Supporting Information

***Rec. Nat. Prod*. 16:6 (2022) 585-591**

New Cyclic Peptides from the Endophytic *Aspergillus versicolor* 0312 with Their Antimicrobial Activity

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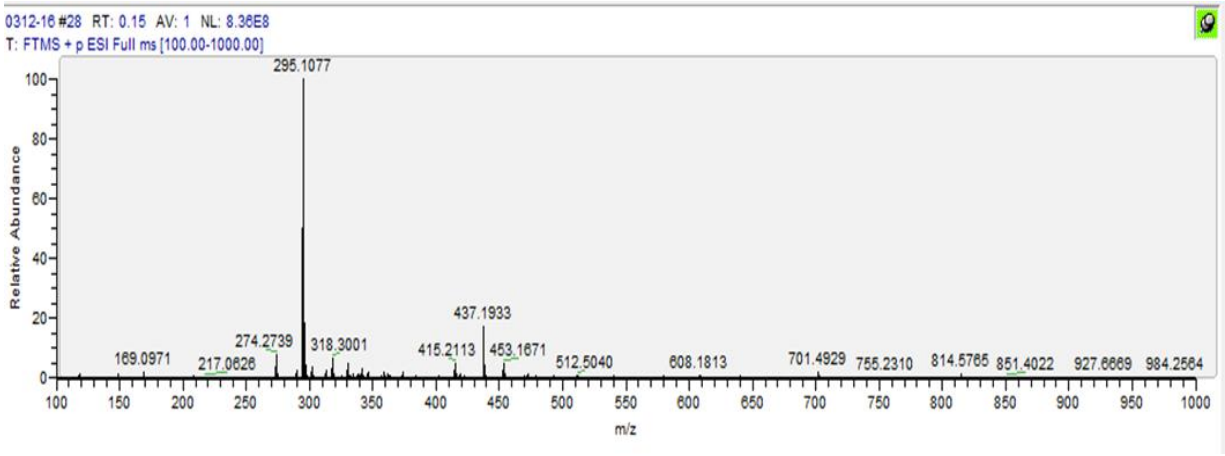

Figure S1: HR-ESI-MS spectrum of **1** (7-hydroxyldehydrocyclopeptin)

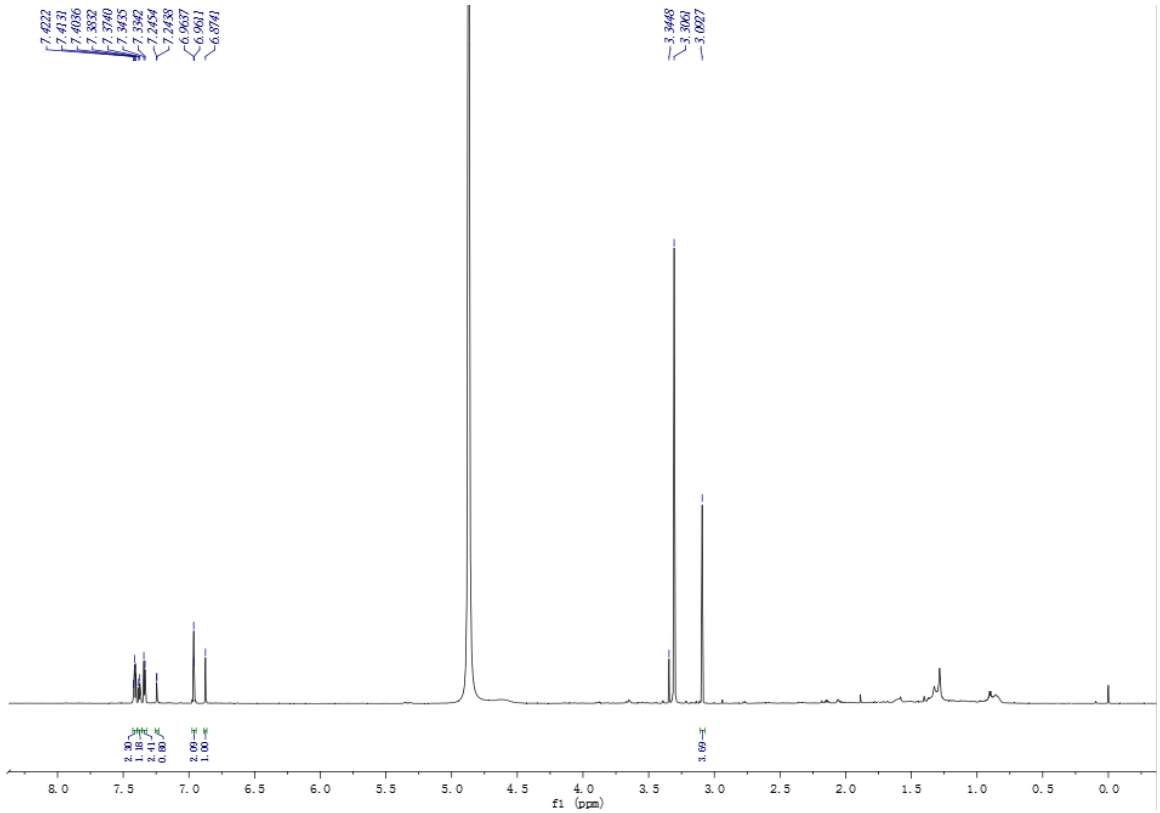

Figure S2: ^{1}H-NMR (800 MHz, CD_3OD) spectrum of **1** (7-hydroxyldehydrocyclopeptin)

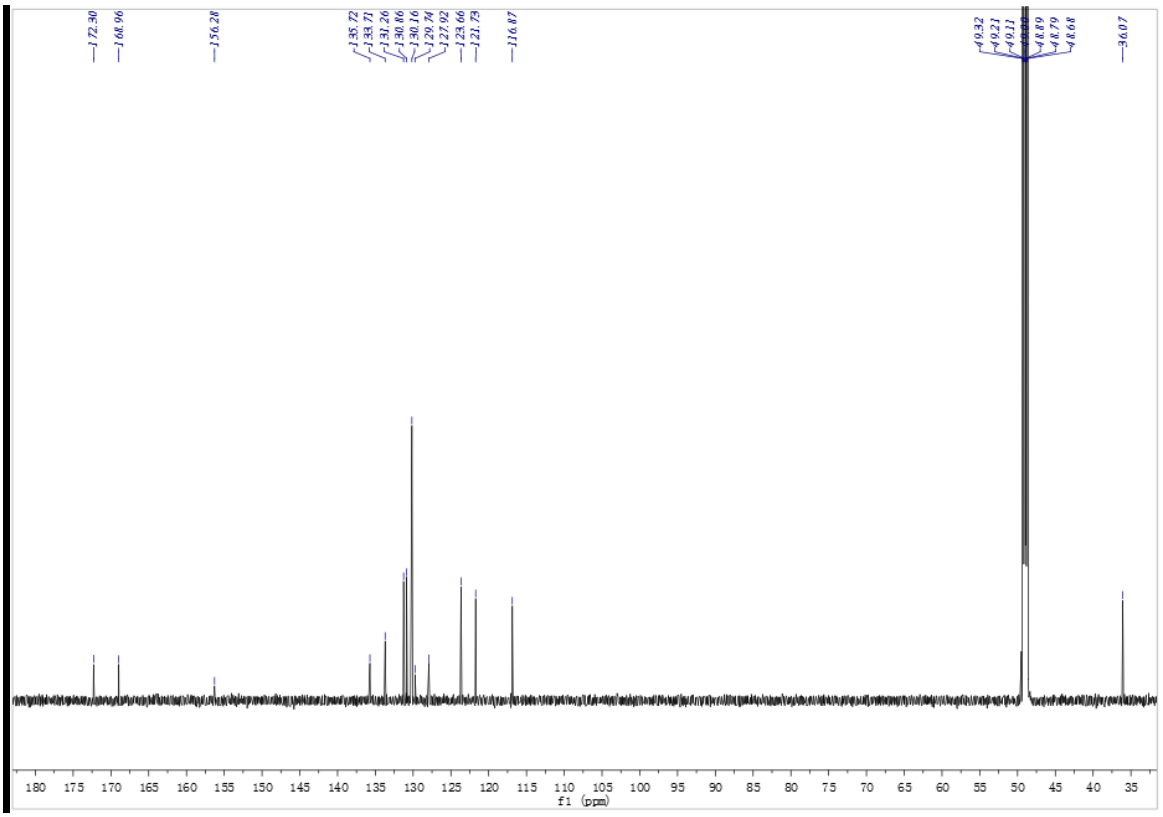

Figure S3: ^{13}C-NMR (200 MHz, CD_3OD) spectrum of **1** (7-hydroxyldehydrocyclopeptin)

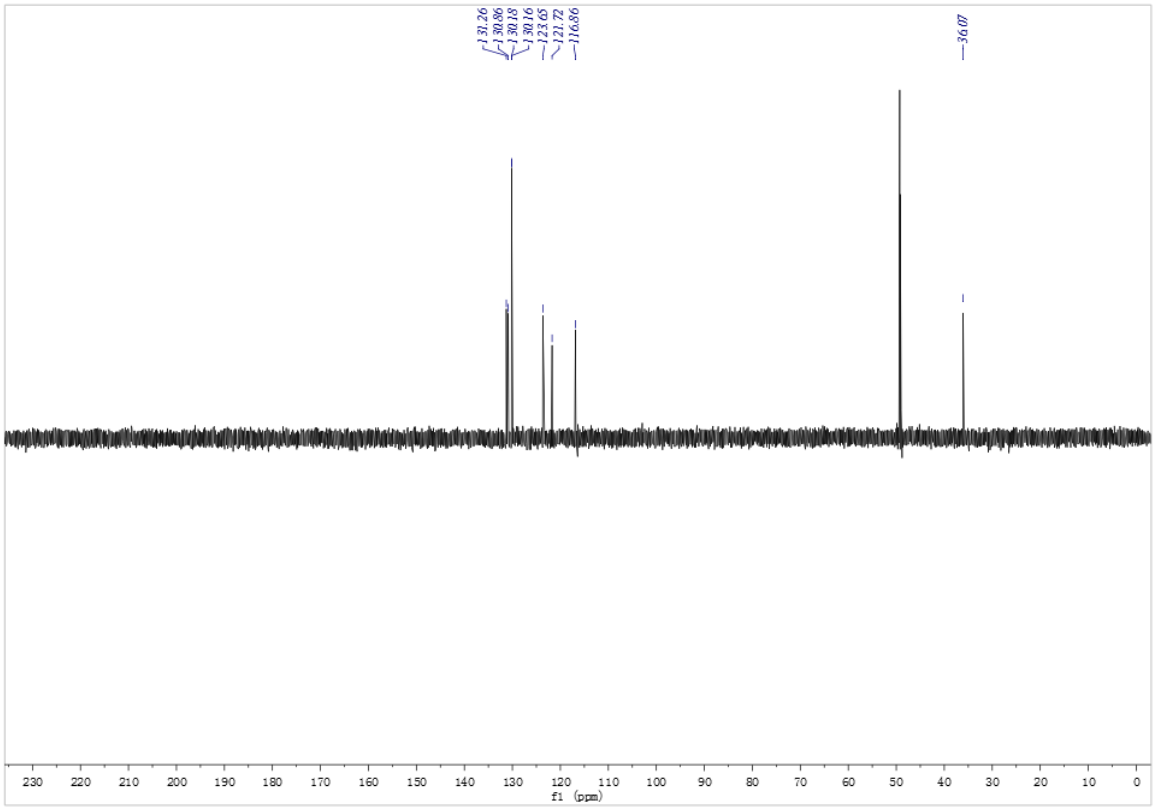

Figure S4: DEPT135 (200 MHz, CD_3OD) spectrum of **1** (7-hydroxyldehydrocyclopeptin)

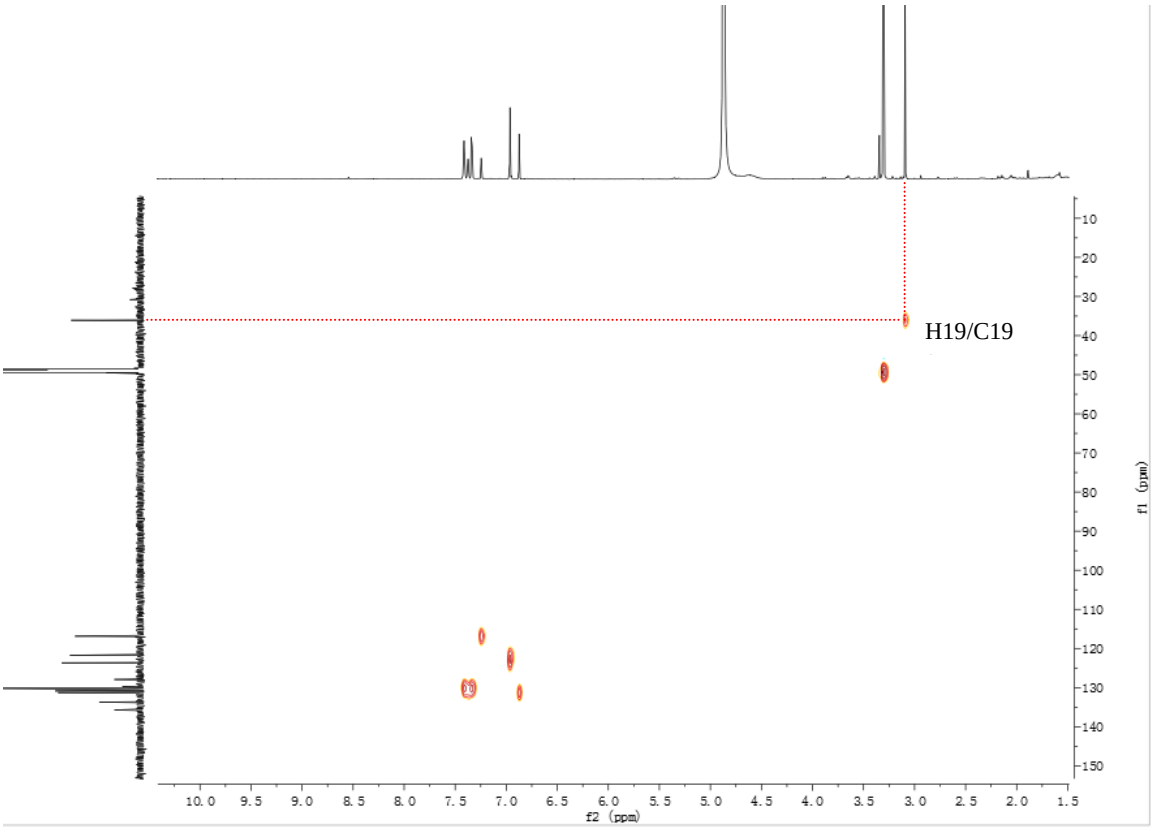

Figure S5: HSQC spectrum of **1** (7-hydroxyldehydrocyclopeptin)

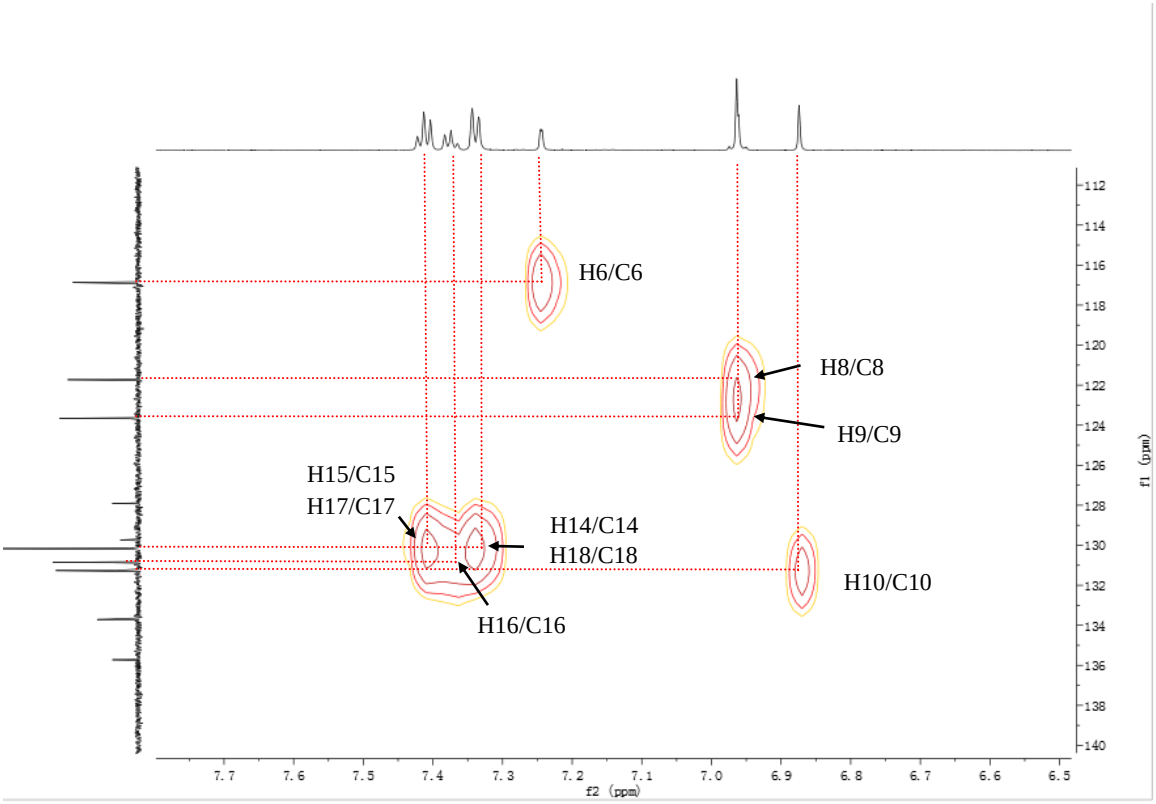

Figure S6: HSQC spectrum of **1** (7-hydroxyldehydrocyclopeptin) (From δ_C110 ppm to δ_C 145 ppm)

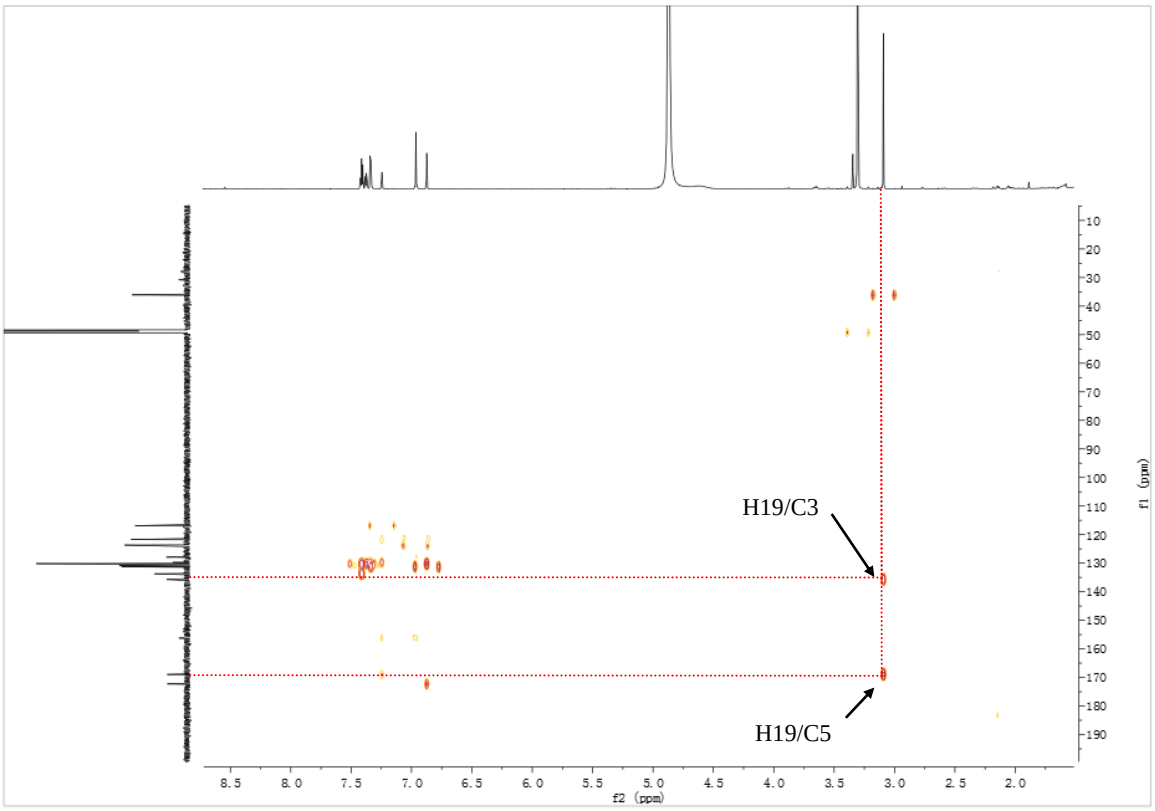

Figure S7: HMBC spectrum of **1** (7-hydroxyldehydrocyclopeptin)

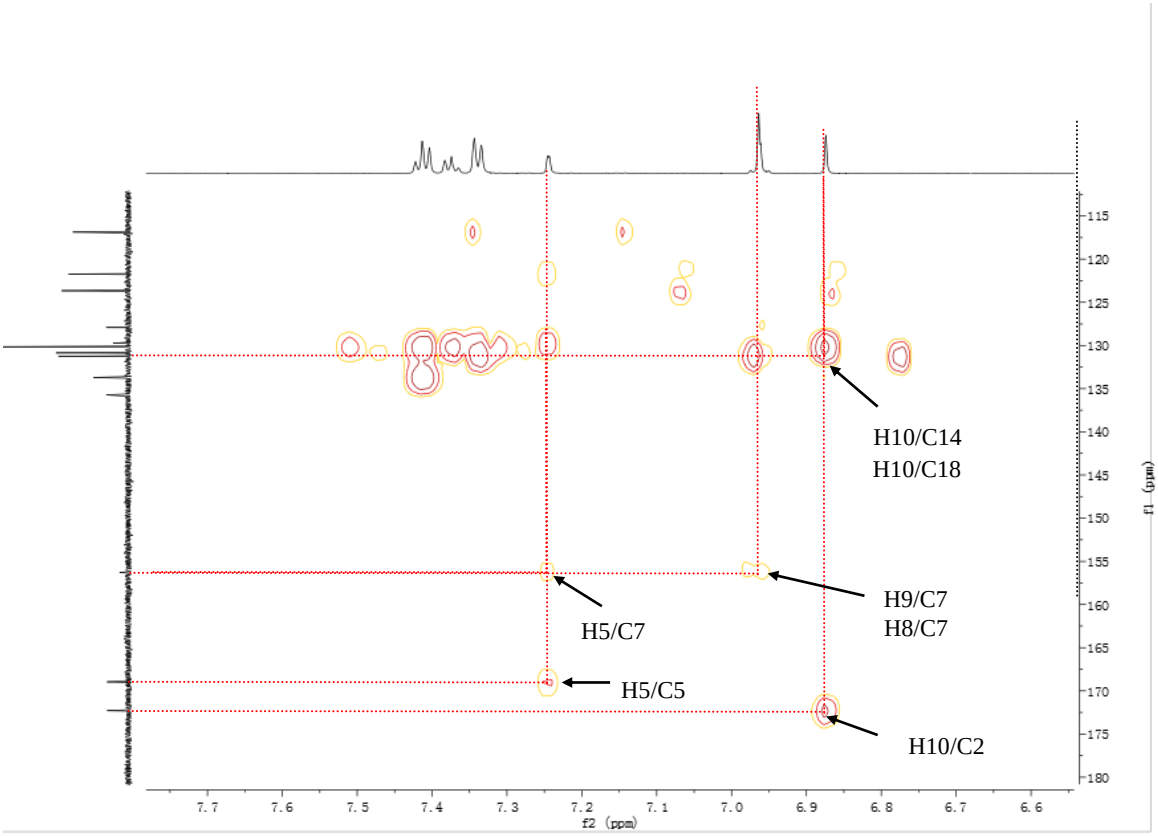

Figure S8: HMBC spectrum of **1** (7-hydroxyldehydrocyclopeptin) (From δ_C 110 ppm to δ_C 180 ppm)

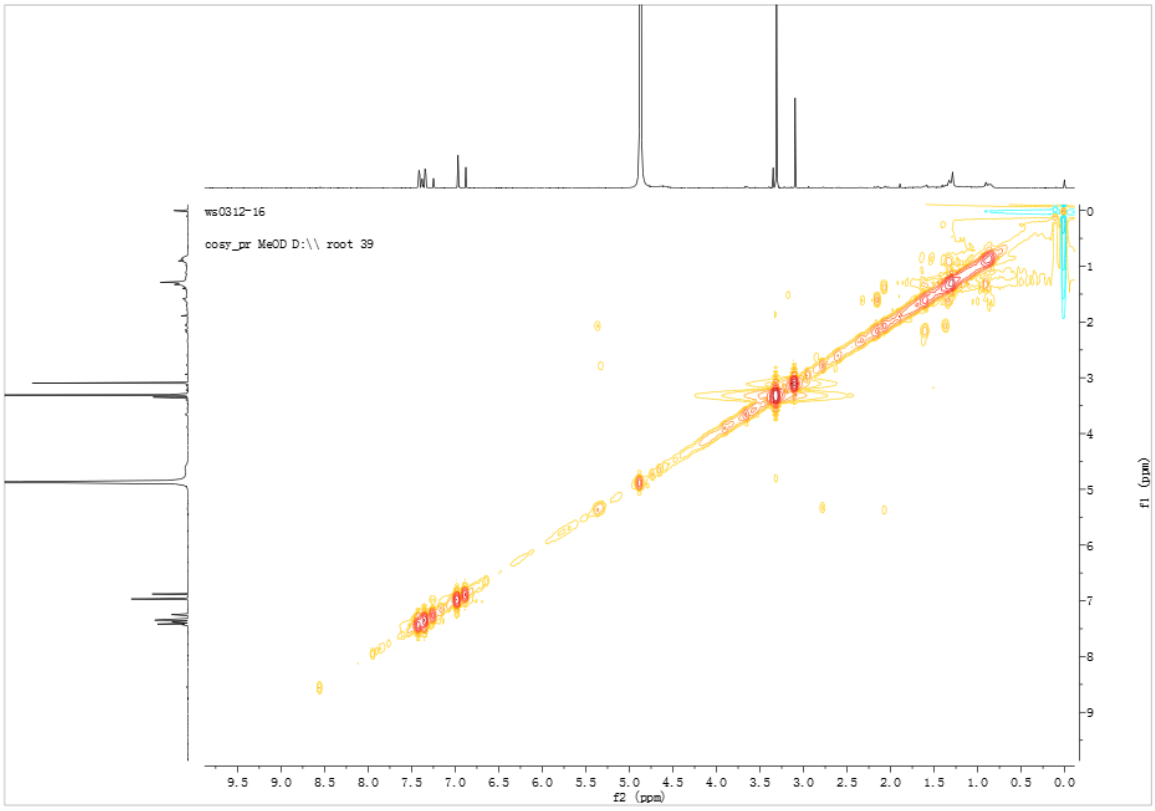

Figure S9: ^{1}H-^{1}H COSY spectrum of **1** (7-hydroxyldehydrocyclopeptin)

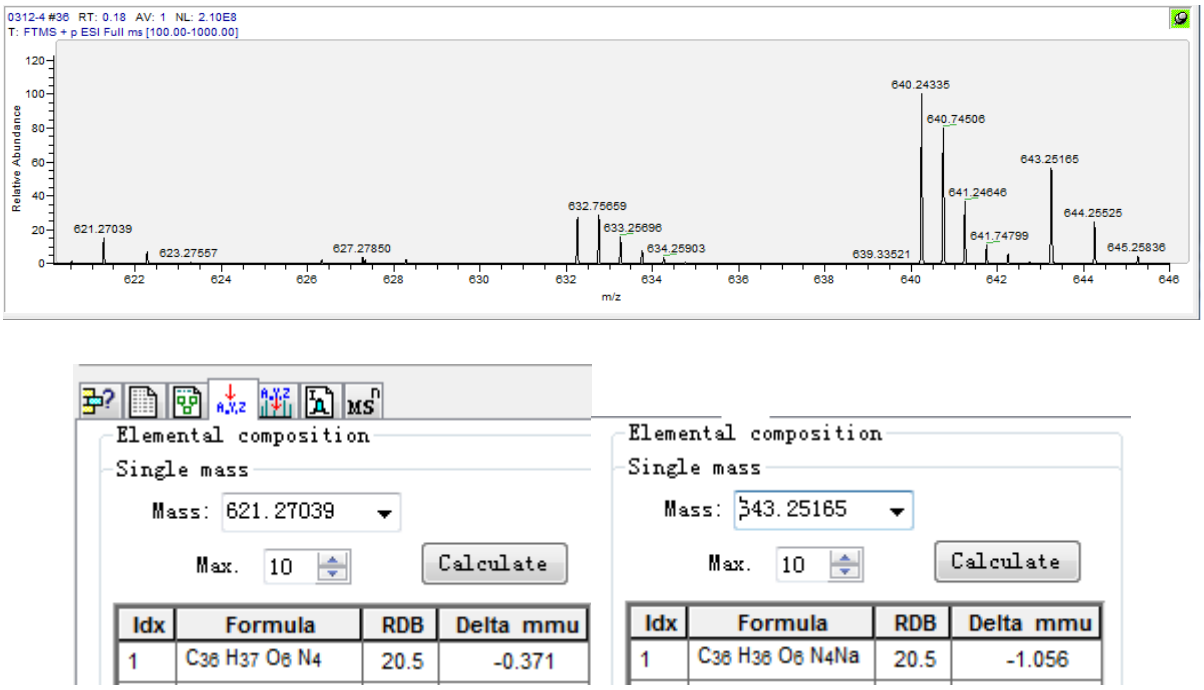

Figure S10: HR-ESI-MS spectrum of **2** (14, 31-dimethoxy-penicopeptide A)

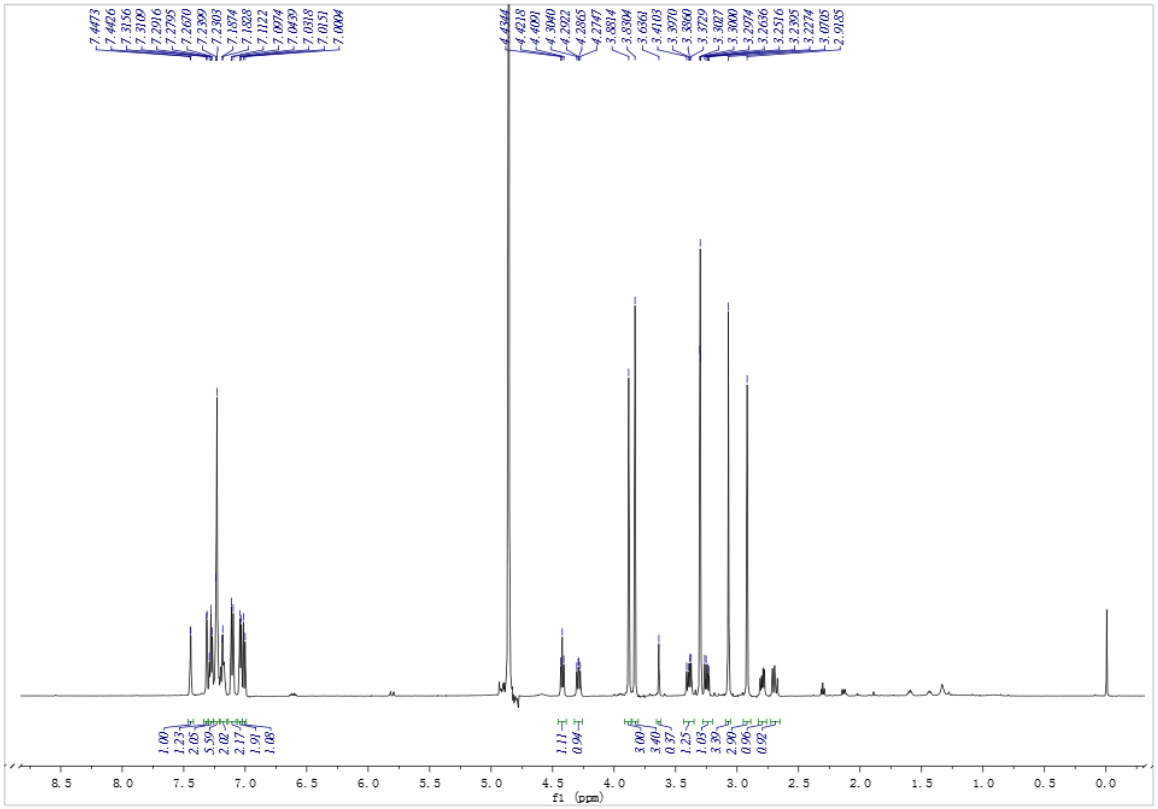

Figure S11: ^{1}H-NMR (800 MHz, CD_3OD) spectrum of **2**(14,31-dimethoxy-penicopeptide A)

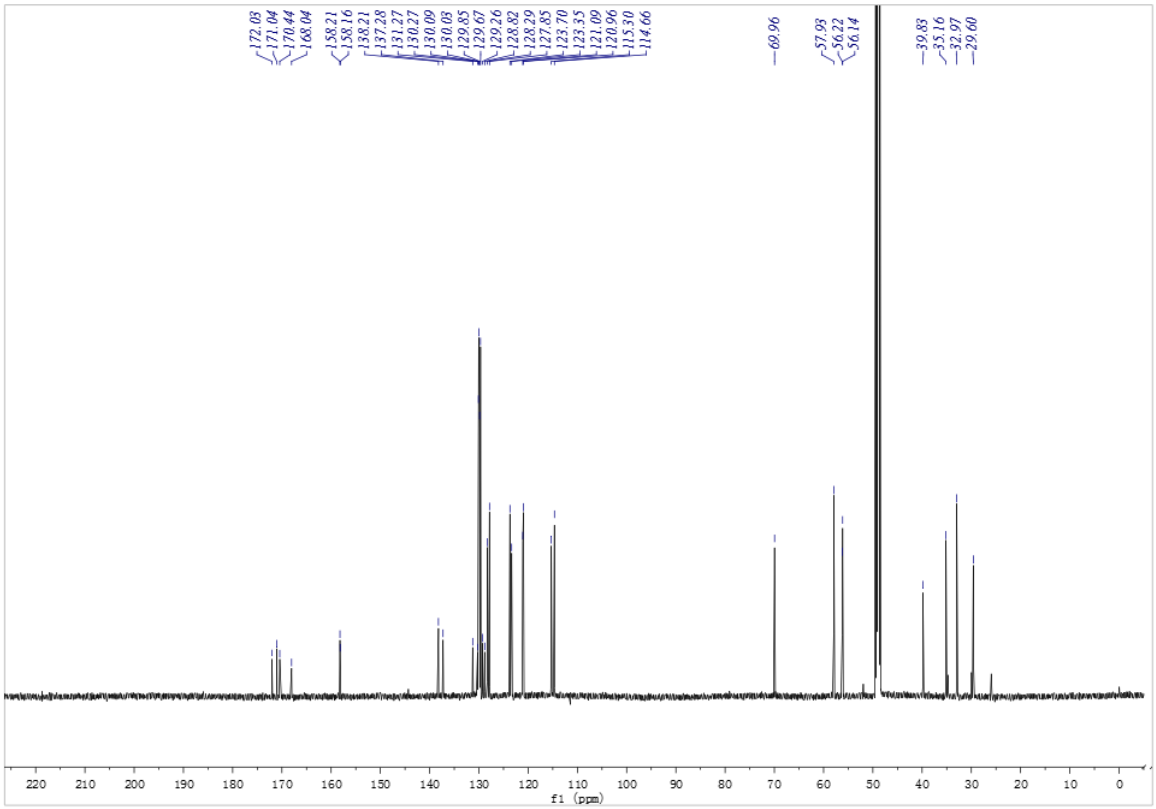

Figure S12: ^{13}C-NMR (200 MHz, CD_3OD) spectrum of **2** (14,31-dimethoxy-penicopeptide A)

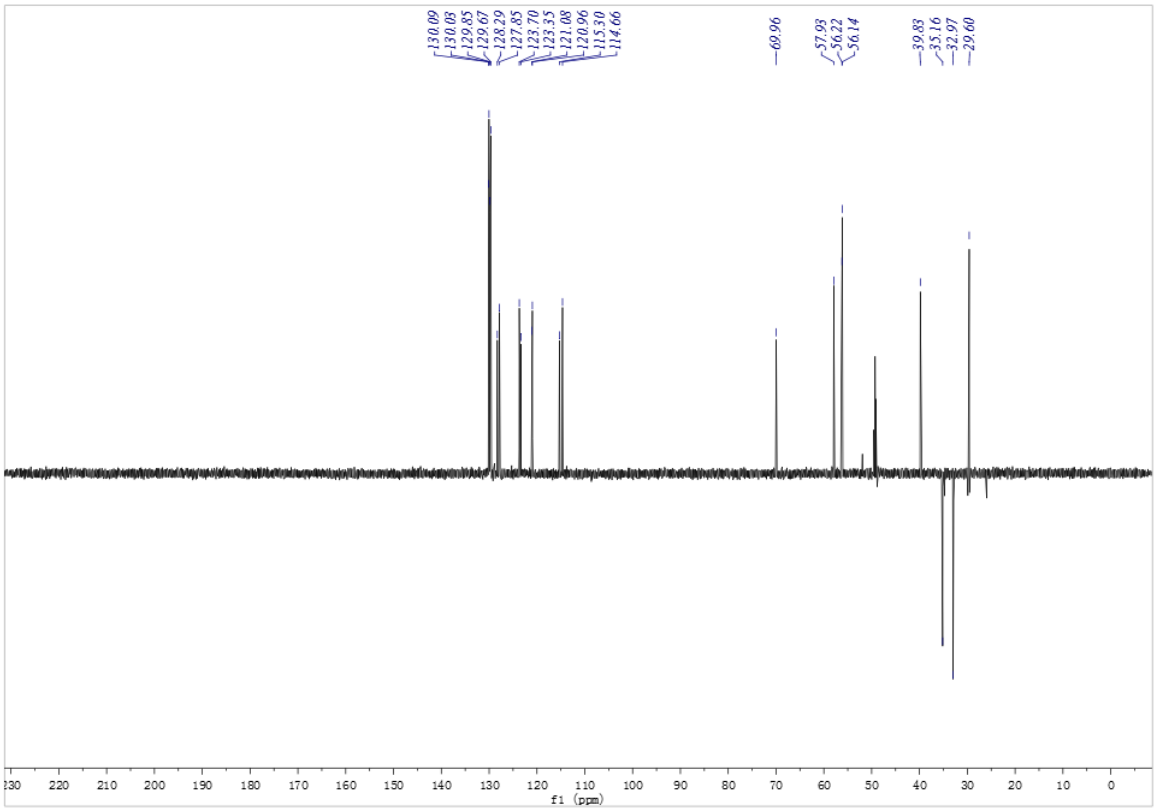

Figure S13: DEPT135 (200 MHz, CD_3OD) spectrum of **2** (14,31-dimethoxy-penicopeptide A)

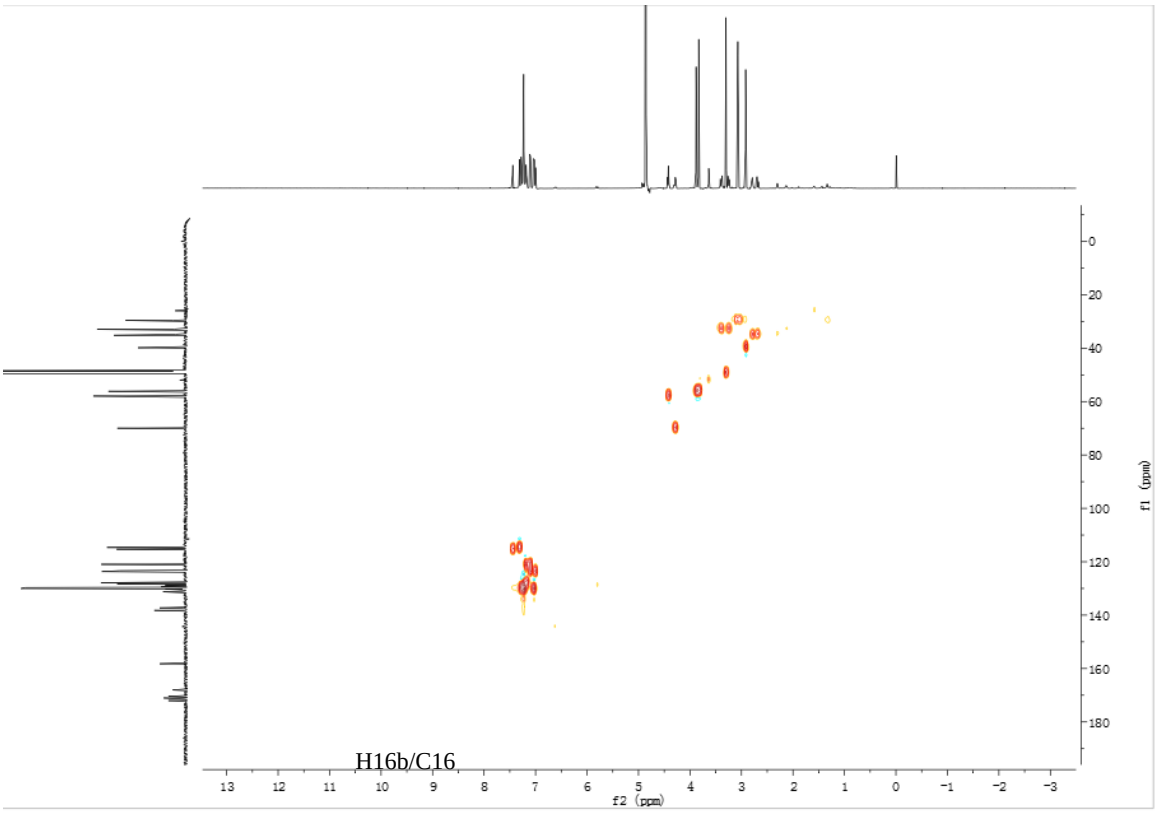

Figure S14: HSQC spectrum of **2** (14,31-dimethoxy-penicopeptide A)

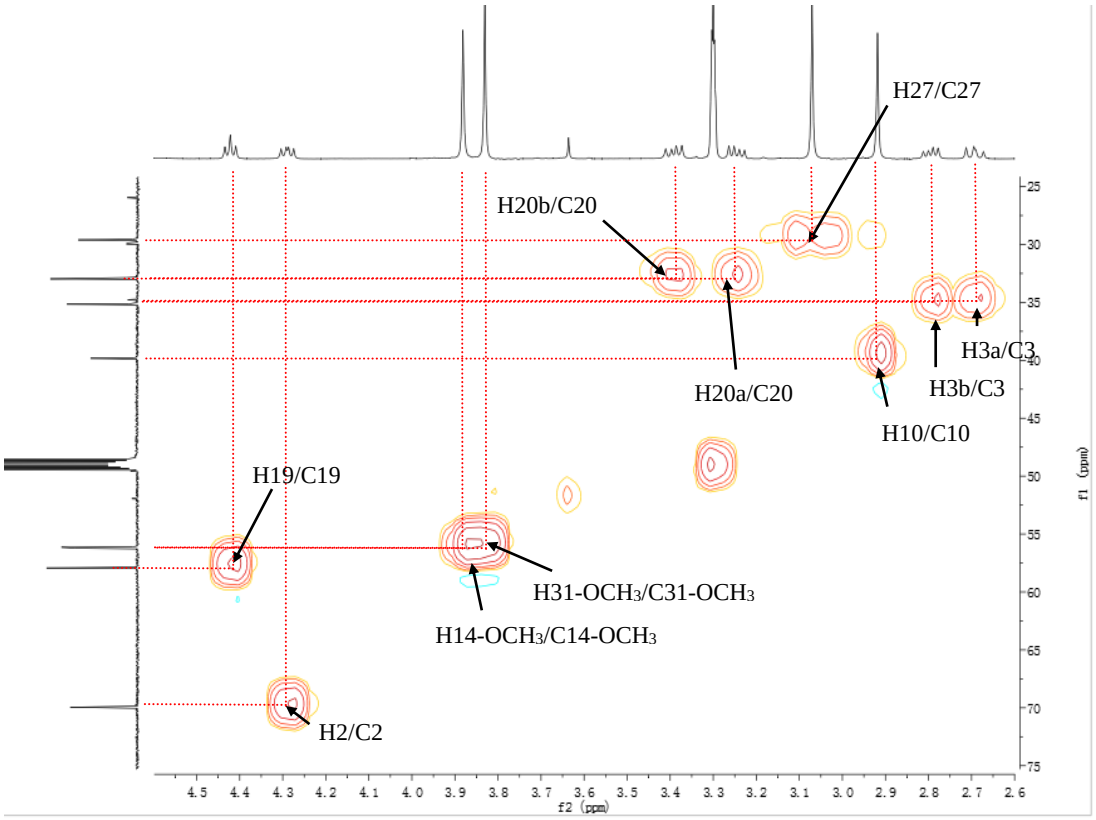

Figure S15: HSQC spectrum of **2** (14,31-dimethoxy-penicopeptide A) (From δ_C 25 ppm to 75 ppm)

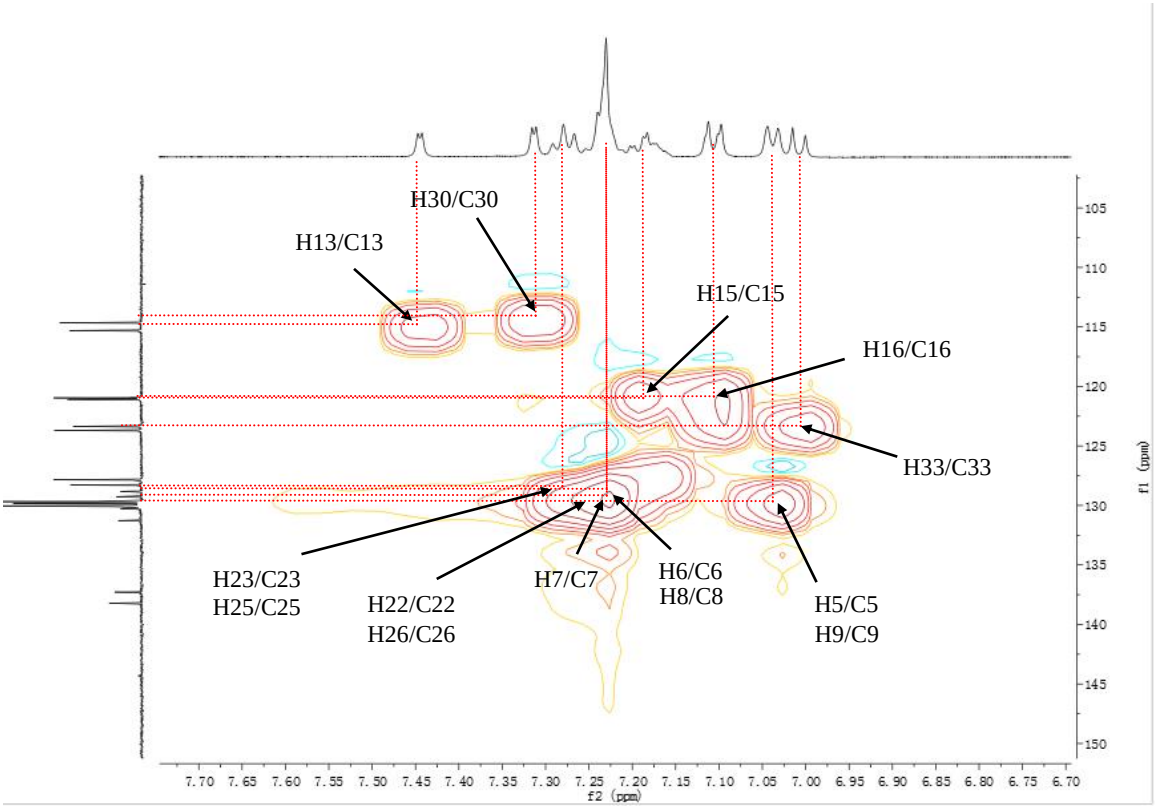

Figure S16: HSQC spectrum of **2** (14,31-dimethoxy-penicopeptide A) (From δ_C 105 ppm to 150 ppm)

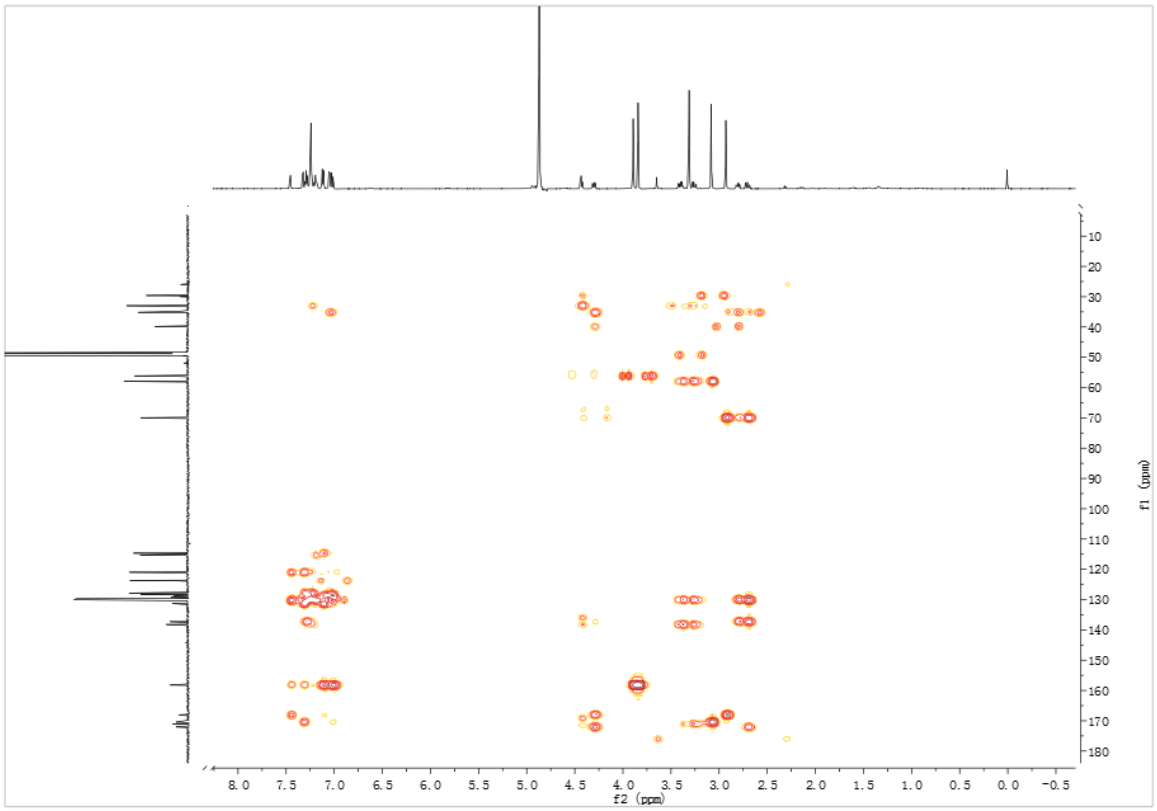

Figure S17: HMBC spectrum of **2** (14,31-dimethoxy-penicopeptide A)

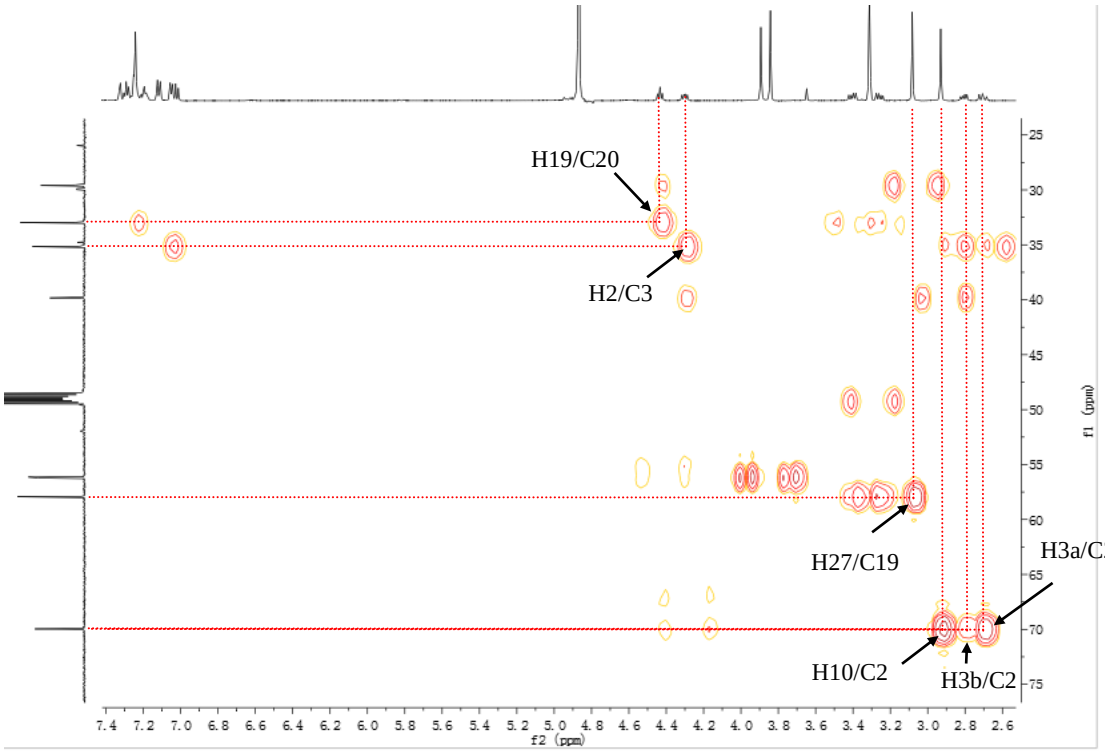

Figure S18: HMBC spectrum of **2** (14,31-dimethoxy-penicopeptide A) (From δ_C 25 ppm to 75 ppm)

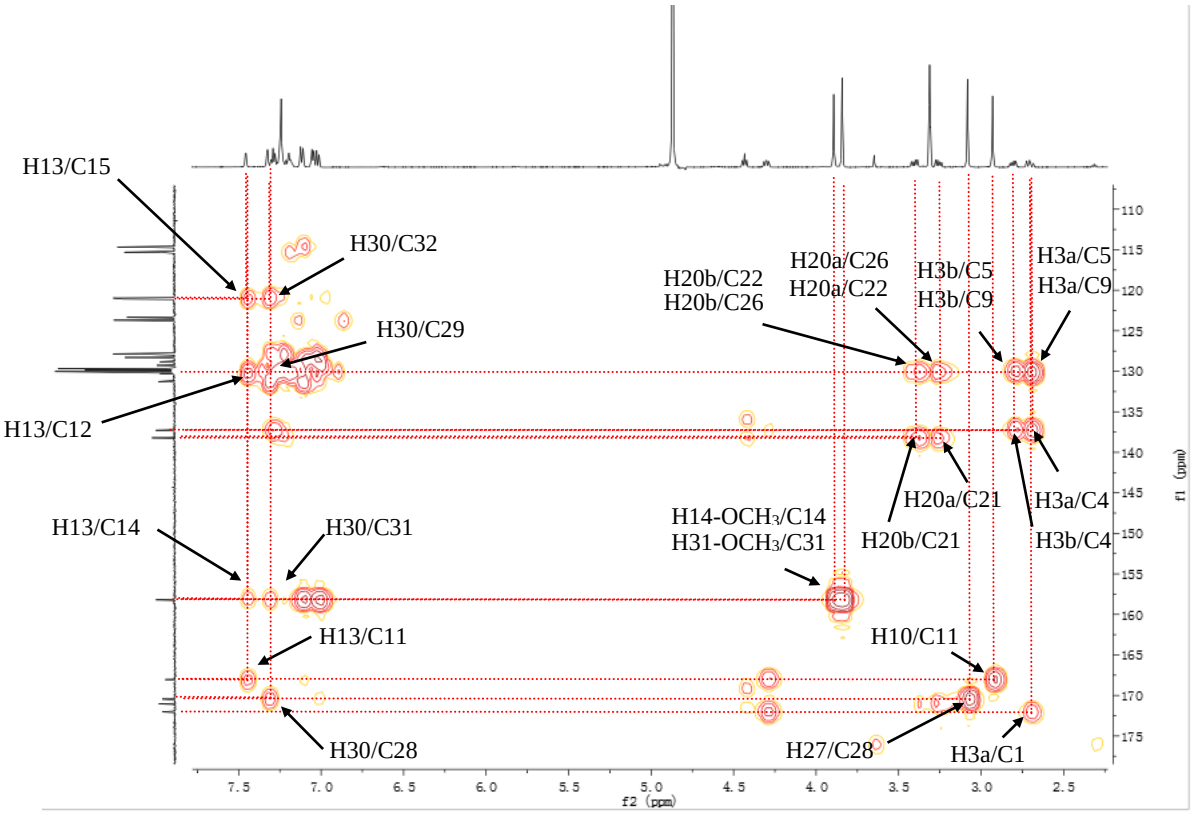

Figure S19: HMBC spectrum of **2** (14,31-dimethoxy-penicopeptide A) (From δ_C 110 ppm to 175 ppm)

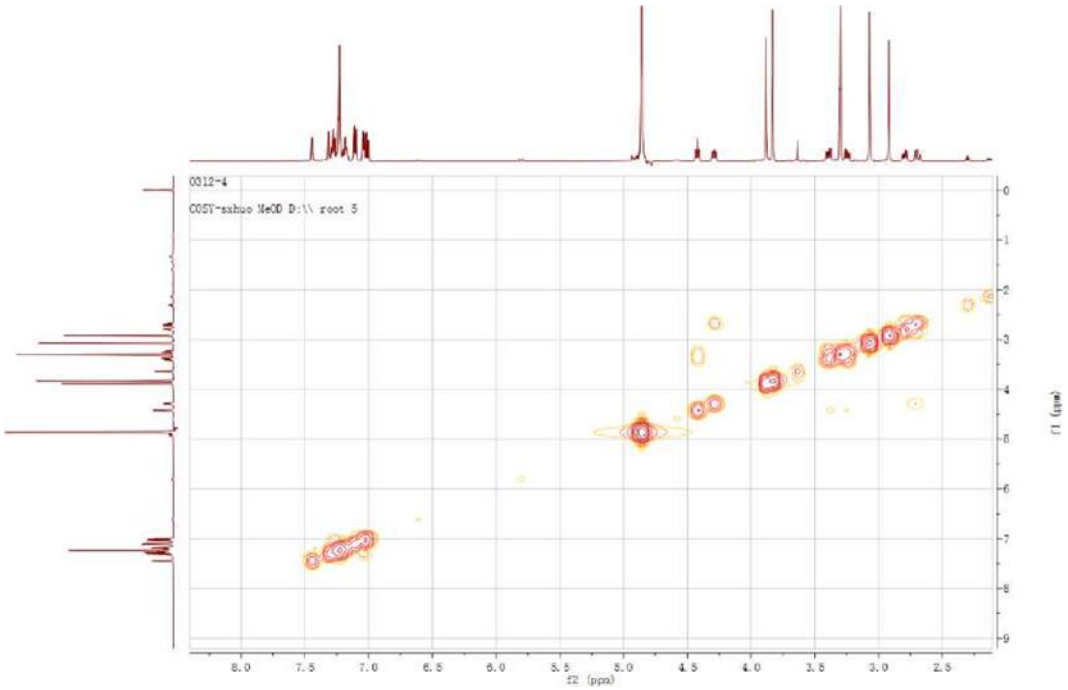

Figure S20: ^{1}H-^{1}H COSY spectrum of **2** (14,31-dimethoxy-penicopeptide A)

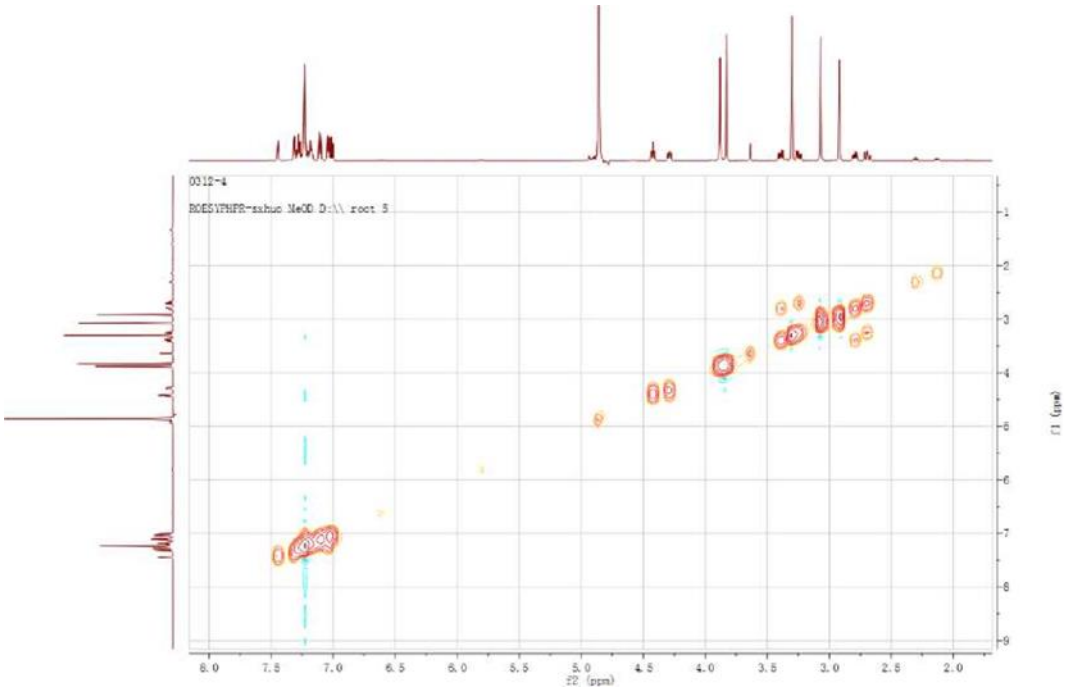

Figure S21: NOESY spectrum of **2** (14,31-dimethoxy-penicopeptide A)

Table S1. ^{1}H NMR and ^{13}C NMR data of compound **1** and **3**(800 MHz and 200 MHz, CD_3OD)

	1			**3**	
No.	δ_C	δ_H **(mult, *J*, Hz)**	**No.**	δ_C	δ_H **(mult, *J*, Hz)**
2	172.3 (C)		2	172.2	
3	135.7 (C)		3	135.4	
5	169.0 (C)		5	168.7	
6	116.9 (CH)	7.25 (1H, d, 1.3)	6	114.8	7.41 (1H, m)
7	156.3 (C)		7	158.1	
8	121.7 (CH)	6.96 (1H, d, 8.6)	8	121.0	7.11 (1H, m)
9	123.7 (CH)	6.96 (1H, d, 8.6)	9	123.6	7.06 (1H, m)
10	131.3 (CH)	6.87 (1H, s)	10	131.5	6.89 (1H, s)
11	129.7 (C)		11	131.1	
12	127.9 (C)		12	127.7	
13	133.7 (C)		13	133.6	
14	130.2 (CH)	7.34 (1H,m)	14	130.2	7.35 (2H, m)
15	130.2 (CH)	7.41 (1H,m)	15	130.3	7.41 (2H, m)
16	130.9 (CH)	7.38 (1H, t, 7.3)	16	131.0	7.40 (1H, m)
17	130.2 (CH)	7.41 (1H, m)	17	130.3	7.41 (2H, m)
18	130.2 (CH)	7.34 (1H, m)	18	130.2	7.35 (2H, m)
19	36.1 (CH_3)	3.10 (3H, s)	19	36.1	3.10 (3H, s)
			7-OCH_3	56.1	3.83 (3H, s)

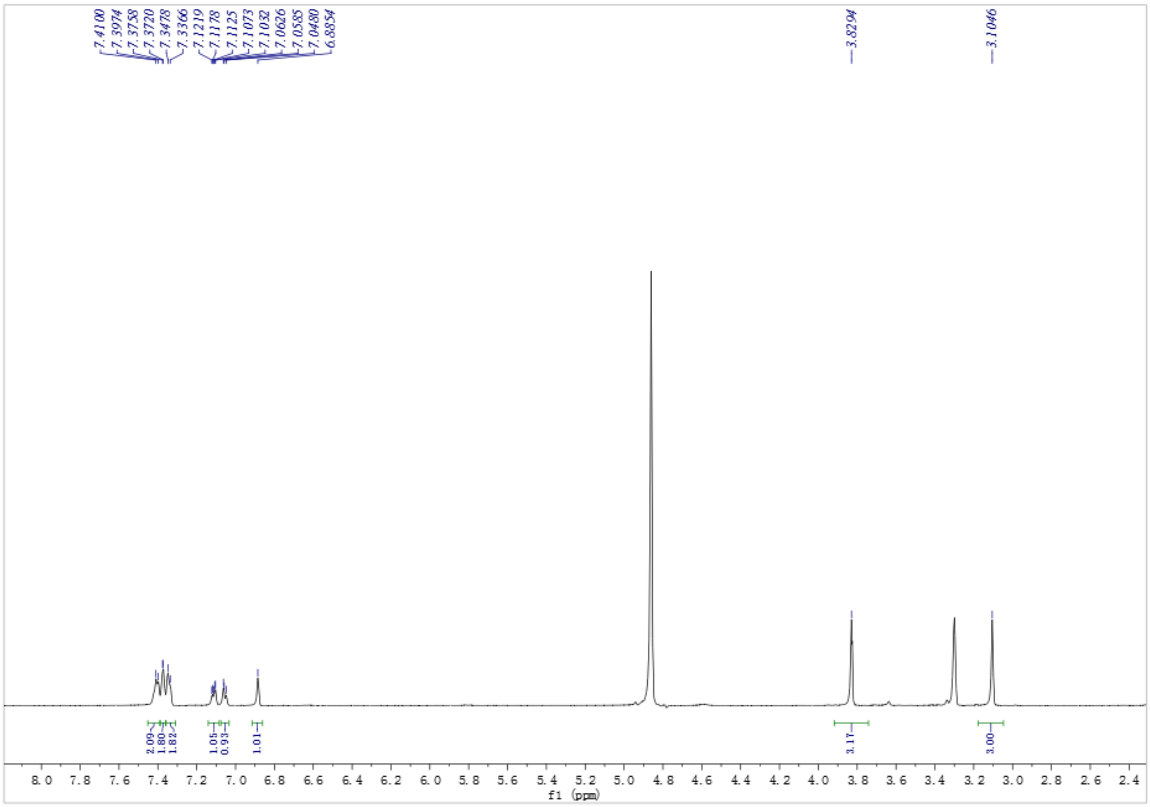

Figure S22: ^{1}H-NMR (800 MHz, CD_3OD) spectrum of **3** (7-methoxydehydrocyclopeptin)

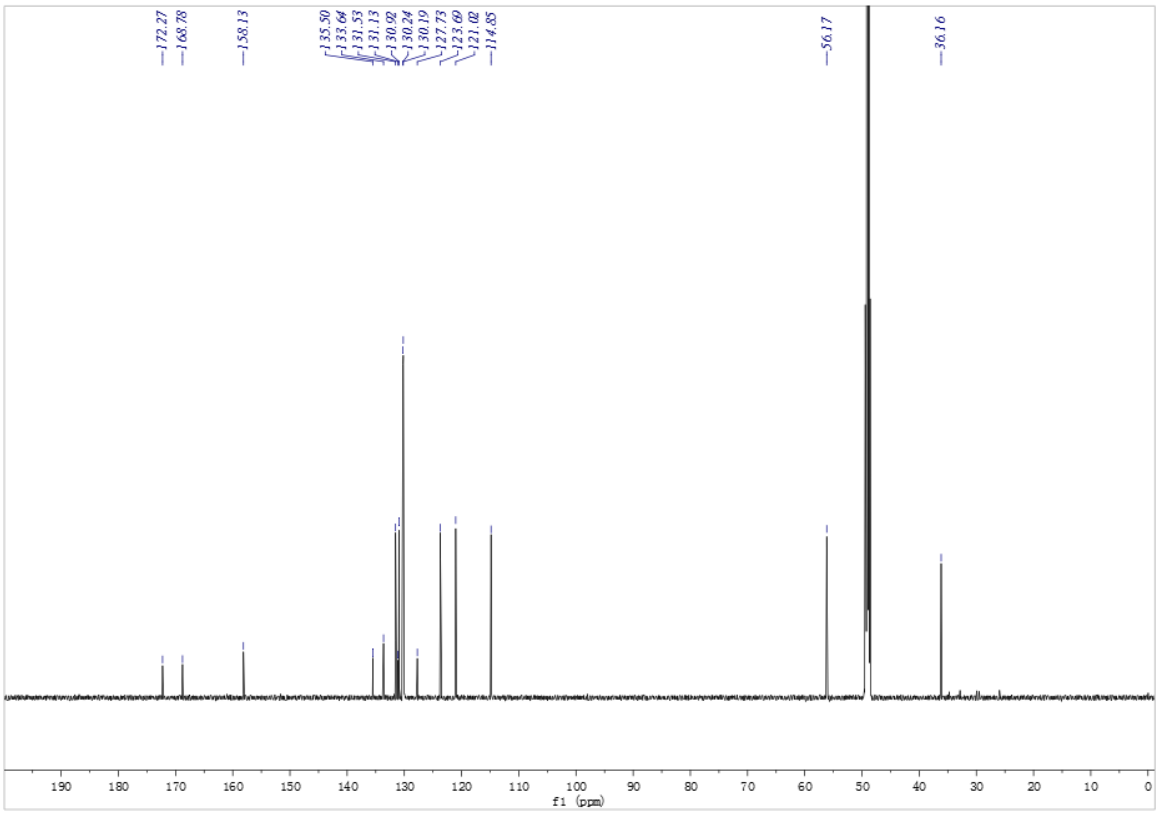

Figure S23: ^{13}C-NMR (200 MHz, CD_3OD) spectrum of **3** (7-methoxydehydrocyclopeptin)

Table S2. ^{1}H NMR and ^{13}C NMR data of compound **2** and **4** (800 MHz and 200 MHz, CD_3OD)

	2			**4**	
No.	**δ_C**	**δ_H (mult, *J*, Hz)**	**No.**	**δ_C**	**δ_H (mult, *J*, Hz)**
1	172.0 (C)		1	170.9 (C)	
2	69.9 (CH)	4.29 (1H, dd, 10.5, 7.1)	2	68.4 (CH)	4.32 (1H, dd, 10.7, 7.0)
3	35.1 (CH_2)	2.69 ($1H_a$, dd, 13.4, 10.7) 2.79 ($1H_b$, dd, 13.4, 7.0)	3	33.7 (CH_2)	2.68 ($1H_a$, dd, 13.4, 11.1), 2.81 ($1H_b$, dd, 13.4, 6.9)
4	137.3 (C)		4	135.7 (C)	
5	130.0 (CH)	7.04 (1H, d , 7.3)	5	128.6 (CH)	7.04 (1H, d, 7.4)
6	129.8 (CH)	7.23 (1H, m)	6	128.4 (CH)	7.24 (3H, m)
7	128.2 (CH)	7.23 (1H, m)	7	126.9 (CH)	7.24 (3H, m)
8	129.8 (CH)	7.23 (1H, m)	8	128.4 (CH)	7.24 (3H, m)
9	130.0 (CH)	7.04 (1H, d, 7.3)	9	128.6 (CH)	7.04 (1H, d, 7.4)
10	39.8 (CH_3)	2.92 (3H, s)	10	38.3 (CH_3)	2.92 (3H, s)
11	168.0 (C)		11	166.9 (C)	
12	128.8 (C)		12	126.4 (C)	
13	115.3 (CH)	7.44 (1H, d, 2.8)	13	130.9 (CH)	7.96 (1H, d, 7.7)
14	158.1 (C)		14	124.4 (CH)	7.35 (1H, t, 7.5)
14-OCH_3	56.2 (CH_3)	3.88 (3H, s)			
15	120.9 (CH)	7.19 (1H, m)	15	132.8 (CH)	7.61 (1H, t, 7.6)
16	123.3 (CH)	7.10 (1H, m)	16	120.2 (CH)	7.17 (1H, d, 8.1)
17	137.2 (C)		17	135.6 (C)	
18	171.0 (C)		18	169.8 (C)	
19	57.9 (CH)	4.42 (1H, t, 7.6)	19	56.5 (CH)	4.43 (1H, t, 7.6)
20	32.9 (CH_2)	3.25 ($1H_a$, dd, 14.5, 7.2) 3.39 ($1H_b$, dd, 14.5, 7.9)	20	31.5 (CH_2)	3.27 ($1H_a$, dd, 14.5, 7.2) 3.41 ($1H_b$, dd, 14.5, 7.9)
21	138.2 (C)		21	136.7(C)	
22	130.0 (CH)	7.23 (1H, m)	22	128.6 (CH)	7.24 (1H, m)
23	129.6 (CH)	7.27 (1H, m)	23	128.2 (CH)	7.24 (1H, m)
24	127.8 (CH)	7.17 (1H, m)	24	126.4 (CH)	7.17 (1H, m)
25	129.6 (CH)	7.27 (1H, m)	25	128.2 (CH)	7.29 (1H, dd, 15.5, 7.7)
26	130.0 (CH)	7.23 (1H, m)	26	128.6 (CH)	7.29 (1H, m)
27	29.6 (CH_3)	3.07(3H, s)	27	28.1 (CH_3)	3.07 (3H, s)
28	170.4 (C)		28	160.3(C)	
29	129.2 (C)		29	128.3(C)	
30	114.6 (CH)	7.31 (1H, d, 2.8)	30	130.4 (CH)	7.83 (1H, d, 7.7)
31	158.1 (C)		31	124.5(CH)	7.29 (1H, m)
31-OCH_3	56.1 (CH_3)	3.83 (3H, s)			
32	121.0 (CH)	7.11 (1H, m)	32	132.3 (CH)	7.53 (1H, t, 7.4)
33	123.7 (CH)	7.01 (1H, d, 8.8)	33	120.6 (CH)	7.08 (1H, d, 8.0)
34	138.2 (C)		34	136.6 (C)	

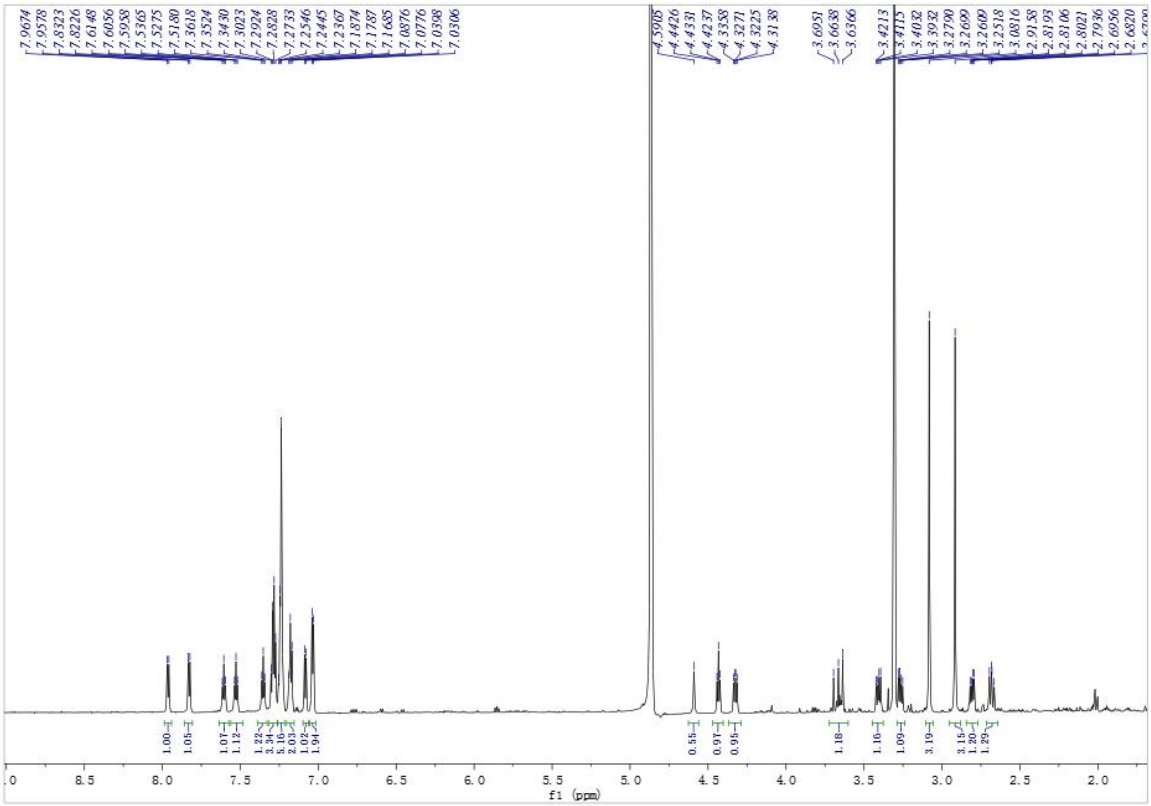

Figure S24: ^{1}H-NMR (800 MHz, CD_3OD) spectrum of **4** (penicopeptide A)

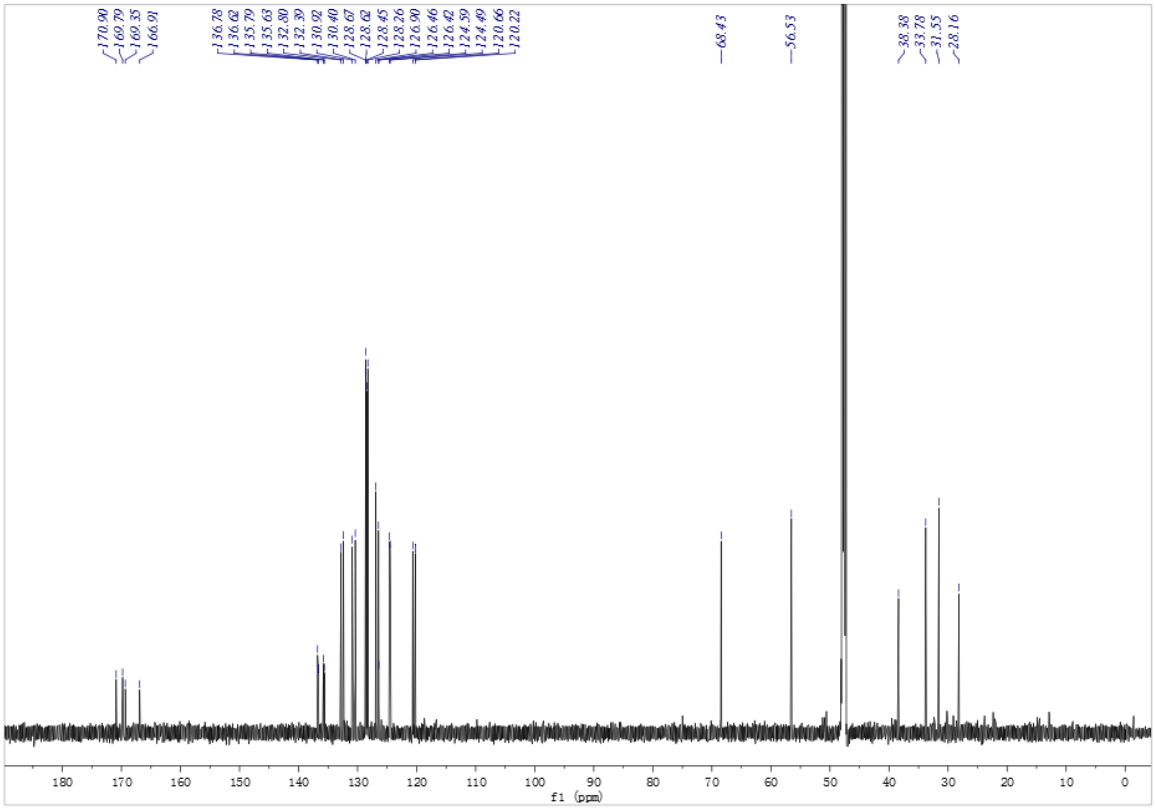

Figure S25: ^{13}C-NMR (200 MHz, CD_3OD) spectrum of **4** (penicopeptide A)

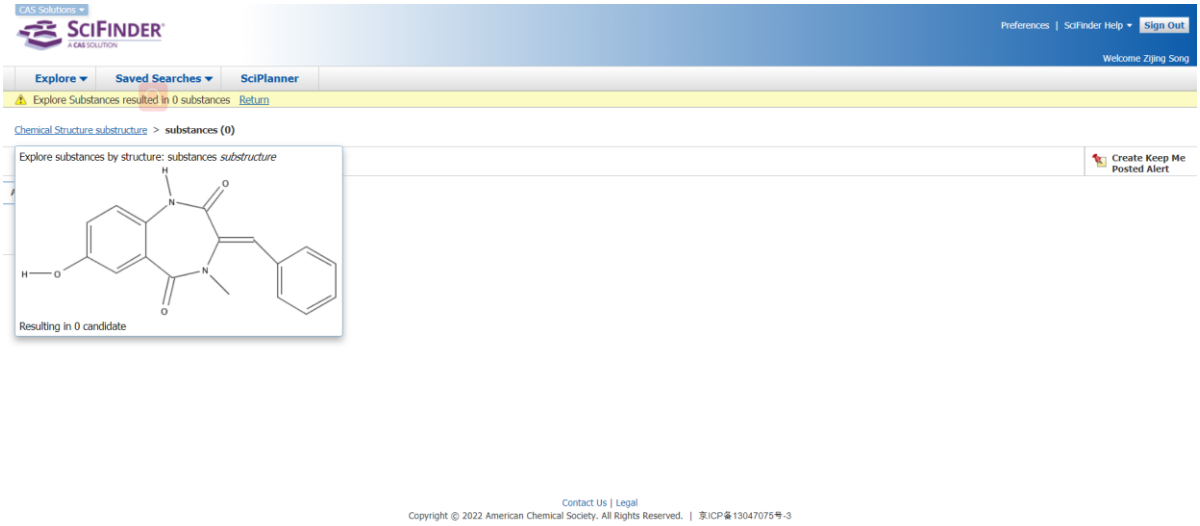

Figure S26: The Scifinder search reports of the compound **1**

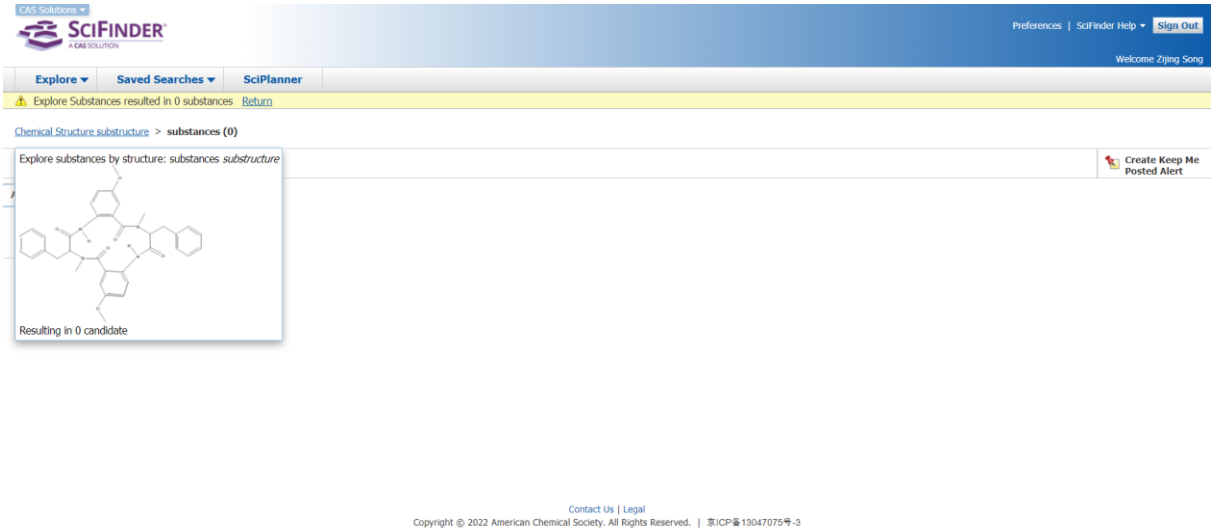

Figure S27: The Scifinder search reports of the compound **2**

VeriGuide - Originality Report
Individual Report

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Similarity Statistics Overview

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Similar Sentence(s) Filtered by User:	16 out of 358 sentences = 4.47%
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Similarity Statistics for Each Source

Entry	Source	From	Similarity
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Figure S28: VeriGuide originality report