Structures of the Largest Amphidinol Homologues from the Dinoflagellate *Amphidinium carterae* and Structure-Activity Relationships

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Supporting Information

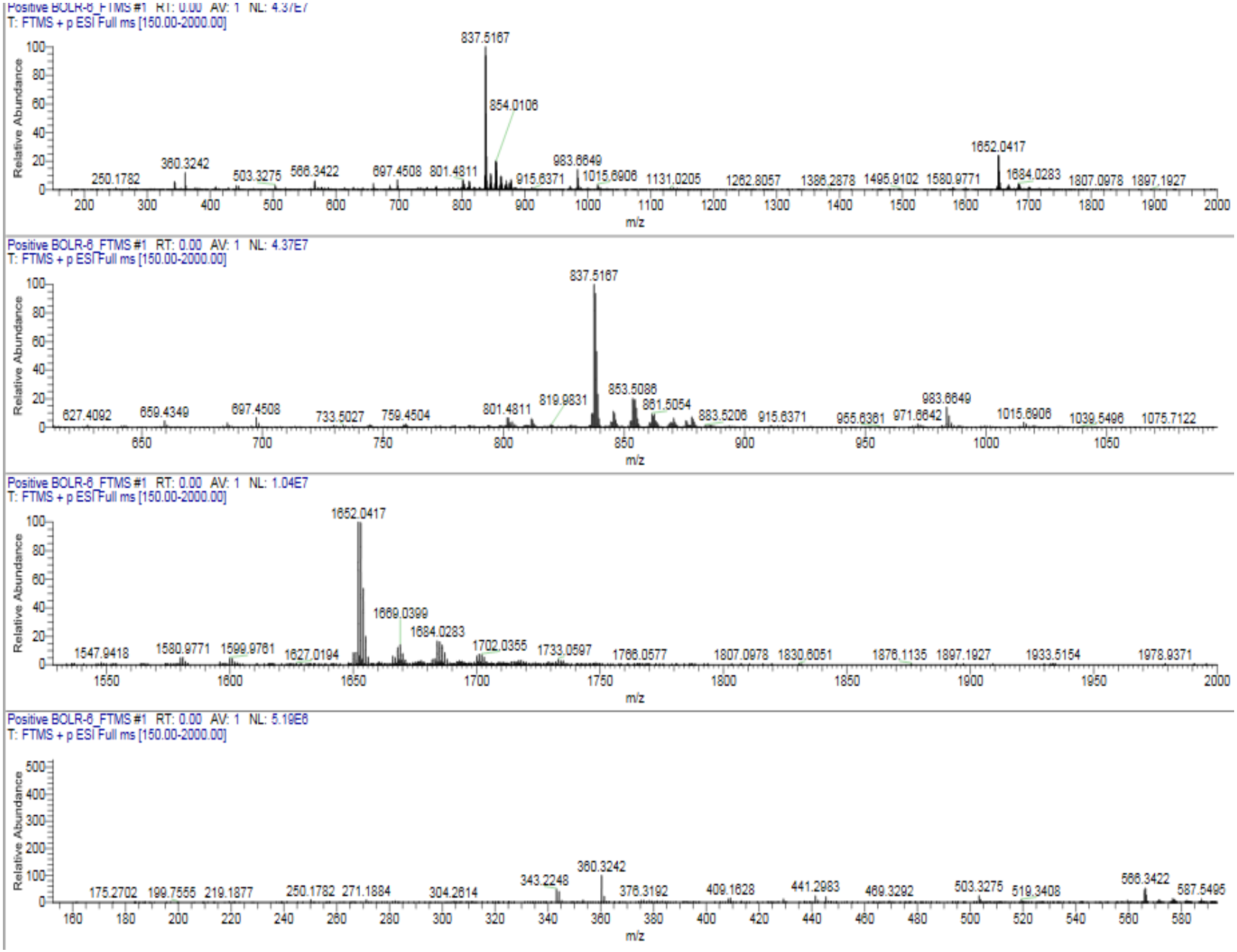


Figure S1. ESI MS of **1** (pos**itive m**ode)

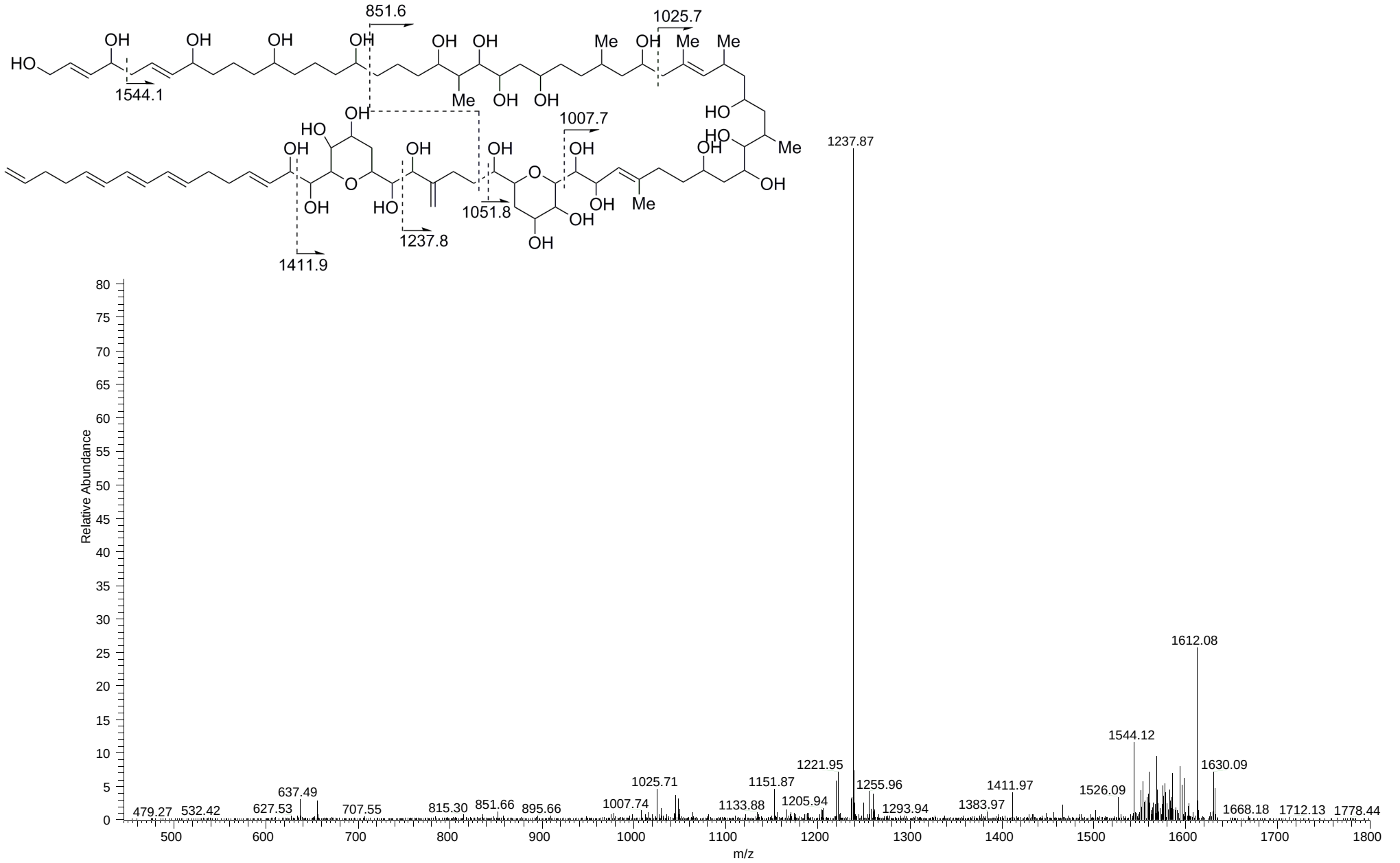


Figure S2. ESI MS/MS (positive) of 1 on the proton adduct ion $[M+H]^+$

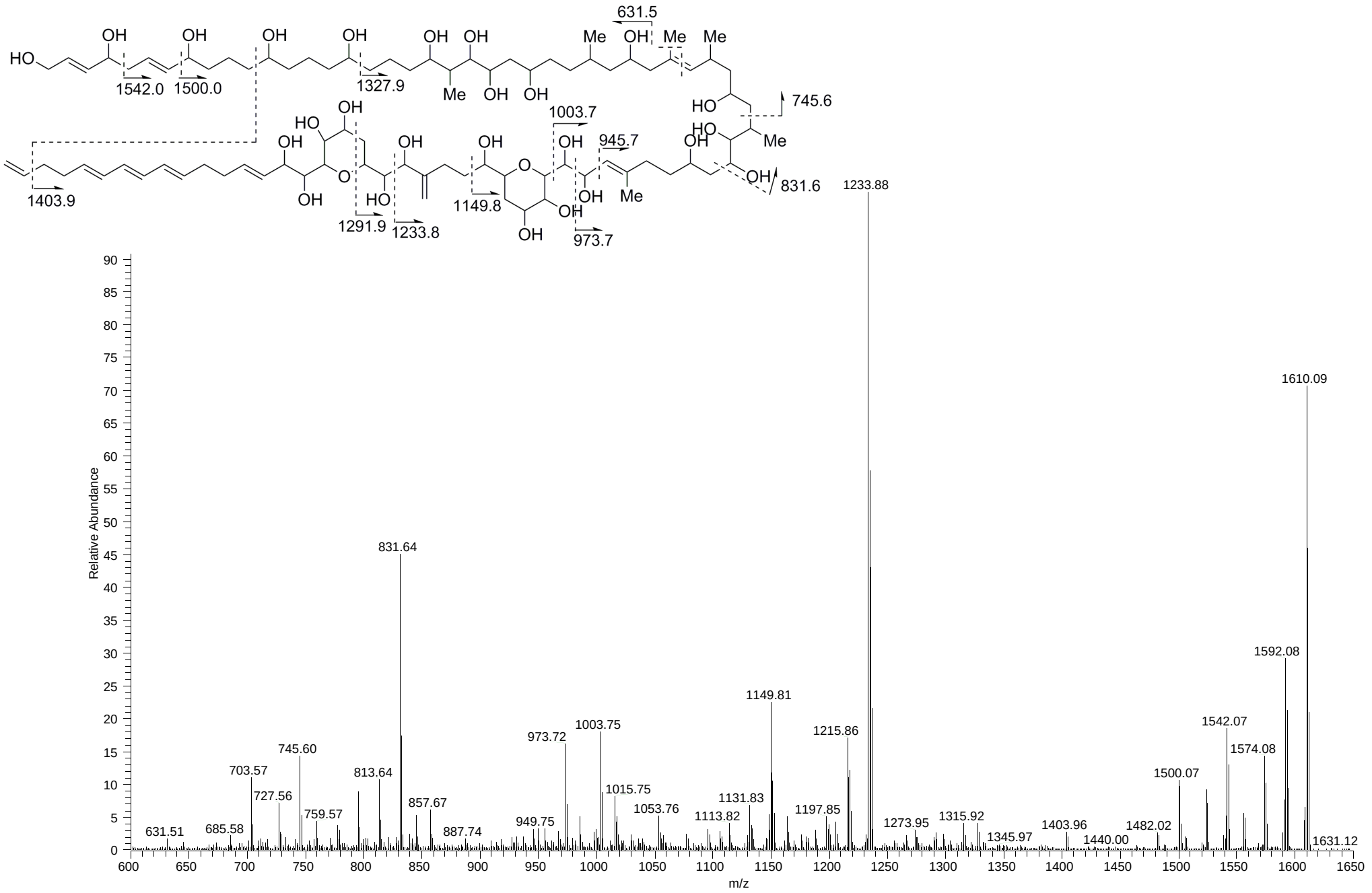


Figure S3. ESI MS/MS (negative) of 1 on the deprotonated ion $[M-H]^-$

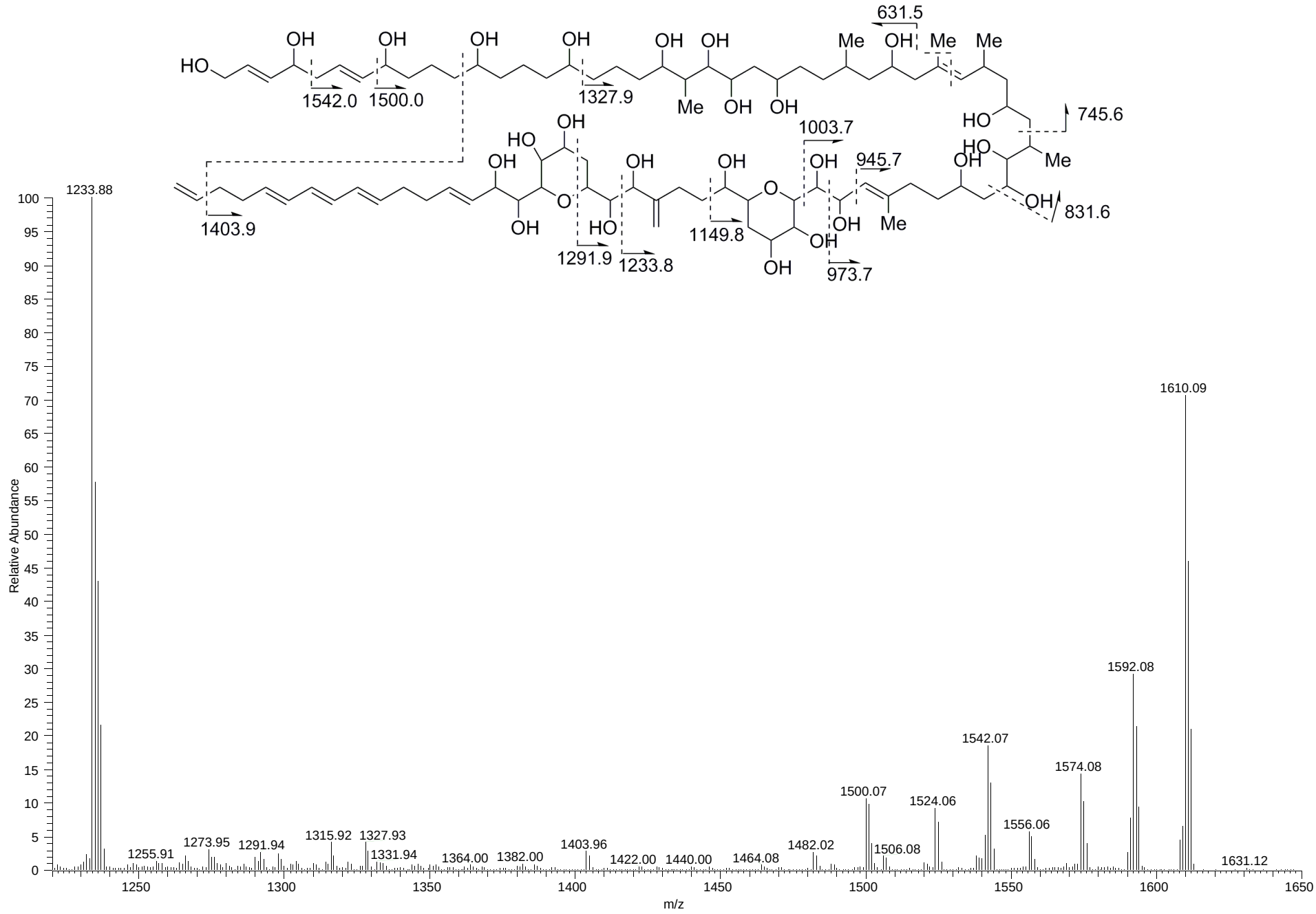


Figure S4 ESI MS/MS (negative) of **1** on the deprotonated ion $[M-H]^-$

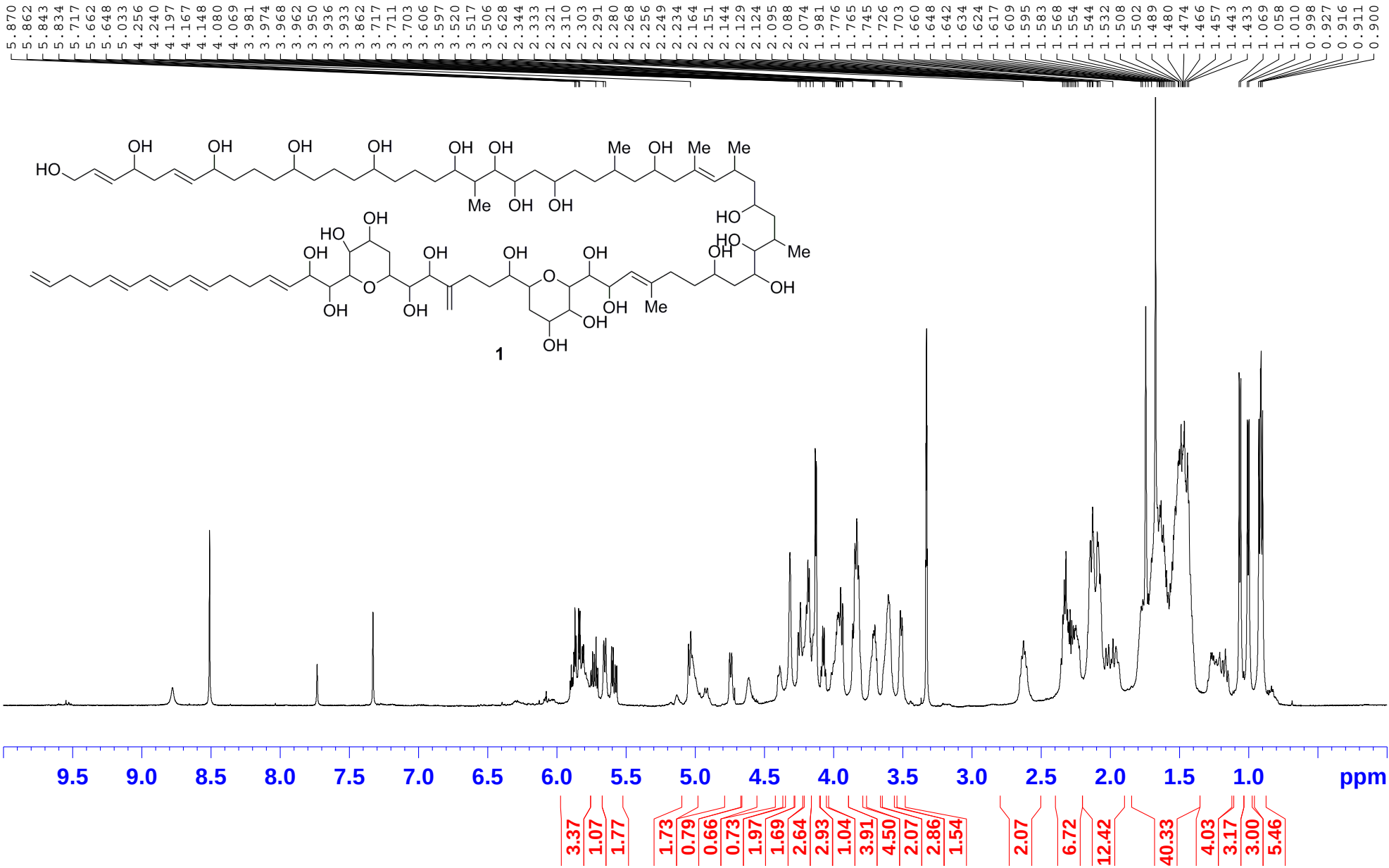


Figure S5. ^{1}H NMR spectrum of **1** in CD_3OD-C_5D_5N (2:1), 600 MHz.

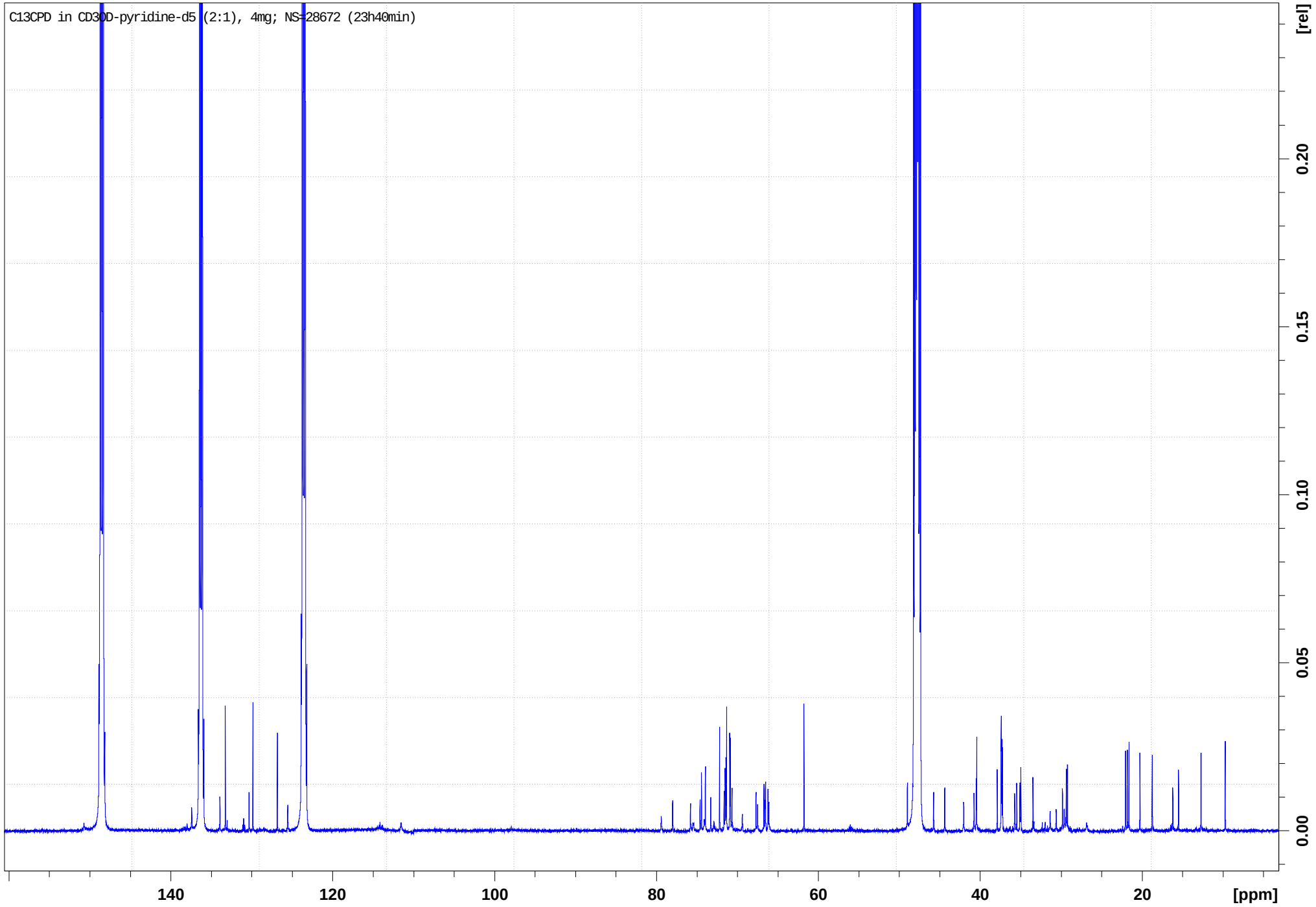


Figure S6. ^{13}C NMR spectrum of **1** in CD_3OD-C_5D_5N (2:1), 150 MHz.

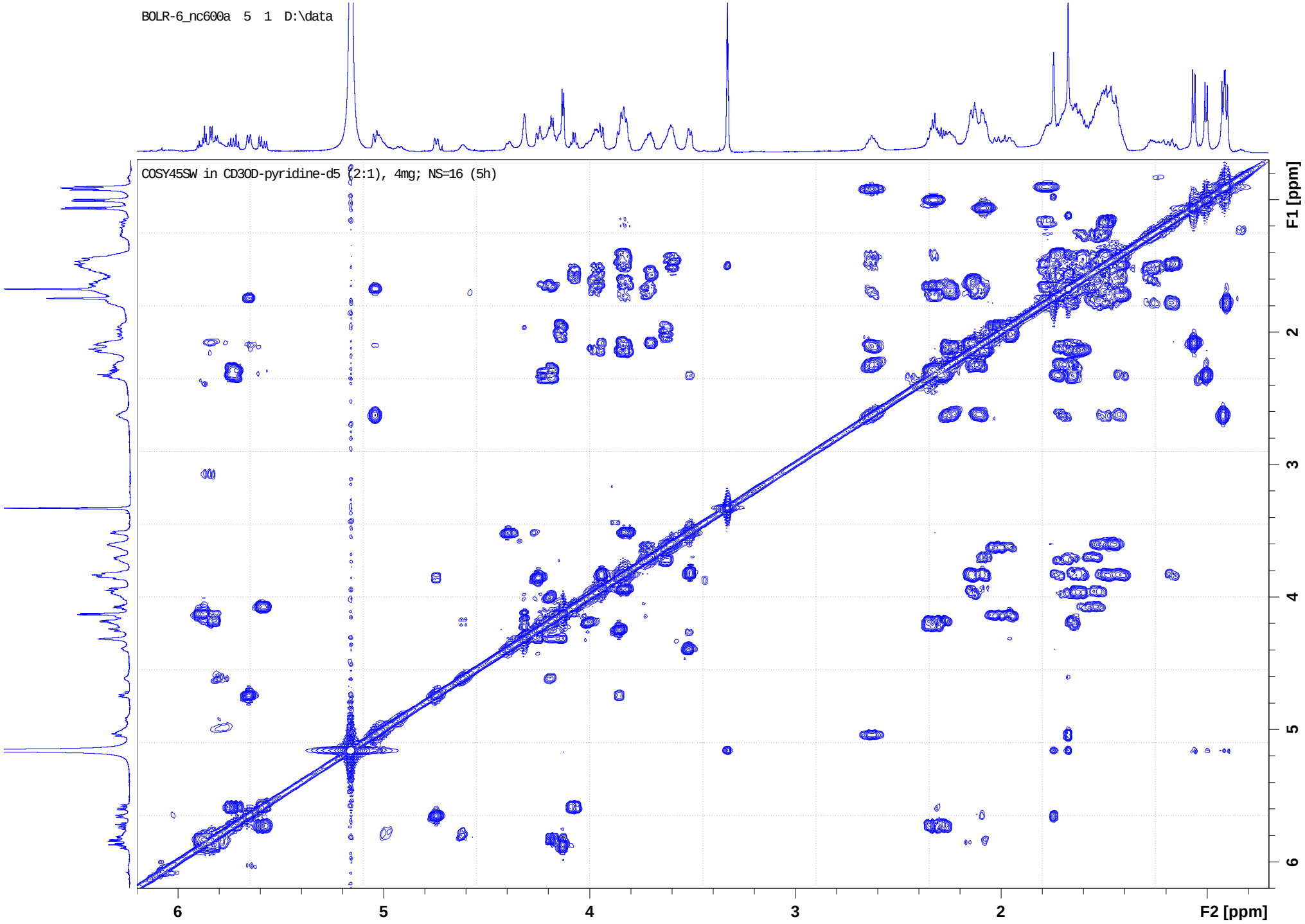


Figure S7. ^{1}H-^{1}H COSY spectrum of **1** in CD_3OD-C_5D_5N (2:1), 600 MHz.

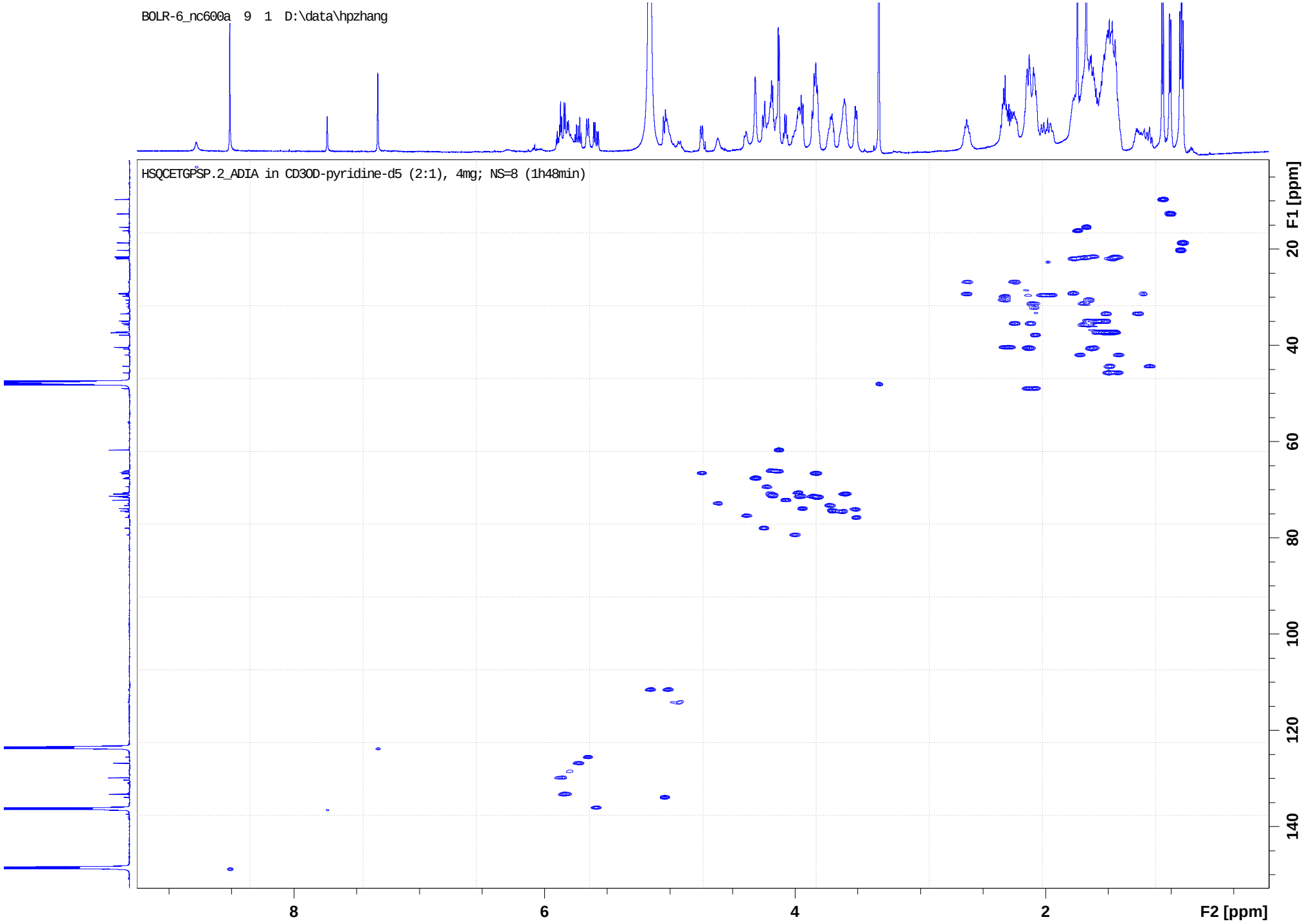


Figure S8. HSQC spectrum of **1** in CD_3OD-C_5D_5N (2:1), 600 MHz.

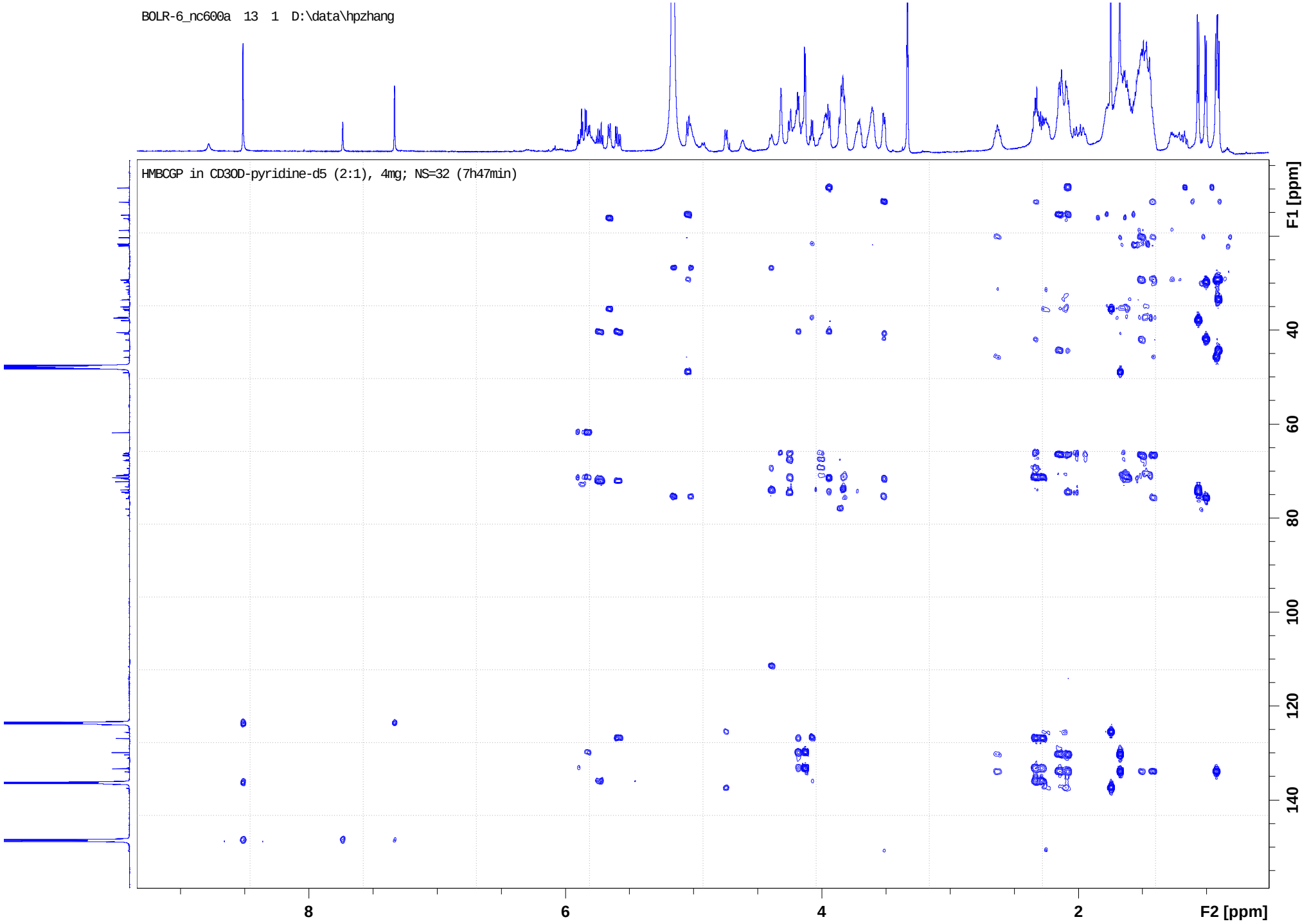


Figure S9. HMBC spectrum of **1** in CD_3OD-C_5D_5N (2:1), 600 MHz.

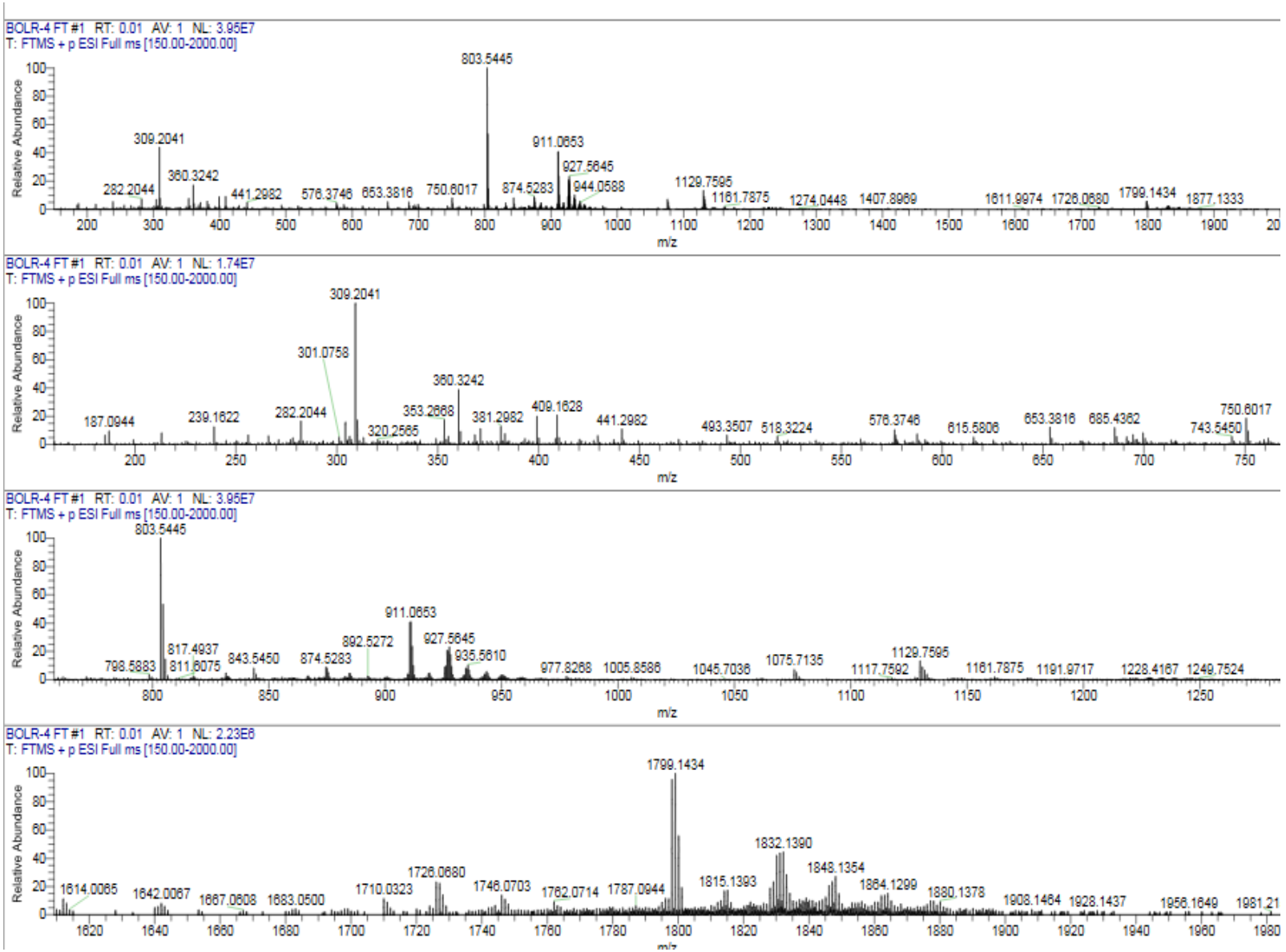


Figure S10. ESI MS of **2** (positive mode).

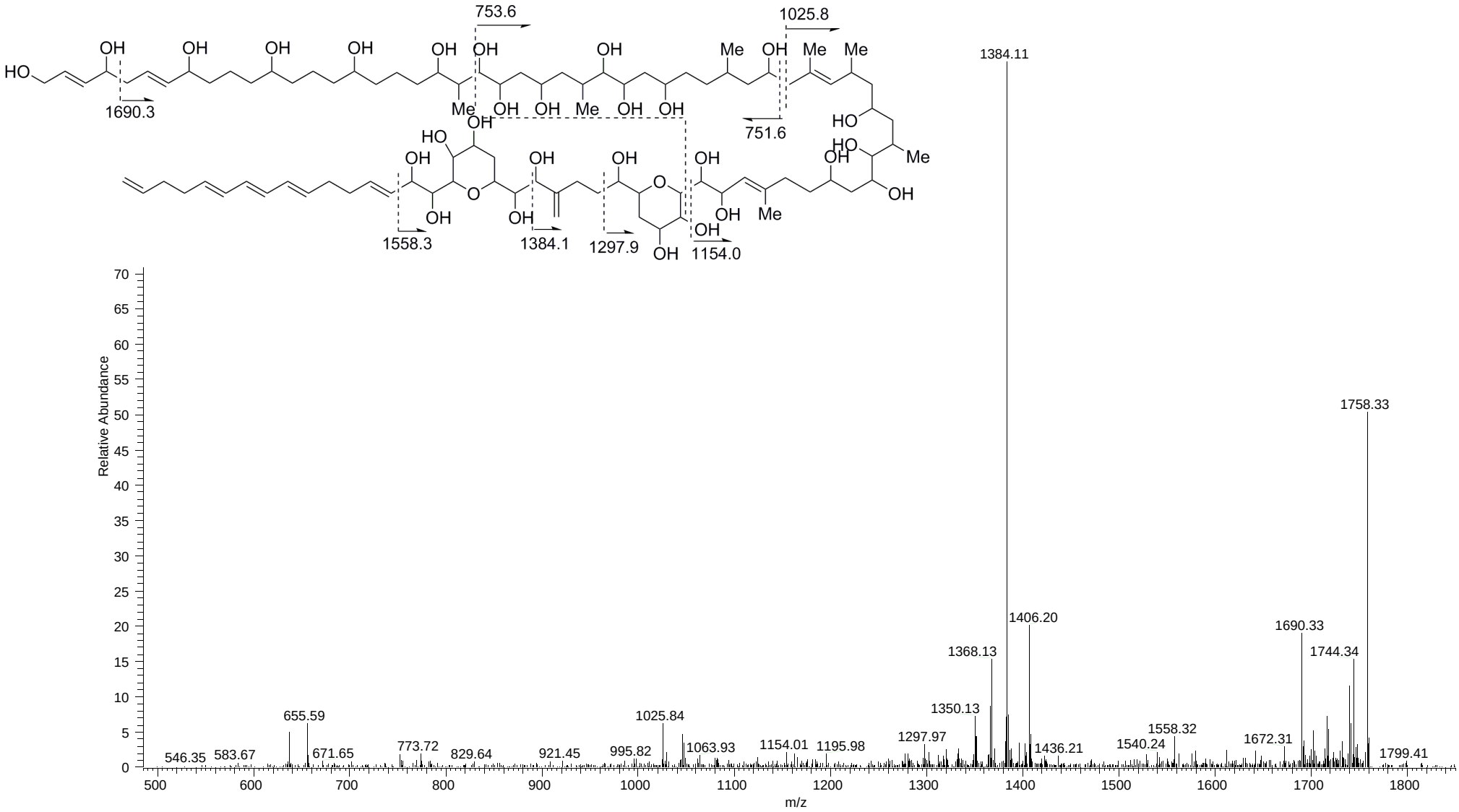
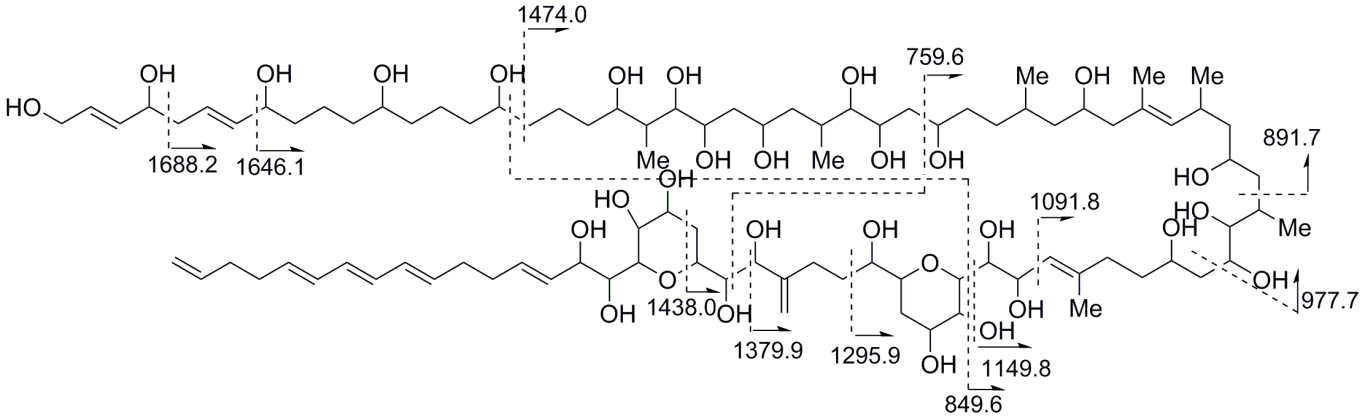


Figure S11. ESI MS/MS (positive) of **2** on the proton adduct ion $[M+H]^+$



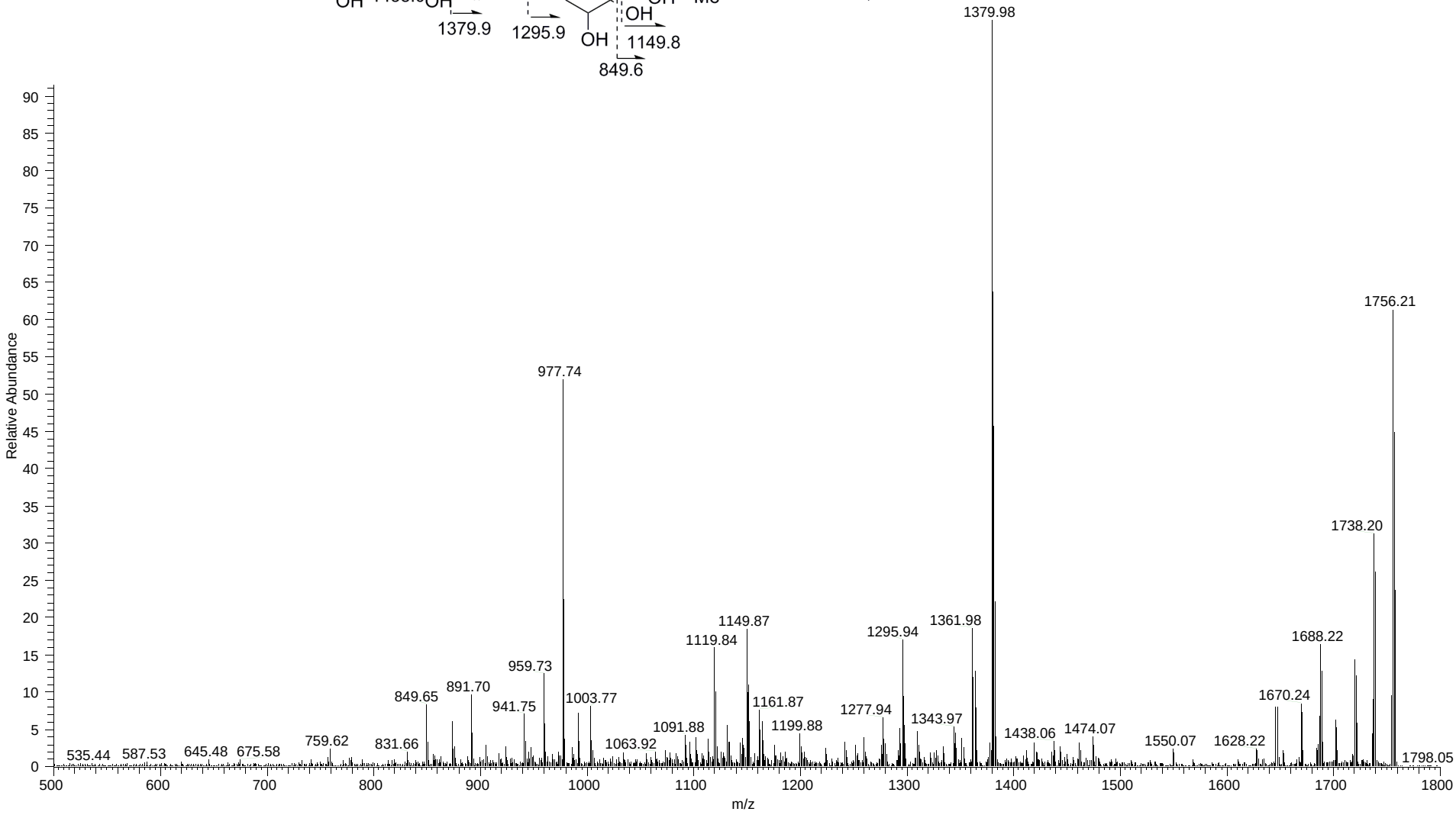


Figure S12. ESI MS/MS (negative) of **2** on the deprotonated ion $[M-H]^-$

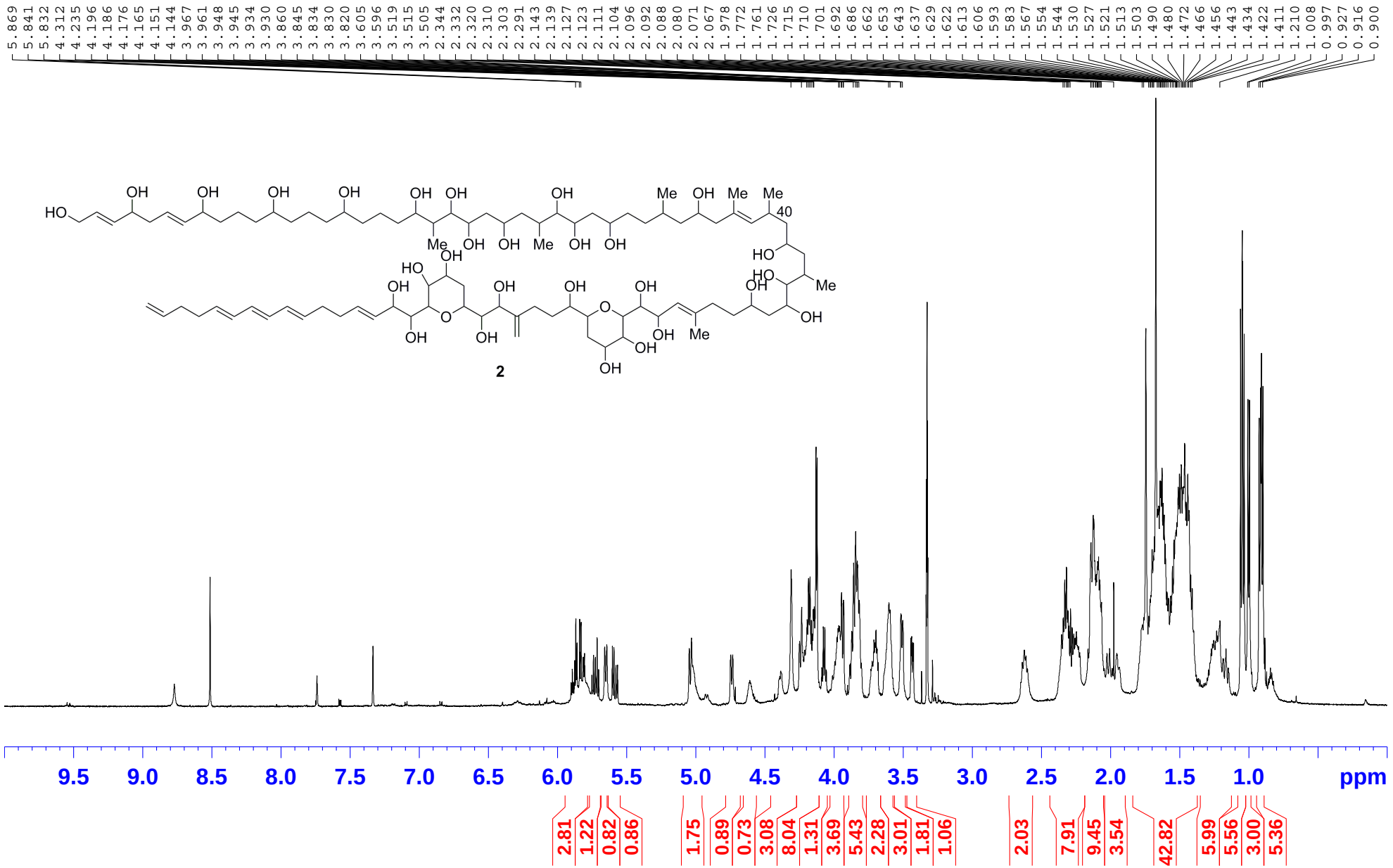


Figure S13. ^{1}H NMR spectrum of **2** in CD_3OD-C_5D_5N (2:1), 600 MHz.

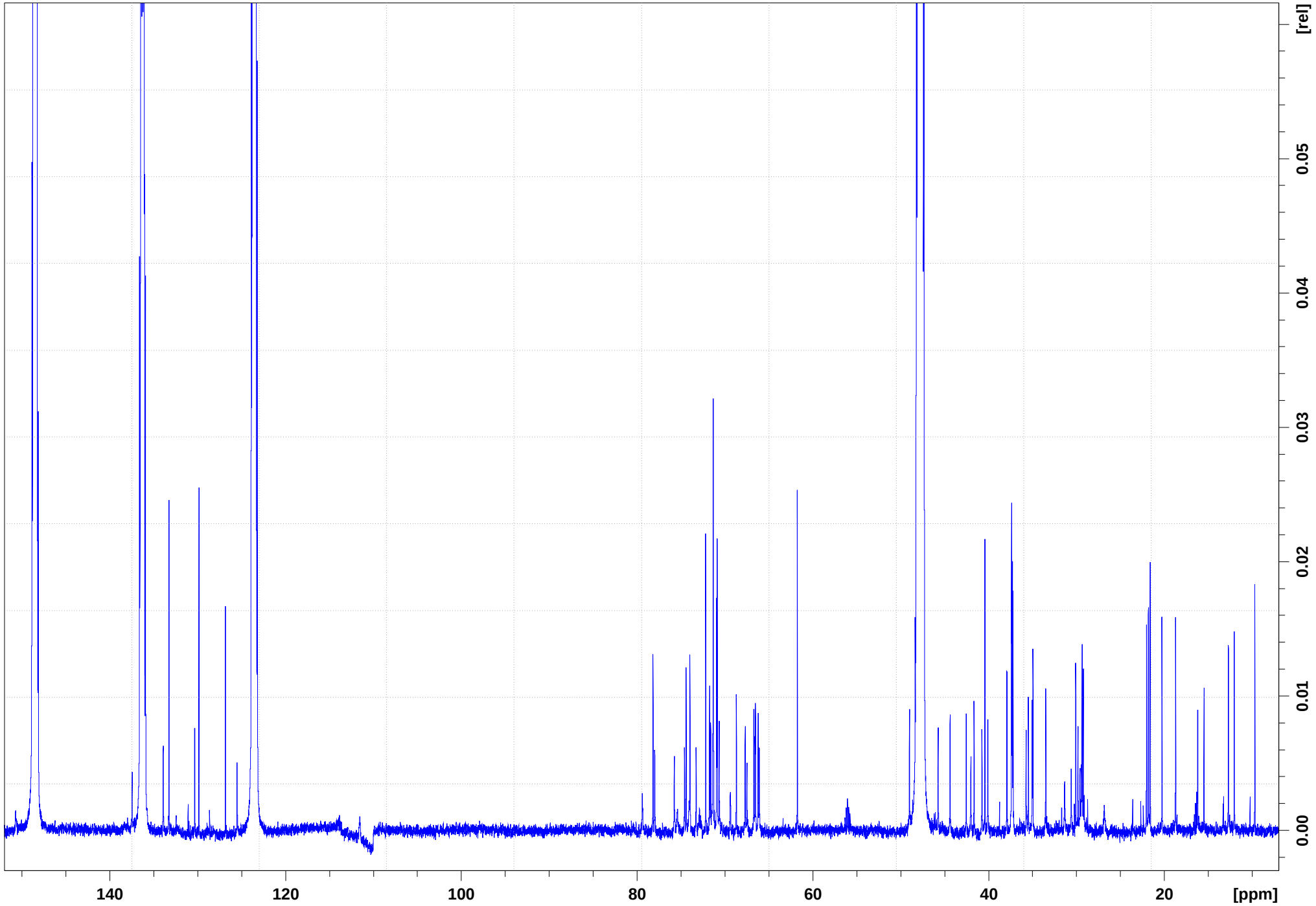


Figure S14. ^{13}C NMR spectrum of **2** in CD_3OD-C_5D_5N (2:1), 150 MHz.

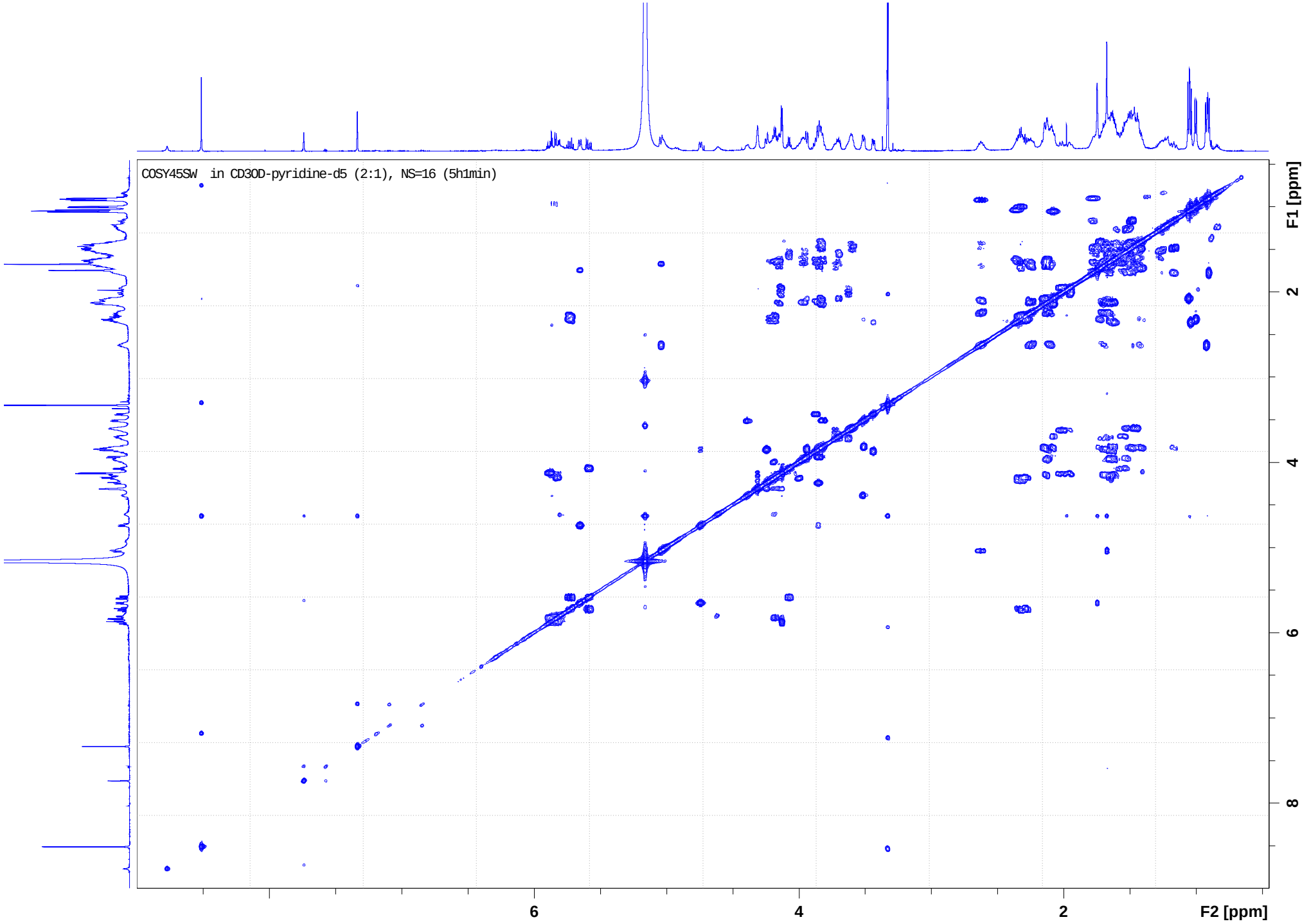


Figure S15. ^{1}H-^{1}H COSY spectrum of **2** in CD_3OD-C_5D_5N (2:1), 600 MHz.

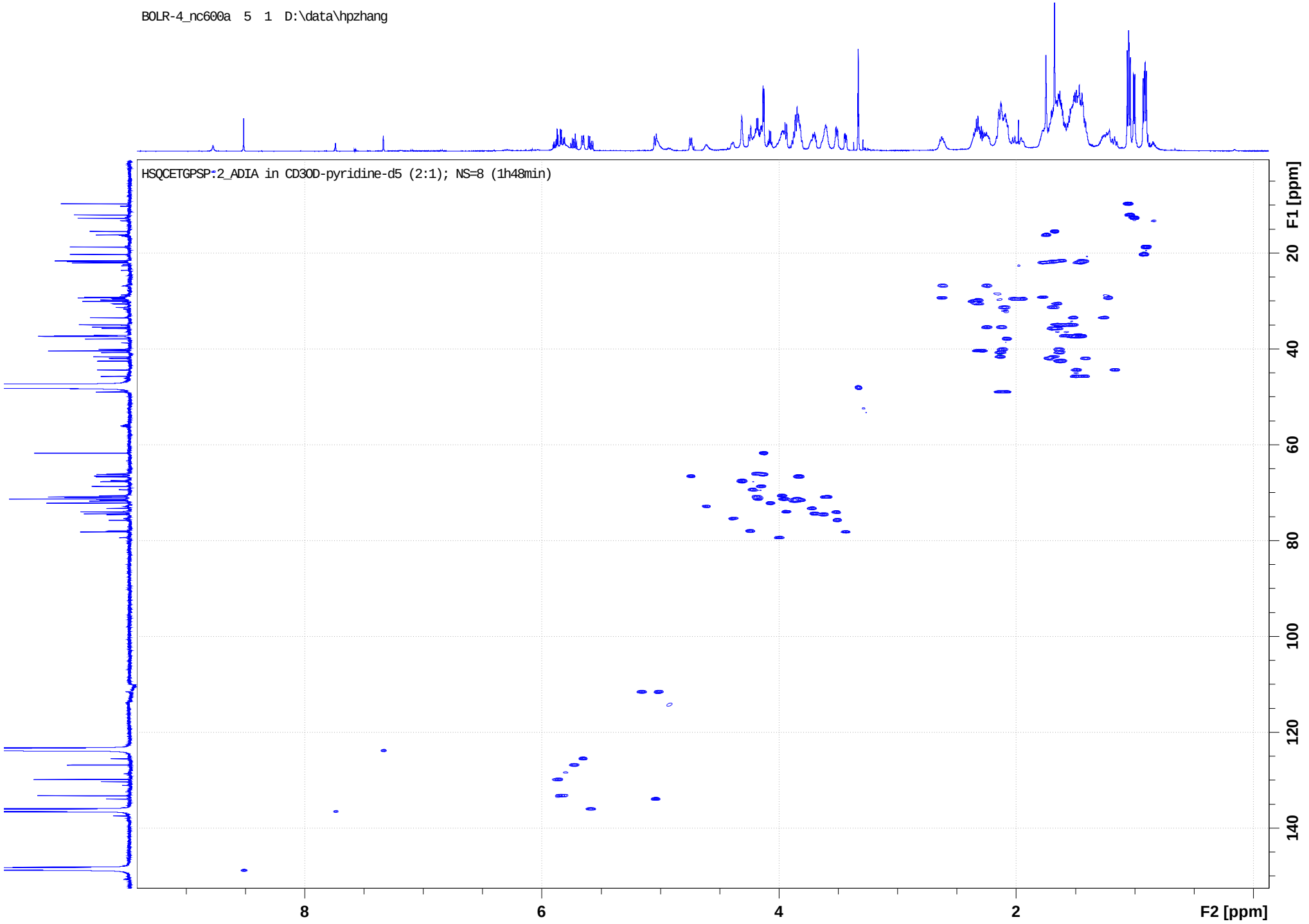


Figure S16. HSQC spectrum of **2** in CD_3OD-C_5D_5N (2:1), 600 MHz.

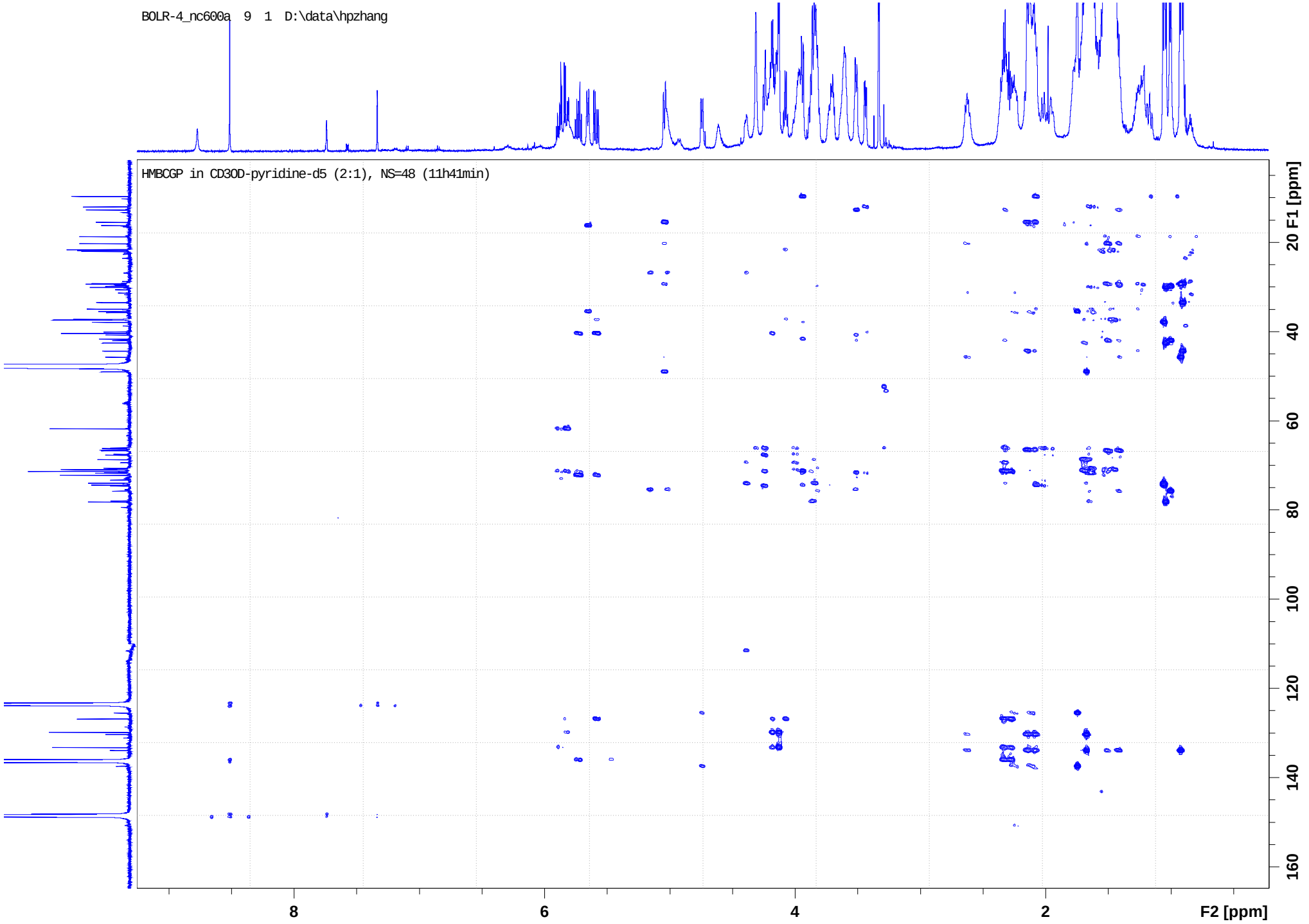


Figure S17. HMBC spectrum of **2** in CD_3OD-C_5D_5N (2:1), 600 MHz.

Table S1. NMR Spectroscopic Data (600 MHz, CD_3OD/C_5D_5N (2:1)) for AM20 (**1**)

Pos.	δ_c, type	δ_H (Jin Hz)	Pos.	δ_c, type	δ_H (Jin Hz)	Pos.	δ_c, type	δ_H (Jin Hz)
1	61.8, CH_2	4.13, d (4)	30	66.6[f], CH	3.84, m	59	74.1, CH	3.53, m
2	129.8, CH	5.91, ddd (5,5,15)	31	48.9, CH_2	2.09, m; 2.15, m	60	69.4, CH	4.23, m
3	133.3, CH	5.88, dd (5, 15)	32	130.3, C		61	30.6, CH_2	1.66, m; 2.33,ddd(10,10,10)
4	71.4, CH	4.17, m	33	133.9, CH	5.04, d (9)	62	66.1, CH	4.19, m
5	40.4, CH_2	2.29, ddd (6,6,6); 2.32, m	34	29.3, CH	2.62, m	63	67.5, CH	4.31, m
6	126.8, CH	5.73, ddd (7,7,15)	35	45.7, CH_2	1.43, m; 1.50, m	64	79.4, CH	4.00, m
7	135.9, CH	5.58, dd (7,15)	36	66.7[f], CH	3.84, m	65	71.4, CH	4.18, m
8	72.2, CH	4.07, ddd (6,6,6)	37	42.0, CH_2	1.42, m; 1.73, m	66	72.9, CH	4.62, m
9	37.2[a], CH_2	1.47, m; 1.55,m	38	29.8, CH	2.33, m	67	128.2, CH	5.80, m
10	21.6[b], CH_2	1.44, m; 162, m	39	75.8, CH	3.52, dd (2,8)	68	134.9, CH	5.82, m
11	37.3[a], CH_2	1.47, m; 1.55, m	40	71.6, CH	3.82, m	69	29.8[g], CH_2	2.04, m; 2.04,m
12	70.8[c], CH	3.60, m	41	40.8[d], CH_2	1.63, m; 2.14,m	70	32.1[g], CH_2	2.04, m; 2.08, m
13	37.4[a], CH_2	1.47, m; 1.55, m	42	70.7, CH	3.98, m	71	135.2, CH	5.60, m
14	21.8[b], CH_2	1.44, m; 1.69, m	43	35.7, CH_2	1.66, m; 1.67, m	72	132.8, CH	6.03, m
15	37.4[a], CH_2	1.47, m; 1.55, m	44	35.4, CH_2	2.13, m; 2.26, m	73	132.9, CH	6.05, m
16	70.9[c], CH	3.60, m	45	137.4, C		74	133.0, CH	6.06, m
17	37.4[a], CH_2	1.47, m; 1.55, m	46	125.5, CH	5.66, d '(8)	75	133.1, CH	5.96, m
18	22.0[b], CH_2	1.44, m; 1.77, m	47	66.5[f], CH	4.74, brd (8)	76	134.8, CH	5.61, m
19	34.9[e], CH_2	1.53,m; 1.66, m	48	71.5, CH	3.85, m	77	31.9[g], CH_2	2.05, m; 2.05, m
20	74.4, CH	3.71, m	49	77.9, CH	4.25, d (4)	78	29.9[g], CH_2	2.01, m; 2.01, m
21	37.9, CH	2.08, m	50	67.7, CH	4.31, m	79	140.1, CH	5.75, m
22	73.9, CH	3.94, m	51	66.2, CH	4.14, m	80	114.1, CH_2	4.85, m; 4.97, m
23	71.4, CH	3.85, m	52	29.4, CH_2	1.96, m; 2.01,ddd (11,11,11)	81	9.7, CH_3	1.06, d (7)
24	40.5[d], CH_2	1.62, m; 2.14, m	53	74.6, CH	3.64, m	82	18.7, CH_3	0.91, d (7)
25	71.4, CH	3.96, m	54	73.3, CH	3.73, m	83	15.5, CH_3	1.67, s
26	35.0[e], CH_2	1.54, m; 1.65, m	55	31.3, CH_2	1.69, m; 2.10,m	84	20.3, CH_3	0.93, d (6)
27	33.5, CH_2	1.27, m; 1.49, m	56	23.4, CH_2	2.26, m; 2.61, m	85	12.7, CH_3	0.99, d (7)
28	29.2, CH	1.79, m	57	150.7, C		86	16.2, CH_3	1.74, s
29	44.4, CH_2	1.17, ddd (3,9,9); 1.49, m	58	75.5, CH	4.39, m	87	111.5, CH_2	5.04, s; 5.31, s

The carbon chemical shifts with superscripts a-g are interchangeable.

Table S2. NMR Spectroscopic Data (600 MHz, CD_3OD/C_5D_5N (2:1)) for AM21 (**2**)

Pos.	δ_c, type	δ_H (Jin Hz)	Pos.	δ_c, type	δ_H (Jin Hz)	Pos.	δ_c, type	δ_H (Jin Hz)
1	61.8, CH_2	4.13, d (4)	33	33.5, CH_2	1.27, m; 1.49, m	65	74.1, CH	3.53, m
2	129.8, CH	5.91, ddd (5,5,15)	34	29.2, CH	1.79, m	66	69.4, CH	4.23, m
3	133.3, CH	5.88, dd (5, 15)	35	44.4, CH_2	1.17, ddd (3,9,9); 1.49, m	67	30.6, CH_2	1.66,m; 2.33,ddd (10,10,10)
4	71.4, CH	4.17, m	36	66.7[f], CH	3.84, m	68	66.1, CH	4.19, m
5	40.4, CH_2	2.29, ddd (6,6,6); 2.32, m	37	48.9, CH_2	2.09, m; 2.05, m	69	67.5, CH	4.31, m
6	126.8, CH	5.73, ddd (7,7,15)	38	130.3, CH		70	79.4, CH	4.00, m
7	135.9, CH	5.58, dd (7,15)	39	133.9, CH	5.04, d (9)	71	71.4, CH	4.18, m
8	72.2, CH	4.07, ddd (6,6,6)	40	29.3, CH	2.62, m	72	72.9, CH	4.62, m
9	37.2[a], CH_2	1.47, m; 1.55, m	41	45.7, CH_2	1.43, m; 1.50, m	73	128.2, CH	5.80, m
10	21.6[b], CH_2	1.44, m; 1.62, m	42	66.5[f], CH	3.84, m	74	134.9, CH	5.82, m
11	37.3[a], CH_2	1.47, m; 1.55, m	43	42.0, CH_2	1.42, m; 1.73, m	75	34.0[g], CH_2	2.04, m; 2.04, m
12	70.8[c], CH	3.60, m	44	29.8, CH	2.33, m	76	34.1[g], CH_2	2.04, m; 2.08, m
13	37.4[a], CH_2	1.47, m; 1.55, m	45	75.8, CH	3.52, dd (2,8)	77	135.2, CH	5.60, m
14	21.8[b], CH_2	1.44, m; 1.69, m	46	71.6, CH	3.82, m	78	132.8, CH_2	6.03, m
15	37.4[a], CH_2	1.47, m; 1.55, m	47	40.8, CH_2	1.63, m; 2.14, m	79	132.9, CH	6.05, m
16	70.9[c], CH	3.60, m	48	70.7, CH	3.98, m	80	133.0, CH	6.06, m
17	37.4[a], CH_2	1.47, m; 1.55, m	49	35.7, CH_2	1.66, m; 1.67,m	81	133.1, CH	5.96, m
18	22.0[b], CH_2	1.44, m; 1.77, m	50	35.4, CH_2	2.13, m; 2.26,m	82	134.8, CH	5.61, m
19	34.9[e], CH_2	1.53, m; 1.66, m	51	137.4, C		83	31.9[g], CH_2	2.05, m; 2.05, m
20	74.4, CH	3.71, m	52	125.5, CH	5.66, d ‘(8)	84	35.2[g], CH_2	2.01, m; 2.01,m
21	37.9, CH	2.08, m	53	66.5[f], CH	4.74, brd (8)	85	140.1, CH	5.75, m
22	73.9, CH	3.94, dd (3,8)	54	71.5, CH	3.85, m	86	114.1, CH_2	4.85, m; 4.97, m
23	71.2, CH	3.86, m	55	77.9, CH	4.25, d (4)	87	9.7, CH_3	1.06, d (7)
24	41.6, CH_2	1.69, m; 2.13, m	56	67.7, CH	4.31, m	88	12.0, CH_3	1.05, d (6)
25	68.9, CH	4.15, m	57	66.2, CH	4.14, m	89	18.7, CH_3	0.91, d (7)
26	42.5, CH	1.64, m; 1.64, m	58	29.4, CH_2	1.96, m; 2.01,ddd (11,11,11)	90	15.5, CH_3	1.67, s
27	30.0, CH	2.35, m	59	74.6, CH	3.64, m	91	20.3, CH_3	0.93, d (6)
28	78.2, CH	3.44, dd (3,8)	60	73.3, CH	3.73, m	92	12.7, CH_3	0.99, d (7)
29	71.7, CH	3.87, m	61	31.3, CH_2	1.69, m; 2.10, m	93	16.2, CH_3	1.74, s
30	40.1, CH_2	1.65, m; 2.12, m	62	23.4, CH_2	2.26, m; 2.61, m	94	111.5, CH_2	5.04, s; 5.31, s
31	71.3, CH	3.96, m	63	150.7, C				
32	34.9[e], CH_2	1.54, m; 1.65, m	64	75.5, CH	4.39, m			

The carbon chemical shifts with superscripts a-g are interchangeable.