Contents **Page Number**

Table S1. NMR spectral data for loggerpeptin A (**1**) at 600 MHz (^{1}H), 150 MHz (^{13}C) in DMSO-d_6

C/H no.		δ_H (*J* in Hz)	δ_C[a]	^{1}H-^{1}H COSY	HMBC[b]	ROESY
Val	1		173.5, s			
	2	4.63, dd (9.5, 4.5)	56.2, d	H-3, NH	1 (Tyr), 3, 4, 5	H-3, H_3-4, H_3-5, H_3-3 (Ala), NH
	3	2.02, m	31.2, d	H-2, H_3-4, H_3-5	4, 5	H-2, H_3-4, H_3-5
	4	0.68, d (6.5)	17.5, q	H-3	2, 3, 5	H_3-4, NH
	5	0.82, d (6.2)	19.6, q	H-3	2, 3, 4	H-2, H-3, N-Me (Tyr),
	NH	7.4, d (9.4)		H-2	2	H-2, H-3, H_3-4, H_3-5, H-2 (Tyr), N-Me (Tyr)
N-Me-Tyr	1		172.2, s			
	2	4.86, dd (11.7, 1.5)	61.3, d	H-3a, H-3b		H-3a, H-3b, H-3b (Phe), H-2 (Phe), H-5/9, H-5/9 (Phe), NH (Val)
	3a	3.07, dd (–13.3, 5.5)	33.1, t	H-2, H-3b	5/9	H-2, H-2 (Phe), H-5/9
	3b	2.66, dd (–14.0, 10.0)		H-2, H-3a	2, 5/9	H-2, H-5/9
	4		127.8, s			
	5/9	6.96, d (8.3)	131.2, d	H-6/8	3, 5/9, 7	H-2, H-3a, H-3b, N-Me, H-6/8, H-2 (Phe)
	6/8	6.74, d (8.3)	115.7, d	H-5/9	4, 6/8, 7	H-5/9, H-3b (Phe)
	7		156.8, s			
	7-OH					
	N-Me	2.72, s	30.7, q		2, 1 (Phe)	H-2, H-2 (Val), H-2 (Phe), H-6 (Ahp), H-5/9, NH (Val)
Phe	1		170.9, s			
	2	4.69, dd (11.4, 3.8)	50.5, d	H-3a, H-3b	2 (Ahp)	H-3a, H-3b, H-3a (Tyr), H-2 (Tyr), H-6 (Ahp), H-5/9, H-5/9 (Tyr), NH (Val)
	3a	2.82, dd (–15.2, 12.2)	35.3, t	H-2, H-3b	5/9	H-2, H-3b, H-6 (Ahp), H-5/9
	3b	1.74, dd (–15.2, 3.1)		H-2, H-3a		H-2, H-3a, H-2 (Tyr), H-6 (Ahp), H-5/9
	4		137.2, s			
	5/9	6.79, d (7.3)	130.1, d	H-6/8	3, 5/9, 7	H-2, H-3a, H-3b, H-4b (Ahp), H-3 (Ahp), H-2 (Tyr), H-6 (Ahp), H-6/8
	6/8	7.13, d (7.3)	128.3, d	H-5/9	4, 6/8	H-5/9
	7	7.10, m	126.6, d		5/9	H-5/9
Ahp	2		170.26, s			
	3	3.58, m	48.9, d	H-4a, H-4b, NH		H-4b, H-5/9 (Phe),H-6/8 (Phe), NH
	4a	2.36, m	21.9 ,t	H-3, H-4b		H-4b, H-5a, H-3 (Thr-1), NH
	4b	1.53, m		H-3, H-4a, H-5a		H-3, H-4b, NH
	5a	1.64, m	29.6, t	H-4b, H-5a, H-6		H-4a, H-4b, H-6
	5b	1.51, m		H-5a, H-6		H-5a, H-6, H-5/9 (Phe)
	6	5.02, br s	74.1, d	H-5a, H-5b		H-4b, H-5a, H-5b, H-3a (Phe), H-3b (Phe),
	6-OH					
	NH	7.03, d (9.0)		H-3	1 (Leu)	H-3, H-4a, H-4b, H-2 (Leu), H-3 (Thr-1), NH (Leu)
Leu	1		171.0, s			
	2	4.16, m	50.7, d	H-3a, H-3b, NH		H_3-5, H-3a, H-4, NH (Ahp), NH
	3a	1.64, m	39.3, t	H-2, H-4		H-2, H-3b, H_3-5, H_3-6
	3b	1.26, m		H-2		H-3a, H_3-6, NH
	4	1.39, m	24.3, d	H-3a, H_3-5, H_3-6		H_3-5, H_3-6, NH
	5	0.68, d (6.8)	21.2, q	H-4	3, 6	H-2, H-3a, H-4
	6	0.79, d (6.8)	23.6, q	H-4	3, 4, 5	H-4

Table S1. Continued

C/H no.		δ$_H$ (*J* in Hz)	δ$_C$[a]	^{1}H-^{1}H COSY	HMBC[b]	ROESY
	NH	8.37, d (8.5)		H-2		H-2, H-3b, H-4, H-2 (Thr-1), H-3 (Thr-1), NH (Ahp)
Thr-1	1		169.3, s			
	2	4.55, d (9.4)	55.1, d	NH	1 (Val)	H-3, H-4 (Leu), H_3-4, NH, NH (Leu)
	3	5.35, br q (6.6)	72.2, d	H_3-4	1 (Val), 4	H-2, H_3-5 (Val), H_3-4, H-2 (Val), NH (Ahp), NH (Leu)
	4	1.15, d (6.6)	18.1, q	H-3	2, 3	H-2, H-3, NH
	NH	7.70, d (9.0)		H-2	1 (Thr-2)	H-2, H_3-4, H-2 (Thr-2), H-3 (Thr-2), H_3-4 (Thr-2), NH (Thr-2)
Thr-2	1		171.1, s			
	2	4.31, dd (8.4, 4.2)	58.1, d	H-3, NH	1	H-3, H_3-4, NH (Thr-1), NH
	3	3.95, m	66.8, d	H-2, H_3-4	1	H-2, H_3-4, NH (Thr-1), NH
	4	0.97, d (6.3)	19.4, q	H-3	2, 3	H-2, H-3, NH
	OH					
	NH	7.81, br		H-2	1 (Ala)	H-3, H_3-4, H-2 (Ala), H_3-3 (Ala)
Ala	1		173.3, s			
	2	4.35, m	48.4, d	H_3-3, NH	1, 3	H_3-3, NH (Thr-2), NH
	3	1.18, d (7.2)	18.4, q	H-2	1, 2	H-2, NH
	NH	8.01, d (7.4)		H-2	1 (Ba)	H-2, H_3-3, H-2 (Ba)
Ba	1		172.3, s			
	2	2.04, m (2H)	37.4, t	H_2-3	1, 3, 4	H-3, NH (Ala)
	3	1.46, m (2H)	18.9, t	H_2-2, H_3-4	1, 2, 4	H-2, H_3-4
	4	0.81, t (7.5)	13.9, q	H_2-3	2	H-2, H-3

[a] Multiplicity derived from HSQC spectrum. [b] Protons showing long-range correlation with indicated carbon.

Table S2. NMR spectral data for loggerpeptin B (**2**) at 600 MHz (^{1}H), 150 MHz (^{13}C) in DMSO-d_6

C/H no.		δ_H (*J* in Hz)	δ_C[a]	^{1}H-^{1}H COSY	HMBC[b]	ROESY
Val	1		169.5, s			
	2	4.66, dd (9.9, 4.7)	55.8, d	H-3, NH	1, 3, 4, 5	H-3, H_3-5, NH
	3	2.06, m	30.8, d	H-2, H_3-4, H_3-5		H-2, H_3-4, H_3-5
	4	0.72, d (6.5)	17.3, q	H-3	2, 3, 5	H-3, NH
	5	0.86, d (6.2)	19.3, q	H-3	2, 3, 4	H-2, NH, N-Me (Tyr)
	NH	7.43, d (9.6)		H-2	1	H-1, H_3-4, H-2 (Tyr), N-Me (Tyr)
N-Me-Tyr	1		170.9, s			
	2	4.90, dd (11.7, 1.8)	60.8, d	H-3a, H-3b		H-2 (Phe), H-5/9, NH (Val)
	3a	3.12, dd (–14.6, 1.5)	32.9, t	H-2, H-3b	5/9	H-2, H-3b, H-5/9
	3b	2.71, m		H-2, H-3a	1, 2, 5/9	H-3a
	4		127.8, s			
	5/9	7.00, d (8.3)	130.3, d	H-6/8	3, 5/9, 7	H-2, H-3a, H-3b, H-6/8, N-Me, H-2 (Phe)
	6/8	6.78, d (8.3)	115.3, d	H-5/9	4	H-5/9
	7		156.8, s			
	7-OH					
	N-Me	2.76, s	30.4, q		2, 1 (Phe)	H-5/9, H_3-4, H_3-5, NH (Val)
Phe	1		170.5, s			
	2	4.75, dd (11.4, 4.0)	50.2, d	H-3a, H-3b		H-3a, H-3b
	3a	2.87, m	35.4, t	H-2, H-3b	5/9	H-3b, H-5,9, H-6 (Ahp)
	3b	1.79, m		H-2, H-3a		H-2, H-3a, H-6 (Ahp)
	4		137.2, s			
	5/9	6.83, d (7.3)	129.4, d	H-6/8	3, 7, 5/9	H-2, H-3a, H-3b, H-6/8, H-6 (Ahp),
	6/8	7.17, d (7.3)	127.7, d	H-5/9	4, 6/8	H-5/9
	7	7.15, m	126.1, d		5/9	H-5/9
Ahp	2		170.5, s			
	3	3.63, m	48.7, d	H-4a, H-4b, NH	1 (Leu)	H-4b, NH
	4a	2.40, m	21.6 ,t	H-3, H-4b, H-5a, H-5b		H-4b, H-5a, NH
	4b	1.58, m		H-4a, H-5a	1 (Leu)	H-3, H-4a, H-6
	5a	1.68, m	29.4, t	H-4b, H-5b, H-6		H-4a, H-6
	5b	1.57, m		H-5a, H-6		H-6
	6	5.06, br s	73.7, d	H-5a, H-5b		H-5a, H-5b, H-3a (Phe), H-3b (Phe), H-5/9 (Phe)
	6-OH					
	NH	7.07, d (9.0)		H-3	2	H-3, H-4a, H-2 (Leu), H-3 (Thr-1), NH (Leu)
Leu	1		173.9, s			
	2	4.19, m	50.4, d	H-3a, H-3b, NH		H-3a, H-3b, H-4, H_3-5, H_3-6, NH
	3a	1.69, m	39.1, t	H-3b, H-4		H-2, H-3b, H-4
	3b	1.31, m		H-2, H-3a		H-3a, NH, NH (Ala)
	4	1.43, m	24.1, d	H-3a, H_3-5, H_3-6		H_3-5, H_3-6, NH
	5	0.72, d (6.5)	20.9, q	H-4	3, 6	H-2, H-3a, H-4

Table S2. Continued

C/H no.		δ$_H$ (*J* in Hz)	δ$_C$[a]	^{1}H-^{1}H COSY	HMBC[b]	ROESY
	6	0.84, d (6.5)	23.3, q	H-4	3, 4, 5	H-3a, H-3b, H-4
	NH	8.42, d (8.5)		H-2		H-2 (Thr-1), H-3 (Thr-1), NH (Ahp)
Thr-1	1		169.4, s			
	2	4.59, d (9.3)	54.6, d	H-3, NH	1	H-3, H_3-4, NH, NH (Leu)
	3	5.38, br q (6.8)	71.8, d	H-2, H_3-4		H-2, H_3-4, NH (Leu)
	4	1.19, d (6.6)	17.8, q	H-3	2, 3	H-2, H-3, NH
	NH	7.73, d (9.0)		H-2		H-2, H-2 (Thr-2), NH (Thr-2)
Thr-2	1		173.0, s			
	2	4.34, dd (8.2, 4.3)	57.8, d	H-3, NH		H-3, H_3-4, NH (Thr-1), NH
	3	3.98, m	66.4, d	H-2, H_3-4		H-2, H_3-4, NH (Thr-1), NH
	4	1.01, d (6.3)	20.1, q	H-3	2, 3	H-2, H-3, NH (Thr-1), NH, NH (Ala)
	O					
	NH	7.89, br		H-2	1 (Ala)	H-2 (Ala), NH (Thr-1), NH (Ala)
Ala-1	1		172.9, s			
	2	4.39, m	48.1, d	H_3-3, NH	1, 3	H_3-3, NH (Thr-2), NH
	3	1.21, d (7.3)	18.2, q	H-2	1, 2	H-2, NH (Thr-2), NH, NH (Thr-1)
	NH	8.07, m		H-2	1 (Ba-1)	H-2, H-2 (Ba-1), NH (Thr-2)
Ba-1	1		172.2, s			
	2	2.08, m (2H)	37.1, t	H_2-3	1, 3, 4	H_2-3, NH (Ala)
	3	1.50, m (2H)	18.7, t	H_2-2, H_3-4	1, 2, 4	
	4	0.84, m	13.8, q	H_2-3	2, 3	
Ala-2	1		174.0, s			
	2	3.62, m	50.0, d	H_3-3, NH	1	H_3-3
	3	1.10, d (6.9)	19.6, q	H-2, NH[c]	1, 2	H-2, H_3-4 (Thr-2)
	NH	7.18, m		H-2[c]		H-2 (Ba-2)
Ba-2	1		170.6, s			
	2	2.02, m (2H)	37.9, t	H_2-3, H_3-4[c]	1, 3, 4	H_2-3, NH (Ala-2)
	3	1.48, m (2H)	19.0, t	H_2-2, H_3-4	1, 2, 4	H_2-2 (Ba-1)
	4	0.84, m	13.8, q	H_2-3	2, 3	

[a]Multiplicity derived from HSQC spectrum. [b] Protons showing long-range correlation with indicated carbon. [c]These couplings were only observed in the TOCSY spectrum.

Table S3. NMR spectral data for loggerpeptin C (**3**) at 600 MHz (^{1}H), 150 MHz (^{13}C) in DMSO-d_6

C/H no.		δ_H (*J* in Hz)	δ_C[a]	^{1}H-^{1}H COSY	HMBC[b]	ROESY
Val	1		172.4, s			
	2	4.59, dd (9.6, 5.0)	55.9, d	H-3, NH	1, 3, 4, 5	H-3, H_3-4, H_3-5, NH
	3	2.05, m	30.6, d	H-2, H_3-4, H_3-5		H-2, H_3-4, H_3-5
	4	0.72, d (6.7)	17.3, q	H-3	2, 3, 5	H-2, H-3, N-Me (Tyr), NH
	5	0.84, d (6.7)	19.3, q	H-3	2, 3, 4	H-2, H-3, H_3-4, N-Me (Tyr)
	NH	7.48, d (9.5)		H-2	1 (Tyr)	H-2, H_3-4, N-Me (Tyr), H-2 (Tyr)
N-Me-Tyr	1		169.7, s			
	2	4.90, dd (11.5, 2.4)	60.9, d	H-3a, H-3b		H-3a, H-3b, H-5/9, NH (Val), H-2 (Phe), H-3b (Phe), H-5/9 (Phe), N-Me
	3a	3.10, dd (–14.3, 2.3)	32.9, t	H-2, H-3b	4, 5/9	H-2, H-3b, H-5/9, H-2 (Phe)
	3b	2.71, m		H-2, H-3a	2, 4, 5/9	H-3a, H-5/9
	4		127.7, s			
	5/9	7.00, d (8.5)	130.4, d	H-6/8	3, 5/9, 7, 6/8	H-2, H-3a, H-3b, N-Me, H-6/8, H-2 (Phe)
	6/8	6.77, d (8.5)	115.3, d	H-5/9	4, 6/8, 7	H-5/9, H-3b (Phe)
	7		156.4, s			
	7-OH					
	N-Me	2.75, s	30.3, q		2, 1 (Phe)	H-2, H-5/9, H_3-4 (Val), H_3-5 (Val), NH (Val)
Phe	1		170.8, s			
	2	4.76, dd (11.9, 4.0)	50.2, d	H-3a, H-3b	1, 3, 2 (Ahp)	H-3a, H-3b, H-5/9, H-2 (Tyr), H-3a (Tyr), H-5/9 (Tyr)
	3a	2.86, dd (–15.3, 11.6)	35.2, t	H-2, H-3b	2, 4, 5/9	H-3b, H-5/9, H-6 (Ahp)
	3b	1.81, dd (–14.2, 3.5)		H-2, H-3a	4, 5/9	H-2, H-3a, H-5/9, H-6 (Ahp), H-2 (Phe)
	4		137.1, s			
	5/9	6.83, d (7.4)	129.5, d	H-6/8	3, 5/9, 7	H-2, H-3a, H-3b, H-6/8, H-5b (Ahp), H-6 (Ahp)
	6/8	7.17, d (7.4)	127.7, d	H-5/9	4, 6/8	H-5/9
	7	7.14, m	126.2, d		5/9	H-5/9
Ahp	2		169.1, s			
	3	3.63, m	48.7, d	H-4a, H-4b, NH	1 (Leu)	H-4b, H-5b, NH
	4a	2.41, m	21.5 ,t	H-3, H-4b, H-5a		H-4b, H-5a, H-5b, NH
	4b	1.58, m		H-3, H-4a, H-5a		H-3, H-4a
	5a	1.69, m	29.3, t	H-4a, H-5b, H-6		H-4a, H-5b, H-6
	5b	1.56, m		H-5a, H-6		H-5a, H-6, H-5/9 (Phe)
	6	5.06, br s	73.7, d	H-5a, H-5b	2	H-5a, H-5b, H-2 (Phe), H-3a (Phe), H-3b (Phe), H-5/9 (Phe)
	6-OH					
	NH	7.09, d (9.0)		H-3		H-3, H-4a, H-2 (Leu), H-3 (Thr), NH (Leu)
Leu	1		173.9, s			
	2	4.18, m	50.5, d	H-3a, H-3b, NH		H-3a, H_3-5, NH, NH (Ahp)
	3a	1.71, m	39.1, t	H-2, H-3b, H-4		H-2, H-3a, H_3-5, H_3-6
	3b	1.31, m		H-2, H-3a		H-3a, NH
	4	1.46, m	24.1, d	H-3a, H_3-5, H_3-6		H_3-5, H_3-6
	5	0.74, d (6.6)	21.1, q	H-4	3, 6	H-2, H-3a, H-4
	6	0.85, d (6.6)	23.3, q	H-4	3, 4, 5	H-4

Table S3. Continued

C/H no.		δ_H (*J* in Hz)	δ_C[a]	^{1}H-^{1}H COSY	HMBC[b]	ROESY
	NH	8.39, d (8.5)		H-2	1 (Thr)	H-2, H-3b, H-4, H-2 (Thr), H-3 (Thr), NH (Ahp)
Thr	1		169.3, s			
	2	4.61, d (9.6)	54.9, d	NH	1, 4	H-3, H_3-4, NH, NH (Leu)
	3	5.41, q (6.6)	71.9, d	H_3-4	1 (Val), 4	H-2, H_3-4, NH (Ahp), NH (Leu)
	4	1.19, d (6.6)	17.7, q	H-3	2, 3	H-2, H-3, NH
	NH	7.05, d (9.0)		H-2		H-2, H_3-4, H-3 (Ala), H-3 (Abu), NH (Abu)
Abu	1		164.7, s			
	2		131.0, s			
	3	6.48, q	129.8, d	H_3-4	1, 4	H_3-4, NH (Thr)
	4	1.63, d (7.0)	12.9, q	H-3	2, 3	H-3, H-4 (Leu), NH
	NH	9.26, br s		H_3-4	1 (Ala)	H-4, H-2 (Ala), H-3 (Ala), NH (Ala), NH (Thr)
Ala	1		172.6, s			
	2	4.33, m	48.8, d	H_3-3, NH	1, 3	H_3-3, NH, NH (Abu)
	3	1.35, d (7.2)	17.9, q	H-2	1, 2	H-2, NH, NH (Abu), H-2 (Val)
	NH	8.10, d (6.6)		H-2	1	H-2, H_3-3, H-2 (Ba)
Ba	1		172.6, s			
	2	2.10, m (2H)	37.0, t	H_2-3	1, 3, 4	H-3, H_3-4, NH (Ala)
	3	1.52, m (2H)	18.6, t	H_2-2, H_3-4	1, 2, 4	H-2, H_3-4
	4	0.86, t (7.5)	13.6, q	H_2-3	2, 3	H-2, H-3

[a] Multiplicity derived from HSQC spectrum. [b] Protons showing long-range correlation with indicated carbon.

Table S4. NMR spectral data for molassamide (**4**) at 600 MHz (^{1}H), 150 MHz (^{13}C) in DMSO-d_6

C/H no.		δ_H (*J* in Hz)	δ_C[a]	^{1}H-^{1}H COSY	HMBC[b]	ROESY
Val	1		173.0, s			
	2	4.55, dd (8.4, 4.4)	57.2, d	NH	1 (Tyr)	
	3	2.02, m	30.3, d	H_3-4, H_3-5	5	H_3-4, H_3-5, 7-OH (Tyr)
	4	0.79, d (7.0)	17.9, q	H-3	3, 5	H-3, N-Me (Tyr), 7-OH (Tyr)
	5	0.87, d (7.0)	19.1, q	H-3	2, 3, 4	H-3, N-Me (Tyr), 7-OH (Tyr)
	NH	7.77, d (8.4)		H-2	1	H-3 (Thr-2), H_3-4 (Thr-2), H-2 (Ala), H_3-3 (Ala), NH (Ala)
N-Me-Tyr	1		169.7, s			
	2	4.88, d (11.0)	60.9, d	H-3a, H-3b	1 (Phe), 3, N-Me	H-3a, H-5/9, H-2 (Phe), H-3b (Phe), H-5/9 (Phe), N-Me
	3a	3.16, dd (–13.3, 5.5)	32.8, t	H-2, H-3b		H-2, H-3b, H-5/9, H-2 (Phe)
	3b	2.68 dd (–15.1, 11.5)		H-2, H-3a	2, 4, 5/9	H-3a, H-5/9
	4		127.8, s			
	5/9	7.02, d (8.3)	130.7, d	H-6/8	3, 5/9, 6, 7	H-2, H-3a, H-3b, H-6/8, N-Me, H-2 (Phe)
	6/8	6.76, d (8.3)	115.3, d	H-5/9	4, 6/8, 7	H-2 (Phe), H-3b (Phe), H-5/9
	7		156.5, s			
	7-OH	4.45				
	N-Me	2.75, s	30.4, q		2, 1 (Phe)	H-2, H-5/9, H_3-4 (Val), H_3-5 (Val)
Phe	1		170.8, s			
	2	4.76, dd (11.0, 3.9)	50.4, d	H-3a, H-3b	1, 3, 4, 2 (Ahp), 6 (Ahp)	H-3b, H-2 (Tyr), H-3a (Tyr), H-6 (Ahp), H-5/9, H-5/9 (Tyr)
	3a	2.87, dd (–14.3, 12.3)	35.2, t	H-2, H-3b	1, 2, 4, 5/9	H-3b, H-6 (Ahp), H-5/9
	3b	1.87, dd (–15.2, 3.1)		H-2, H-3a	2, 4, 5/9	H-2, H-3a, H-2 (Tyr), H-6 (Ahp), H-5/9
	4		137.2, s			
	5/9	6.84, d (7.4)	129.5, d	H-6/8	3, 5/9, 7	H-2, H-3a, H-6/8, H-4b (Ahp), H-5b (Ahp), H-6 (Ahp), H-2 (Tyr)
	6/8	7.18, d (7.4)	127.8, d	H-5/9	4, 6/8	H-5/9
	7	7.15, m	126.3, d		5/9	H-5/9
Ahp	2		169.2, s			
	3	3.83, m	48.4, d	H-4b, NH	2, 5	H-4a, H-4b, NH, H-7 (Phe)
	4a	2.35, m	21.7 ,t	H-4b		H-4b, H-5a
	4b	1.56, m		H-3, H-4a, H-5a	2, 3, 6	H-4a, H-5a, H-3 (Abu)
	5a	1.72, m	29.4, t	H-5a, H-6		H-4a, H-4b, H-6
	5b	1.58, m		H-5a, H-6		H-9, H-5/9 (Phe)
	6	5.09, br s	73.9, d	H-5a, H-5b	2, 4	H-5a, H-5b, H-3a (Phe), H-3b (Phe), H-5/9 (Phe)
	6-OH					
	NH	7.13, d (9.0)		H-3		H-3, H-4a, H-4b
Abu	1		163.2, s			
	2		130.2, s			
	3	6.56, q	132.0, d	H_3-4	1, 4	H_3-4, H-3 (Ahp), NH
	4	1.51, d	13.1, q	H-3	1, 2, 3	H-3, NH
	NH	8.90, br s		H_3-4	1	H-3, H_3-4, H_3-4 (Thr-2)
Thr-1	1		169, s			

Table S4. Continued

C/H no.		δ_H (*J* in Hz)	δ_C[a]	^1H-^1H COSY	HMBC[b]	ROESY
	2	4.60, br	55.5, d	NH		H-3, H_3-4, H_3-4 (Abu), NH
	3	5.42, br	71.8, d			H-2, H_3-4
	4	1.27, d (6.0)	17.9, q	H-3	2, 3	H-2, H-3, NH
	NH	7.69, br d (6.0)		H-2		H-2, H_3-4, H-3 (Thr-2), H-2 (Val)
Thr-2	1		173.0, s			
	2	4.39, dd (8.4, 4.2)	57.7, d	H-3, NH		H-3
	3	4.09, br	66.6, d	H_3-4		H-2, H_3-4, H-2 (Ala), OH, H-5/9 (Tyr), NH (Thr-1), NH (Val)
	4	1.04, d (6.3)	19.1, q	H-3	2, 3	H-2, H-3, OH, H-5/9 (Tyr), NH (Thr-1), NH (Ala), NH (Val)
	OH	4.50, br				H-3, H_3-4, NH (Thr-1), NH (Val)
	NH	7.63, br		H-2		
Ala	1		172.9, s			
	2	4.37, m	48.1, d	H_3-3, NH	1, 3	H_3-3, H-2 (Ba), H_3-4 (Thr-2), NH, NH (Val)
	3	1.21, d (7.0)	17.9, q	H-2	1, 2	H-2, NH, NH (Val)
	NH	8.05, d (7.4)		H-2	2, 3, 1 (Ba)	H-2, H_3-3, H-2 (Ba), NH (Val)
Ba	1		172.3, s			
	2	2.08, m (2H)	37.0, t	H_2-3	1, 3, 4	H-3, NH (Ala)
	3	1.50, m (2H)	18.7, t	H_2-2, H_3-4	1, 2, 4	H-2, H_3-4
	4	0.84, t (7.5)	13.6, q	H_2-3	2, 3	H-2, H-3

[a] Multiplicity derived from HSQC spectrum. [b] Protons showing long-range correlation with indicated carbon.

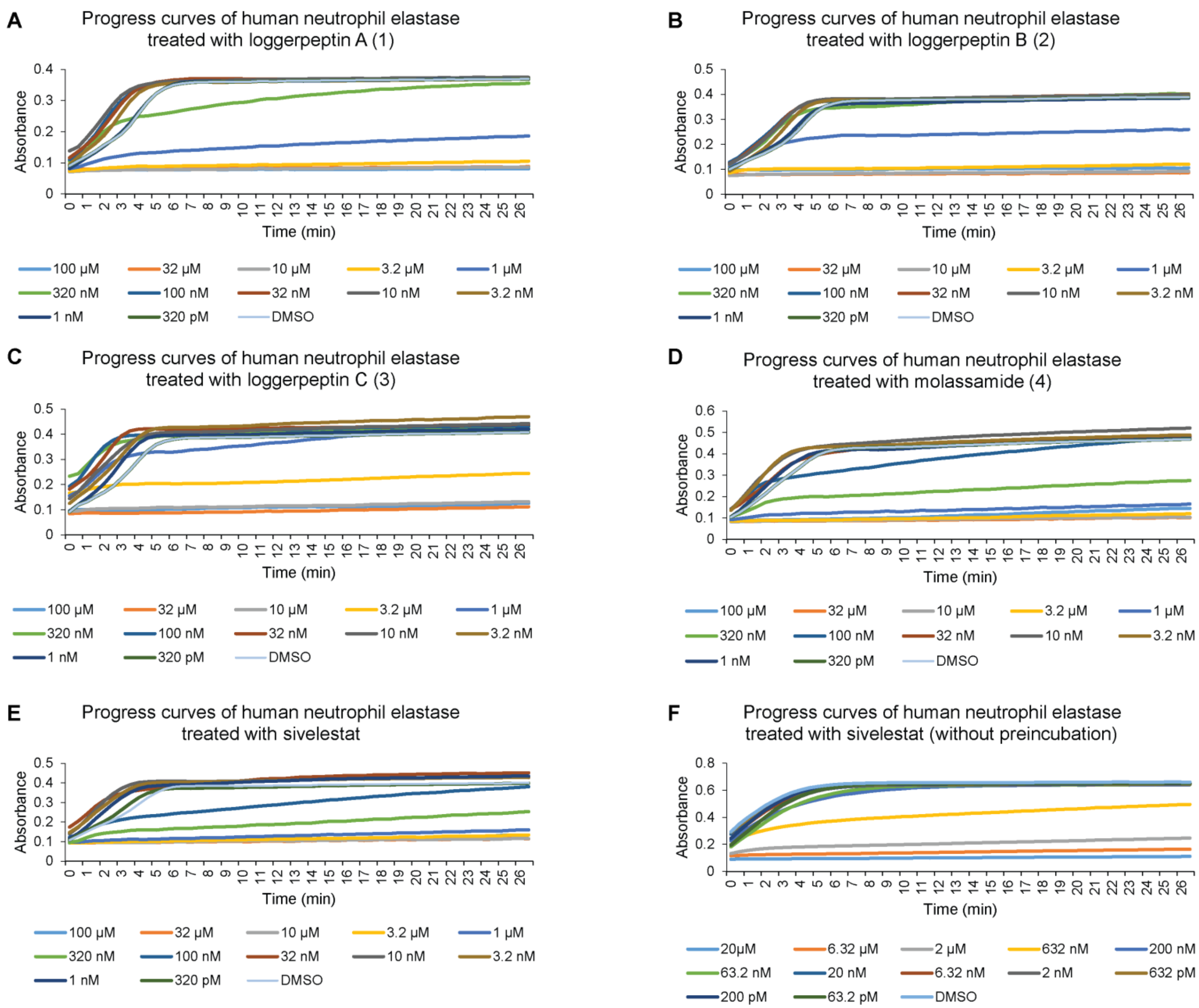


Figure S1. Progress curves of HNE treated with loggerpeptins A−C (**1**−**3**), molassamide (**4**) and sivelestat. Panels A–E were obtained by pre-incubating HNE with the inhibitors for 15 min whereas panel F was obtained without pre-incubation step.

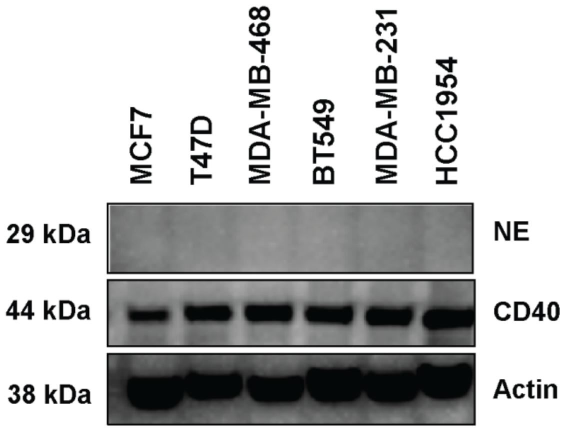


Figure S2. The expression levels of NE and CD40 in a panel of breast cancer cell lines assessed by Western blot. Actin was used as a loading control.

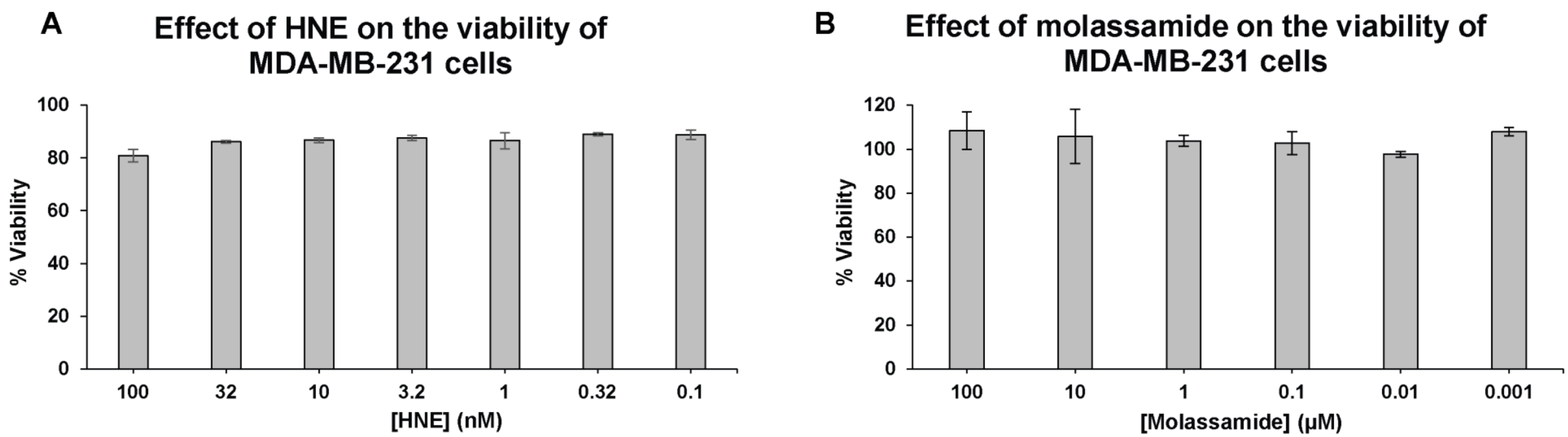


Figure S3. The effects of HNE and molassamide (**4**) on cell viability. MDA-MB-231 cells were seeded in 96-well plates. Following 24 h incubation, the cells were treated with different concentrations of **4**, HNE, or solvent control for 48 h. The cell viability was measured using 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT assay).

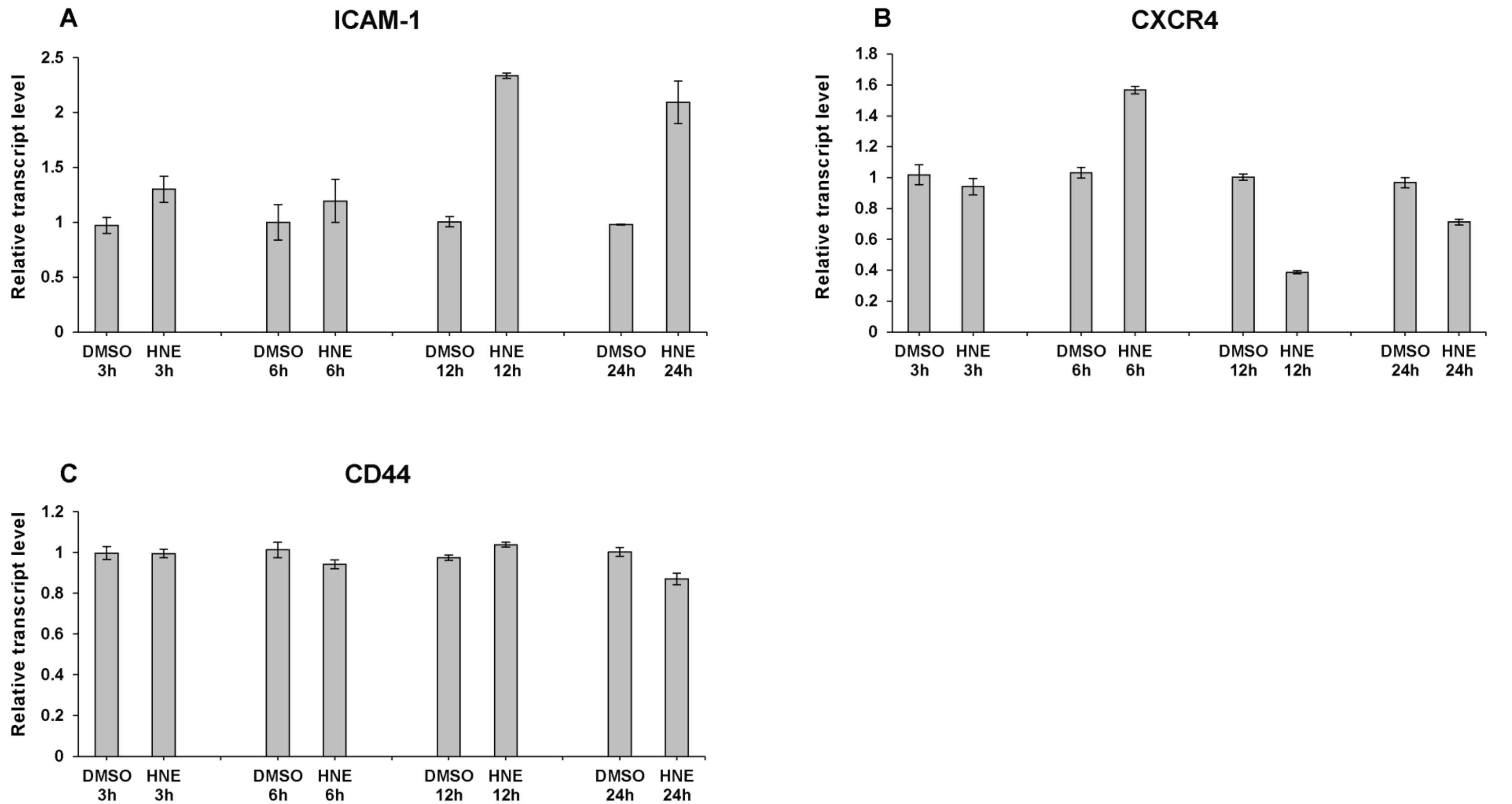


Figure S4. The effects of HNE on expression levels of NFκB target genes in MDA-MB-231 cells assessed by RT-qPCR. MDA-MB-231 cells were seeded in 6-well plates, incubated overnight, then starved for additional 24 h. The media was then replaced with serum free DMEM supplemented with DMSO or 100 nM HNE and the cells were incubated for the indicated time points. Following the incubation periods, the RNA was isolated, cDNA was synthesized, and the expression levels of each target gene were assessed by RT-qPCR.

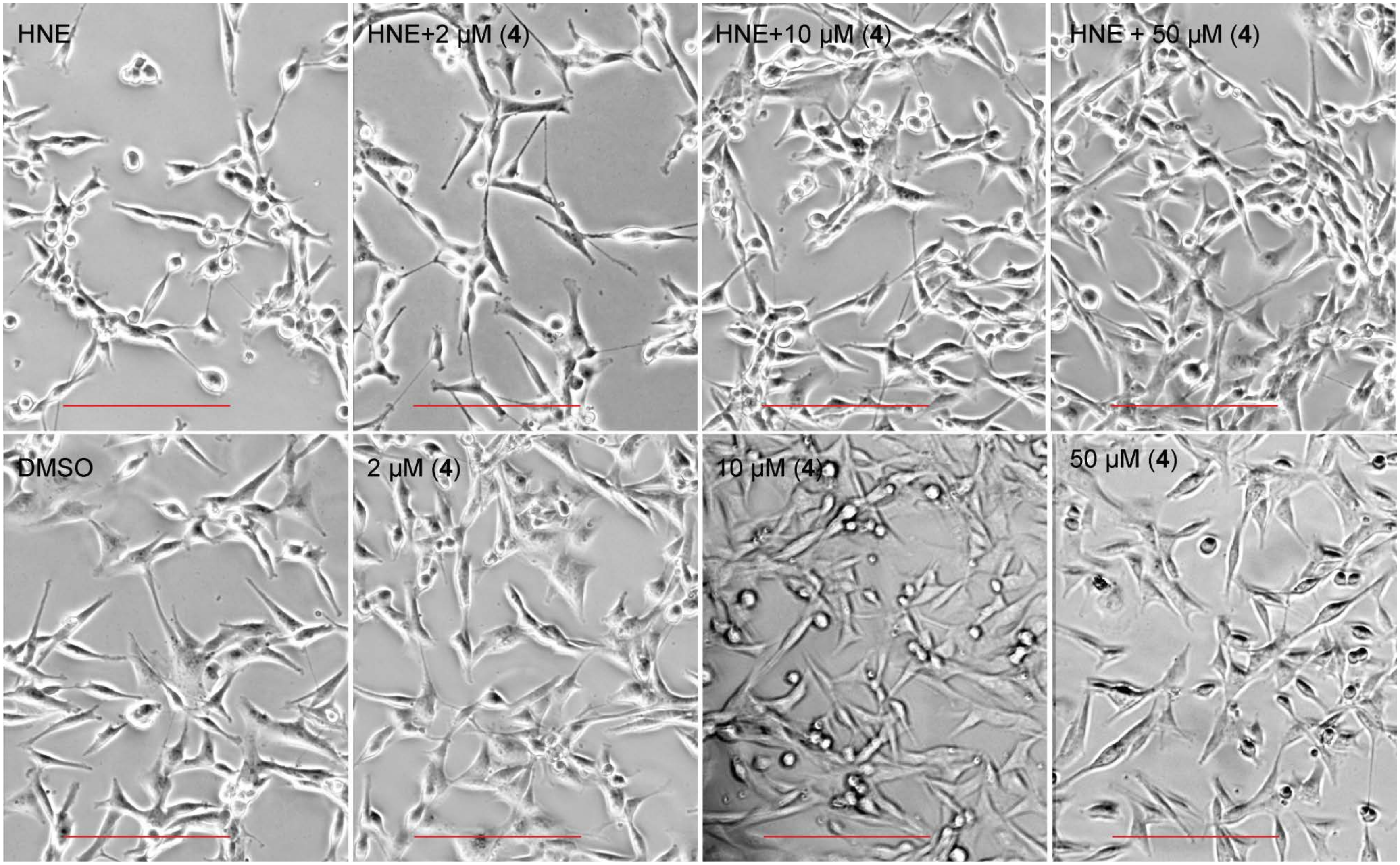


Figure S5. The effects of molassamide (**4**) on HNE-induced morphological changes in MDA-MB-231 cells. MDA-MB-231 cells were treated with **4** for 3 h in the presence or absence of 100 nM HNE. Scale bar 200 μm.

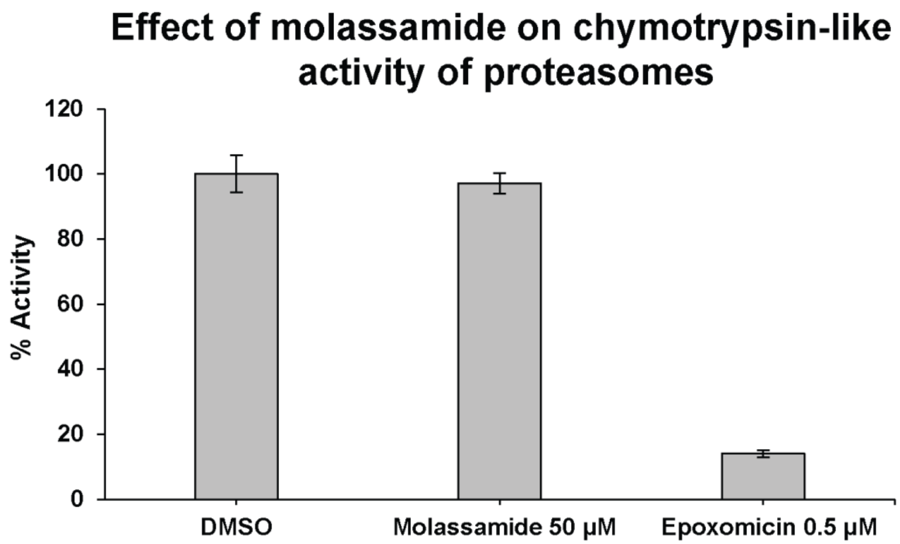
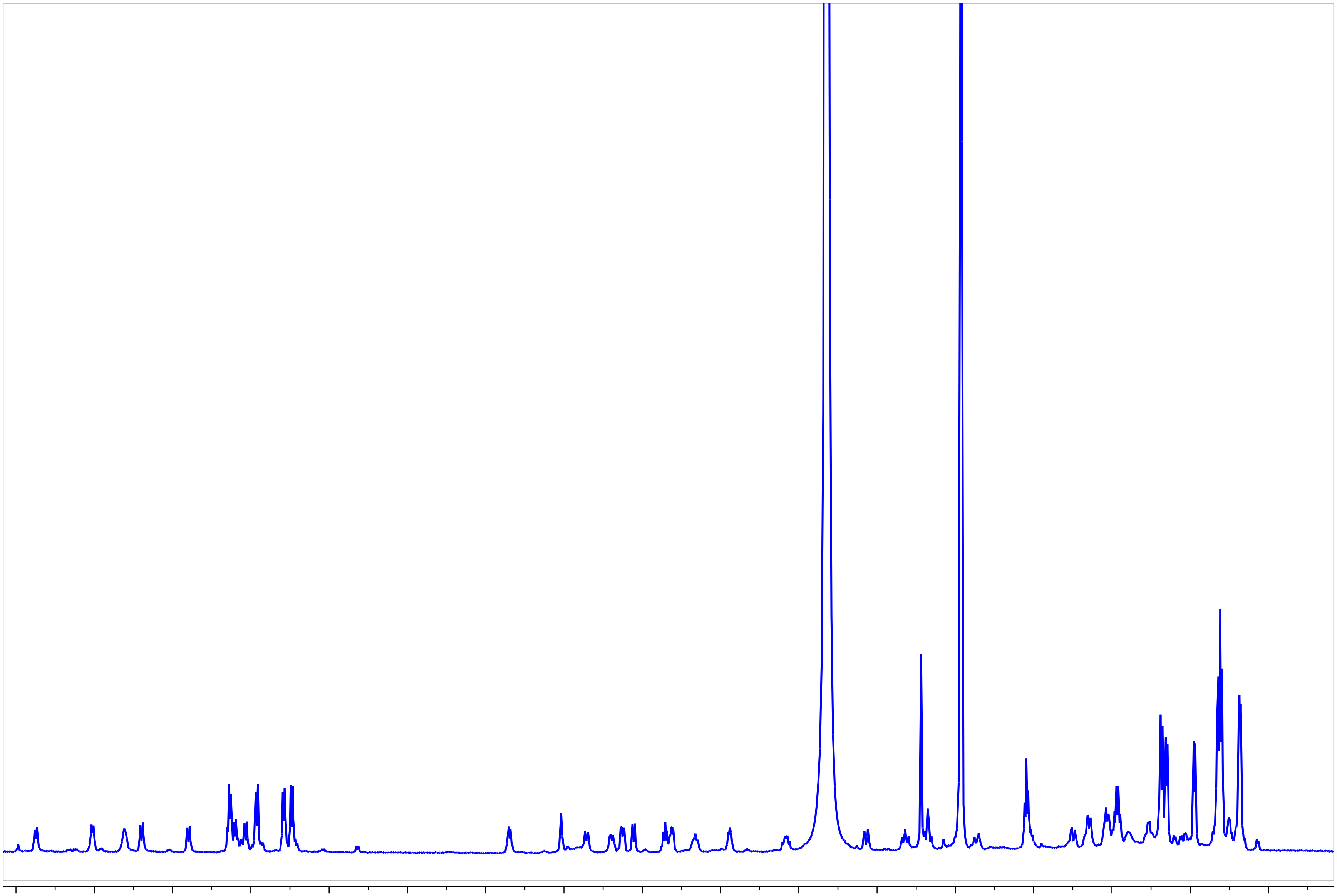
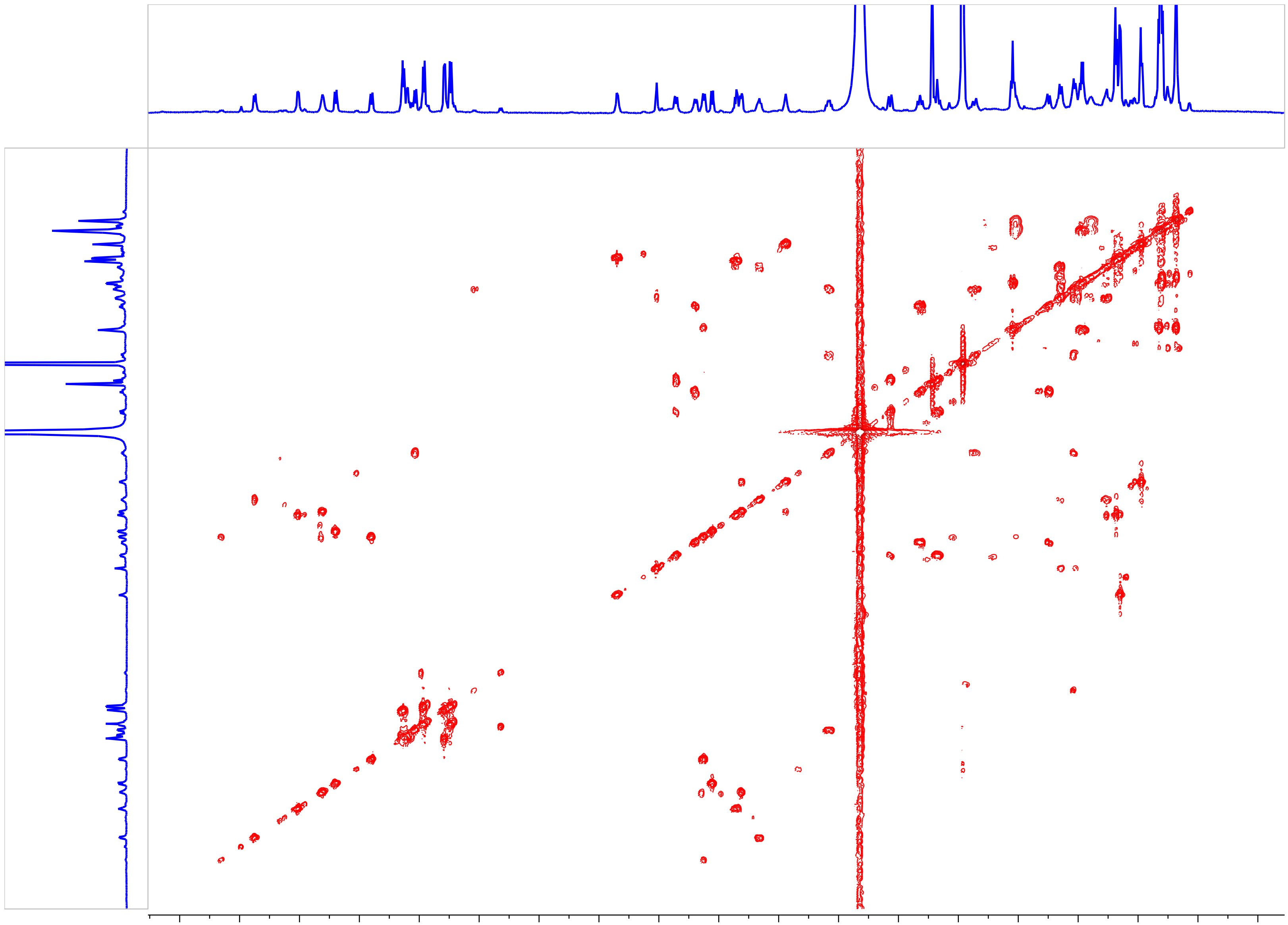


Figure S6. The effect of molassamide (**4**) on the chymotrypsin-like activity of proteasomes *in vitro* assessed using proteasome 20S assay kit (EnzoLife Sciences).

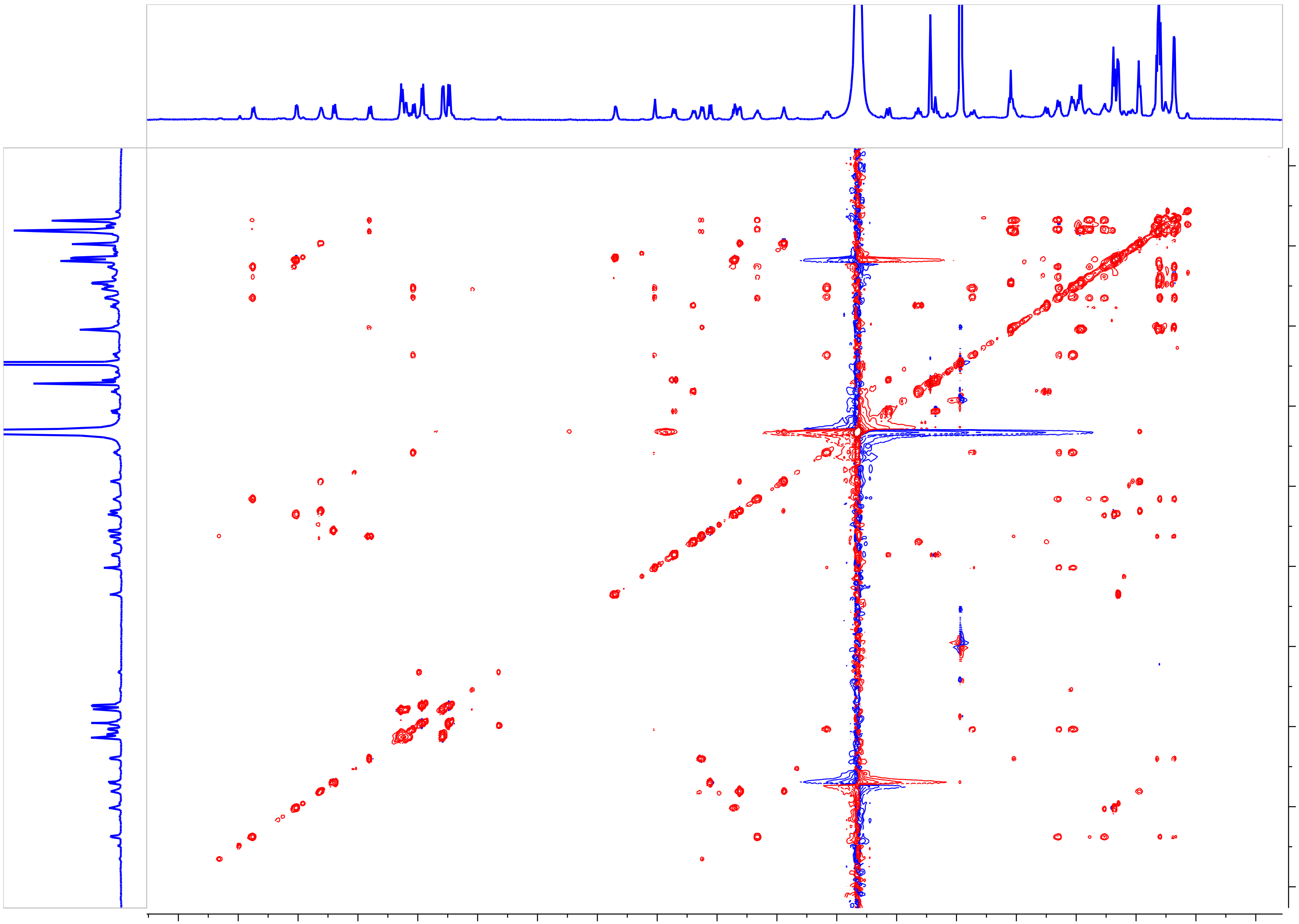
^{1}H NMR Spectrum of Loggerpeptin A (**1**) in DMSO-d_6, 600 MHz



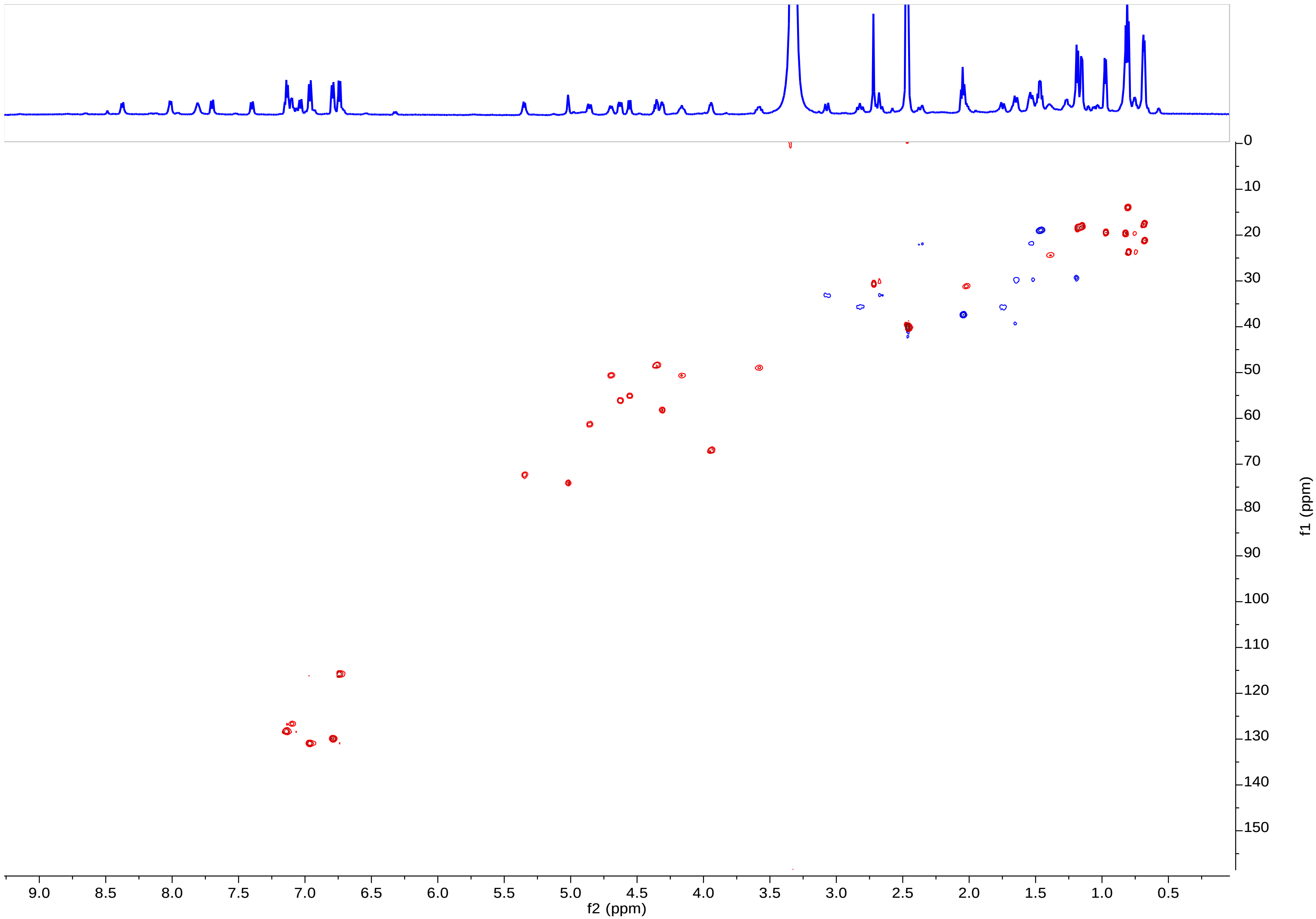
COSY Spectrum of Loggerpeptin A (**1**) in DMSO-d_6, 600 MHz



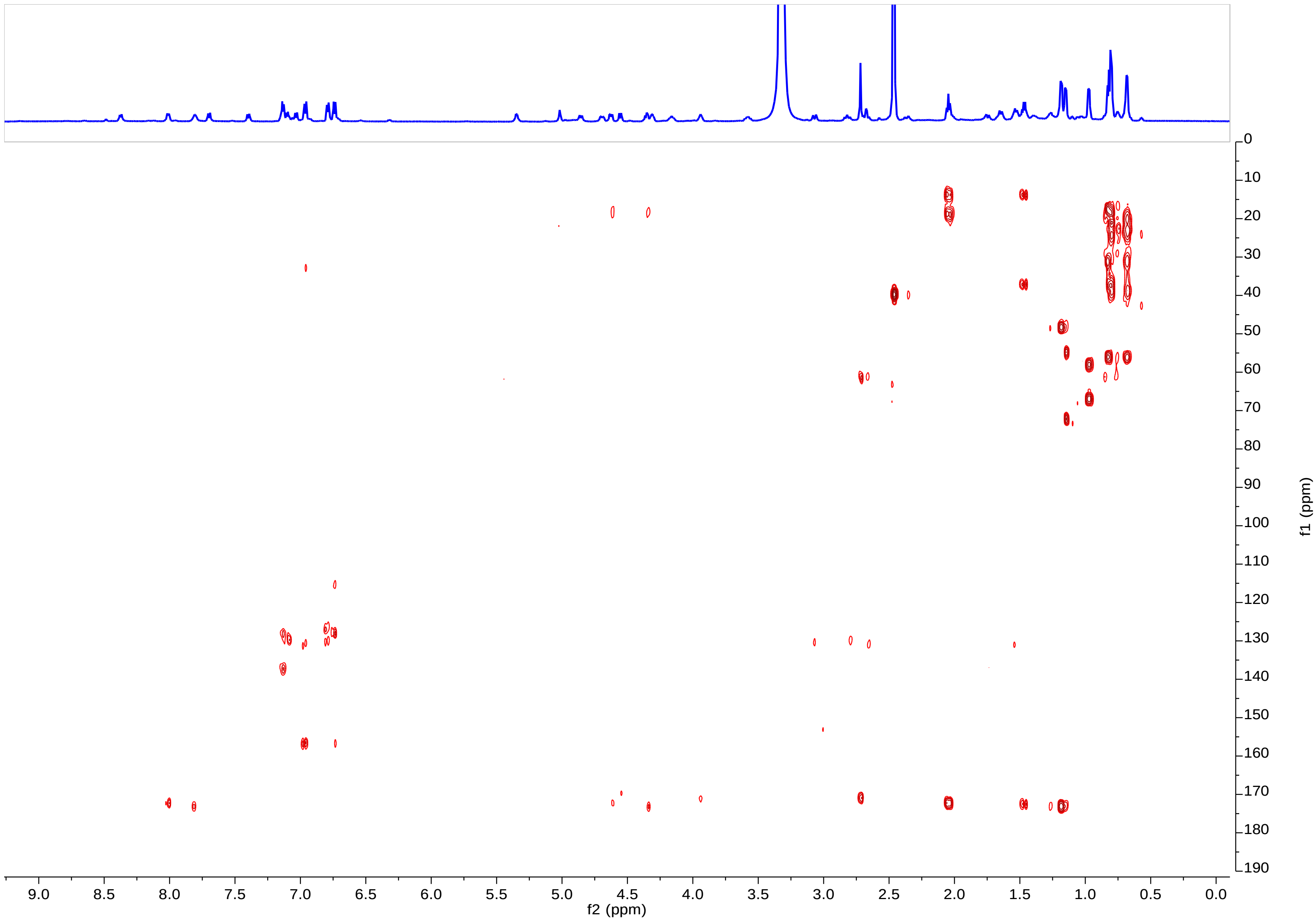
TOCSY Spectrum of Loggerpeptin A (**1**) in DMSO-d_6, 600 MHz



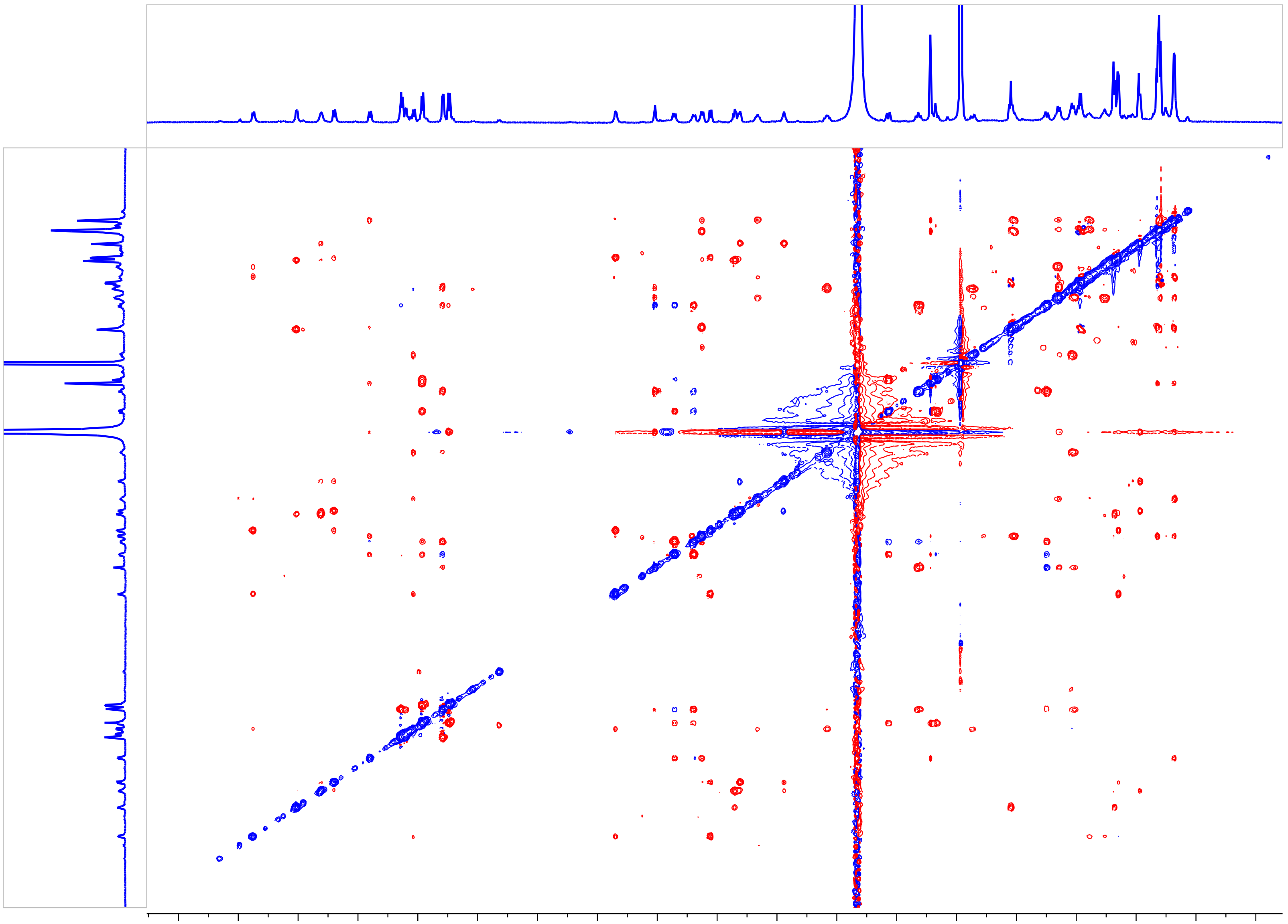
HSQC Spectrum of Loggerpeptin A (**1**) in DMSO-d_6, 600 MHz



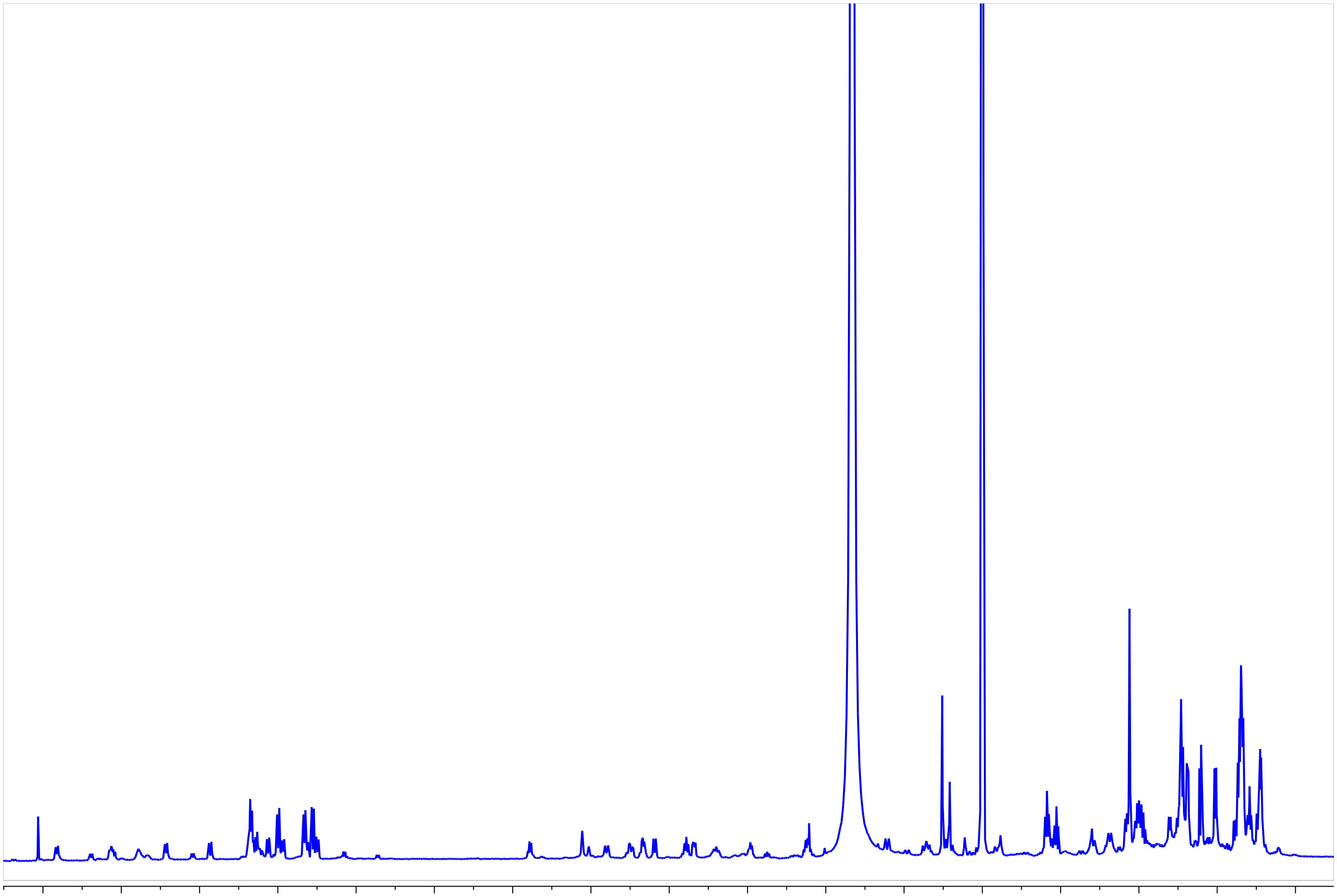
HMBC Spectrum of Loggerpeptin A (**1**) in DMSO-d_6, 600 MHz



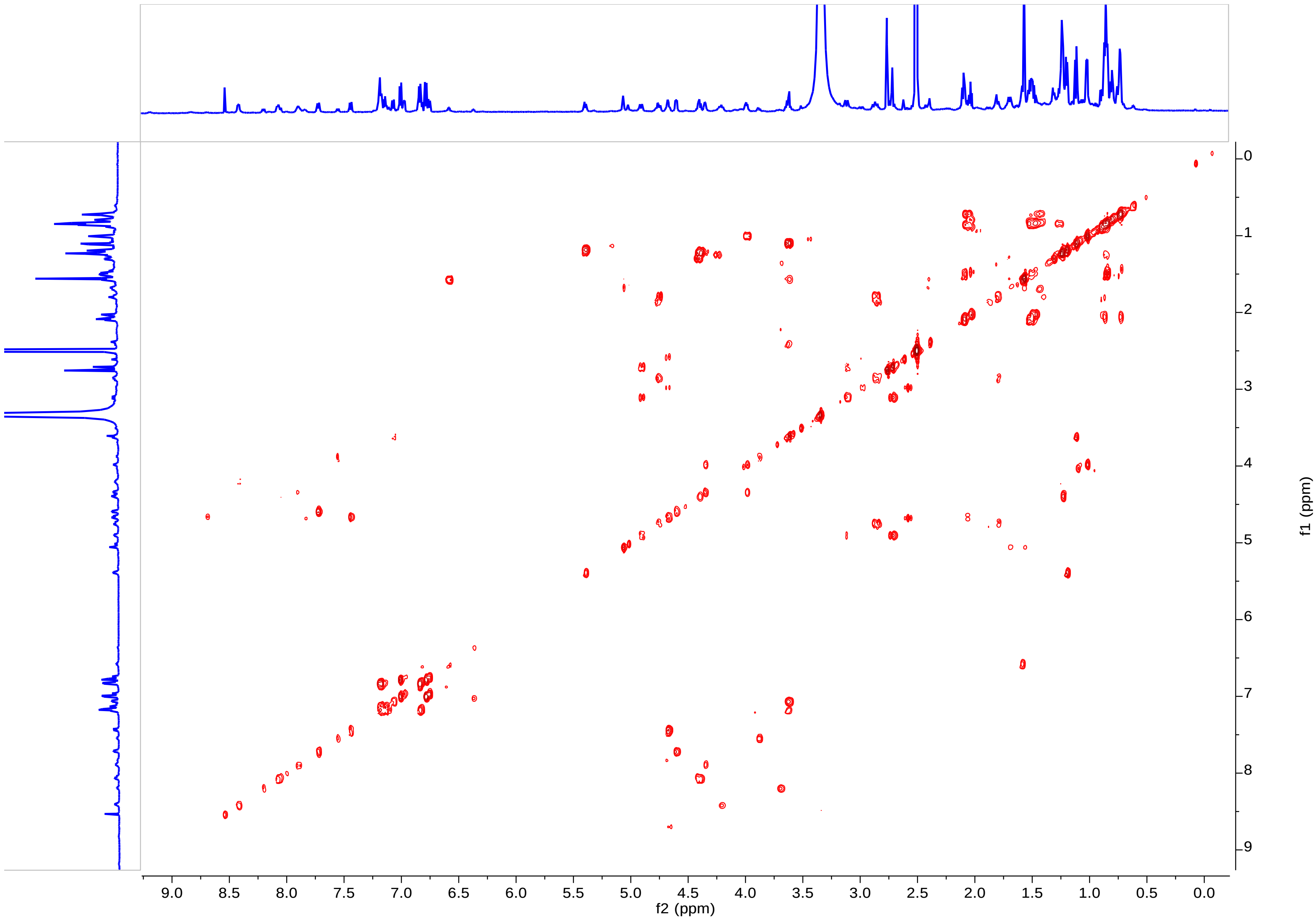
ROESY Spectrum of Loggerpeptin A (**1**) in DMSO-d_6, 600 MHz



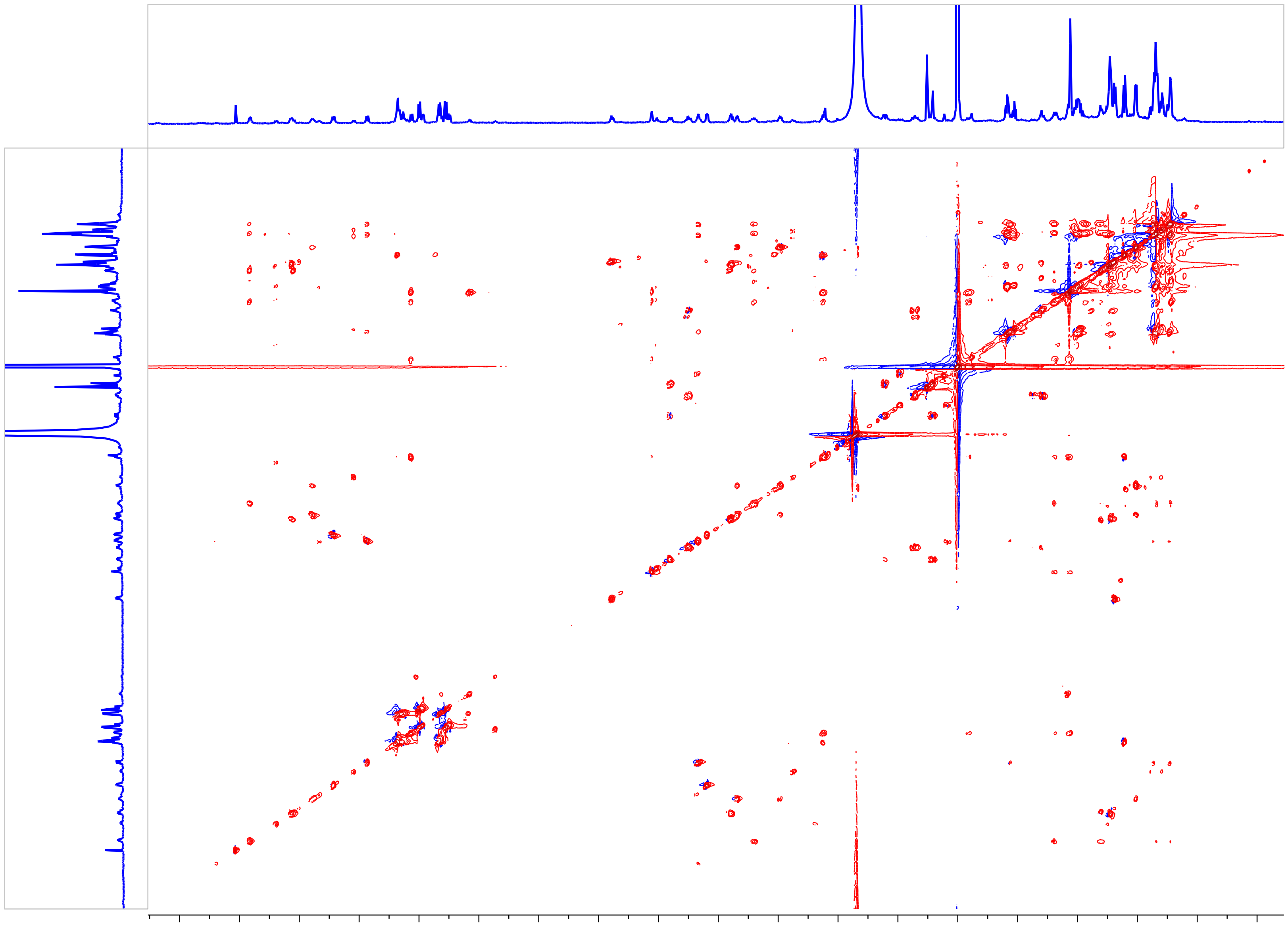
^{1}H NMR Spectrum of Loggerpeptin B (**2**) in DMSO-d_6, 600 MHz



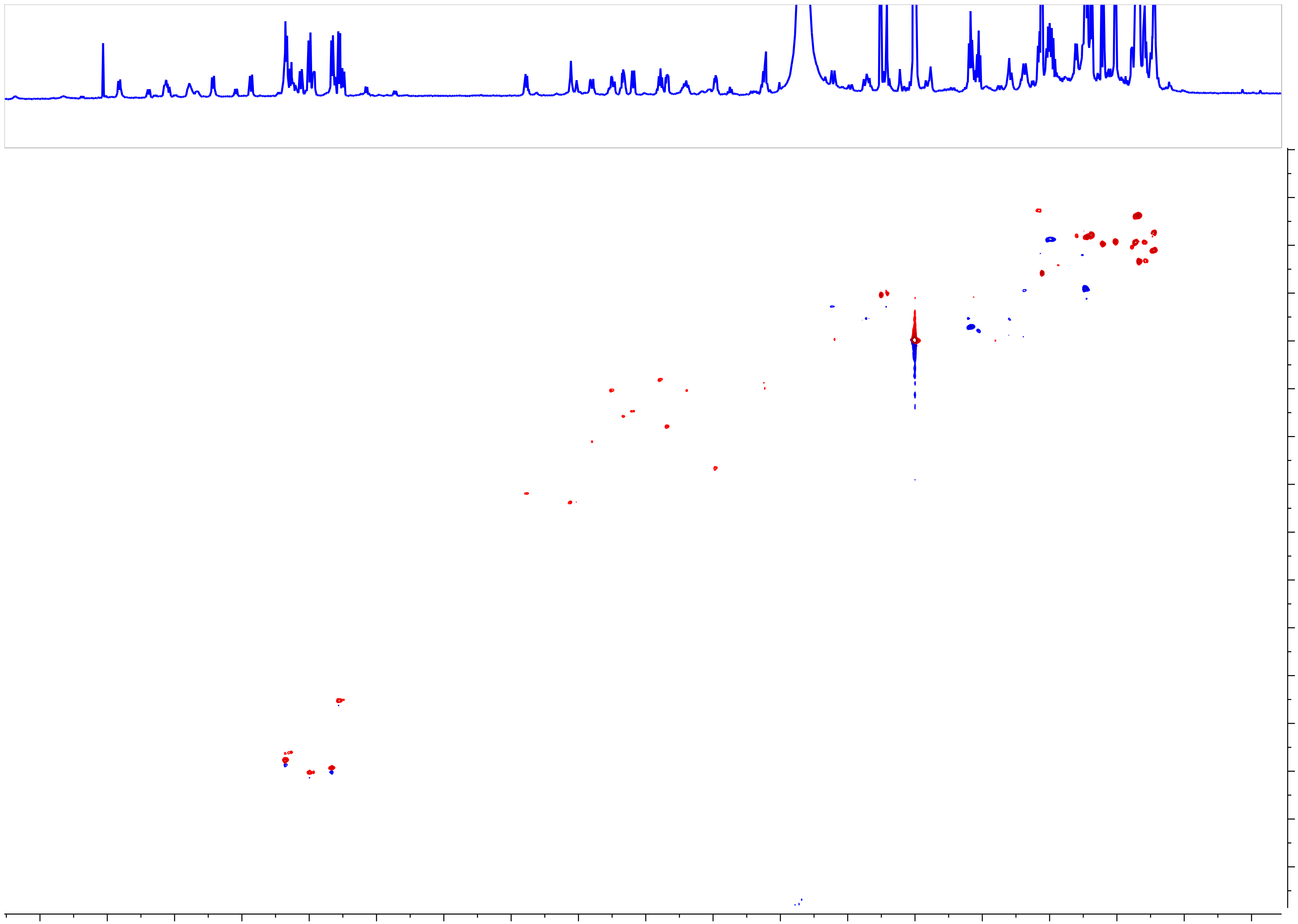
COSY Spectrum of Loggerpeptin B (**2**) in DMSO-d_6, 600 MHz



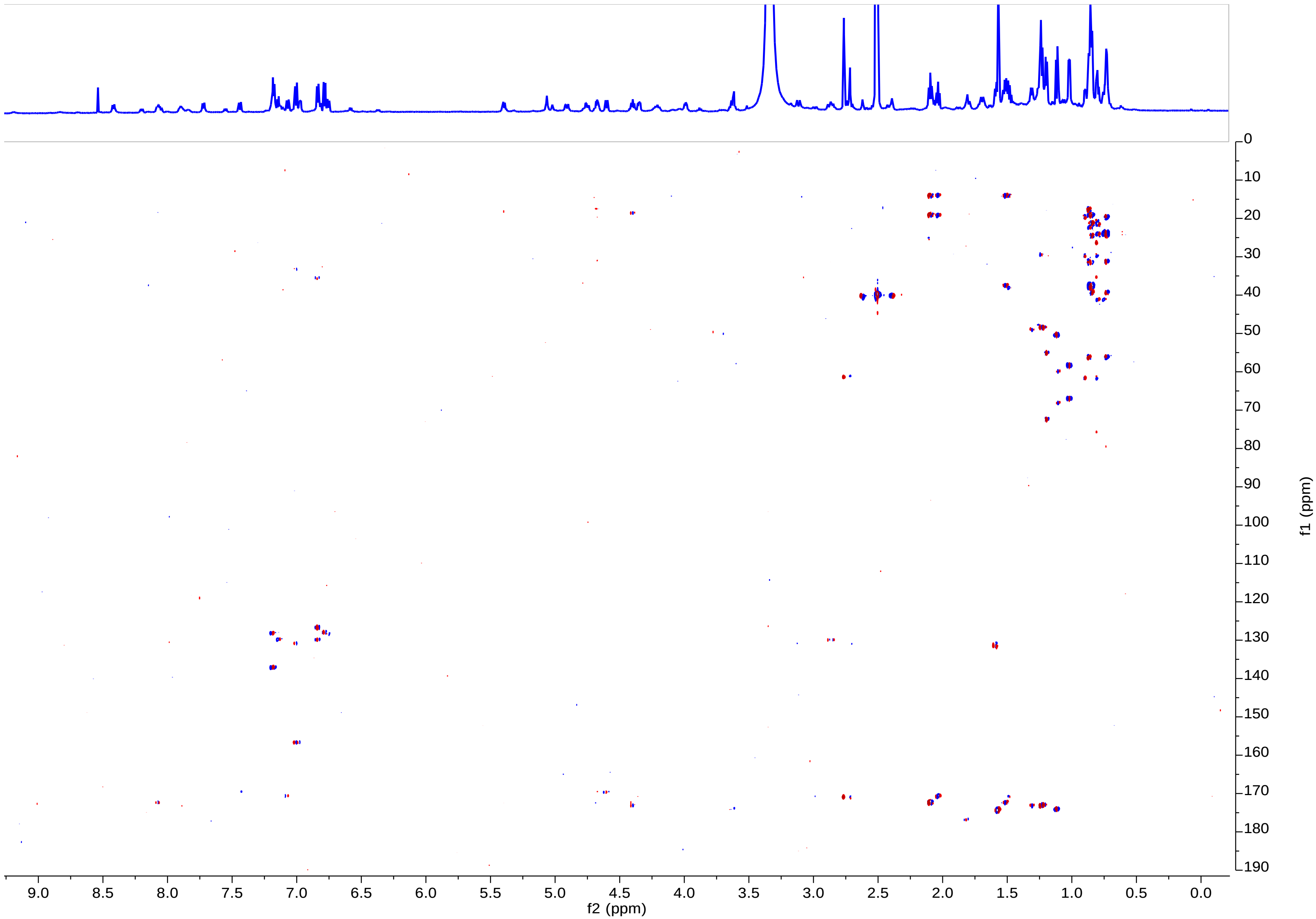
TOCSY Spectrum of Loggerpeptin B (**2**) in DMSO-d_6, 600 MHz



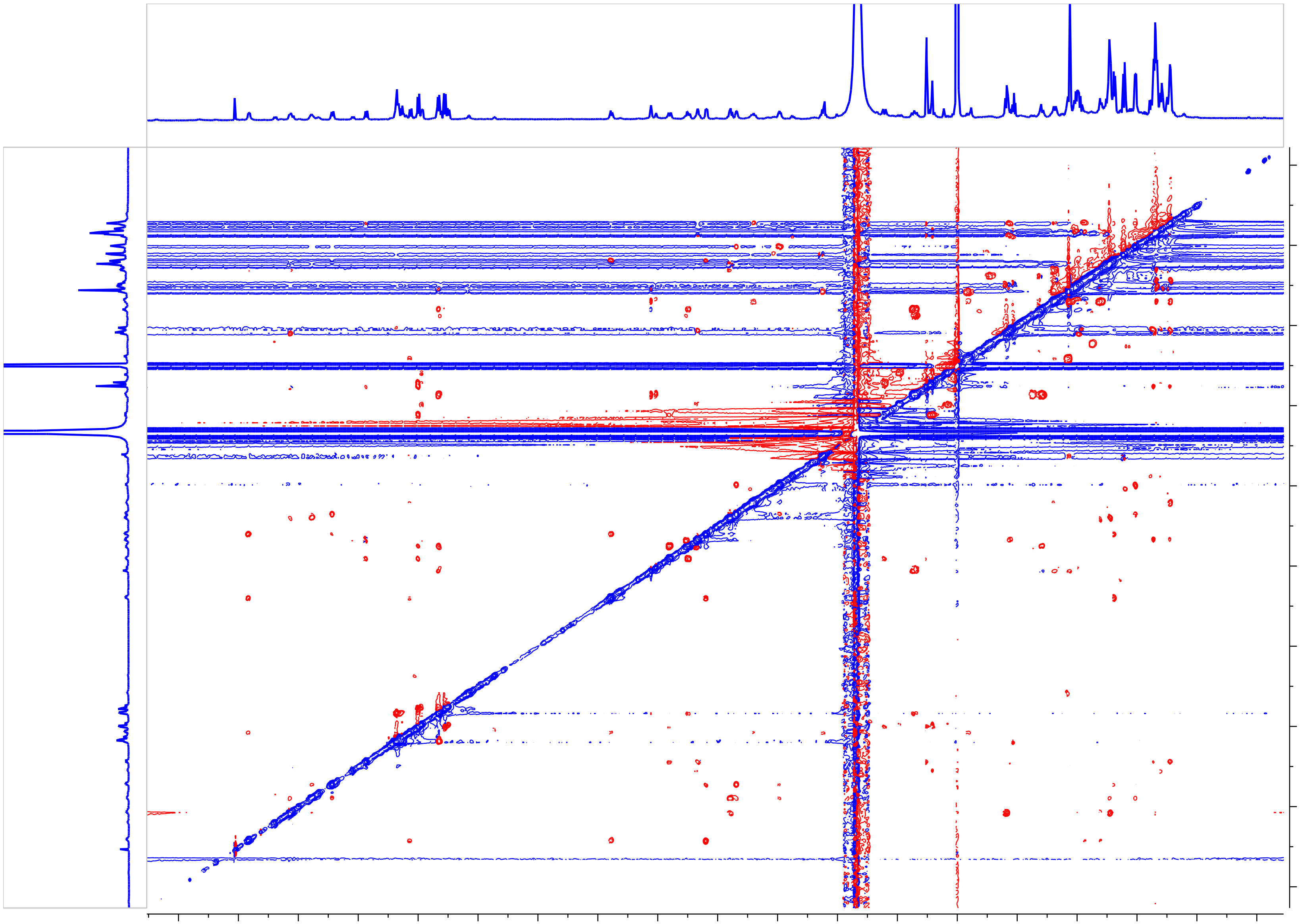
HSQC Spectrum of Loggerpeptin B (**2**) in DMSO-d_6, 600 MHz



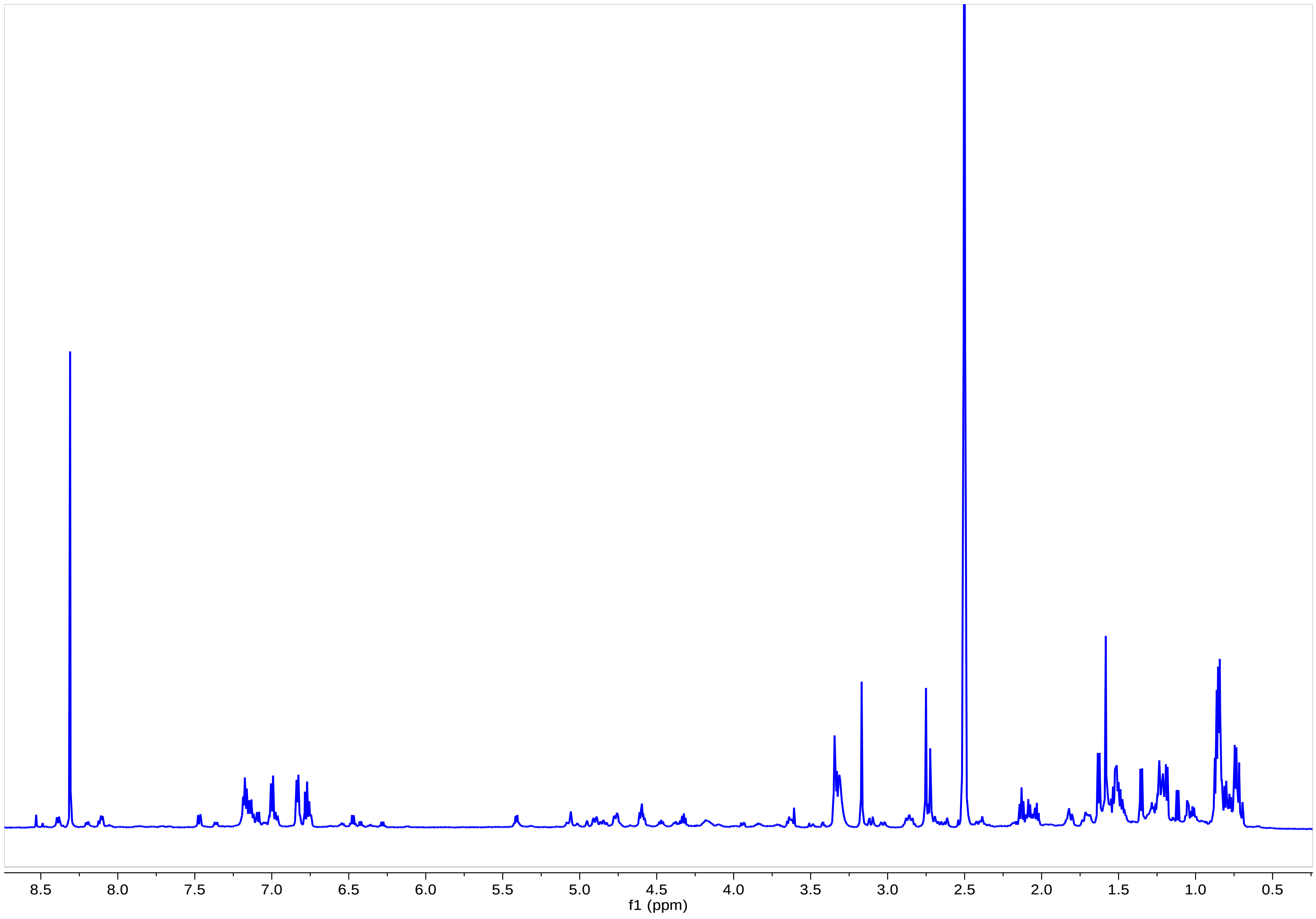
HMBC Spectrum of Loggerpeptin B (**2**) in DMSO-d_6, 600 MHz



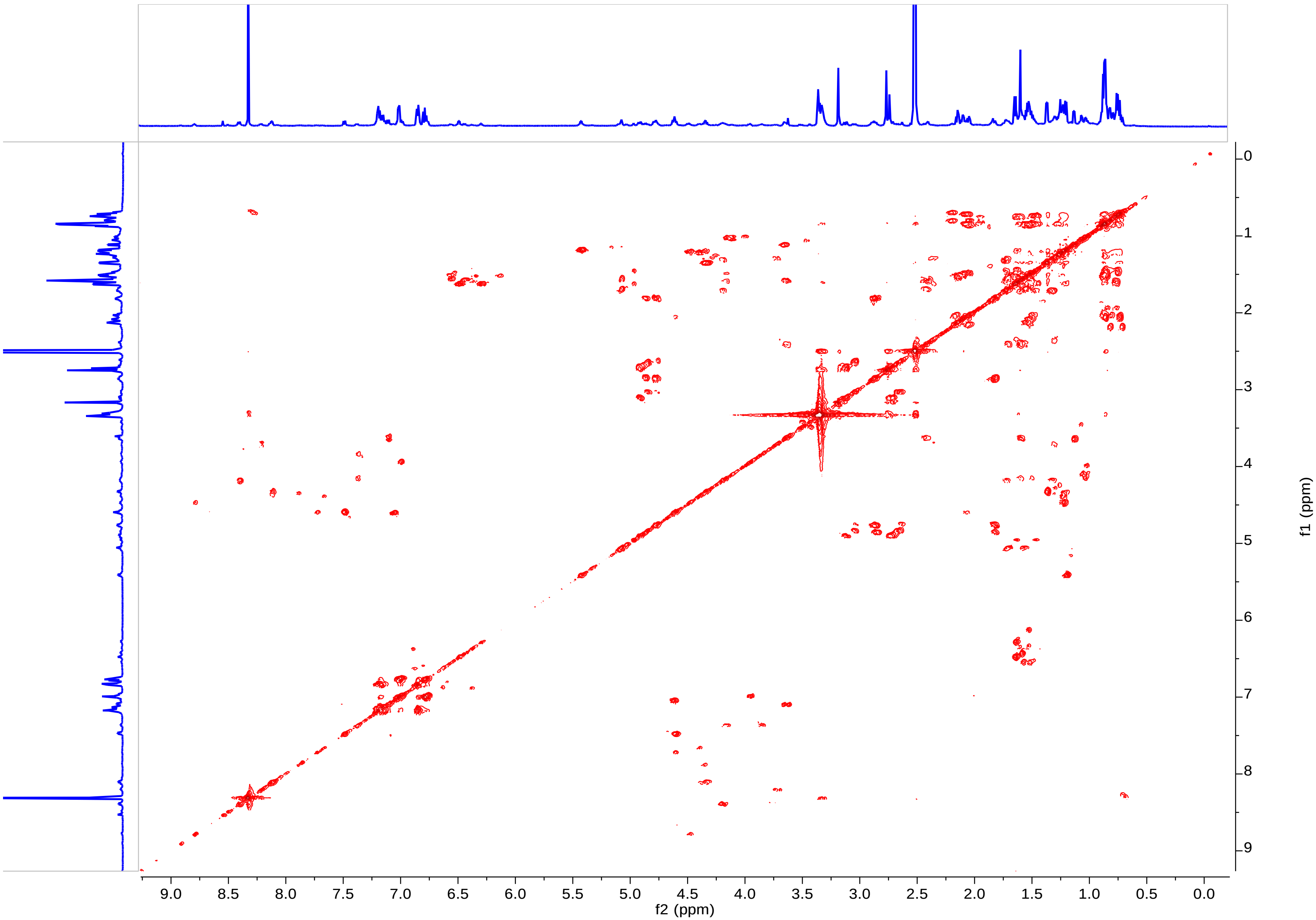
ROESY Spectrum of Loggerpeptin B (**2**) in DMSO-d_6, 600 MHz



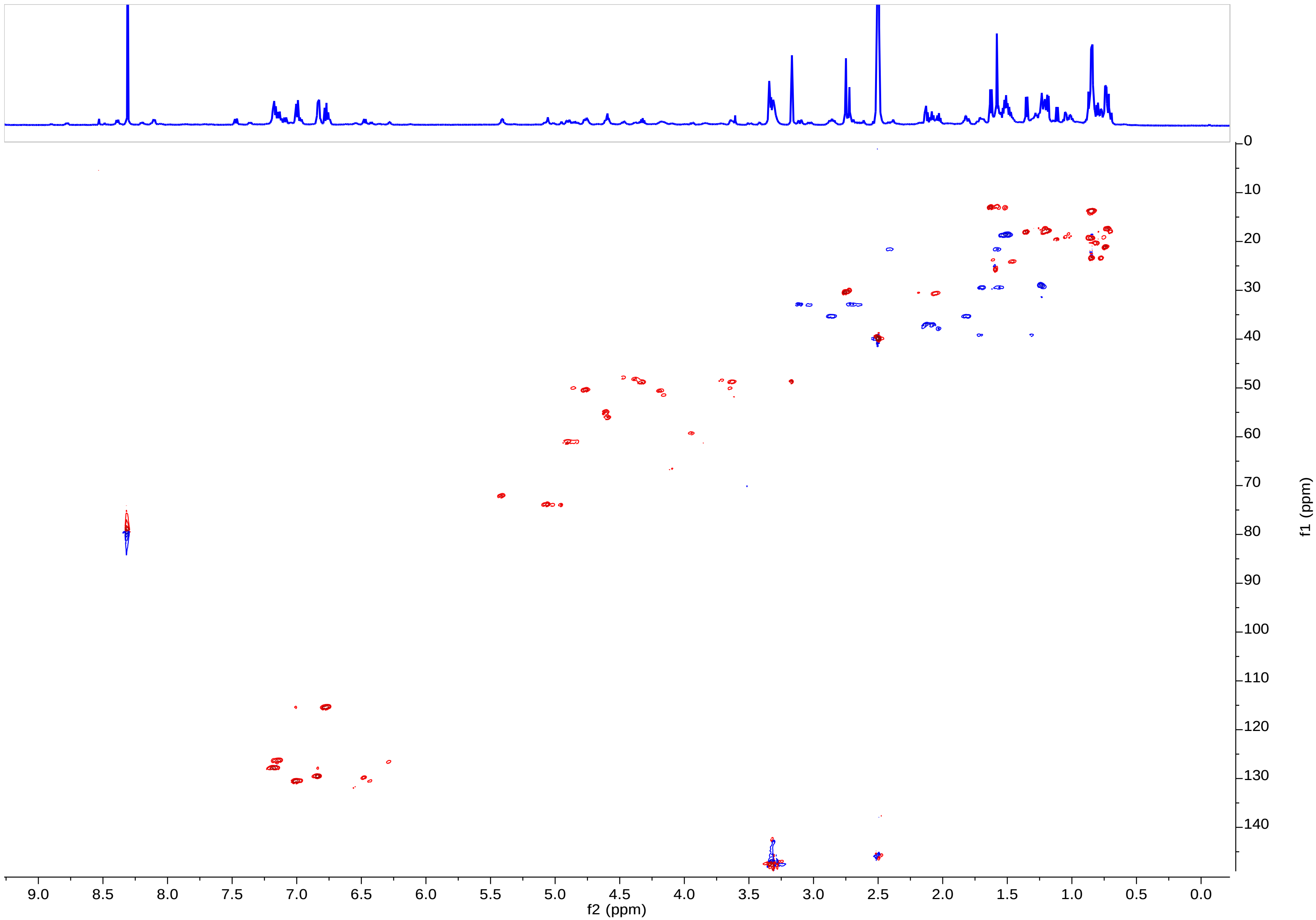
^{1}H NMR Spectrum of Loggerpeptin C (**3**) in DMSO-d_6, 600 MHz



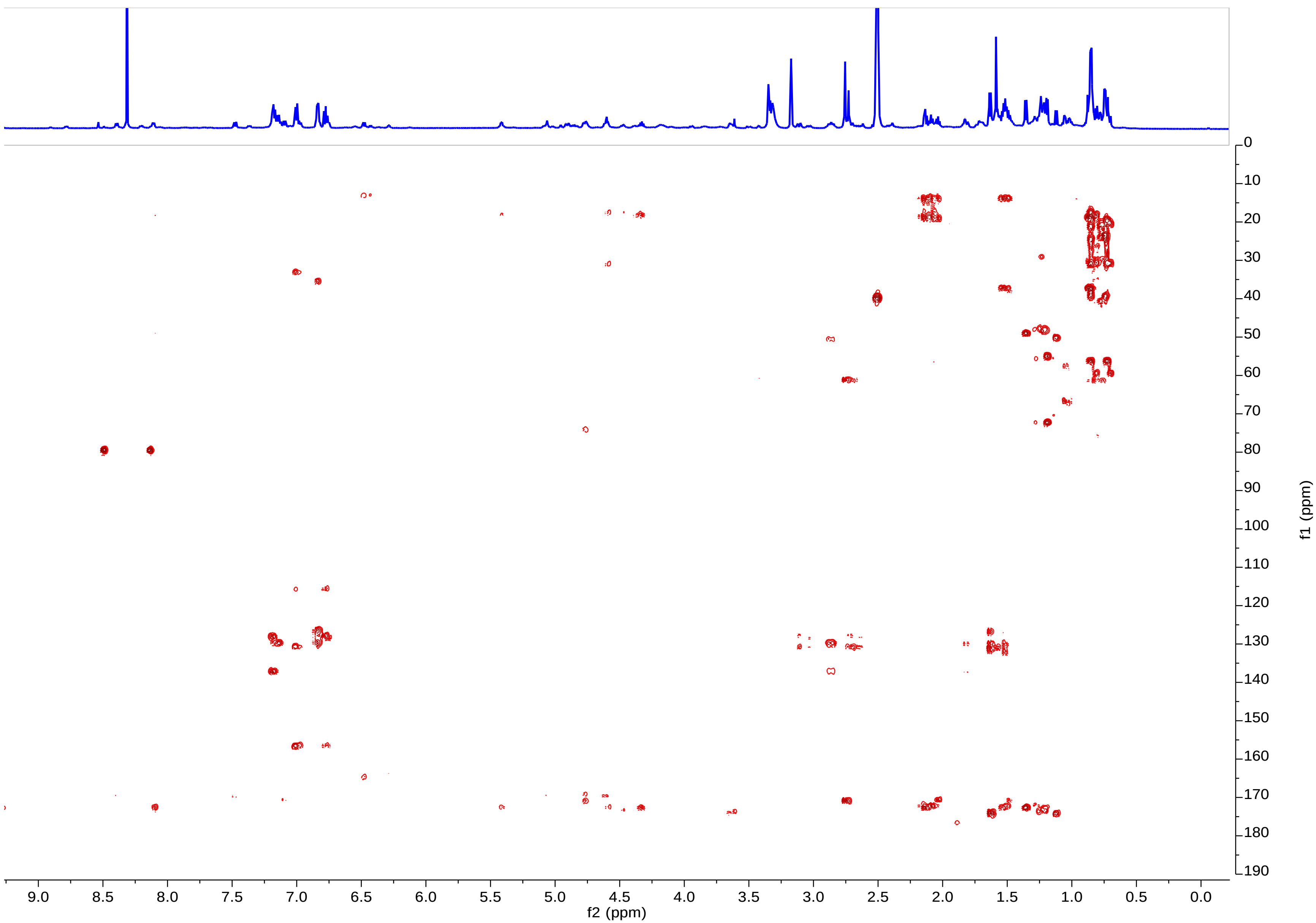
COSY Spectrum of Loggerpeptin C (**3**) in DMSO-d_6, 600 MHz



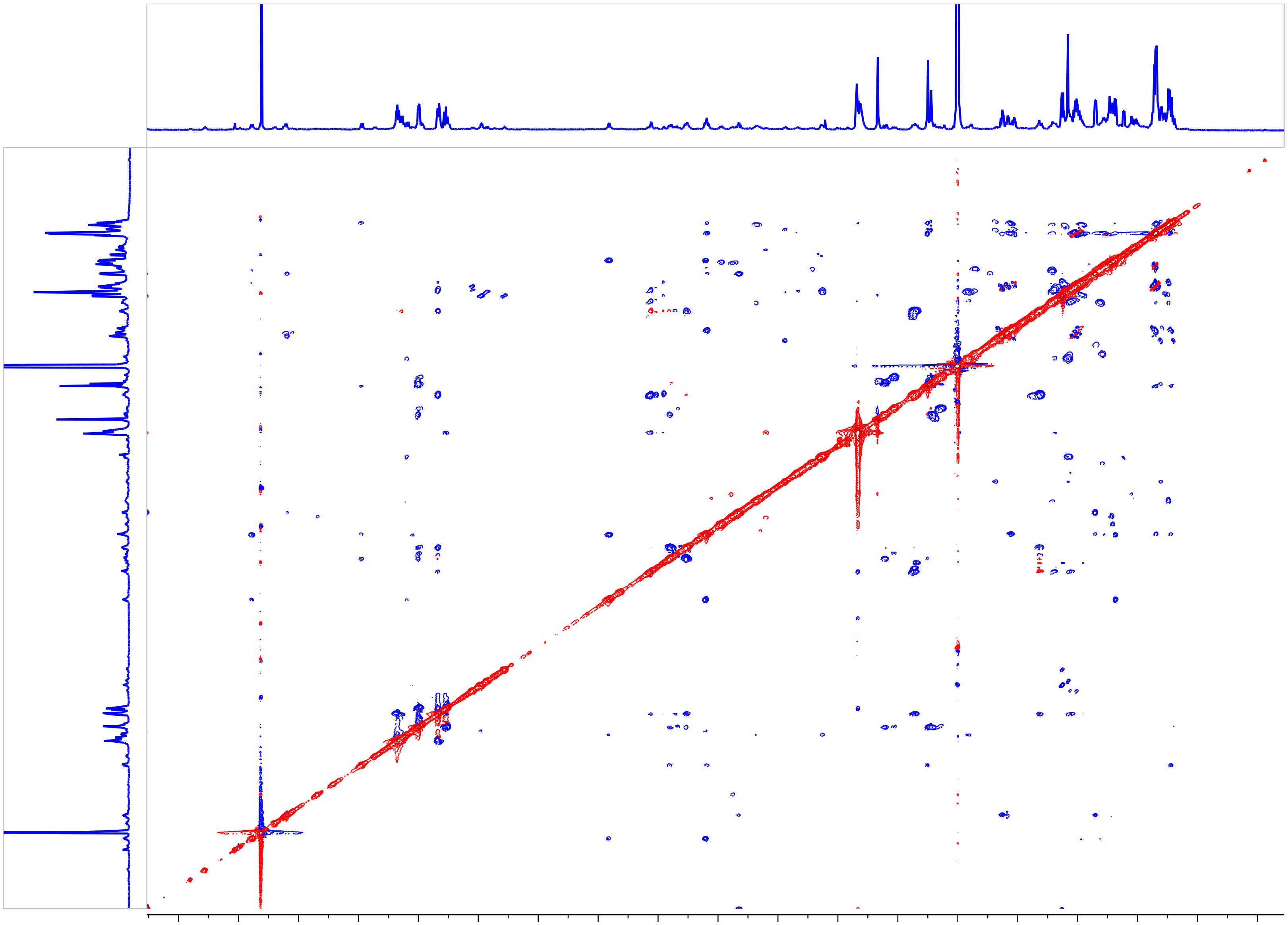
HSQC Spectrum of Loggerpeptin C (**3**) in DMSO-d_6, 600 MHz



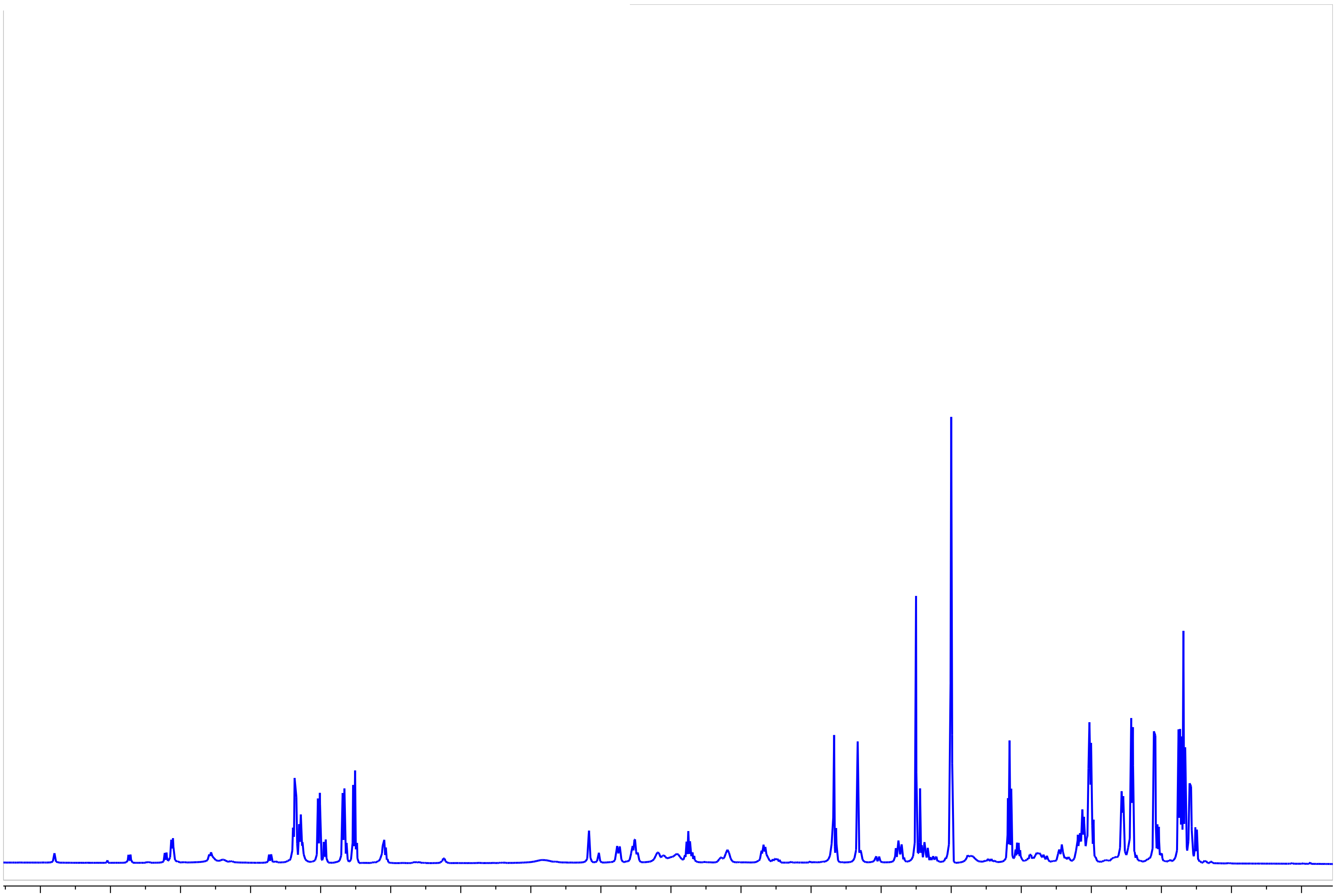
HMBC Spectrum of Loggerpeptin C (**3**) in DMSO-d_6, 600 MHz



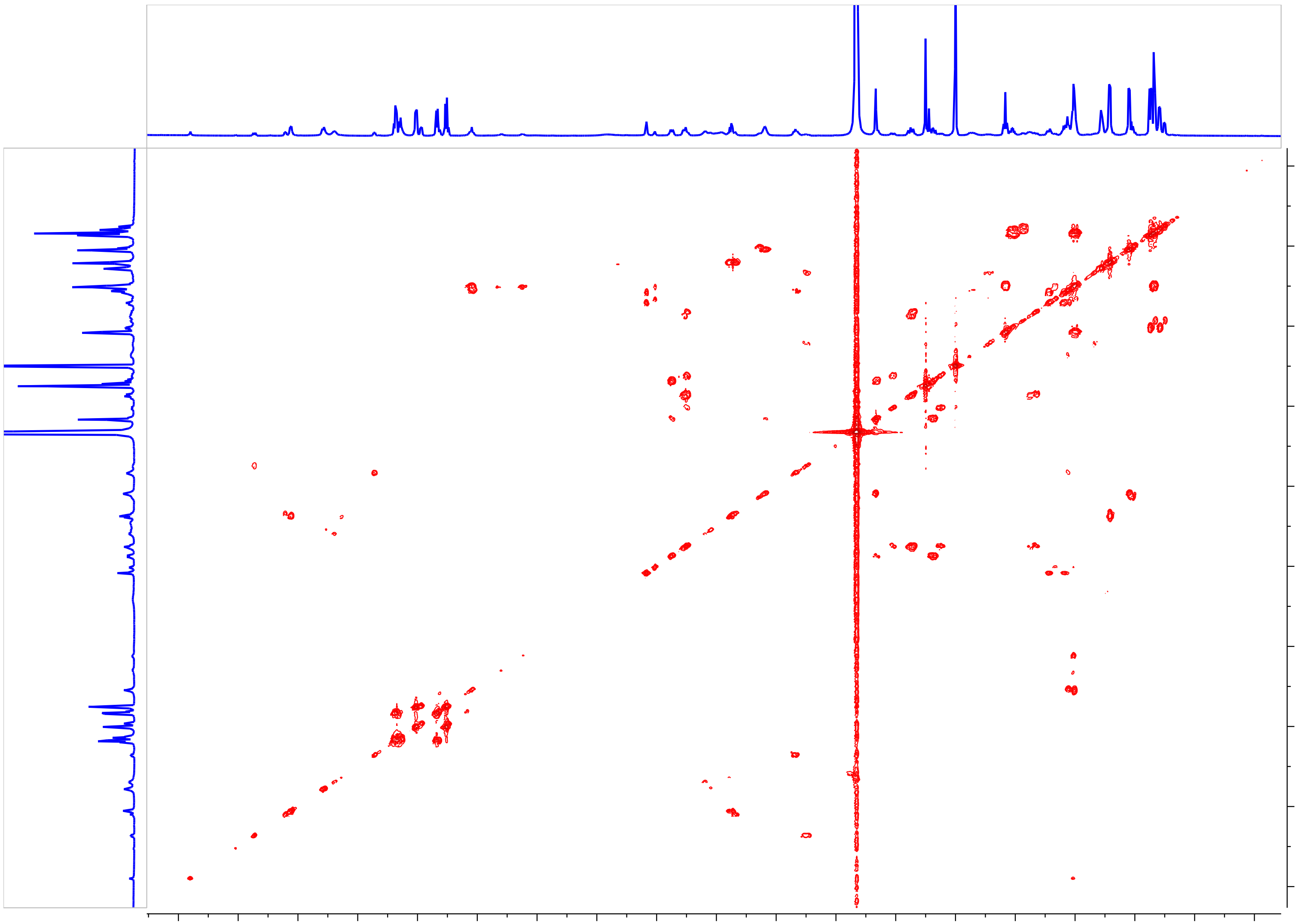
ROESY Spectrum of Loggerpeptin C (**3**) in DMSO-d_6, 600 MHz



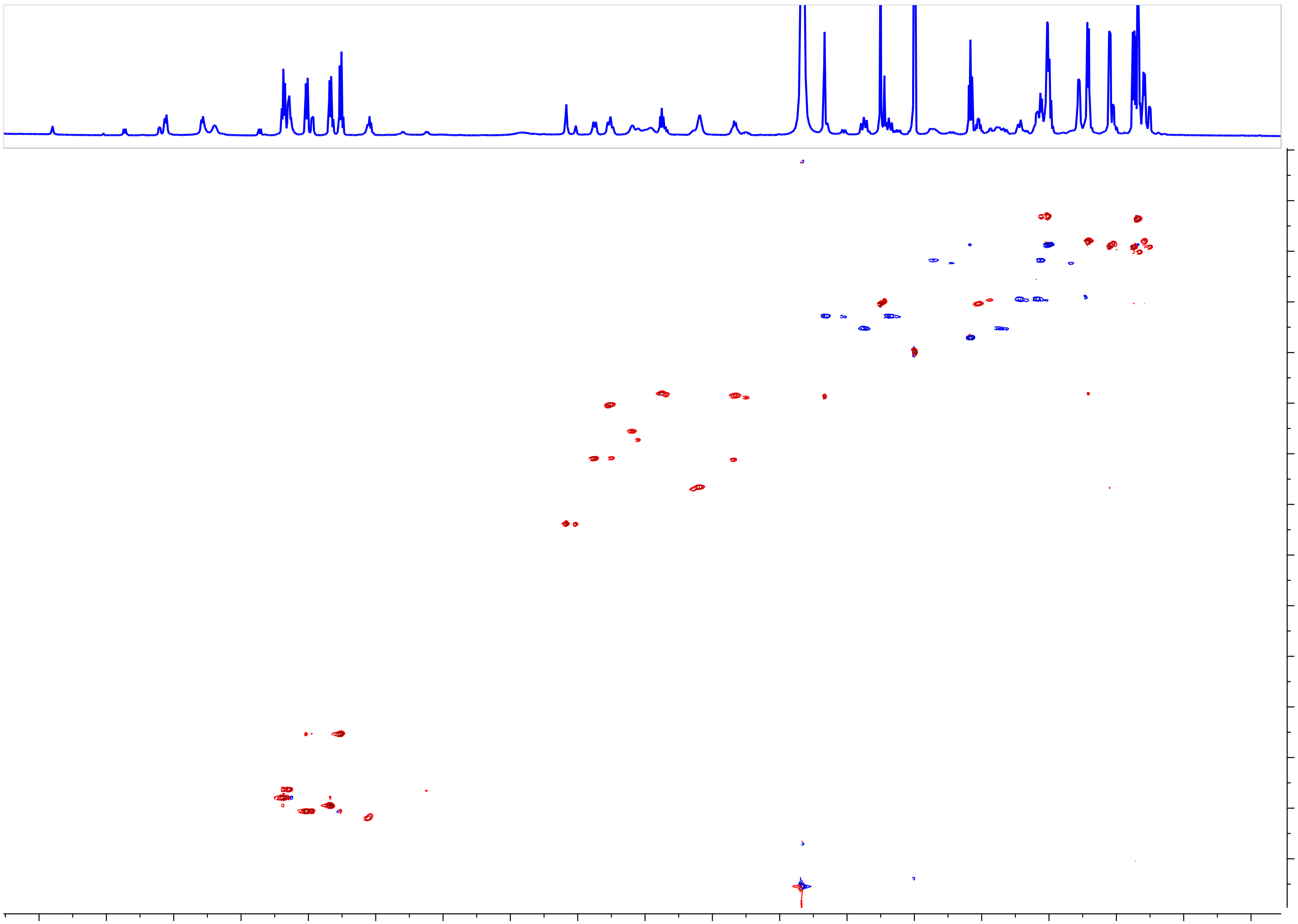
[1]H NMR Spectrum of Molassamide (**4**) in DMSO-d_6, 600 MHz



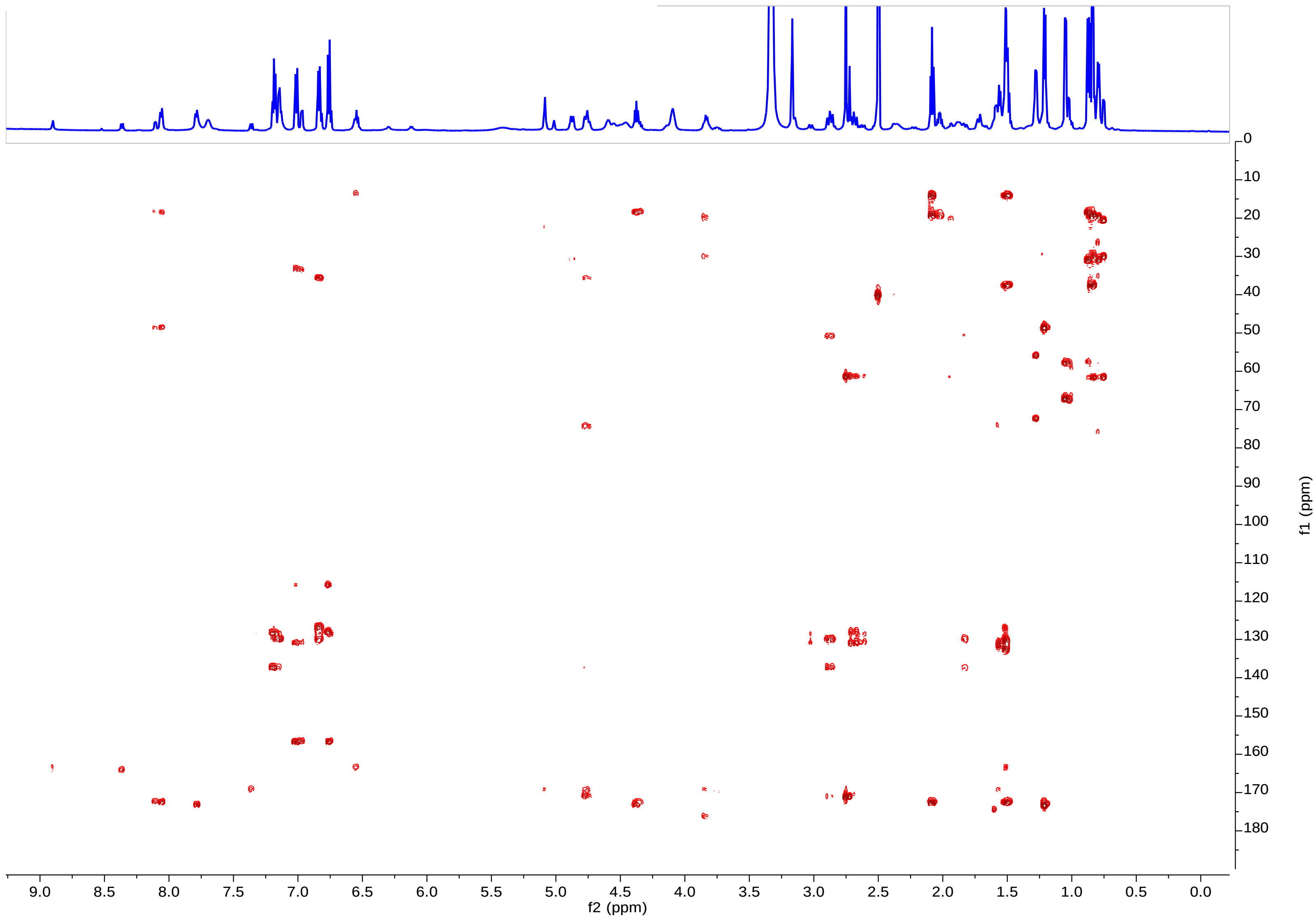
COSY Spectrum of Molassamide (**4**) in DMSO-d_6, 600 MHz



HSQC Spectrum of Molassamide (**4**) in DMSO-d_6, 600 MHz



HMBC Spectrum of Molassamide (**4**) in DMSO-d_6, 600 MHz



ROESY Spectrum of Molassamide (**4**) in DMSO-d_6, 600 MHz