Supporting Information

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Anthraquinones and Macrocyclic Lactones from Endophytic Fungus *Penicillium roseopurpureum* and Their Bioactivities

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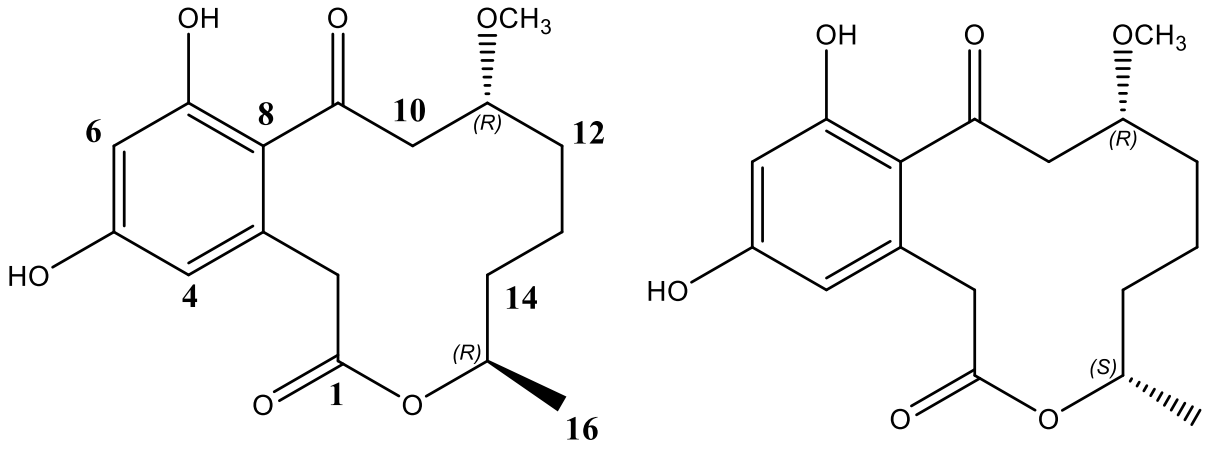

Figure S 1: Chemical structures of compound **1a** and **1b**.

Table S 1: ^{1}H and ^{13}C NMR data for compound **1**.

No	1a		1b	
	δ_C, Type[a]	**δ_H (*J* in Hz)[b]**	**δ_C, Type[a]**	**δ_H (*J* in Hz)[b]**
1	170.3 s	-	169.7 s	-
2	39.5 t	3.83 (d, 15.7), 3.54 (d, 15.8)	39.5 t	3.83 (d, 15.7), 3.54 (d, 15.8)
3	136.6 s	-	136.6 s	-
4	111.0 d	6.16 (d, 2.4)	111.4 d	6.16 (d, 2.4)
5	160.0 s	-	160.0 s	-
6	101.9 d	6.30 (d, 2.3)	101.9 d	6.30 (d, 2.3)
7	158.9 s	-	158.9 s	-
8	118.2 s	-	118.2 s	-
9	202.7 s	-	202.7 s	-
10	48.5 t	3.24 (m), 2.85 (m)	48.5 t	3.24 (m), 2.85 (m)
11	76.5 d	3.50 (m)	76.5 d	3.50 (m)
12	30.7 t	1.51 (m), 1.33 (m)	30.7 t	1.51 (m), 1.33 (m)
13	17.6 t	1.28 (2H, m)	17.6 t	1.28 (2H, m)
14	30.7 t	1.71 (m), 1.42 (m)	30.7 t	1.52 (m), 1.35 (m)
15	72.7 d	4.73 (ddt, 8.9, 6.2, 3.5)	69.8 d	4.86 (td, 6.7, 3.7)
16	21.1 q	1.04 (3H, d, 6.4)	18.7 q	1.02 (3H, d, 6.4)
5-OH	-	9.94 (s)	-	9.94 (s)
7-OH	-	10.20 (s)	-	10.20 (s)
11-OMe	55.6 q	3.23 (3H, s)	55.6 q	3.18 (3H, s)

[a]Chemical shifts were measured at 600 MHz in DMSO-d_6
[b]Chemical shifts were measured at 150 MHz in DMSO-d_6

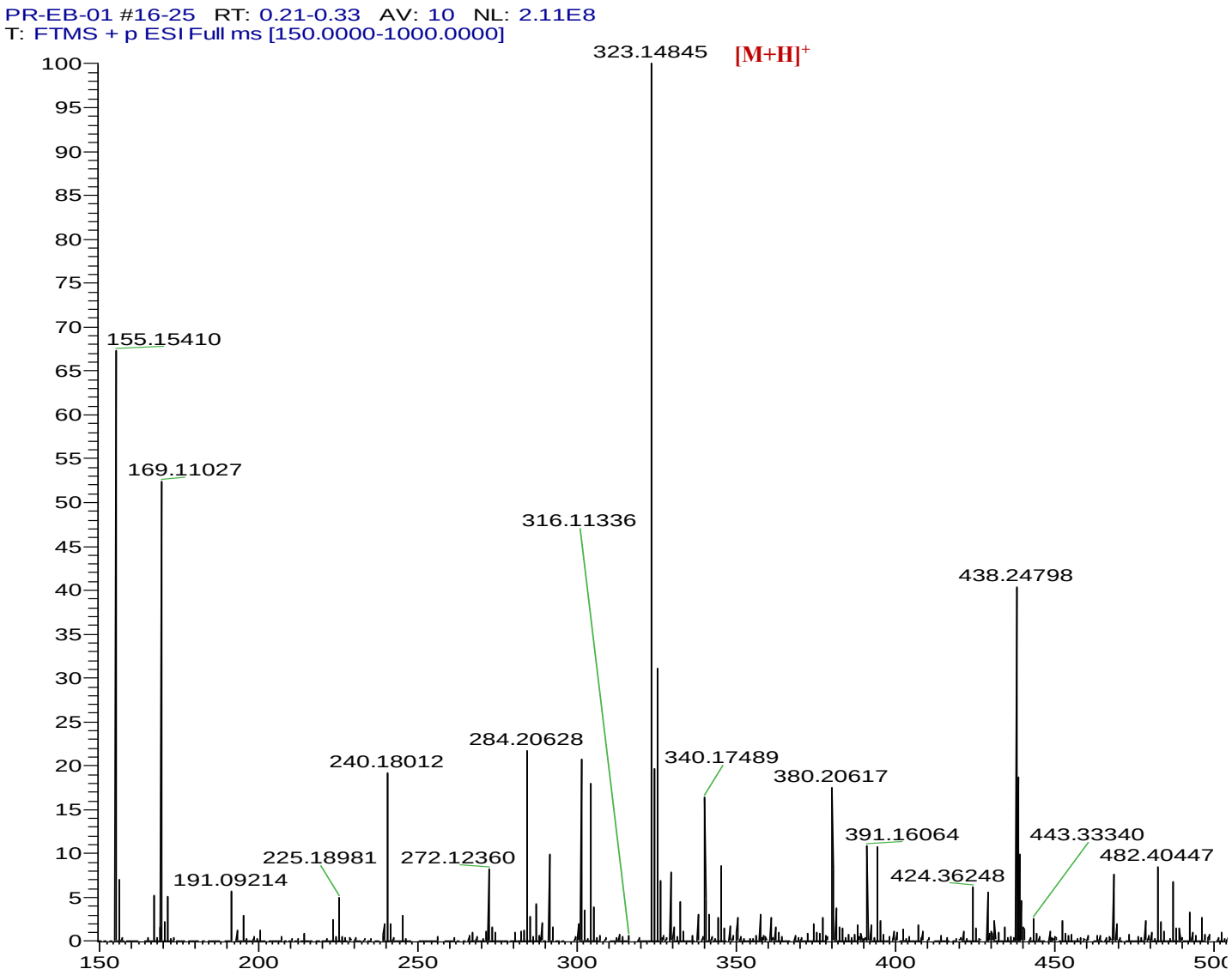

Figure S 2: HR-ESI-MS spectrum of compound **1** (positive mode).

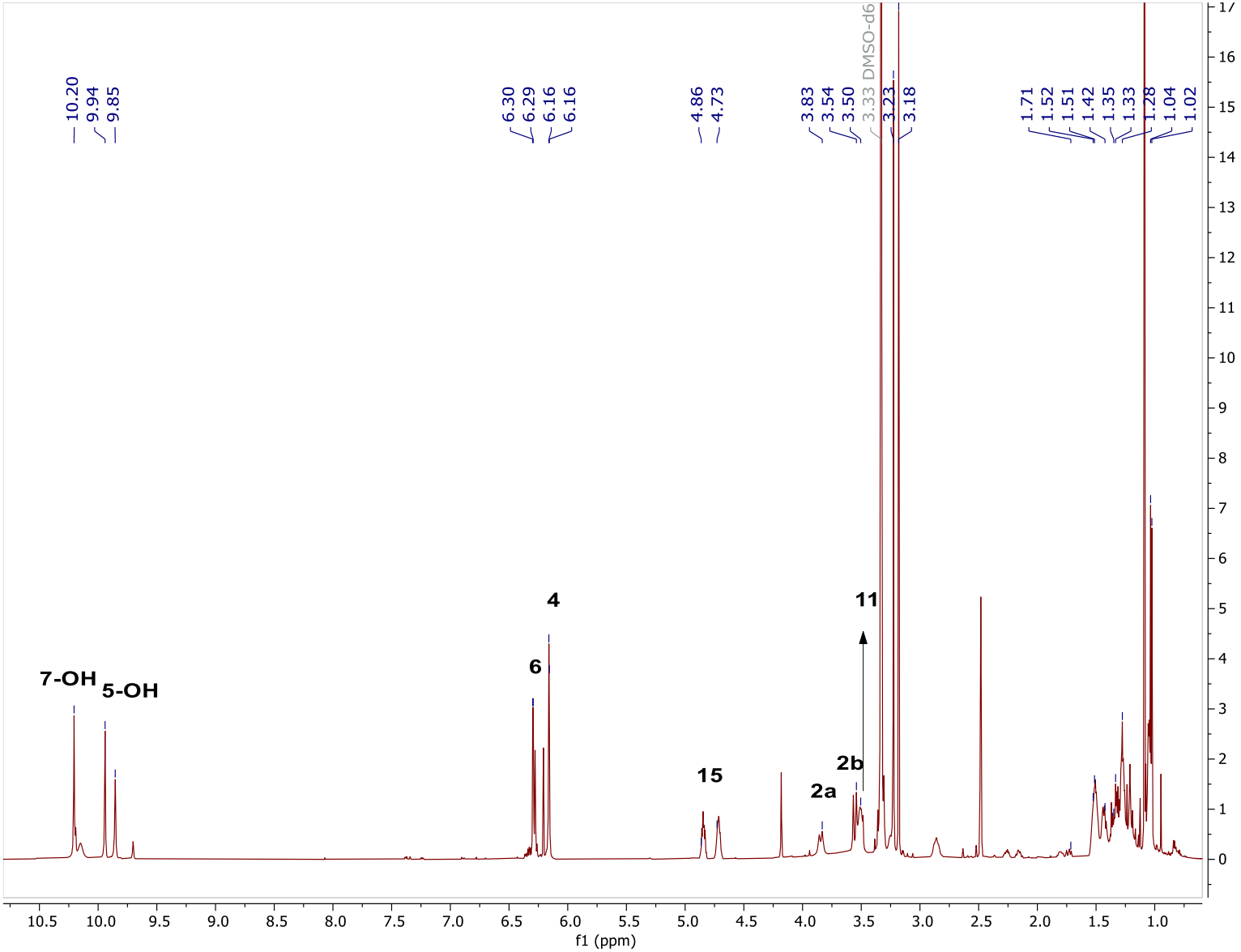

Figure S 3: ^{1}H NMR spectrum of compound **1** (in DMSO-d_6, ^{1}H: 600 MHz).

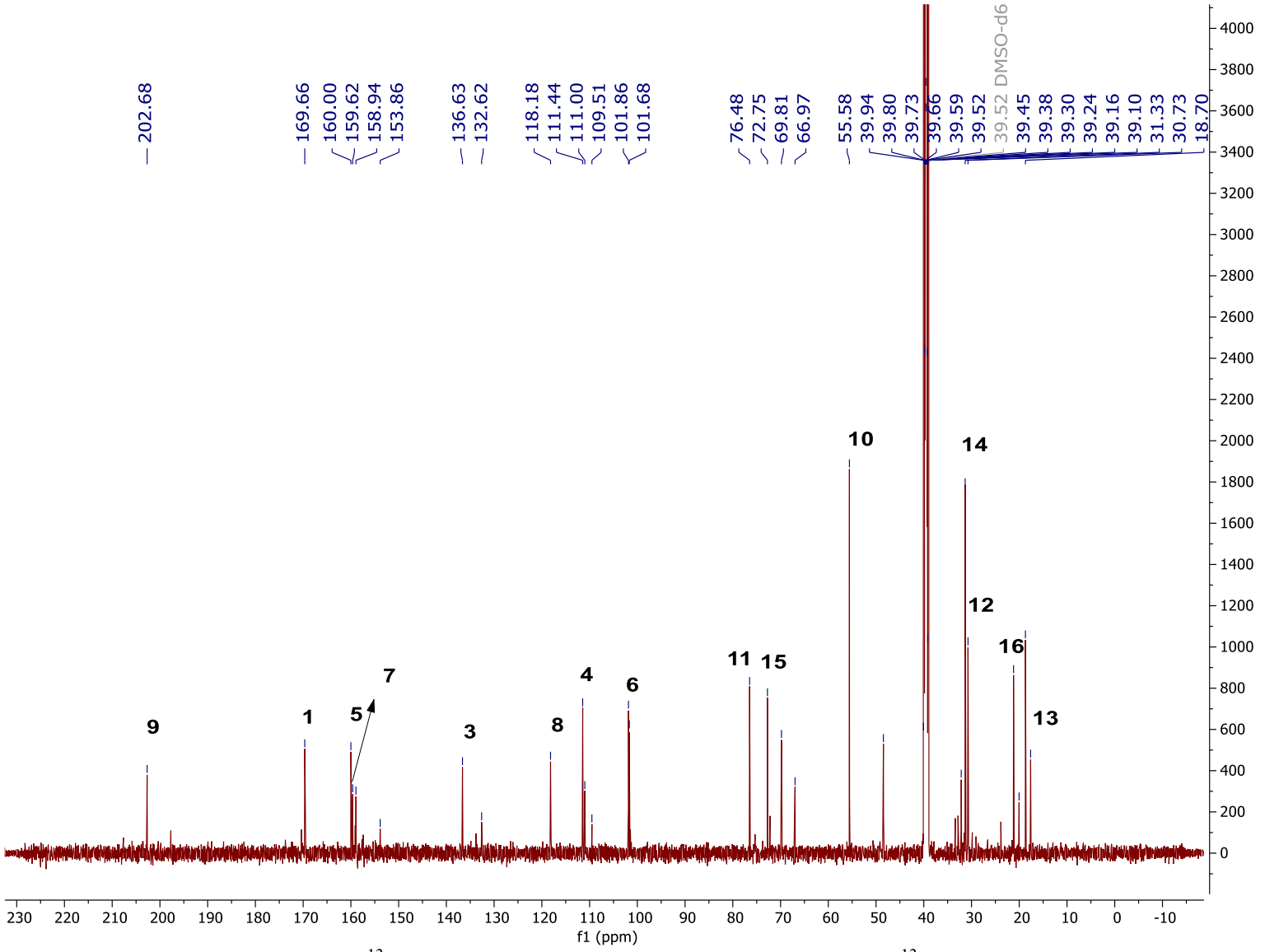

Figure S 4: ^{13}C NMR spectrum of compound **1** (in DMSO-d_6, ^{13}C:150 MHz).

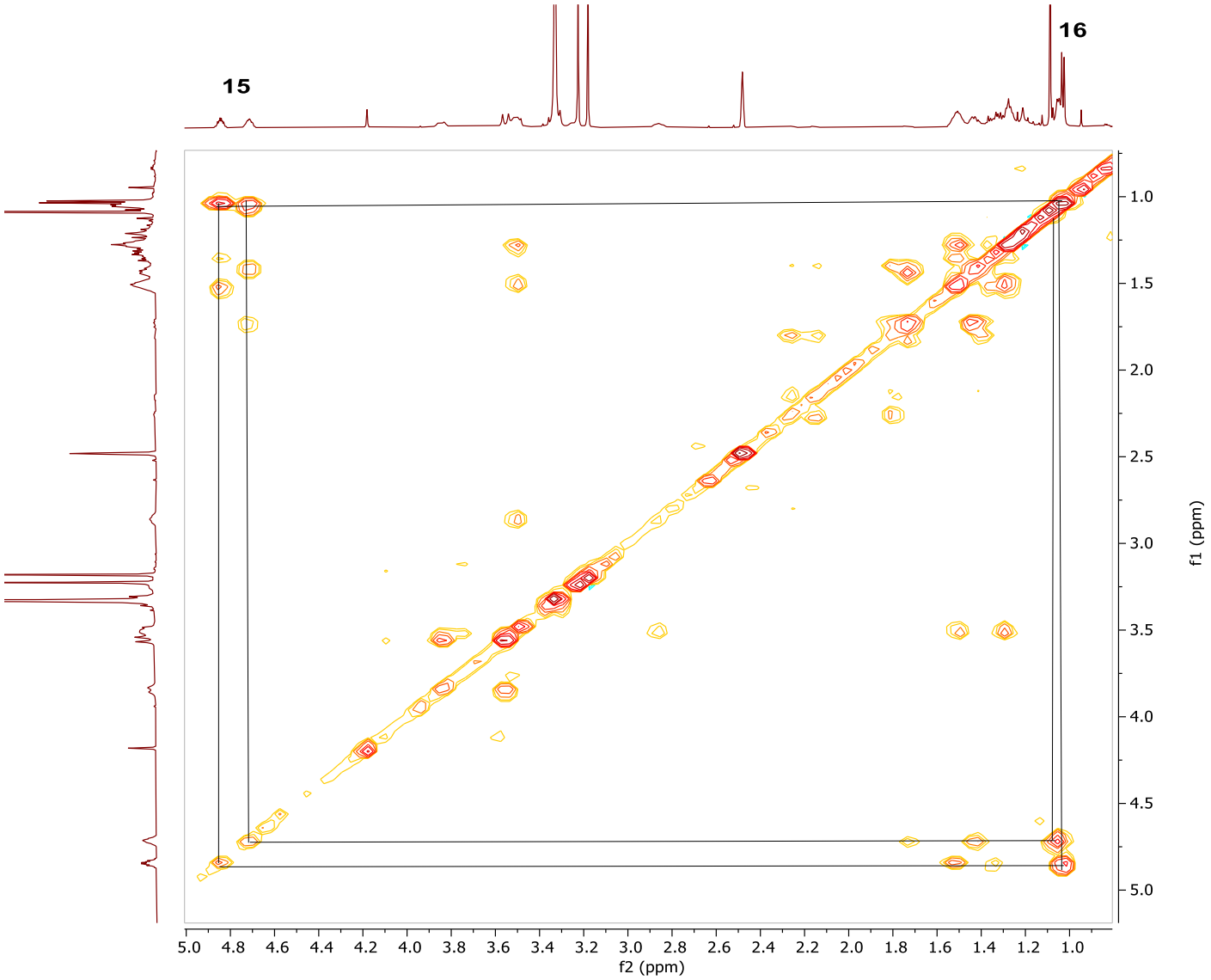

Figure S 5: COSY spectrum of compound **1**.

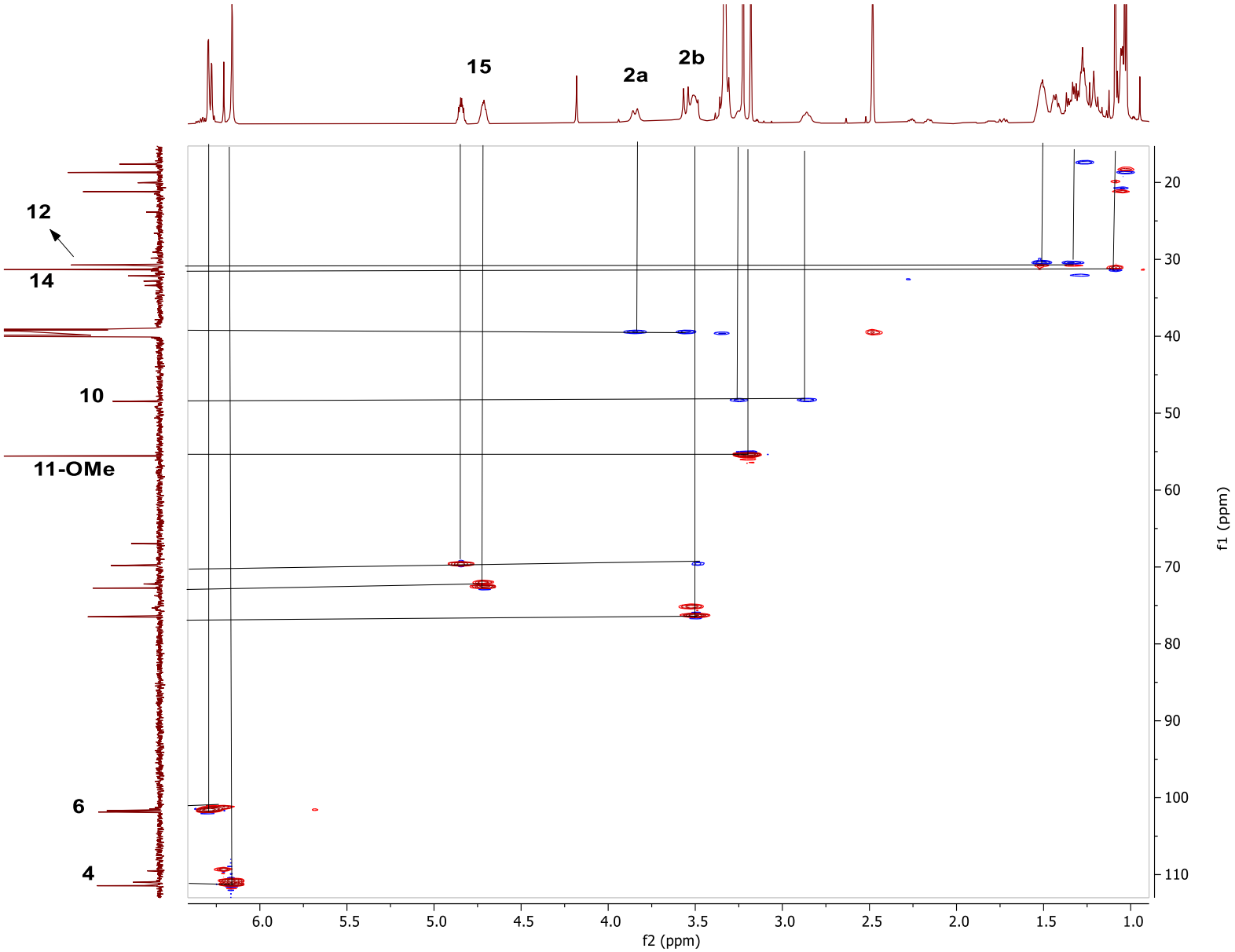

Figure S 6: HSQC spectrum of compound **1**.

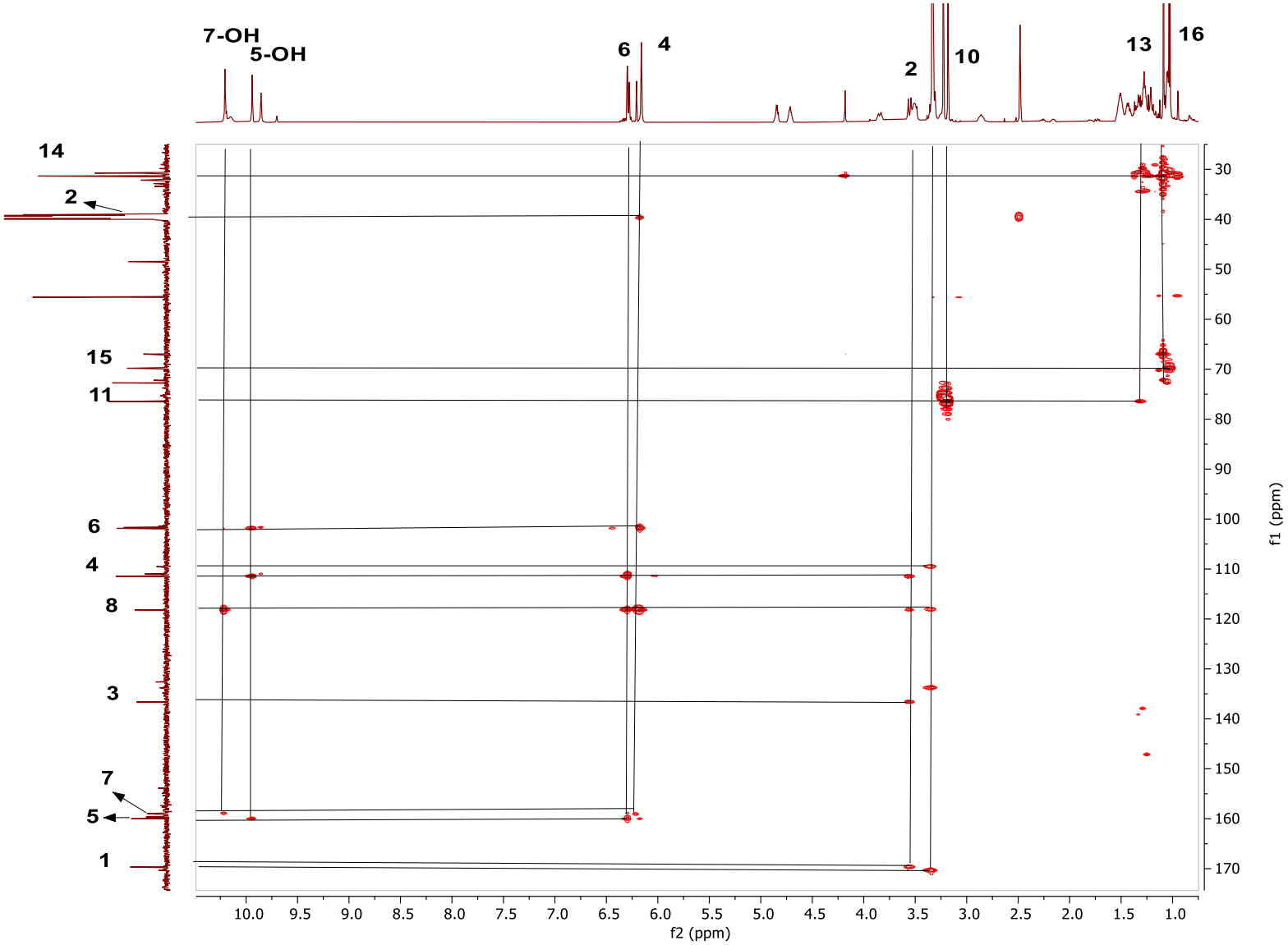

Figure S 7: HMBC spectrum of compound **1**.

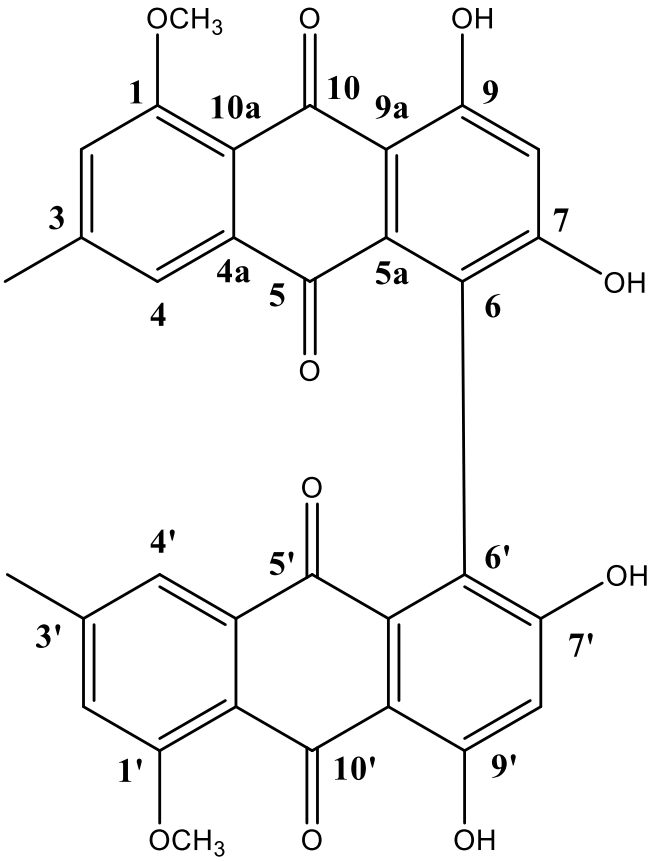

Figure S 8: Chemical structure of compound **2**.

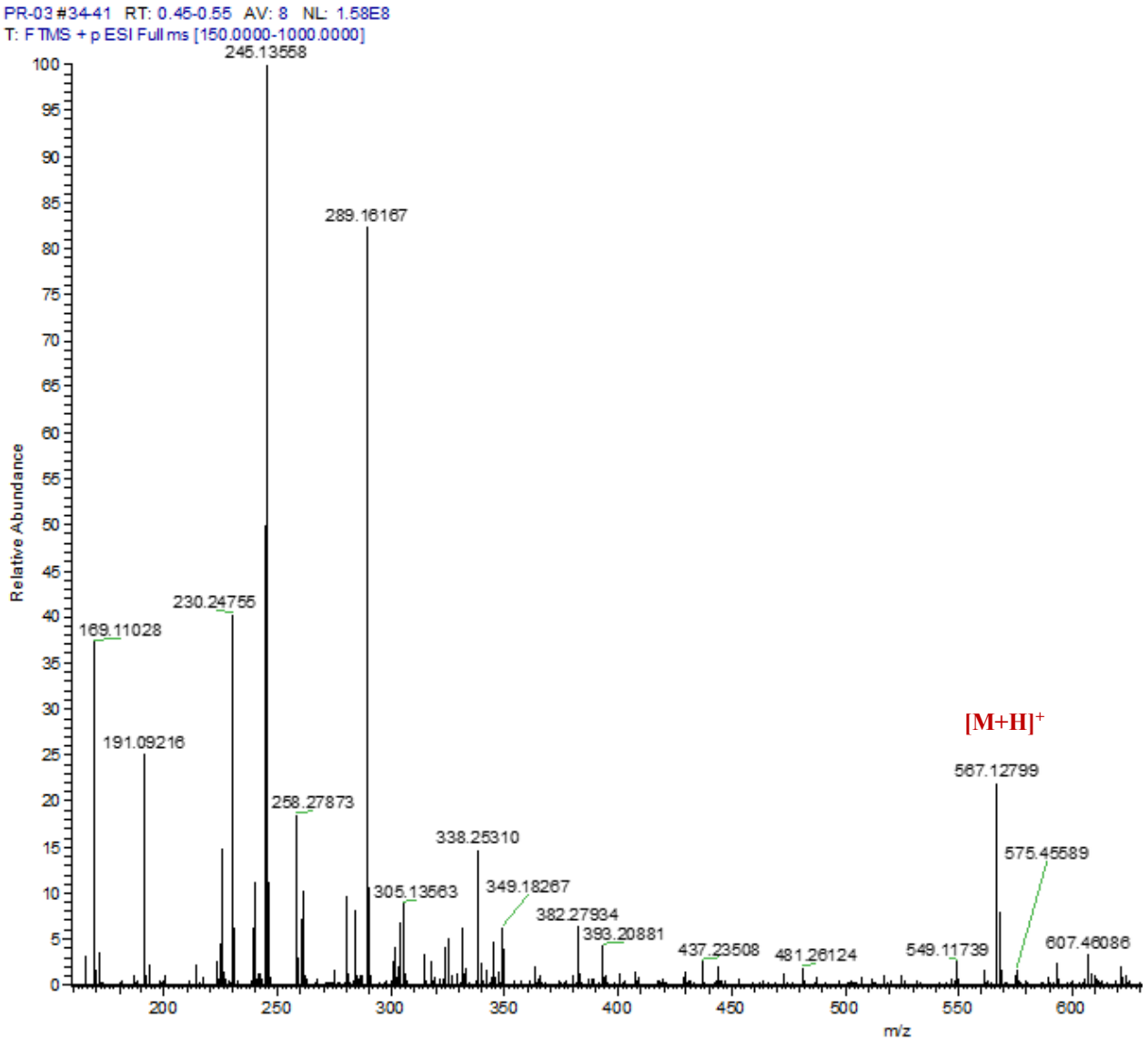

Figure S 9: HR-ESI-MS spectrum of compound **2** (positive mode).

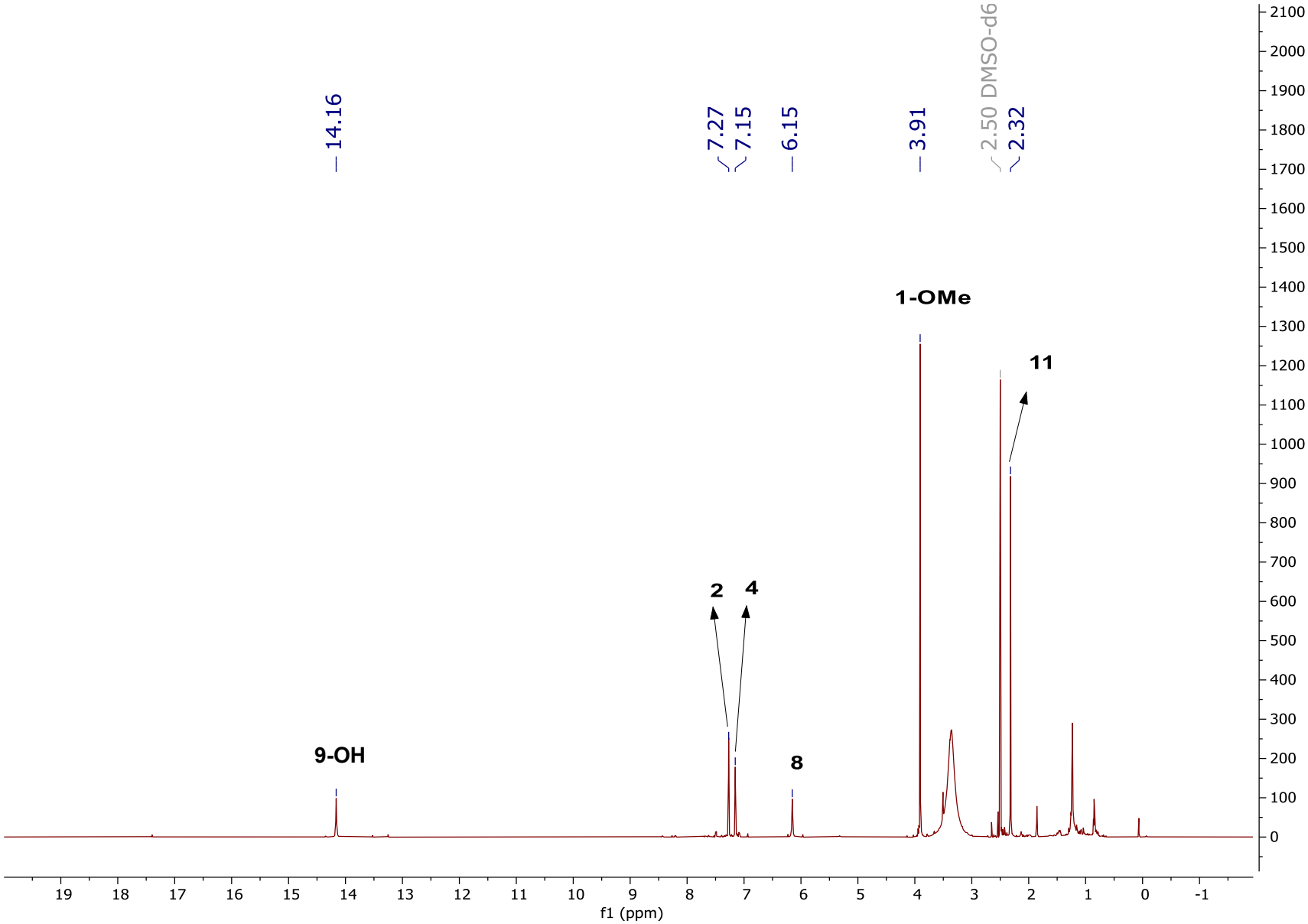

Figure S 10: ^{1}H NMR spectrum of compound **2** (in DMSO-d_6, ^{1}H: 600 MHz).

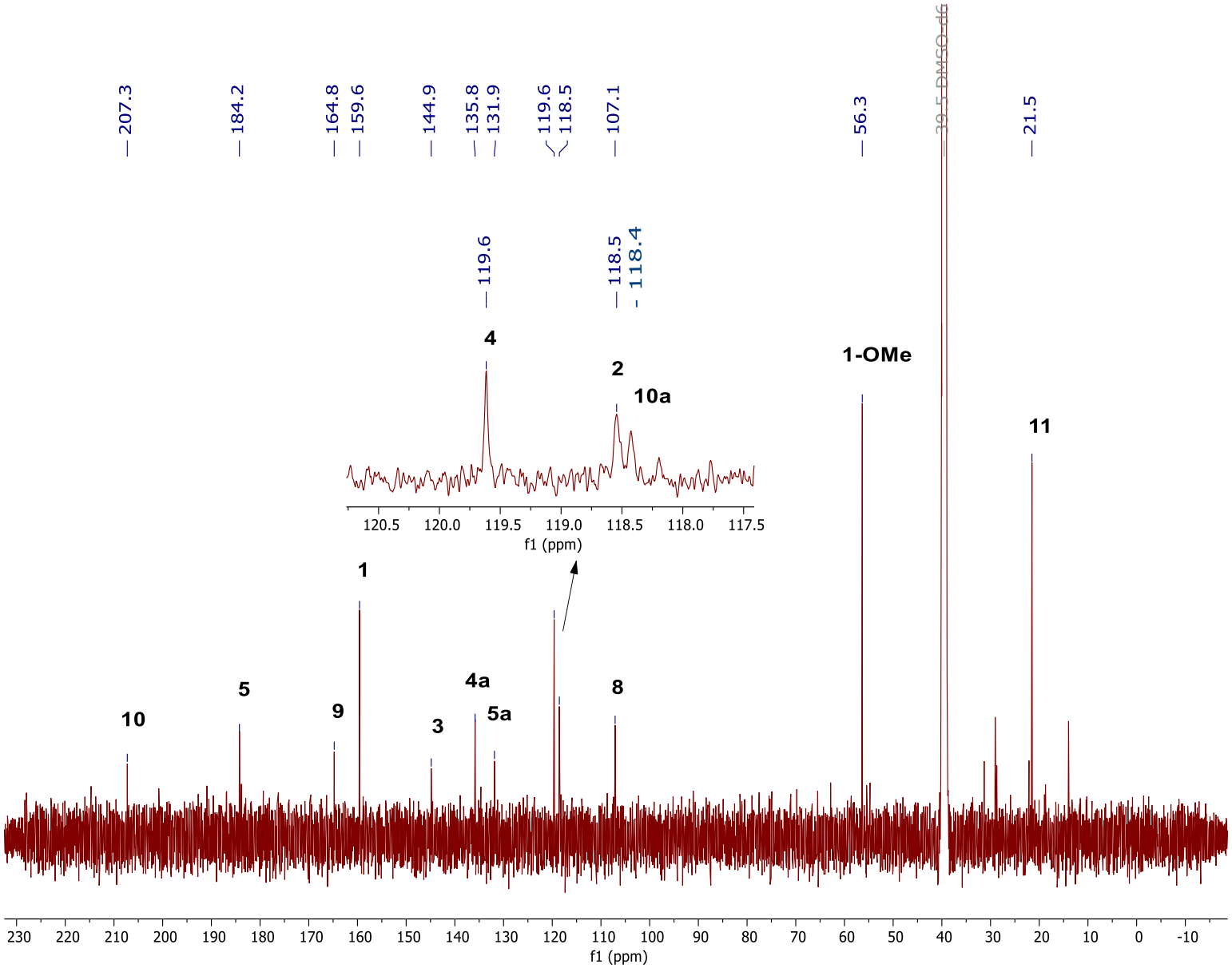

Figure S 11: ^{13}C NMR spectrum of compound **2** (in DMSO-d_6, ^{13}C:150 MHz).

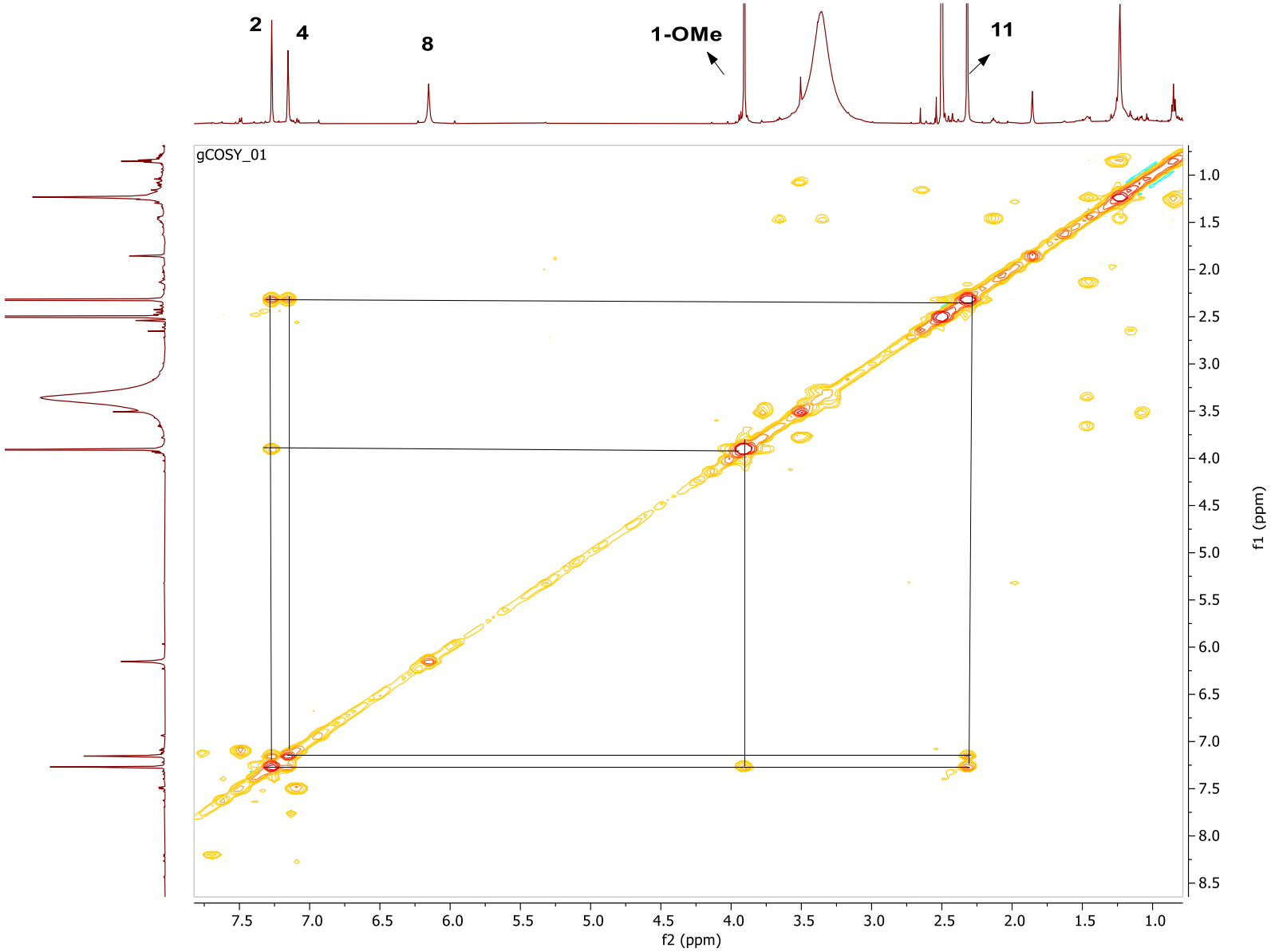

Figure S 12: COSY spectrum of compound **2**.

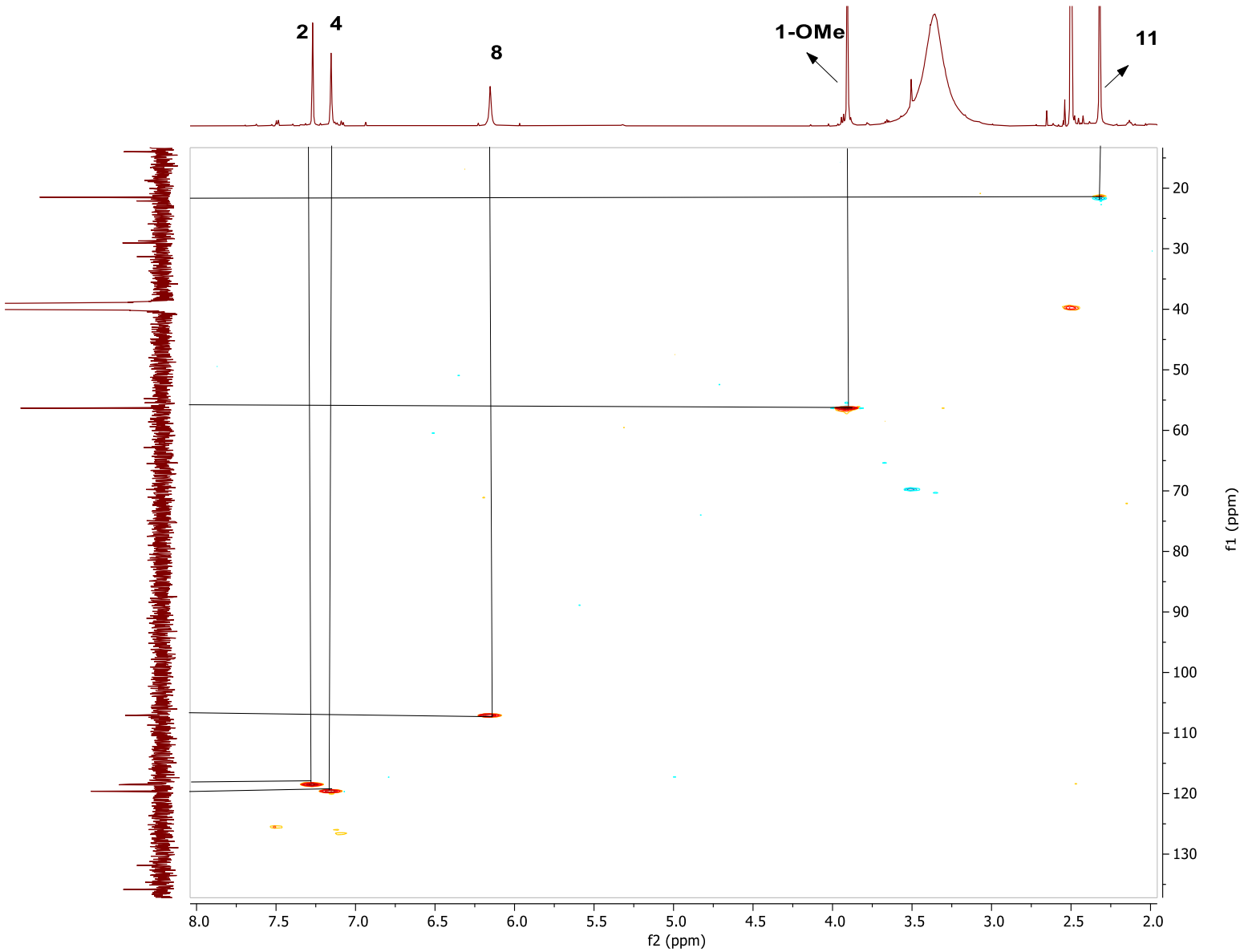

Figure S 13: HSQC spectrum of compound **2**.

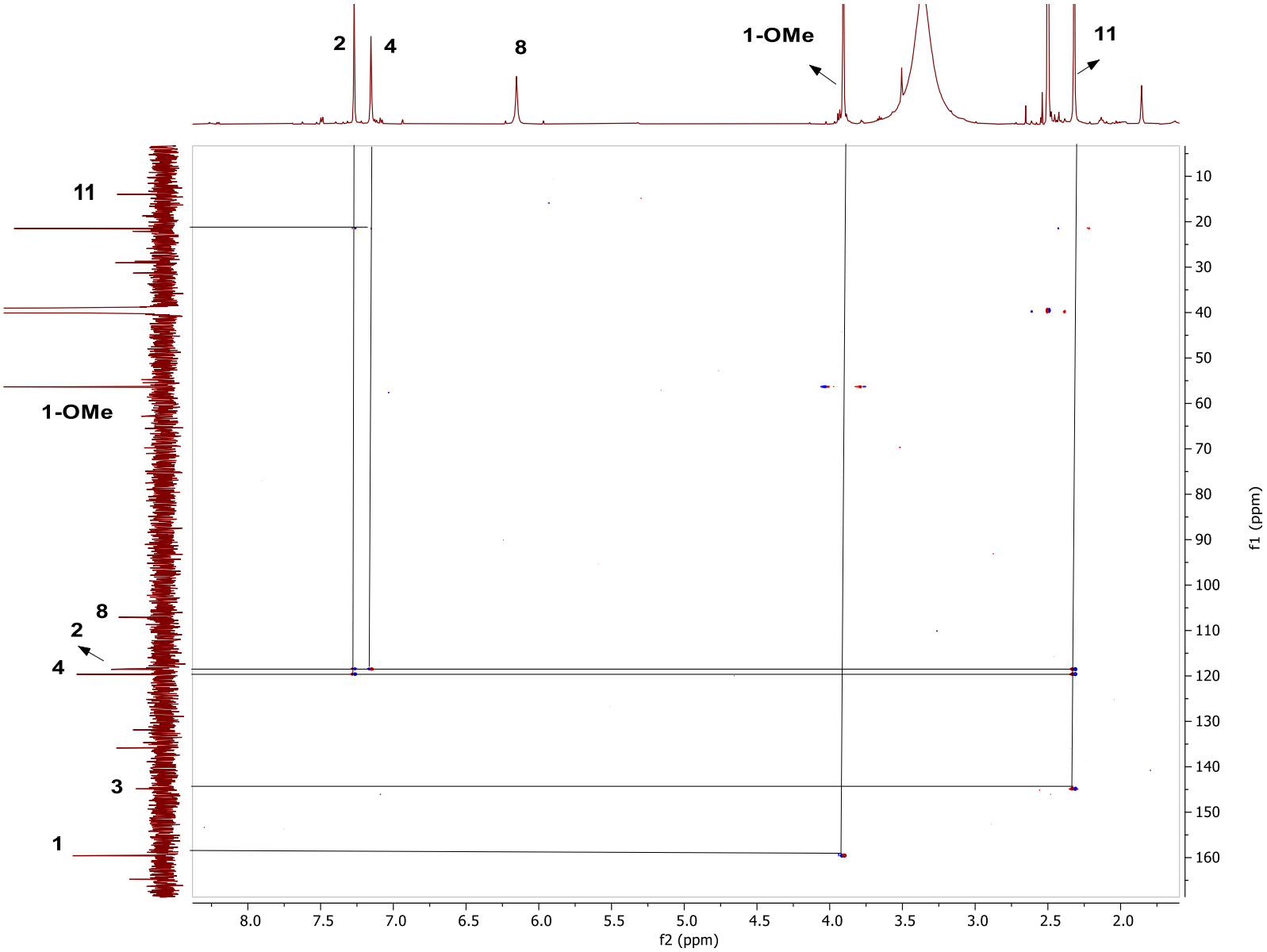

Figure S 14: HMBC spectrum of compound **2**.

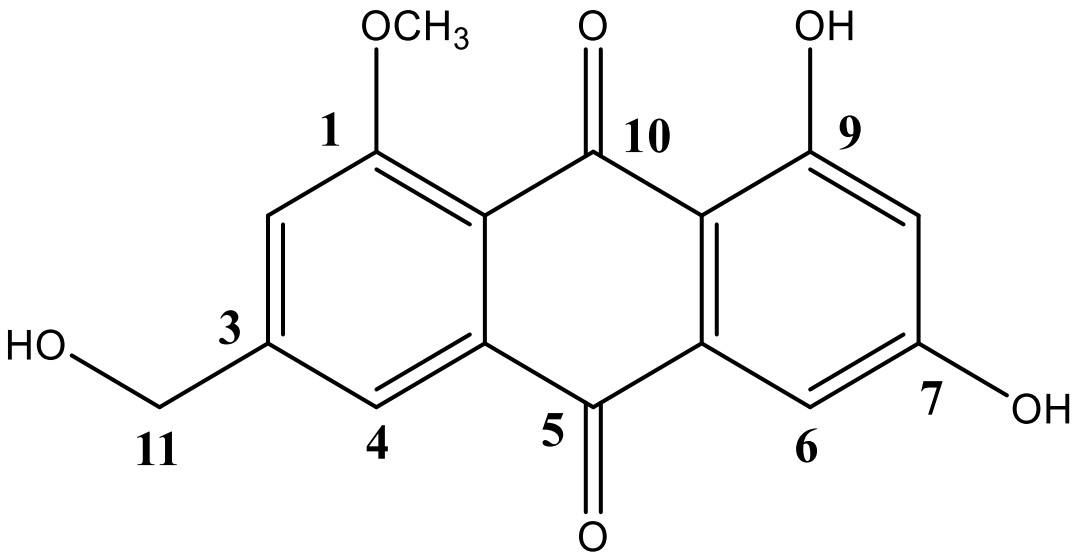

Figure S 15: Chemical structure of compound **3**.

Table S 2: ^{1}H and ^{13}C NMR data for compound **3**.

	3	
No	**δ_C, Type[a]**	**δ_H (J in Hz)[b]**
1	160.6 s	-
2	116.2 d	7.47 (d, 1.5)
3	151.3 s	-
4	116.8 d	7.72 (d, 1.5)
4a	134.7 s	-
5	182.5 s	-
5a	134.0 s	-
6	107.7 d	7.02 (d, 2.4)
7	164.7 s	-
8	108.3 d	6.52 (d, 2.4)
9	165.4 s	-
9a	109.7 s	-
10	186.0 s	-
10a	118.4 s	-
11	62.3 t	4.63 (2H, s)
1-OMe	56.4 q	3.93 (3H, s)
7-OH	-	-
9-OH	-	13.28 (s)
11-OH	-	-

[a]Chemical shifts were measured at 400 MHz in DMSO-d_6
[b]Chemical shifts were measured at 100 MHz in DMSO-d_6

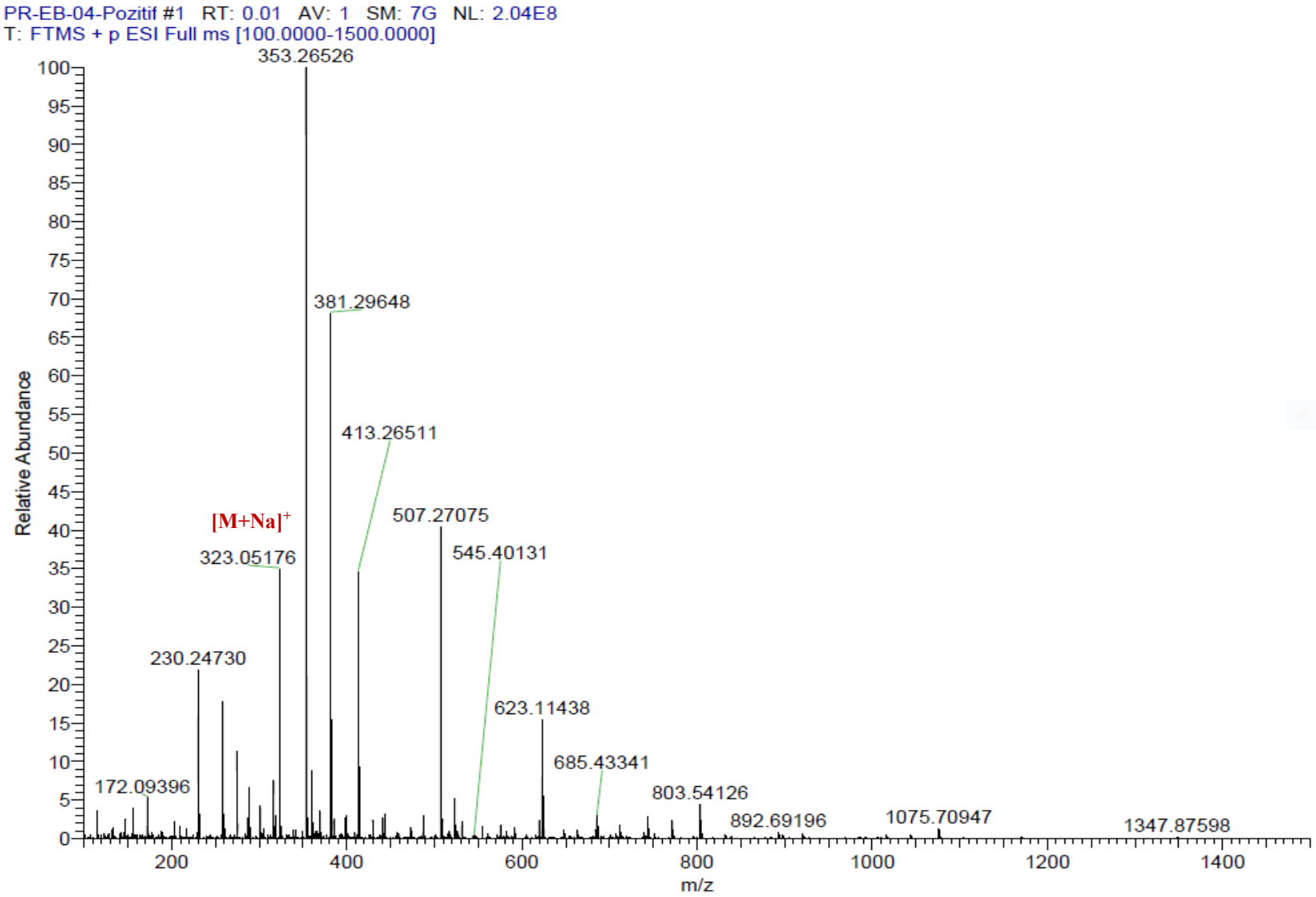

Figure S 16: HR-ESI-MS spectrum of compound **3** (positive mode).

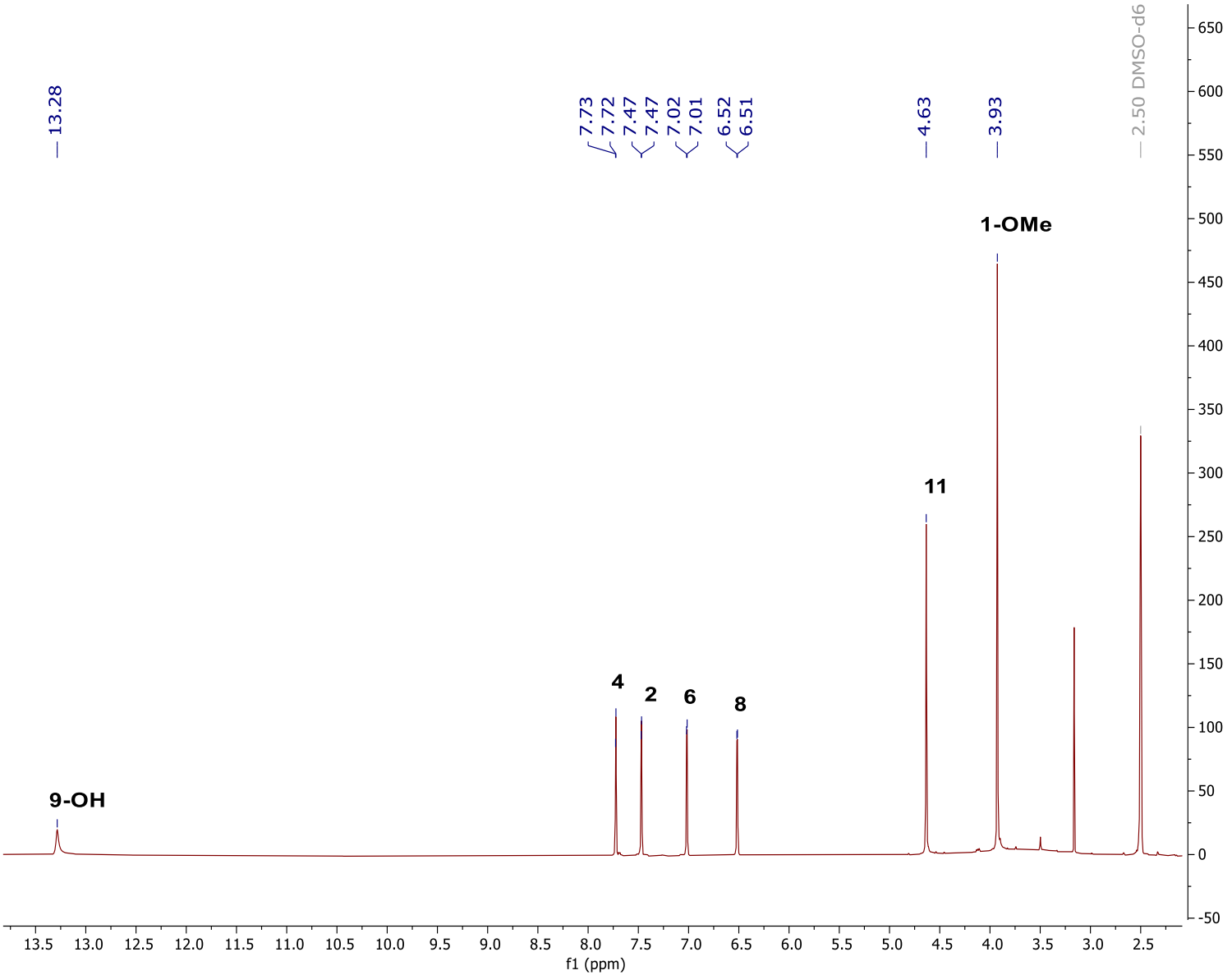

Figure S 17: ^{1}H NMR spectrum of compound **3** (in DMSO-d_6, ^{1}H: 400 MHz).

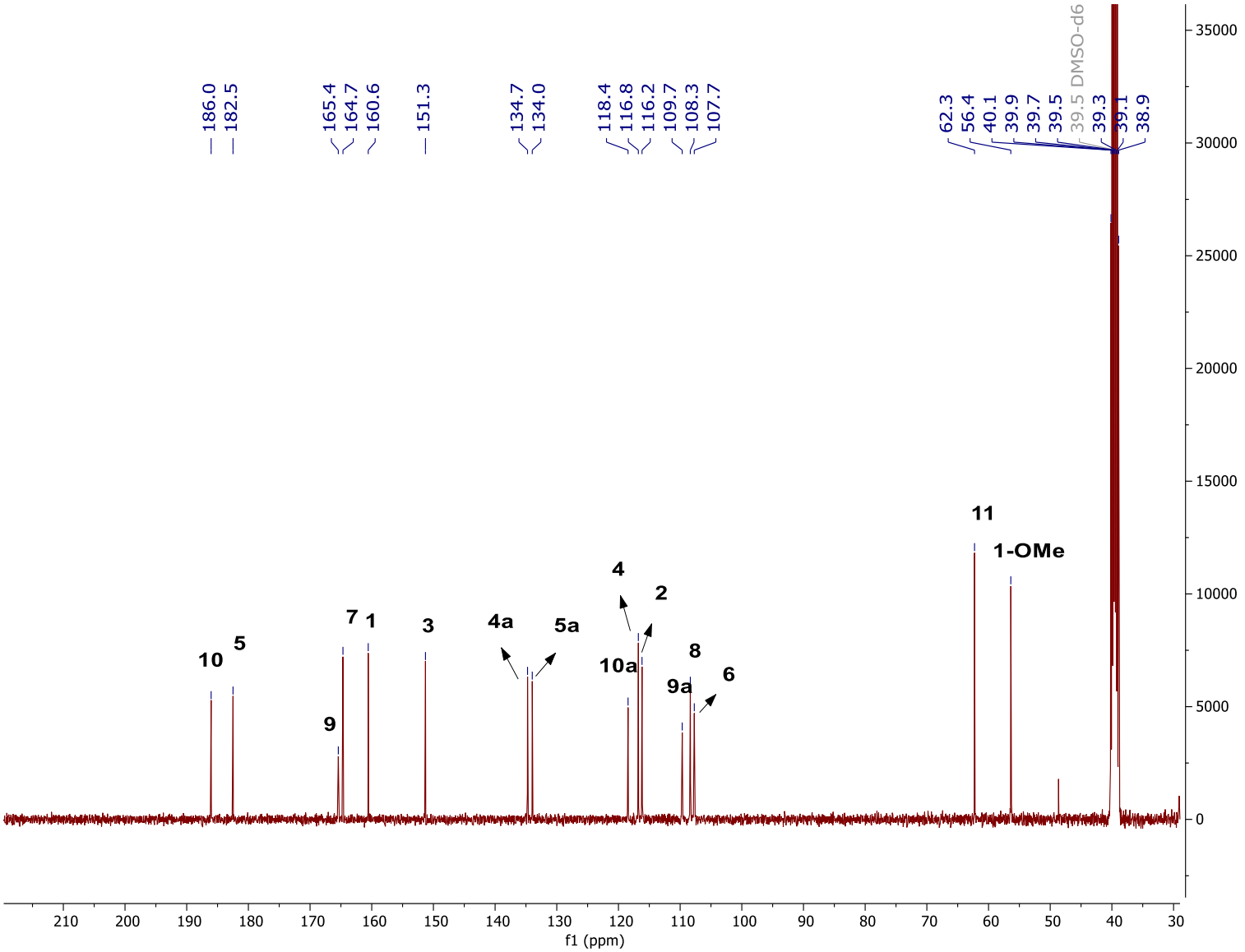

Figure S 18: ^{13}C NMR spectrum of compound **3** (in DMSO-d_6, ^{13}C:100 MHz).

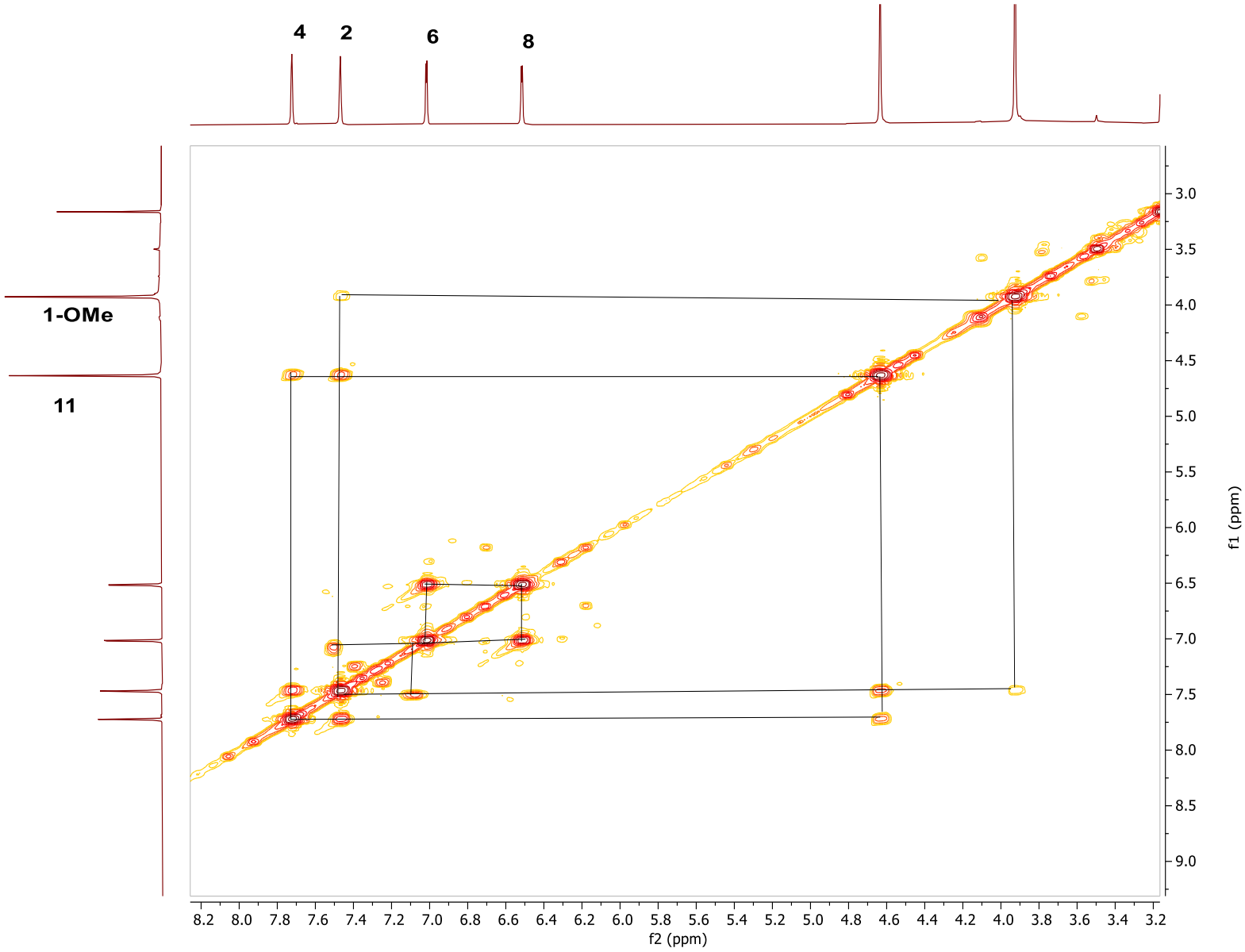

Figure S 19: COSY spectrum of compound **3**.

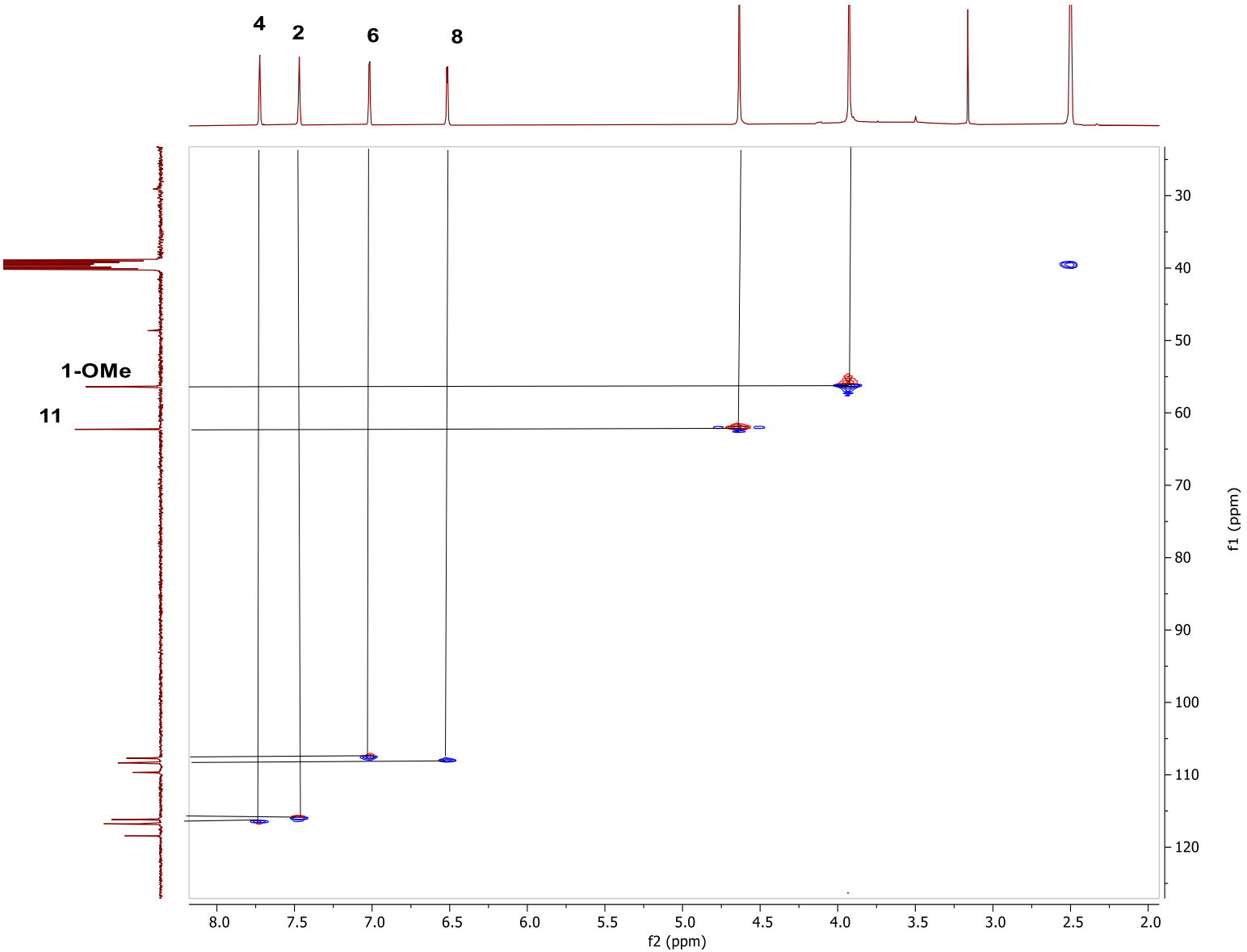

Figure S 20: HSQC spectrum of compound **3**.

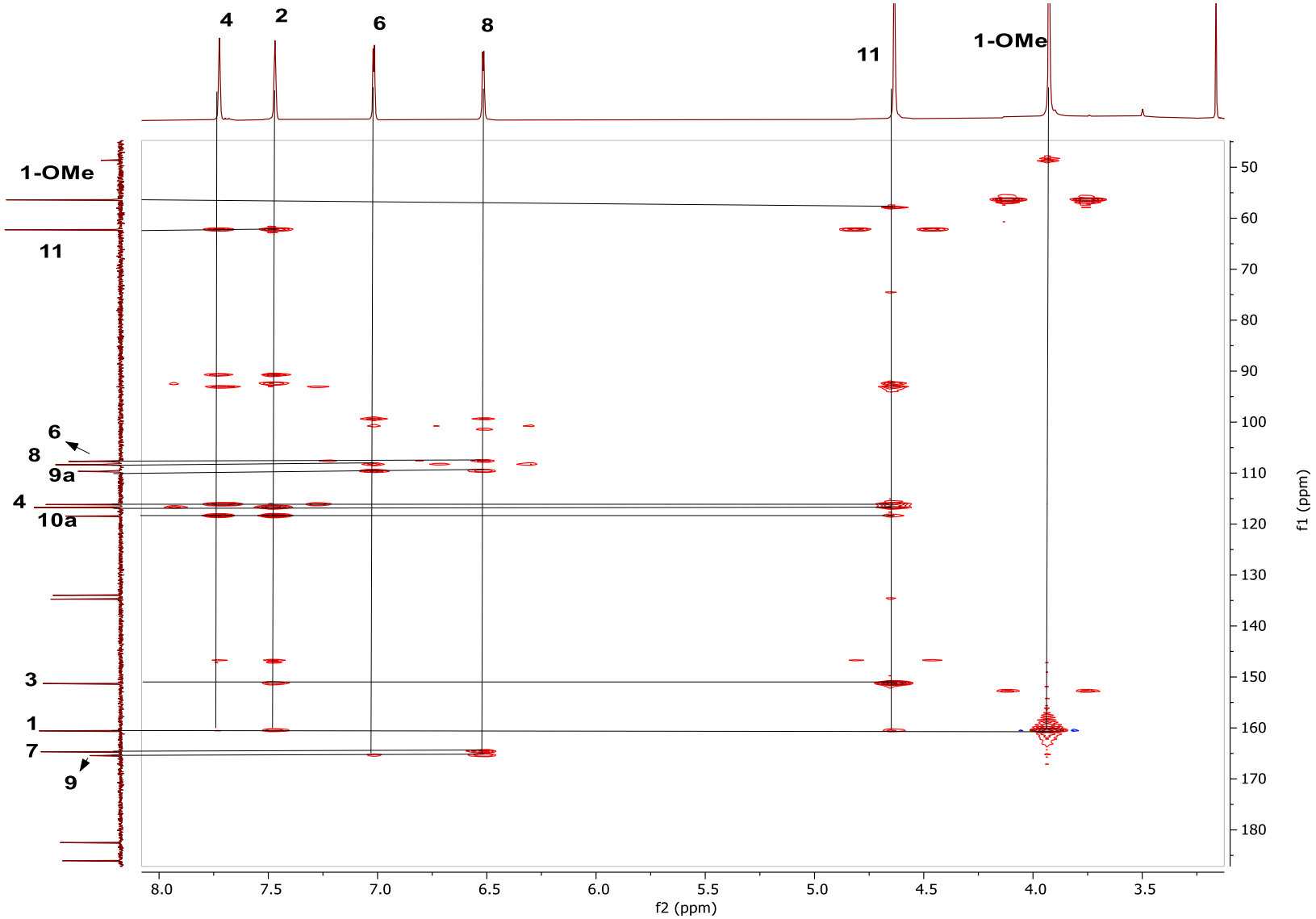

Figure S 21: HMBC spectrum of compound **3**.

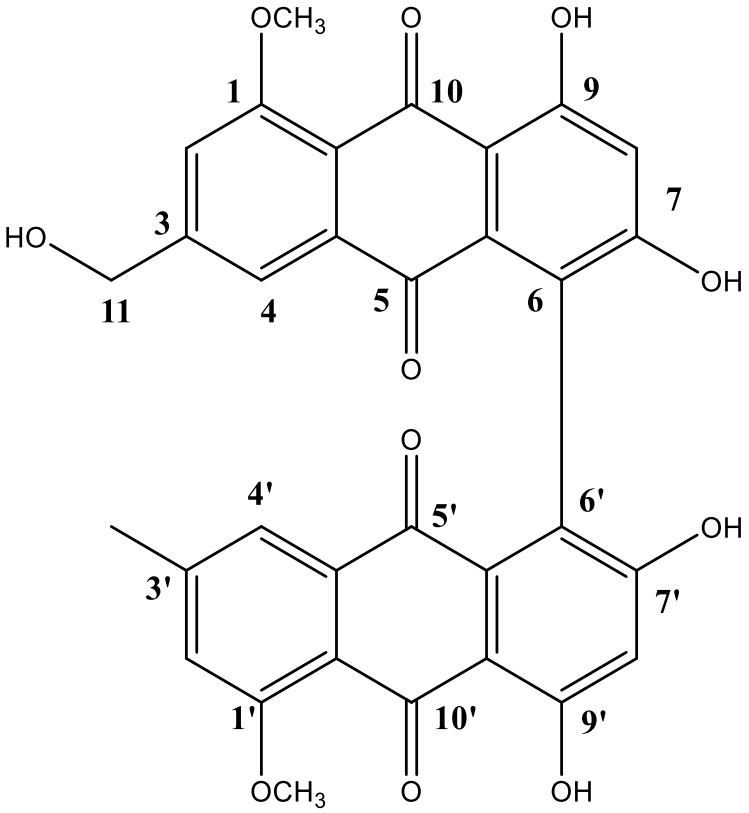

Figure S 22: Chemical structure of compound **4**.

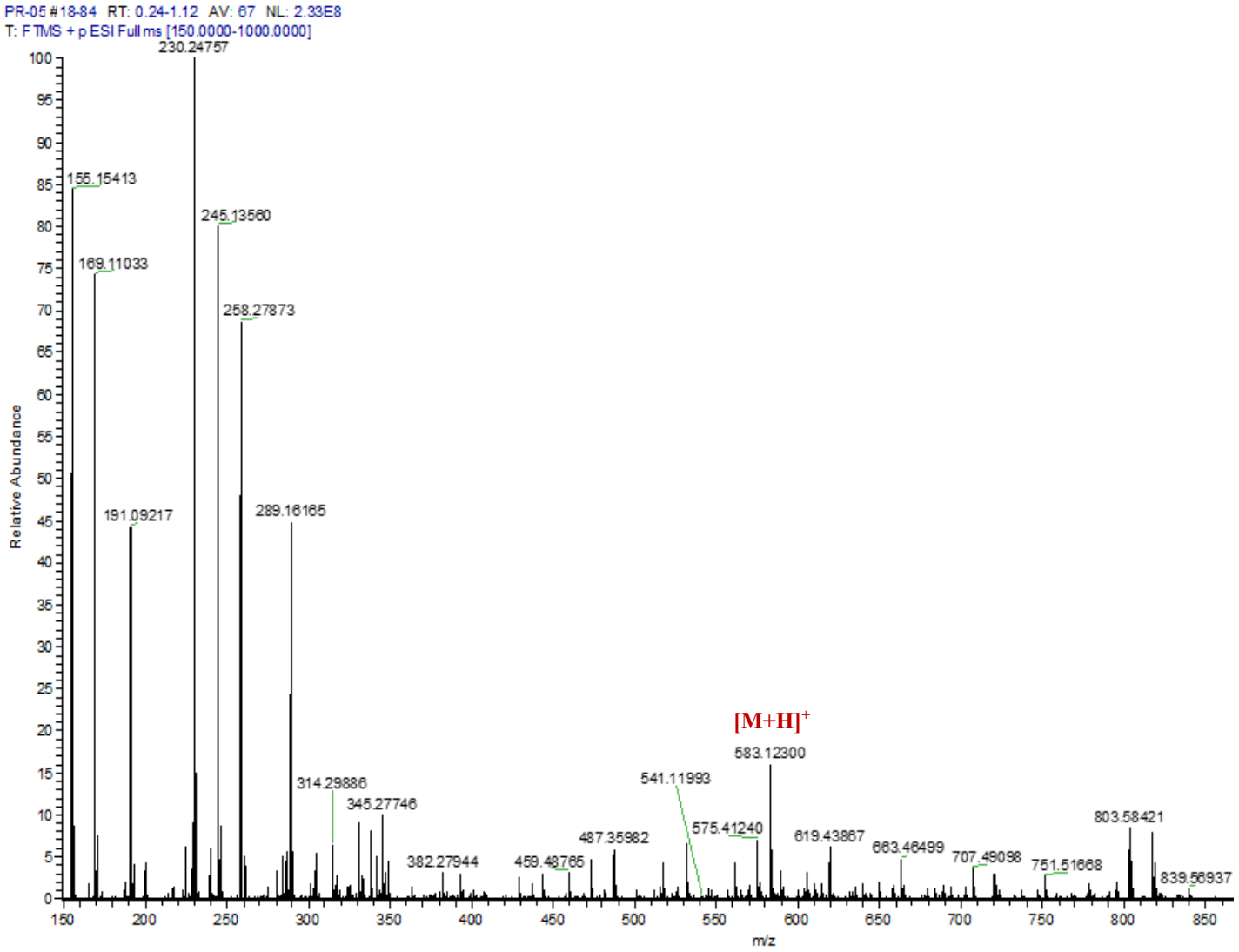

Figure S 23: HR-ESI-MS spectrum of compound **4** (positive mode).

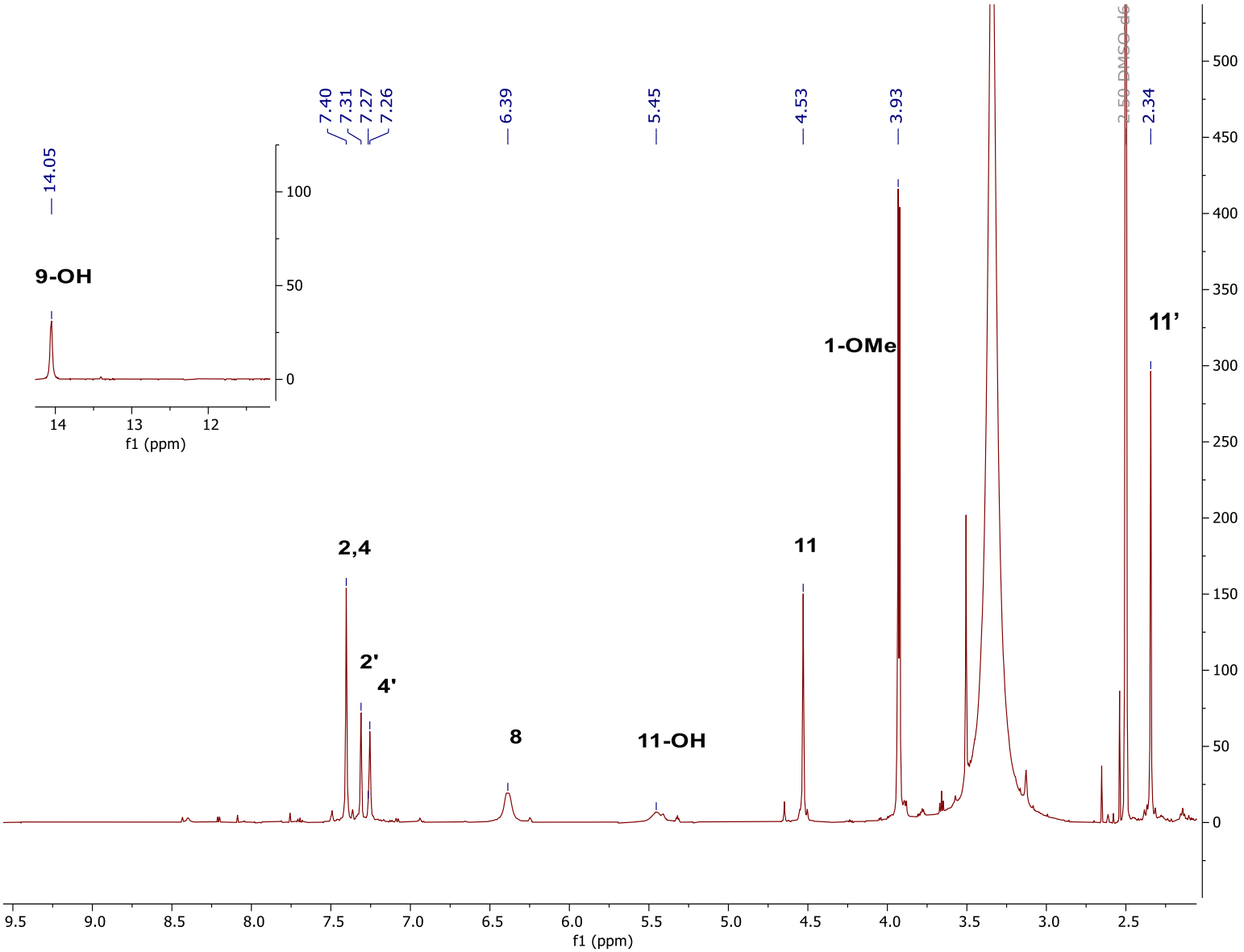

Figure S 24: ^{1}H NMR spectrum of compound **4** (in DMSO-d_6, ^{1}H: 600 MHz).

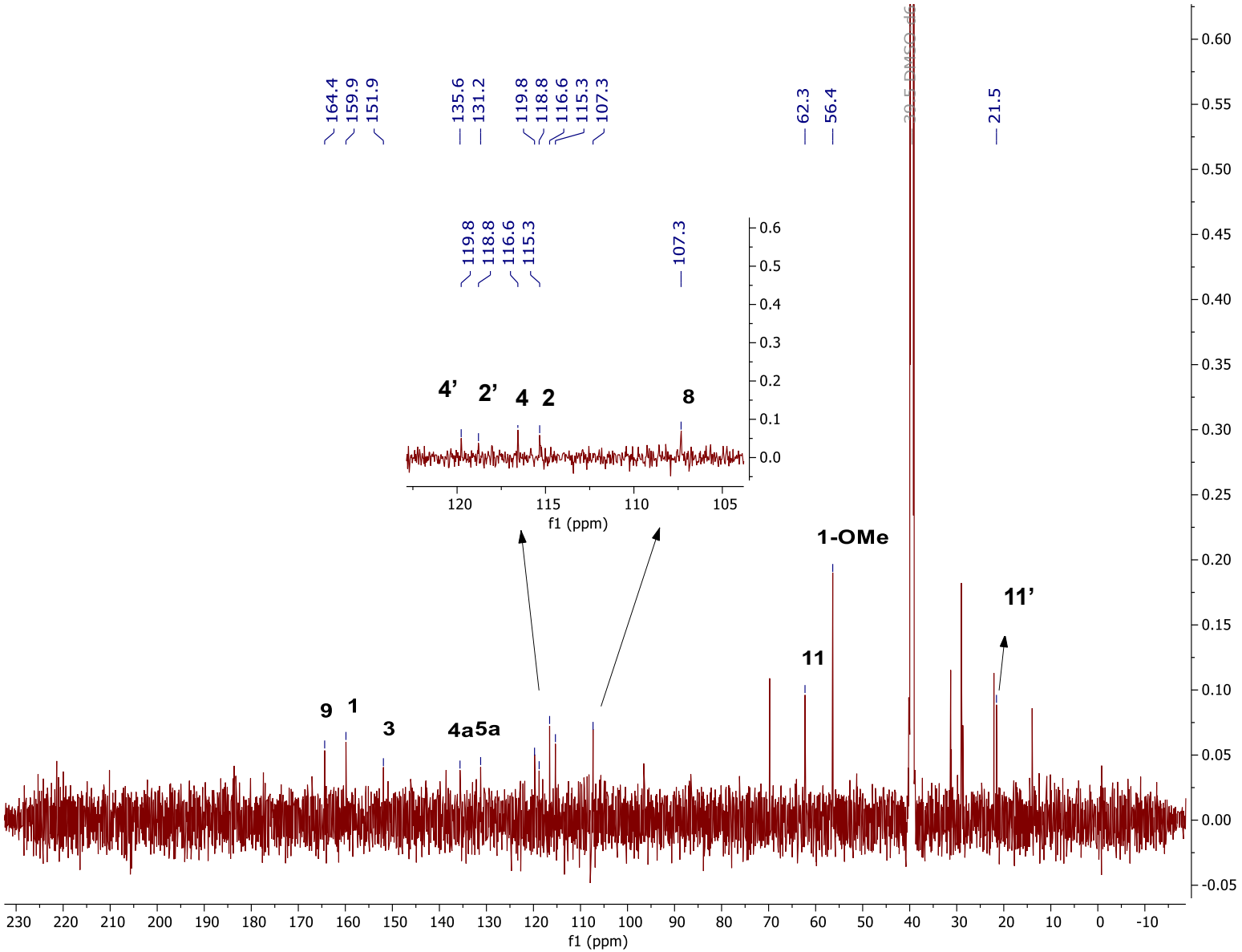

Figure S 25: ^{13}C NMR spectrum of compound **4** (in DMSO-d$_6$, ^{13}C:150 MHz).

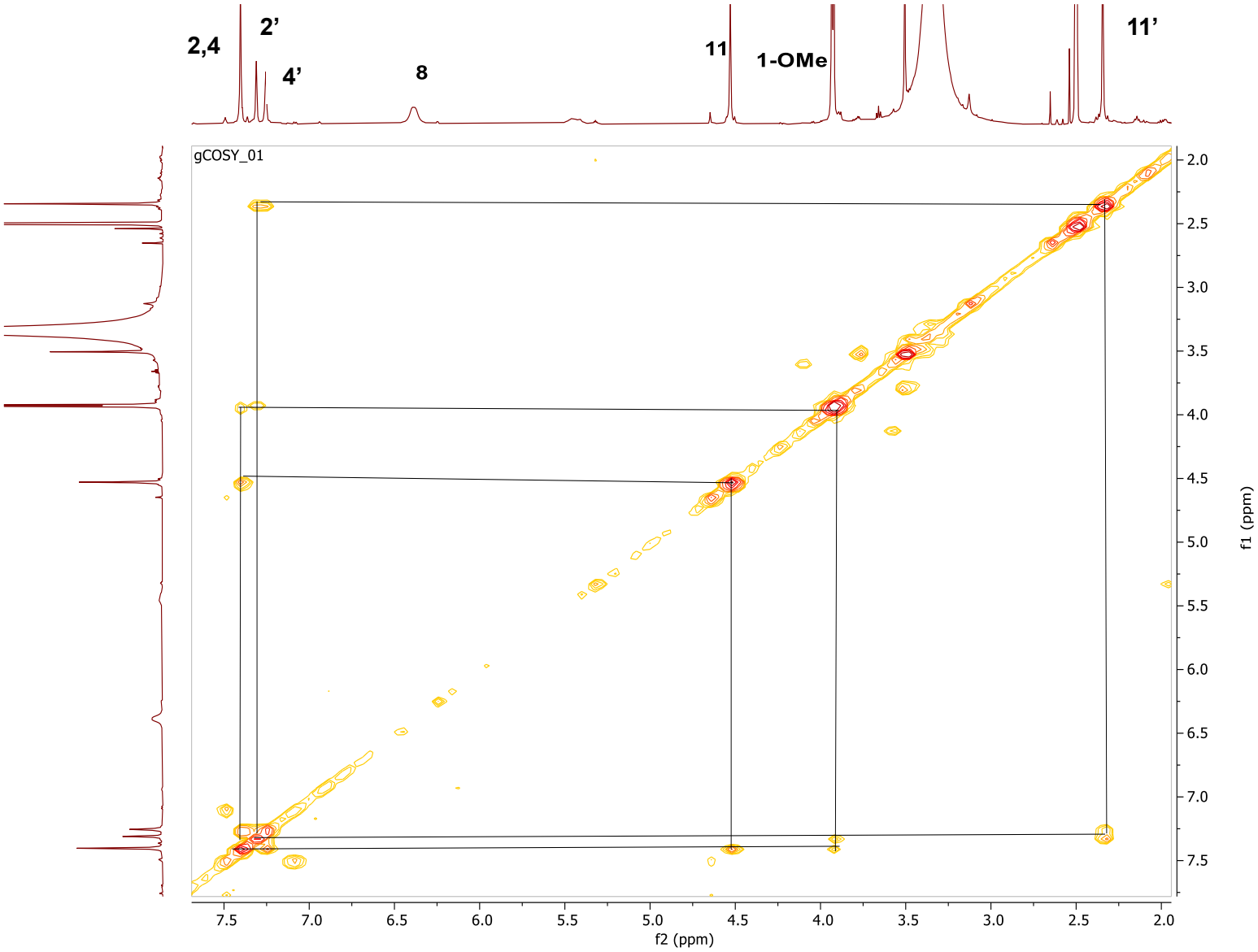

Figure S 26: COSY spectrum of compound **4**.

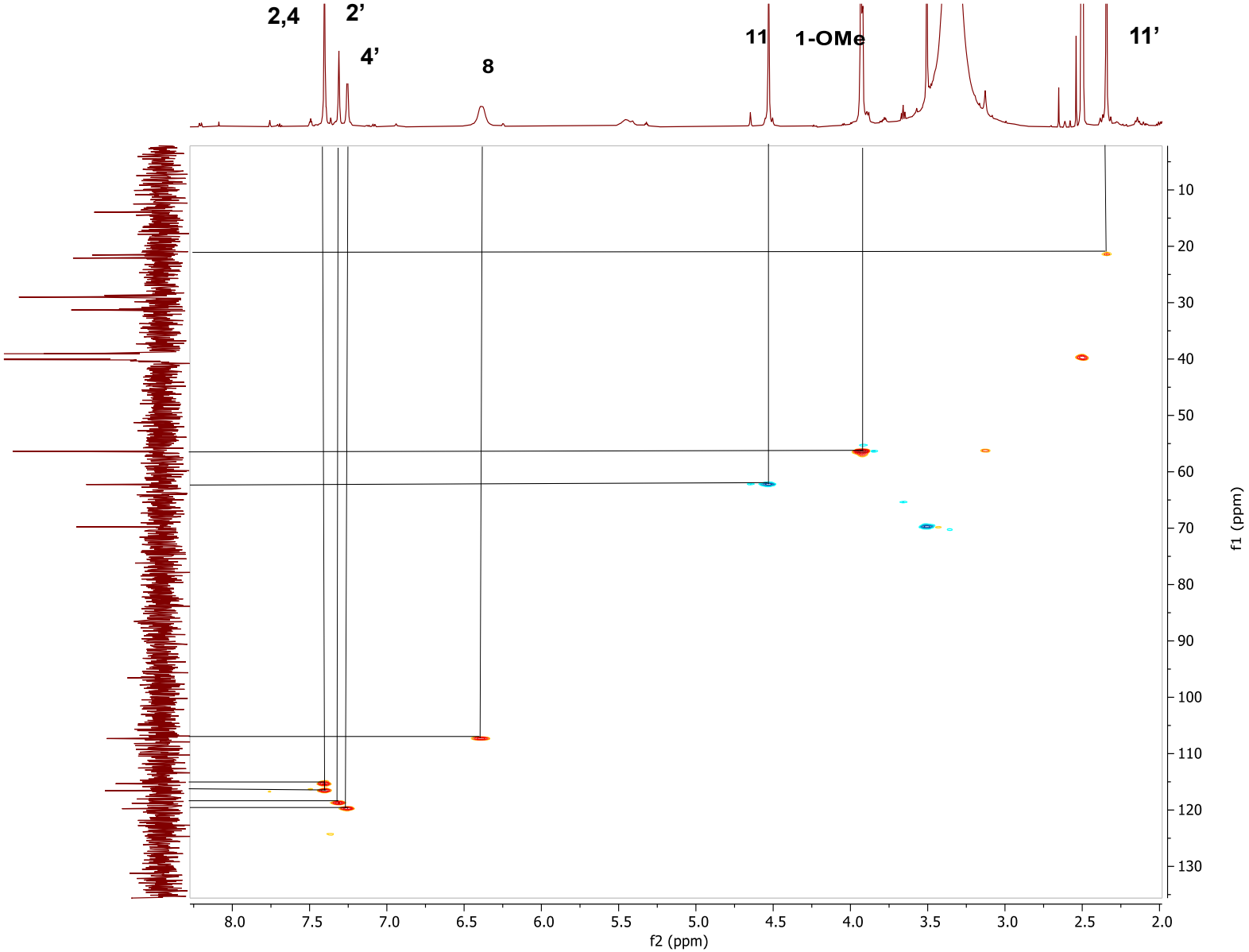

Figure S 27: HSQC spectrum of compound **4**.

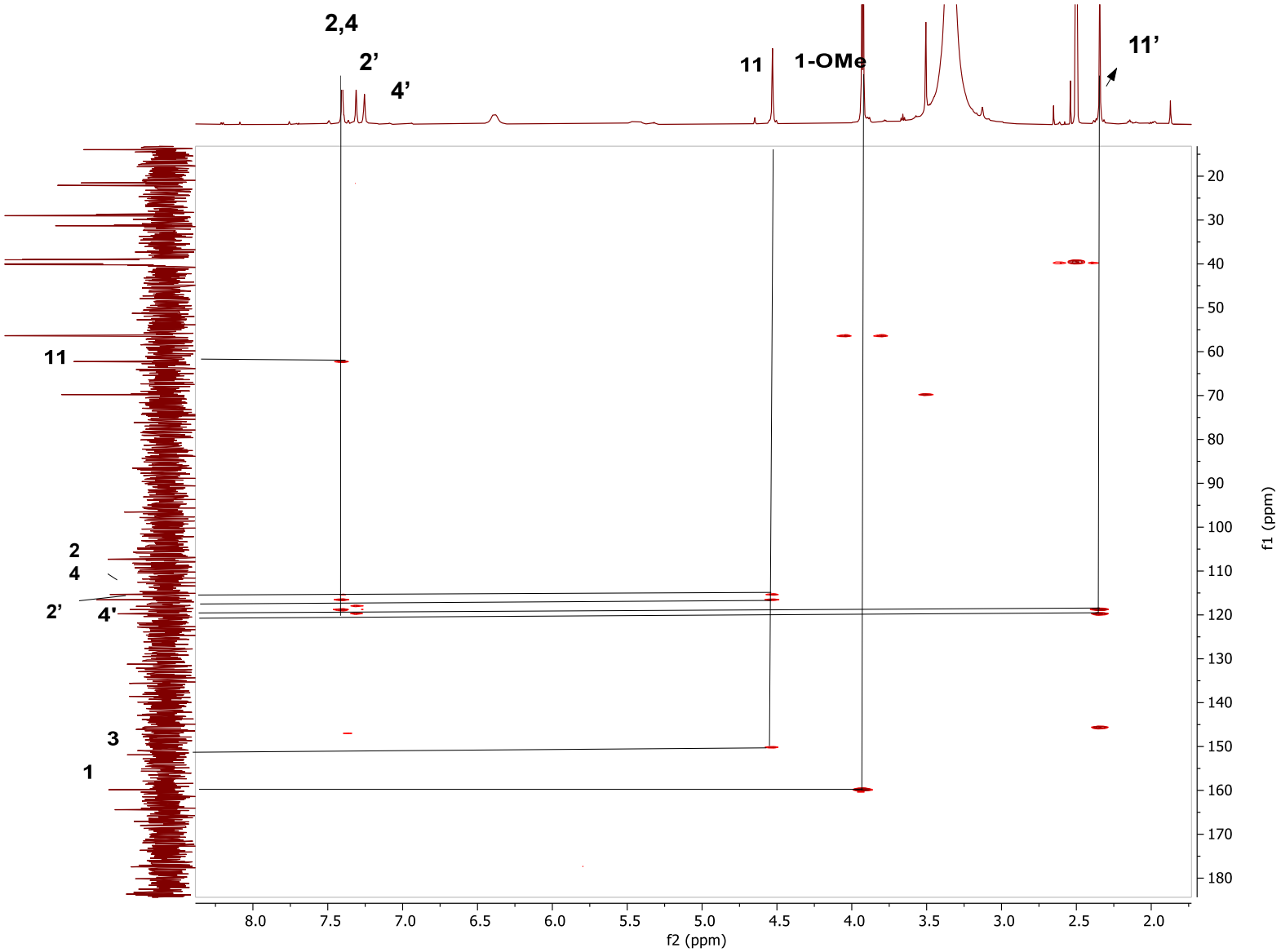

Figure S 28: HMBC spectrum of compound **4**.

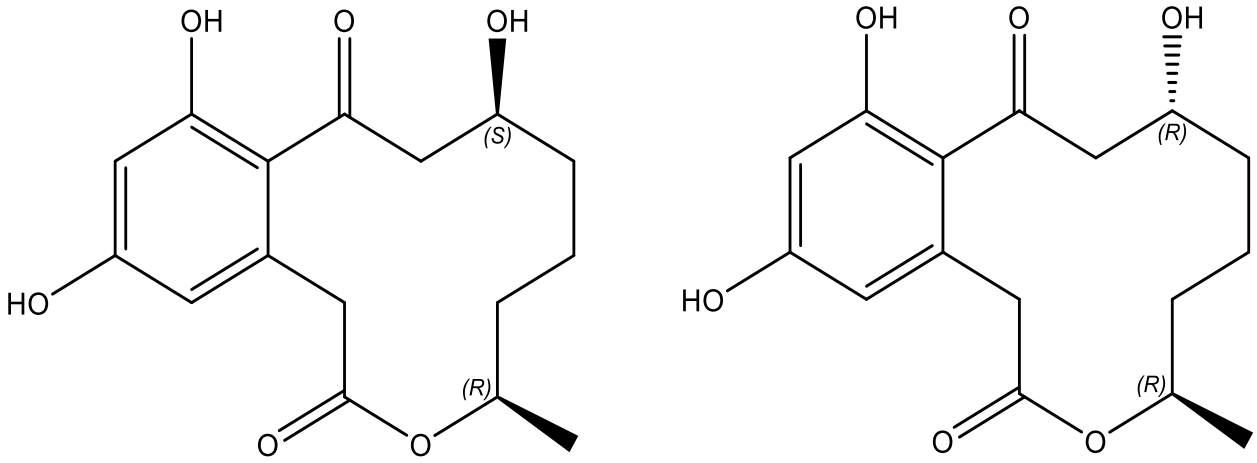

Figure S 29: Chemical structures of compound **5a** and **5b**.

Table S 3: ^{1}H and ^{13}C NMR data for compound **5**.

	5a		**5b**	
No	**δ_C, Type[a]**	**δ_H (*J* in Hz)[b]**	**δ_C, Type[a]**	**δ_H (*J* in Hz)[b]**
1	169.9 s	-	170.2 s	-
2	38.9 t	3.77 (m), 3.56 (d, 15.6)	38.9 t	3.77 (m), 3.56 (d, 15.6)
3	136.0 s	-	136.0 s	-
4	111.4 d	6.15 (d, 2.3)	110.8 d	6.15 (d, 2.3)
5	159.7 s	-	159.4 s	-
6	101.8 d	6.26 (d, 2.2)	101.7 d	6.28 (d, 2.3)
7	157.6 s	-	158.5 s	-
8	118.8 s	-	118.8 s	-
9	203.5 s	-	204.2 s	-
10	53.2 t	3.14 (d, 13.4), 2.85 (s)	53.9 t	3.14 (d, 13.4), 2.85 (s)
11	65.0 d	3.87 (s)	65.9 d	3.77 (d, 13.6)
12	34.4 t	1.47 (m), 1.21 (m)	34.4 t	1.47 (m), 1.21 (m)
13	21.7 t	1.06 (s), 1.05 (s)	21.7 t	1.06 (s), 1.05 (s)
14	31.1 t	1.46 (m), 1.21 (m)	30.5 t	1.58 (m), 1.32 (m)
15	70.2 d	4.84 (m)	72.8 d	4.71 (m)
16	18.0 q	1.06 (3H, s)	18.8 q	1.06 (3H, s)
5-OH	-	9.87 (brs)	-	9.81 (brs)
7-OH	-	10.03 (brs)	-	10.09 (brs)
11-OH	-	4.60 (d, 5.2)	-	4.58 (d, 5.8)

[a]Chemical shifts were measured at 600 MHz in DMSO-d_6
[b]Chemical shifts were measured at 150 MHz in DMSO-d_6

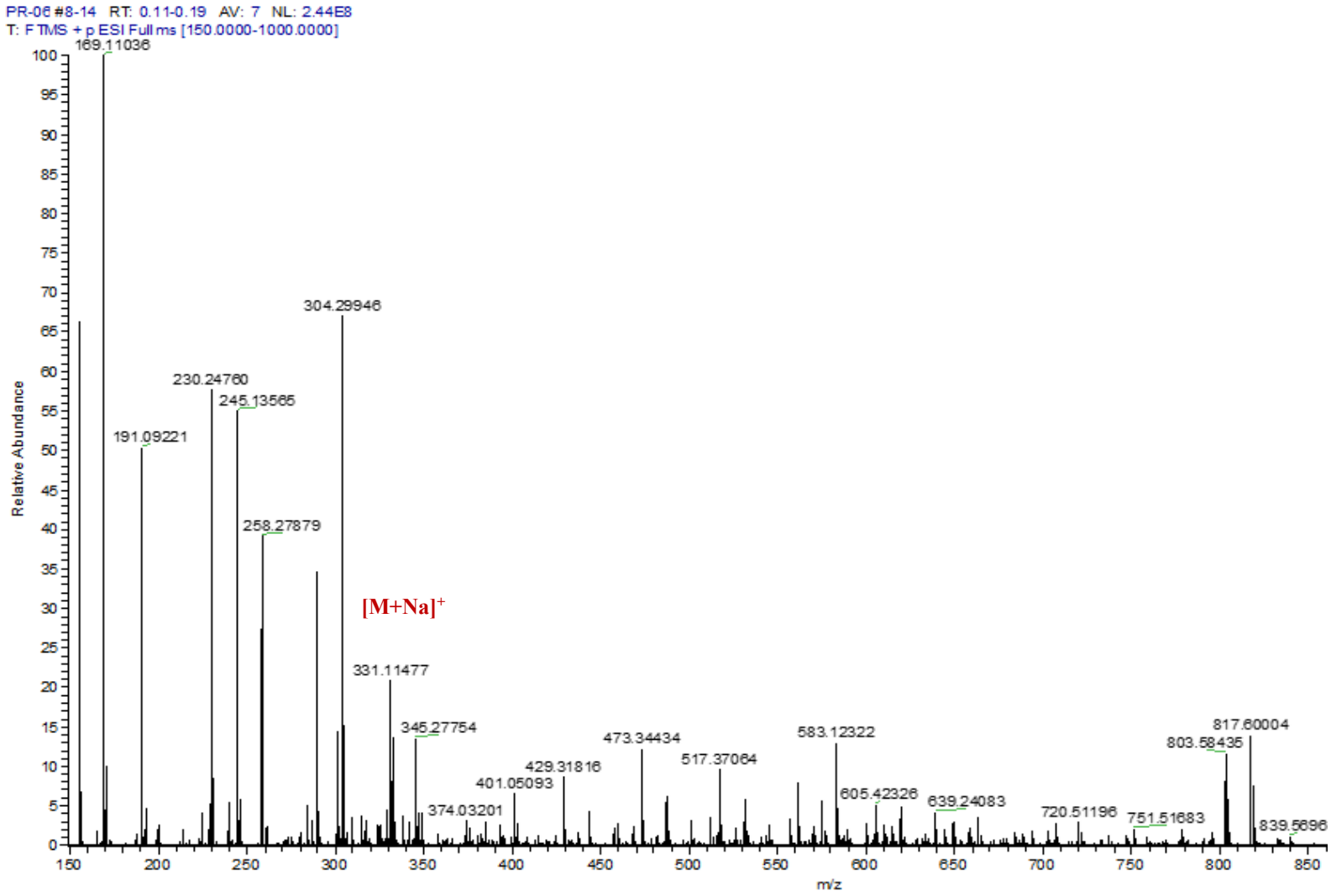

Figure S 30: HR-ESI-MS spectrum of compound **5** (positive mode).

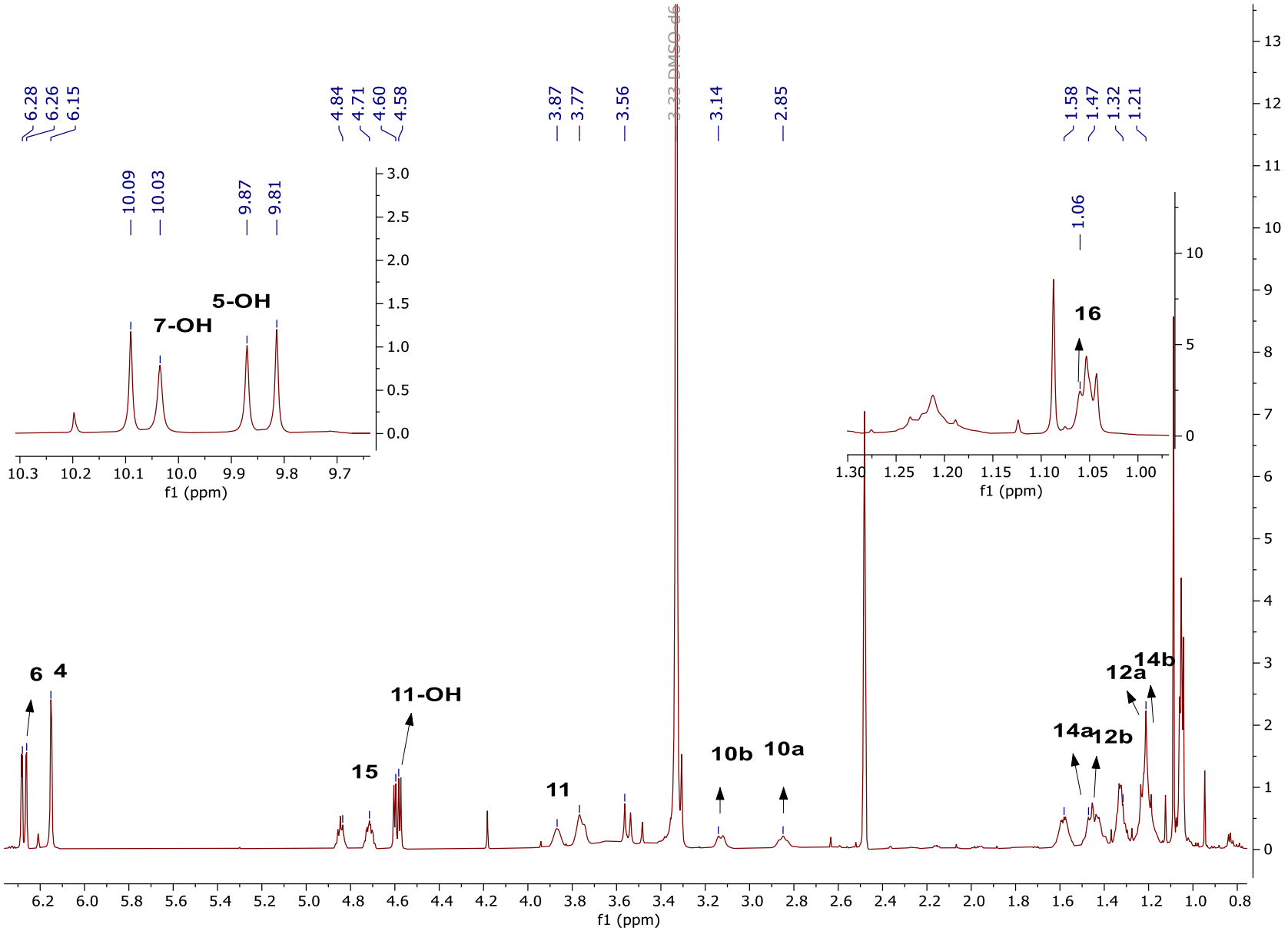

Figure S 31: ^{1}H NMR spectrum of compound **5** (in DMSO-d_6, ^{1}H: 600 MHz).

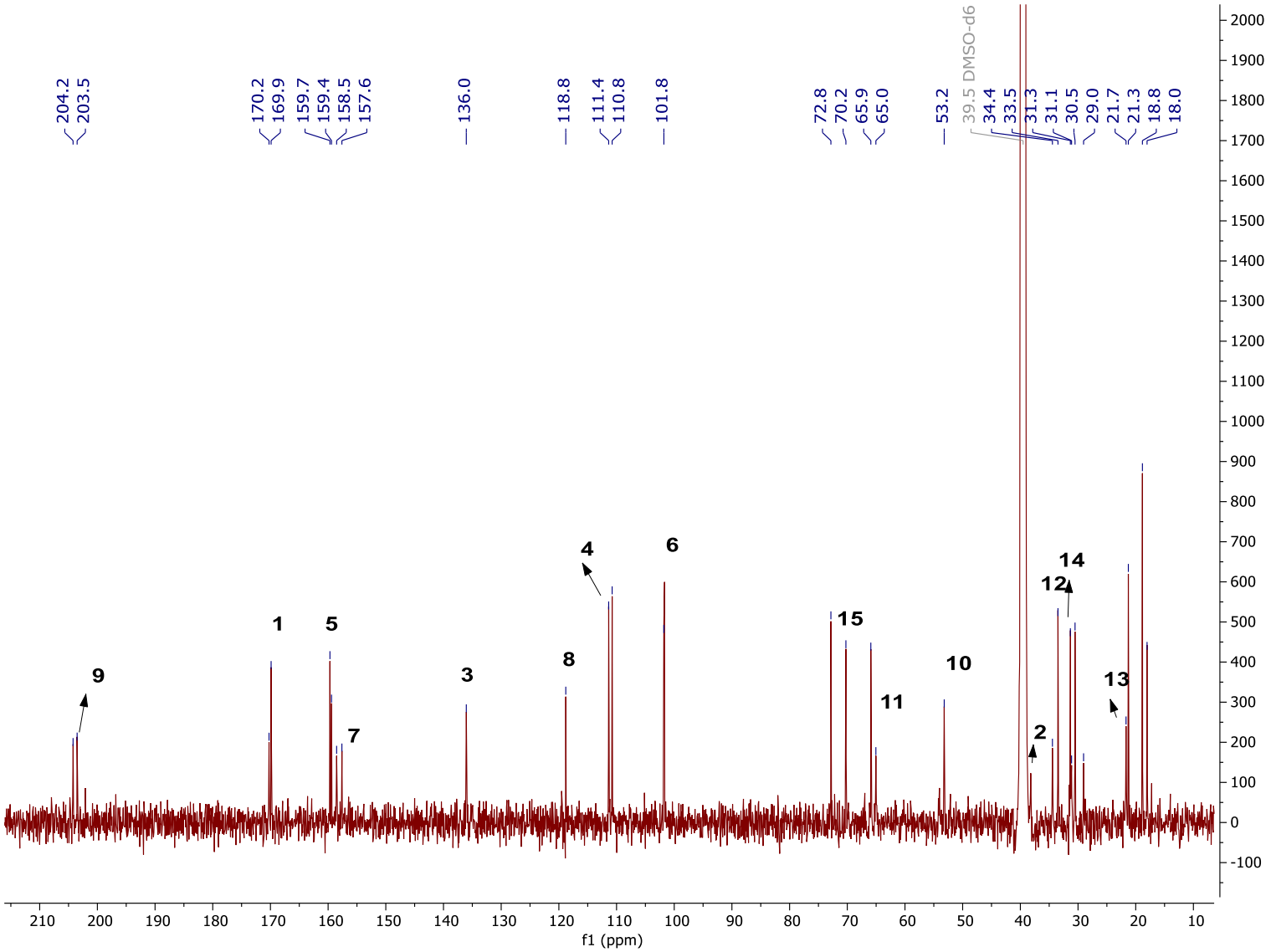

Figure S 32: ^{13}C NMR spectrum of compound **5** (in DMSO-d_6, ^{13}C:150 MHz).

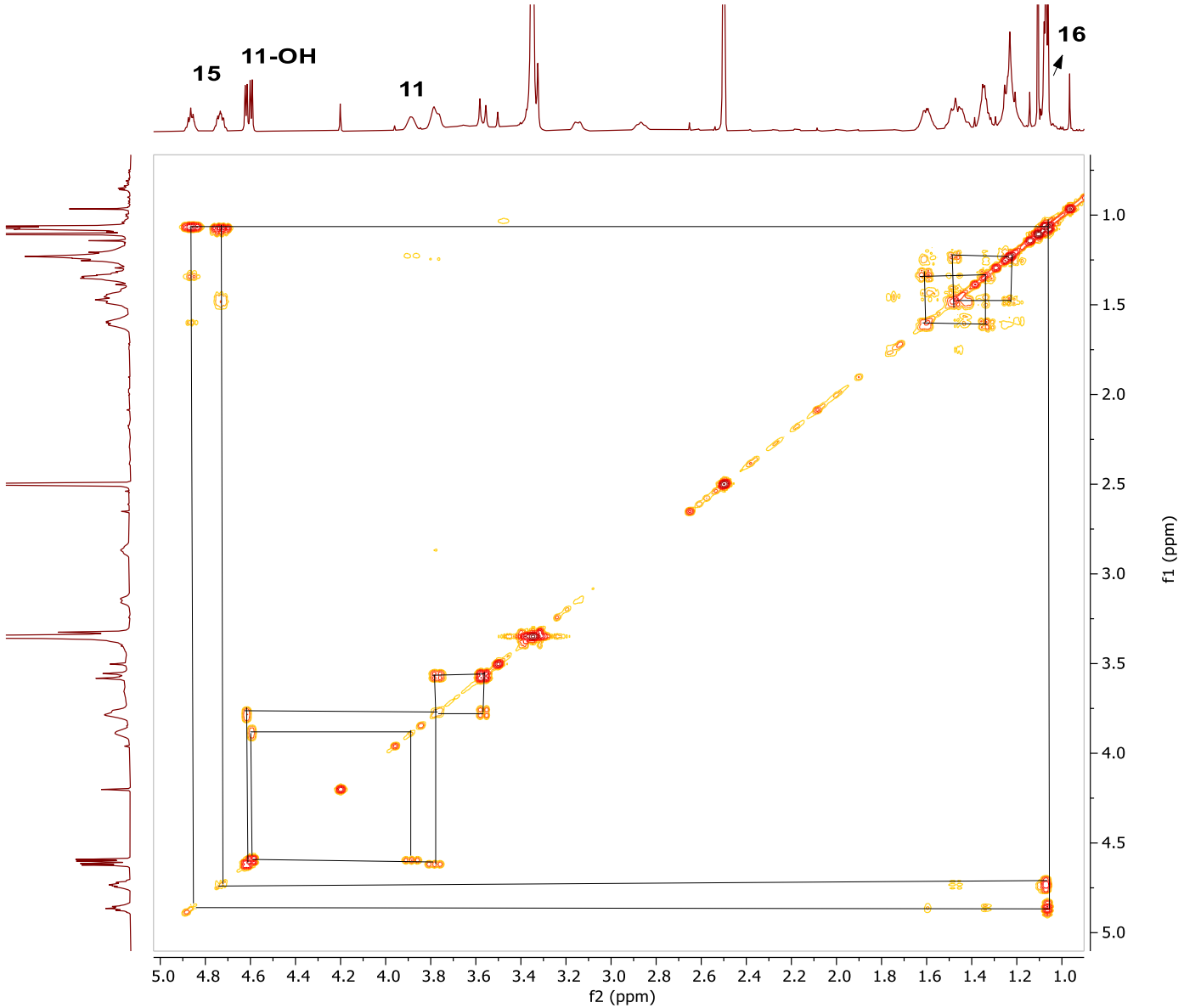

Figure S 33: COSY spectrum of compound **5**.

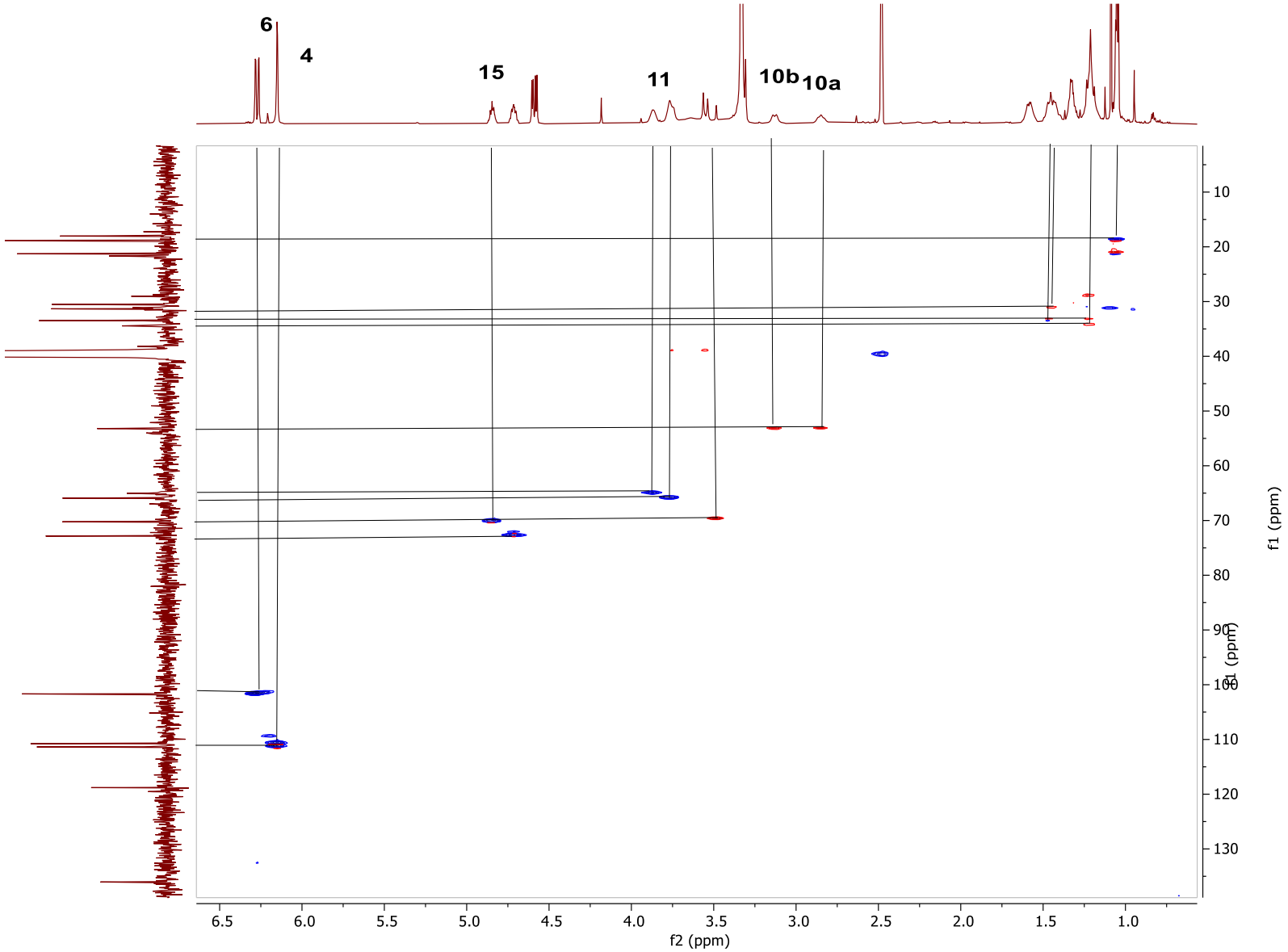

Figure S 34: HSQC spectrum of compound **5**.

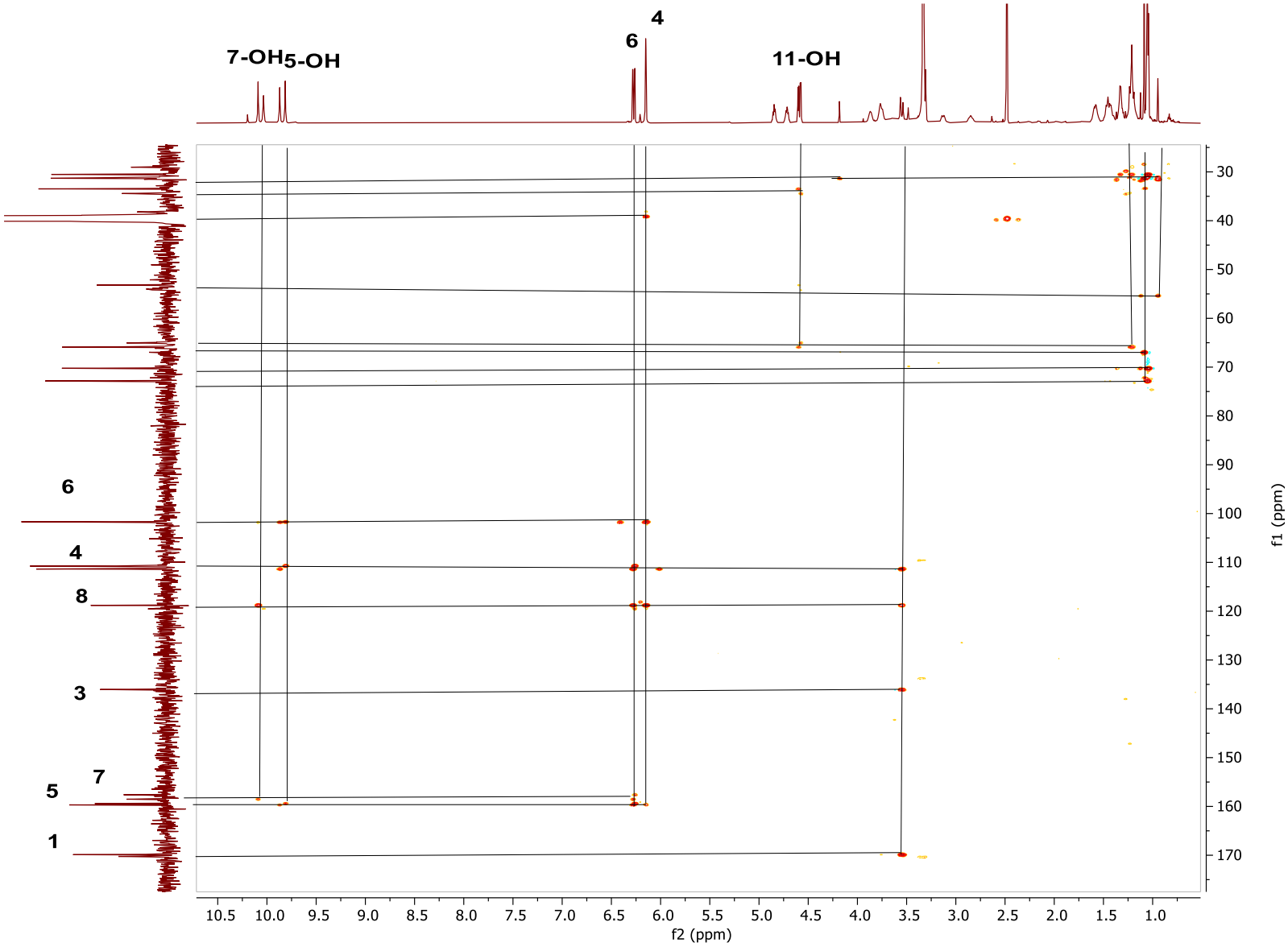

Figure S 35: HMBC spectrum of compound **5**.

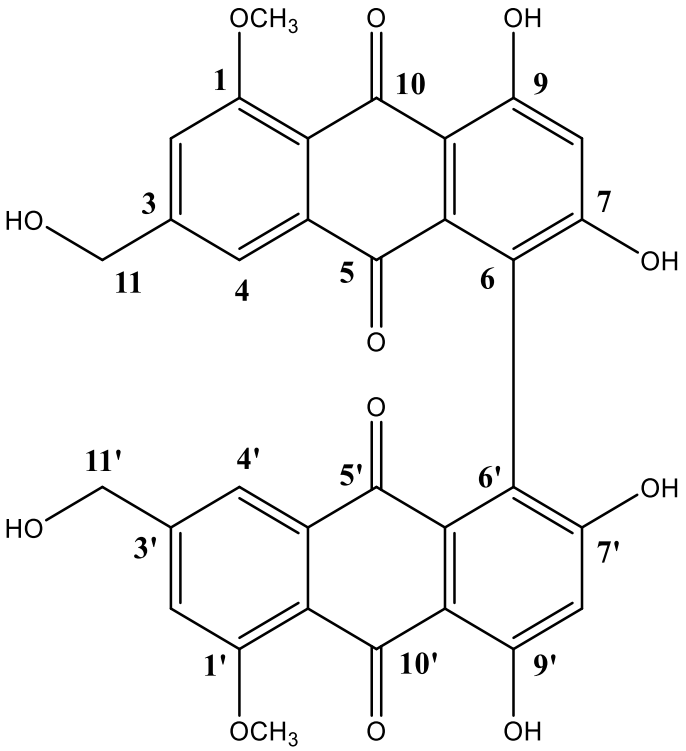

Figure S 36: Chemical structure of compound **6**.

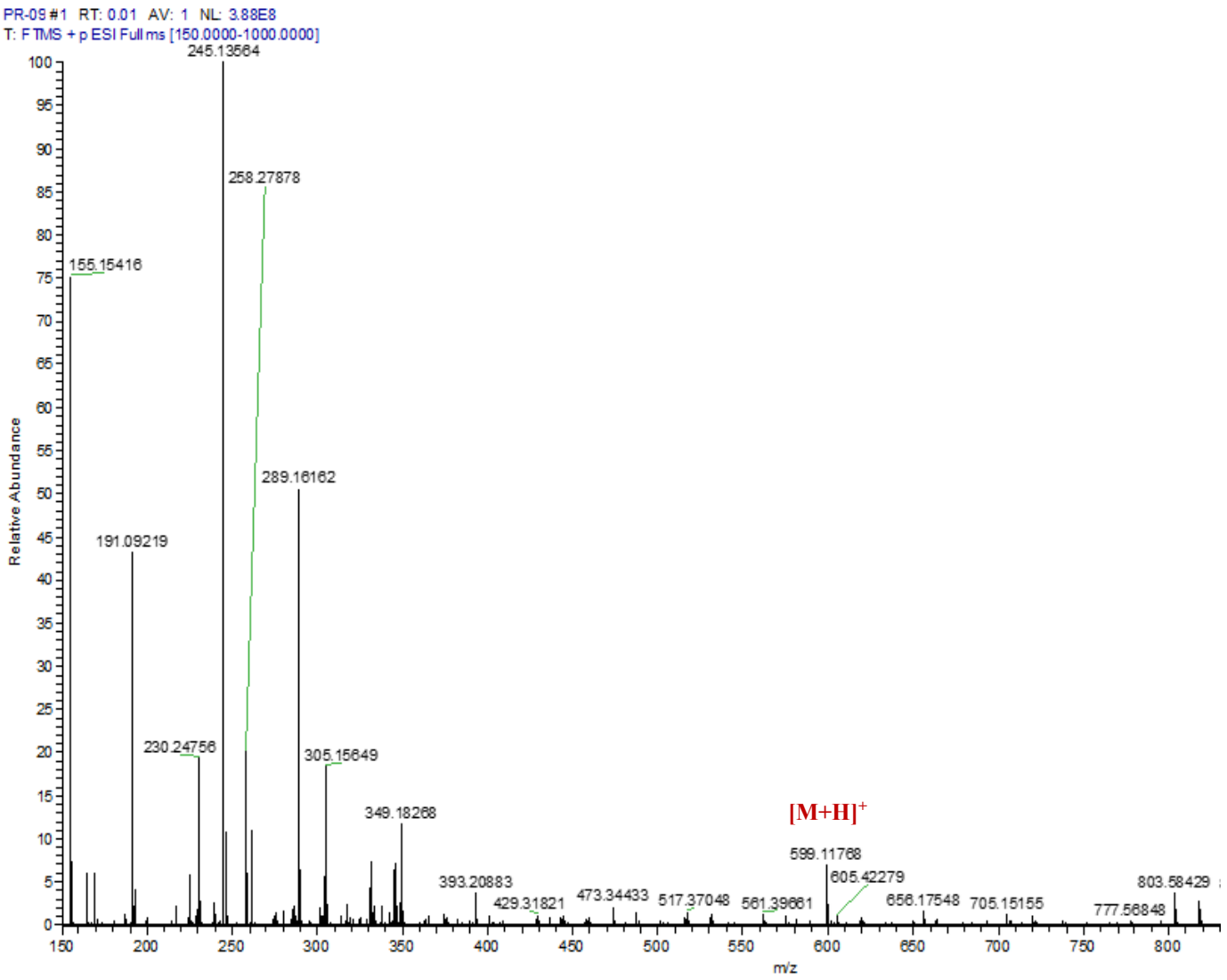

Figure S 37: HR-ESI-MS spectrum of compound **6** (positive mode).

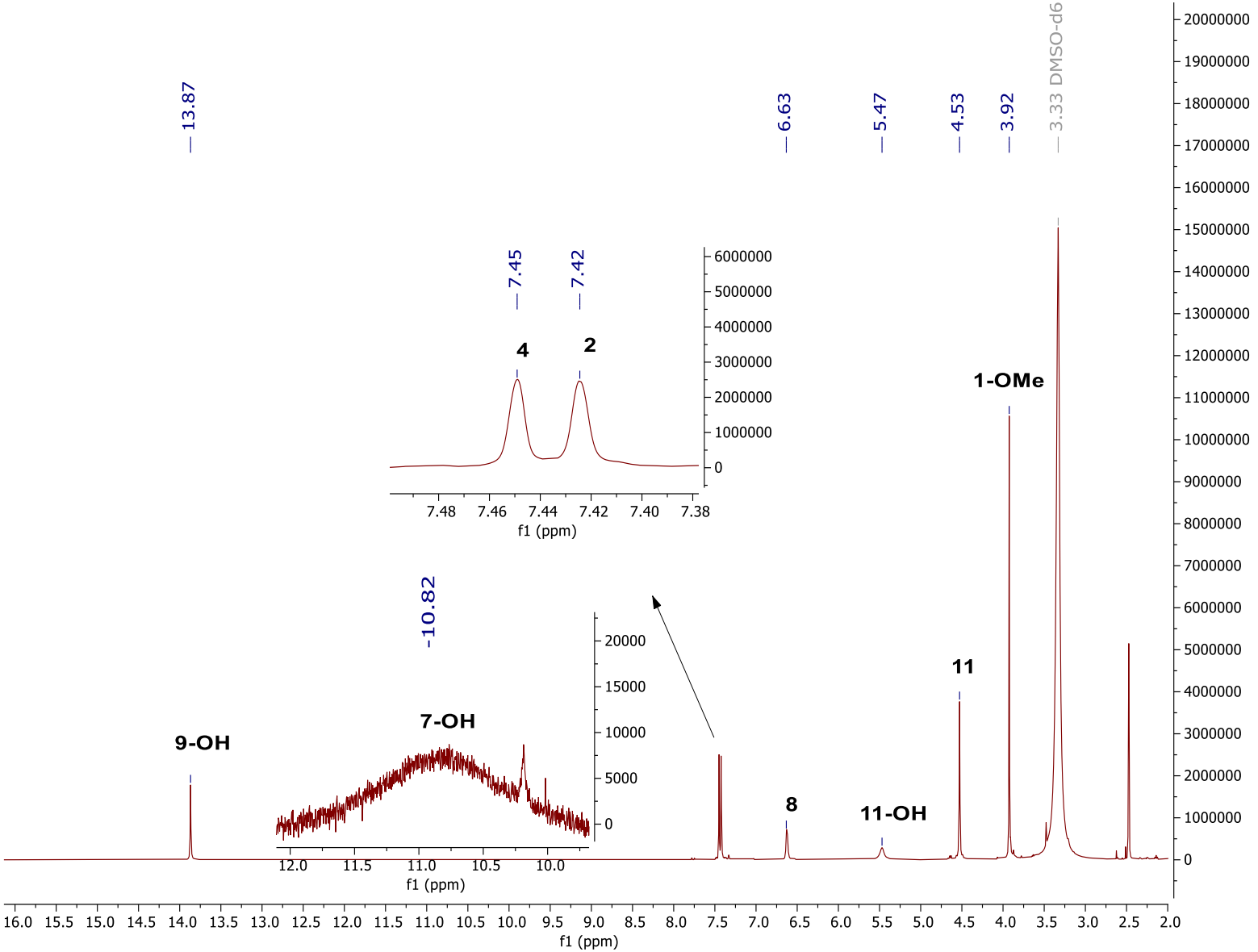

Figure S 38: ^{1}H NMR spectrum of compound **6** (in DMSO-d_6, ^{1}H: 500 MHz).

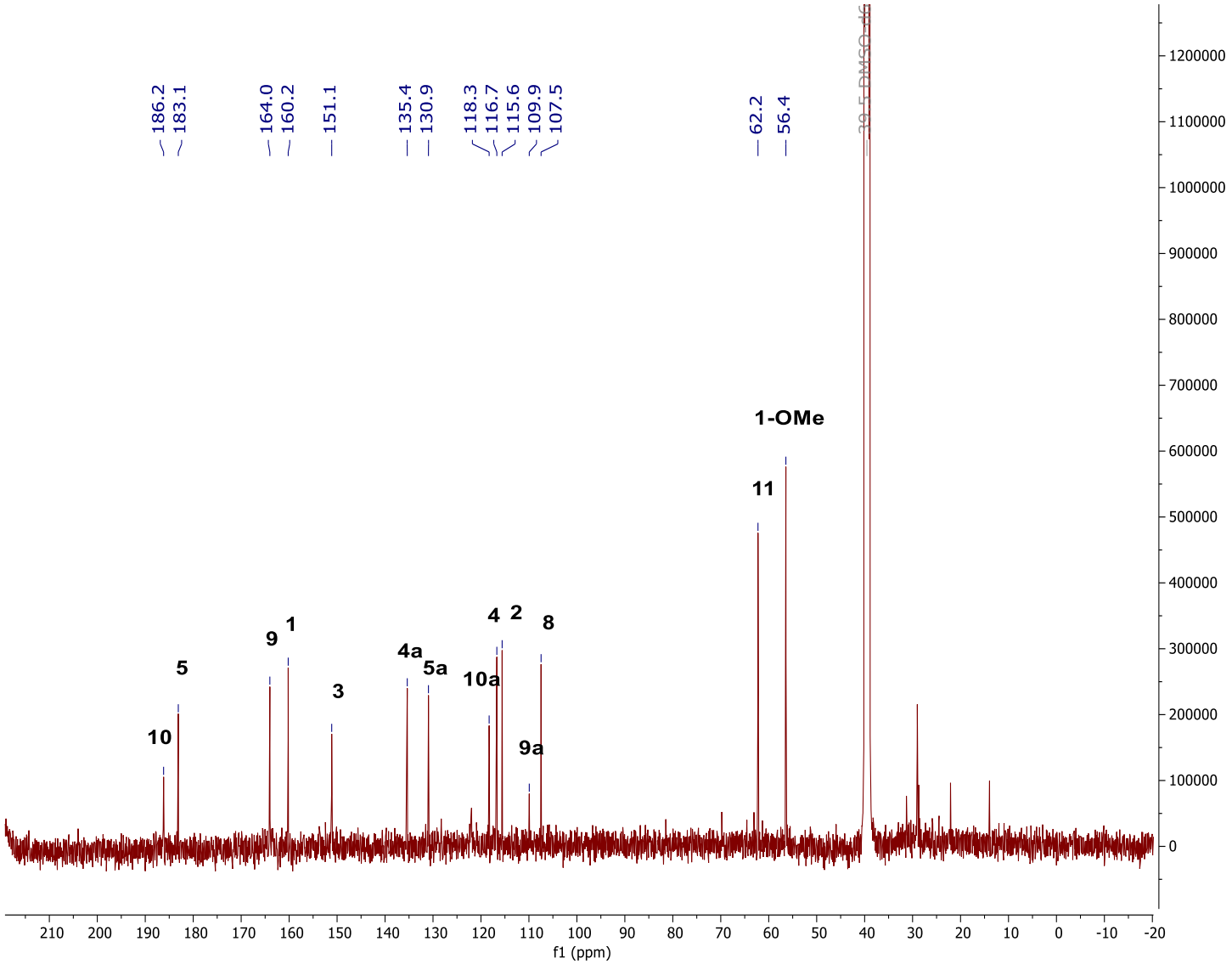

Figure S 39: ^{13}C NMR spectrum of compound **6** (in DMSO-d_6, ^{13}C:125 MHz).

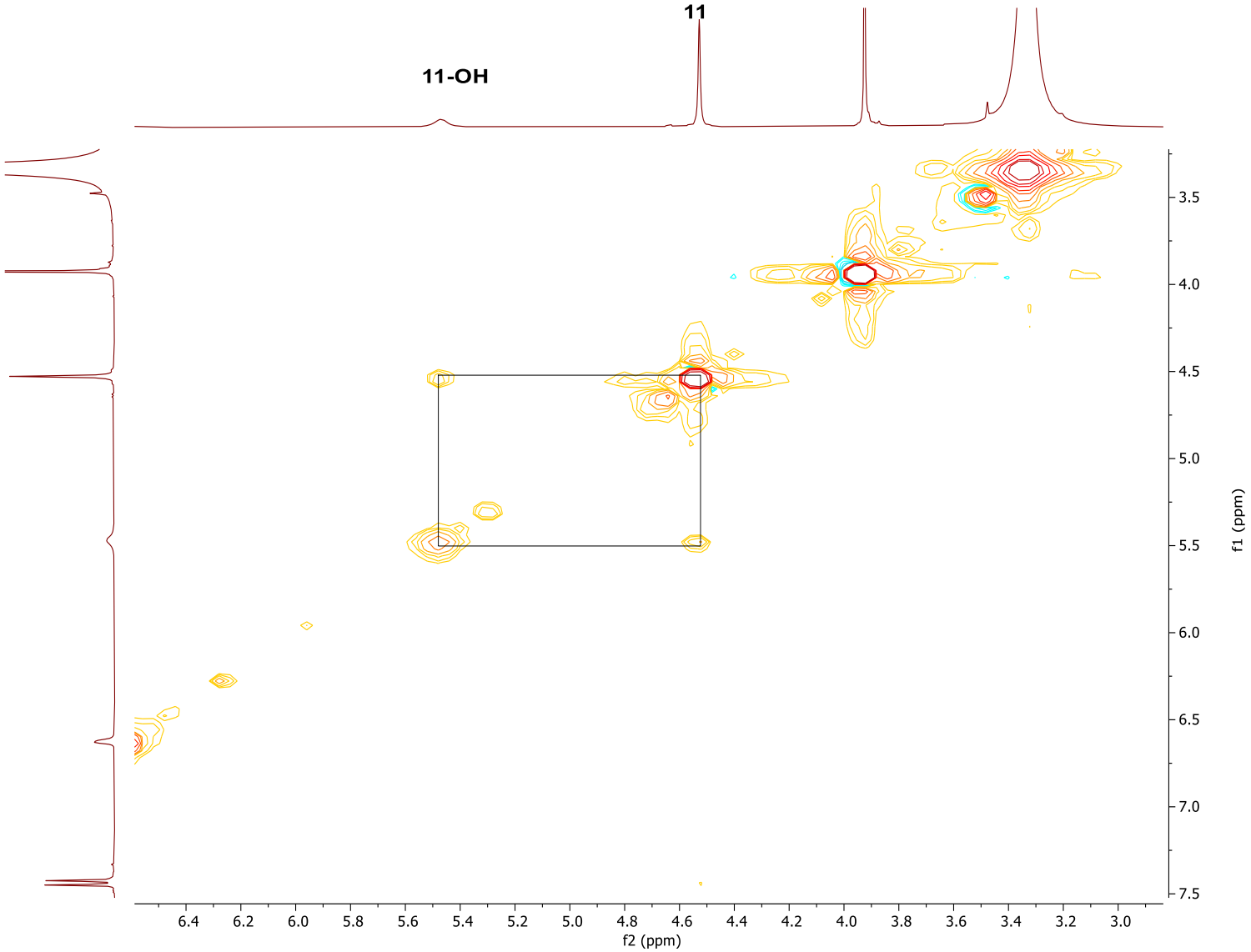

Figure S 40: COSY spectrum of compound **6**.

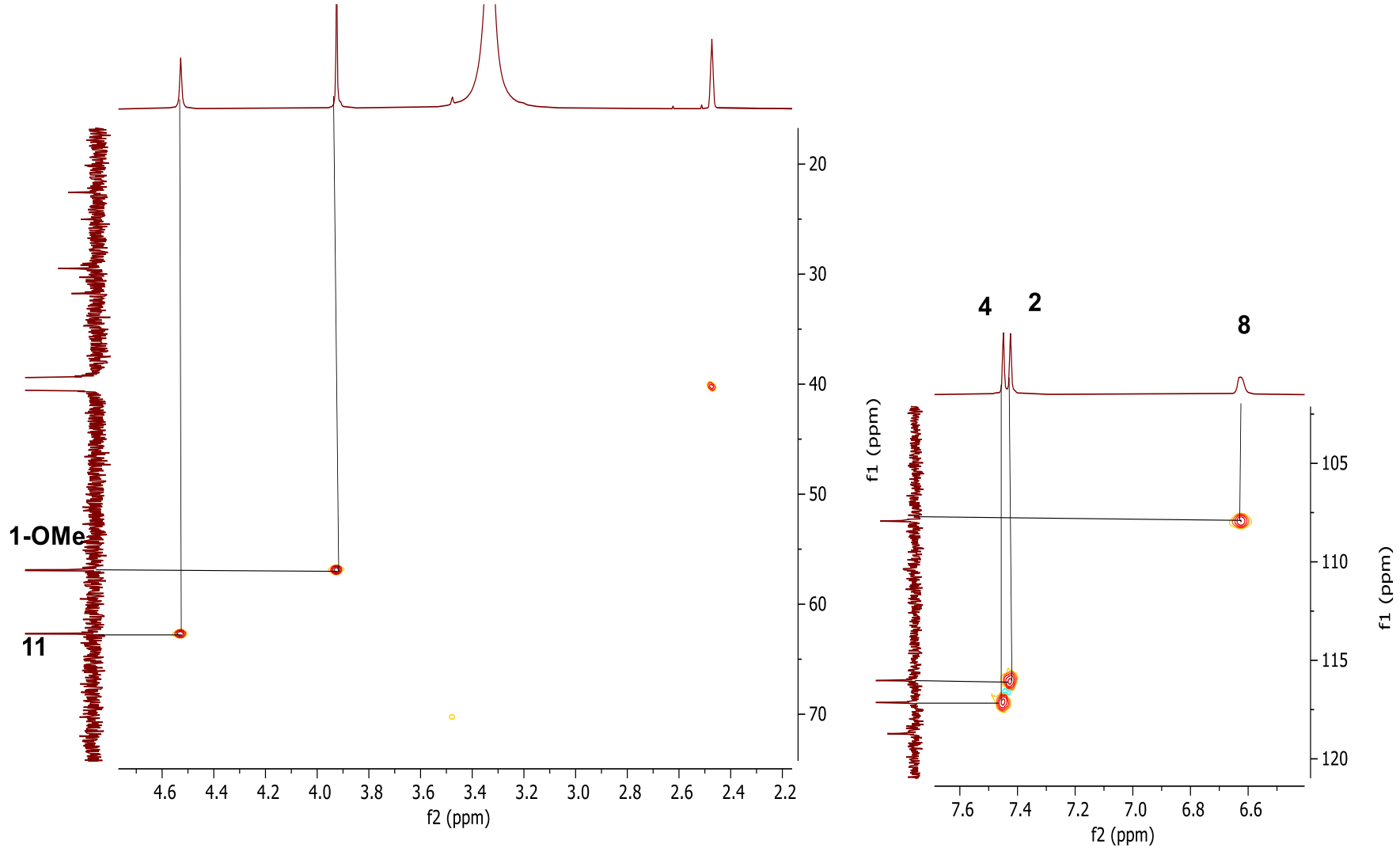

Figure S 41: HSQC spectrum of compound **6**.

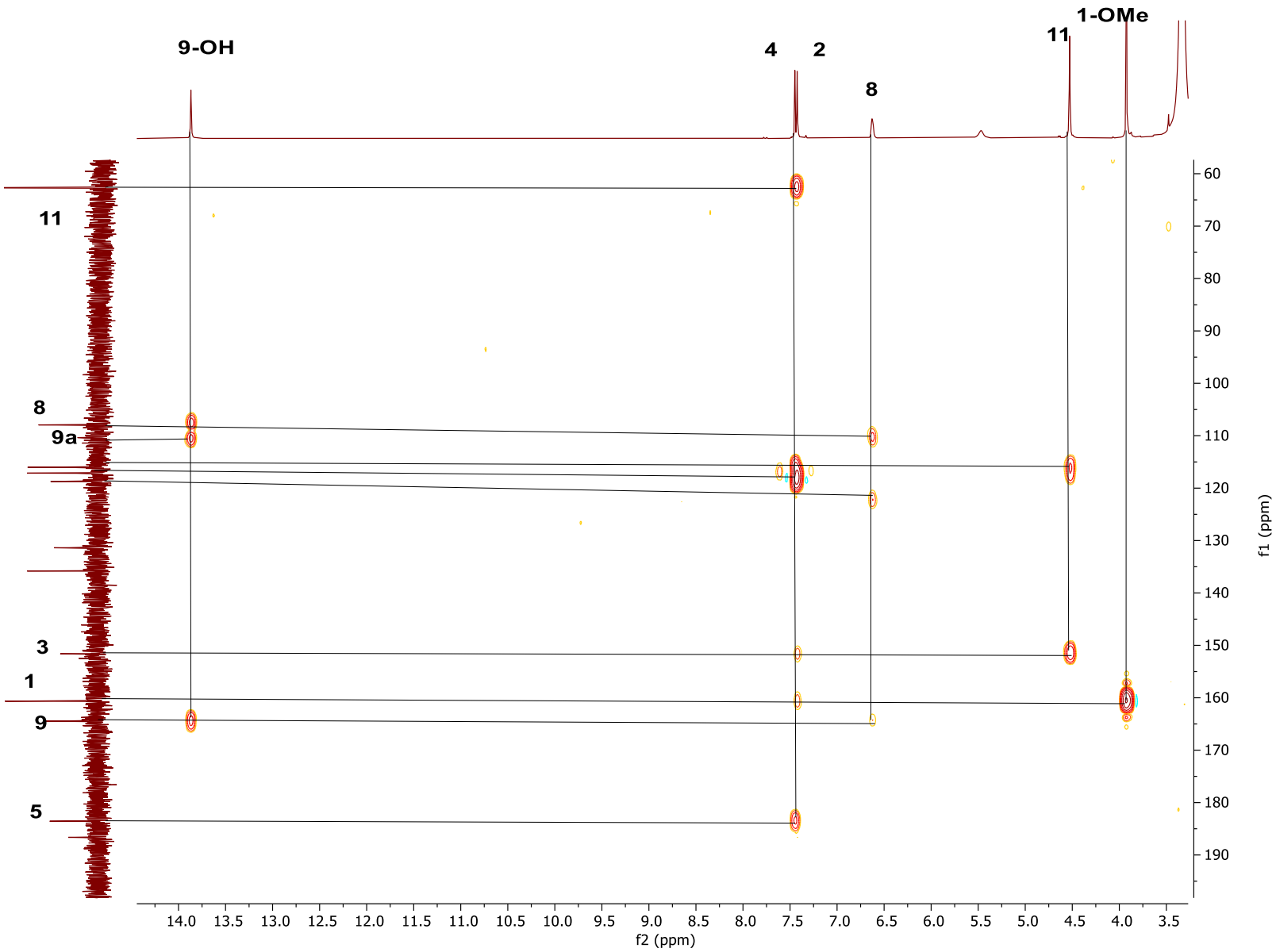

Figure S 42: HMBC spectrum of compound **6**.

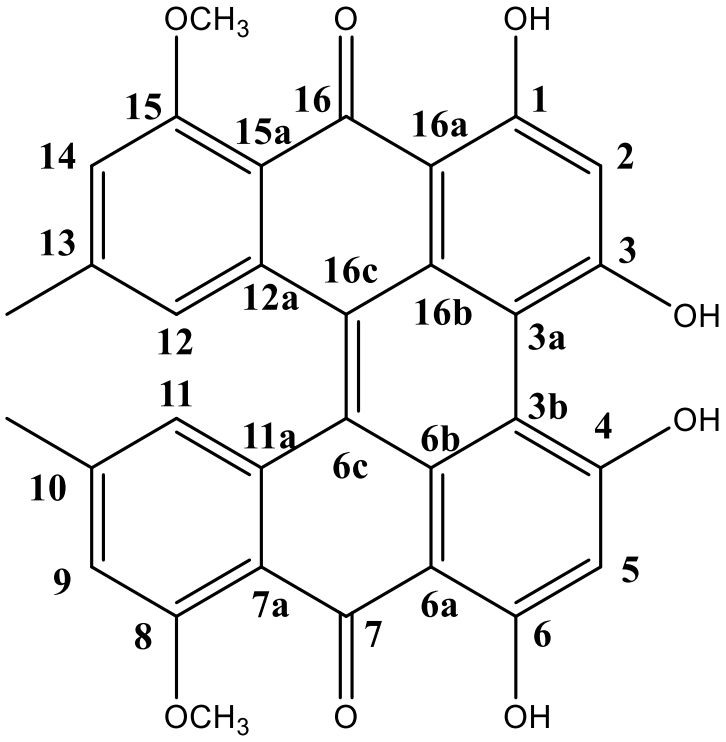

Figure S 43: Chemical structure of compound **7**.

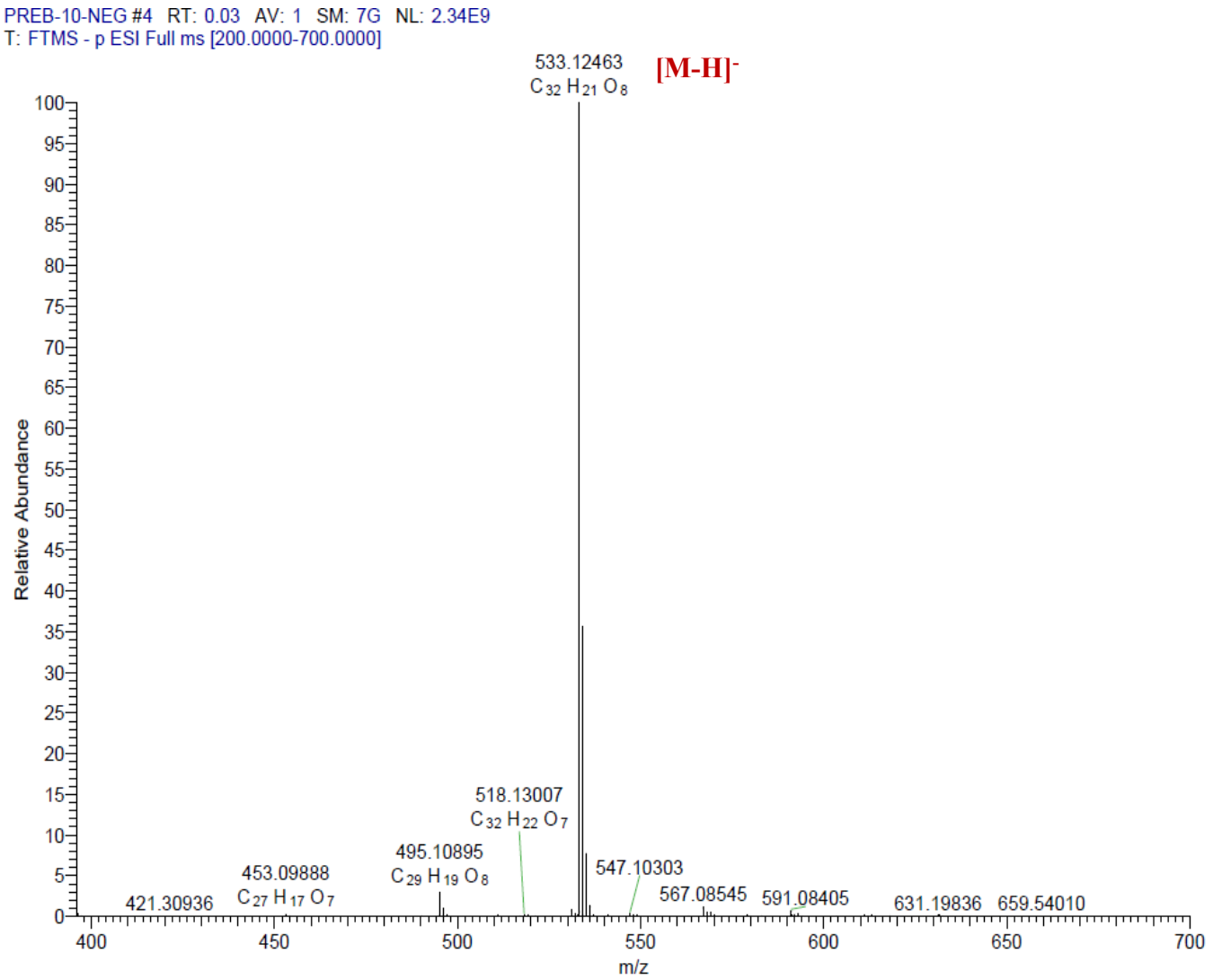

Figure S 44: HR-ESI-MS spectrum of compound **7** (negative mode).

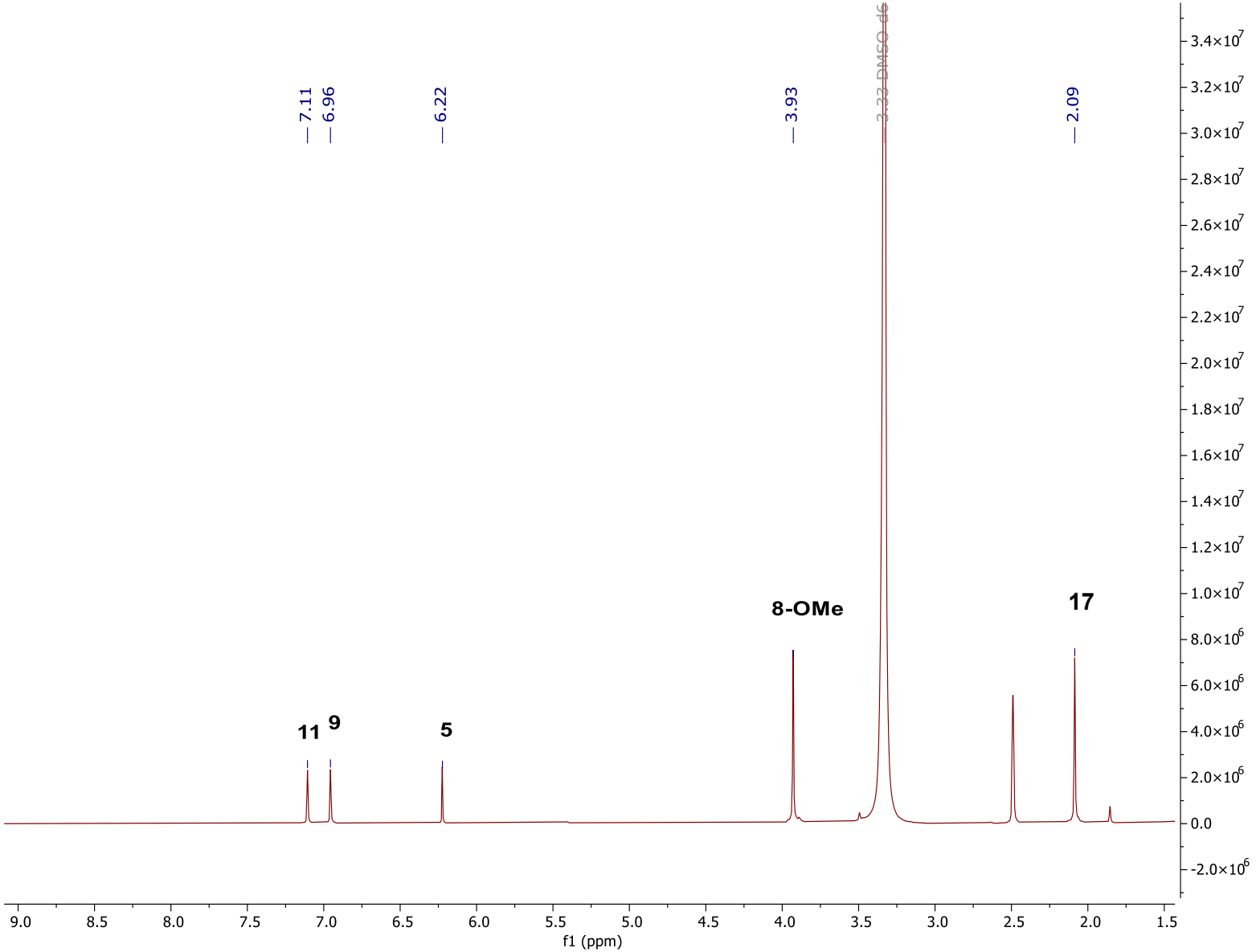

Figure S 45: ^{1}H NMR spectrum of compound **7** (in DMSO-d_6, ^{1}H: 500 MHz).

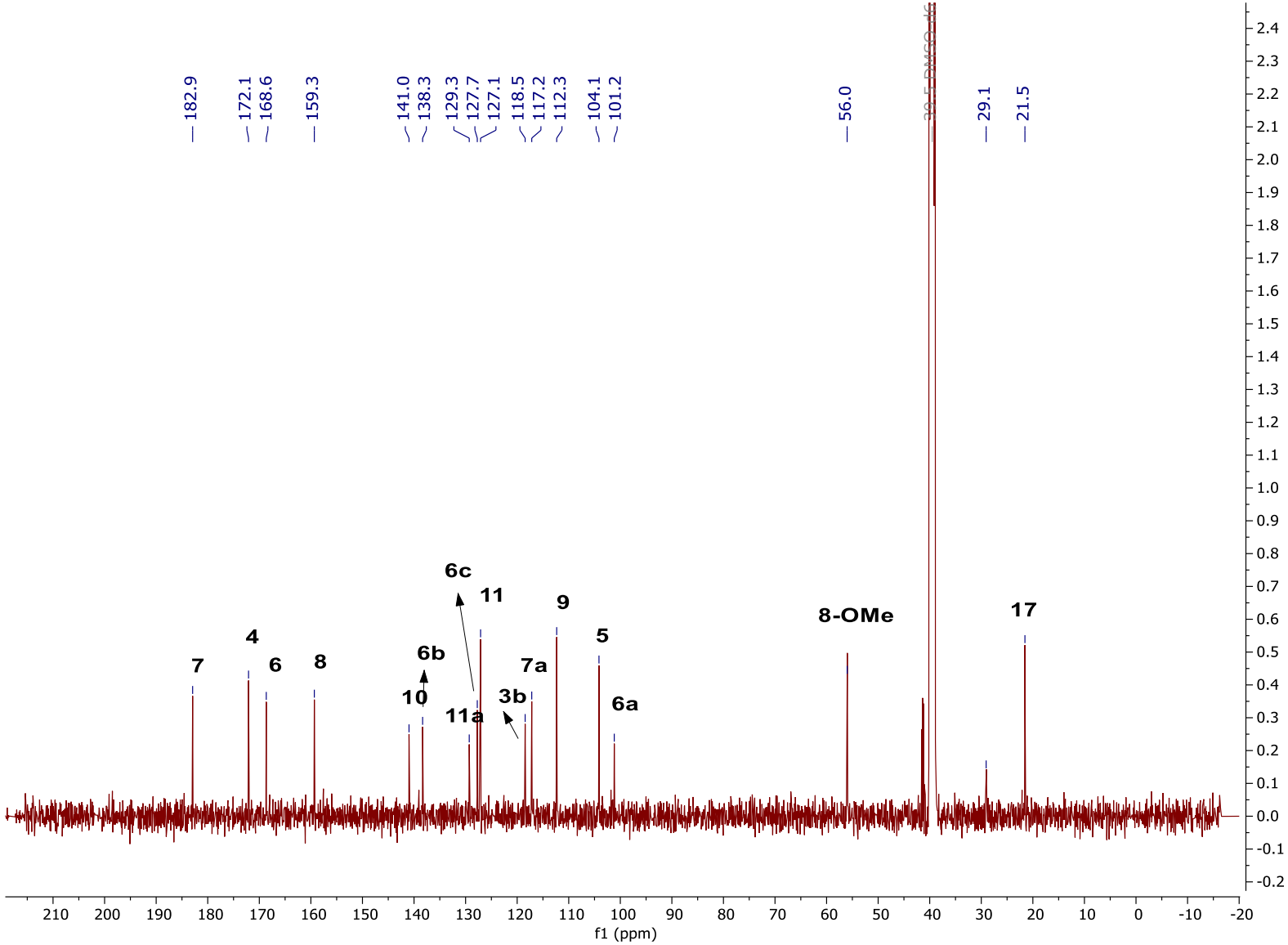

Figure S 46: ^{13}C NMR spectrum of compound **7** (in DMSO-d_6, ^{13}C:125 MHz).

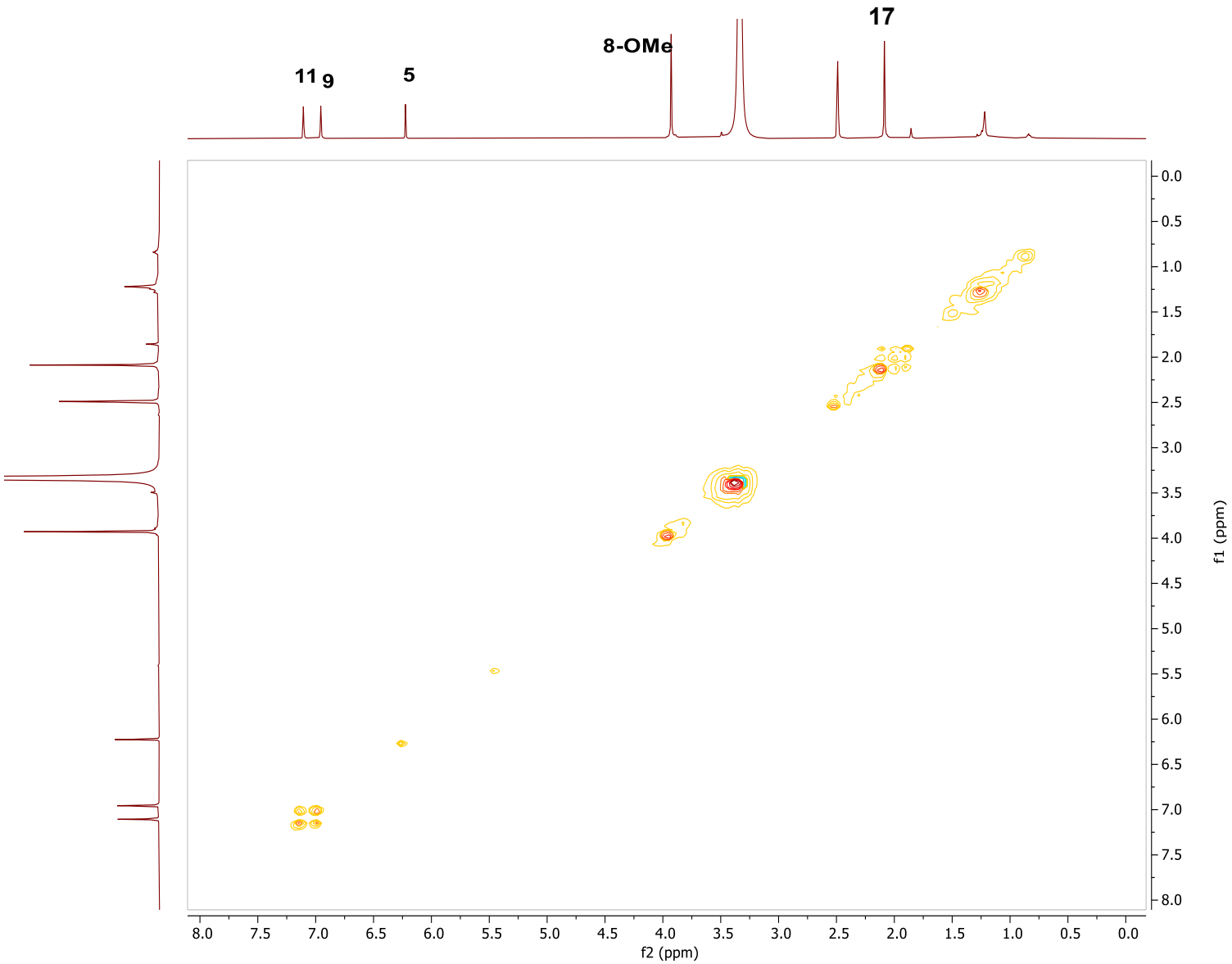

Figure S 47: COSY spectrum of compound **7**.

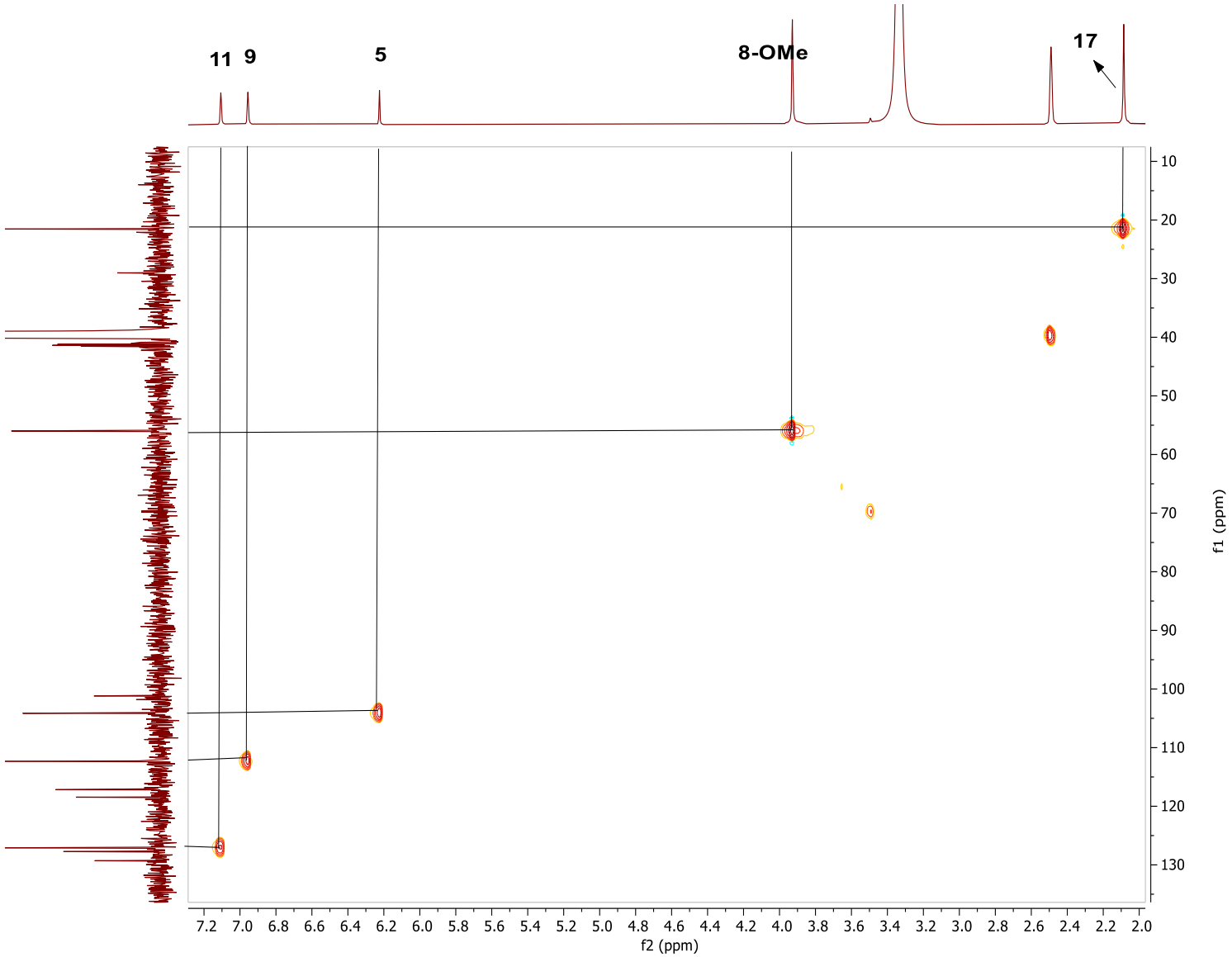

Figure S 48: HSQC spectrum of compound **7**.

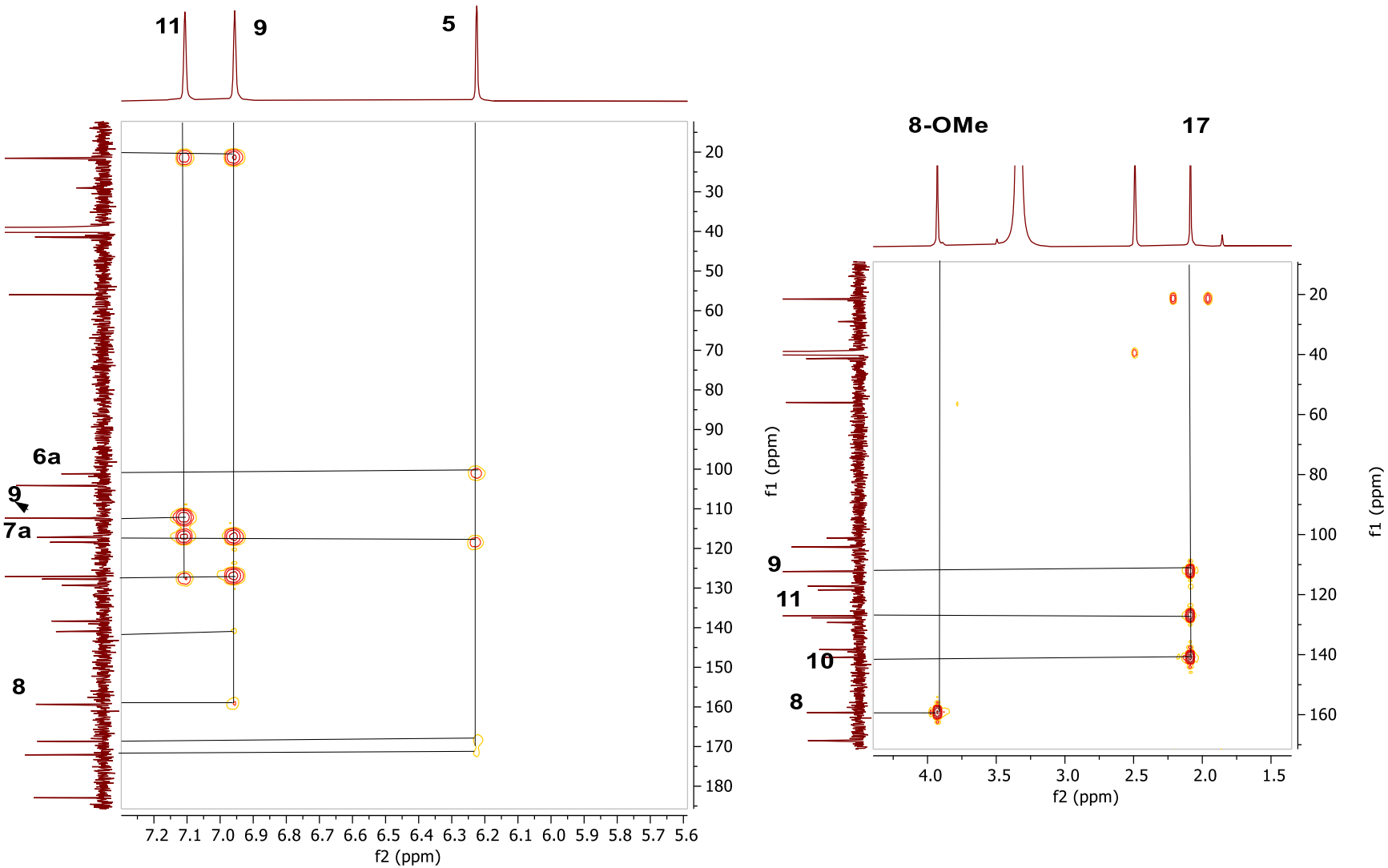

Figure S 49: HMBC spectrum of compound **7**.

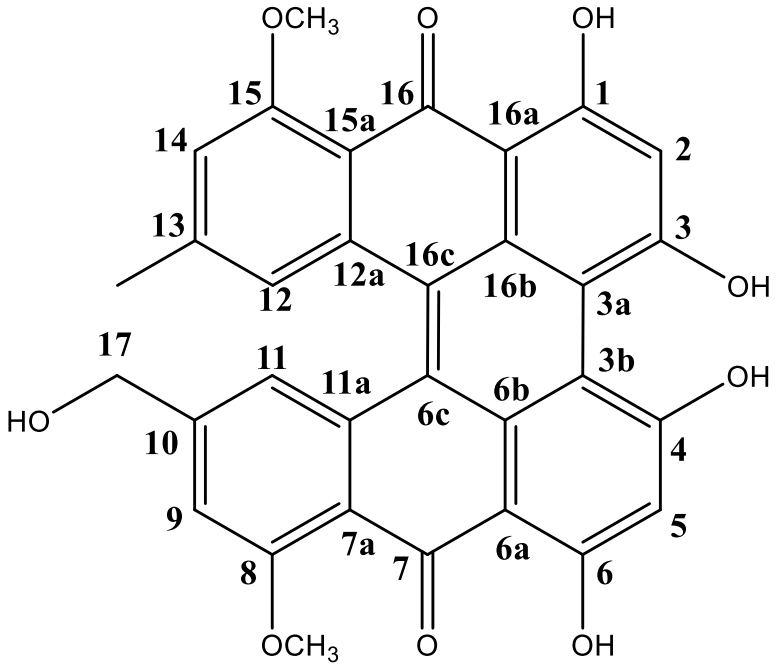

Figure S 50: Chemical structure of compound **8**.

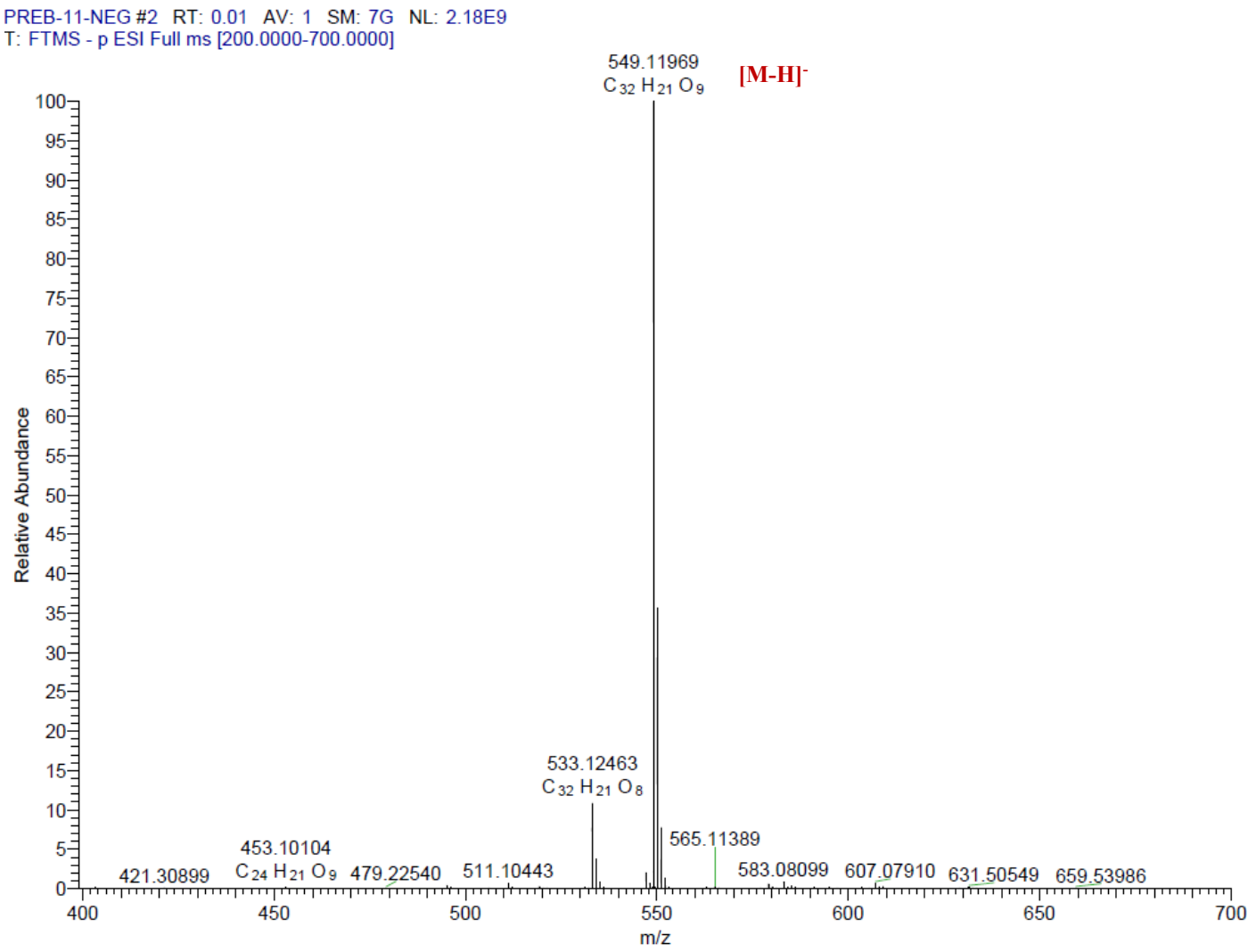

Figure S 51: HR-ESI-MS spectrum of compound **8** (negative mode).

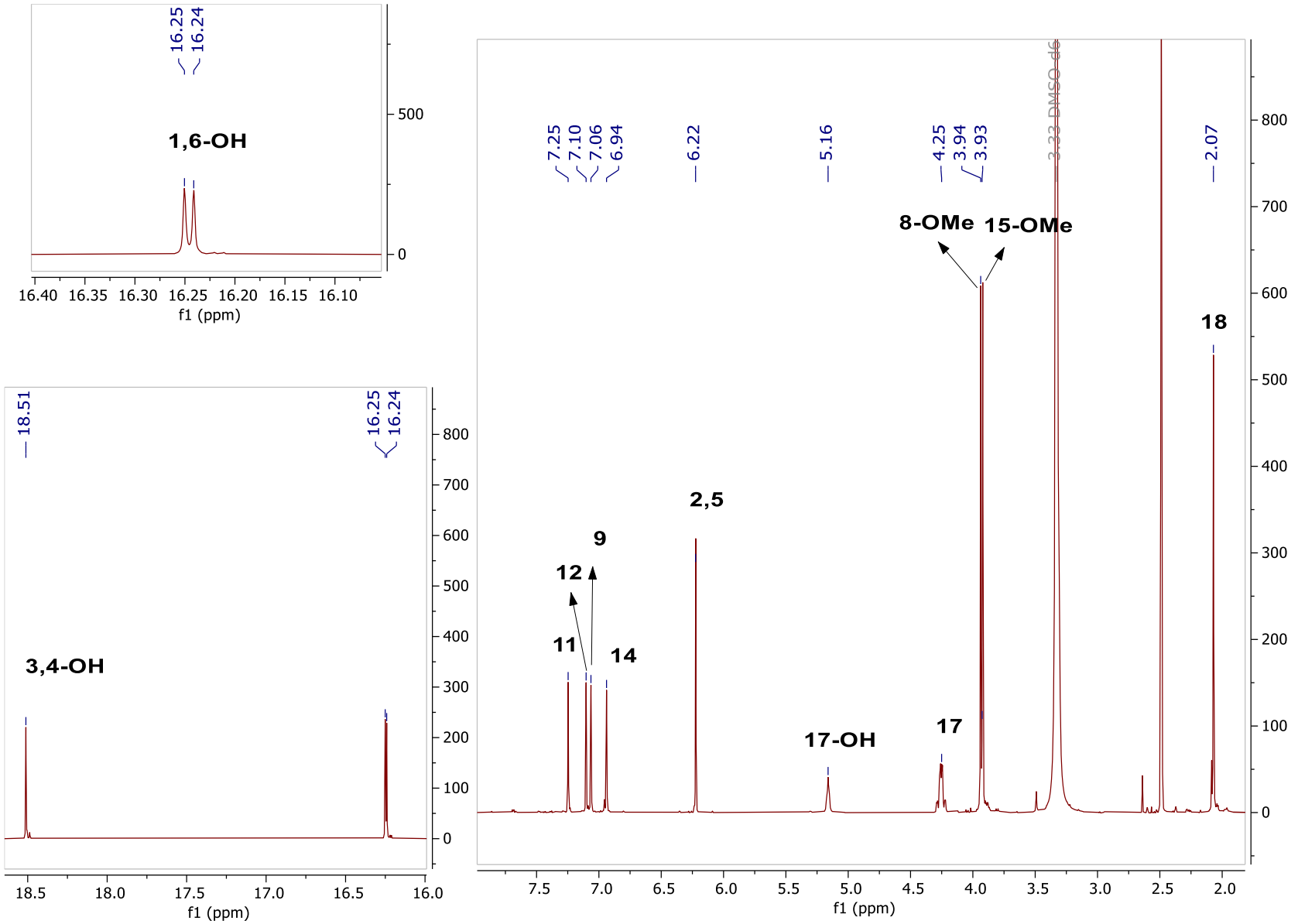

Figure S 52: ^{1}H NMR spectrum of compound **8** (in DMSO-d_6, ^{1}H: 500 MHz).

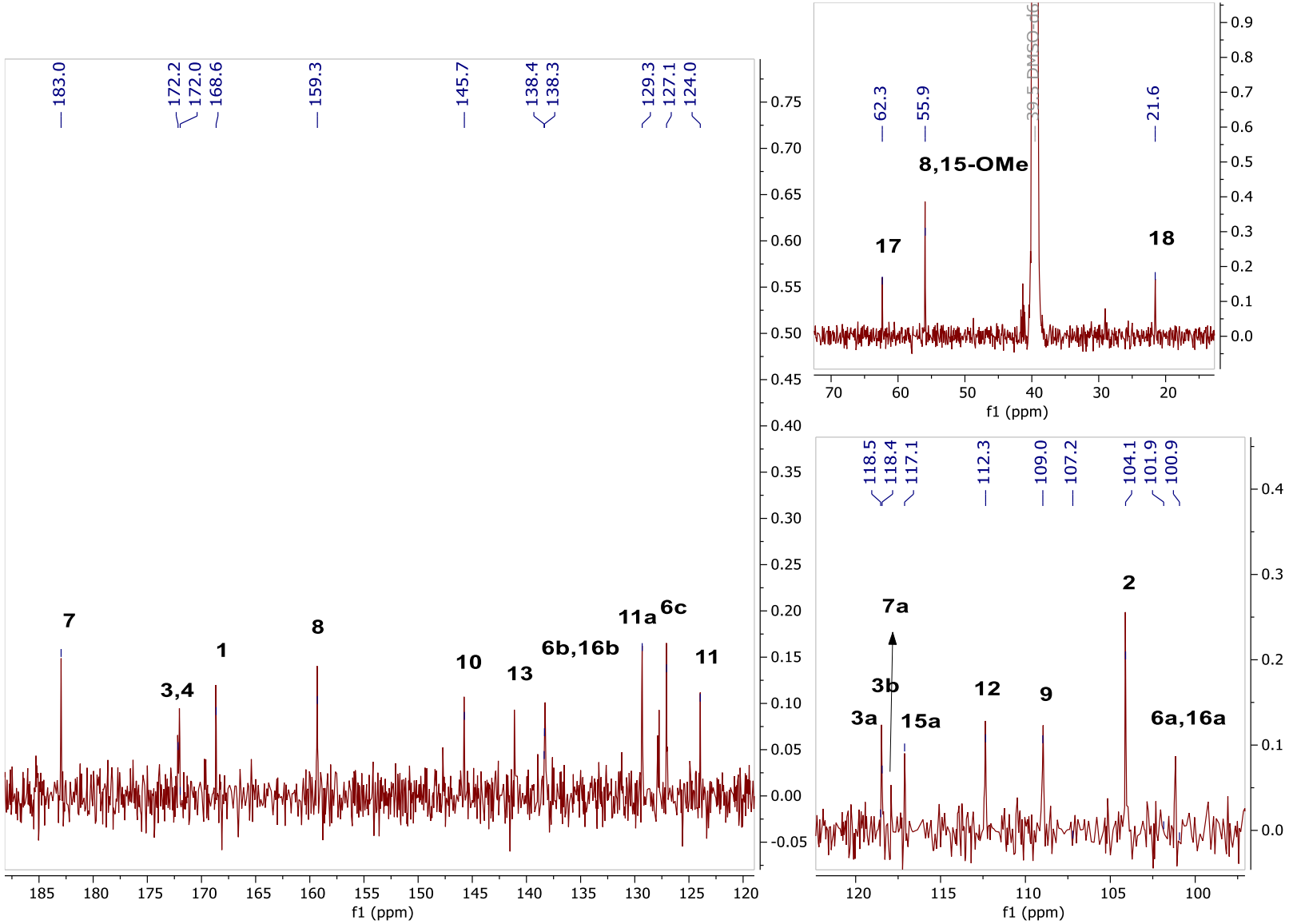

Figure S 53: ^{13}C NMR spectrum of compound **8** (in DMSO-d_6, ^{13}C:125 MHz).

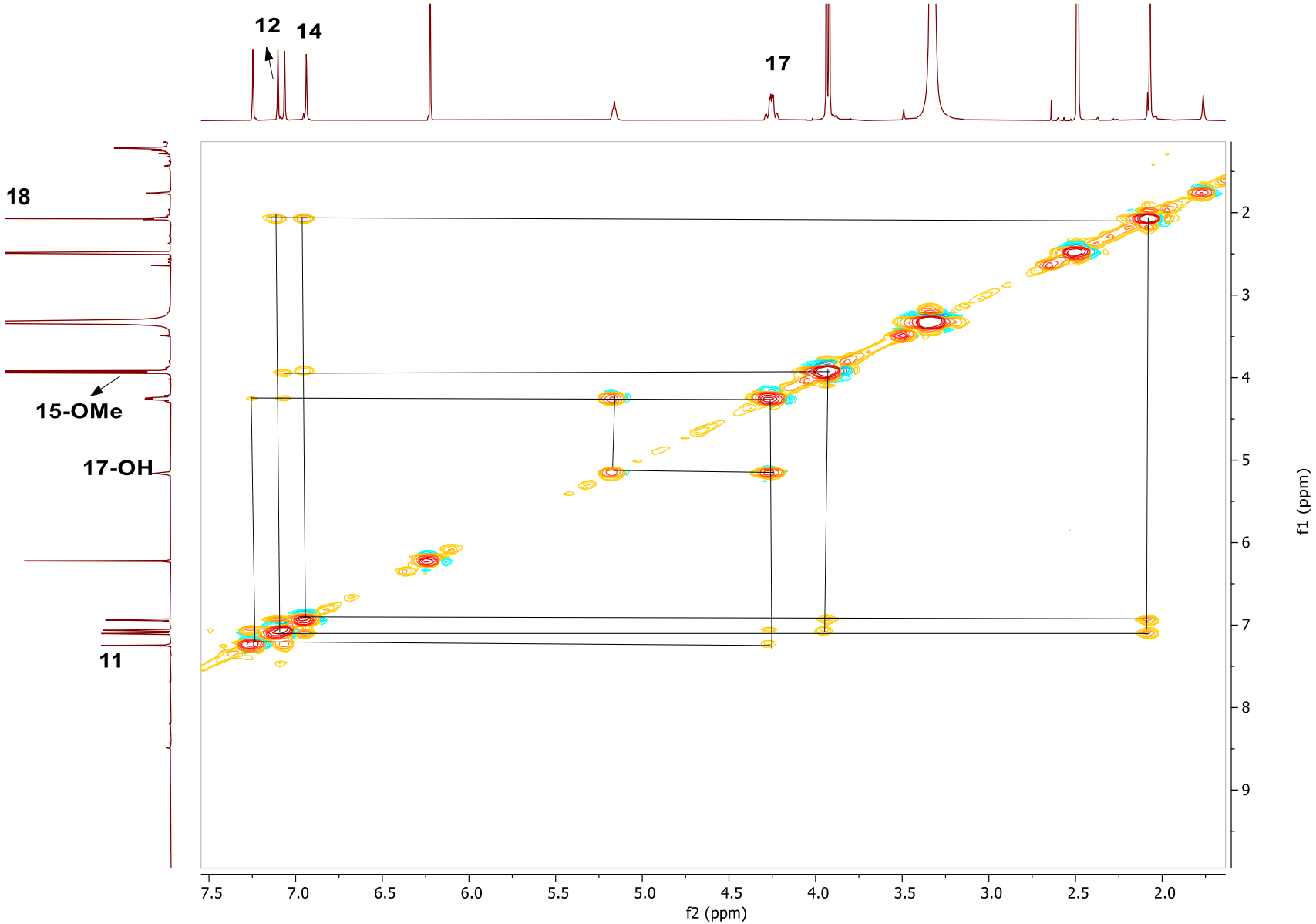

Figure S 54: COSY spectrum of compound **8**.

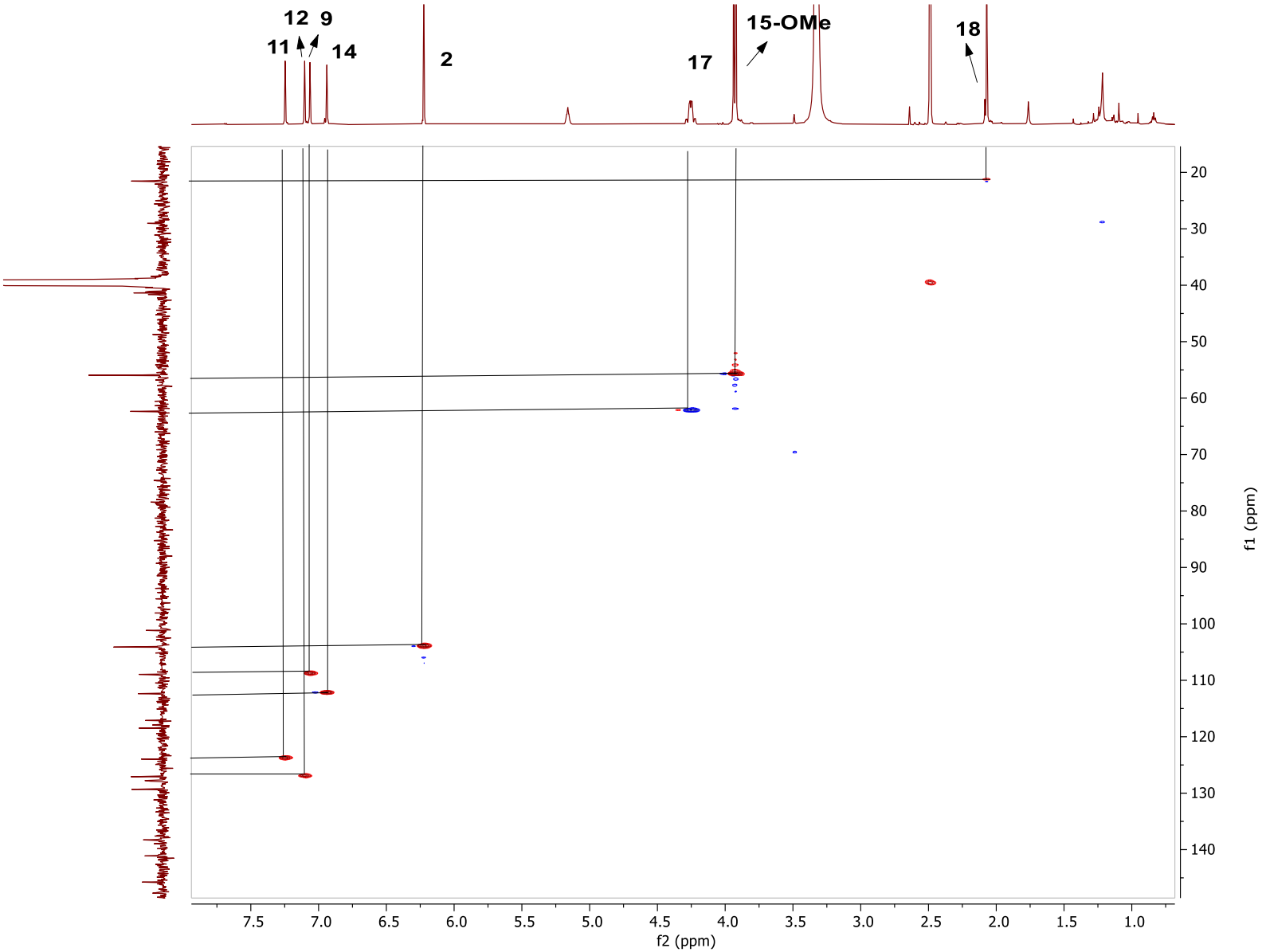

Figure S 55: HSQC spectrum of compound **8**.

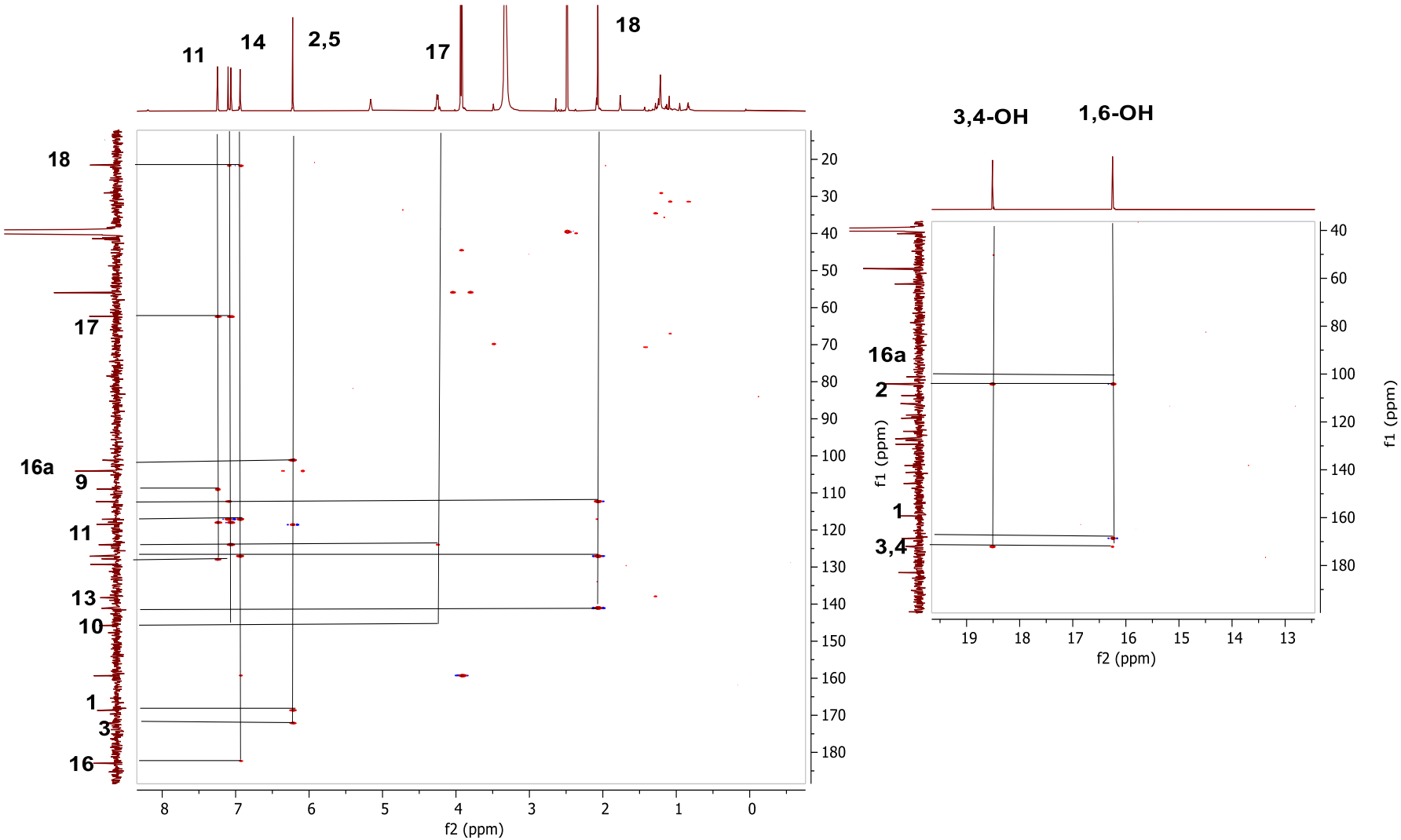

Figure S 56: HMBC spectrum of compound **8**.

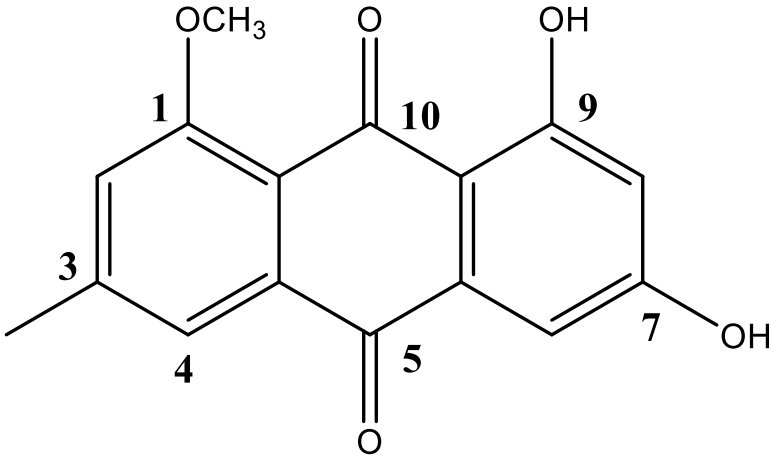

Figure S 57: Chemical structure of compound **9**.

Table S 4: ^{1}H and ^{13}C NMR data for compound **9**.

	9	
No	**δ_C, Type[a]**	**δ_H (*J* in Hz)[b]**
1	160.6 s	-
2	119.8 d	7.43 (d, 1.5)
3	146.9 s	-
4	120.1 d	7.60 (d, 1.6)
4a	134.1 s	-
5	186.2 s	-
5a	110.0 s	-
6	107.2 d	7.03 (d, 2.4)
7	164.5 s	-
8	108.3 d	6.54 (d, 2.4)
9	164.5 s	-
9a	117.7 s	-
10	182.5 s	-
10a	134.6 s	-
11	21.7 q	2.46 (3H, s)
1-OMe	56.5 q	3.93 (3H, s)
7-OH	-	-
9-OH	-	13.28 (s)

[a]Chemical shifts were measured at 500 MHz in DMSO-d_6
[b]Chemical shifts were measured at 125 MHz in DMSO-d_6

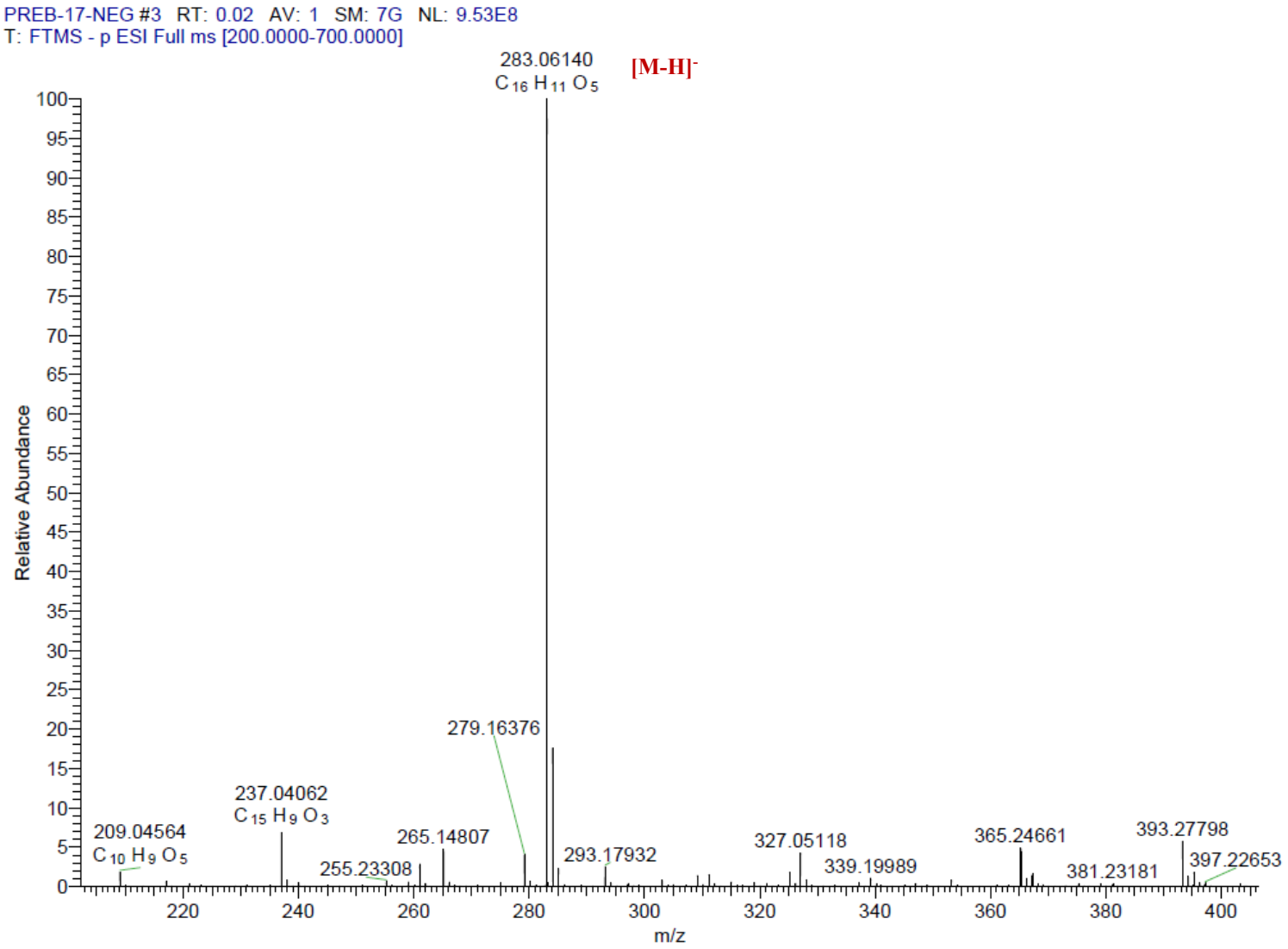

Figure S 58: HR-ESI-MS spectrum of compound **9** (positive mode).

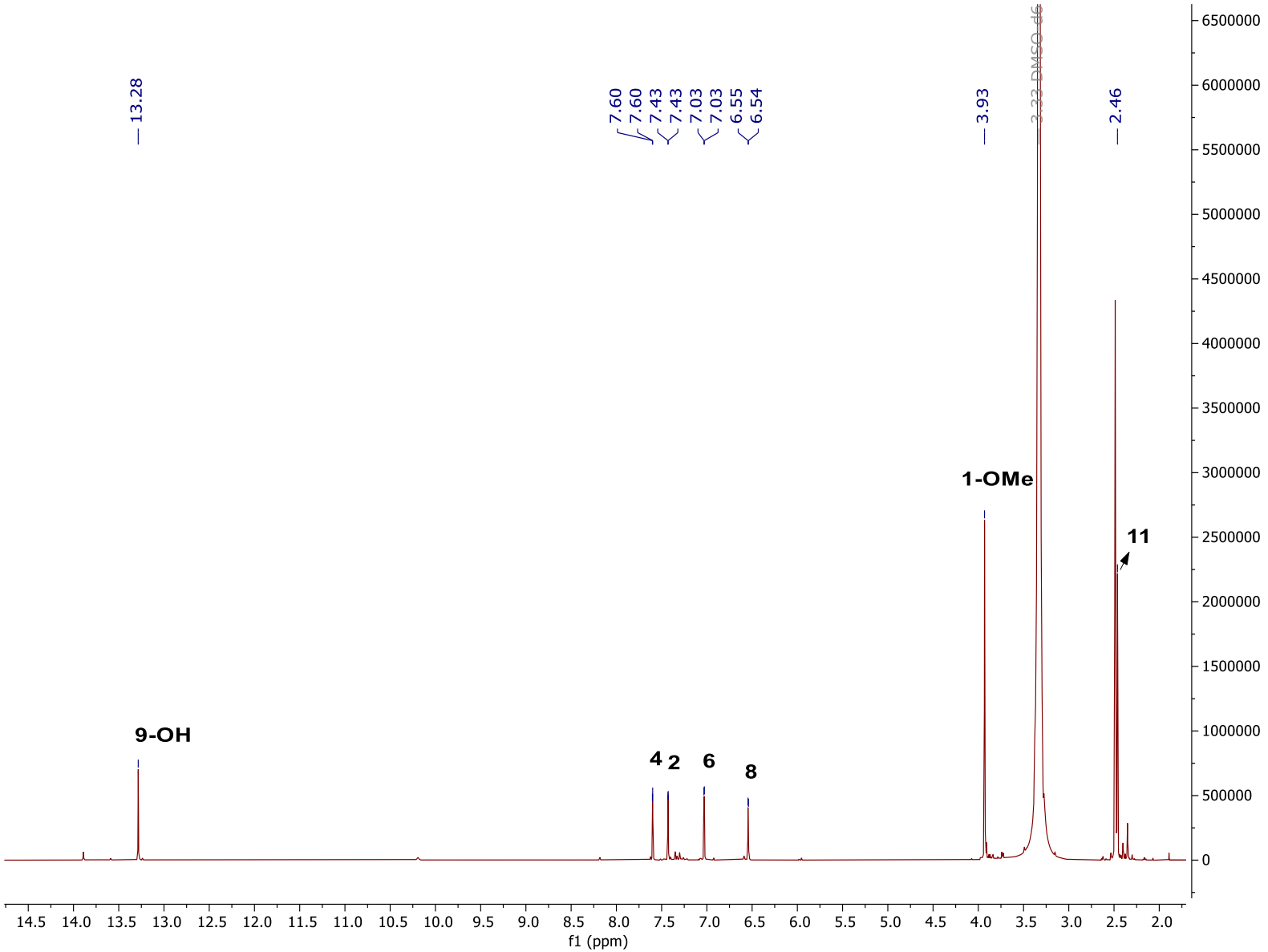

Figure S 59: ^{1}H NMR spectrum of compound **9** (in DMSO-d_6, ^{1}H: 500 MHz).

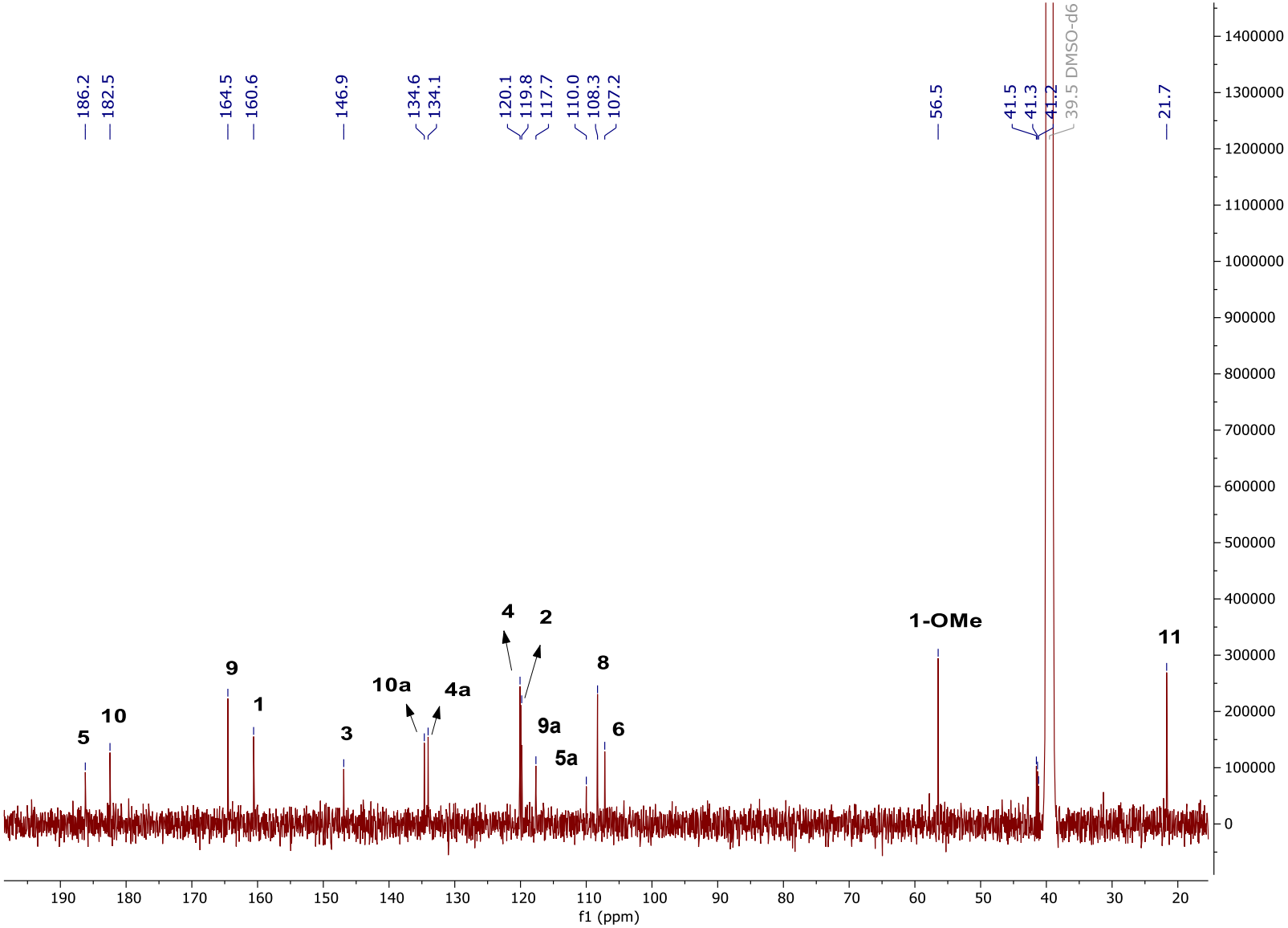

Figure S 60: ^{13}C NMR spectrum of compound **9** (in DMSO-d_6, ^{13}C:125 MHz).

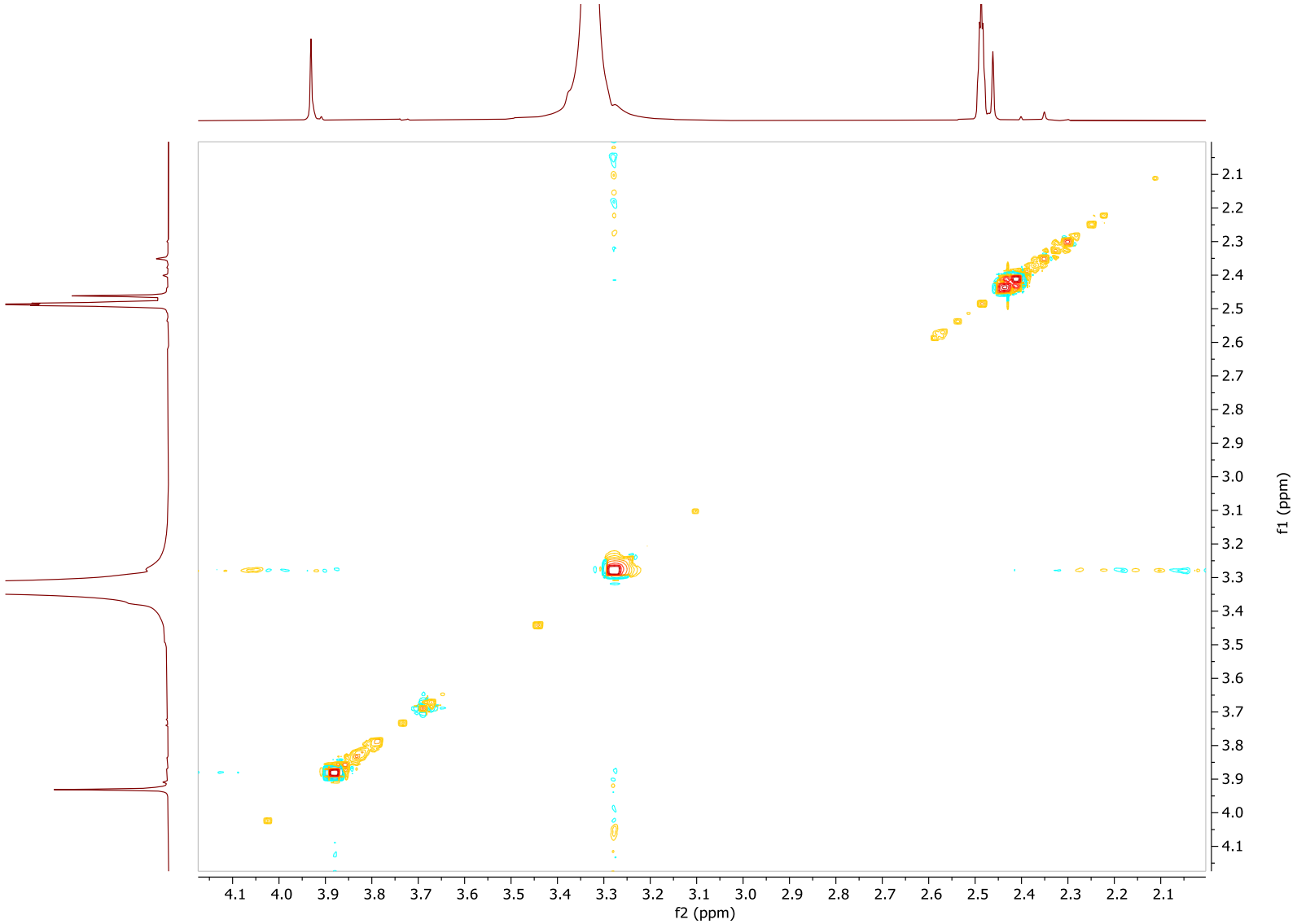

Figure S 61: COSY spectrum of compound **9**.

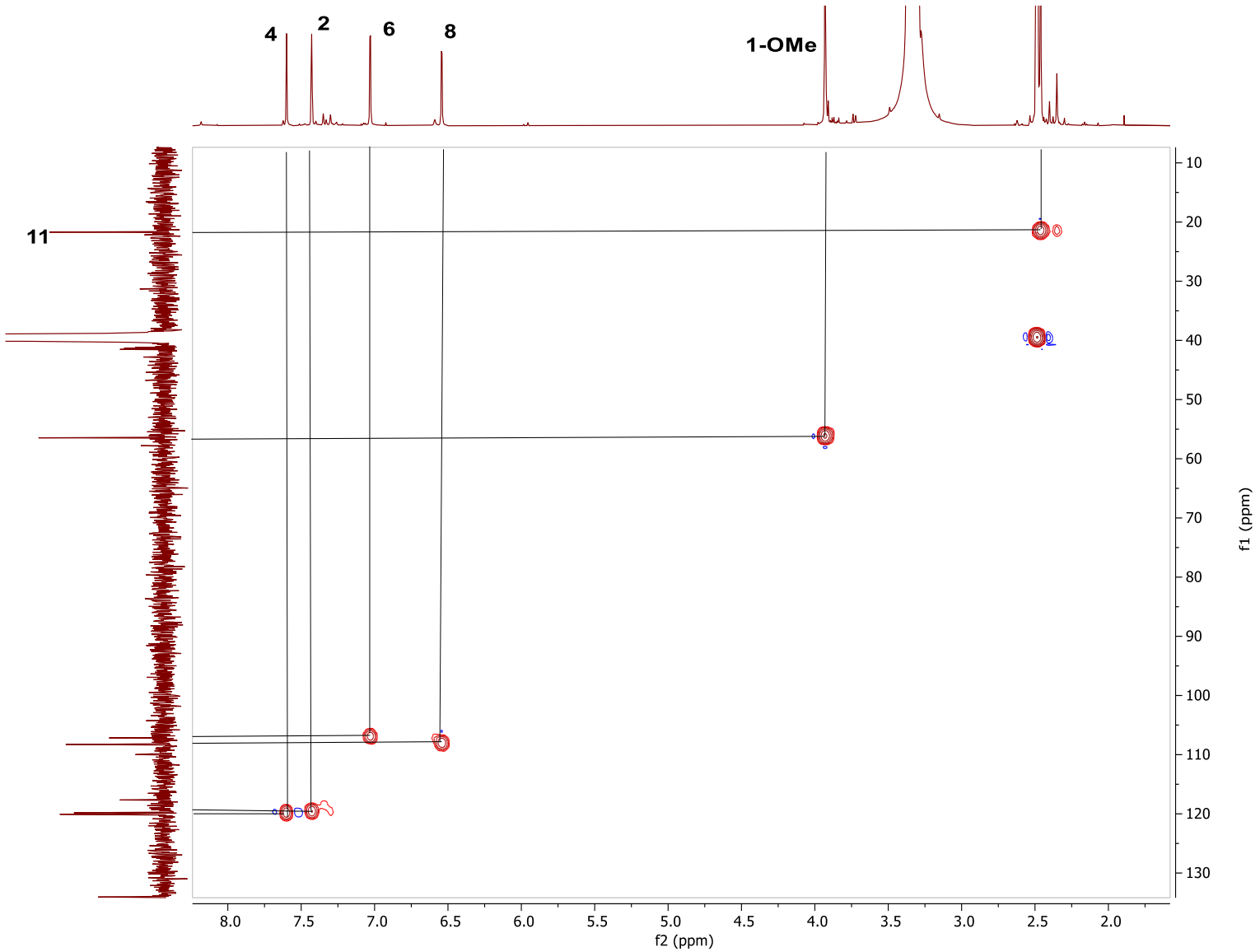

Figure S 62: HSQC spectrum of compound **9**.

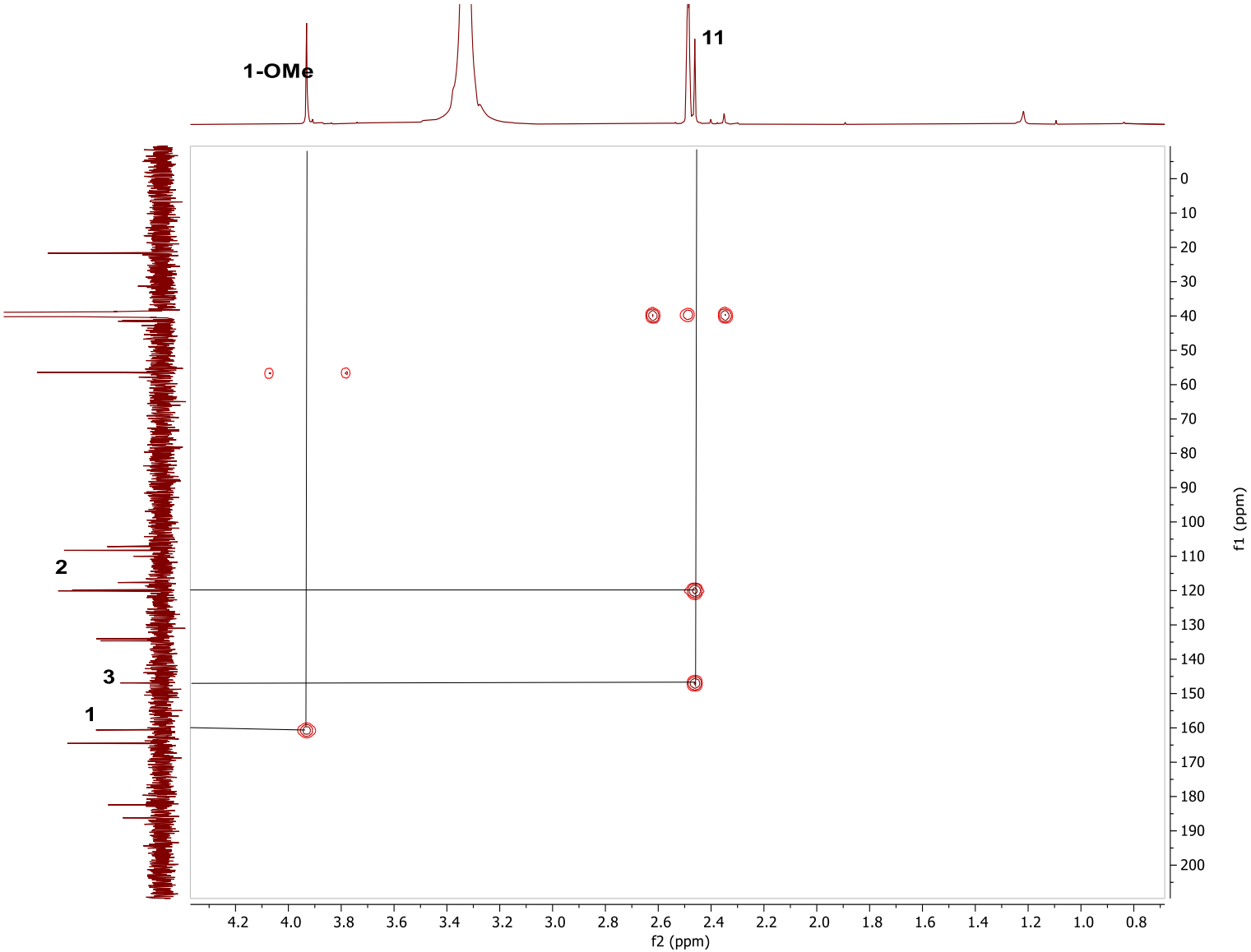

Figure S 63: HMBC spectrum of compound **9**.