Supplementary information for

Antimicrobial Bacillus probiotics as animal growth promoters

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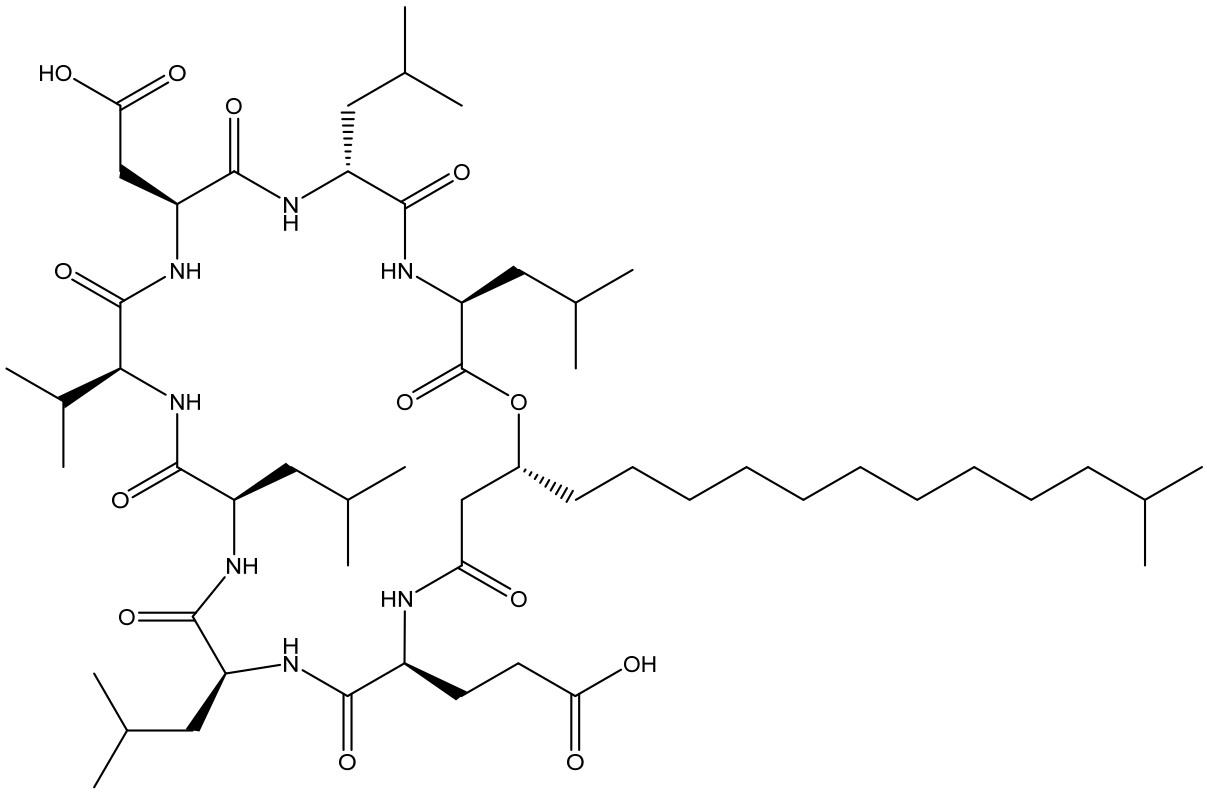
Table S1 Experimental NMR data of C16 Surfactin C in DMSO - d_6 at 25°C



Position		δ_C	δ_H (J in Hz)
Glu1	NH	-	8.44, (d), 6.6
	CO	172.2	-

	α-C	51.1	4.04, (q), 4.8
	β-C	39.5	1.63, (m)
	γ-C	39.3	1.63, (m)
	COOH		
Leu2	NH	-	8.13 d, 7.2
	CO	173.6	-
	α-C	52.3	4.16, (m)
	β-C	24.5	1.47, (m)
	γ-C	39.8	1.50, (m)
	δ_1-C	23.7	0.87, (m)
	δ_2-C	23.4	0.86, (m)
Leu3	NH	-	7.60, (s)
	CO	157.5	-
	α-C	51.4	4.32, (q), 5.6
	β-C	24.7	1.52, (m)
	γ-C	39.0	1.26, (m)
	δ_1-C	23.8	0.86, (m)
	δ_2-C	22.9	0.82, (m)
Val4	NH	-	8.00, (s)
	CO	-	-
	α-C	51.2	4.02, (t), 7.6
	β-C	30.3	2.02, (m)
	γ_1-C	22.9	0.90, (m)
	γ_2-C	22.6	0.76, (m)
Asp5	NH	-	8.19, (s)
	CO		-
	α-C	49.9	4.55, (m)
	β-C	35.9	2.63, (t), 8.0
	COOH		
Leu6	NH	-	7.61, (s)
	CO		-
	α-C	51.6	4.33, (m)
	β-C	40.3	1.46, (m)
	γ-C	23.4	1.14, (m)
	δ_1-C	23.1	0.89, (m)
	δ_2-C	22.3	0.88, (m)
Leu7	NH	-	7.90, (s)
	CO		-
	α-C	52.3	4.14, (m)
	β-C	30.1	1.25, (m)
	γ-C	41.6	1.56, (m)
	δ_1-C	23.1	0.83, (m)
	δ_2-C	22.7	0.80, (m)
Fatty acid part	C1	171.4	-
	C2	41.7	2.38, (m)
	C3	71.6	5.06, (m)
	C4	33.7	1.51, (m)
	C5-15	22.3	0.80, (m)
	C16	29.7	2.03, (m)
	C17	22.1	0.80, (m)
	C18	24.3	0.81, (m)

Figure S1 (+)-LRESIMS spectrum of compound 1

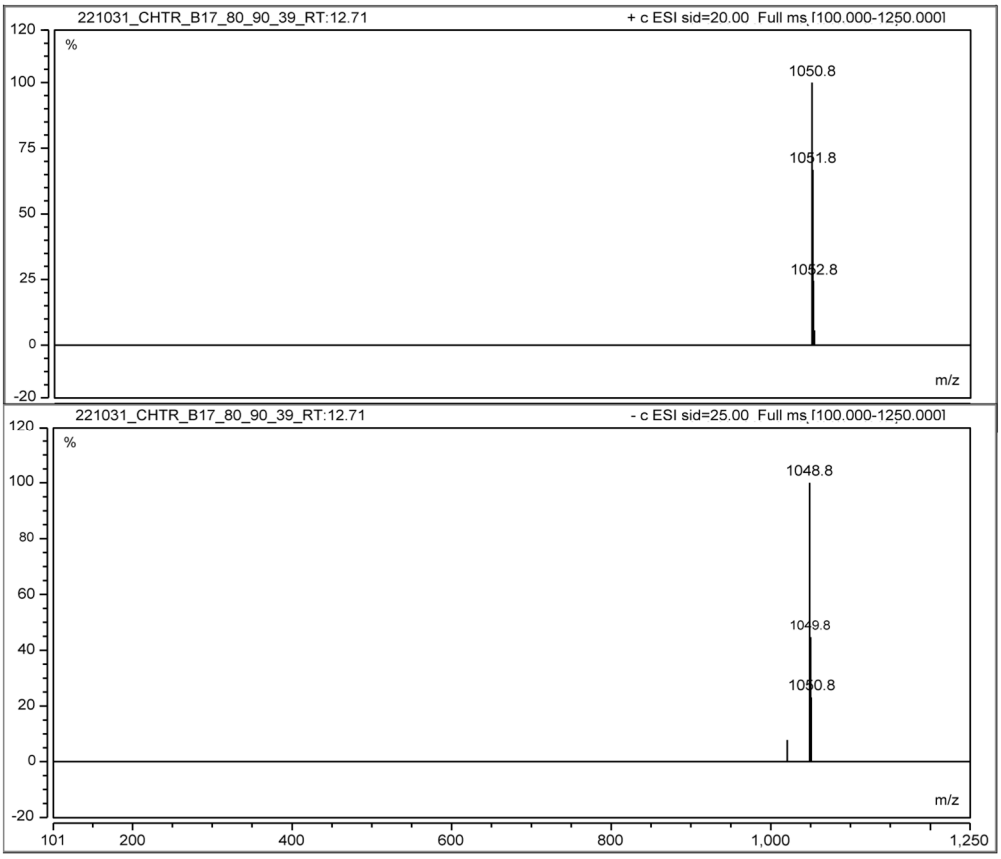


Figure S2 ^{1}H NMR (800 MHz, DMSO) spectrum of compound 1

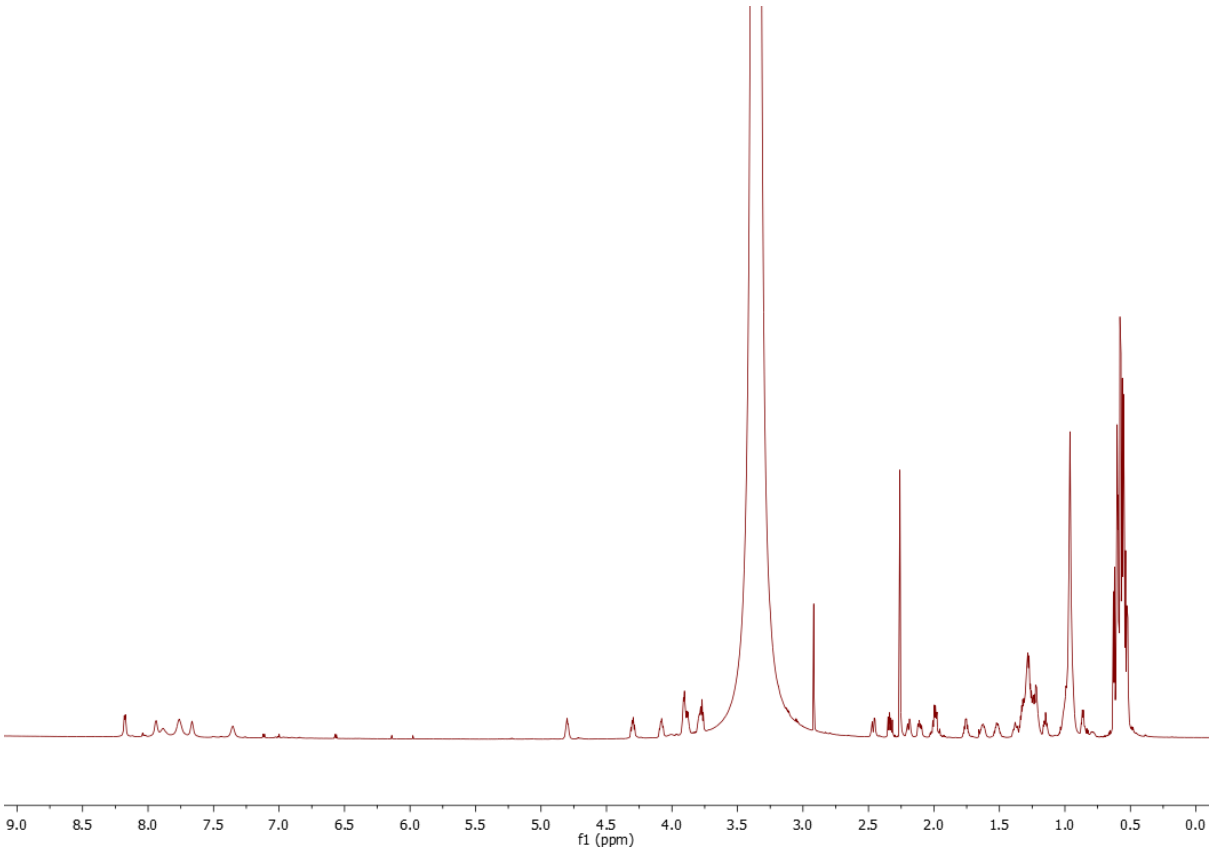


Figure S3 ^{1}H - ^{1}H COSY spectrum of compound 1 in DMSO

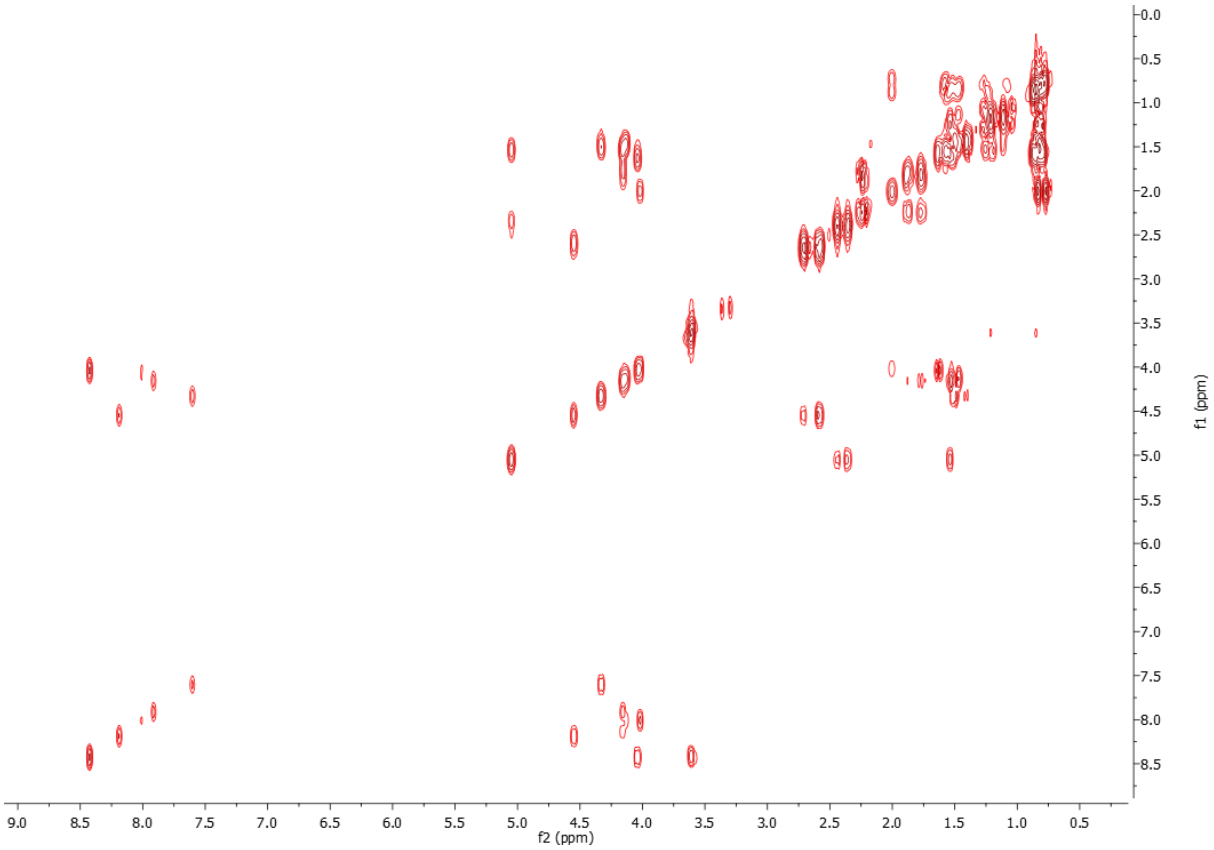


Figure S4 HSQC spectrum of compound 1 in DMSO

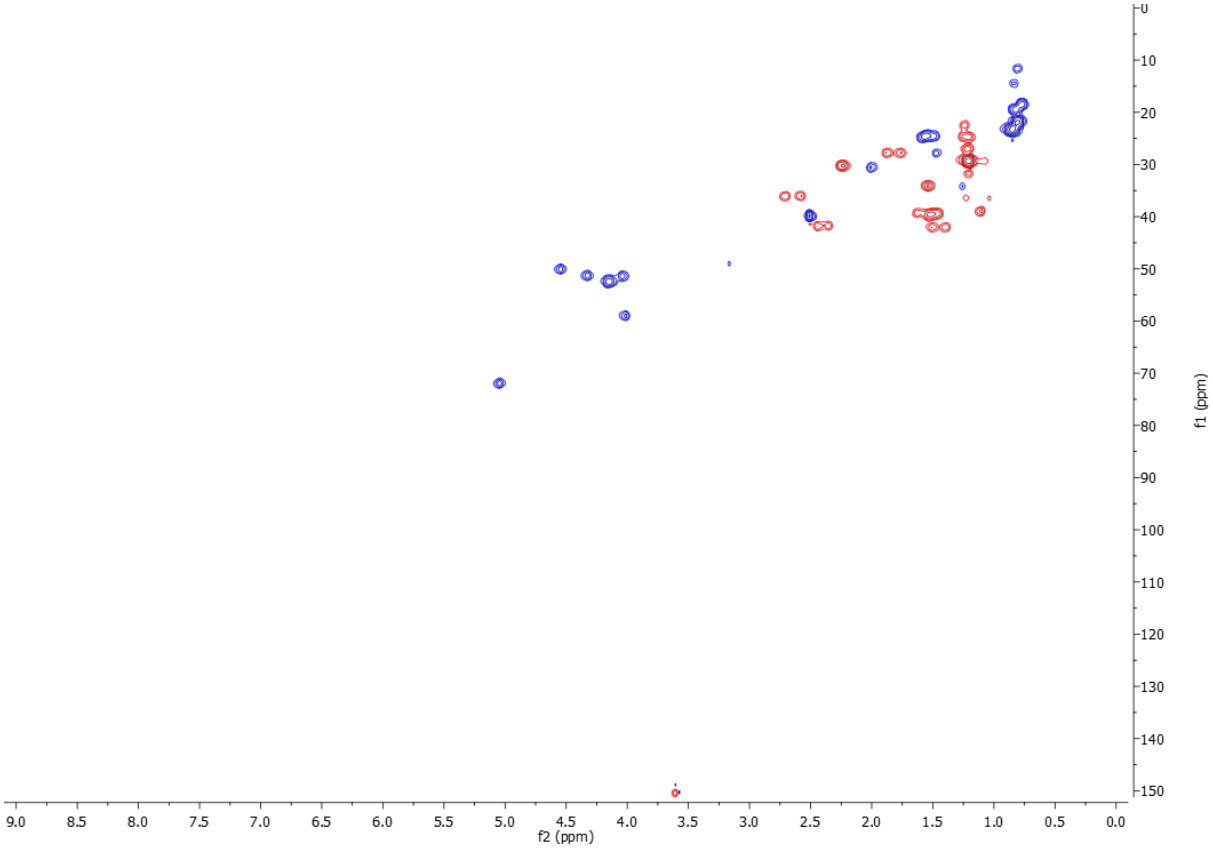


Figure S5 HMBC spectrum of compound 1 in DMSO

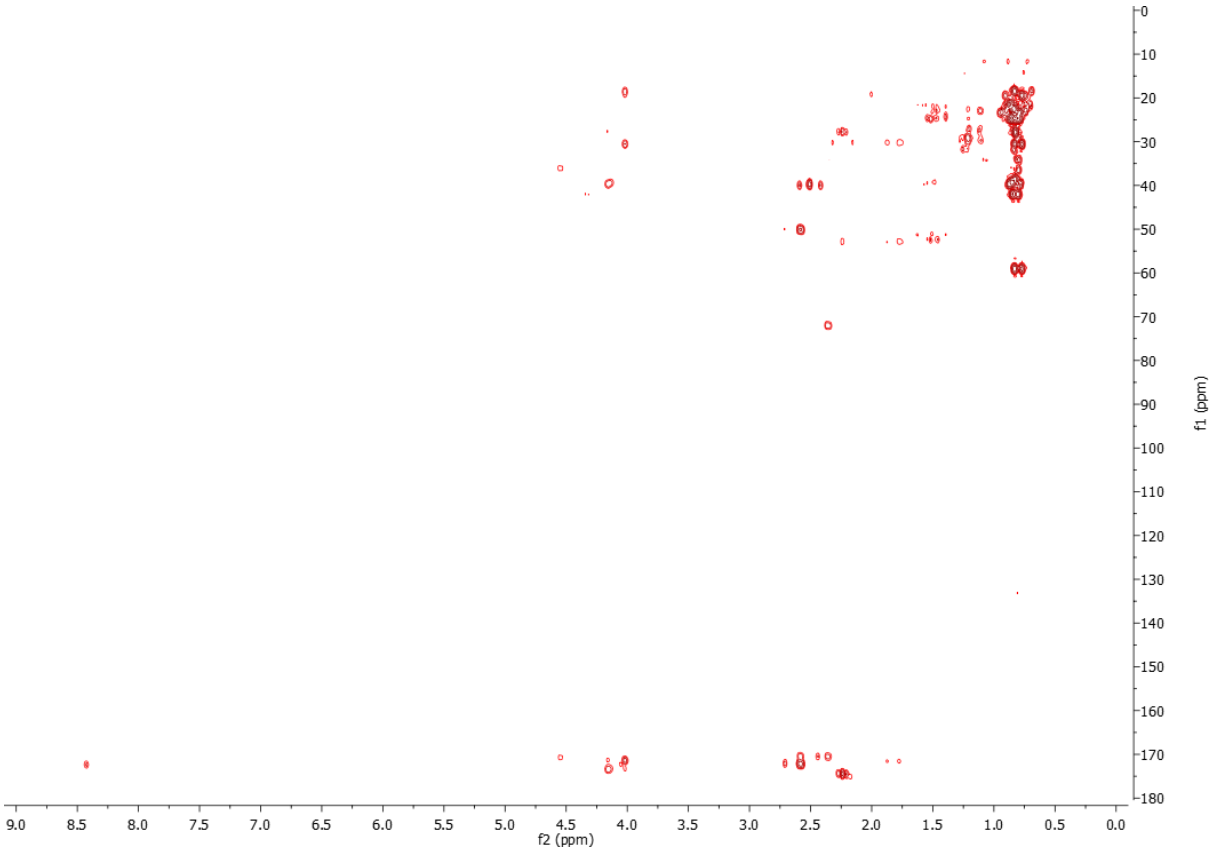
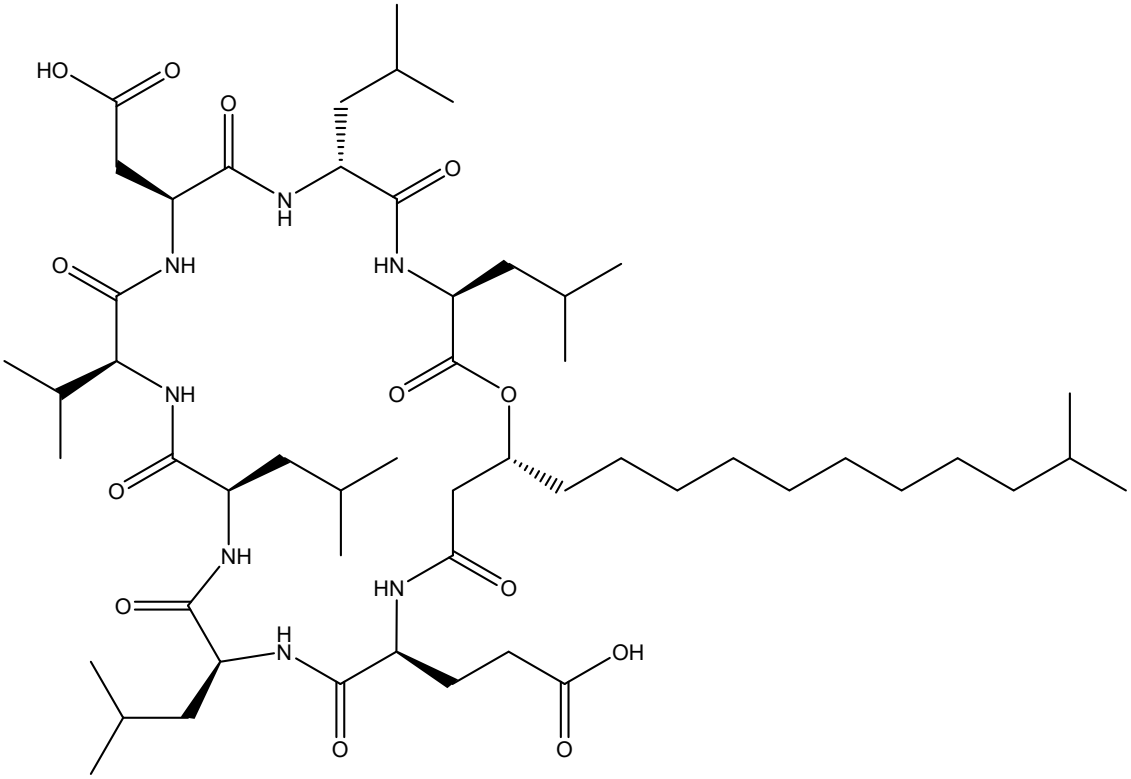


Table S2 Experimental NMR data of compound 2 in DMSO - d_6 at 25°C



Position		δ_C	δ_H (J in Hz)
Glu1	NH	-	8.14, (d), 6.6
	CO	170.5	-
	α-C	50.2	4.55, (q), 4.8
	β-C	36.3	2.58, (m)
	γ-C	40.3	2.74, (dd), 4.8/12.8
	COOH	172.3	12.0
Leu2	NH	-	8.44, d, 7.2
	CO	172.4	-
	α-C	51.5	4.08, (m)
	β-C	39.0	1.66 (m)
	γ-C	28.5	1.55 (m)
	δ_1-C	22.5	0.83, (m)
	δ_2-C	22.5	0.83, (m)
Leu3	NH	-	7.60, (s)
	CO	172.2	-
	α-C	51.2	4.37, (q), 5.6
	β-C	42.1	1.50, (m)
	γ-C	39.8	1.60, (m)
	δ_1-C	22.5	0.87, (m)
	δ_2-C	22.5	0.87, (m)
Val4	NH	-	8.05, (s)
	CO	171.1	-
	α-C	59.0	4.04, (t), 7.6
	β-C	30.6	2.01, (m)
	γ_1-C	18.6	0.81, (m)
	γ_2-C	19.5	0.89, (m)

Asp5	NH	-	7.99, (s)
	CO	173.4	-
	α-C	52.7	4.17, (m)
	β-C	30.1	1.80, (m) / 2.24, (t), 8.0
	COOH	174.5	12.33, (s)
Leu6	NH	-	7.81, (s)
	CO	171.1	-
	α-C	52.8	4.17, (m)
	β-C	39.9	1.50 (m)/1.61 (m)
	γ-C	21.9	0.80
	δ_1-C	18.1	0.81 (m)
	δ_2-C	19.2	0.88 (m)
Leu7	NH	-	7.81, (s)
	CO	173.4	-
	α-C	52.8	4.17, (m)
	β-C	39.9	1.50 (m)/1.61 (m)
	γ-C	21.9	0.80
	δ_1-C	18.1	0.81 (m)
	δ_2-C	19.2	0.88 (m)
Fatty acid part	C1	170.3	-
	C2	41.9	2.50 (m)/2.33 (m)
	C3	71.8	5.08, (m)
	C4	39.3	1.53, (m)
	C5-15	26.1	0.84, (m)
	C16	24.6	1.62, (m)
	C17	23.2	0.91, (m)
	C18	23.2	0.91, (m)

Figure S6 (+)-LRESIMS spectrum of compound 2

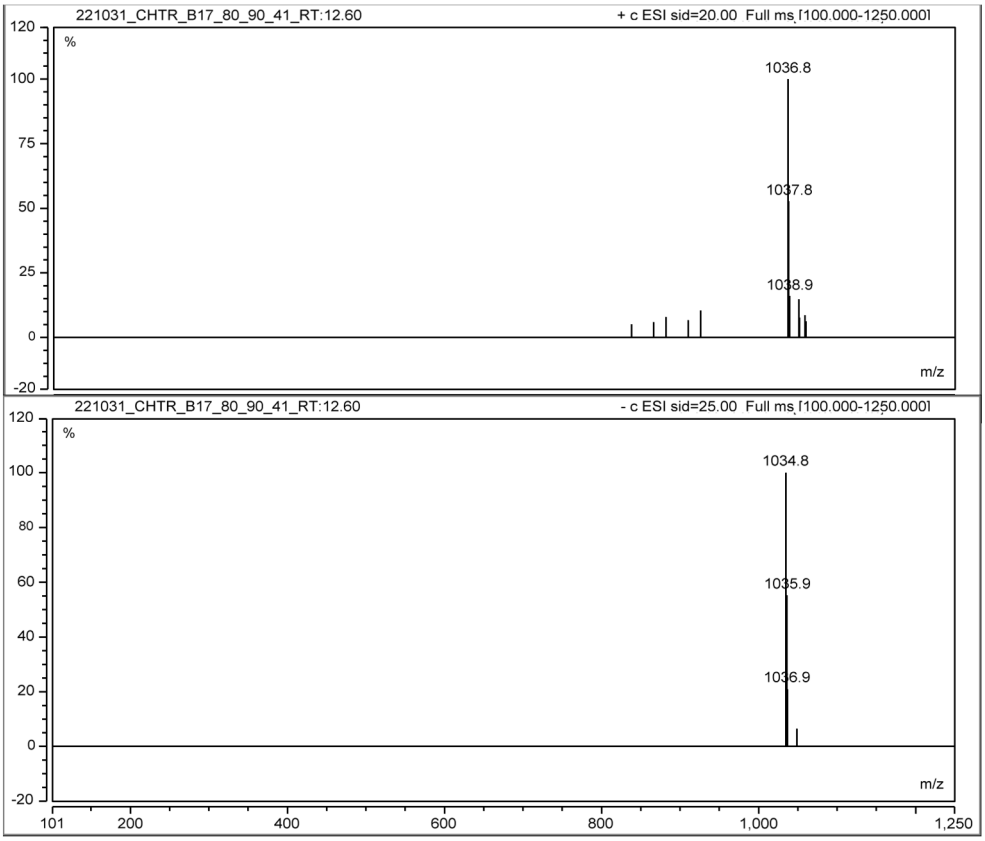


Figure S7 ^{1}H NMR (800 MHz, DMSO) spectrum of compound 2

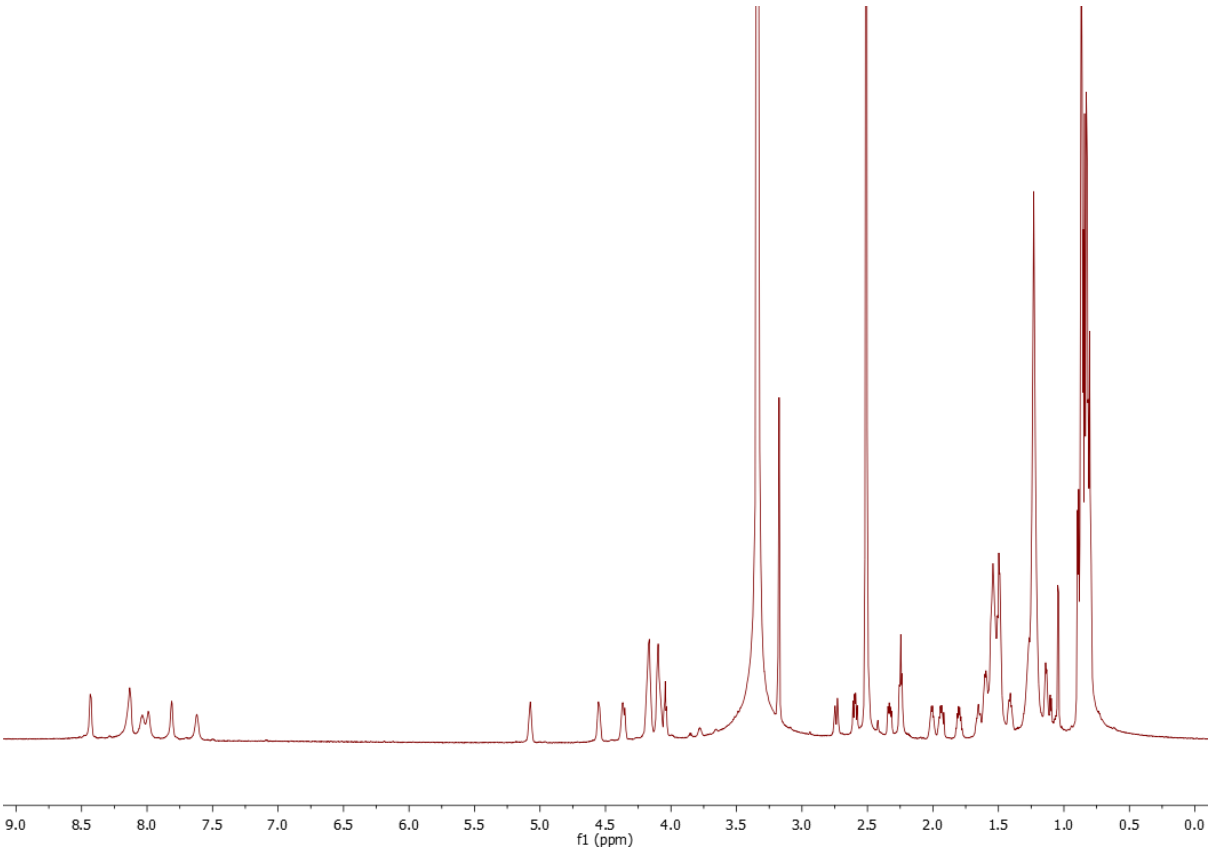


Figure S8 $^{1}H-^{1}H$ COSY spectrum of compound 2 in DMSO

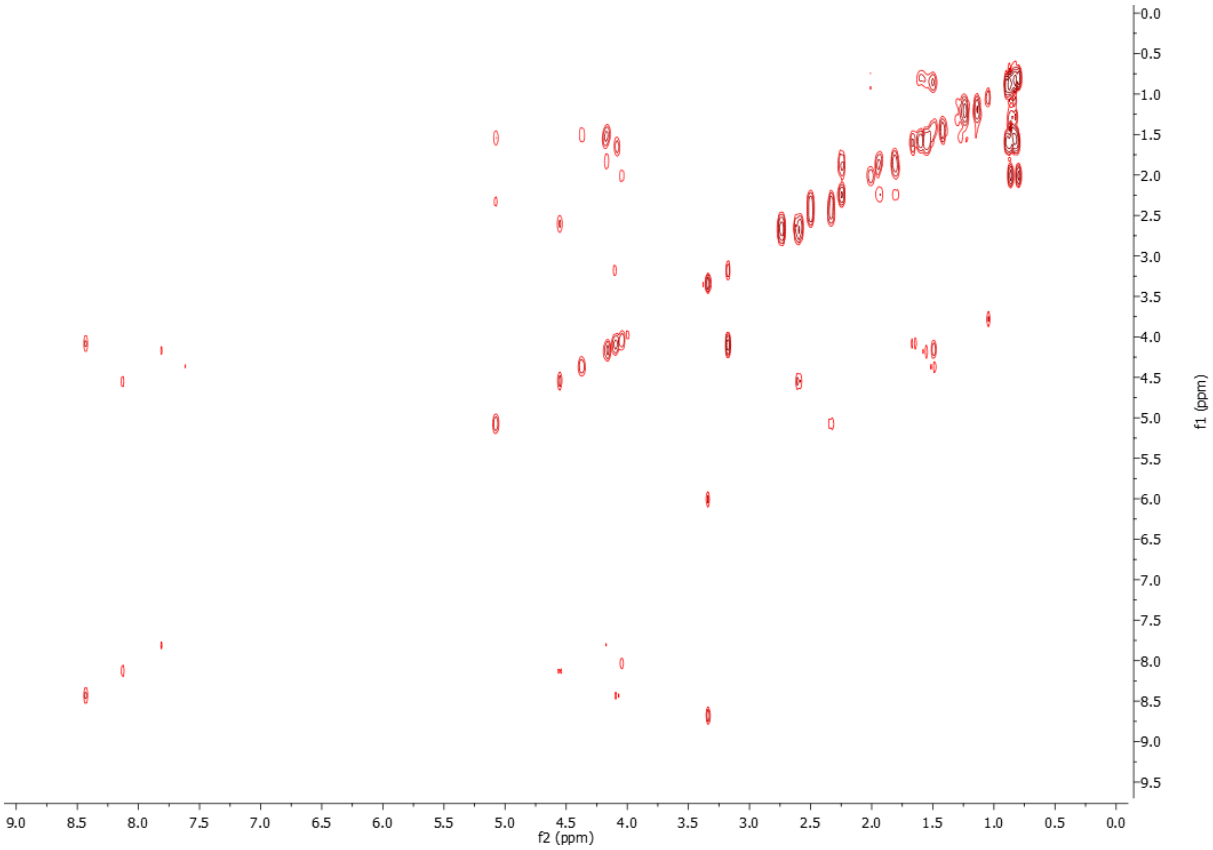


Figure S9 HSQC spectrum of compound 2 in DMSO

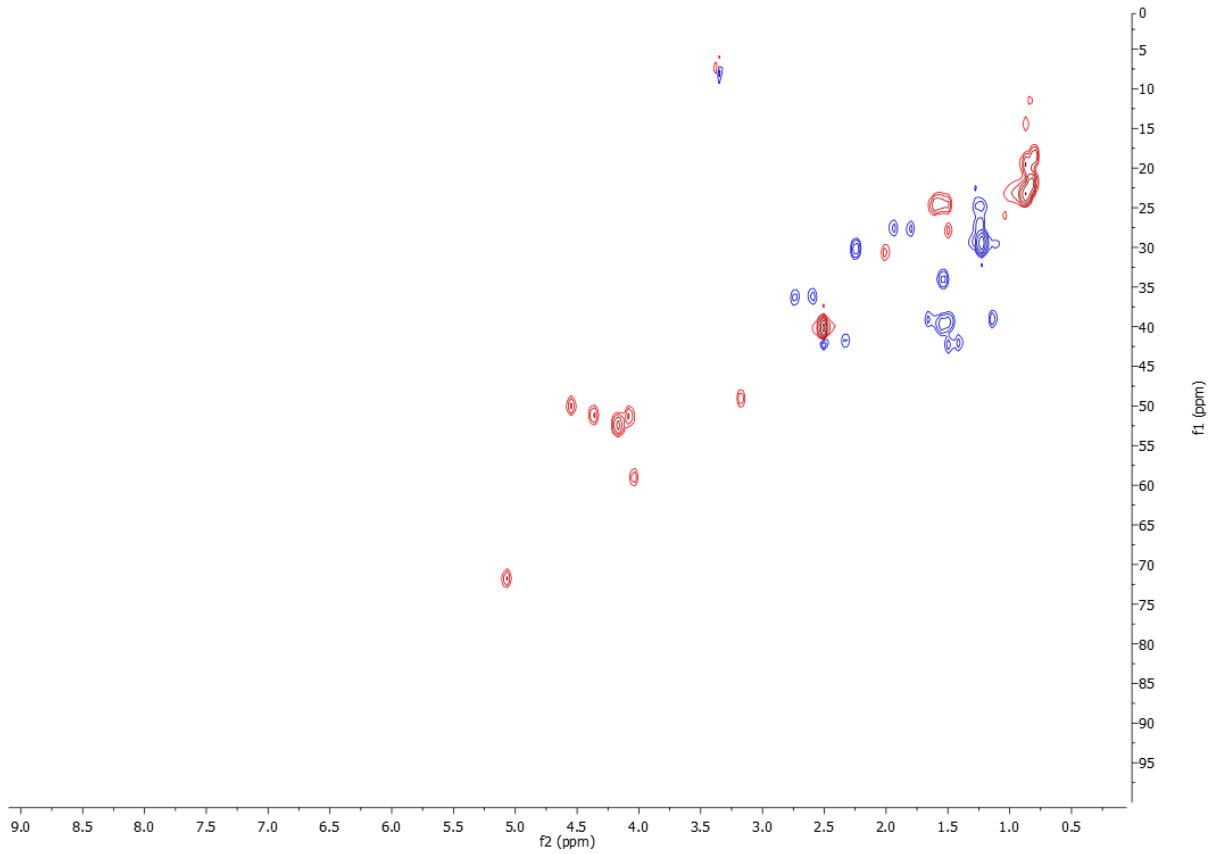


Figure S10 HMBC spectrum of compound 2 in DMSO

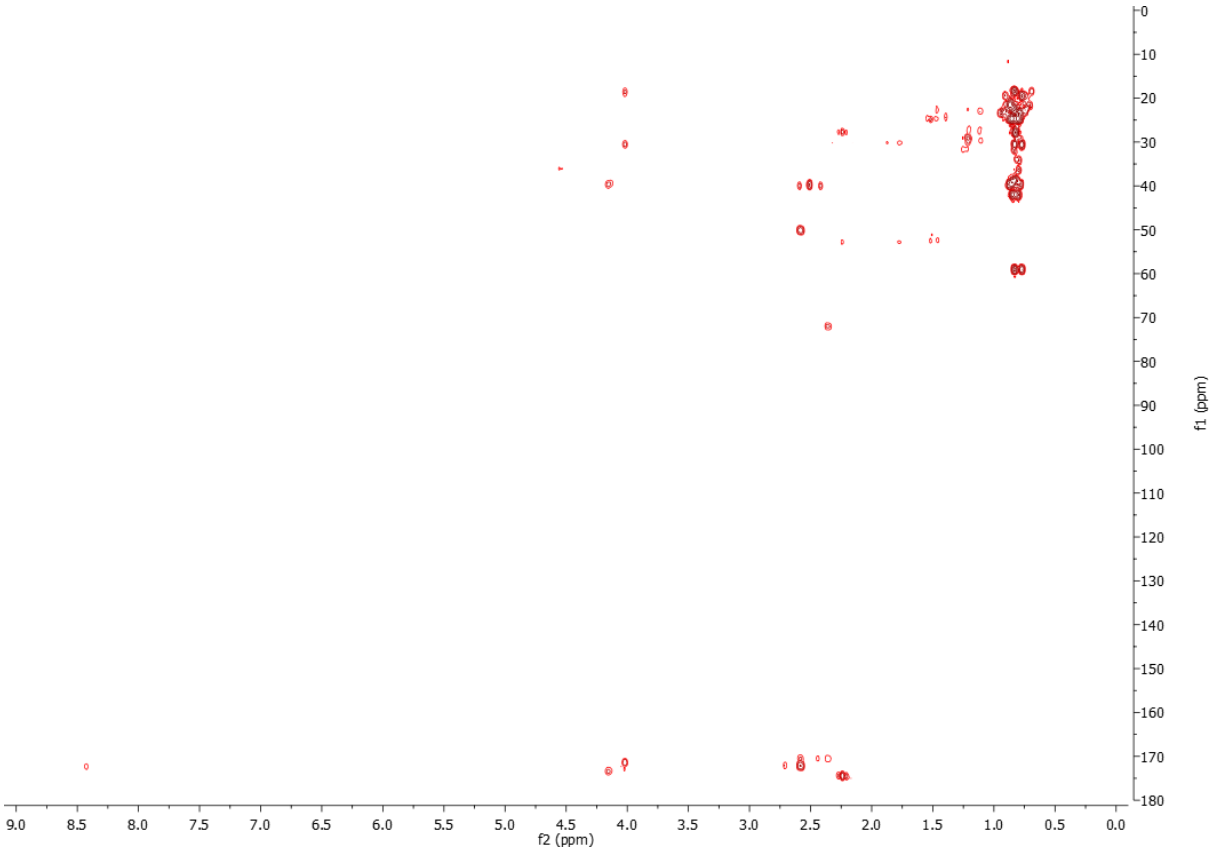
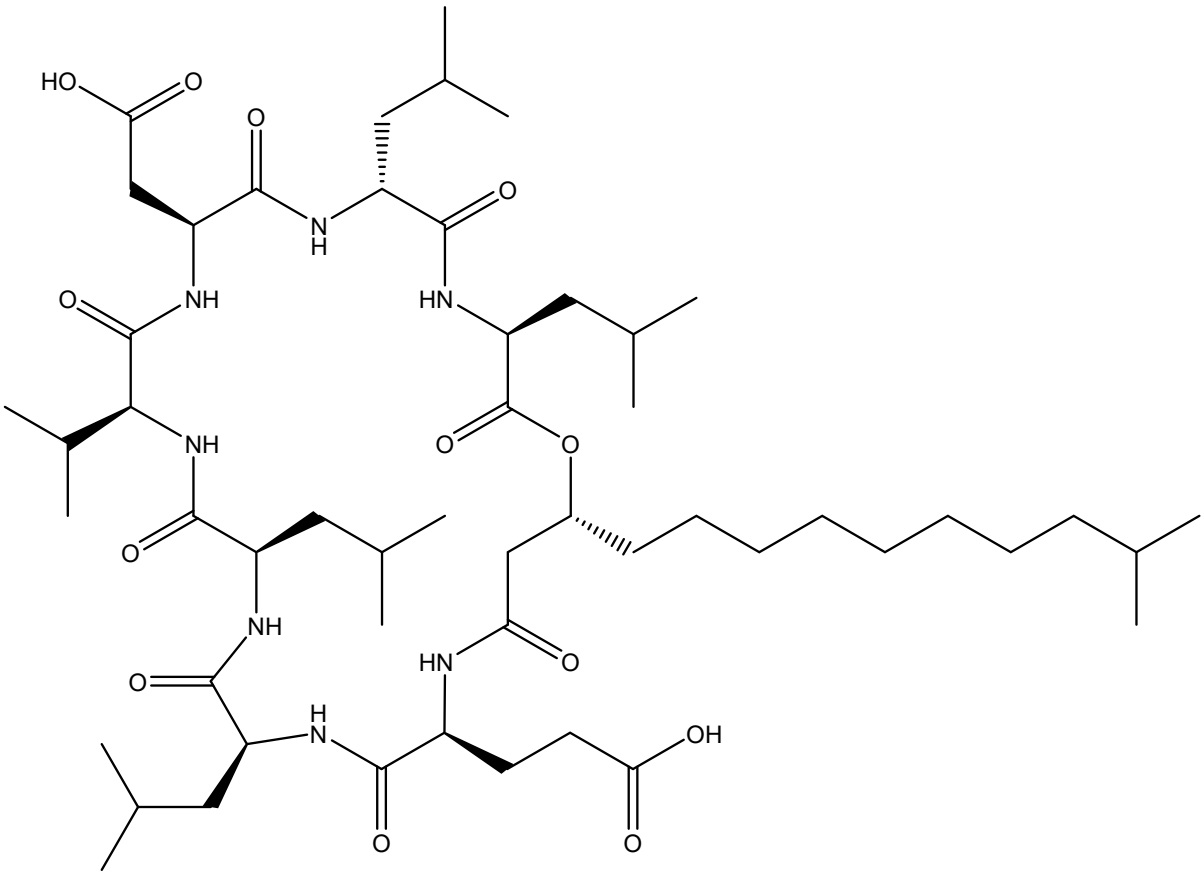


Table S3 Experimental NMR data of compound 3 in DMSO - d_6 at 25°C



Position		δ_C	δ_H (J in Hz)
Glu1	NH	-	8.42, (d), 6.6
	CO	172.2	-
	α-C	51.1	4.04, (q), 4.8
	β-C	39.5	1.63, (m)
	γ-C	39.3	1.63, (dd), 4.8/12.8
	COOH	172.3	12.0
Leu2	NH	-	8.14, d, 7.2
	CO	173.6	-
	α-C	52.3	4.16, (m)
	β-C	24.5	1.47, (m)
	γ-C	39.8	1.50, (m)
	δ_1-C	23.7	0.87, (m)
	δ_2-C	23.4	0.86, (m)
Leu3	NH	-	7.60, (s)
	CO	157.5	-
	α-C	51.4	4.35, (q), 5.6
	β-C	24.7	1.52, (m)
	γ-C	39.0	1.26, (m)
	δ_1-C	23.8	0.86, (m)
	δ_2-C	22.9	0.82, (m)
Val4	NH	-	8.00, (s)
	CO	-	-
	α-C	51.2	4.04, (t), 7.6
	β-C	30.3	2.02, (m)

	γ_1-C	22.9	0.90, (m)
	γ_2-C	22.6	0.76, (m)
Asp5	NH	-	8.16, (s)
	CO		-
	α-C	49.9	4.54, (m)
	β-C	35.9	2.60, (m)
	COOH		12.33 (s)
Leu6	NH	-	7.60, (s)
	CO		-
	α-C	51.6	4.36, (m)
	β-C	40.3	1.46, (m)
	γ-C	23.4	1.14, (m)
	δ_1-C	23.1	0.89, (m)
	δ_2-C	22.3	0.88, (m)
Leu7	NH	-	7.88, (s)
	CO		-
	α-C	52.3	4.16, (m)
	β-C	30.1	1.25, (m)
	γ-C	41.6	1.56, (m)
	δ_1-C	23.1	0.83, (m)
	δ_2-C	22.7	0.80, (m)
Fatty acid part	C1	171.4	-
	C2	41.7	2.34, (m)
	C3	71.6	5.06, (m)
	C4	33.7	1.51, (m)
	C5-15	22.3	0.80, (m)
	C16	29.7	2.03, (m)
	C17	22.1	0.80, (m)
	C18	24.3	0.81, (m)

Figure S11 (+)-LRESIMS spectrum of compound 3

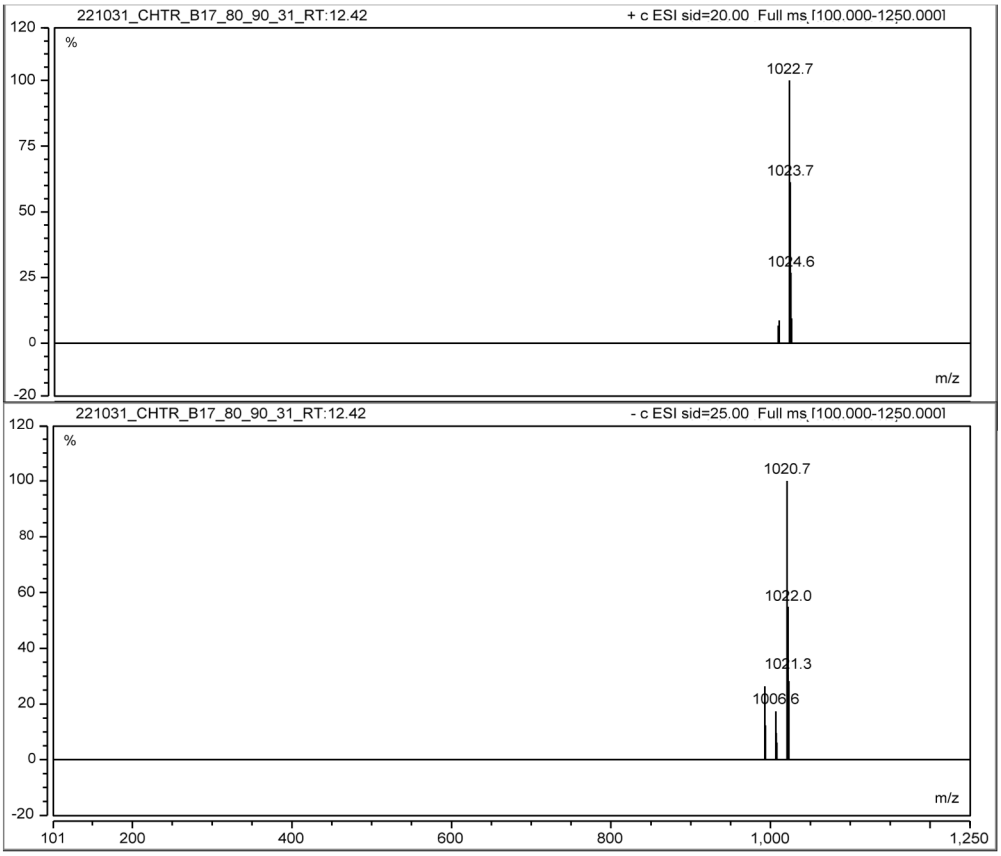


Figure S12 ^{1}H NMR (800 MHz, DMSO) spectrum of compound 3

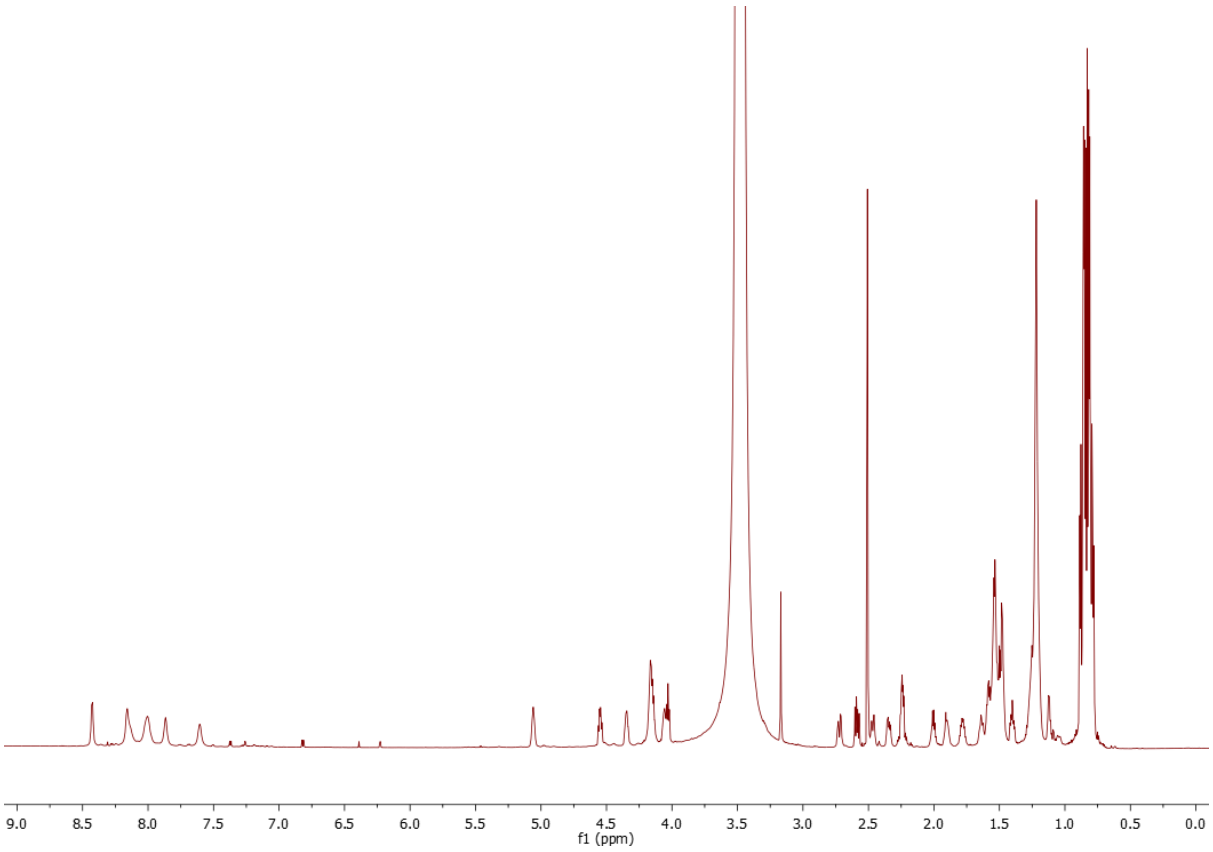


Figure S13 $^{1}H-^{1}H$ COSY spectrum of compound 3 in DMSO

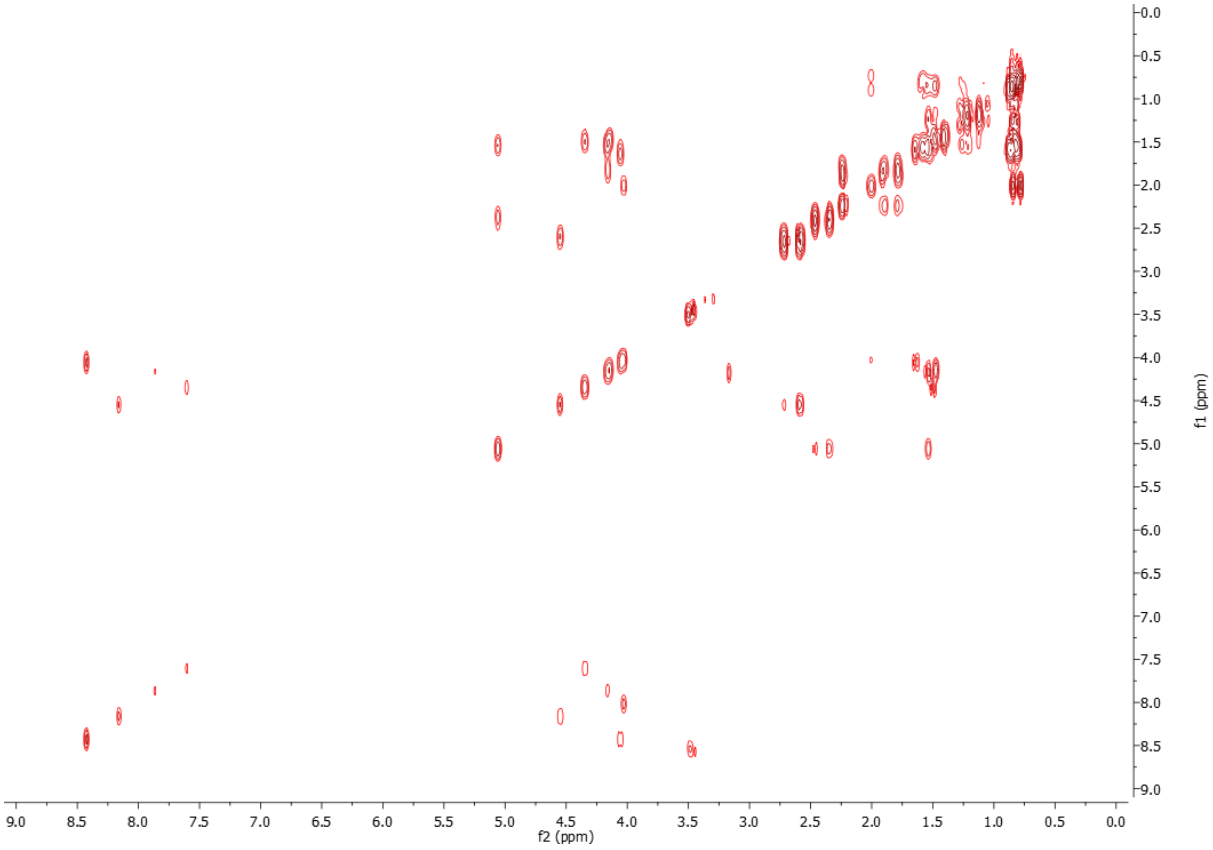


Figure S14 HSQC spectrum of compound 3 in DMSO

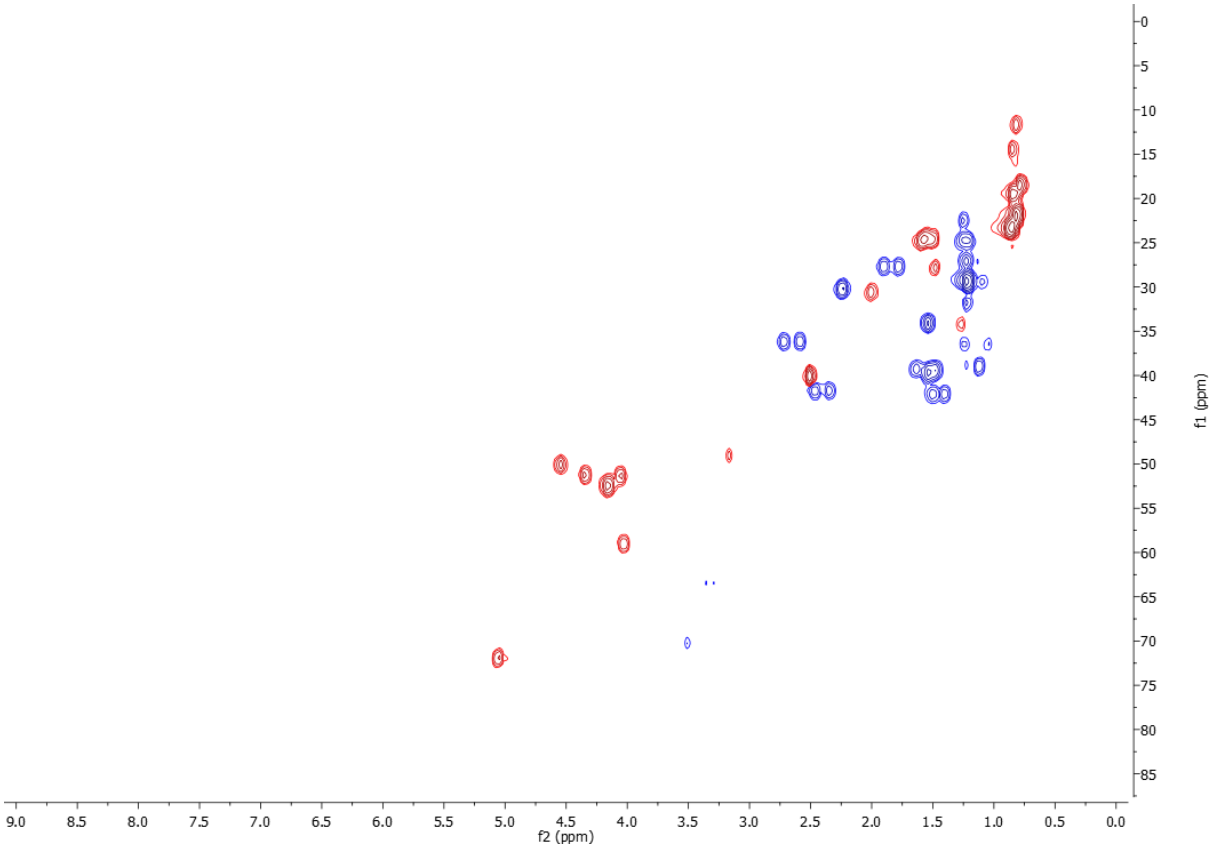


Figure S15 HMBC spectrum of compound 3 in DMSO

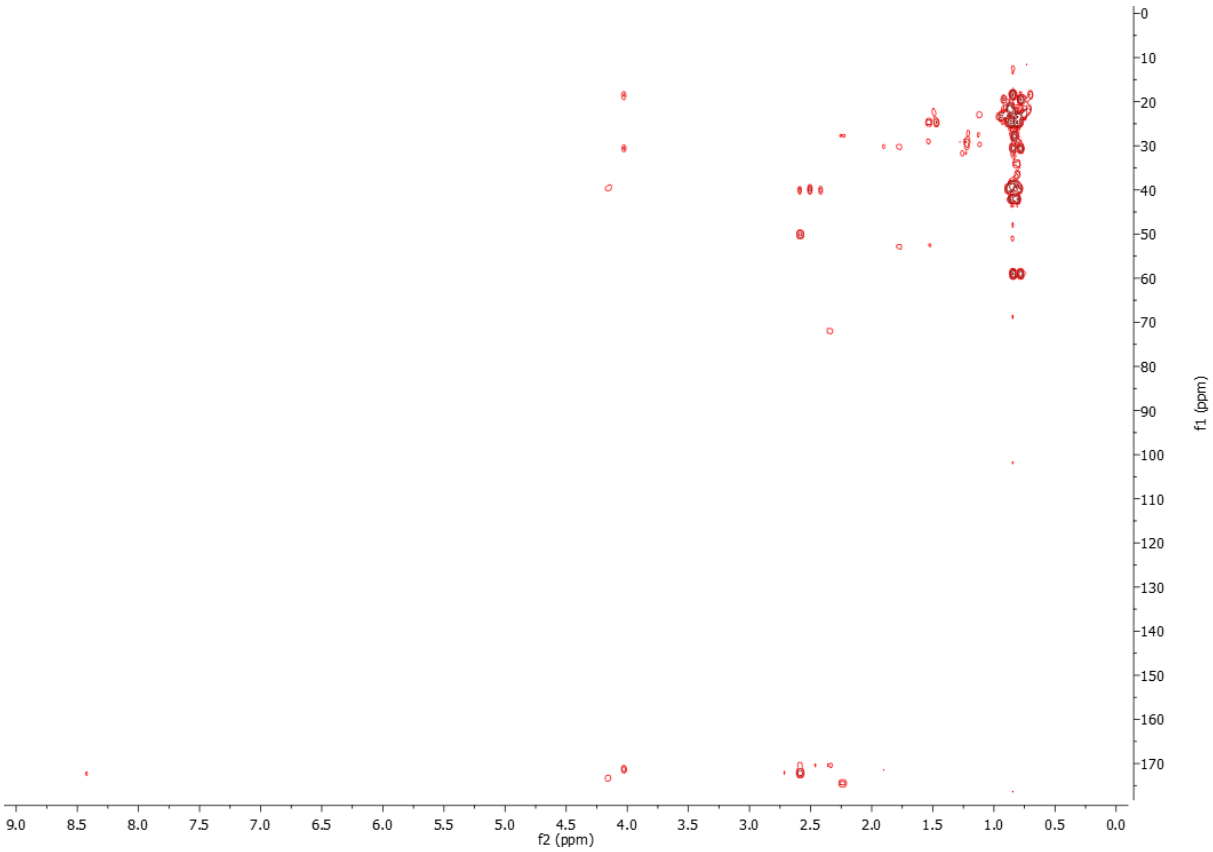
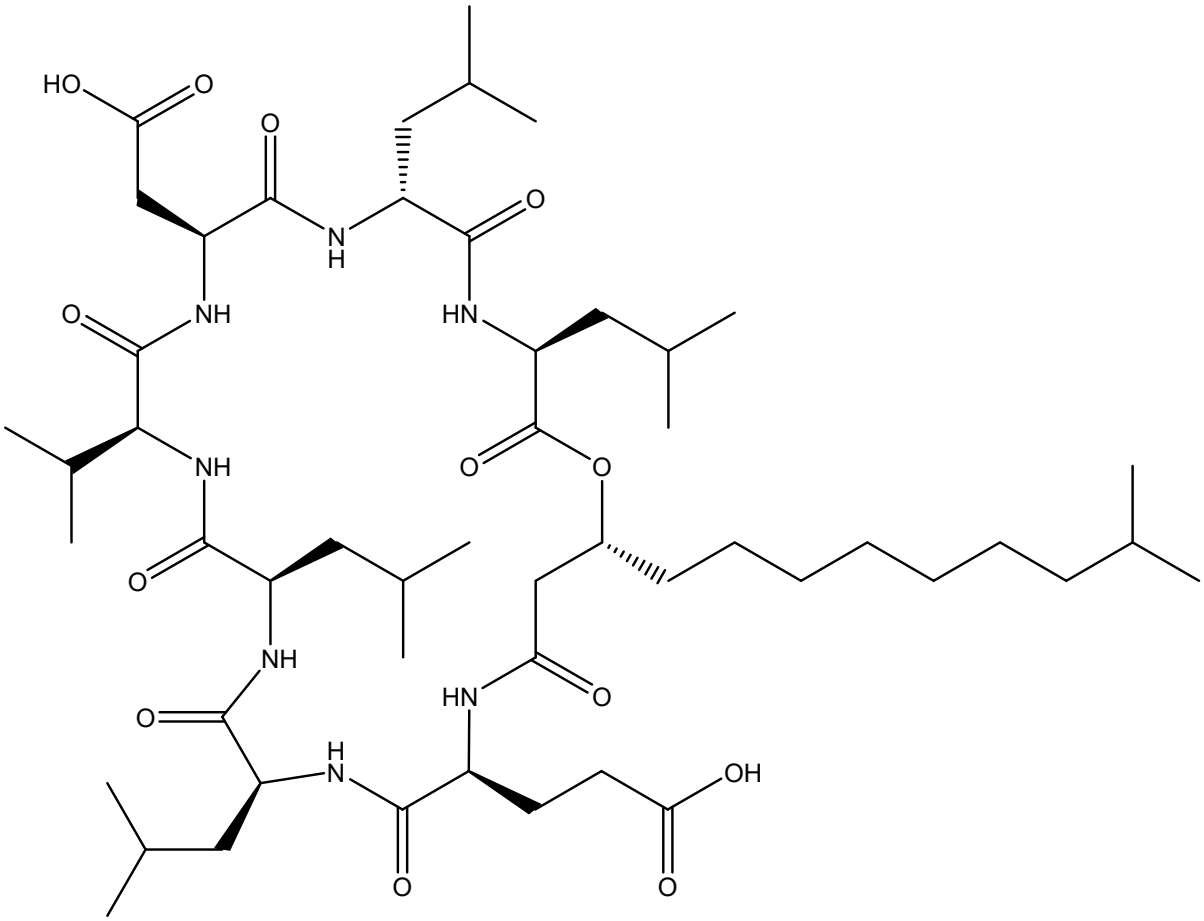


Table S4 Experimental NMR data of compound 4 in DMSO - d_6 at 25°C



Position		δ_C	δ_H (J in Hz)
Glu1	NH	-	8.44, (d), 6.6
	CO	172.2	-
	α-C	51.1	4.04, (q), 4.8
	β-C	39.5	1.63, (m)
	γ-C	39.3	1.63, (dd), 4.8
	COOH		12.0
Leu2	NH	-	8.13, (d), 7.2
	CO	173.6	-
	α-C	52.3	4.16, (m)
	β-C	24.5	1.47, (m)
	γ-C	39.8	1.50, (m)
	δ_1-C	23.7	0.87, (m)
	δ_2-C	23.4	0.86, (m)
Leu3	NH	-	7.61, (s)
	CO	157.5	-
	α-C	51.4	4.35, (q), 5.6
	β-C	24.7	1.53, (m)
	γ-C	39.0	1.21, (m)
	δ_1-C	23.8	0.86, (m)
	δ_2-C	22.9	0.82, (m)

Val4	NH	-	8.00, (s)
	CO	-	-
	α-C	51.2	4.04, (t), 7.6
	β-C	30.3	2.00, (m)
	γ_1-C	22.9	0.90, (m)
	γ_2-C	22.6	0.76, (m)
Asp5	NH	-	8.17, (s)
	CO		-
	α-C	49.9	4.55, (m)
	β-C	35.9	2.60, (m)
	COOH		12.33, (s)
Leu6	NH	-	7.61, (s)
	CO		-
	α-C	51.6	4.34, (m)
	β-C	40.3	1.47, (m)
	γ-C	23.4	1.13, (m)
	δ_1-C	23.1	0.89, (m)
	δ_2-C	22.3	0.88, (m)
Leu7	NH	-	7.88, (s)
	CO		-
	α-C	52.3	4.16, (m)
	β-C	30.1	1.22, (m)
	γ-C	41.6	1.56, (m)
	δ_1-C	23.1	0.83, (m)
	δ_2-C	22.7	0.80, (m)
Fatty acid part	C1	171.4	-
	C2	41.7	2.35, (m)
	C3	71.6	5.06, (m)
	C4	33.7	1.53, (m)
	C5-15	22.3	0.80, (m)
	C16	29.7	2.03, (m)
	C17	22.1	0.80, (m)
	C18	24.3	0.81, (m)

Figure S16 (+)-LRESIMS spectrum of compound 4

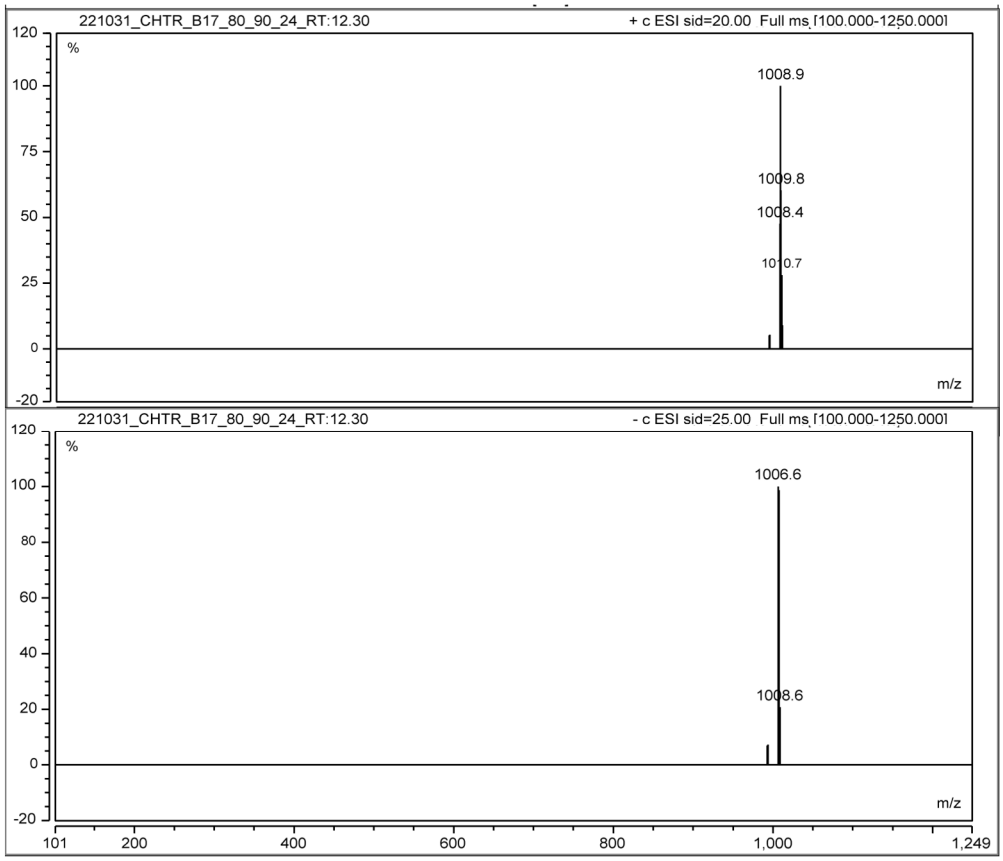


Figure S17 ^{1}H NMR (800 MHz, DMSO) spectrum of compound 4

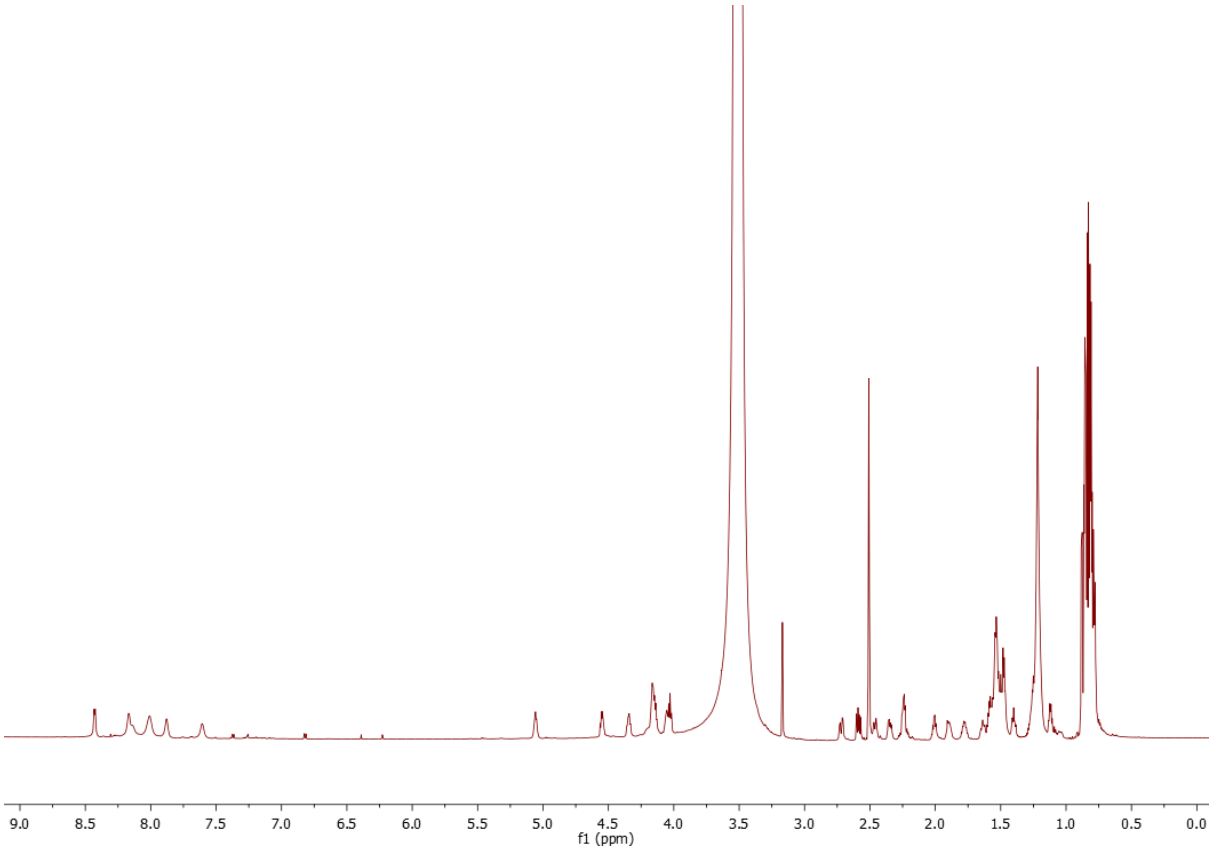


Figure S18 ^{1}H $^{-1}$H COSY spectrum of compound 4 in DMSO

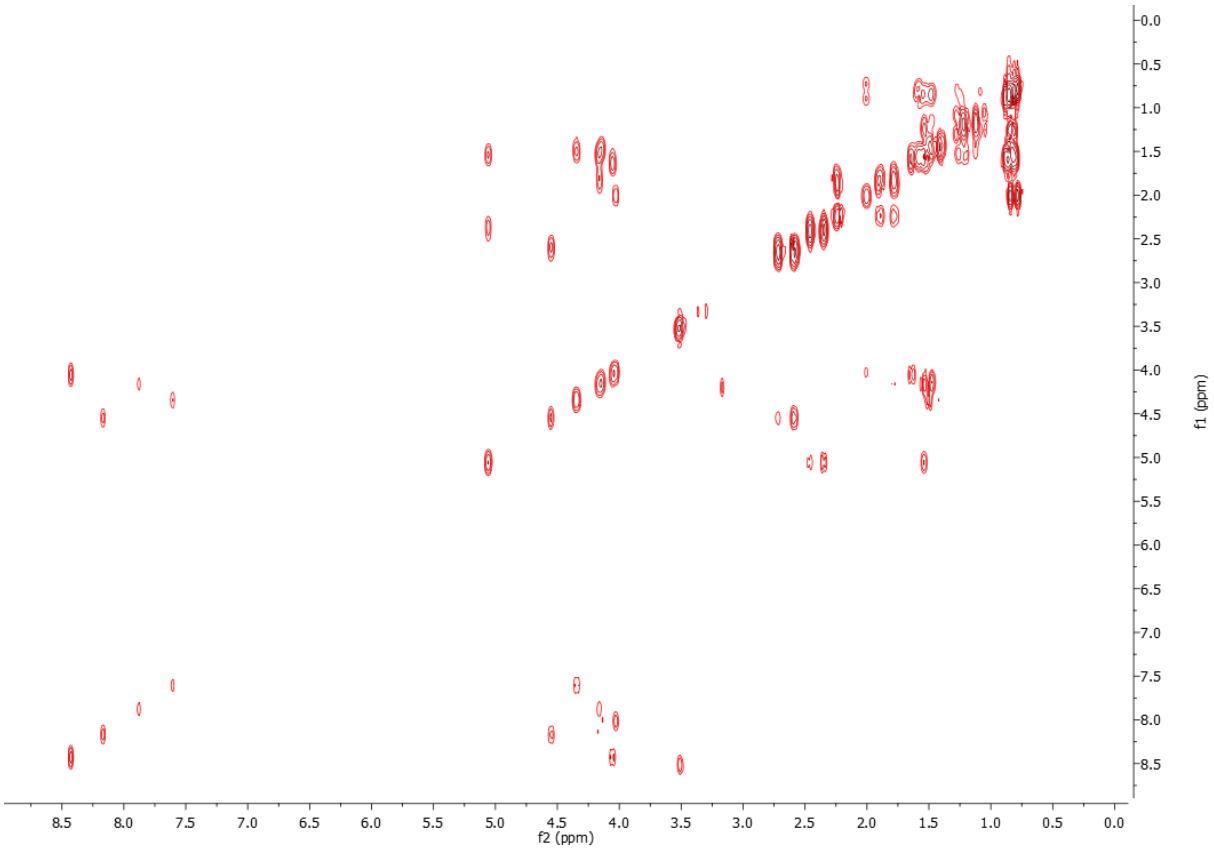


Figure S19 HSQC spectrum of compound 4 in DMSO

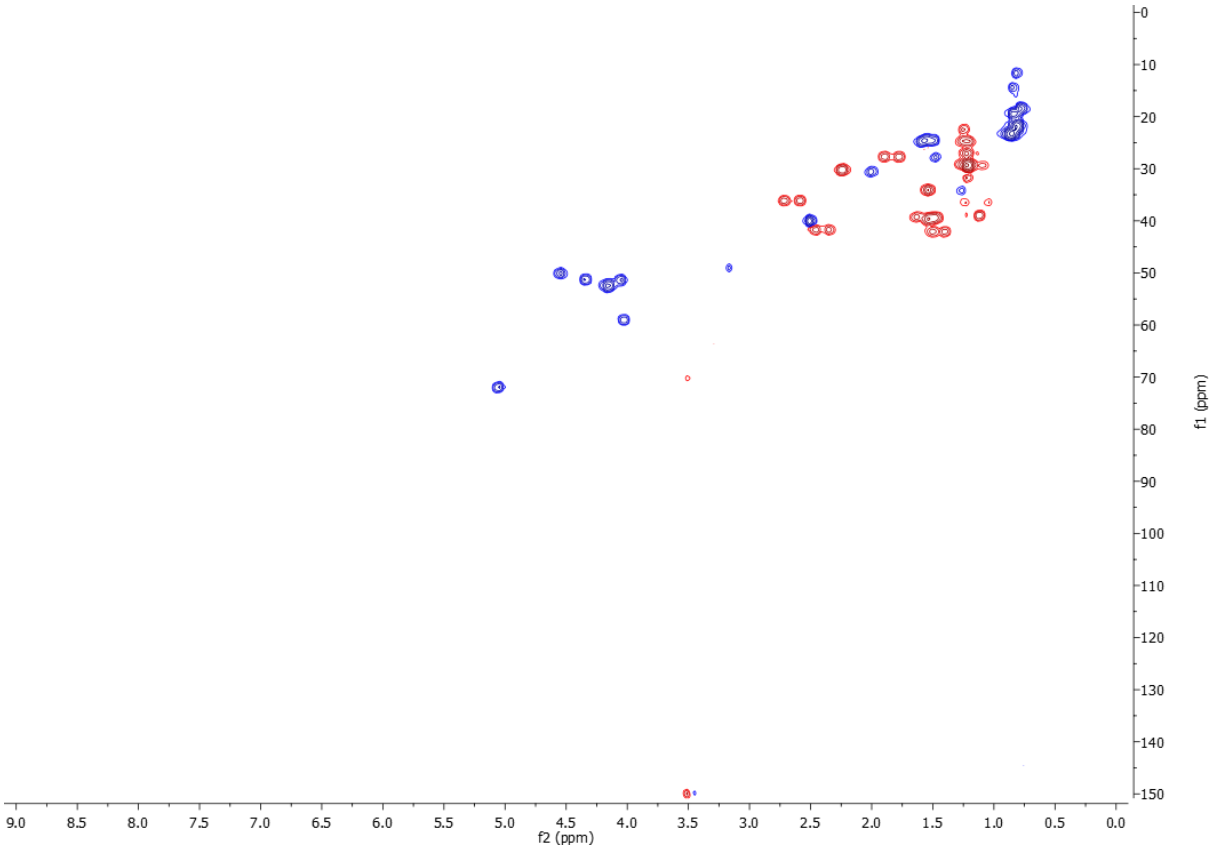


Figure S20 HMBC spectrum of compound 4 in DMSO

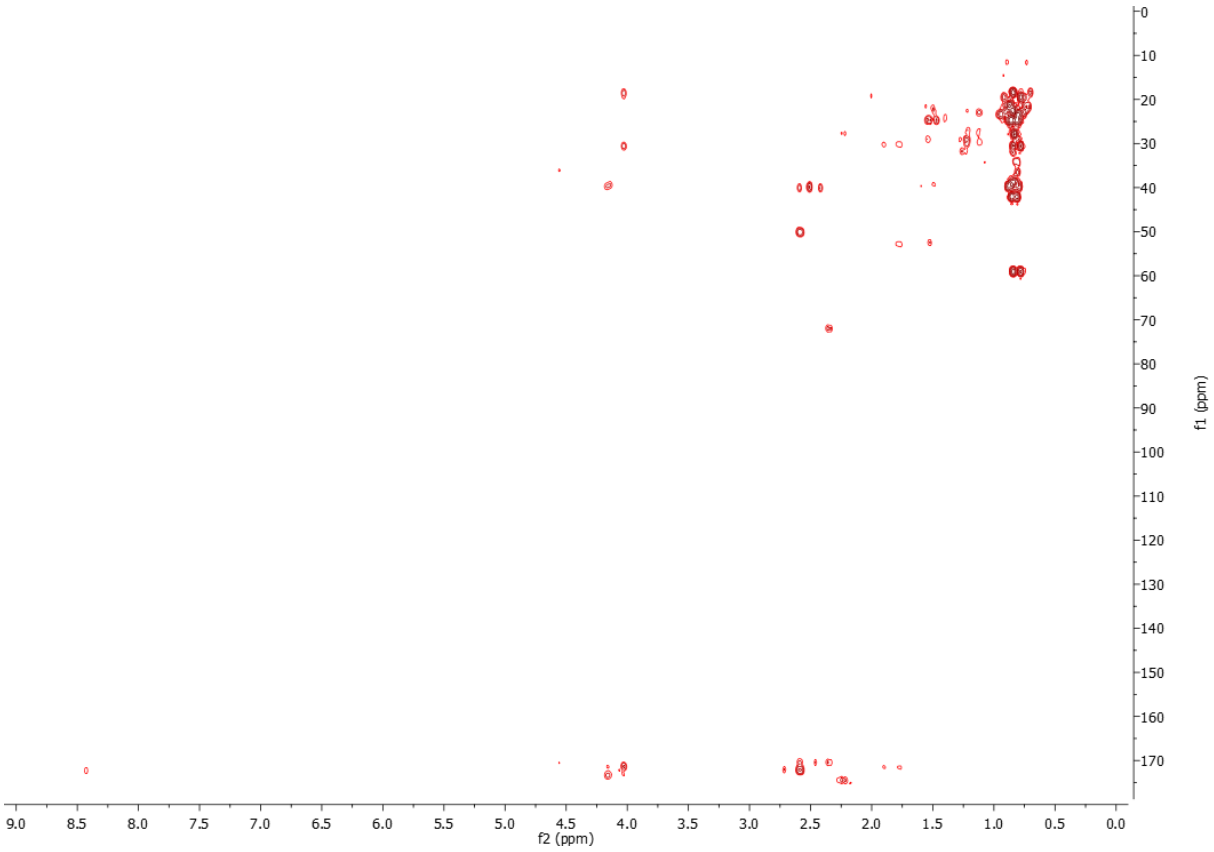
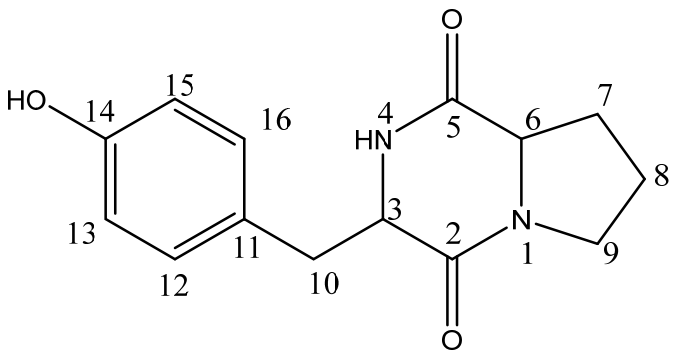


Table S5 Experimental NMR data of compound 5 in DMSO - d_6 at 25°C



Position	δ_C	C-type	δ_H (J in Hz)
1	- (N)	-	-
2	165.3	CO	-
3	56.4	CH	4.25
4	-	NH	7.86
5	169.8	CO	-
6	59.0	C	4.05
7	45.0	CH2	3.43, 3.28
8	22.0	CH2	1.74
9	28.3	CH2	2.01, 1.41
10	35.5 (C-1)	CH2	2.93
11	127.1	C	-
12	131.9	CH	7.06
13	114.6	CH	6.64

14	155.6	COH	9.11
15	114.6	CH	6.64
16	131.9	CH	7.06

Figure S21 (+)-LRESIMS spectrum of compound 5

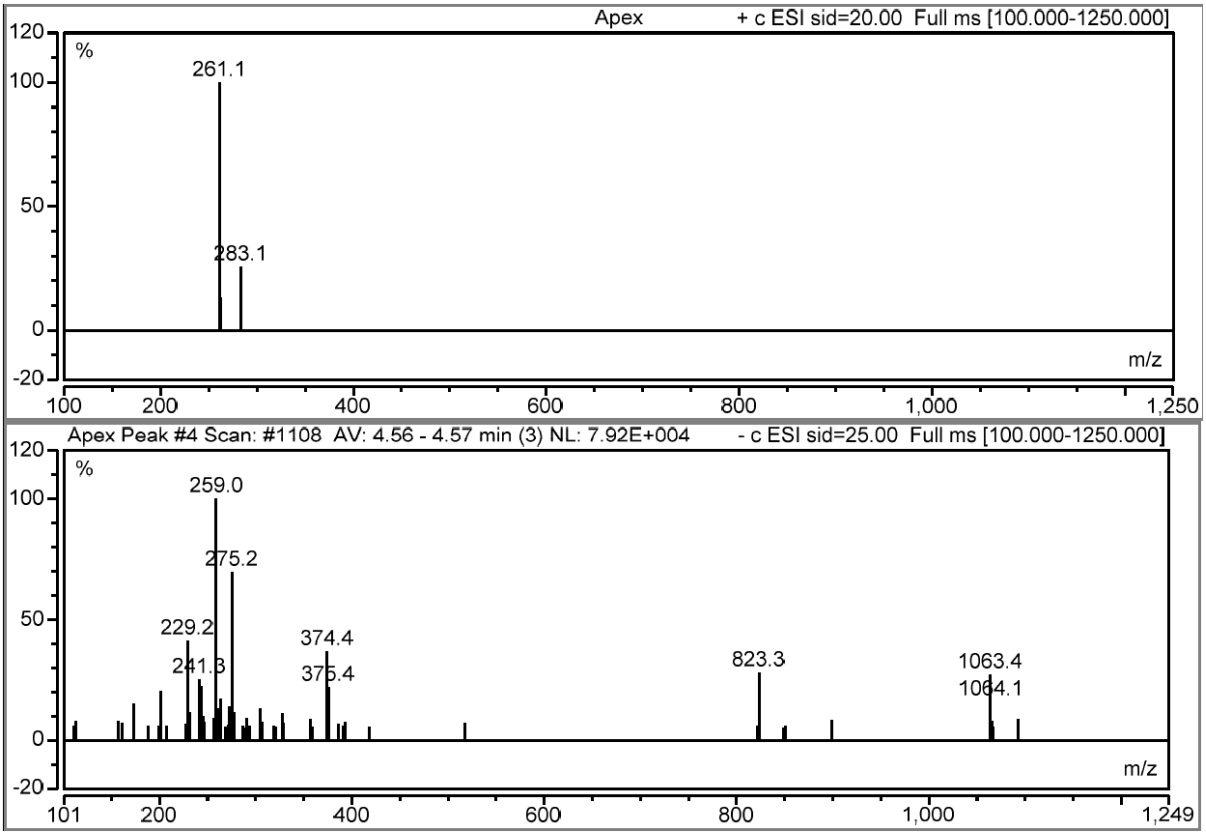


Figure S22 ^{1}H NMR (800 MHz, DMSO) spectrum of compound 5

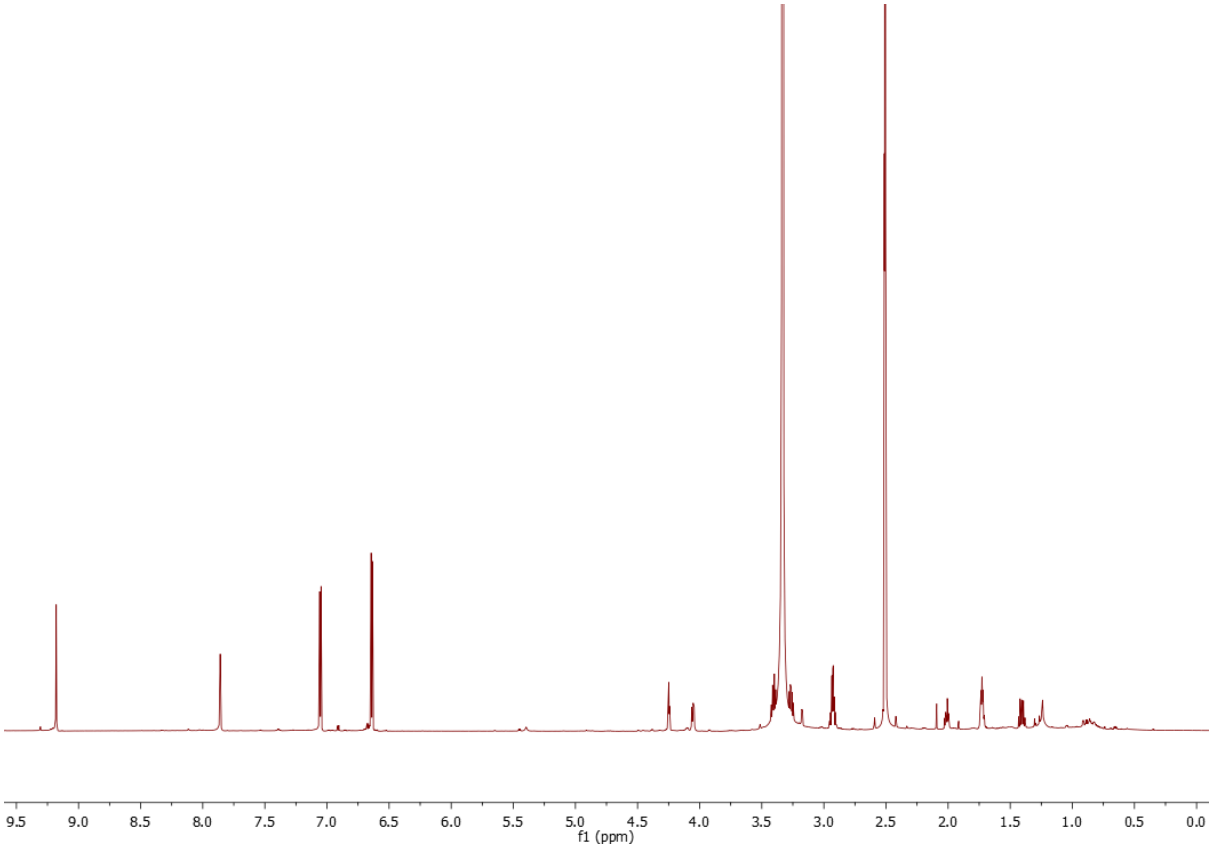


Figure S23 $^{1}H-^{1}H$ COSY spectrum of compound 5 in DMSO

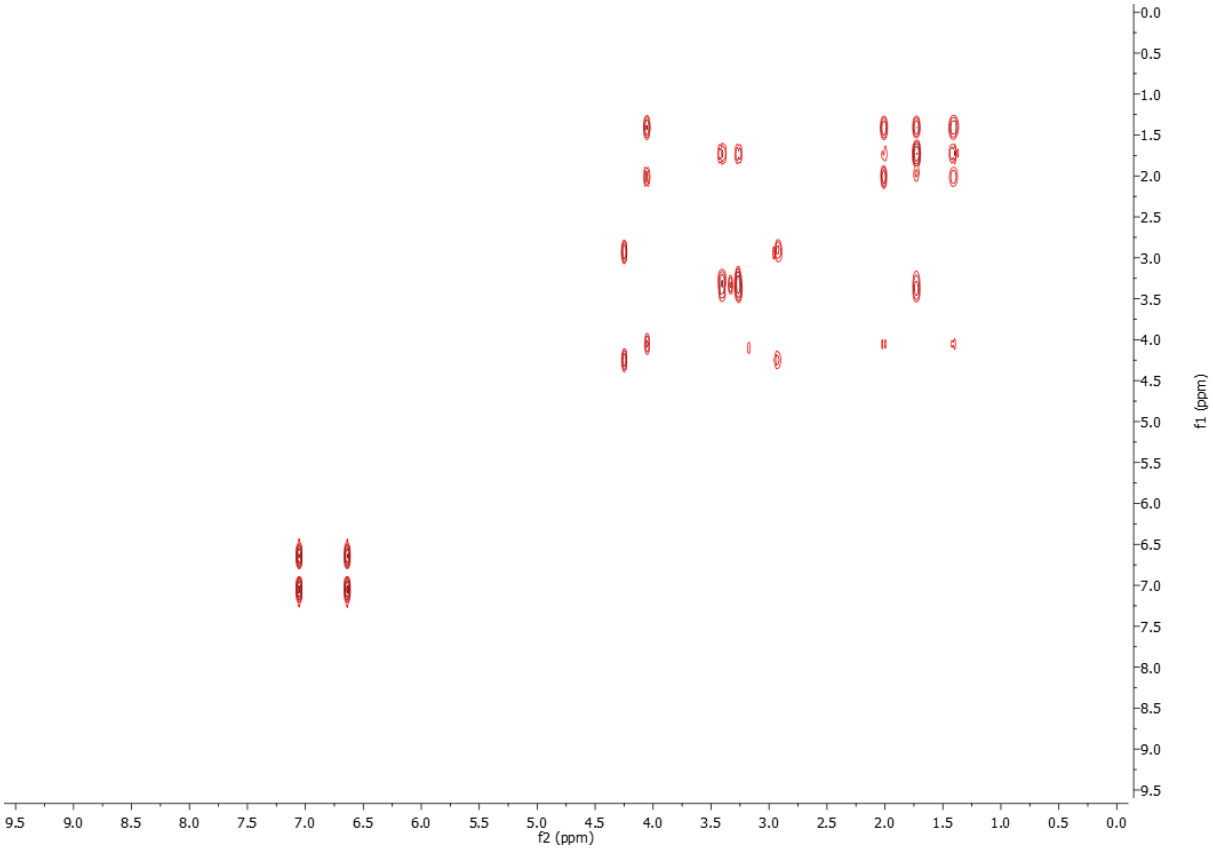


Figure S24 HSQC spectrum of compound 5 in DMSO

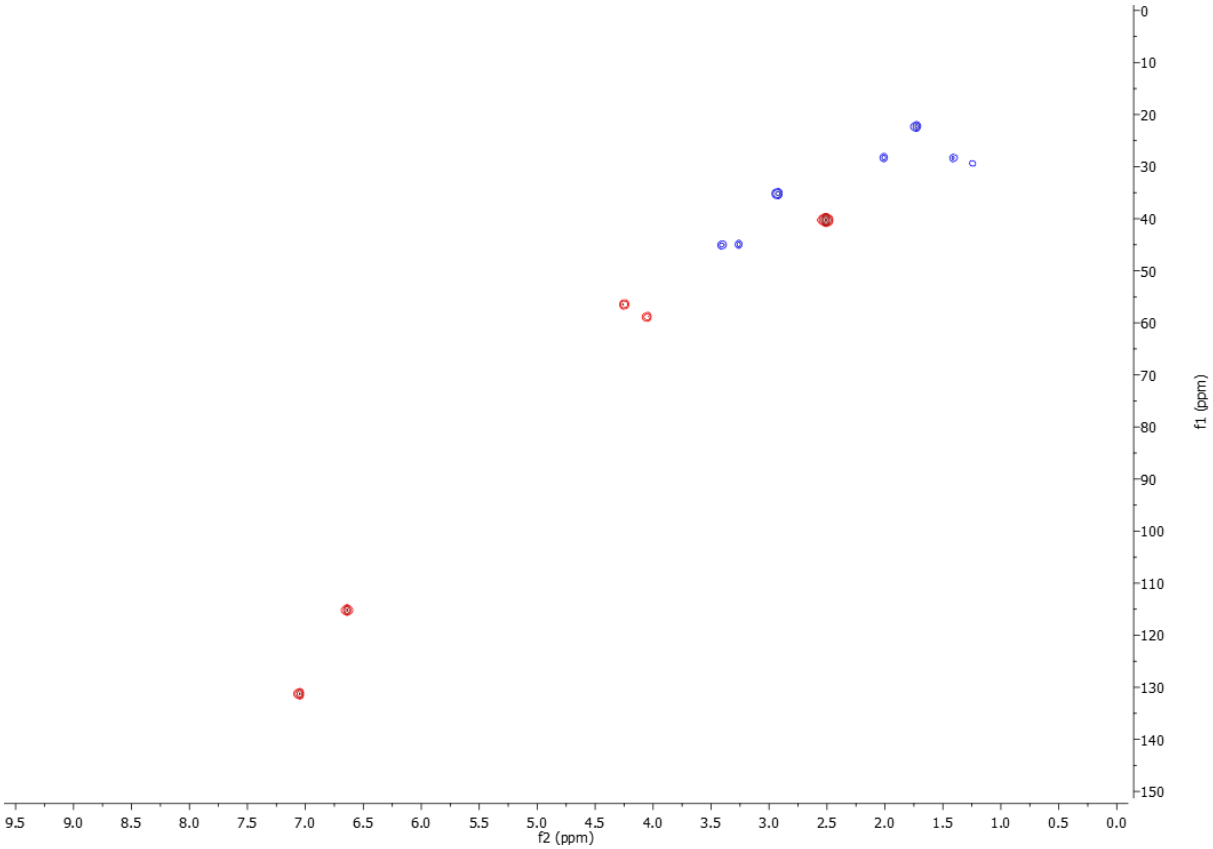


Figure S25 HMBC spectrum of compound 5 in DMSO

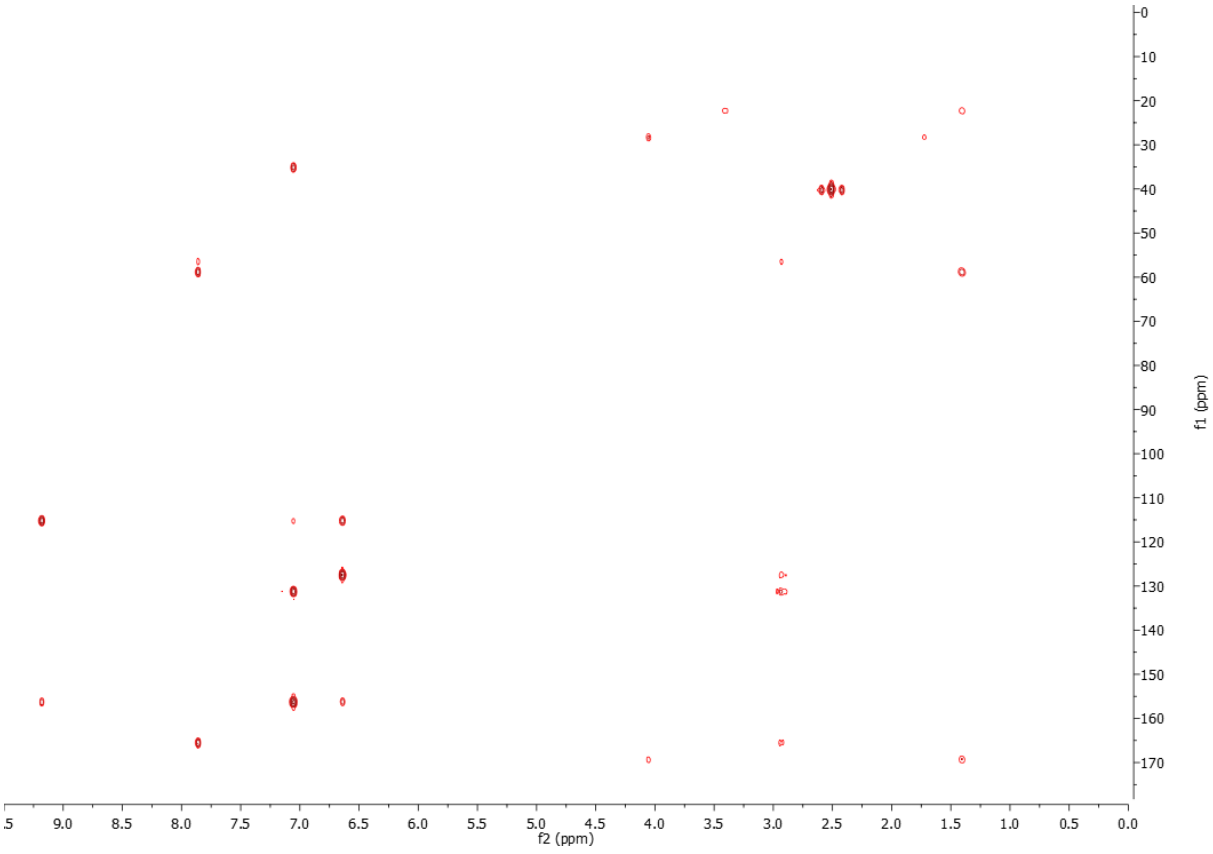
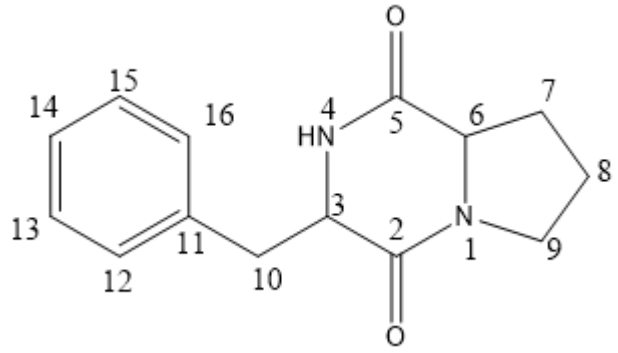


Table S6 Experimental NMR data of compound 6 in DMSO - d_6 at 25°C



Position	δ_C	C-type	δ_H (J in Hz)
1	- (N)	-	-
2	169.3 (C-2)	C=O	-
3	(C-3)	CH	4.36
4	- (N)	-	8.00
5	165.6 (C)	-	-
6	58.7 (C)	CH	4.05
7	28.9	CH2	2.01, 1.45
8	22.6	CH2	1.72
9	44.3	CH2	3.37, 3.25
10	36.7	CH2	3.06
1	138.0	C	-
12	130.0	CH	7.28, s
13	128.0	CH	7.20, s
14	128.0	CH	7.20, s
15	128.0	CH	7.20, s
16	130.0	CH	7.20, s

Figure S26 (+)-LRESIMS spectrum of compound 6

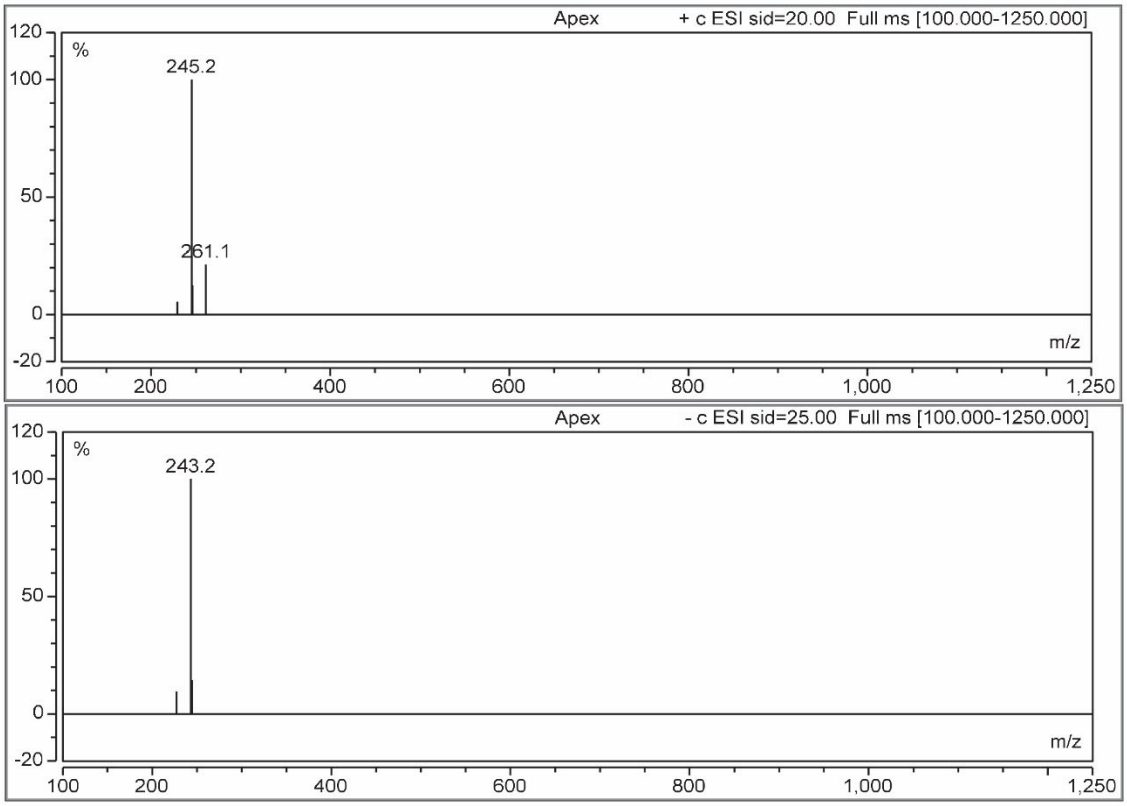


Figure S27 ^{1}H NMR (800 MHz, DMSO) spectrum of compound 6

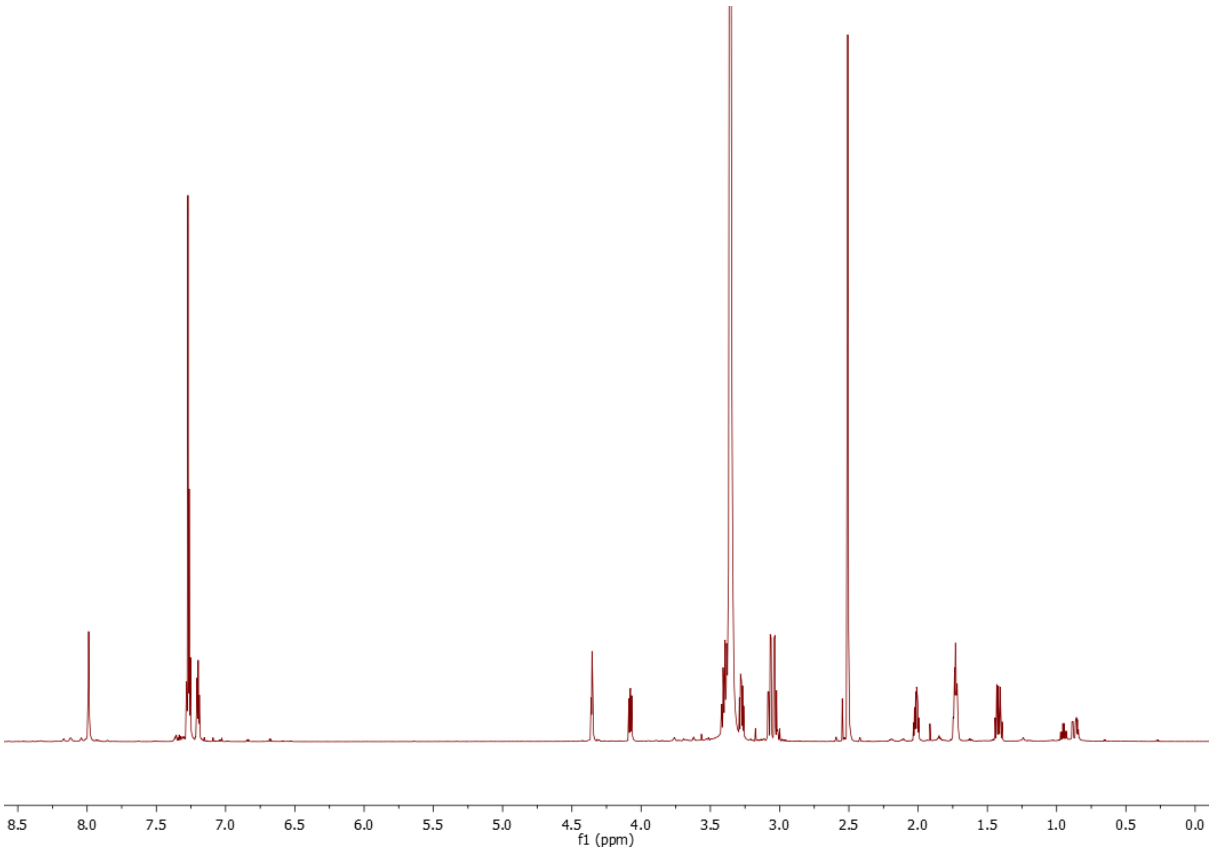


Figure S28 ^{1}H $-^{1}$H COSY spectrum of compound 6 in DMSO

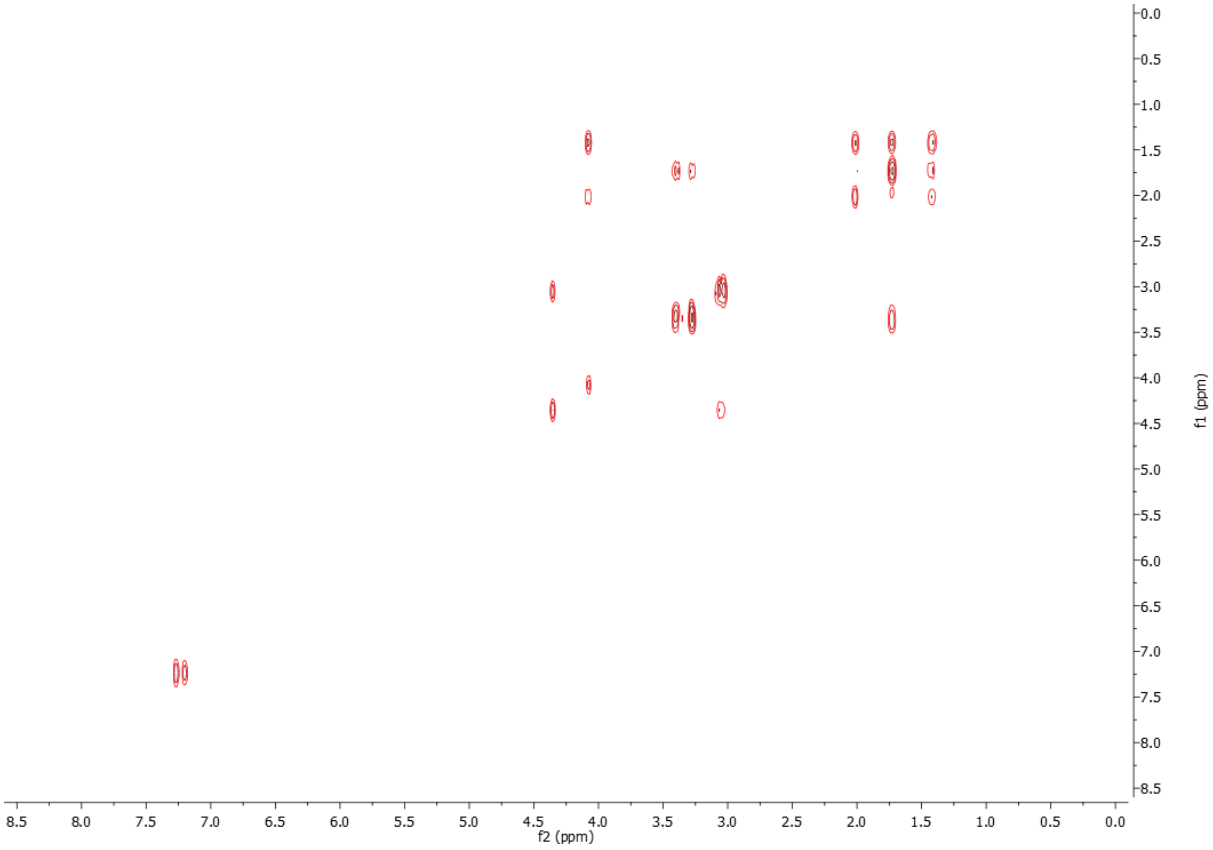


Figure S29 HSQC spectrum of compound 6 in DMSO

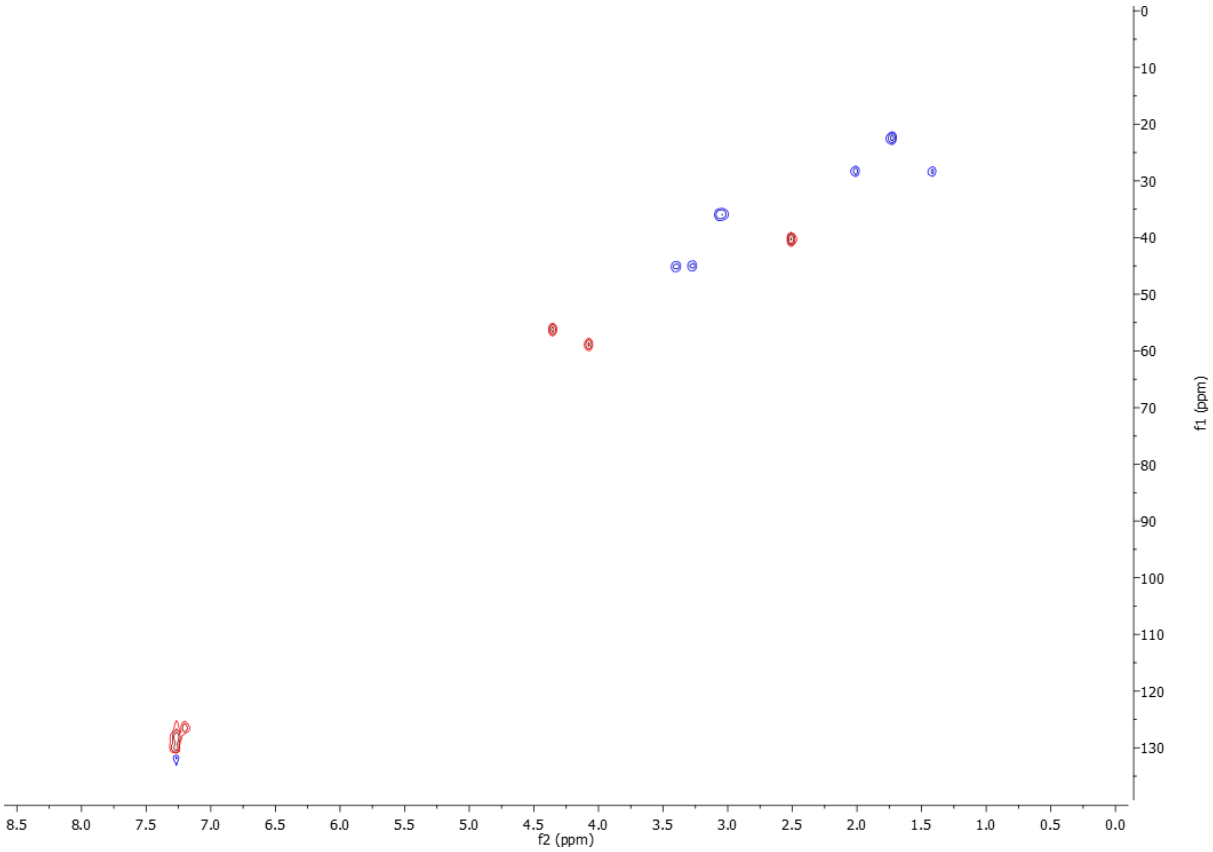


Figure S30 HMBC spectrum of compound 6 in DMSO

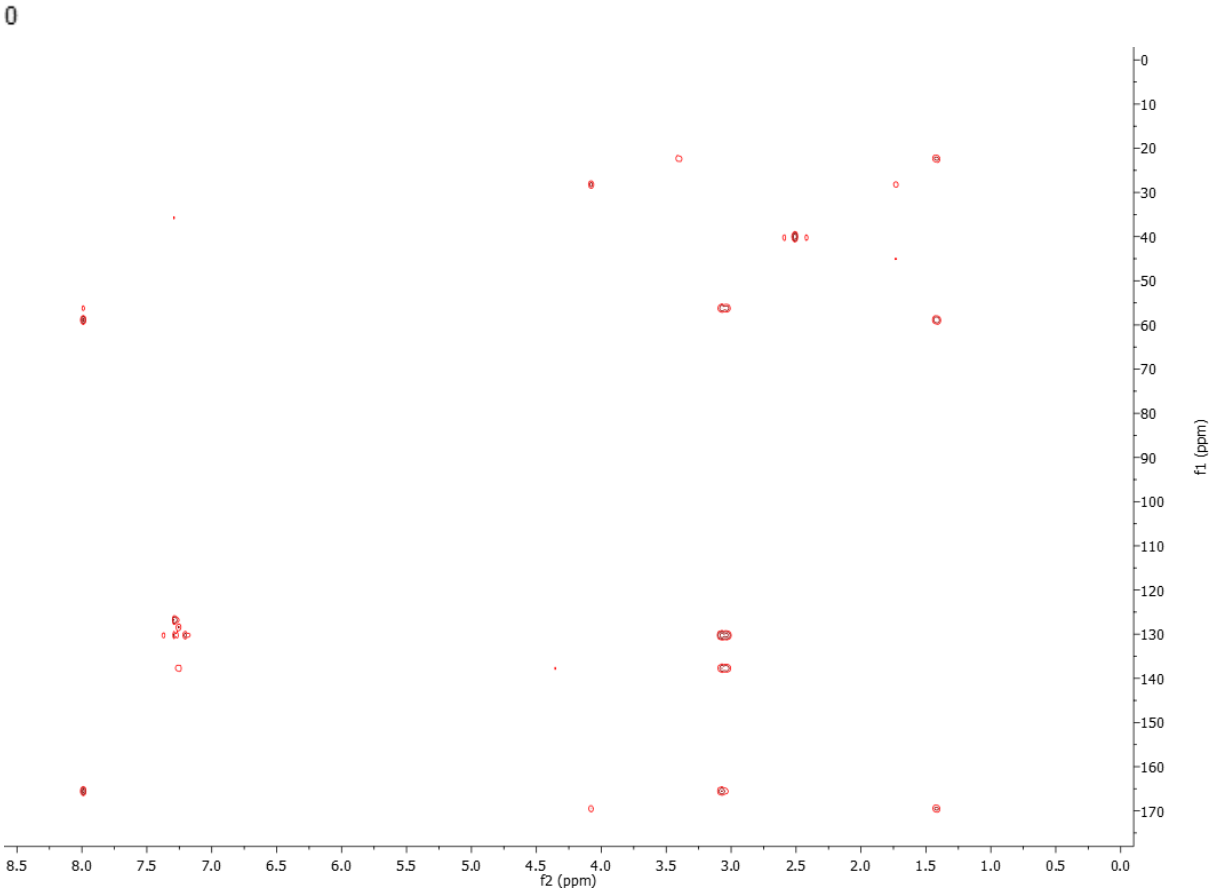
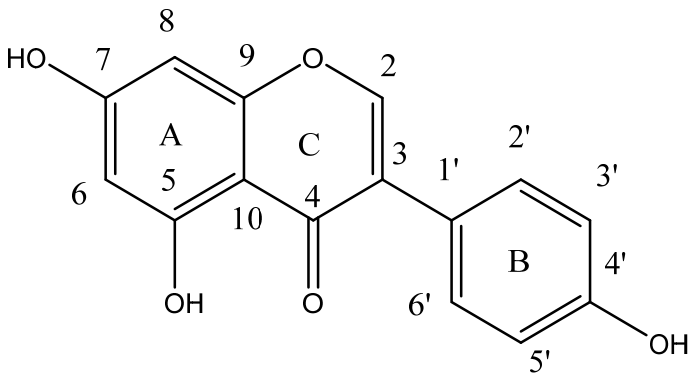


Table S7 Experimental NMR data of compound 7 in DMSO - d_6 at 25°C



Part (ring)	Position	δ_C	δ_H (J in Hz)
C	2	154.8	8.32, s
C	3	121.3	-
C	4	180.1	-
A	5	162.6	12.99, s
A	6	99.9	6.25, *d*, 1.8J)
A	7	164.8	11.01
A	8	94.2	6.35,

			d, 1.8J
A, C	9	158.0	-
A, C	10	105.4	-
B	1’	122.0	-
B			7.37,
	2’	129.9	(doublet)
B			6.82,
	3’	114.9	(doublet)
B	4’	157.0	
B			6.82,
	5’	114.9	(doublet)
B			7.37,
	6’	129.9	(doublet)
	7-OH	-	11.01, s
	5-OH	-	12.99, s
	4’-OH		9.68, s

Figure S31 (+)-LRESIMS spectrum of compound 7

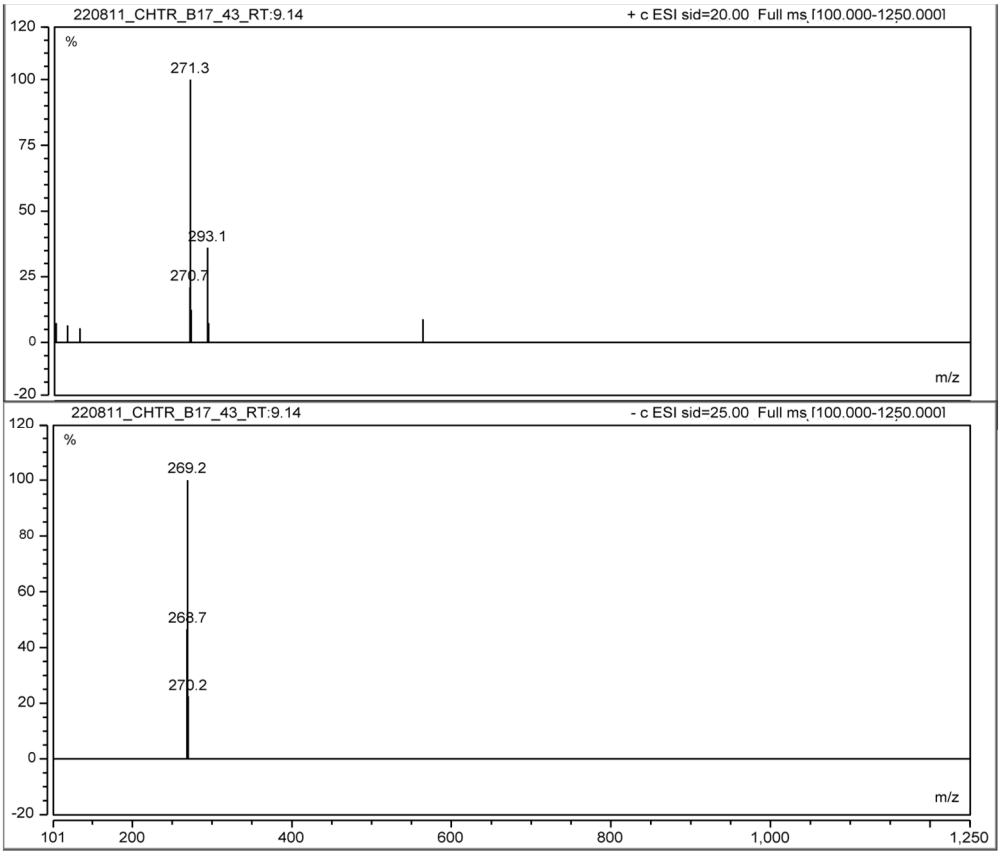


Figure S32 ^{1}H NMR (800 MHz, DMSO) spectrum of compound 7

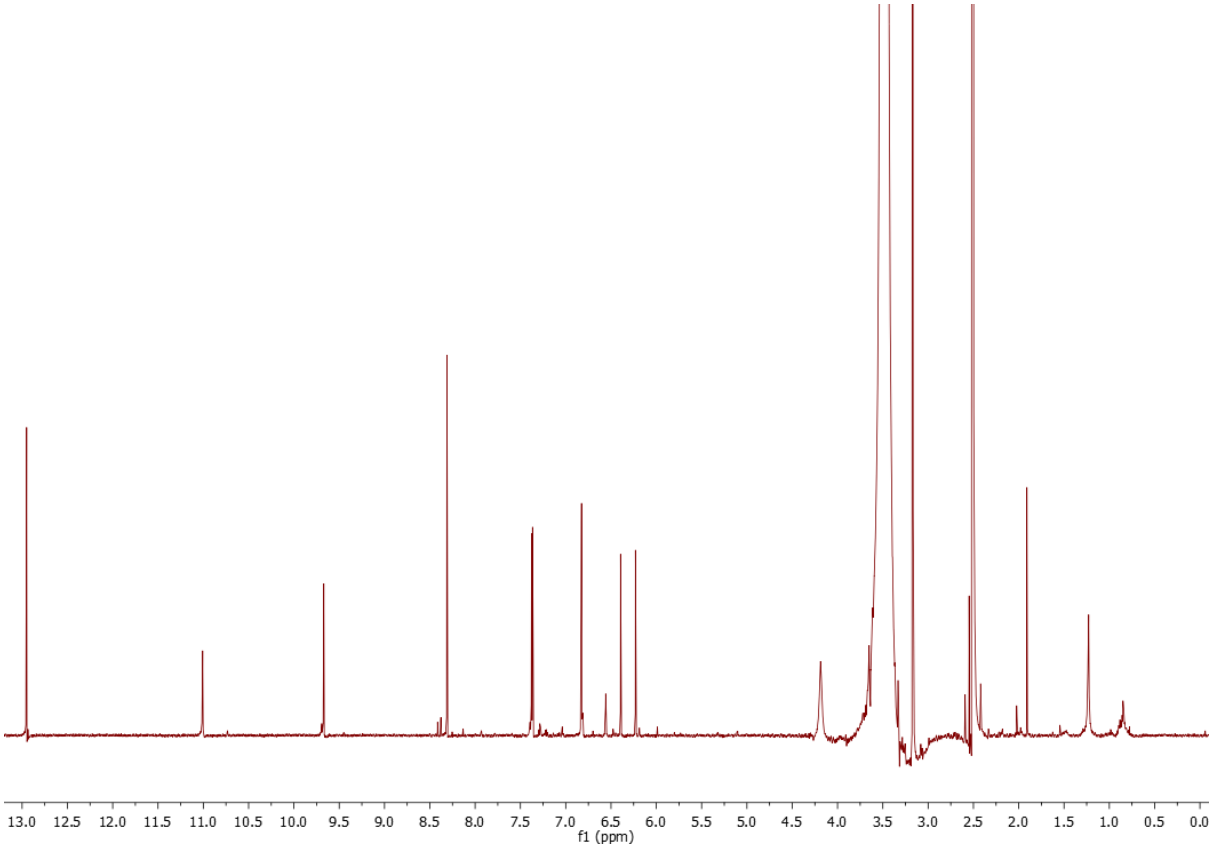


Figure S33 $^{1}H-^{1}H$ COSY spectrum of compound 7 in DMSO

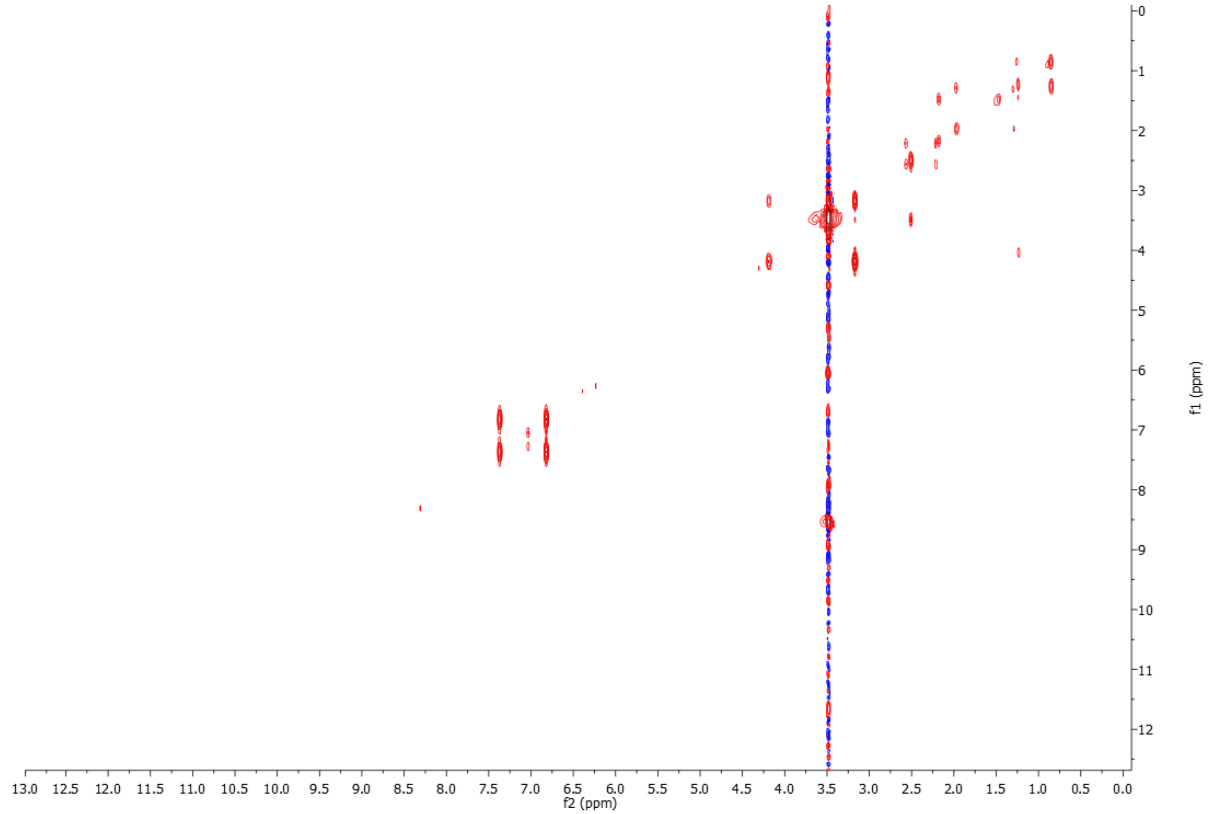


Figure S34 HSQC spectrum of compound 7 in DMSO

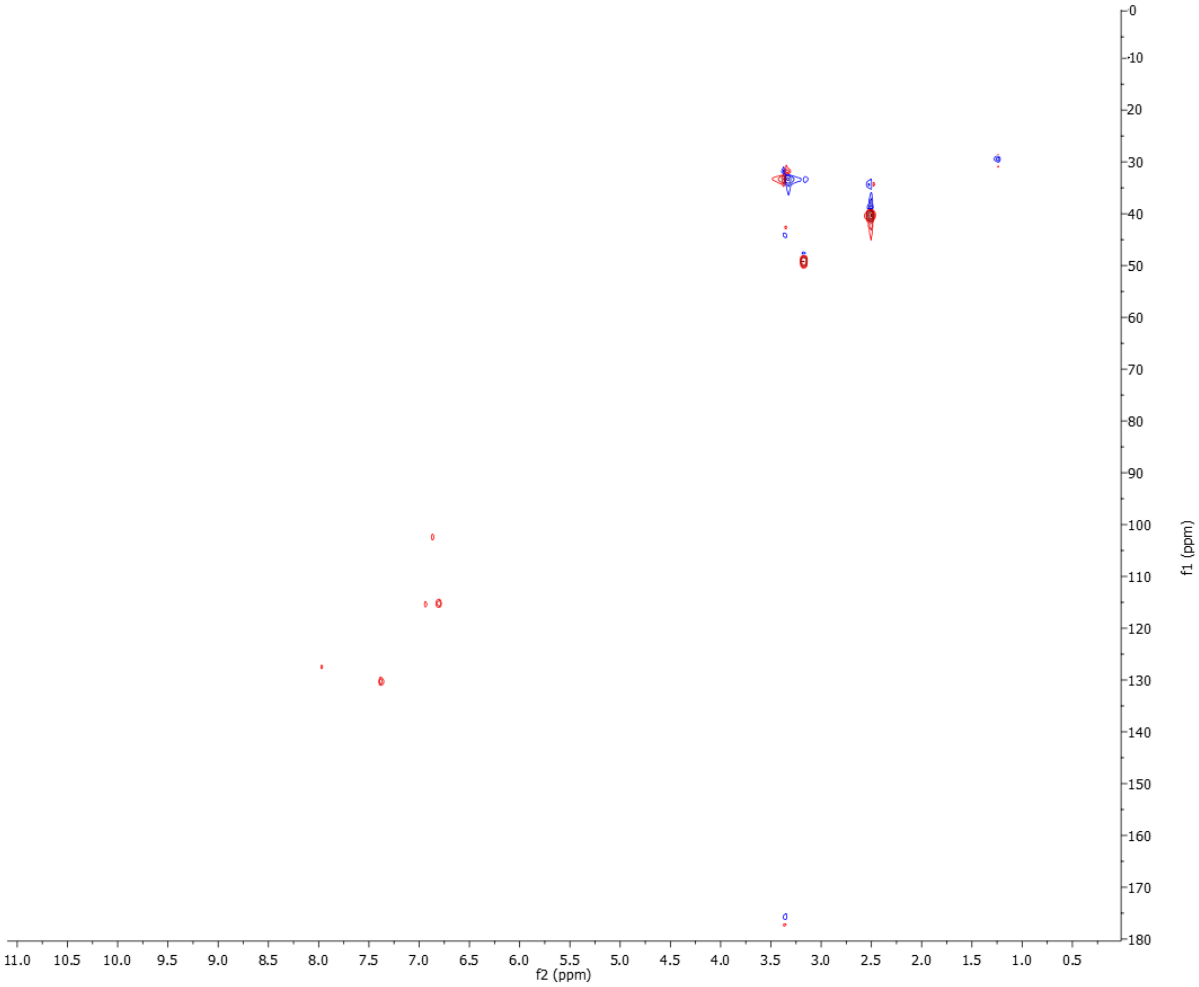


Figure S35 HMBC spectrum of compound 7 in DMSO

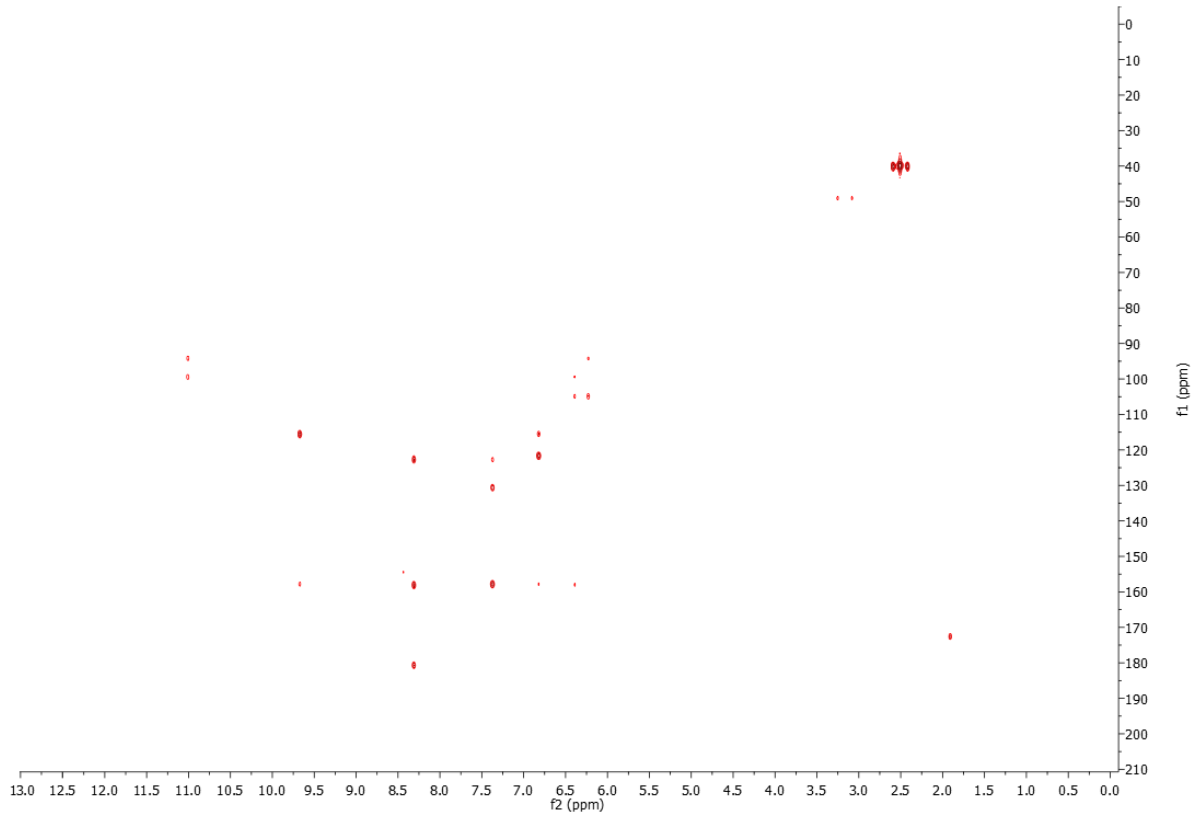
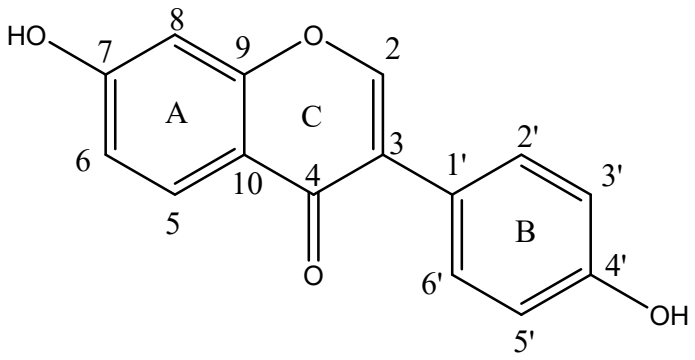


Table S8 Experimental NMR data of compound 8 in DMSO - d_6 at 25°C



Part (ring)	Position	δ_C	δ_H (J in Hz)
C	2		
C	3	123.9	-
C	4	175.6	-
A	5	128.8	7.94, d, 7.9J
A	6	115.3	6.94, dd, 2.27J, 8.88J
A	7	163.3	-
A	8	102.6	6.82, *d*, 3.28*J*
A, C	9	157.7	-
A, C	10	117.3	-
B	1’	123.9	-
B	2’	130.8	7.38, *d*, 8.8*J*
B	3’	115.6	6.80, *d*, 8.8*J*
B	4’	157.7	-

B	5’	115.6	6.80, *d*, 8.8*J*
B	6’	130.8	7.38, *d*, 8.8*J*
	7-OH	-	10.76, *s*
	4’-OH	-	9.53, *s*

Figure S36 (+)-LRESIMS spectrum of compound 8

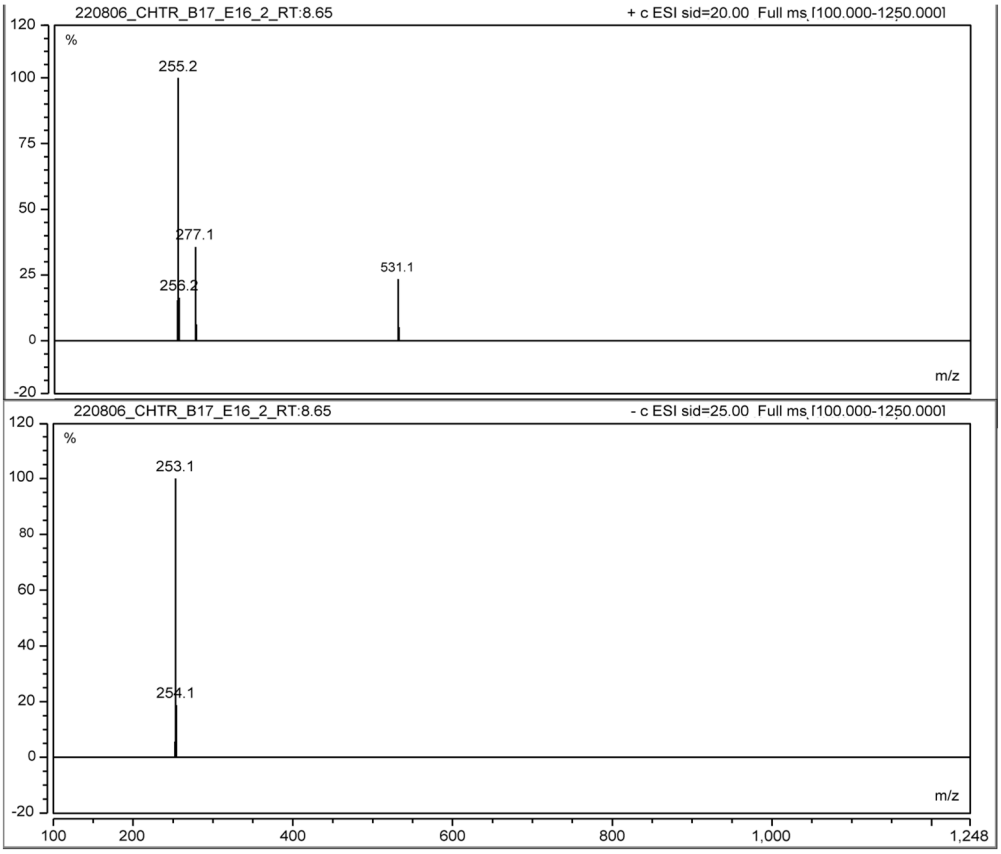


Figure S37 ^{1}H NMR (800 MHz, DMSO) spectrum of compound 8

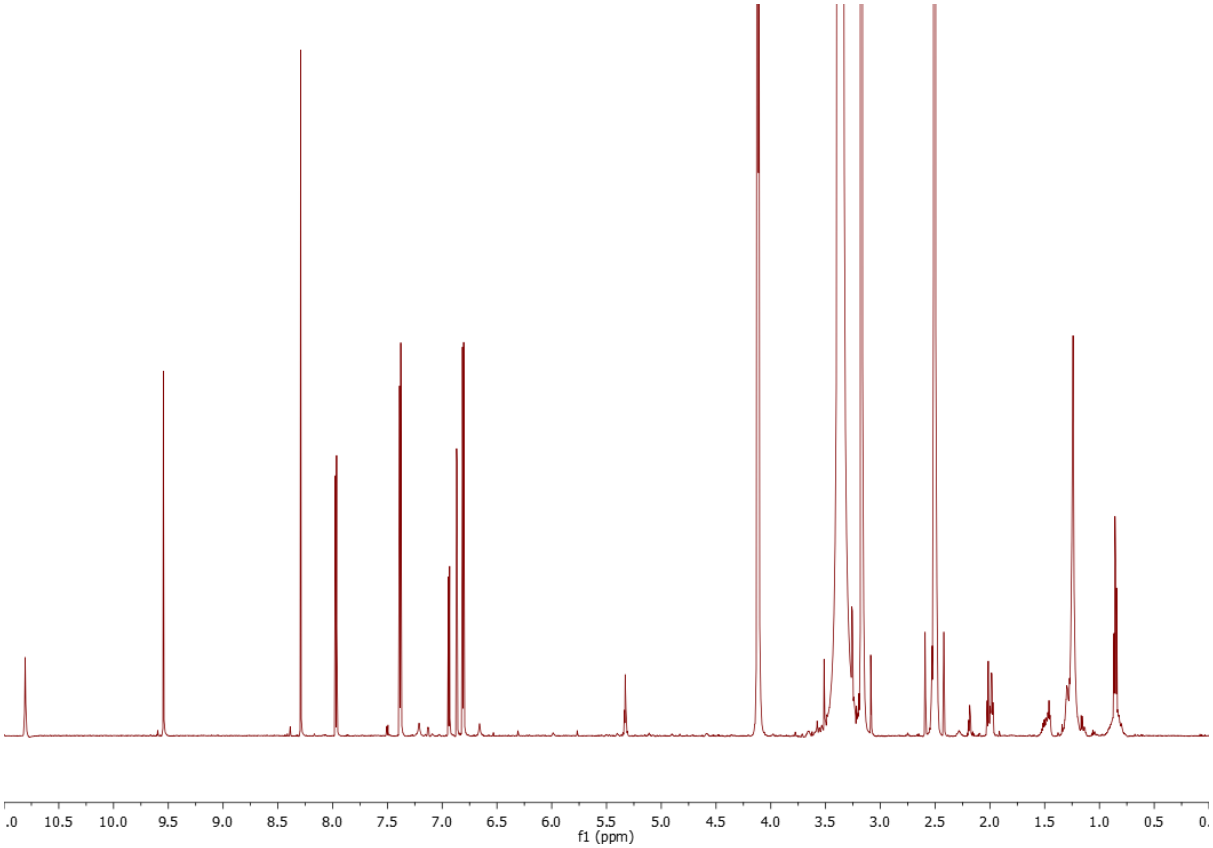


Figure S38 $^{1}H-^{1}H$ COSY spectrum of compound 8 in DMSO

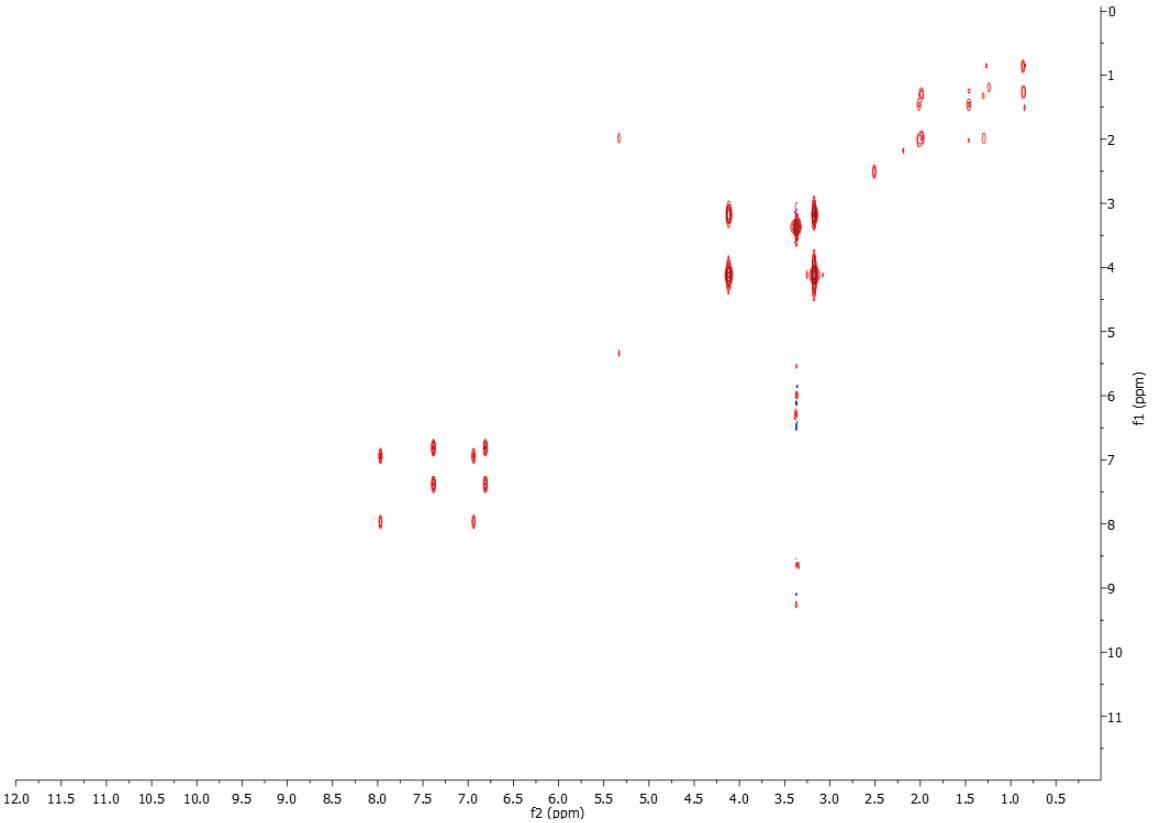


Figure S39 HSQC spectrum of compound 8 in DMSO

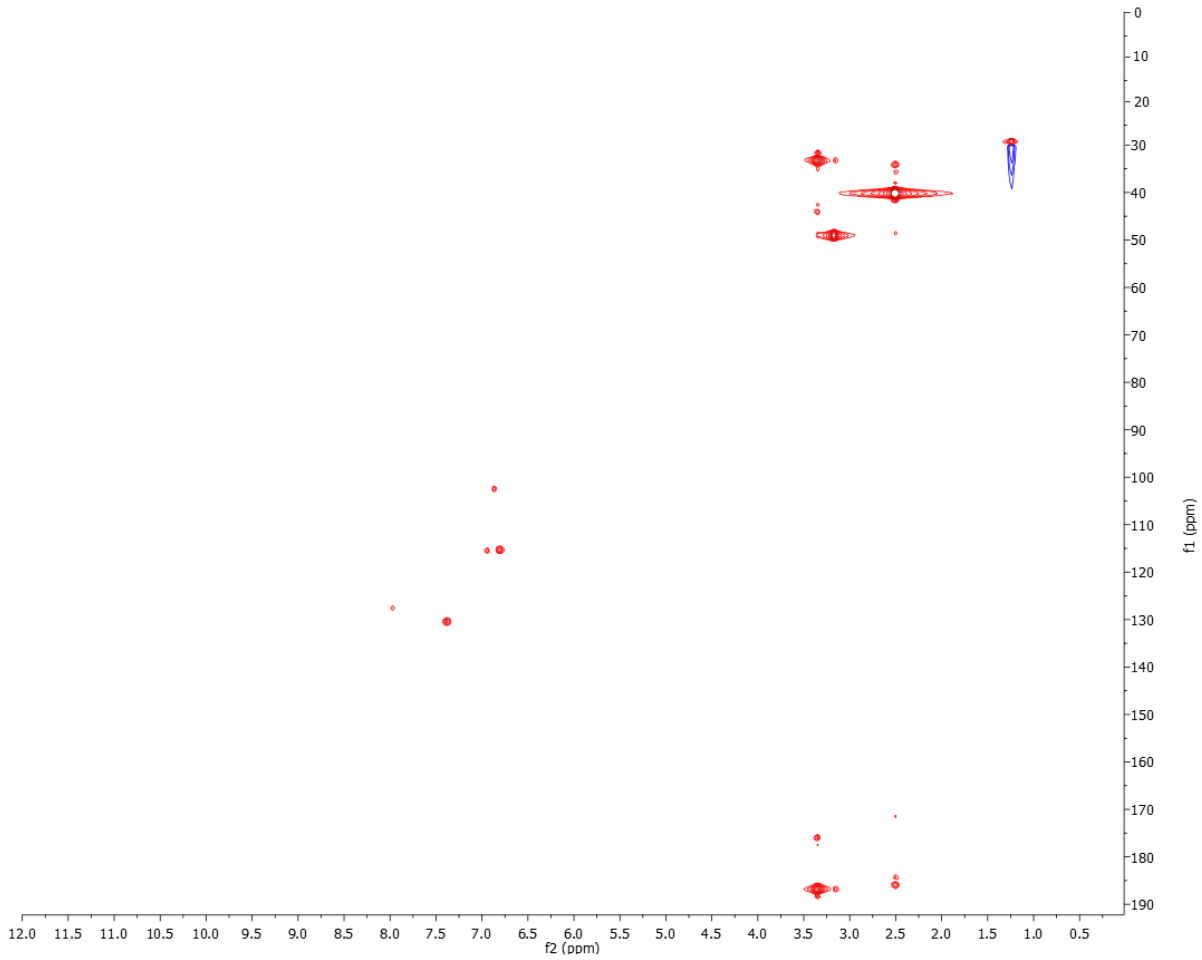


Figure S40 HMBC spectrum of compound 8 in DMSO

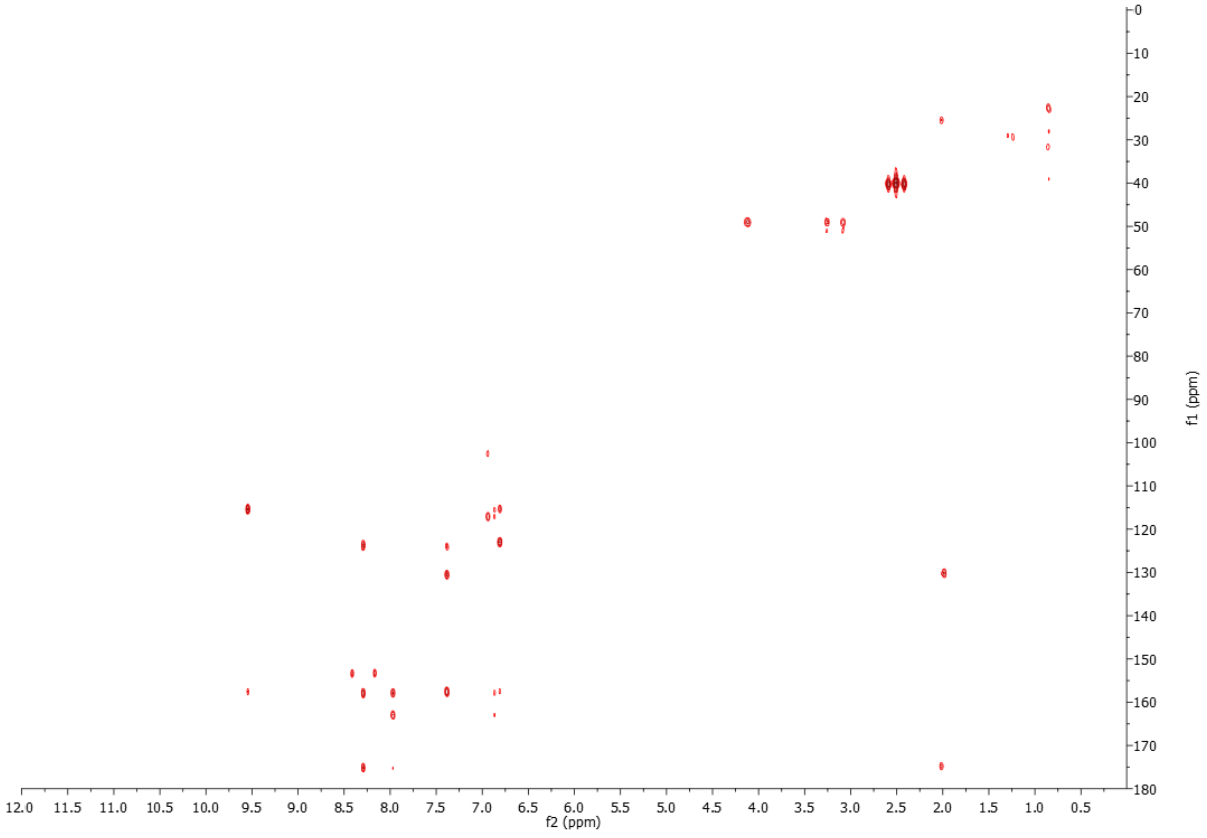


Figure S41 LC-MS chromatograms of caecum extracts produced from a single animal sample fed with *Bacillus* composition F1.

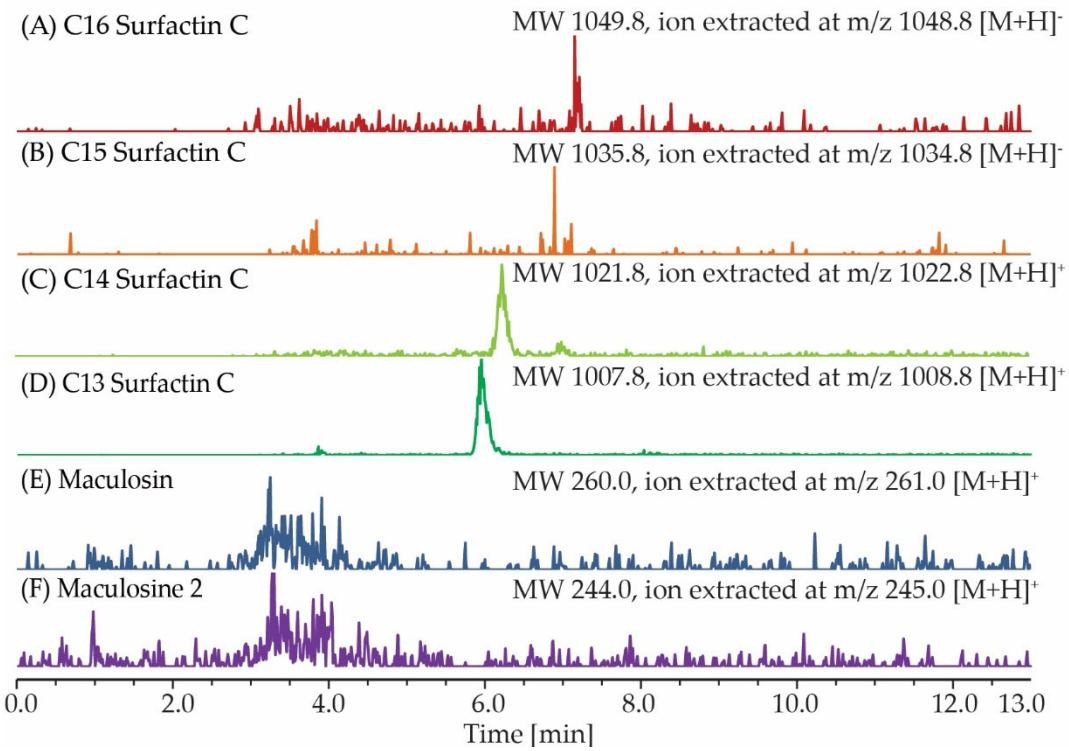


Table S9 Antimicrobial activity of EtoAc and Crude extracts of *Bacillus* strains

EtoAc Extract

Strain	200µg/mL					100µg/mL					50µg/mL					25µg/mL				
	C.P	E.C	P.A	S.A	S.E	C.P	E.C	P.A	S.A	S.E	C.P	E.C	P.A	S.A	S.E	C.P	E.C	P.A	S.A	S.E
BPR-17	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	×	✓	×	✓	✓	×	✓	×
BPR-16	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	×	✓	×	✓	✓	×	✓	×
BPR-14	✓	✓	×	✓	×	✓	✓	×	✓	×	✓	✓	×	✓	×	✓	✓	×	✓	×
BPR-13	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×
BPR-12	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×
BPR-11	✓	✓	×	✓	×	✓	✓	×	✓	×	✓	✓	×	✓	×	✓	✓	×	✓	×

Crude Extract

Strain	800µg/mL					400µg/mL					200µg/mL					100µg/mL				
	C.P	E.C	P.A	S.A	S.E	C.P	E.C	P.A	S.A	S.E	C.P	E.C	P.A	S.A	S.E	C.P	E.C	P.A	S.A	S.E
BPR-17	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×
BPR-16	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×
BPR-14	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×
BPR-13	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×
BPR-12	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×
BPR-11	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×

Figure S42 Stacked ^{1}H NMR spectra of *Bacillus* EtoAC extracts