Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supplementary Information

Penaloidines A and B: two unprecedented pyridine alkaloids from *Penicillium* sp. KYJ-6

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Content

Table S1. Crystal data and structure refinement for Penaloidine A (**1**).

Identification code	global	
Empirical formula	C13 H16 N2 O3	
Formula weight	248.28	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 9.0646(2) Å	α= 90°.
	b = 13.3250(3) Å	β= 90°.
	c = 20.6396(4) Å	γ = 90°.
Volume	2492.97(9) $Å^3$	
Z	8	
Density (calculated)	1.323 Mg/m^3	
Absorption coefficient	0.782 mm^{-1}	
F(000)	1056	
Crystal size	0.650 x 0.530 x 0.470 mm^3	
Theta range for data collection	3.95 to 72.12°.	
Index ranges	-11<=h<=11, -15<=k<=16, -25<=l<=24	
Reflections collected	27321	
Independent reflections	4905 [R(int) = 0.0330]	
Completeness to theta = 72.12°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.71 and 0.58	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4905 / 0 / 332	
Goodness-of-fit on F^2	1.068	
Final R indices [I>2sigma(I)]	R1 = 0.0262, wR2 = 0.0680	
R indices (all data)	R1 = 0.0263, wR2 = 0.0681	
Absolute structure parameter	0.01(3)	
Extinction coefficient	0.0153(6)	
Largest diff. peak and hole	0.224 and -0.239 $e.Å^{-3}$	

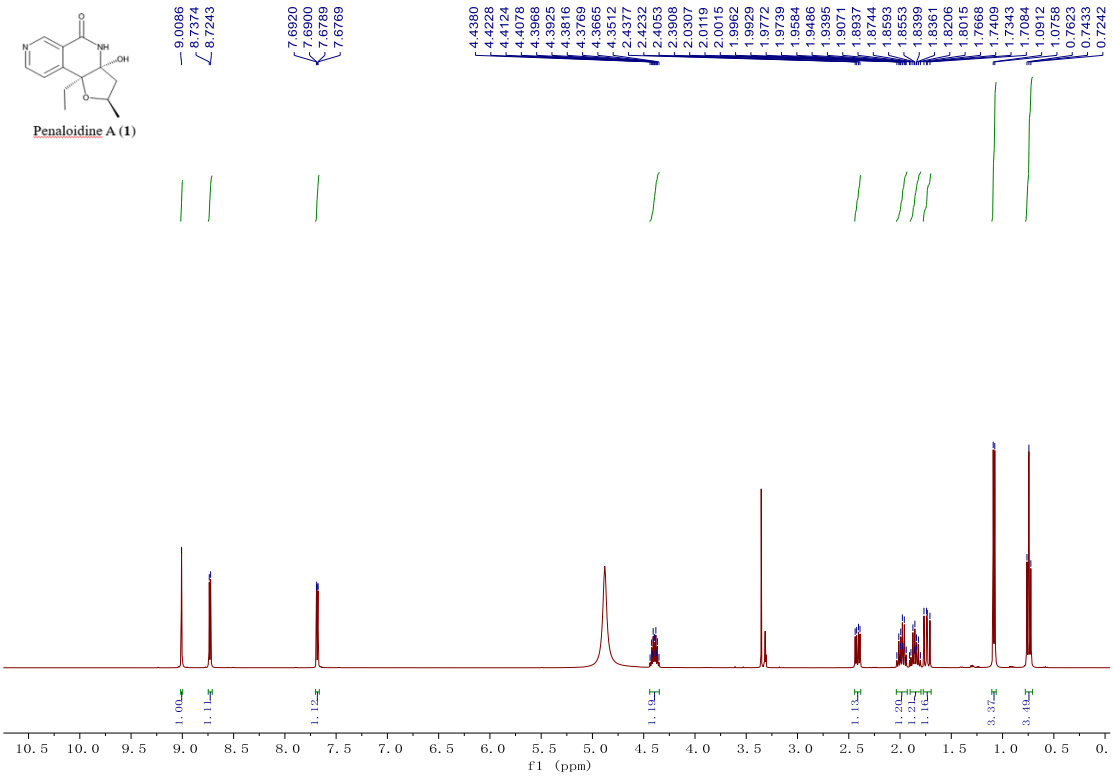


Figure S1. ^{1}H NMR spectrum of penaloidine A (**1**) in methanol-d_4 (400 MHz).

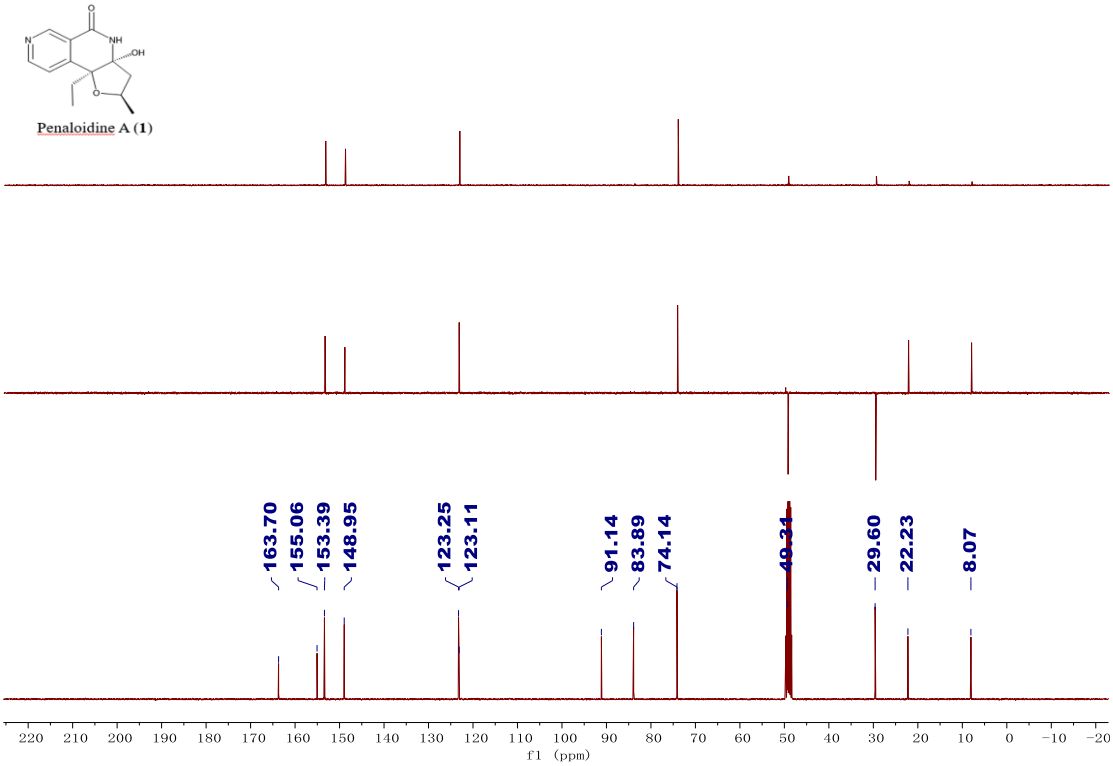


Figure S2. 13C and DEPT NMR spectrum of penaloidine A (**1**) in methanol-d_4 (100 MHz).

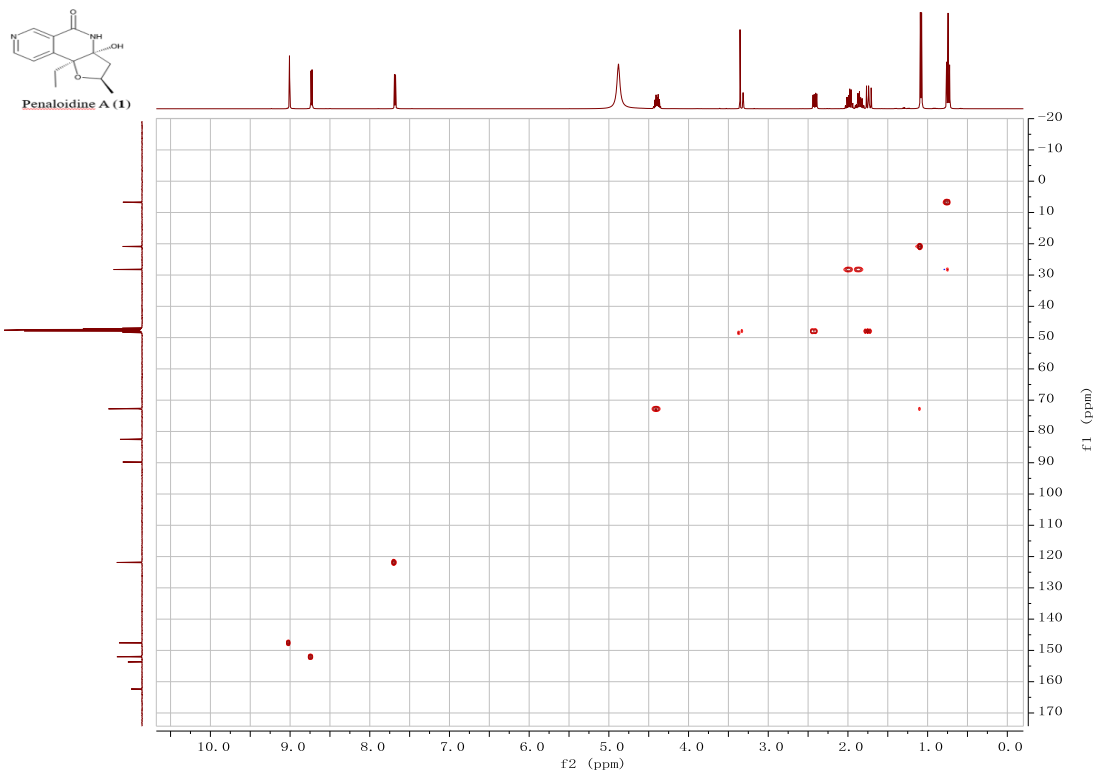


Figure S3. HSQC spectrum of penaloidine A (**1**) in methanol-d_4 (400 MHz).

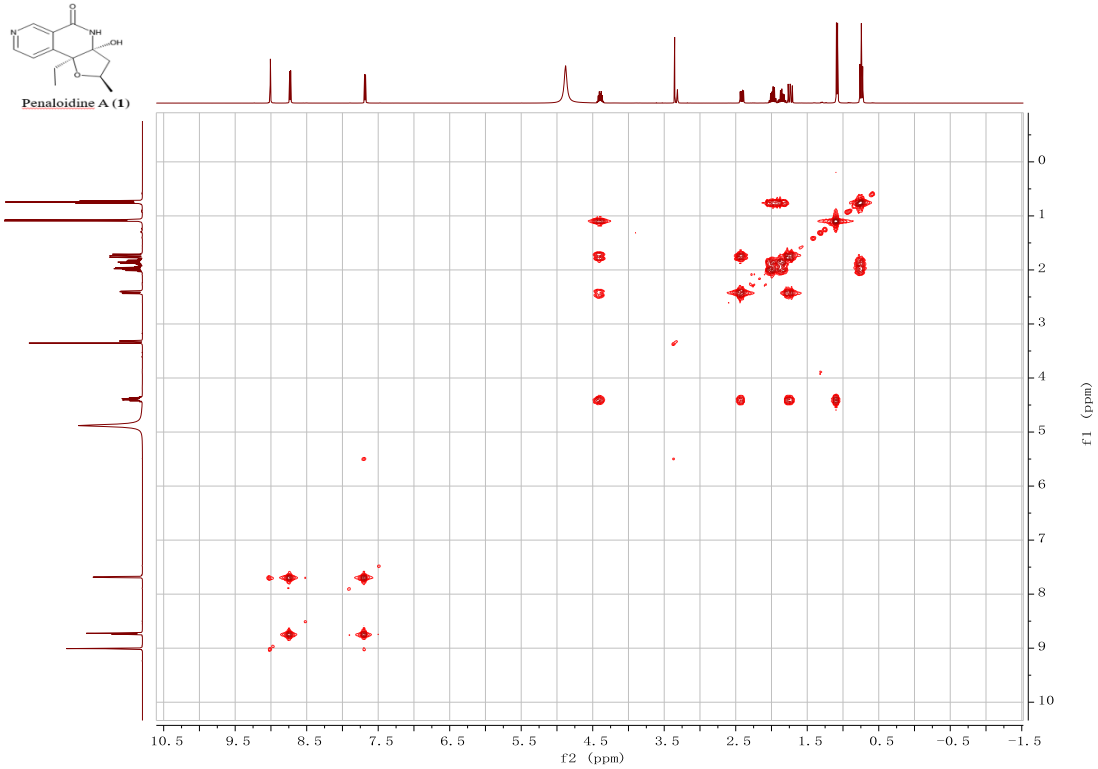


Figure S4. ^{1}H-^{1}H COSY spectrum of penaloidine A (**1**) in methanol-d_4 (400 MHz).

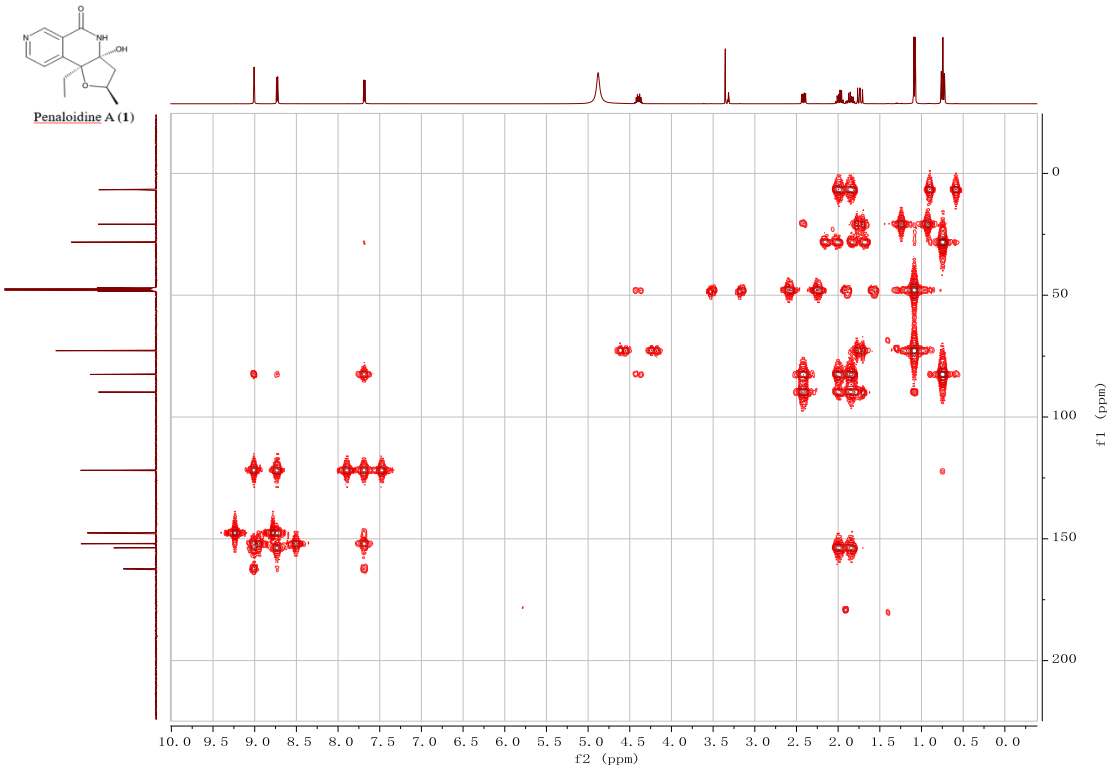


Figure S5. HMBC spectrum of penaloidine A (**1**) in methanol-d_4 (400 MHz).

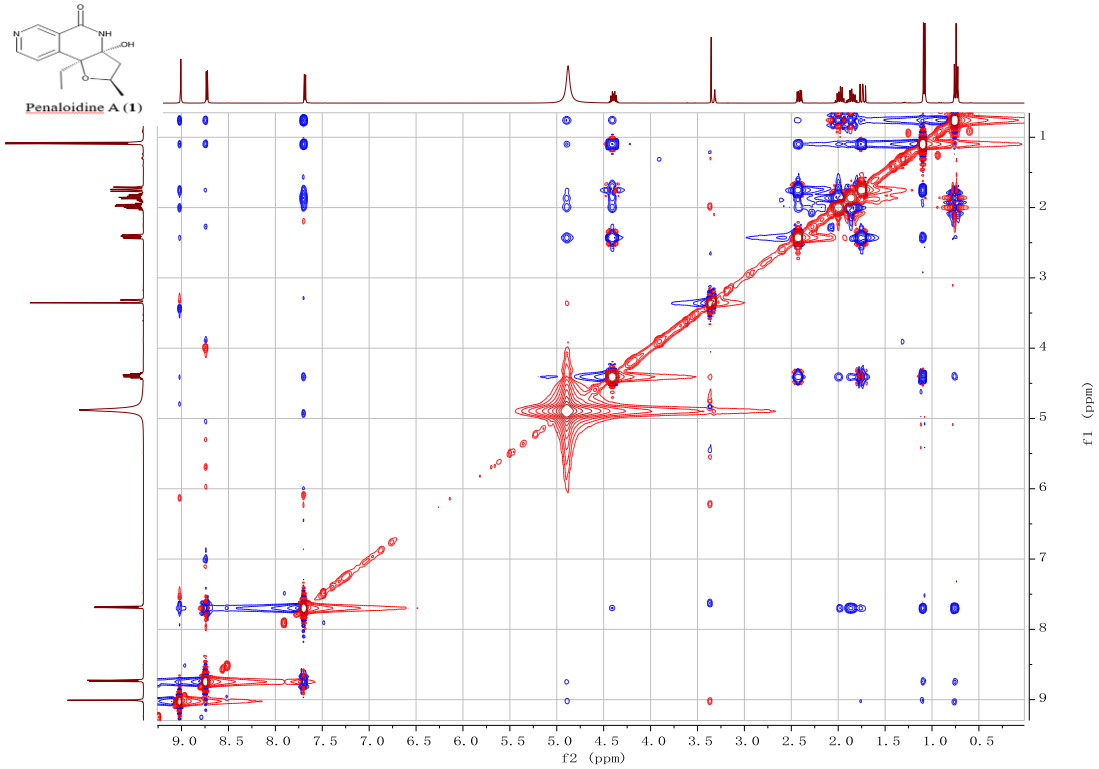
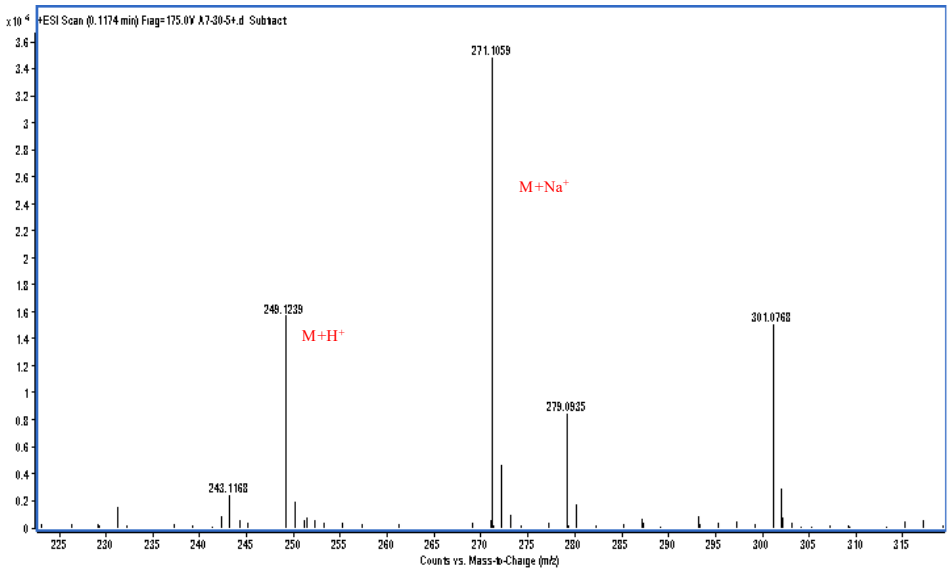


Figure S6. NOESY spectrum of penaloidine A (**1**) in methanol-d_4 (400 MHz).



MS Formula Results: + Scan (0.1174 min) Sub (A7-30-5+.d)

m/z	Ion	Formula	Abundance
249.1239	(M+H)+	C13 H17 N2 O3	15727.1

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C13 H16 N2 O3	C13 H17 N2 O3	91.91		249.1234	-2.23	97.39	87.01	86.83

m/z	Ion	Formula	Abundance
271.1059	(M+Na)+	C13 H16 N2 Na O3	34895.6

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C13 H16 N2 O3	C13 H16 N2 Na O3	81.68		271.1053	-2.25	97.53	82.93	48.47

Figure S7. HRESIMS spectrum of penaloidine A (**1**).

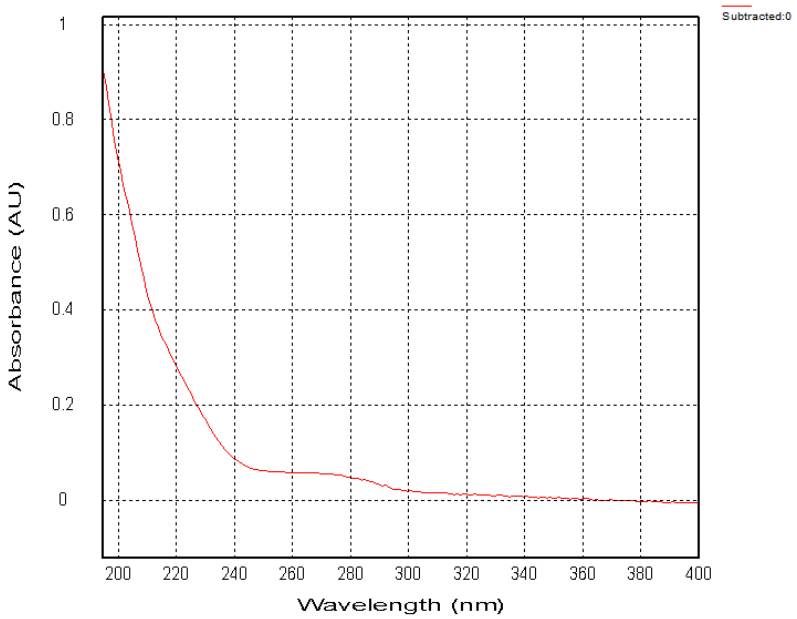


Figure S8. UV Spectrum of penaloidine A (**1**) in methanol

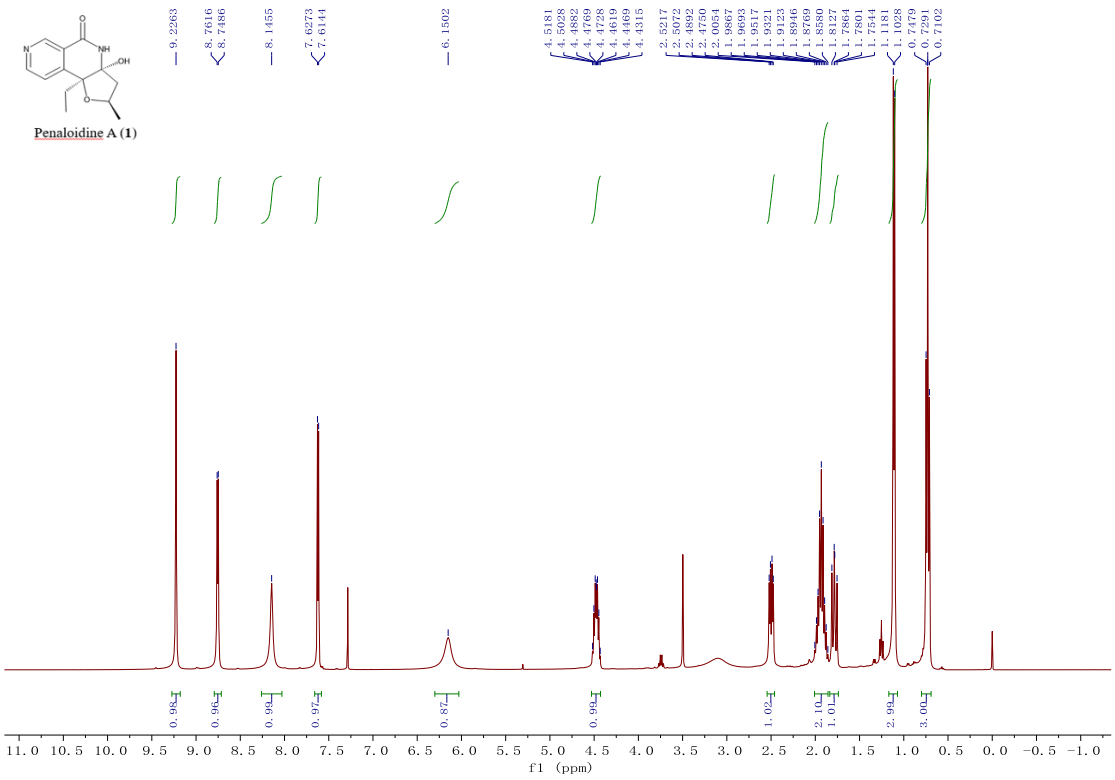


Figure S9. ^{1}H NMR spectrum of penaloidine A (**1**) in $CDCl_3$ (400 MHz).

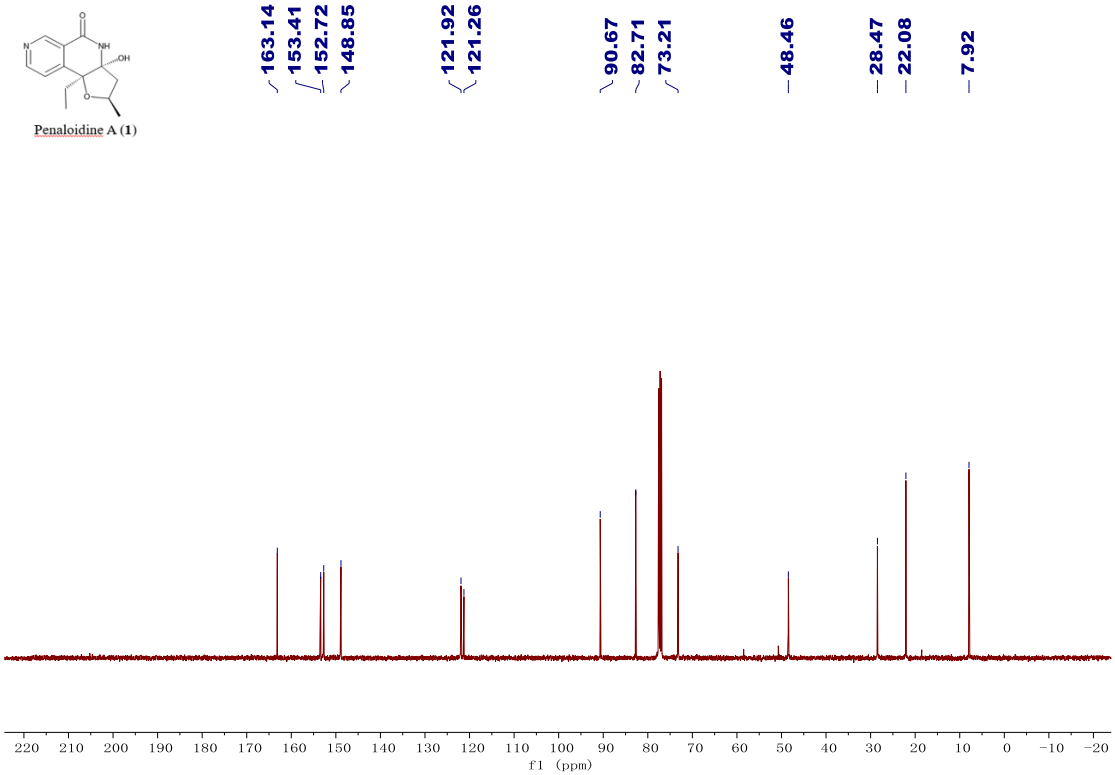


Figure S10. ^{13}C NMR spectrum of penaloidine A (**1**) in $CDCl_3$ (400 MHz).

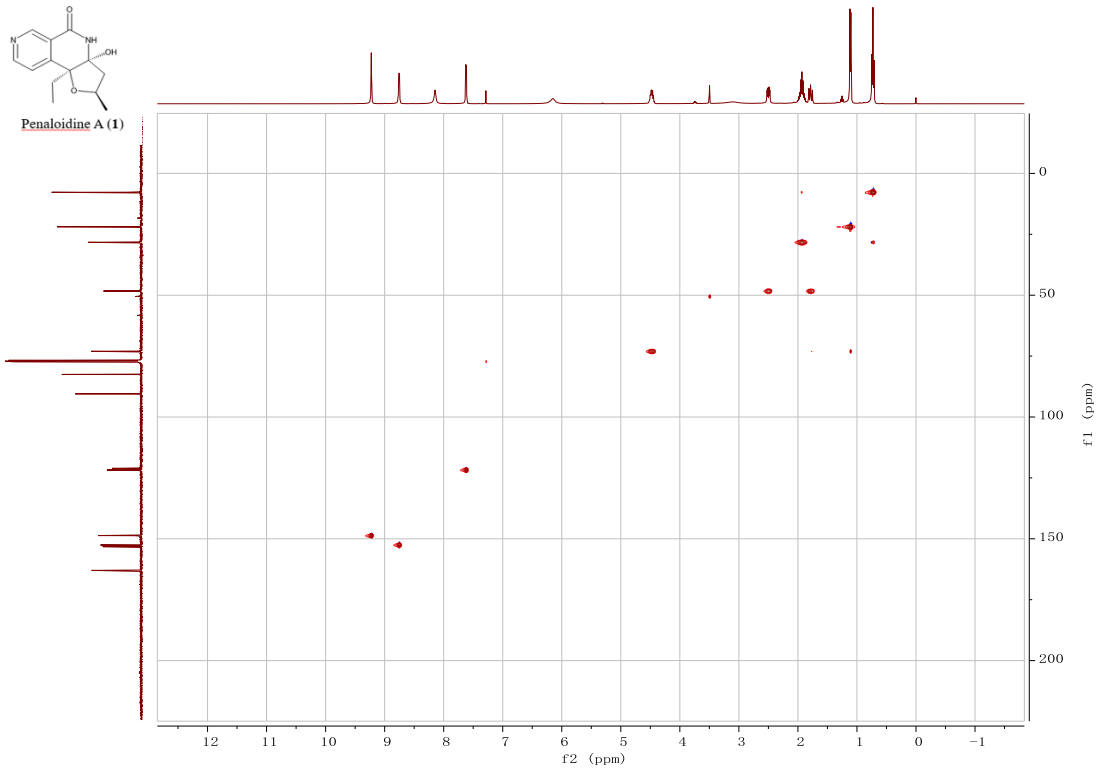


Figure S11. HSQC spectrum of penaloidine A (**1**) in $CDCl_3$ (400 MHz).

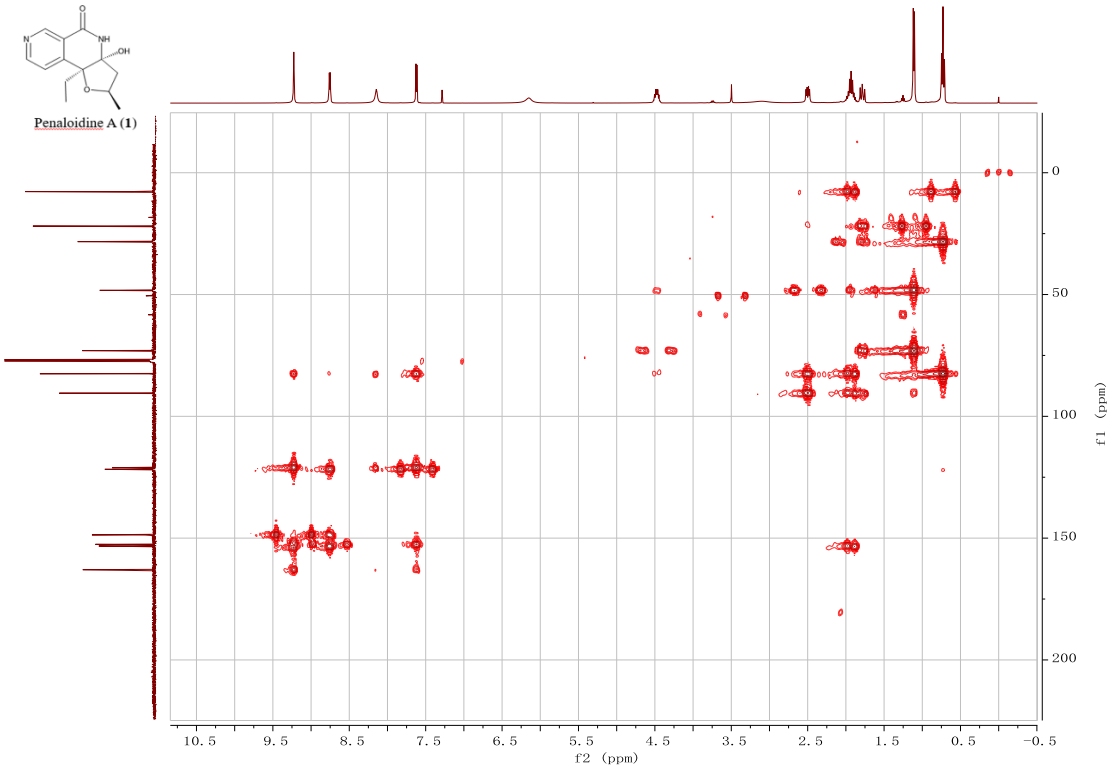


Figure S12. HMBC spectrum of penaloidine A (**1**) in $CDCl_3$ (400 MHz).

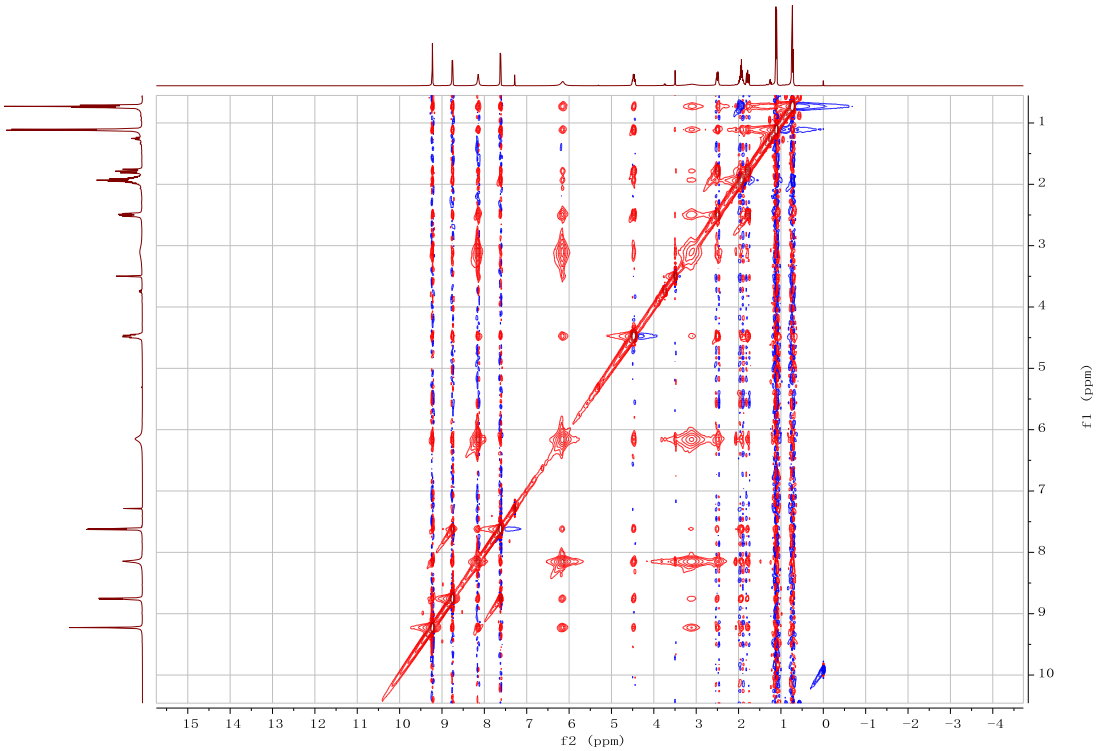


Figure S13. NOESY spectrum of penaloidine A (**1**) in $CDCl_3$ (400 MHz).

Table S2 ^{1}H NMR (400MHz) and ^{13}C NMR (100MHz) spectroscopic data in $CDCl_3$ of penaloidine A (**1**).

Pos.	**1** (in $CDCl_3$)	
	δ_H (J in Hz)	δ_C
1	8.75, d (5.1)	152.7, CH
2	9.2, brs	148.9, CH
3		121.3, C
4		163.1, C
5		90.7, C
6a	1.78, dd (10.5,13.0)	48.5, CH_2
6b	2.49, dd (5.8, 13.0)	
7	4.47, m	73.2, CH
8		82.7, C
9		153.4, C
10	7.68, brd (5.1)	121.9, CH
11	1.93, m	28.5, CH_2
12	0.72, t (7.5)	7.9, CH_3
13	1.10, d (6.1)	22.1, CH_3
-NH-	8.75, s	
OH-5	6.15, s	

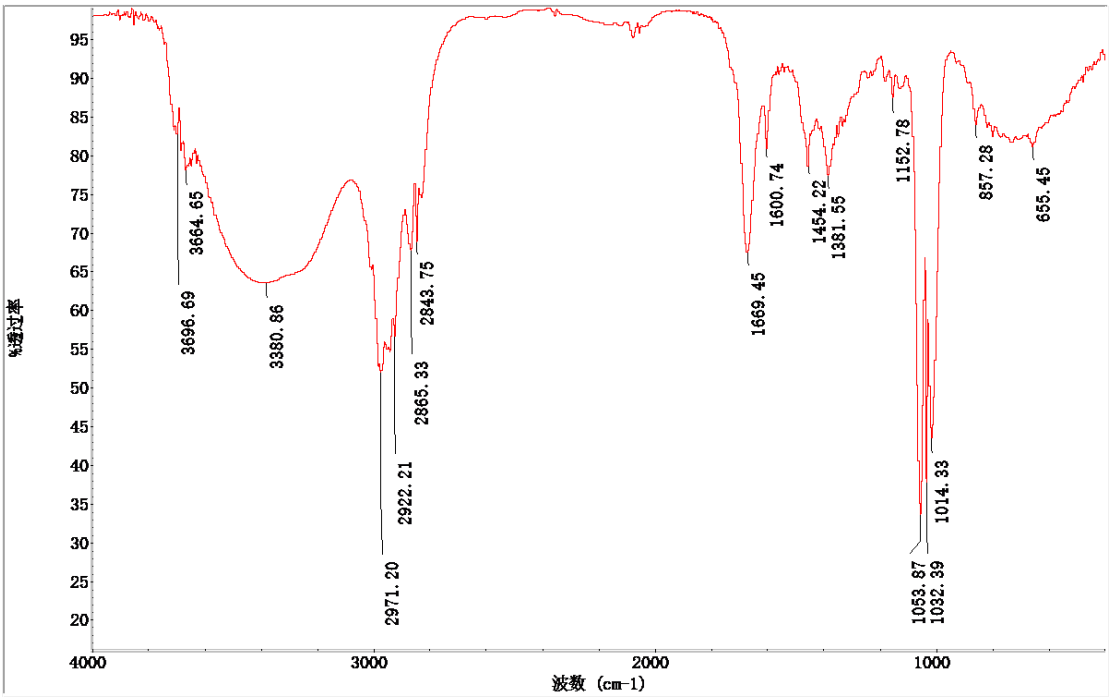


Figure S14. IR spectrum of penaloidine A (**1**)

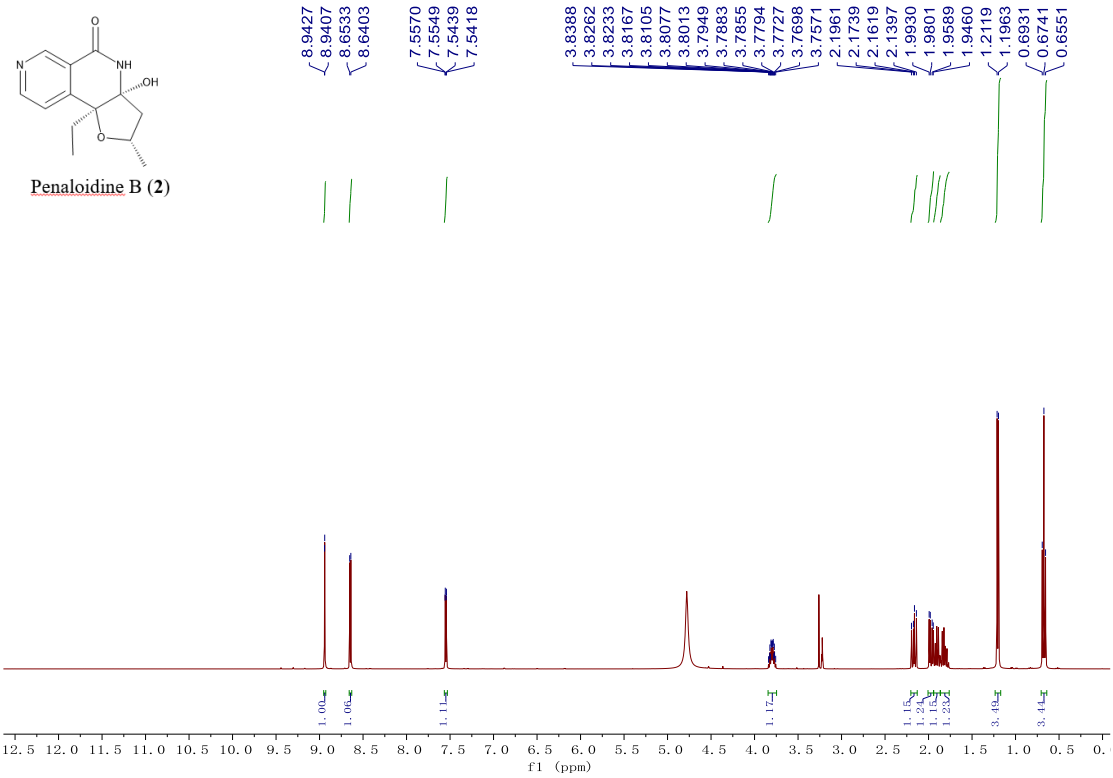


Figure S15. ^{1}H NMR spectrum of penaloidine B (**2**) in methanol-*d4* (400 MHz).

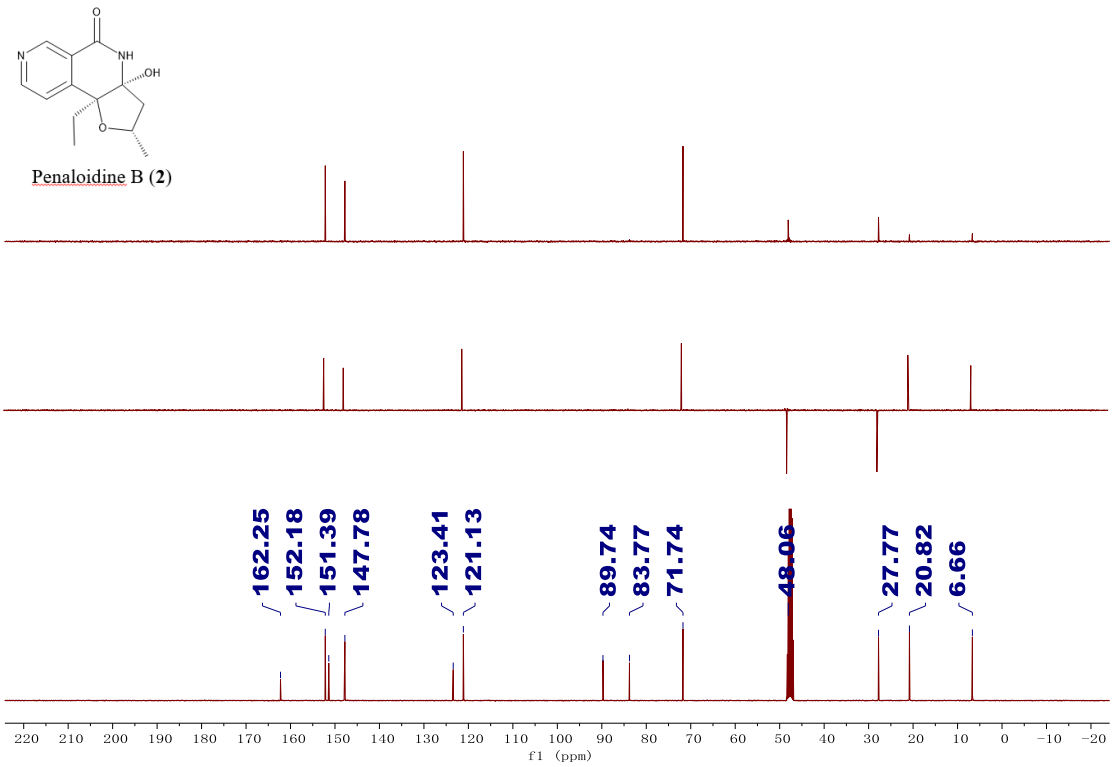


Figure S16. ^{13}C and DEPT NMR spectrum of penaloidine B (**2**) in methanol-*d4* (100 MHz).

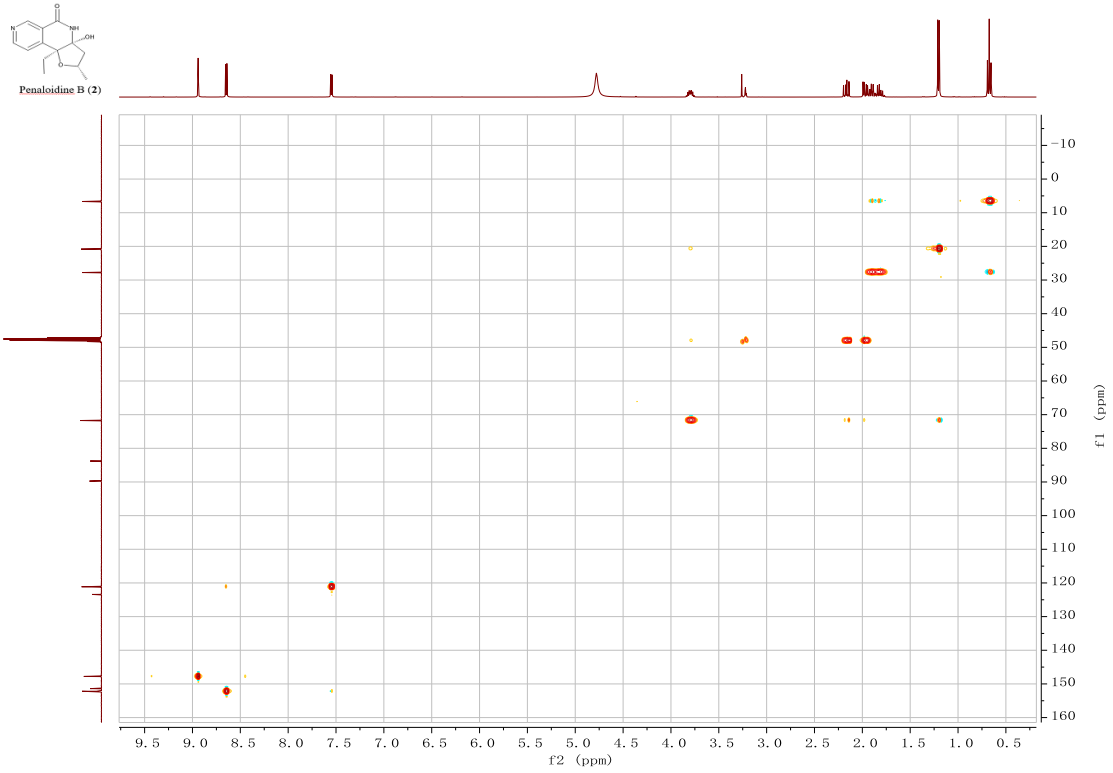


Figure S17. HSQC spectrum of penaloidine B (**2**) in methanol-*d4* (400 MHz).

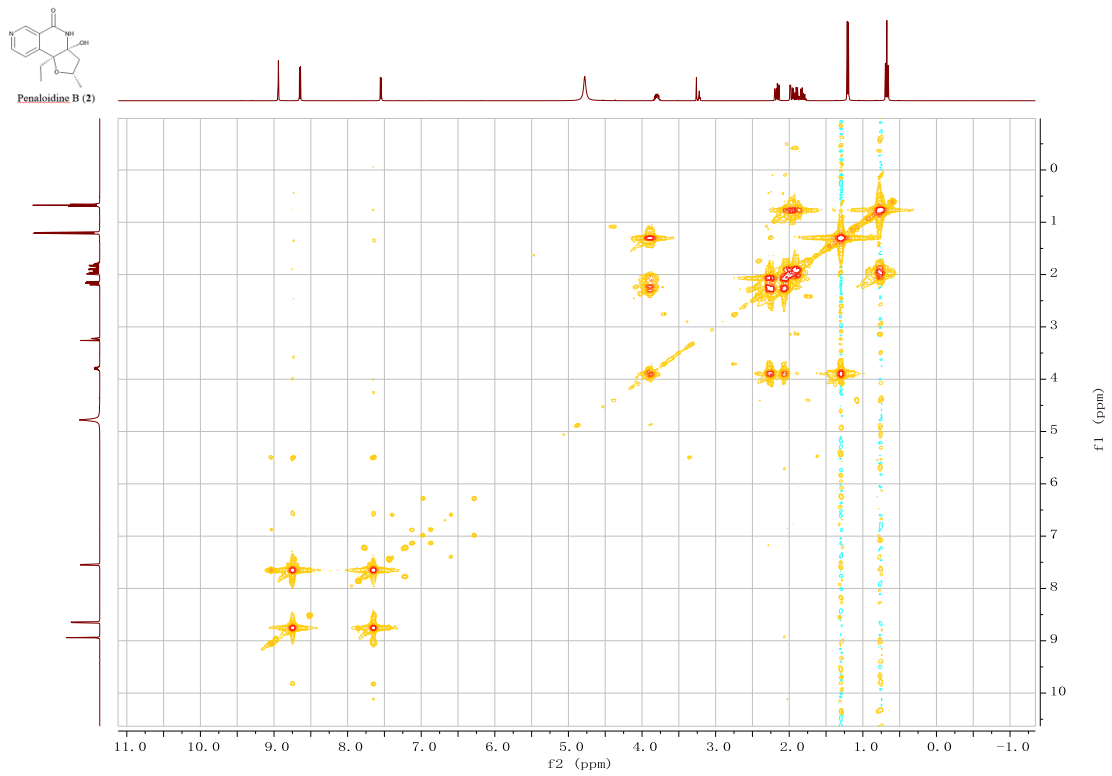


Figure S18. ^{1}H-^{1}H COSY spectrum of penaloidine B (**2**) in methanol-*d4* (400 MHz)

Figure S19. HMBC spectrum of penaloidine B (**2**) in methanol-*d4* (400 MHz).

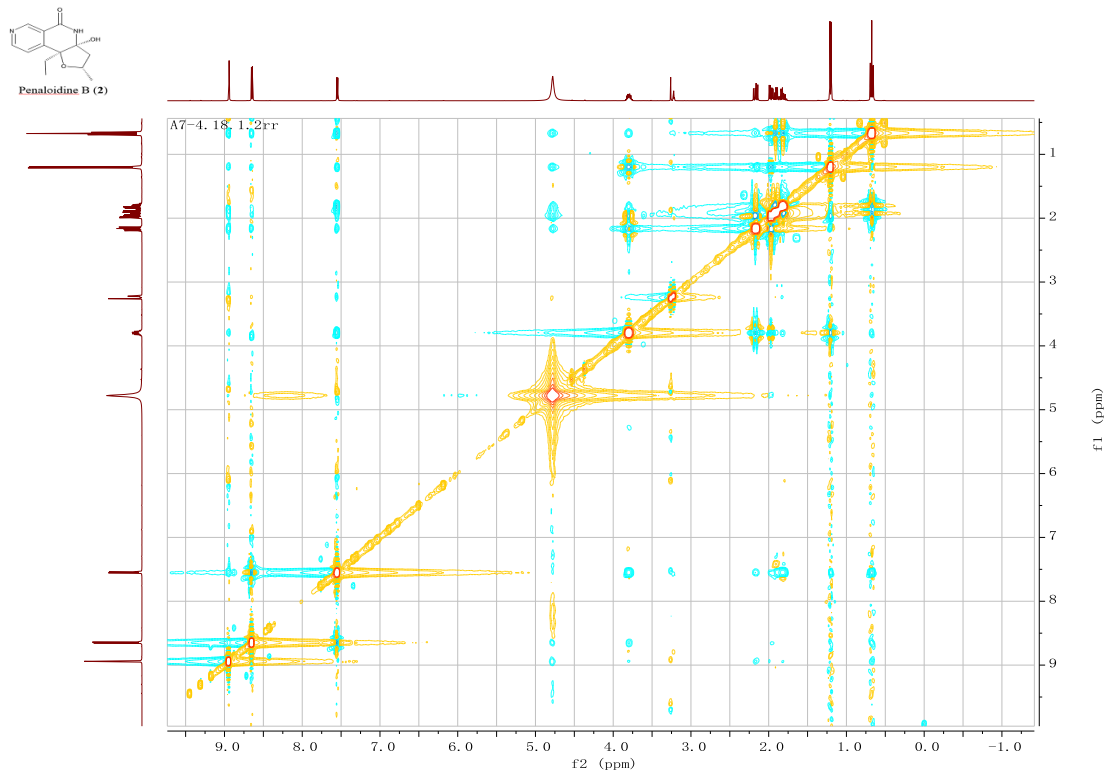
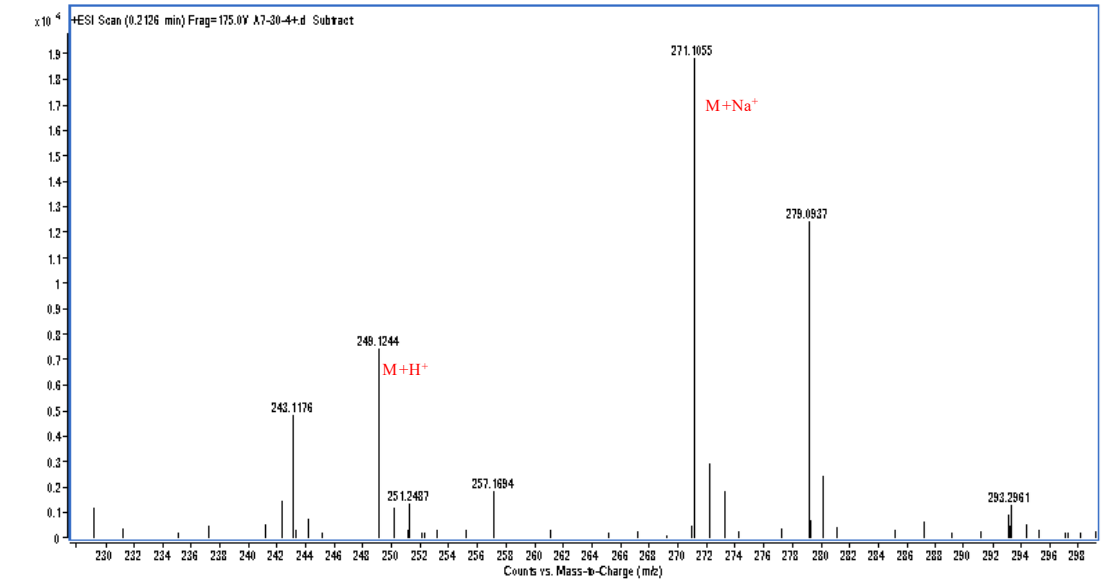


Figure S20. NOESY spectrum of penaloidine B (**2**) in methanol-*d4* (400 MHz).



MS Formula Results: + Scan (0.2126 min) Sub (A7-30-4+.d)

m/z	Ion	Formula	Abundance
249.1244	(M+H)+	C13 H17 N2 O3	7463.1

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C13 H16 N2 O3	C13 H17 N2 O3	81.23		249.1234	-4.17	91.13	91.03	49.65

m/z	Ion	Formula	Abundance
271.1055	(M+Na)+	C13 H16 N2 Na O3	18867.5

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C13 H16 N2 O3	C13 H16 N2 Na O3	68.68		271.1053	-0.95	99.72	32.51	50

Figure S21. HRESIMS spectrum of penaloidine B (**2**).

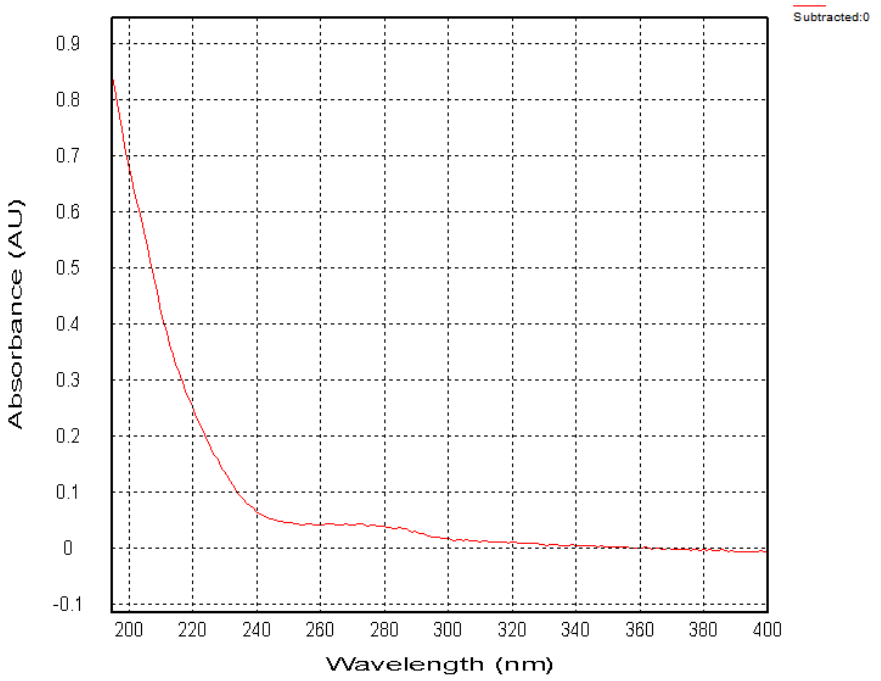


Figure S22. UV Spectrum of penaloidine B (**2**) in methanol

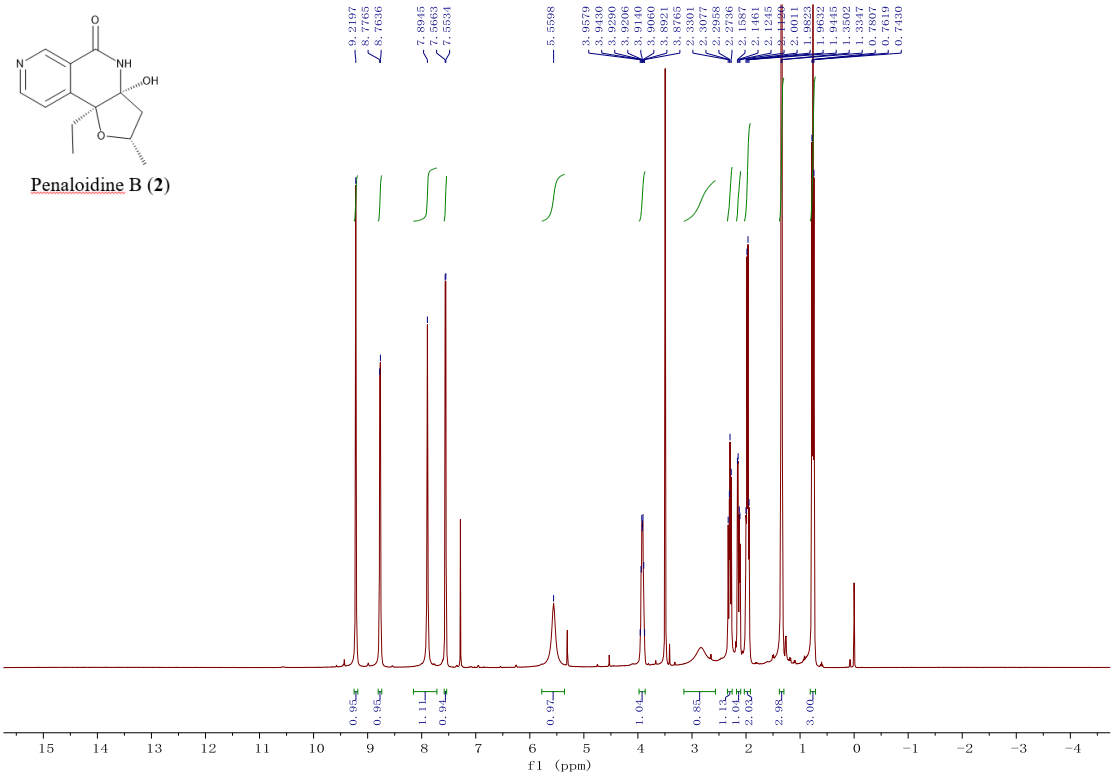


Figure S23. ^{1}H NMR spectrum of penaloidine B (**2**) in $CDCl_3$ (400 MHz).

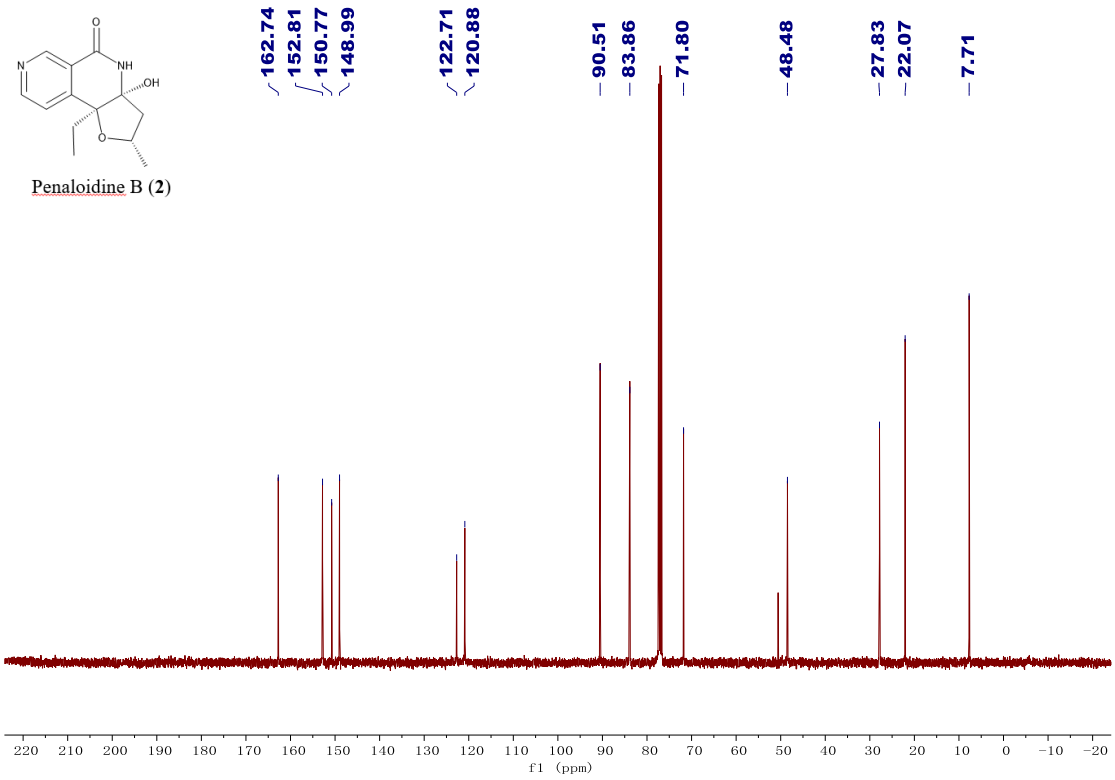


Figure S24. ^{13}C NMR spectrum of penaloidine B (**2**) in $CDCl_3$ (400 MHz).

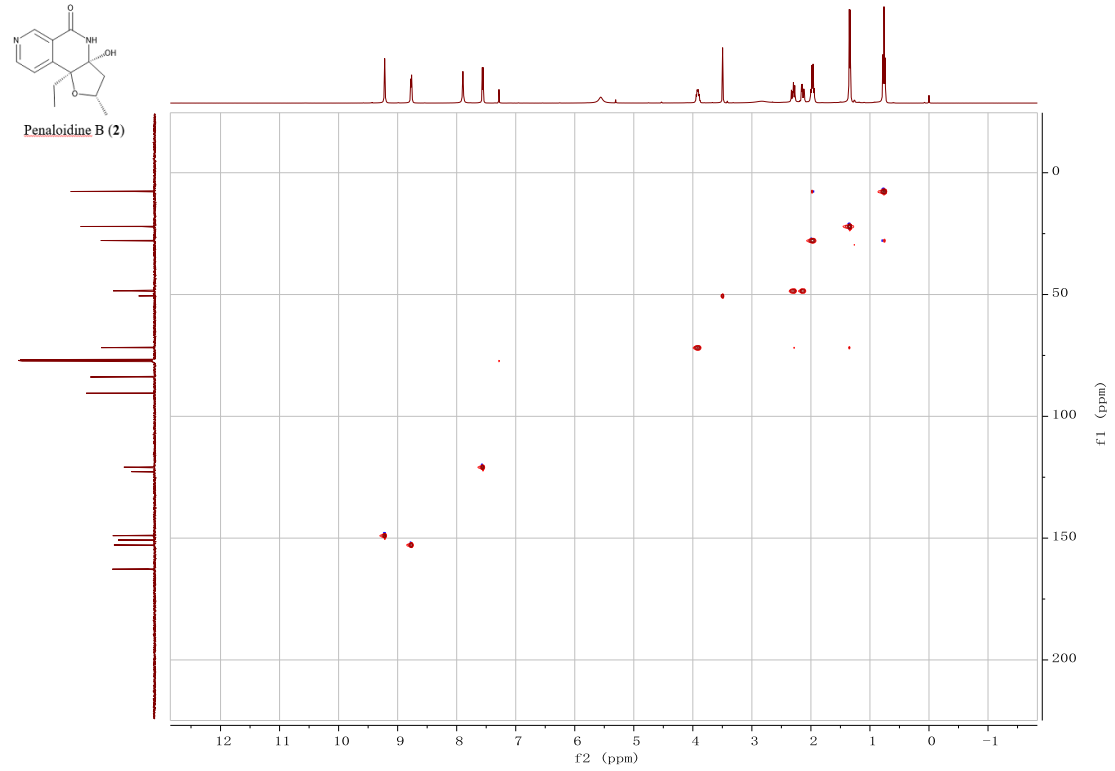


Figure S25. HSQC spectrum of penaloidine B (**2**) in $CDCl_3$ (400 MHz).

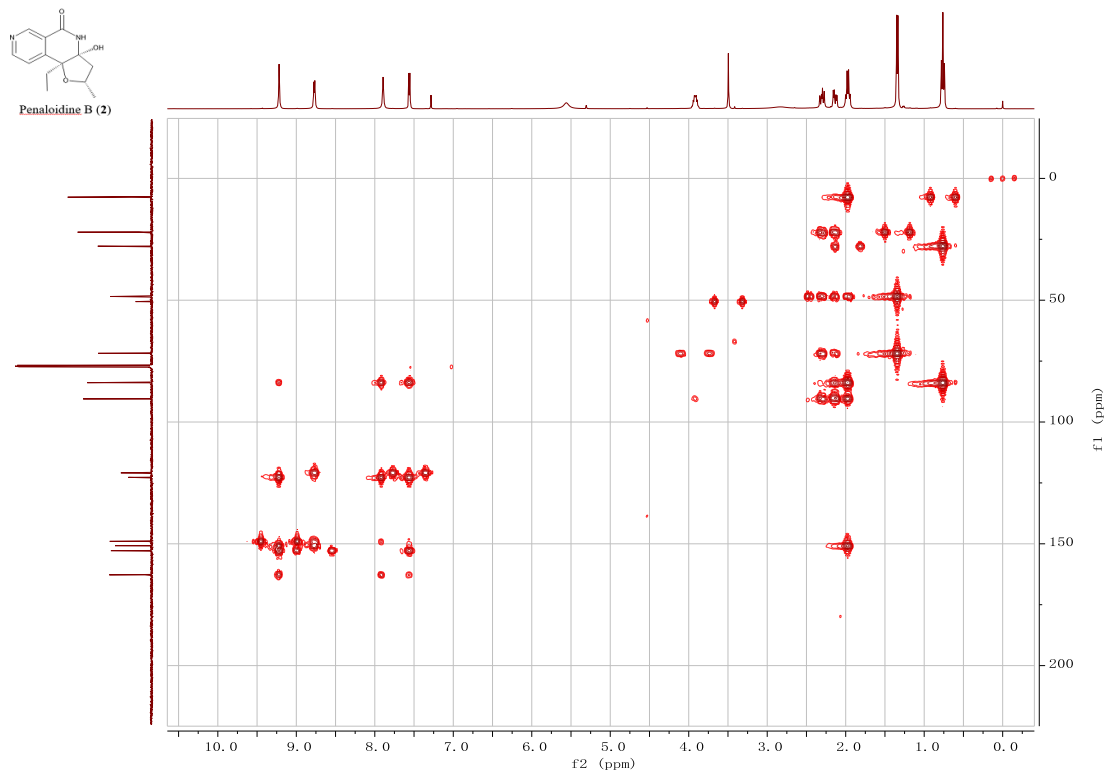


Figure S26. HMBC spectrum of penaloidine B (**2**) in $CDCl_3$ (400 MHz).

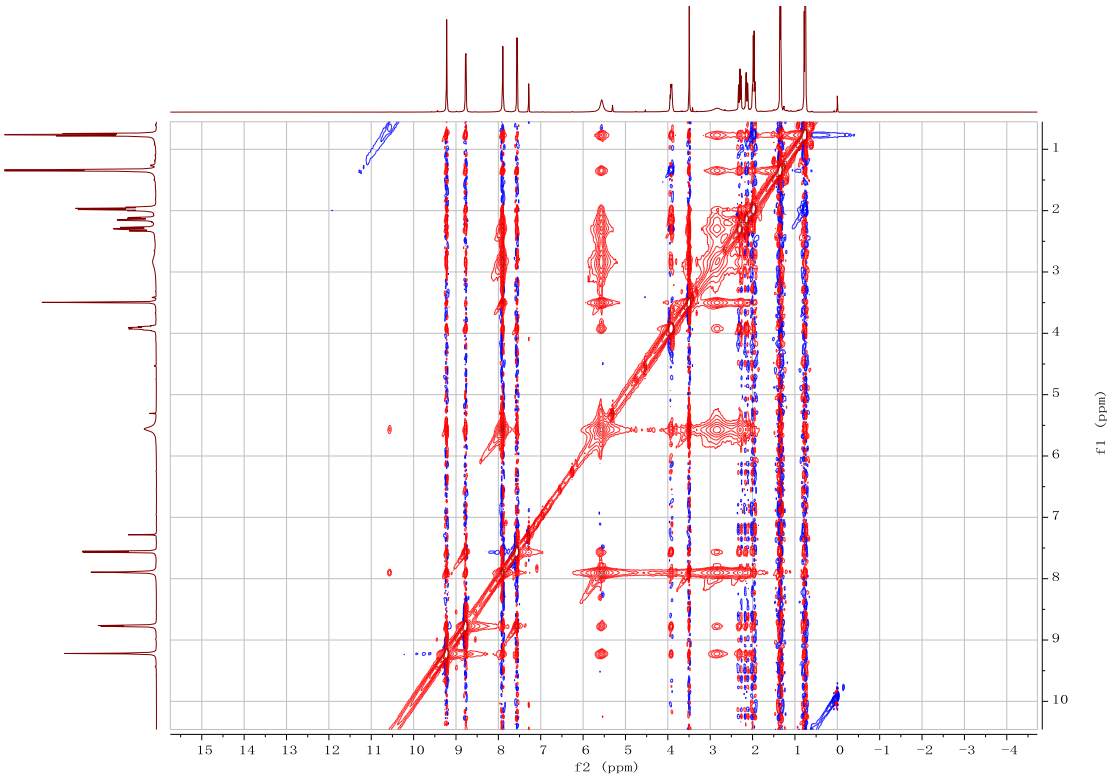


Figure S27. NOESY spectrum of penaloidine B (**2**) in $CDCl_3$ (400 MHz).

Table S3 ^{1}H NMR (400MHz) and ^{13}C NMR (100MHz) spectroscopic data in $CDCl_3$ of penaloidine B (**2**).

Pos.	**2** (in $CDCl_3$)	
	δ_H (J in Hz)	δ_C
1	8.76, d (5.2)	152.8, CH
2	9.2, brs	148.9, CH
3		122.7, C
4		162.7, C
5		90.5, C
6a	2.13, dd (5.0, 13.7)	48.5, CH_2
6b	2.29, dd (8.9, 13.6)	
7	3.92, m	71.8, CH
8		83.9, C
9		150.8, C
10	7.56, brd (5.2)	120.9, CH
11	1.97, m	27.8, CH_2
12	0.76, t (7.5)	7.7, CH_3
13	1.34, d (6.2)	22.1 CH_3
-NH-	7.89, s	
OH-5	5.56, s	

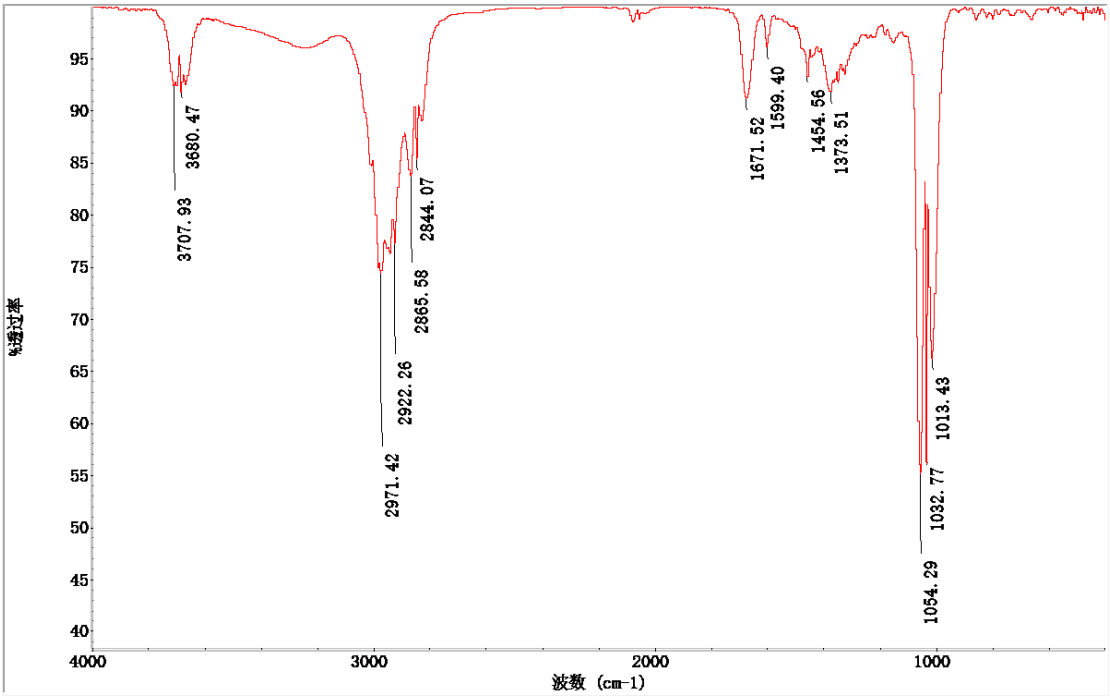


Figure S28. IR spectrum of penaloidine B (**2**)

NMR Computational Methods

Table S4. Energy (298.15K) analysis for a (5R,7R,8S)-1, b (5S,7R,8S)-1, c (5R,7S,8S)-1 and d (5S,7S,8R)-1

Conf.	G (Hartree)	△G (Kcal/mol)	Boltzmann Distribution
a			
a1	-840.017919	0.002332	0.041764086
a2	-840.017949	0.002362	0.040457317
a3	-840.016993	0.001406	0.111415391
a4	-840.015587	0	0.494290024
a5	-840.016021	0.000434	0.312073181
b			
b1	-840.00761	0.004058	0.012926388

b2	-840.006687	0.003135	0.034374691
b3	-840.003552	0	0.952698921
c			
c1	-840.00761	0.004058	0.012926388
c2	-840.006687	0.003135	0.034374691
c3	-840.003552	0	0.952698921
d			
d1	-840.017919	0.002332	0.039752833
d2	-840.017949	0.002362	0.038508995
d3	-840.017738	0.002151	0.048157474
d4	-840.016993	0.001406	0.106049908
d5	-840.015587	0	0.470486265
d6	-840.016021	0.000434	0.297044525

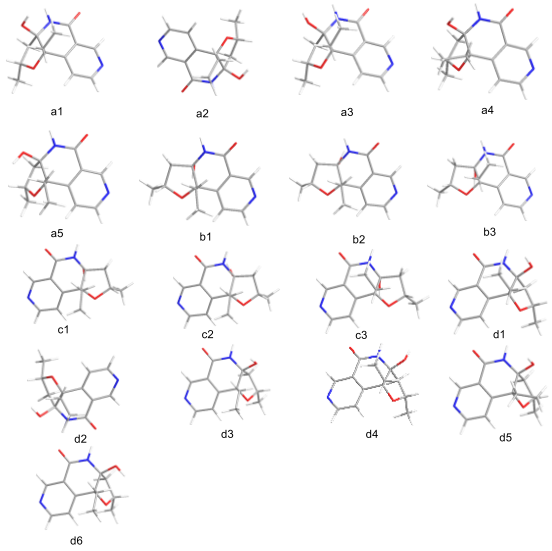


Figure S29. Mpw1pw91/6-311+G(d,p) (chloroform) optimized lowest energy conformers for 1(a-d).

		DP4+	100.00%	0.00%	0.00%	0.00%
Nuclei	sp2?	xperimenta	Isomer 1	Isomer 2	Isomer 3	Isomer 4
C	x	153.4	160.7	161.6	161.5	161.7
C	x	149	155.6	155.7	155.7	155.6
C	x	123.1	129.8	129.5	129.4	124.8
C	x	163.7	167.3	173.1	173.1	167.3
C		91.1	95.2	91.8	91.6	95.2
C		49.3	49.2	42.8	42.5	49.1
C		74.1	77.5	77.6	77.4	77.6
C		83.9	86.3	90.5	90.3	90.3
C	x	155.1	162.3	156.1	156.0	162.2
C	x	123.3	127.2	124.6	124.5	127.3
C		29.6	32.7	35.5	35.2	32.5
C		8.1	10.5	11.4	11.1	10.4
C		22.2	23.1	23.3	23.0	23.1
H	x	8.65	9.16	9.18	9.14	9.16
H	x	8.94	9.36	9.44	9.40	9.37
H		1.96	1.77	1.91	1.86	1.77
H		2.17	2.23	2.76	2.71	2.23
H		3.79	4.49	4.76	4.71	4.72
H	x	7.55	7.90	7.73	7.69	7.69
H		1.86	1.89	2.04	1.99	1.88
H		0.67	0.99	0.75	0.69	1.00
H		1.2	1.16	1.39	1.34	1.16
			a	b	c	d

Functional	Solvent?	Basis Set		
mPW1PW91	PCM	6-311+G(d,p)		
	Isomer 1	Isomer 2	Isomer 3	Isomer 4
sDP4+ (H data)	78.42%	8.43%	8.47%	4.68%
sDP4+ (C data)	95.44%	0.00%	0.00%	4.56%
sDP4+ (all data)	99.72%	0.00%	0.00%	0.28%
uDP4+ (H data)	90.23%	0.30%	1.27%	8.20%
uDP4+ (C data)	97.71%	0.00%	0.00%	2.29%
uDP4+ (all data)	99.79%	0.00%	0.00%	0.21%
DP4+ (H data)	99.28%	0.04%	0.15%	0.54%
DP4+ (C data)	99.89%	0.00%	0.00%	0.11%
DP4+ (all data)	100.00%	0.00%	0.00%	0.00%

Figure S30. DP4+ evaluation of theoretical and experimental data of penaloidine A (**1**)

Table S5. Calculated (calc.) and experimental (exp.) ^{1}H NMR chemical shift values of **a**-**d** of **1** at the mPW1PW91/6-311+G(d,p) level in chloroform and total absolute deviation (TAD) and mean absolute error (MAE).

H	exp.	calc. **a**	|calc. **a**- exp.|	calc. **b**	|calc.**b**- exp.|	calc.**c**	|calc.**c**- exp.|	calc.**d**	|calc.**d** exp.|
1	8.65	9.16	0.51	9.18	0.53	9.14	0.49	9.16	0.51
2	8.94	9.36	0.42	9.44	0.50	9.40	0.46	9.37	0.43
3	1.96	1.77	0.19	1.91	0.05	1.86	0.10	1.77	0.19
4	2.17	2.23	0.06	2.76	0.59	2.71	0.54	2.23	0.06
5	3.79	4.49	0.70	4.76	0.97	4.71	0.92	4.72	0.93
6	7.55	7.90	0.35	7.73	0.18	7.69	0.14	7.69	0.14
7	1.86	1.89	0.03	2.04	0.18	1.99	0.13	1.88	0.02
8	0.67	0.99	0.32	0.75	0.08	0.69	0.02	1.00	0.33
9	1.2	1.16	0.04	1.39	0.19	1.34	0.14	1.16	0.04
TAD			2.62		3.27		2.94		2.65
MAE			0.29		0.36		0.33		0.29

Table S6. Energy (298.15K) analysis for a (5R,7S,8S)-2, b (5S,7S,8S)-2, c (5S,7R,8R)-2 and d (5R,7R,8R)-2

Conf.	G (Hartree)	△G (Kcal/mol)	Boltzmann Distribution
a			
a1	-840.017731	0.004427	0.007039332
a2	-840.016462	0.003158	0.027009786
a3	-840.017576	0.004272	0.00829587
a4	-840.016533	0.003229	0.025052276
a5	-840.016602	0.003298	0.023285931
a6	-840.014894	0.00159	0.142268804
a7	-840.013304	0	0.767048
b			
b1	-840.006211	0.000264	0.43051616
b2	-840.005947	0	0.56948384
c			
c1	-840.017731	0.004427	0.008206921
c2	-840.016462	0.003158	0.031489803
c3	-840.017576	0.004272	0.009671877
c4	-840.016533	0.003229	0.029207607
c5	-840.016602	0.003298	0.027148285
c6	-840.043974	0.03067	6.87443E-15
c7	-840.013304	0	0.894275508
d			
d1	-840.006211	0.000264	0.43051616
d2	-840.005947	0	0.56948384

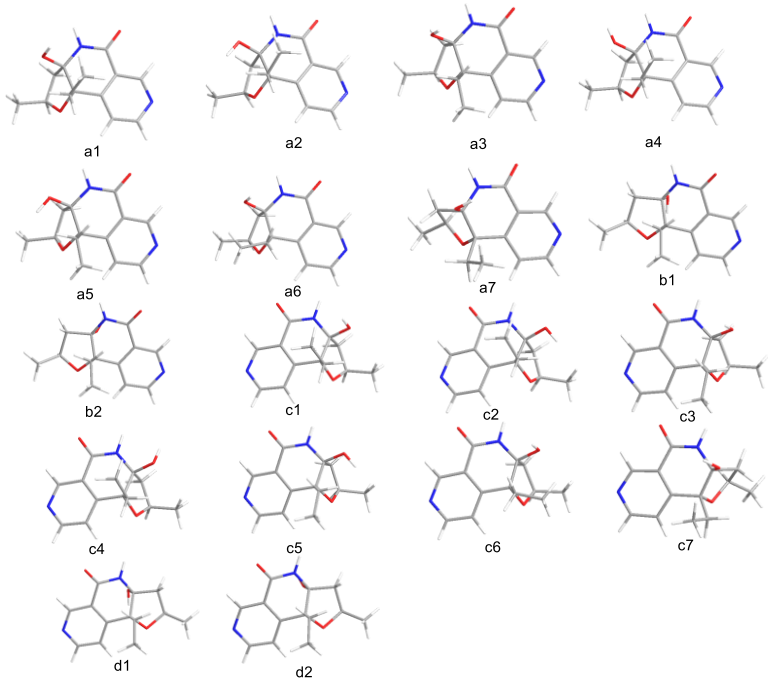


Figure S31. Mpw1pw91/6-311+G(d,p) (chloroform) optimized lowest energy conformers for 2 (a-d).

		DP4+	100.00%	0.00%	0.00%	0.00%
Nuclei	sp2?	xperimenta	Isomer 1	Isomer 2	Isomer 3	Isomer 4
C	x	152.2	158.9	160.2	160.8	160.2
C	x	147.8	155.0	156.4	157.2	156.4
C	x	123.4	125.7	127.9	125.6	127.9
C	x	162.3	167.2	172.1	167.2	172.1
C		89.8	95.7	93.4	95.5	93.4
C		48.1	50.3	44.0	50.6	44.0
C		71.8	76.1	81.0	76.1	81.0
C		83.8	85.2	89.8	85.0	89.8
C	x	151.4	155.3	158.8	154.2	158.8
C	x	121.1	127.7	125.5	128.1	125.5
C		27.8	34.4	37.3	34.7	37.3
C		6.7	11.2	8.8	11.1	8.8
C		20.8	22.1	23.9	22.0	23.9
H	x	8.65	9.18	9.02	9.18	9.02
H	x	8.94	9.33	9.41	9.67	9.41
H		1.96	2.05	2.26	2.04	2.26
H		2.17	2.32	2.39	2.37	2.39
H		3.79	4.07	4.69	4.09	4.69
H	x	7.55	7.81	7.73	7.79	7.73
H		1.86	2.28	1.76	2.34	1.76
H		0.67	0.86	1.00	0.79	0.85
H		1.2	1.25	1.51	1.24	1.51

a b c d

Functional	Solvent?	Basis Set
mPW1PW91	PCM	6-311+G(d,p)

	Isomer 1	Isomer 2	Isomer 3	Isomer 4
sDP4+ (H data)	69.54%	2.35%	26.03%	2.08%
sDP4+ (C data)	98.62%	0.32%	0.73%	0.32%
sDP4+ (all data)	99.70%	0.01%	0.28%	0.01%
uDP4+ (H data)	94.32%	0.85%	2.68%	2.15%
uDP4+ (C data)	75.12%	0.08%	24.72%	0.08%
uDP4+ (all data)	99.07%	0.00%	0.93%	0.00%
DP4+ (H data)	98.85%	0.03%	1.05%	0.07%
DP4+ (C data)	99.75%	0.00%	0.24%	0.00%
DP4+ (all data)	100.00%	0.00%	0.00%	0.00%

Figure S32. DP4+ evaluation of theoretical and experimental data of penaloidine B (**2**)

Table S7. Calculated (calc.) and experimental (exp.) ^{13}C NMR chemical shift values of **a**-**b** of **2** at the mPW1PW91/6-311+G(d,p) level in chloroform and total absolute deviation (TAD) and mean absolute error (MAE).

C	exp.	calc. **a**	|calc. **a**-exp.|	calc. **b**	|calc.**b**- exp.|	calc. **c**	|calc.**c**-exp.|	calc. **d**	|calc.**d**-exp.|
1	152.2	158.9	6.7	160.2	8	160.8	8.6	160.2	8
2	147.8	155.0	7.2	156.4	8.6	157.2	9.4	156.4	8.6
3	123.4	125.7	2.3	127.9	4.5	125.6	2.2	127.9	4.5
4	162.3	167.2	4.9	172.1	9.8	167.2	4.9	172.1	9.8
5	89.8	95.7	5.9	93.4	3.6	95.5	5.7	93.4	3.6
6	48.1	50.3	2.2	44.0	4.1	50.6	2.5	44.0	4.1
7	71.8	76.1	4.3	81.0	9.2	76.1	4.3	81.0	9.2
8	83.8	85.2	1.4	89.8	6	85.0	1.2	89.8	6
9	151.4	155.3	3.9	158.8	7.4	154.2	2.8	158.8	7.4
10	121.1	127.7	6.6	125.5	4.4	128.1	7	125.5	4.4
11	27.8	34.4	6.6	37.3	9.5	34.7	6.9	37.3	9.5
12	6.7	11.2	4.5	8.8	2.1	11.1	4.4	8.8	2.1
13	20.8	22.1	1.3	23.9	3.1	22.0	1.2	23.9	3.1
TAD			57.8		80.3		61.1		80.3
MAE			4.5		6.2		4.7		6.2

Table S8. Calculated (calc.) and experimental (exp.) ^{1}H NMR chemical shift values of **a**-**d** of **2** at the mPW1PW91/6-311+G(d,p) level in chloroform and total absolute deviation (TAD) and mean absolute error (MAE).

H	exp.	calc. **a**	|calc. **a**- exp.|	calc. **b**	|calc.**b**- exp.|	calc. **c**	|calc.**c**- exp.|	calc. **d**	|calc.**d**- exp.|
1	8.65	9.18	0.53	9.02	0.37	9.18	0.53	9.02	0.37
2	8.94	9.33	0.39	9.41	0.47	9.67	0.73	9.41	0.47
3	1.96	2.05	0.09	2.26	0.3	2.04	0.08	2.26	0.3
4	2.17	2.32	0.15	2.39	0.22	2.37	0.2	2.39	0.22
5	3.79	4.07	0.28	4.69	0.9	4.09	0.3	4.69	0.9
6	7.55	7.81	0.26	7.73	0.18	7.79	0.24	7.73	0.18
7	1.86	2.28	0.42	1.76	0.1	2.34	0.48	1.76	0.1
8	0.67	0.86	0.19	1.00	0.33	0.79	0.12	0.85	0.18
9	1.2	1.25	0.05	1.51	0.31	1.24	0.04	1.51	0.31
TAD			2.36		3.18		2.72		3.03
MAE			0.26		0.35		0.30		0.34

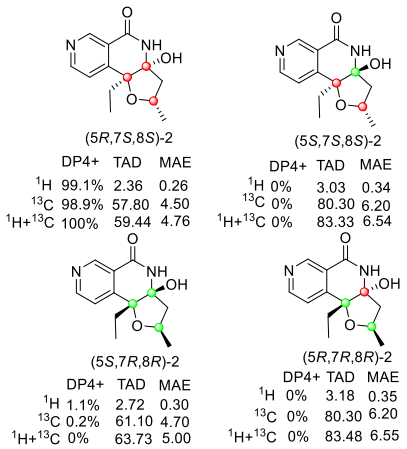


Figure S33. Total absolute deviation (TAD), mean absolute error (MAE), and DP4+ probability analyses for **2** and its three diastereomers.

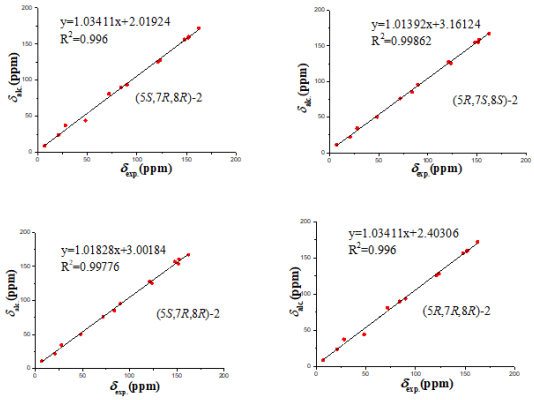


Figure S34. Linear correlations between the experimental and calculated ^{13}CNMR chemical shifts for **2** and its three diastereomers at the PCM/mPW1PW91/6-311+G(d,p) level.

ECD calculation details for compounds 1-2

The ECD spectra were simulated by overlapping Gaussian functions for each transition according to:

$$\Delta\varepsilon(E)=\frac{1}{2.296\times10^{-39}\sqrt{\pi}\sigma}\sum_{i}^{A}\Delta E_i R_i e^{[-(E-\Delta Ei)^2/\sigma^2]}$$

The σ represented the width of the band at 1/e height, and ΔE_i and R_i were the excitation energies and rotational strengths for transition i, respectively. R_{vel} had been used in this work.

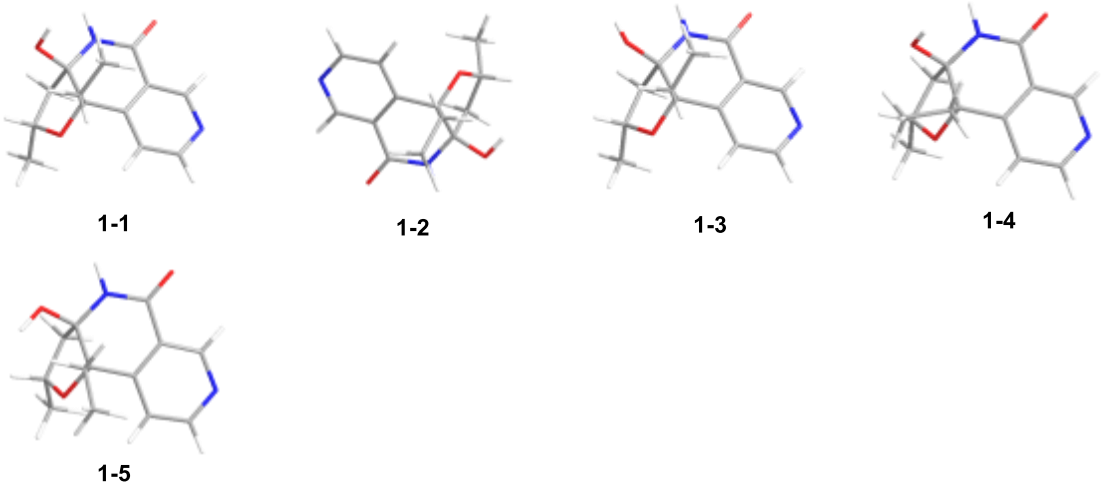


Figure S35. Optimized geometries of predominant conformers for **1**.

Table S9. Cartesian Coordinates of the Lowest Energy Conformers for Compound **1.**

1-1					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-3.40423	1.287448	-0.356581
2	6	0	-2.621633	2.095413	0.389278
3	6	0	-1.319859	1.785282	0.752003
4	6	0	-0.764575	0.570298	0.323425
5	6	0	-1.560095	-0.276333	-0.459648
6	6	0	-2.856981	0.116679	-0.764723
7	6	0	0.65019	0.165145	0.710942
8	6	0	1.216408	-0.924403	-0.259584
9	7	0	0.260873	-1.857672	-0.770912
10	6	0	-1.065195	-1.576256	-0.956913

11	8	0	1.481707	1.343414	0.507399
12	6	0	2.423127	1.069713	-0.542165
13	6	0	1.846641	-0.077401	-1.351223
14	8	0	2.239801	-1.726621	0.303736
15	6	0	0.742887	-0.187779	2.212098
16	6	0	-0.129732	-1.348883	2.671525
17	6	0	2.647543	2.327076	-1.360455
18	8	0	-1.806005	-2.376847	-1.511677
19	1	0	-3.081859	3.029583	0.700152
20	1	0	-0.744667	2.483196	1.353962
21	1	0	-3.513244	-0.51125	-1.36287
22	1	0	0.587385	-2.738237	-1.17365
23	1	0	3.364829	0.770064	-0.066517
24	1	0	1.08898	0.286667	-2.056243
25	1	0	2.622932	-0.597764	-1.922098
26	1	0	1.78889	-2.411939	0.823248
27	1	0	1.788267	-0.40027	2.47121
28	1	0	0.486762	0.69491	2.813709
29	1	0	0.042912	-1.542614	3.735437
30	1	0	-1.193345	-1.123349	2.549424
31	1	0	0.090382	-2.270902	2.128579
32	1	0	3.039737	3.12907	-0.726036
33	1	0	3.353481	2.148377	-2.176883
34	1	0	1.705691	2.695152	-1.782007

1-2					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-3.399483	1.236556 -0	0.20465
2	6	0	-2.618488	2.001096	0.588043
3	6	0	-1.308801	1.684599	0.915709
4	6	0	-0.745146	0.510228	0.397373
5	6	0	-1.53999	-0.293061	-0.433297
6	6	0	-2.844969	0.10121	-0.695646
7	6	0	0.680851	0.094076	0.732357
8	6	0	1.251649	-0.866207	-0.353928
9	7	0	0.307708	-1.799125	-0.88808
10	6	0	-1.031876	-1.554654	-1.01409
11	8	0	1.50849	1.288266	0.64983
12	6	0	2.284646	1.251892	-0.559465
13	6	0	1.757777	0.106936	-1.407709
14	8	0	2.341607	-1.662321	0.085596
15	6	0	0.786481	-0.418183	2.185701
16	6	0	0.051231	-1.718777	2.478828
17	6	0	2.204412	2.599269	-1.253104
18	8	0	-1.776182	-2.343454	-1.580647
19	1	0	-3.08786	2.904589	0.968181
20	1	0	-0.73673	2.345321	1.56064
21	1	0	-3.50125	-0.495799	-1.324457
22	1	0	0.659847	-2.678567	-1.268297
23	1	0	3.323191	1.058047	-0.26634
24	1	0	0.943218	0.450822	-2.057155
25	1	0	2.542086	-0.308735	-2.049348
26	1	0	2.945891	-1.091586	0.590503
27	1	0	1.843566	-0.542253	2.453916

28	1	0	0.419215	0.353407	2.875865
29	1	0	0.184716	-1.990233	3.531331
30	1	0	-1.023316	-1.624511	2.297812
31	1	0	0.43568	-2.545922	1.875939
32	1	0	2.583097	3.389126	-0.595625
33	1	0	2.786782	2.604084	-2.179223
34	1	0	1.166314	2.859712	-1.487491

1-3					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-3.428855	1.247645	-0.343479
2	6	0	-2.658454	2.059476	0.410969
3	6	0	-1.353924	1.762636	0.775615
4	6	0	-0.781898	0.557795	0.340204
5	6	0	-1.565225	-0.293039	-0.449011
6	6	0	-2.866677	0.085002	-0.754286
7	6	0	0.640685	0.171739	0.720648
8	6	0	1.222411	-0.902778	-0.257083
9	7	0	0.275385	-1.850593	-0.766047
10	6	0	-1.055951	-1.587995	-0.940753
11	8	0	1.446879	1.369407	0.516858
12	6	0	2.383502	1.122398	-0.541257
13	6	0	1.827834	-0.035993	-1.350204
14	8	0	2.258928	-1.67778	0.32485
15	6	0	0.748878	-0.191225	2.217406
16	6	0	-0.017597	-1.436664	2.642494
17	6	0	2.571186	2.387313	-1.357123
18	8	0	-1.788798	-2.40265	-1.486289
19	1	0	-3.13072	2.985569	0.727397
20	1	0	-0.789037	2.46305	1.384297
21	1	0	-3.51471	-0.549996	-1.353879
22	1	0	0.577571	-2.766685	-1.098145
23	1	0	3.336544	0.842932	-0.075974
24	1	0	1.057415	0.313014	-2.048909
25	1	0	2.611999	-0.534794	-1.929116
26	1	0	2.599886	-2.26686	-0.366217
27	1	0	1.806412	-0.315381	2.485135
28	1	0	0.408533	0.654609	2.829709
29	1	0	0.126758	-1.612757	3.71359
30	1	0	-1.092018	-1.326391	2.469364
31	1	0	0.32974	-2.328003	2.113188
32	1	0	2.950284	3.196112	-0.723414
33	1	0	3.273683	2.227785	-2.180382
34	1	0	1.617252	2.734636	-1.769022

1-4					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	3.555636	-1.228778	-0.111242
2	6	0	2.649722	-2.180115	0.19675
3	6	0	1.303843	-1.92092	0.406958
4	6	0	0.835202	-0.602114	0.293563
5	6	0	1.76085	0.393872	-0.038594

6	6	0	3.091808	0.039517	-0.222589
7	6	0	-0.632243	-0.261442	0.541363
8	6	0	-1.008991	1.095269	-0.147997
9	7	0	0.025894	2.082361	-0.186514
10	6	0	1.363597	1.80439	-0.202875
11	8	0	-1.407051	-1.285334	-0.132826
12	6	0	-2.145931	-0.670463	-1.201476
13	6	0	-1.43763	0.632921	-1.528904
14	8	0	-2.100307	1.774976	0.441765
15	6	0	-0.917634	-0.315158	2.062019
16	6	0	-2.377142	-0.536811	2.448302
17	6	0	-2.219557	-1.624481	-2.378447
18	8	0	2.190993	2.694173	-0.34727
19	1	0	3.04442	-3.189597	0.274768
20	1	0	0.628359	-2.735955	0.652237
21	1	0	3.845432	0.781599	-0.476278
22	1	0	-0.226193	3.057886	-0.357142
23	1	0	-3.157717	-0.473073	-0.827064
24	1	0	-0.567328	0.450301	-2.171536
25	1	0	-2.102352	1.334156	-2.044166
26	1	0	-1.746581	2.197029	1.242904
27	1	0	-0.362341	-1.147323	2.515228
28	1	0	-0.536792	0.592829	2.546019
29	1	0	-2.470339	-0.55943	3.539282
30	1	0	-3.034435	0.252859	2.080068
31	1	0	-2.745731	-1.494846	2.068553
32	1	0	-2.717301	-2.554564	-2.083709
33	1	0	-2.76907	-1.181769	-3.214256
34	1	0	-1.217179	-1.902499	-2.722393

1-5					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	3.381098	-1.0127	-0.63687
2	6	0	2.515446	-2.023018	-0.408776
3	6	0	1.196601	-1.835968	-0.022277
4	6	0	0.717119	-0.529939	0.150469
5	6	0	1.597299	0.531461	-0.107583
6	6	0	2.903665	0.245978	-0.481299
7	6	0	-0.713879	-0.244832	0.596323
8	6	0	-1.177416	1.13694	0.035244
9	7	0	-0.183243	2.163058	0.09282
10	6	0	1.161489	1.94105	-0.016692
11	8	0	-1.595145	-1.207465	-0.032806
12	6	0	-2.214183	-0.602616	-1.184771
13	6	0	-1.592823	0.774457	-1.381217
14	8	0	-2.301724	1.693852	0.701047
15	6	0	-0.868518	-0.331829	2.133389
16	6	0	-0.579173	-1.697994	2.747929
17	6	0	-2.04598	-1.512886	-2.387865
18	8	0	1.964928	2.86309	-0.046523
19	1	0	2.921705	-3.021404	-0.547505
20	1	0	0.555613	-2.697309	0.142138
21	1	0	3.620945	1.038086	-0.682894
22	1	0	-0.493528	3.13243	0.170484

23	1	0	-3.281543	-0.504385	-0.954744
24	1	0	-0.727283	0.71922	-2.052591
25	1	0	-2.309949	1.475154	-1.822168
26	1	0	-2.955425	0.984354	0.826979
27	1	0	-0.231042	0.41638	2.62033
28	1	0	-1.904303	-0.097168	2.406342
29	1	0	-0.848164	-1.690627	3.809597
30	1	0	-1.159625	-2.488264	2.262657
31	1	0	0.48283	-1.95061	2.687402
32	1	0	-2.495543	-2.491734	-2.190203
33	1	0	-2.515405	-1.083985	-3.278021
34	1	0	-0.98663	-1.693273	-2.600432

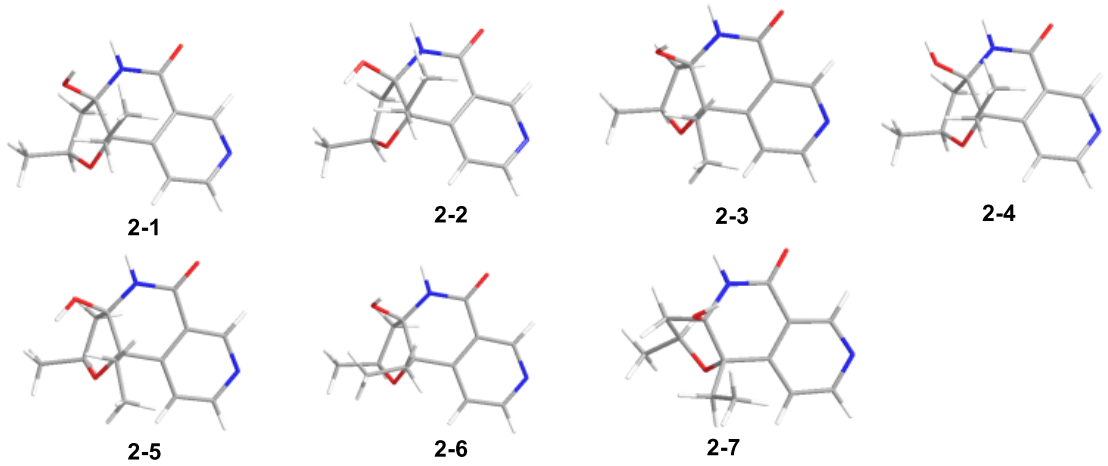


Figure S36. Optimized geometries of predominant conformers for **2**.

Table S10. Cartesian Coordinates of the Lowest Energy Conformers for Compound **2.**

2-1					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	3.567632	-1.047027	-0.556647
2	6	0	2.783736	-2.075289	-0.169336
3	6	0	1.444765	-1.939155	0.164168
4	6	0	0.851481	-0.669861	0.09503
5	6	0	1.649082	0.407311	-0.312899
6	6	0	2.983864	0.174447	-0.618513
7	6	0	-0.607062	-0.453716	0.473772
8	6	0	-1.168806	0.862788	-0.152332
9	7	0	-0.234783	1.942644	-0.25854
10	6	0	1.11519	1.780895	-0.412225
11	8	0	-1.356609	-1.53739	-0.141006
12	6	0	-2.133625	-1.027502	-1.23517
13	6	0	-1.662365	0.391172	-1.509041
14	8	0	-2.271305	1.4168	0.542137
15	6	0	-0.813191	-0.589288	1.999293
16	6	0	-0.038163	0.398458	2.862184
17	6	0	-3.608578	-1.126564	-0.869509
18	8	0	1.8446	2.740955	-0.620887
19	1	0	3.274453	-3.044079	-0.130817
20	1	0	0.871242	-2.810368	0.468083
21	1	0	3.642414	0.981282	-0.931837

22	1	0	-0.584693	2.894214	-0.386258
23	1	0	-1.949325	-1.662978	-2.108384
24	1	0	-0.835443	0.355802	-2.229874
25	1	0	-2.448492	1.020284	-1.939922
26	1	0	-1.899486	1.902016	1.296375
27	1	0	-1.883065	-0.503384	2.229555
28	1	0	-0.546903	-1.606661	2.31703
29	1	0	-0.288922	0.243416	3.916843
30	1	0	1.041982	0.258364	2.759919
31	1	0	-0.275067	1.436141	2.616513
32	1	0	-3.883568	-2.17401	-0.70304
33	1	0	-4.242449	-0.724489	-1.665293
34	1	0	-3.834082	-0.599956	0.062922

2-2					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	3.469621	-1.263703	-0.47255
2	6	0	2.665033	-2.173389	0.118022
3	6	0	1.353035	-1.918008	0.48703
4	6	0	0.814429	-0.649327	0.233481
5	6	0	1.634071	0.307577	-0.383709
6	6	0	2.938896	-0.03834	-0.706202
7	6	0	-0.611324	-0.291513	0.629885
8	6	0	-1.152143	0.877959	-0.238675
9	7	0	-0.191951	1.900814	-0.52426
10	6	0	1.149438	1.675173	-0.67403
11	8	0	-1.470703	-1.411985	0.293741
12	6	0	-2.009775	-1.22289	-1.025114
13	6	0	-1.627002	0.172211	-1.501648
14	8	0	-2.254815	1.561699	0.334889
15	6	0	-0.731107	-0.091798	2.157255
16	6	0	0.014145	1.107441	2.726865
17	6	0	-3.512134	-1.45248	-0.969617
18	8	0	1.913044	2.561772	-1.03146
19	1	0	3.117317	-3.145502	0.29547
20	1	0	0.761262	-2.695563	0.961296
21	1	0	3.614317	0.673662	-1.174577
22	1	0	-0.531466	2.846856	-0.702212
23	1	0	-1.564351	-1.979526	-1.681236
24	1	0	-0.815259	0.079759	-2.234514
25	1	0	-2.452241	0.687891	-2.005223
26	1	0	-2.865306	0.890624	0.685787
27	1	0	-1.790367	-0.011035	2.433739
28	1	0	-0.383067	-0.996306	2.674339
29	1	0	-0.130481	1.151637	3.811493
30	1	0	1.089948	1.039578	2.541985
31	1	0	-0.354107	2.0482	2.309096
32	1	0	-3.72799	-2.461992	-0.603335
33	1	0	-3.967346	-1.335923	-1.957648
34	1	0	-3.998134	-0.759726	-0.275406

2-3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	3.561239	-0.841713	-0.776009
2	6	0	2.715291	-1.892454	-0.803388
3	6	0	1.374431	-1.810204	-0.458193
4	6	0	0.846832	-0.576242	-0.048979
5	6	0	1.706887	0.529876	-0.045348
6	6	0	3.038065	0.350133	-0.40062
7	6	0	-0.611771	-0.424265	0.37078
8	6	0	-1.093672	1.046949	0.131049
9	7	0	-0.120647	2.060481	0.404223
10	6	0	1.2303	1.88627	0.287415
11	8	0	-1.412064	-1.247554	-0.509937
12	6	0	-2.075792	-0.410965	-1.473539
13	6	0	-1.531066	1.003632	-1.320808
14	8	0	-2.210486	1.43272	0.912688
15	6	0	-0.847945	-0.874392	1.832976
16	6	0	-0.543873	-2.337542	2.138655
17	6	0	-3.577853	-0.51667	-1.247473
18	8	0	2.004225	2.82032	0.446629
19	1	0	3.15511	-2.834582	-1.11956
20	1	0	0.751265	-2.698814	-0.508818
21	1	0	3.740101	1.180765	-0.40649
22	1	0	-0.433959	3.018302	0.573238
23	1	0	-1.846612	-0.797561	-2.472761
24	1	0	-0.669547	1.127375	-1.989173
25	1	0	-2.267379	1.769232	-1.587256
26	1	0	-1.864437	1.604004	1.804609
27	1	0	-0.270329	-0.243416	2.519684
28	1	0	-1.908181	-0.735185	2.079144
29	1	0	-0.879118	-2.580807	3.152671
30	1	0	-1.061099	-3.00939	1.44728
31	1	0	0.529158	-2.543518	2.097777
32	1	0	-3.906142	-1.552725	-1.385953
33	1	0	-4.130011	0.118056	-1.94687
34	1	0	-3.855369	-0.241765	-0.225228

2-4					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	3.579624	-1.045773	-0.538377
2	6	0	2.802747	-2.068465	-0.122802
3	6	0	1.465246	-1.93092	0.215966
4	6	0	0.865159	-0.666352	0.122087
5	6	0	1.655892	0.404597	-0.312215
6	6	0	2.990394	0.171842	-0.619342
7	6	0	-0.595524	-0.449963	0.495051
8	6	0	-1.16584	0.84828	-0.15954
9	7	0	-0.234467	1.932812	-0.280799
10	6	0	1.116938	1.773892	-0.424183
11	8	0	-1.332189	-1.554242	-0.102209
12	6	0	-2.099971	-1.07711	-1.215395
13	6	0	-1.644294	0.342788	-1.511956
14	8	0	-2.272137	1.3878	0.54379
15	6	0	-0.807742	-0.550522	2.021517

16	6	0	-0.129532	0.533576	2.848512
17	6	0	-3.578306	-1.186436	-0.866892
18	8	0	1.842773	2.735946	-0.637843
19	1	0	3.298066	-3.03407	-0.065381
20	1	0	0.897348	-2.797495	0.54283
21	1	0	3.644096	0.976105	-0.948604
22	1	0	-0.561333	2.897591	-0.336206
23	1	0	-1.896688	-1.727158	-2.073521
24	1	0	-0.811245	0.304125	-2.225558
25	1	0	-2.434438	0.952218	-1.962897
26	1	0	-2.615166	2.127712	0.018748
27	1	0	-1.883893	-0.542137	2.238986
28	1	0	-0.463343	-1.529935	2.379889
29	1	0	-0.343936	0.37722	3.910913
30	1	0	0.957327	0.512467	2.726149
31	1	0	-0.489607	1.53148	2.58428
32	1	0	-3.842687	-2.232935	-0.679072
33	1	0	-4.206388	-0.811397	-1.68038
34	1	0	-3.82278	-0.640335	0.049302

2-5					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	3.460556	-0.922216	-0.898268
2	6	0	2.595395	-1.956813	-0.835918
3	6	0	1.28062	-1.838126	-0.410305
4	6	0	0.807239	-0.580065	-0.014314
5	6	0	1.686856	0.510257	-0.095502
6	6	0	2.988444	0.292256	-0.525336
7	6	0	-0.617073	-0.370635	0.489751
8	6	0	-1.084678	1.078665	0.160807
9	7	0	-0.092142	2.082311	0.395073
10	6	0	1.252645	1.883347	0.241602
11	8	0	-1.526846	-1.20291	-0.265098
12	6	0	-1.950432	-0.482953	-1.439449
13	6	0	-1.498843	0.969241	-1.299672
14	8	0	-2.211846	1.509549	0.908576
15	6	0	-0.748692	-0.701772	1.995417
16	6	0	-0.461996	-2.151359	2.37541
17	6	0	-3.456005	-0.638353	-1.584163
18	8	0	2.057102	2.796262	0.367429
19	1	0	2.999003	-2.917277	-1.145311
20	1	0	0.63966	-2.714622	-0.385388
21	1	0	3.705844	1.106463	-0.59549
22	1	0	-0.404026	3.022538	0.641488
23	1	0	-1.465344	-0.943985	-2.307755
24	1	0	-0.648091	1.140668	-1.971235
25	1	0	-2.279402	1.68274	-1.586095
26	1	0	-2.855288	0.779584	0.910917
27	1	0	-0.096729	-0.046409	2.585901
28	1	0	-1.777793	-0.507408	2.320755
29	1	0	-0.713183	-2.314499	3.428951
30	1	0	-1.057814	-2.84867	1.778898
31	1	0	0.596426	-2.397975	2.255249
32	1	0	-3.72227	-1.69819	-1.659753

33	1	0	-3.823213	-0.122439	-2.476343
34	1	0	-3.984842	-0.246524	-0.709651

2-6					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	3.667456	-1.138932	-0.360919
2	6	0	2.780434	-2.153333	-0.285493
3	6	0	1.423927	-1.973812	-0.061437
4	6	0	0.923919	-0.671291	0.093902
5	6	0	1.830063	0.392345	0.00686
6	6	0	3.173432	0.114114	-0.212065
7	6	0	-0.556986	-0.418242	0.373624
8	6	0	-0.953809	1.033217	-0.050012
9	7	0	0.050333	2.032193	0.163418
10	6	0	1.396414	1.79619	0.135956
11	8	0	-1.302292	-1.308429	-0.489968
12	6	0	-1.874847	-0.555125	-1.572252
13	6	0	-1.299439	0.852907	-1.517565
14	8	0	-2.088361	1.55727	0.609354
15	6	0	-0.850312	-0.768611	1.853174
16	6	0	-2.307514	-1.075988	2.183967
17	6	0	-3.391704	-0.598797	-1.447408
18	8	0	2.20095	2.714518	0.214644
19	1	0	3.200392	-3.147655	-0.411556
20	1	0	0.765287	-2.836551	-0.009764
21	1	0	3.912479	0.909032	-0.281366
22	1	0	-0.227939	3.014809	0.196216
23	1	0	-1.590439	-1.043664	-2.510818
24	1	0	-0.393236	0.887786	-2.135812
25	1	0	-1.991863	1.606551	-1.907467
26	1	0	-1.786707	1.805304	1.49935
27	1	0	-0.288093	-1.668104	2.138086
28	1	0	-0.481328	0.031247	2.50726
29	1	0	-2.396885	-1.338016	3.243672
30	1	0	-2.967493	-0.225883	2.003058
31	1	0	-2.675459	-1.9282	1.604246
32	1	0	-3.742579	-1.635965	-1.47994
33	1	0	-3.871241	-0.044091	-2.259513
34	1	0	-3.733261	-0.187748	-0.49288

2-7					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	3.662487	-0.353637	-0.802219
2	6	0	3.00599	-1.527431	-0.881192
3	6	0	1.658696	-1.675796	-0.584463
4	6	0	0.914476	-0.560303	-0.16175
5	6	0	1.575116	0.67062	-0.116449
6	6	0	2.928787	0.72382	-0.435462
7	6	0	-0.563675	-0.672715	0.162303
8	6	0	-1.207417	0.652753	0.718023
9	7	0	-0.436152	1.853822	0.553157
10	6	0	0.87984	1.926095	0.207716

11	8	0	-1.198686	-0.905988	-1.133563
12	6	0	-2.086301	0.182894	-1.418073
13	6	0	-2.50151	0.735306	-0.073061
14	8	0	-1.51299	0.649402	2.094152
15	6	0	-0.917857	-1.917301	1.02347
16	6	0	-0.141821	-2.08121	2.32619
17	6	0	-3.252527	-0.316763	-2.248757
18	8	0	1.45459	3.006765	0.177376
19	1	0	3.604806	-2.374255	-1.205268
20	1	0	1.198565	-2.652592	-0.698482
21	1	0	3.478655	1.662176	-0.414248
22	1	0	-0.875397	2.751133	0.771251
23	1	0	-1.523534	0.931277	-1.98911
24	1	0	-2.918096	1.745829	-0.144722
25	1	0	-3.267513	0.102069	0.393106
26	1	0	-0.725154	1.01508	2.531656
27	1	0	-1.992152	-1.902722	1.250527
28	1	0	-0.785138	-2.830969	0.428662
29	1	0	-0.506152	-2.965053	2.860897
30	1	0	0.926388	-2.230373	2.14561
31	1	0	-0.255558	-1.226155	2.994783
32	1	0	-2.893649	-0.73534	-3.195056
33	1	0	-3.958175	0.490108	-2.467311
34	1	0	-3.78635	-1.122766	-1.733557