Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers. This journal is © the Partner Organisations 2022

Supplementary Information

Penaloidines A and B: two unprecedented pyridine alkaloids from

Penicillium sp. KYJ-6

Dong Gan, Li Zhu, Xiao-Ran Zhang, Chen-Zhe Li, Cheng-Yao Wang, Le Cai*, Zhong-Tao Ding*

Functional Molecules Analysis and Biotransformation Key Laboratory of Universities

in Yunnan Province, Key Laboratory of Medicinal Chemistry for Natural Resource,

Ministry of Education, School of Chemical Science and Technology, Yunnan University,

Kunming 650091, People's Republic of China;

*Corresponding Authors. E-mail: ztding@ynu.edu.cn (Zhong-Tao Ding) E-mail: caile@ynu.edu.cn (Le Cai)

Content

Table S1. Crystal data and structure refinement for Penaloidine A (1). 4
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) 5
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)7
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) 10
Figure S12. HMBC spectrum of penaloidine A (1) in CDCl ₃ (400 MHz) 10
Figure S13. NOESY spectrum of penaloidine A (1) in CDCl ₃ (400 MHz) 11
Table S2 ¹ H NMR (400MHz) and ¹³ C NMR (100MHz) spectroscopic data in CDCl ₃ of
penaloidine A (1)
Figure S14. IR spectrum of penaloidine A (1) 12
Figure S15. ¹ H NMR spectrum of penaloidine B (2) in methanol- <i>d4</i> (400 MHz) 12
Figure S16. ¹³ C and DEPT NMR spectrum of penaloidine B (2) in methanol- <i>d4</i> (100 MHz).
= 13
Figure S17. HSQC spectrum of penaloidine B (2) in methanol- $d4$ (400 MHz)
Figure S18. ¹ H- ¹ H COS Y spectrum of penaloidine B (2) in methanol- $a4$ (400 MHz)
Figure S19. HMBC spectrum of penaloidine B (2) in methanol- <i>d4</i> (400 MHz)
Figure S20. NOESY spectrum of penaloidine B (2) in methanol-d4 (400 MHz) 15
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) 17
Figure S25. HSQC spectrum of penaloidine B (2) in CDCl ₃ (400 MHz) 17
Figure S26. HMBC spectrum of penaloidine B (2) in CDCl ₃ (400 MHz) 18
Figure S27. NOESY spectrum of penaloidine B (2) in CDCl ₃ (400 MHz)18

Table S3 ¹ H NMR (400MHz) and ¹³ C NMR (100MHz) spectroscopic data in CDCl ₃ of
penaloidine B (2)
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 19
Figure S29. Mpw1pw91/6-311+G(d,p) (chloroform) optimized lowest energy conformers for 1(a-d)
Figure S30. DP4+ evaluation of theoretical and experimental data of penaloidine A (1) 20
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).21
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 21
Figure S31. Mpw1pw91/6-311+G(d,p) (chloroform) optimized lowest energy conformers for 2 (a-d)
Figure S32. DP4+ evaluation of theoretical and experimental data of penaloidine B (2) 22
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).23
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).23
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
Figure S35. Optimized geometries of predominant conformers for 1
Table S9. Cartesian Coordinates of the Lowest Energy Conformers for Compound 1
Figure S36. Optimized geometries of predominant conformers for 2
Table S10. Cartesian Coordinates of the Lowest Energy Conformers for Compound 2

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	P212121			
Unit cell dimensions	a = 9.0646(2) Å	<i>α</i> = 90°.		
	b = 13.3250(3) Å	$\beta = 90^{\circ}$.		
	c = 20.6396(4) Å	$\gamma = 90^{\circ}.$		
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 m	n ³		
Theta range for data collection	3.95 to 72.12°.			
Index ranges	-11<=h<=11, -15<=k<=1	6, -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 equ	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	a / 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				

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





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. ¹H-¹H 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	lon	Formula	Abundance /						
P		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	lon	Formula	Abundance /						
ė		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
	÷	V	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 S10. ¹³C NMR spectrum of penaloidine A (1) in CDCl₃ (400 MHz).



Figure S11. HSQC spectrum of penaloidine A (1) in CDCl₃ (400 MHz).



Figure S12. HMBC spectrum of penaloidine A (1) in CDCl₃ (400 MHz).



Figure S13. NOESY spectrum of penaloidine A (1) in CDCl₃ (400 MHz). **Table S2** ¹H NMR (400MHz) and ¹³C NMR (100MHz) spectroscopic data in CDCl₃ of penaloidine A (1).

Pos.	1 (in CDCl ₃)					
	$\delta_{\rm H}(J \text{ in Hz})$	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				
ба	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 S15. ¹H NMR spectrum of penaloidine B (2) in methanol-d4 (400 MHz).



Figure S16. ¹³C 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. ¹H-¹H 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).



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



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



Figure S23. ¹H NMR spectrum of penaloidine B (2) in CDCl₃ (400 MHz).



Figure S25. HSQC spectrum of penaloidine B (2) in CDCl₃ (400 MHz).



Figure S26. HMBC spectrum of penaloidine B (2) in CDCl₃ (400 MHz).



Figure S27. NOESY spectrum of penaloidine B (2) in CDCl₃ (400 MHz).

2 (in CDCl₃) Pos. $\delta_{\rm H}(J \text{ in Hz})$ $\delta_{\rm C}$ 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 48.5, CH₂ 6а 2.13, dd (5.0, 13.7) 6b 2.29, dd (8.9, 13.6) 7 71.8, CH 3.92, m 8 83.9, C 9 150.8, C 10 7.56, brd (5.2) 120.9, CH 11 1.97, m 27.8, CH₂ 12 0.76, t (7.5) 7.7, CH₃ 13 1.34, d (6.2) 22.1 CH₃ -NH-7.89, s OH-5 5.56, s m 1671. 52 _____ 1599. 40 _____ 95 1454. 56 1373. 51 3680.47 90 85 2844.07 3707.93 80 75 2865.58 要 立 選い 70 2922.26 65 1013.43 60 2971.42 1032.77 55 50 1054.29 45 40 1000 4000 3000 2000

Table S3 ¹H NMR (400MHz) and ¹³C NMR (100MHz) spectroscopic data in CDCl₃ of penaloidine B (2).

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

波数 (cm-1)

Conf.	G (Hartree)	$\triangle G$ (Kcal/mol)	Boltzmann Distribution					
a								
al	-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).

Dirt Dirt <thdirt< th=""> Dirt Dirt <thd< th=""><th></th><th>-</th><th>22</th><th></th><th>~</th><th>L</th><th></th><th>- D</th><th></th><th>12.</th><th></th><th>. v</th><th></th><th></th></thd<></thdirt<>		-	22		~	L		- D		12.		. v		
Nuclei sperimenta Isomer 1 Isomer 2 Isomer 3 Isomer 3				DF	4+	100.	00%	o. 0 Illi	0%	0. O	0%	0. O)%	l
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Nucl	ei	sp2?	xperi	menta	Isom	er 1	Isome	er 2	Isome	r 3	Isome	r 4	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	C		x	15	3.4	1	60.7	10	51.6	16	1.5	16	1.7	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	C		x	1.	49	1	55.6	1	55.7	15	5.7	15	5.6	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	С		x	123	3.1	1	29.8	1:	29.5	12	9.4	12	4.8	
C 91.1 95.2 91.8 91.6 95.2 C 140.3 49.2 42.8 42.5 49.1 C 33.6 162.3 90.6 96.6 90.2 C x 125.3 127.2 134.6 124.5 197.3 C x 125.2 23.1 123.5 123.5 23.0 23.0 C 8.1 10.5 11.4 11.1 10.4 30.4 C 22.2 23.1 23.3 23.0 23.0 23.1 H x 8.94 9.36 9.44 9.40 9.37 H 3.79 4.49 4.76 4.71 4.72 H x 7.66 1.06 1.09 1.06 H x 7.66 1.09 1.06 1.09	С		x	16	3.7	1	67.3	13	73.1	17	3.1	16	7.3	
C 49.3 49.2 42.8 42.8 42.5 49.1 C 43.6 77.5 77.6 77.6 77.6 77.6 77.6 C 43.6 42.8 42.8 77.5 77.6 77.6 77.6 C 43.6 142.8 162.3 164.6 196.3 196.3 196.3 196.3 196.3 C x 123.3 114.6 114.6 114.5 112.3 112.4 112.4 112.3 112.4 111.1 10.0 11.4 11.1 10.0 11.4 11.1 10.0 11.4 11.1 10.0 11.4 11.1 10.0 11.6 1.77 1.96 1.77 1.96 1.77 1.96 1.77 1.96 1.77 1.96 1.77 1.96 1.77 1.96 1.77 1.96 1.97 1.96 1.99 1.98 1.99 1.98 1.99 1.98 1.99 1.94 1.99 1.98 1.99 1.94 1.99 1.98 1.99 1.98 1.99 1.98 1.99 1.98 <td< td=""><td>С</td><td></td><td></td><td>91</td><td>. 1</td><td></td><td>95.2</td><td>5</td><td>91.8</td><td>9</td><td>1.6</td><td>9</td><td>5.2</td><td></td></td<>	С			91	. 1		95.2	5	91.8	9	1.6	9	5.2	
C 74.1 77.5 77.6 77.4 77.7 77.6 C x 135.3 162.3 196.6 90.5 90.3 90.5 C x 135.3 162.3 196.6 195.0 192.2 194.6 195.0 192.2 C x 123.3 123.2 134.6 195.6 195.5 122.2 C 22.2 23.1 23.3 23.0 23.1 23.3 23.0 23.1 H x 8.94 9.36 9.44 9.40 9.37 191 1.86 1.77 H x 8.94 9.36 9.44 9.40 9.37 H x 8.94 9.36 9.44 9.40 9.37 H 2.17 2.33 2.70 2.71 2.32 14.9 1.76 H x 1.86 1.99 2.04 1.99 1.86 1.99 1.48 1.16 H x 1.86 1.99 2.04 1.99 1.85 1.16 1.99 1.48 </td <td>С</td> <td></td> <td></td> <td>49</td> <td>. 3</td> <td></td> <td>49.2</td> <td></td> <td>42.8</td> <td>- 4</td> <td>2.5</td> <td>4</td> <td>9.1</td> <td></td>	С			49	. 3		49.2		42.8	- 4	2.5	4	9.1	
C x 135.3 166.3 190.5 90.3 90.3 160.2 C x 123.4 155.4 165.2 156.6 156.0 162.2 C x 123.4 127.7 136.6 156.0 162.2 23.4 C x 123.4 127.7 136.6 135.0 127.2 23.4 C x 22.2 23.1 23.3 23.0 23.1 H x 8.65 9.16 9.14 9.16 9.16 H x 8.65 9.16 9.14 9.16 1.77 H x 8.65 1.77 1.91 1.86 1.77 H x 7.75 4.76 4.71 4.76 7.76 H x 7.75 4.70 4.73 1.69 1.765 H x 1.96 1.77 1.91 1.86 1.769 H x 1.96 1.77 1.91 1.34 1.16 H x 1.96 1.16 1.3	C			74	. 1		77.5		77.6	7	7.4	7	7.6	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C			83	. 9		86. 3		90.5	9	0.3	9	0.3	
C X 123.3 124.6 </td <td>C</td> <td></td> <td>x</td> <td>15</td> <td>5.1</td> <td>1</td> <td>62.3</td> <td>1:</td> <td>56.1</td> <td>15</td> <td>6.0</td> <td>16</td> <td>2.2</td> <td></td>	C		x	15	5.1	1	62.3	1:	56.1	15	6.0	16	2.2	
C 29% 0 32.7 33.2 <	C		x	12	3. 3	1	27.2	13	24.6	12	4. 0	12	1.3	
C 3.1 1.1.3 1.1.3 1.1.4 1.1.7 1.1.7 1.1.4 1.1.7 1.1.7 1.1.77 1.1.4 1.1.77 1.1.4 1.1.77 1.1.4 1.1.6 1.1.77 1	0			29	. 0		10 5		35.5	3	0.2	3	2.0	
C 1 20.1 2	C			0.	2		22 1		22 2	1	2 0	2	2 1	
H x 8.65 9.16 9.18 9.14 9.14 9.16 9.17 H 1.96 1.77 1.91 1.86 1.77 1.77 1.77 1.77 1.77 1.77 1.77 1.77 1.77 1.77 1.78 1.91 1.86 1.77 1.72 1.73 7.69 7.79 7.75 7.69 7.69 7.69 7.69 7.69 7.69 1.91 1.86 1.77 1.73 7.69 7.69 7.69 7.69 7.69 7.69 7.69 7.69 7.69 7.69 1.88 1.88 1.86 1.89 2.04 1.99 1.88 1.16 1.39 1.34 1.16 H 1.2 1.16 1.39 1.34 1.16 1.39 1.34 1.16 H 1.2 1.16 1.39 1.34 1.16 3.34 1.16 H 1.2 1.16 1.39 1.34 1.16 3.34 1.16 H 1.2 1.16 1.39 1.34 1.16 3.34 1.16 <	C						20. 1		20.0	-	3. 0	-	J. 1	
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 7.99 H 0.67 0.99 0.75 0.69 1.00 H 1.2 0 0 1.17 1.99 1.86 H 0.67 0.69 1.100 1.13 1.100 1.12 a b C D E F Functional Solvent? Basis Set 1.99 1.80 mPW1PW91 PCM 6-311+G(d, p) 1 1 sDP4+ (C data)	н		×	8	65		9.16		9.18	9	14	9	16	
H 1.96 1.77 1.91 1.86 1.77 H 2.17 2.13 2.76 2.71 2.23 H 3.79 4.49 4.76 4.71 4.72 H 1.86 1.99 2.04 1.99 1.88 H 1.27 1.16 1.39 1.34 1.16 H 1.2 1.16 1.39 1.34 1.16 H 1.2 1.16 1.39 1.34 1.16 A B C D E F Functional Solvent? Basis Set 6-311+G(d, p) Isomer 1 Isomer 2 Isomer 3 Isomer 4 1 sDP4+ (H data) 495.44% 0.00% 0.00% 4.63% sDP4+ (C data) 497.71% 0.00% 0.00% 0.23% uDP4+ (All	н		x	8	94		9.36		9.44	9	40	9	37	
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 7.99 H x 7.55 7.90 7.73 7.69 7.99 1.86 H 0.67 0.99 0.75 0.69 1.00 1.16 1.39 1.34 1.109 H 1.2 1.12 1.16 1.39 1.34 1.100 1.10 H 1.2 1.2 1.150mer 1.50mer 1.	H			1.	96		1.77		1.91	1	. 86	1	. 77	
H x 3, 79 4, 49 4, 76 4, 71 4, 72 H x 7, 55 7, 69 7, 69 7, 69 7, 69 7, 69 H x 1, 86 1, 89 2, 04 1, 99 1, 88 H x 1, 2 1, 19 1, 39 1, 34 1, 16 H x 1, 2 1, 16 1, 39 1, 34 1, 16 H x 1, 2 1, 16 1, 39 1, 34 1, 16 A B C D E F Functional Solvent? Basis Set 6-311+G(d, p) Isomer 1 Isomer 2 Isomer 3 Isomer 4 1 sDP4+ (H data) d 7,74 d 6.6% sDP4+ (C data) d 99,72% d 0.00% d 0.28% uDP4+ (H data) d 99,72% d 0.00% d 0.28% uDP4+ (C data) d 99,73% d 0.00% d 0.29% uDP4+ (all data) d 99,74% <td>Н</td> <td></td> <td></td> <td>2.</td> <td>17</td> <td></td> <td>2.23</td> <td></td> <td>2.76</td> <td>2</td> <td>. 71</td> <td>2</td> <td>. 23</td> <td></td>	Н			2.	17		2.23		2.76	2	. 71	2	. 23	
H x 7.55 7.90 7.73 7.69 7.99 H 0.67 1.90 1.99 1.99 1.99 1.99 1.99 H 0.67 0.99 0.75 0.69 1.00 1.00 1.00 H 1.2 1.2 1.10 1.39 1.34 1.10 1.00 H 1.2 1.2 1.10 1.10 1.10 1.10 1.10 H 1.2 1.10 1.10 1.10 1.10 1.10 1.10 SDP4+ (1.14 1.10 1.10 1.10 1.10	н			3.	79		4.49		4.76	4	. 71	4	. 72	
H 1.86 1.99 2.04 1.99 1.88 H 0.67 0.69 0.09 0.75 0.69 1.09 H 1.2 1.16 1.39 1.34 1.16 A B C D E F Punctional Solvent? Basis Set 6-311+G(d, p) MWIPW91 PCM 6-311+G(d, p) 1.99 1.46 SDP4+ (H data) d/78.42% d/8.43% d/8.47% d/4.66% sDP4+ (C data) d/95.44% 0.00% 0.00% d/4.28% uDP4+ (C data) d/97.71% 0.00% d/4.00% 0.28% uDP4+ (C data) d/97.71% 0.00% 0.00% 0.21% DP4+ (C data) d/99.28% 0.04% 0.00% 0.21% DP4+ (C data) d/99.28% 0.04% 0.00% 0.04% 0.21% DP4+ (C data) d/99.89% 0.00% d/0.00% 0.00% 0.00% 0.00% DP4+ (C data) d/99.89% 0.00% d/0.00% 0.00% 0.00% 0.00% 0.00% 0.00% <td>н</td> <td></td> <td>x</td> <td>7.</td> <td>55</td> <td></td> <td>7.90</td> <td></td> <td>7.73</td> <td>7</td> <td>. 69</td> <td>7</td> <td>. 69</td> <td></td>	н		x	7.	55		7.90		7.73	7	. 69	7	. 69	
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 1.69 1.16 A B C D E F Functional Solvent? Basis Set 6-311+G(d, p) B C D E F B C D E F SDP4+ H data d 78.42% d 8.43% d 8.47% d 4.68% SDP4+ C data d 99.72% d 0.00% d 0.28% uDP4+ (altaa) d 99.73% d 0.00% d 0.28% uDP4+ (clata) d 99.73% d 0.00% d 0.21% DP4+ (clata) d 99.73% d 0.00% d 0.00% 0.21% DP4+ (clata) d 99.83% d 0.00% 0.00% 0.00% 0.00% 0.00% 0.00%	Н			1.	86		1.89		2.04	1	. 99	1	. 88	
H 1.2 1.16 1.39 1.34 1.16 a b c d 1.34 1.16 a b c d d 1.16 A B C D E F Functional Solvent? Basis Set 6-311+G(d, p) Isomer 1 Isomer 2 Isomer 3 Isomer 4 1 sDP4+ (H data) d 78.42% d 8.43% d 8.47% d 4.63% sDP4+ (C data) d 95.44% d 0.00% d 0.00% d 2.28% uDP4+ (C data) d 99.72% d 0.00% d 0.28% uDP4+ (H data) d 99.73% d 0.00% d 0.28% uDP4+ (C data) d 99.73% d 0.00% d 0.28% uDP4+ (H data) d 99.73% d 0.00% d 0.28% uDP4+ (All data) d 99.73% d 0.00% d 0.21% uDP4+ (C data) <	H			0.	67		0.99		0.75	0	. 69	1	. 00	
A B C D E F Functional mPW1PW91 Solvent? PCM Basis Set 6=311+G(d, p) Isomer 1 Isomer 2 Isomer 3 Isomer 4 I SDP4+ (H data) 178.42% d8.43% d8.47% d4.68% sDP4+ (C data) 95.44% 0.00% 0.00% d 0.28% uDP4+ (all data) 99.72% 0.00% 0.00% d 0.28% uDP4+ (C data) 99.73% 0.00% 0.00% d 0.28% uDP4+ (cl lata) 99.73% 0.00% 0.00% d 0.21% DP4+ (C data) 99.88% 0.00% 0.00% 0.11% DP4+ (C data) 99.88% 0.00% 0.00% 0.00% 0.00% DP4+ (c data) 99.88% 0.00% 0.00% 0.00% 0.00% 0.00%	H			1.	.2		1.16		1.39	1	. 34	1	. 16	
A B C D E F Functional Solvent? Basis Set mPW1PW91 PCM 6-311+G(d, p) Isomer 1 Isomer 2 Isomer 3 Isomer 4 1 sDP4+ (H data) d178.42% d18.43% d18.47% d14.63% sDP4+ (C data) d195.44% d10.00% d10.00% d14.56% sDP4+ (all data) d190.23% d10.00% d10.28% uDP4+ (all data) d197.71% d10.00% d10.23% uDP4+ (all data) d199.72% d10.00% d10.00% d10.21% uDP4+ (all data) d199.73% d10.00% d10.00% d10.23% uDP4+ (H data) d199.73% d10.00% d10.00% d10.21% uDP4+ (all data) d100.00% d10.00% d10							2		h		0		d	
Functional Solvent? Basis Set mPW1PW91 PCM 6-311+G(d, p) Isomer 1 Isomer 2 Isomer 3 Isomer 4 1 sDP4+ (H data) d178.42% d18.43% d18.47% d14.63% sDP4+ (C data) d195.44% d10.00% d10.00% d14.56% sDP4+ (all data) d190.23% d10.30% d1.27% d18.20% uDP4+ (H data) d190.71% d10.00% d10.00% d12.29% uDP4+ (all data) d199.79% d10.00% d10.01% d10.21% uDP4+ (H data) d199.71% d10.00% d10.00% d10.21% uDP4+ (H data) d199.79% d10.00% d10.01% d10.21% uDP4+ (c data) d199.28% d10.00% d10.00% d10.00% uDP4+ (C data) d199.89% d10.00% d10.00% d10.00% uDP4+ (c data) d100.00% d10.00% d10.00% d10.00%		А		В	(5		D		Е		F		
Functional Solvent? Basis Set mPW1PW91 PCM 6-311+G(d, p) Isomer 1 Isomer 2 Isomer 3 Isomer 4 sDP4+ (H data) d 78.42% d 8.43% d 8.47% d 4.68% sDP4+ (C data) d 95.44% d 0.00% d 0.00% d 4.56% sDP4+ (all data) d 99.72% d 0.00% d 0.00% d 0.23% uDP4+ (Alt data) d 90.23% d 0.30% d 1.27% d 8.20% uDP4+ (c data) d 99.79% d 0.00% d 0.00% d 0.23% uDP4+ (c data) d 99.73% d 0.00% d 0.00% d 0.23% uDP4+ (c data) d 99.73% d 0.00% d 0.00% d 0.23% uDP4+ (c data) d 99.73% d 0.00% d 0.00% d 0.23% uDP4+ (c data) d 99.73% d 0.00% d 0.00% d 0.23% uDP4+ (c data) d 99.28% d 0.00% d 0.15% d 0.54% DP4+ (C data) d 99.89% d 0.00% d 0.00% d 0.11% DP4+ (c data) <		P				0 1	. 0			D ·	0			
mPW1PW91 PCM 6-311+G(d, p) Isomer 1 Isomer 2 Isomer 3 Isomer 4 1 sDP4+ (H data) d178.42% d18.43% d18.47% d14.63% sDP4+ (C data) d195.44% d10.00% d10.00% d14.56% sDP4+ (a11 data) d199.72% d10.00% d10.28% uD94 uDP4+ (H data) d190.23% d10.00% d10.28% uD94 uDP4+ (C data) d197.71% d10.00% d10.00% d10.21% uDP4+ (a11 data) d199.79% d10.00% d10.00% d10.21% uDP4+ (c data) d199.79% d10.00% d10.00% d10.21% DP4+ (c data) d199.79% d10.00% d10.00% d10.00% DP4+ (C data) d199.89% d10.00% d10.00% d10.00% DP4+ (c data) d100.00% d10.00% d10.00% d10.00%		Fur	ictional			Solv	ent?			Bası	s Se	et.		
Isomer 1 Isomer 2 Isomer 3 Isomer 4 Isomer 4 sDP4+ (H data) d 78.42% d 8.43% d 8.47% d 4.68% sDP4+ (C data) d 95.44% d 0.00% d 0.00% d 4.68% sDP4+ (all data) d 99.72% d 0.00% d 0.28% uDP4+ (all data) d 99.73% d 0.00% d 0.28% uDP4+ (c data) d 99.73% d 0.00% d 0.28% uDP4+ (c data) d 99.73% d 0.00% d 0.28% uDP4+ (c data) d 99.73% d 0.00% d 0.28% uDP4+ (c data) d 99.73% d 0.00% d 0.21% uDP4+ (c data) d 99.79% d 0.00% d 0.21% uDP4+ (c data) d 99.28% d 0.00% d 0.54% DP4+ (mF	W1PW91			P	CM			6-311+	-G(d	. n)		
Isomer 1 Isomer 2 Isomer 3 Isomer 4 Isomer 4 sDP4+ (H data) d178.42% d18.43% d18.47% d14.63% sDP4+ (C data) d195.44% d10.00% d10.00% d14.56% sDP4+ (all data) d199.72% d10.00% d10.28% d12.28% uDP4+ (H data) d190.23% d10.30% d1.27% d18.20% uDP4+ (C data) d197.71% d10.00% d10.00% d12.29% uDP4+ (all data) d199.78% d10.00% d10.10% d10.21% DP4+ (Alta) d199.71% d10.00% d10.00% d10.21% DP4+ (C data) d199.28% d10.00% d10.21% d10.21% DP4+ (C data) d199.89% d10.00% d10.00% d10.00% DP4+ (all data) d100.00% d10.00% d10.00% d10.00%												, F,		
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+ (all data) # 99.72% # 0.00% # 0.28% uDP4+ uDP4+ (C data) # 97.71% # 0.00% # 0.00% # 2.29% uDP4+ (cl data) # 99.79% # 0.00% # 0.15% # 2.29% uDP4+ (cl data) # 99.79% # 0.00% # 0.15% # 0.21% uDP4+ (cl data) # 99.28% # 0.00% # 0.15% # 0.54% DP4+ (C data) # 99.89% # 0.00% # 0.00% # 0.11% DP4+ (cl1 data) # 100.00% # 0.00% # 0.00% # 0.00%														
sDP4+ (H data) d 78.42% d 8.43% d 8.47% d 4.68% sDP4+ (C data) g 95.44% d 0.00% d 0.00% d 4.56% sDP4+ (all data) g 99.72% d 0.00% d 0.00% d 0.28% uDP4+ (H data) g 90.23% d 0.30% d 1.27% d 8.20% uDP4+ (C data) g 97.71% d 0.00% d 0.00% d 2.29% uDP4+ (cl data) g 97.79% d 0.00% d 0.00% d 2.29% uDP4+ (cl data) g 99.78% d 0.00% d 0.10% d 2.29% uDP4+ (cl data) g 99.78% d 0.00% d 0.15% d 0.21% DP4+ (all data) g 99.28% d 0.00% d 0.15% d 0.54% DP4+ (C data) g 99.89% d 0.00% d 0.00% 0.11% DP4+ (all data) g 99.89% d 0.00% d 0.00% 0.00%					Ison	er 1	Iso	mer 2	Iso	mer 3	Is	omer 4	1	
sDP4+ (C data) 95.44% 0.00% 0.00% 1.56% sDP4+ (all data) 99.72% 0.00% 0.00% 0.23% uDP4+ (l data) 99.72% 0.30% 1.27% 8.20% uDP4+ (C data) 97.71% 0.30% 1.27% 8.20% uDP4+ (cl data) 97.71% 0.00% 0.00% 1.27% 8.20% uDP4+ (cl 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% 0.15% 0.11% DP4+ (all data) 99.89% 0.00% 0.00% 0.00% 0.00%		sDP4+	+ (H dat	a)	1 78.	42%	₫ 8.	43%	₫ 8.	47%	dí 4	. 68%		
sDP4+ (all data) # 99.72% d 0.00% d 0.00% d 0.28% uDP4+ (H data) # 90.23% d 0.30% d 1.27% d 8.20% uDP4+ (C data) # 97.71% d 0.00% d 0.00% d 2.29% uDP4+ (cll data) # 97.79% d 0.00% d 0.21% uDP4+ (H data) # 99.28% d 0.04% d 0.15% d 0.54% DP4+ (C data) # 99.89% d 0.00% d 0.00% d 0.11% DP4+ (cll data) # 99.89% d 0.00% d 0.00% d 0.00%		sDP4+	+ (C dat	:a)	9 5.	44%	₫ 0.	00%	₫ 0.	00%	₫ 4	. 56%		
uDP4+ (H data) 10.23% 10.30% 11.27% 18.20% uDP4+ (C data) 197.71% 10.00% 10.00% 12.29% uDP4+ (all data) 199.79% 10.00% 10.00% 10.21% DP4+ (H data) 199.28% 10.04% 10.15% 10.54% DP4+ (C data) 199.89% 10.00% 0.00% 10.11% DP4+ (all data) 100.00% 10.00% 0.00% 10.00%		sDP4+	(all da	ita)	1 99.	72%	₫ 0.	00%	₫ 0.	00%	dí C). 28%		
uDP4+ (C data) 197.71% 10.00% 10.00% 12.29% uDP4+ (all data) 199.79% 10.00% 10.00% 10.21% DP4+ (H data) 199.28% 10.04% 10.15% 10.54% DP4+ (C data) 199.89% 10.00% 10.00% 10.11% DP4+ (all data) 100.00% 10.00% 0.00% 0.00%		uDP4+	H dat	a)	d 90.	23%	₫ 0.	30%	₫ 1.	27%	afi 8	3. 20%		
uDP4+ (all data) 199.79% 10.00% 10.00% 10.21% DP4+ (H data) 199.28% 10.04% 10.15% 10.54% DP4+ (C data) 199.89% 10.00% 10.00% 10.11% DP4+ (all data) 100.00% 10.00% 10.00% 0.00%		uDP4+	· (C dat	a)	9 7.	71%	₫ 0.	00%	₫ 0.	00%	đl 2	2. 29%		
DP4+ (H data) 199.28% all 0.04% all 0.15% all 0.54% DP4+ (C data) 199.89% all 0.00% all 0.00% all 0.11% DP4+ (all data) 100.00% all 0.00% all 0.00% all 0.00%		uDP4+	(all da	ita)	1 99.	79%	ⅆ 0.	00%	đ 0.	00%	dí O	. 21%		
DP4+ (C data) 199.89% 10.00% 10.00% 10.11% DP4+ (all data) 100.00% 10.00% 10.00% 10.00%		DP4+	(H dat	a)	1 99.	28%	₫ 0.	04%	₫ 0.	15%	dí O	. 54%	Γ	
DP4+ (all data) #100.00% # 0.00% # 0.00% # 0.00%		DP4+	(C dat	a)	d 99.	89%	₫ 0.	00%	₫ 0.	00%	dil C). 11%	T	
		DP4+	(all da	ta)	100.	00%	₫ 0.	00%	₫ 0.	00%	dl C	. 00%	Τ	

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

absol	lute erro	r (MAE).							
Н	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 S5. Calculated (calc.) and experimental (exp.) ¹H 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).

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)	$\triangle G$ (Kcal/mol)	Boltzmann Distribution					
a								
al	-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%	dl 0. 00%	₫ 0.00%	. 00%
Nuclei	sp2?	xperimenta	Isomer 1	Isomer 2	Isomer 3	Isomer 4
С	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
С		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
С	x	121.1	127.7	125.5	128.1	125. 5
С		27.8	34.4	37.3	34.7	37.3
С		6.7	11.2	8.8	11.1	8.8
С		20.8	22. 1	23.9	22. 0	23. 9
Н	x	8.65	9.18	9.02	9.18	9.02
Н	x	8.94	9.33	9.41	9.67	9.41
Н		1.96	2.05	2.26	2.04	2.26
Н		2.17	2.32	2.39	2.37	2.39
Н		3.79	4.07	4.69	4.09	4.69
Н	x	7.55	7.81	7.73	7.79	7.73
Н		1.86	2.28	1.76	2.34	1.76
Н		0.67	0.86	1.00	0.79	0.85
Н		1.2	1,25	1.51	1 24	1 51
			d	D D	C C	u

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

	Isomer 1	Isomer 2	Isomer 3	Isomer 4
sDP4+ (H data)	4 69. 54%	ⅆ 2.35%	ⅆ 26. 03%	ⅆ 2.08%
sDP4+ (C data)	d 98. 62%	d 0. 32%	d 0. 73%	d 0. 32%
sDP4+ (all data)	d 99. 70%	d 0. 01%	d 0. 28%	d 0. 01%
uDP4+ (H data)	4 94. 32%	dl 0.85%	ⅆ 2.68%	ⅆ 2.15%
uDP4+ (C data)	4 75. 12%	dl 0. 08% 📶	ⅆ 24. 72%	1 0. 08%
uDP4+ (all data)	🚽 99. 07%	d 0. 00%	d. 93% 📶	. 00%
DP4+ (H data)	4 98. 85%	d 0. 03%	1.05%	ⅆ 0.07%
DP4+ (C data)	4 99. 75%	ⅆ 0. 00%	0.24%	ⅆ 0.00%
DP4+ (all data)	1 00. 00%	1 0. 00%	1 0. 00%	0.00%

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

С	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 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).

Table S8. Calculated (calc.) and experimental (exp.) ¹H 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).

Н	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 ¹³CNMR 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

1-5

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

$$\Delta \varepsilon(E) = \frac{1}{2.296 \times 10^{-39} \sqrt{\pi}\sigma} \sum_{i}^{A} \Delta E_{i} R_{i} e^{\left[-(E - \Delta E_{i})^{2}/\sigma^{2}\right]}$$

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	Atomic	Atomic	Coo	ordinates (Angstro	oms)		
Number	Number	Туре	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	Atomic	Atomic	Coo	rdinates (Angstro	oms)		
Number	Number	Туре	Х	Y	Ζ		
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	Atomic	Atomic	Coo	rdinates (Angstre	oms)		
Number	Number	Туре	Х	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	Atomic	Atomic	Coo	rdinates (Angstr	oms)		
Number	Number	Туре	Х	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	Atomic	Atomic	Coo	Coordinates (Angstroms)				
Number	Number	Туре	Х	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	Atomic	Atomic	Coo	rdinates (Angstro	oms)		
Number	Number	Туре	Х	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

Г

<i>L-L</i>							
Center	Atomic	Atomic	Coo	Coordinates (Angstroms)			
Number	Number	Туре	Х	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		

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Туре	Х	Y	Ζ
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	Atomic	Atomic	Coo	Coordinates (Angstroms)			
Number	Number	Туре	Х	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	Atomic	Atomic	Coo	rdinates (Angstr	oms)		
Number	Number	Туре	Х	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	Atomic	Atomic	Coo	rdinates (Angstro	oms)
Number	Number	Туре	Х	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	Atomic	Atomic	Coo	rdinates (Angstro	oms)	
Number	Number	Туре	Х	Y	Ζ	
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