Supporting Information

Seven New Cyclic Octapeptides from the Mangrove rhizo-sphere-derived *Streptomyces* sp. GXIMD 03507

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Table Contents

Table S1. ^{1}H (500MHz) and ^{13}C (126MHz) NMR data of compound 2 in $CDCl_3$

Pos.	δ_H, mult (J in Hz)	δ_C, type	Pos.	δ_H, mult (J in Hz)	δ_C, type	Pos.	δ_H, mult (J in Hz)	δ_C, type
QXA/ QXA'			Ala			Cys'		
2/2'		142.8 [a] /143.3 [a], C	1		173.3, C	1		170.2, C
3/3'	9.53 [a], s/9.62 [a], s	143.6 [b] /143.6 [b], CH	2	4.92, q (8.1, 7.6)	46.4, CH	2	5.67, m	53.6, CH
4a/4a'		143.8 [c] /143.9 [c], C	3	1.31, d (8.0)	18.0, CH_3	3	2.74, m	31.6, CH_2
5/5'	8.14 [b], m/8.14 [b], m	129.3 [d] /129.4 [d], CH	NH	7.67, m			3.29, d (11.5)	
6/6'	7.87 [c], m/7.87 [c], m	132.1 [e] /132.1 [e], CH				N-Me	3.02, overlapped	30.8, CH_3
7/7'	7.83 [d], m/7.83 [d], m	131.1 [f] /131.1 [f], CH						
8/8'	8.20 [e], m/8.20 [e], m	129.9 [g] /130.2 [g], CH						
8a/8a'		140.3 [h] /140.4 [h], C						
9/9'		164.0/162.1, C						
Ser			Ala'			Val		
1		169.9, C	1		172.6, C	1		172.6, C
2	4.76, m	54.9, CH	2	5.01, m	46.6, CH	2	4.76, m	62.5, CH
3	3.89, d (11.9)	63.0, CH_2	3	1.42, d (6.6)	18.4, CH_3	3	2.16, m	27.2, CH
	4.20, d (11.0)		NH	7.67, m		4	0.97, overlapped	20.0, CH_3
NH	8.84, d (7.6)					5	0.71, d (6.4)	18.6, CH_3
						N-Me	2.96, overlapped	31.6, CH_3
Dha			Cys			Val'		
1		163.4, C	1		169.0, C	1		172.6, C
2		133.8, C	2	5.55, d (10.7)	54.9, CH	2	4.63, d (10.0)	63.0, CH
3	5.61, s	104.0, CH_2	3	4.50, d (10.6)	52.9, CH	3	2.10, m	27.2, CH
	6.74, s		S-Me	1.90, s	12.1, CH_3	4	1.02, overlapped	20.0, CH_3
NH	10.51, s		N-Me	3.02, overlapped	31.6, CH_3	5	0.80, d (6.4)	19.2, CH_3
						N-Me	3.04, overlapped	30.6, CH_3

a*−*h **Assignments for overlapping ^{1}H and ^{13}C NMR resonances with the same superscript may be interchanged**

Table S2. ^{1}H (500MHz) and ^{13}C (126MHz) NMR data of compound 3 in $CDCl_3$

Pos.	δ_H, mult (J in Hz)	δ_C, type	Pos.	δ_H, mult (J in Hz)	δ_C, type	Pos.	δ_H, mult (J in Hz)	δ_C, type
QXA/ QXA'			Ala			Cys'		
2/2'		142.6 [a] /142.5 [a], C	1		173.3, C	1		170.4, C
3/3'	9.62 [a], s/9.58 [a], s	143.9 [b] /143.7 [b], CH	2	4.94, q (6.8)	46.3, CH	2	5.81, dd (11.8, 2.8)	53.2, CH
4a/4a'		144.2 [c] /143.6 [c], C	3	1.42, d (6.7)	18.6, CH_3	3	2.94, d (8.7)	29.1, CH_2
5/5'	8.19 [b], m/8.11 [b], m	132.3 [d] /132.2 [d], CH	NH	7.78, d (7.3)			3.26, dd (14.9, 2.7)	
6/6'	7.85 [c], m/7.85 [c], m	130.0 [e] /129.4 [e], CH				N-Me	2.94, s	30.0, CH_3
7/7'	7.88 [d], m/7.84 [d], m	129.7 [f] /129.9 [f], CH						
8/8'	8.17 [e], m/8.14 [e], m	131.3 [g] /131.3 [g], CH						
8a/8a'		140.4 [h] /140.4 [h], C						
9/9'		164.4/164.0, C						
Ser			Ala'			Val		
1		169.0, C	1		173.0, C	1		170.7, C
2	4.83, dd (12.4, 8.1)	55.1, CH	2	4.94, q (6.8)	46.4, CH	2	5.05, m	62.9, CH
3	3.90, dd (9.5, 4.6)	63.6, CH_2	3	1.36, d (6.7)	18.4, CH_3	3	2.35, m	28.1, CH
	4.16, dd (11.5, 4.3)		NH	7.19, d (7.2)		4	1.06, d (6.6)	20.5, CH_3
NH	8.98, d (7.1)					5	0.88, d (6.7)	19.1, CH_3
						N-Me	3.07, s	31.6, CH_3
Ser'			Cys			Val'		
1		167.6, C	1		168.6, C	1		173.1, C
2	4.94, q (6.8)	52.7, CH	2	6.06, d (9.9)	57.7, CH	2	4.83, dd (12.4, 8.1)	62.1, CH
3	4.57, dd (11.2, 5.7)	65.1, CH_2	3	4.63, d (10.0)	52.4, CH	3	2.16, m	27.2, CH
	4.76, dd (11.4, 2.1)		S-Me	1.89, s	13.5, CH_3	4	1.03, d (6.6)	19.9, CH_3
NH	8.76, d (7.0)		N-Me	2.94, s	31.6, CH_3	5	0.81, d (6.6)	18.9, CH_3
						N-Me	3.00, s	31.2, CH_3

a*−*h **Assignments for overlapping ^{1}H and ^{13}C NMR resonances with the same superscript may be interchanged.**

Table S3. ^{1}H (800MHz) and ^{13}C (201MHz) NMR data of compound 4 in DMSO-d_6

Pos.	δ_H, mult (J in Hz)	δ_C, type	Pos.	δ_H, mult (J in Hz)	δ_C, type	Pos.	δ_H, mult (J in Hz)	δ_C, type
QXA/ QXA'			Ala			Cys'		
2/2'		143.2 [a] /143.1 [a], C	1		172.2, C	1		169.2, C
3/3'	9.54 [a], s/9.47 [a], s	143.4 [b] /143.3 [b], CH	2	4.91, dq (14.4, 7.3)	45.5, CH	2	5.43, m	53.2, CH
4a/4a'		143.5 [c] /143.5 [c], C	3	1.20, d (6.8)	16.7, CH_3	3	2.87, m	29.7, CH_2
5/5'	8.15 [b], m/8.15 [b], m	129.3 [d] /128.9 [d], CH	NH	8.70, d (8.0)			2.67, m	
6/6'	7.89 [c], m/7.89 [c], m	132.1 [e] /131.8 [e], CH				N-Me	2.91, overlapped	31.0, CH_3
7/7'	7.89 [d], m/7.89 [d], m	131.4 [f] /131.4 [f], CH						
8/8'	8.20 [e], m/8.20 [e], m	131.2 [g] /131.2 [g], CH						
8a/8a'		139.5 [h] /139.5 [h], C						
9/9'		162.3/162.5, C						
Dha			Ala'			Val		
1		162.5, C	1		172.0, C	1		171.5, C
2		133.4, C	2	4.79, m	45.3, CH	2	4.39 overlapped	62.9, CH
3	6.57, m	103.6, CH_2	3	1.28, d (6.3)	17.4, CH_3	3	2.14, m	26.8, CH
	5.95, m		NH	8.35, m		4	0.93, m	19.9, CH_3
NH	10.42, s					5	0.74, m	18.7, CH_3
						N-Me	2.97, overlapped	30.2, CH_3
Ser			Cys			Val'		
1		168.6, C	1		168.6, C	1		171.2, C
2	5.48, m	54.6, CH	2	5.31, d (10.6)	54.8, CH	2	4.39, overlapped	62.7, CH
3	3.76, m	61.7, CH_2	3	4.50, d (10.2)	52.6, CH	3	2.14, m	26.8, CH
	3.83, m		S-Me	1.87, s	11.9, CH_3	4	0.91, m	19.8, CH_3
NH	8.70, d (8.0)		N-Me	2.96, overlapped	30.8, CH_3	5	0.70, m	18.7, CH_3
						N-Me	2.92, overlapped	30.5, CH_3

a*–*h **Assignments for overlapping ^{1}H and ^{13}C NMR resonances with the same superscript may be interchanged.**

Table S4. ^{1}H (800MHz) and ^{13}C (201MHz) NMR data of compound 5 in $CDCl_3$

Pos.	δ_H, mult (J in Hz)	δ_C, type	Pos.	δ_H, mult (J in Hz)	δ_C, type	Pos.	δ_H, mult (J in Hz)	δ_C, type
QXA/ QXA'			Ala			Cys'		
2/2'		143.3 [a] /143.3 [a], C	1		173.3, C	1		168.4, C
3/3'	9.69 [a], s/9.66 [a], s	143.9 [b] /143.7 [b], CH	2	5.05, overlapped	46.8, CH	2	5.51, overlapped	52.6, CH
4a/4a'		144.4 [c] /144.2 [c], C	3	1.47, d (6.8)	18.8, CH_3	3	2.88, br s	32.7, CH_2
5/5'	8.20 [b], m/8.20 [b], m	129.8 [d] /129.6 [d], CH	NH	8.68, overlapped			3.10, br s	
6/6'	7.88 [c], m7.88 [c], m	131.2 [e] /131.2 [e], CH				N-Me	3.01, overlapped	29.9, CH_3
7/7'	7.90 [d], m/7.90 [d], m	132.4 [f] /132.2 [f], CH						
8/8'	8.23 [e], m /8.23 [e], m	130.2 [g] /130.2 [g], CH						
8a/8a'		140.4 [h] /140.4 [h], C						
9/9'		162.3/163.9, C						
Dha			Ala'			Val		
1		162.9, C	1		172.7, C	1		170.5, C
2		134.2, C	2	5.05, overlapped	46.2, CH	2	4.87, overlapped	63.3, CH
3	5.51, overlapped	102.5, CH_2	3	1.32, br s	18.3, CH_3	3	2.37, m	27.9, CH
	6.79, s		NH	8.68, overlapped		4	1.08, br s	20.7, CH_3
NH	10.60, s					5	0.89, d (7.04)	18.8, CH_3
						N-Me	3.01, overlapped	30.7, CH_3
Ser			Cys			Val'		
1		167.5, C	1		170.5, C	1		170.5, C
2	4.50, br s	52.7, CH	2	5.77, br s	55.7, CH	2	4.52, overlapped	64.2, CH
3	4.88, br s	64.9, CH_2	3	4.52, overlapped	52.4, CH	3	2.37, m	27.9, CH
	4.50, br s		S-Me	2.07, s	12.0, CH_3	4	0.98, m	19.7, CH_3
NH	8.68, overlapped		N-Me	3.01, overlapped	29.9, CH_3	5	0.81, d (7.04)	18.8, CH_3
						N-Me	2.88, overlapped	30.7, CH_3

a*−*h **Assignments for overlapping ^{1}H and ^{13}C NMR resonances with the same superscript may be interchanged**

Table S5. ^{1}H (800MHz) and ^{13}C (201MHz) NMR data of compound 6 in $CDCl_3$

Pos.	δ_H, mult (J in Hz)	δ_C, type	Pos.	δ_H, mult (J in Hz)	δ_C, type	Pos.	δ_H, mult (J in Hz)	δ_C, type
QXA/ QXA'			Ala/Ala'			Val/ Val'		
2/2'		142.7, C	1		172.5, C	1		173.8, C
3/3'	9.56, s	143.7, CH	2	4.94, overlapped	46.4, CH	2	4.82, br s	63.0, CH
4a/4a'		144.1, C	3	1.40, d (6.7)	18.6, CH_3	3	2.23, br s	27.5, CH
5/5'	8.12, m	129.5, CH	NH	7.96, br s		4	1.05, m	20.2, CH_3
6/6'	7.82, br s	132.2, CH				5	0.87, m	19.5, CH_3
7/7'	7.85, br s	131.2, CH				N-Me	3.05, s	31.6, CH_3
8/8'	8.13, br s	130.0, CH						
8a/8a'		140.4, C						
9/9'		164.4 [a] /164.1 [a], C						
Ser/ Ser'			Cys/ Cys'					
1		169.4, C	1		169.9, C			
2	4.94, br s	55.2, CH	2	5.96, br s	54.3, CH			
3	3.99, br s	64.1, CH_2	3	2.83, br s	39.3, CH_2			
	4.15, br s			3.15, br s				
NH	9.03, s		N-Me	2.94, s	30.8, CH_3			

a **Assignments for overlapping ^{1}H and ^{13}C NMR resonances with the same superscript may be interchanged.**

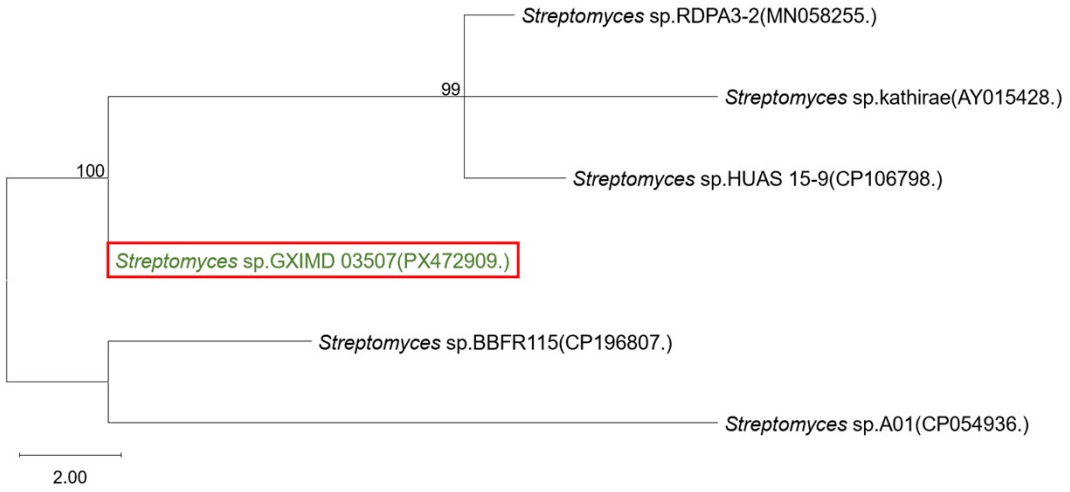
Table S6. ^{1}H (500MHz) and ^{13}C (126MHz) NMR data of compound 7 in $CDCl_3$

Pos.	δ_H, mult (J in Hz)	δ_C, type	Pos.	δ_H, mult (J in Hz)	δ_C, type	Pos.	δ_H, mult (J in Hz)	δ_C, type
QXA/ QXA'			Ala/Ala'			Val/ Val'		
2/2'		142.8 [a] /142.6 [a], C	1		172.8/172.7, C	1		170.2, C
3/3'	9.64 [a], m/9.60 [a], d (3.0)	143.8 [b] /143.6 [b], CH	2	4.96, m/4.81, d (7.7)	47.3/46.6, CH	2	4.94, m	62.0, CH
4a/4a'		144.2 [c] /144.1 [c], C	3	1.44, t (6.0)	18.5/17.9, CH_3	3	2.25, dt (12.4, 6.5) /	27.5/27.4, CH
5/5'	8.15, m	129.5 [d] /129.7 [d], CH	NH	7.88, q (8.1)/8.44, m			2.34, m	
6/6'	7.88, m	132.3 [e] /132.1 [e], CH				4	1.12, m/1.06, m	20.5/20.1, CH_3
7/7'	7.88, m	131.3 [f] /131.2 [f], CH				5	0.85, d (6.7)/1.00, m	19.5/18.8, CH_3
8/8'	8.17, m	130.1 [g] /129.9 [g], CH				N-Me	3.06, s/3.12, s	31.3, CH_3
8a/8a'		140.5 [h] /140.5 [h], C						
9/9'		164.7/163.8, C						
Ser/ Ser'			Cys/ Cys'					
1		168.1, C	1		169.6, C			
2	4.96, m/4.87, d (5.5)	55.5/51.8, CH	2	6.33, s	53.6, CH			
3	4.50, t (9.7)/4.03, m	65.3/64.7, CH_2	3	3.01, m/3.07, d (7.1)	39.4/38.0, CH_2			
	4.60, d (11.0)/			3.26, m				
	4.11, dd (11.9, 6.2)		N-Me	2.97, s/3.02, s	30.5, CH_3			
NH	8.88, d (6.9)/9.13, d (6.4)							

a*−*h **Assignments for overlapping ^{1}H and ^{13}C NMR resonances with the same superscript may be interchanged.**

Table S7. The amino acids configurations of compounds 1-7

Compounds	amino acids configurations			
	Ser	Ala	N-Me-Cys	N-Me-Val
1		L	L	L
2	D	L	L	L
3	D	L	L	L
4	D	L	L	L
5	D	L	L	L/D
6	D	L	L	L
7	D	L	L	L



The strain analyzed in this study is marked in green bold text and with a red box.

Figure S1. Phylogram generated by the concatenation of the GXIMD 03507 of the *Streptomyces* sp.

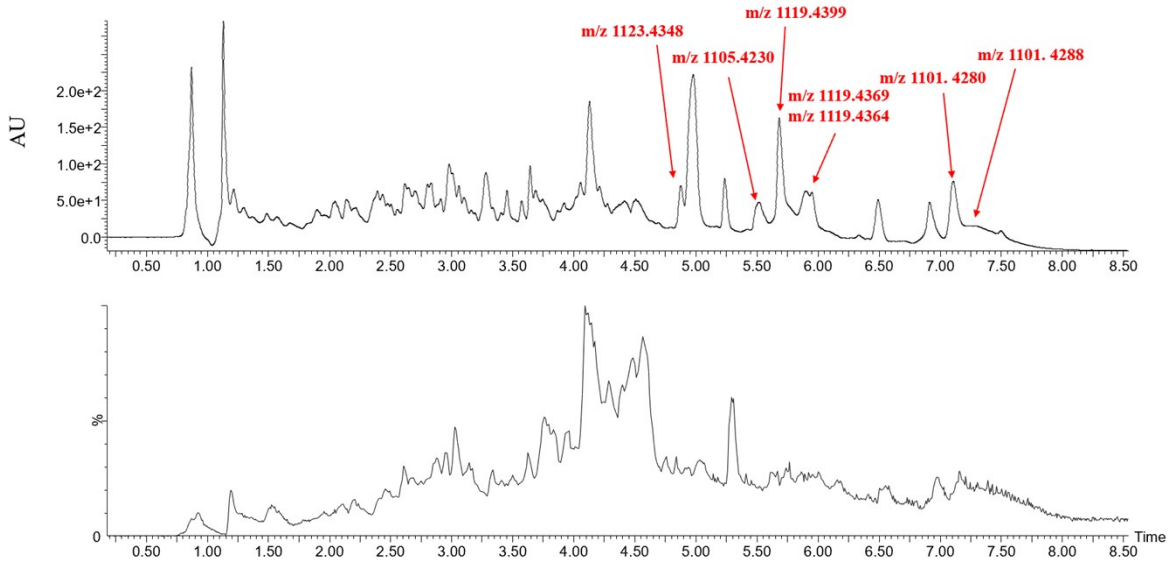


Figure S2. LC-MS and UV spectra of crude extract

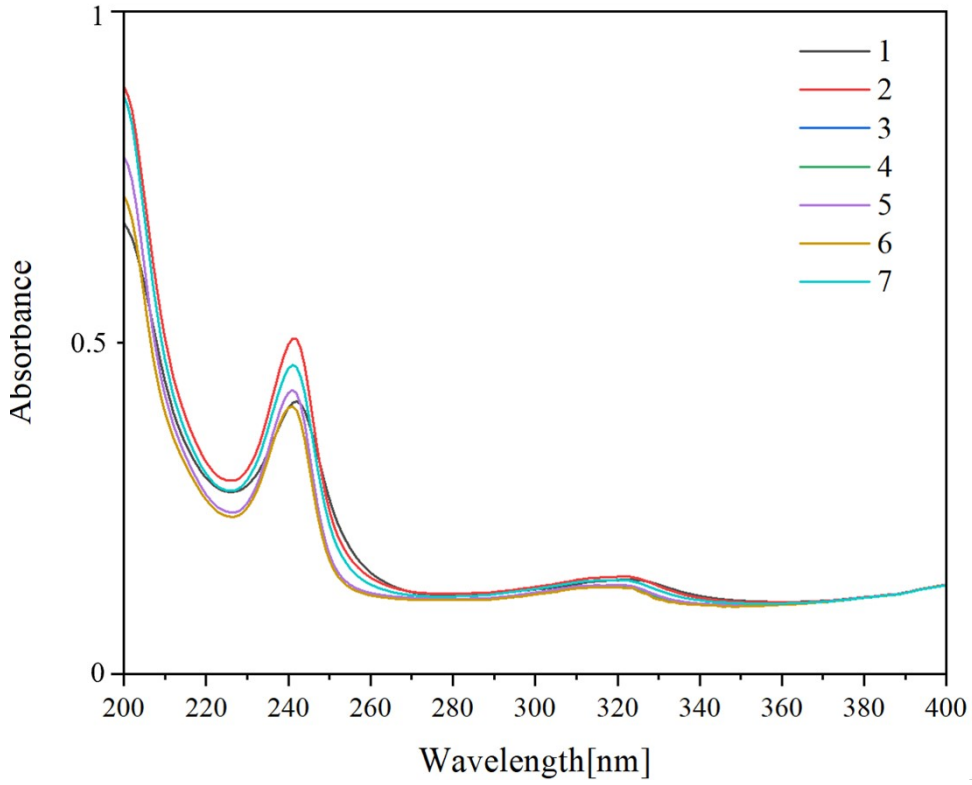


Figure S3. The UV spectra of compounds 1-7

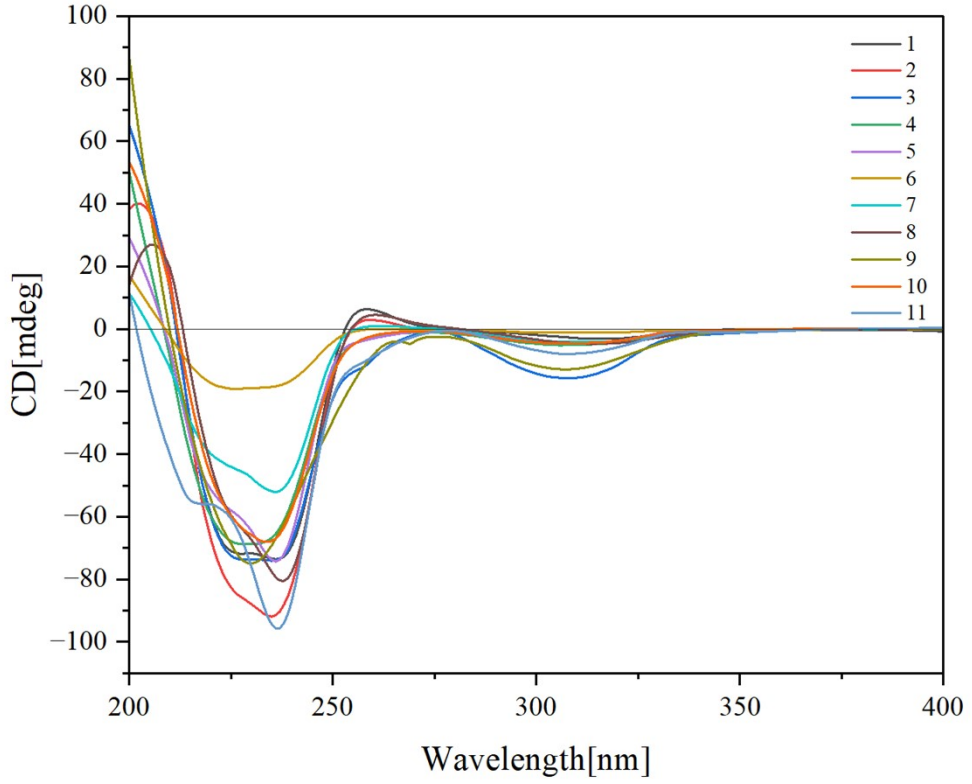


Figure S4. The ECD spectra of compounds 1-11

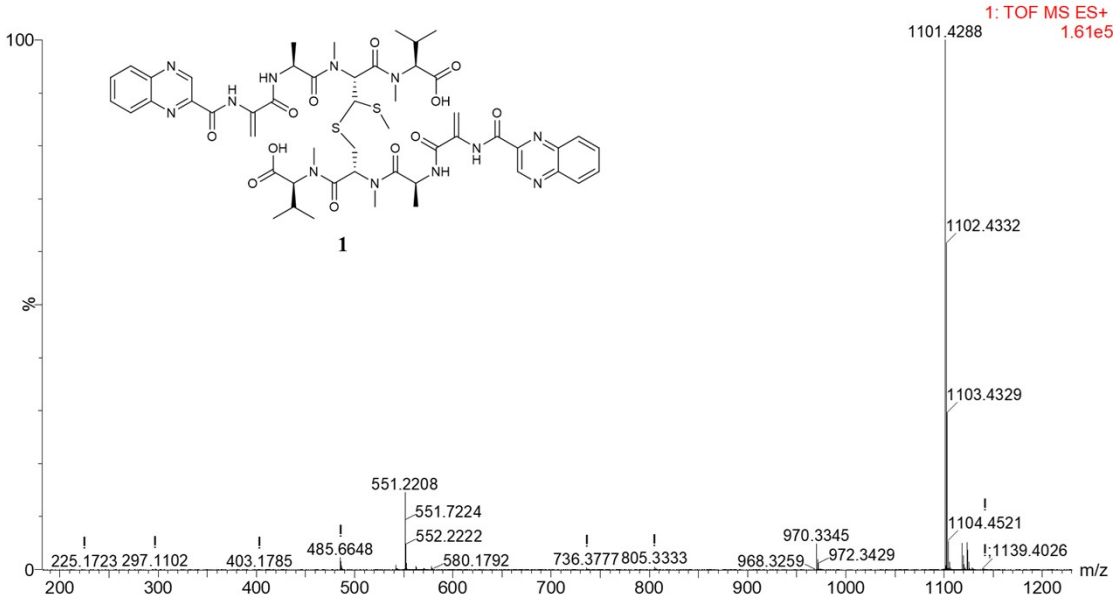


Figure S5. The (+)-HRESIMS spectrum of compound 1

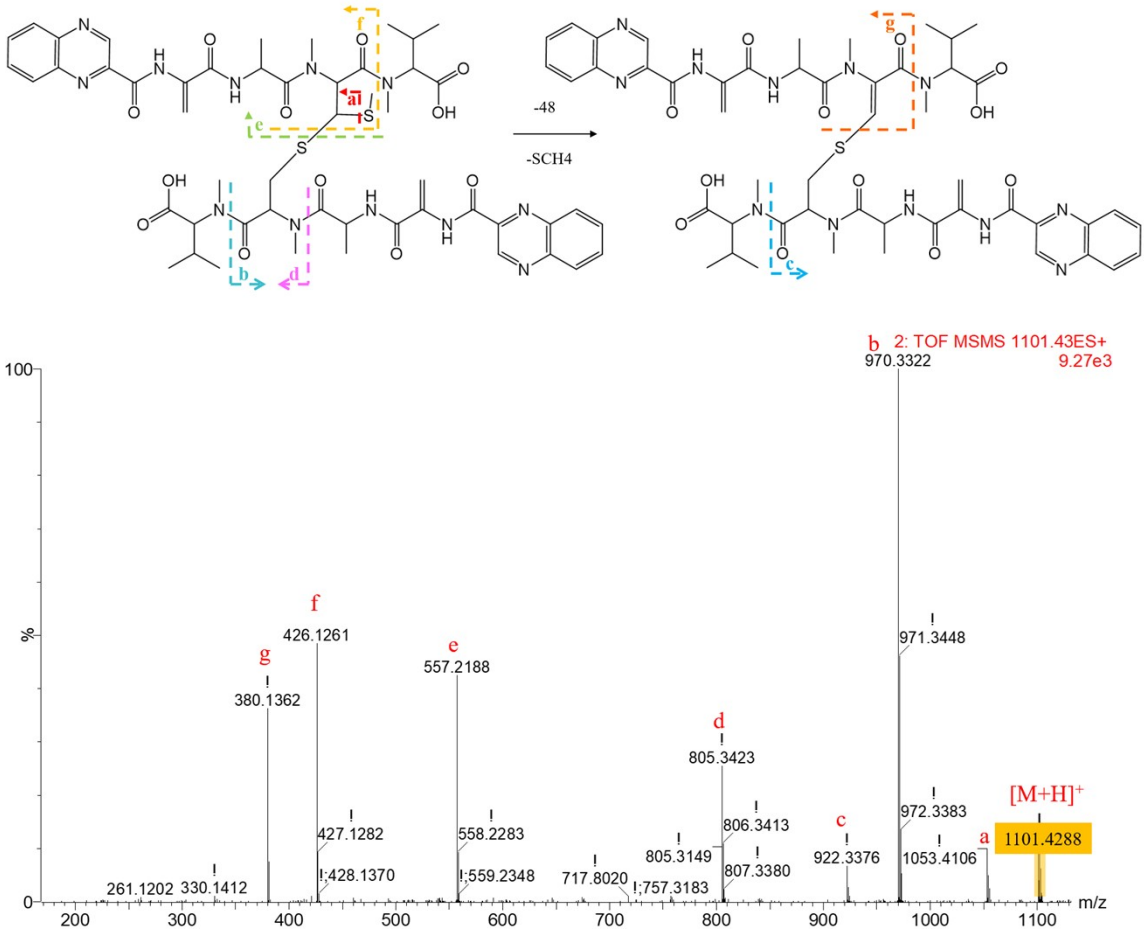


Figure S6. MS/MS fragmentation analysis of compound 1

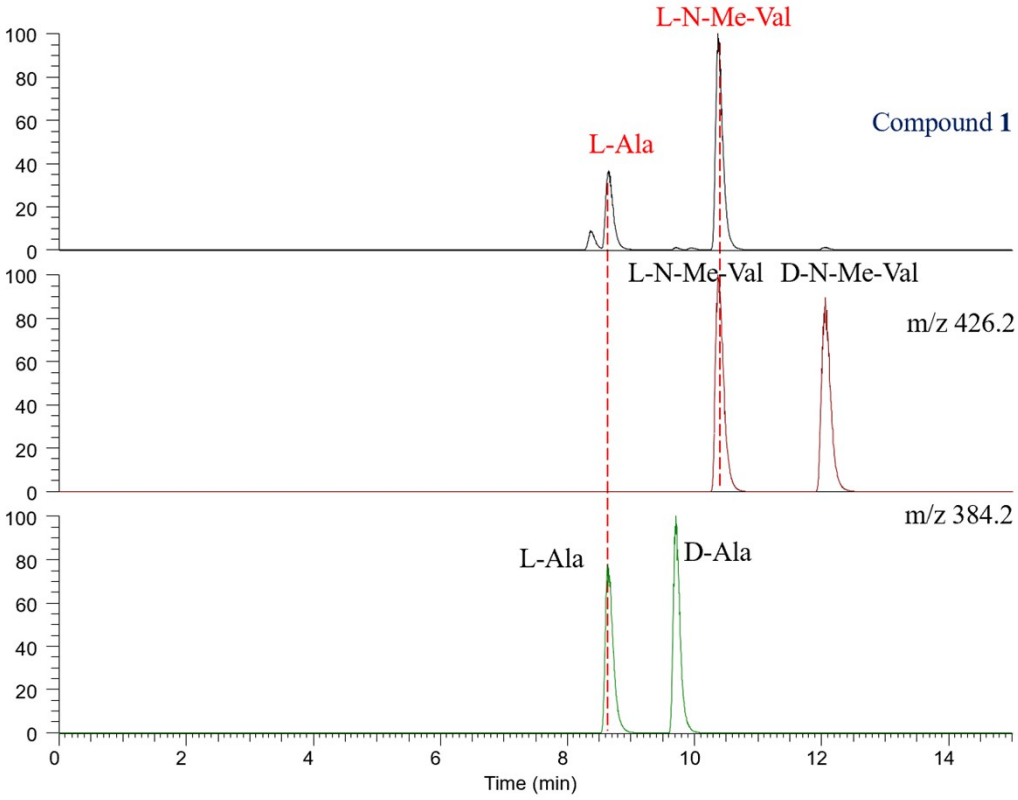


Figure S7. Marfey's analysis of compound 1

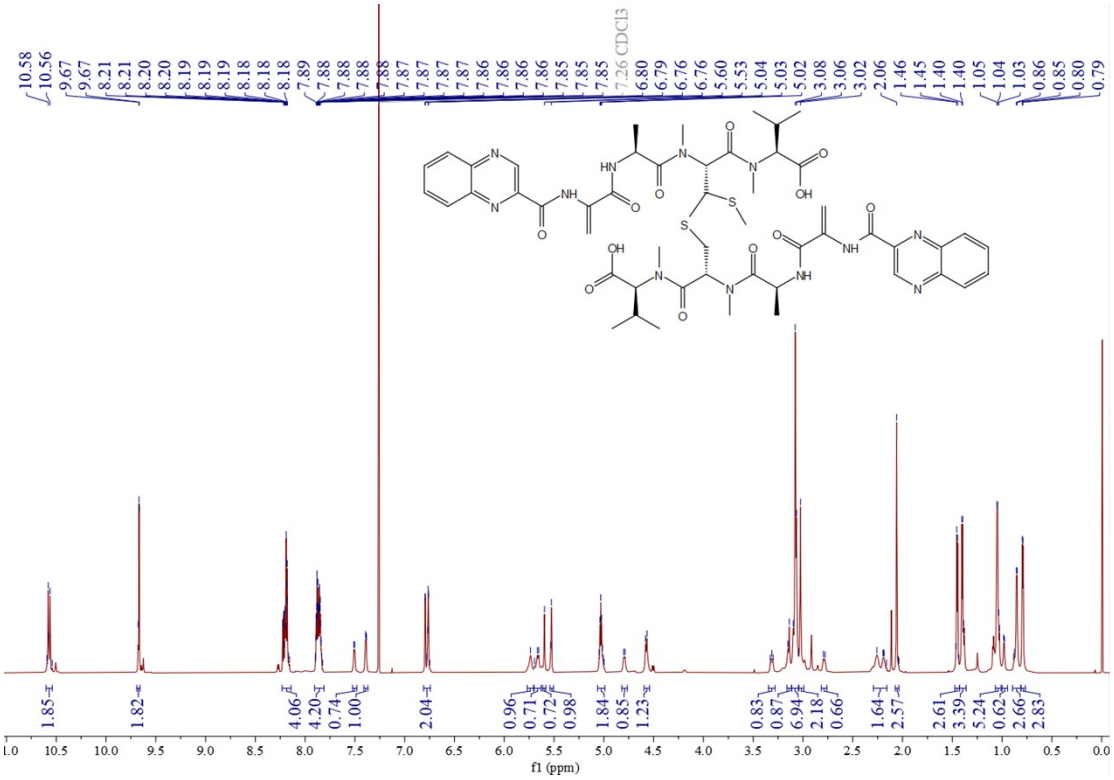


Figure S8. ^{1}H NMR spectrum of (1) at 800 MHz in $CDCl_3$

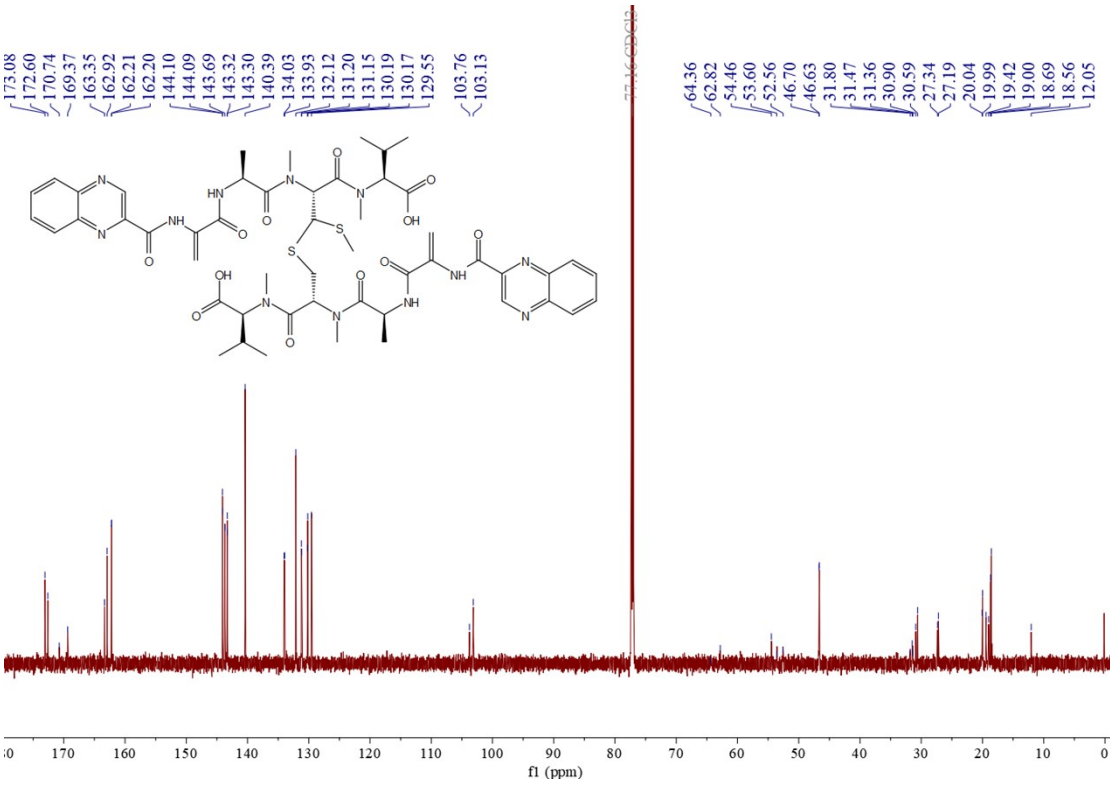


Figure S9. ^{13}C NMR spectrum of (1) at 201 MHz in $CDCl_3$

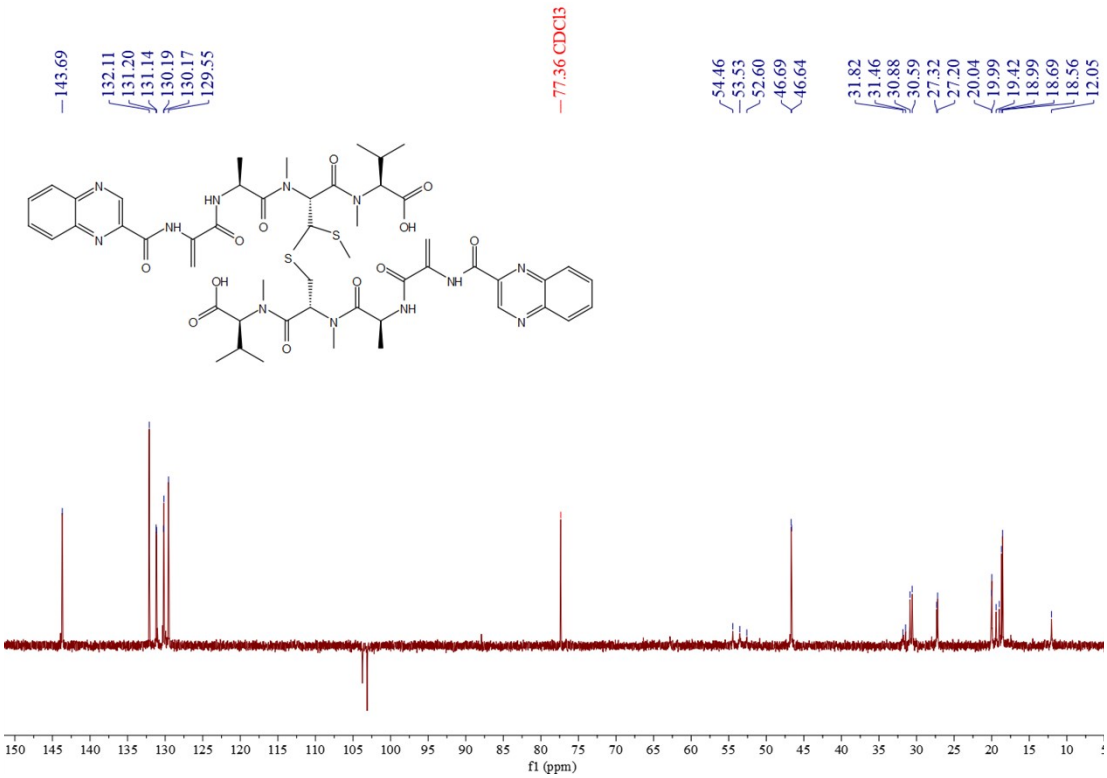


Figure S10. DEPT-135 NMR spectrum of (1) in $CDCl_3$

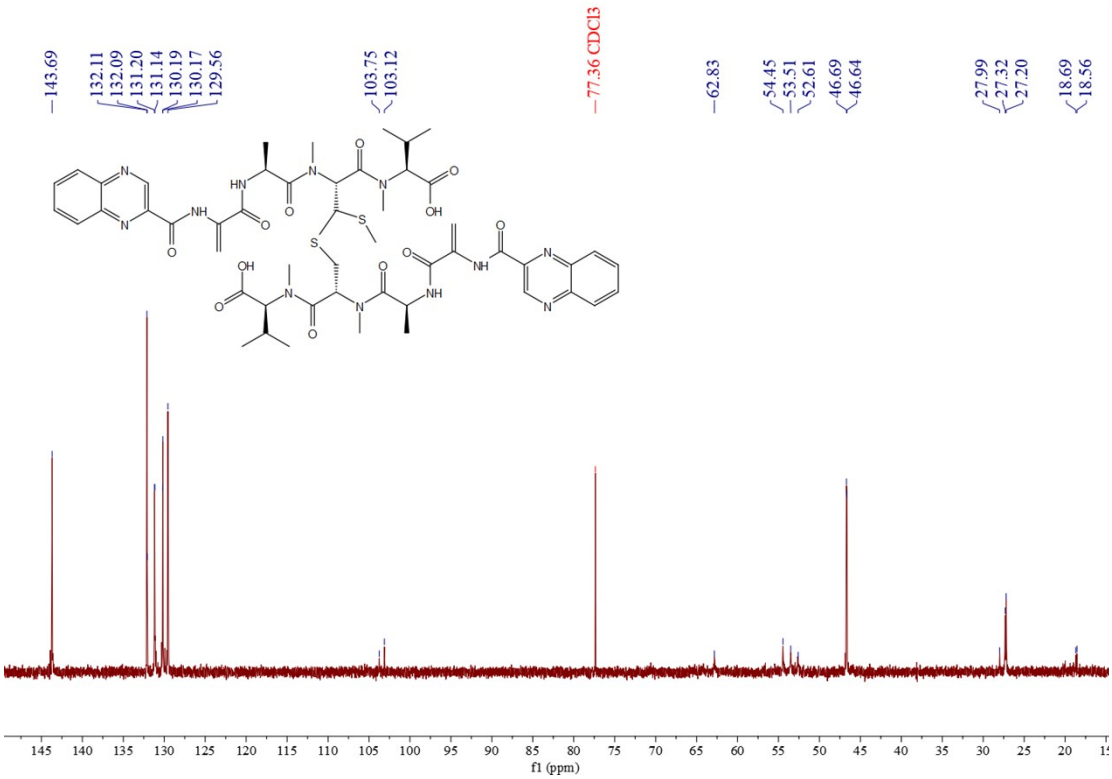


Figure S11. DEPT-90 NMR spectrum of (1) in $CDCl_3$

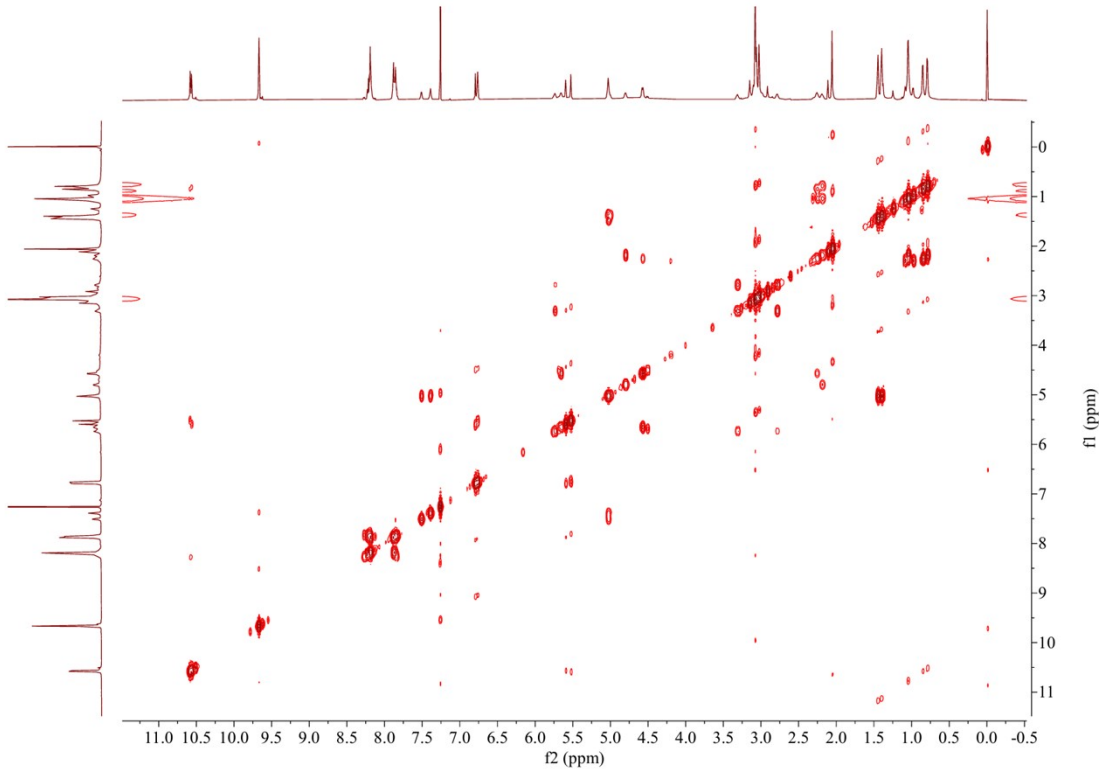


Figure S12. COSY NMR spectrum of (1) in $CDCl_3$

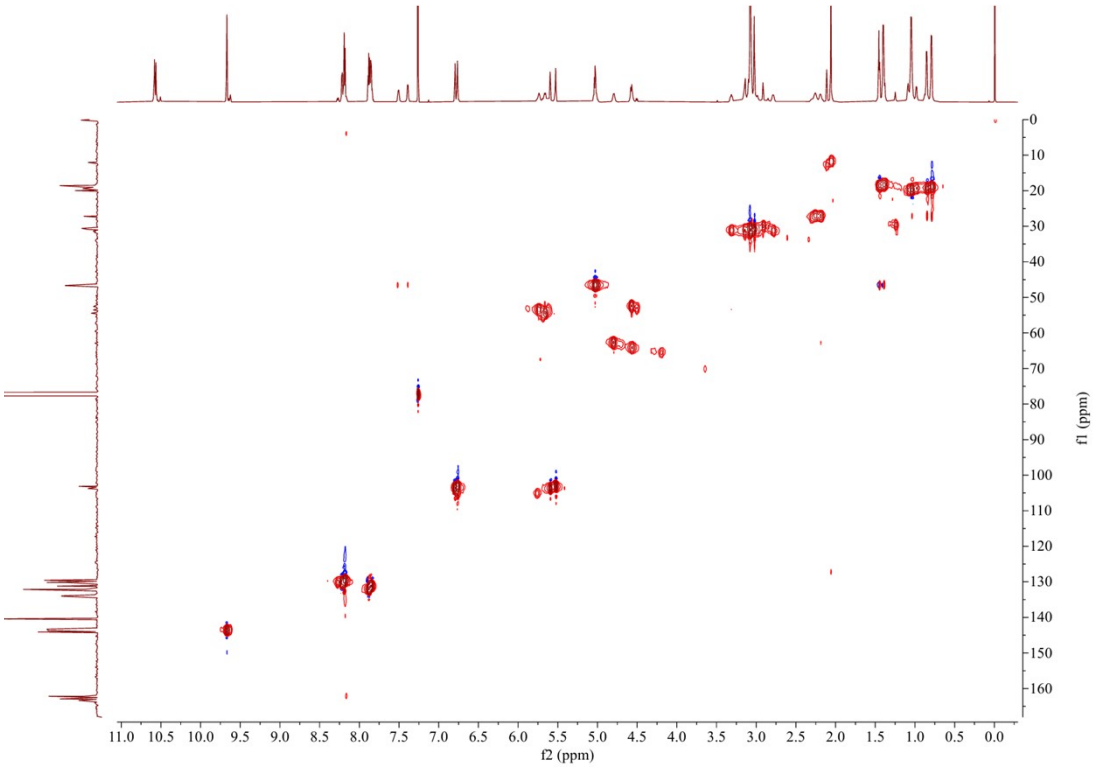


Figure S13. HSQC NMR spectrum of (1) in $CDCl_3$

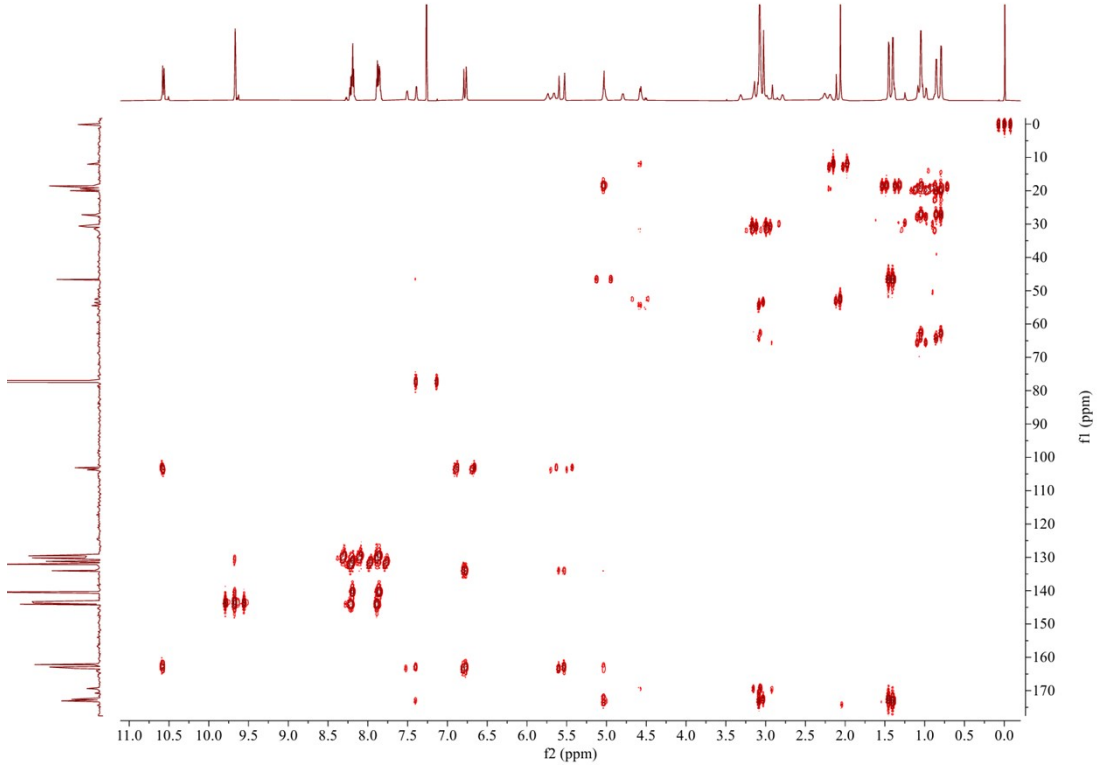


Figure S14. HMBC NMR spectrum of (1) in $CDCl_3$

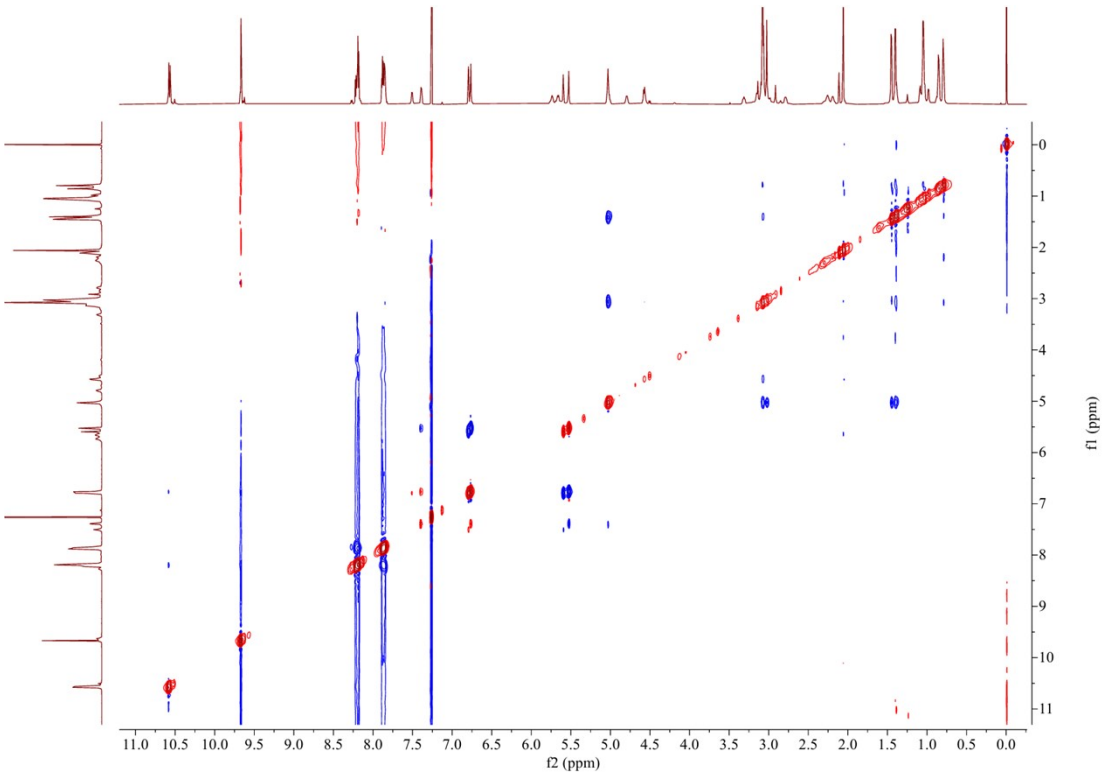


Figure S15. ROESY NMR spectrum of (1) in $CDCl_3$

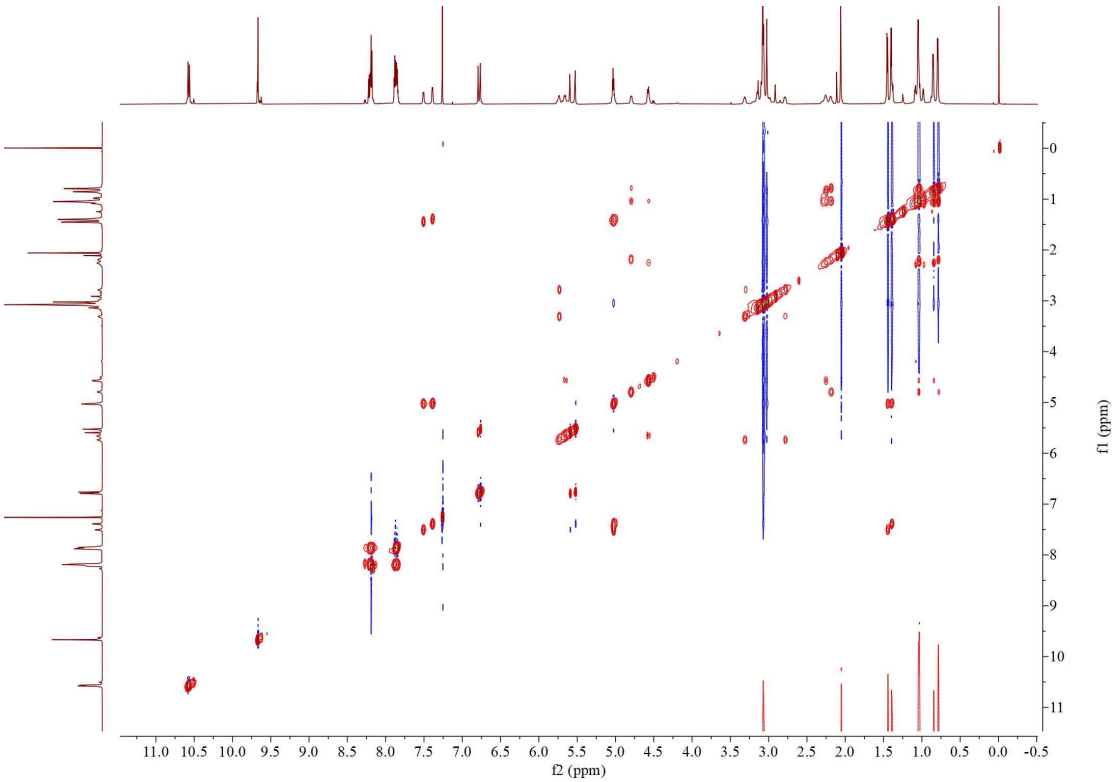


Figure S16. TOCSY NMR spectrum of (1) in $CDCl_3$

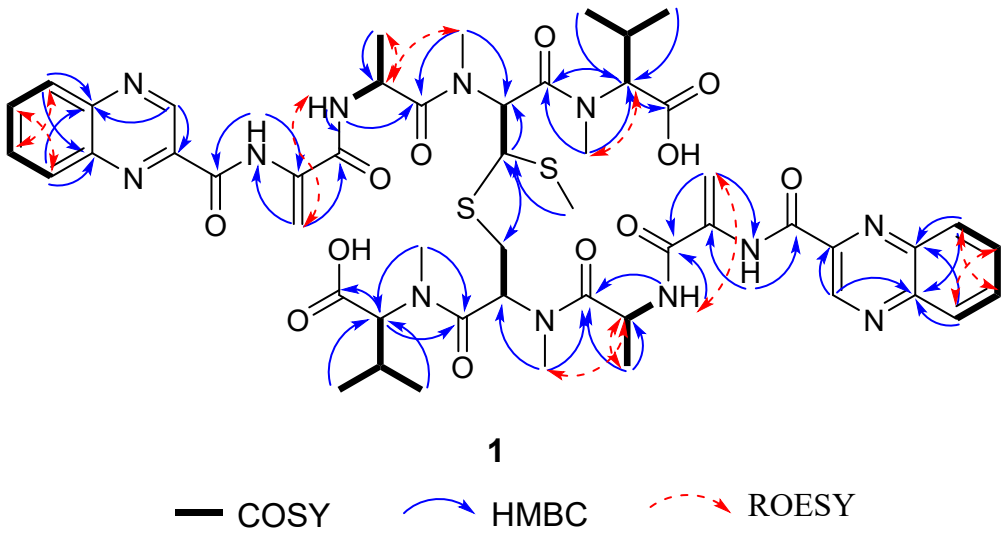


Figure S17. Key COSY, HMBC, ROESY correlations of compounds 1

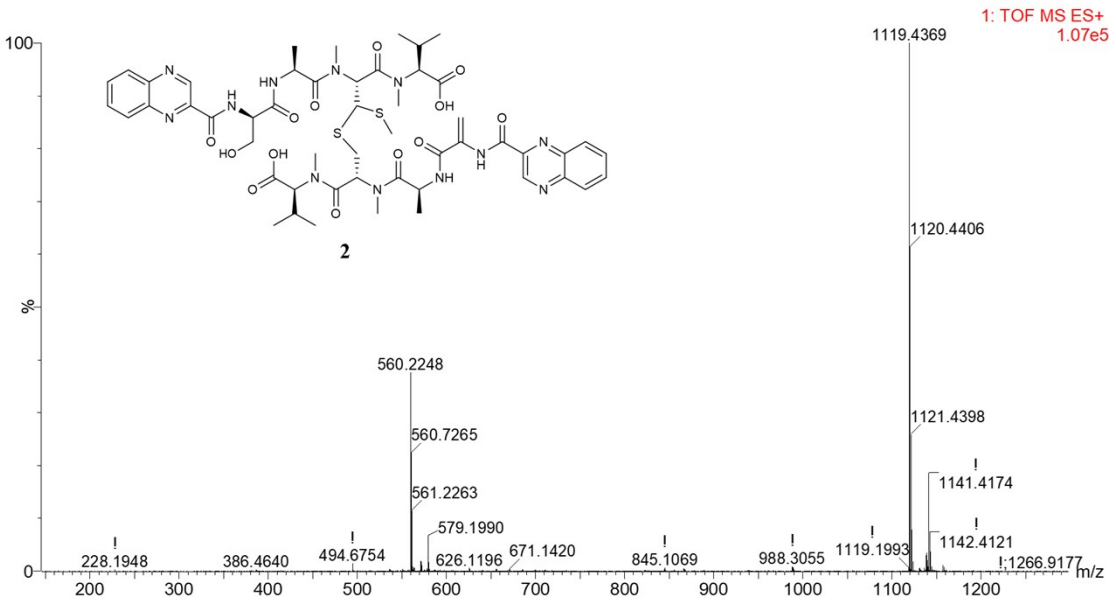


Figure S18. The (+)-HRESIMS spectrum of compound 2

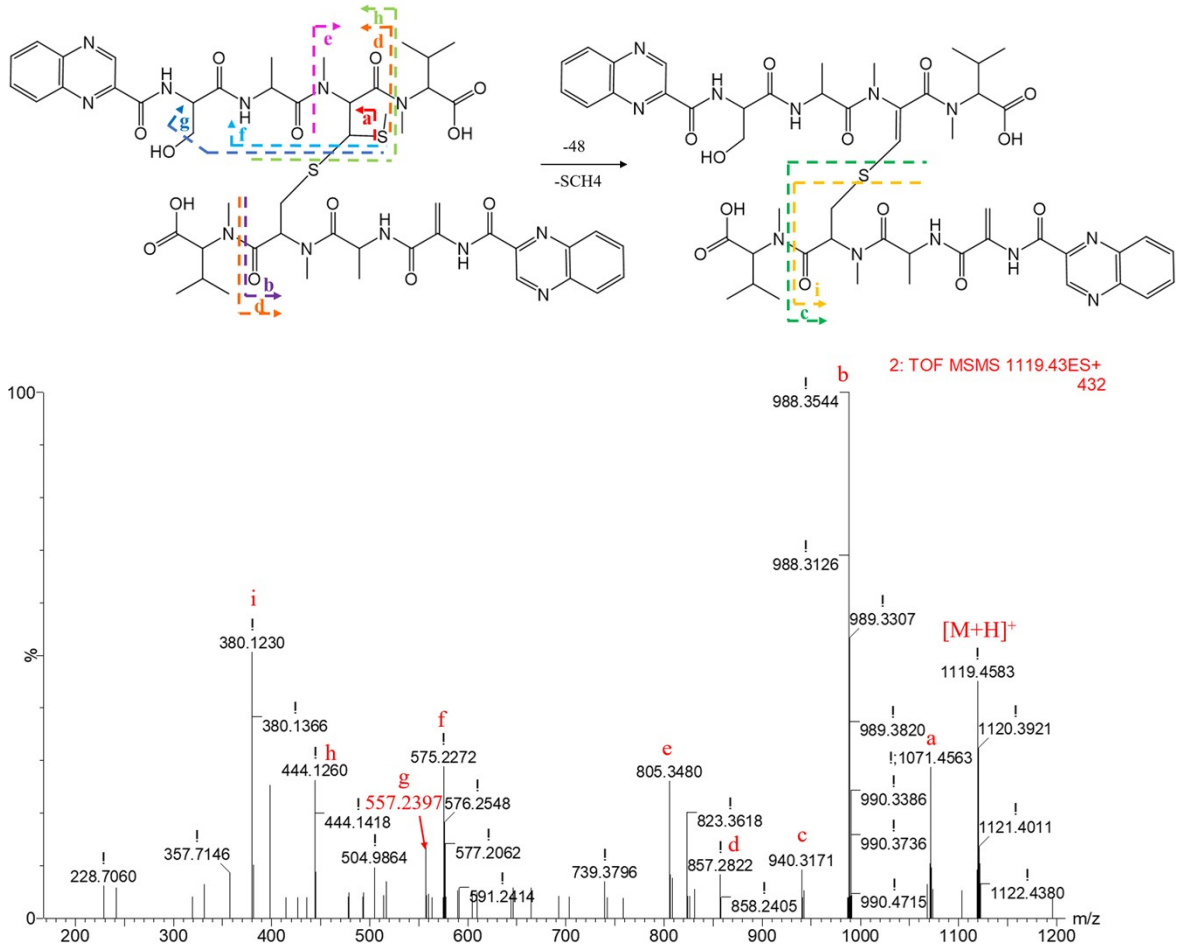


Figure S19. MS/MS fragmentation analysis of compound 2

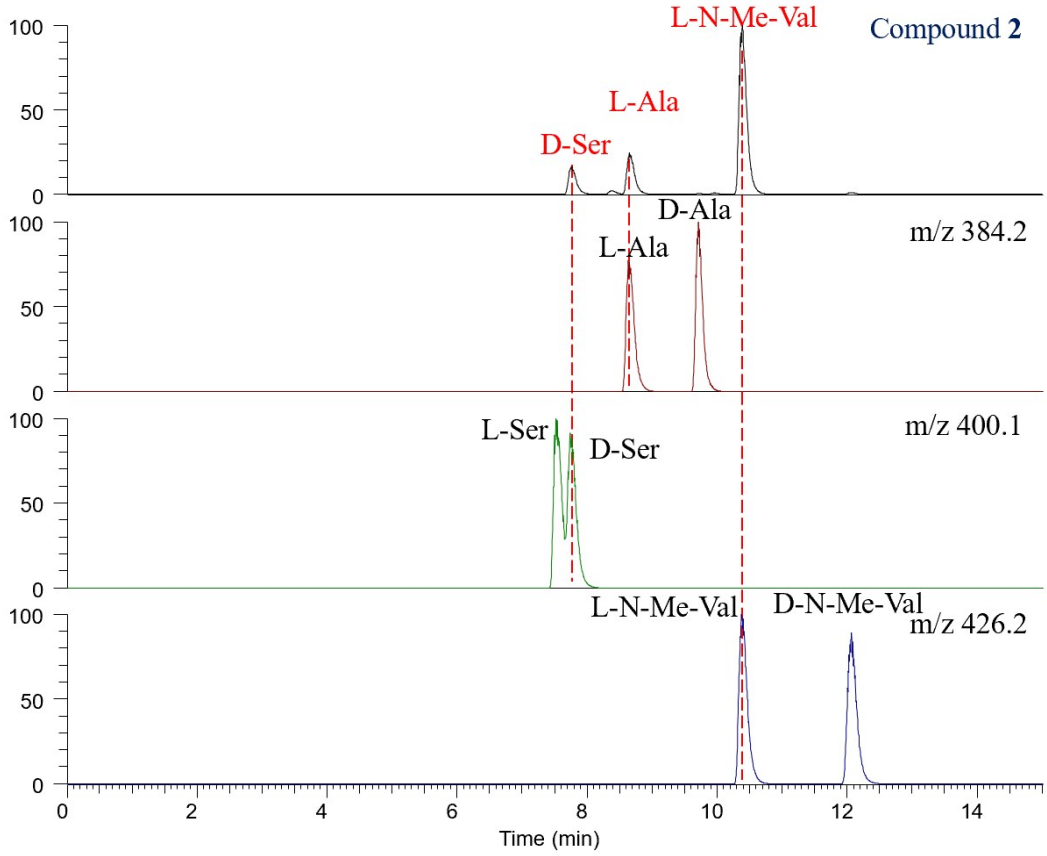


Figure S20. Marfey's analysis of compound 2

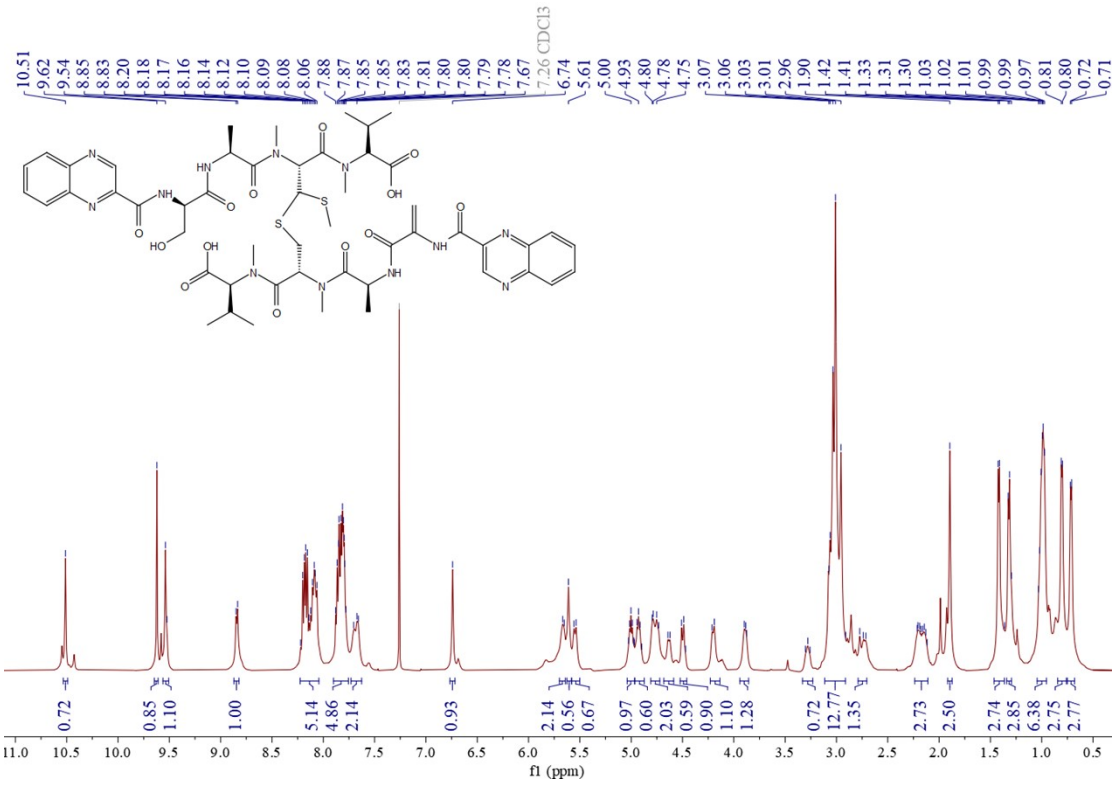


Figure S21. ^{1}H NMR spectrum of (2) at 500 MHz in $CDCl_3$

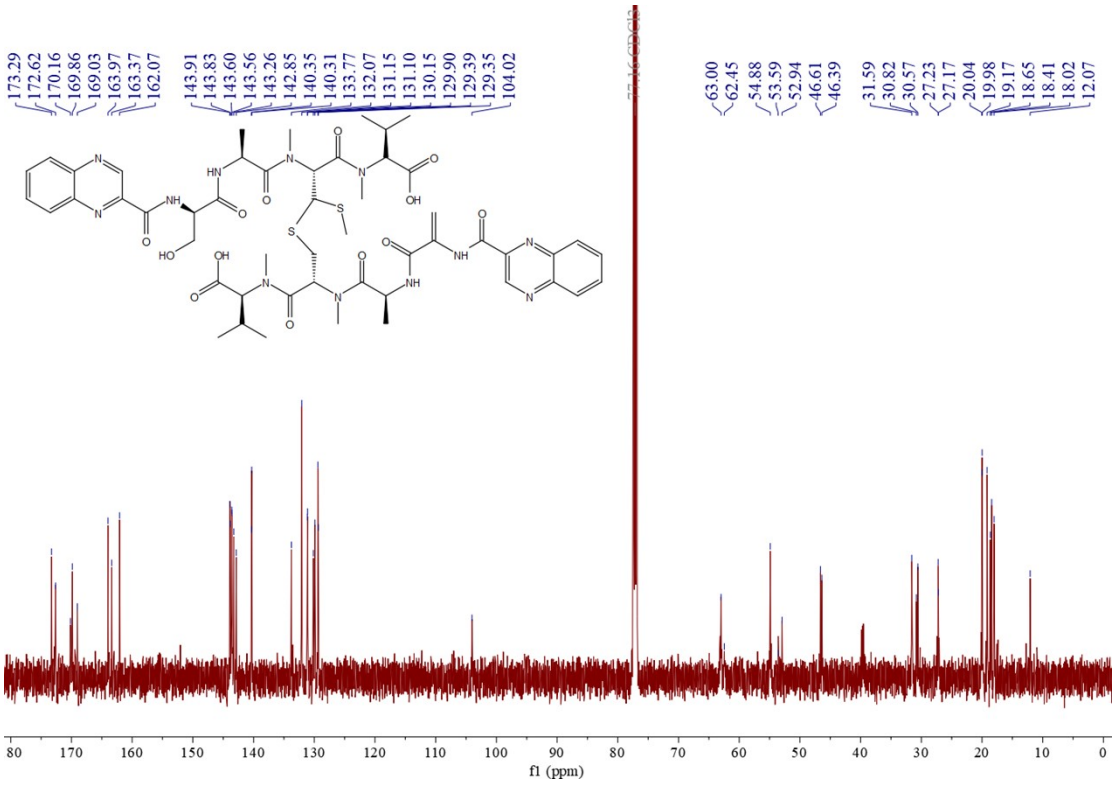


Figure S22. ^{13}C NMR spectrum of (2) at 126 MHz in $CDCl_3$

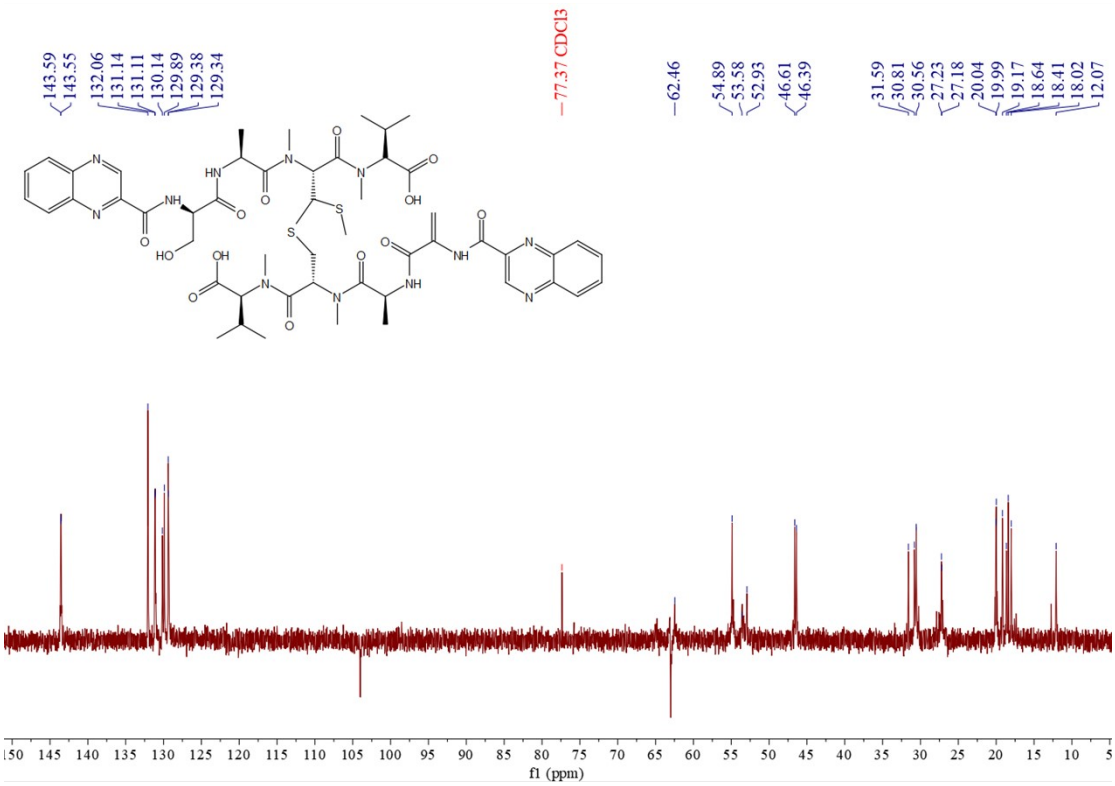


Figure S23. DEPT-135 NMR spectrum of (2) in $CDCl_3$

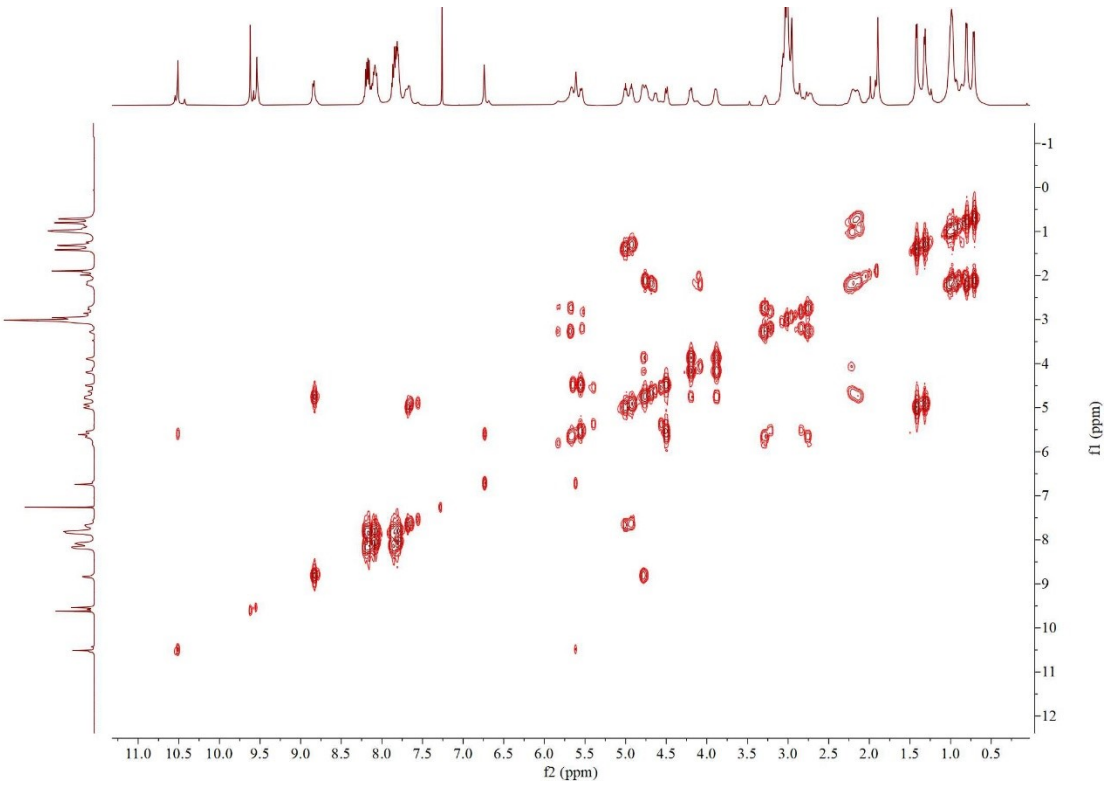


Figure S24. COSY NMR spectrum of (2) in $CDCl_3$

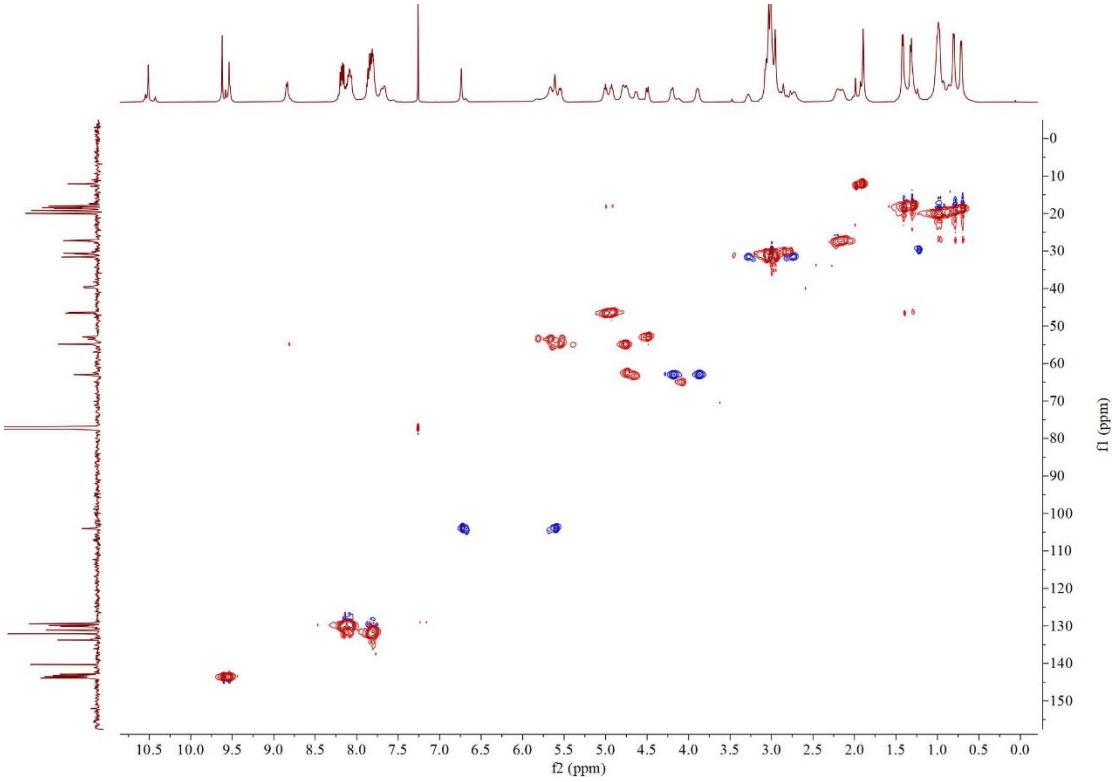


Figure S25. HSQC NMR spectrum of (2) in $CDCl_3$

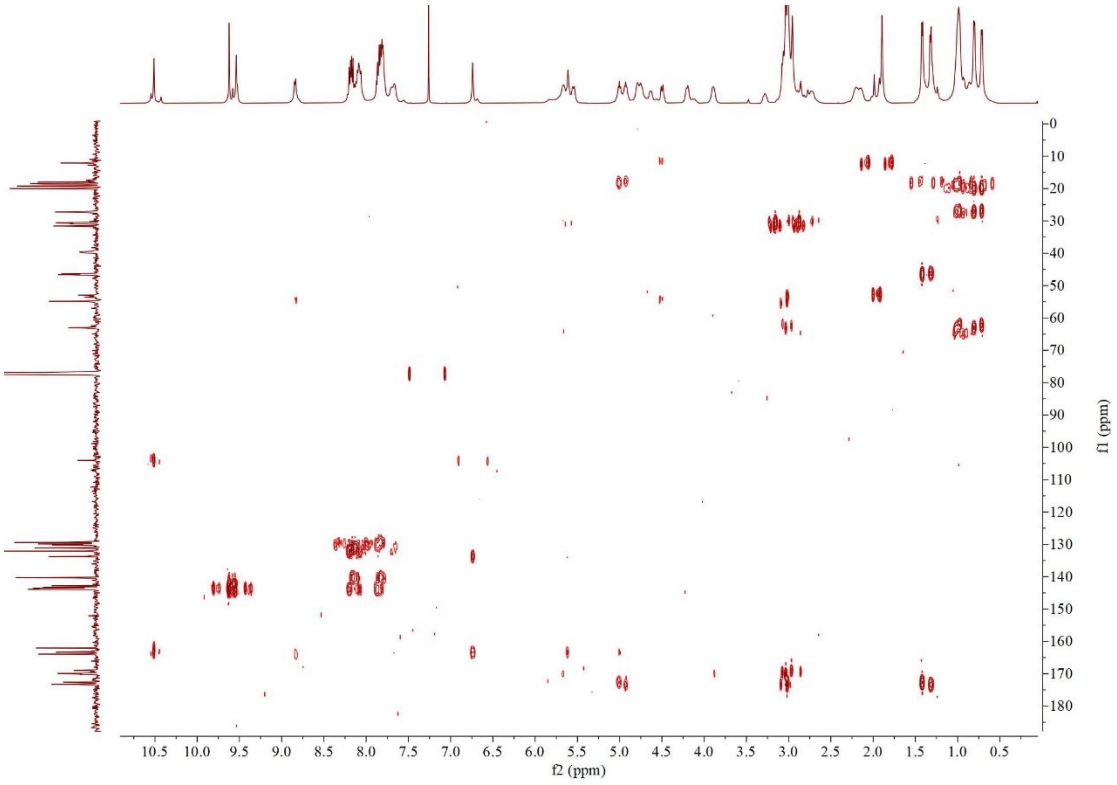


Figure S26. HMBC NMR spectrum of (2) in $CDCl_3$

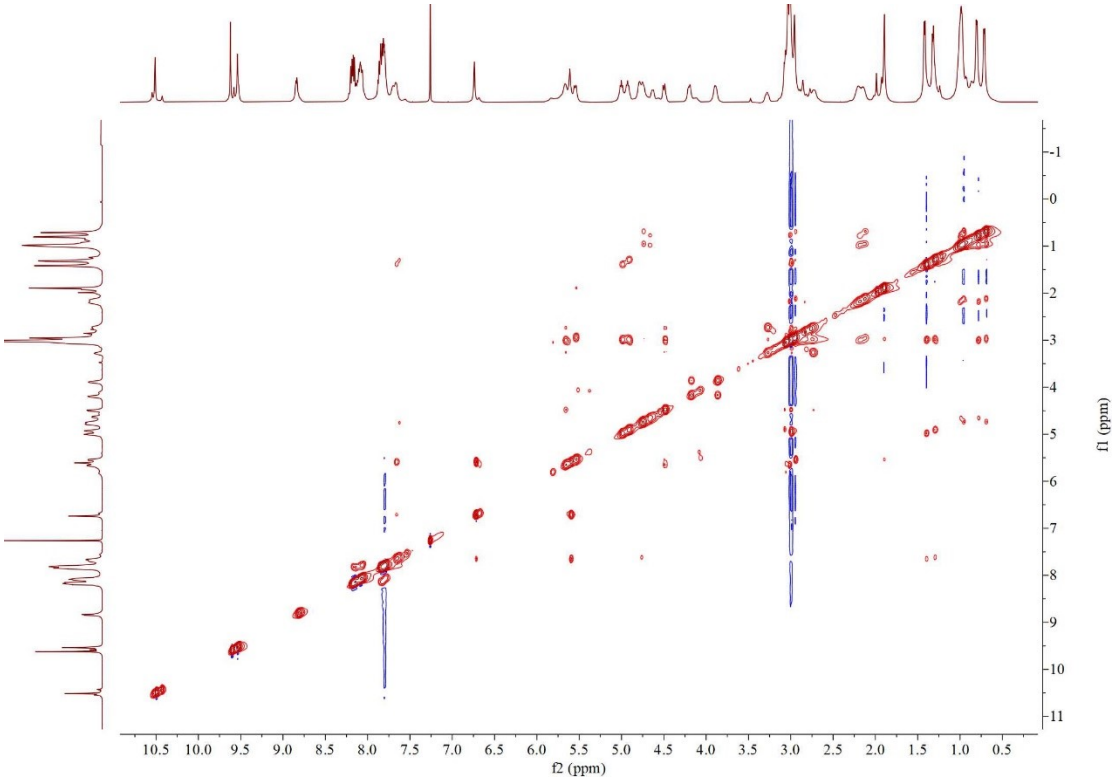


Figure S27. NOESY NMR spectrum of (2) in $CDCl_3$

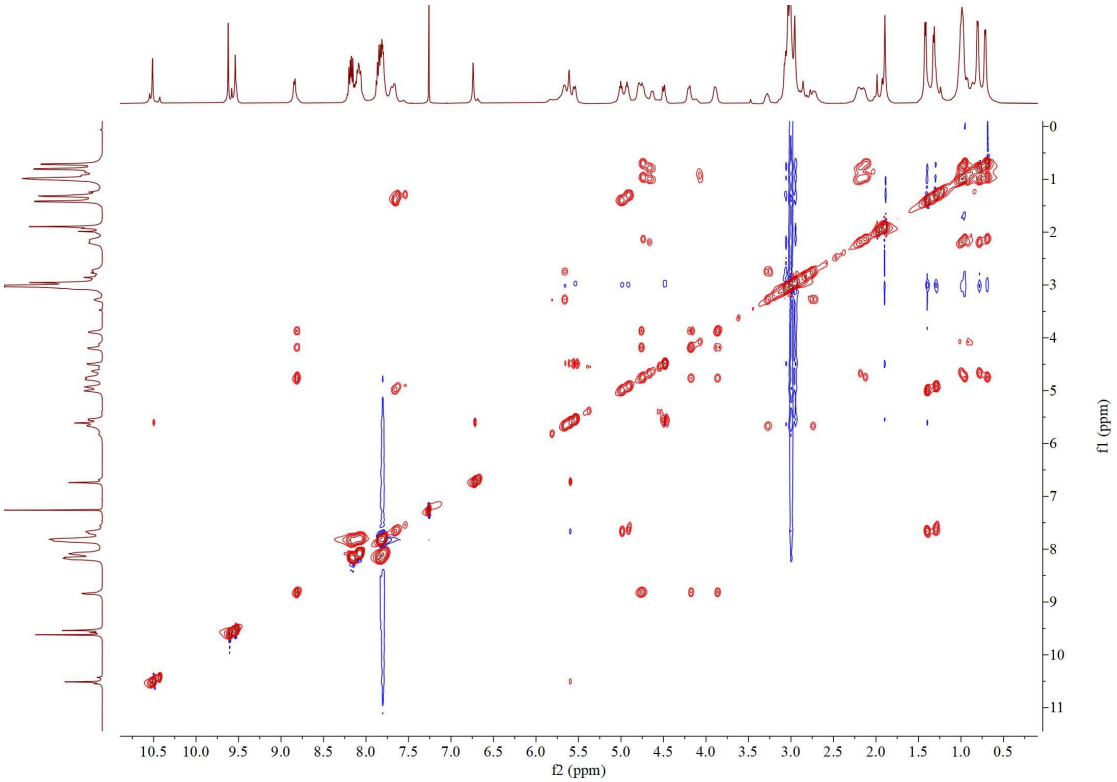


Figure S28. TOCSY NMR spectrum of (2) in $CDCl_3$

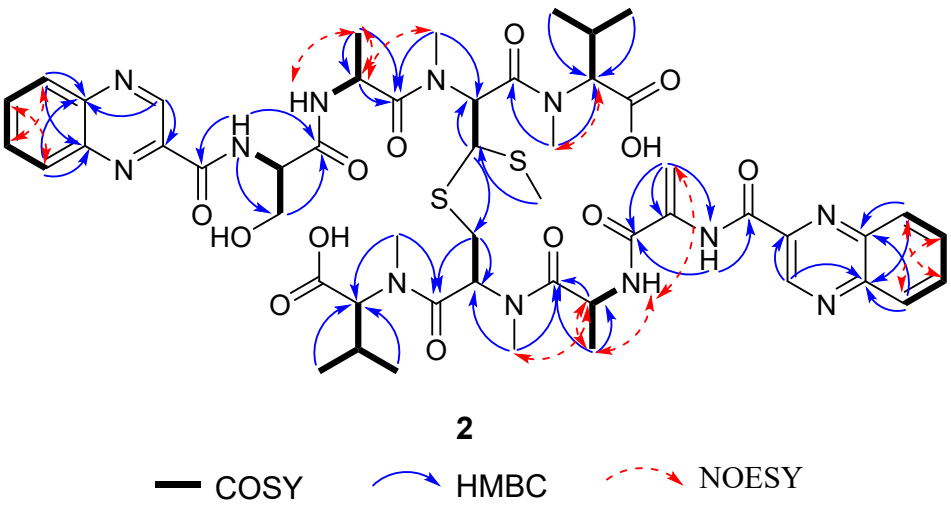


Figure S29. Key COSY, HMBC, NOESY correlations of compounds 2

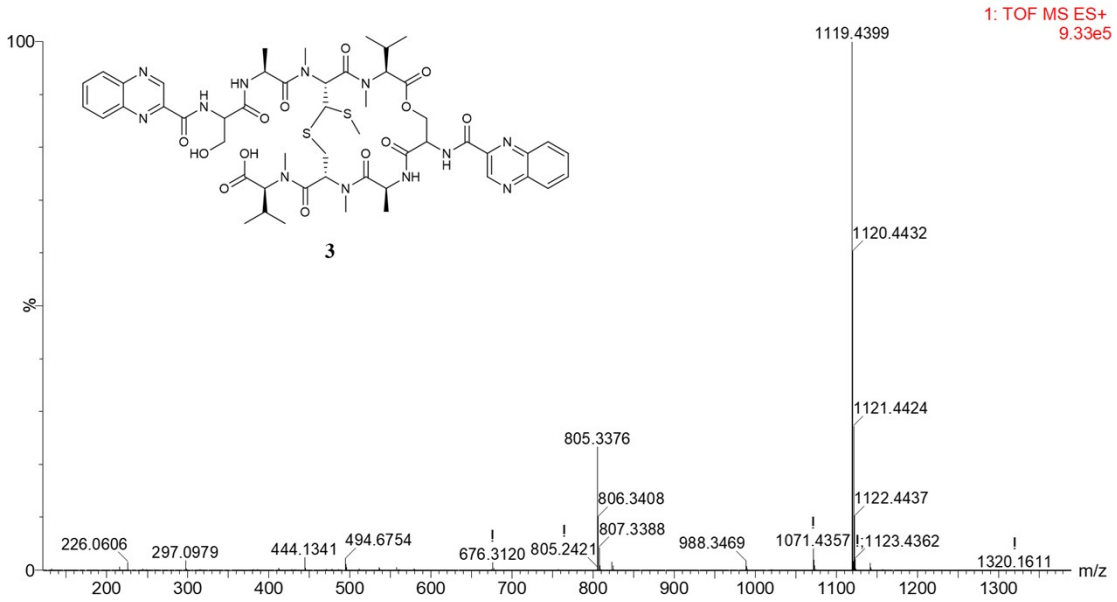


Figure S30. The (+)-HRESIMS spectrum of compound 3

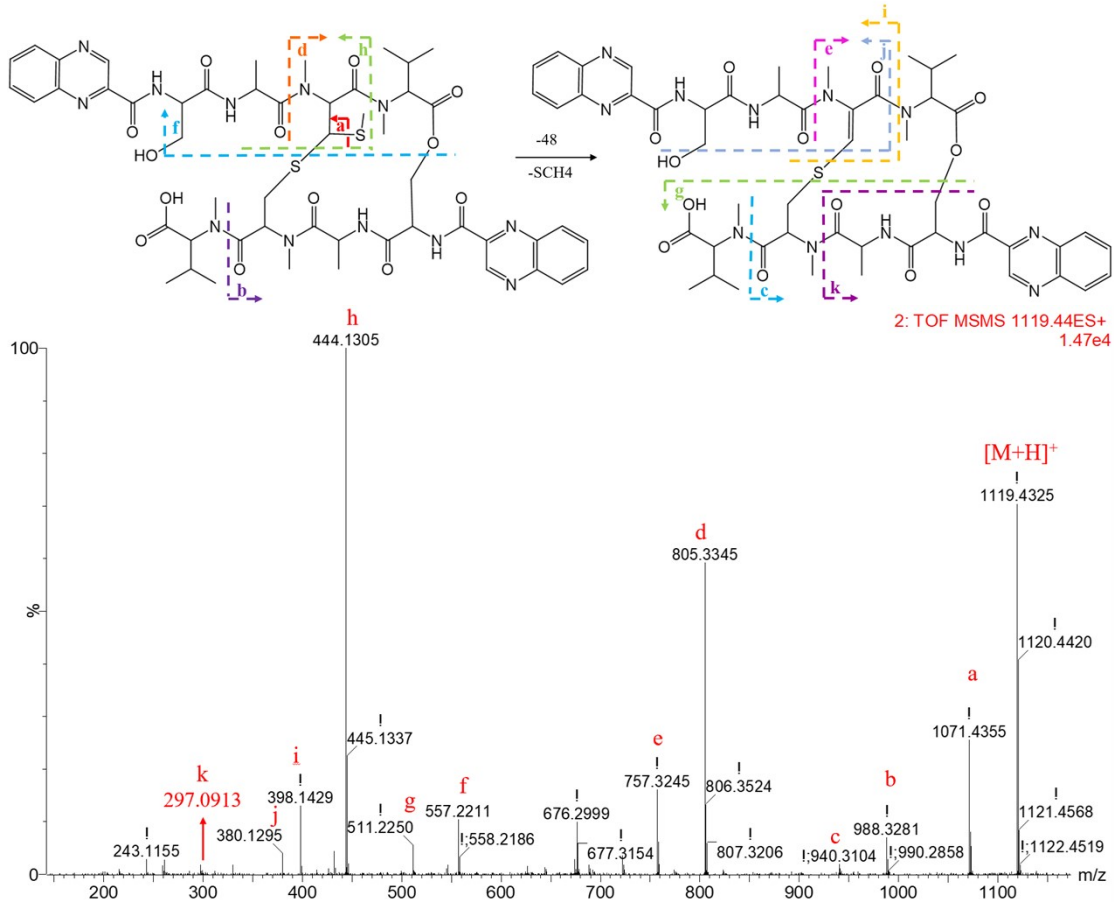


Figure S31. MS/MS fragmentation analysis of compound 3

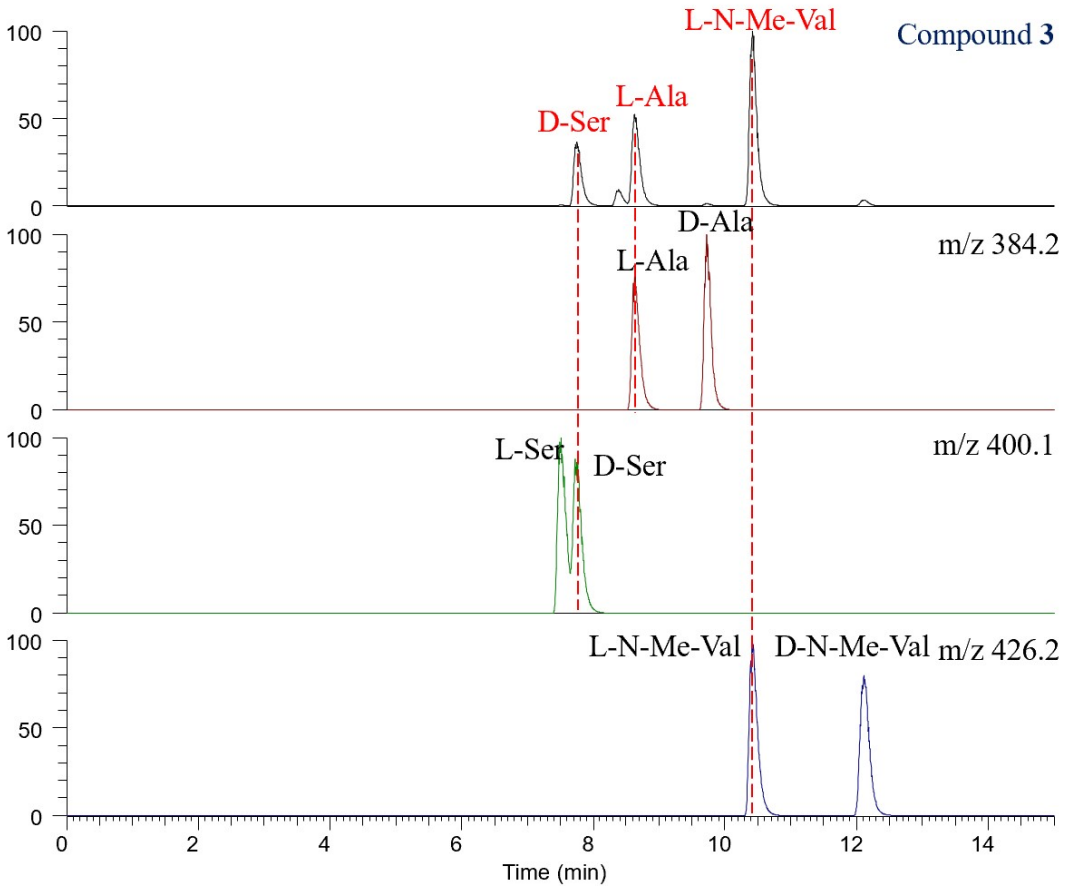


Figure S32. Marfey's analysis of compound 3

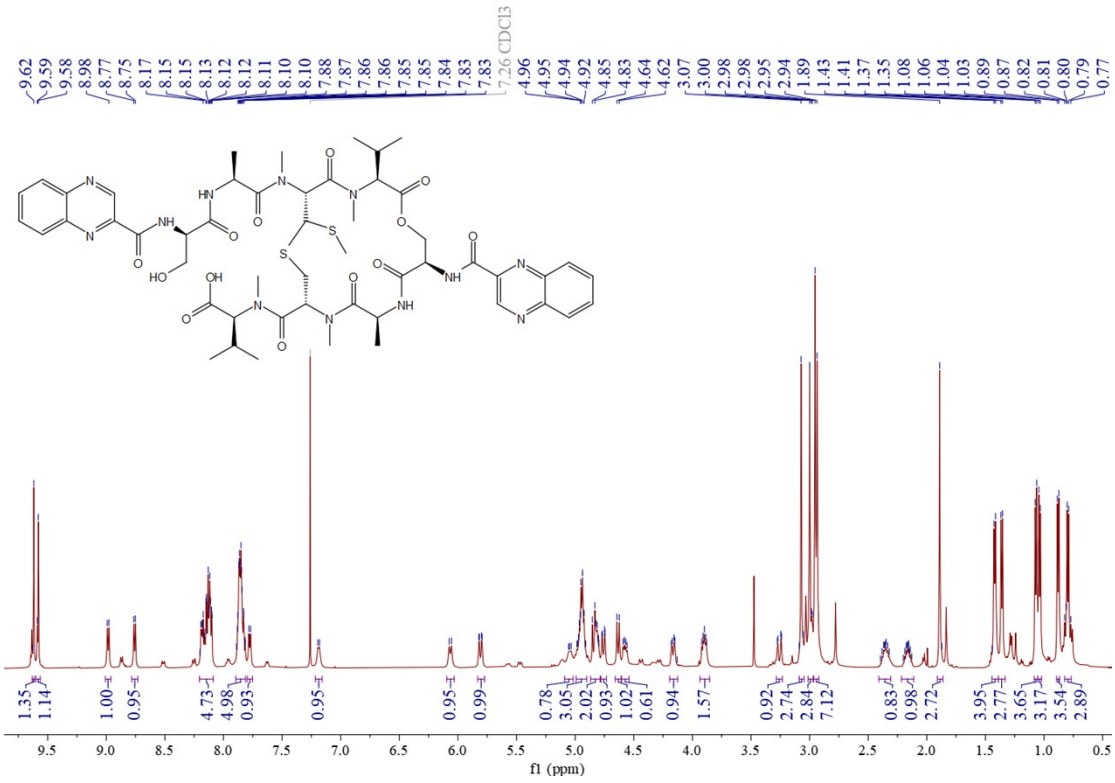


Figure S33. ^{1}H NMR spectrum of (3) at 500 MHz in $CDCl_3$

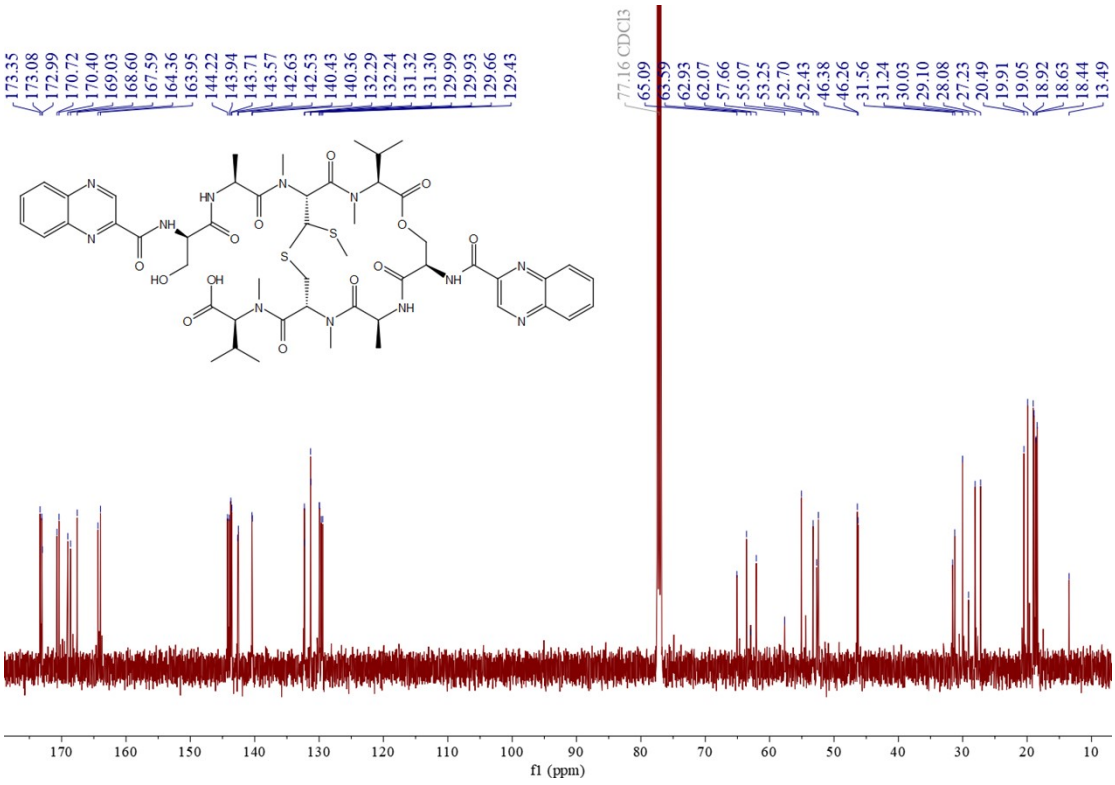


Figure S34. ^{13}C NMR spectrum of (3) at 126 MHz in $CDCl_3$

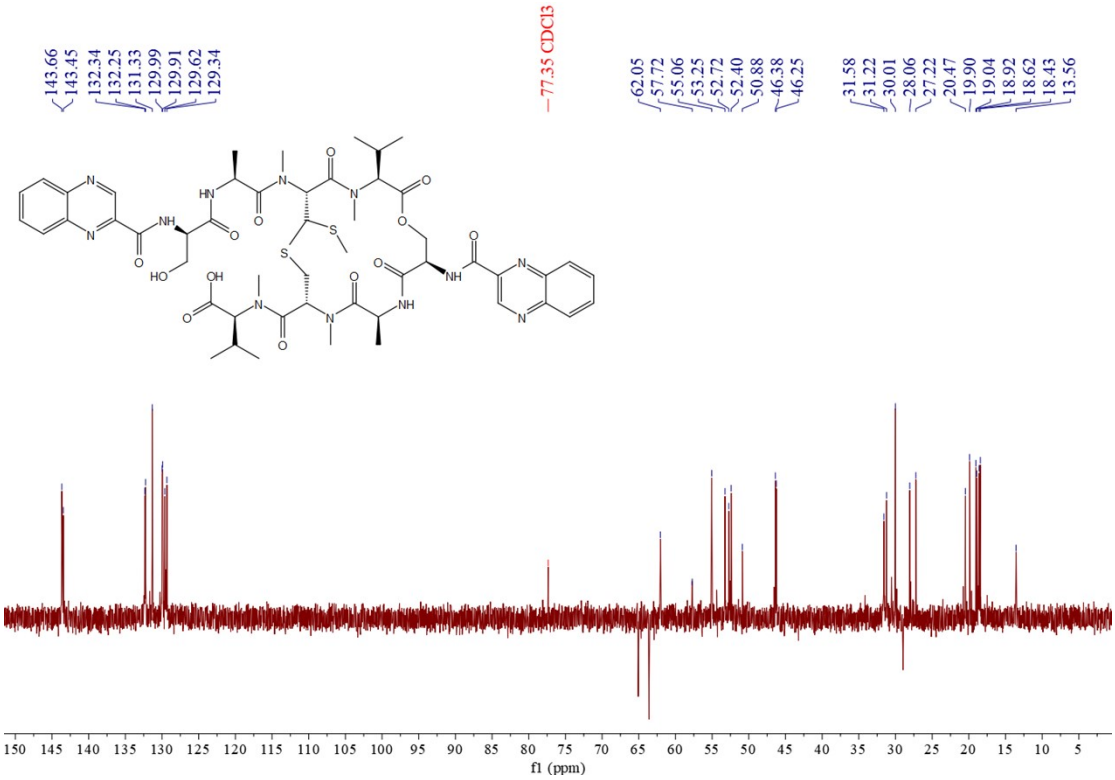


Figure S35. DEPT-135 NMR spectrum of (3) in $CDCl_3$

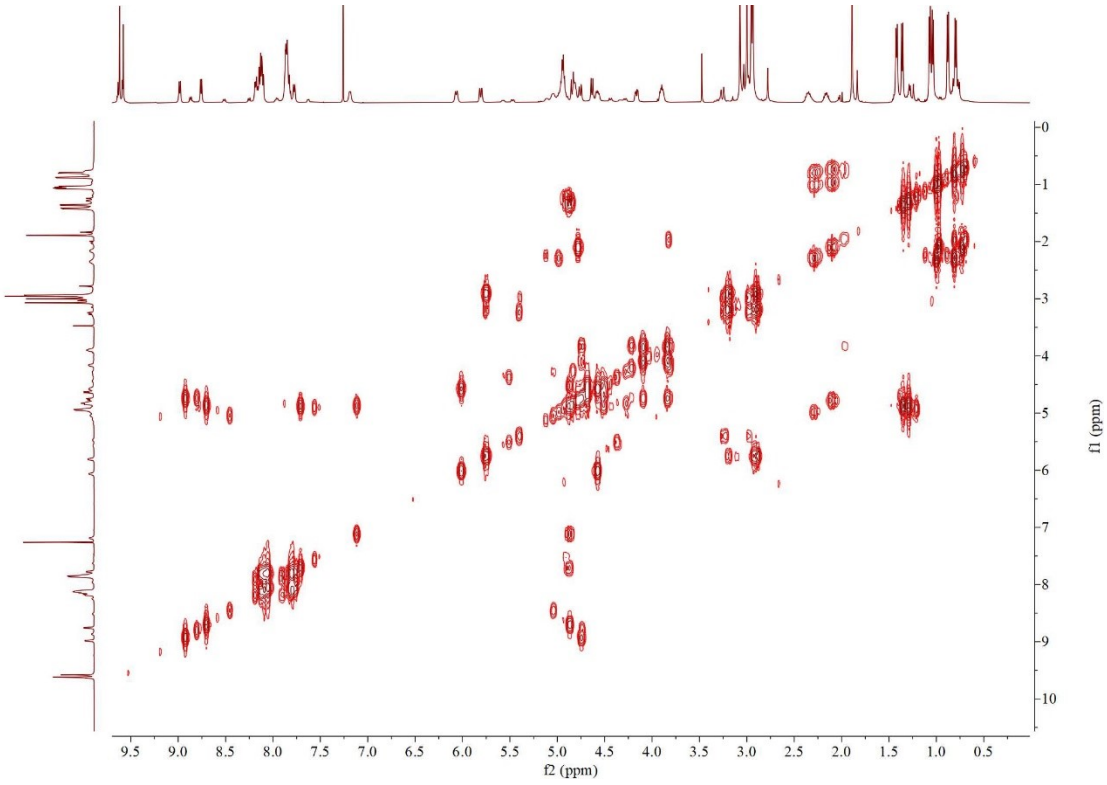


Figure S36. COSY NMR spectrum of (3) in $CDCl_3$

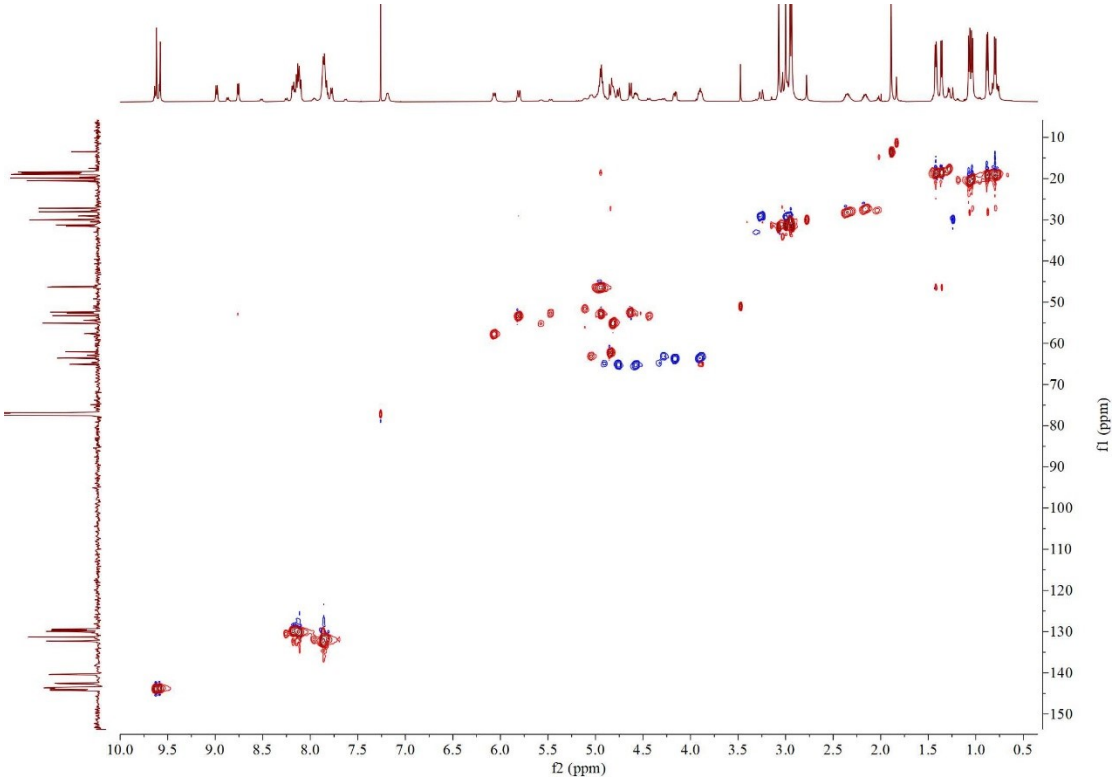


Figure S37. HSQC NMR spectrum of (3) in $CDCl_3$

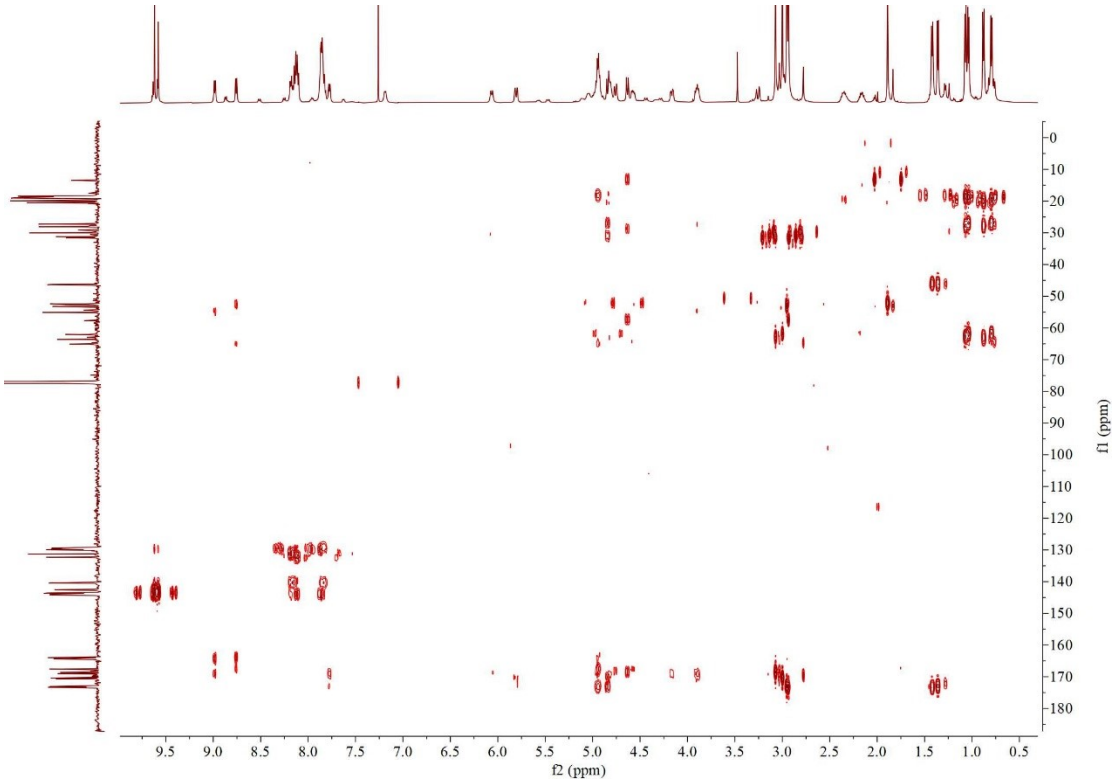


Figure S38. HMBC NMR spectrum of (3) in $CDCl_3$

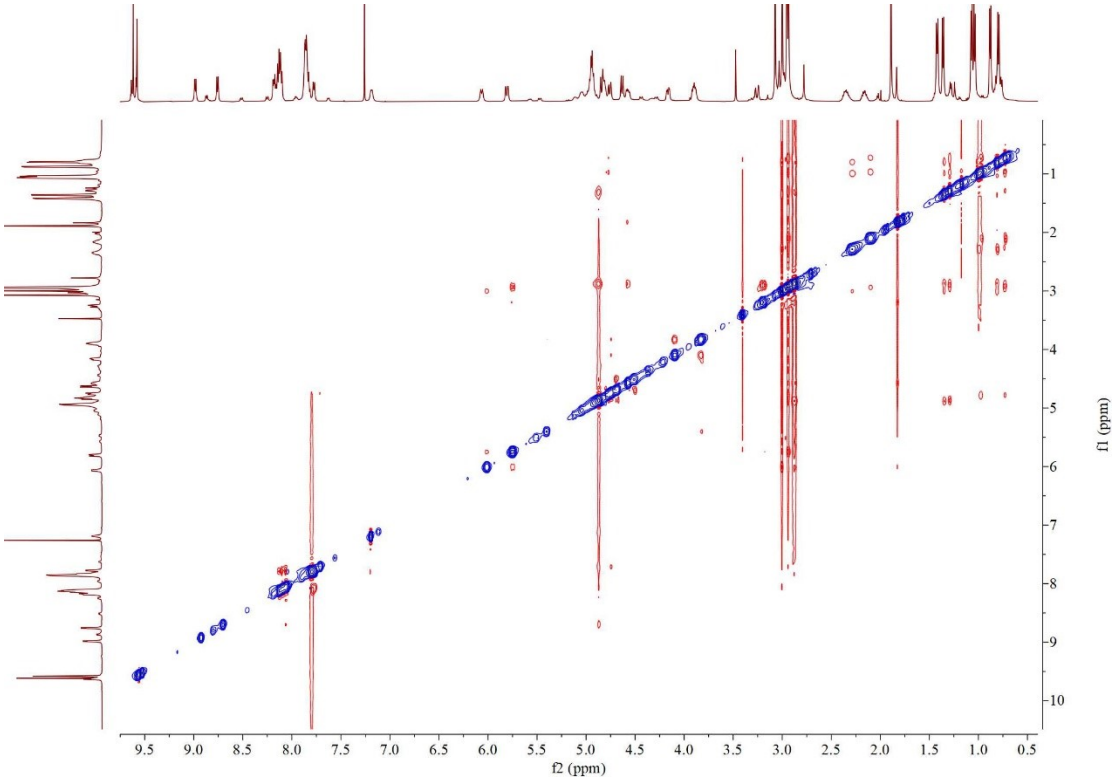


Figure S39. ROESY NMR spectrum of (3) in $CDCl_3$

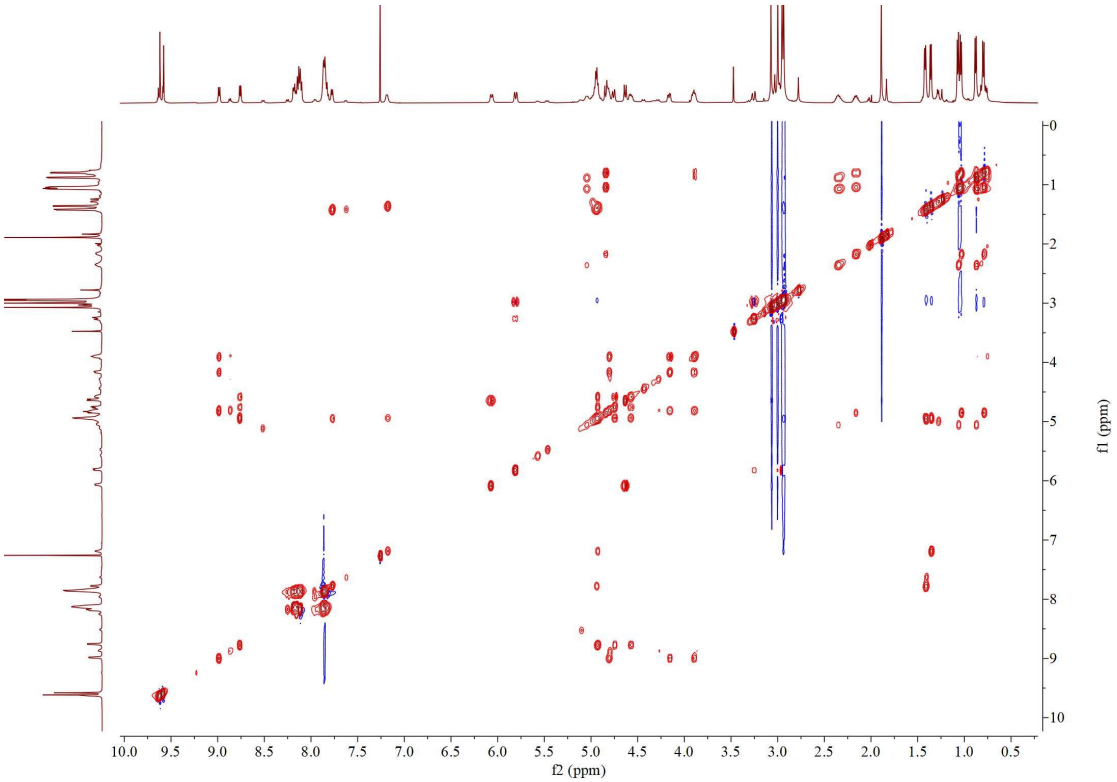


Figure S40. TOCSY NMR spectrum of (3) in $CDCl_3$

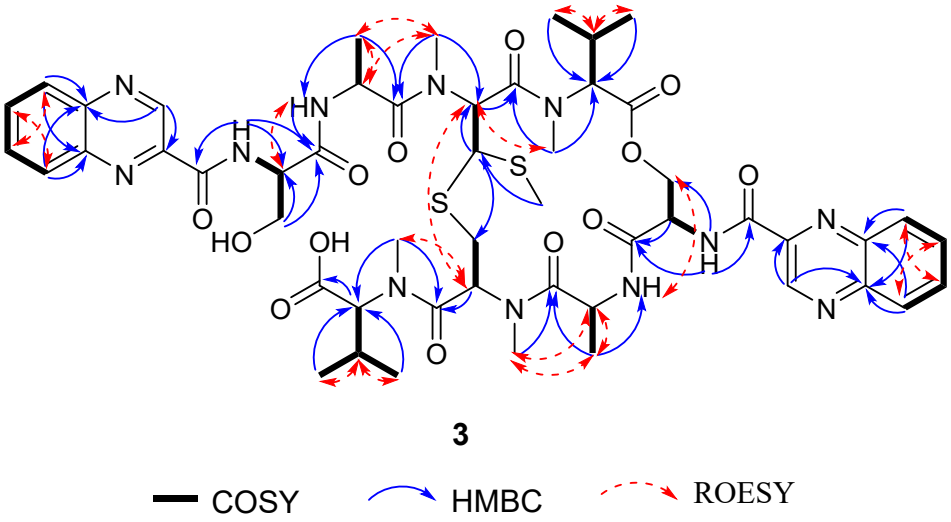


Figure S41. Key COSY, HMBC, ROESY correlations of compounds 3

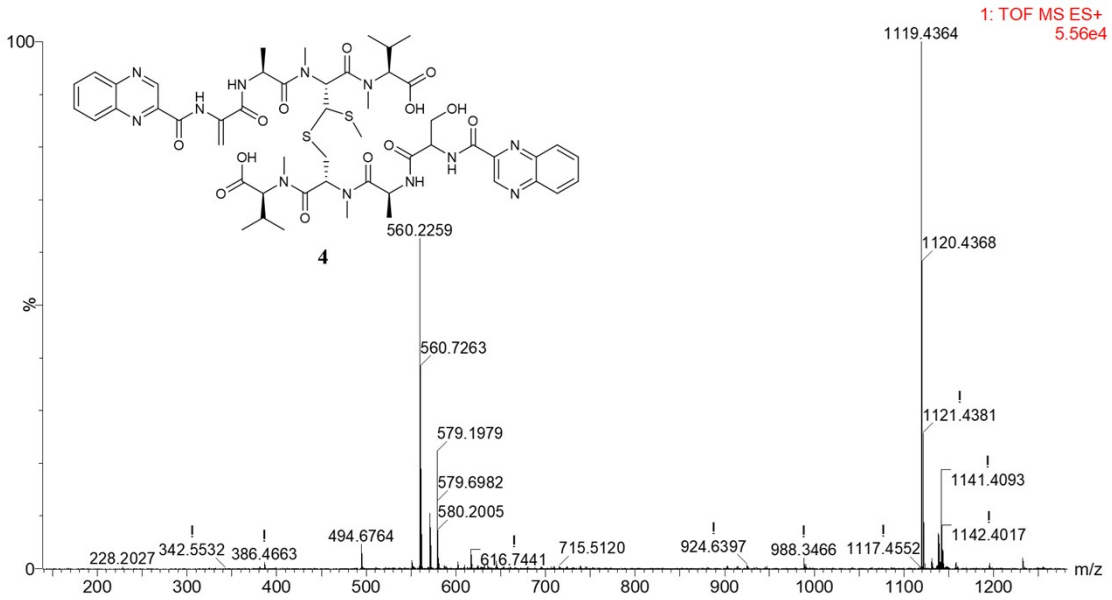


Figure S42. The (+)-HRESIMS spectrum of compound 4

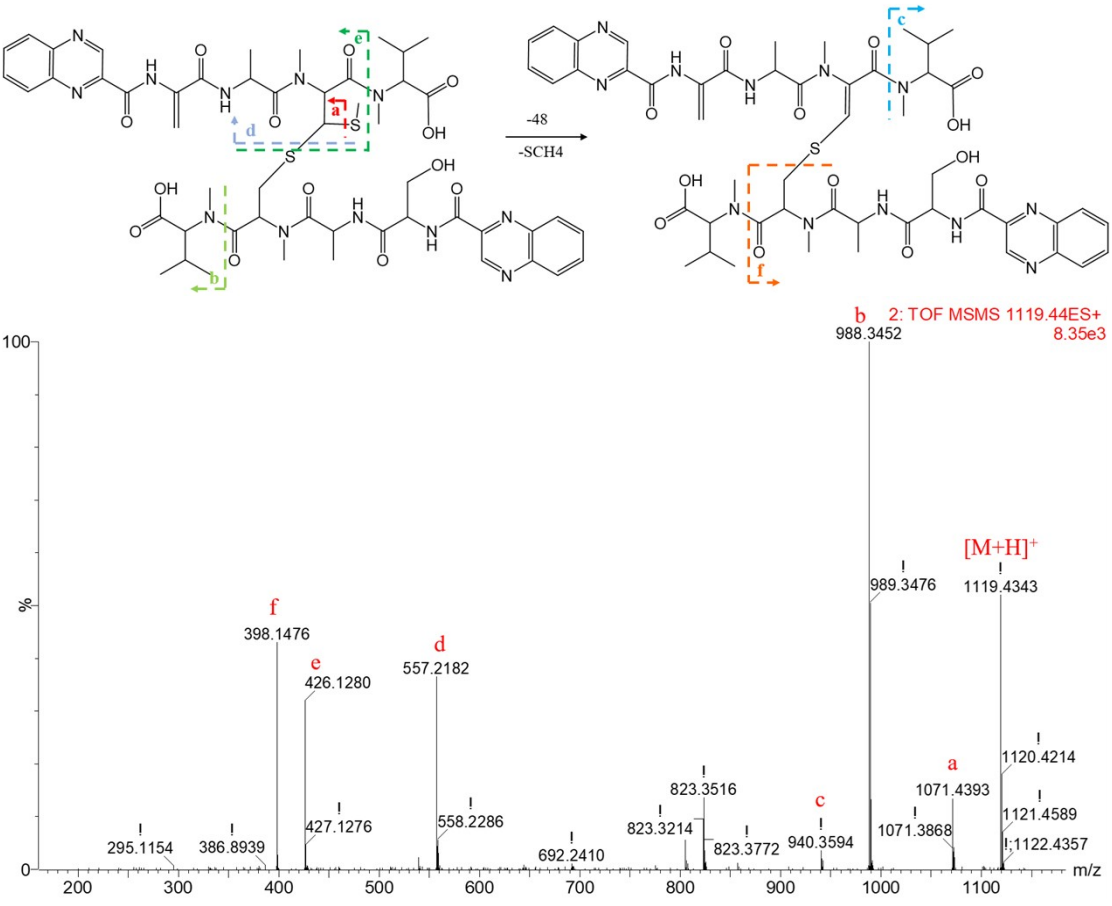


Figure S43. MS/MS fragmentation analysis of compound 4

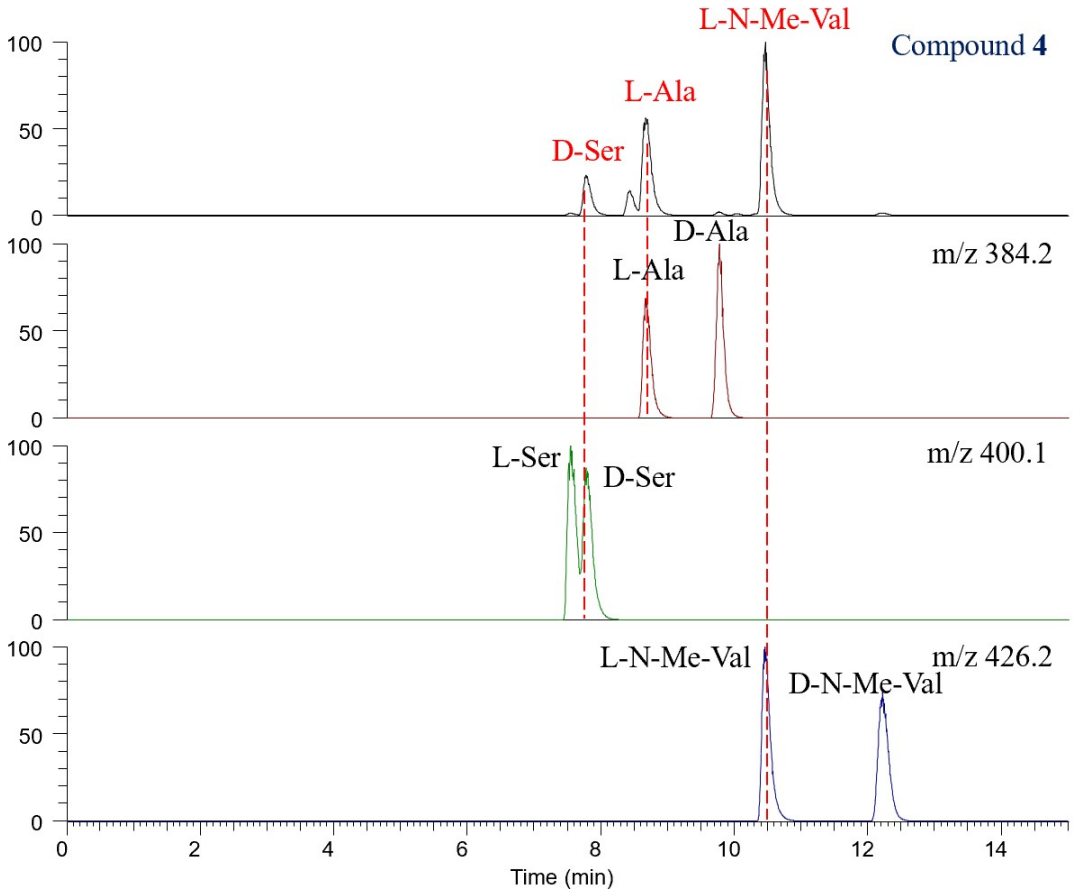


Figure S44. Marfey's analysis of compound 4

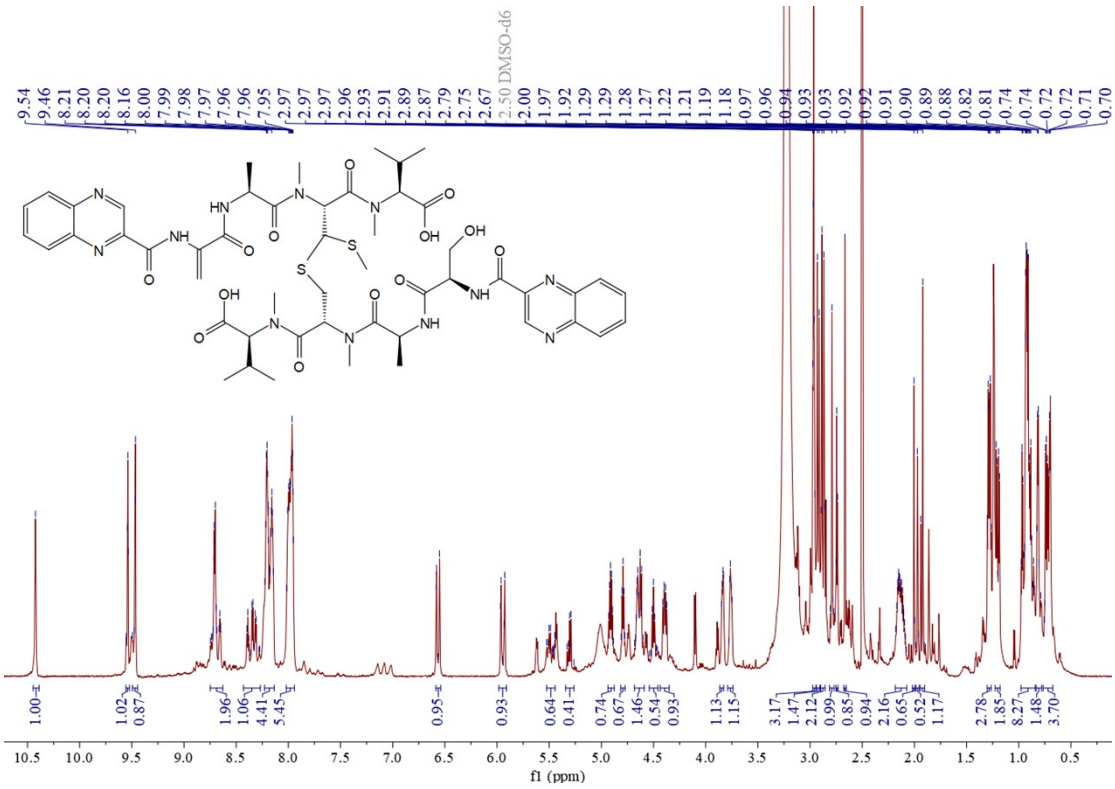


Figure S45. ^{1}H NMR spectrum of (4) at 800 MHz in DMSO-d_6

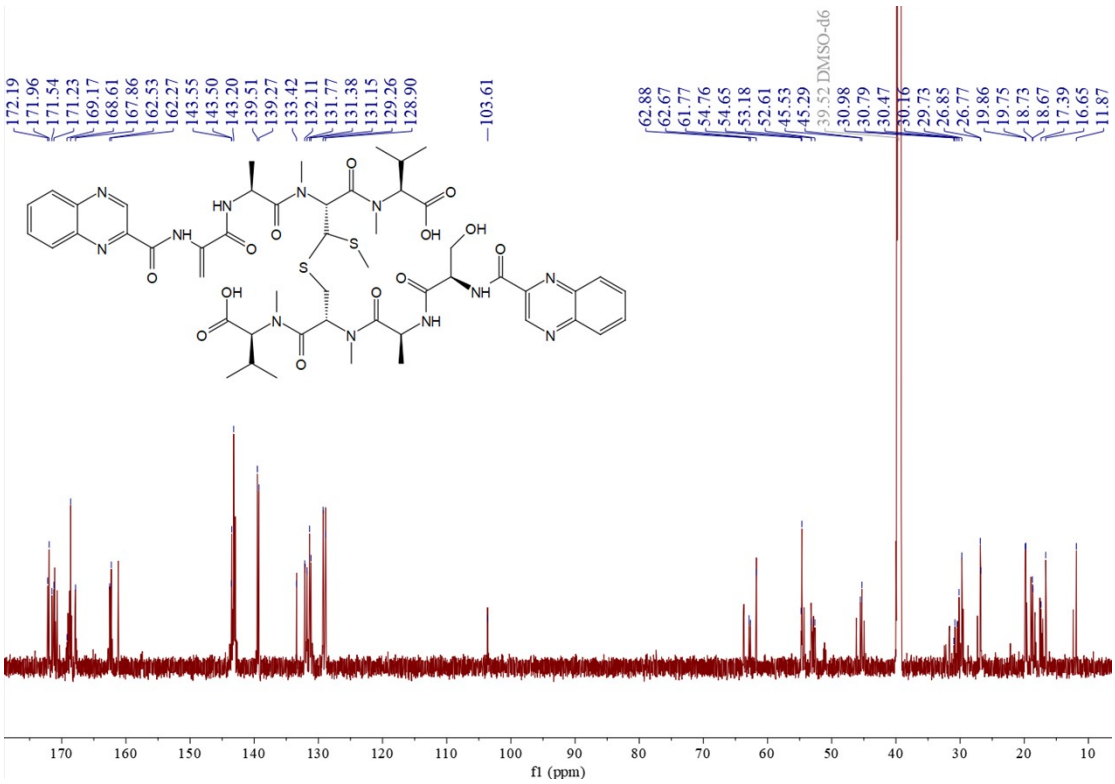


Figure S46. ^{13}C NMR spectrum of (4) at 201 MHz in DMSO-d_6

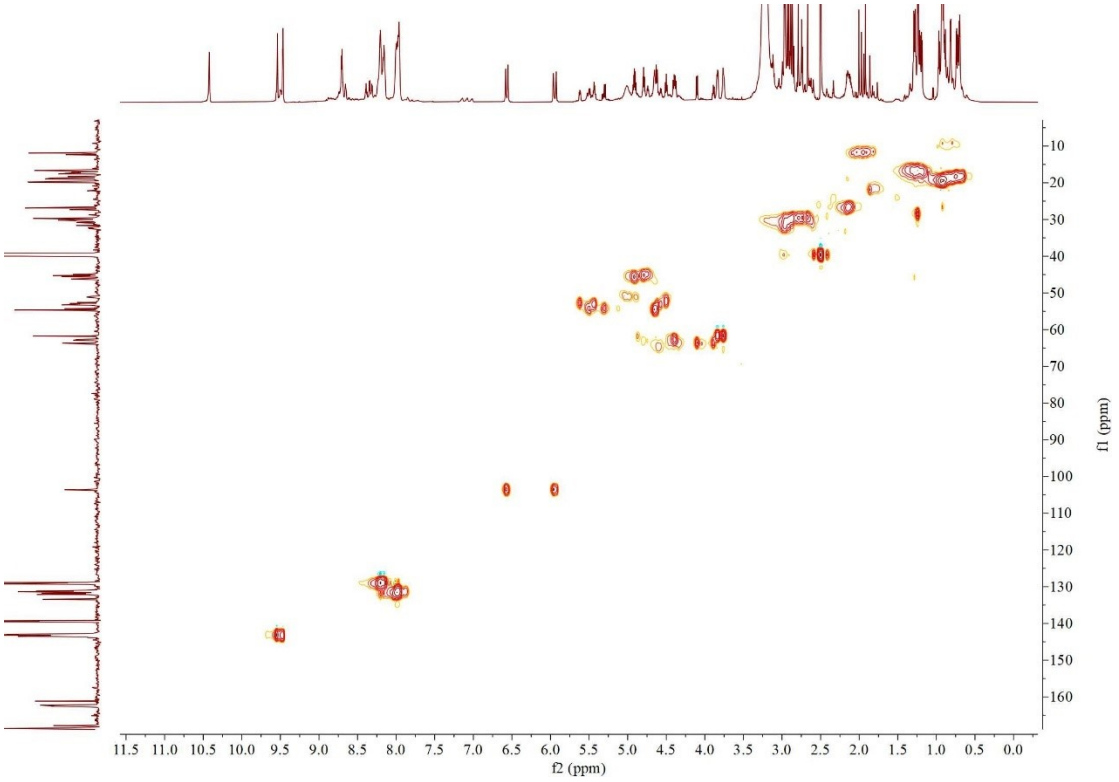


Figure S47. HSQC NMR spectrum of (4) in DMSO-d_6

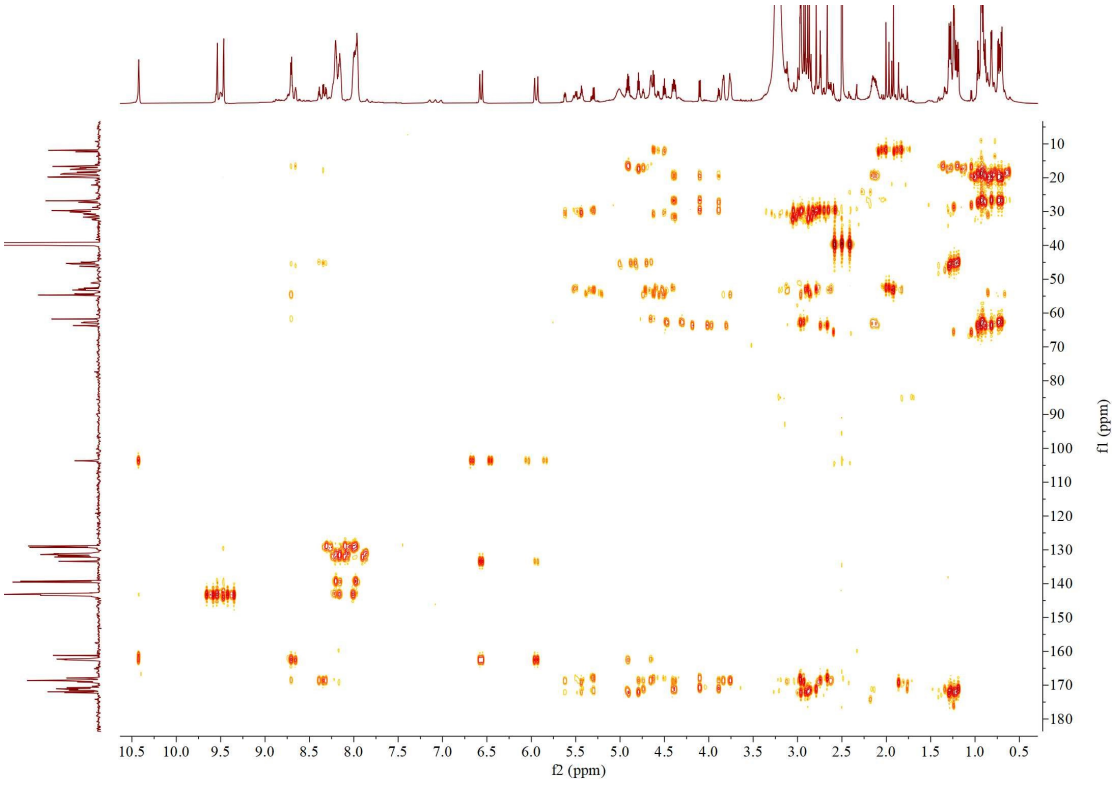


Figure S48. HMBC NMR spectrum of (4) in DMSO-d_6

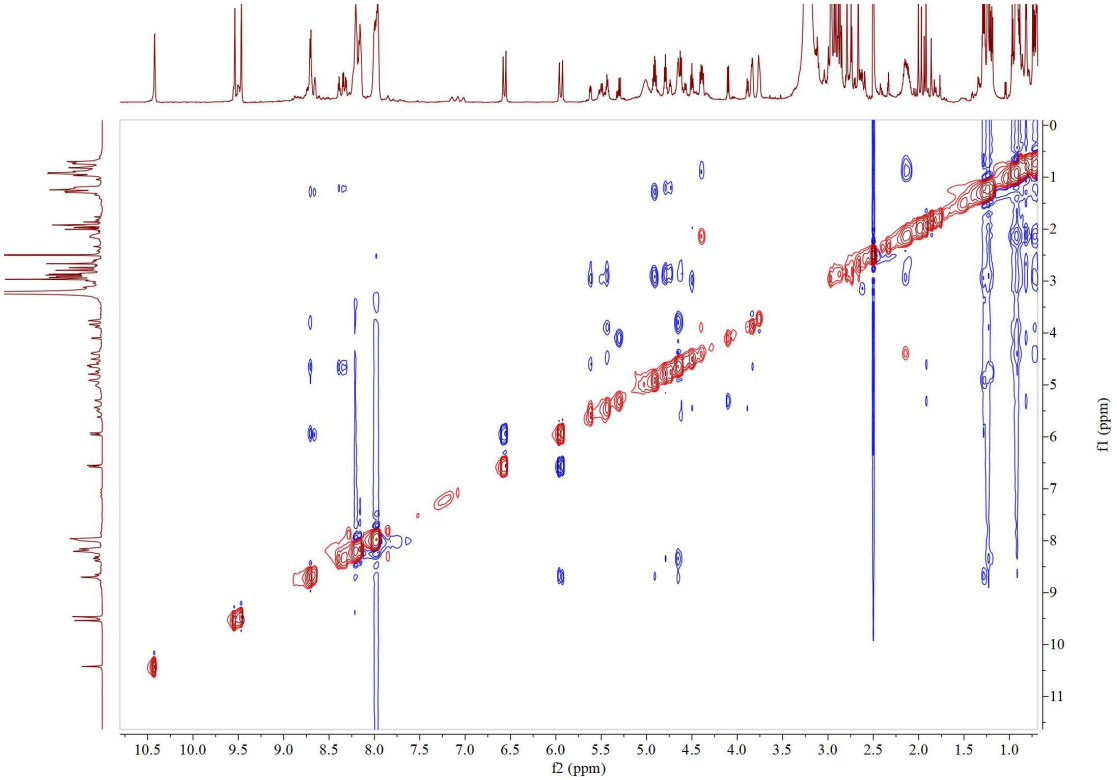


Figure S49. ROESY NMR spectrum of (4) in DMSO-d_6

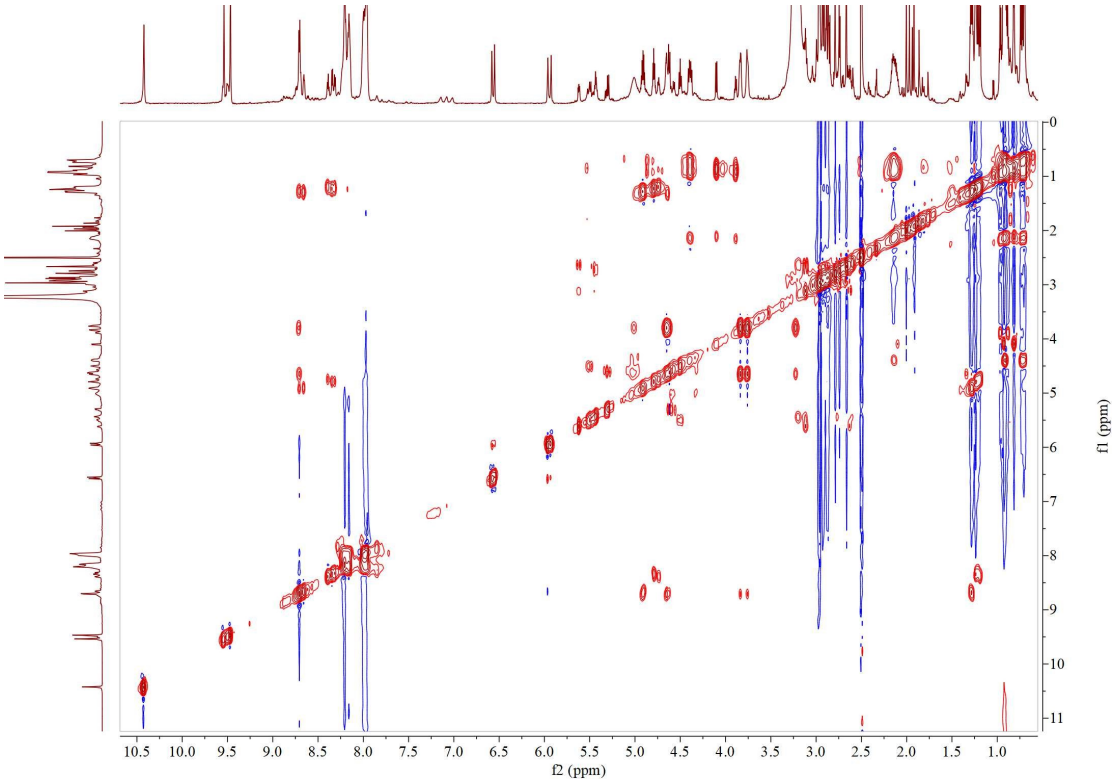


Figure S50. TOCSY NMR spectrum of (4) in DMSO-d_6

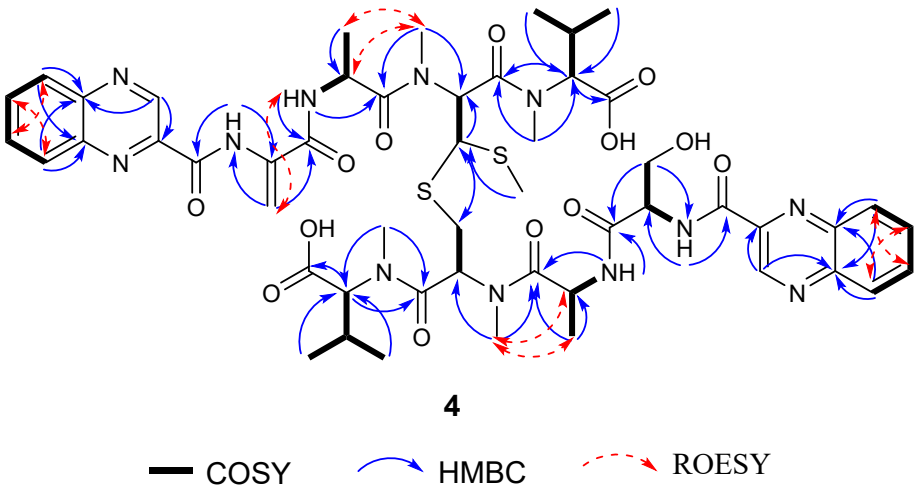


Figure S51. Key COSY, HMBC, ROESY correlations of compounds 4

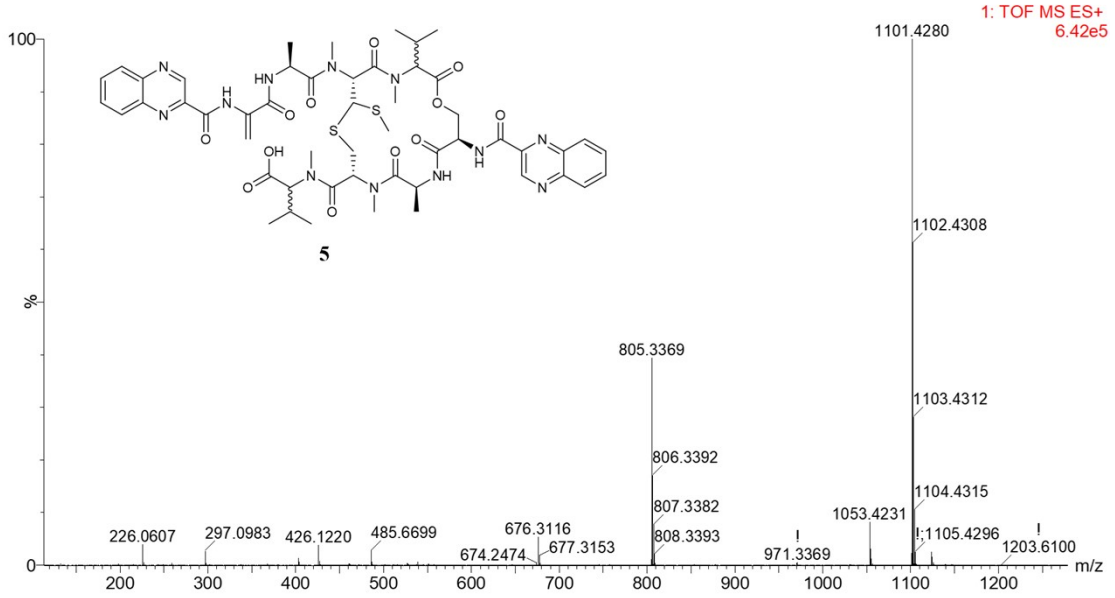


Figure S52. The (+)-HRESIMS spectrum of compound 5

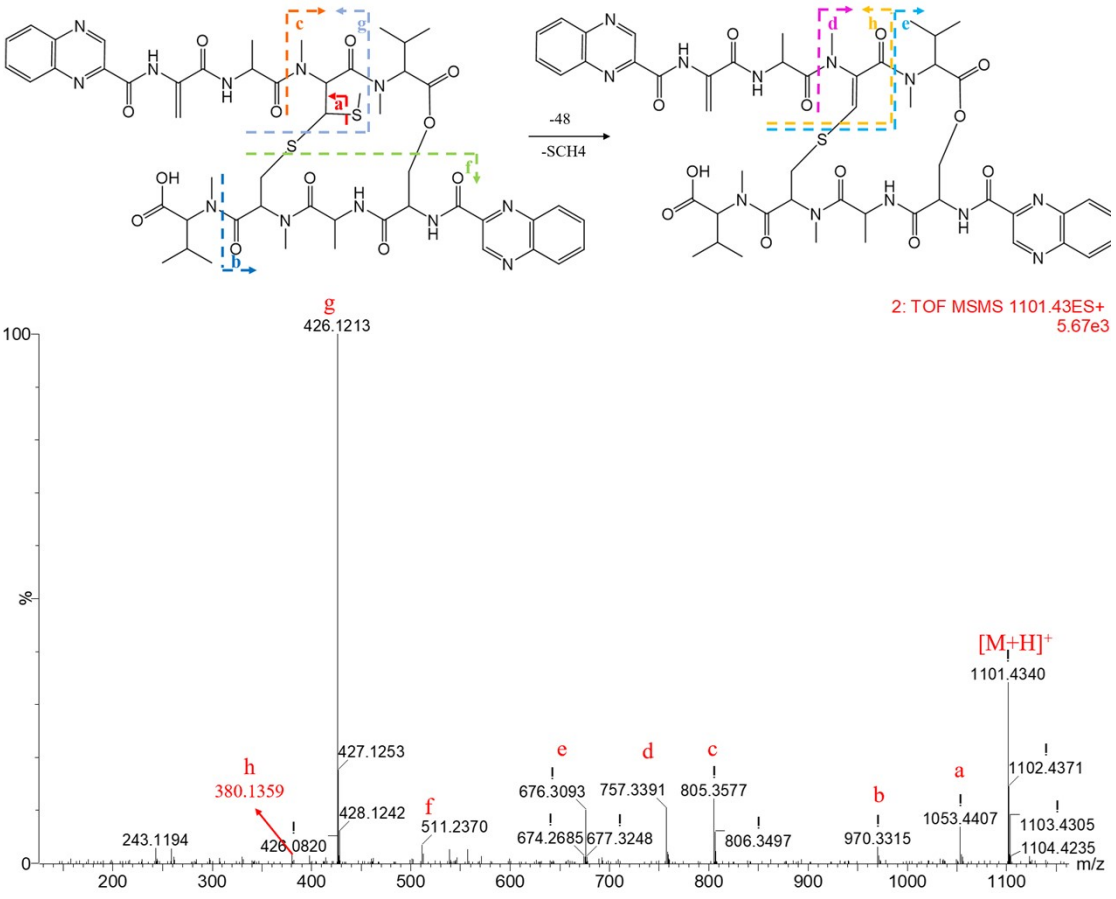


Figure S53. MS/MS fragmentation analysis of compound 5

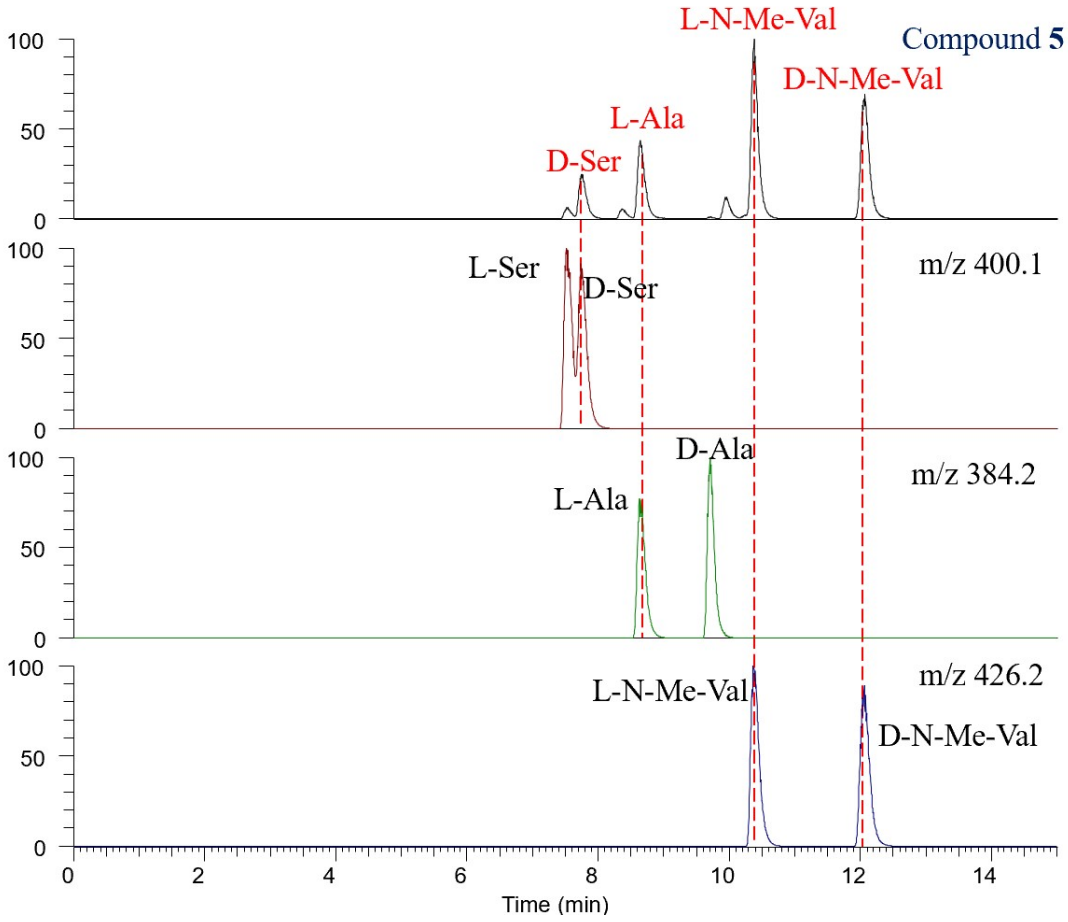


Figure S54. Marfey's analysis of compound 5

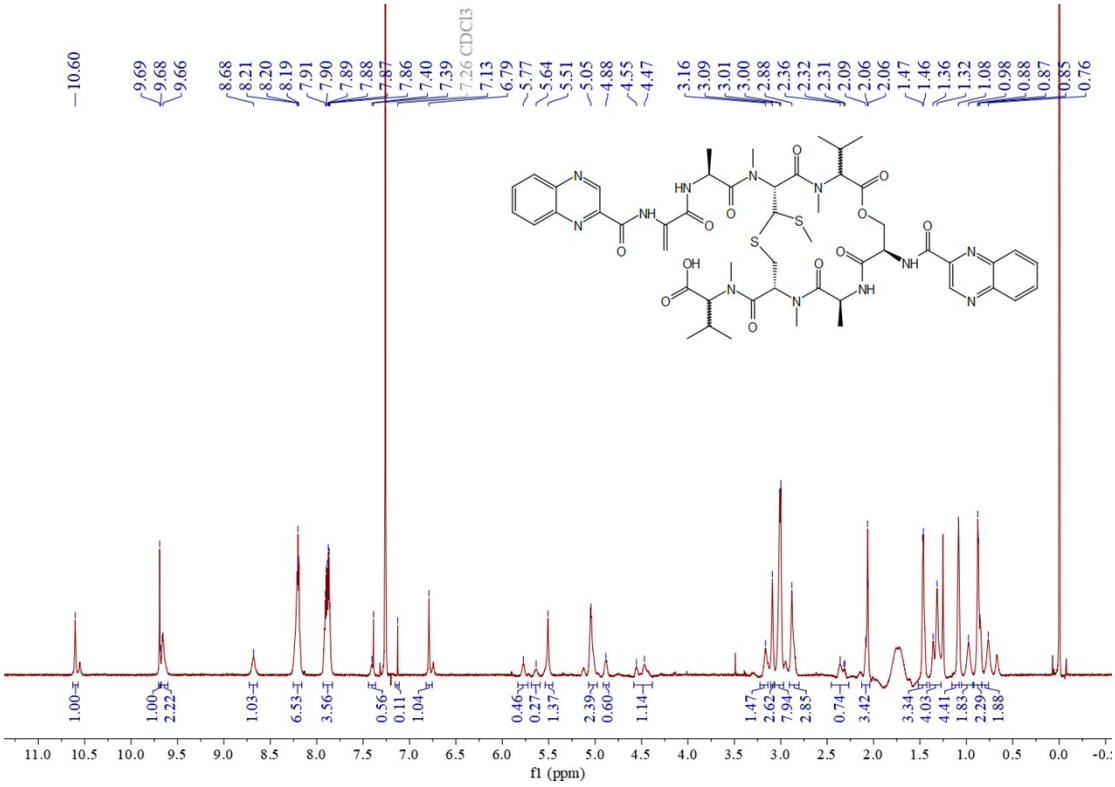


Figure S55. ^{1}H NMR spectrum of (5) at 800 MHz in $CDCl_3$

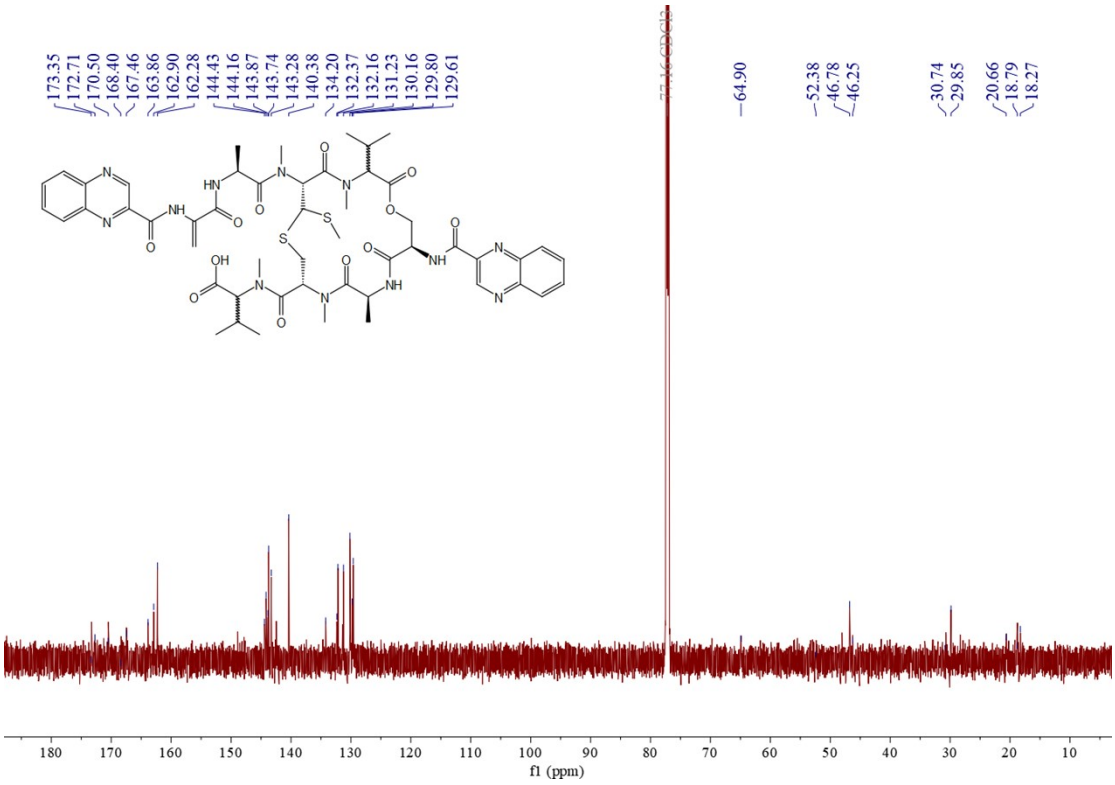


Figure S56. ^{13}C NMR spectrum of (5) at 201 MHz in $CDCl_3$

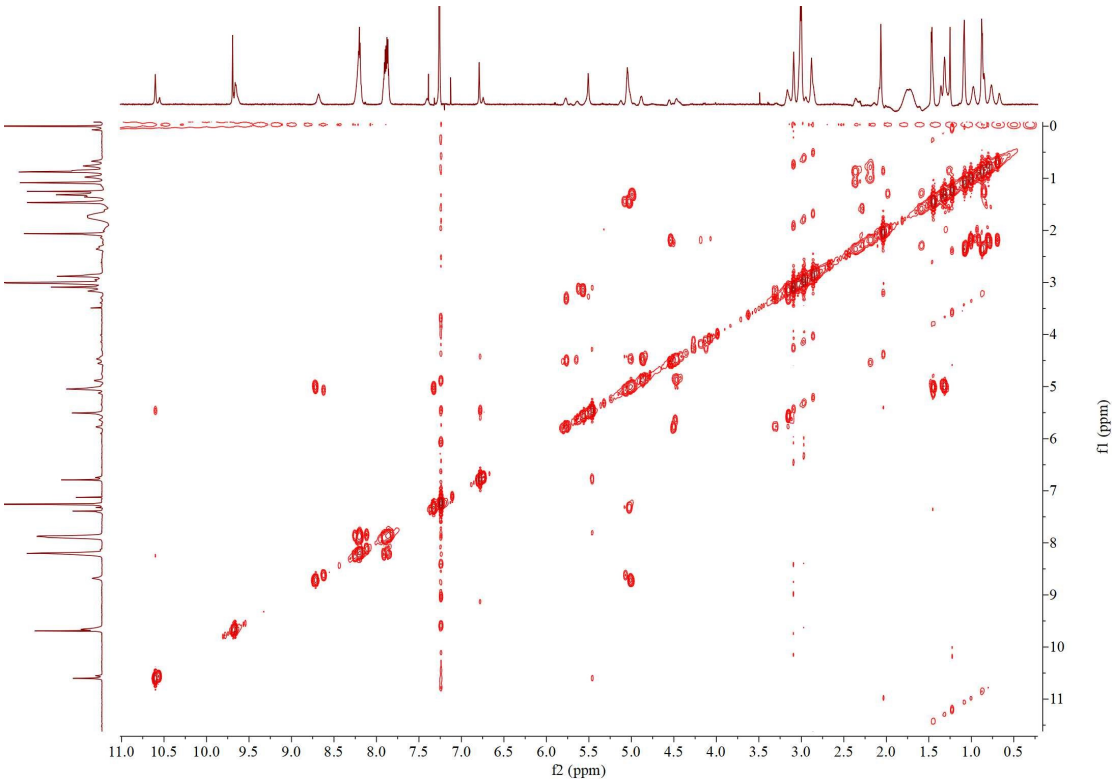


Figure S57. COSY NMR spectrum of (5) in $CDCl_3$

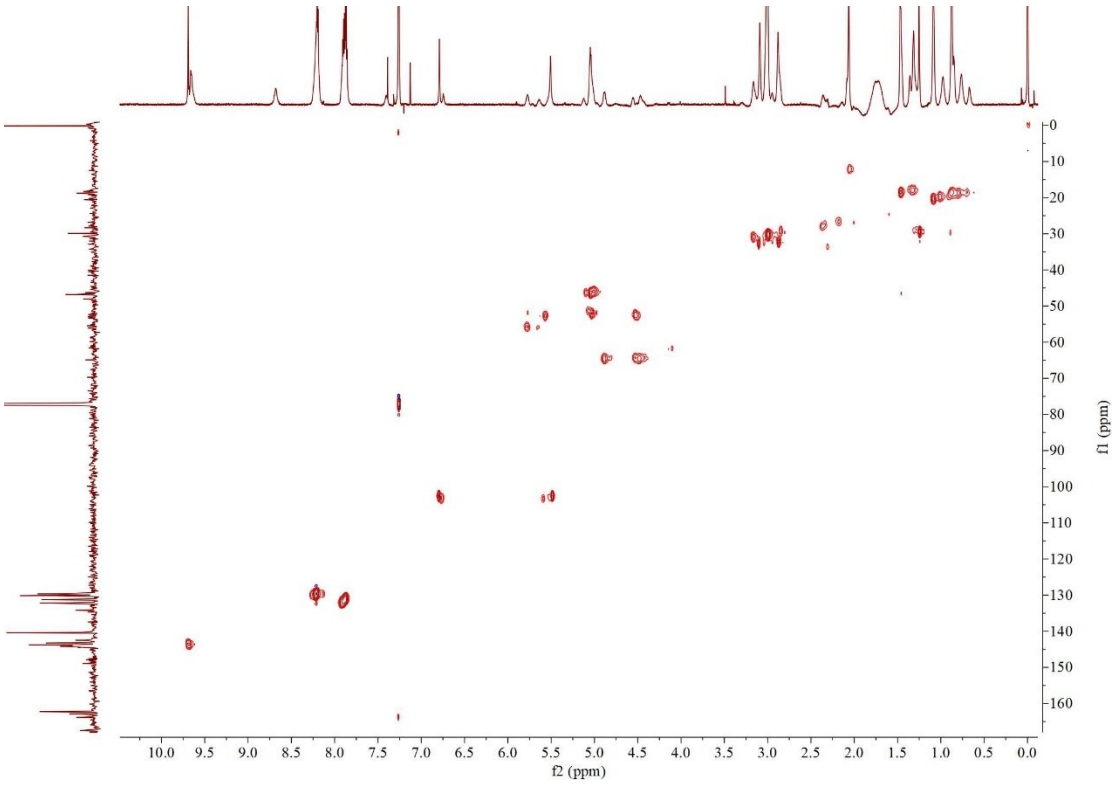


Figure S58. HSQC NMR spectrum of (5) in $CDCl_3$

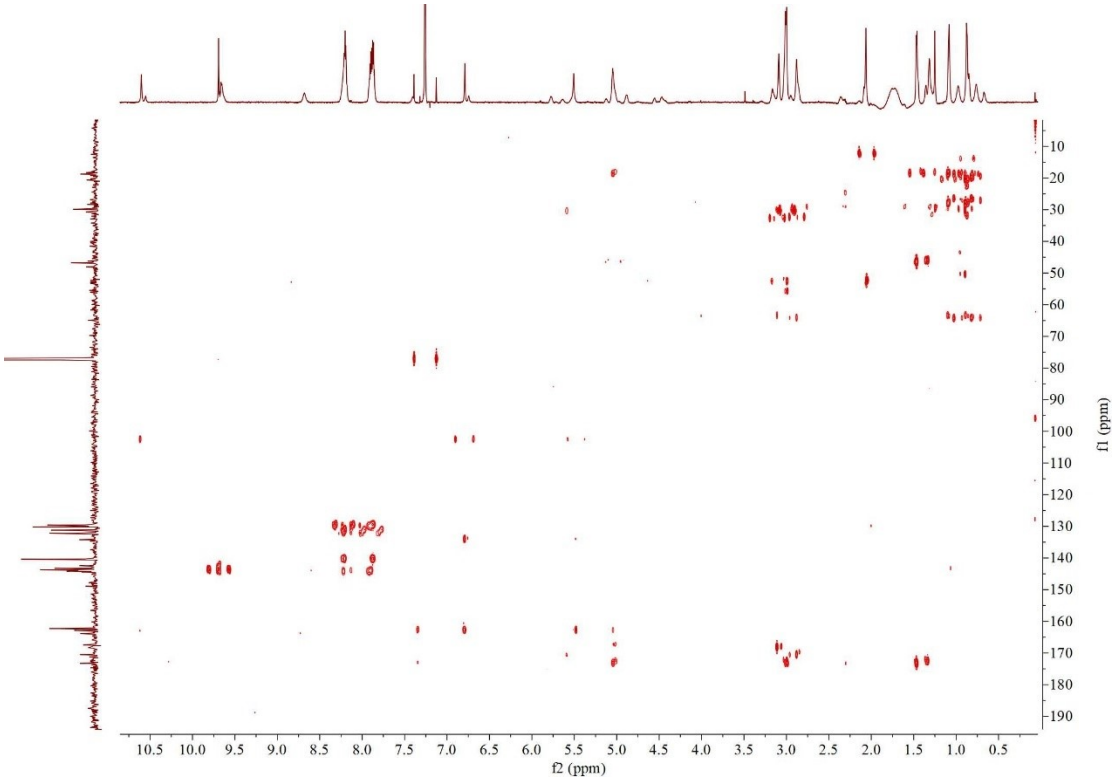


Figure S59. HMBC NMR spectrum of (5) in $CDCl_3$

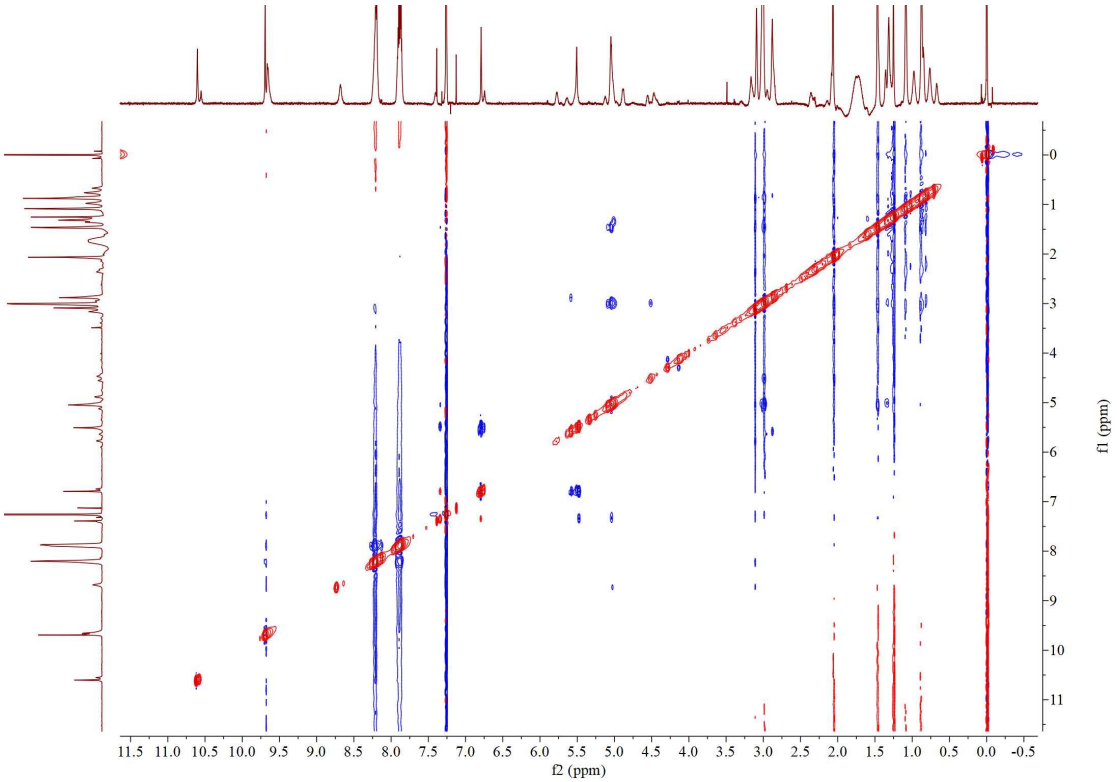


Figure S60. ROESY NMR spectrum of (5) in $CDCl_3$

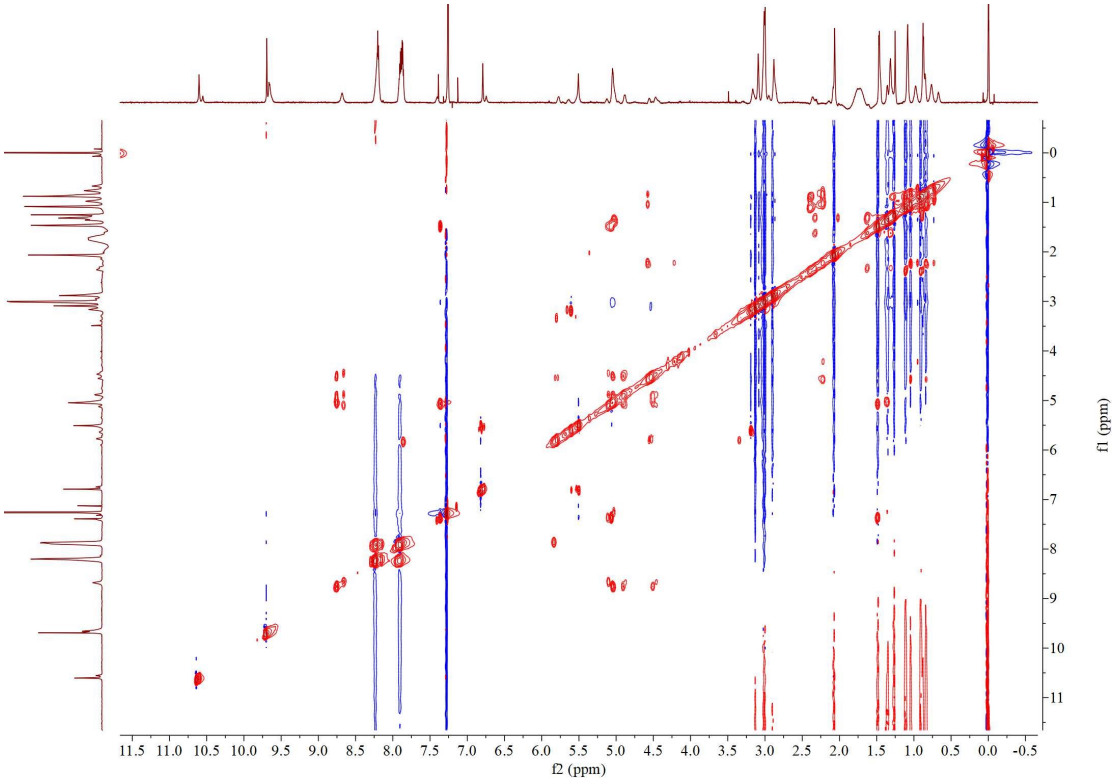


Figure S61. TOCSY NMR spectrum of (5) in $CDCl_3$

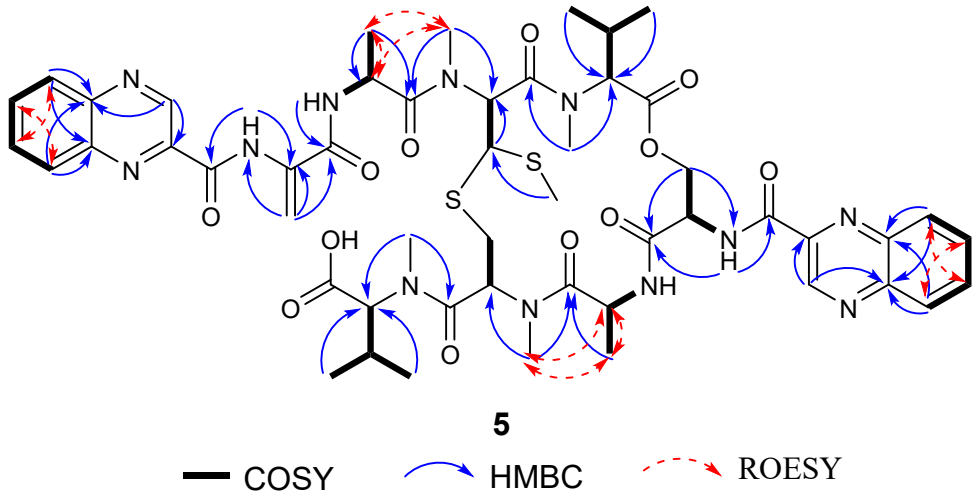


Figure S62. Key COSY, HMBC, ROESY correlations of compounds 5

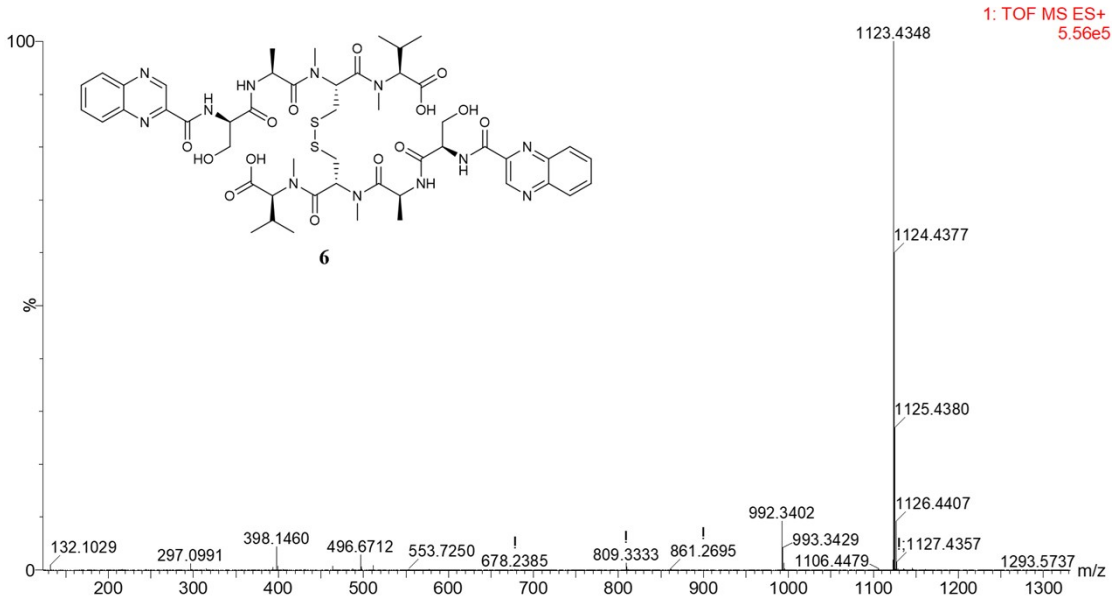


Figure S63. The (+)-HRESIMS spectrum of compound 6

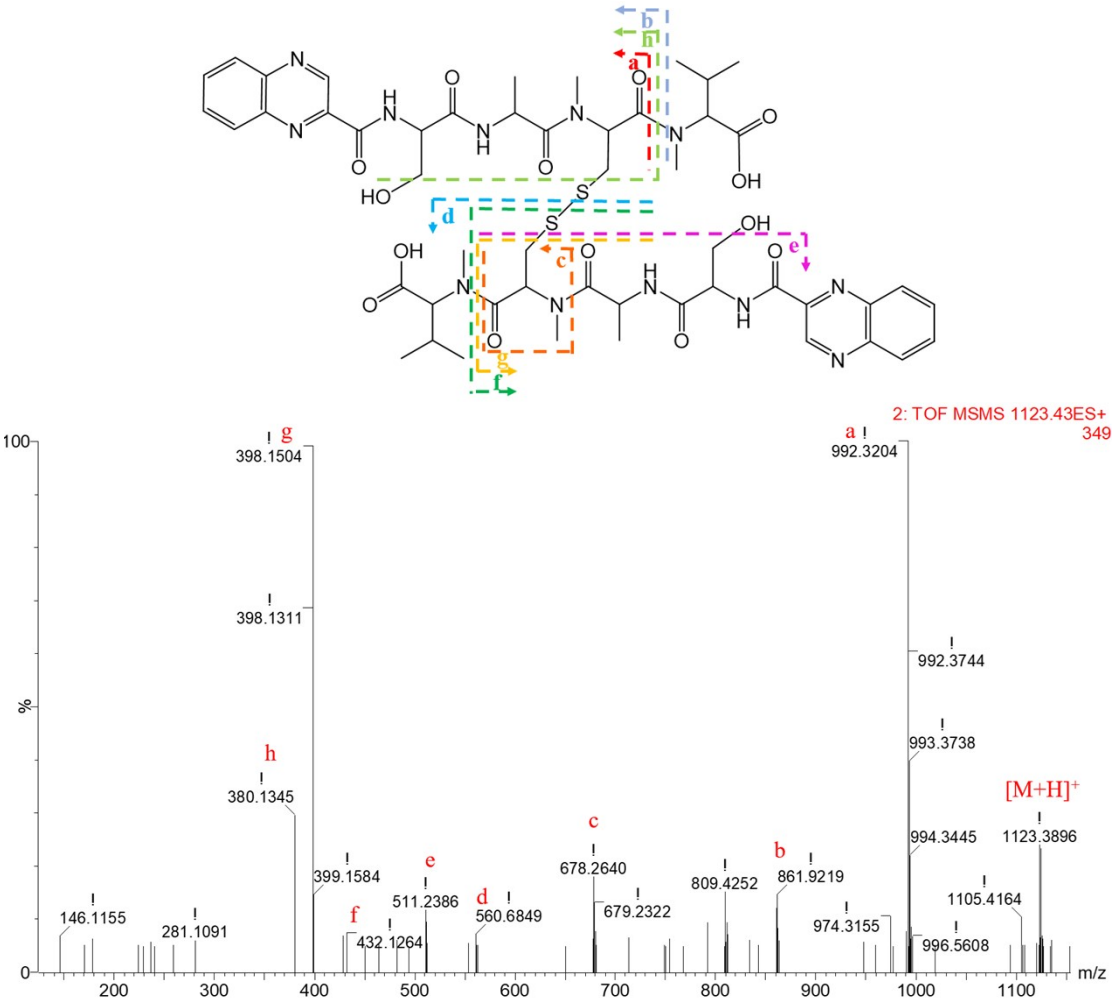


Figure S64. MS/MS fragmentation analysis of compound 6

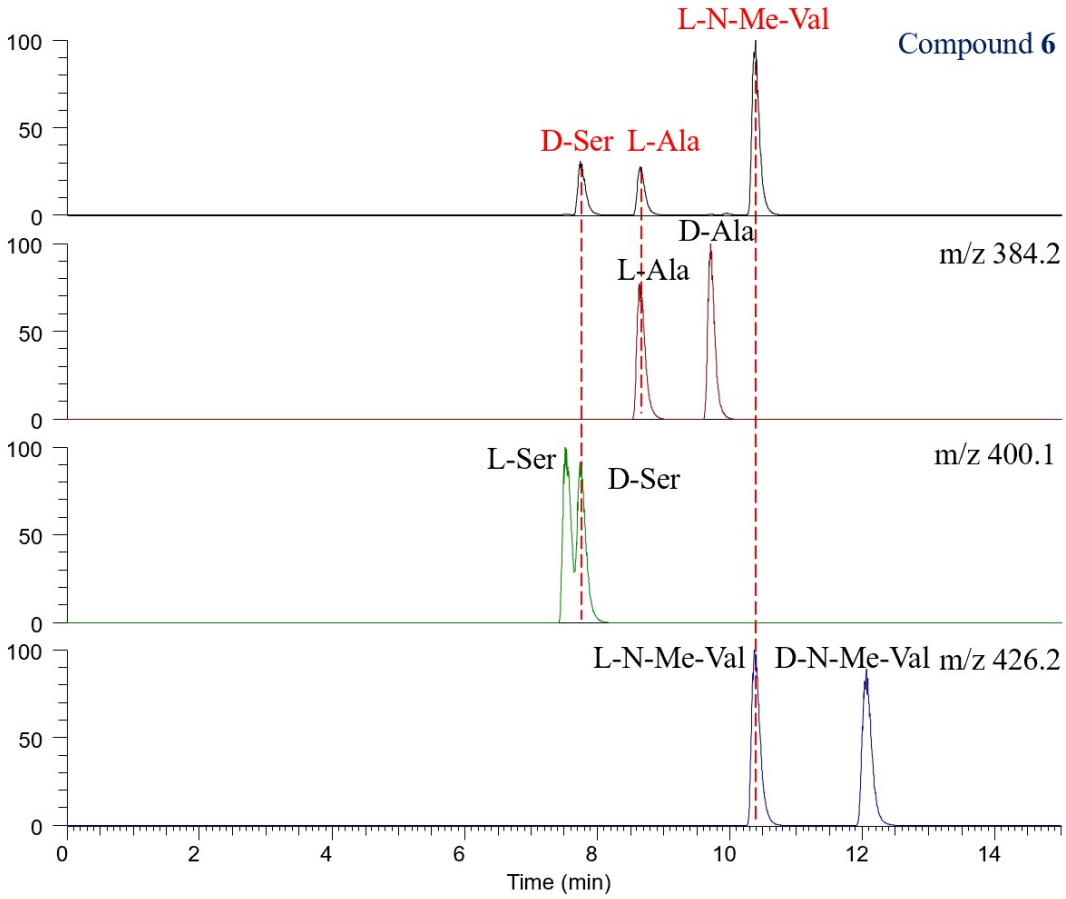


Figure S65. Marfey's analysis of compound 6

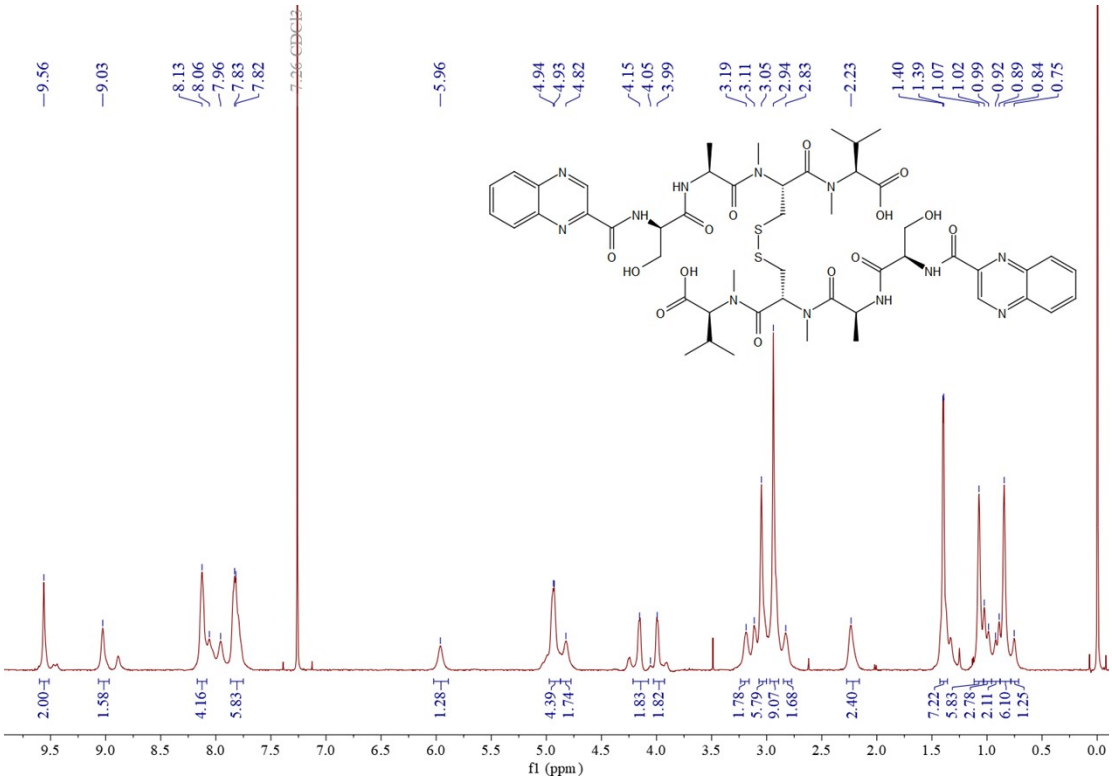


Figure S66. ^{1}H NMR spectrum of (6) at 800 MHz in $CDCl_3$

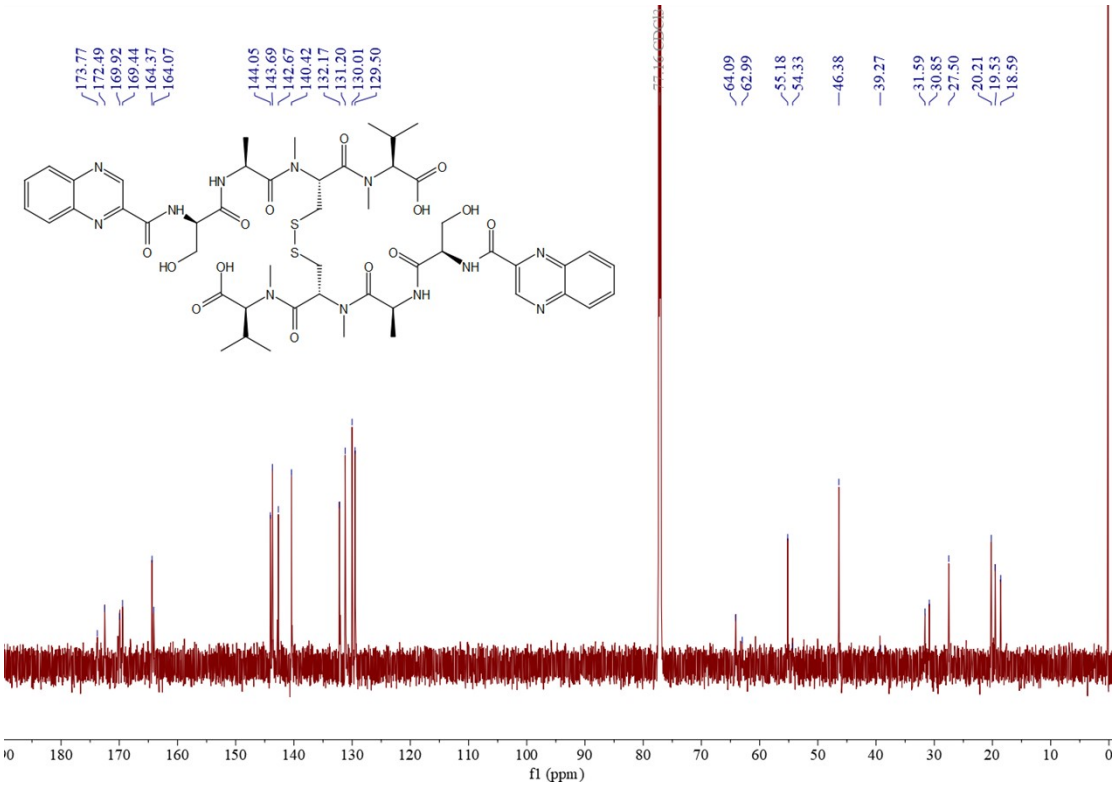


Figure S67. ^{13}C NMR spectrum of (6) at 201 MHz in $CDCl_3$

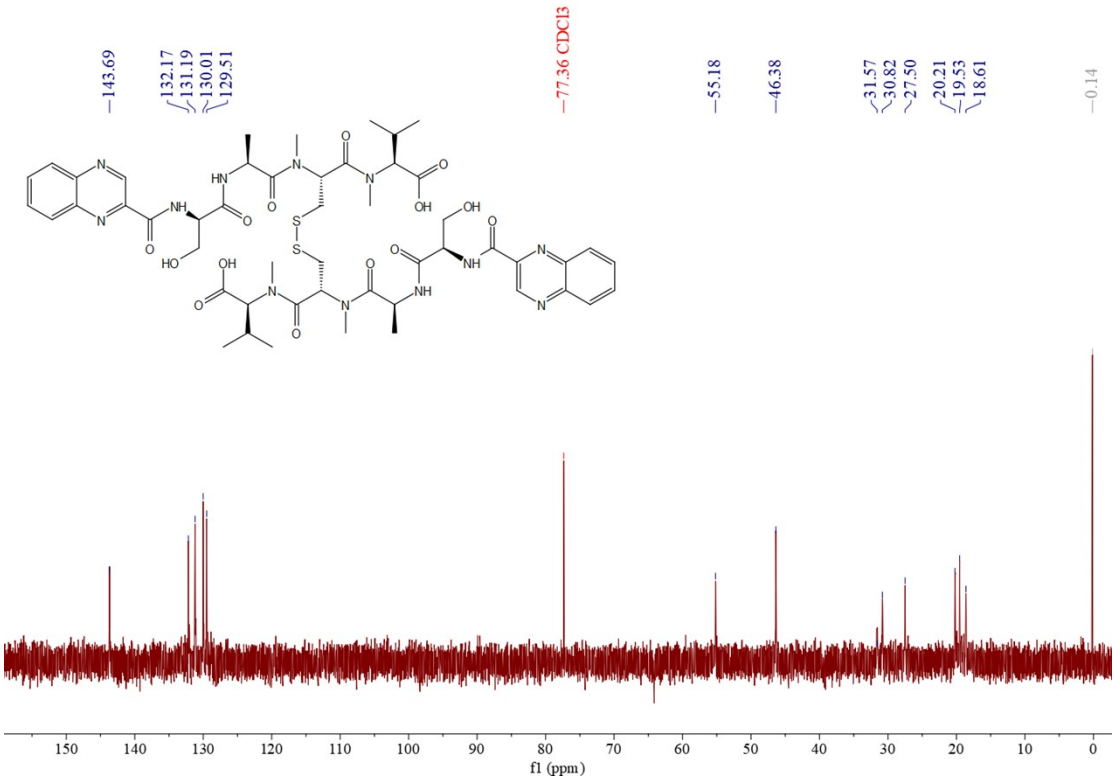


Figure S68. DEPT-135 spectrum of (6) at 201 MHz in $CDCl_3$

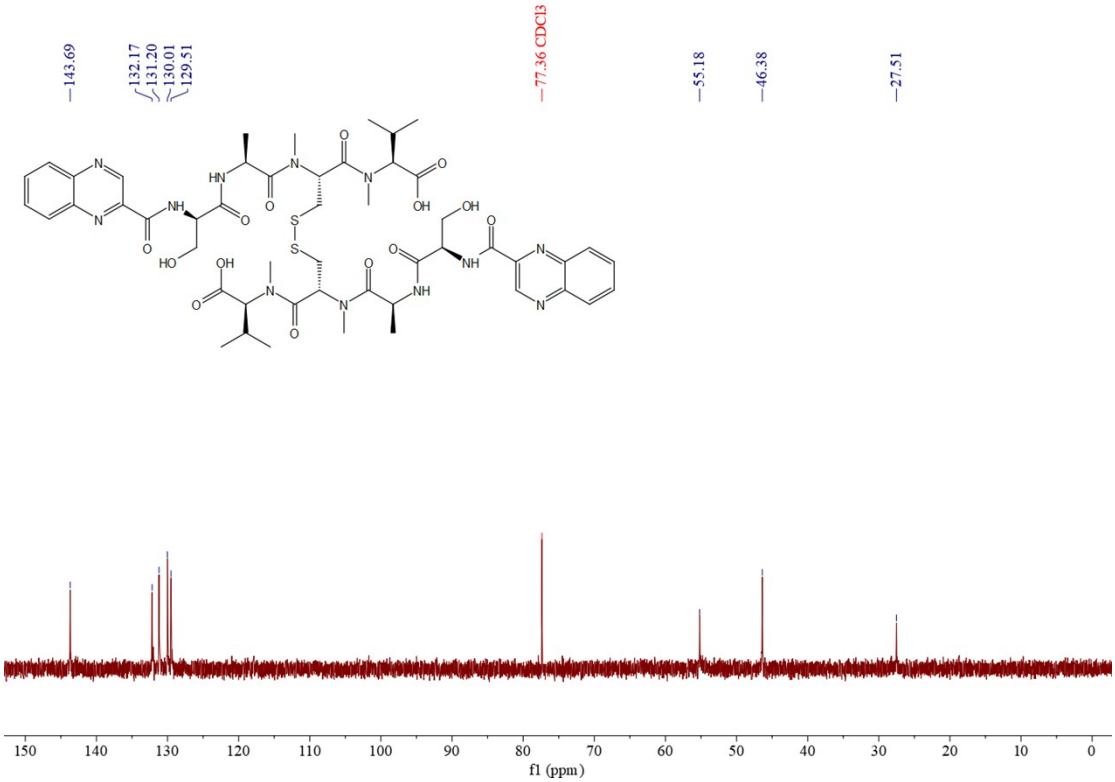


Figure S69. DEPT-90 spectrum of (6) at 201 MHz in $CDCl_3$

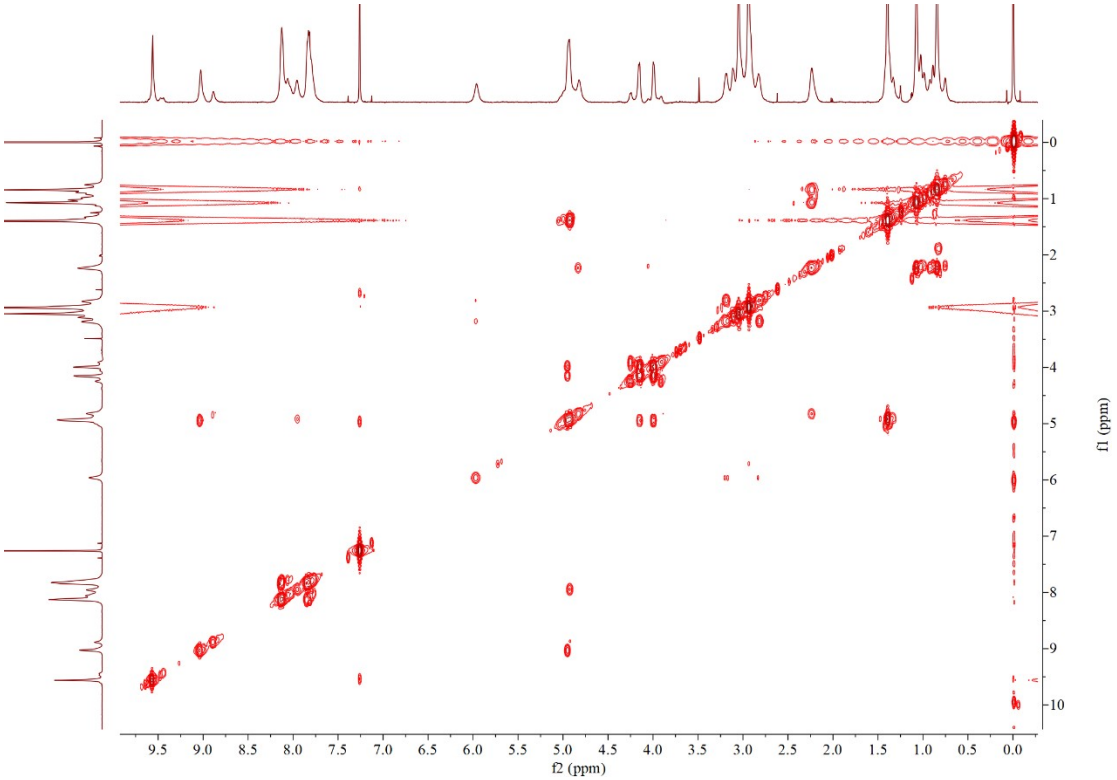


Figure S70. COSY NMR spectrum of (6) in $CDCl_3$

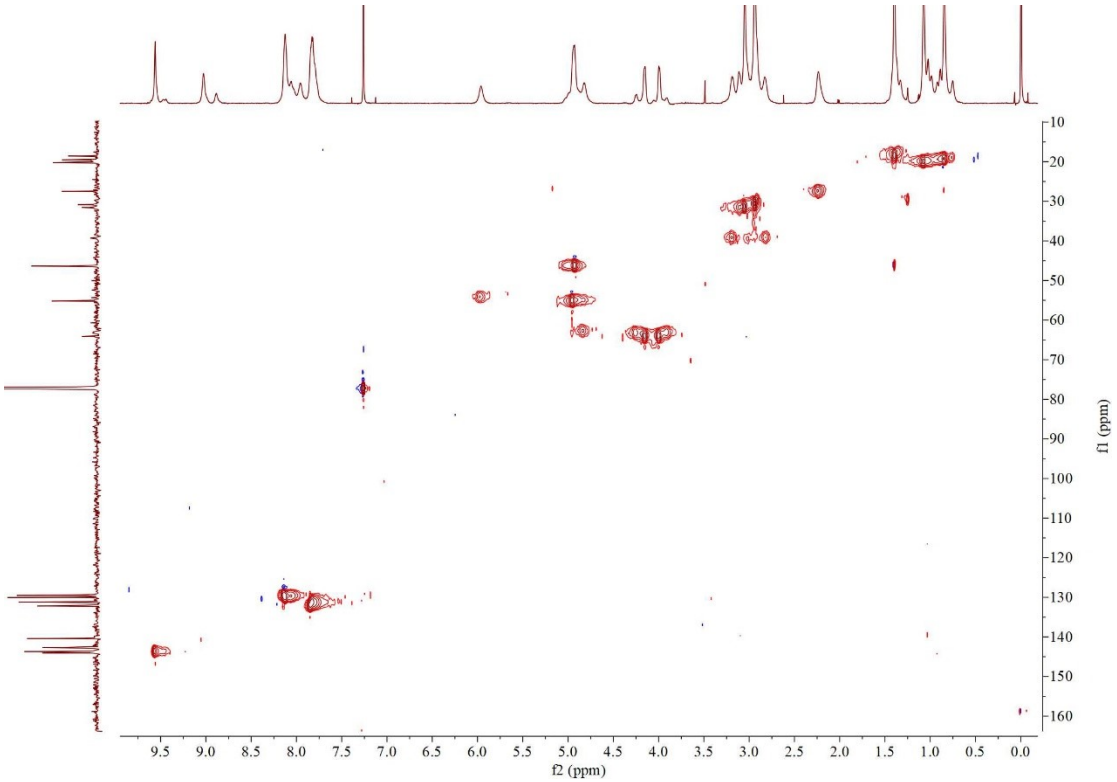


Figure S71. HSQC NMR spectrum of (6) in $CDCl_3$

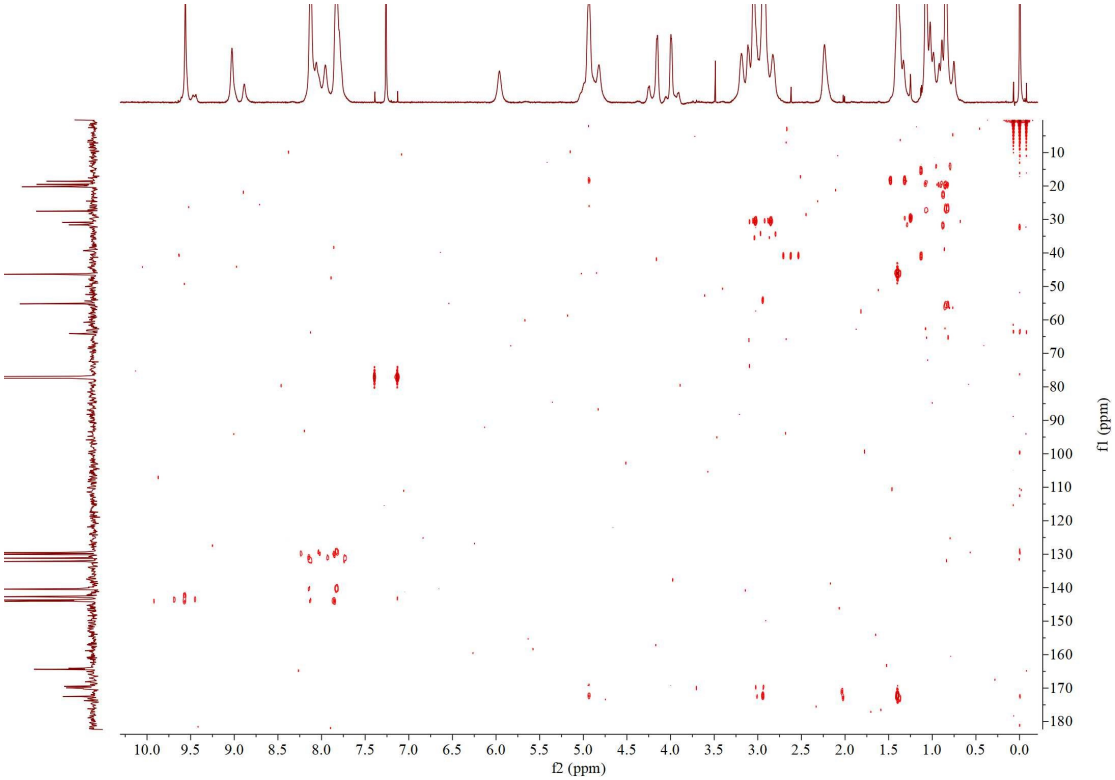


Figure S72. HMBC NMR spectrum of (6) in $CDCl_3$

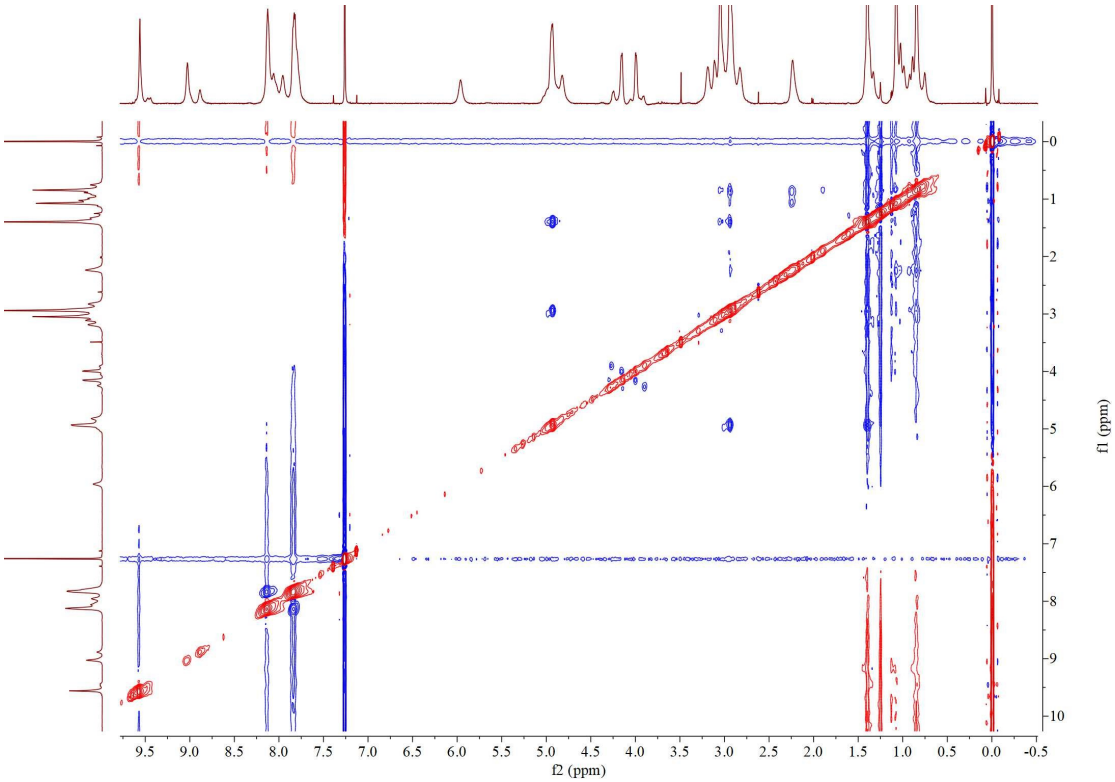


Figure S73. ROESY NMR spectrum of (6) in $CDCl_3$

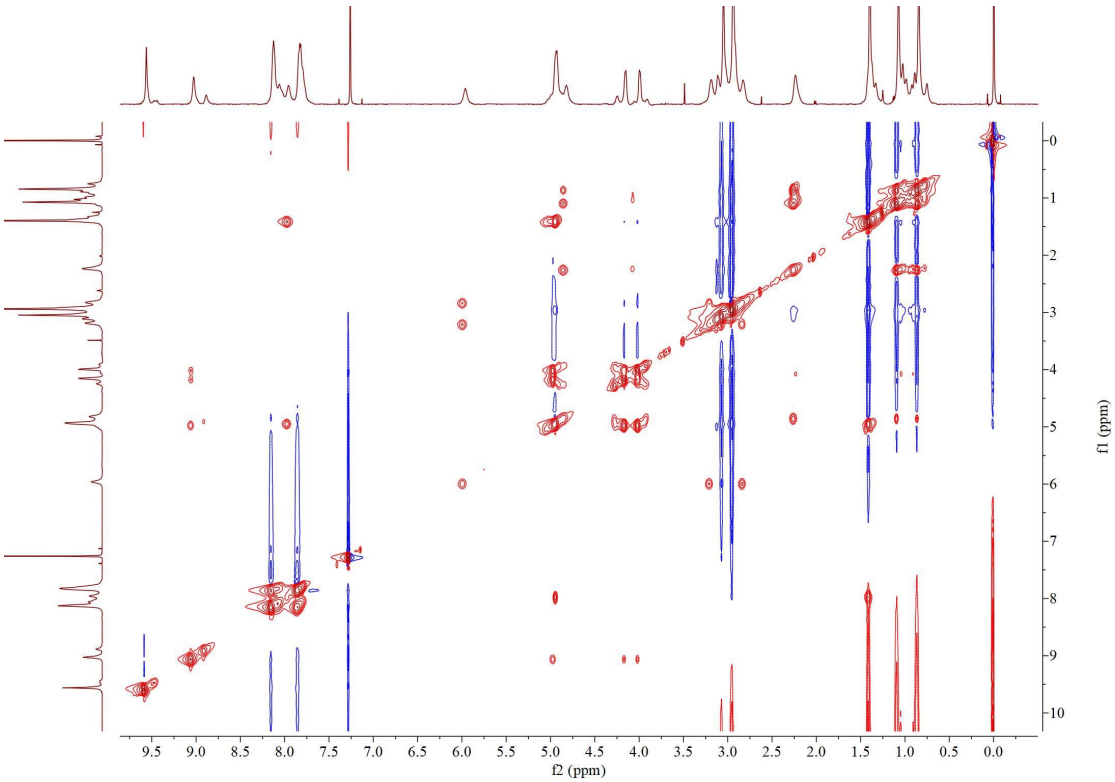


Figure S74. TOCSY NMR spectrum of (6) in $CDCl_3$

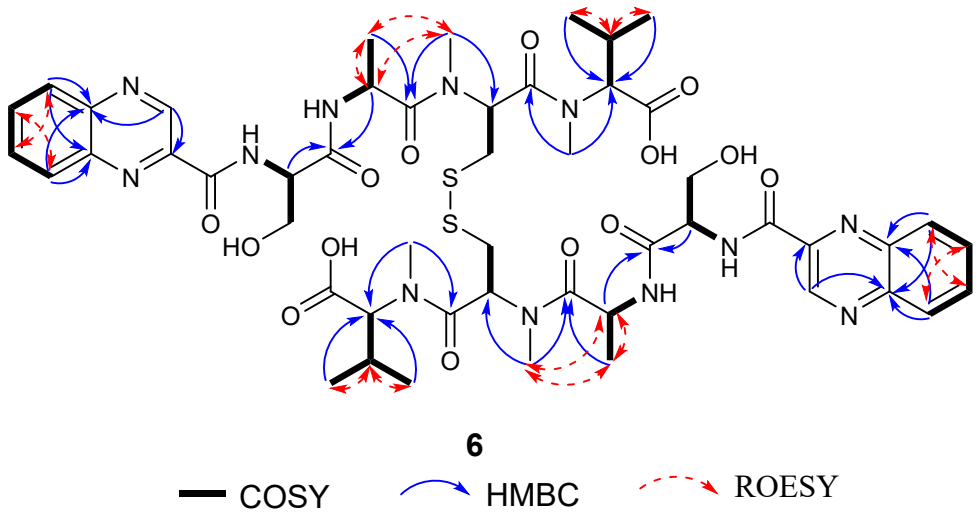


Figure S75. Key COSY, HMBC, ROESY correlations of compounds 6

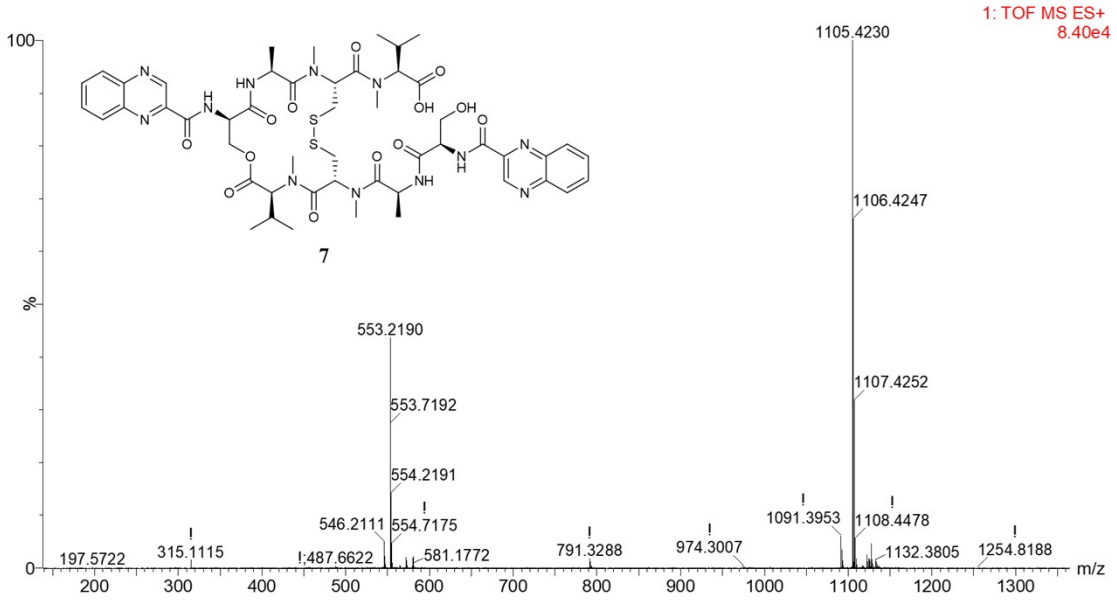


Figure S76. The (+)-HRESIMS spectrum of compound 7

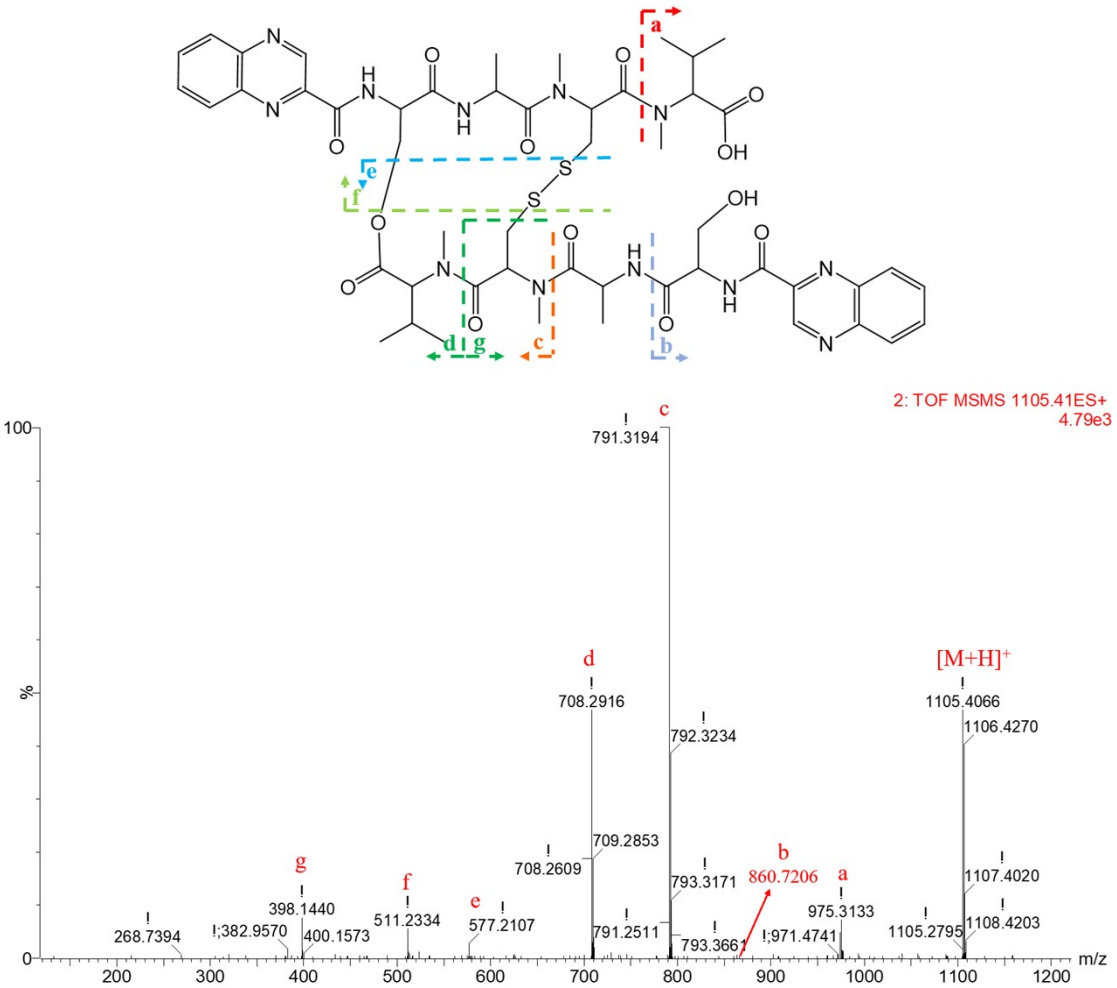


Figure S77. MS/MS fragmentation analysis of compound 7

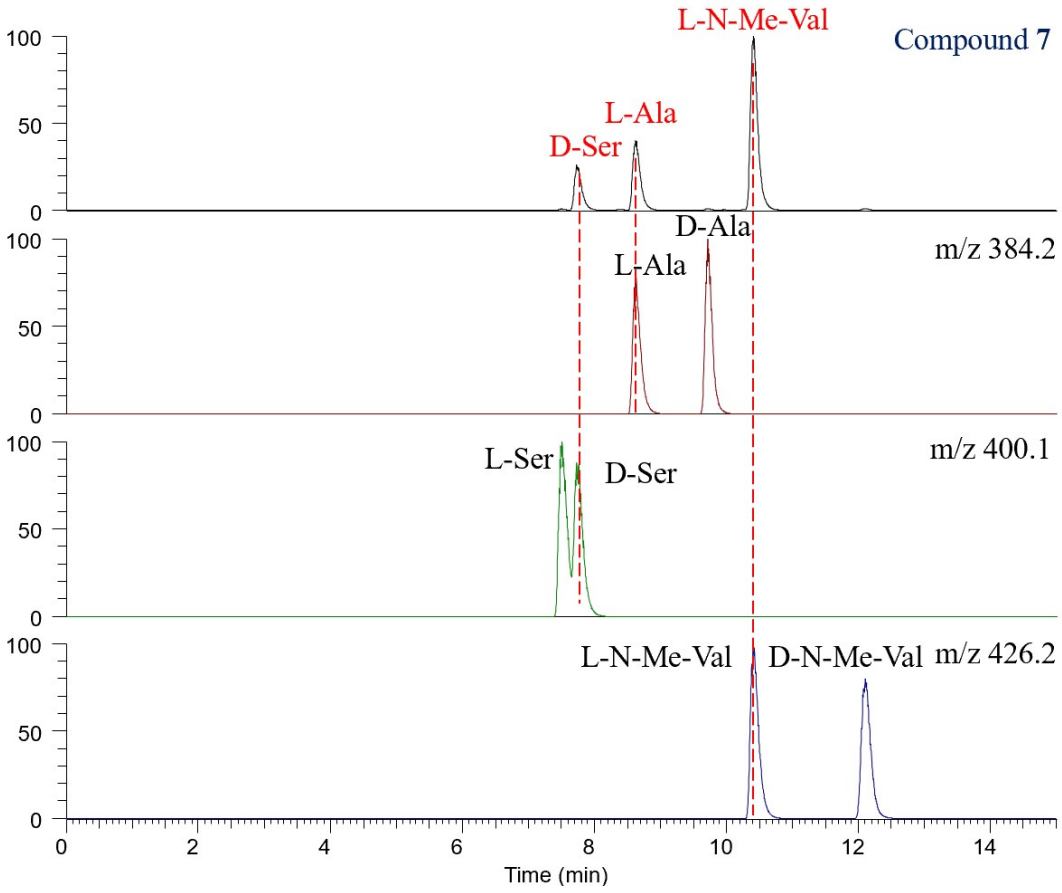


Figure S78. Marfey's analysis of compound 7

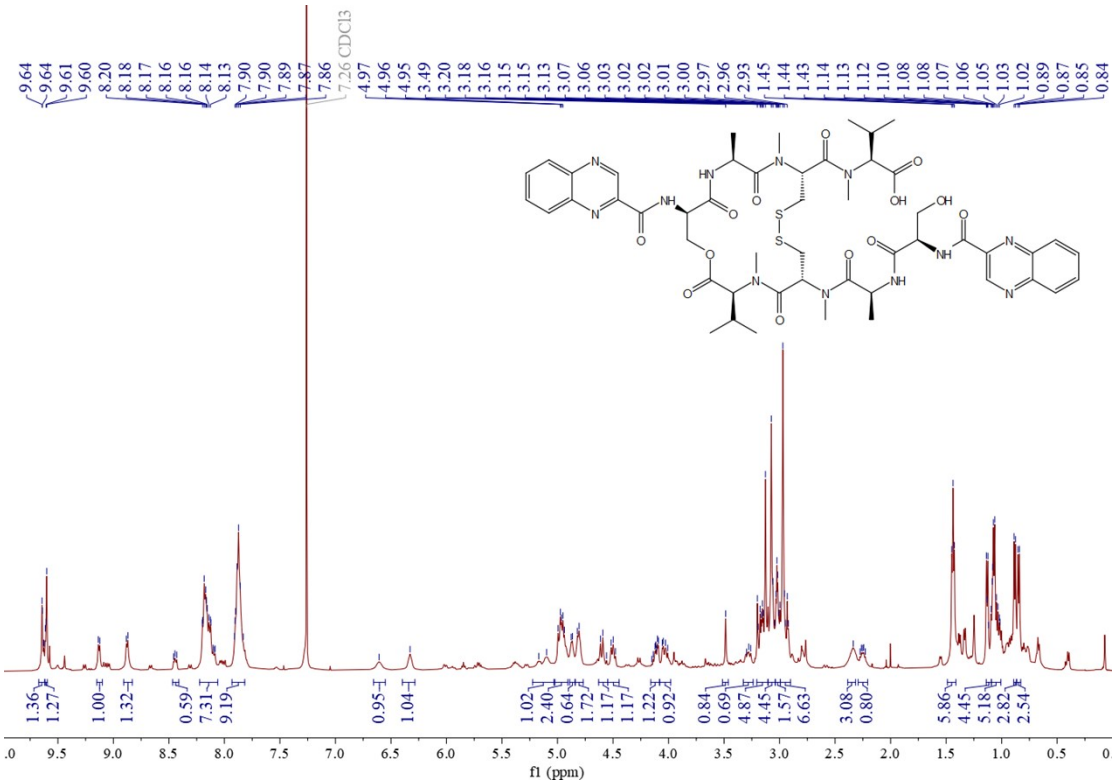


Figure S79. ^{1}H NMR spectrum of (7) at 500 MHz in $CDCl_3$

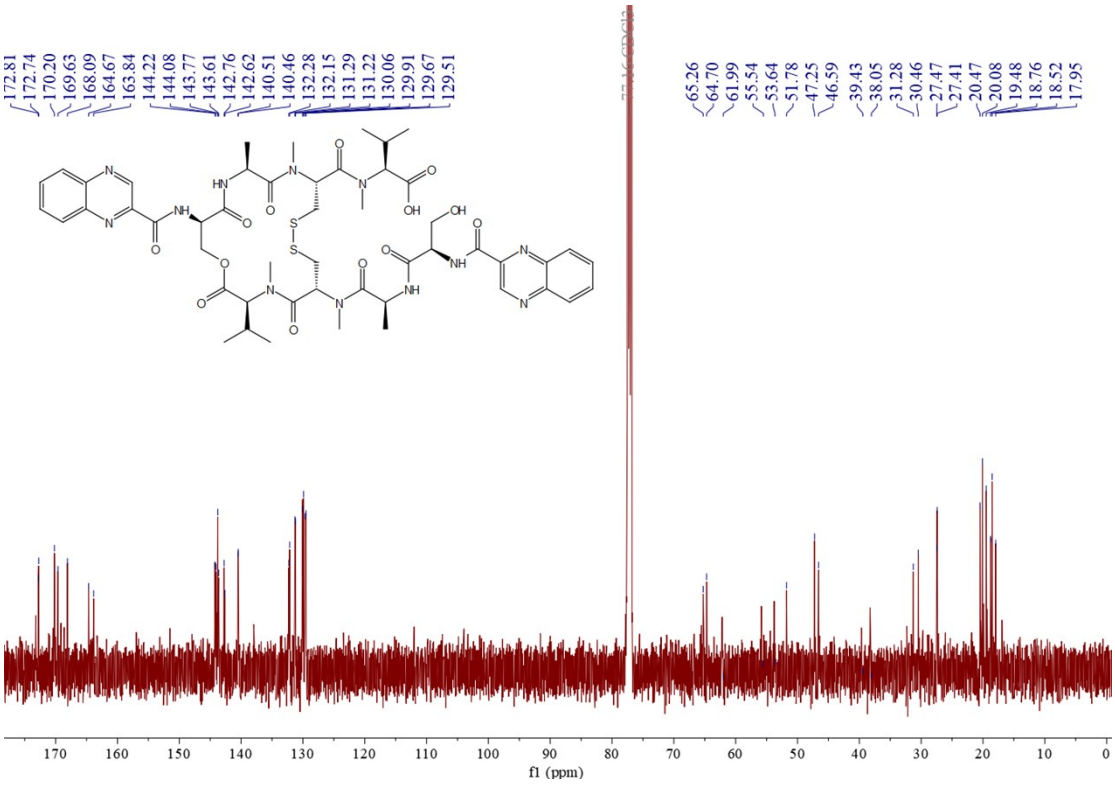


Figure S80. ^{13}C NMR spectrum of (7) at 126 MHz in $CDCl_3$

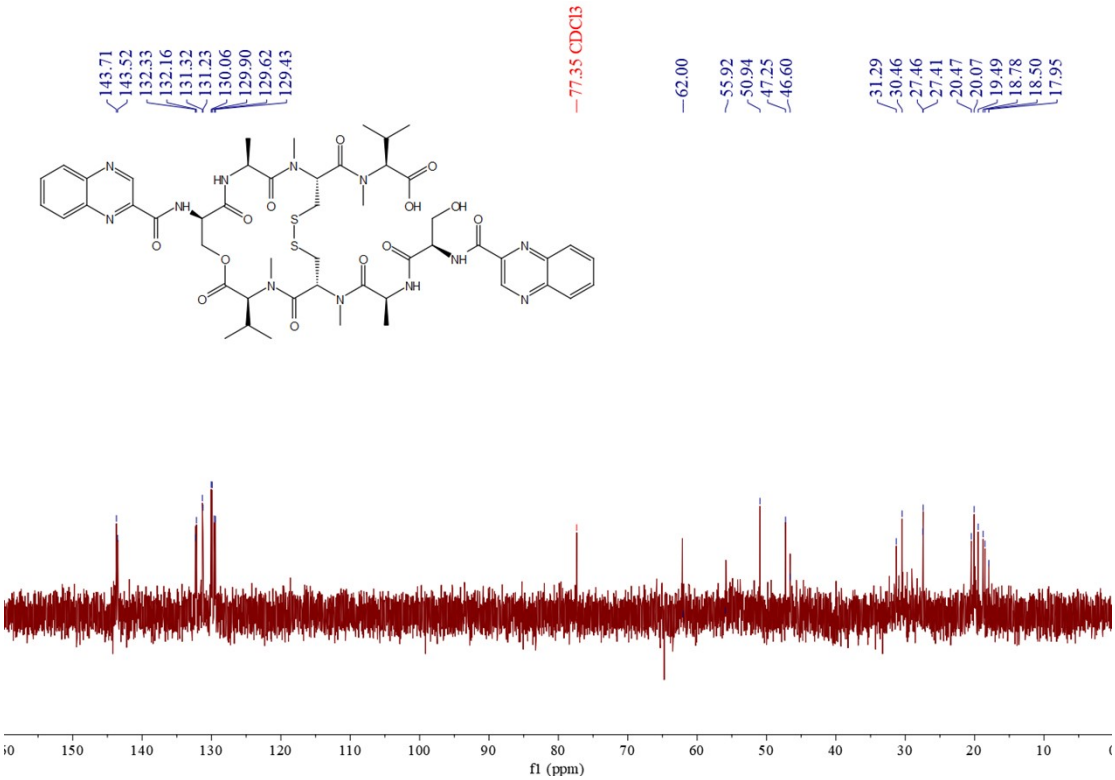


Figure S81. DEPT-135 spectrum of (7) at 126 MHz in $CDCl_3$

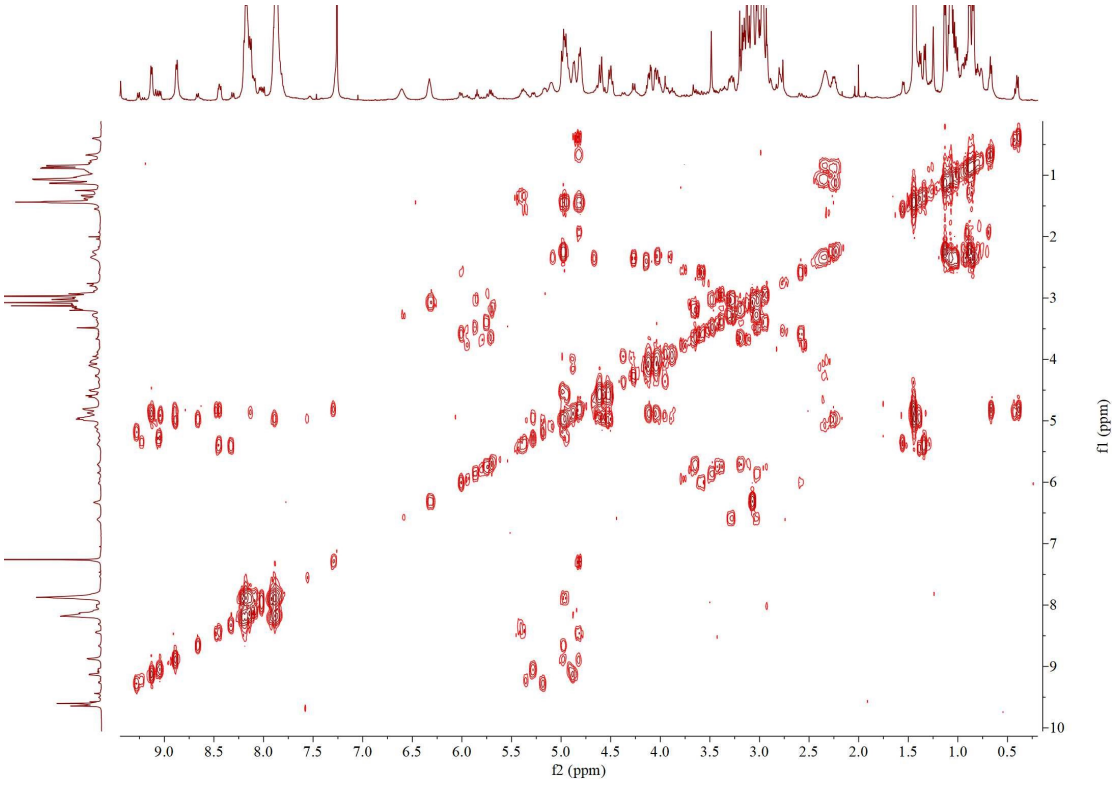


Figure S82. COSY NMR spectrum of (7) in $CDCl_3$

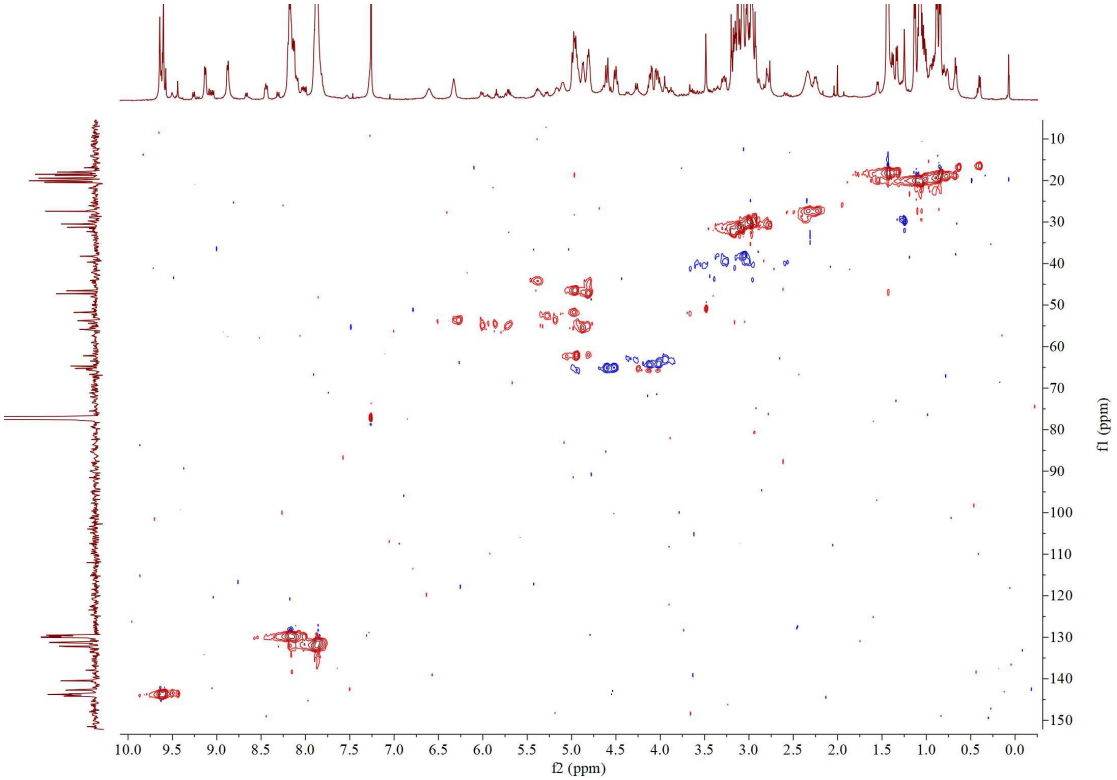


Figure S83. HSQC NMR spectrum of (7) in $CDCl_3$

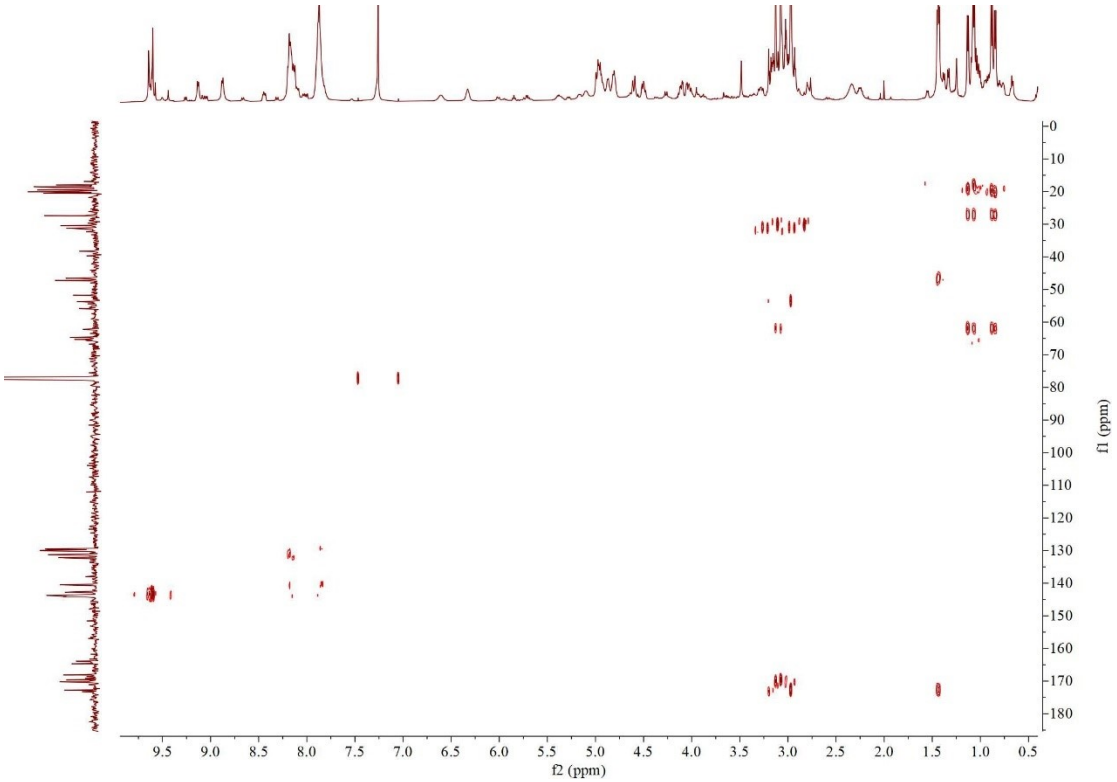


Figure S84. HMBC NMR spectrum of (7) in $CDCl_3$

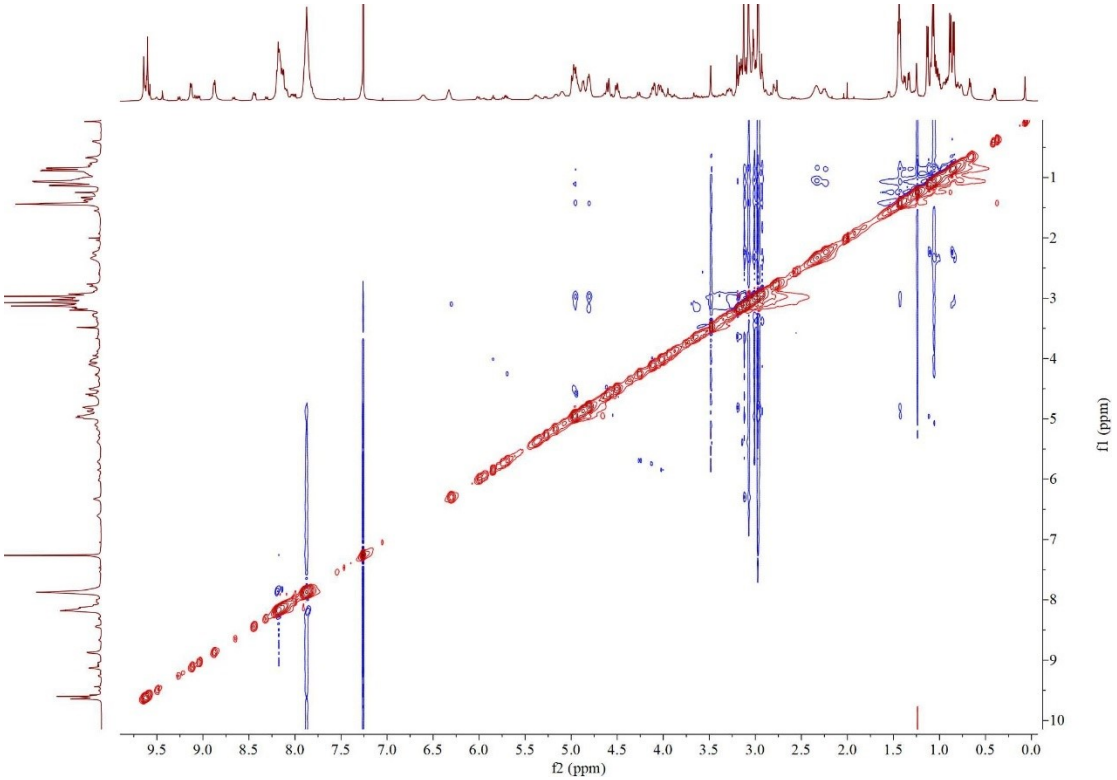


Figure S85. ROESY NMR spectrum of (7) in $CDCl_3$

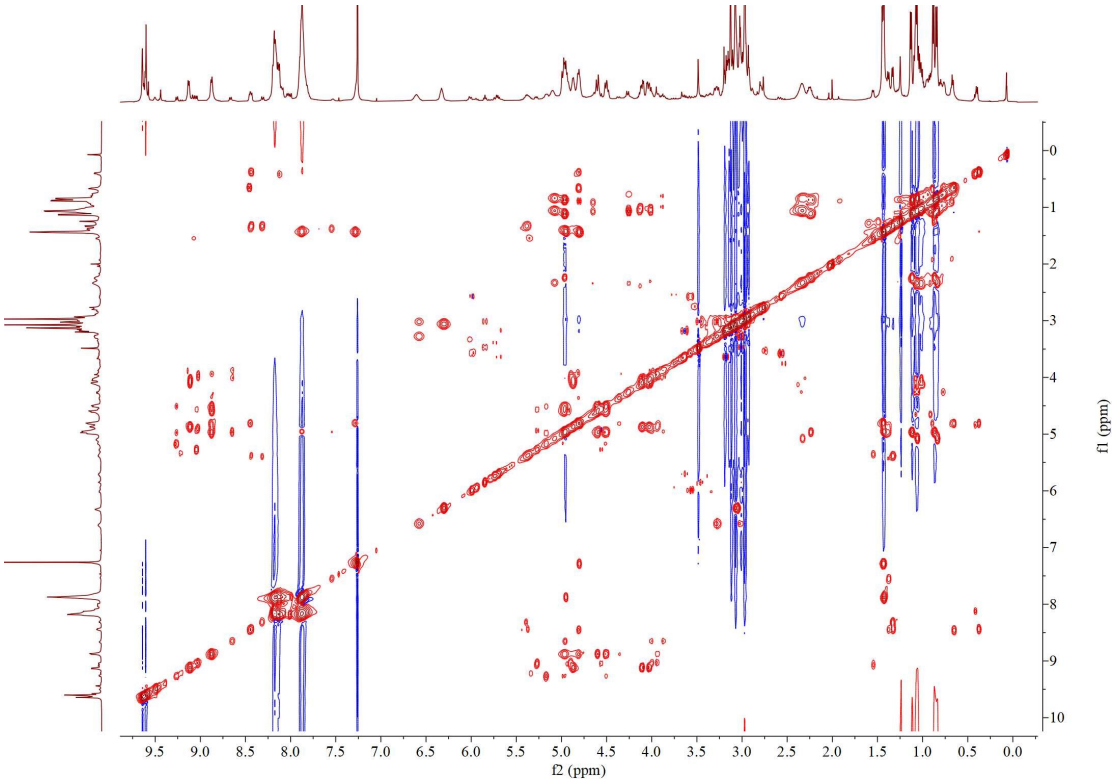


Figure S86. TOCSY NMR spectrum of (7) in $CDCl_3$

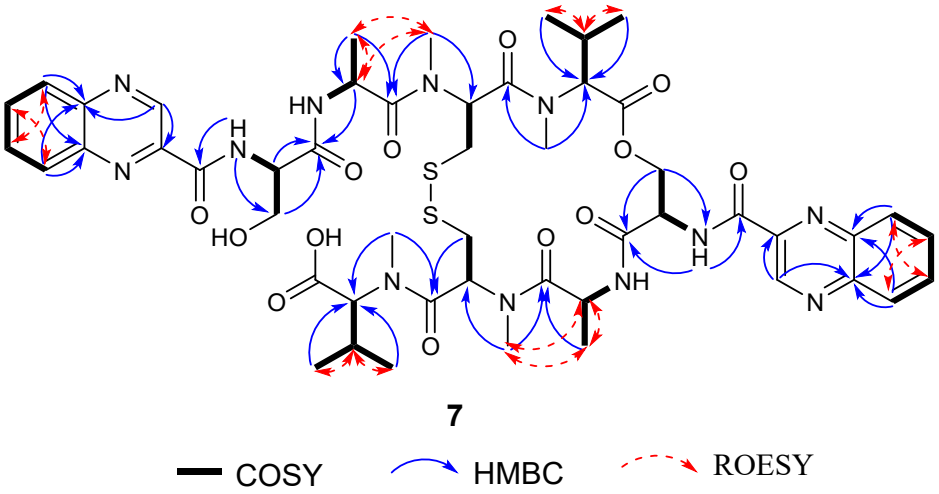


Figure S87. Key COSY, HMBC, ROESY correlations of compounds 7

Fraction: Fr. 7.1 Liquid Chromatography Conditions:50% aqueous MeCN with 0.1% formic acid

t_R: 11.7 min 45.7 min Weight: 12.3 mg 7.6 mg

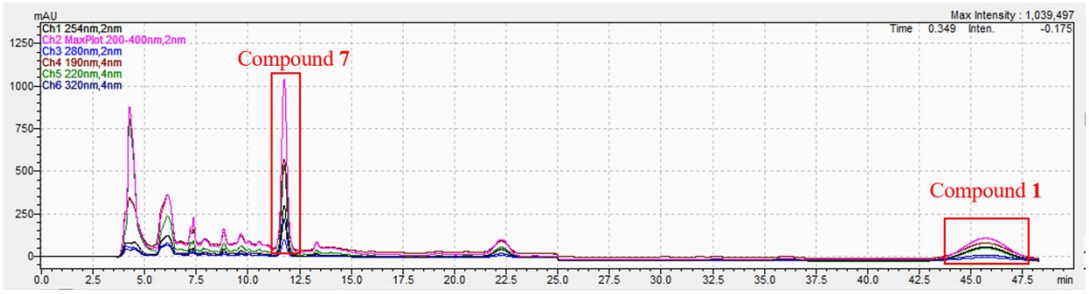


Figure S88. Preparative HPLC chromatogram of compounds 1 and 7

Fraction: Fr. 9.1 Liquid Chromatography Conditions:44% aqueous MeCN with 0.1% formic acid

t_R: 26.4 min 28.7 min Weight: 36.1 mg 10.1 mg

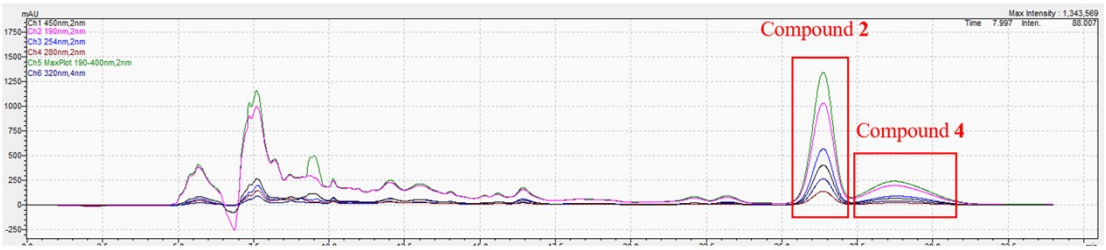


Figure S89. Preparative HPLC chromatogram of compounds 2 and 4

Fraction: Fr. 5.2 Liquid Chromatography Conditions:75% aqueous MeOH with 0.1% formic acid

t_R: 20.6 min Weight: 18.7 mg

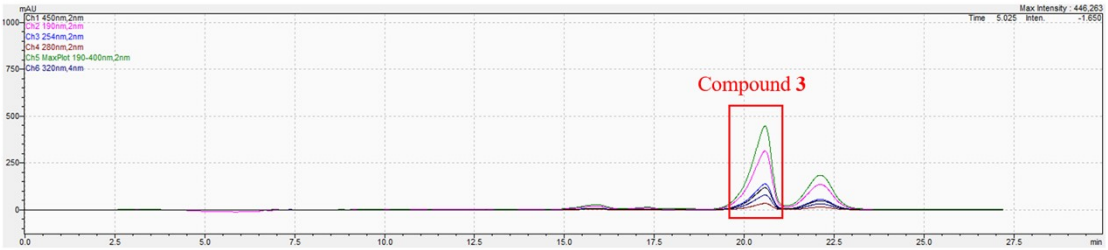


Figure S90. Preparative HPLC chromatogram of compound 3

Fraction: Fr. 5.2 Liquid Chromatography Conditions:52% aqueous MeCN with 0.1% formic acid

t_R: 41.6 min Weight: 4.7 mg

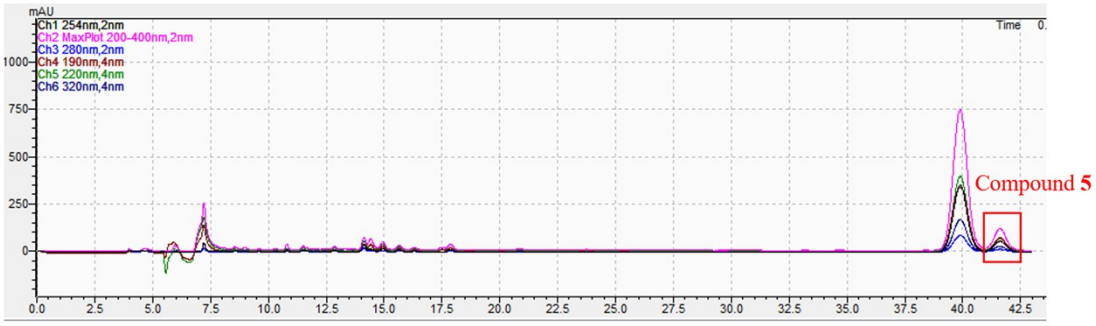


Figure S91. Preparative HPLC chromatogram of compound 5

Fraction: Fr. 10.1 Liquid Chromatography Conditions:37% aqueous MeCN with 0.1% formic acid

t_R: 23.1 min Weight: 5 mg

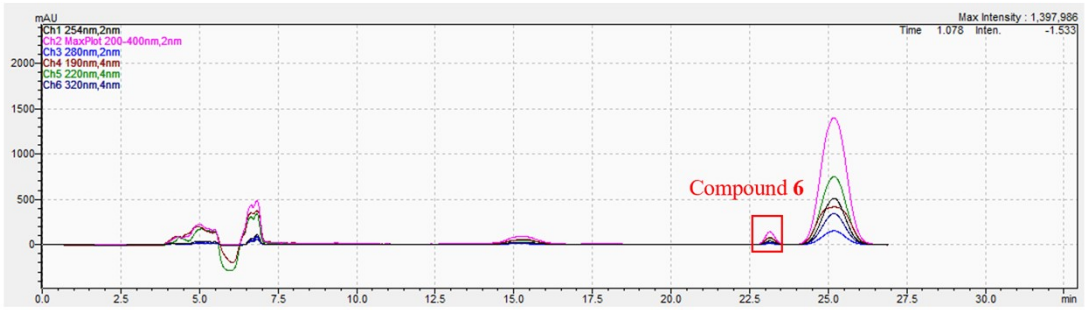


Figure S92. Preparative HPLC chromatogram of compound 6

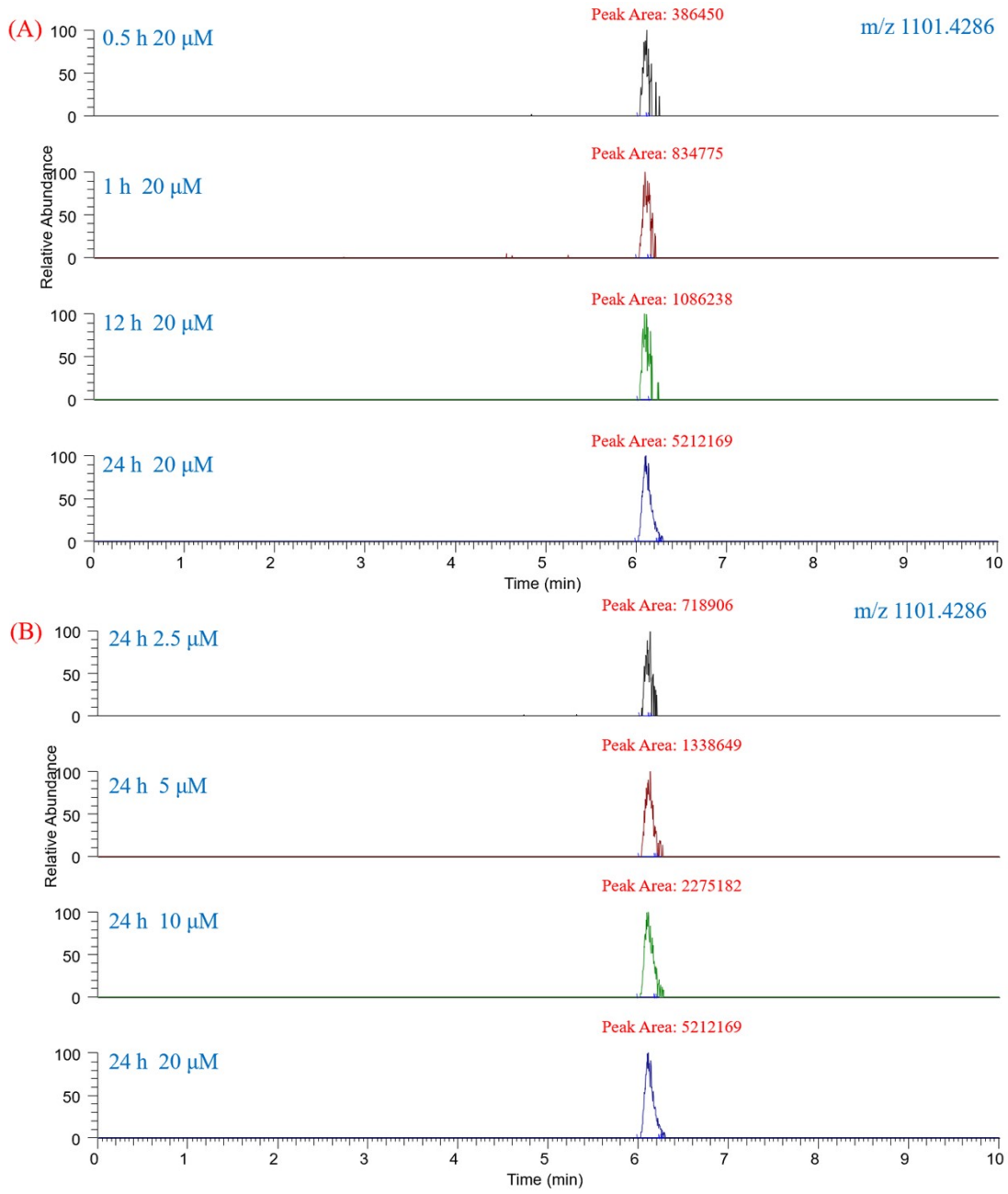


Figure S93. UPLC-HRMS analysis of intracellular compound 11 with peak areas labeled

(A) Time-dependent accumulation at 20 μM (0.5, 1, 12, and 24 h). (B) Concentration-dependent accumulation at 24 h (2.5, 5, 10, and 20 μM). Extracted ion chromatograms are shown at *m/z* 1101.42.

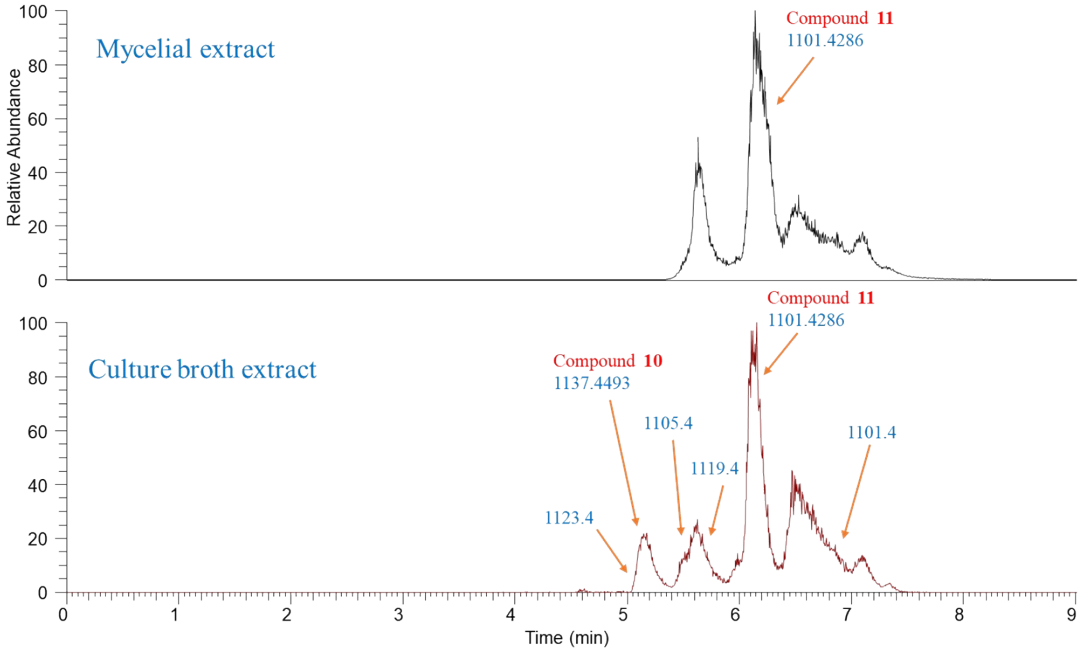


Figure S94. UPLC-HRMS extracted ion chromatograms (*m*/*z* 1101-1138) of compound 10 and compound 11 in the culture broth extract and mycelial extract