

Supporting Information

Rec. Nat. Prod. 18:1 (2024) 95-106

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

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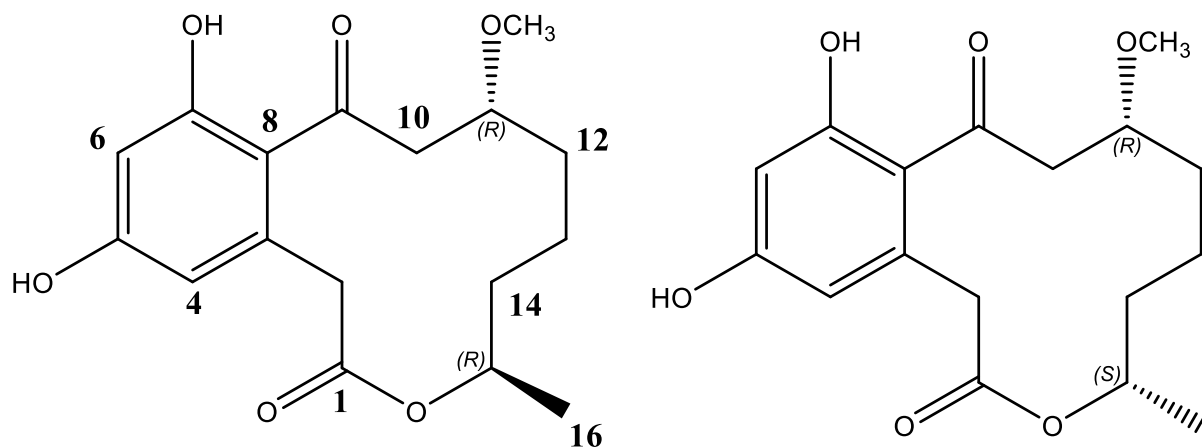


Figure S 1: Chemical structures of compound **1a** and **1b**.

Table S 1: ^1H 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)

^aChemical shifts were measured at 600 MHz in DMSO- d_6

^bChemical shifts were measured at 150 MHz in DMSO- d_6

PR-EB-01 #16-25 RT: 0.21-0.33 AV: 10 NL: 2.11E8
T: FTMS + p ESI Full ms [150.0000-1000.0000]

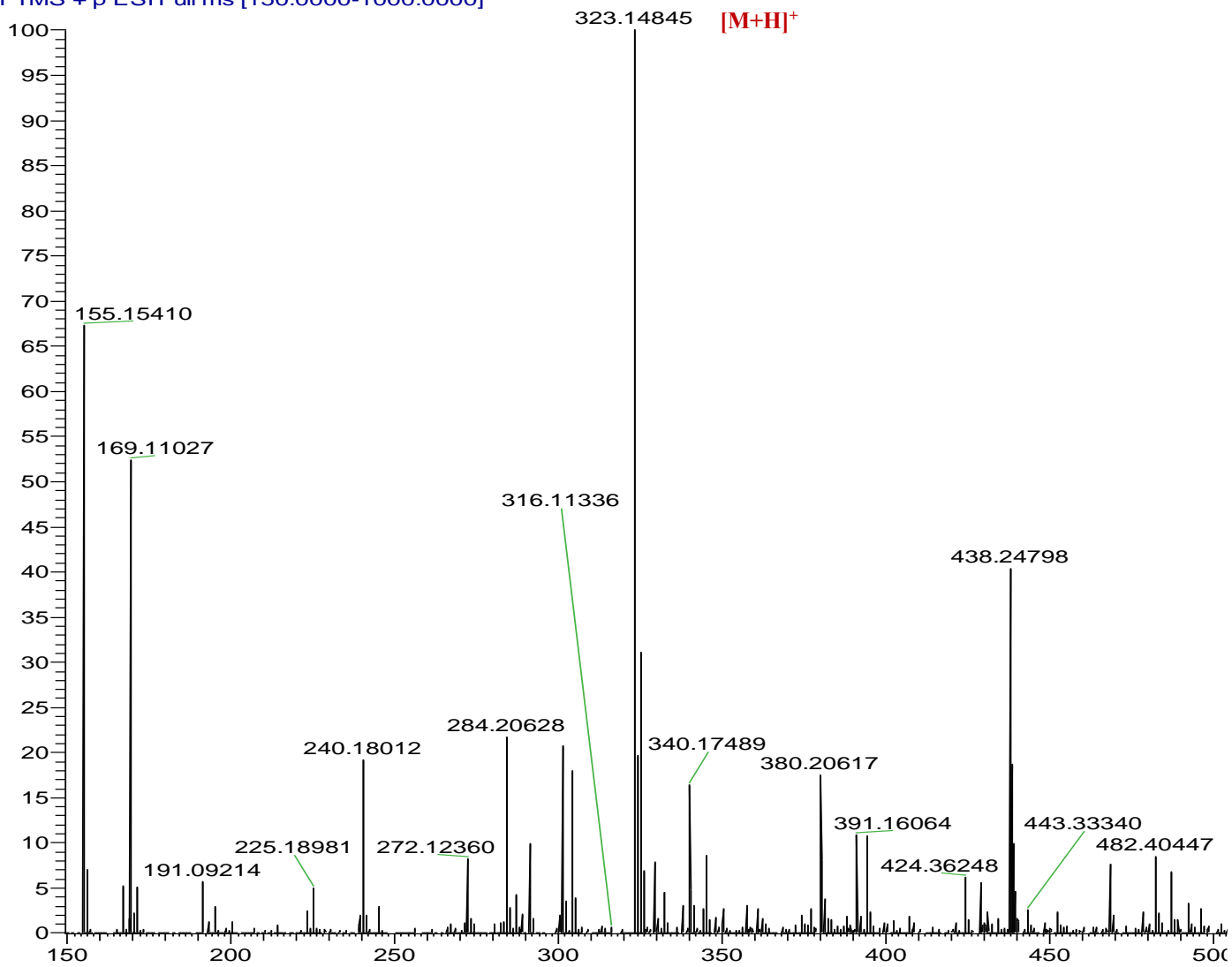


Figure S 2: HR-ESI-MS spectrum of compound 1 (positive mode).

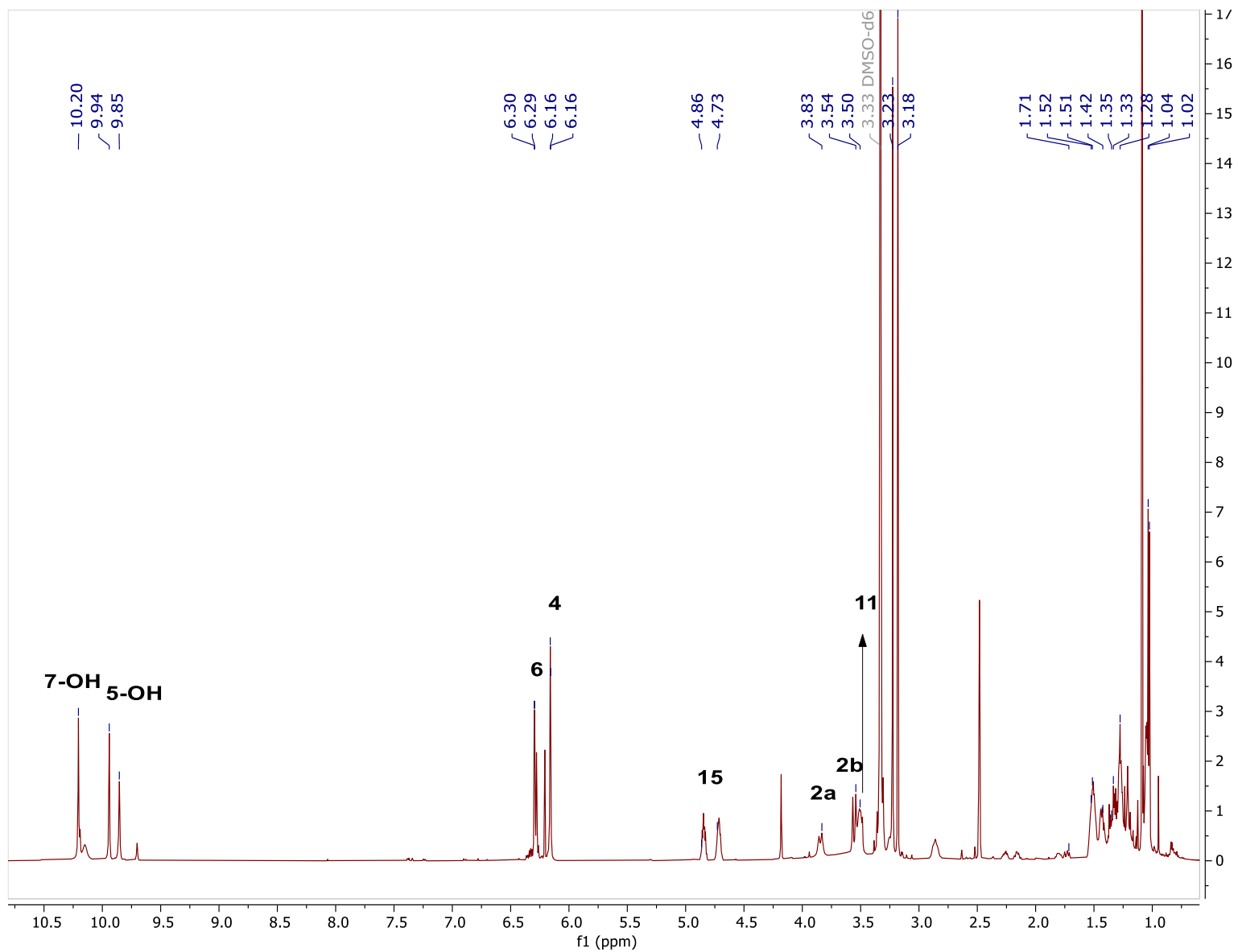


Figure S 3: ^1H NMR spectrum of compound **1** (in DMSO-d_6 , ^1H : 600 MHz).

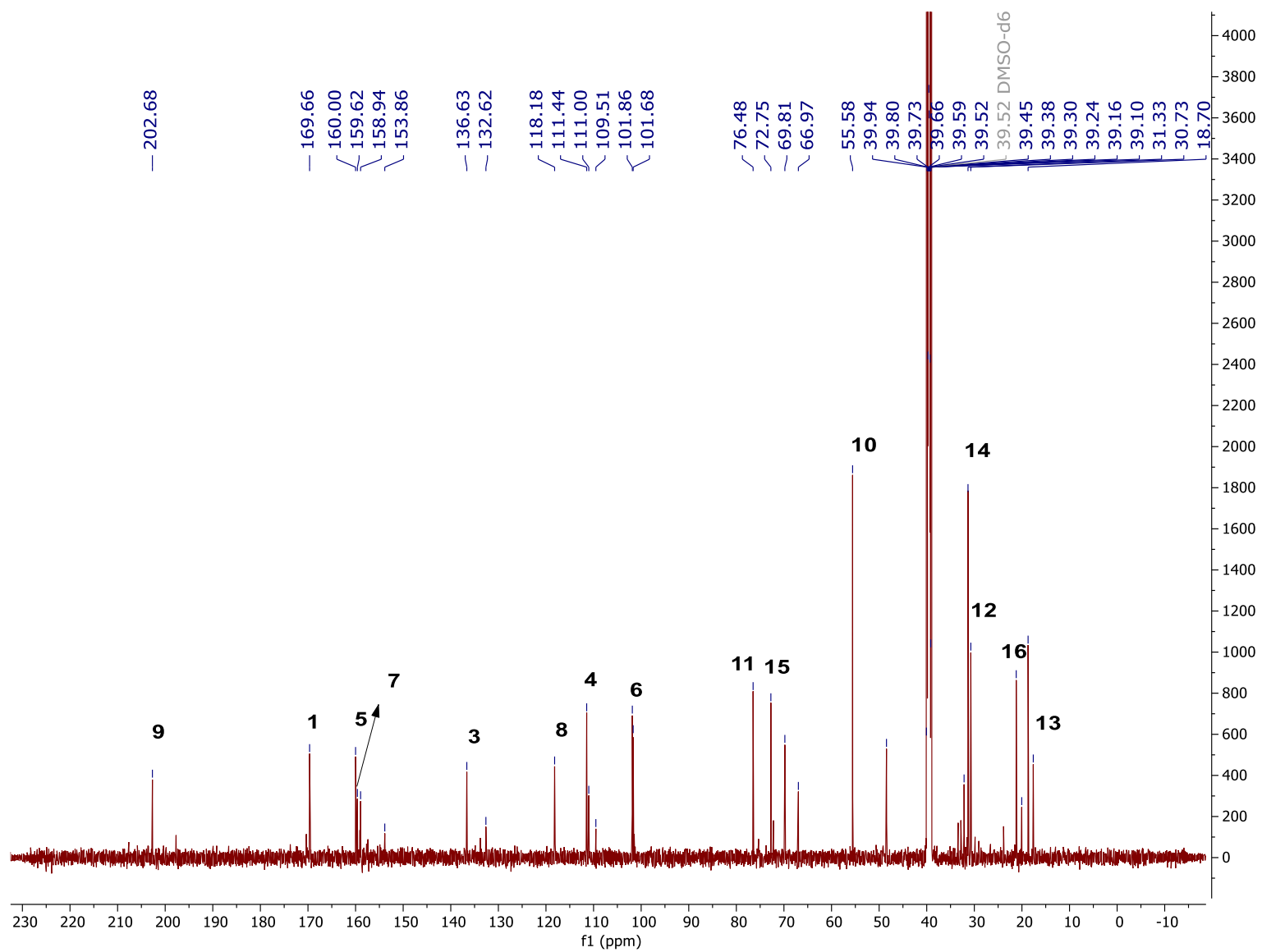


Figure S 4: ^{13}C NMR spectrum of compound **1** (in DMSO-d_6 , ^{13}C :150 MHz).

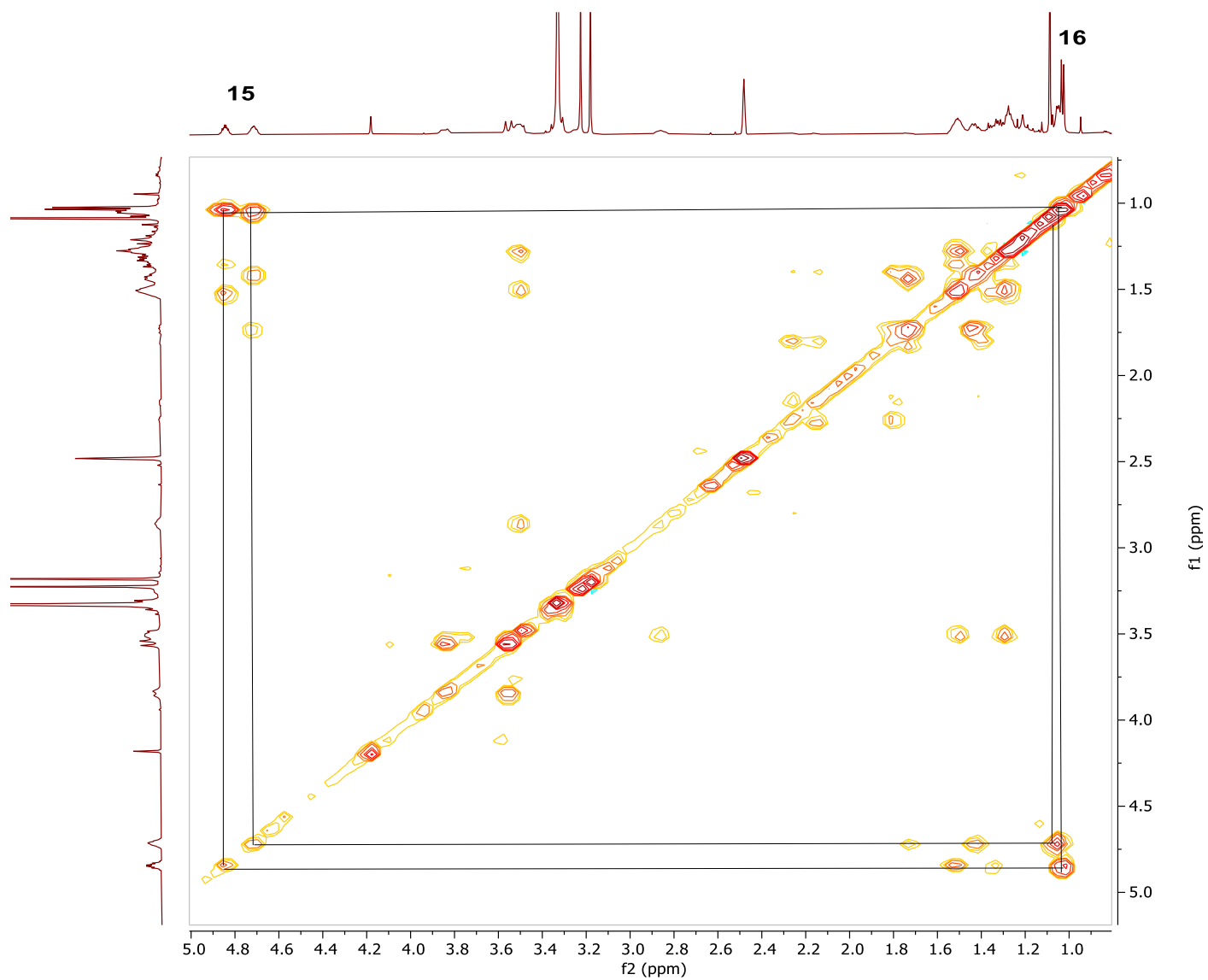


Figure S 5: COSY spectrum of compound **1**.

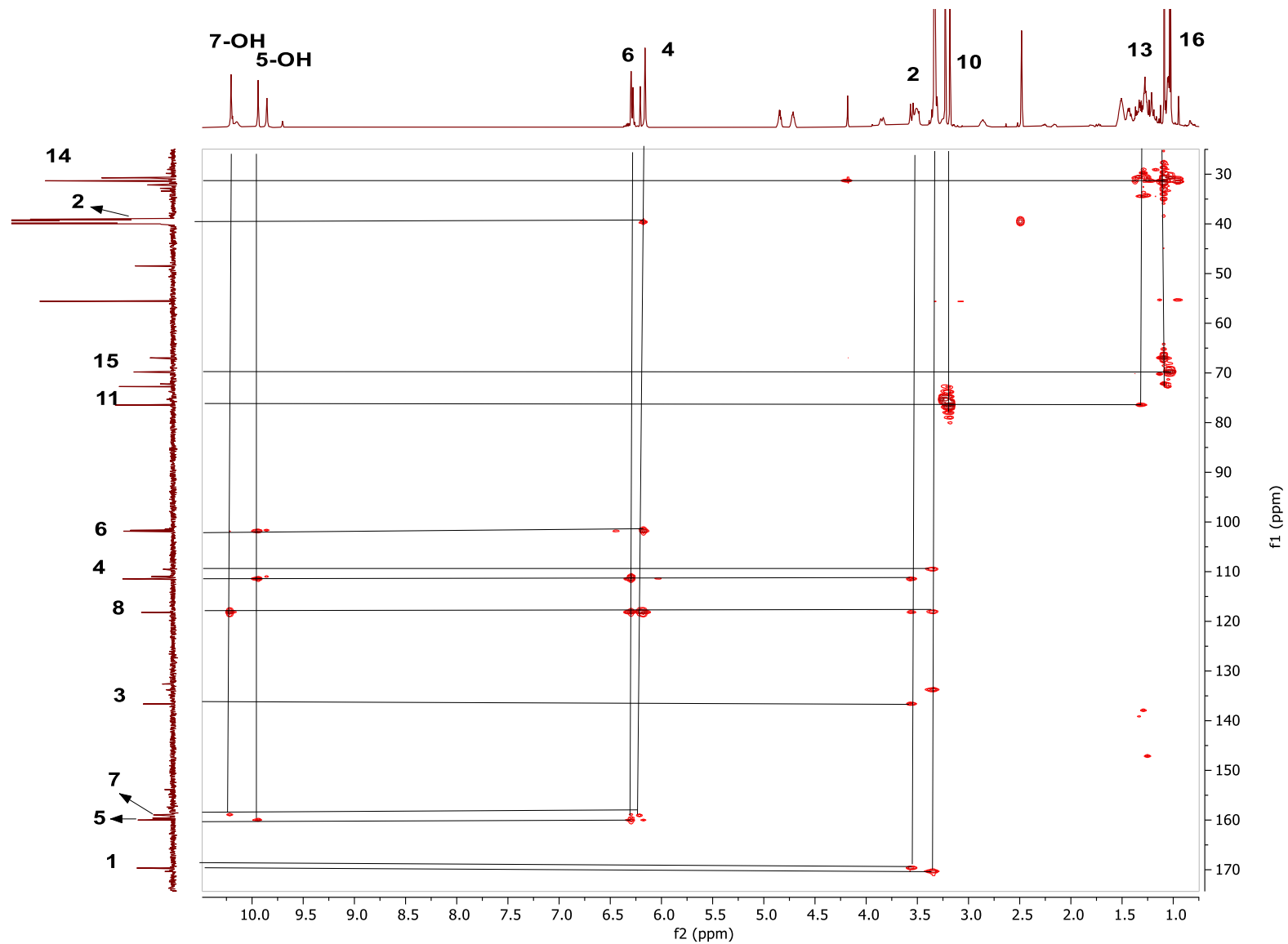


Figure S 7: HMBC spectrum of compound 1.

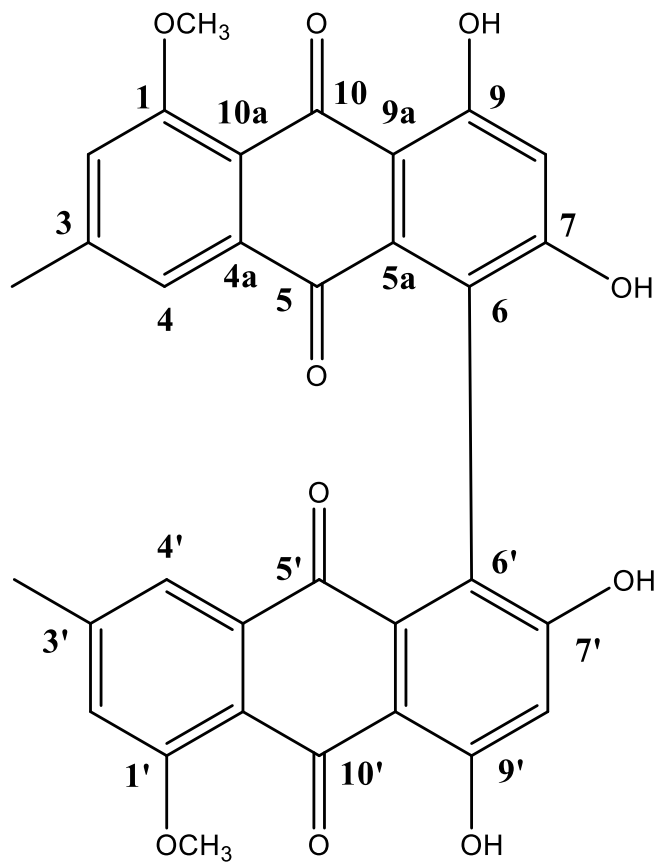


Figure S 8: Chemical structure of compound 2.

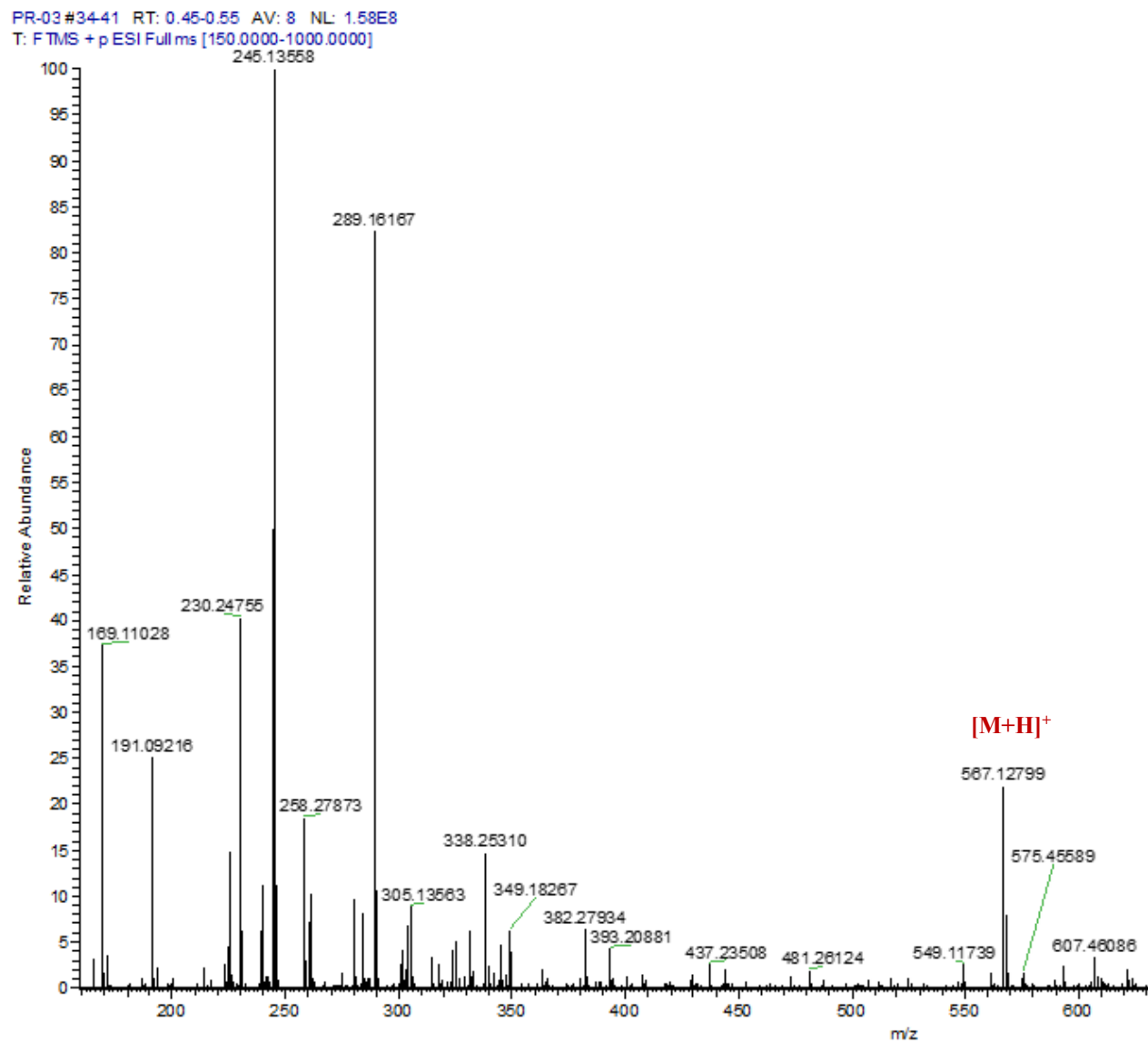


Figure S 9: HR-ESI-MS spectrum of compound **2** (positive mode).

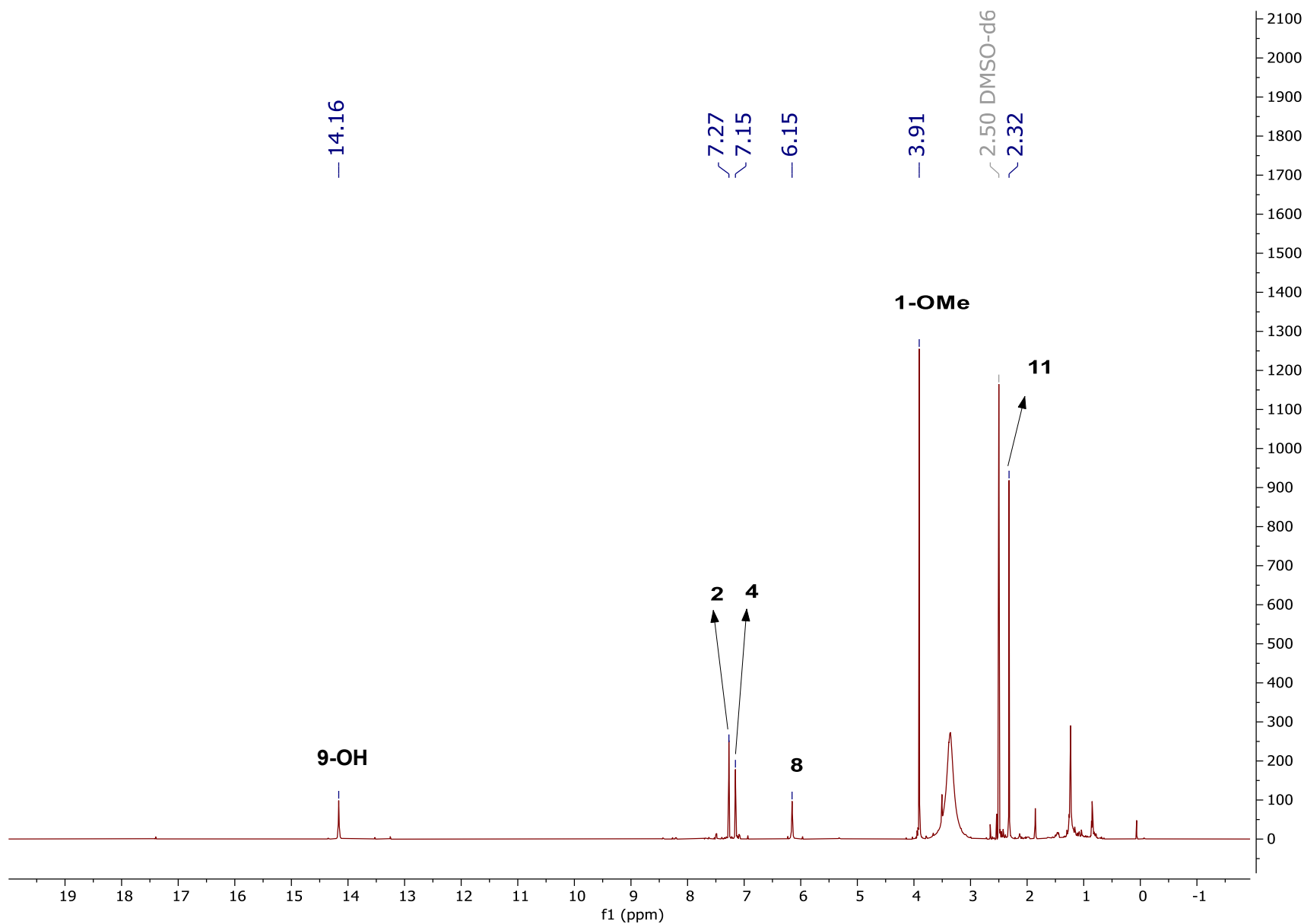


Figure S 10: ^1H NMR spectrum of compound **2** (in DMSO-d_6 , ^1H : 600 MHz).

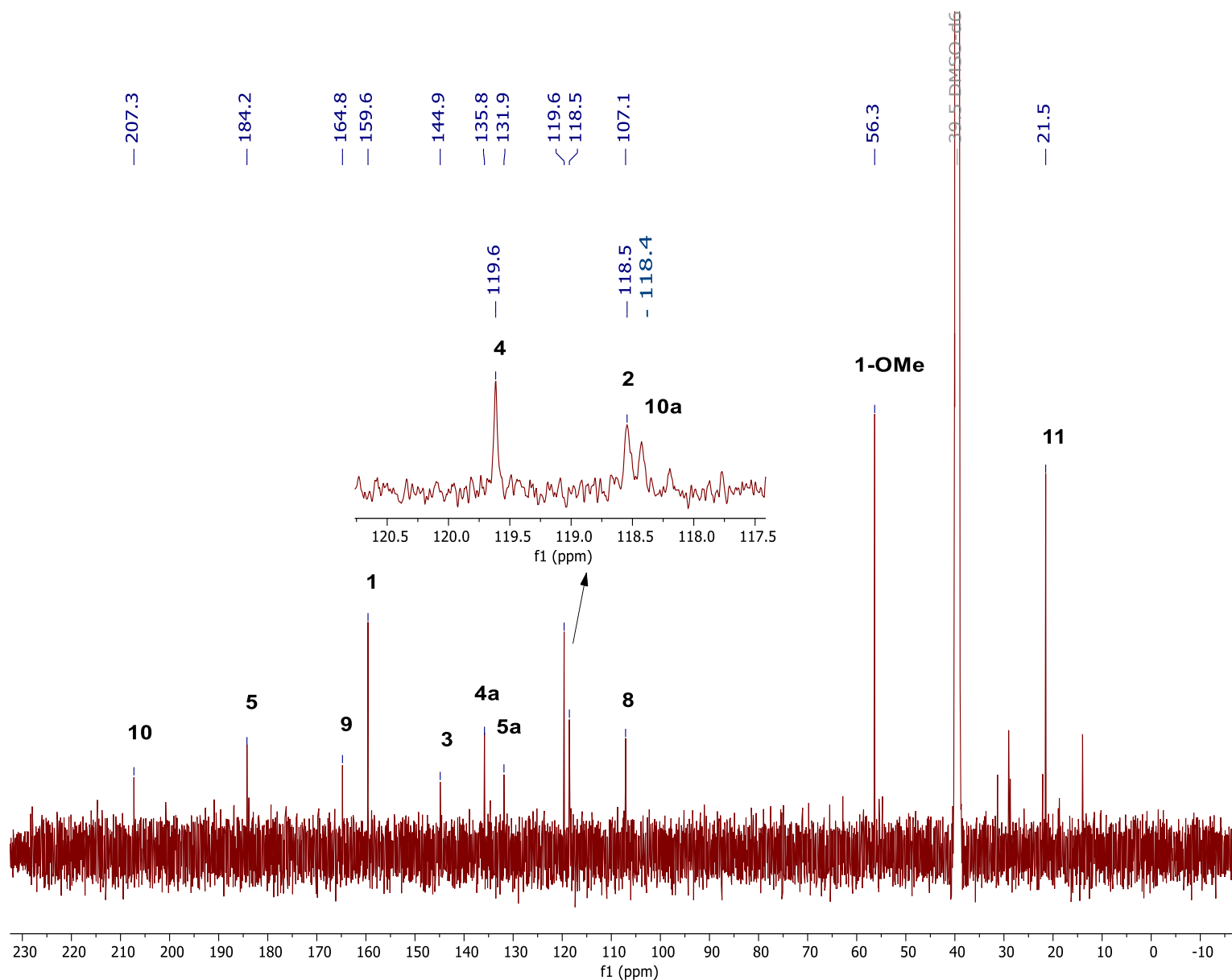


Figure S 11: ^{13}C NMR spectrum of compound 2 (in DMSO-d_6 , ^{13}C :150 MHz).

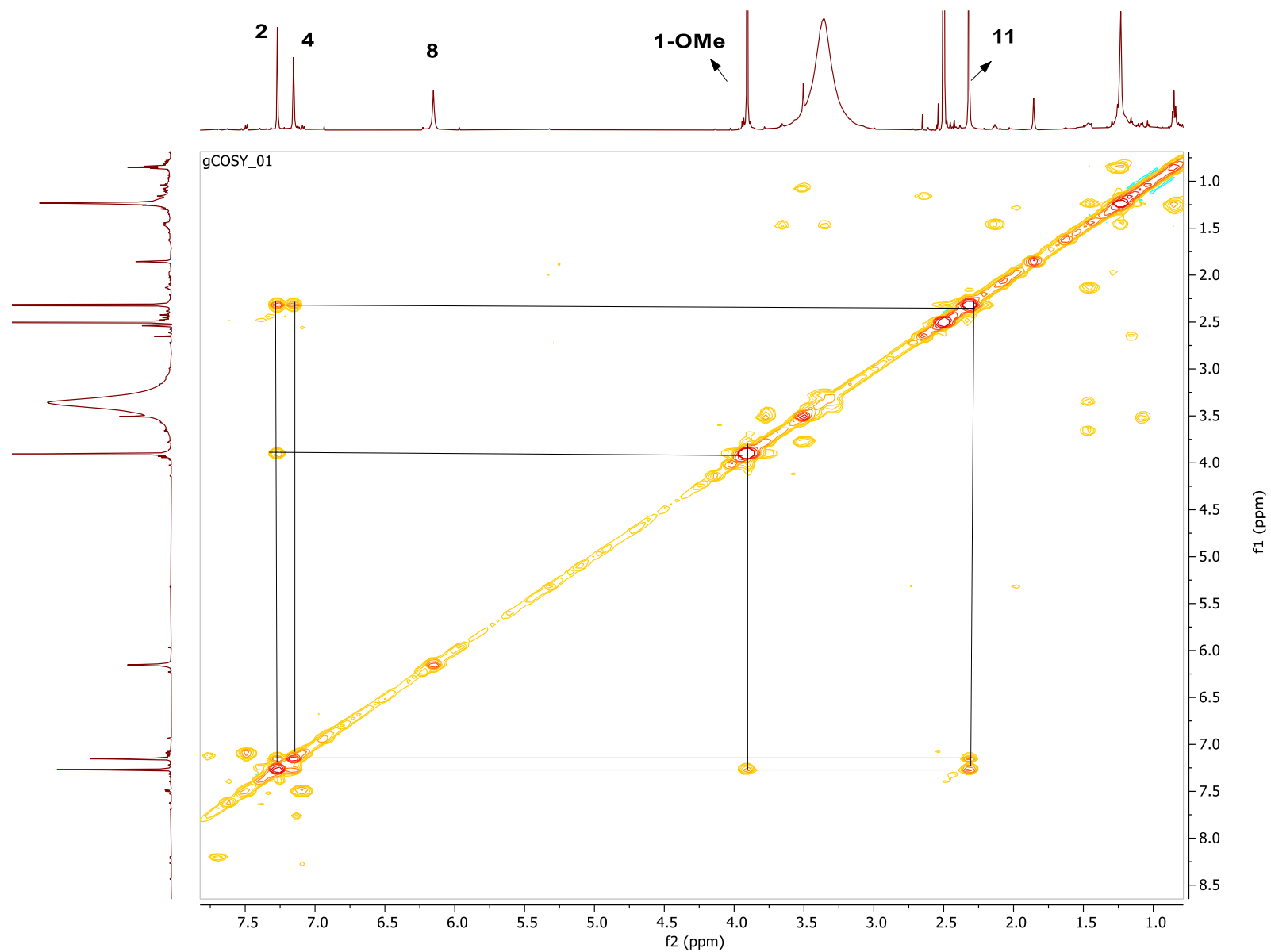


Figure S 12: COSY spectrum of compound **2**.

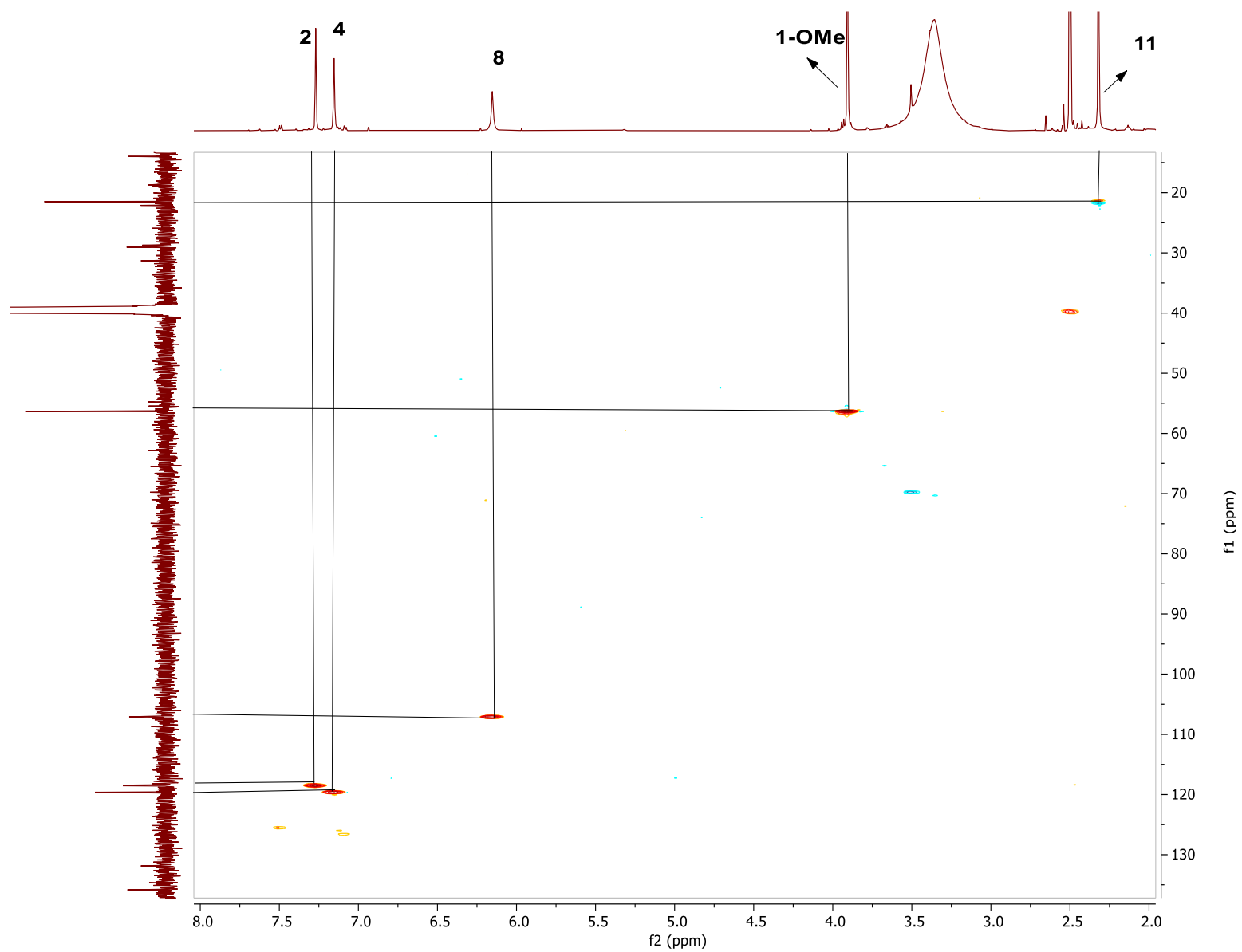


Figure S 13: HSQC spectrum of compound 2.

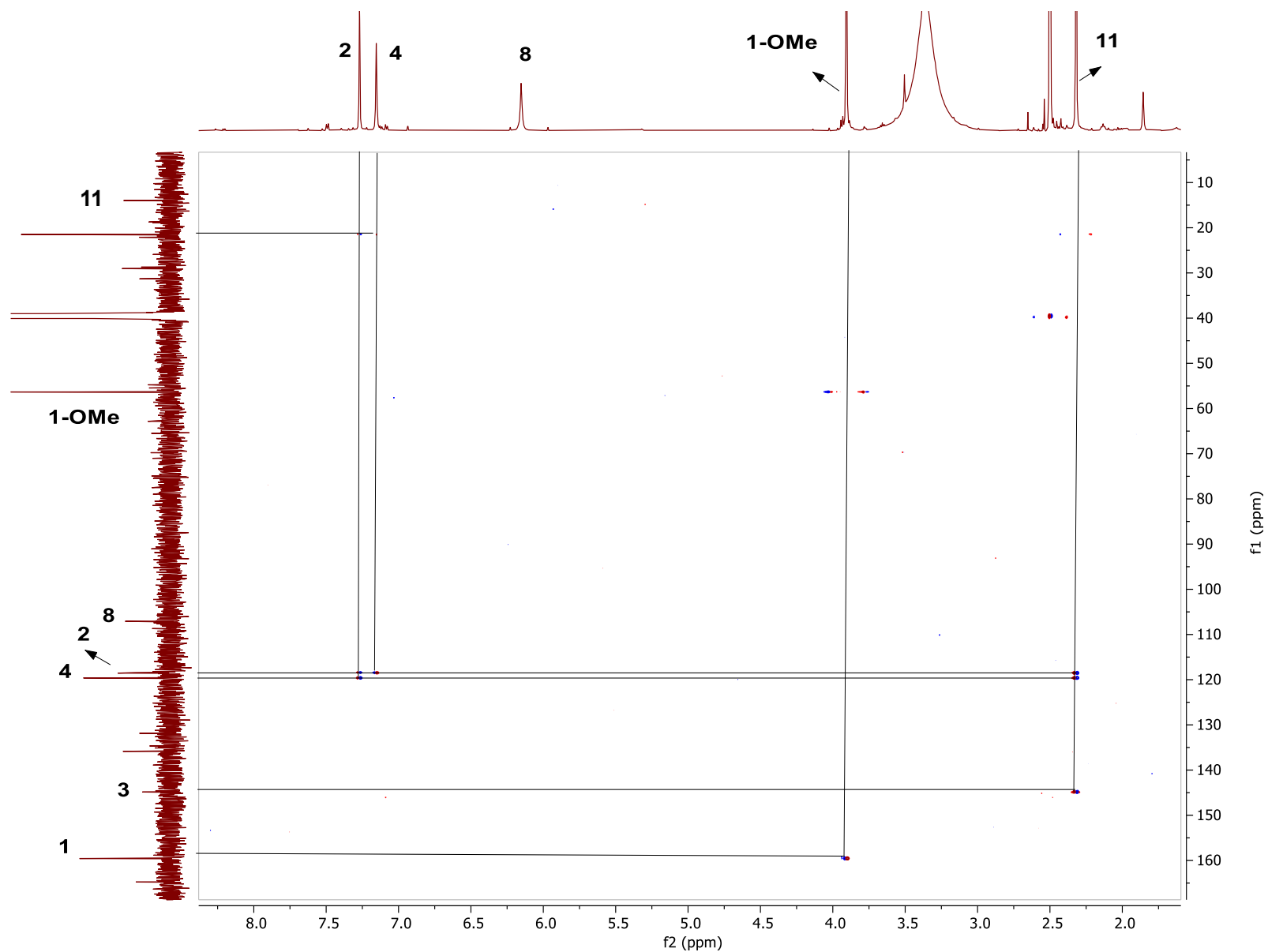


Figure S 14: HMBC spectrum of compound 2.

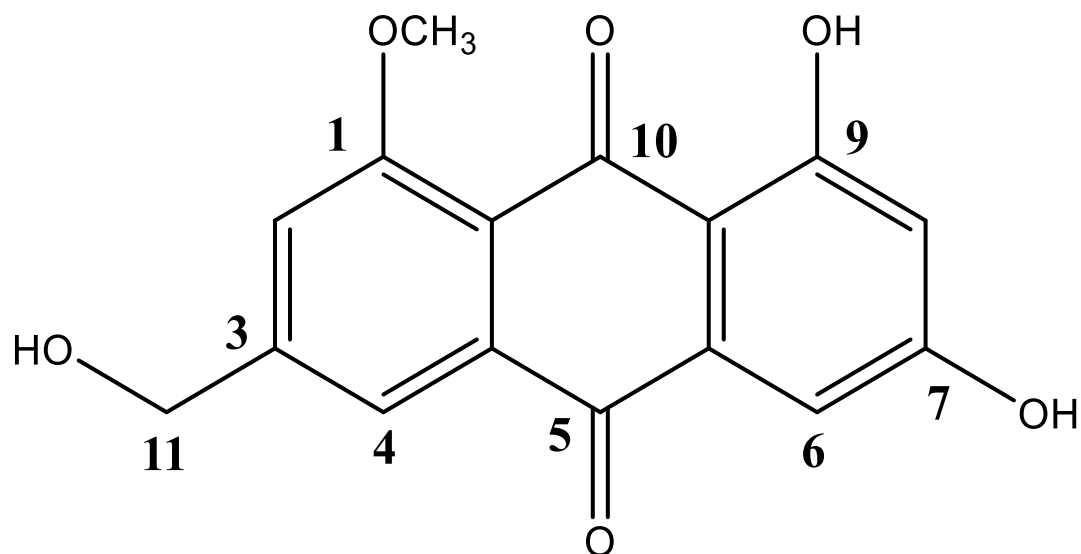


Figure S 15: Chemical structure of compound **3**.

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

No	3	
	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	-	-

^aChemical shifts were measured at 400 MHz in DMSO- d_6

^bChemical shifts were measured at 100 MHz in DMSO- d_6

PR-EB-04-Pozitif #1 RT: 0.01 AV: 1 SM: 7G NL: 2.04E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]

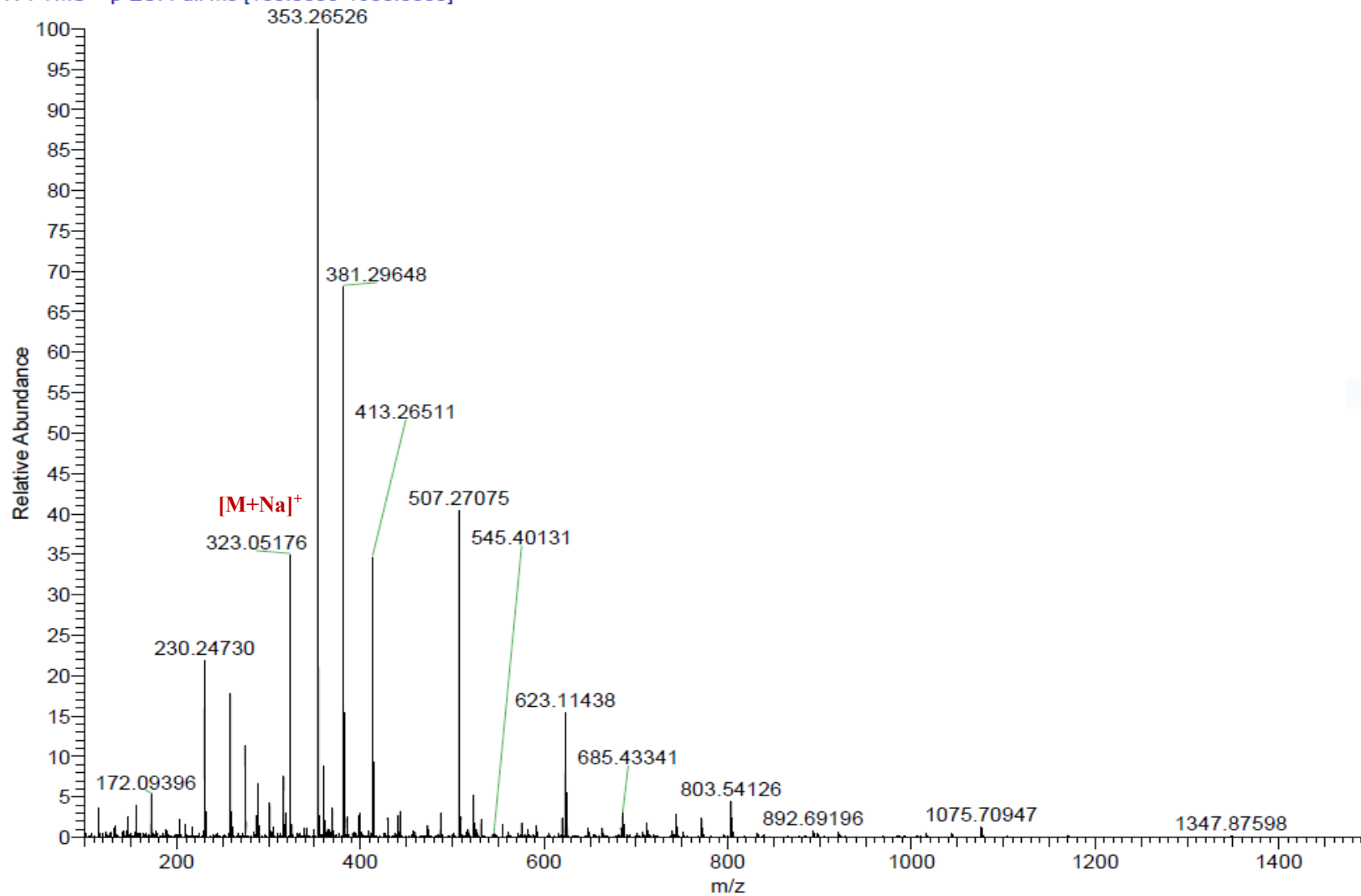


Figure S 16: HR-ESI-MS spectrum of compound 3 (positive mode).

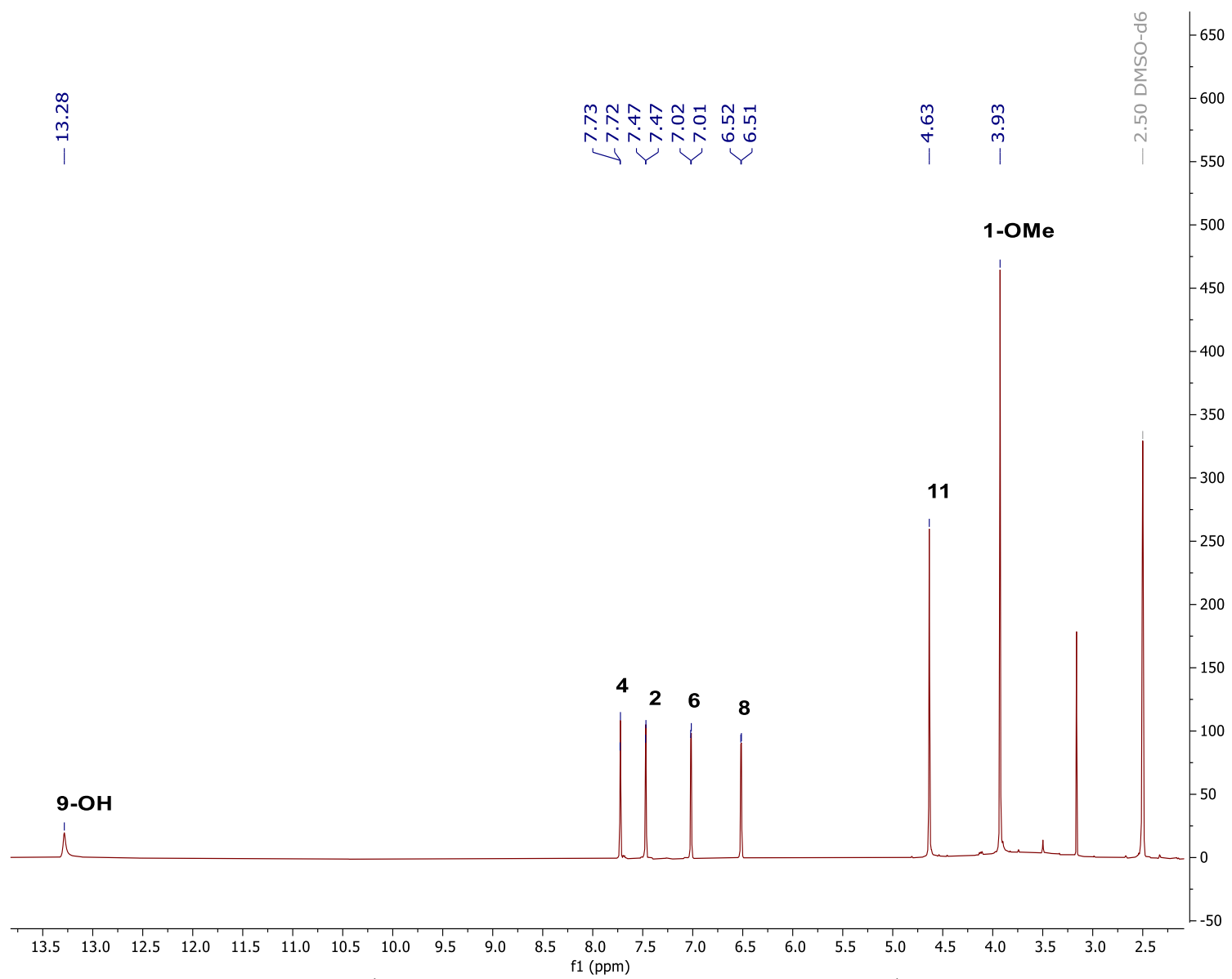


Figure S 17: ^1H NMR spectrum of compound **3** (in DMSO-d_6 , ^1H : 400 MHz).

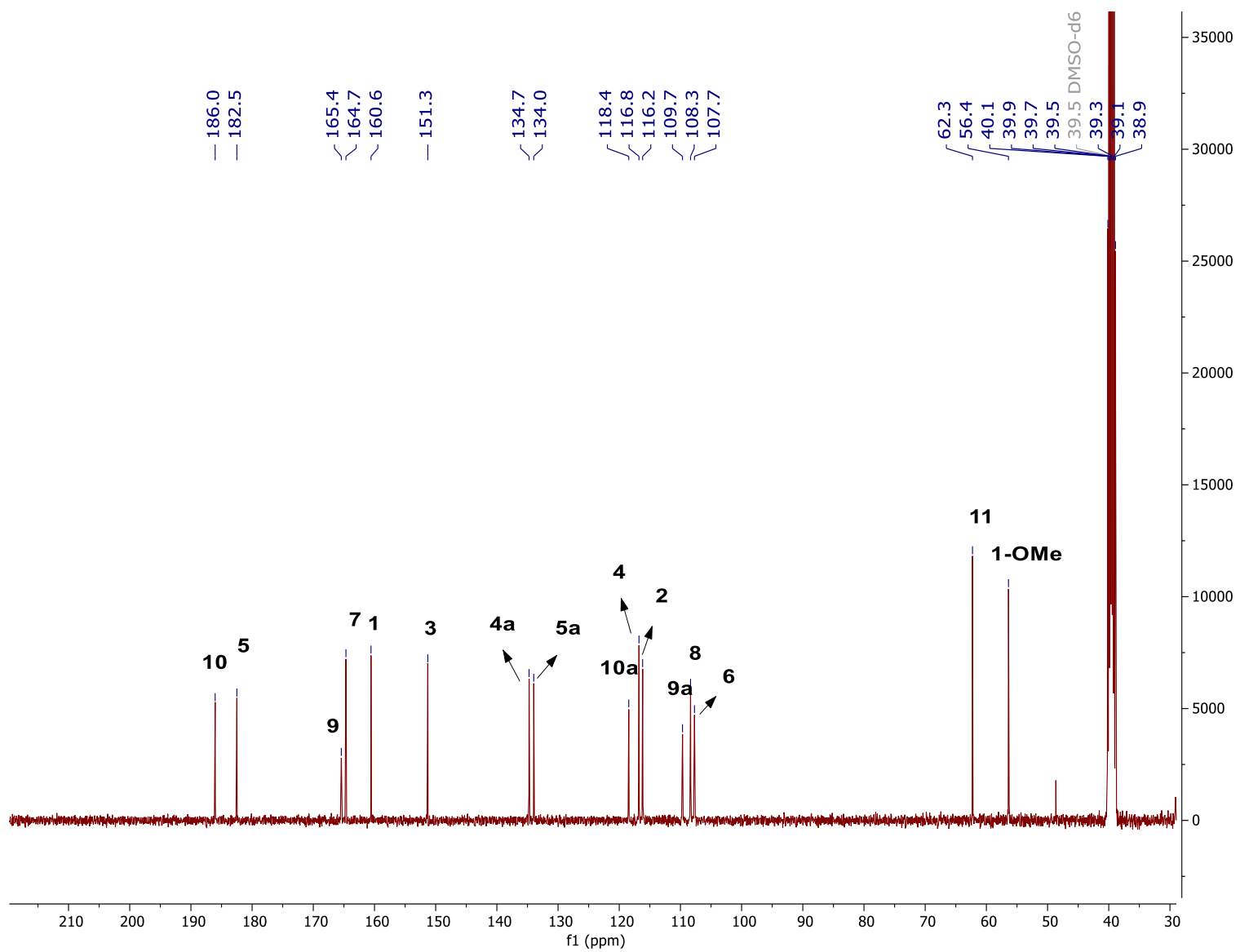


Figure S 18: ^{13}C NMR spectrum of compound **3** (in DMSO- d_6 , ^{13}C :100 MHz).

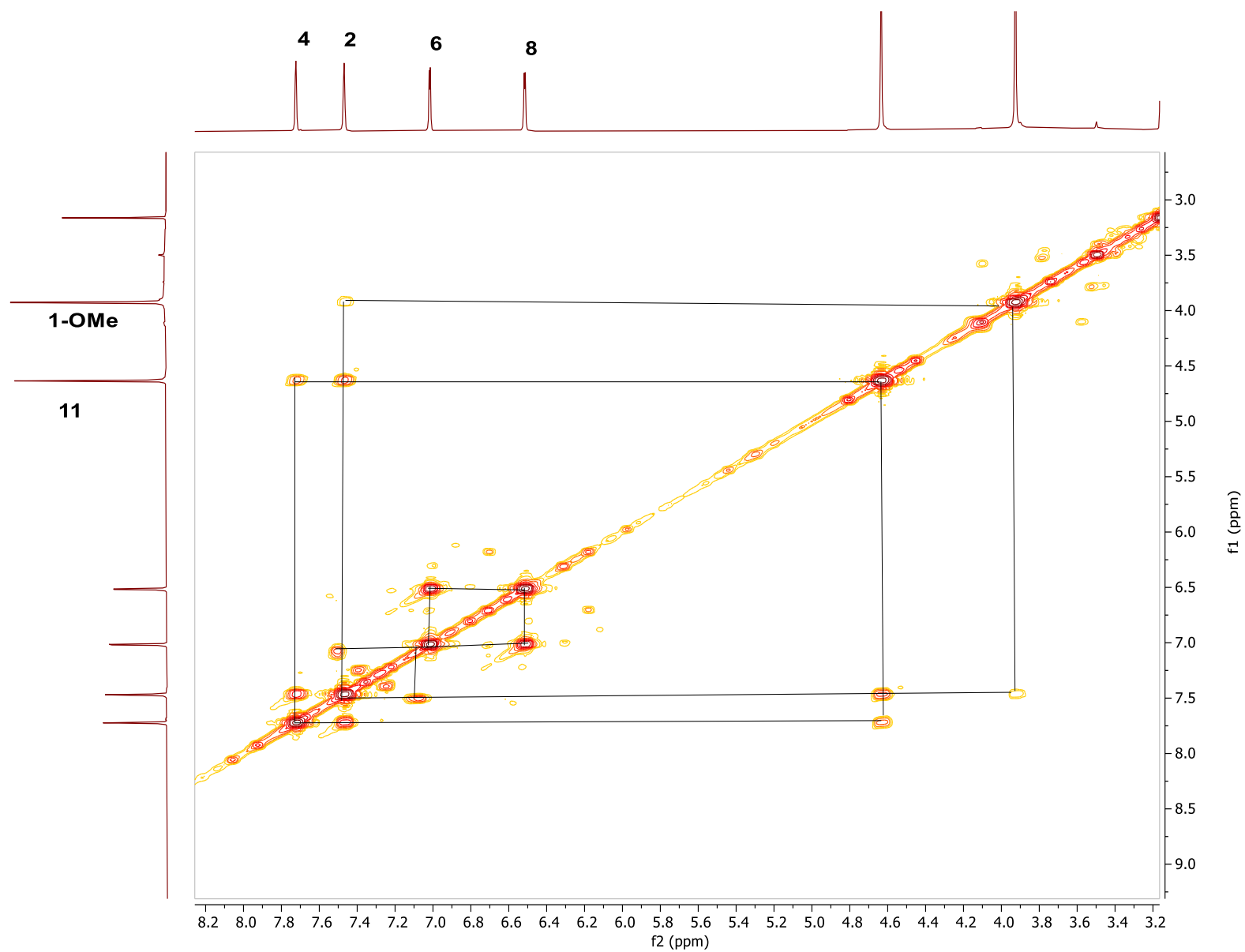


Figure S 19: COSY spectrum of compound 3.

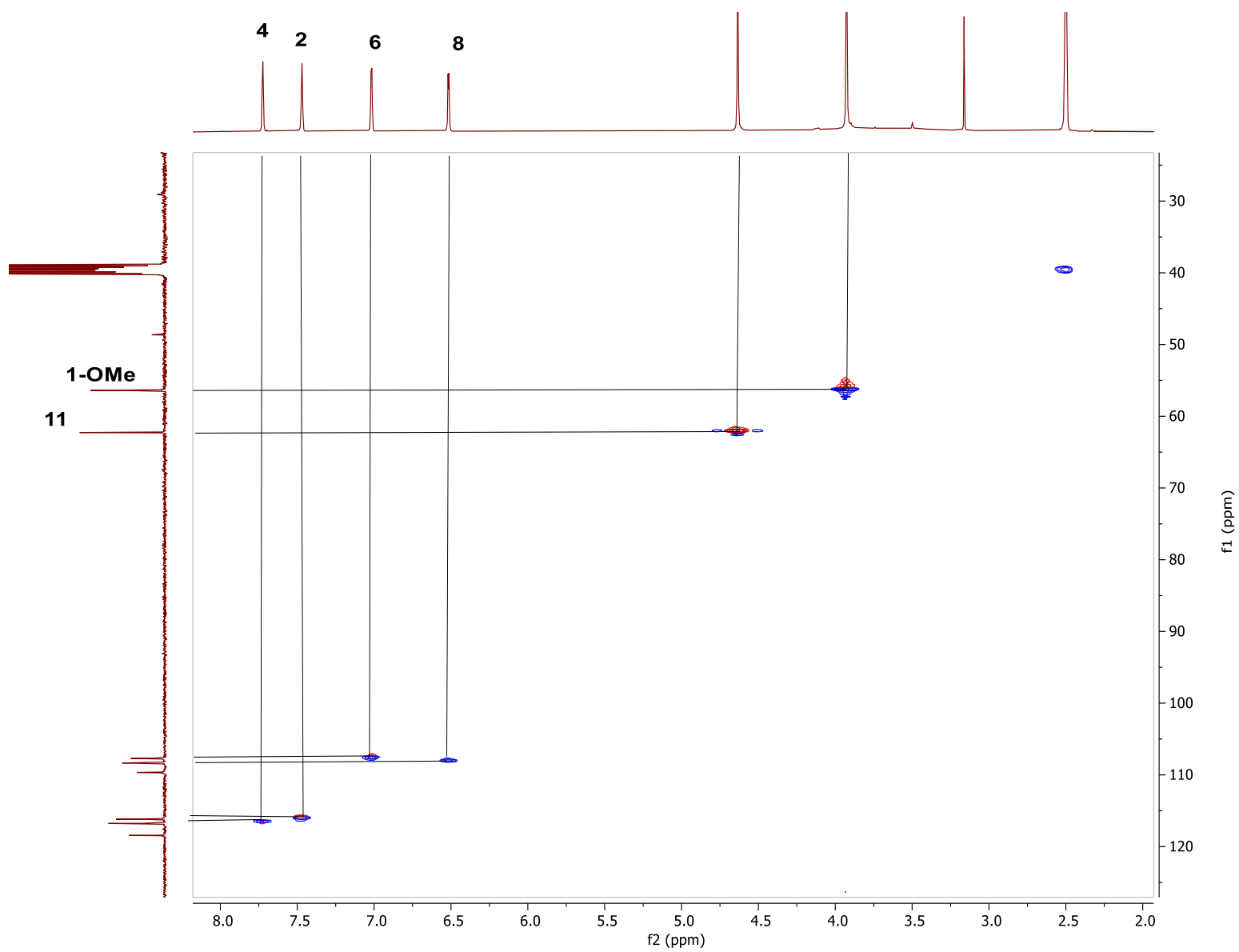


Figure S 20: HSQC spectrum of compound 3.

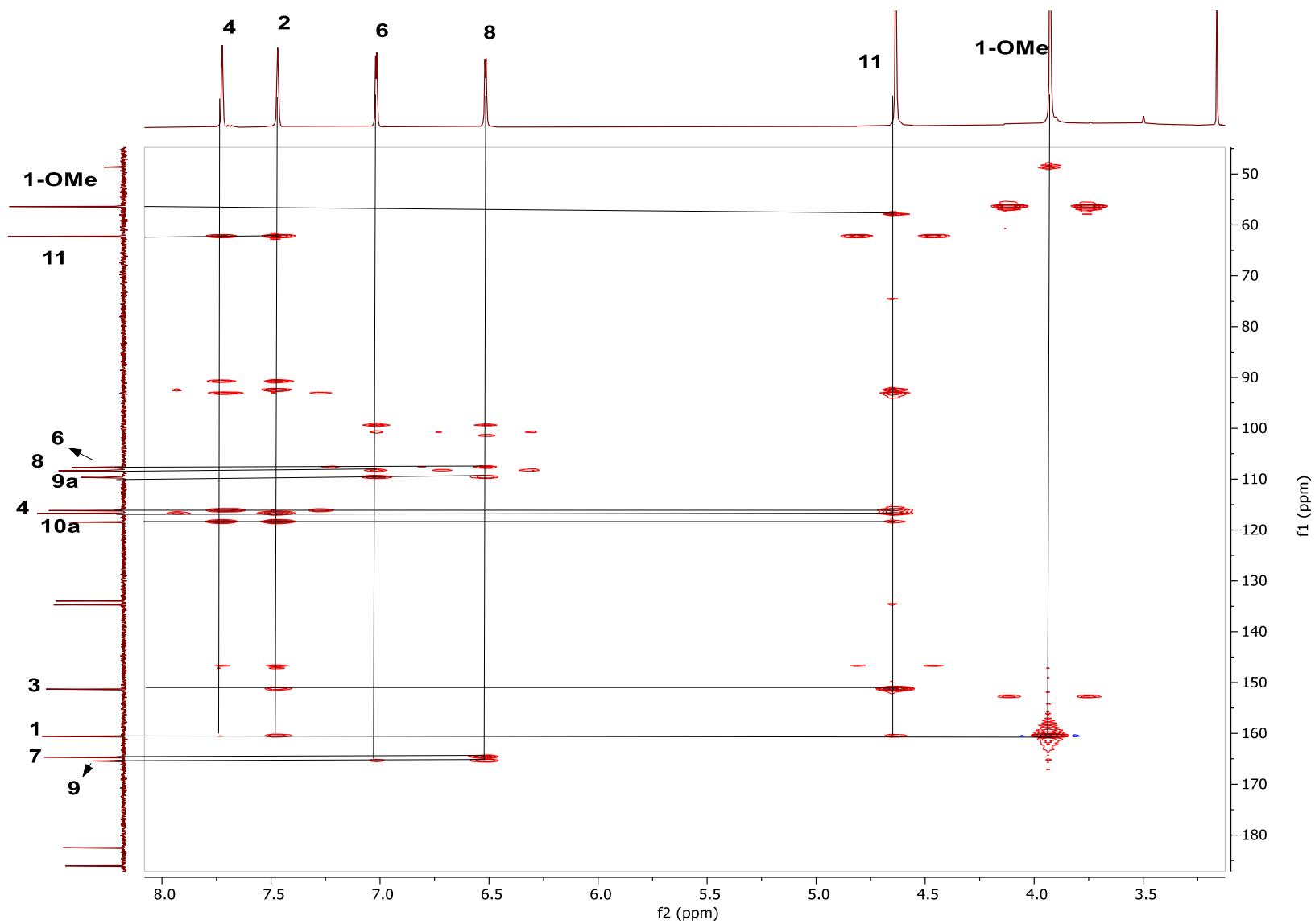


Figure S 21: HMBC spectrum of compound 3.

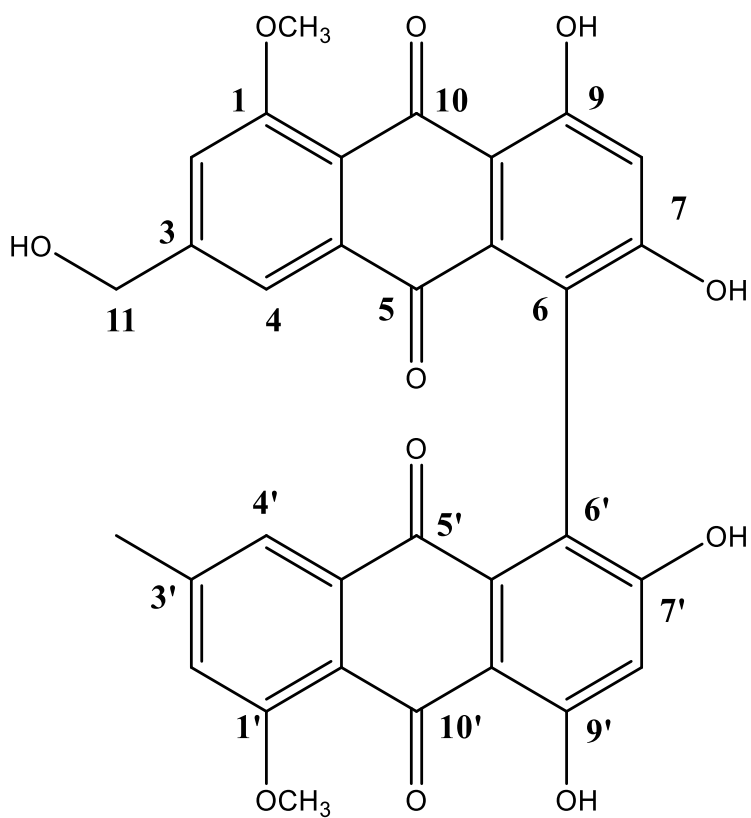


Figure S 22: Chemical structure of compound 4.

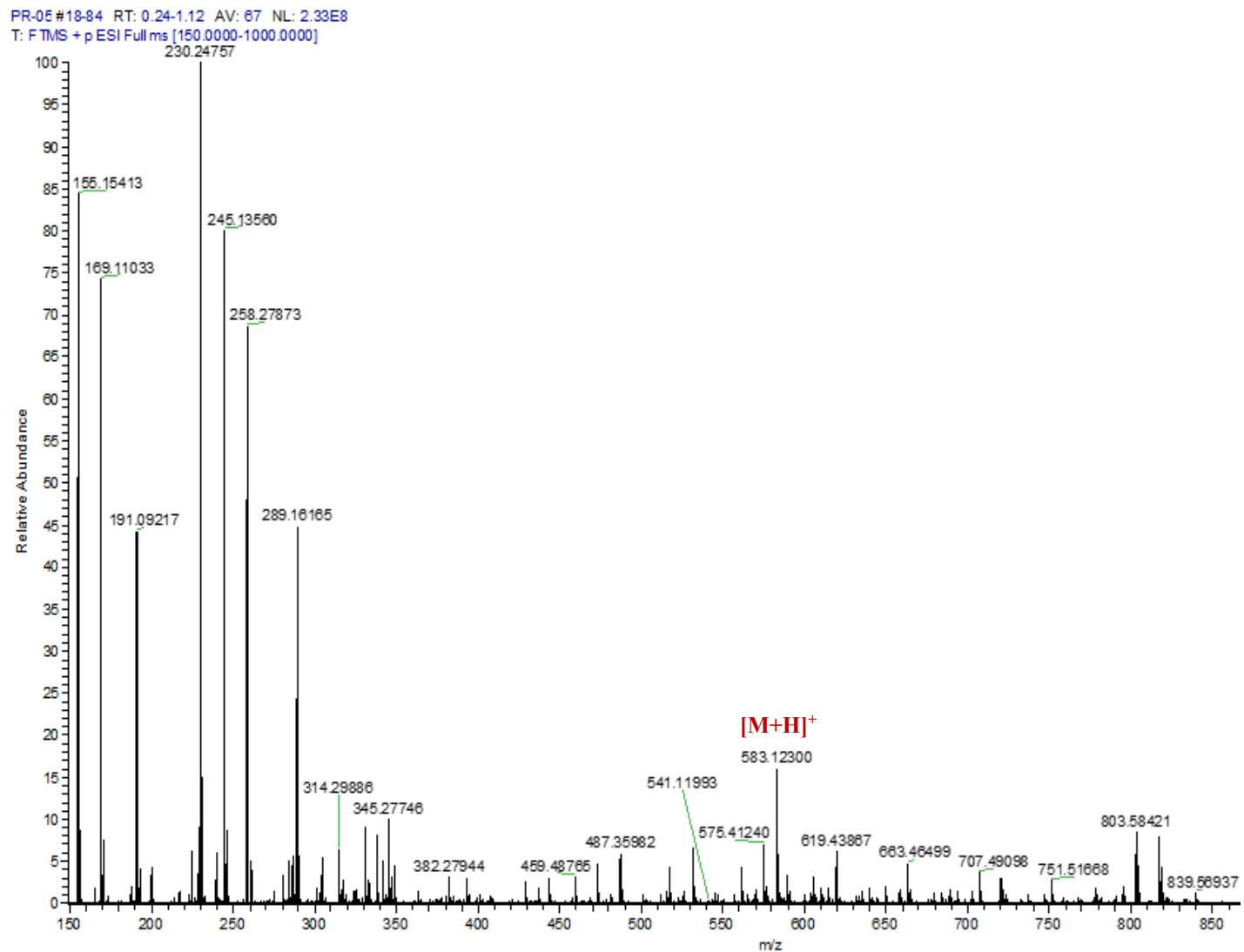


Figure S 23: HR-ESI-MS spectrum of compound **4** (positive mode).

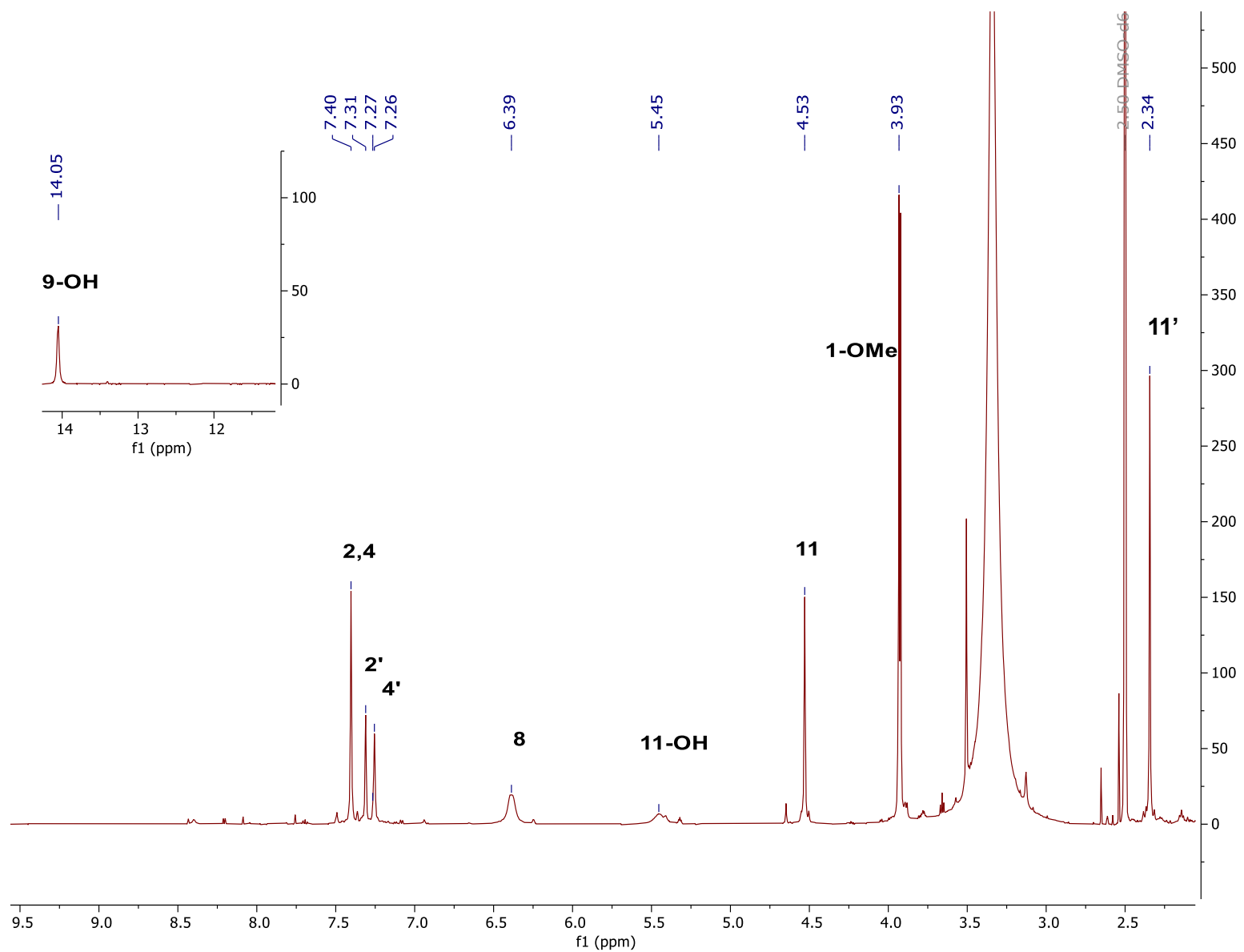


Figure S 24: ^1H NMR spectrum of compound 4 (in DMSO-d_6 , ^1H : 600 MHz).

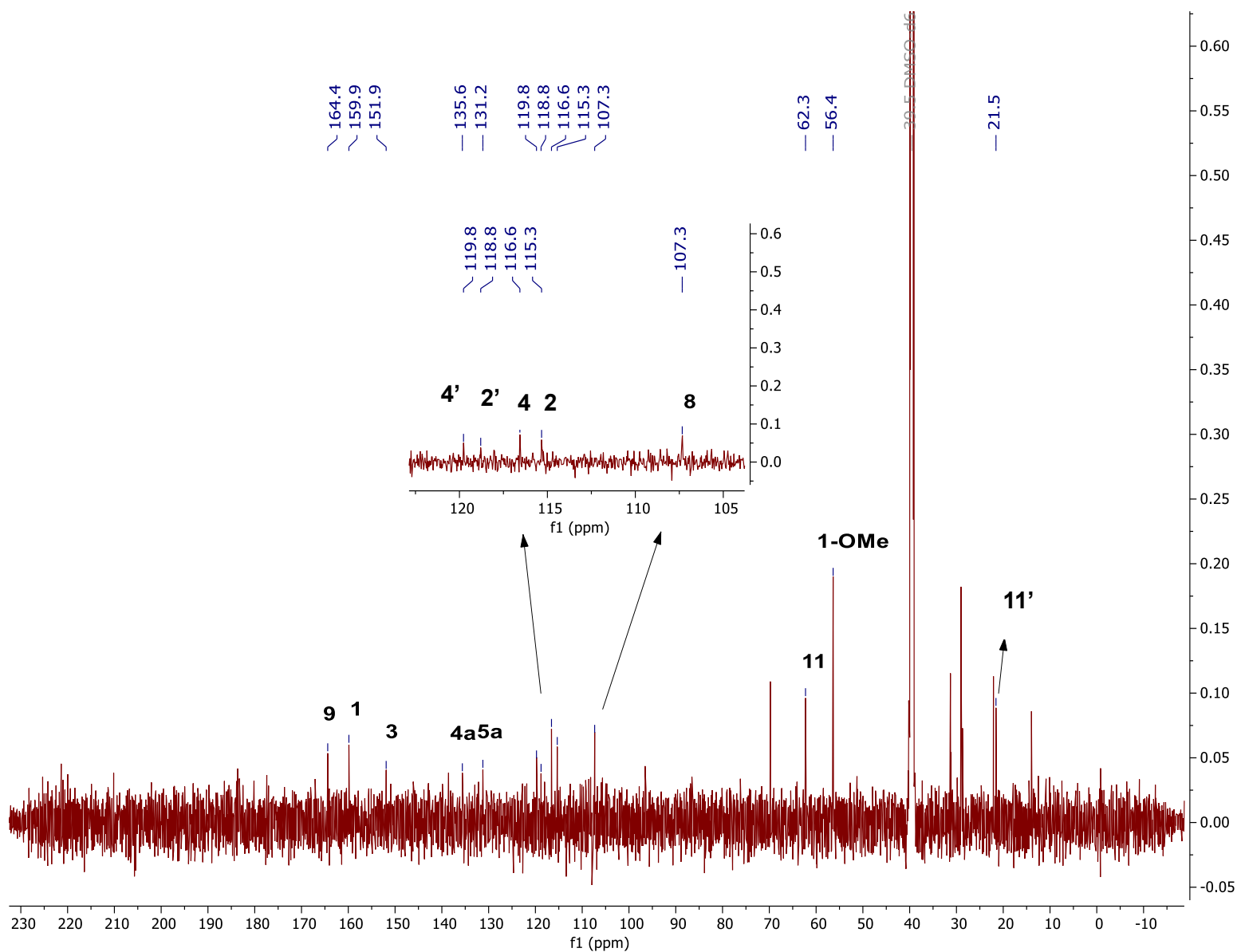


Figure S 25: ^{13}C NMR spectrum of compound **4** (in DMSO-d_6 , ^{13}C :150 MHz).

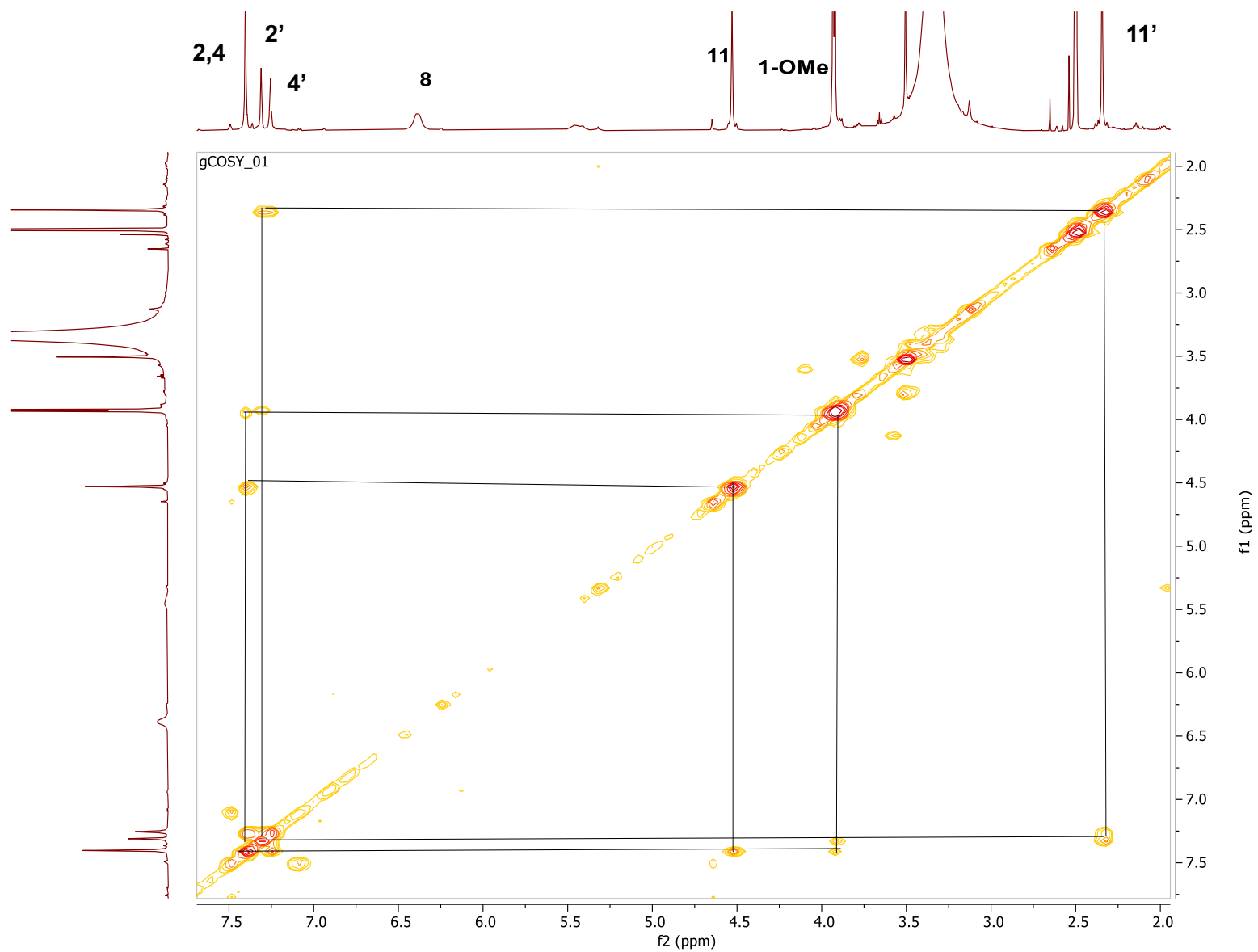


Figure S 26: COSY spectrum of compound 4.

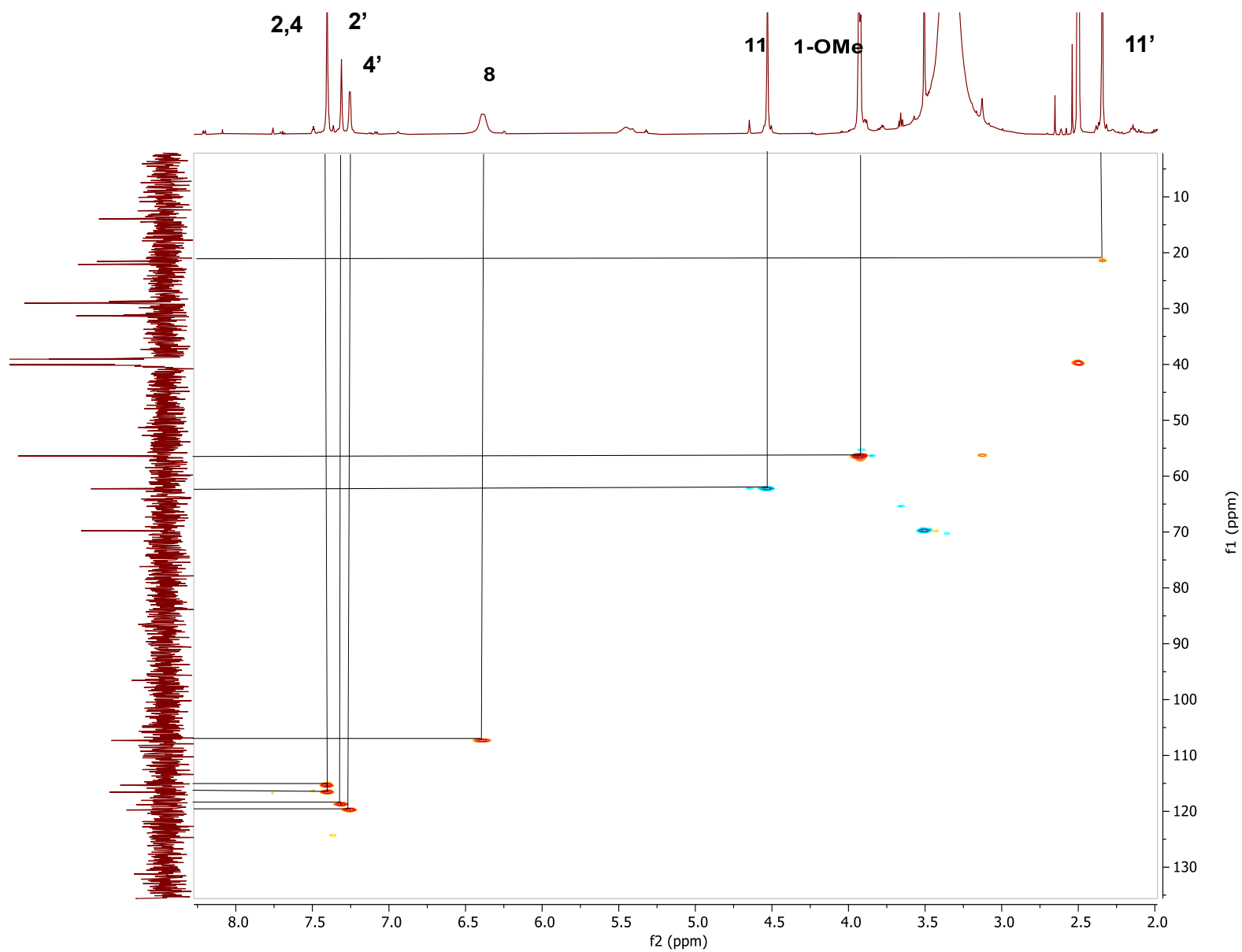


Figure S 27: HSQC spectrum of compound 4.

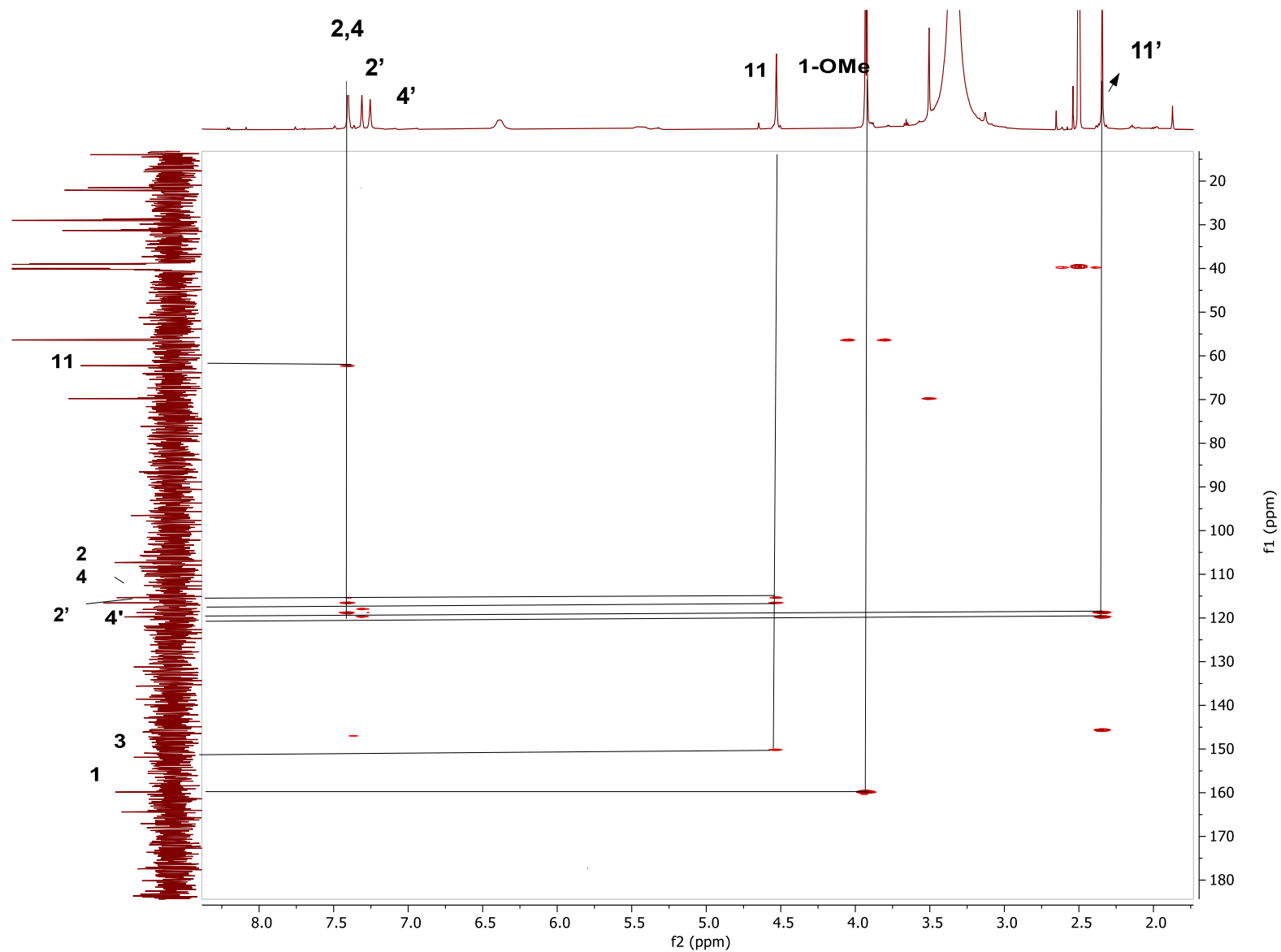


Figure S 28: HMBC spectrum of compound 4.

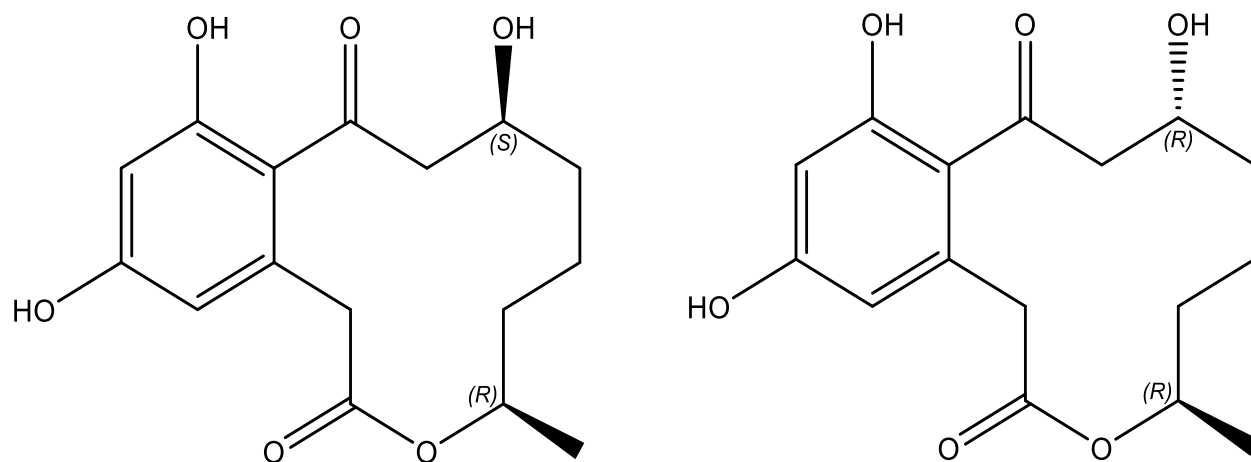


Figure S 29: Chemical structures of compound **5a** and **5b**.

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

No	5a		5b	
	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)

^aChemical shifts were measured at 600 MHz in DMSO- d_6

^bChemical shifts were measured at 150 MHz in DMSO- d_6

PR-06 #8-14 RT: 0.11-0.19 AV: 7 NL: 2.44E8
T: F TMS + p ESI Full ms [150.0000-1000.0000]

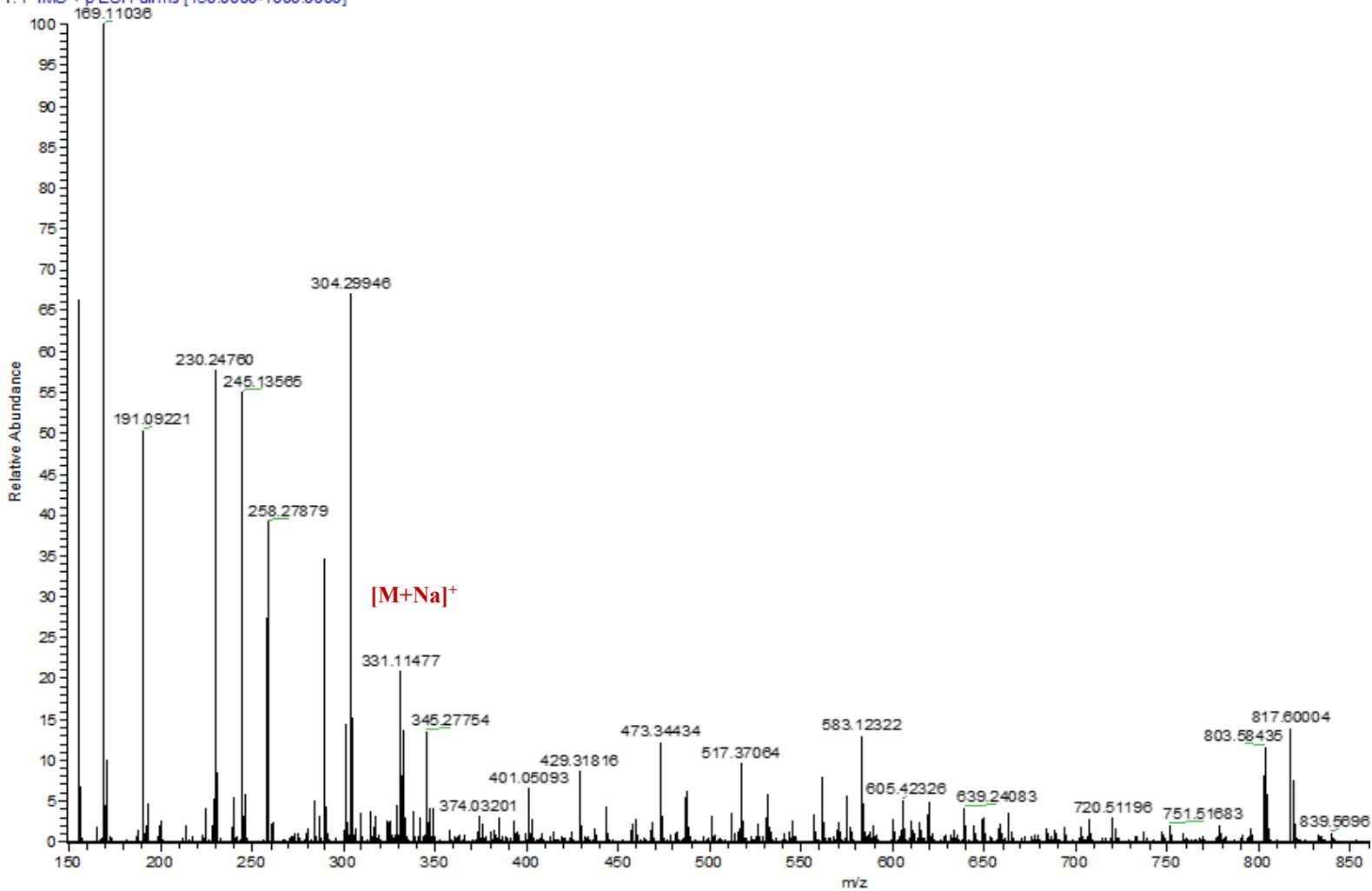


Figure S 30: HR-ESI-MS spectrum of compound 5 (positive mode).

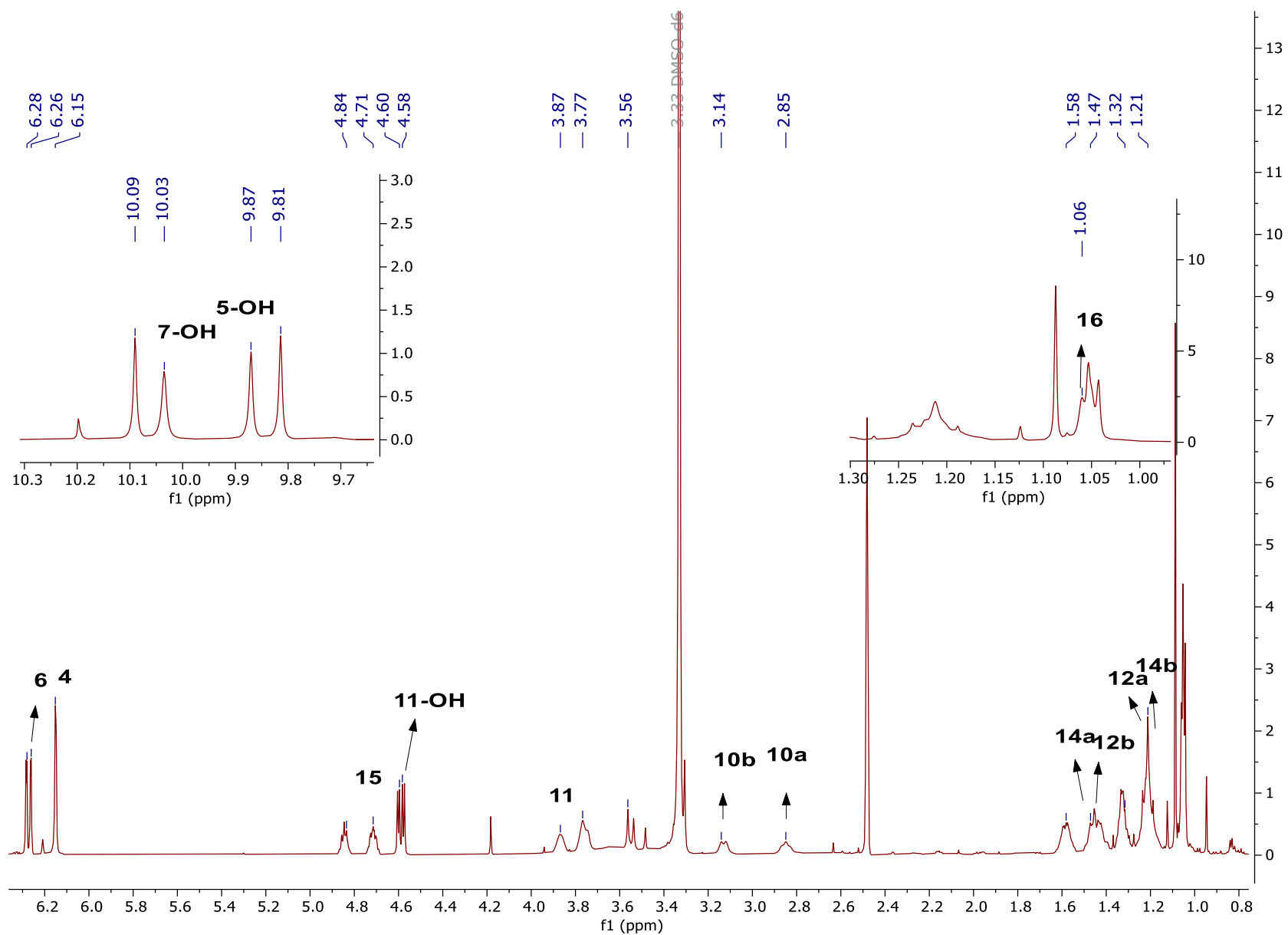


Figure S 31: ^1H NMR spectrum of compound 5 (in DMSO-d_6 , ^1H : 600 MHz).

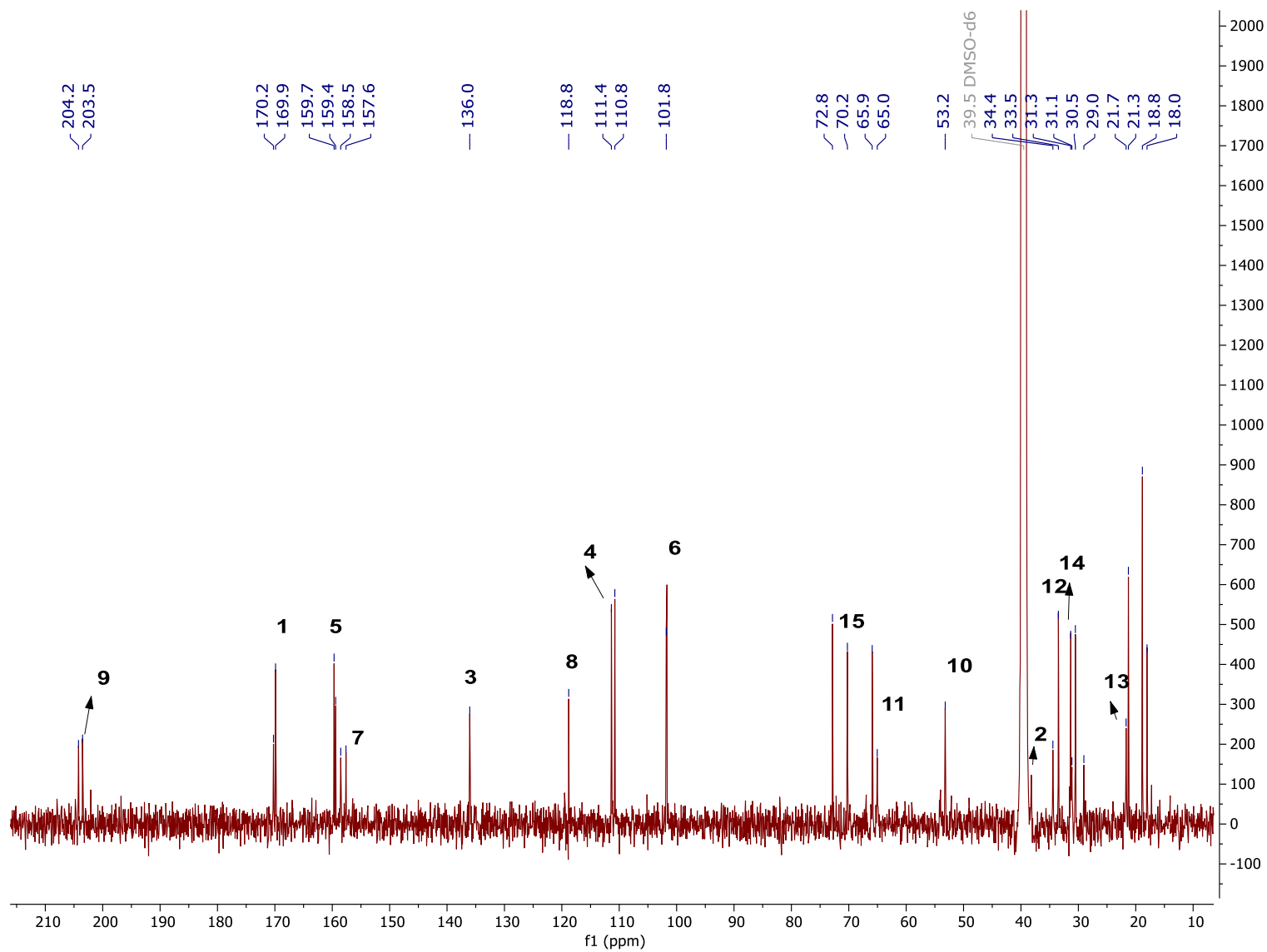


Figure S 32: ^{13}C NMR spectrum of compound **5** (in DMSO- d_6 , ^{13}C :150 MHz).

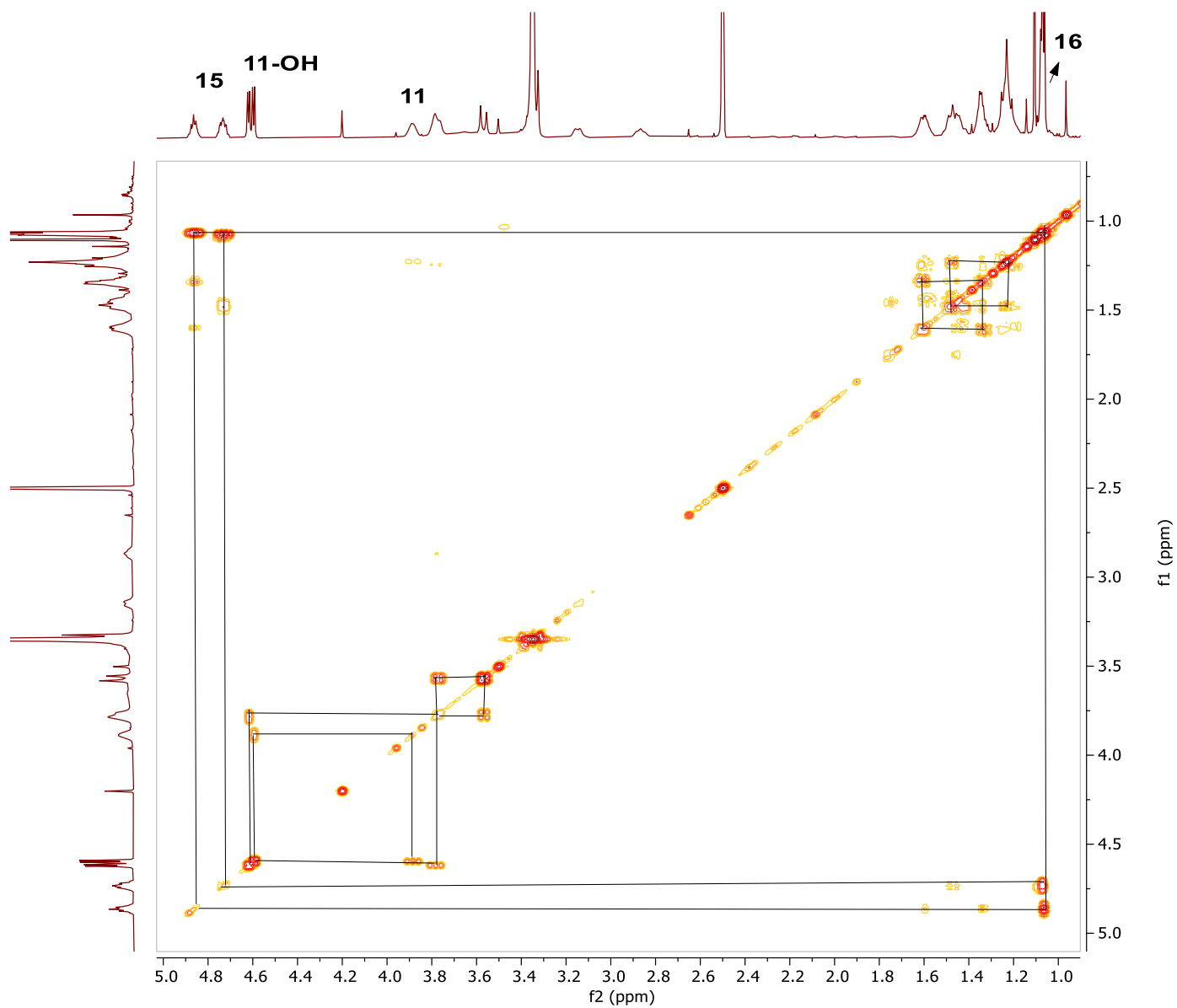


Figure S 33: COSY spectrum of compound 5.

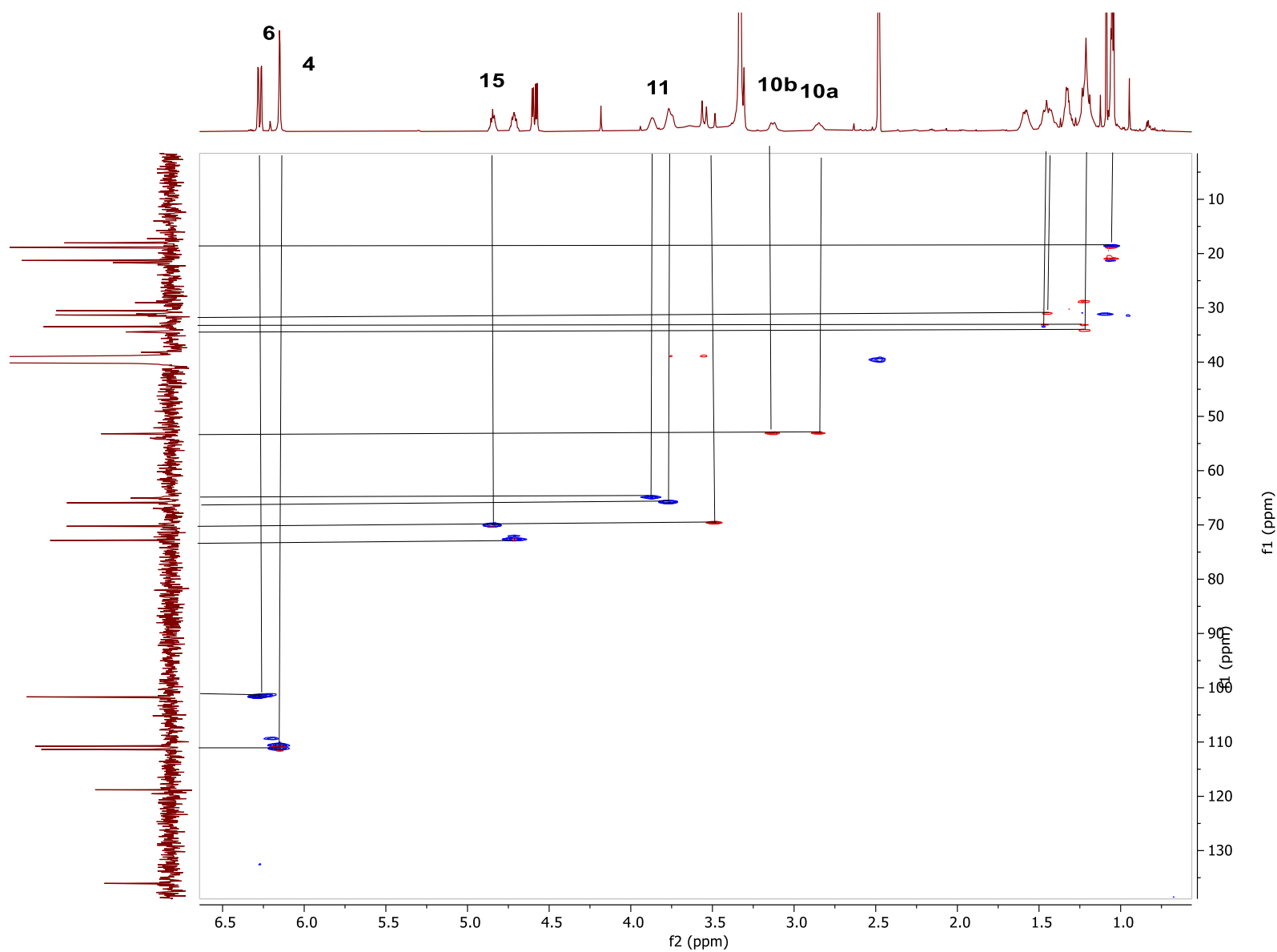


Figure S 34: HSQC spectrum of compound **5**.

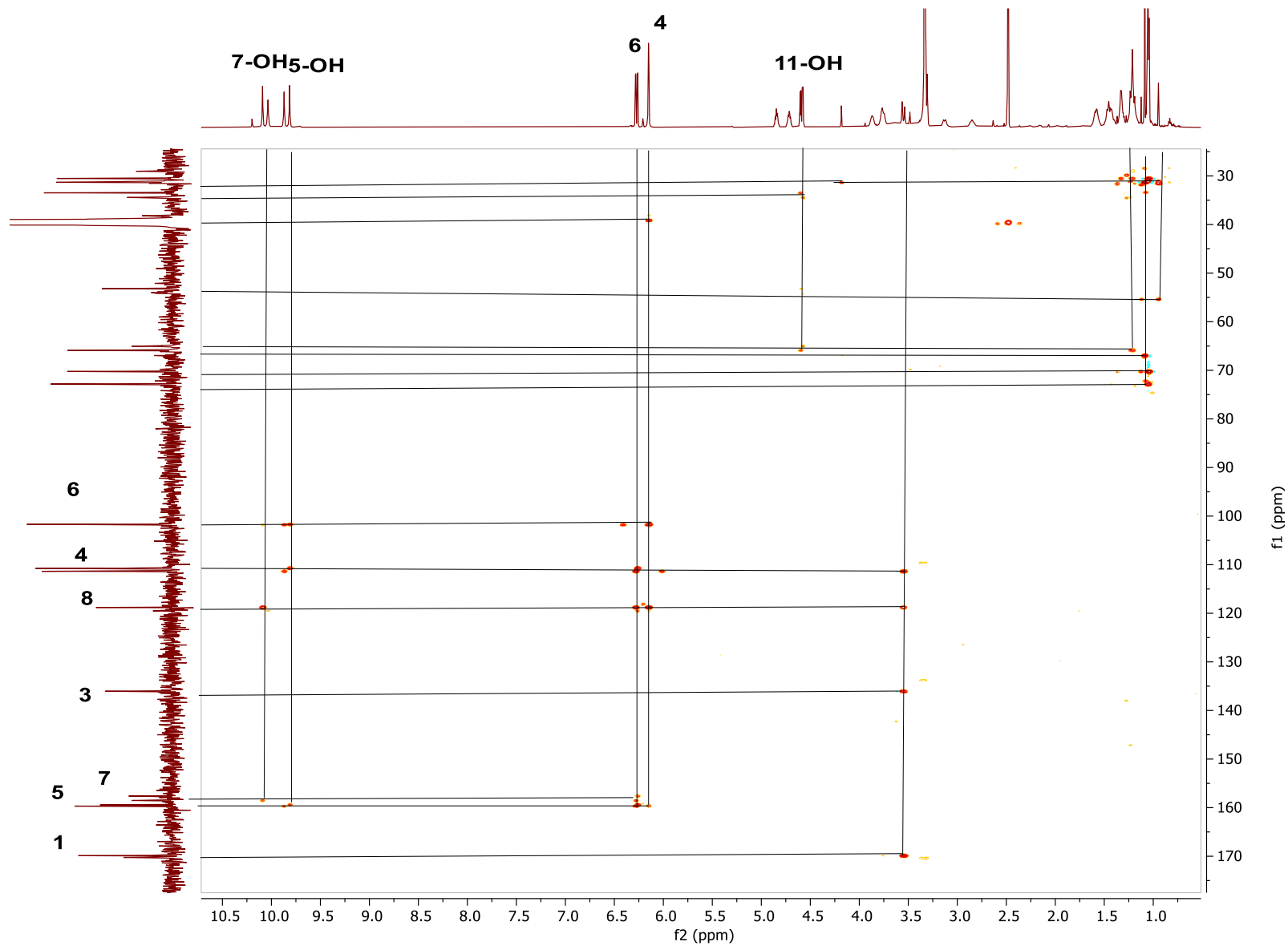


Figure S 35: HMBC spectrum of compound 5.

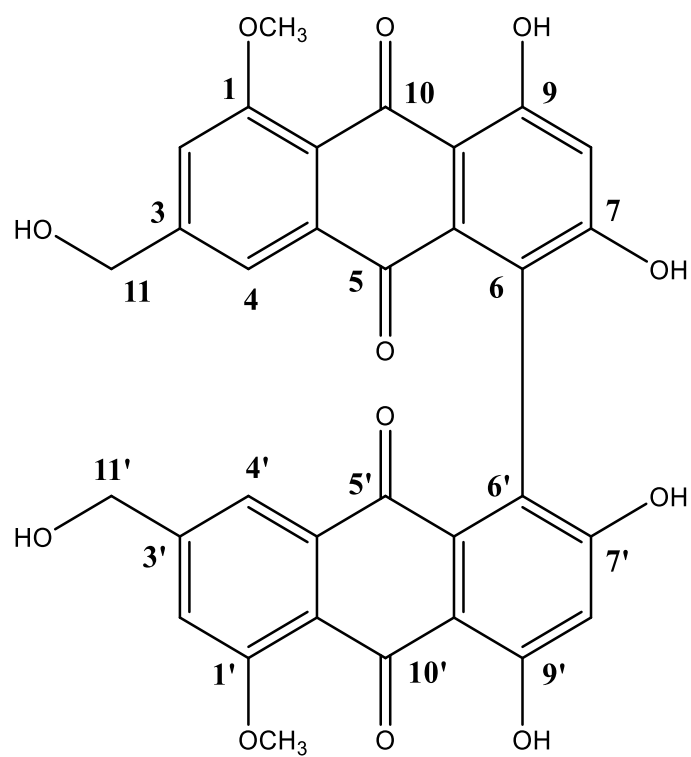


Figure S 36: Chemical structure of compound 6.

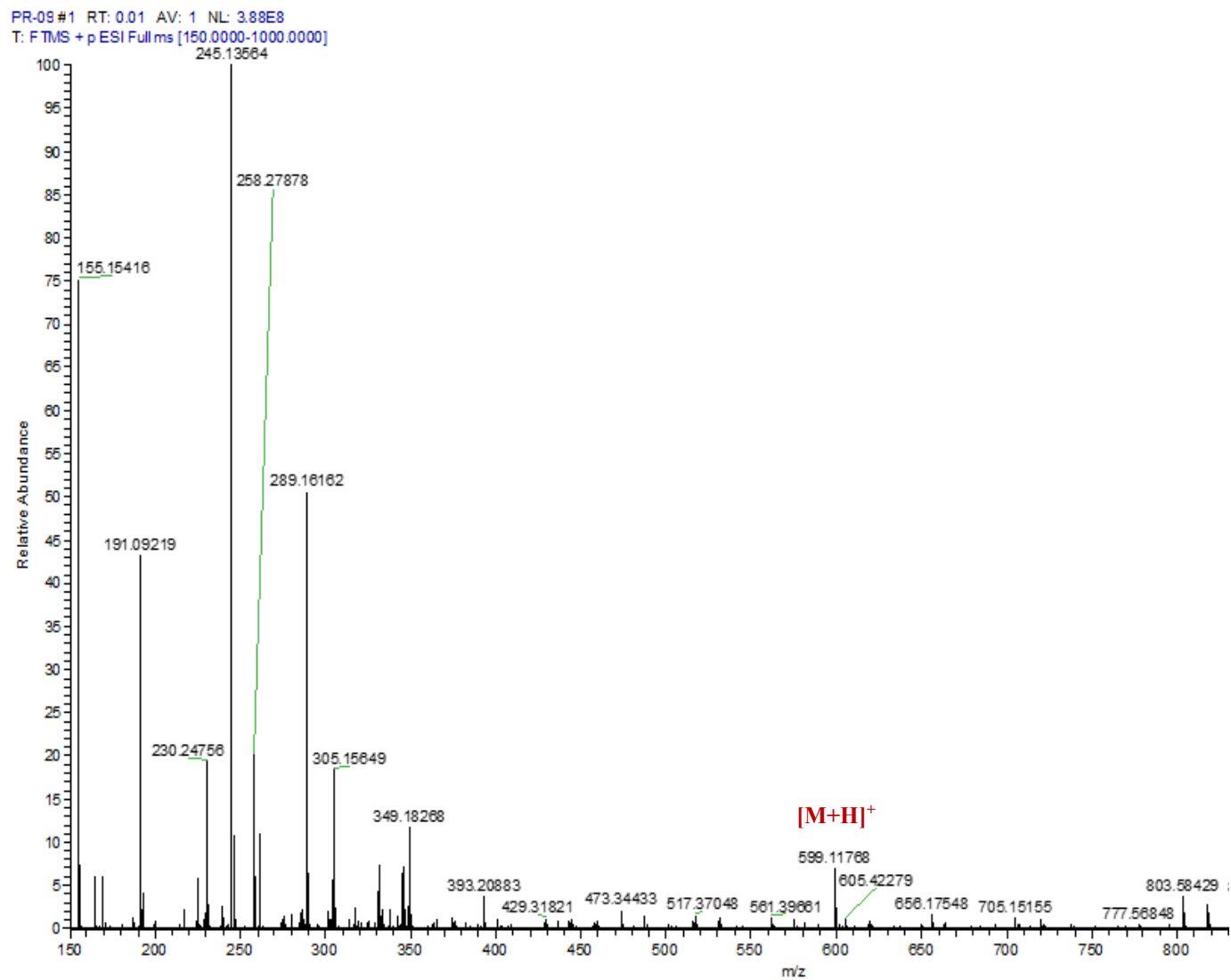


Figure S 37: HR-ESI-MS spectrum of compound **6** (positive mode).

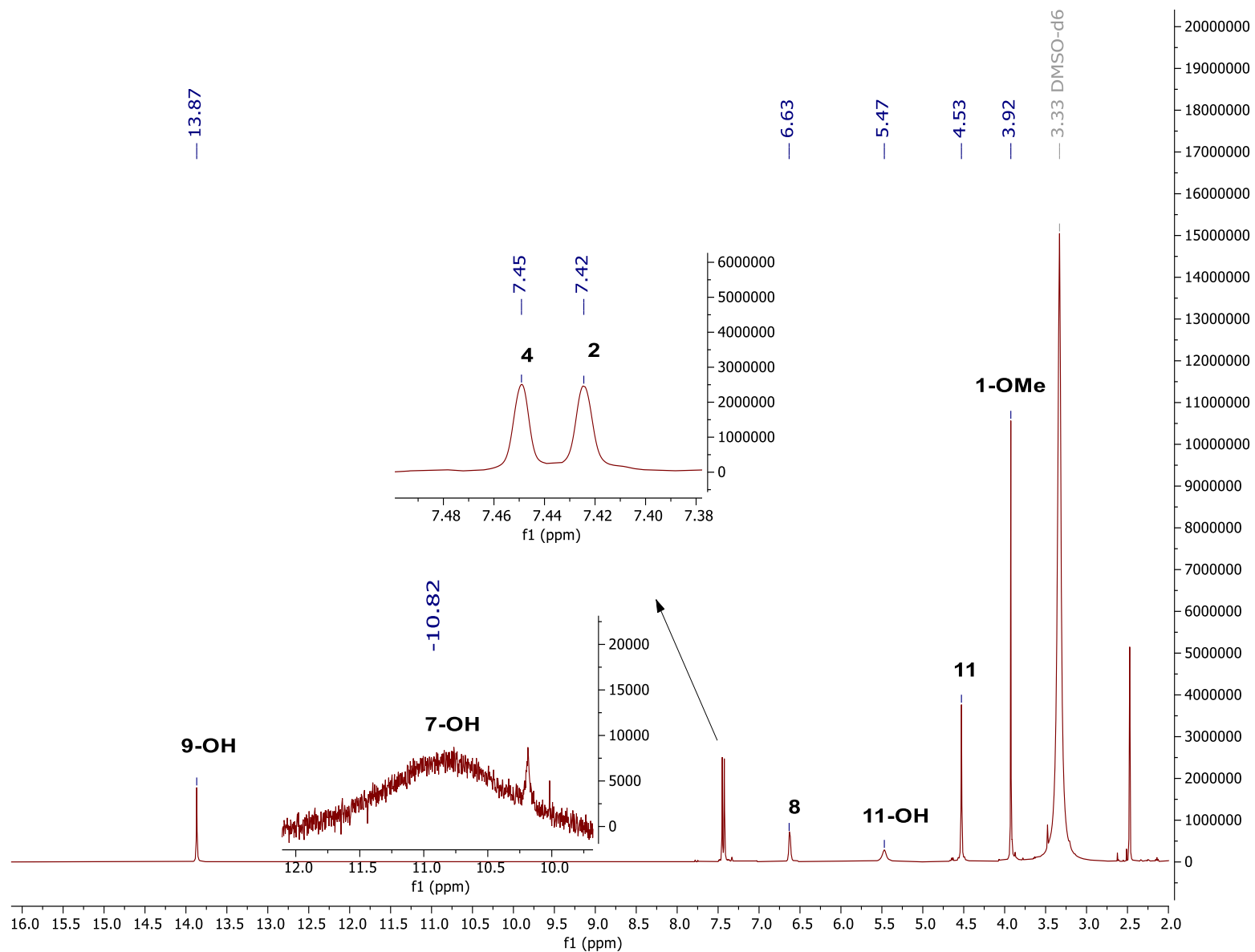


Figure S 38: ^1H NMR spectrum of compound **6** (in DMSO-d_6 , ^1H : 500 MHz).

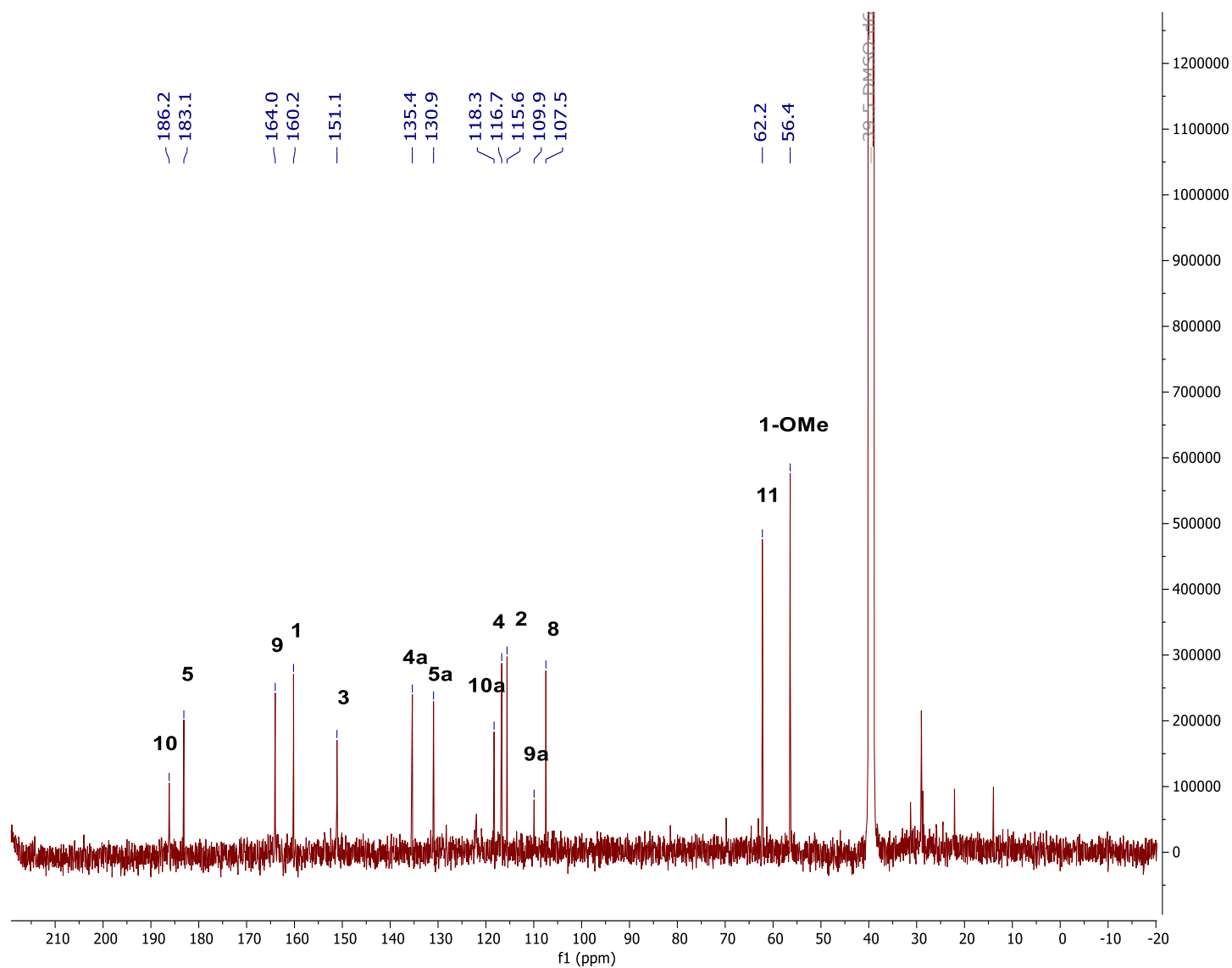


Figure S 39: ^{13}C NMR spectrum of compound **6** (in DMSO-d_6 , ^{13}C :125 MHz).

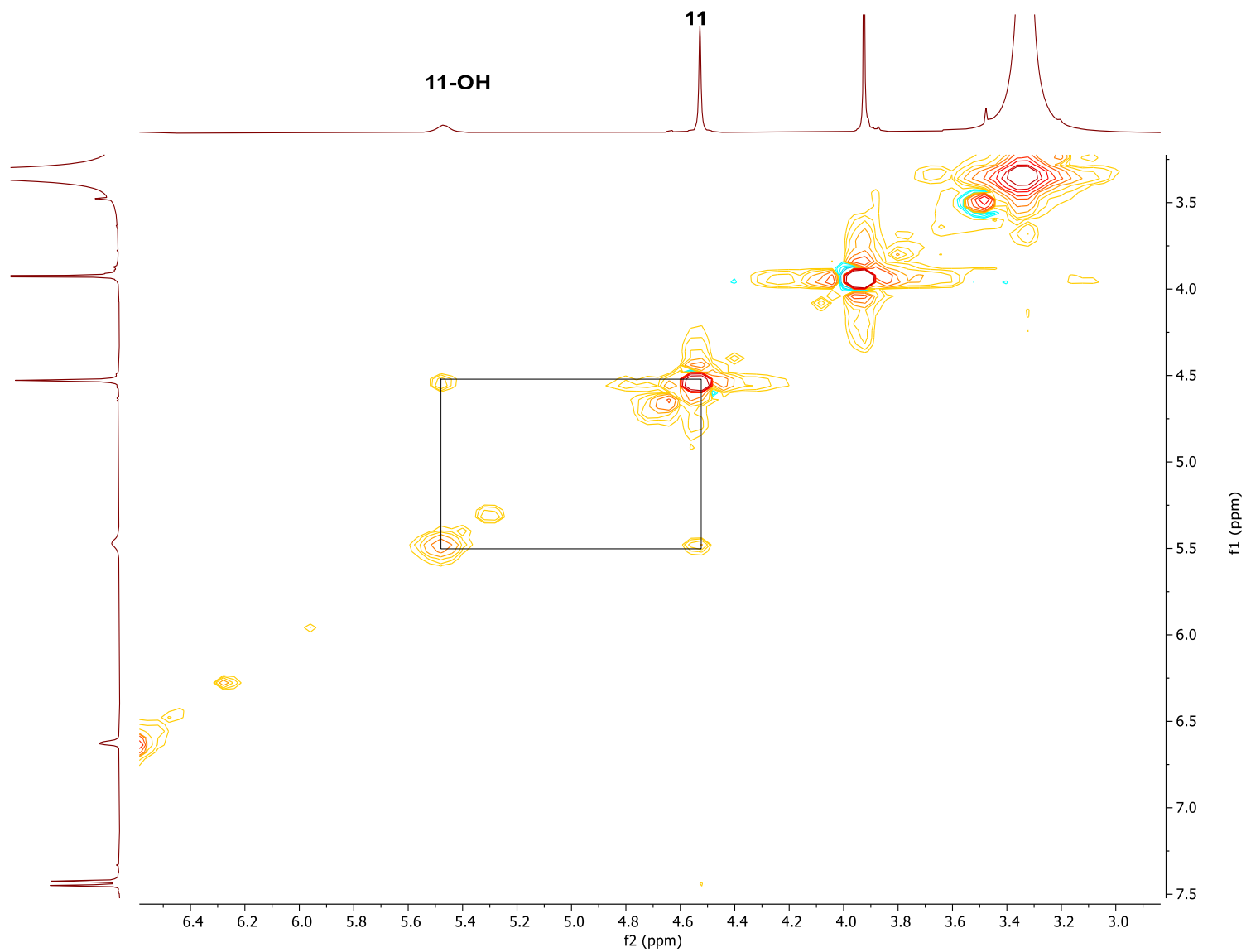


Figure S 40: COSY spectrum of compound **6**.

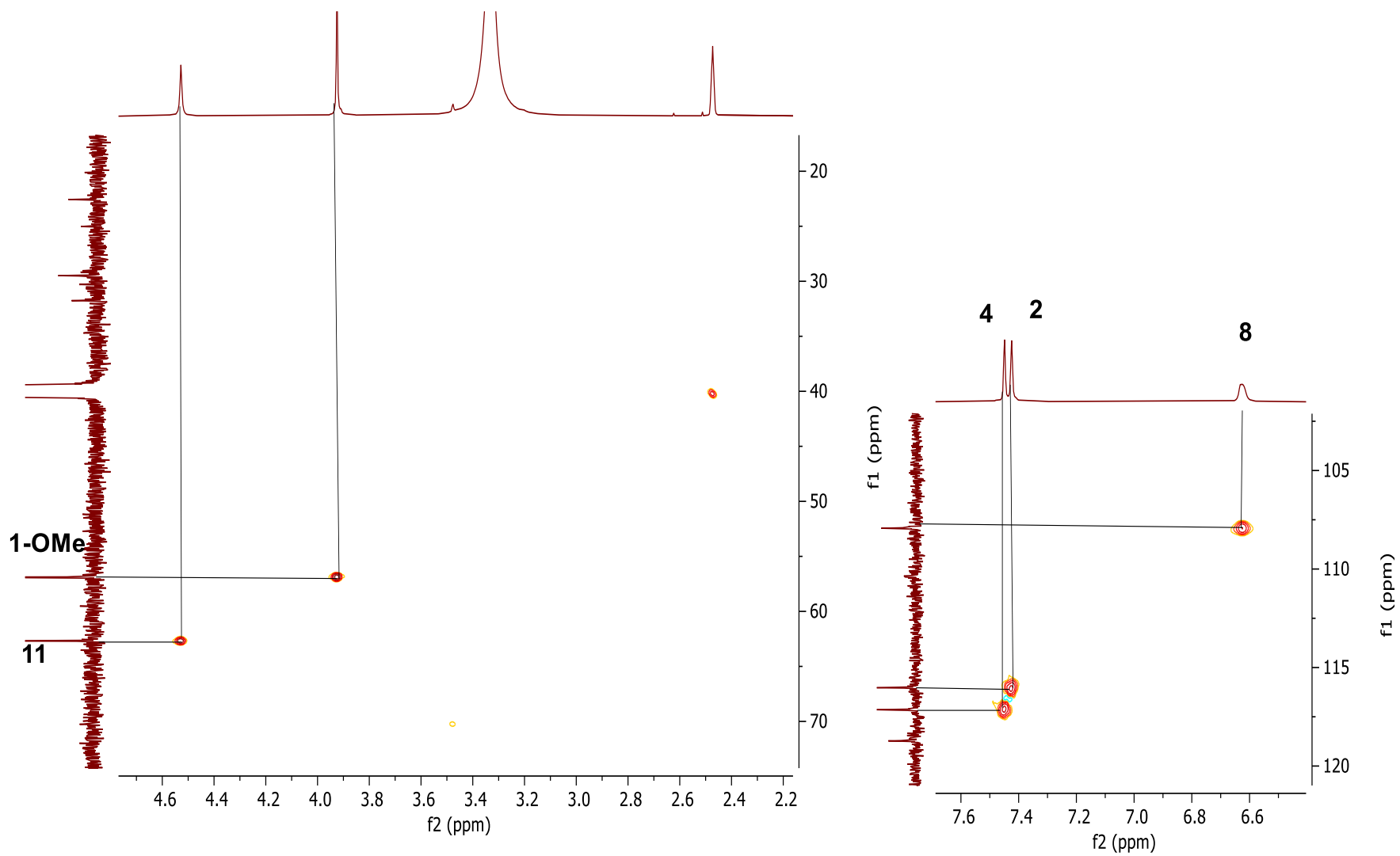


Figure S 41: HSQC spectrum of compound **6**.

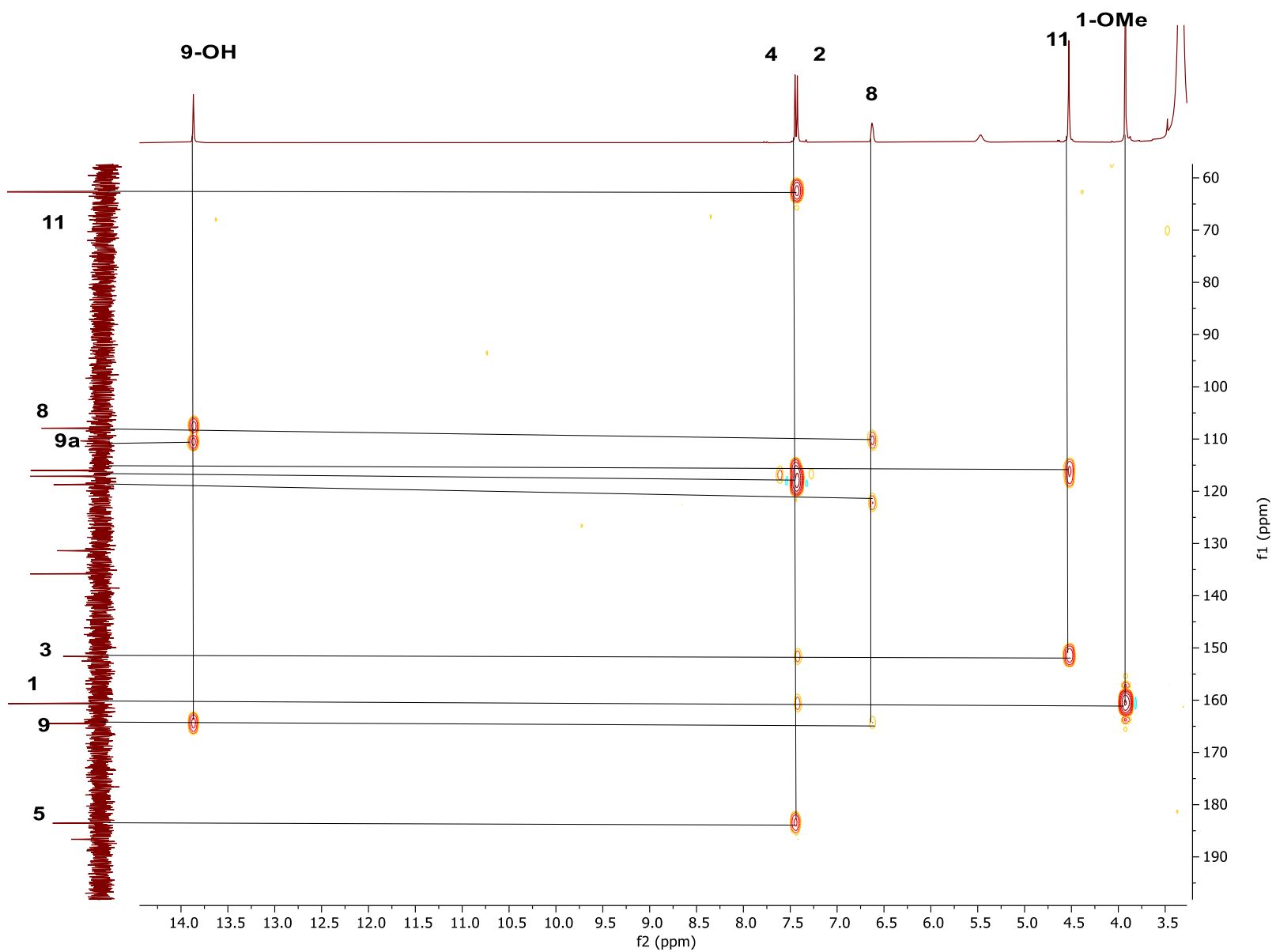


Figure S 42: HMBC spectrum of compound 6.

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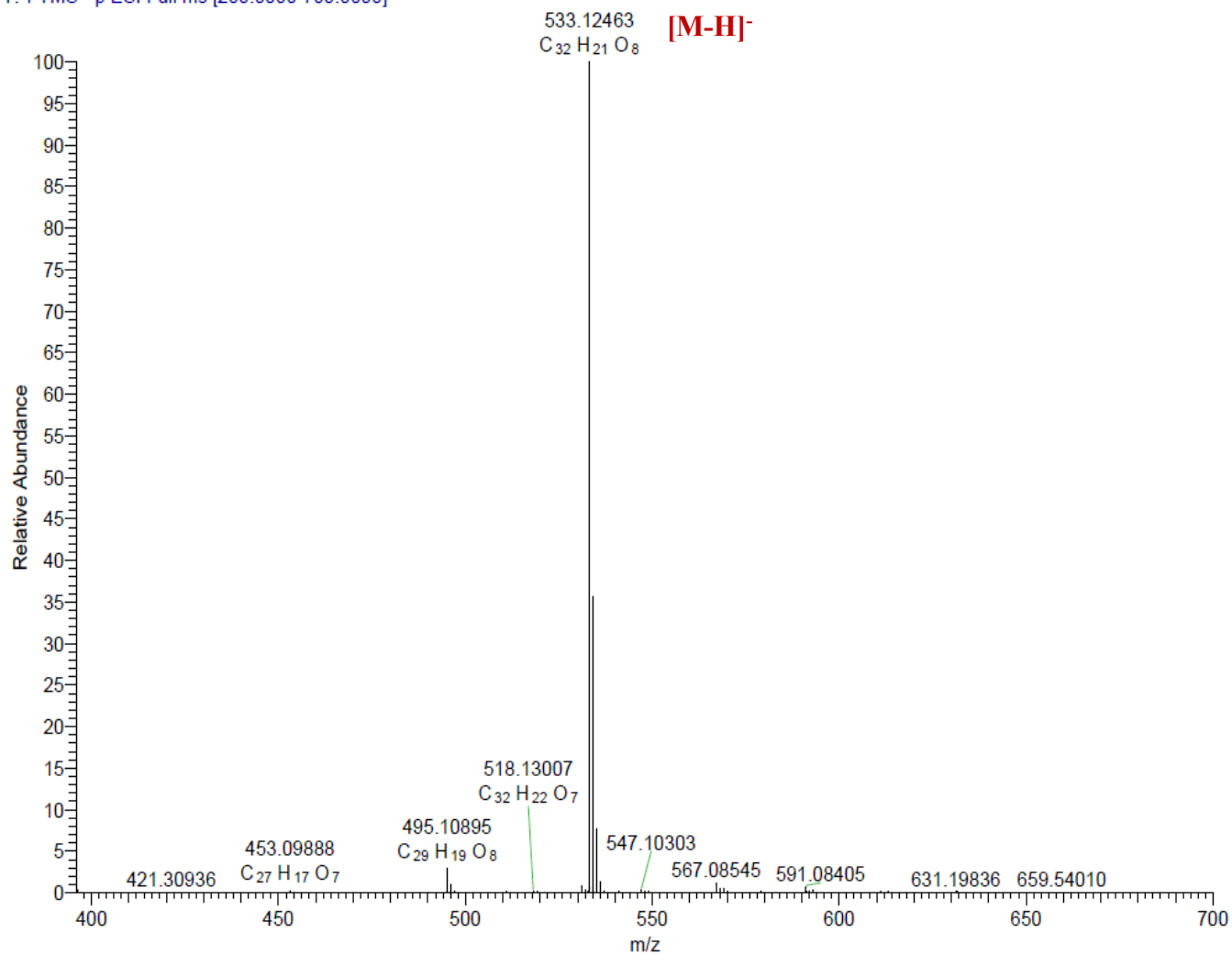


Figure S 44: HR-ESI-MS spectrum of compound 7 (negative mode).

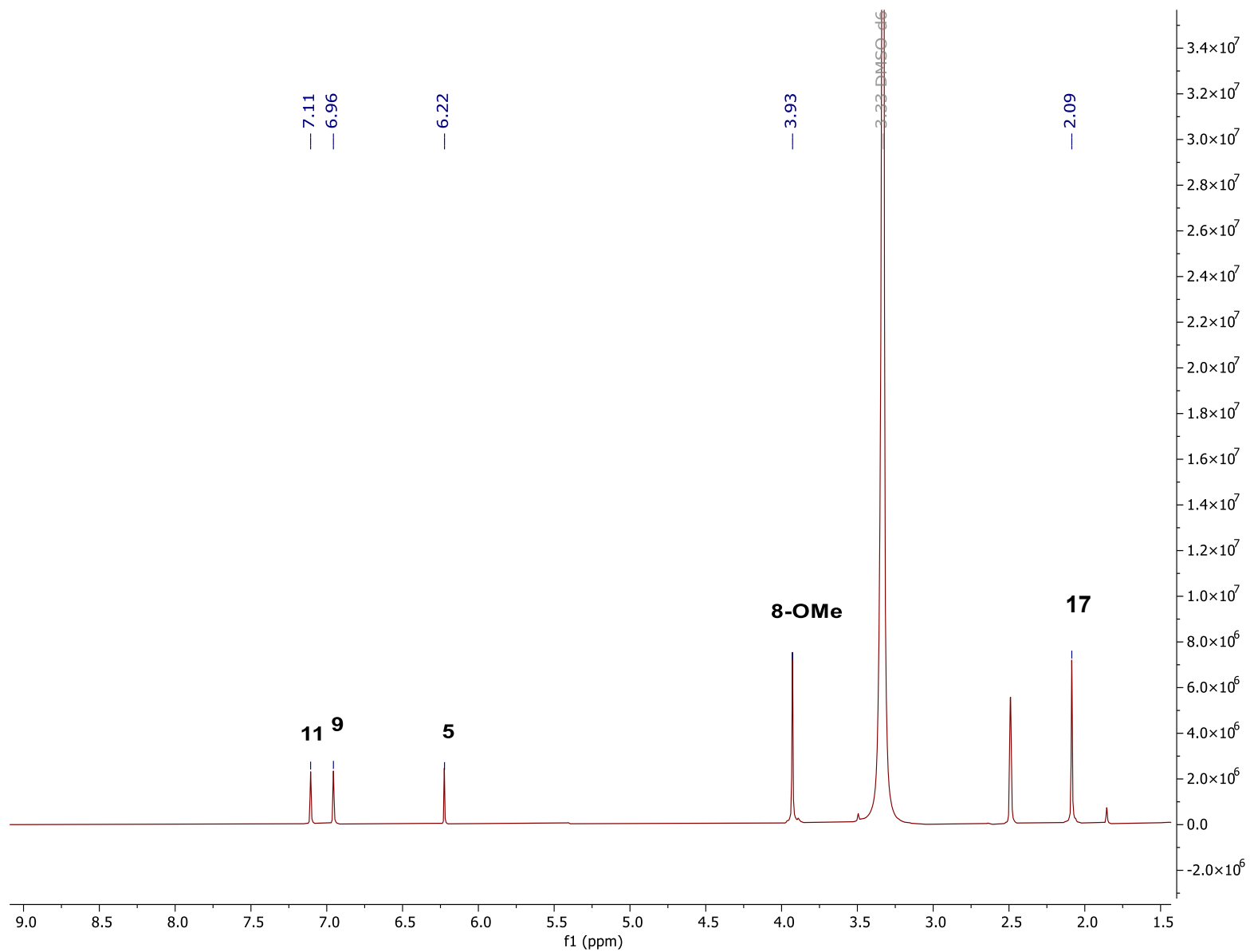


Figure S 45: ^1H NMR spectrum of compound 7 (in DMSO-d_6 , ^1H : 500 MHz).

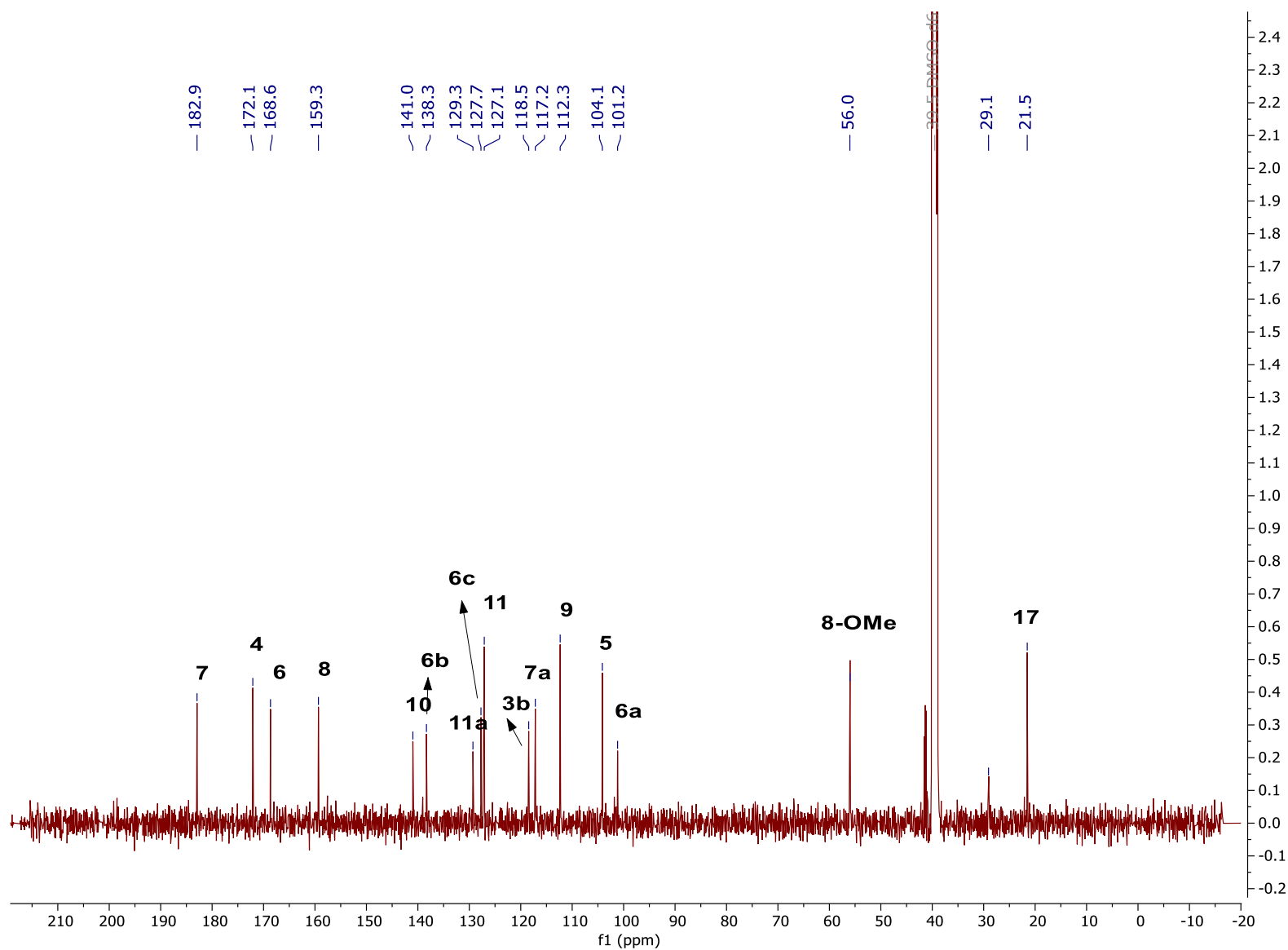


Figure S 46: ^{13}C NMR spectrum of compound 7 (in DMSO-d_6 , ^{13}C :125 MHz).

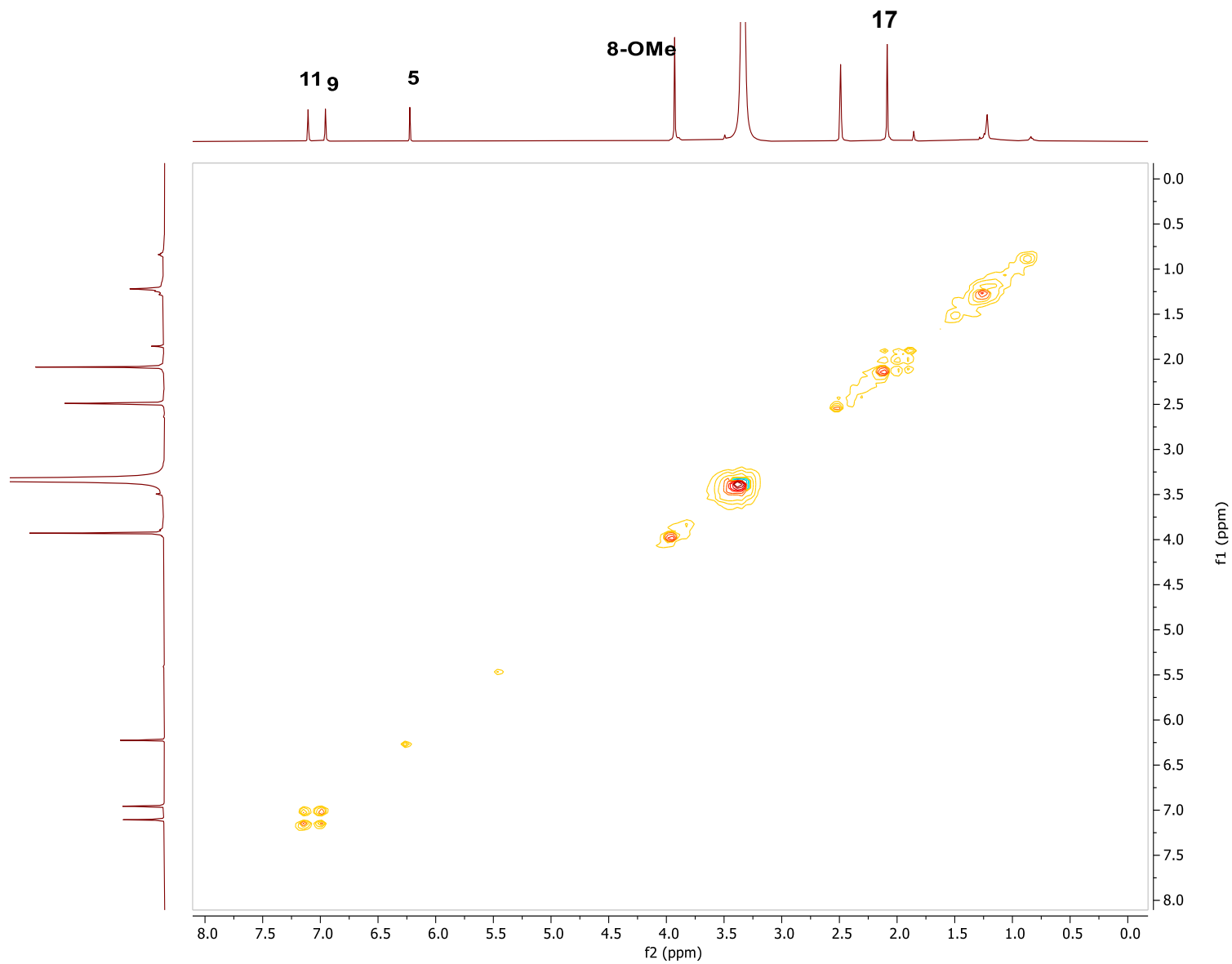


Figure S 47: COSY spectrum of compound 7.

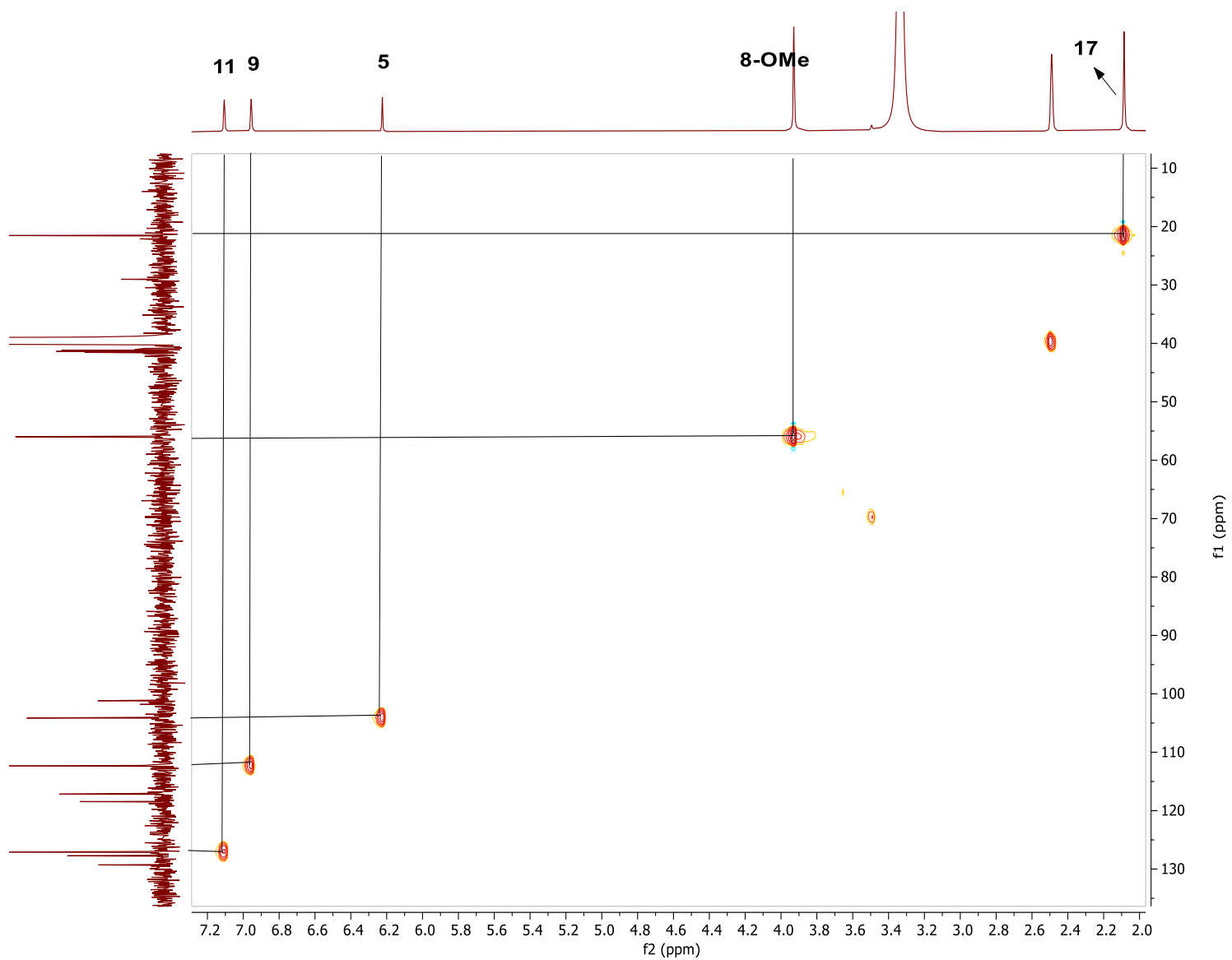


Figure S 48: HSQC spectrum of compound 7.

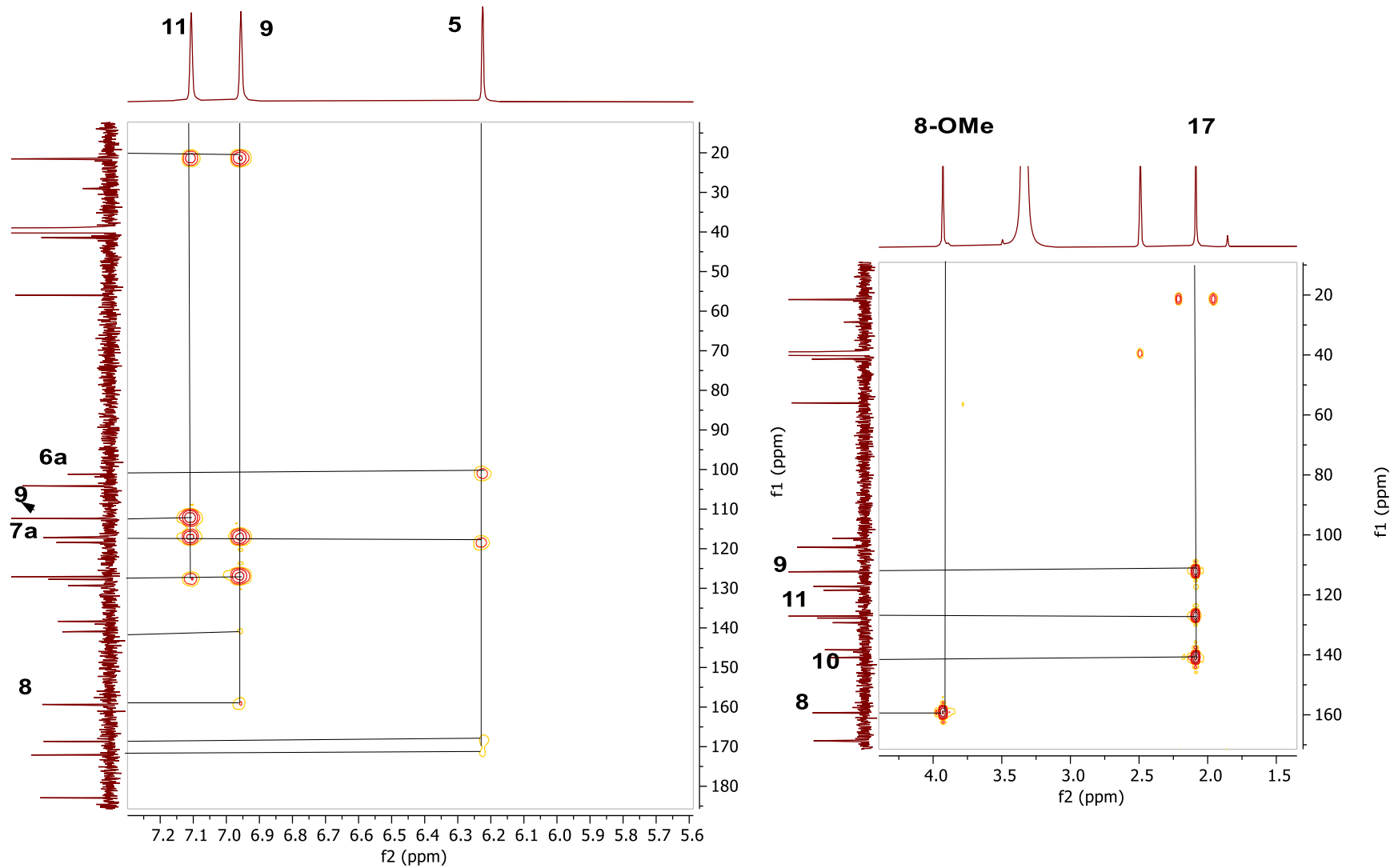


Figure S 49: HMBC spectrum of compound 7.

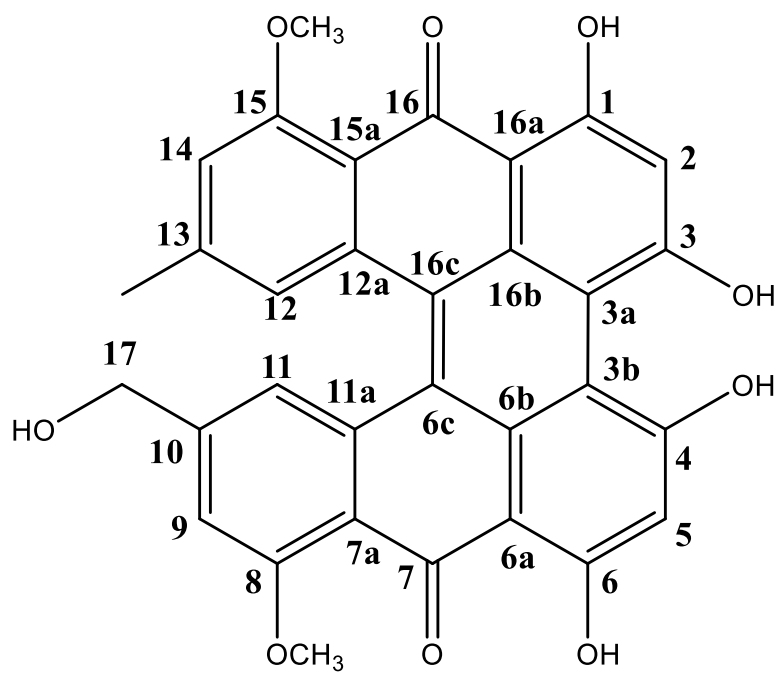


Figure S 50: Chemical structure of compound 8.

PREB-11-NEG #2 RT: 0.01 AV: 1 SM: 7G NL: 2.18E9
T: FTMS - p ESI Full ms [200.0000-700.0000]

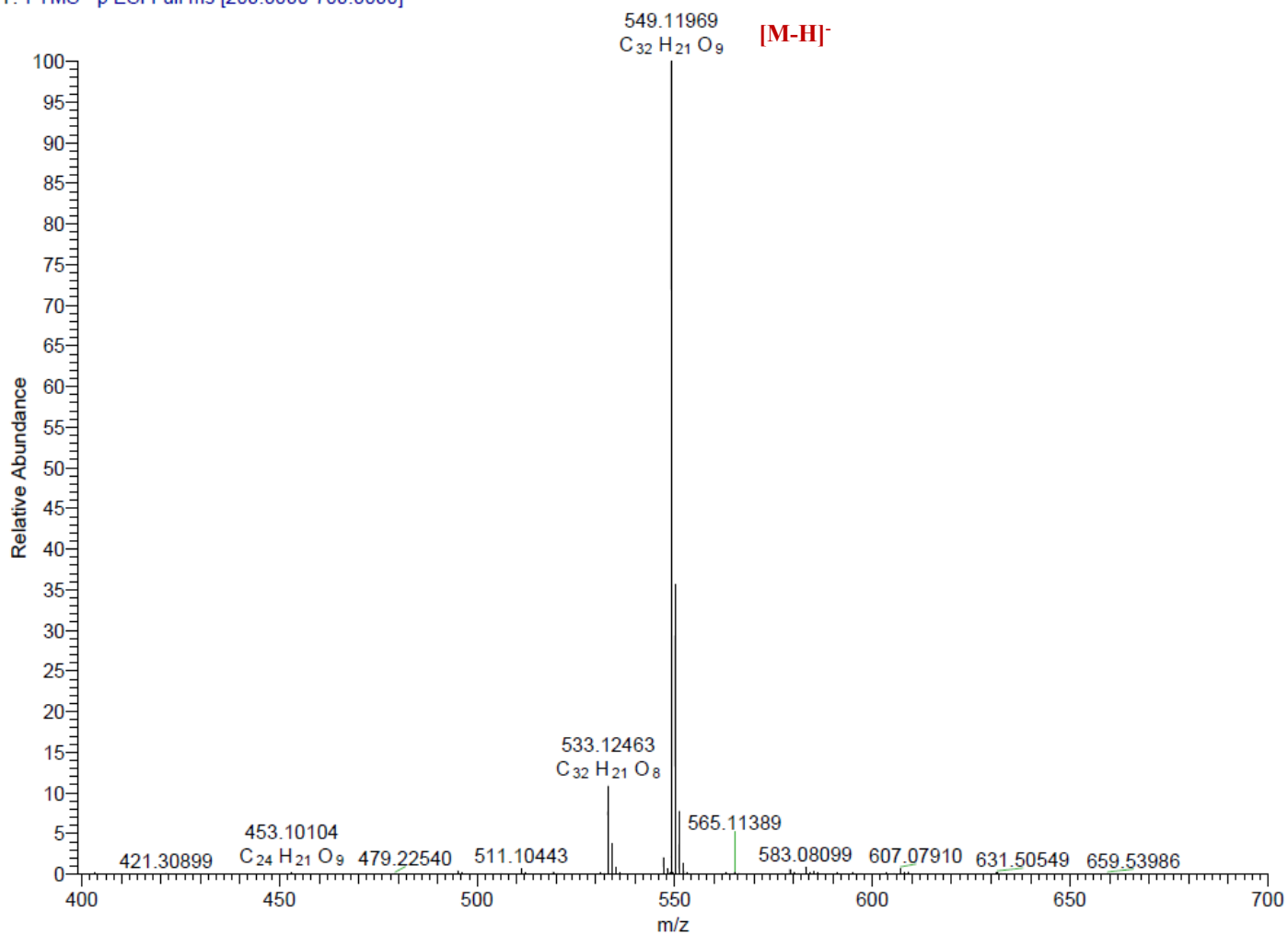


Figure S 51: HR-ESI-MS spectrum of compound **8** (negative mode).

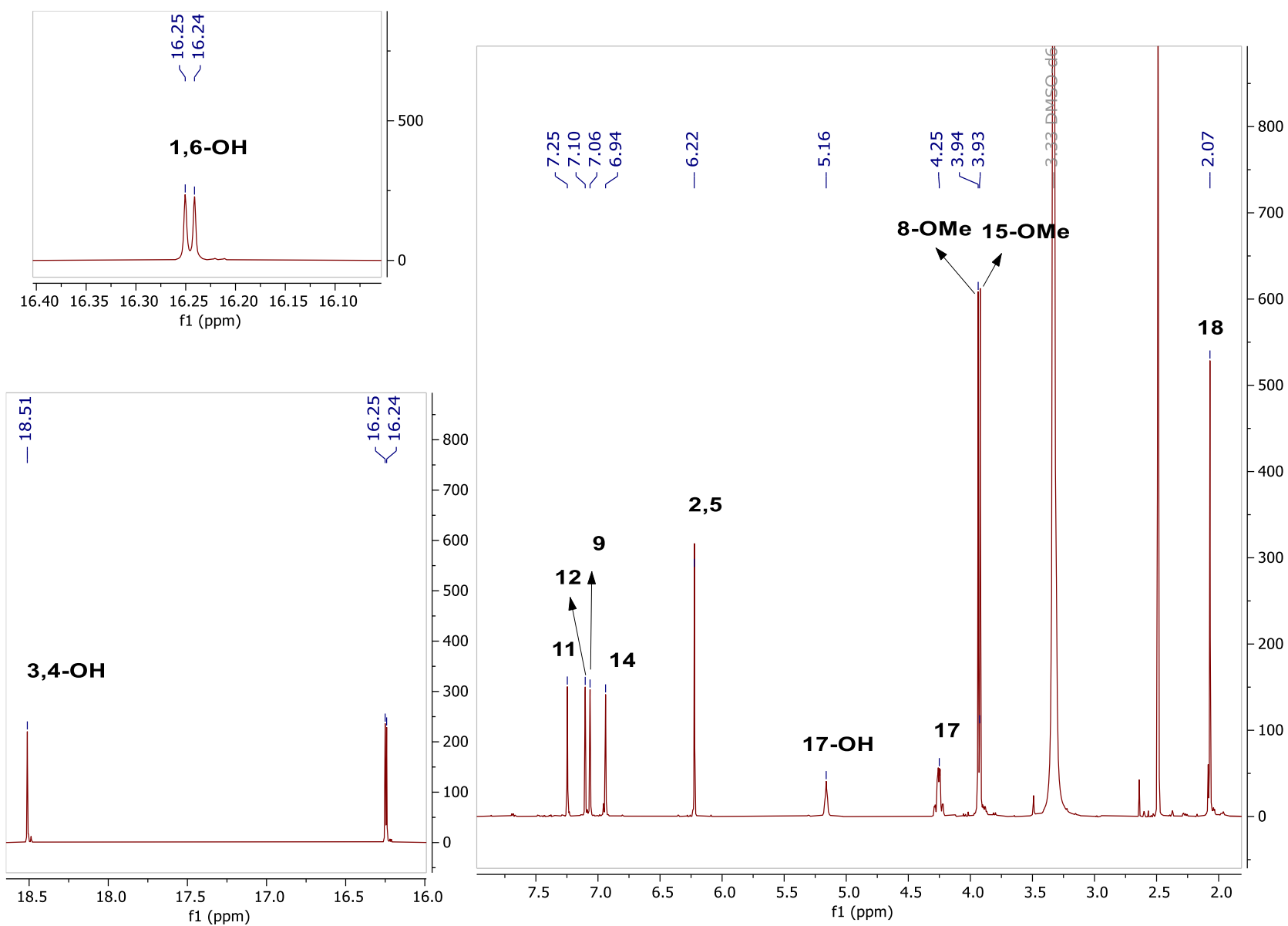


Figure S 52: ^1H NMR spectrum of compound **8** (in DMSO-d_6 , ^1H : 500 MHz).

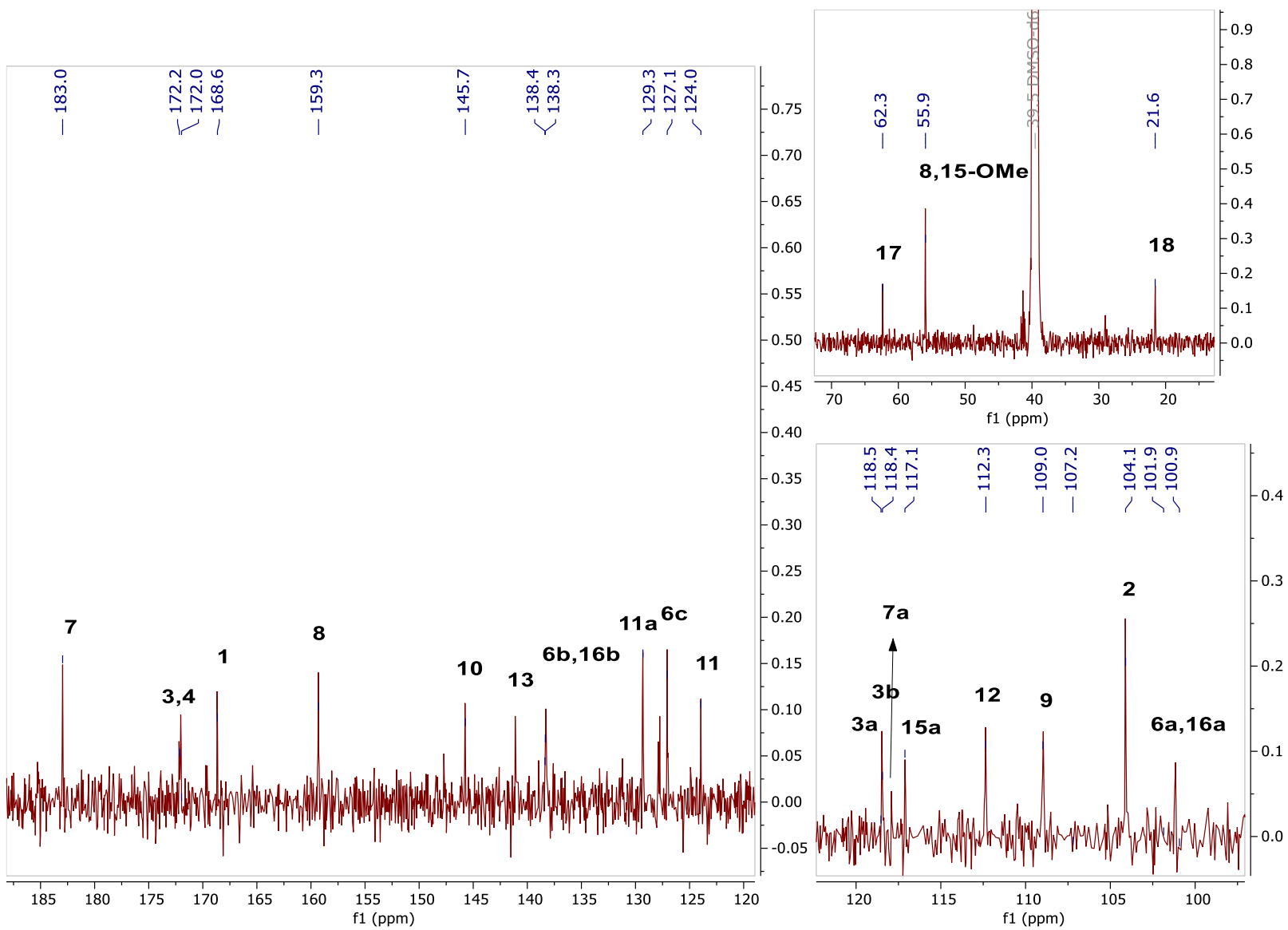


Figure S 53: ^{13}C NMR spectrum of compound **8** (in DMSO-d_6 , ^{13}C :125 MHz).

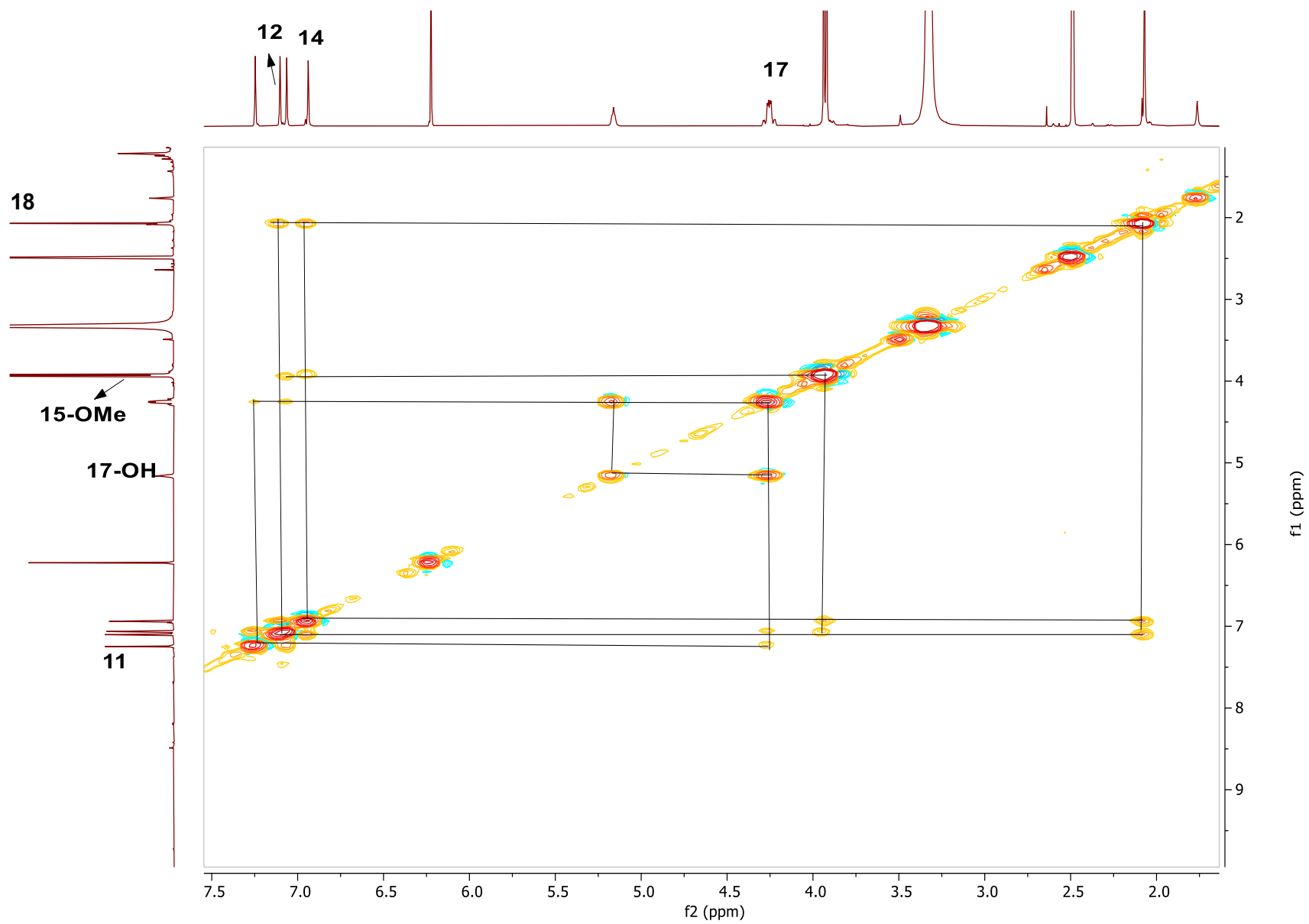


Figure S 54: COSY spectrum of compound **8**.

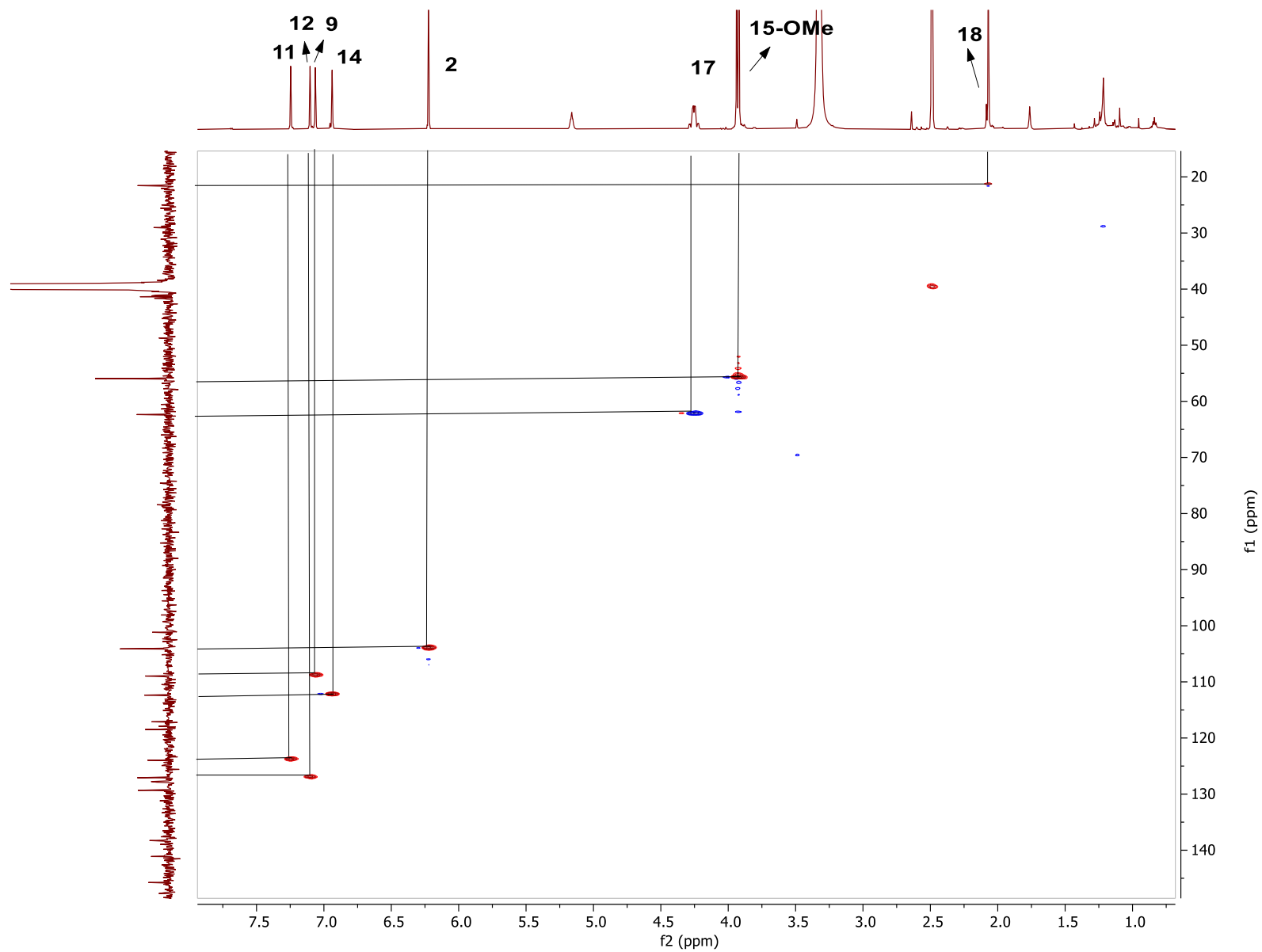


Figure S 55: HSQC spectrum of compound **8**.

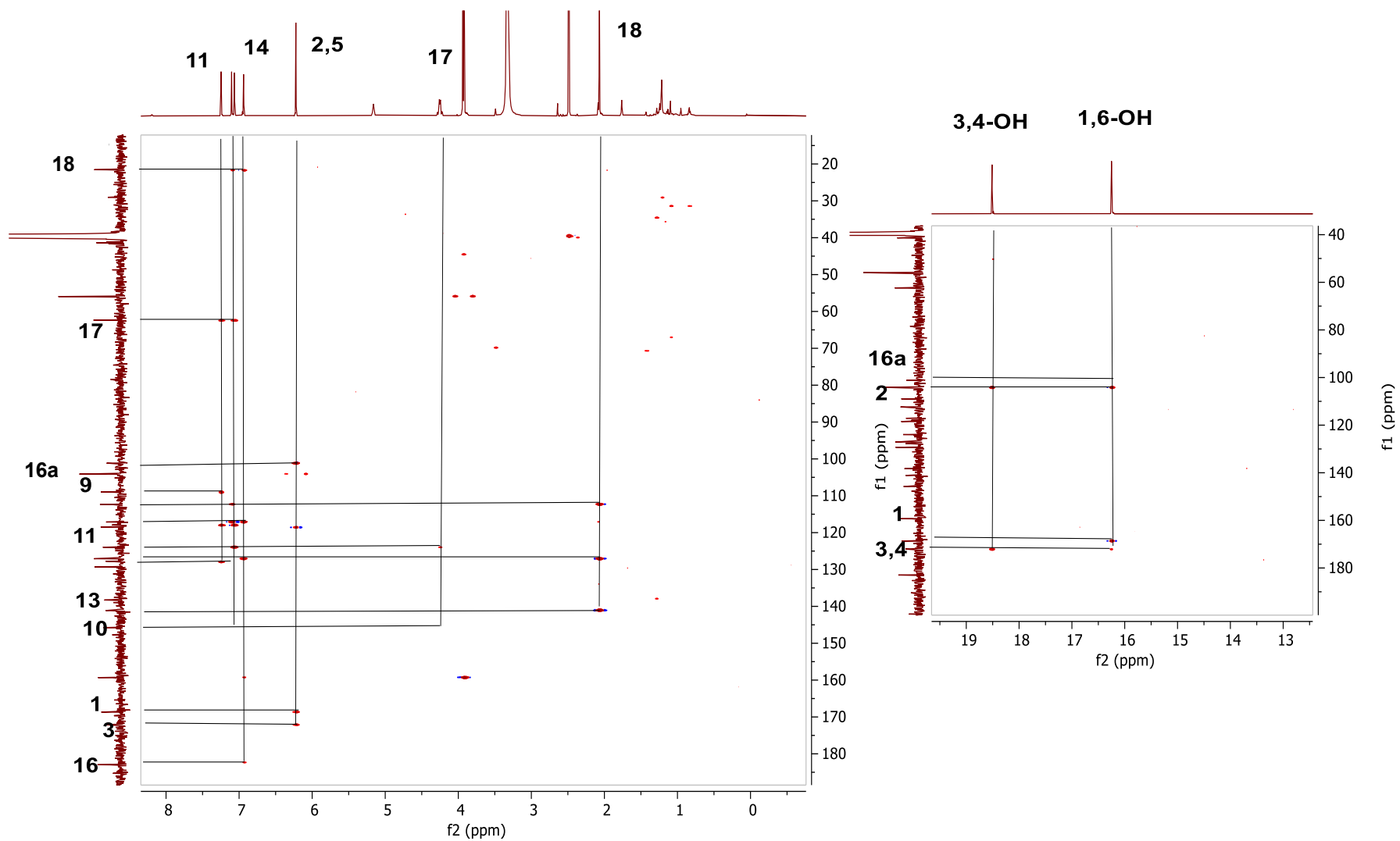


Figure S 56: HMBC spectrum of compound **8**.

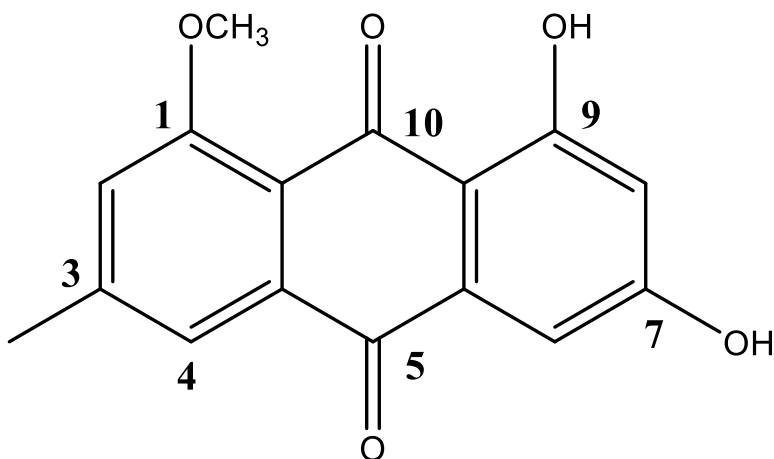


Figure S 57: Chemical structure of compound **9**.

Table S 4: ^1H 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)

^aChemical shifts were measured at 500 MHz in DMSO- d_6

^bChemical shifts were measured at 125 MHz in DMSO- d_6

PREB-17-NEG #3 RT: 0.02 AV: 1 SM: 7G NL: 9.53E8
T: FTMS - p ESI Full ms [200.0000-700.0000]

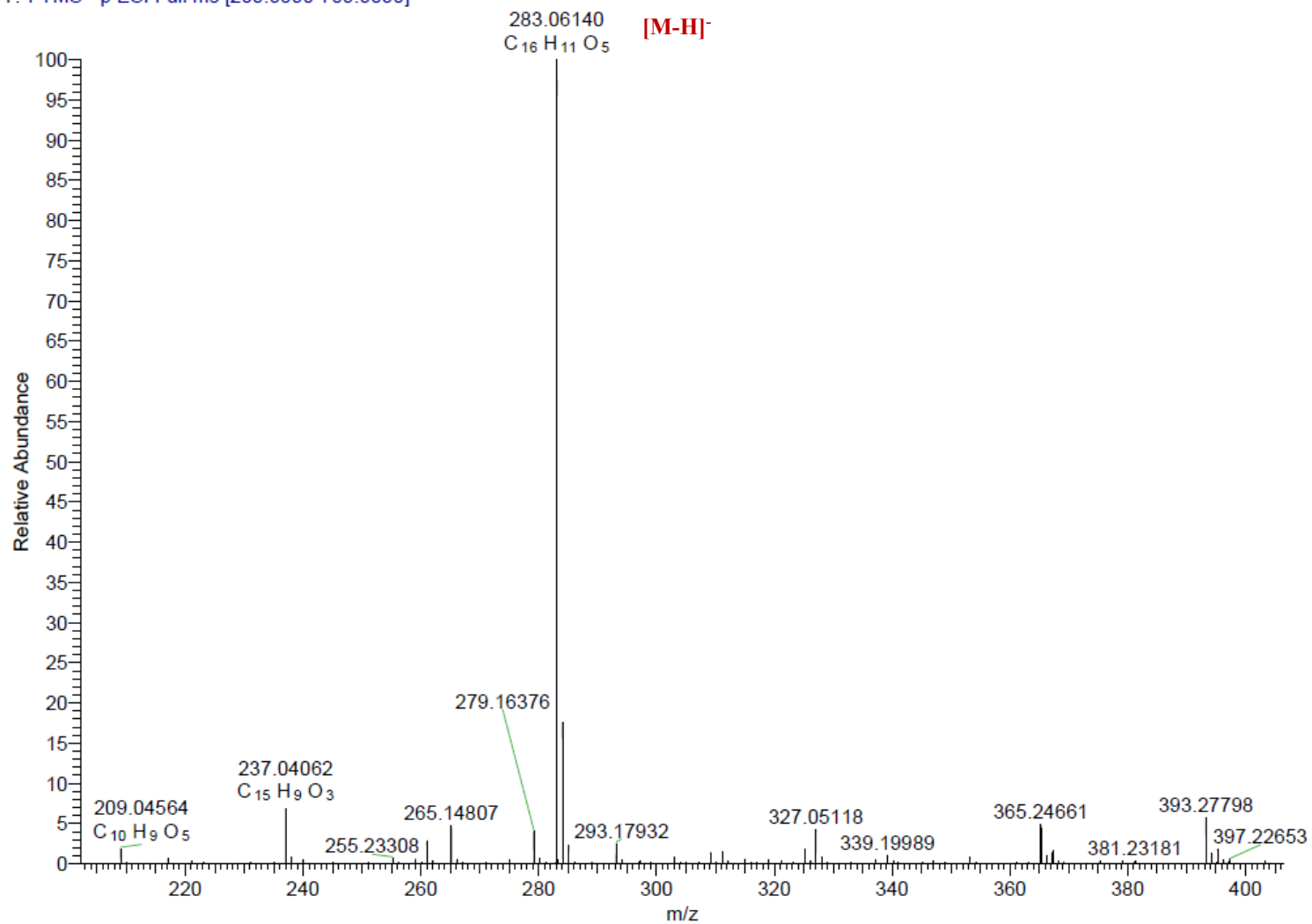


Figure S 58: HR-ESI-MS spectrum of compound **9** (positive mode).

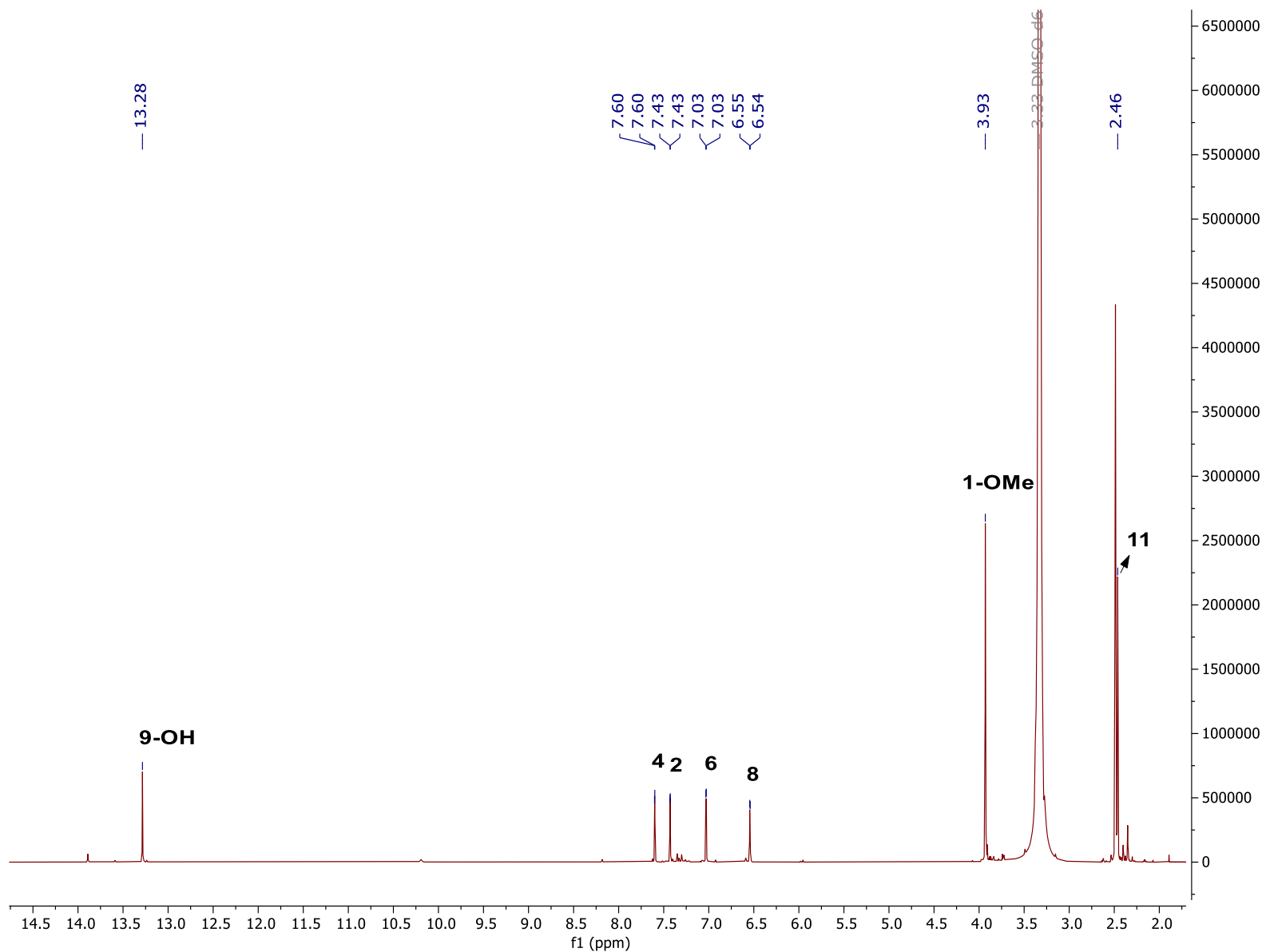


Figure S 59: ^1H NMR spectrum of compound **9** (in DMSO-d_6 , ^1H : 500 MHz).

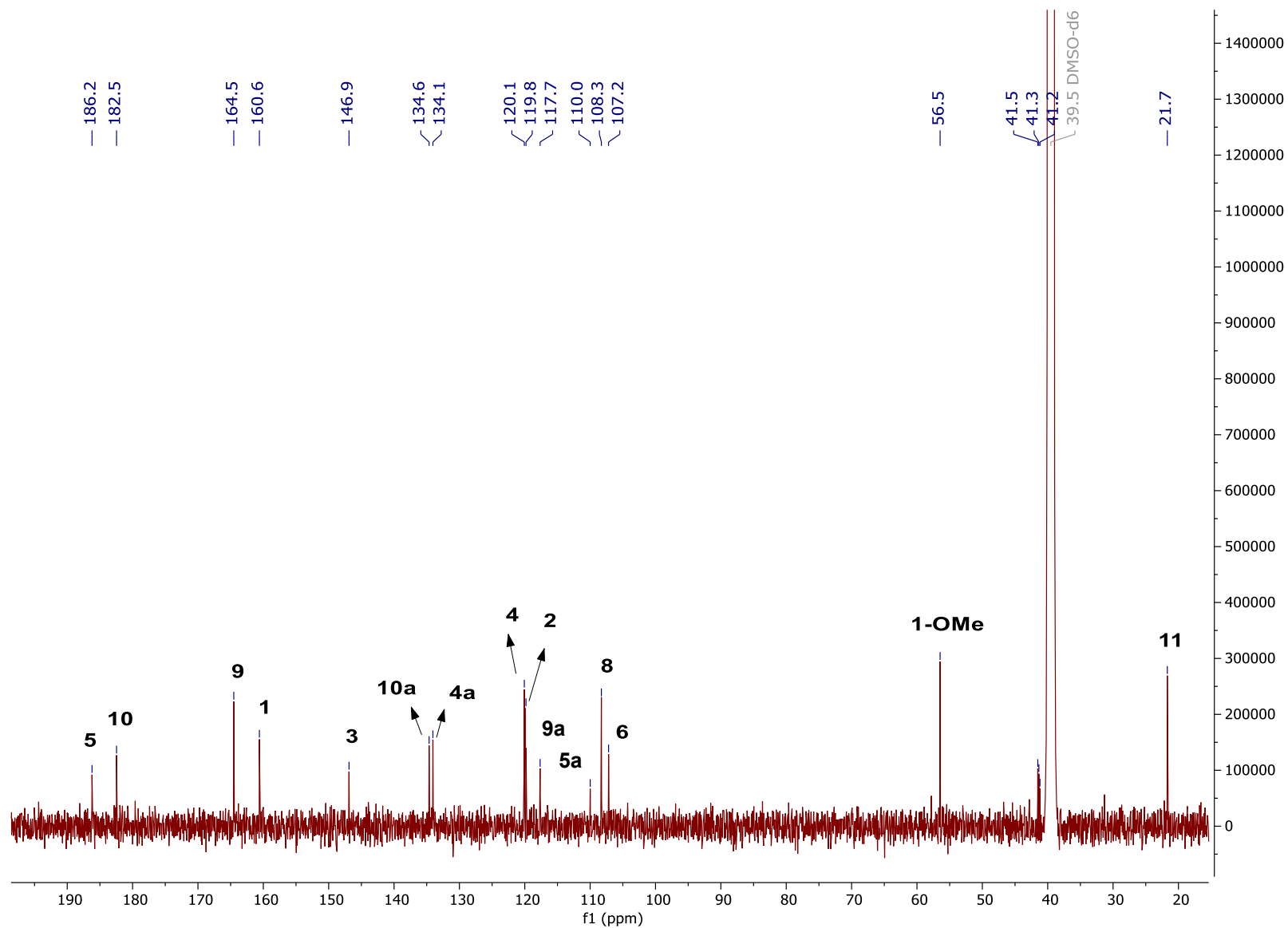


Figure S 60: ^{13}C NMR spectrum of compound **9** (in DMSO- d_6 , ^{13}C :125 MHz).

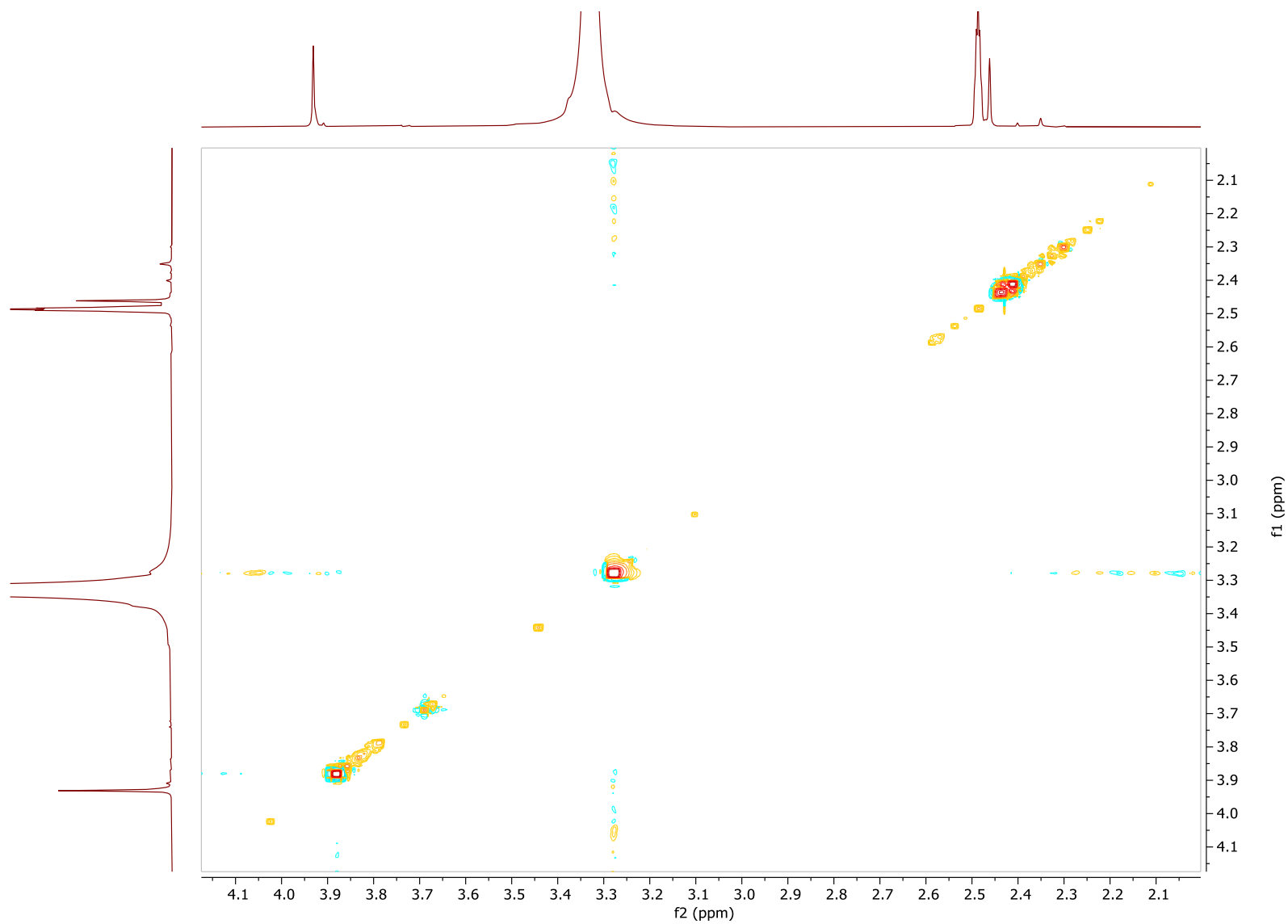


Figure S 61: COSY spectrum of compound **9**.

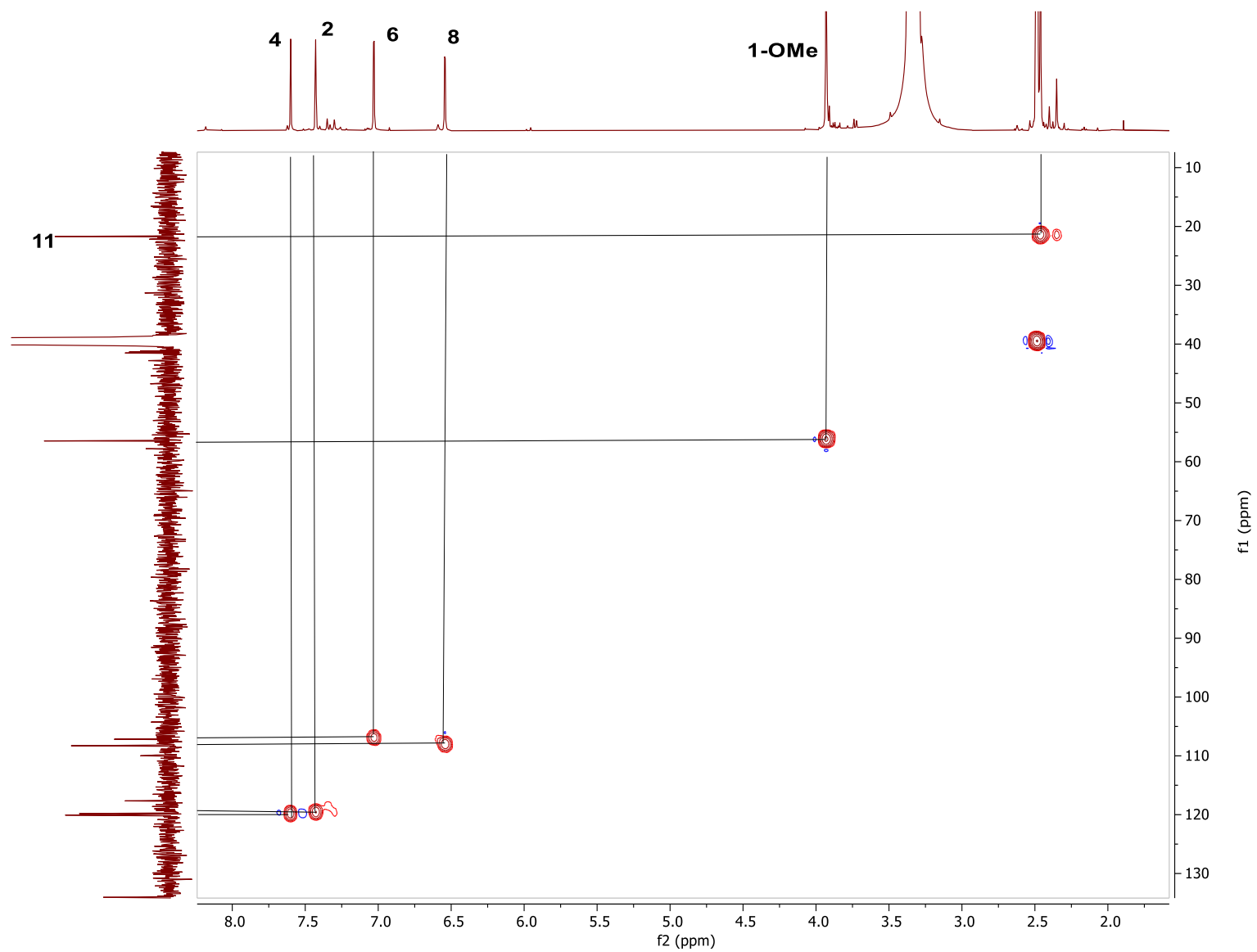


Figure S 62: HSQC spectrum of compound 9.

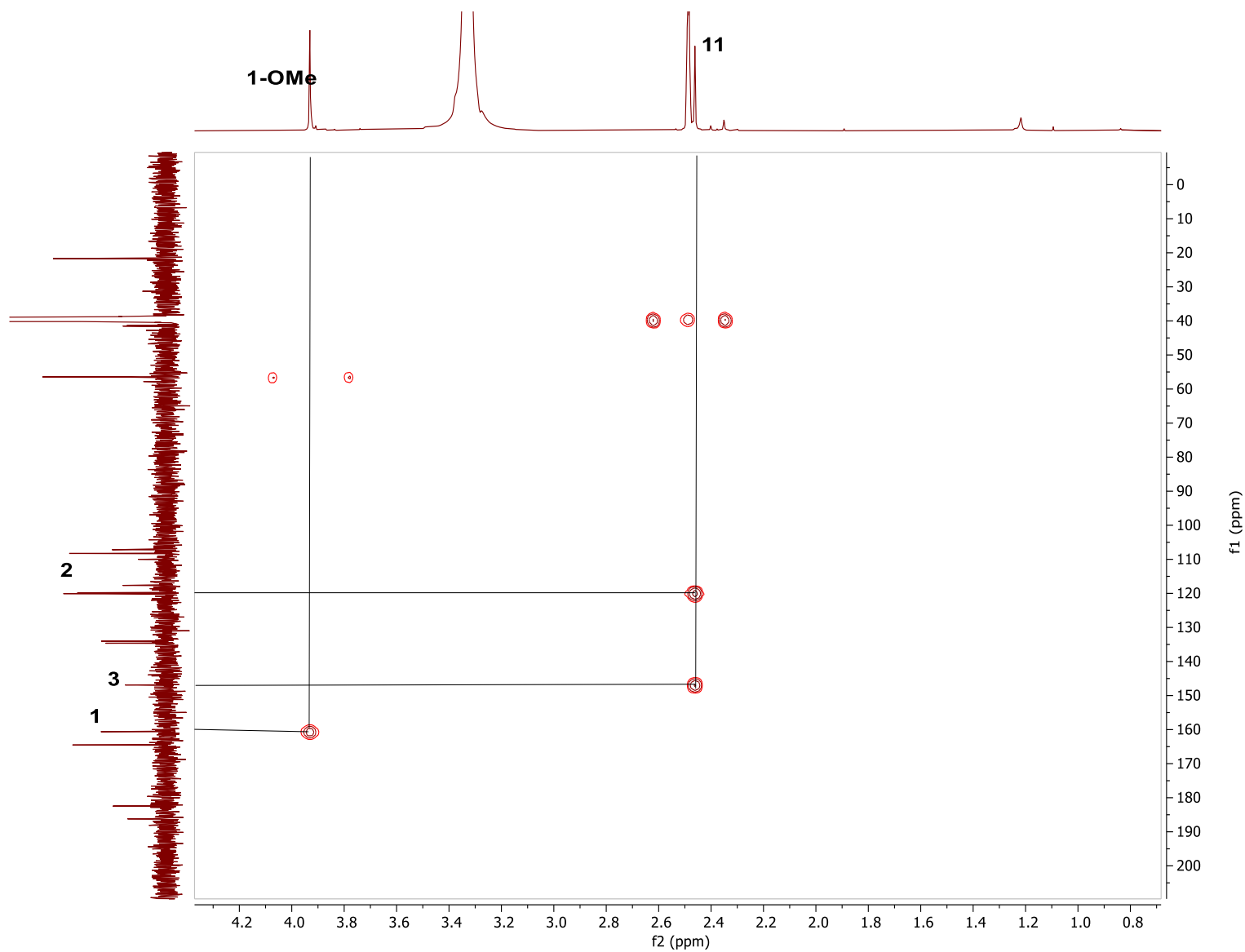


Figure S 63: HMBC spectrum of compound **9**.