

Supporting Information

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A New Butoxy Substituted Indolediketopiperazine from the Marine Derived Fungus *Aspergillus* sp. 66may

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Mass Spectrum SmartFormula Report

Analysis Info		Acquisition Date	5/6/2023 4:07:04 PM
Analysis Name	D:\Data\202304\16-1_000001.d	Operator	
Method	4_17_Mass_range_pos_7T	Instrument	solariX
Sample Name	16-1		
Comment			

Acquisition Parameter					
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n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
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Broadband High Mass	1000.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a	Calibration Date	Mon Mar 20 10:54:37
Pulse Program	basic	n/a	n/a	Data Acquisition Size	2028576
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Ion Accumulation Time	0.200 sec	n/a	n/a		
Flight Time to Acq. Cell	0.001 sec				

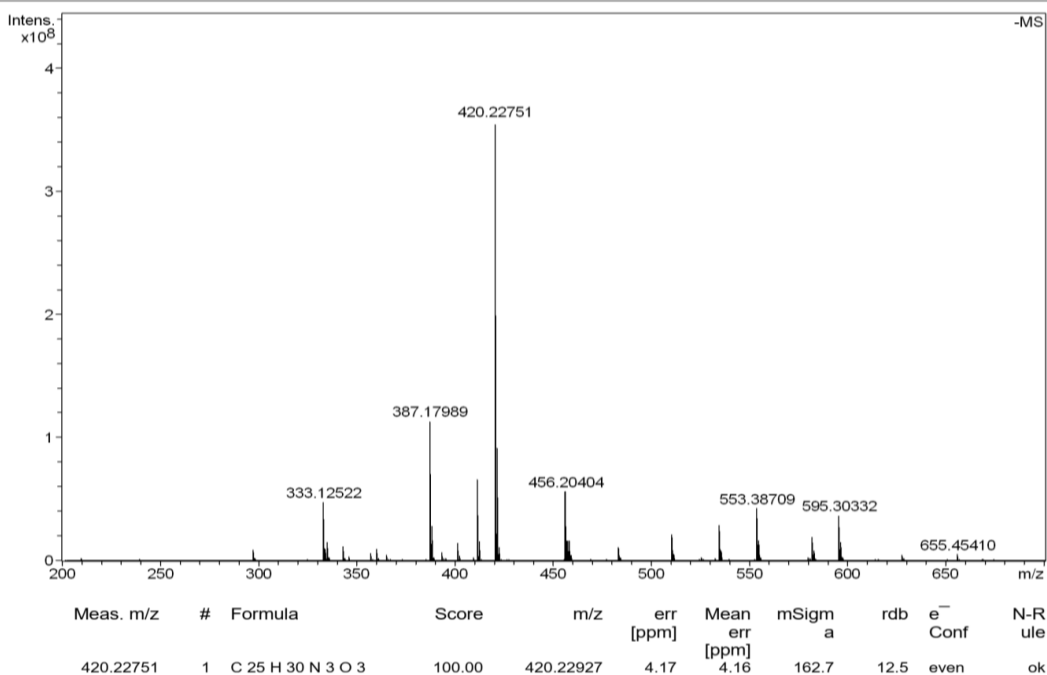


Figure S1: HRESIMS spectrum for n-butoxybrevianamide V (1)

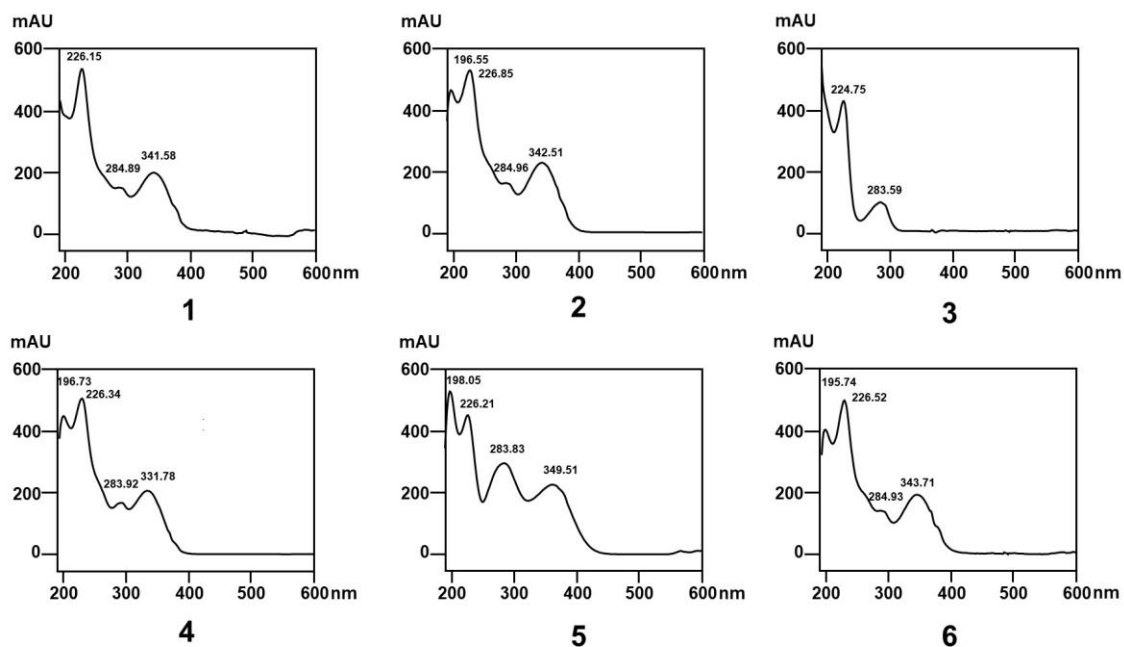


Figure S2: The UV characteristics of compounds **1–6**.

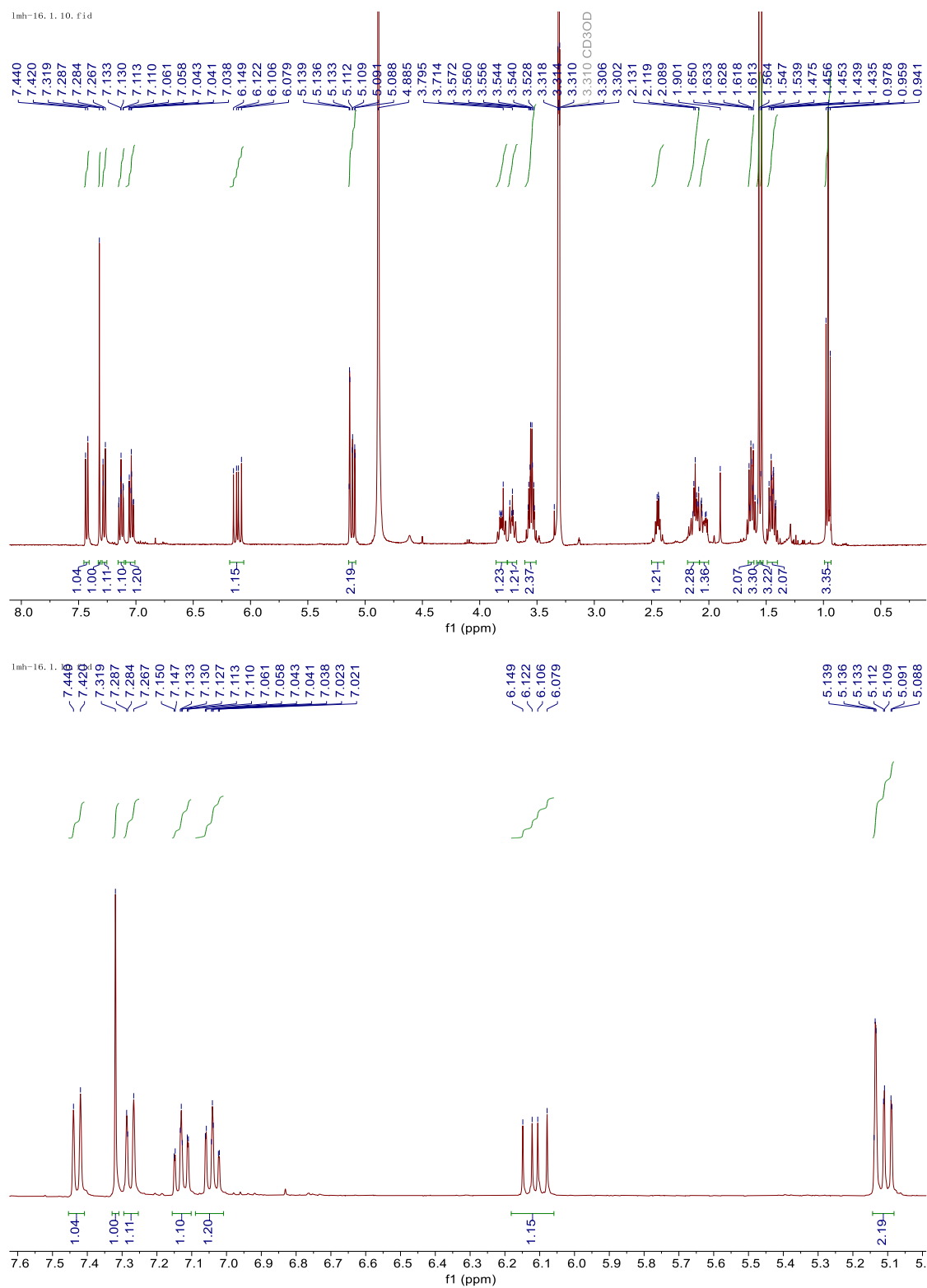


Figure S3: The ^1H NMR (400 MHz) and the expanded ^1H NMR (400 MHz) spectra of n-butoxylbrevianamide **V** (**1**) in CD_3OD (5-7.6 ppm range).

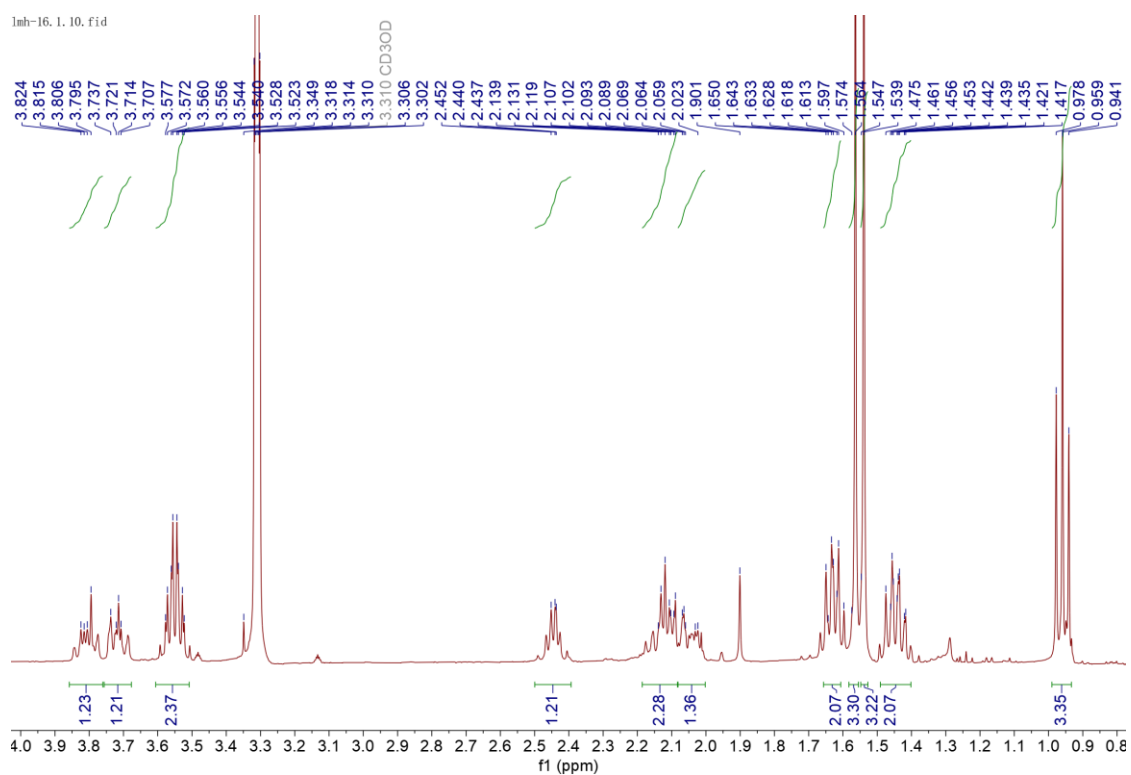
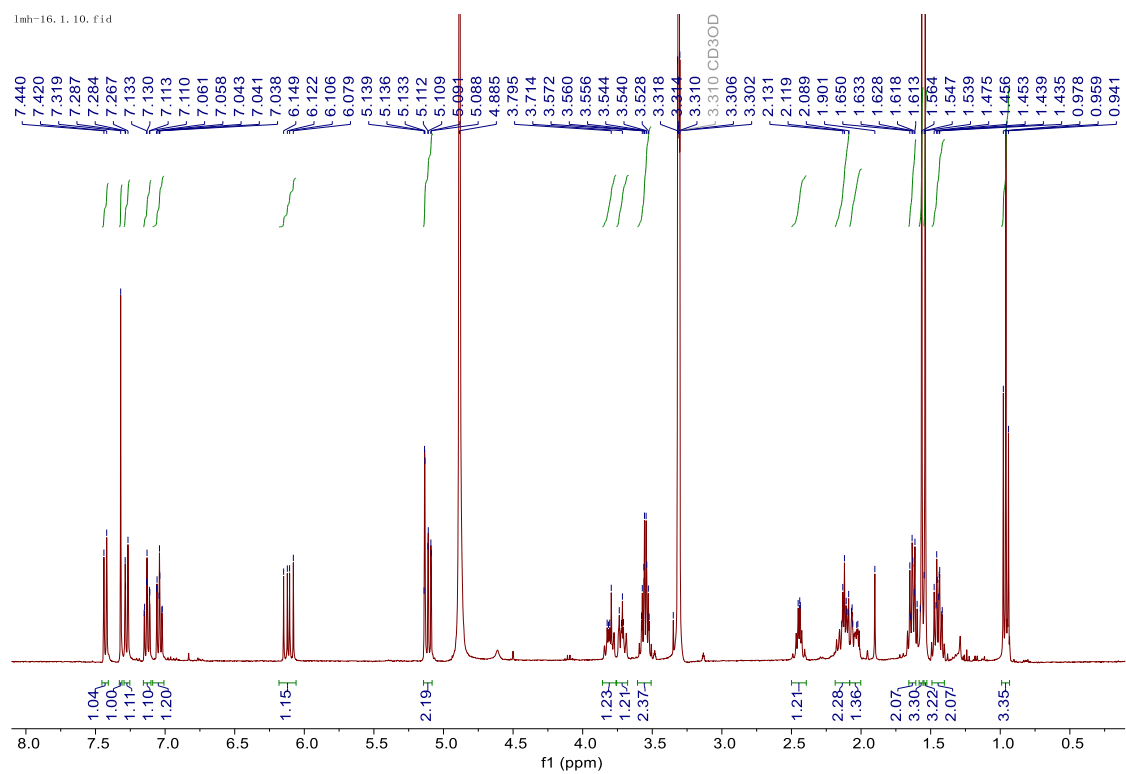


Figure S4: The ^1H NMR (400 MHz) and the expanded ^1H NMR (400 MHz) spectra of n-butoxylbrevianamide **V** (**1**) in CD_3OD (0.8-4 ppm range).

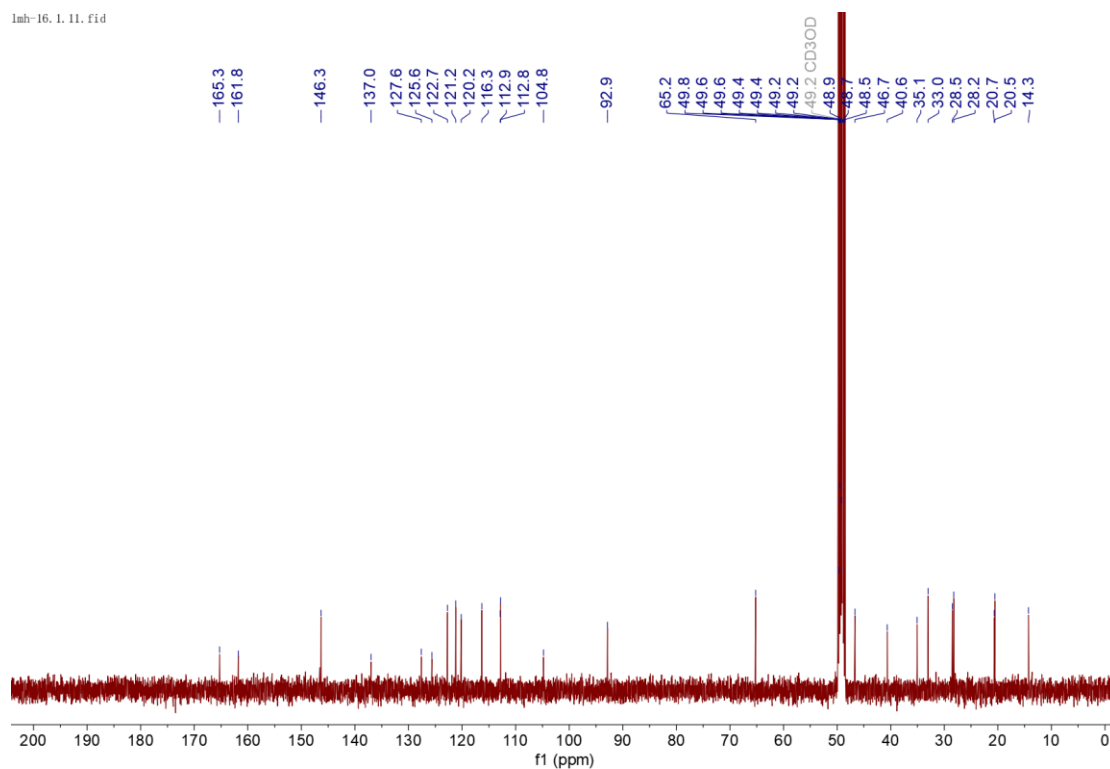


Figure S5: The ^{13}C NMR (100 MHz) spectrum of n-butoxybrevianamide V (**1**) in CD_3OD .

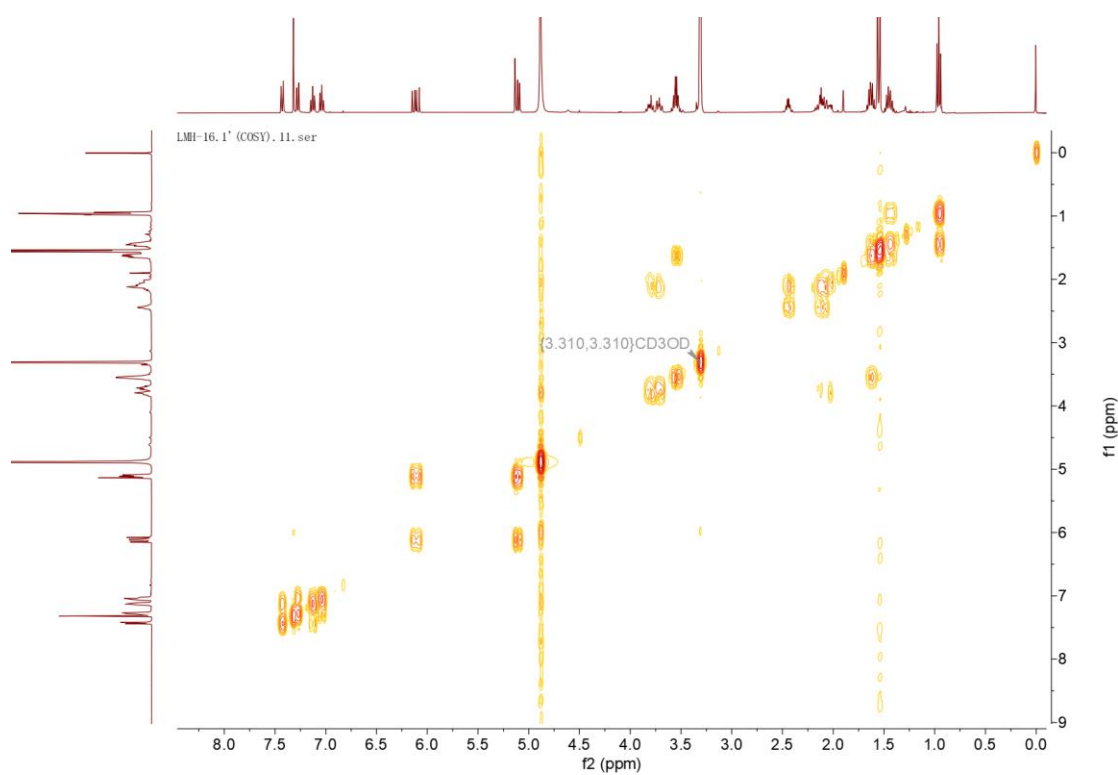


Figure S6: The ^1H - ^1H COSY spectrum of n-butoxybrevianamide V (**1**) in CD_3OD .

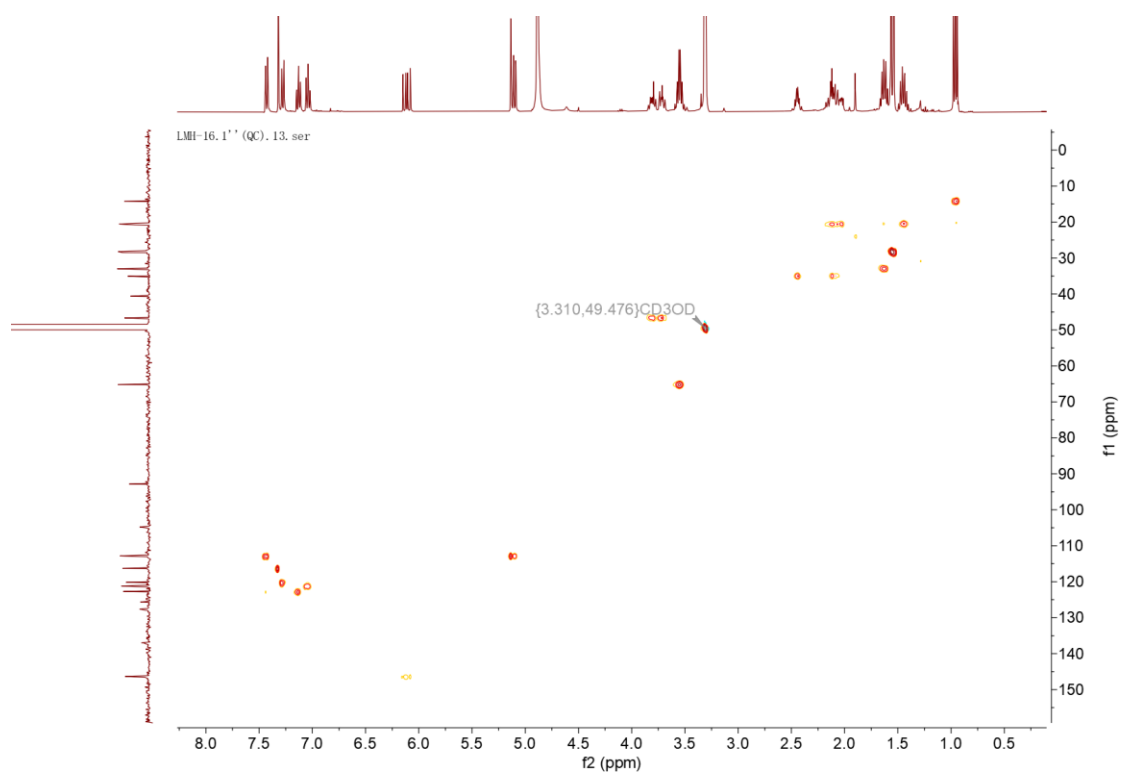


Figure S7: The HSQC spectrum of n-butoxybrevianamide V (**1**) in CD₃OD.

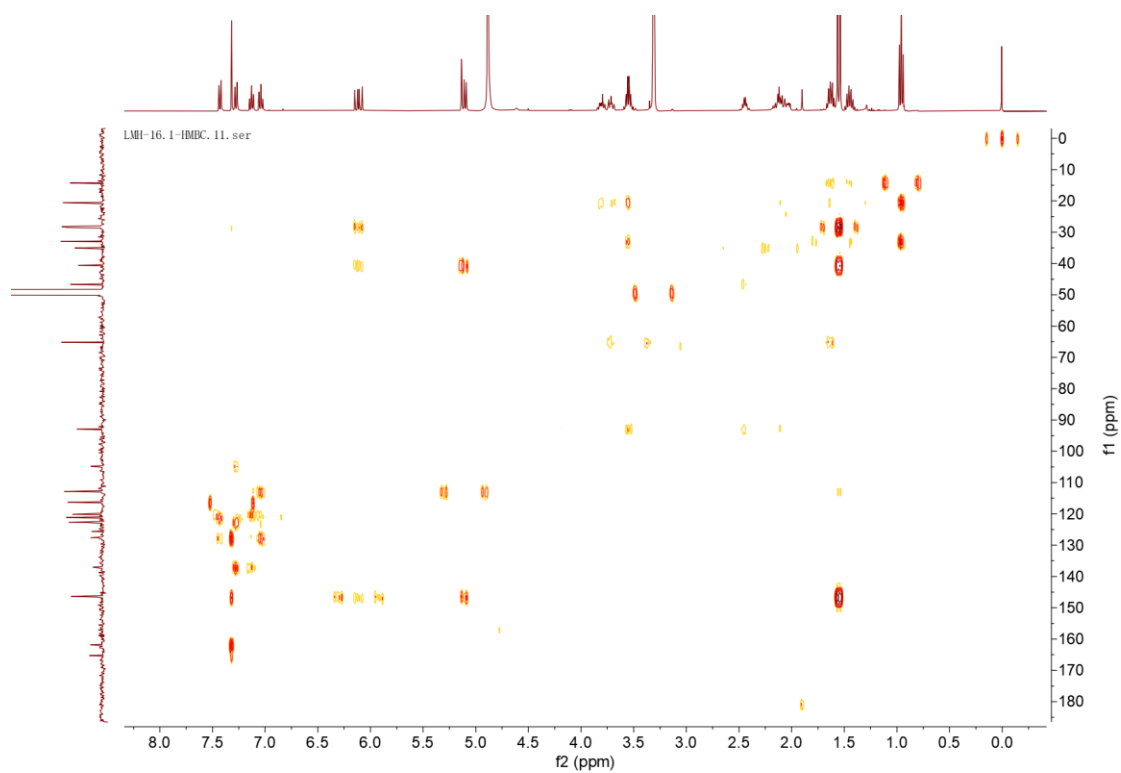


Figure S8: The HMBC spectrum of n-butoxybrevianamide V (**1**) in CD₃OD.

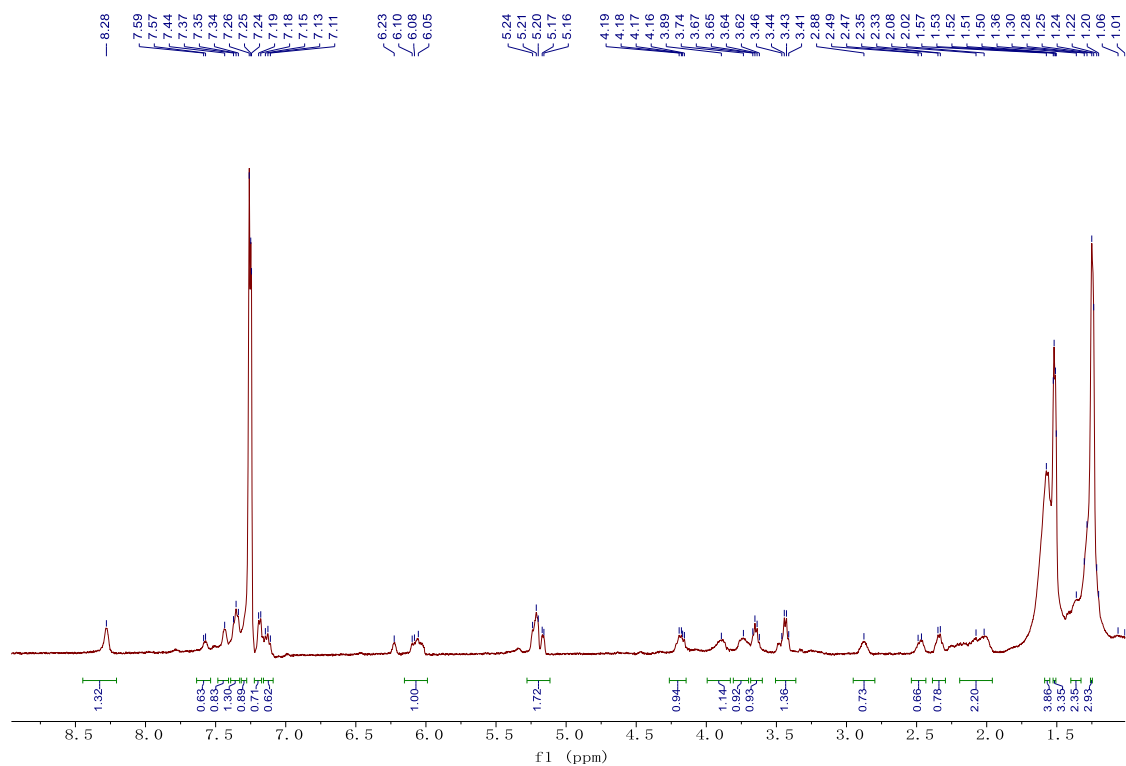


Figure S9: The ^1H NMR (400 MHz) spectrum of n-butoxybrevianamide V (**1**) in CDCl_3 .

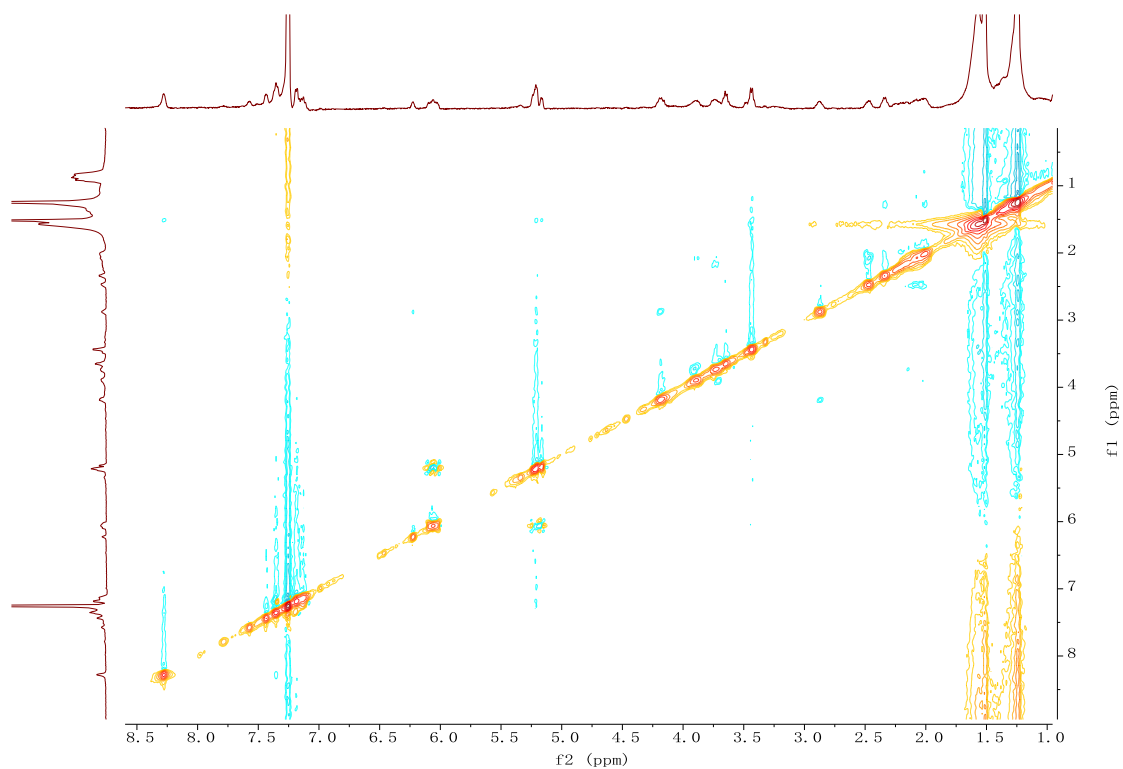


Figure S10: The NOESY spectrum of n-butoxybrevianamide V (**1**) in CDCl_3 .

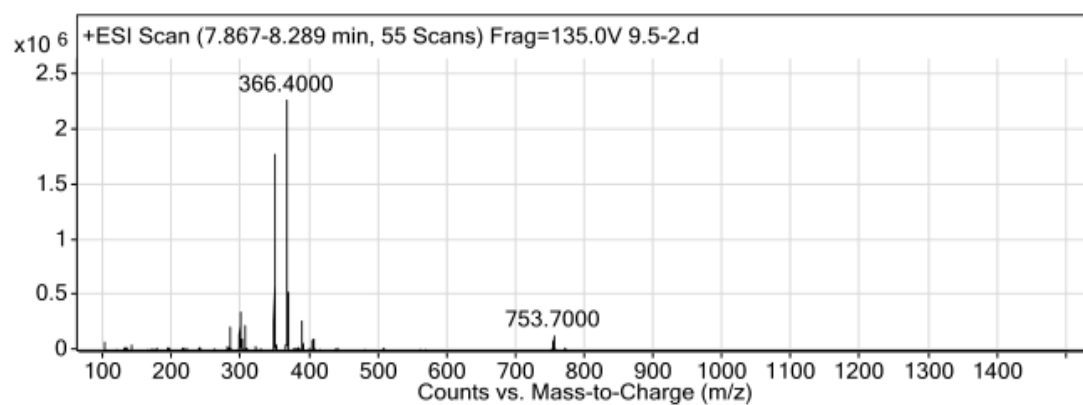


Figure S11: ESIMS spectrum for Brevianamide Q (**2**).

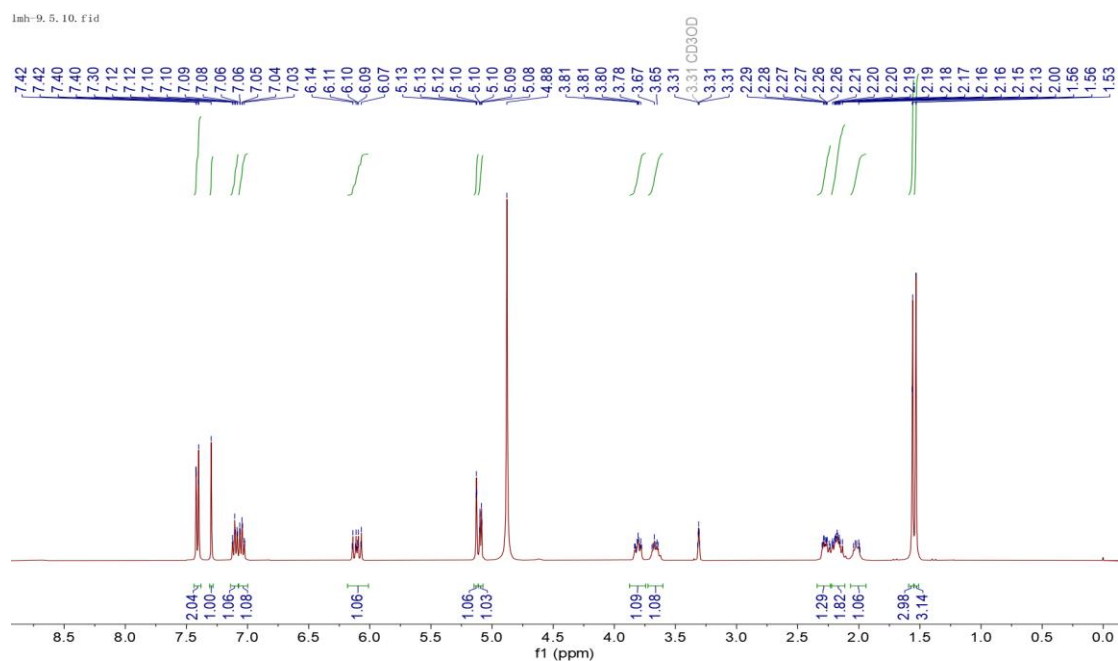


Figure S12: The ^1H NMR (400 MHz) spectrum of Brevianamide Q (**2**) in CD_3OD .

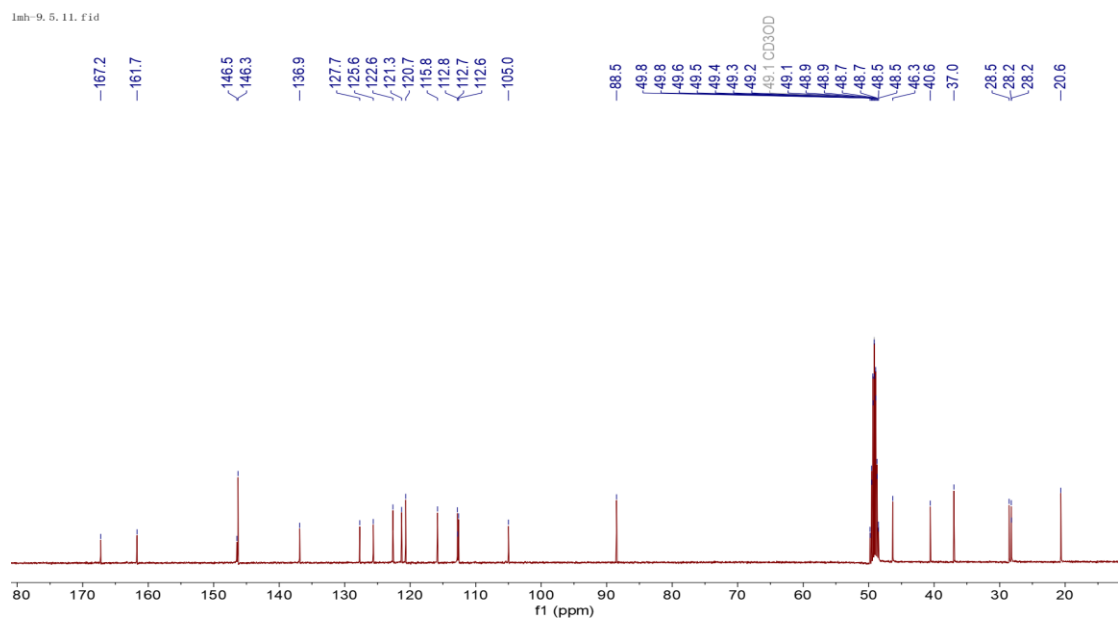


Figure S13: The ^{13}C NMR (100 MHz) spectrum of Brevianamide Q (**2**) in CD_3OD .

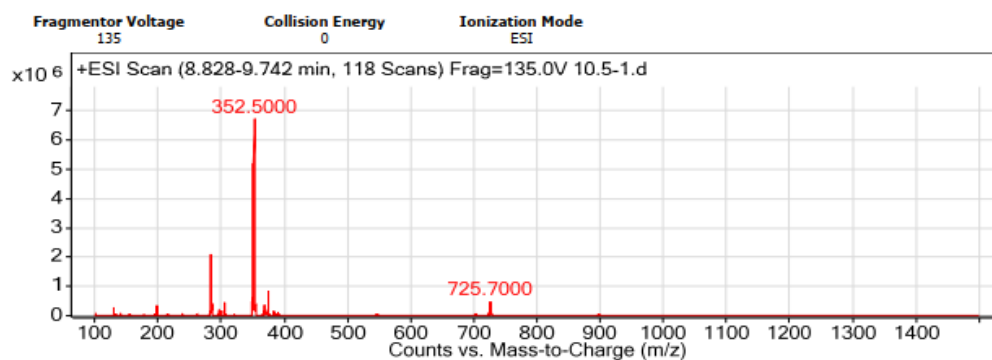


Figure S14: ESIMS spectrum for epi-deoxybrevianamide E (**3**).

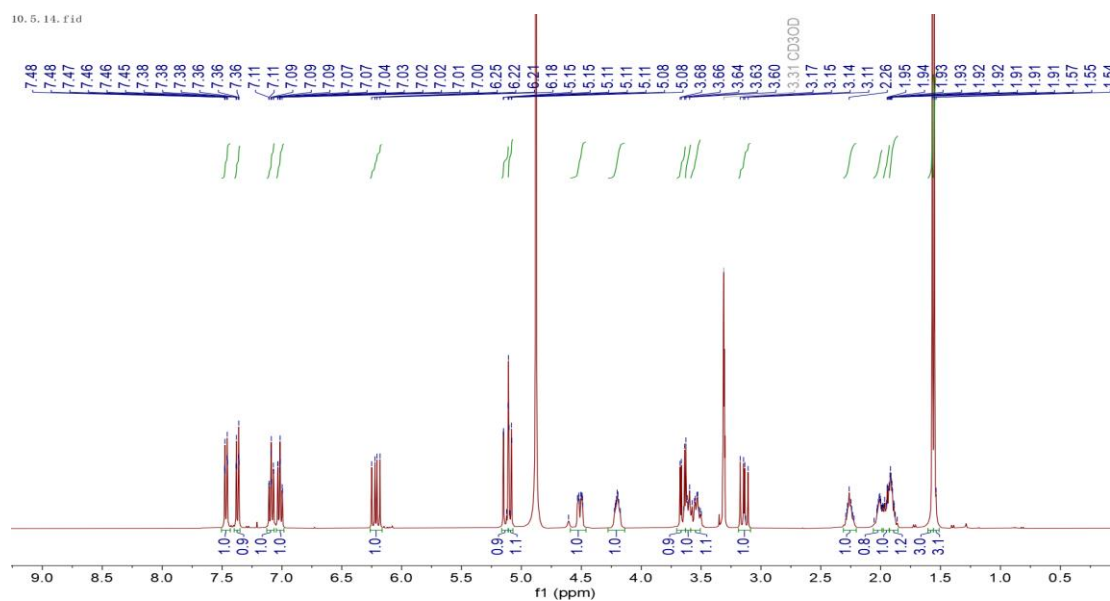


Figure S15: The ^1H NMR (400 MHz) spectrum of epi-deoxybrevianamide E (**3**) in CD_3OD .

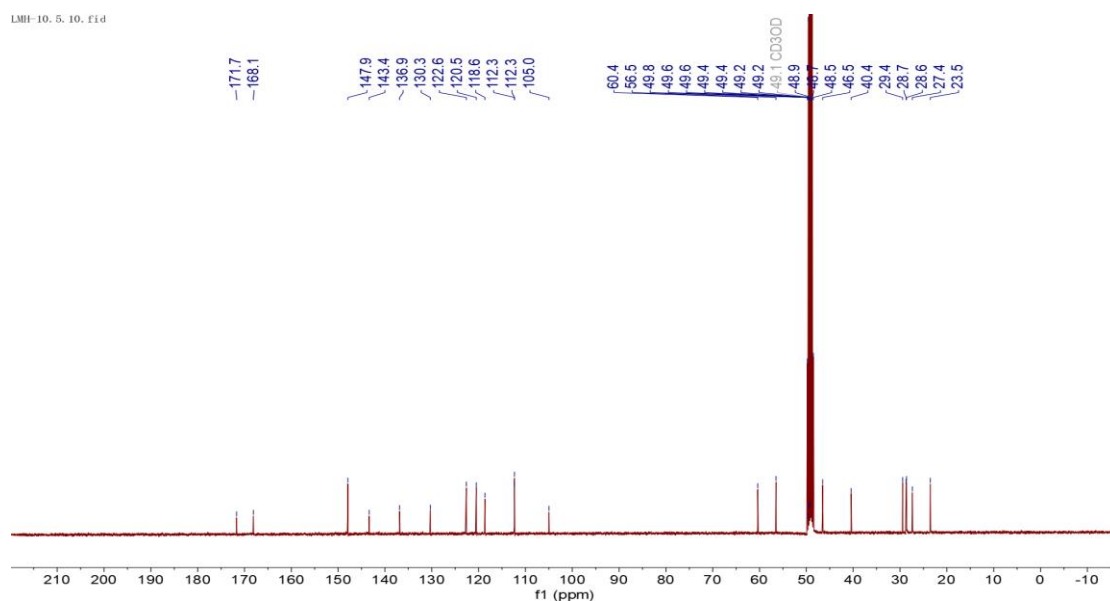


Figure S16: The ^{13}C NMR (100 MHz) spectrum of epi-deoxybrevianamide E (**3**) in CD_3OD .

CD₃OD.

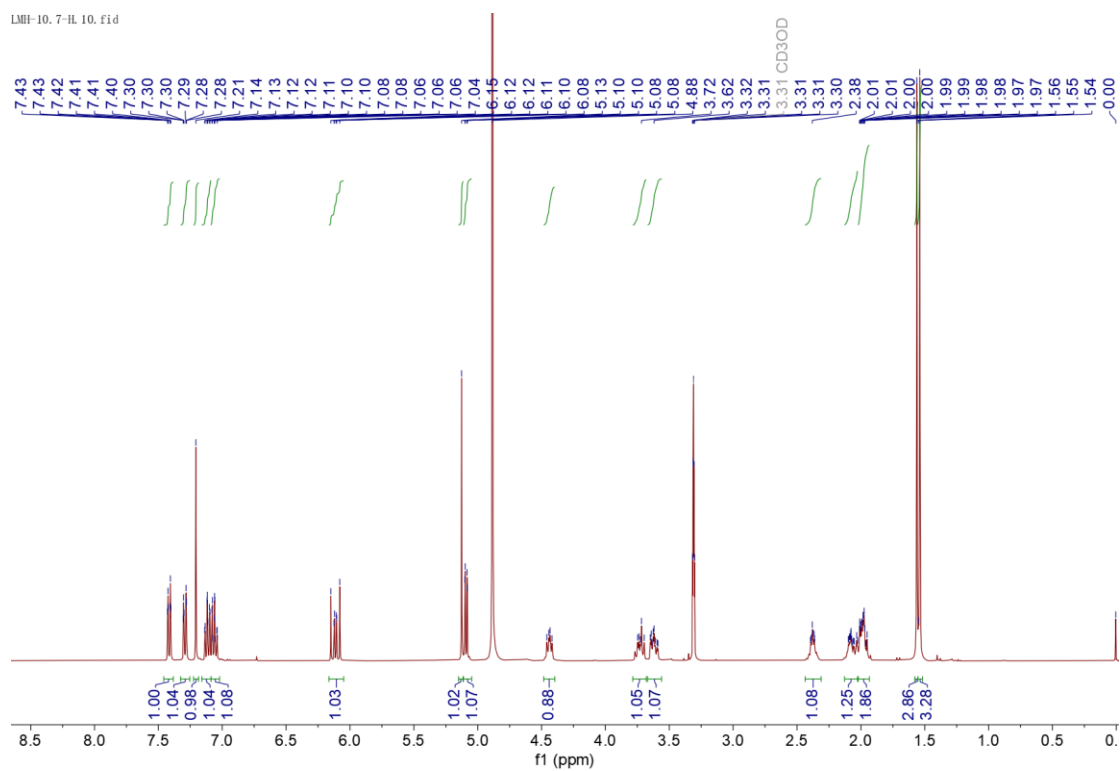


Figure S17: The ¹H NMR (400 MHz) spectrum of Brevianamide V (**4**) in CD₃OD.

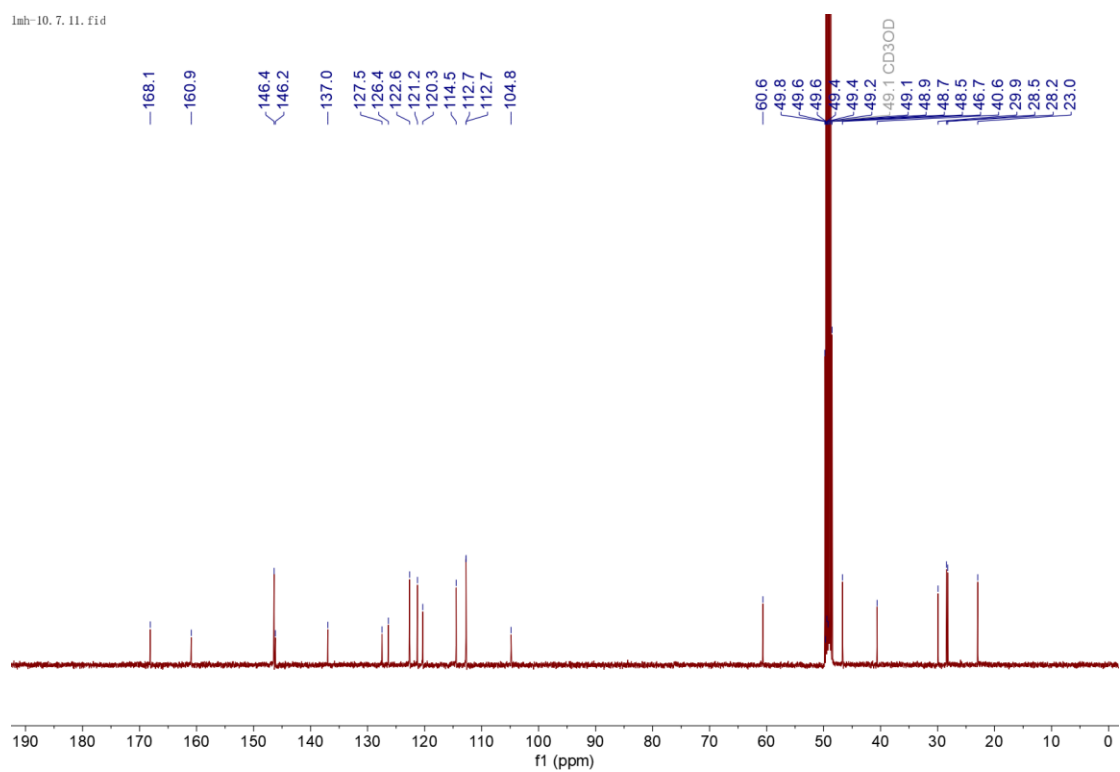


Figure S18: The ^{13}C NMR (100 MHz) spectrum of Brevianamide V (**4**) in CD_3OD .

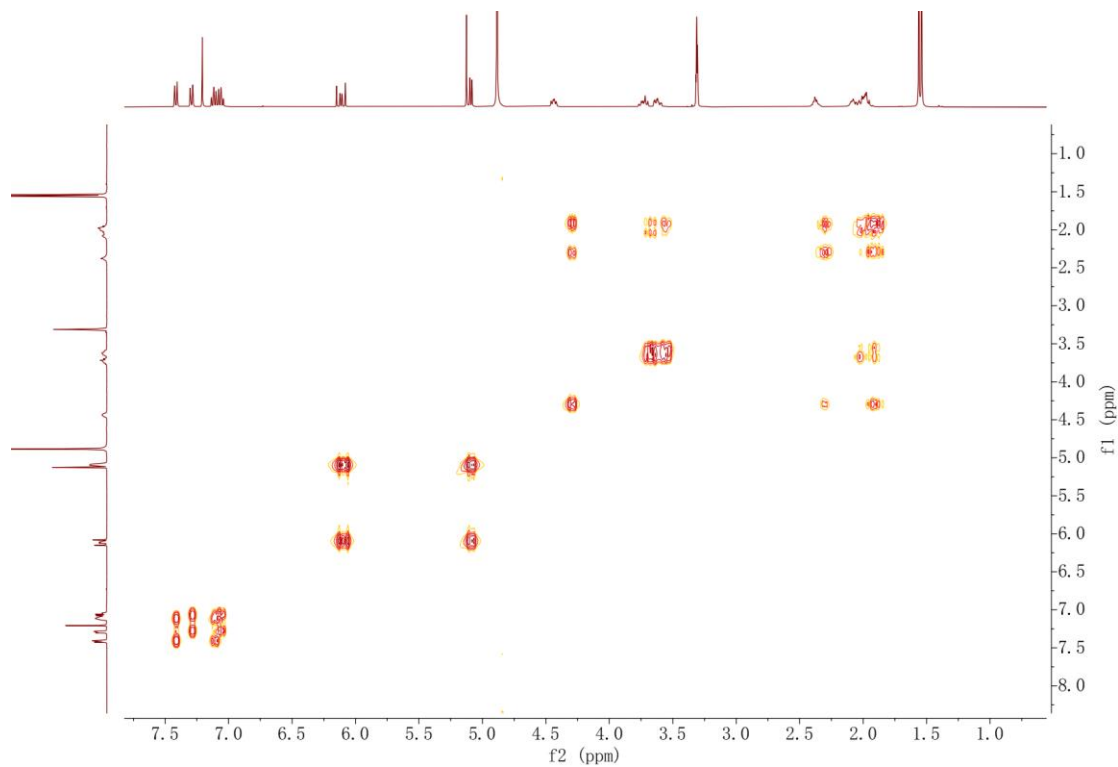


Figure S19: The ^1H - ^1H -COSY spectrum of Brevianamide V (**4**) in CD_3OD .

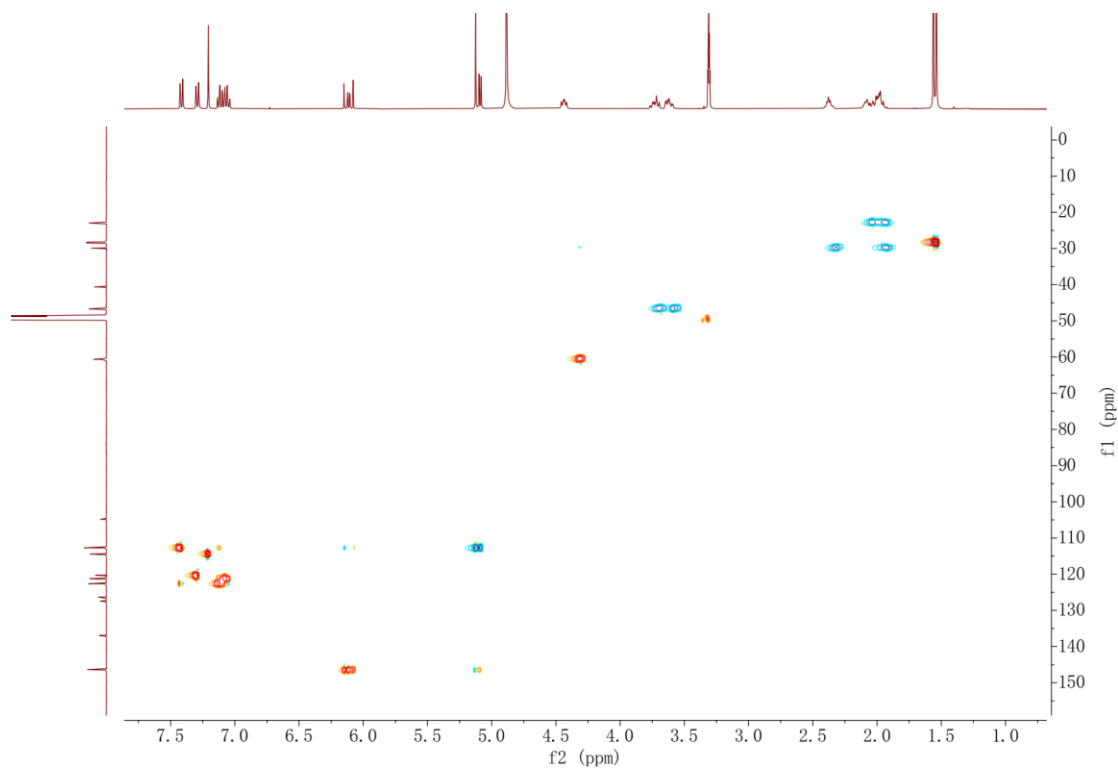


Figure S20: The HSQC spectrum of Brevianamide V (**4**) in CD₃OD.

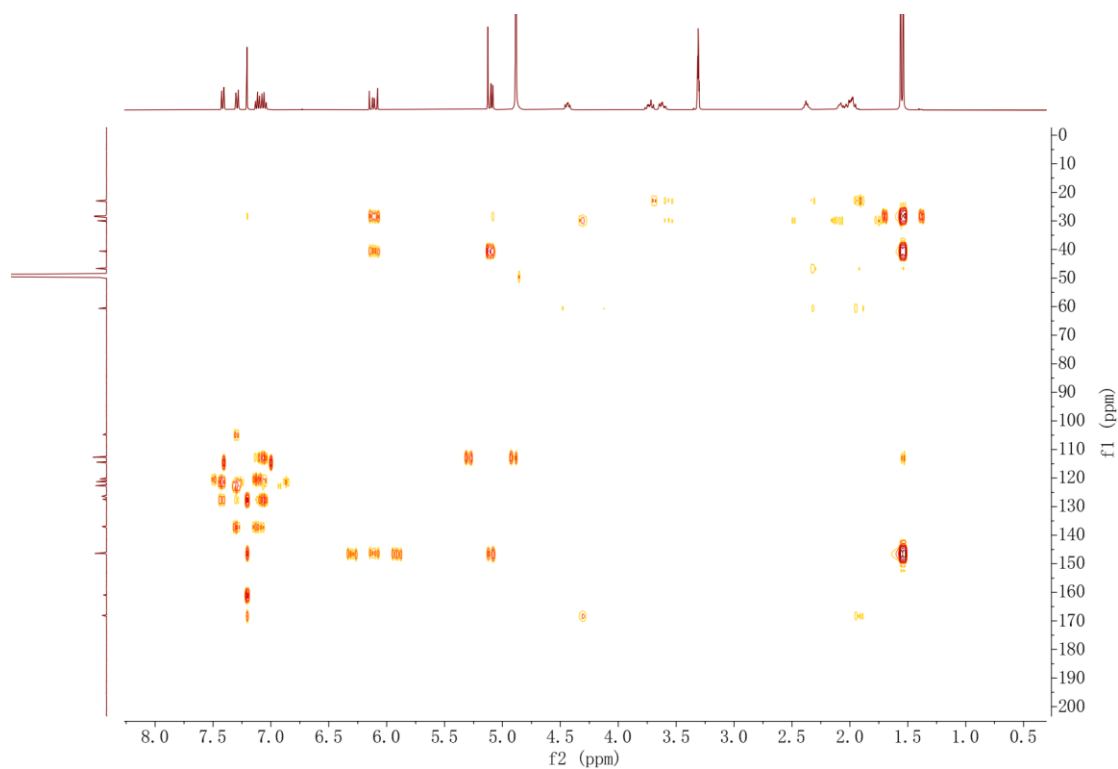


Figure S21: The HMBC spectrum of Brevianamide V (**4**) in CD₃OD.

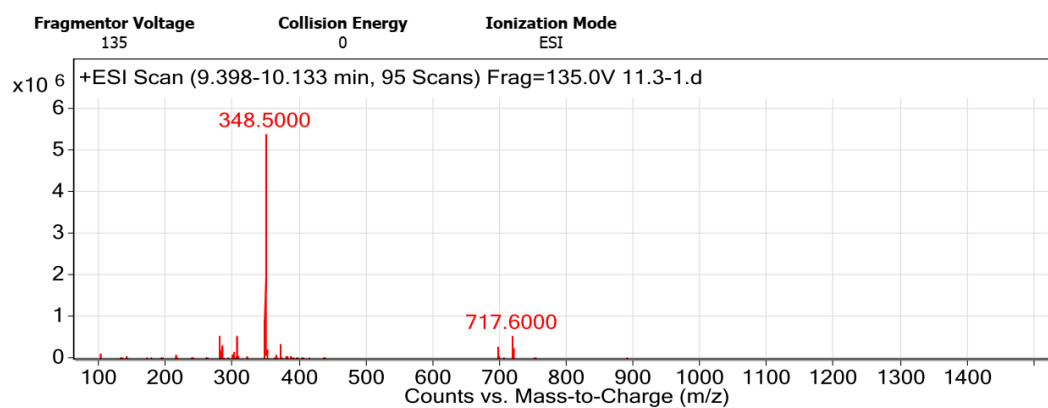


Figure S22: ESIMS spectrum for Brevianamide K (**5**).

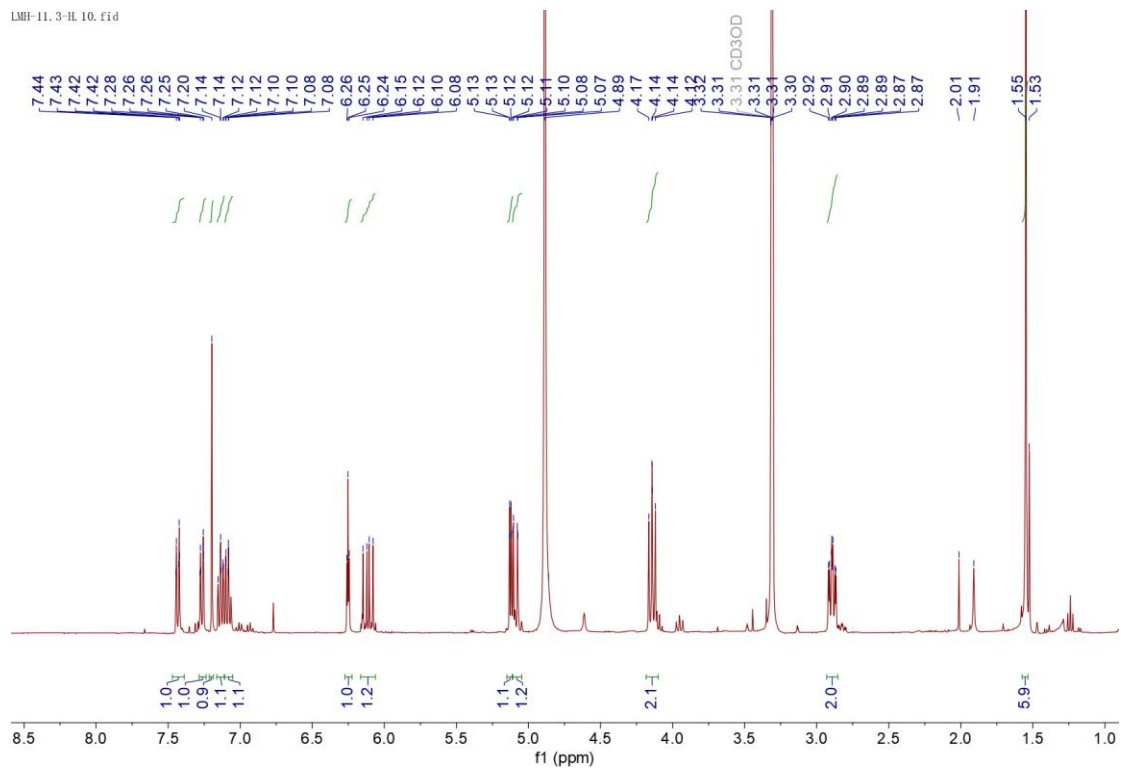


Figure S23: The ^1H NMR (400 MHz) spectrum of Brevianamide K (**5**) in CD_3OD .

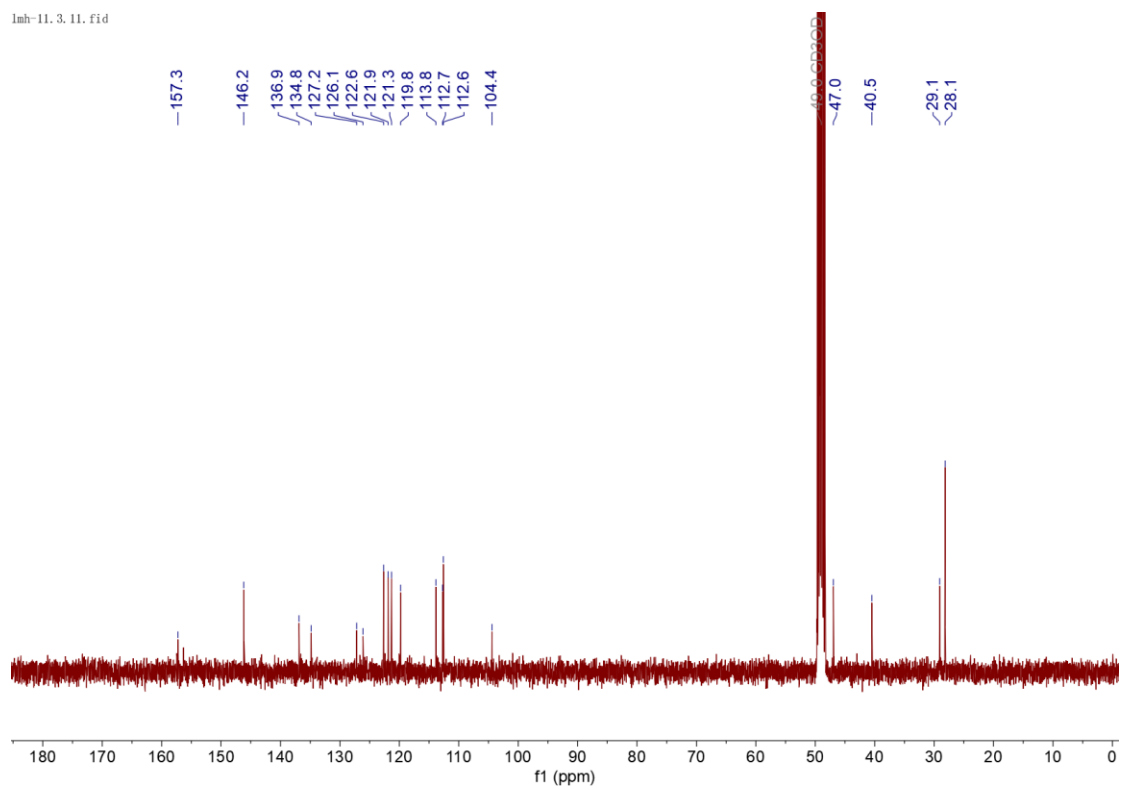


Figure S24: The ^{13}C NMR (100 MHz) spectrum of Brevianamide K (**5**) in CD_3OD .

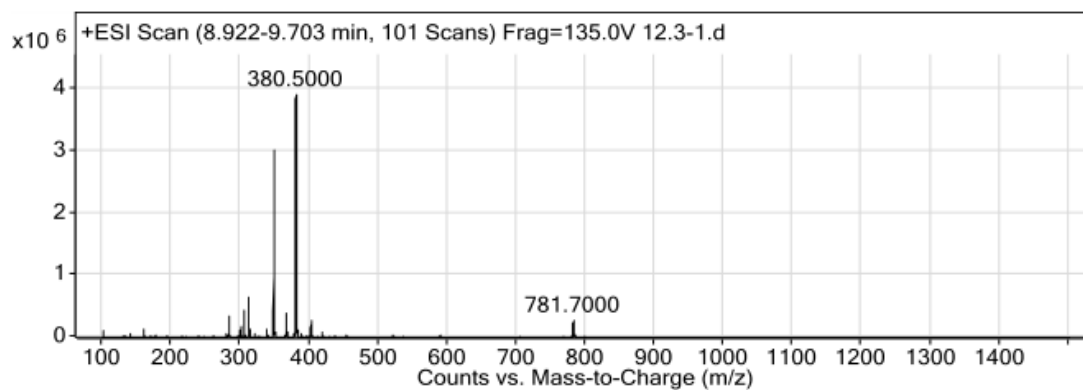


Figure S25: ESIMS spectrum for Brevianamide R (**6**).

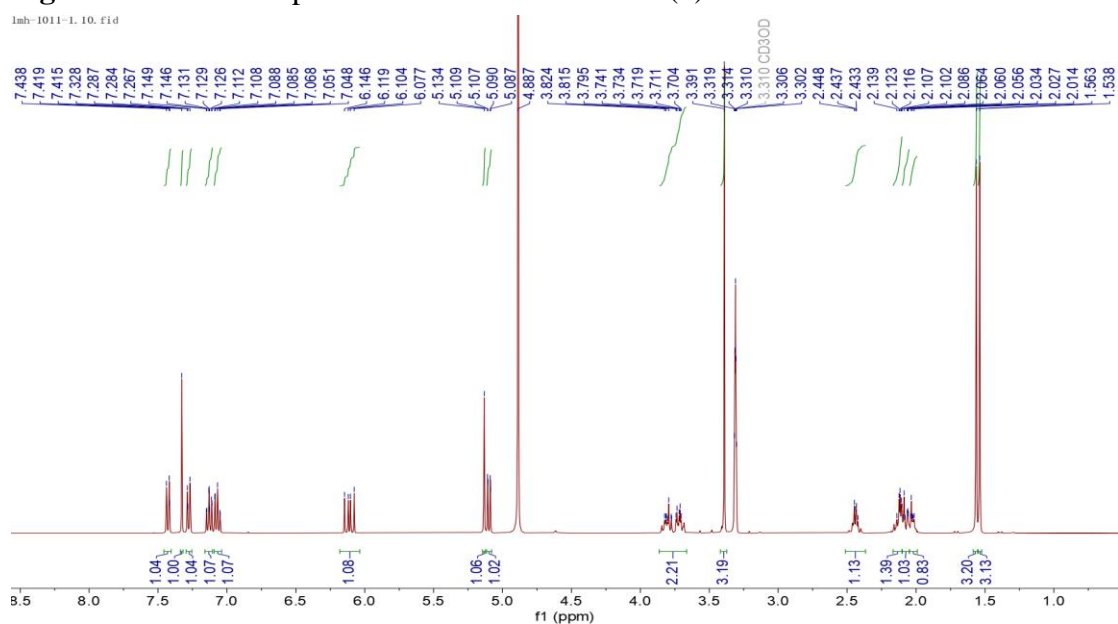


Figure S26: The ^1H NMR (400 MHz) spectrum of Brevianamide R (**6**) in CD_3OD .

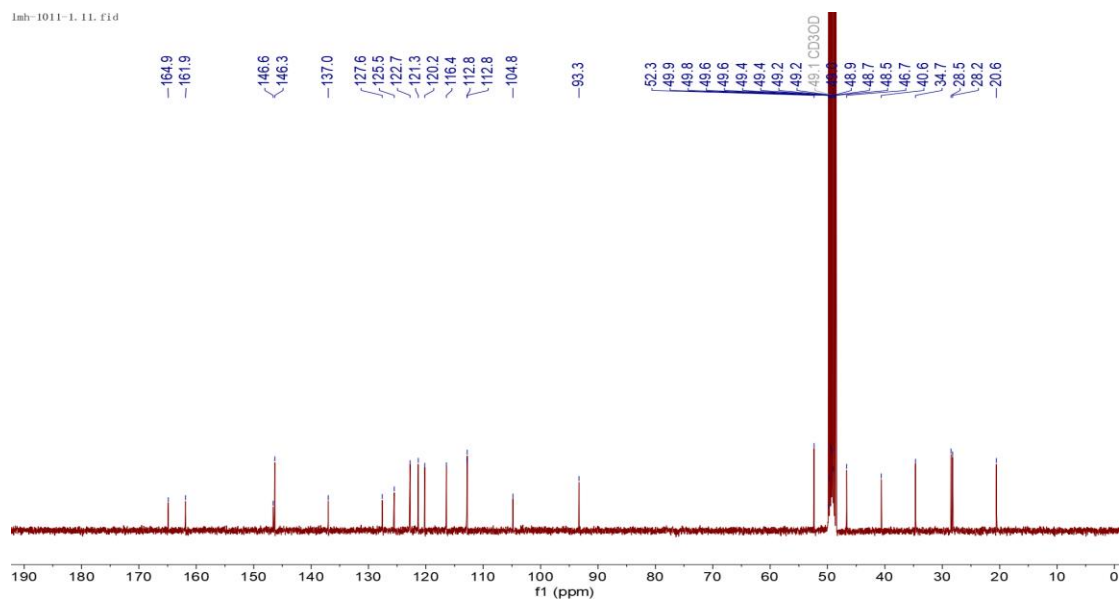


Figure S27: The ^{13}C NMR (100 MHz) spectrum of Brevianamide R (**6**) in CD_3OD .

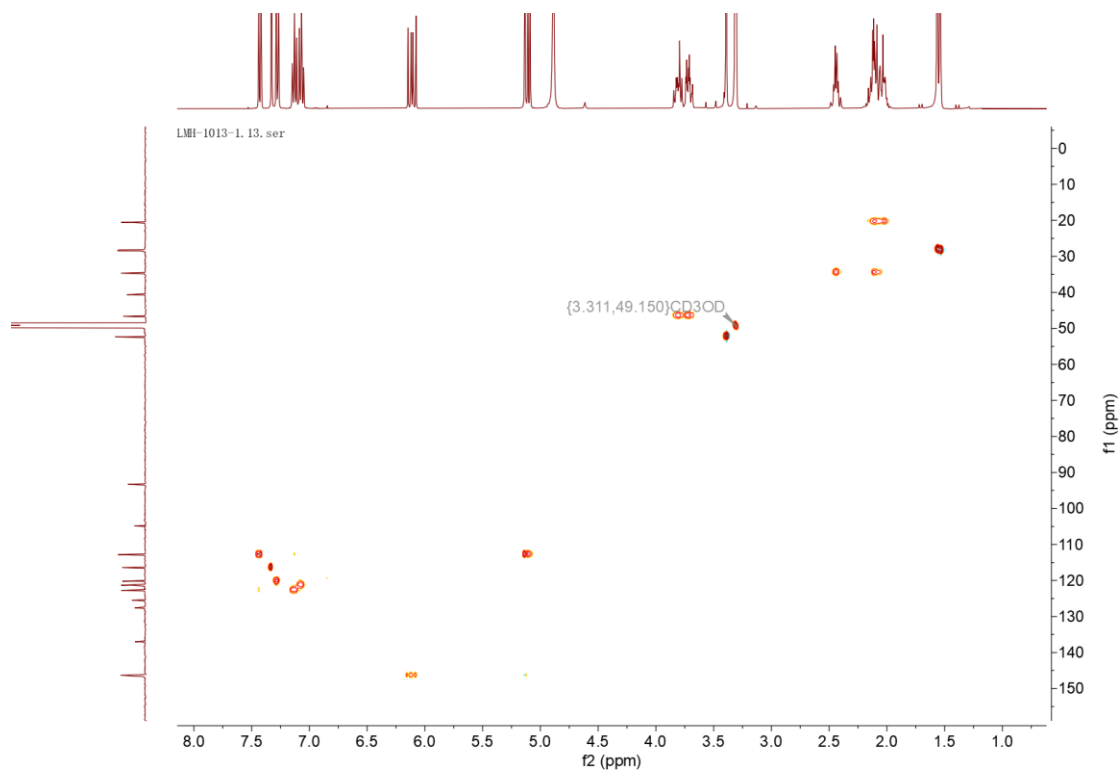


Figure S28: HSQC spectrum of Brevianamide R (**6**) in CD_3OD .

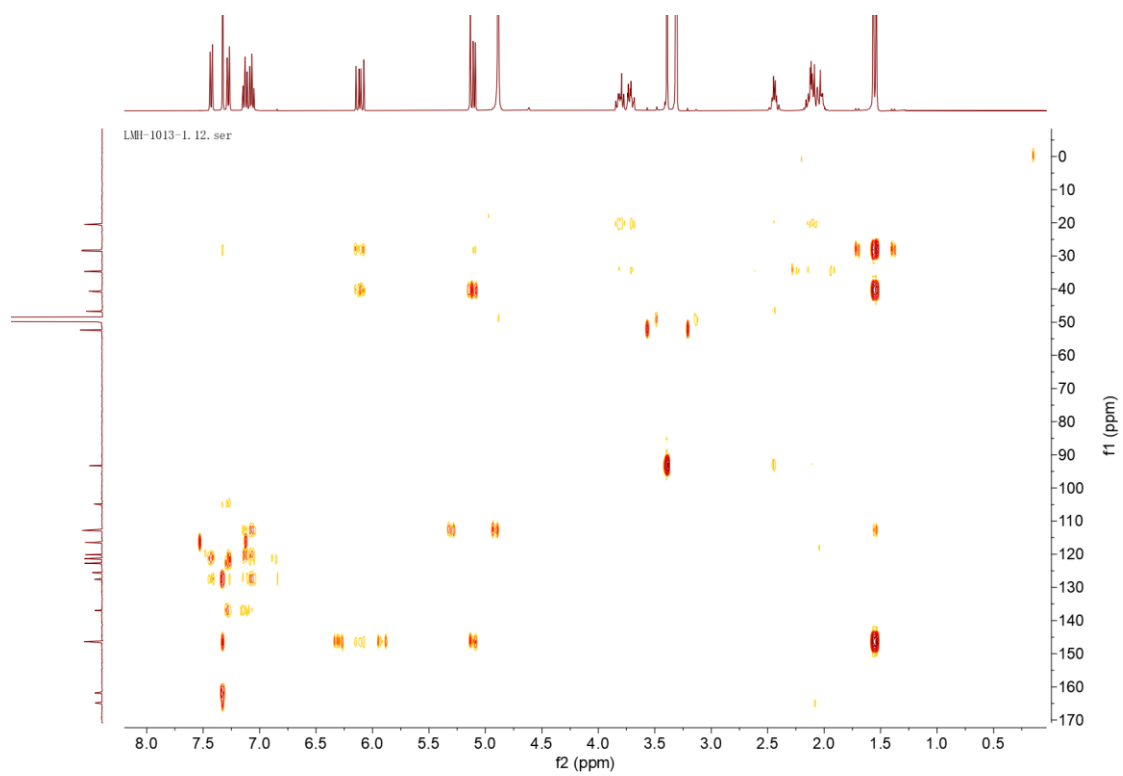


Figure S29: HMBC spectrum of Brevianamide R (**6**) in CD₃OD.

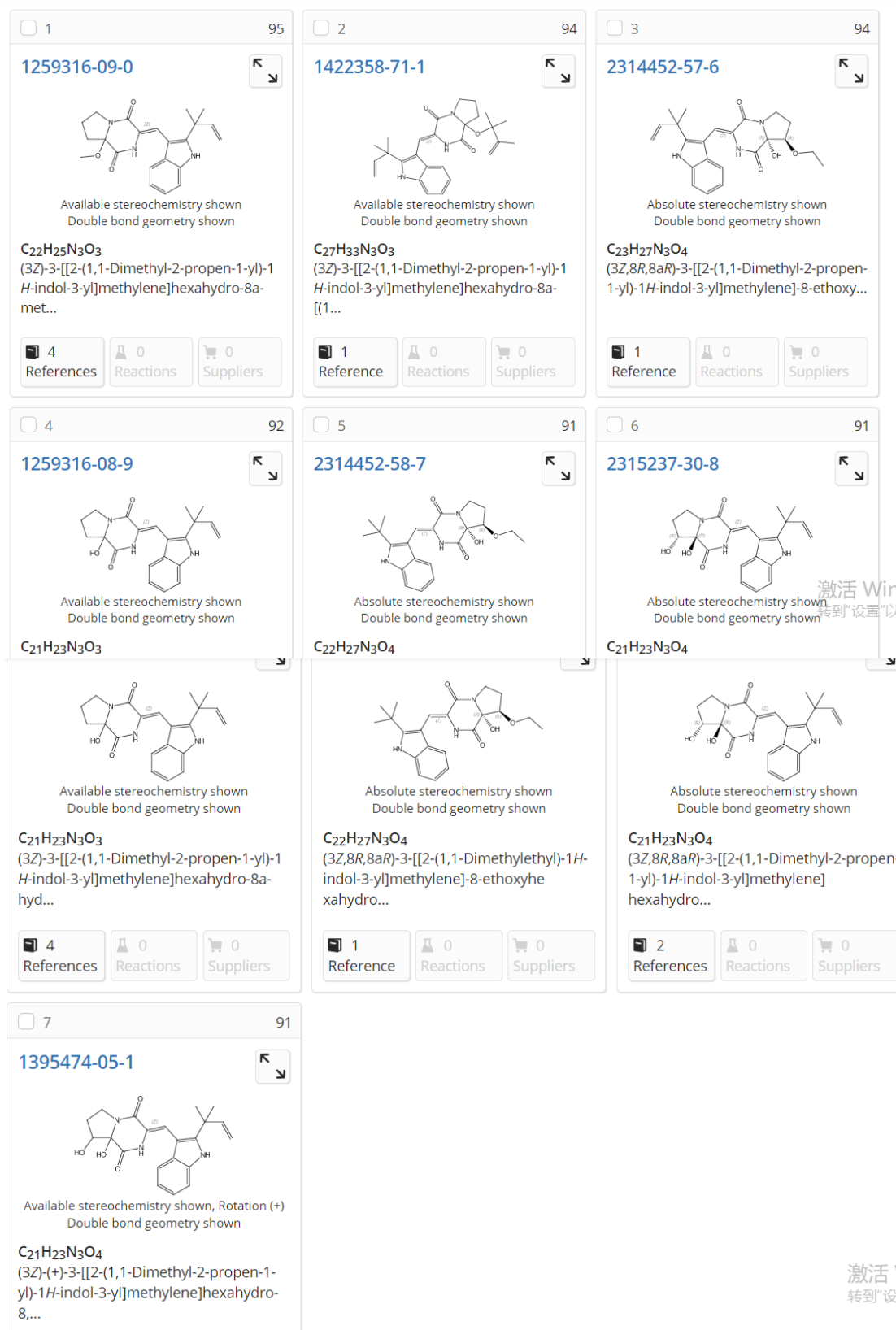
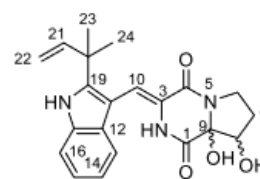
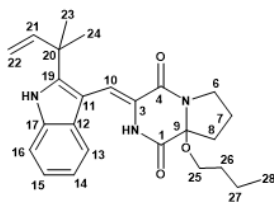


Figure S30: The similarity search report for compound **1** through scifinder.

n-butoxybrevianamide V



NO.	n-butoxybrevianamide V		(±)-brevianamide X	
	δ_{H} , mult. (<i>J</i> in Hz)	δ_{C}	δ_{H} , mult. (<i>J</i> in Hz)	δ_{C}
1		165.3, C		165.7, C
3		125.5, C		125.1, C
4		161.8, C		161.3, C
6	3.71, m; 3.81, m	46.7, CH ₂	3.96, m; 3.72, m	44.7, CH ₂
7	2.01, m; 2.12, m	20.5, CH ₂	1.93, m; 2.41, m	29.0, CH ₂
8	2.12, m; 2.44, m	35.1, CH ₂	4.41, m	76.4, CH
9		92.9, C		91.0, C
10	7.32, s	116.3, CH	7.29, s	115.1, CH
11		104.8, C		104.5, C
12		127.6, C		127.4, C
13	7.28, (d, 8.0)	120.2, CH	7.37, d (7.9)	120.2, CH
14	7.04, (t, 8.0)	121.2, CH	7.07, dd (7.9, 7.9)	121.3, CH
15	7.13, (t, 8.0)	122.7, CH	7.12, dd (7.9, 7.9)	122.6, CH
16	7.43, (d, 8.0)	112.9, CH	7.43, d (7.9)	112.6, CH
17		137.0, C		136.8, CH
19		146.5, C		146.2, CH
20		40.6, C		40.5, C
21	6.12, (dd, 17.2, 10.8)	146.3, CH	6.11, dd (17.3, 10.6)	146.1, CH
22	5.10, (d, 10.8); 5.12, (d, 17.6)	112.8, CH ₂	5.10, d (10.6); 5.13, d (17.3)	112.6, CH ₂
23	1.56, s	28.2, CH ₃	1.57, s	28.1, CH ₃
24	1.54, s	28.5, CH ₃	1.54, s	28.3, CH ₃
25	3.55, m	65.2, CH ₂		
26	1.63, m	33.0, CH ₂		
27	1.45, m	20.7, CH ₂		
28	0.96, (t, 7.2)	14.3, CH ₃		

Figure S31: The NMR data comparison of compound **1** with that of breviaamide X.

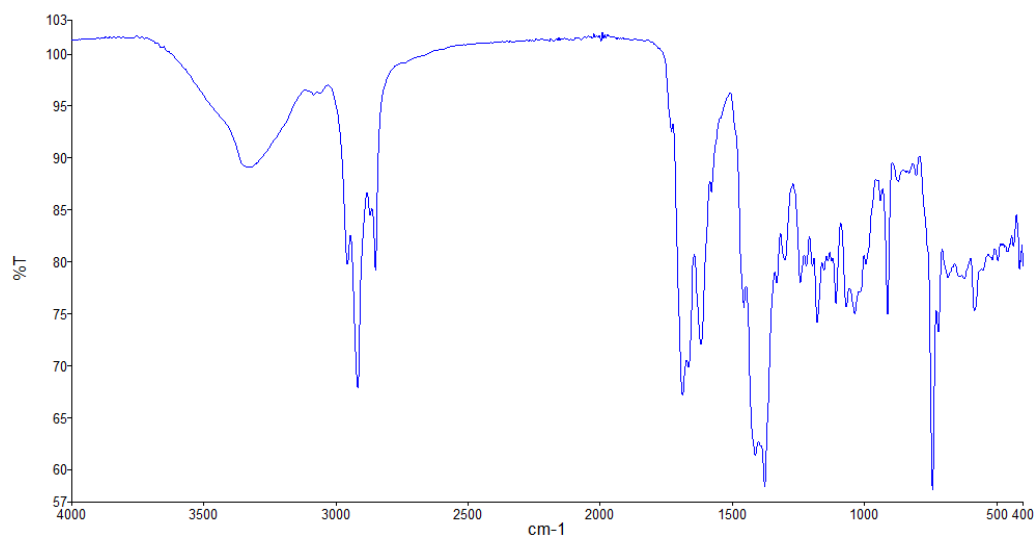


Figure S32: The IR spectrum of compound **1**.