

Supporting information

Unguiculin A and Ptilomycalin E-H, Novel Antimalarial Guanidine Alkaloids from the Marine Sponge *Monanchora unguiculata*

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In-situ Monanchora unguiculata photo



S0. Observed data for known compounds.

(-)-*Crambescidin* 800 (**6**) : yellow oil, $[\alpha]_D^{20}$ -7.8 (c 4.1, MeOH); ^1H and ^{13}C NMR data see **Supporting Information**; HRESIMS m/z 801.62347 $[\text{M} + \text{H}]^+$ (calc for $\text{C}_{45}\text{H}_{81}\text{N}_6\text{O}_6$, 801.6212).

(-)-*Crambescidin* 359 (**7**) : yellow oil, $[\alpha]_D^{20}$ -12.7 (c 0.4, MeOH); ^1H data see **Supporting Information**; HRESIMS m/z 360.26724 $[\text{M} + \text{H}]^+$ (calc for $\text{C}_{21}\text{H}_{34}\text{N}_3\text{O}_2$, 360.2646).

(-)-*Crambescidic acid* (**8**) : yellow oil, $[\alpha]_D^{20}$ -6.6 (c 0.9, MeOH); ^1H data see **Supporting Information**; HRESIMS m/z 658.47943 $[\text{M} + \text{H}]^+$ (calc for $\text{C}_{38}\text{H}_{64}\text{N}_3\text{O}_6$, 658.4790).

(-)-*Fromiamycalin* (**9**) : yellow oil, $[\alpha]_D^{20}$ -1.3 (c 1.3, MeOH); ^1H data see **Supporting Information**; HRESIMS m/z 783.60980 $[\text{M} + \text{H}]^+$ (calc for $\text{C}_{45}\text{H}_{79}\text{N}_6\text{O}_5$, 783.6106).

Figure S1: HRMS-HRMS spectrum for unguiculin A (**1**)

160127_PMA_PEC_Mona_pos #15828 RT: 24.50 AV: 1 NL: 8.46E6
T: FTMS + c ESI d Full ms2 468.44@hcd30.00 [50.00-495.00]

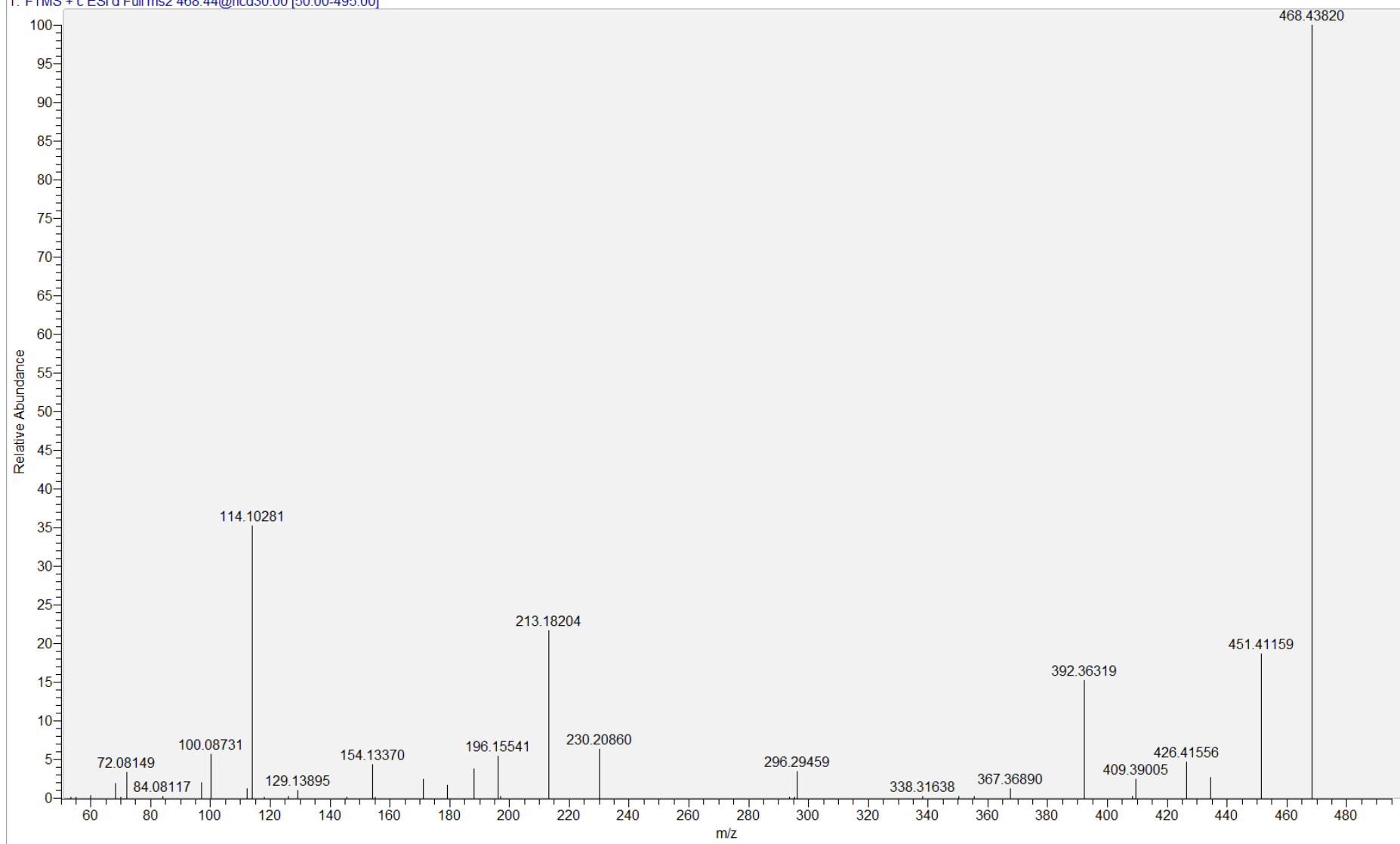


Figure S2: ^1H NMR (500 MHz, MeOD) spectrum for unguiculin A (**1**)

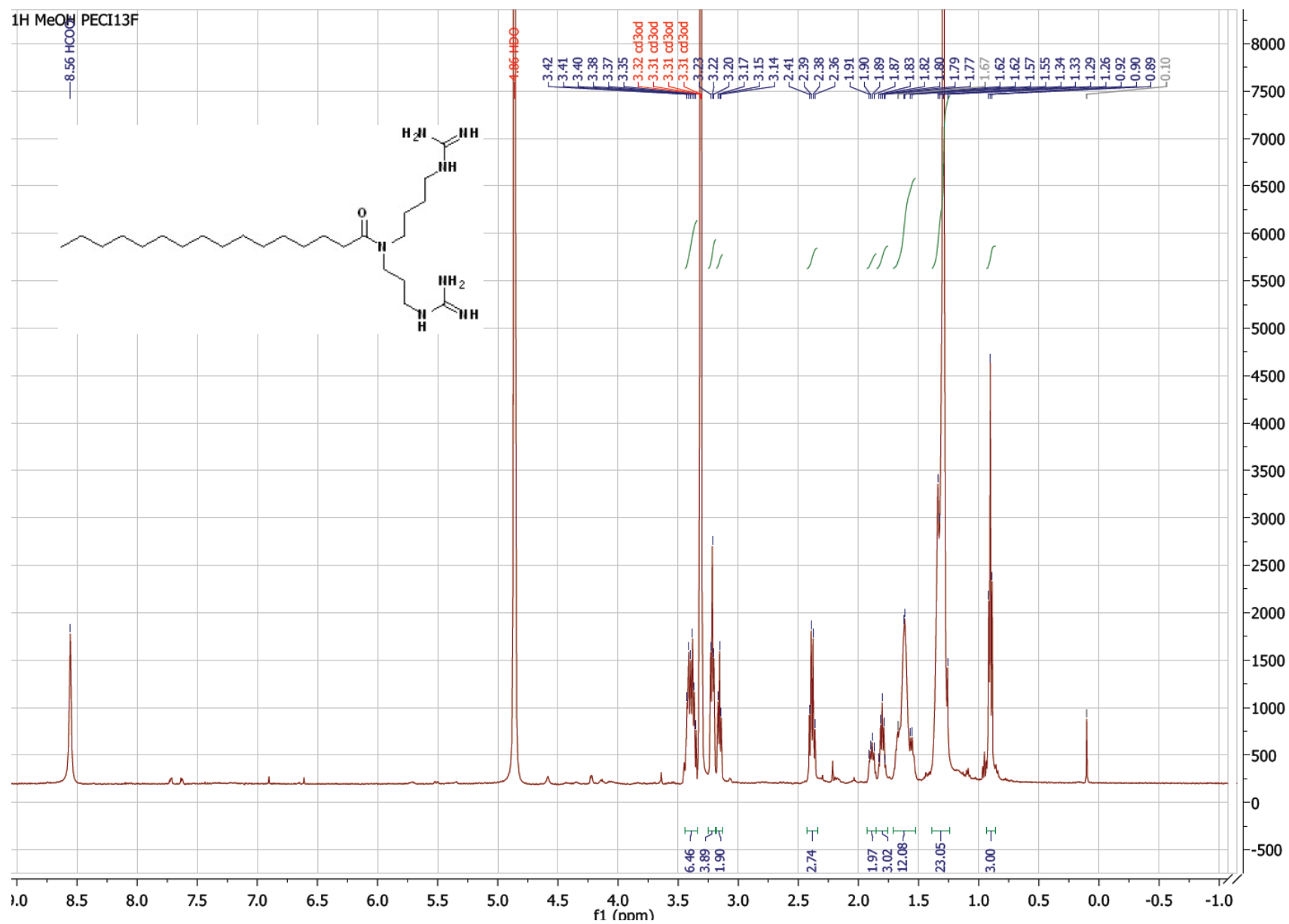


Figure S3: ^{13}C NMR (125 MHz, MeOD) spectrum for unguiculin A (1)

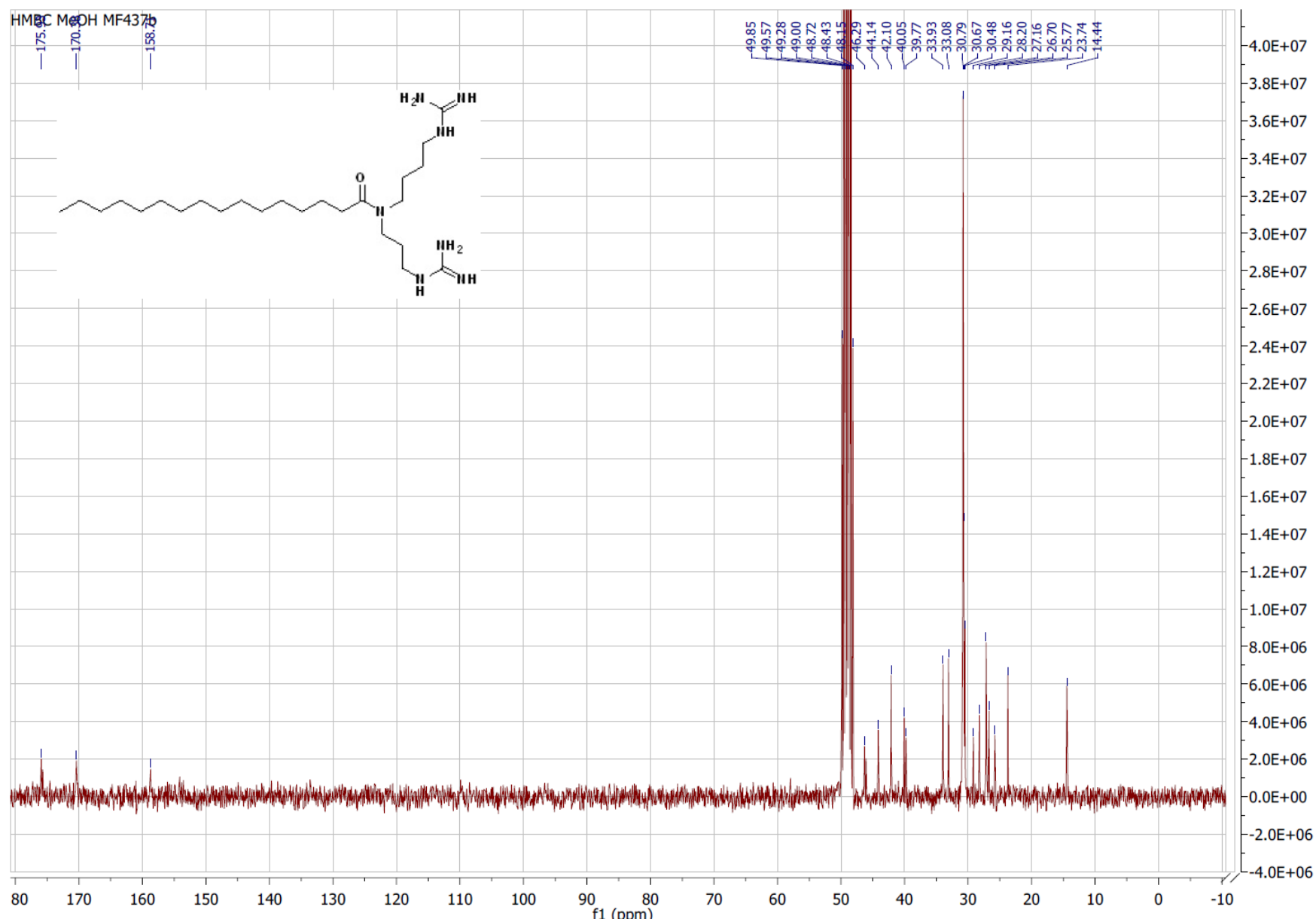


Figure S4: ^1H - ^1H COSY NMR (500 MHz, MeOD) spectrum for unguiculin A (**1**)

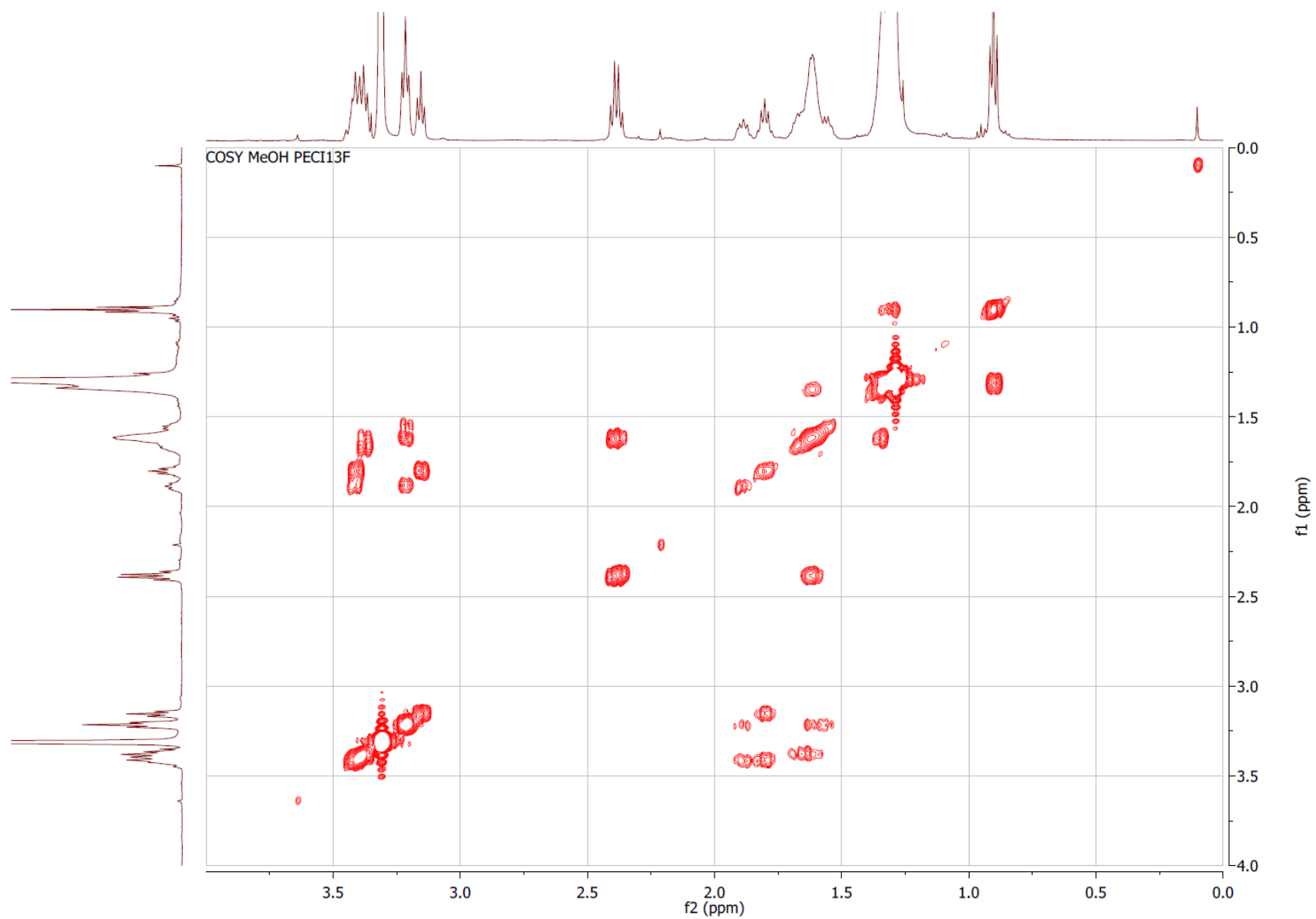


Figure S5: HSQC NMR (500 MHz, MeOD) spectrum for unguiculin A (**1**)

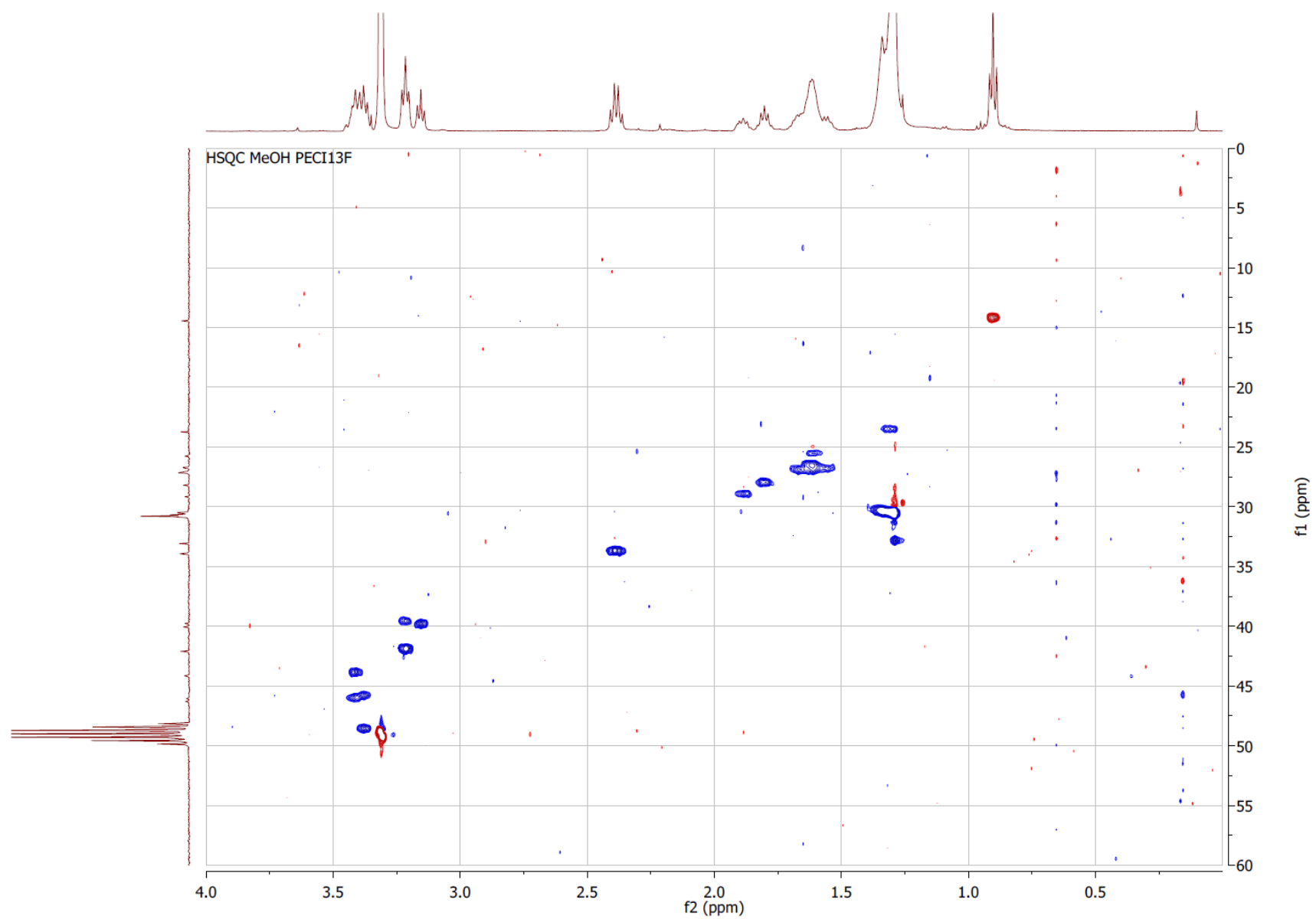


Figure S6: ^1H - ^{13}C HMBC NMR (500 MHz, MeOD) spectrum for unguiculin A (**1**)

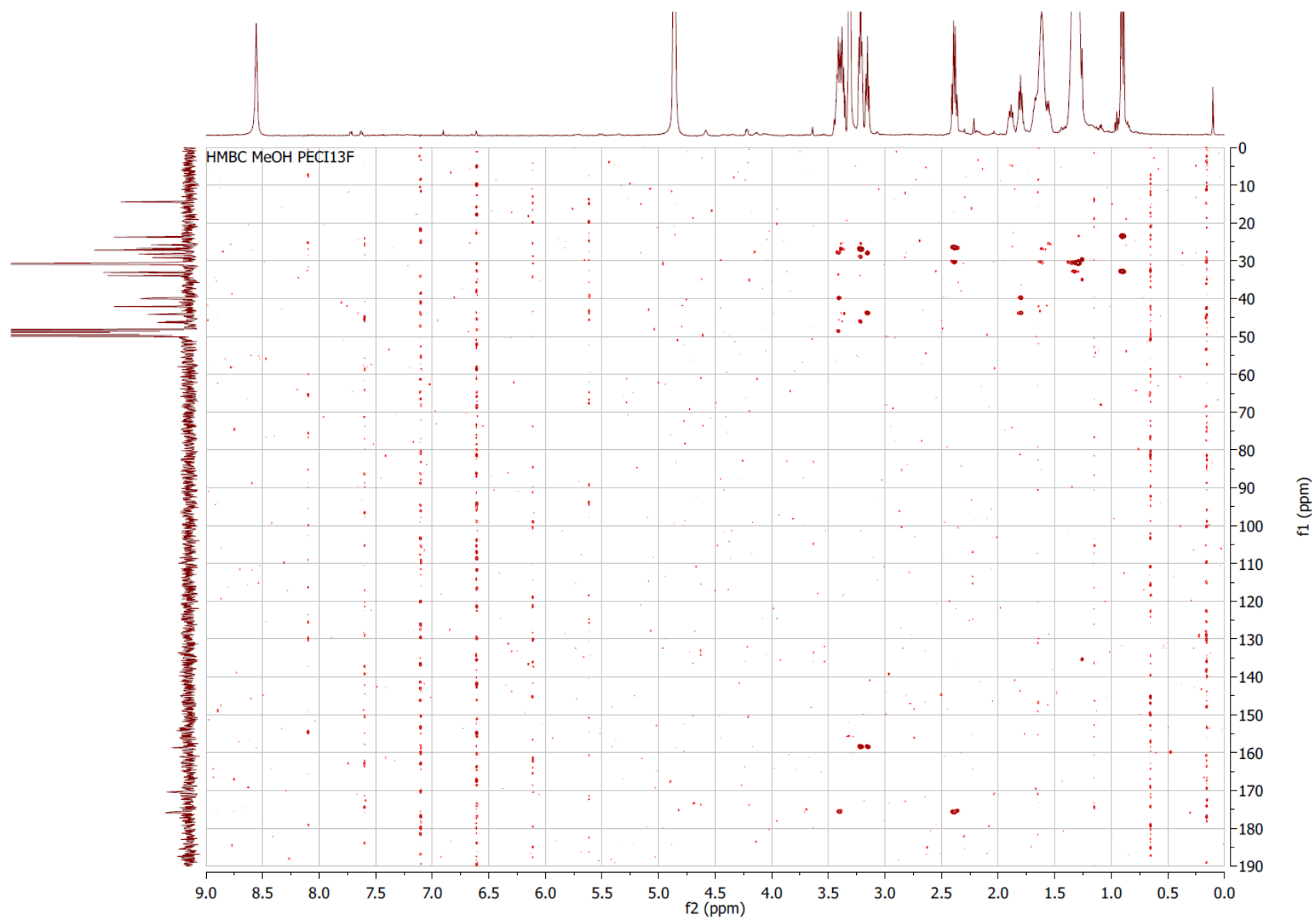


Figure S7: ^1H - ^1H TOCSY NMR (500 MHz, MeOD) spectrum for unguiculin A (**1**)

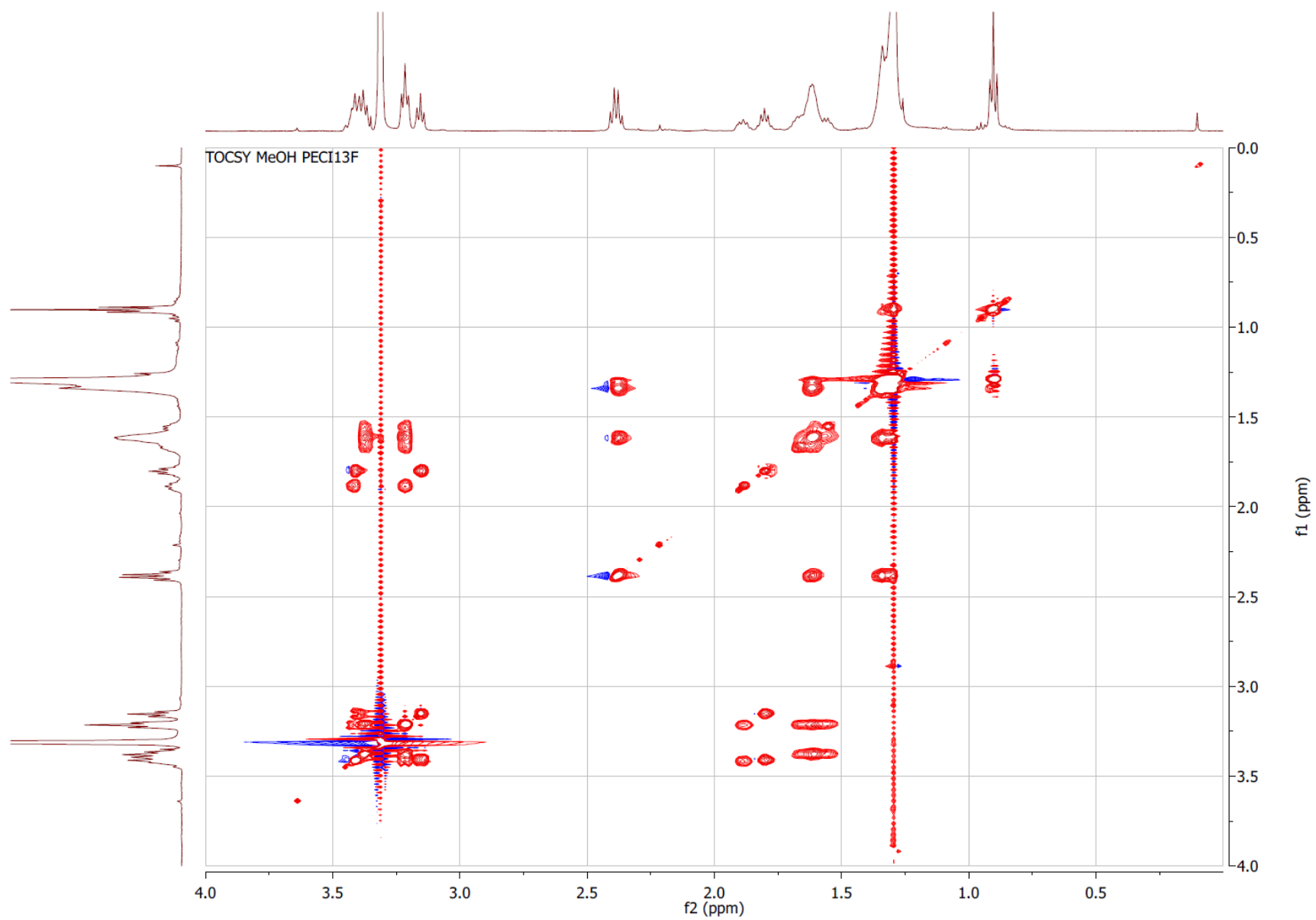


Figure S8: ^1H - ^1H NOESY NMR (500 MHz, MeOD) spectrum for unguiculin A (**1**)

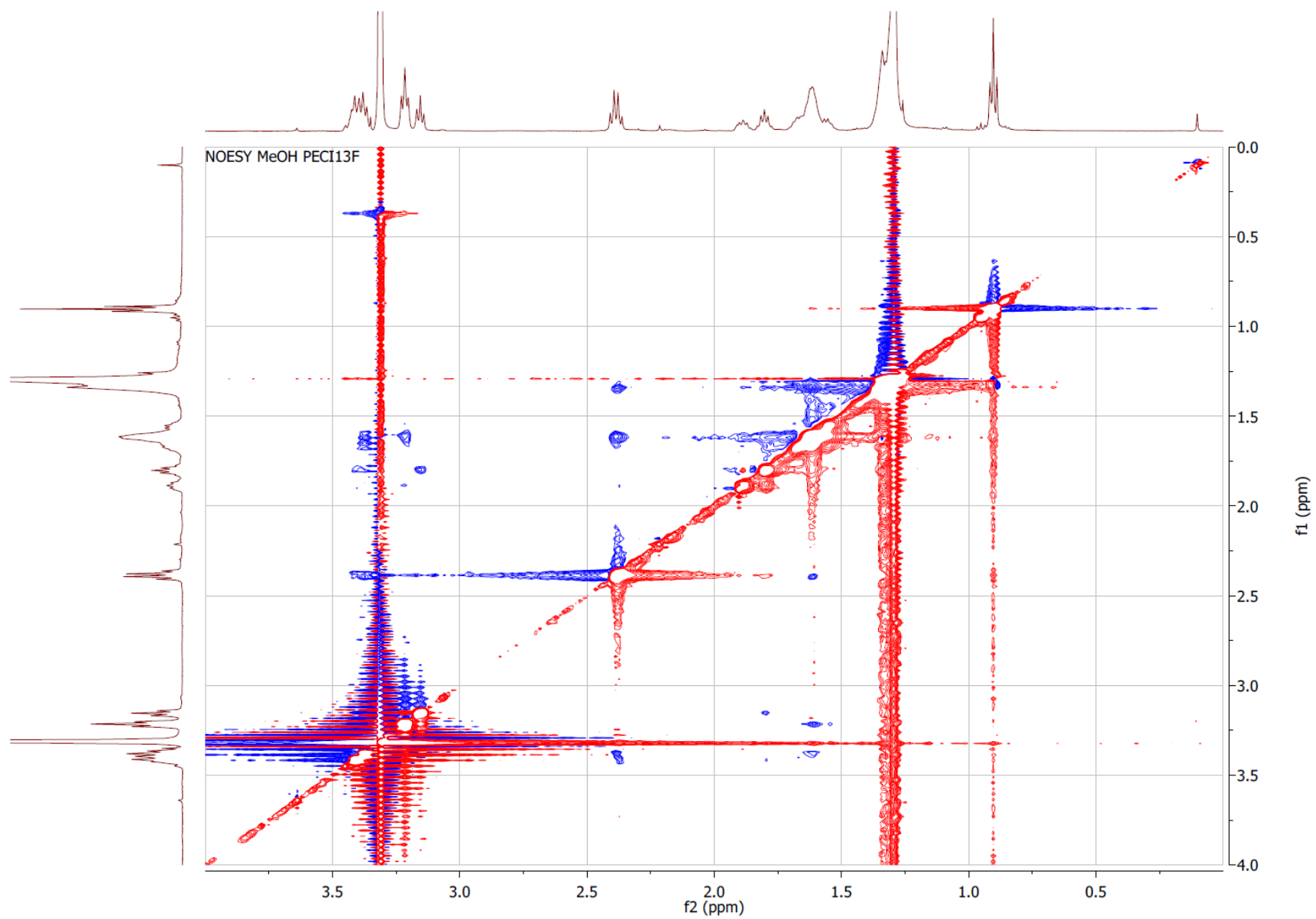


Figure S9: HRMS-HRMS spectrum for ptilomycalin E (**2**)

160127_PMA_PEC_Mona_pos #14285 RT: 22.27 AV: 1 NL: 5.82E6
T: FTMS + c ESI d Full ms2 869.67@hcd30.00 [60.33-905.00]

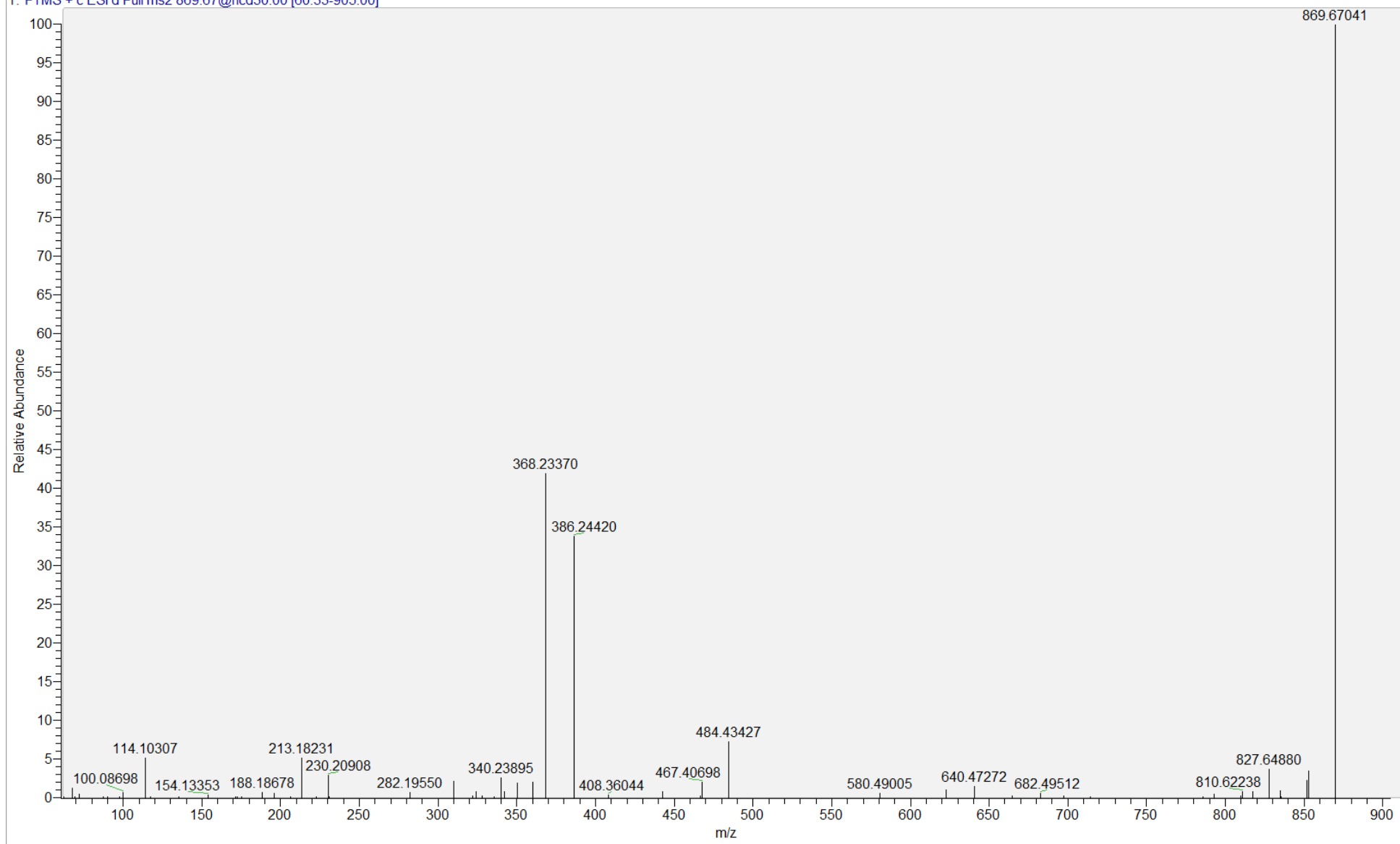


Figure S10: IR spectrum for ptilomycalin E (2)

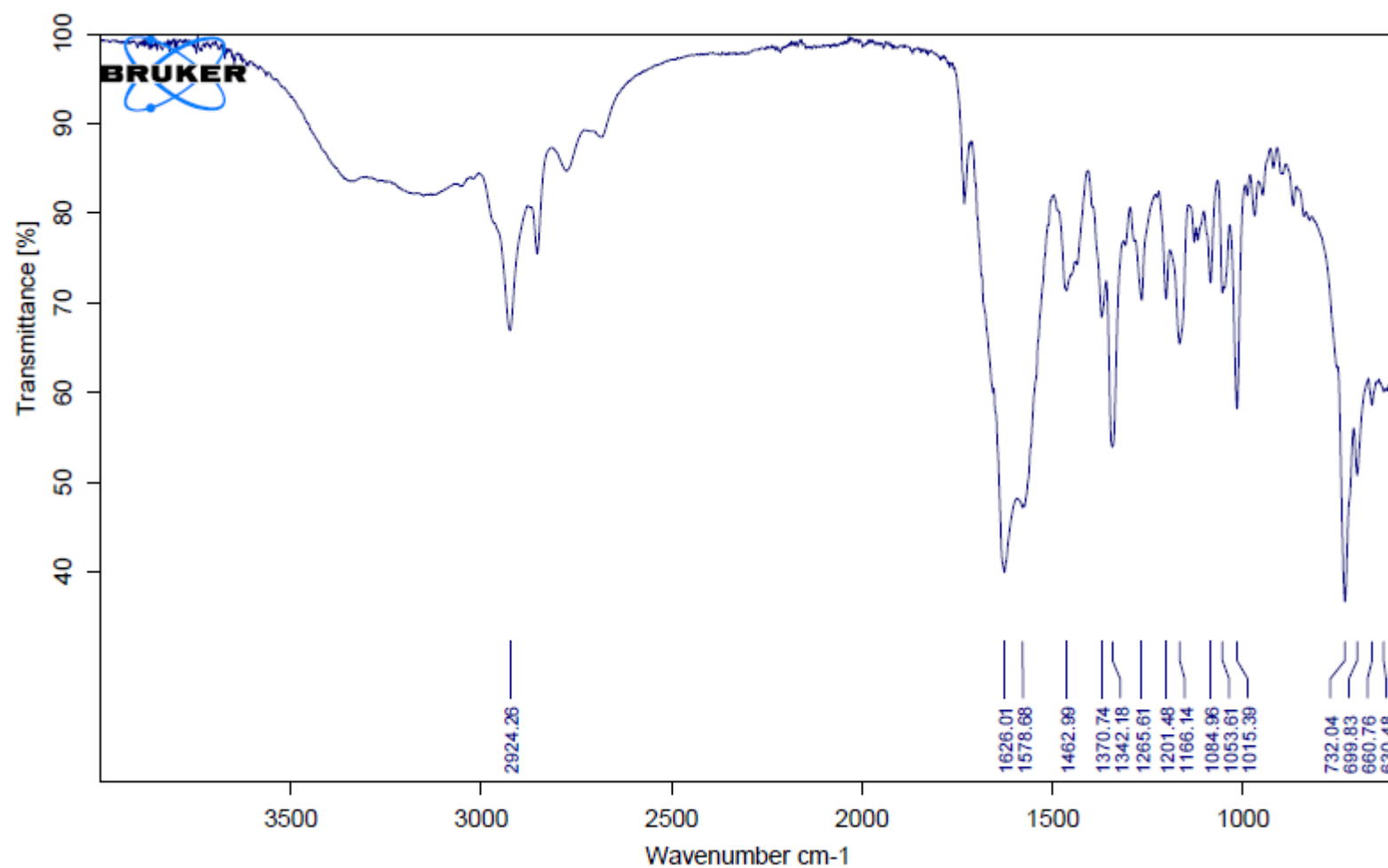


Figure S11: ^1H NMR (500 MHz, MeOD) spectrum for ptilomycin E (2)

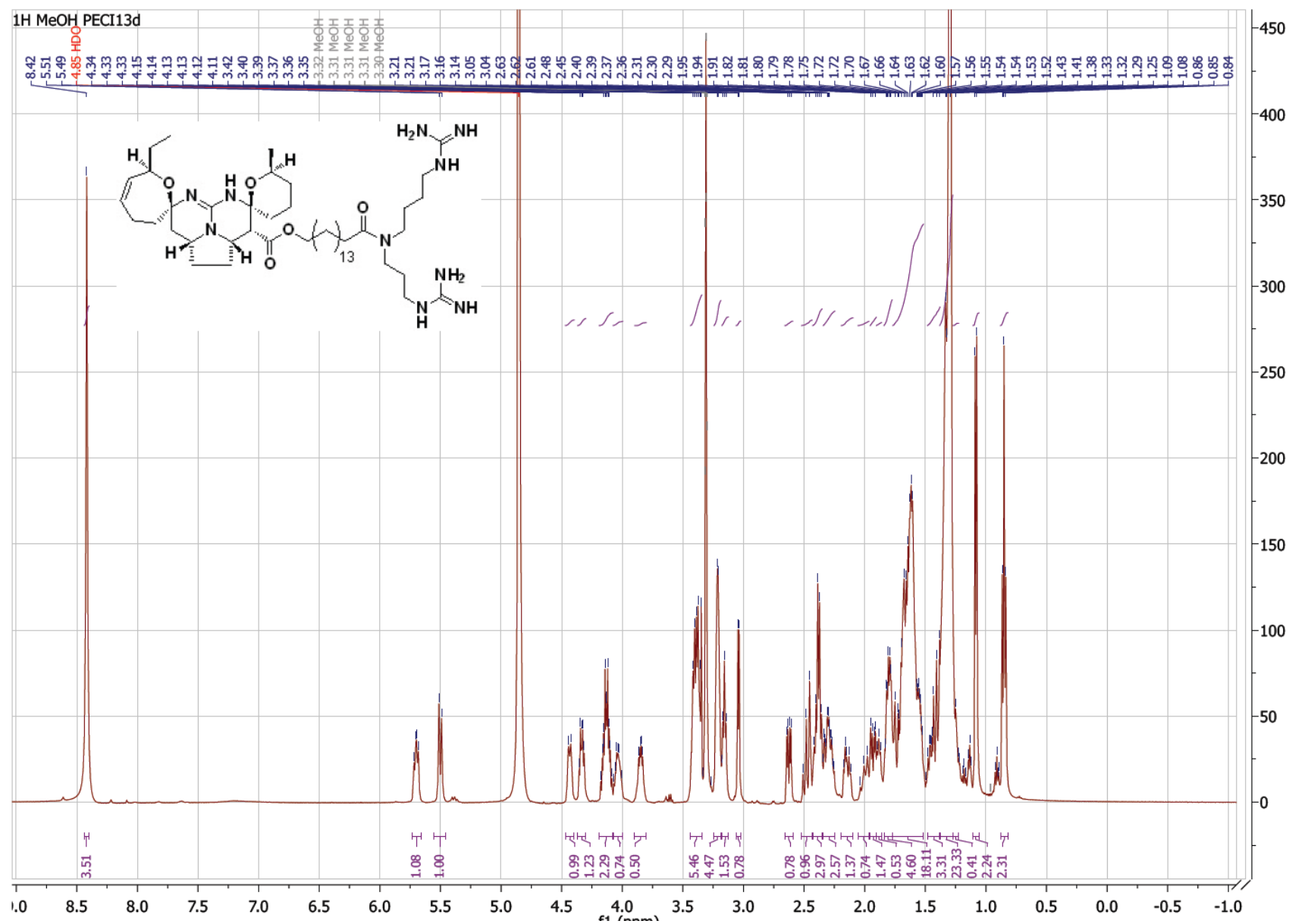


Figure S12: ^{13}C NMR (125 MHz, MeOD) spectrum for ptilomycalin E (**2**)

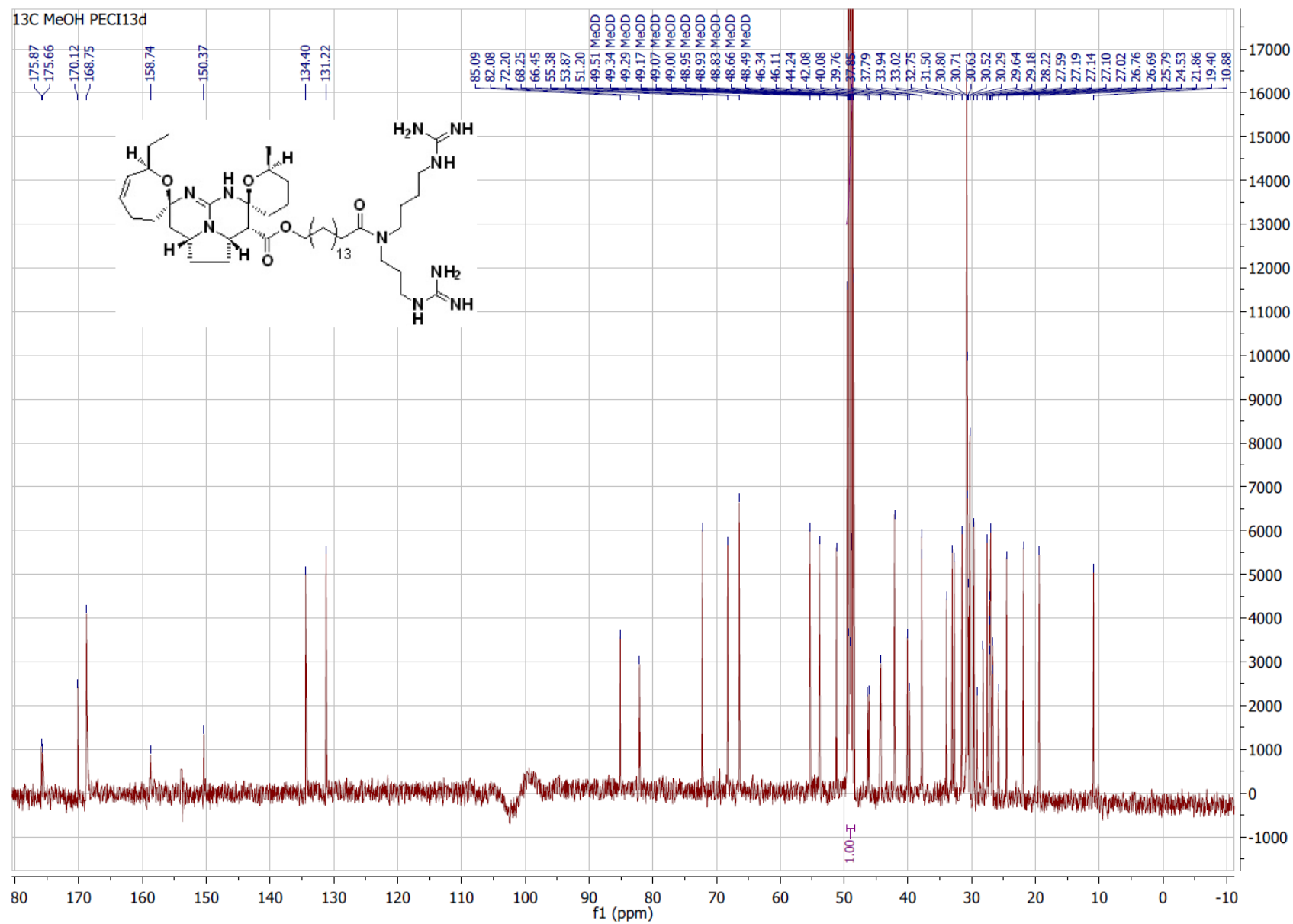


Figure S13: ^1H - ^1H COSY NMR (500 MHz, MeOD) spectrum for ptilomycalin E (**2**)

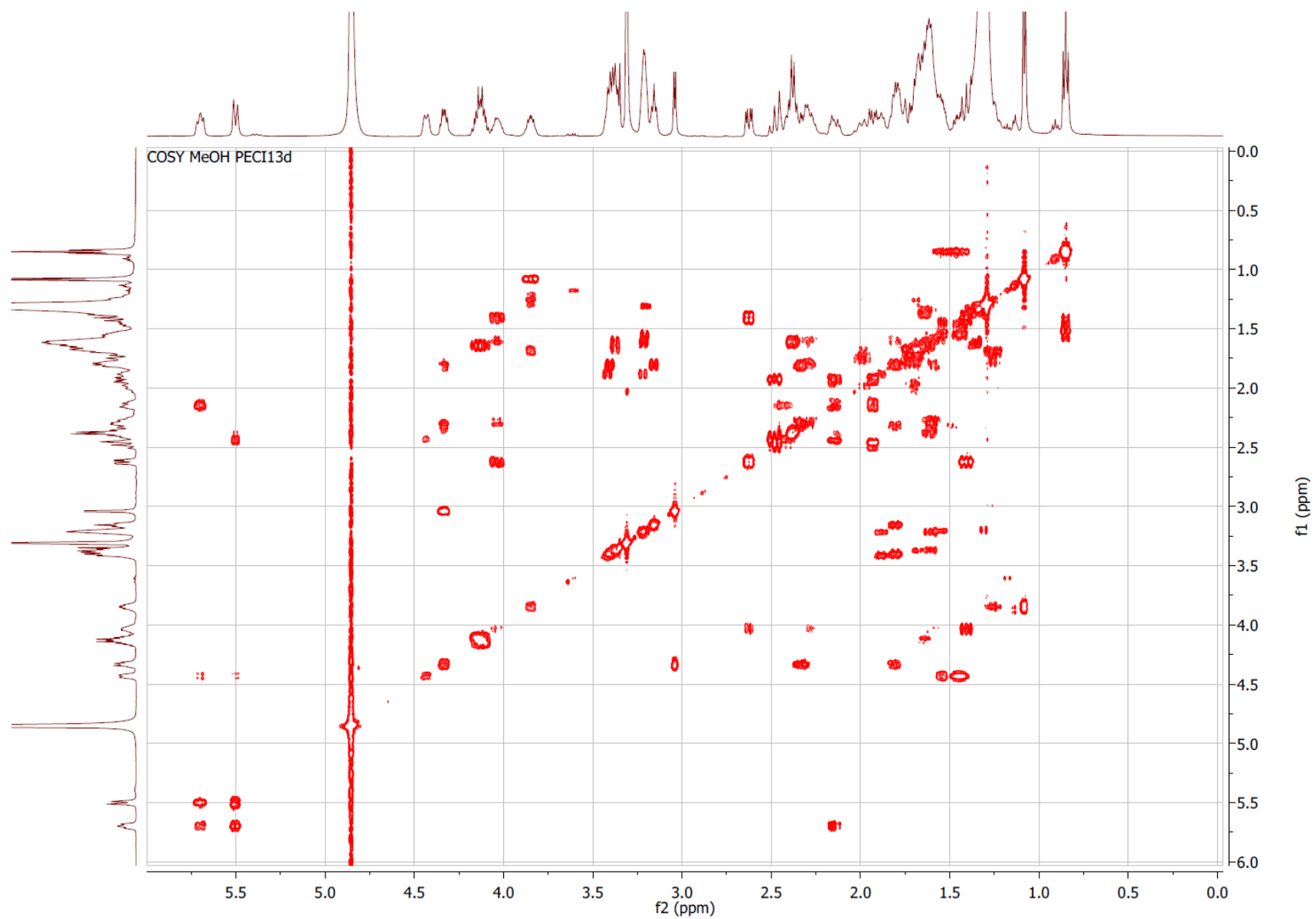


Figure S14: HSQC NMR (500 MHz, MeOD) spectrum for ptilomycalin E (**2**)

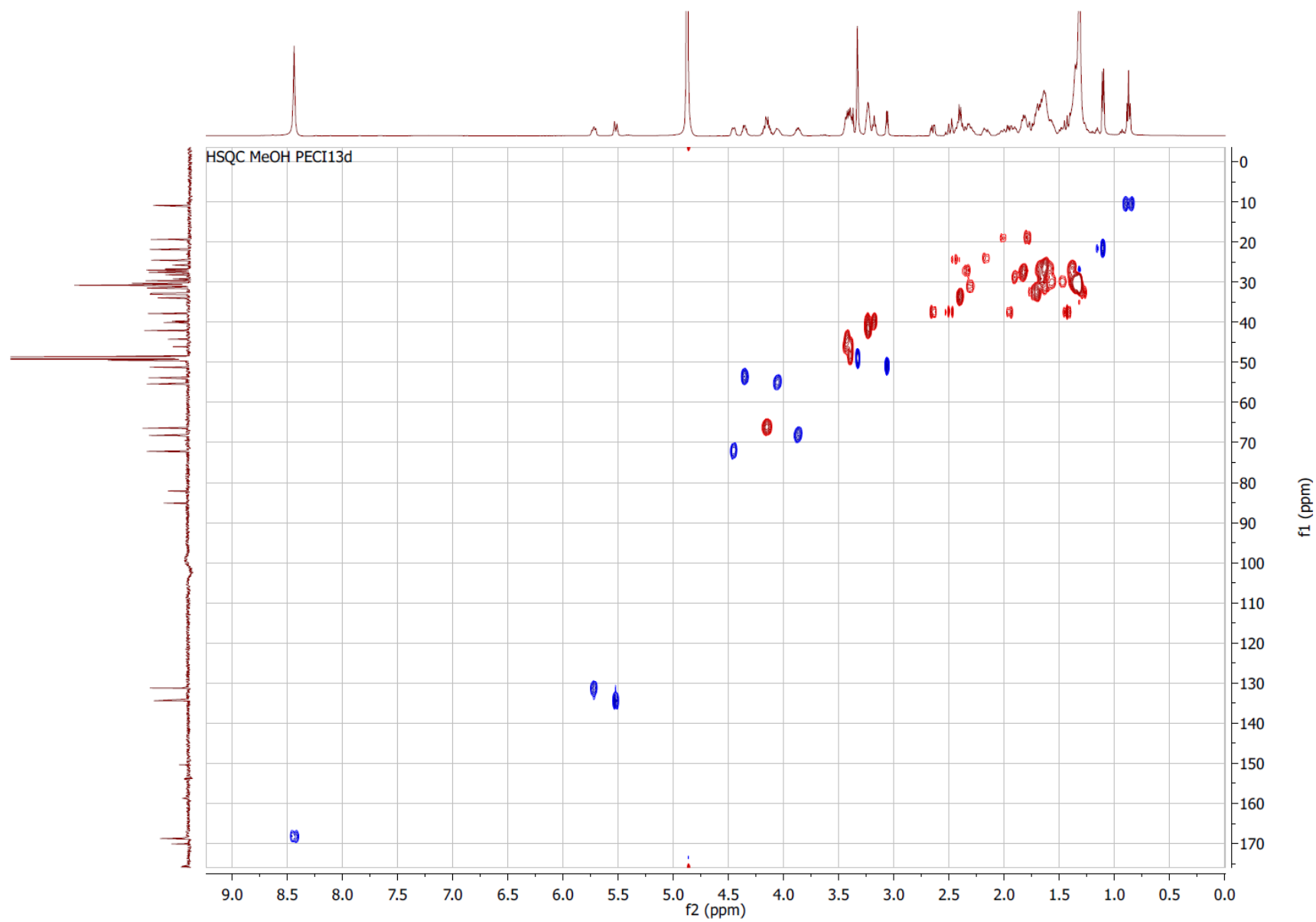


Figure S15: ^1H - ^{13}C HMBC NMR (500 MHz, MeOD) spectrum for pilomycalin E (**2**)

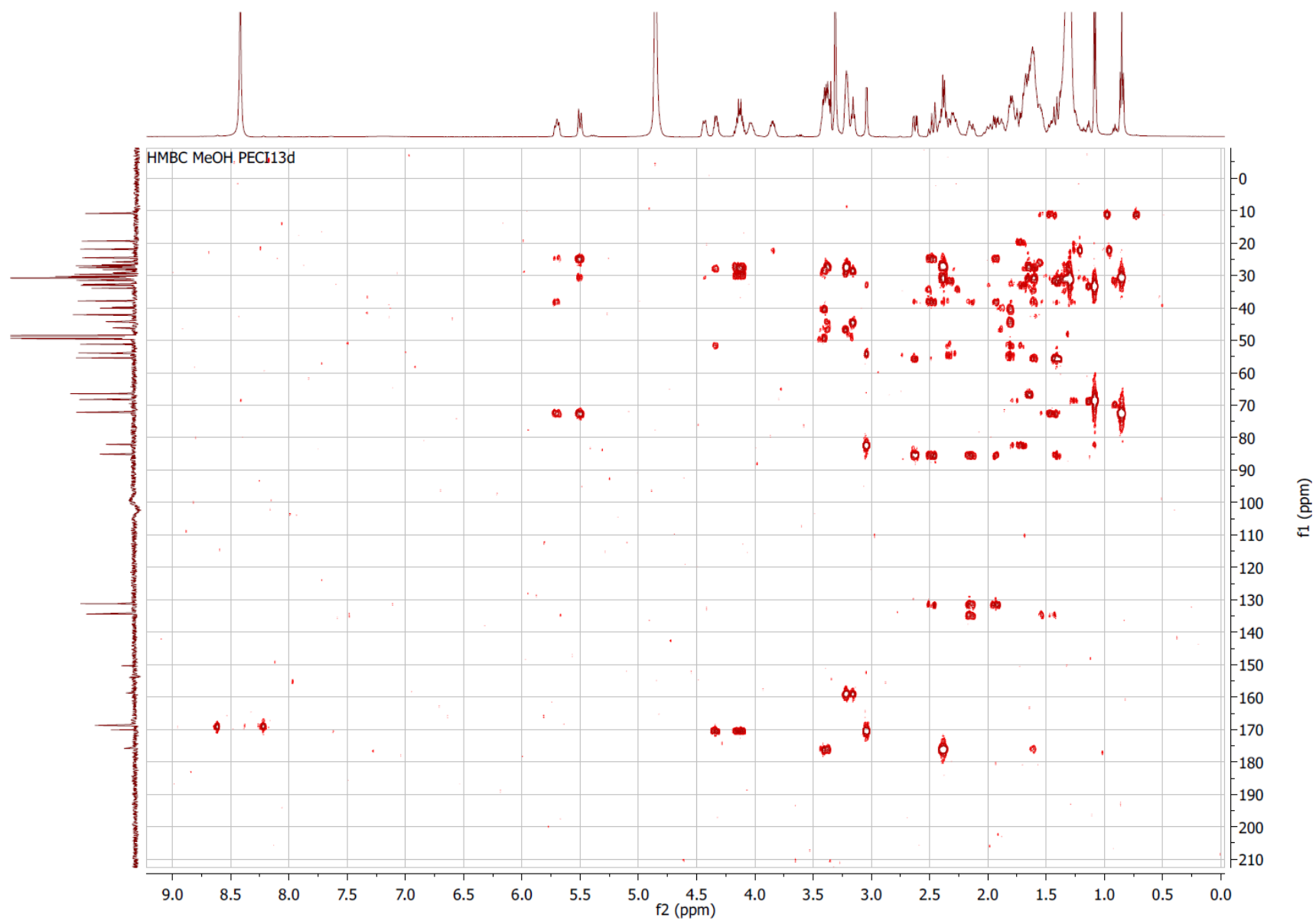


Figure S16: HRMS-HRMS spectrum for ptilomycalin F (**3**)

160127_PMA_PEC_Mona_pos #19685 RT: 30.48 AV: 1 NL: 7.60E6
T: FTMS + c ESI d Full ms2 428.33@hcd30.00 [59.33-890.00]

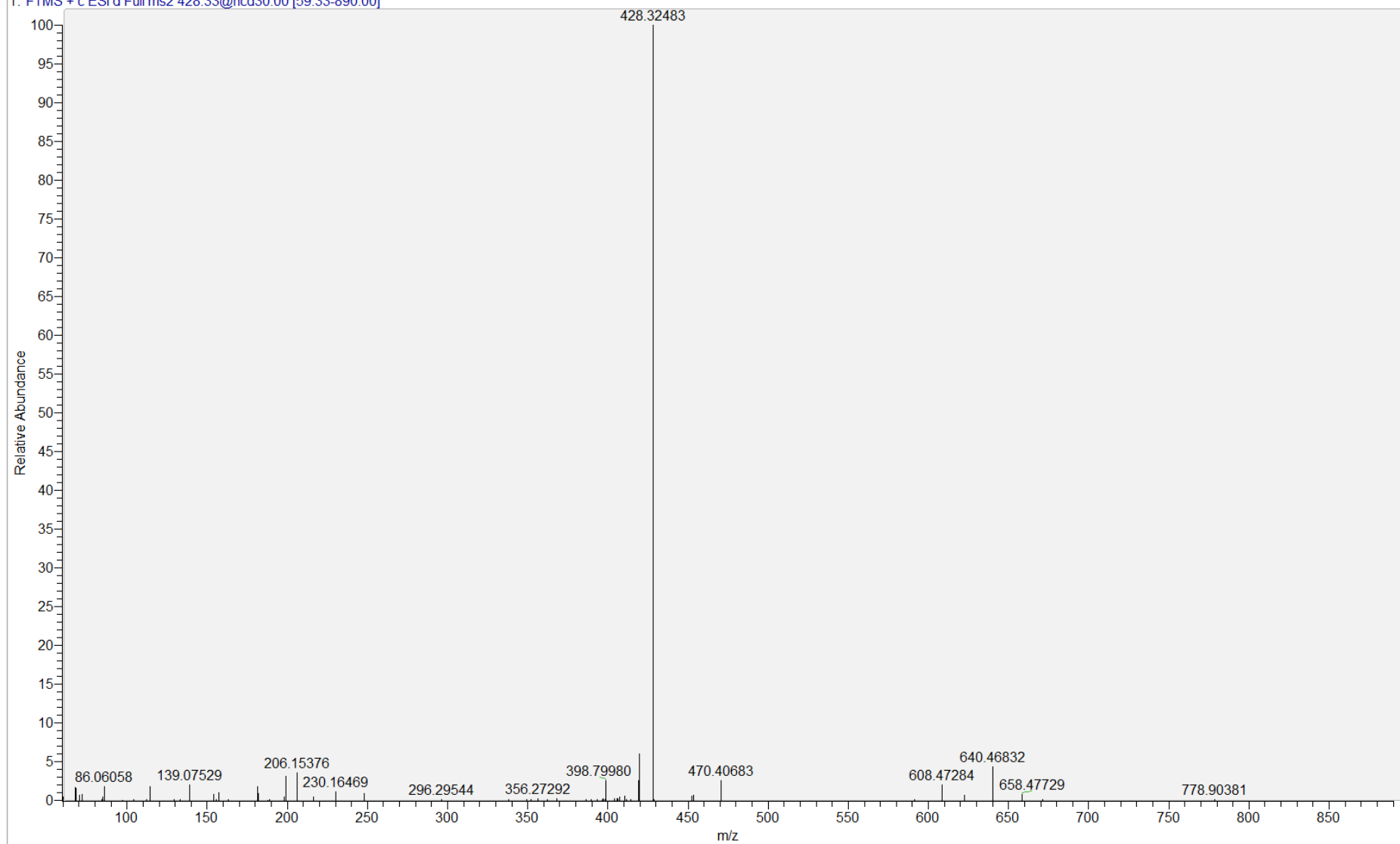


Figure S17: ^1H NMR (500 MHz, MeOD) spectrum for ptilomycalin F (**3**)

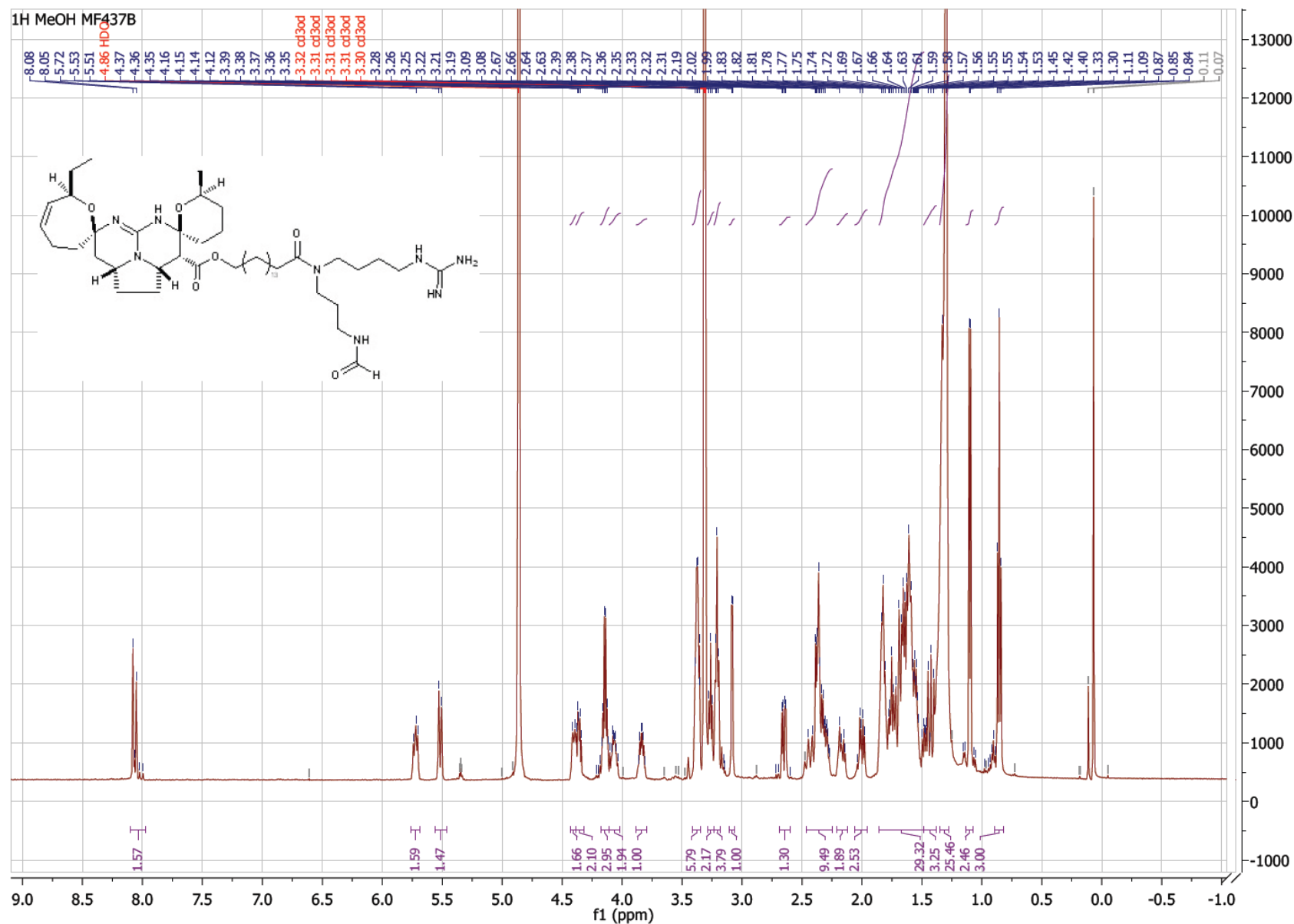


Figure S18: ^{13}C NMR (125 MHz, MeOD) spectrum for ptilomycalin F (**3**)

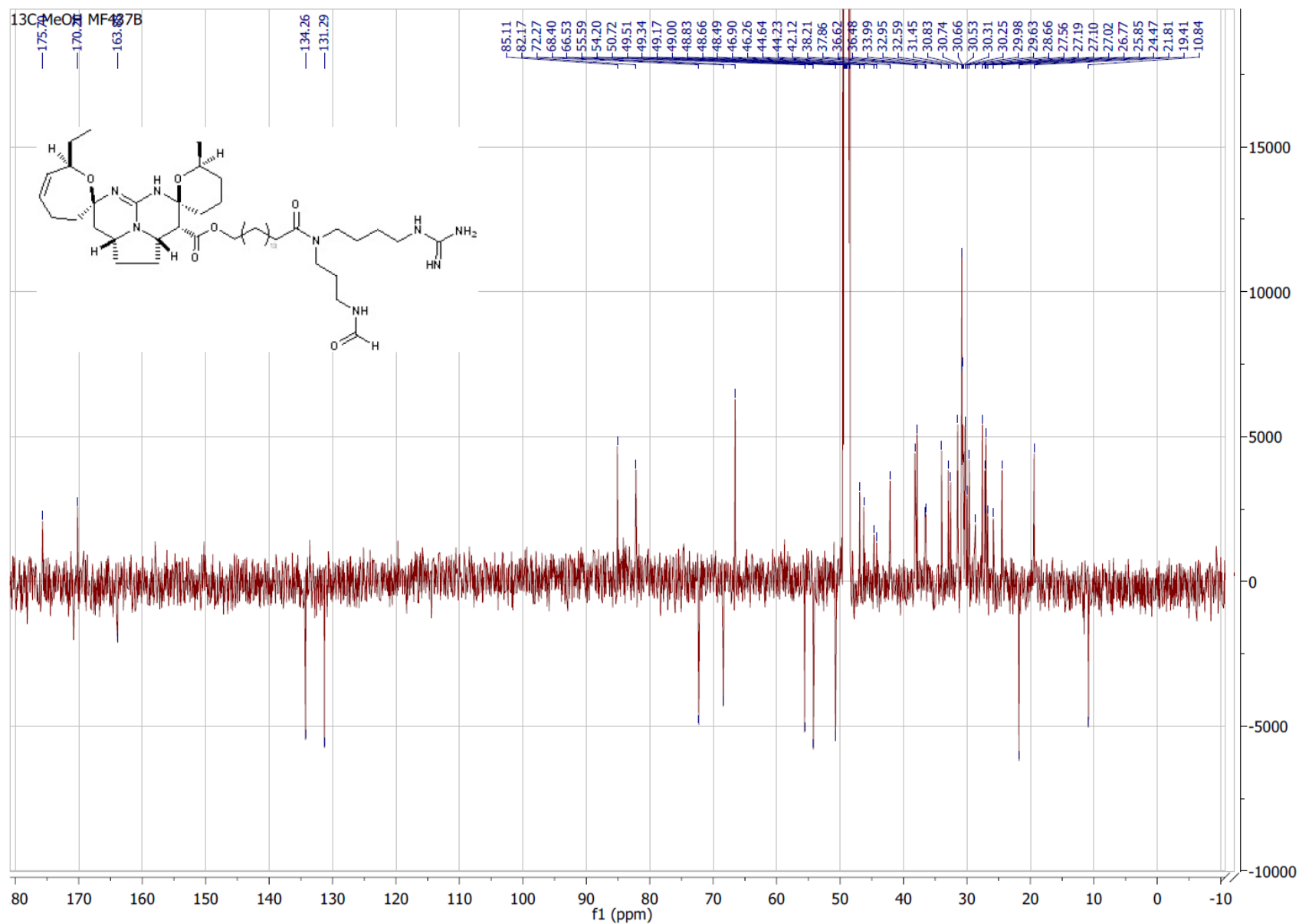


Figure S19: ^1H - ^1H COSY NMR (500 MHz, MeOD) spectrum for ptilomycalin F (**3**)

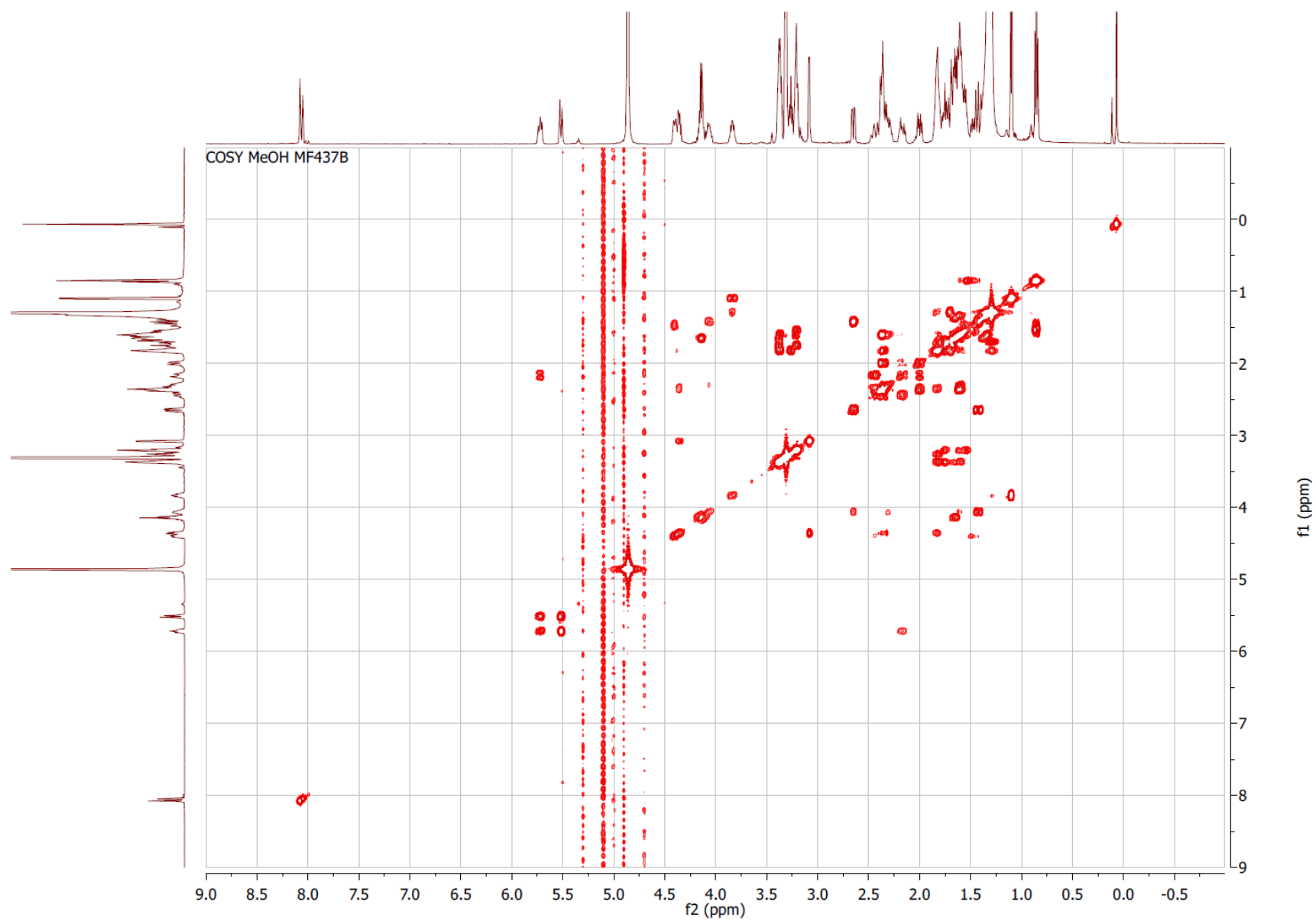


Figure S20: HSQC NMR (500 MHz, MeOD) spectrum for ptilomycalin F (**3**)

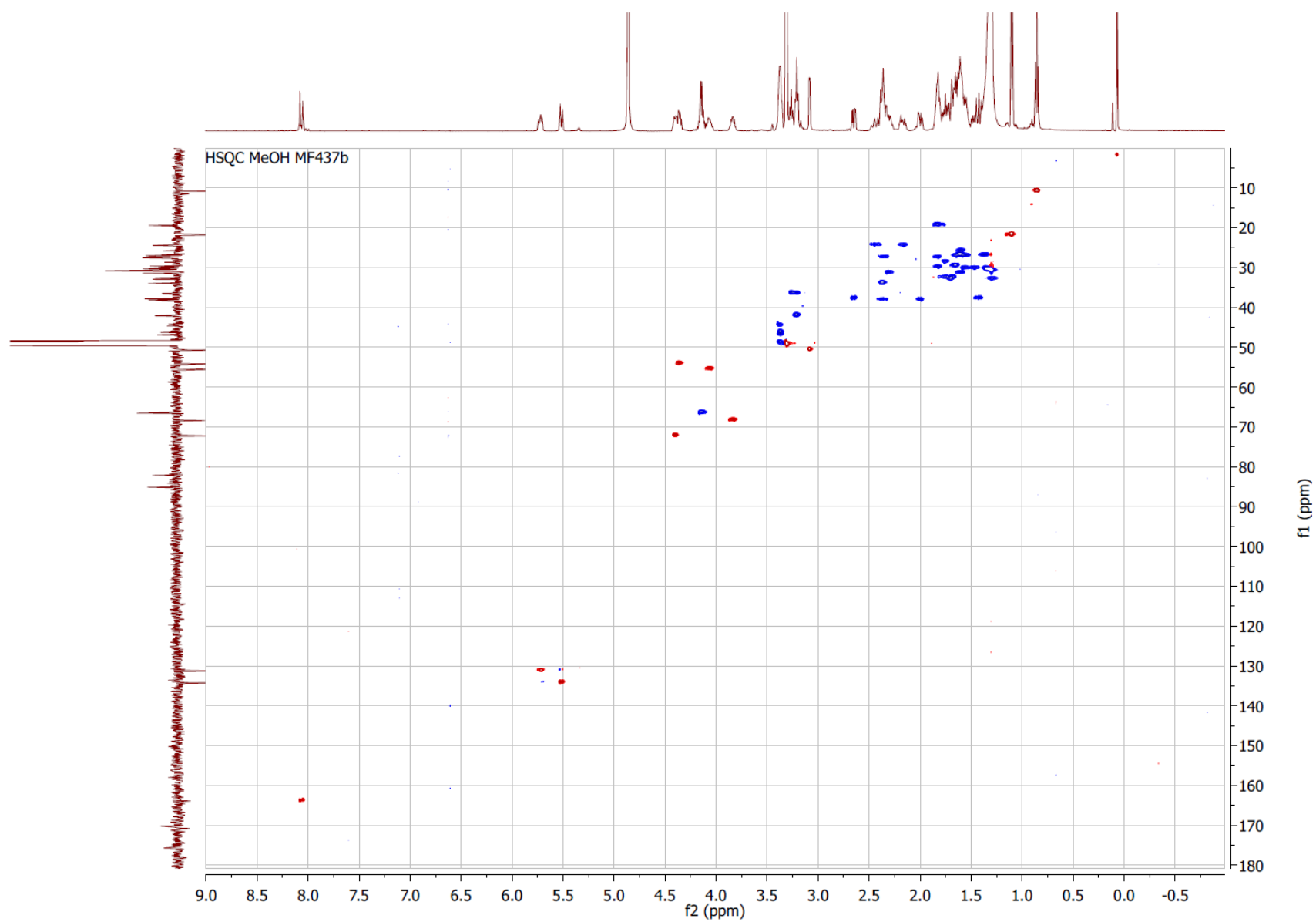


Figure S21: ^1H - ^{13}C HMBC NMR (500 MHz, MeOD) spectrum for ptilomycalin F (**3**)

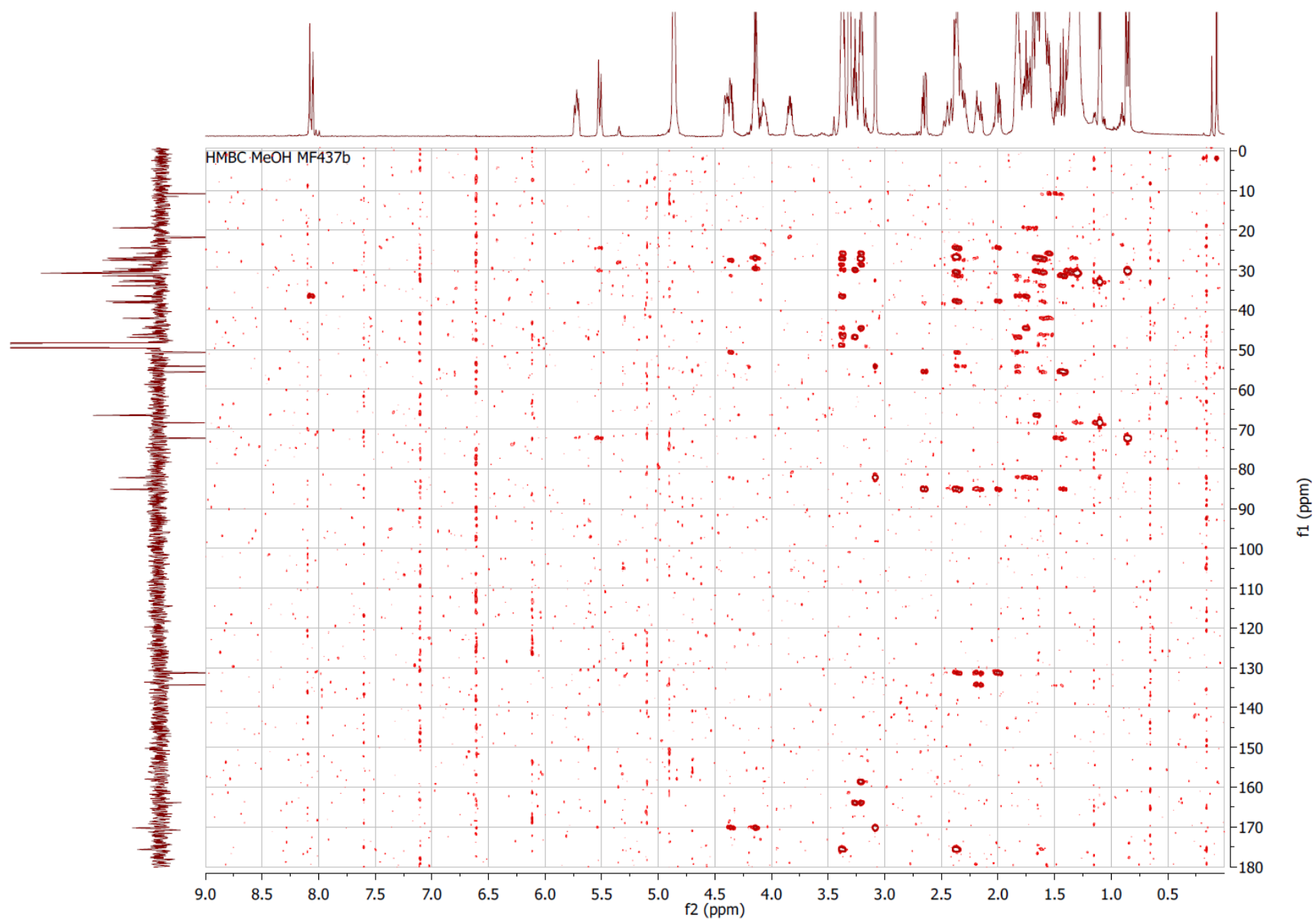


Figure S22: ^1H - ^1H TOCSY NMR (500 MHz, MeOD) spectrum for ptilomycalin F (**3**)

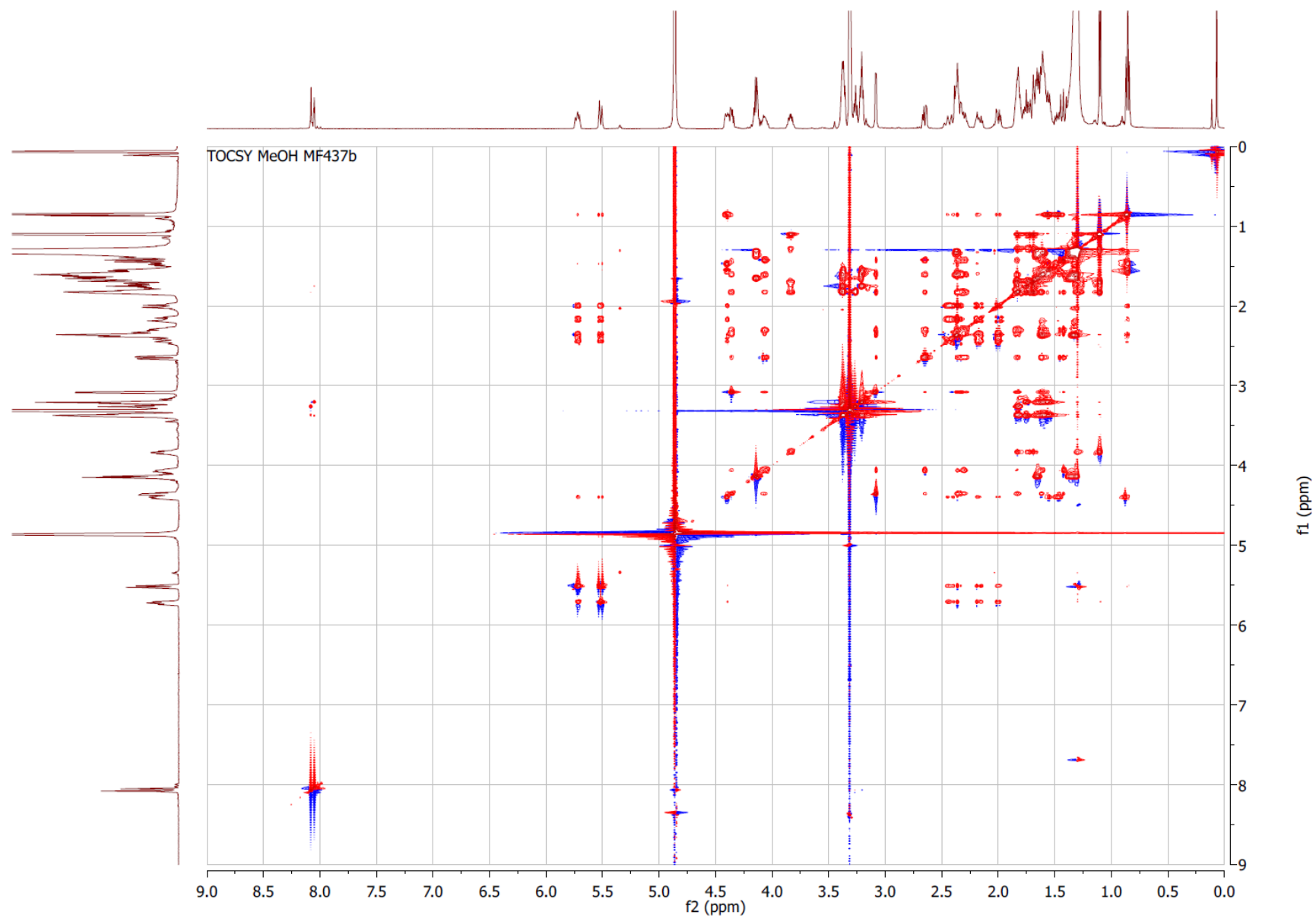


Figure S23: ^1H - ^1H NOESY NMR (500 MHz, MeOD) spectrum for ptilomycalin F (**3**)

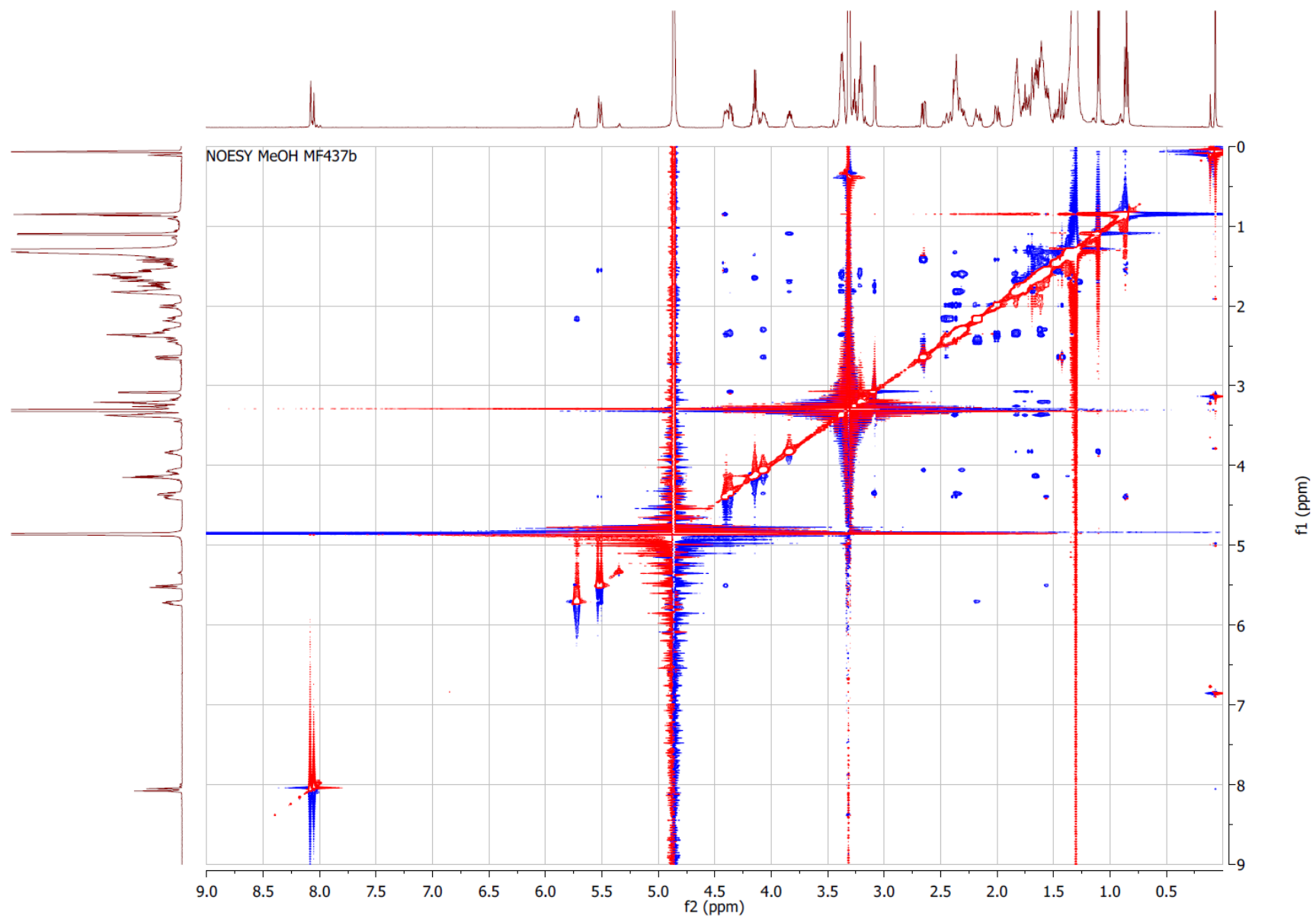


Figure S24: UPLC-HRMS of the ptilomycalins G (**4**; RT 20.99 min; Area 12107) and H (**5**; RT 20.94 min; Area 6475) mixture (approximately 2:1 mixture)

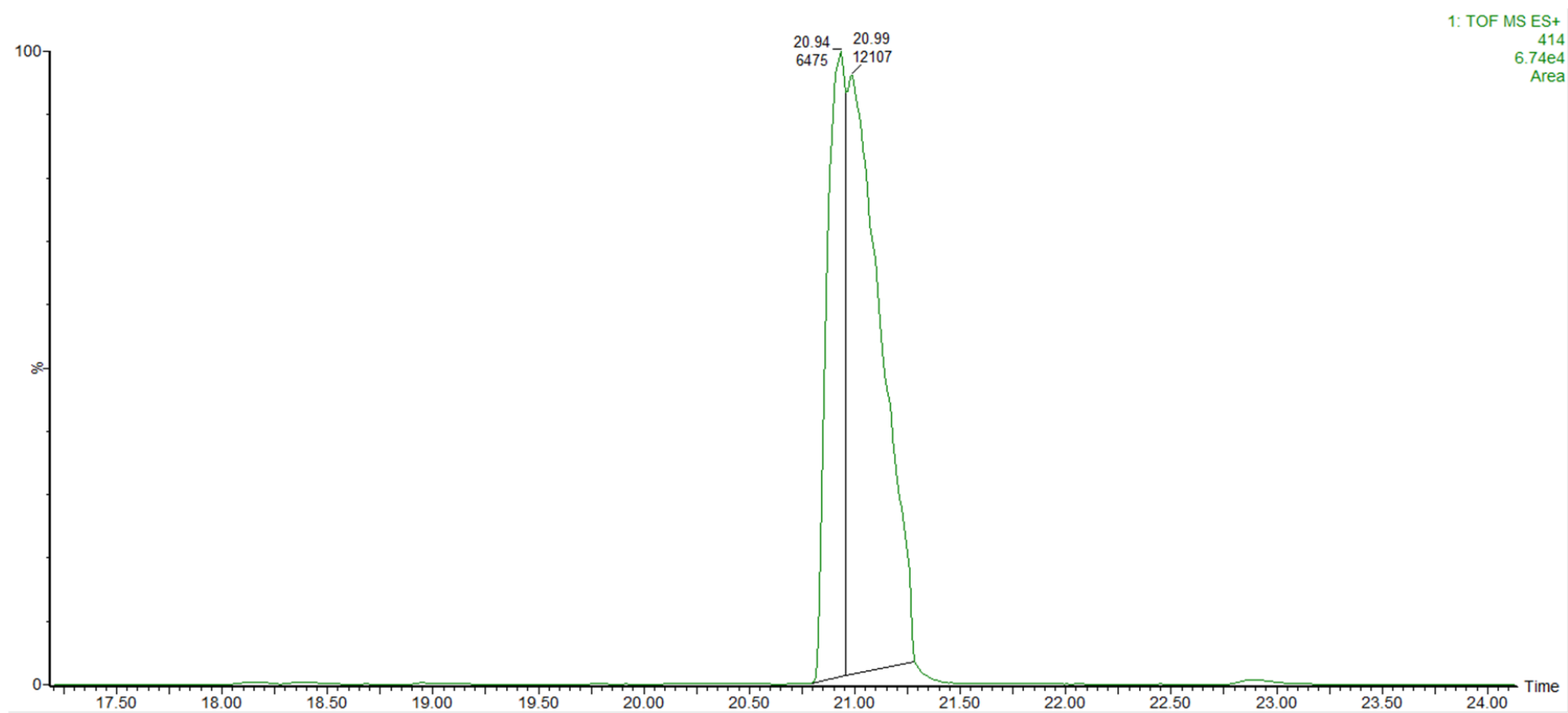


Figure S25: HRMS-HRMS spectrum for ptilomycalin G and ptilomycalin H (4+5)

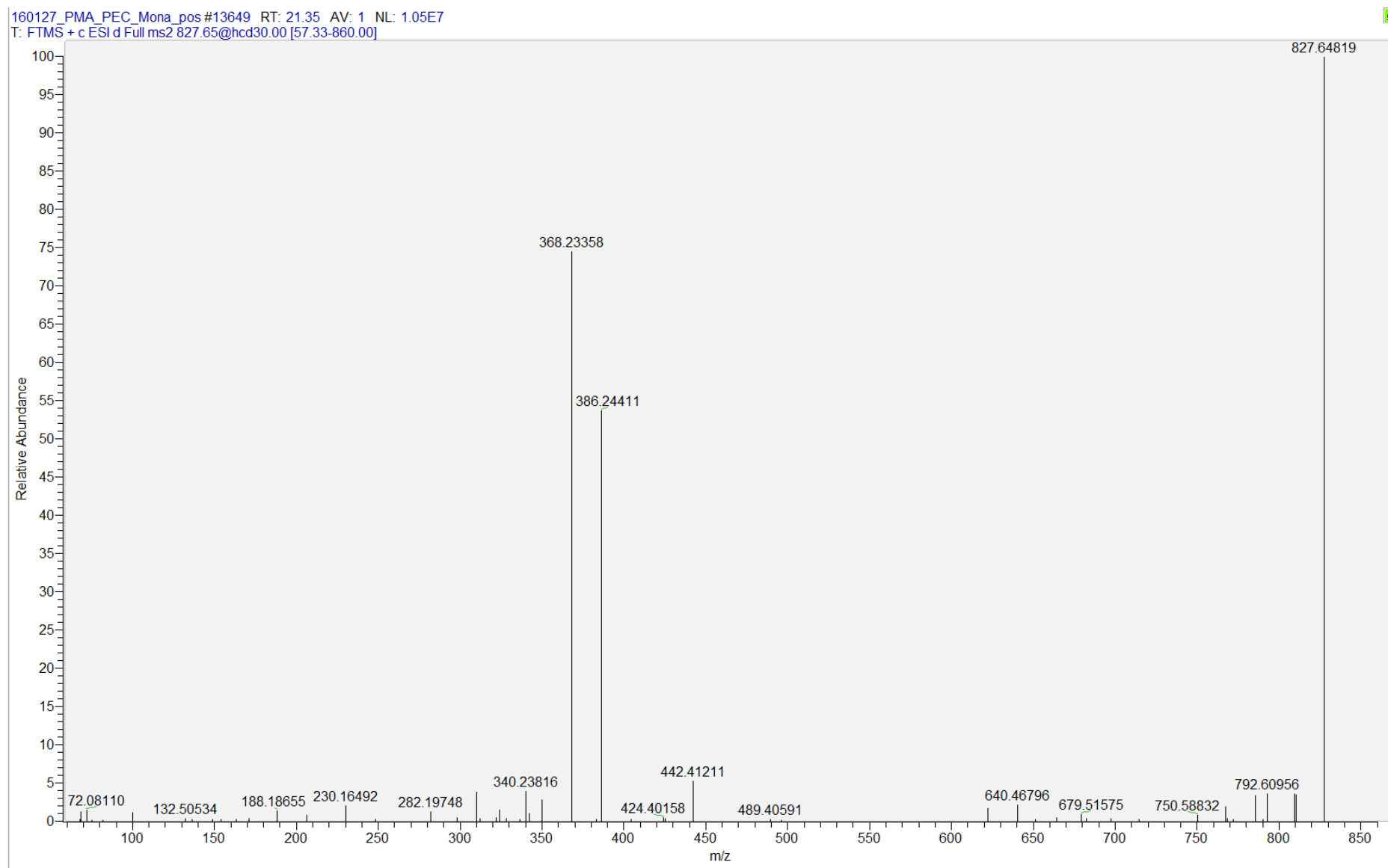


Figure S26: ^1H NMR (500 MHz, MeOD) spectrum for ptilomycalin G and ptilomycalin H (**4 + 5**)

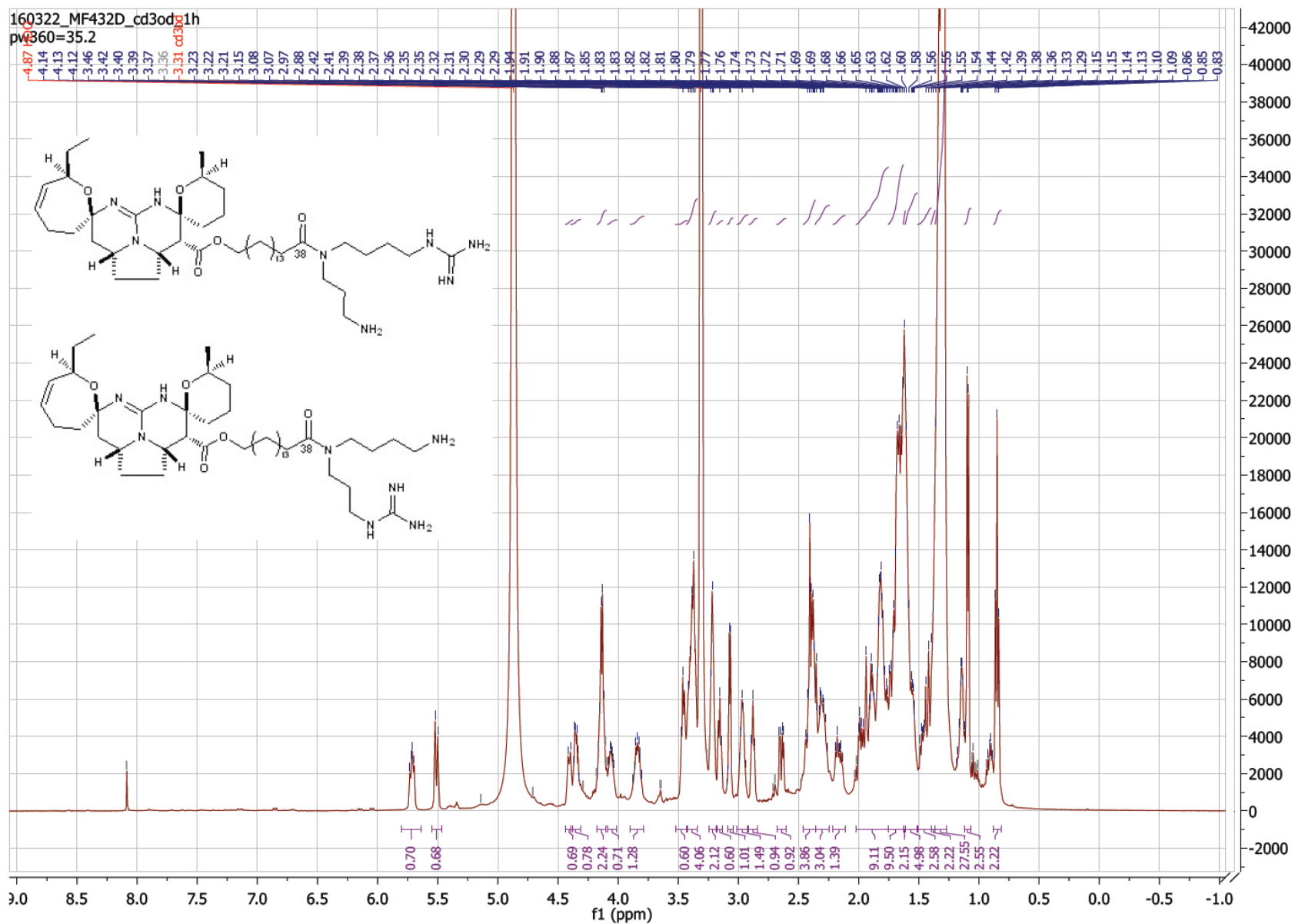


Figure S27: ^1H - ^1H COSY NMR (500 MHz, MeOD) spectrum for ptilomycalin G and ptilomycalin H (4 + 5)

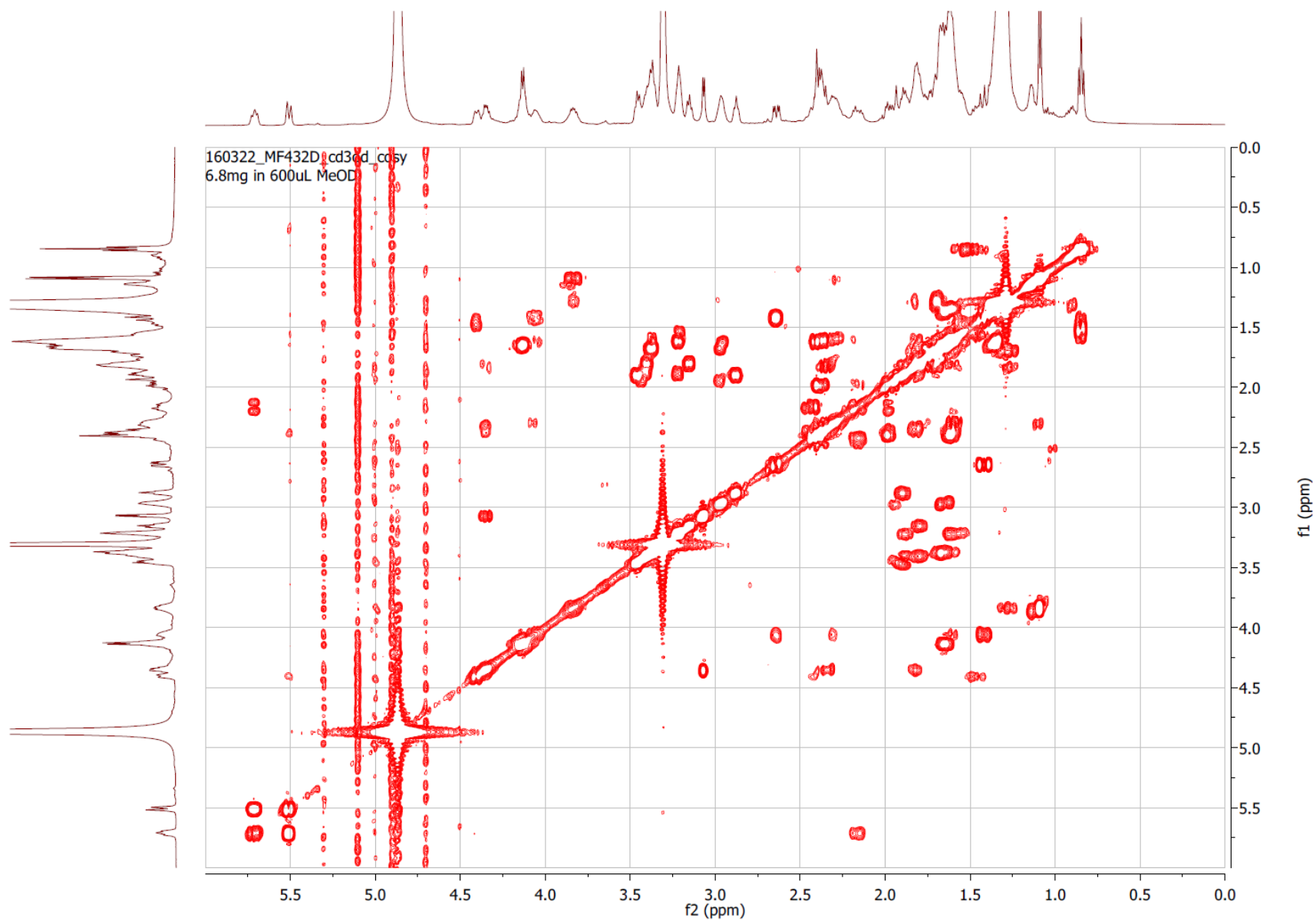


Figure S28: HSQC NMR (500 MHz, MeOD) spectrum for ptilomycalin G and ptilomycalin H (4 + 5)

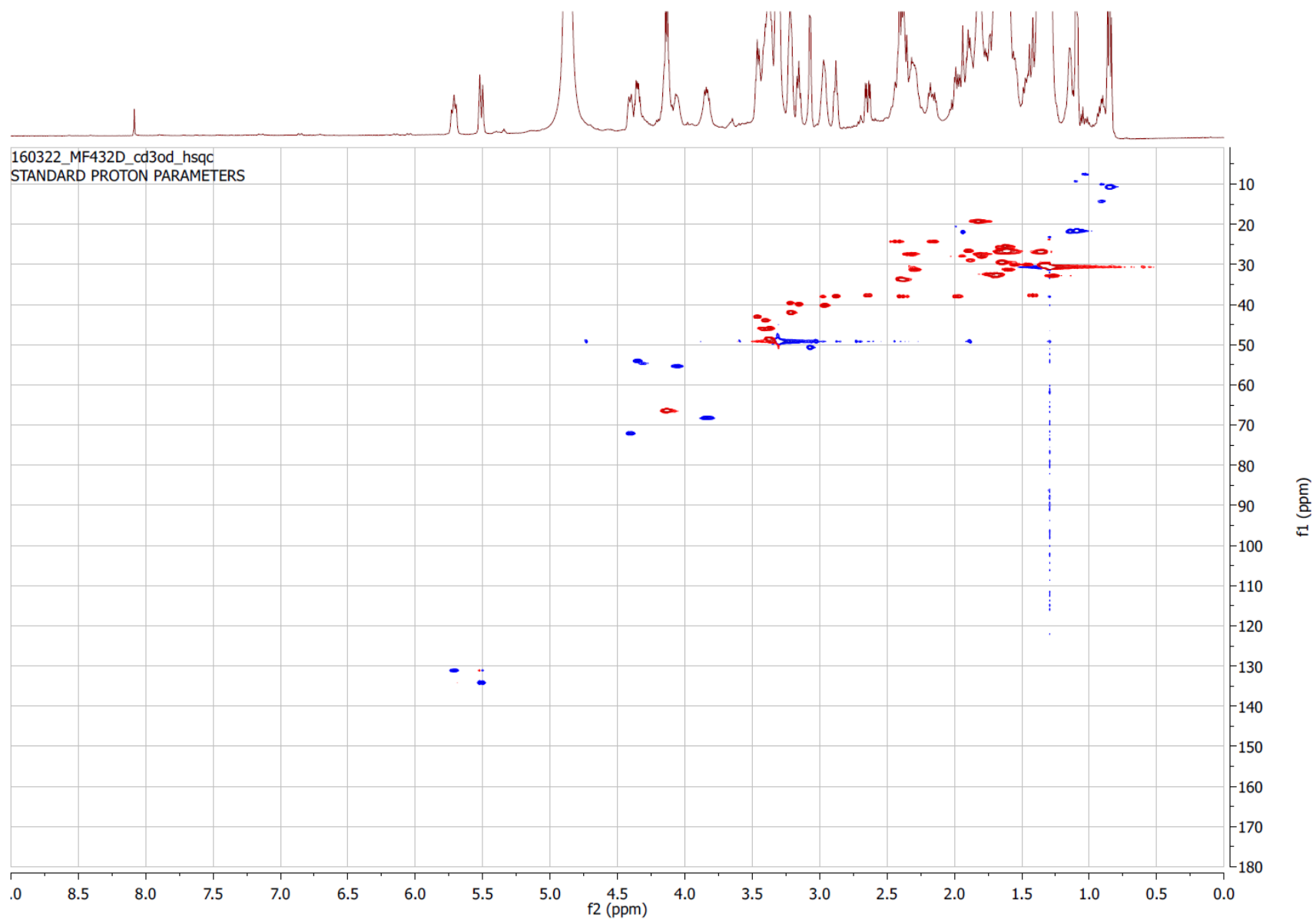


Figure S29: ^1H - ^{13}C HMBC NMR (500 MHz, MeOD) spectrum for ptilomycalin G and ptilomycalin H (4 + 5)

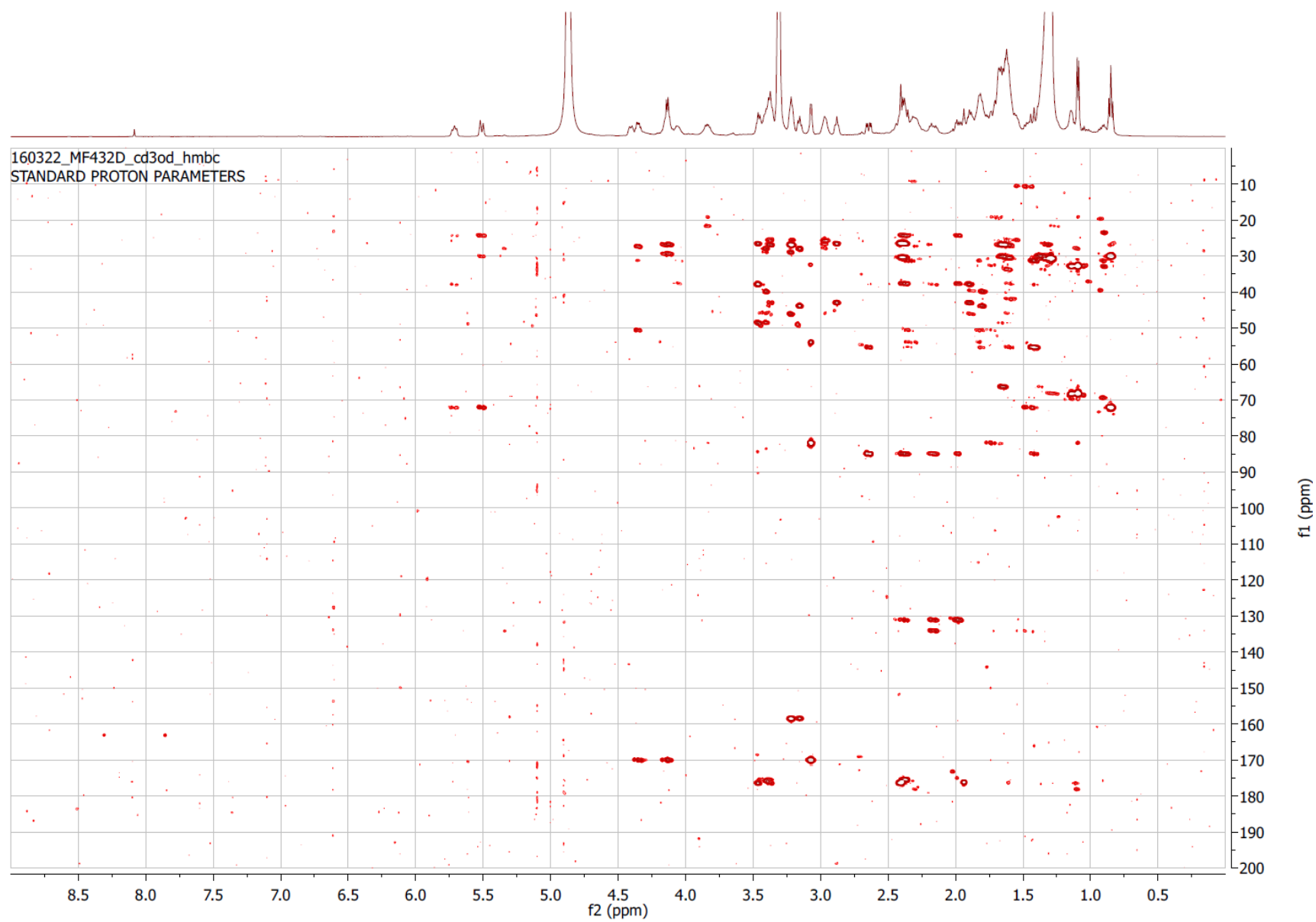


Figure S30: ^1H - ^1H TOCSY NMR (500 MHz, MeOD) spectrum for ptilomycalin G and ptilomycalin H (4 + 5)

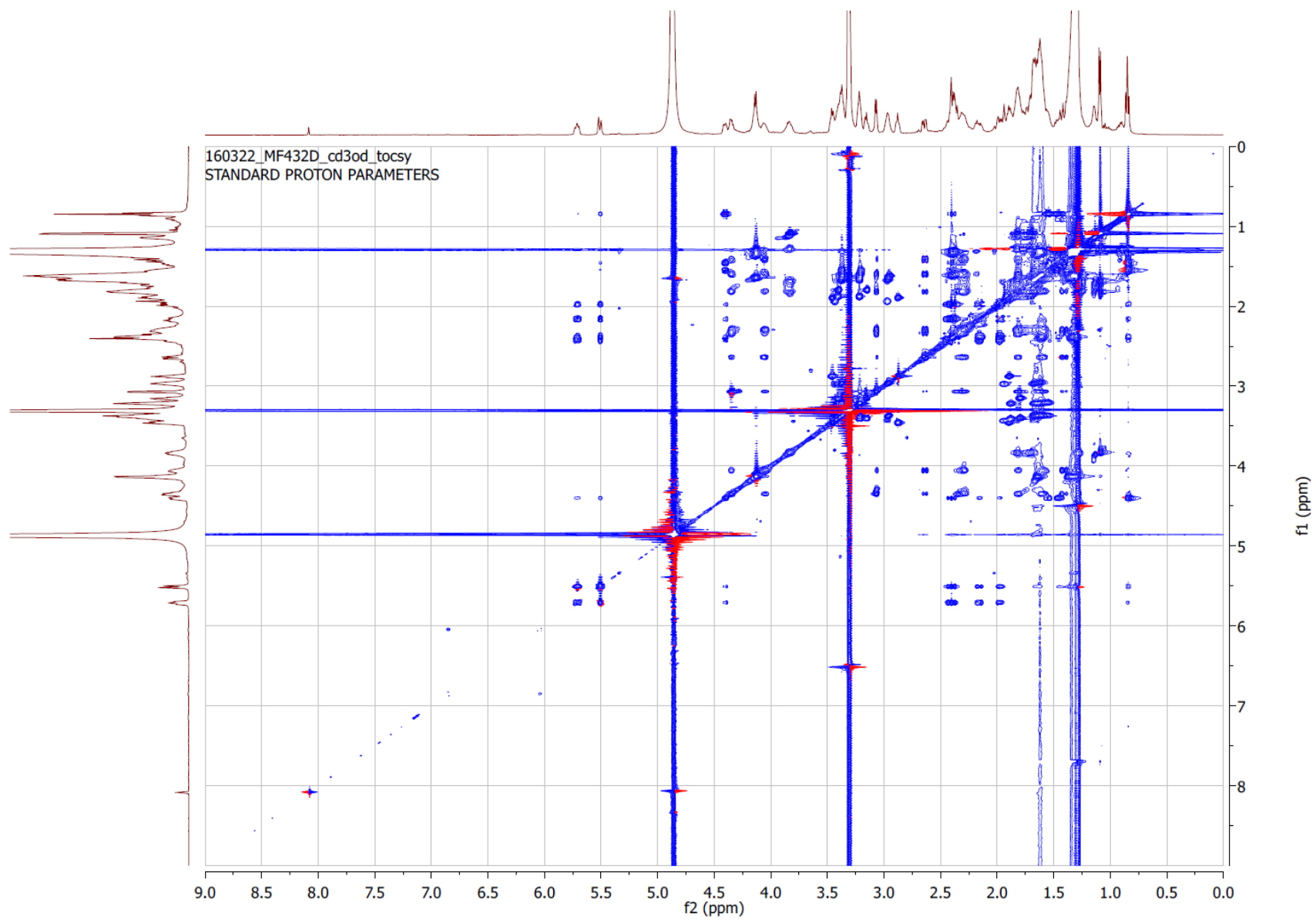


Figure S31: ^1H - ^1H NOESY NMR (500 MHz, MeOD) spectrum for ptilomycalin G and ptilomycalin H (4 + 5)

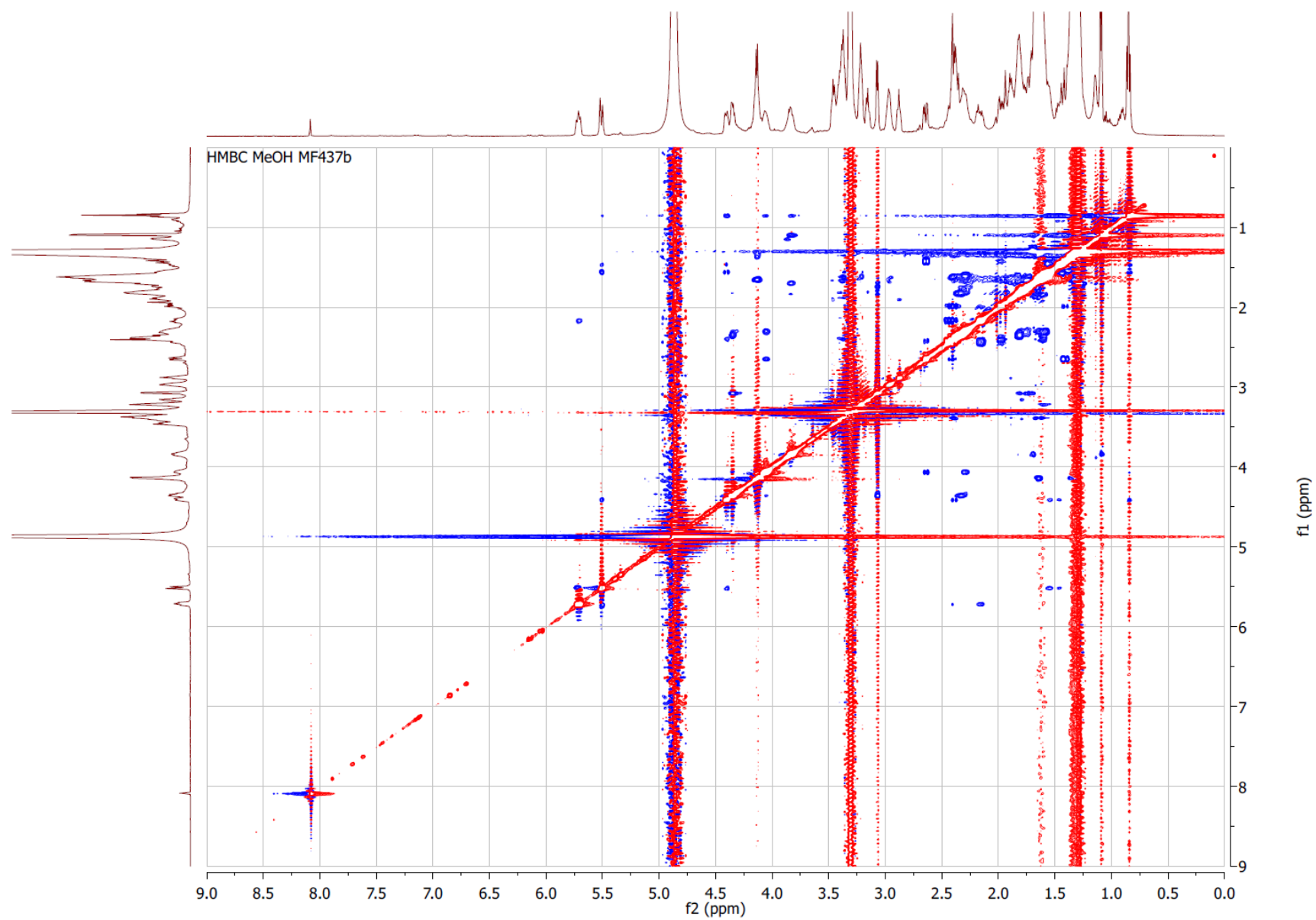


Figure S32: ^1H NMR (500 MHz, MeOD) spectrum for crambescidin 800 (**7**)

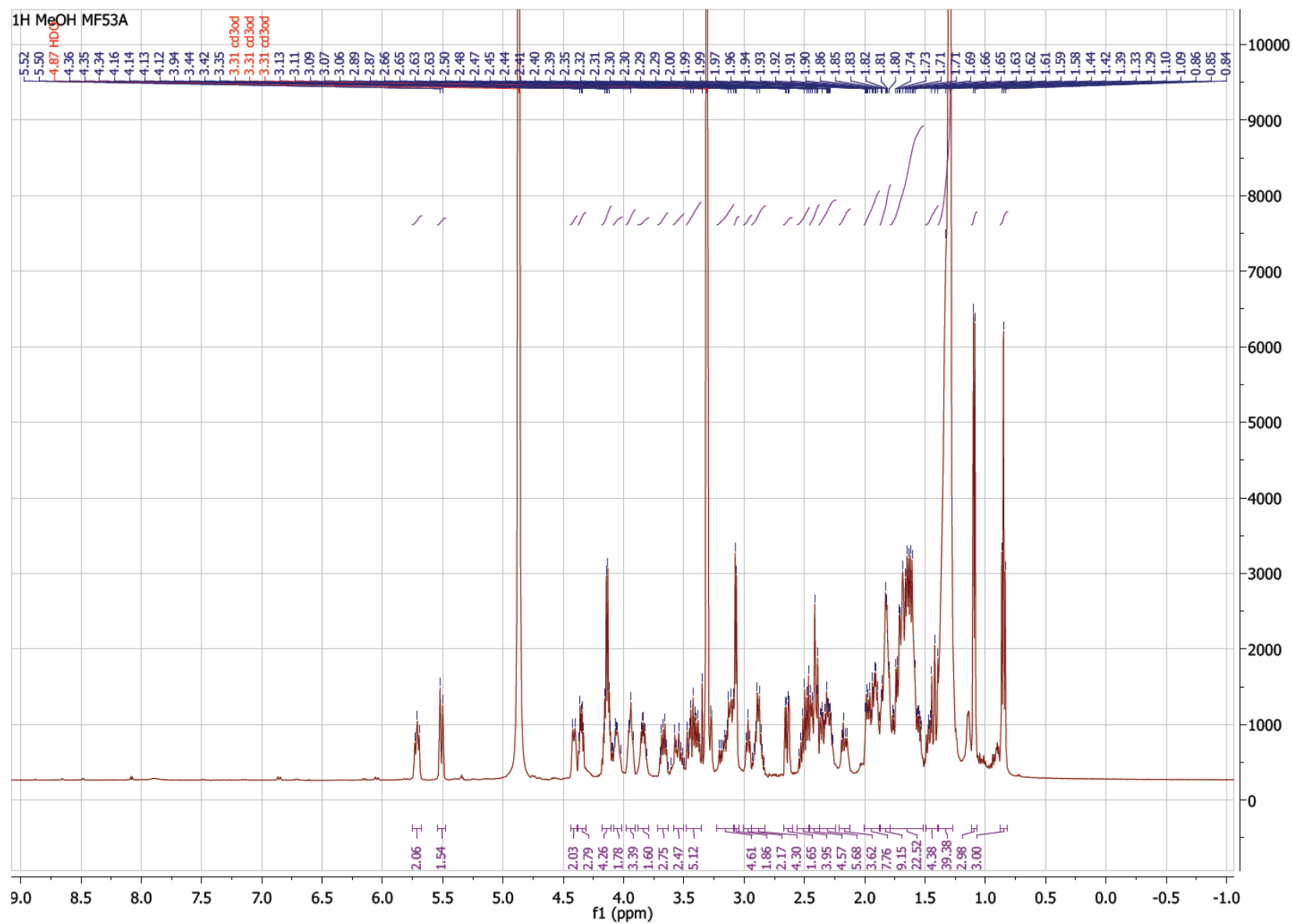


Figure S33: ^{13}C NMR (125 MHz, MeOD) spectrum for crambescidin 800 (**7**)

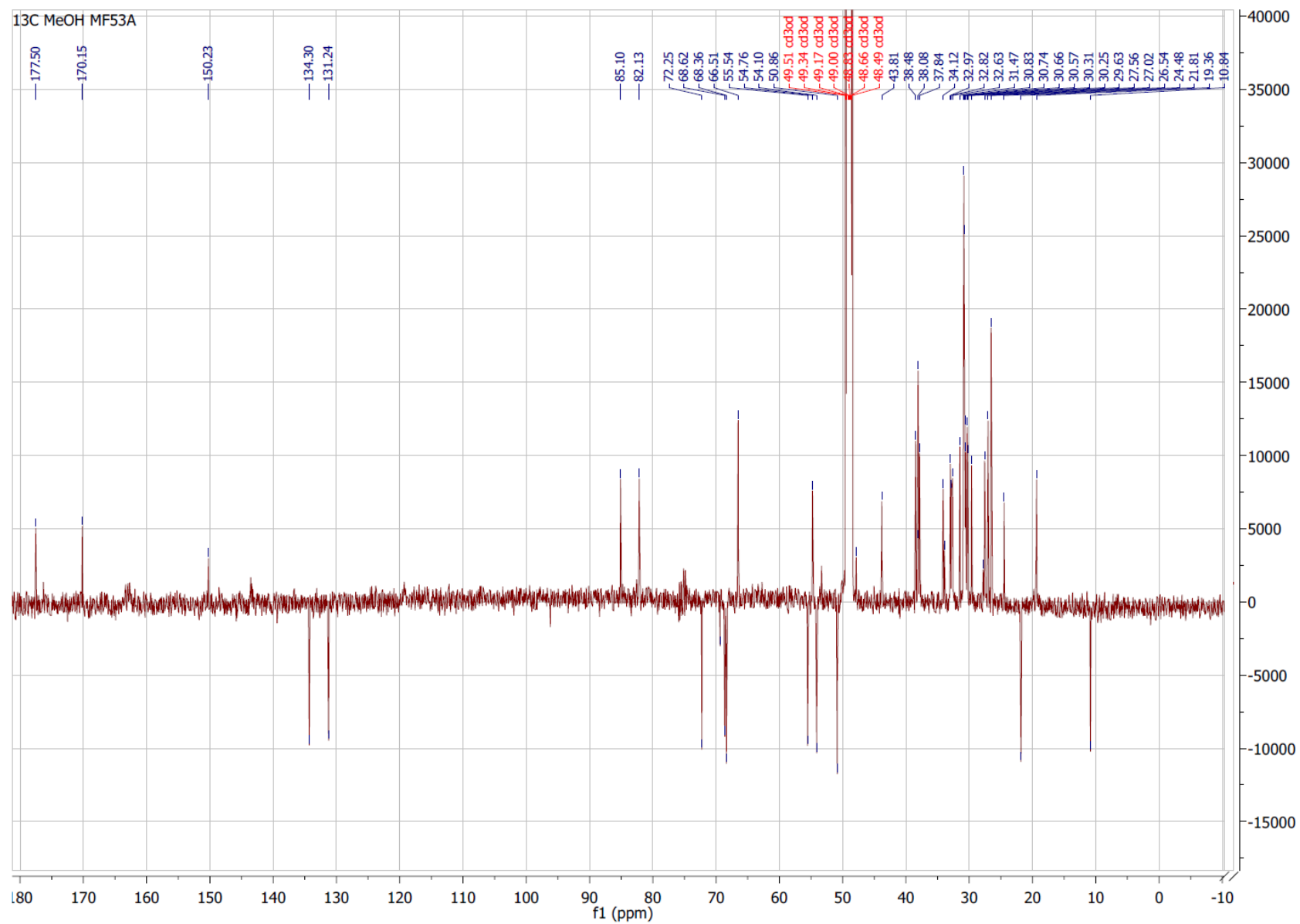


Figure S34: ^1H NMR (500 MHz, MeOD) spectrum for crambescidin 359 (**7**)

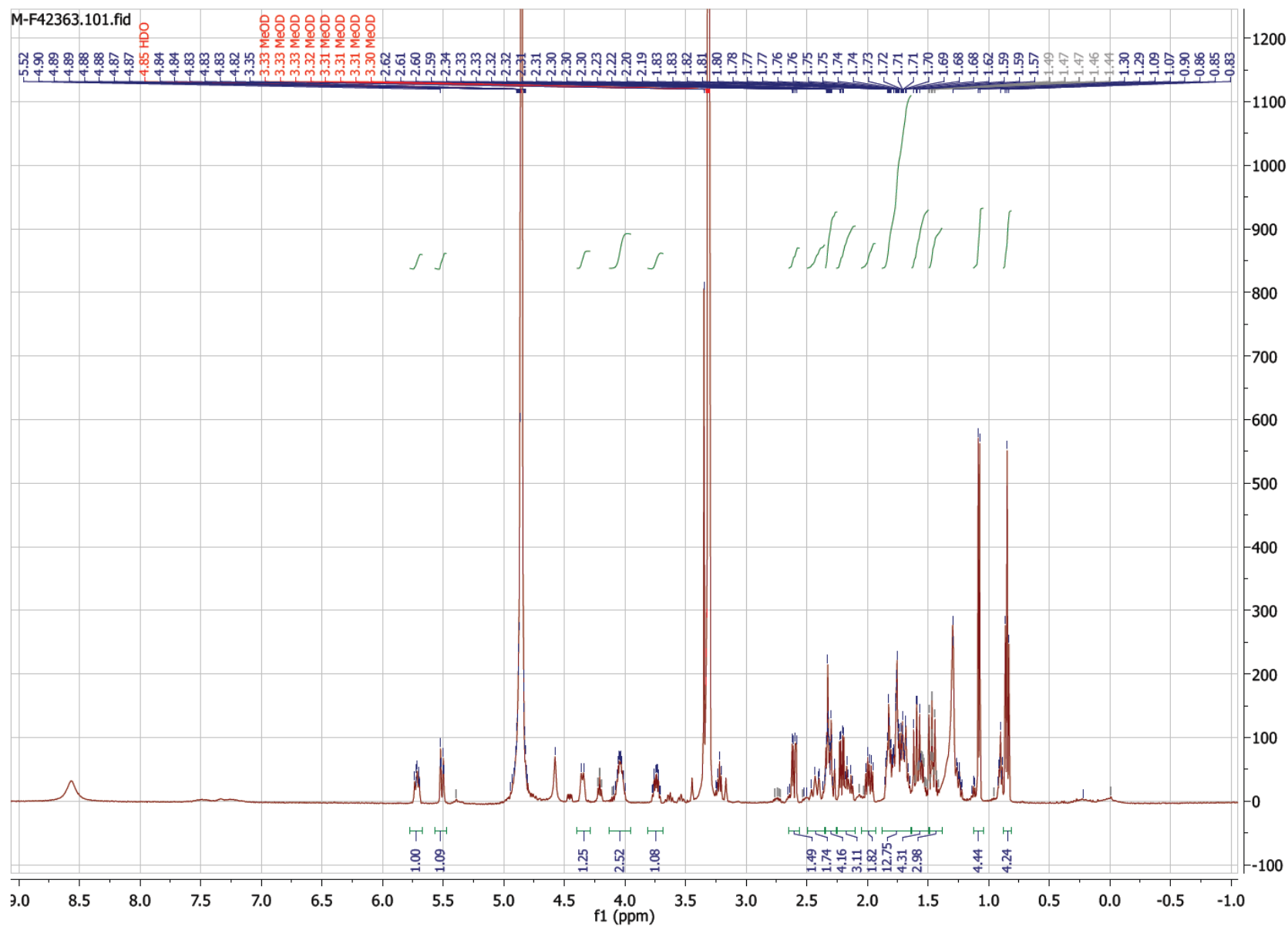


Figure S35: ^1H NMR (500 MHz, MeOD) spectrum for crambescidic acid (**8**)

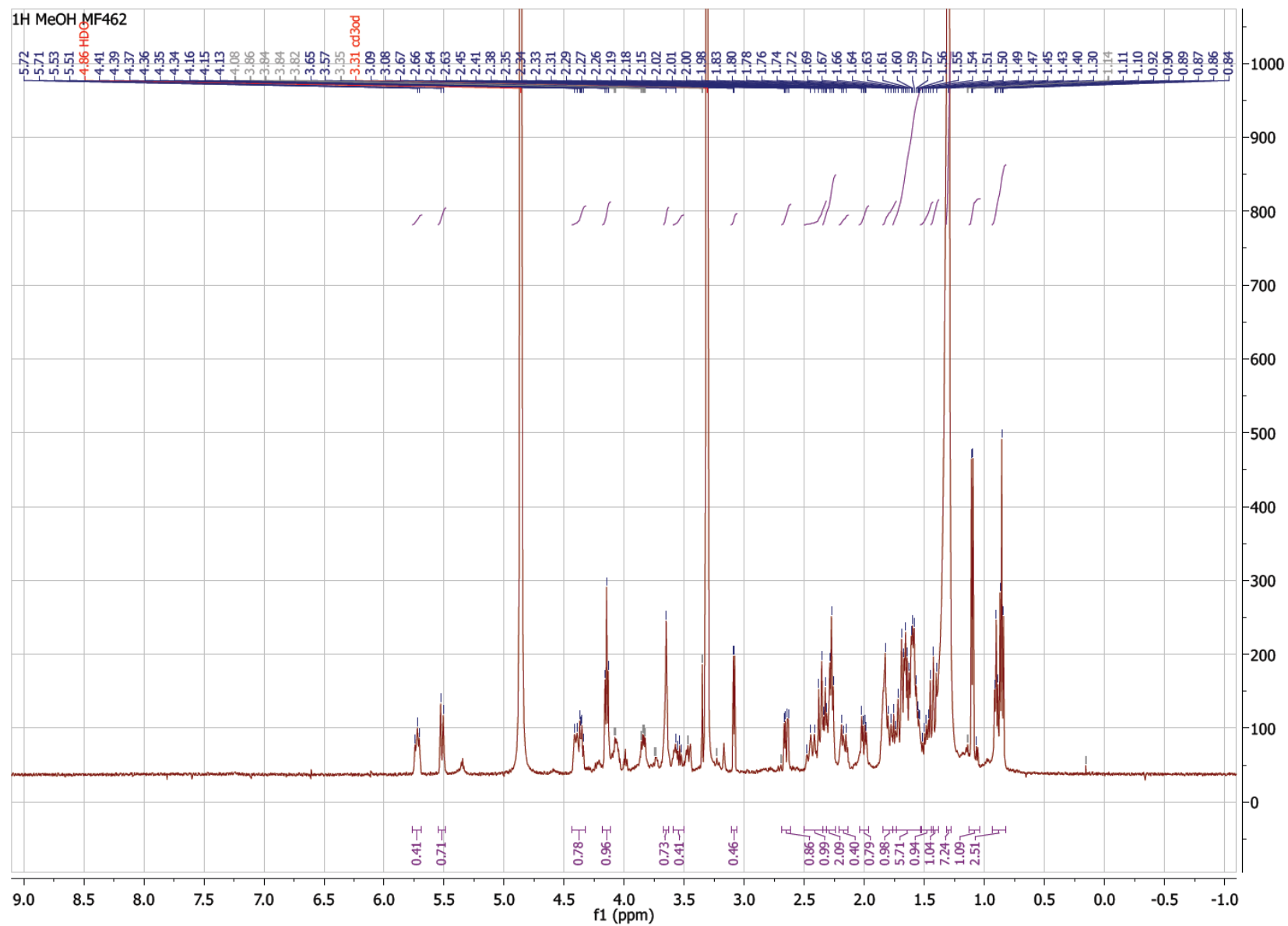


Figure S36: ^1H NMR (500 MHz, MeOD) spectrum for fromiamycalin (**9**)

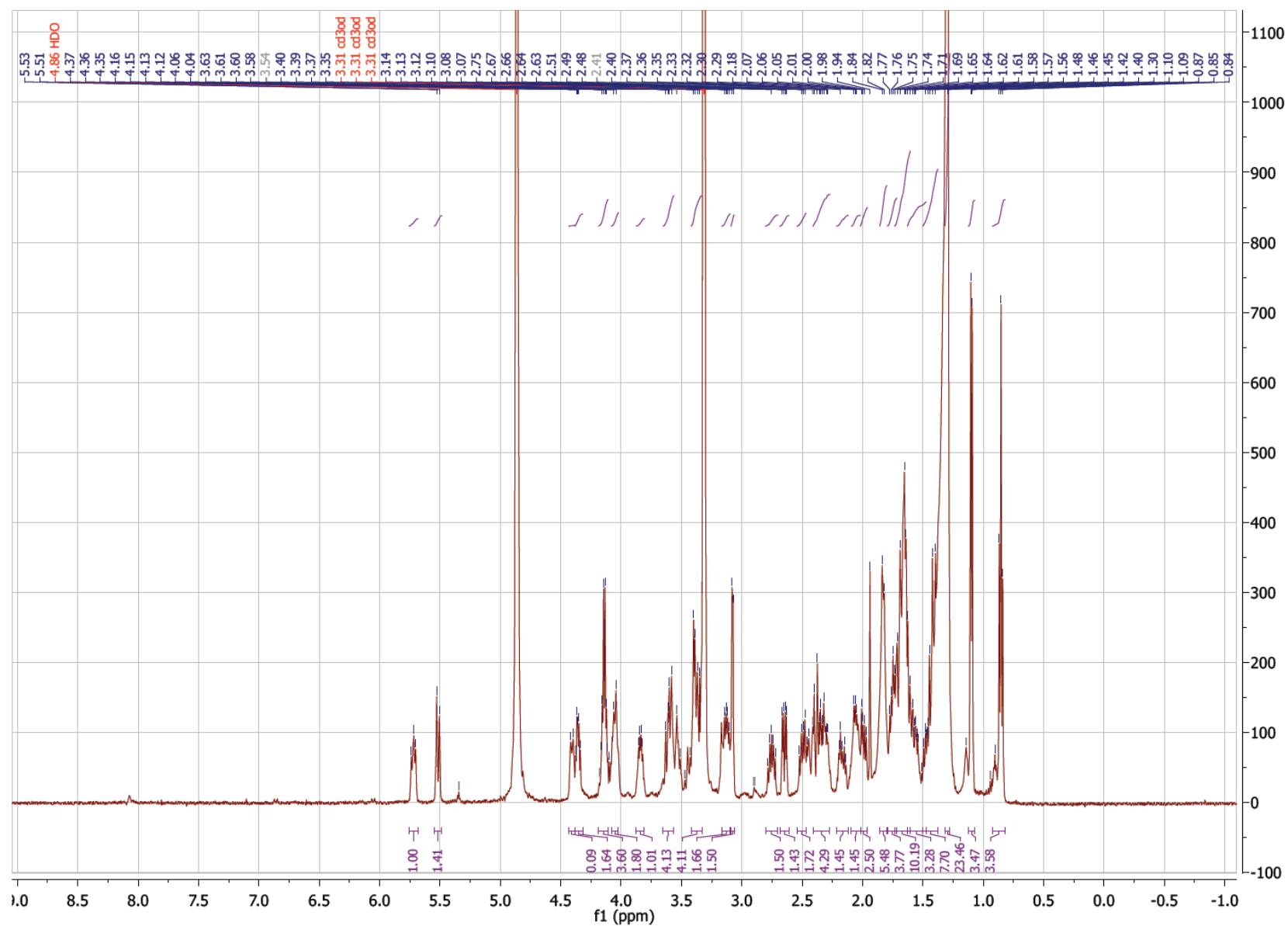


Table S1: 1D and 2D NMR (500 MHz, CD₃OD) data for ptilomycalin E (2)

position	δC , type	δH (J in Hz)	COSY (1H - 1H)	HMBC (1H - ^{13}C)
1	10.9, CH ₃	0.87 (t, 7.3)	H2	2, 3
2	29.6, CH ₂	1.47 (m)	H1, H3	1, 3, 4
3	72.2, CH	4.45 (brd, 9.4)	H2, H4	2
4	134.4, CH	5.52 (brd, 11.0)	H5	2, 3, 6
5	131.2, CH	5.72 (brdd, 9.9 ; 7.8)	H4, H6a	3, 6, 7
6	24.5, CH ₂	2.17 (m) ; 2.46 (m)	H5, H7	4, 5, 7, 8
7	37.9, CH ₂	2.00 (m) ; 2.49 (m)	H6	5, 6, 8, 9
8	85.1, C	-	-	-
9	37.8, CH ₂	1.43 (m) ; 2.65 (dd, 13.0 ; 4.8)	H10	7, 8, 10
10	55.4, CH	4.06 (m)	H9, H11	-
11	31.5, CH ₂	1.61 (m) ; 2.31 (m)	H10, H12	9, 10
12	27.6, CH ₂	1.83 (m) ; 2.33 (m)	H11, H13	10, 11, 13, 14
13	53.9, CH	4.36 (dt, 9.2 ; 5.4)	H12, H14	12, 14, 22
14	51.2, CH	3.06 (d, 5.1)	H13, H15	13, 15, 16, 22
15	82.1, C	-	-	-
16	32.8, CH ₂	1.72 (m)	H17	14, 15, 17
17	19.4, CH ₂	1.78 (m) ; 2.00 (m)	H16, H18	16, 18
18	33.0, CH ₂	1.28 (m) ; 1.72 (m)	H17, H19	17, 19, 20
19	68.3, CH ₂	3.87, (m)	H18, H20	20
20	21.9, CH ₃	1.10 (d, 6.2)	H19	18, 19
21	150.4, C	-	-	-
22	170.1, C	-	-	-
23	66.5, CH ₂	4.14 (m)	H24	22, 24
24	27.0, CH ₂	1.66 (m)	H23, H25	23
25 – 35	30.0 – 31.0, CH ₂	1.31 (m)	-	-
36	26.7, CH ₂	1.63 (m)	H35, H37	37, 38
37	33.9, CH ₂	2.40 (m)	H36	36, 38
38	175.7, C	-	-	-
39	44.2, CH ₂ (2a) 46.1, CH ₂ (2b)	3.42 (m) (2a) 3.43 (m) (2b)	H40	38, 40, 41, 43
40	28.2, CH ₂ (2a) 29.2, CH ₂ (2b)	1.82 (m) (2a) 1.90 (m) (2b)	H39, H41	39, 41
41	40.1, CH ₂ (2a) 39.8, CH ₂ (2b)	3.18 (t, 6.7) (2a) 3.23 (m) (2b)	H40	39, 40, 42
42	158.7, C	-	-	-
43	49.0, CH ₂ (2a) 46.3, CH ₂ (2b)	3.40 (m) (2a) 3.40 (m) (2b)	H44	38, 44
44	27.1, CH ₂	1.66 (m)	H43	43
45	27.1, CH ₂	1.61 (m)	H46	44
46	42.1, CH ₂	3.23 (m)	H45	44, 45, 47
47	158.7, C	-	-	-

Table S2: 1D and 2D NMR (500 MHz, CD₃OD) data for ptilomycalin F (3)

position	δ C, type	δ H (J in Hz)	COSY (^1H - ^1H)	HMBC (^1H - ^{13}C)
1	10.8, CH ₃	0.85 (t, 7.3)	H2	2, 3
2	30.3, CH ₂	1.47 (m) ; 1.56 (m)	H1, H3	1, 3, 4
3	72.3, CH	4.45 (brd, 9.5)	H2, H4	2
4	134.3, CH	5.52 (brd, 11.0)	H5	2, 3, 6
5	131.3, CH	5.72 (m)	H4, H6a	3, 6, 7
6	24.5, CH ₂	2.16 (m) ; 2.44 (m)	H5, H7	4, 5, 7, 8
7	38.2, CH ₂	2.00 (m) ; 2.36 (m)	H6	5, 6, 8, 9
8	85.1, C	-	-	-
9	37.8, CH ₂	1.42 (m) ; 2.65 (dd, 12.9 ; 4.8)	H10	7, 8, 10
10	55.6, CH	4.07 (m)	H9, H11	-
11	31.4, CH ₂	1.61 (m) ; 2.31 (m)	H10, H12	9, 10
12	27.5, CH ₂	1.82 (m) ; 2.35 (m)	H11, H13	10, 11, 13, 14
13	54.2, CH	4.36 (dt, 9.5 ; 5.6)	H12, H14	12, 14, 22
14	50.7, CH	3.08 (d, 5.0)	H13, H15	13, 15, 16, 22
15	82.2, C	-	-	-
16	32.9 CH ₂	1.70 (m)	H17	14, 15, 17
17	19.4, CH ₂	1.82 (m) ; 1.77 (m)	H16, H18	16, 18
18	32.9, CH ₂	1.29 (m) ; 1.70 (m)	H17, H19	17, 19, 20
19	68.4, CH ₂	3.83 (m)	H18, H20	20
20	21.8, CH ₃	1.10 (d, 6.2)	H19	18, 19
21	150.4, C	-	-	-
22	170.2, C	-	-	-
23	66.5, CH ₂	4.14 (m)	H24	22, 24
24	29.6, CH ₂	1.66 (m)	H23, H25	23
25 – 35	30.0 – 31.0, CH ₂	1.31 (m)	-	-
36	26.8, CH ₂	1.60 (m)	H35, H37	37, 38
37	34.0, CH ₂	2.37 (m)	H36	36, 38
38	175.7, C	-	-	-
39	46.9, CH ₂	3.36 (m)	H40	38, 40, 41, 43
40	30.0, CH ₂	1.82 (m)	H39, H41	39, 41
41	36.5, CH ₂ (3a) 36.6, CH ₂ (3b)	3.26 (t, 6.8) (3a) 3.21, t (6.8) (3b)	H40	39, 40, 42
42	163.9, CH (3a) 164.0, CH (3b)	8.08 (s) (3a) 7.98 (s) (3b)	-	41
43	46.2, CH ₂	3.36 (m)	H44	38, 44
44	25.8, CH ₂	1.60 (m)	H43	43
45	27.1, CH ₂	1.62 (m)	H46	44
46	42.1, CH ₂	3.21 (m)	H45	44, 45, 47
47	158.7, C	-	-	-

Table S3: 1D and 2D NMR (500 MHz, CD₃OD) data for ptilomycalin G (4)

position	δC , type	δH (J in Hz)	COSY (1H - 1H)	HMBC (1H - ^{13}C)
1	10.7, CH ₃	0.85, (t, 7.3)	H2	2, 3
2	30.1, CH ₂	1.46 (m) ; 1.55 (m)	H1, H3	1, 3, 4
3	72.1, CH	4.41 (brd, 10.3)	H2, H4	2
4	134.1, CH	5.51 (brd 10.9)	H5	2, 3, 6
5	131.1, CH	5.71 (m)	H4, H6a	3, 6, 7
6	24.3, CH ₂	2.16 (m) ; 2.42 (m)	H5, H7	4, 5, 7, 8
7	38.0, CH ₂	1.98 (m) ; 2.38 (m)	H6	5, 6, 8, 9
8	84.9, C	-	-	-
9	37.7, CH ₂	1.42 (m) ; 2.64 (dd, 12.8 ; 4.7)	H10	7, 8, 10
10	55.4, CH	4.06 (m)	H9, H11	-
11	31.3, CH ₂	1.60 (m) ; 2.30 (m)	H10, H12	9, 10
12	27.4, CH ₂	1.81 (m) ; 2.32 (m)	H11, H13	10, 11, 13, 14
13	54.0, CH	4.35 (dt 9.7 ; 5.3)	H12, H14	12, 14, 22
14	50.7, CH	3.07 (d, 5.0)	H13, H15	13, 15, 16, 22
15	81.9, C	-	-	-
16	32.7, CH ₂	1.70 (m)	H17	14, 15, 17
17	19.2, CH ₂	1.82 (m) ; 1.76 (m)	H16, H18	16, 18
18	32.8, CH ₂	1.28 (m) ; 1.70 (m)	H17, H19	17, 19, 20
19	68.2, CH ₂	3.83 (m)	H18, H20	20
20	21.7, CH ₃	1.09 (d, 6.1)	H19	18, 19
21	150.3, C	-	-	-
22	170.0, C	-	-	-
23	66.4, CH ₂	4.14 (m)	H24	22, 24
24	29.4, CH ₂	1.65 (m)	H23, H25	23
25 – 35	30.0 – 31.0, CH ₂	1.31 (m)	-	-
36	26.6, CH ₂	1.60 (m)	H35, H37	37, 38
37	33.7, CH ₂	2.39 (m)	H36	36, 38
38	176.3, C	-	-	-
39	46.1, CH ₂ (4a) 43.0, CH ₂ (4b)	3.42 (m) (4a) 3.46 (t, 6.5) (4b)	H40	38, 40, 41, 43
40	27.9, CH ₂ (4a) 26.6, CH ₂ (4b)	1.95 (m) (4a) 1.90 (m) (4b)	H39, H41	39, 41
41	38.0, CH ₂ (4a) 37.9, CH ₂ (4b)	2.98 (m) (4a) 2.88 (t, 6.9) (4b)	H40	39, 40
42	48.5, CH ₂	3.38 (m)	H43	38, 43
43	26.6, CH ₂	1.68 (m)	H42	42
44	26.8, CH ₂	1.60 (m)	H45	43
45	42.0, CH ₂	3.22 (m)	H44	43, 44, 46
46	158.5, C	-	-	-

Table S4: 1D and 2D NMR (500 MHz, CD₃OD) data for ptilomycalin H (5)

position	δC , type	δH (J in Hz)	COSY (1H - 1H)	HMBC (1H - ^{13}C)
1	10.7, CH ₃	0.85 (t, 7.3)	H2	2, 3
2	30.1, CH ₂	1.46 (m) ; 1.55 (m)	H1, H3	1, 3, 4
3	72.1, CH	4.41 (brd, 10.3)	H2, H4	2
4	134.1, CH	5.51 (brd, 10.9)	H5	2, 3, 6
5	131.1, CH	5.71 (m)	H4, H6a	3, 6, 7
6	24.3, CH ₂	2.16 (m) ; 2.42 (m)	H5, H7	4, 5, 7, 8
7	38.0, CH ₂	1.98 (m) ; 2.38 (m)	H6	5, 6, 8, 9
8	84.9, C	-	-	-
9	37.7, CH ₂	1.42 (m) ; 2.64 (dd, 12.8 ; 4.7)	H10	7, 8, 10
10	55.4, CH	4.06 (m)	H9, H11	-
11	31.3, CH ₂	1.60 (m) ; 2.30 (m)	H10, H12	9, 10
12	27.4, CH ₂	1.81 (m) ; 2.32 (m)	H11, H13	10, 11, 13, 14
13	54.0, CH	4.35 (dt, 9.7 ; 5.3)	H12, H14	12, 14, 22
14	50.7, CH	3.07 (d, 5.0)	H13, H15	13, 15, 16, 22
15	81.9, C	-	-	-
16	32.7, CH ₂	1.70 (m)	H17	14, 15, 17
17	19.2, CH ₂	1.82 (m) ; 1.76 (m)	H16, H18	16, 18
18	32.8, CH ₂	1.28 (m) ; 1.70, (m)	H17, H19	17, 19, 20
19	68.2, CH ₂	3.83 (m)	H18, H20	20
20	21.7, CH ₃	1.09 (d, 6.1)	H19	18, 19
21	150.3, C	-	-	-
22	170.0, C	-	-	-
23	66.4, CH ₂	4.14 (m)	H24	22, 24
24	29.4, CH ₂	1.65 (m)	H23, H25	23
25 – 35	30.0 – 31.0, CH ₂	1.31 (m)	-	-
36	26.6, CH ₂	1.60 (m)	H35, H37	37, 38
37	33.7, CH ₂	2.39 (m)	H36	36, 38
38	176.3, C	-	-	-
39	49.1, CH ₂ (5a) 43.9, CH ₂ (5b)	3.40 (m)	H40	38, 40, 41, 43
40	29.0, CH ₂ (5a) 28.0, CH ₂ (5b)	1.89 (m) (5a) 1.80 (m) (5b)	H39, H41	39, 41
41	39.6, CH ₂ (5a) 39.9, CH ₂ (5b)	3.22 (m) (5a) 3.15 (t, 6.8) (5b)	H40	39, 40, 42
42	158.5, C	-	-	-
43	48.5, CH ₂	3.38 (s)	H44	38, 44
44	25.7, CH ₂	1.67 (m)	H43	43
45	26.7, CH ₂	1.63 (m)	H46	44
46	40.2, CH ₂	2.96 (m)	H45	44, 45