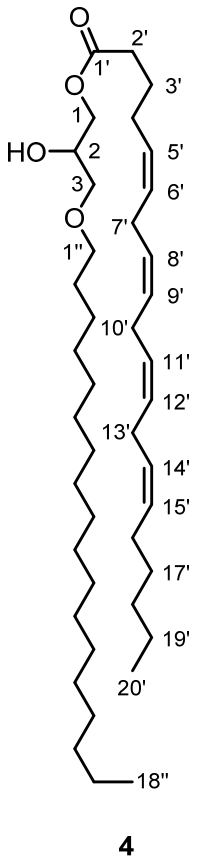


Fig. S26. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of monoalkylmonoacylglycerol **4**.



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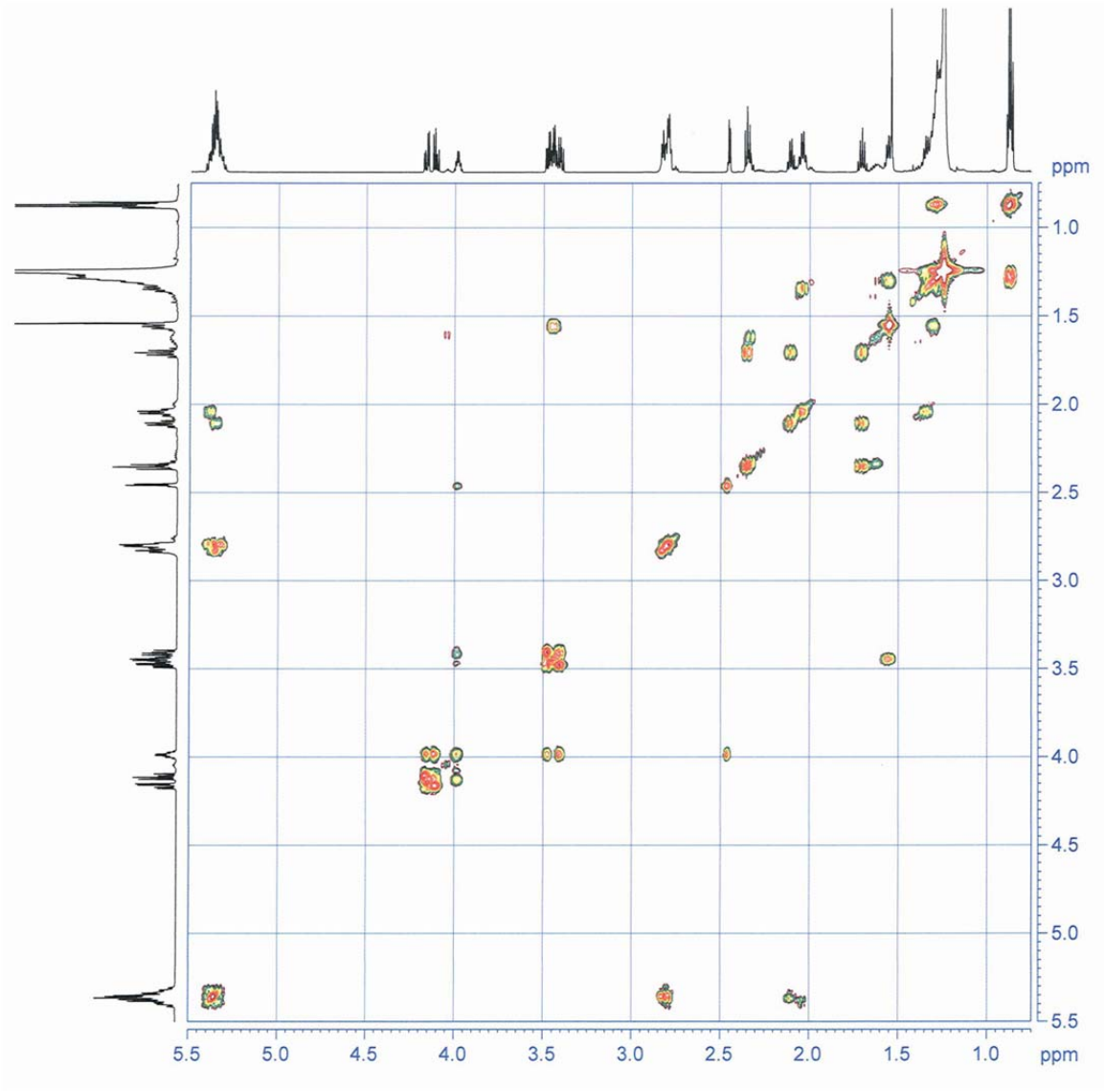
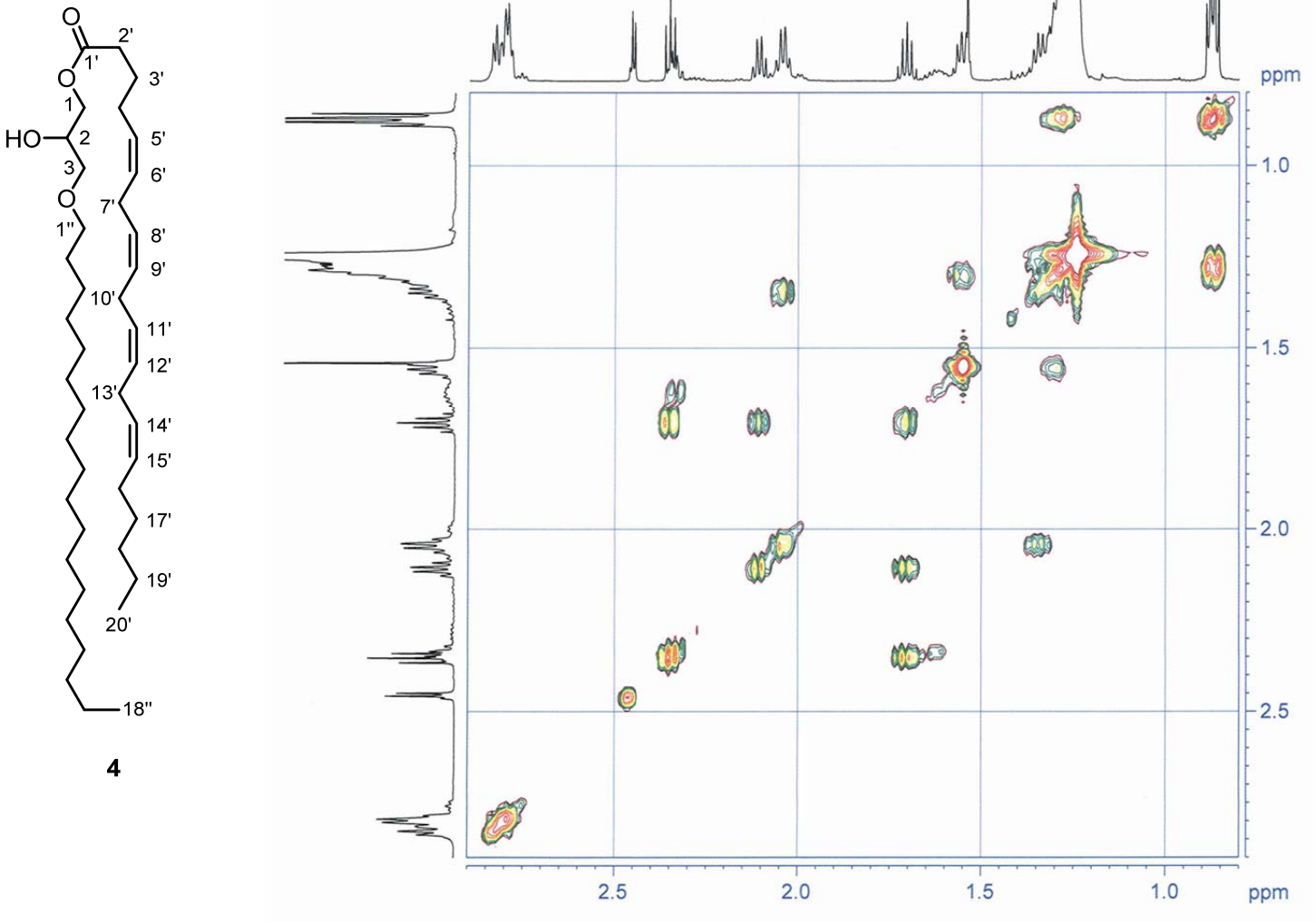


Fig. S27. COSY spectrum of monoalkylmonoacylglycerol **4**.



4

Fig. S28. Details of the COSY spectrum of monoalkylmonoacylglycerol **4**.

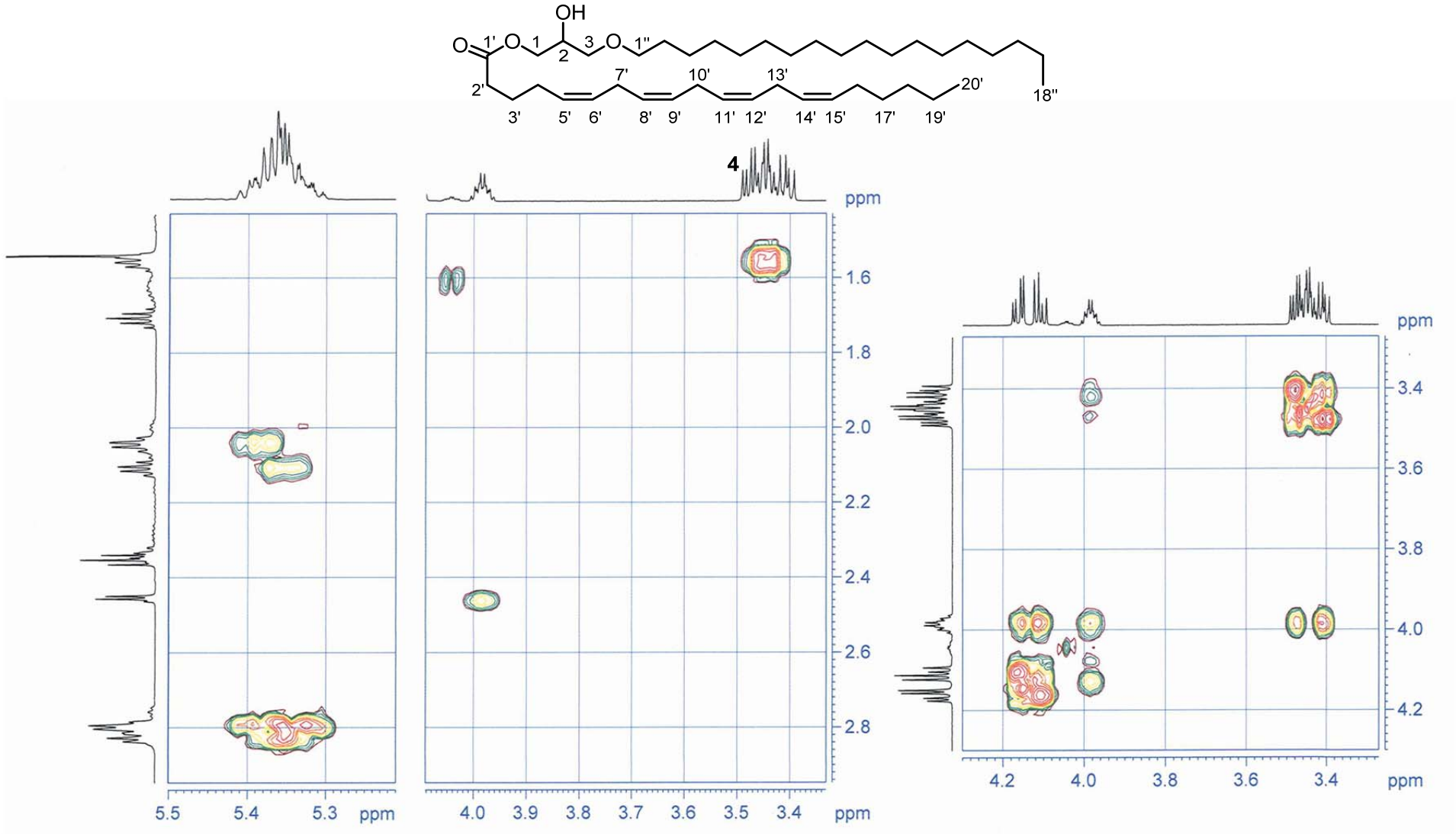


Fig. S29. Details of the COSY spectrum of monoalkylmonoacylglycerol **4**.

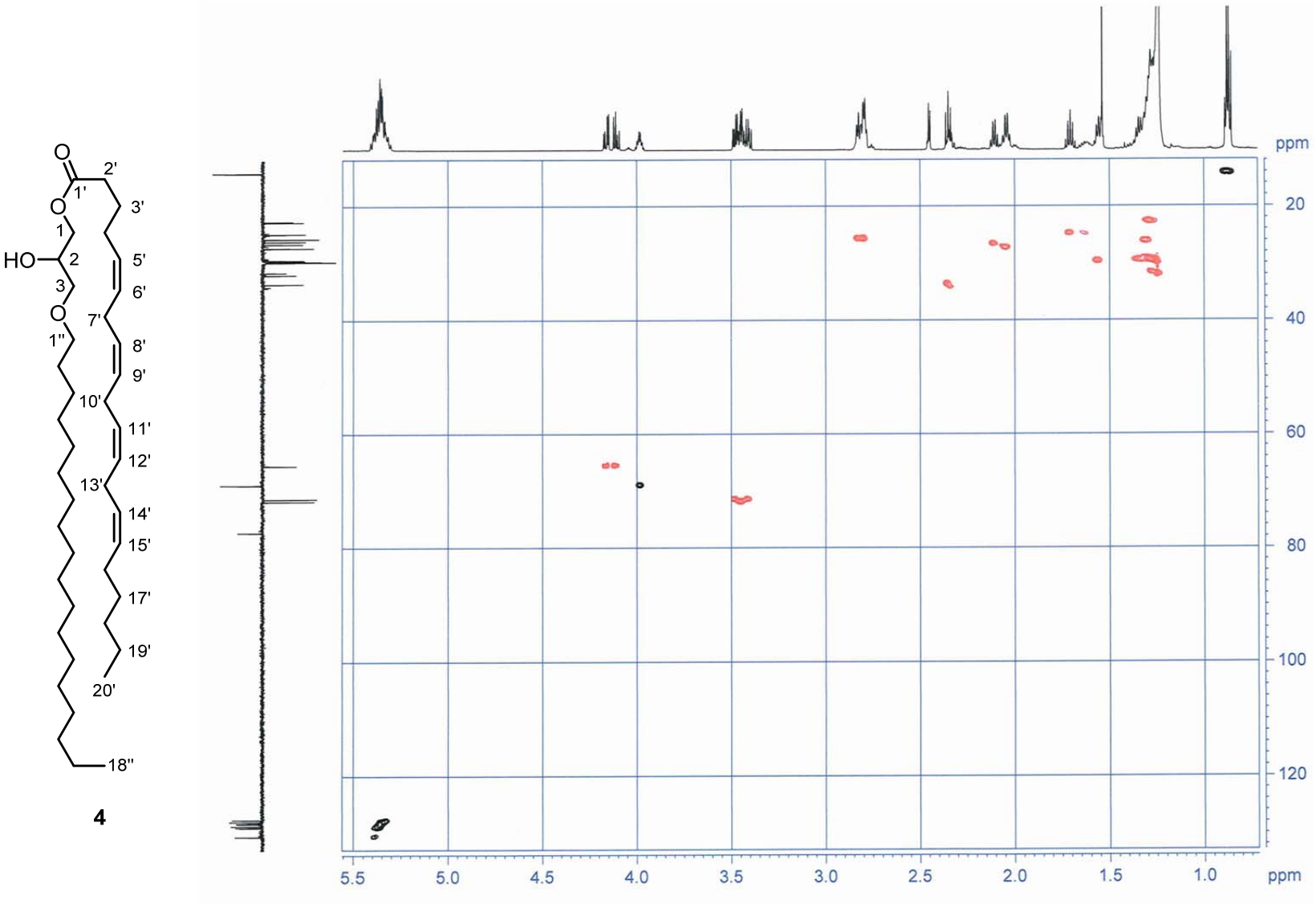


Fig. S30. HSQC spectrum of monoalkylmonoacylglycerol **4**.

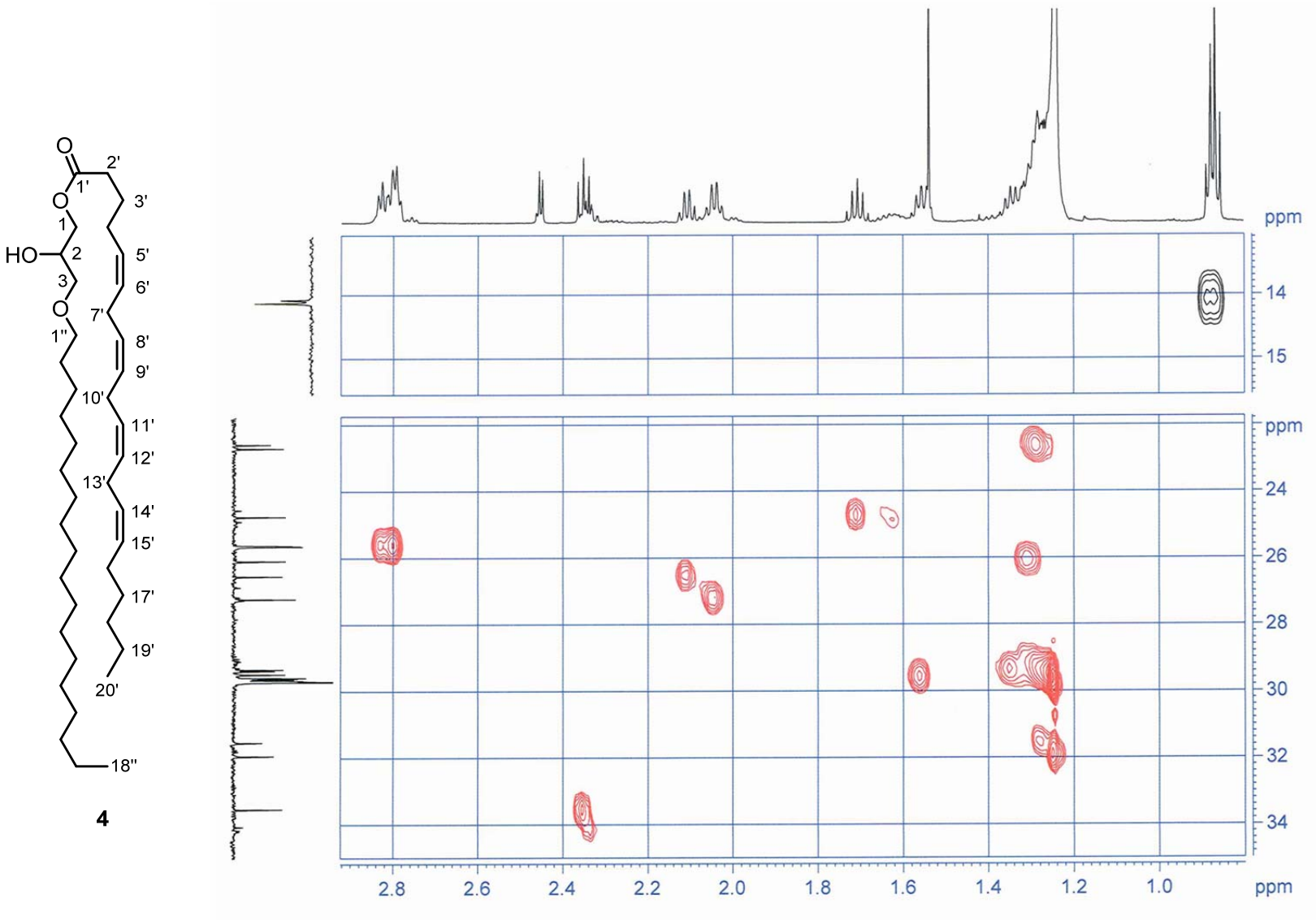
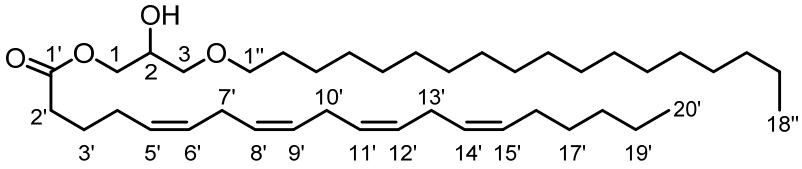


Fig. S31. Details of the HSQC spectrum of monoalkylmonoacylglycerol **4**.



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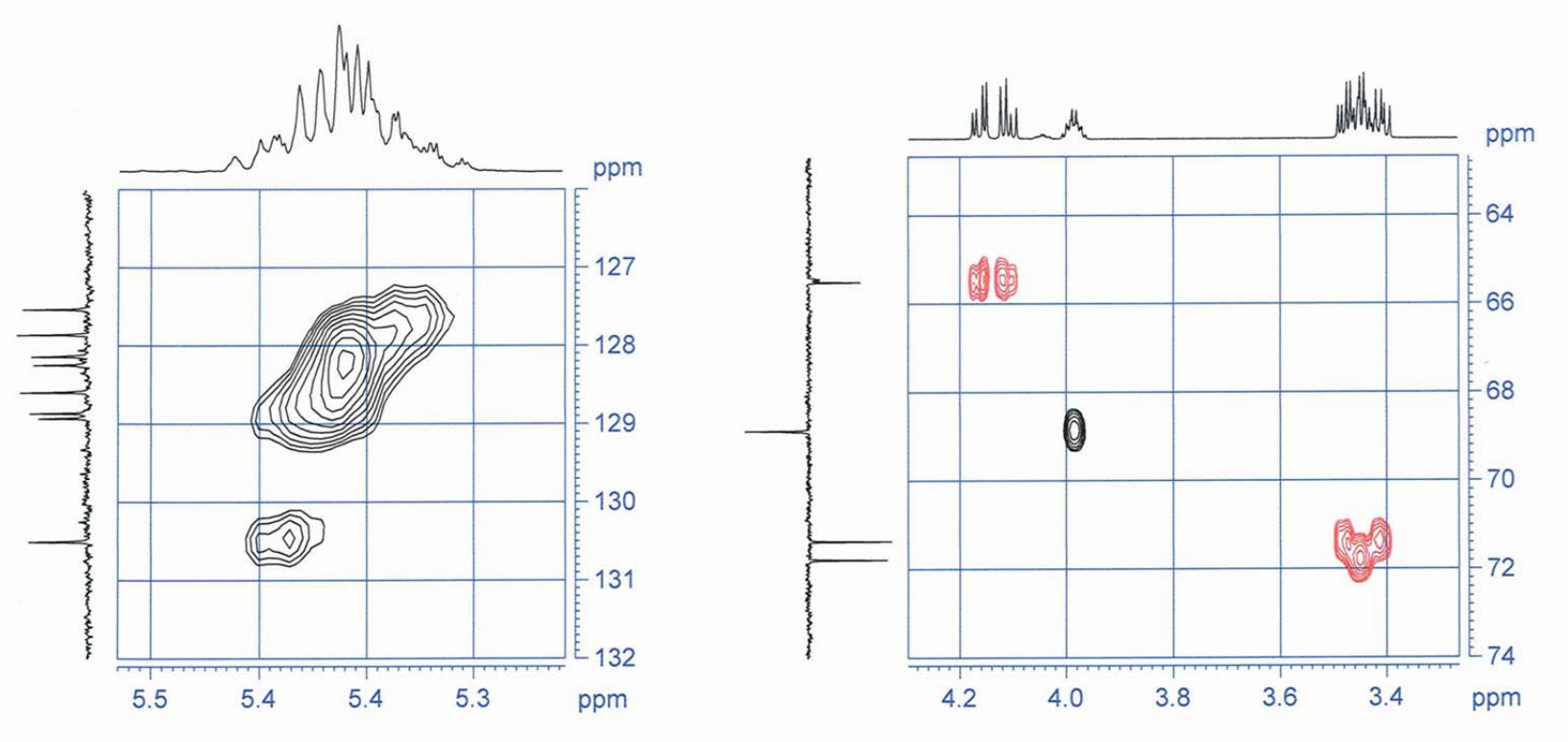


Fig. S32. Details of the HSQC spectrum of monoalkylmonoacylglycerol **4**.

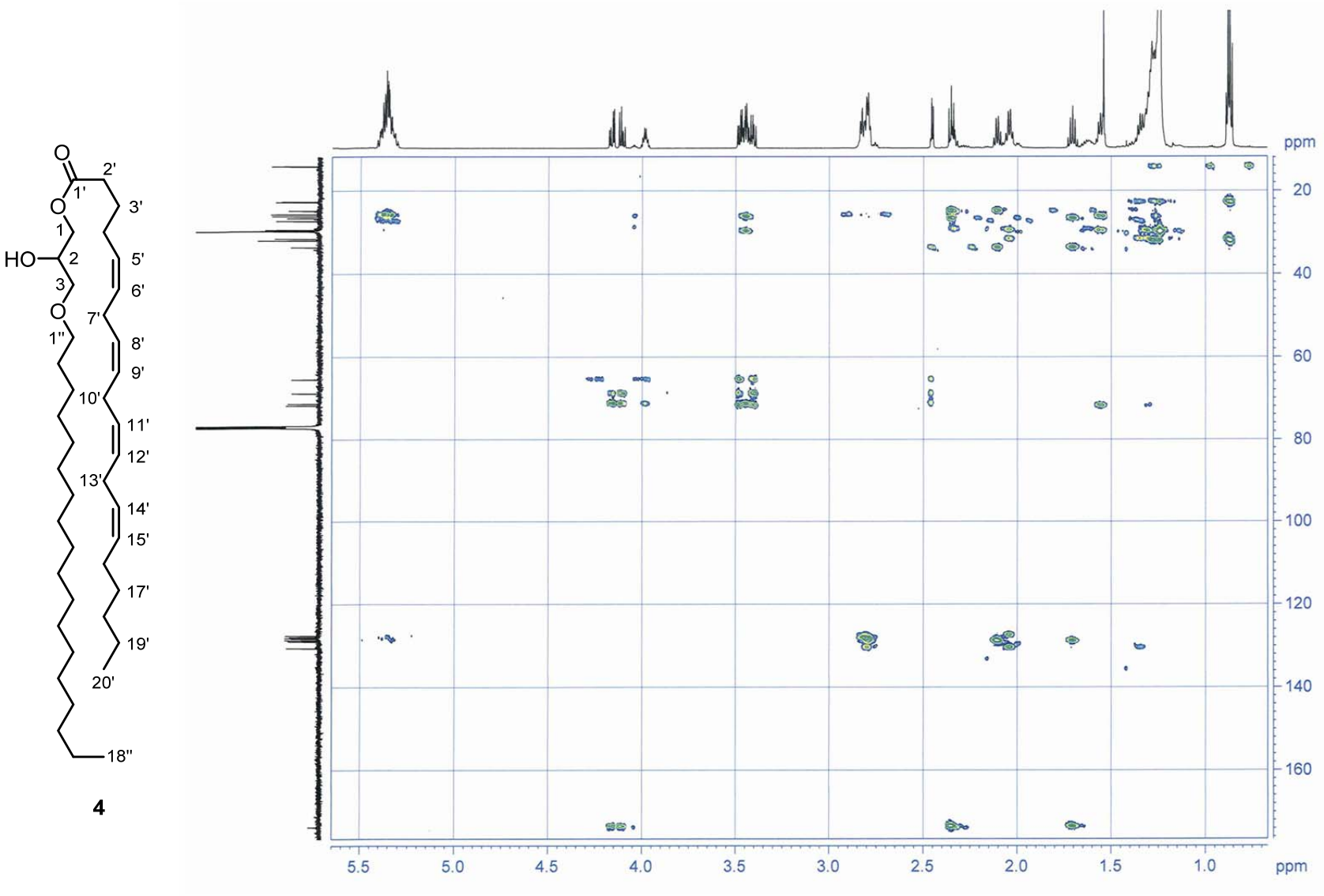


Fig. S33. HMBC spectrum of monoalkylmonoacylglycerol **4**.

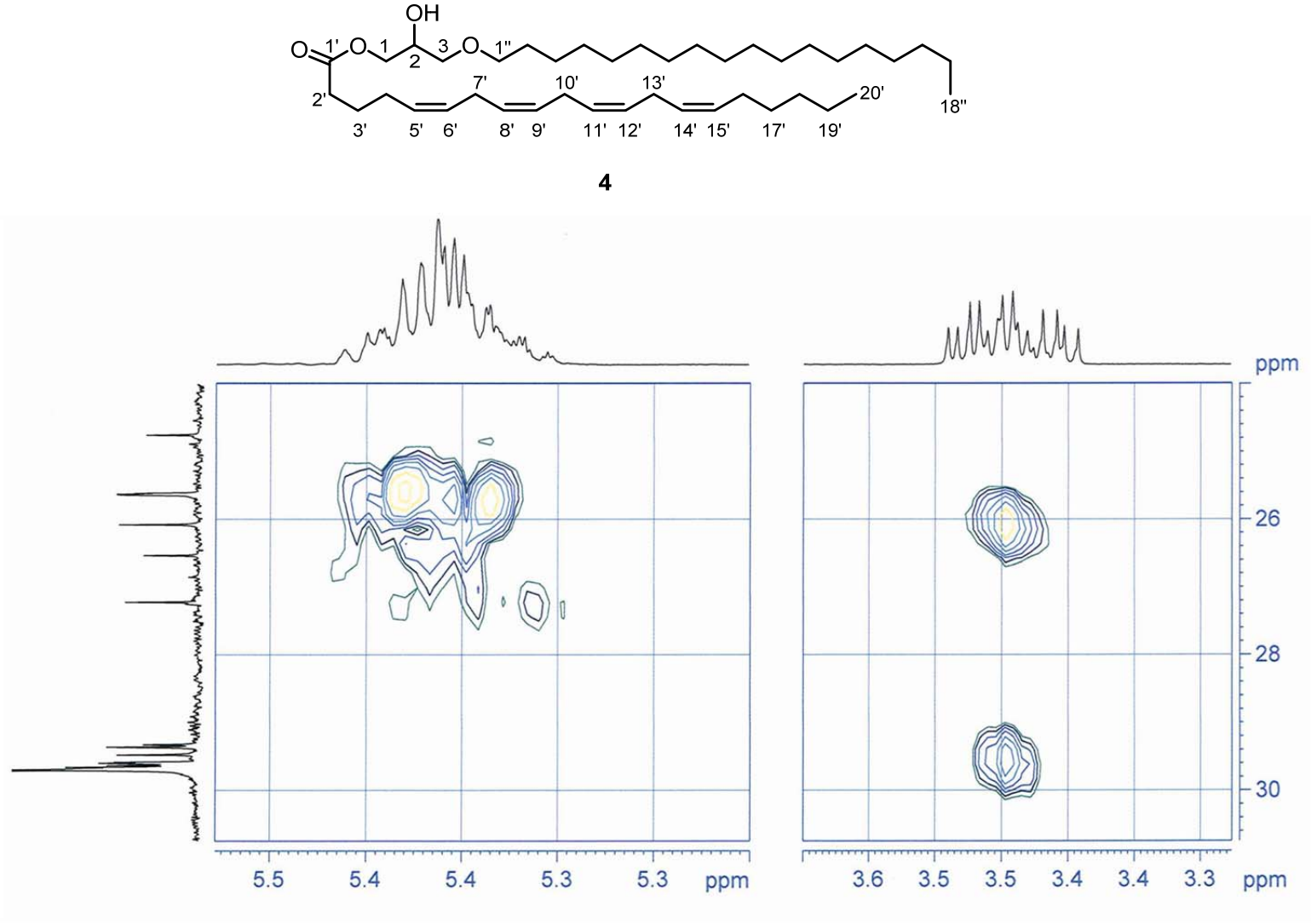


Fig. S34. Details of the HMBC spectrum of monoalkylmonoacylglycerol **4**.

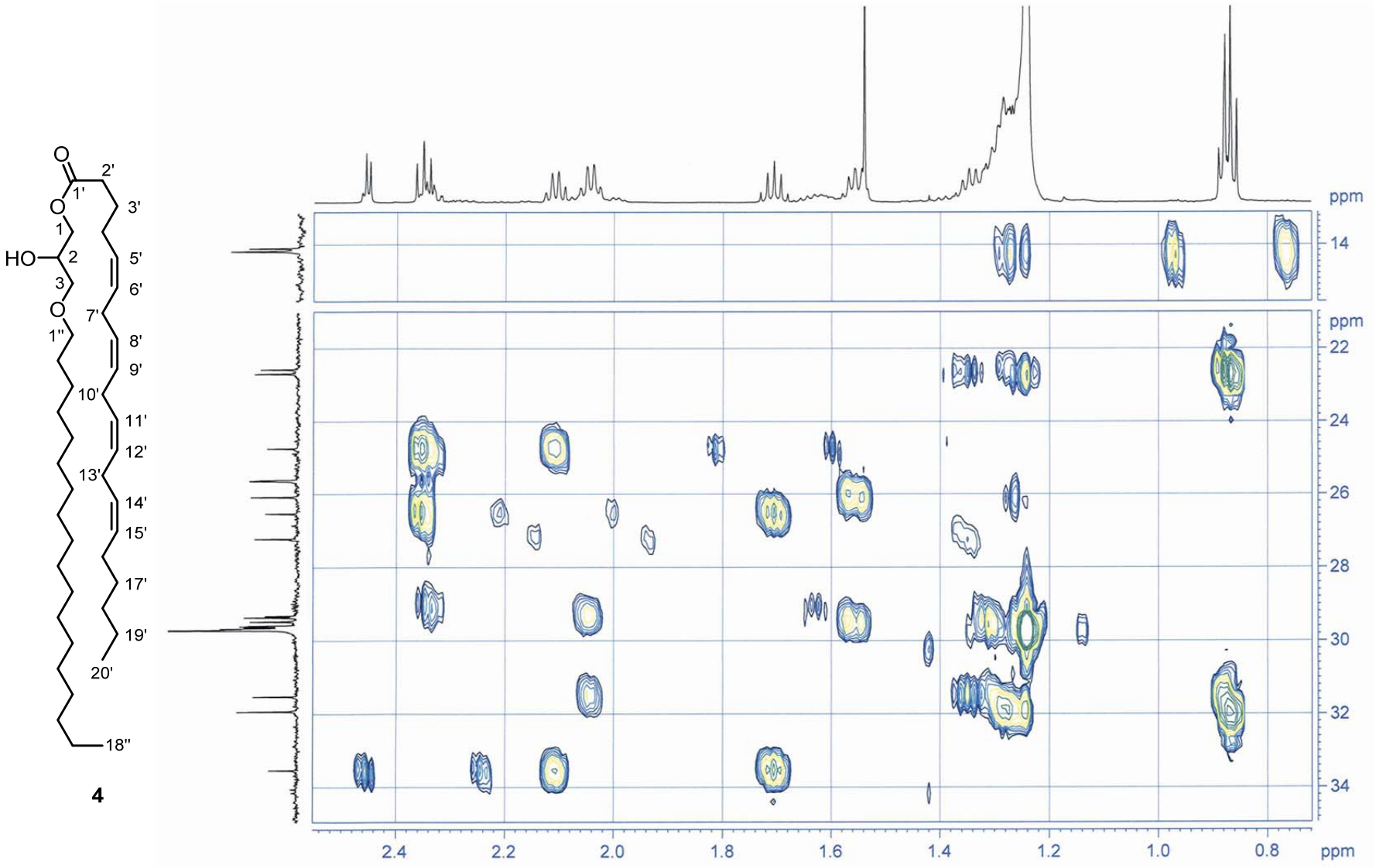


Fig. S35. Details of the HMBC spectrum of monoalkylmonoacylglycerol **4**.

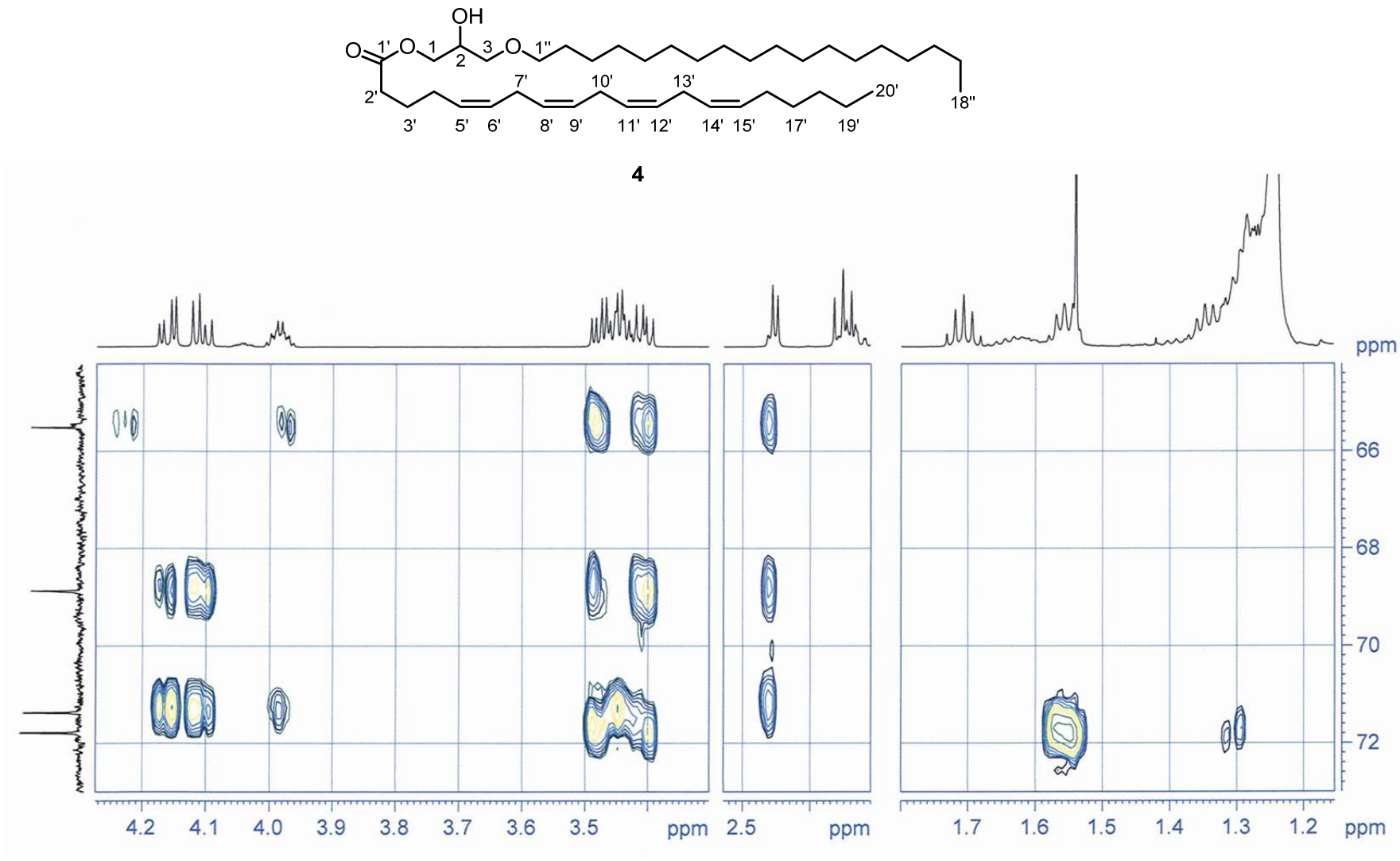


Fig. S36. Details of the HMBC spectrum of monoalkylmonoacylglycerol **4**.

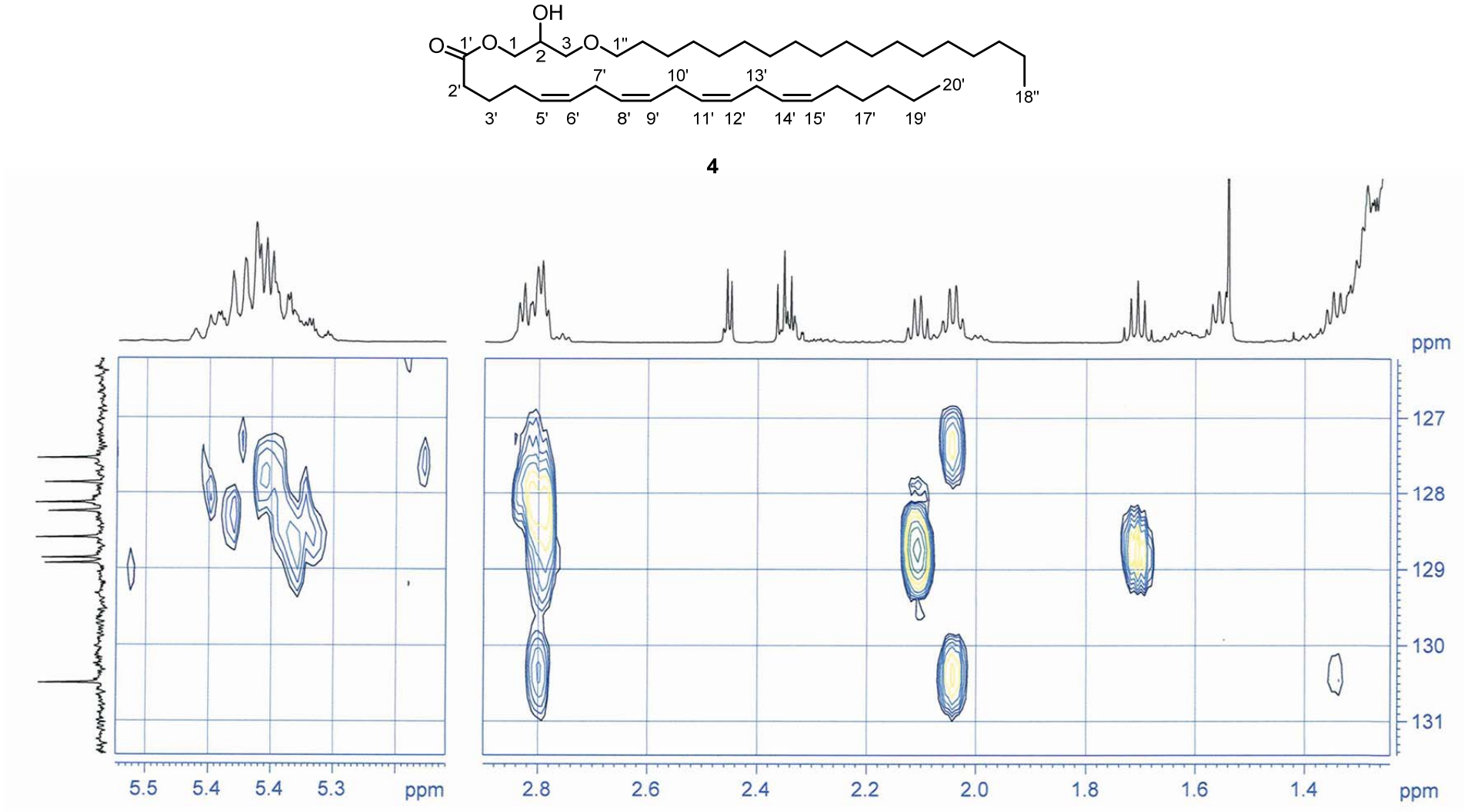


Fig. S37. Details of the HMBC spectrum of monoalkylmonoacylglycerol **4**.

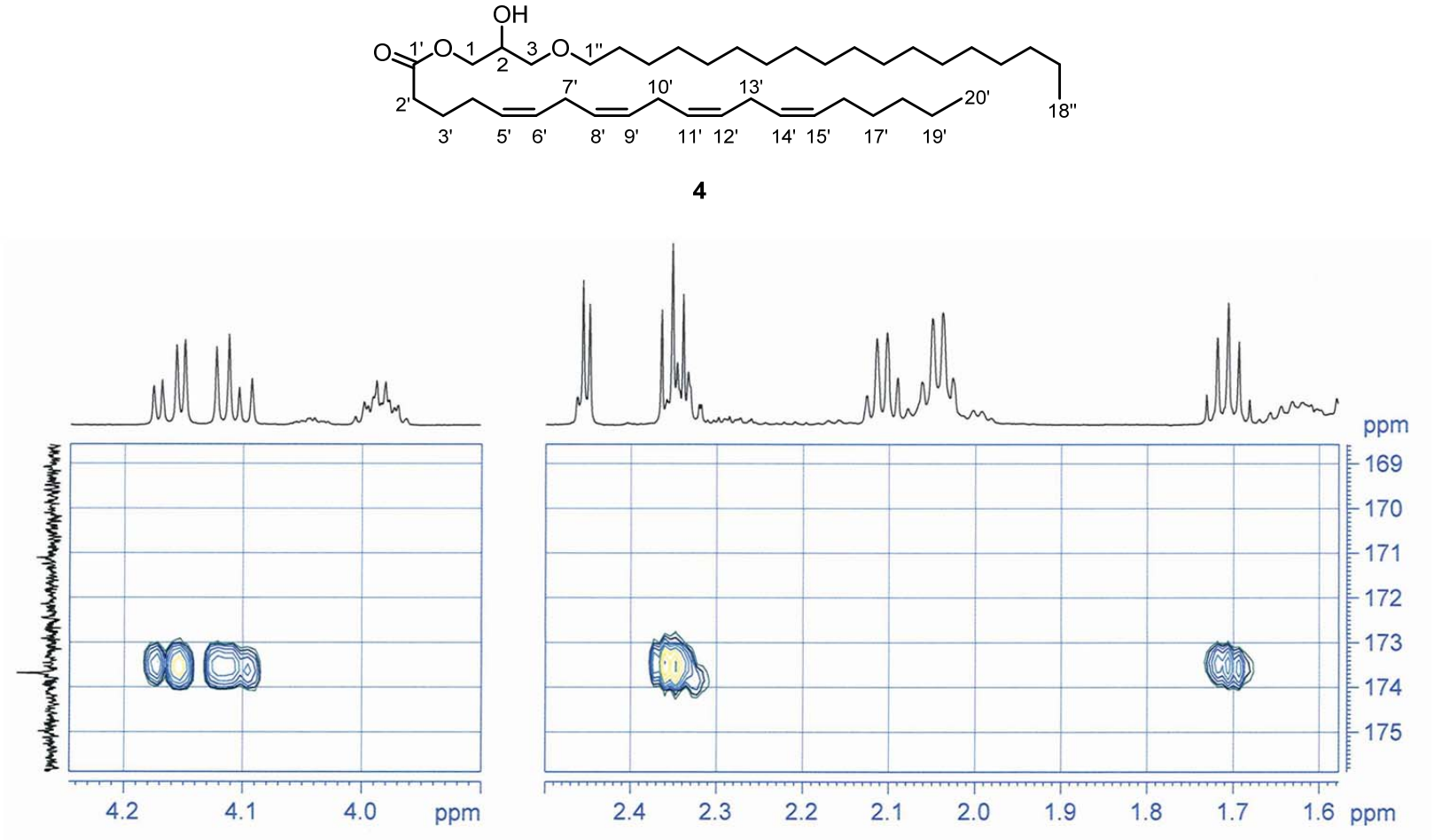
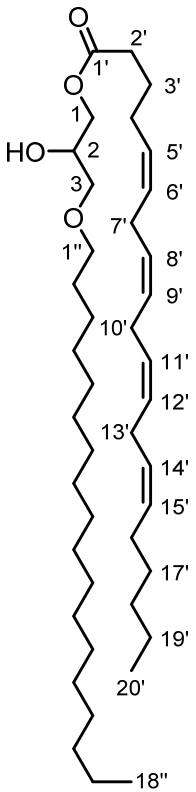


Fig. S38. Details of the HMBC spectrum of monoalkylmonoacylglycerol **4**.



4

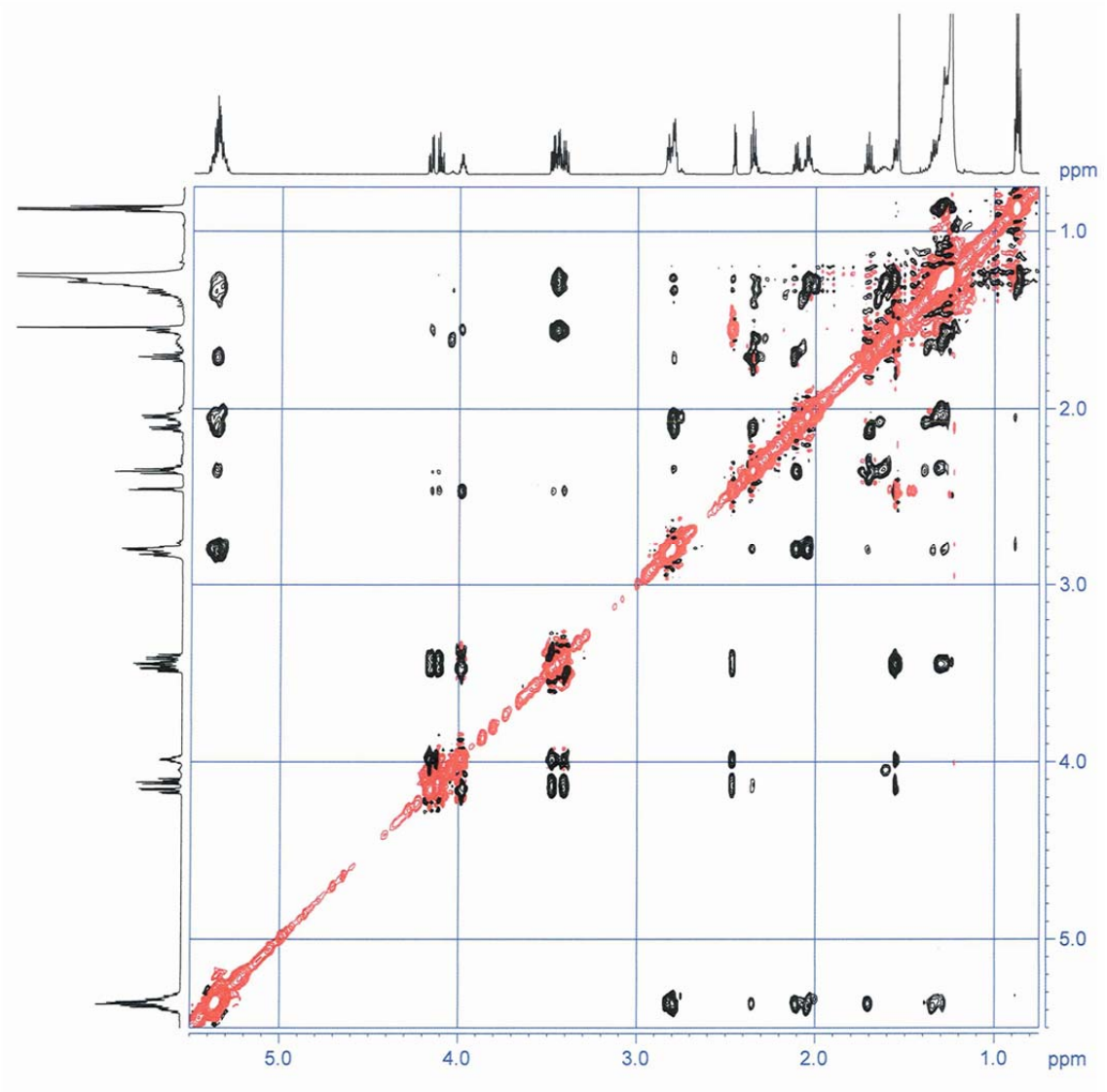
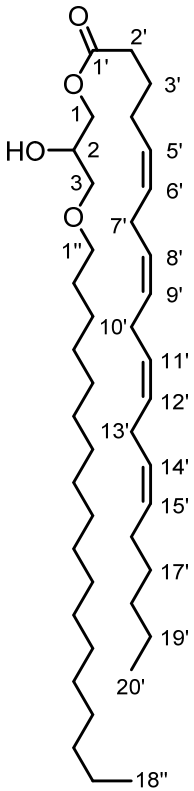


Fig. S39. NOESY spectrum of monoalkylmonoacylglycerol **4**.



4

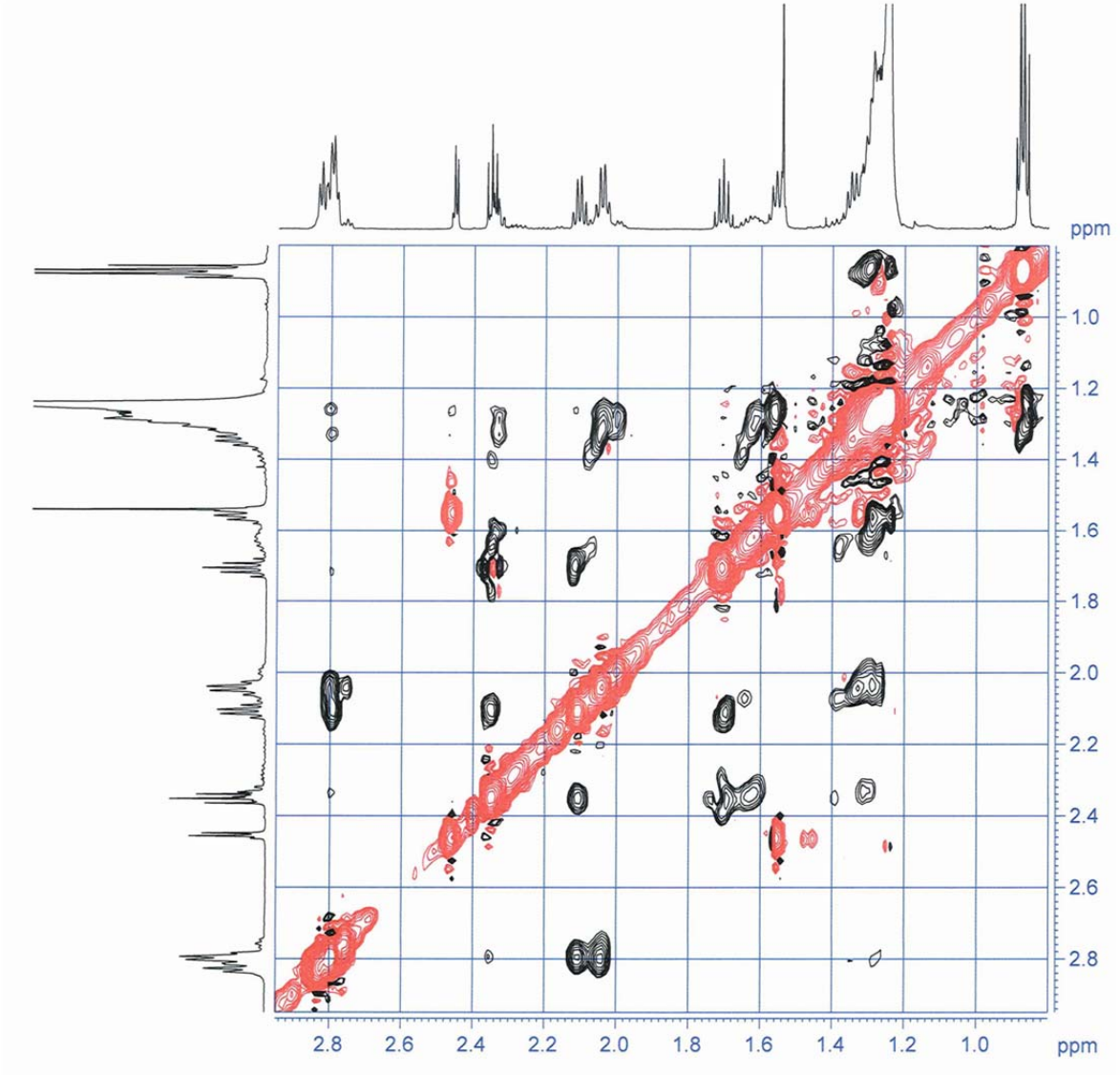


Fig. S40. Details of the NOESY spectrum of monoalkylmonoacylglycerol **4**.

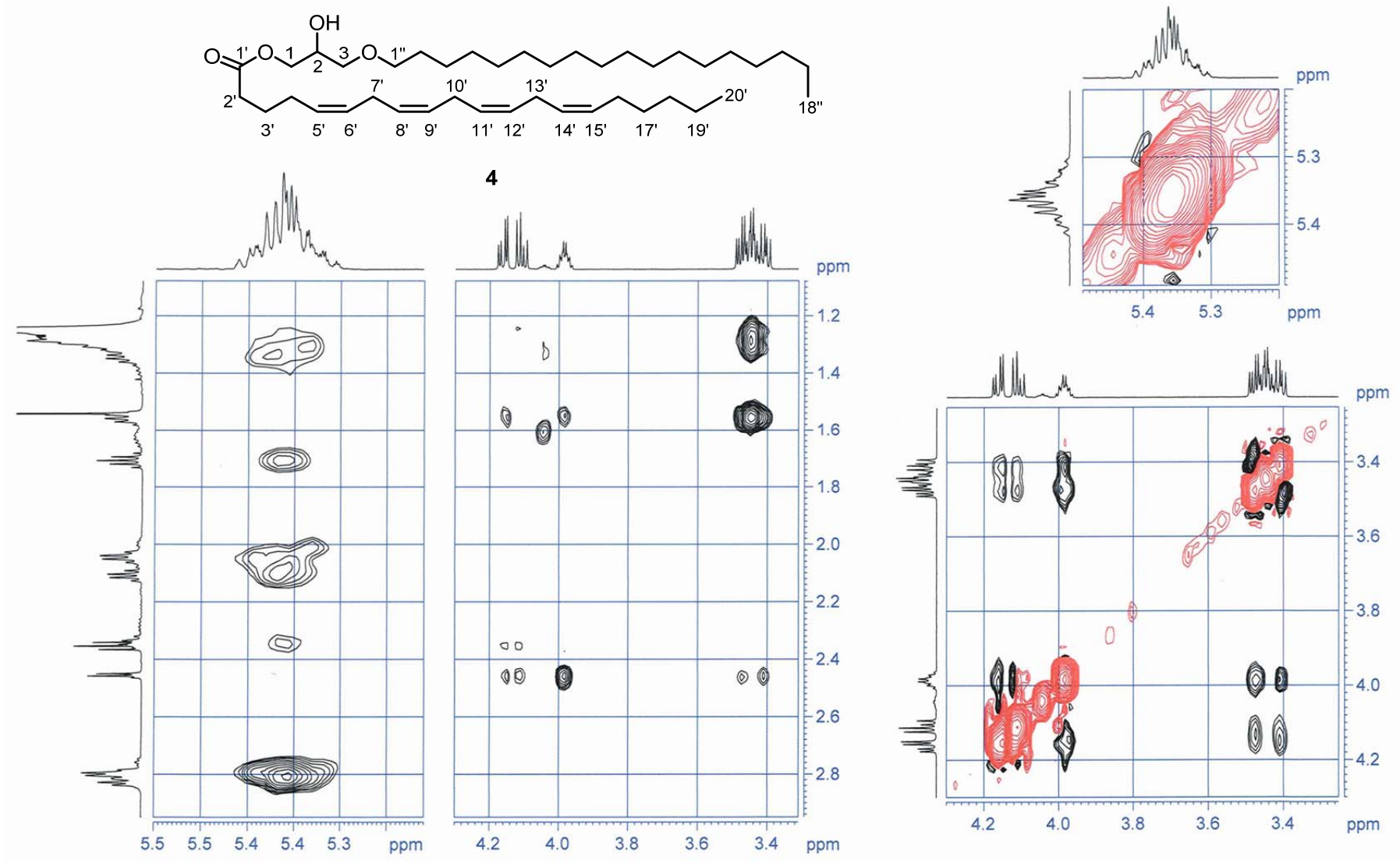


Fig. S41. Details of the NOESY spectrum of monoalkylmonoacylglycerol **4**.

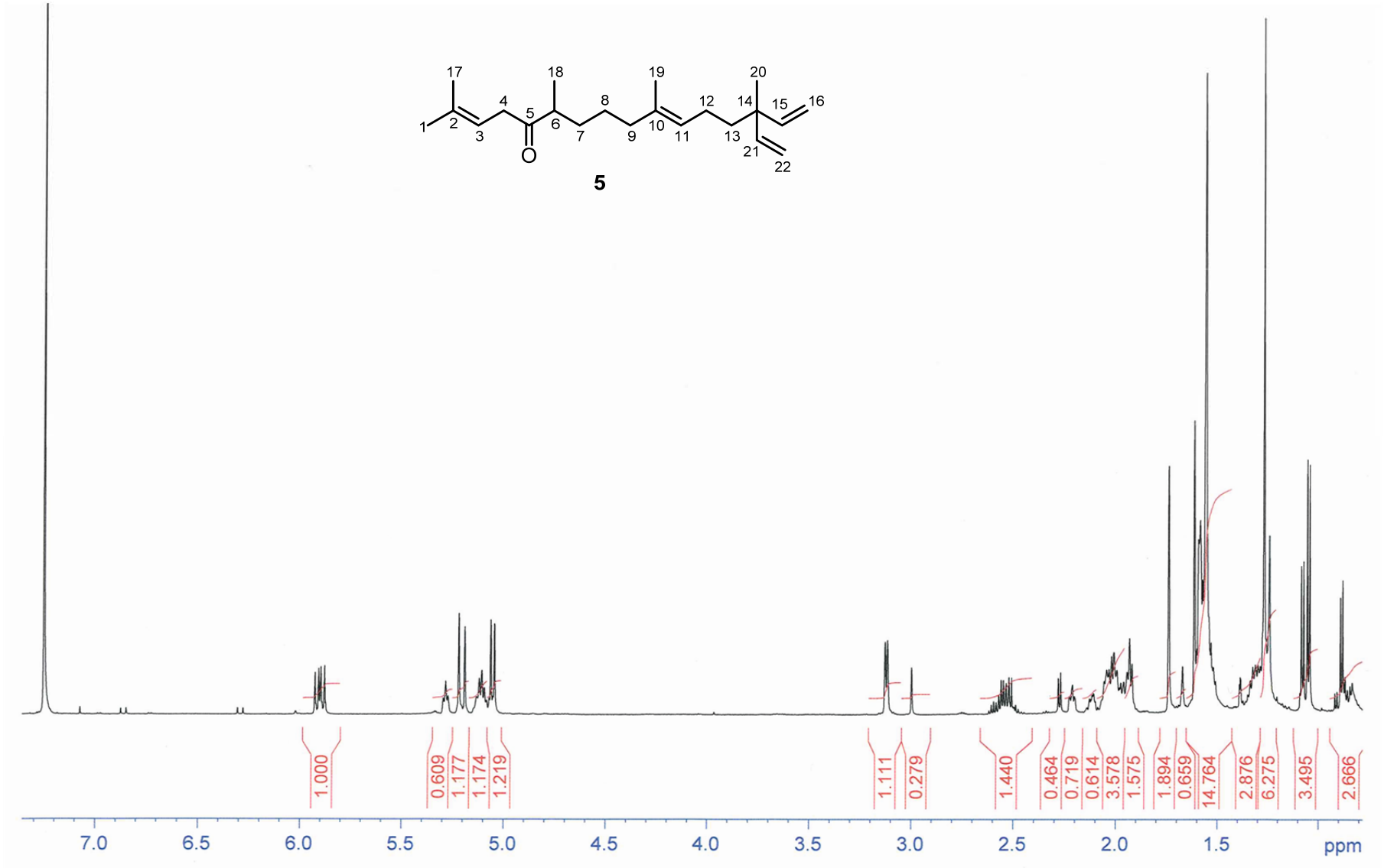


Fig. S42. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound **5**.

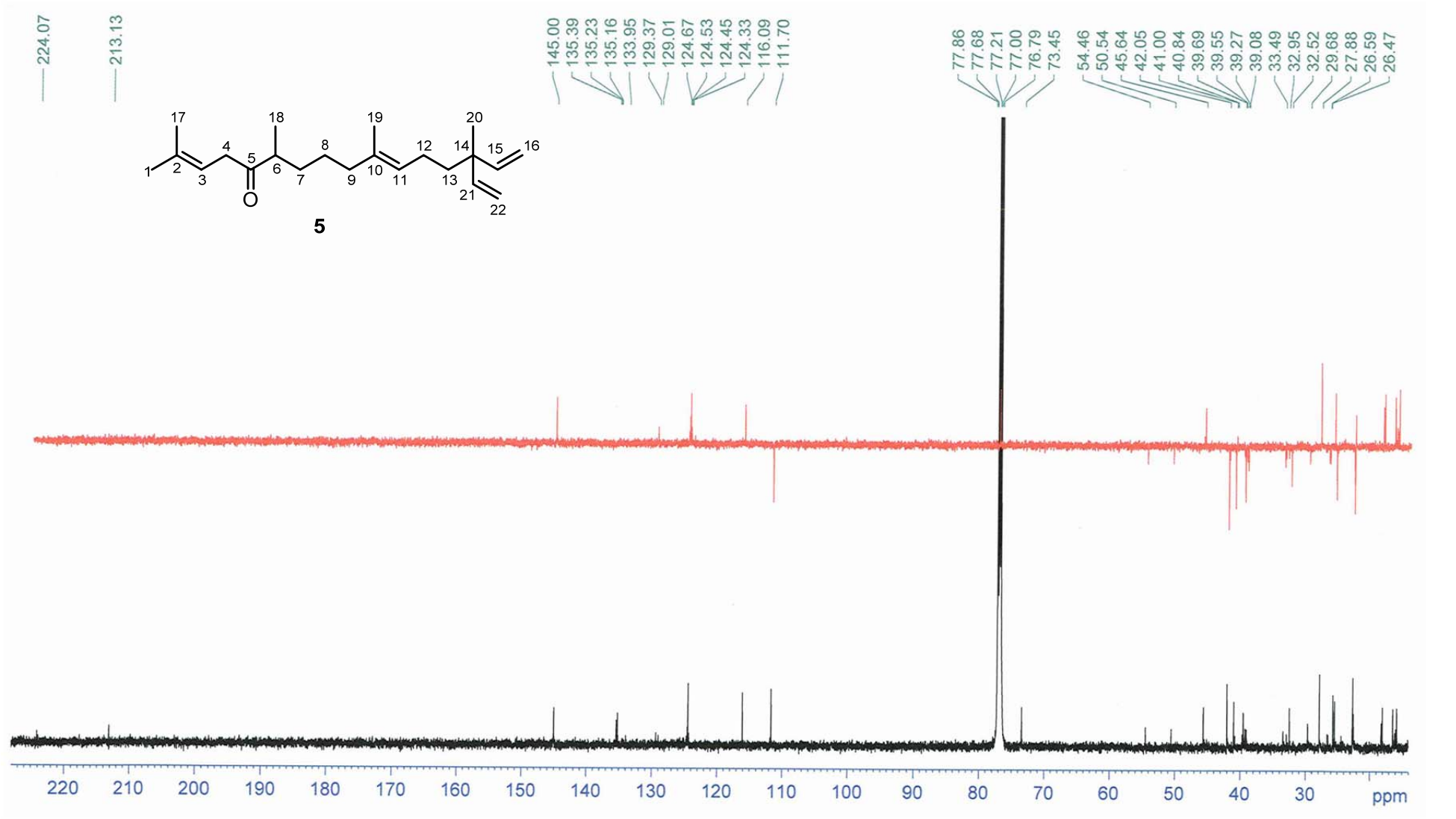


Fig. S43. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound **5**.

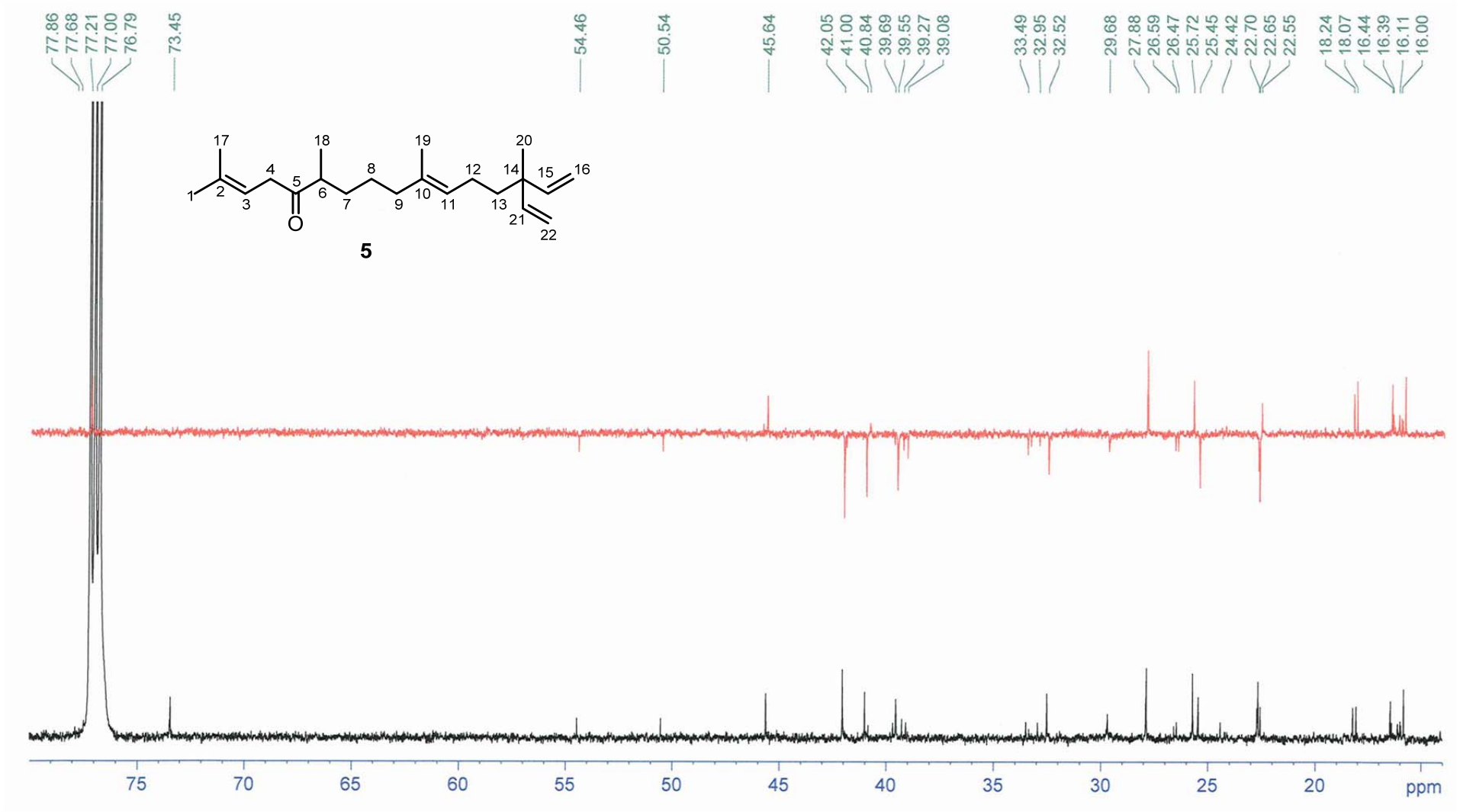
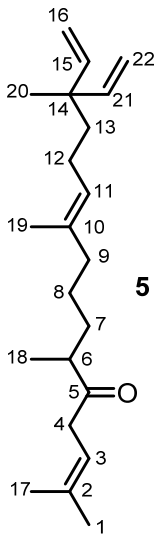


Fig. S44. Details of the ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound **5**.



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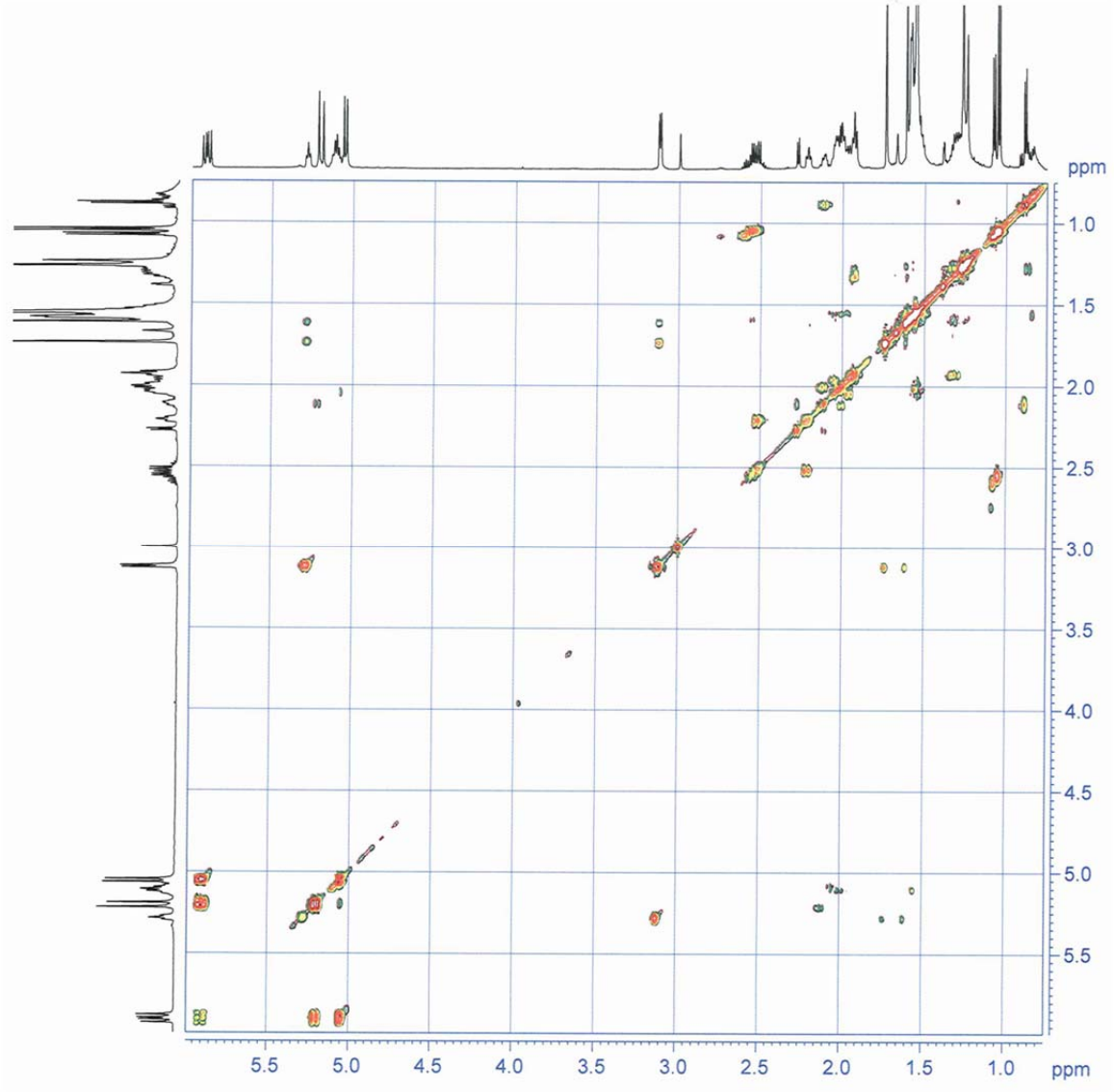


Fig. S45. COSY spectrum of compound **5**.

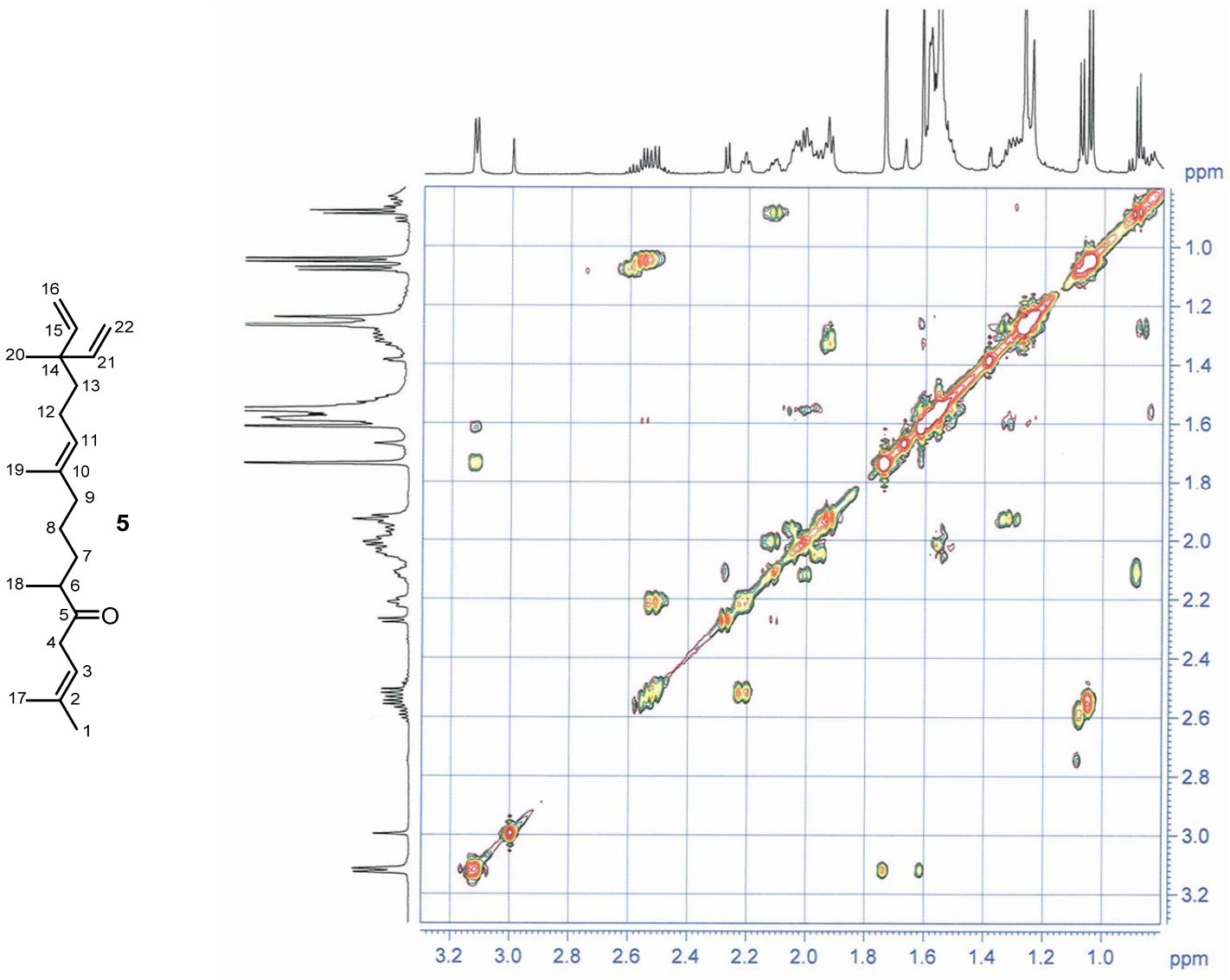
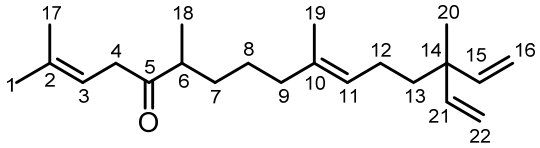


Fig. S46. Details of the COSY spectrum of compound **5**.



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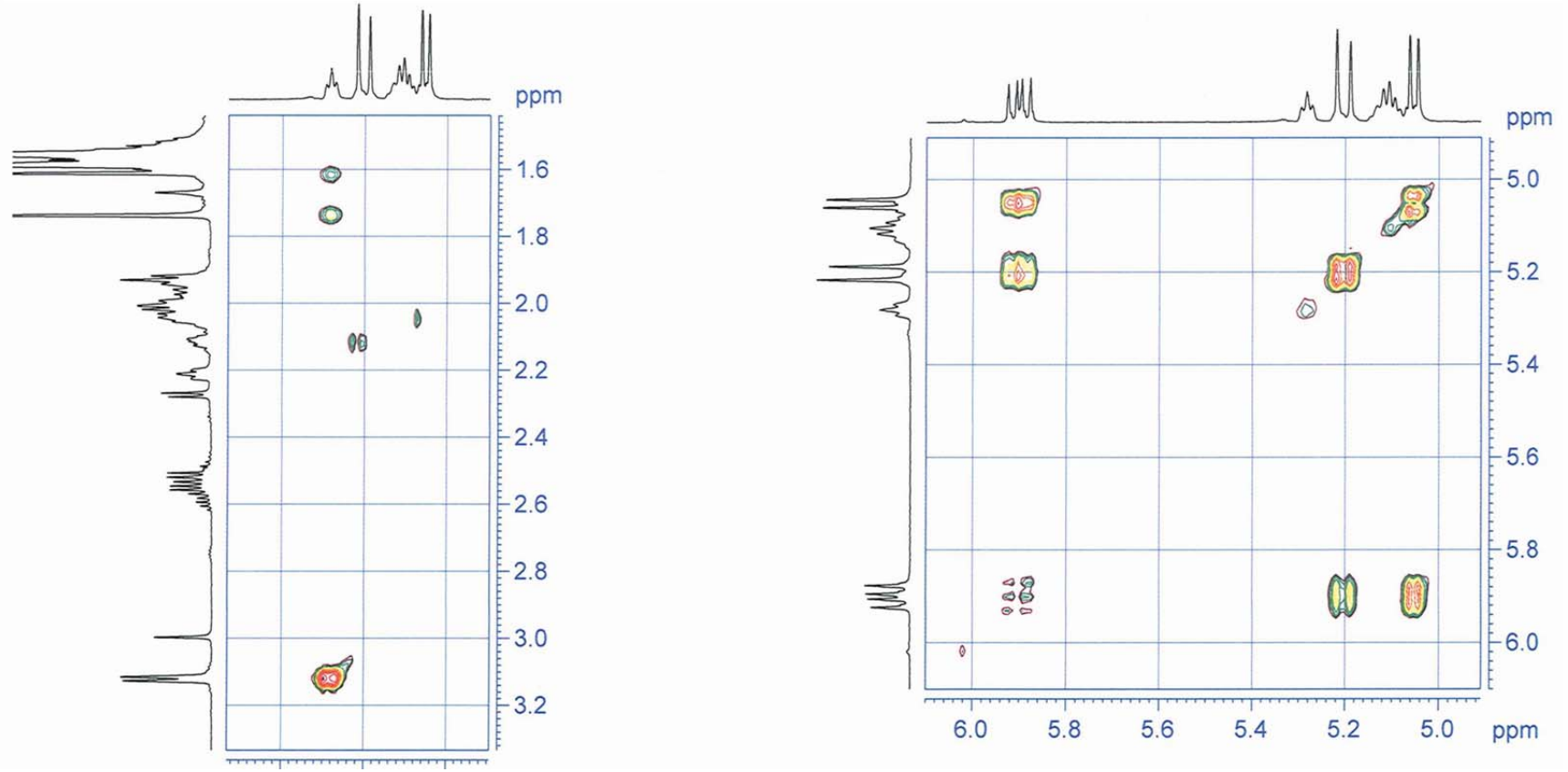


Fig. S47. Details of the COSY spectrum of compound **5**.

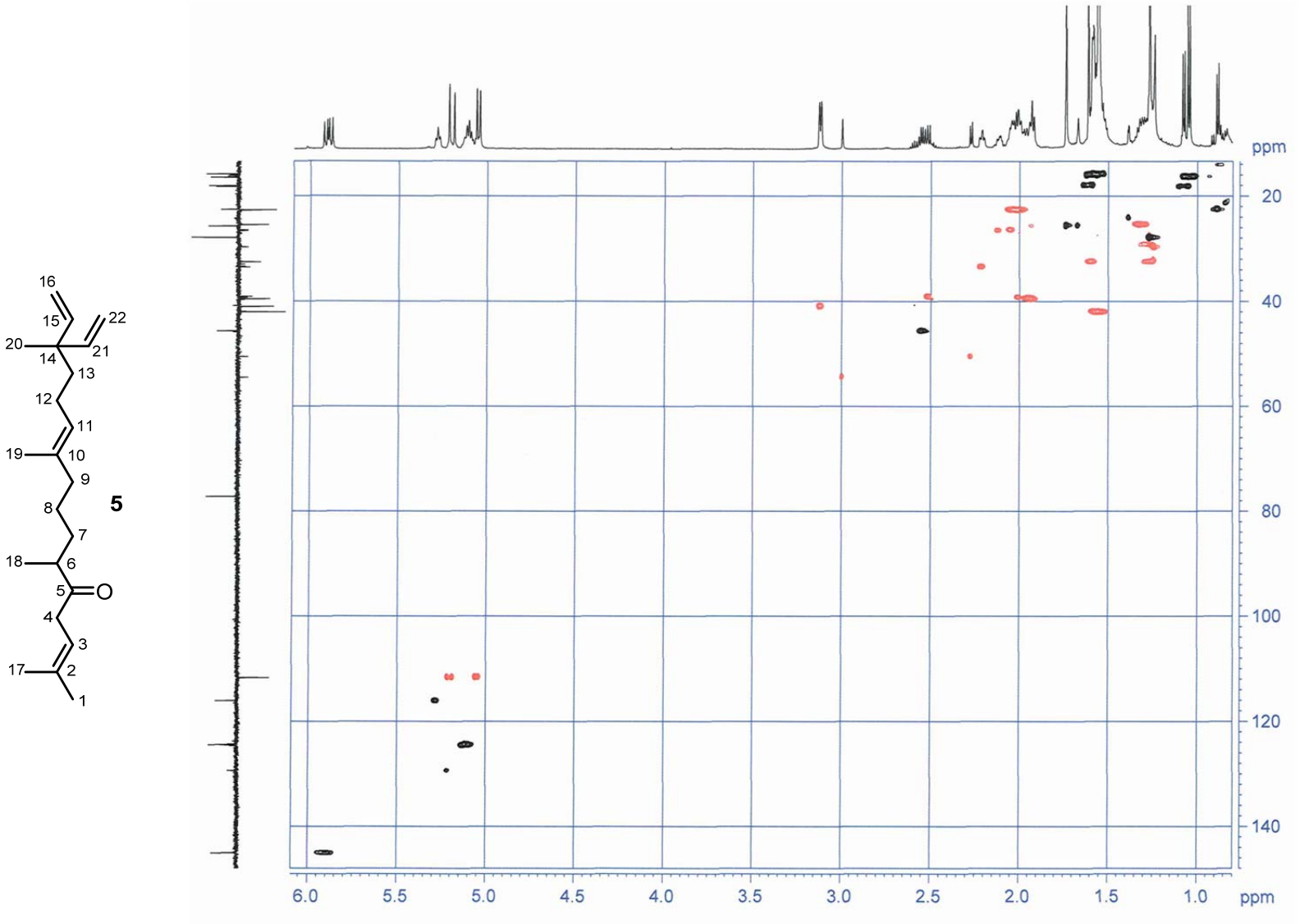


Fig. S48. HSQC spectrum of compound **5**.

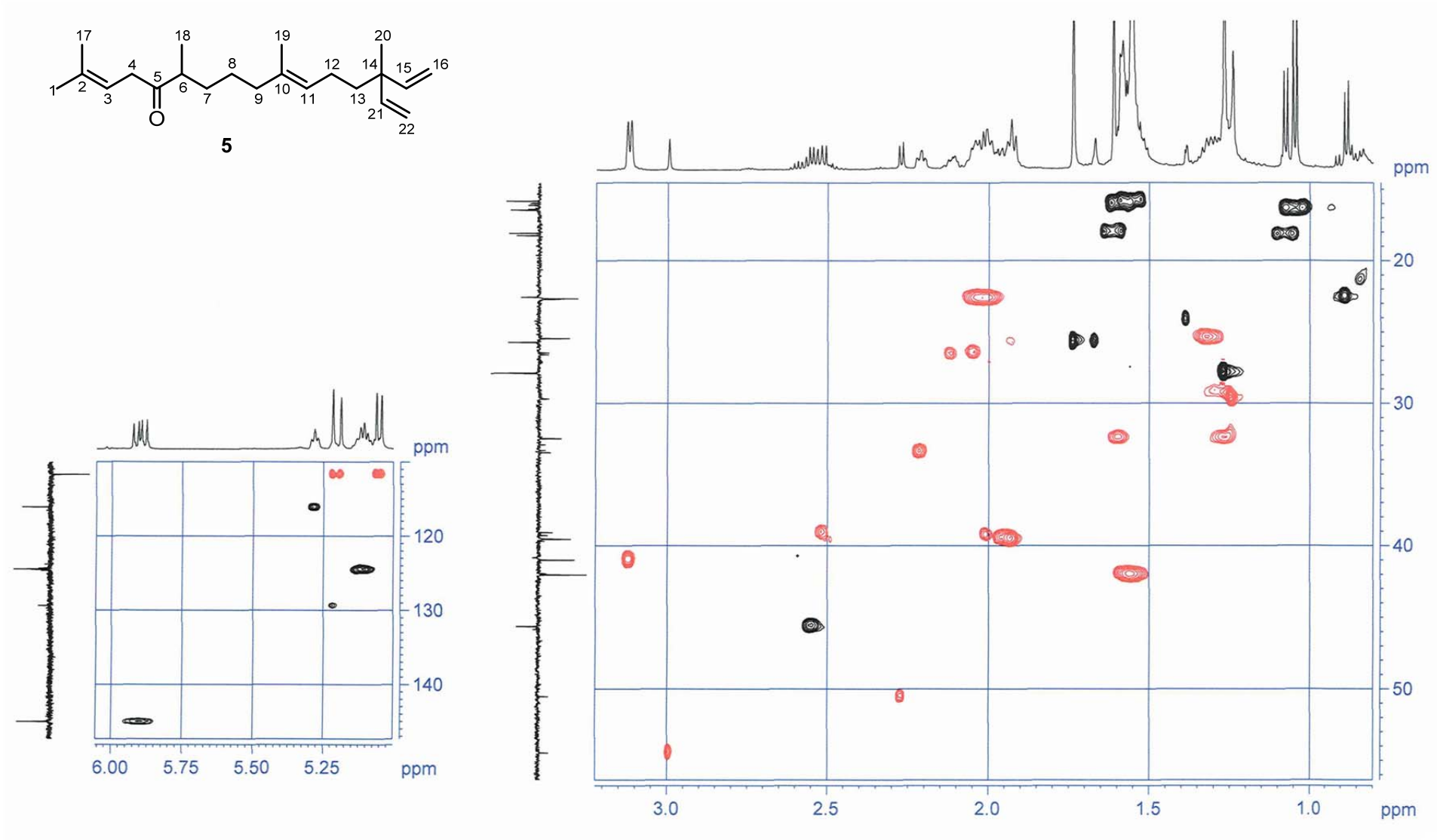


Fig. S49. Details of the HSQC spectrum of compound **5**.

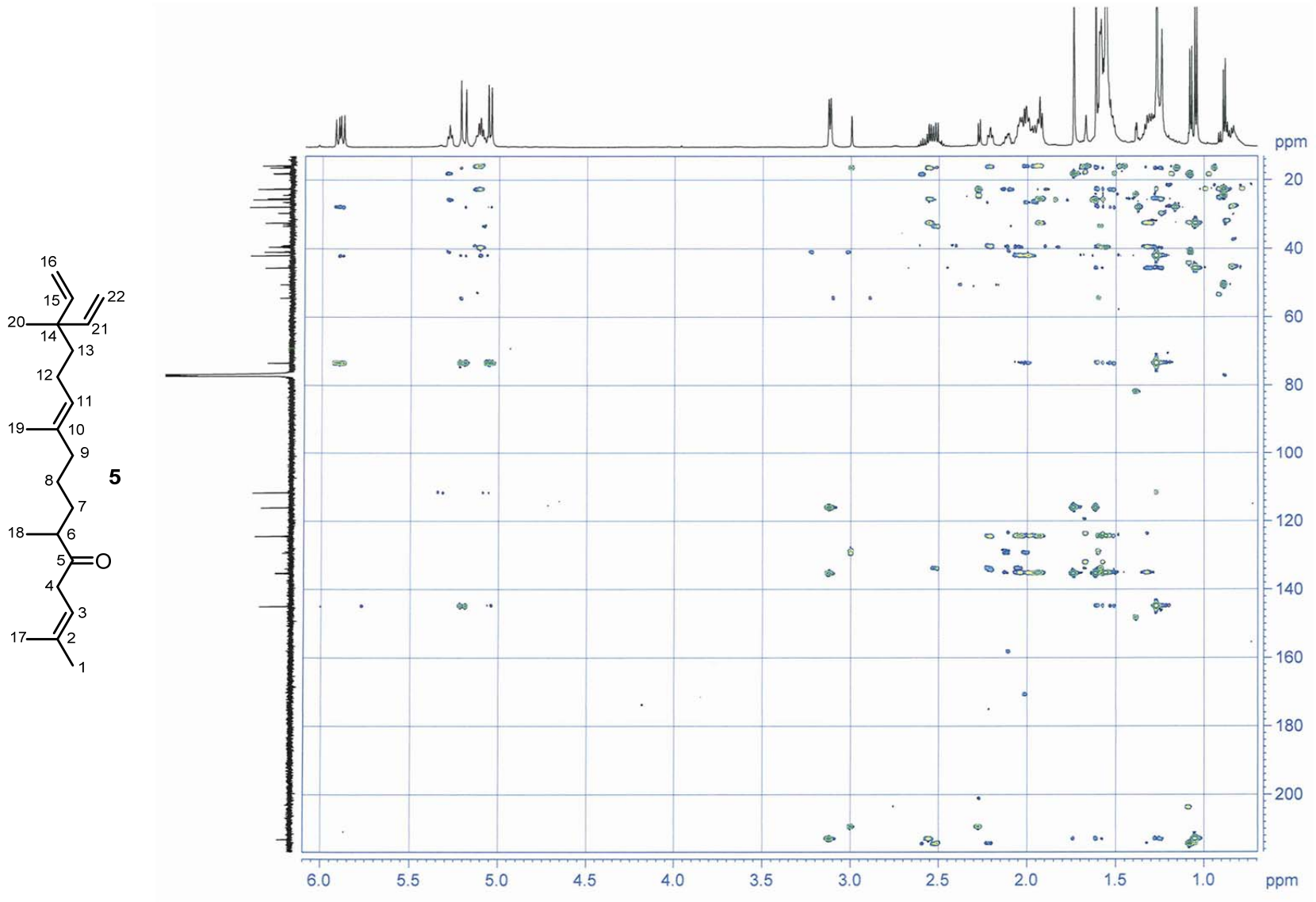
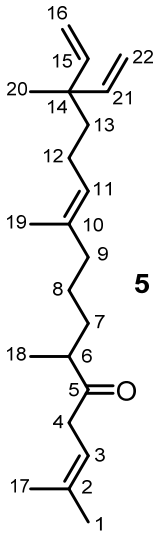


Fig. S50. HMBC spectrum of compound **5**.



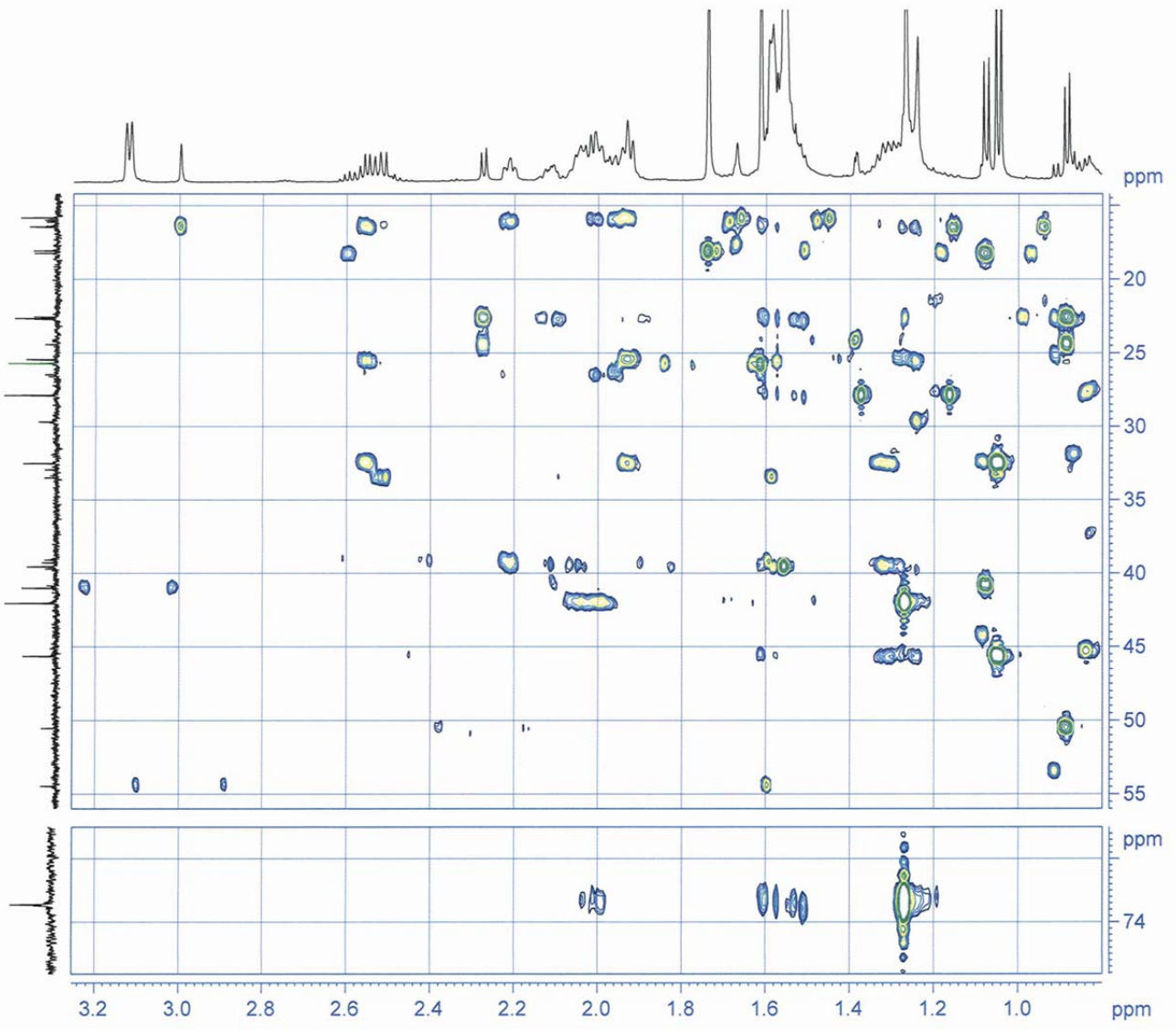
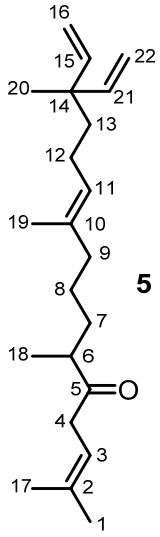


Fig. S51. Details of the HMBC spectrum of compound **5**.



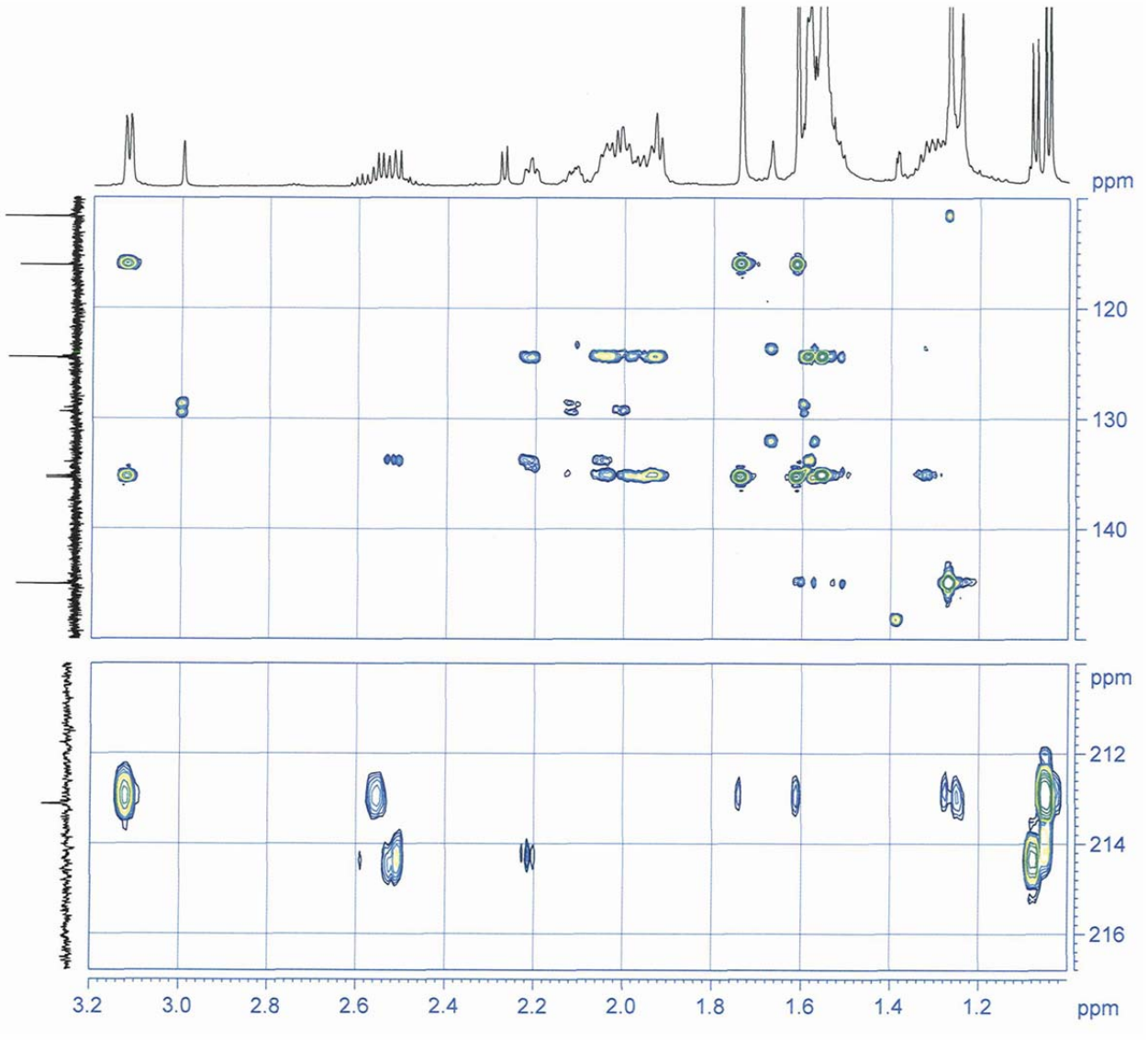
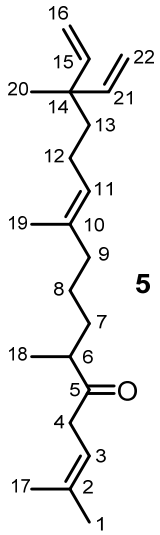


Fig. S52. Details of the HMBC spectrum of compound **5**.



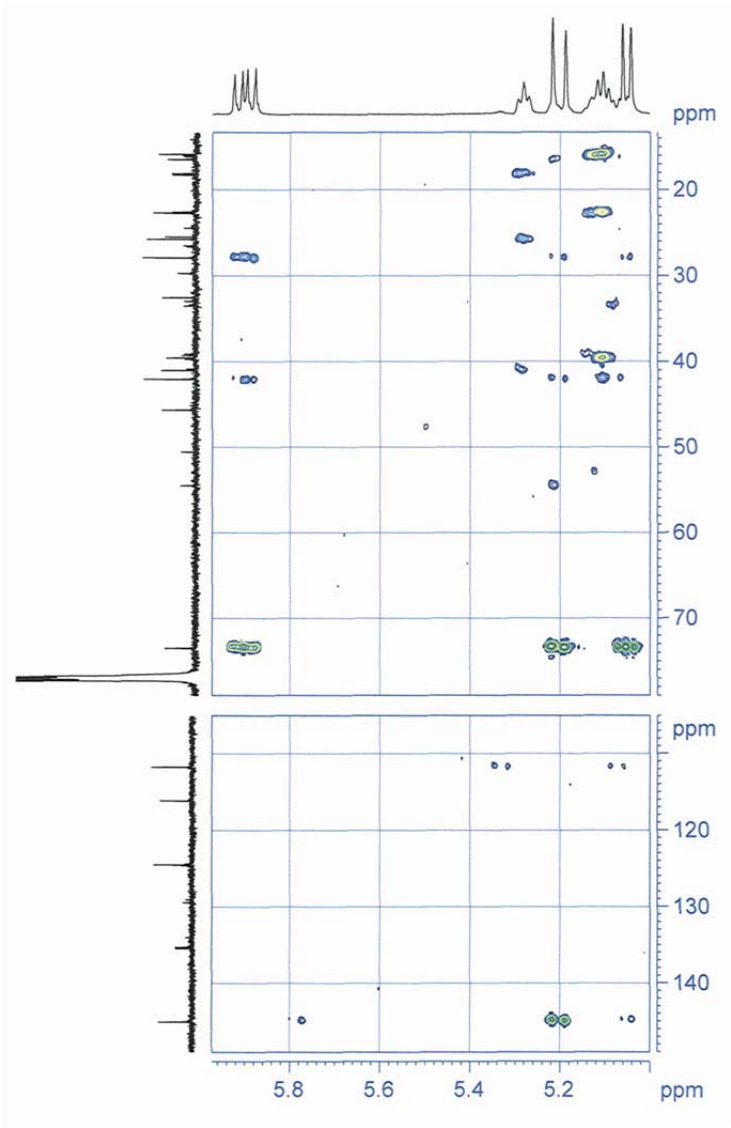
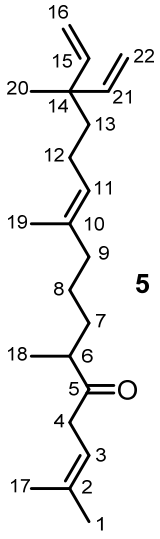


Fig. S53. Details of the HMBC spectrum of compound **5**.



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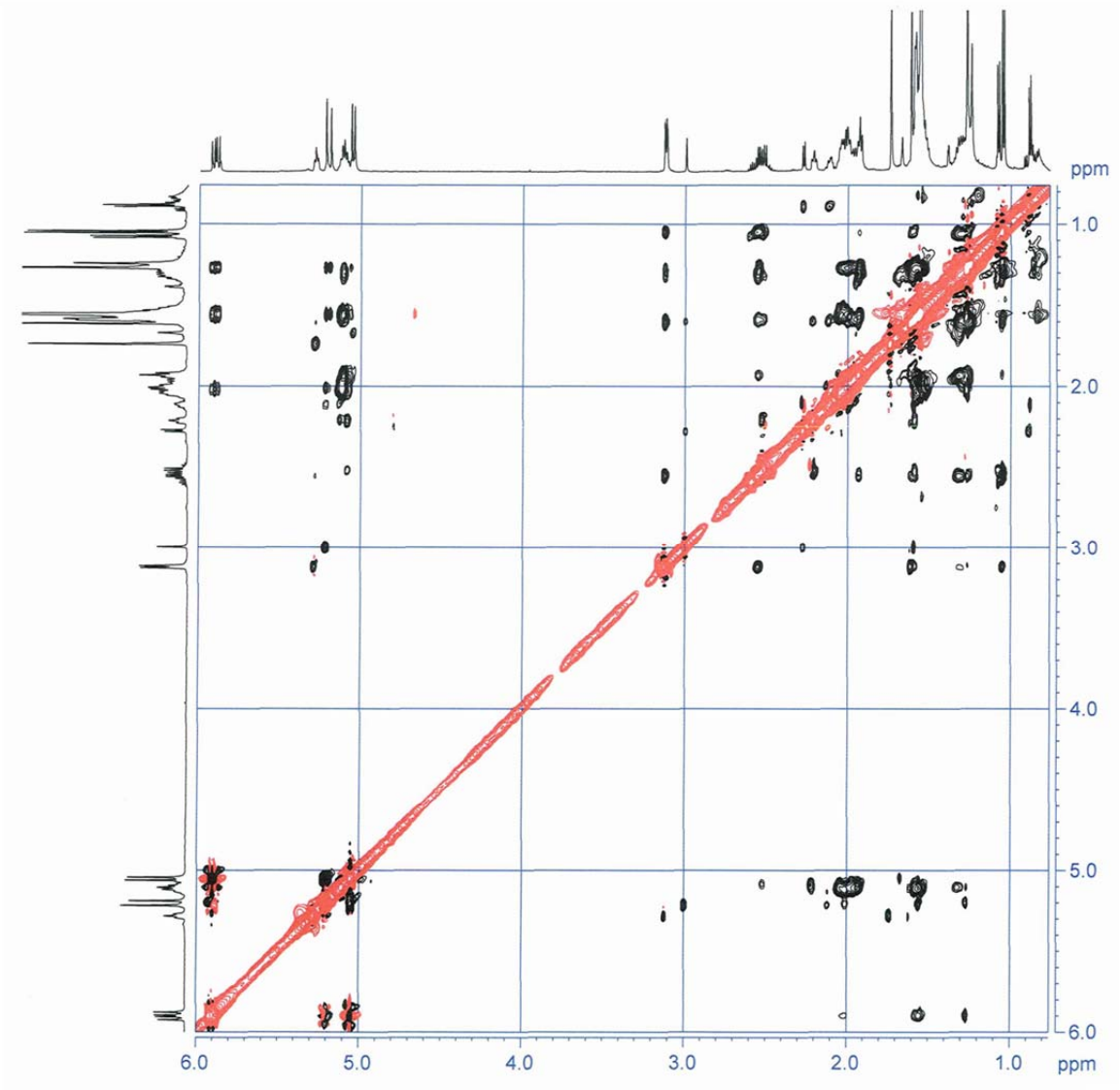
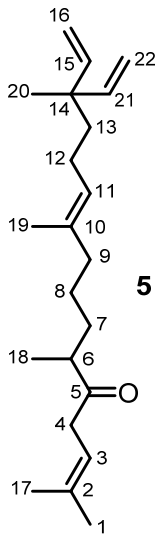


Fig. S54. NOESY spectrum of compound **5**.



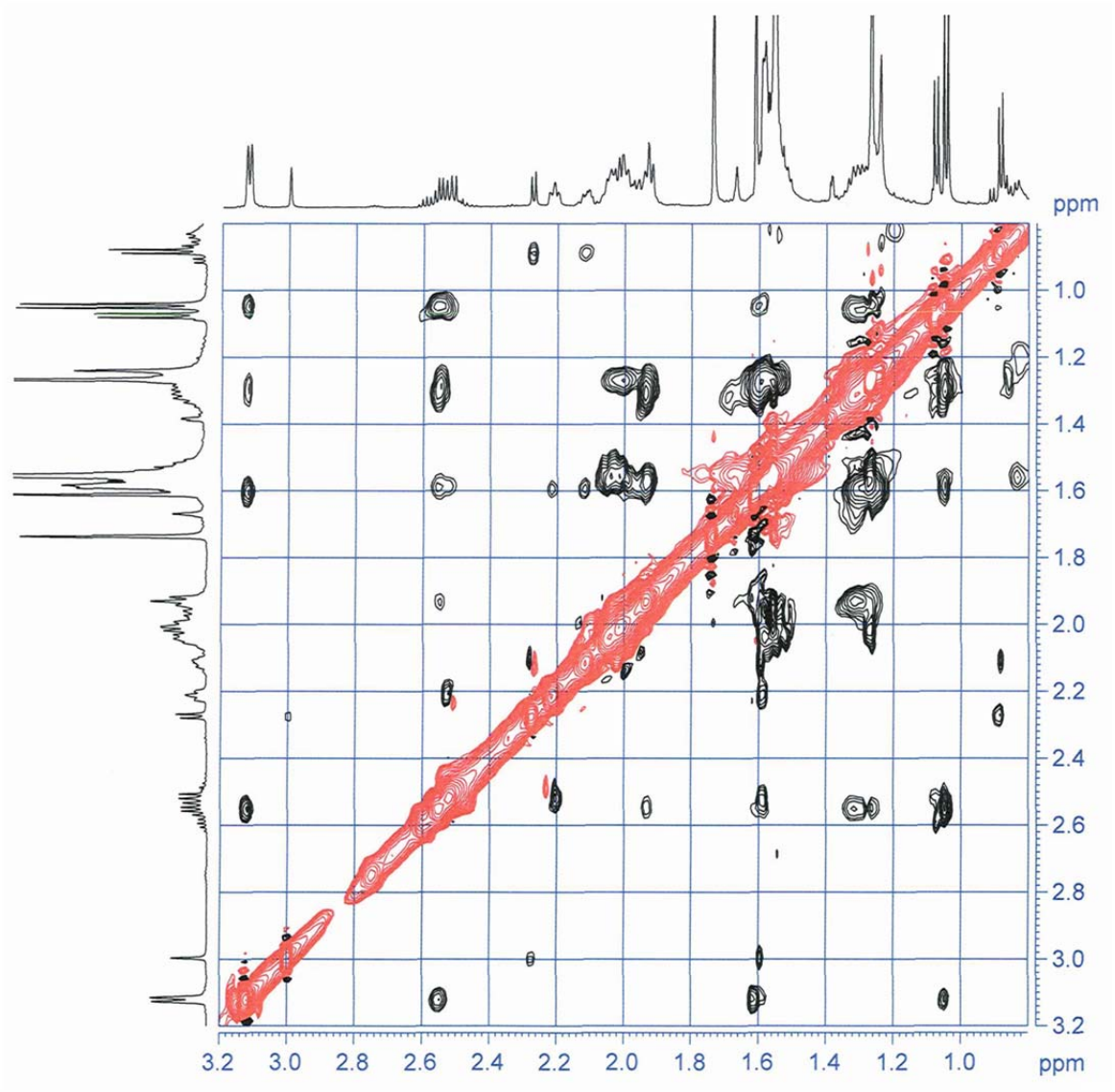


Fig. S55. Details of the NOESY spectrum of compound **5**.

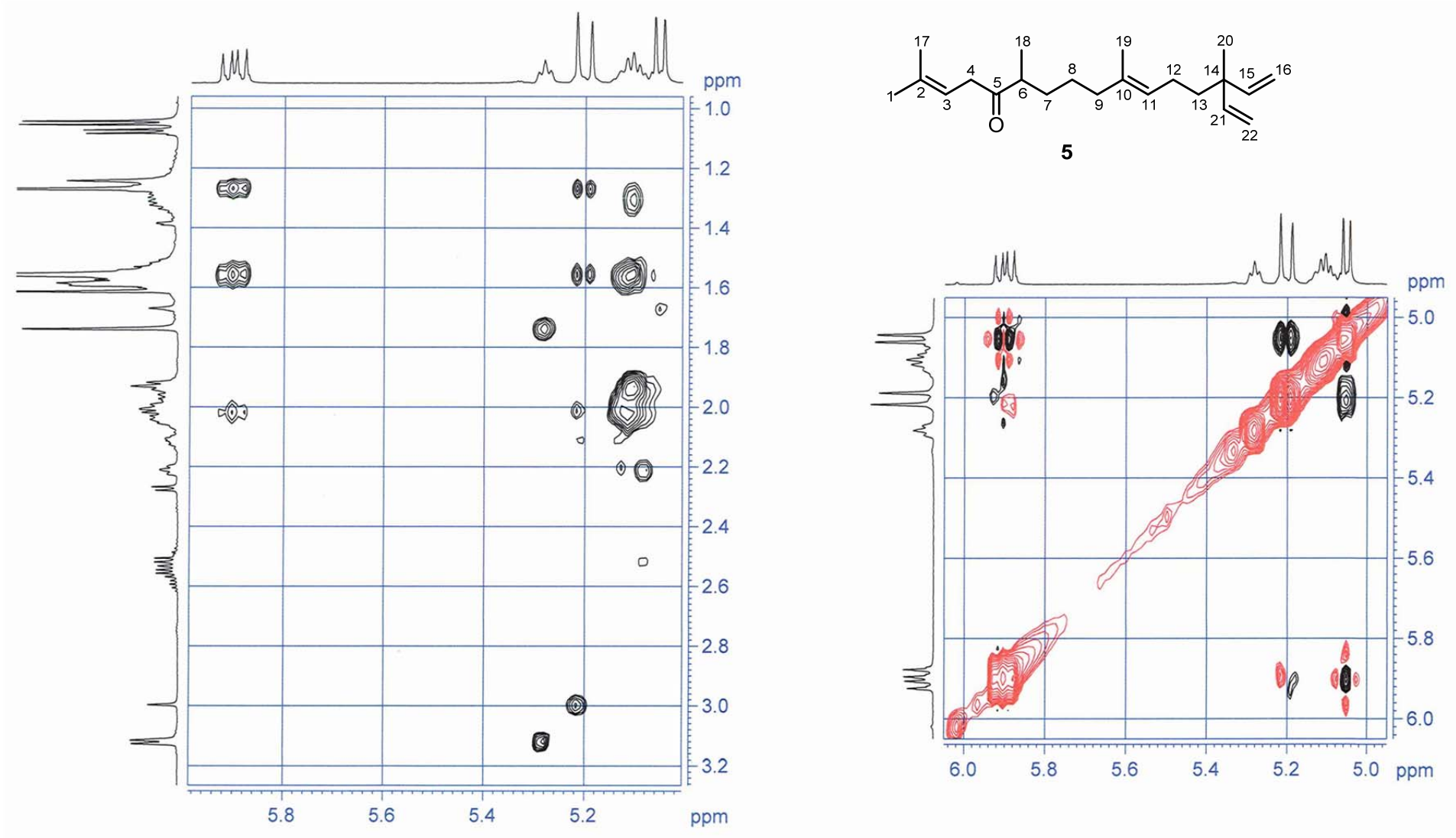


Fig. S56. Details of the NOESY spectrum of compound **5**.

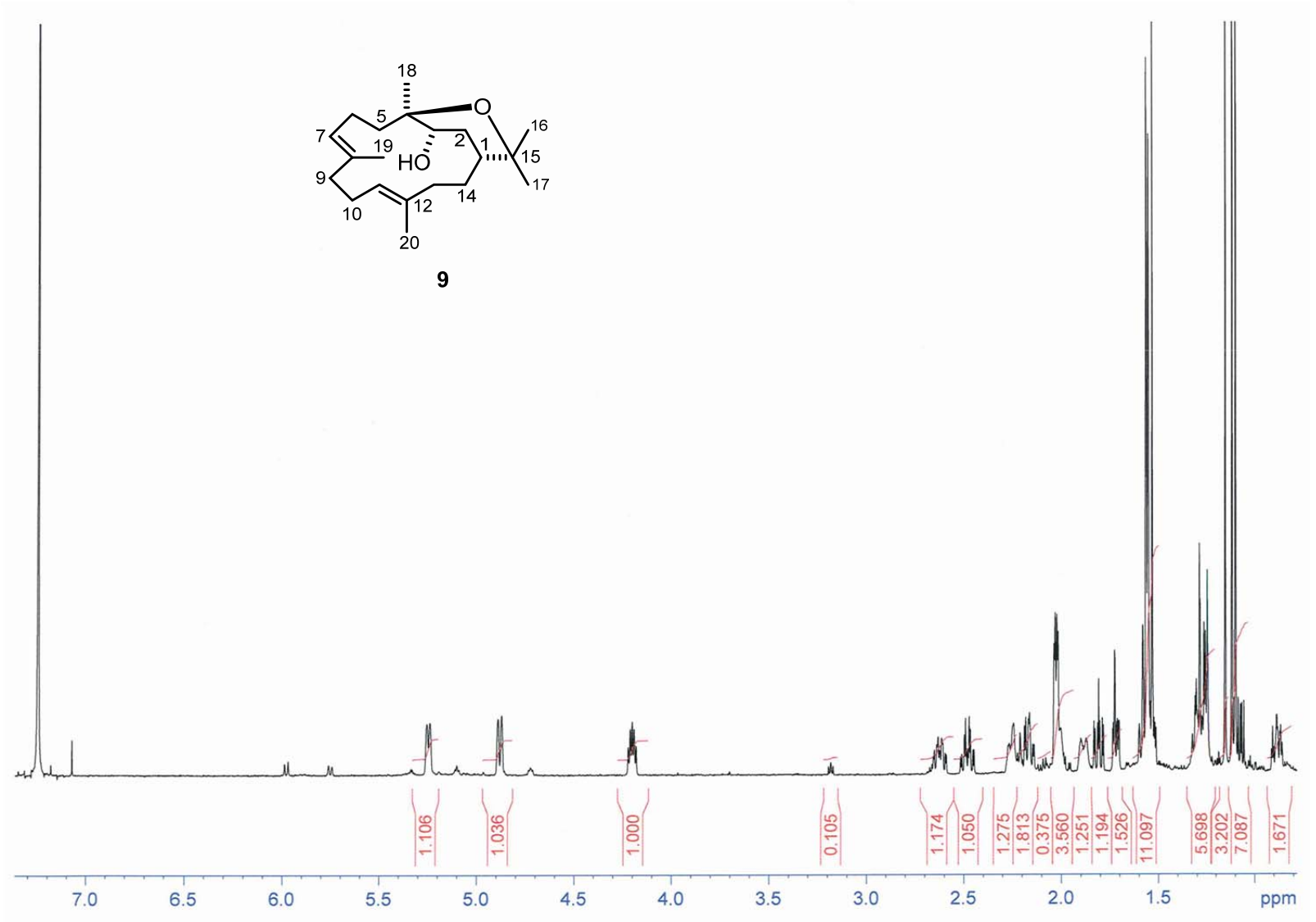


Fig. S57. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of isodecaryiol (**9**).

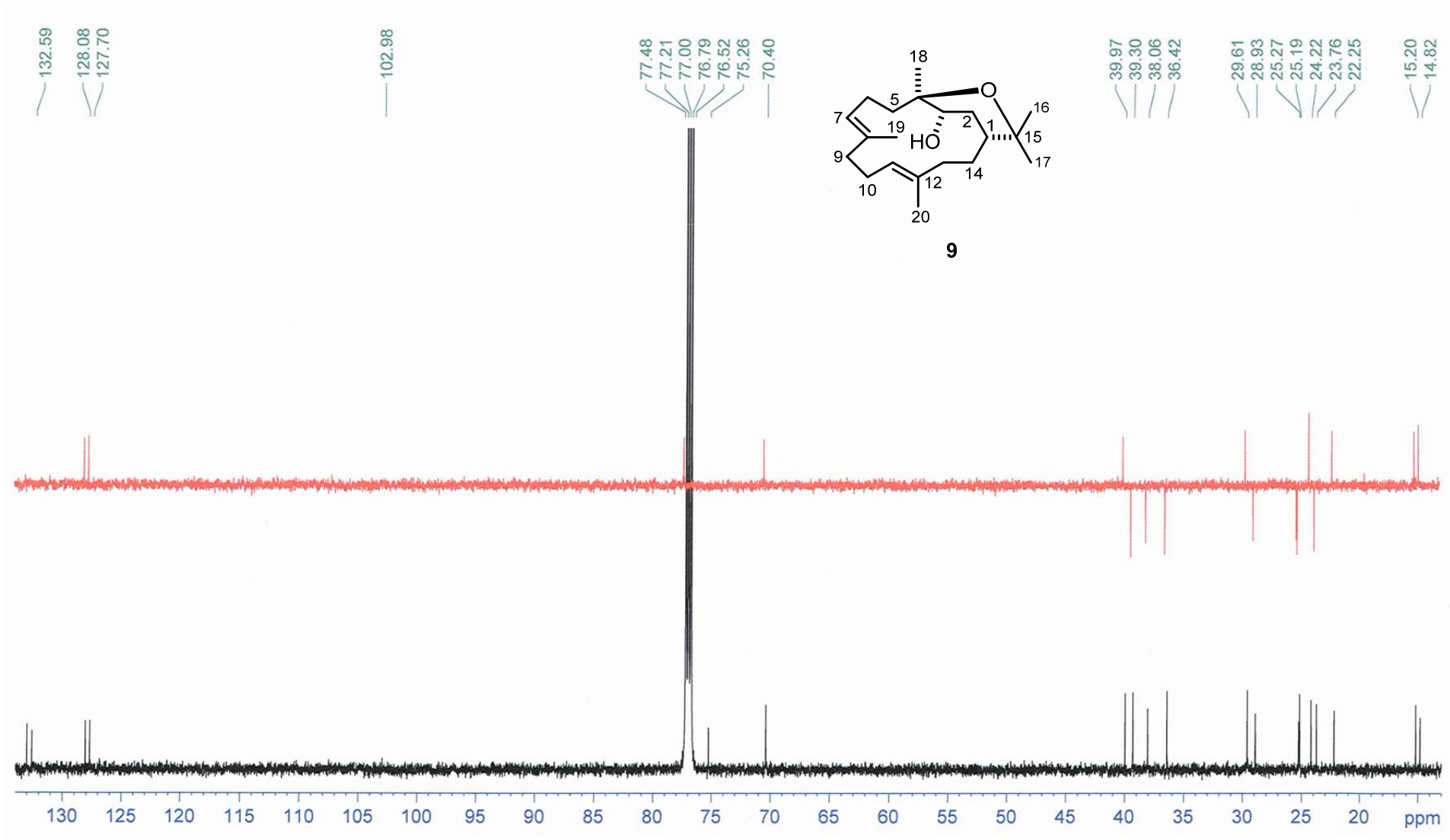


Fig. S58. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of isodecaryiol (**9**).

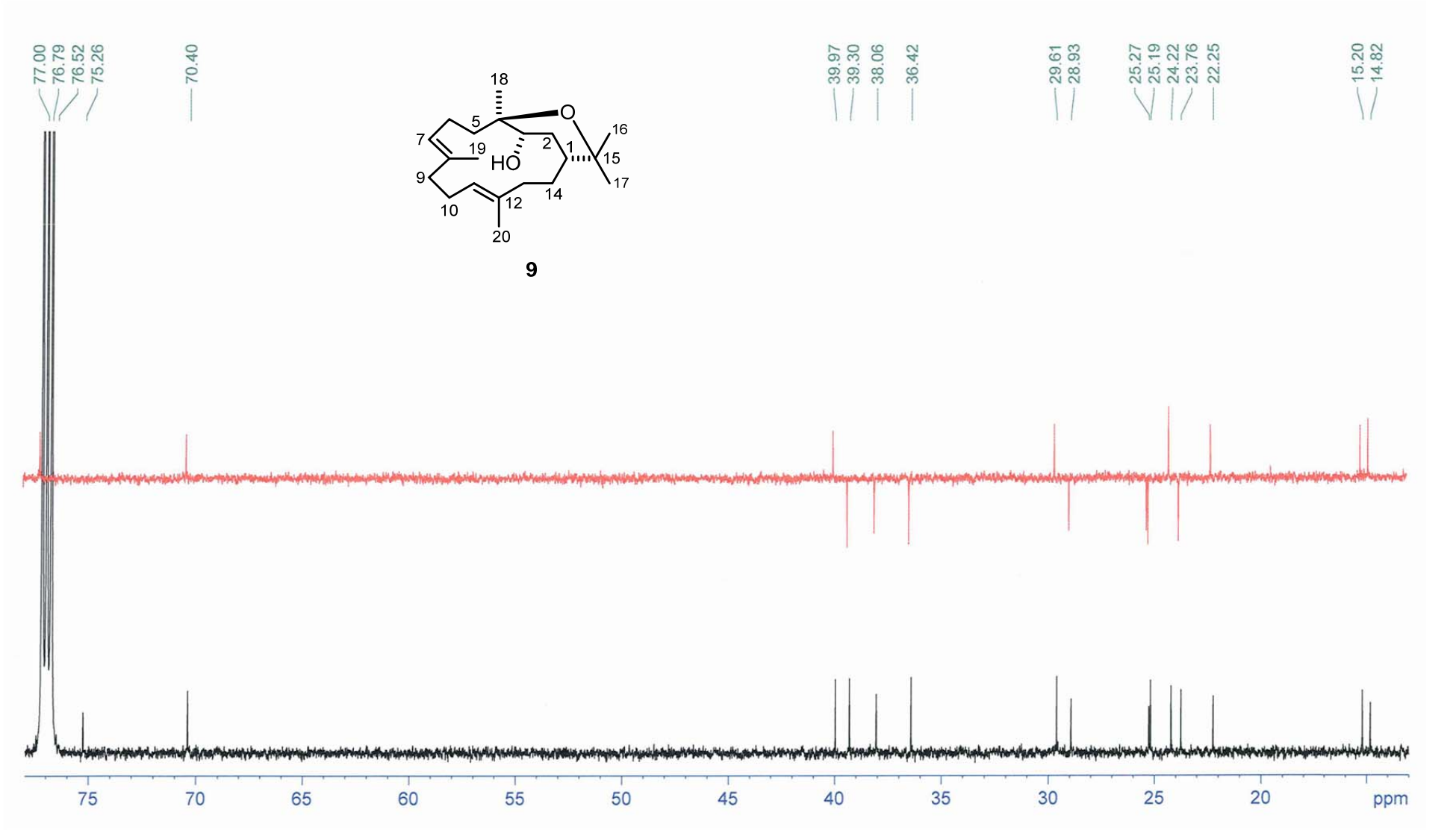


Fig. S59. Details of the ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of isodecaryiol (**9**).

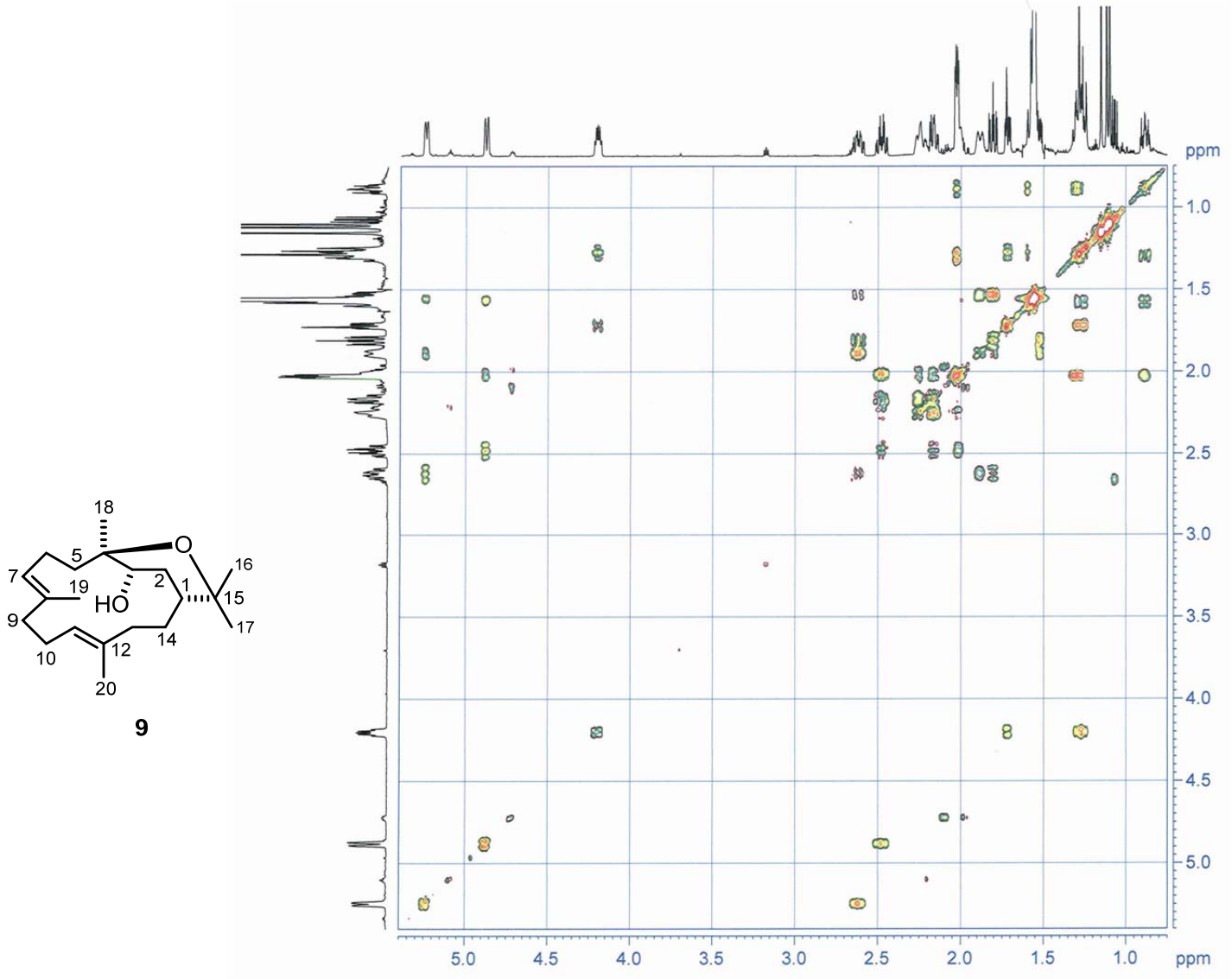


Fig. S60. COSY spectrum of isodecaryiol (**9**).

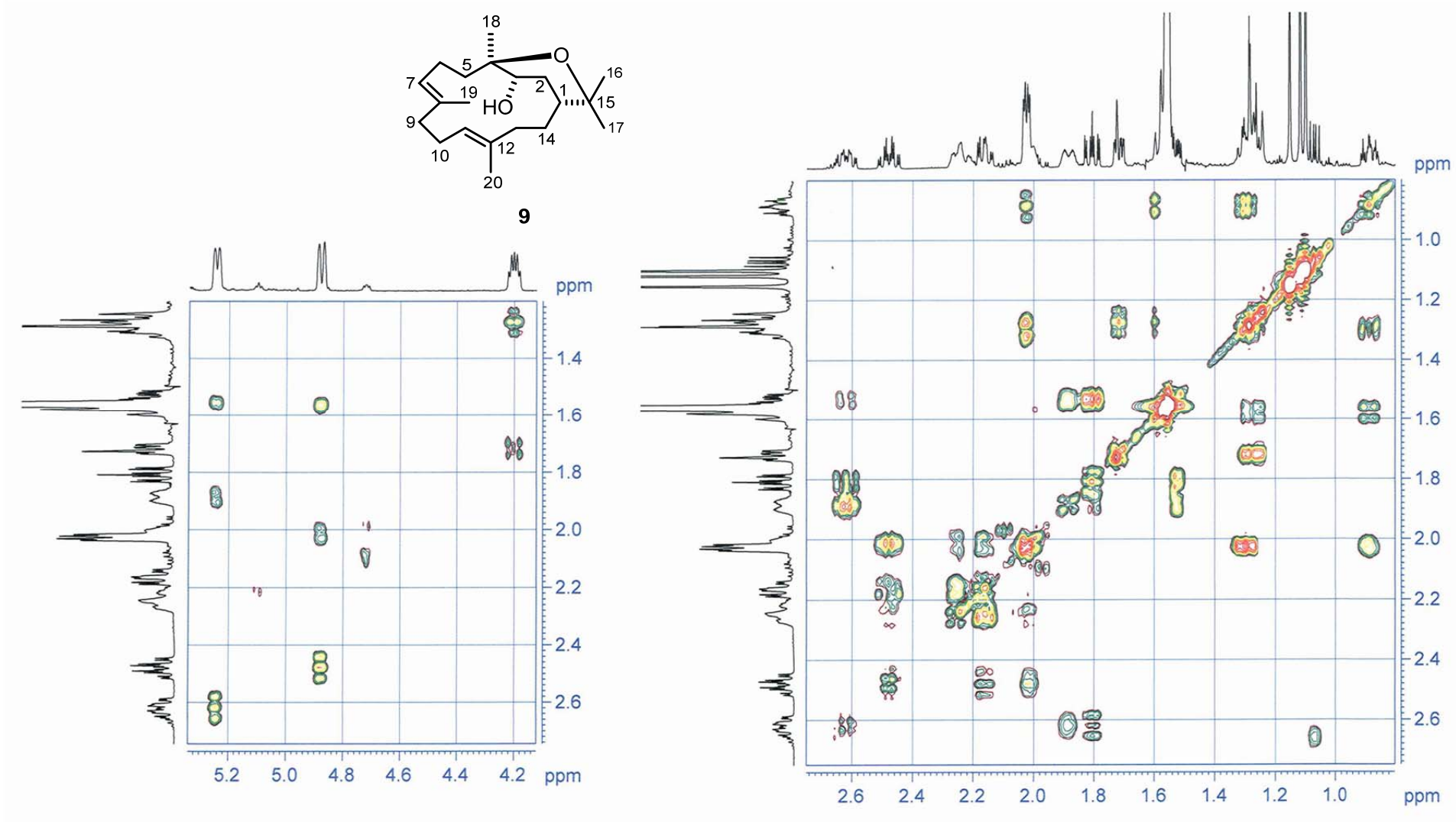
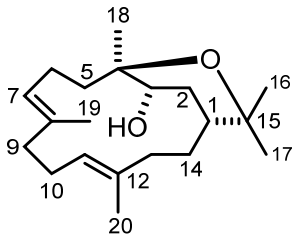


Fig. S61. Details of the COSY spectrum of isodecaryiol (**9**).



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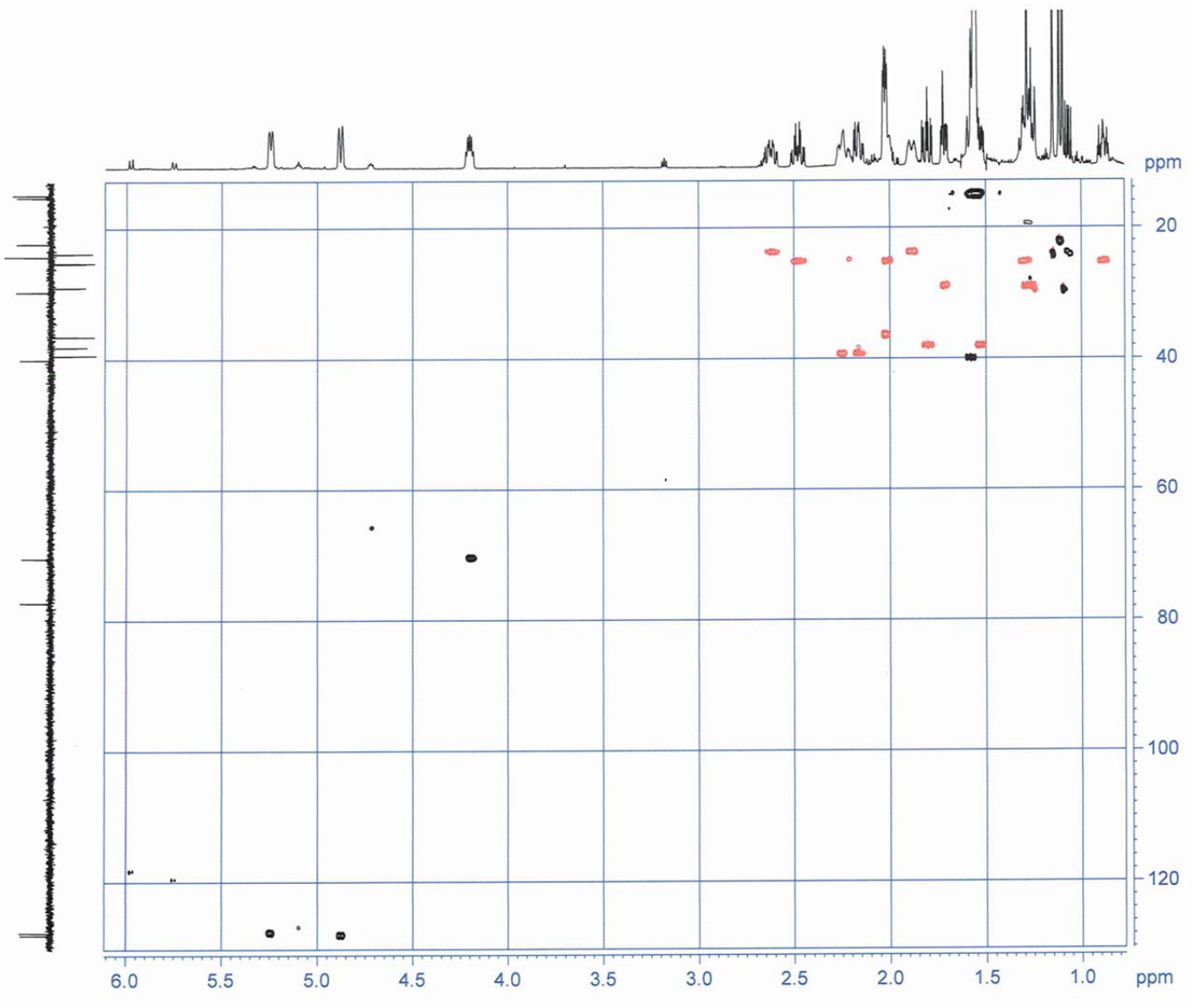


Fig. S62. HSQC spectrum of isodecaryiol (**9**).

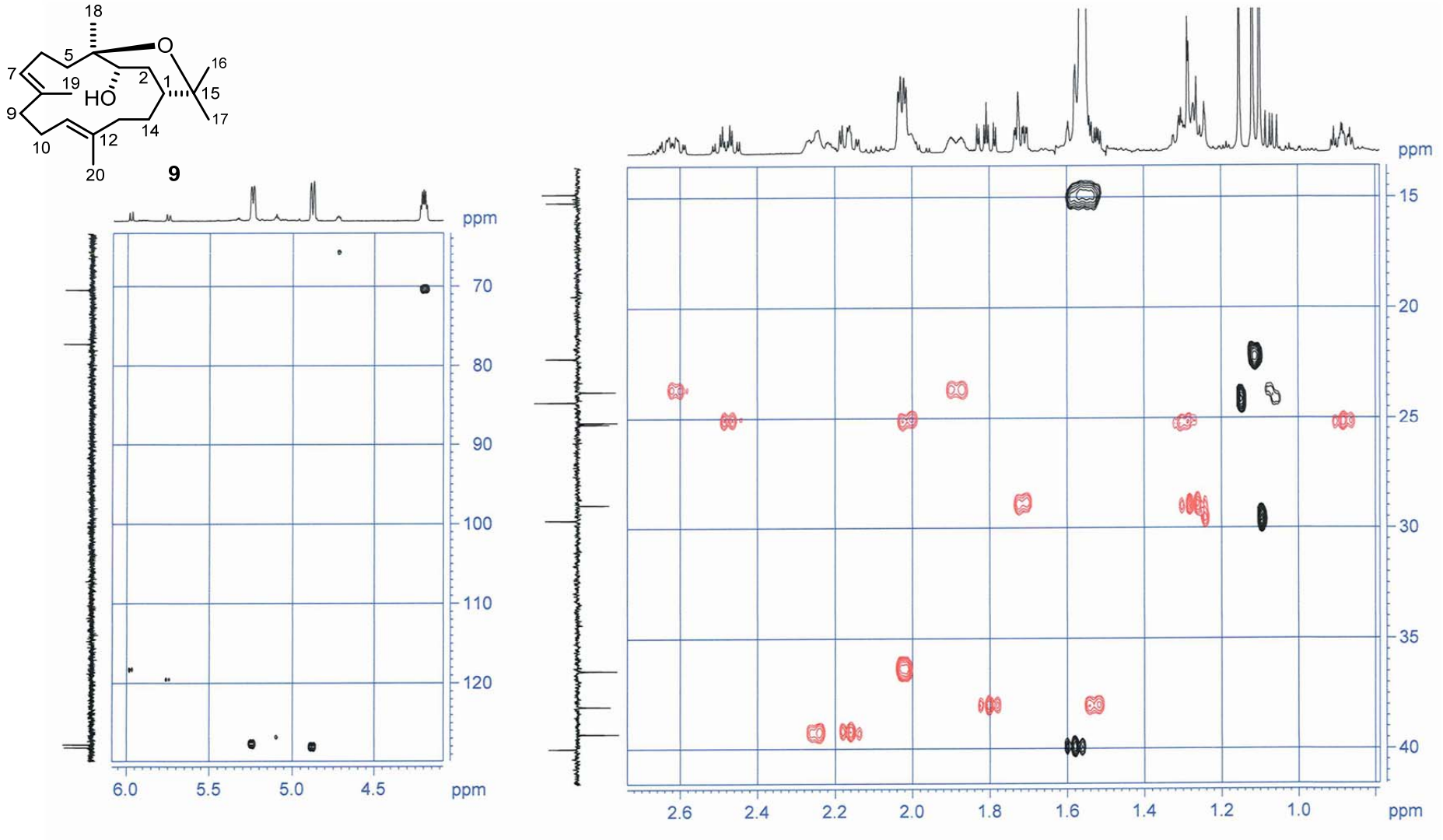


Fig. S63. Details of the HSQC spectrum of isodecaryiol (**9**).

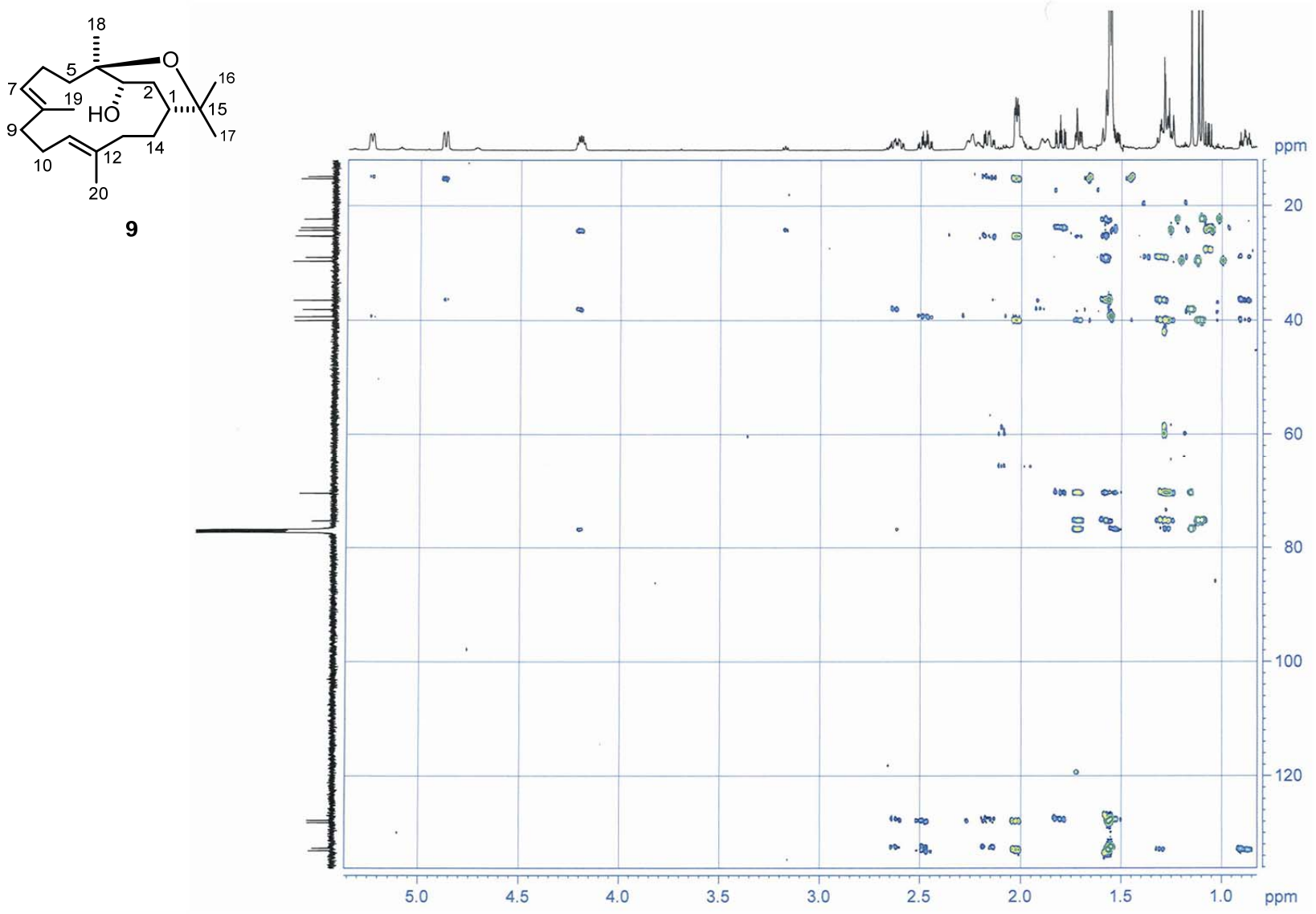


Fig. S64. HMBC spectrum of isodecaryiol (**9**).

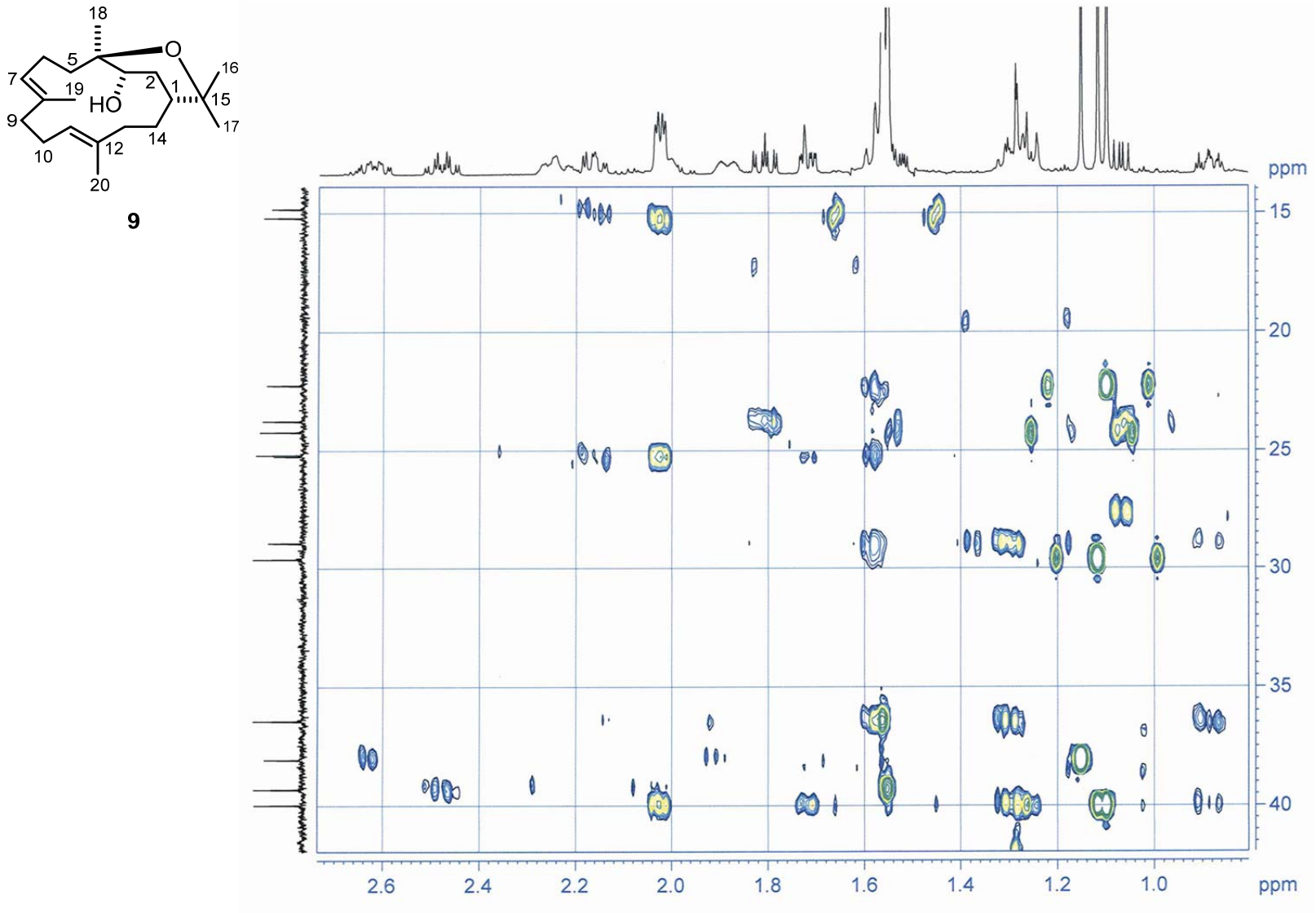


Fig. S65. Details of the HMBC spectrum of isodecaryiol (**9**).

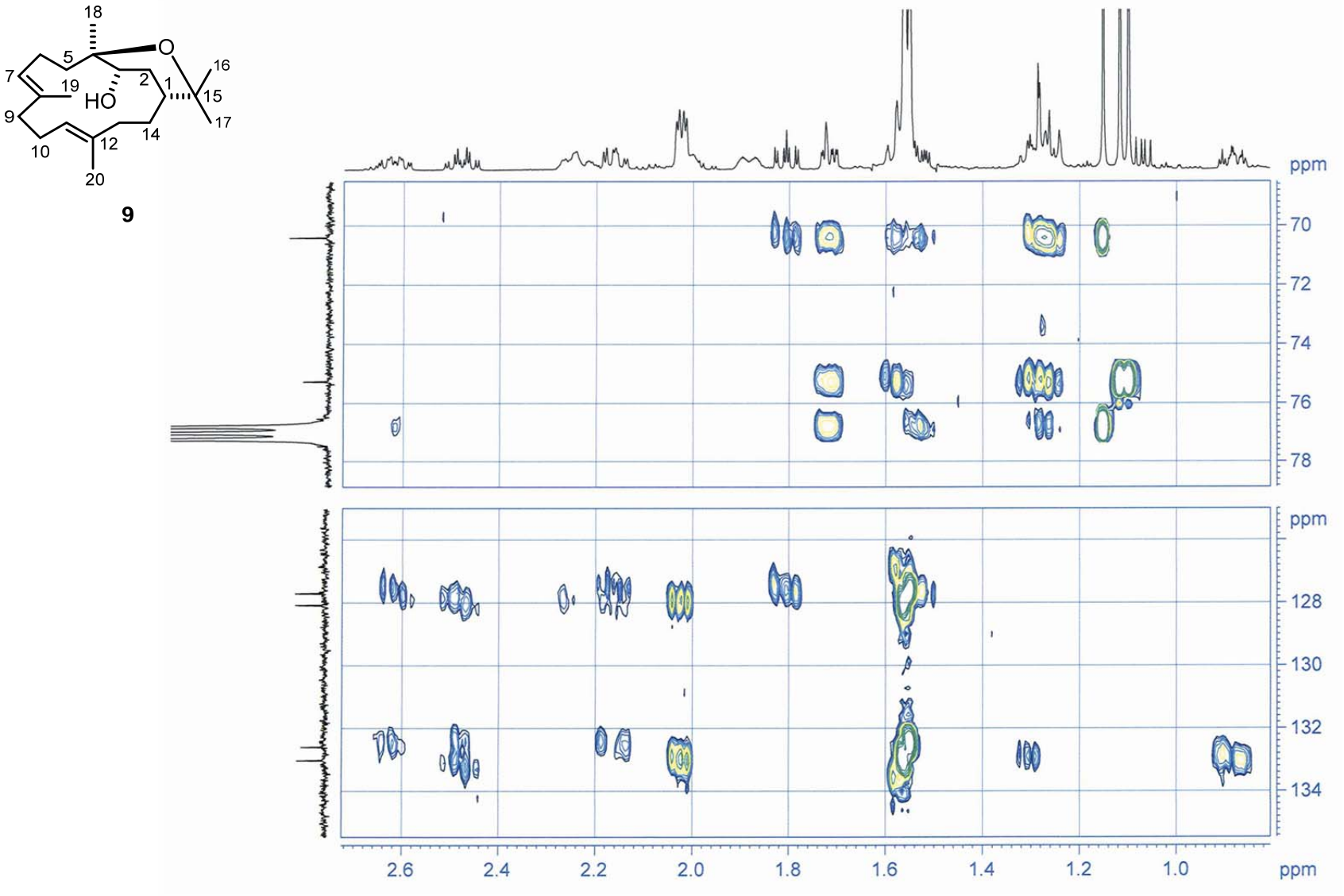
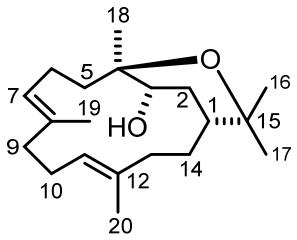


Fig. S66. Details of the HMBC spectrum of isodecaryiol (**9**).



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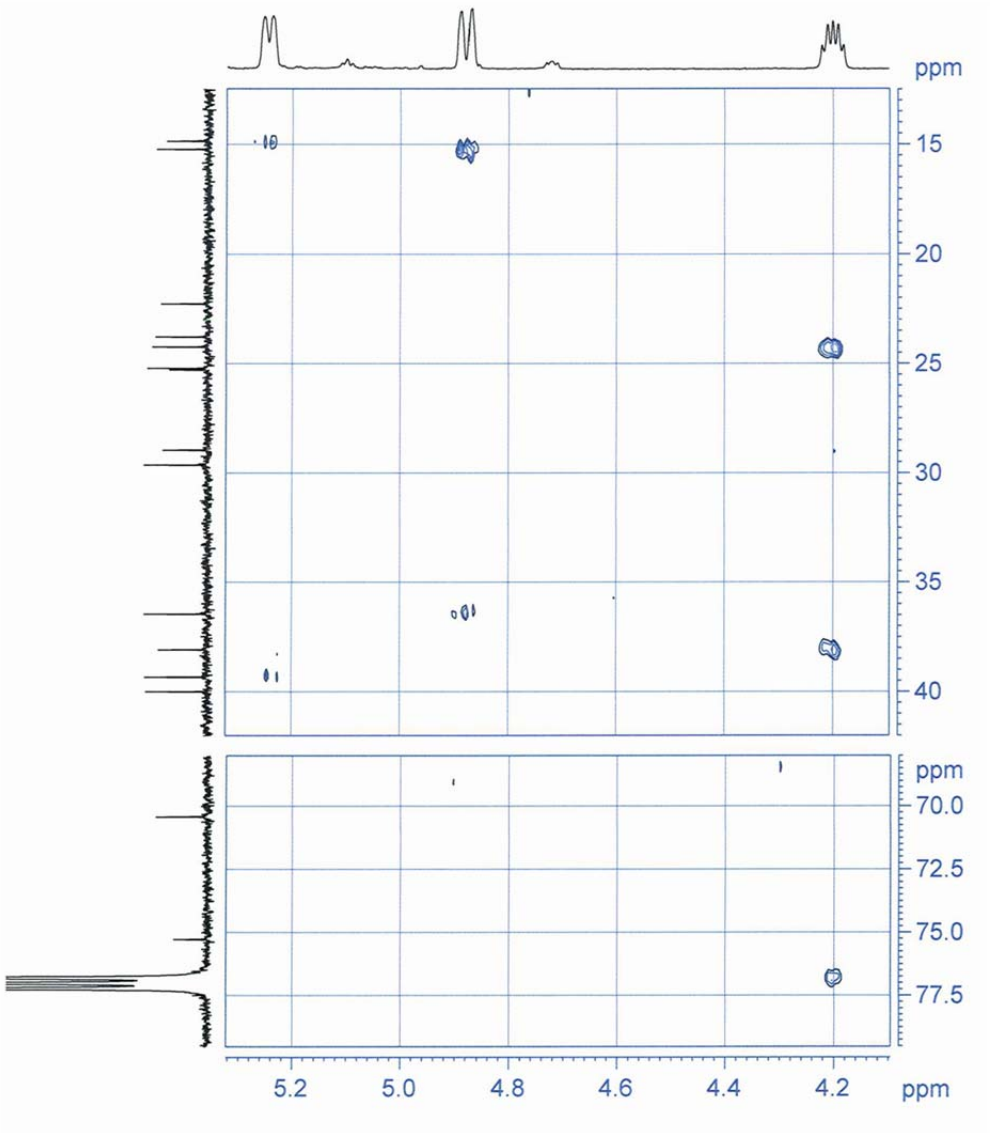
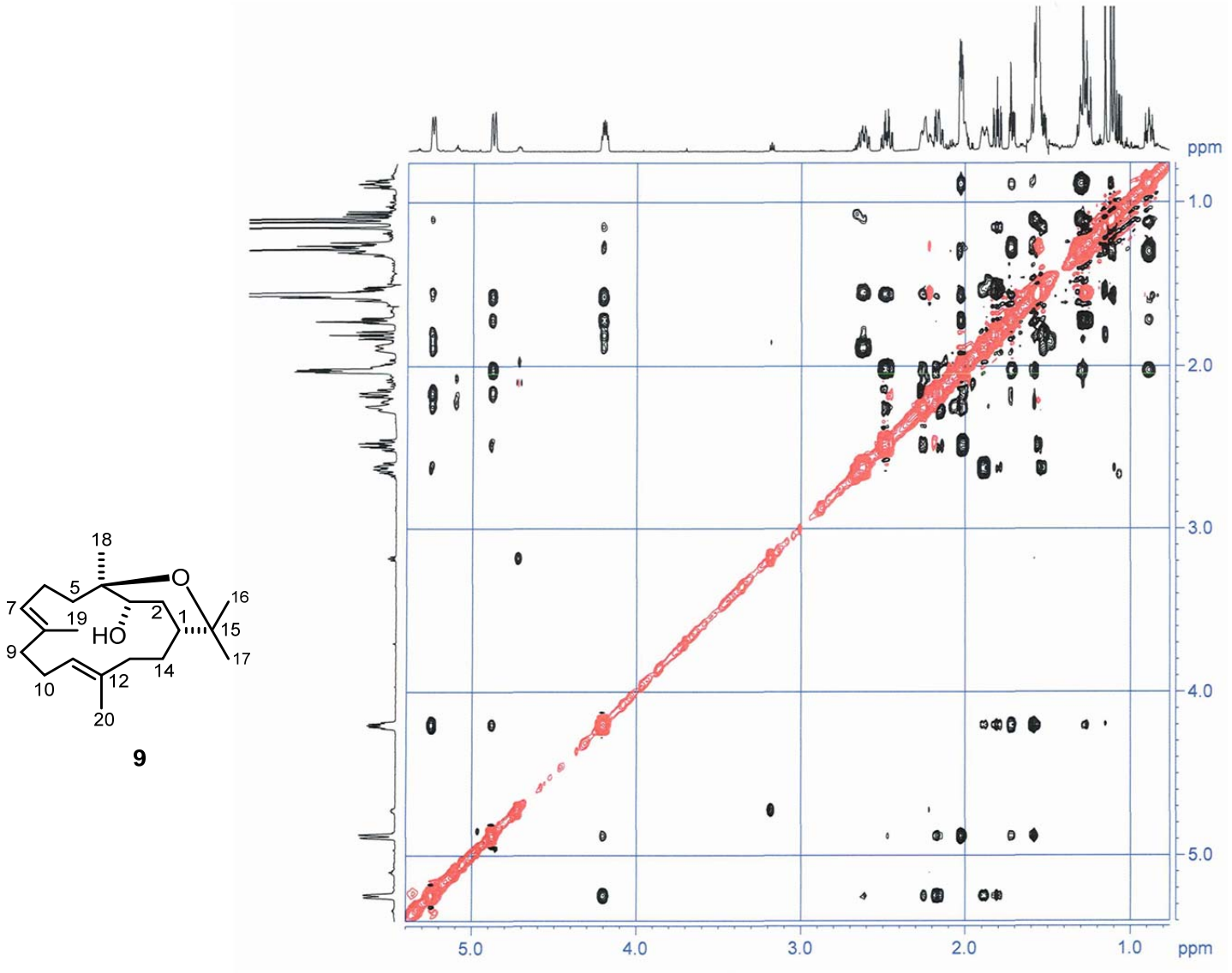
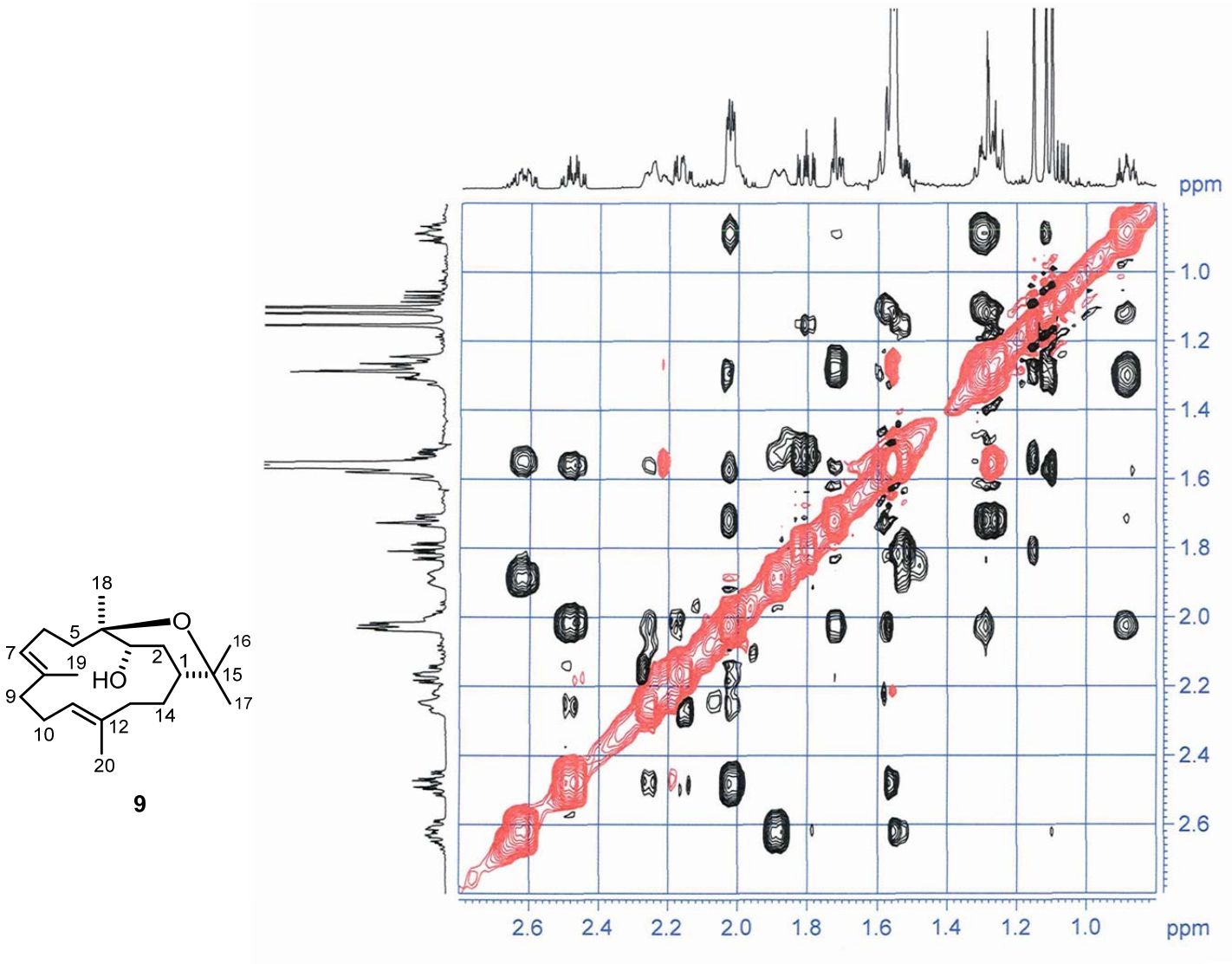


Fig. S67. Details of the HMBC spectrum of isodecaryiol (**9**).



9

Fig. S68. NOESY spectrum of isodecaryiol (**9**).



9

Fig. S69. Details of the NOESY spectrum of isodecaryiol (**9**).

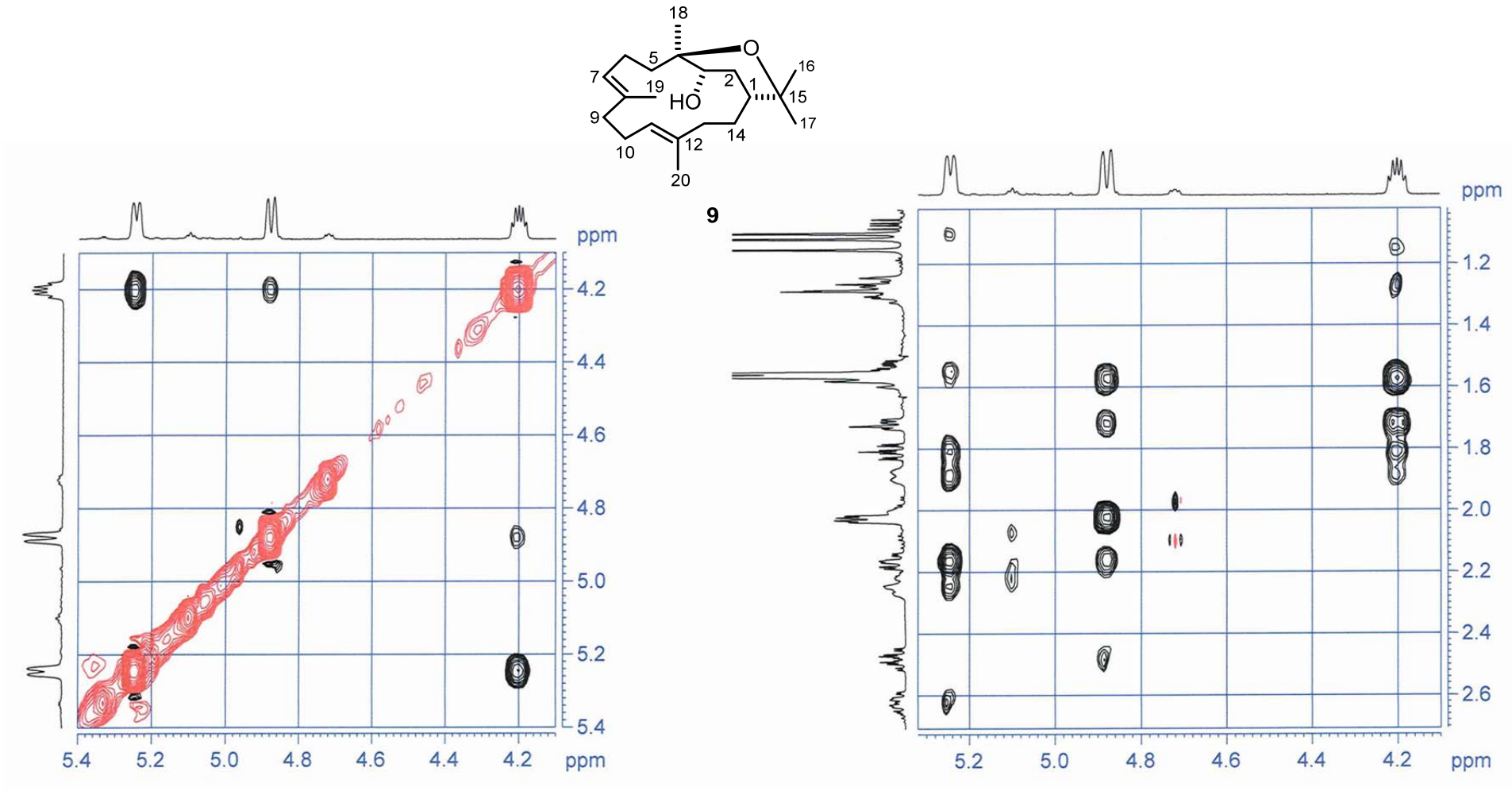


Fig. S70. Details of the NOESY spectrum of isodecaryiol (**9**).

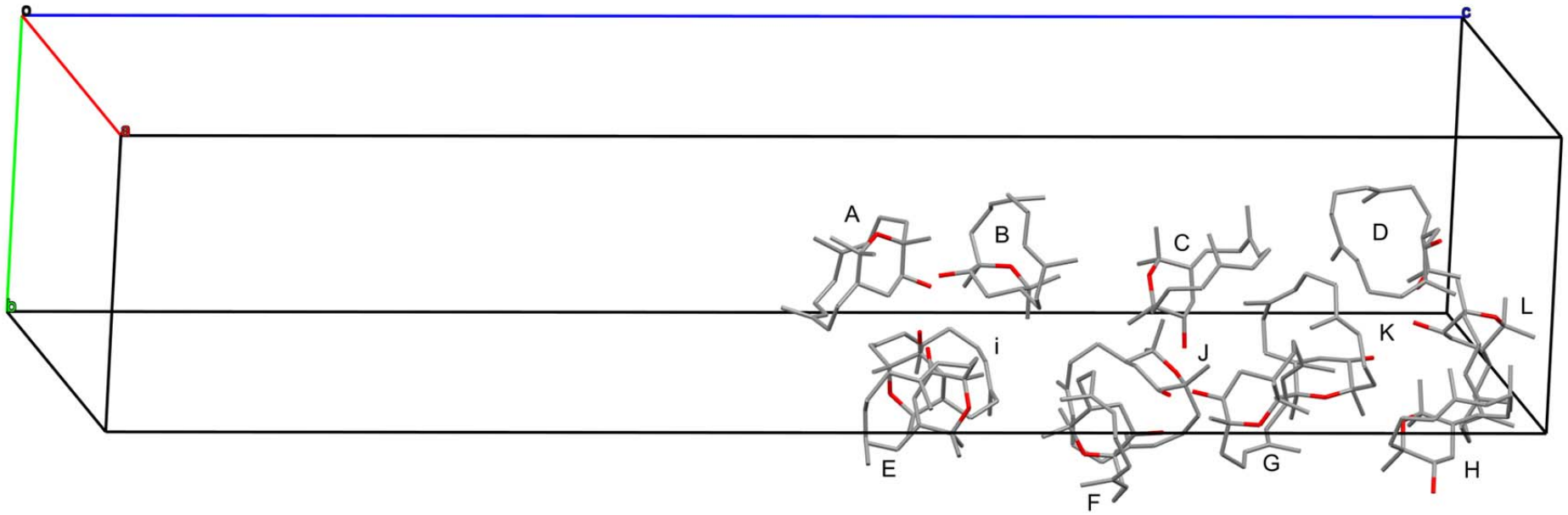


Fig. S71. X-ray crystal structure of isodecaryiol (**9**): Fragment of the crystal packing showing the 12 symmetry-independent molecules A–L.

Antimalaria Assay

Parasite culture. The chloroquine resistant strain (FCM29) of *P. falciparum* was provided by Mr. Michel Ratsimbason, Centre National d'Application de Recherche Pharmaceutique (CNARP), Antananarivo, Madagascar. The strain was maintained *in vitro* by using the Trager and Jensen's method reported earlier.[8, 9] The culture media consisted of standard RPMI 1640 (Sigma, St. Louis, MO) supplemented with 10% heat-inactivated (56 °C, 1 h) human type O+ serum, 25 mM $NaHCO_3$, 2 mM glutamine, and 1 M HEPES (Sigma, St. Louis, MO). The culture was maintained in type AB+ human red blood cell suspensions collected from healthy local donors and prepared in citrate-phosphate-dextrose anticoagulant (Sigma, St. Louis, MO) at a hematocrit of 2%. The parasite density was maintained below 2% parasitemia under an atmosphere of a gas mixture containing CO_2 (5%), O_2 (5%), and N_2 (90%) and at 37 °C. For each experiment the sample of stock sorbitol-synchronized culture was further diluted in culture medium containing sufficient non-infected type AB+ human erythrocytes to yield a final hematocrit of 2% and a parasitemia of 1%.

Fluorimetric susceptibility test. The synchronized ring form cultures (hematocrit 2% and parasitemia 1%) were used to test serial dilutions of extracts in 96-well culture plates. Culture of *P. falciparum* was placed in a humidified, air-sealed container, flushed with the gas mixture described above, and incubated at 37 °C. Parasites were allowed to grow for a 48-hour incubation period, after which a 150 µL aliquot of culture was transferred to a new 96-well flat bottom plate. Fifty microliters of the fluorochrome mixture, which consists of PicoGreen® (Molecular Probes, Inc., Eugene, OR), 10 mM Tris-HCl, 1 mM EDTA, pH 7.5 (TE buffer), and 2% Triton X-100 diluted with double-distilled water, was then added to liberate and label the parasitic DNA. The plates were then incubated for 5−30 minutes in the dark. The fluorescence signal, measured as relative fluorescence units (RFU) was quantified with a fluorescence microplate reader (FLx 800; Bio-Tek Instruments, Inc., Winooski, VT) at 485/20 nm excitation and 528/20 nm emission. Simultaneously, the RFU from positive (quinine: IC_{50} = 3.5 µg/mL) and negative (solvent, MeOH) control samples were also performed.

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