Supporting Information

Strepyrrolins A–E, five pyrrole-sesquiterpene hybrids from Streptomyces sp. KIB 015, revealing a new formation logic of pyrroles by isotope labeling

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Scheme S1. Hypothetical formation mechanisms of compounds 3 and 4 from epoxide 8.

No.	$\delta_{ ext{H}}$	δς	НМВС	COSY	ROESY
2	7.06 (1H, overlapped)	126.93 (CH)	C-3, C-4, C-5	H-3	
3	6.24 (1H, dd, <i>J</i> = 3.6, 2.6 Hz)	111.25 (CH)	C-4, C-2, C-5		
4	7.07 (1H, overlapped)	119.04 (CH)	C-3, C-2, C-5, C-6	H-3	
5		133.00 (C)			
6		189.58 (C)			
7	3.48 (2H, br s)	49.61 (CH ₂)	C-6, C-8, C-9, C-18		H-4
8		136.23 (C)			
9	5.41 (1H, dd, J = 9.0, 1.4 Hz)	131.53 (CH)	C-18, C-7, C-11, C-10, C-8, C-6	H-7	H-7
10	4.27 (1H, t like, J = 8.7 Hz)	77.02 (CH)	C-11, C-12, C-15, C-8, C-9, C-16	H-9	
11	2.41 (1H, td, J = 8.7, 1.0 Hz)	65.51 (CH)	C-14, C-13, C-15, C-10, C-12, C-9	H-10	H-9
12		81.37 (C)			
13a	1.83 (1H, m)	40 60 (CH.)	C-14, C-12		H-10
13b	1.70 (1H, m)	40.00 (CH ₂)	C-14, C-15, C-11, C-12		
14a	1.89 (1H, m)	25 61 (CH ₂)	C-15, C-16	H-15	H-10
14b	1.72 (1H, m)	25.01 (CH ₂)	C-15, C-12, C-16	H-15	
15	2.74 (1H, ddd, J = 9.5, 8.7, 4.5 Hz)	55.45 (CH)	C-14, C-17, C-13, C-11, C-10	H-11	H-11
16		84.30 (C)			
17	1.26 (3H, s)	31.86 (CH ₃)	C-20, C-15, C-16		
18	1.78 (3H, br d, <i>J</i> = 1.0 Hz)	17.39 (CH₃)	C-7, C-9, C-8	H-9	H-10
19	1.15 (3H, s)	24.55 (CH ₃)	C-11, C-12, C-13		H-10, H-11
20	1.22 (3H, s)	24.07 (CH₃)	C-17, C-15, C-16		H-10

 Table S1. Detailed 2D-NMR data of compound 1.

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No.	$\delta_{ extsf{H}}$	δ _c	НМВС	COSY	ROESY
2	7.03 (1H, dd, <i>J</i> = 2.1, 1.5 Hz)	126.14 (CH)	C-3, C-4, C-5	H-3	
3	6.22 (1H, dd, <i>J</i> = 3.6, 1.2 Hz)	111.03 (CH)	C-4, C-2, C-5		
4	6.96 (1H, dd, <i>J</i> = 3.6, 1.2 Hz)	117.01 (CH)	C-3, C-2, C-5	H-3	H-7
5		135.16 (C)			
6		182.13 (C)			
7	6.70 (1H, br t, <i>J</i> = 1.2 Hz)	122.84 (CH)	C-18, C-9, C-10, C-8, C-6	H ₃ -18	
8		157.39 (C)			
9a	3.33 (1H, overlapped)	42 72 (CH_)	C-18, C-11, C-10, C-7, C-8, C-6	H-7, H-10	H ₃ -19
9b	2.65 (1H, dd, J = 12.9, 9.9 Hz)	42.73 (CH2)	C-18, C-11, C-10, C-7, C-8, C-6	H-10	H ₃ -18
10	3.91 (1H, ddd, <i>J</i> = 9.6, 8.1, 3.6 Hz)	81.04 (CH)	C-9, C-11, C-12, C-16, C-8		H ₃ -19
11	2.42 (1H, t like, J = 7.9 Hz)	65.34 (CH)	C-14, C-13, C-9, C-15, C-10, C-12	H-10	
12		82.04 (C)			
13a	1.77 (1H, m)	40.22 (СH ₂)	C-14, C-15, C-12		H-10
13b	1.66 (1H, overlapped)	40.22 (CH2)	C-14, C-15, C-12	H-11	
14a	1.85 (1H, m)	25 32 (CH ₂)	C-13, C-15, C-11, C-12, C-16	H-15	
14b	1.67 (1H, overlapped)	25.52 (CH2)	C-13, C-15, C-11, C-12, C-16	H-15, H-11	
15	2.70 (1H, ddd, <i>J</i> = 9.6, 7.8, 4.5 Hz)	55.24 (CH)	C-20, C-14, C-17, C-13, C-11, C-10	H-11	H-11
16		84.30 (C)			
17	1.27 (3H, s)	31.89 (CH₃)	C-20, C-15, C-16		H-10
18	2.08 (3H, br d, <i>J</i> = 1.2 Hz)	27.59 (CH ₃)	C-9, C-10, C-7, C-8, C-6		H-7
19	1.44 (3H, s)	24.69 (CH ₃)	C-13, C-11, C-12		
20	1.17 (3H, s)	24.50 (CH ₃)	C-17, C-15, C-16		

 Table S2. Detailed 2D-NMR data of compound 2.



No.	$\delta_{ ext{H}}$	δς	НМВС	COSY	ROESY
2	7.06 (1H, dd, <i>J</i> = 2.4, 1.2 Hz)	126.57 (CH)	C-3, C-4, C-5, C-6	H-3	
3	6.23 (1H, dd, <i>J</i> = 3.8, 2.4 Hz)	111.23 (CH)	C-4, C-2, C-5		
4	6.98 (1H, dd, <i>J</i> = 3.8, 1.2 Hz)	117.37 (CH)	C-3, C-2, C-5	H-3	H-7
5		135.40 (C)			
6		182.37 (C)			
7	6.62 (1H, s)	122.22 (CH)	C-8, C-9, C-18		
8		150.63 (C)			
9	7.66 (1H, d, J = 15.8 Hz)	130.55 (CH)	C-18, C-11, C-7, C-8		H-11
10	6.08 (1H, dd, <i>J</i> = 15.8, 9.7 Hz)	142.37 (CH)	C-15, C-11, C-12, C-8	H-9	
11	2.56 (1H, dd, <i>J</i> = 9.7, 7.1 Hz)	57.68 (CH)	C-13, C-15, C-16, C-12, C-19, C-9, C-10	H-10	
12		82.56 (C)			
13a	1.72 (1H, dd, <i>J</i> = 8.2, 5.4 Hz)	41 14 (CLL)	C-14, C-15, C-11, C-12		
13b	1.67 (1H, dd, <i>J</i> = 8.2, 4.5 Hz)	41.14 (CH ₂)	C-14, C-15, C-11, C-12	H ₂ -14	H-10, H-15
14	1.78 (2H, m)	25.17 (CH ₂)	C-13, C-15, C-16, C-12	H-15	
15	2.03 (1H, dt, J = 9.1, 7.1 Hz)	56.14 (CH)	C-14, C-17, C-13, C-11, C-16, C-12, C-10	H-11	H-10
16		73.25 (C)			
17	1.20 (3H, s)	28.31 (CH₃)	C-20, C-15, C-16		
18	2.11 (3H, br d, <i>J</i> = 1.0 Hz)	21.53 (CH ₃)	C-7, C-8. C-9		H-7, H-10
19	1.14 (3H, s)	24.17 (CH₃)	C-11, C-12, C-13		H-10
20	1.17 (3H, s)	28.66 (CH₃)	C-17, C-15, C-16		

 Table S3. Detailed 2D-NMR data of compound 3.



No.	$\delta_{ extsf{H}}$	δ _c	НМВС	COSY	ROESY
2	7.06 (1H, dd, <i>J</i> = 2.4, 1.4 Hz)	126.46 (CH)	C-3, C-4, C-5	H-3	
3	6.23 (1H, dd, <i>J</i> = 3.9, 2.4 Hz)	111.20 (CH)	C-4, C-2, C-5		
4	6.97 (1H, dd, <i>J</i> = 3.9, 1.4 Hz)	117.24 (CH)	C-3, C-2, C-5, C-6	H-3	H-7
5		135.48 (C)			
6		182.41 (C)			
7	6.59 (1H, s)	121.63 (CH)	C-18, C-9, C-8, C-6	H-9	
8		150.90 (C)			
9	7.66 (1H, d, <i>J</i> = 15.8 Hz)	130.30 (CH)	C-18, C-11, C-12, C-7, C-8		
10	6.12 (1H, dd, <i>J</i> = 15.8, 11.1 Hz)	140.34 (CH)	C-15, C-11, C-12, C-9, C-8	H-9	H ₃ -18
11	2.59 (1H, dd, J = 11.1, 5.8 Hz)	60.34 (CH)	C-14, C-13, C-12, C-15, C-9, C-10	H-10	H-9
12		83.04 (C)			
13a	1.83 (1H, m)	20 22 (CLL)	C-14, C-19, C-15, C-12		H-10
13b	1.78 (1H, m)	38.33 (CH ₂)	C-14, C-11, C-15, C-12		H-15
14	1.91 (2H, m)	23.63 (CH ₂)	C-13, C-15, C-11, C-12, C-16	H-13a, b	
15	2.67 (1H, ddd, <i>J</i> = 10.2, 9.6, 5.8 Hz)	54.51 (CH)	C-14, C-20, C-17, C-13, C-11, C-16, C-10	H ₂ -14	H-11
16		72.80 (C)			
17	1.19 (3H, s)	30.45 (CH ₃)	C-20, C-15, C-16, C-9		H-10
18	2.09 (3H, br d, <i>J</i> = 1.0 Hz)	21.67 (CH ₃)	C-6, C-7, C-8, C-9	H-7	H-7
19	1.15 (3H, s)	26.71 (CH₃)	C-11, C-12, C-13		H-10; H-11
20	1.22 (3H, s)	28.25 (CH₃)	C-15, C-16, C-17		

 Table S4. Detailed 2D-NMR data of compound 4.



No.	$\delta_{ extsf{H}}$	δ	НМВС	COSY	ROESY
2	7.06 (1H, dd, <i>J</i> = 2.2, 1.2 Hz)	126.47 (CH)	C-3, C-4, C-5	H-3	
3	6.23 (1H, dd, <i>J</i> = 3.7, 2.2 Hz)	111.19 (CH)	C-4, C-2, C-5		
4	6.97 (1H, dd, <i>J</i> = 3.7, 1.2 Hz)	117.28 (CH)	C-3, C-2, C-5	H-3	H-7
5		135.48 (C)			
6		182.36 (C)			
7	6.59 (1H, br s)	122.32 (CH)	C-18, C-9, C-8, C-6	H ₃ -18	H ₃ -18
8		150.48 (C)			
9	7.66 (1H, d, J = 15.8 Hz)	130.26 (CH)	C-18, C-11, C-7, C-8		H-11
10	5.90 (1H, dd, <i>J</i> = 15.8, 9.0 Hz)	138.60 (CH)	C-11. C-12, C-15, C-8	H-9	H ₃ -18
11	3.14 (1H, d, <i>J</i> = 9.0 Hz)	60.28 (CH)	C-14, C-13, C-12, C-9, C-10	H-11	H ₃ -19
12		82.50 (C)			
13	1.75 (2H, m)	38.69 (CH ₂)	C-14, C-11, C-12		H-10
14a	2.48 (1H, m)	20.06 (CUL)	C-13, C-15, C-16	H ₂ -13	
14b	2.36 (1H, m)	28.80 (CH ₂)	C-13, C-12, C-15, C-16	H ₂ -13	
15		137.49 (C)			
16		126.86 (C)			
17	1.61 (3H, s)	21.22 (CH ₃)	C-15, C-16		
18	2.07 (3H, br d, J = 0.9 Hz)	21.44 (CH ₃)	C-7, C-8, C-9		
19	1.23 (3H, s)	25.24 (CH₃)	C-11, C-12, C-13		H-10
20	1.65 (3H, s)	21.23 (CH ₃)	C-15, C-16		

 Table S5. Detailed 2D-NMR data of compound 5.



labeling substrates	Solvent used to dissolve the labeling substrate	Quality of labeling substrate used	Final concentration of the feeding experiment	fermentation medium	fermentation scale in total	yield of compound 3
[¹³ C ₅ , ¹⁵ N]-L-Pro	dd H ₂ O	100 mg	666 mg/L	M15A ^a	150 mL	NP ^d
[¹³ C ₅ , ¹⁵ N]-L-Glu	0.5N HCl	500 mg	625 mg/L	M15A ^a	800 mL	0.8 mg
¹³ C ₆ -glucose	dd H ₂ O	1000 mg	1250 mg/L	M15B ^b	800 mL	1.0 mg
¹³ C ₂ -Gly	dd H ₂ O	500 mg	625 mg/L	M15A ^a	800 mL	0.5 mg
¹³ C ₂ -sodium acetate	dd H ₂ O	1000 mg	1250 mg/L	M15B ^b	800 mL	0.8 mg
¹³ C ₃ -glycerol	dd H ₂ O	1000 mg	1250 mg/L	M15B ^b	800 mL	1.0 mg
[¹³ C ₃ , ¹⁵ N]-L-Ala	dd H ₂ O	500 mg	714 mg/L	M15A ^a	700 mL	0.6 mg
¹⁵ NH ₄ Cl	dd H ₂ O	450 mg	500 mg/L	M15A ^a	900 mL	NP ^d
¹⁵ NH₄Cl	dd H ₂ O	450 mg	500 mg/L	M15 ^c	900 mL	NP ^d

 Table S6. Details of feeding experiments using several isotope labeling substrates.

^{*a*} Medium M15A: glucose 30 g/L, beef extract 1 g/L, peptone 1 g/L, NaCl 5 g/L, CaCO₃ 3 g/L, pH 7.2 ^{*b*} Medium M15B: glucose 12 g/L, beef extract 5 g/L, peptone 1 g/L, NaCl 5 g/L, CaCO₃ 3 g/L, pH 7.2 ^{*c*} Medium M15: glucose 30 g/L, beef extract 5 g/L, peptone 1 g/L, NaCl 5 g/L, CaCO₃ 3 g/L, pH 7.2 ^{*d*}NP: Not to be purified.

Table S7. Energies and populations of predominant conformers of (10*S*, 11*R*, 12*S*, 15*R*)-**1** at M06-2X/6-31G(d,p) theory level in gas.

Conformers	Structures	E (Hartree)	E (kcal/mol)	Population (%)
а	A A A	-1020.543899	-640400.9603	48.51
Ь		-1020.540591	-640398.8846	1.46
с	大大	-1020.543929	-640400.9787	50.03

Conformers	Structures	E (Hartree)	E (kcal/mol)	Population (%)
а	A A	-1020.725693	-640515.0377	23.61
b	A A	-1020.725332	-640514.8109	16.10
c	1 the	-1020.723932	-640513.9327	3.66
d	A A	-1020.724043	-640514.0023	4.11
e	HAN H	-1020.725491	-640514.9108	19.06
f	J. Wet	-1020.725034	-640514.624	11.75
g	1 tot	-1020.72386	-640513.8873	3.39
h	1 the	-1020.725453	-640514.8873	18.32

Table S8. Energies and populations of predominant conformers of (11*S*, 12*S*, 15*R*)-**3** at B3LYP/6-31G(d,p) theory level in gas.

Conformers	Structures	E (Hartree)	E (kcal/mol)	Population (%)
a	ALT	-1020.55242	-640406.3074	95.59
b	SXX	-1020.548958	-640404.1345	2.44
С	文で	-1020.548691	-640403.967	1.84
d	the the	-1020.546184	-640402.3942	0.13

Table S9. Energies and populations of predominant conformers of (11*S*, 12*S*, 15*S*)-**4** at CAM-B3LYP/def2-TZVP theory level in gas.

Table S10. Energies and populations of predominant conformers of (11*S*, 12*S*)-**5** at CAM-B3LYP/def2-TZVP theory level in gas.

Conformers	Structures	E (Hartree)	E (kcal/mol)	Population (%)
а	4XXX	-944.0982086	-592430.5656	93.36
b	At St	-944.0957124	-592428.9992	6.64

	Conformer (10 <i>S</i> , 11 <i>R</i> , 12 <i>S</i> , 15 <i>R</i>)- 1-a					
Center	Atomic	Atomic		Coordinates (Angstroms)		
Number	Number	Туре	Х	Y	Z	
1	6	0	6.606840	-0.871758	-0.468339	
2	6	0	5.323483	-1.253528	-0.021958	
3	6	0	4.489767	-0.156911	-0.176800	
4	7	0	5.242940	0.860647	-0.702283	
5	6	0	6.520066	0.446116	-0.882735	
6	6	0	3.072688	0.084960	0.092269	
7	6	0	2.256251	-1.083900	0.630918	
8	8	0	2.584705	1.181785	-0.131486	
9	6	0	0.894967	-0.652220	1.110620	
10	6	0	0.914330	0.169598	2.372040	
11	6	0	-0.189781	-0.968926	0.399300	
12	6	0	-1.598712	-0.506578	0.623146	
13	6	0	-2.078853	0.408263	-0.533105	
14	6	0	-3,504627	-0.095355	-0.831988	
15	6	0	-3 434465	-1 574046	-0 402874	
16	8	0	-2 508120	-1 602316	0.687949	
17	6	0	-2 242525	1 886779	-0 158073	
18	6	0	-3 529235	1 877240	0.669101	
19	6	0	-4 443031	0.869390	-0.052356	
20	6	0	-4 734559	-2 183834	0.032330	
20	6	0	-2 879/193	_2.103034	-1 55295/	
21	0 0	0	-2 567671	2.422773	_1 2/2762	
22	6	0	-1.036360	2.013047	0 528274	
23	1	0	7 /07076	_1 /12127	-0.486500	
24	1	0	5.022440		0.480599	
25	1	0	1 2/6527	1 760275		
20	1	0	7 272060	1 106888	-1 286274	
27	1	0	2 821125	_1 560202	1 /268/2	
20	1	0	2.031135	-1.300203	_0 176021	
20	1	0	_0.076108	0 202272	2 810650	
21	1	0	1 2/1121	1 150706	2.810050	
22	1	0	1.541121	_0.21/102	2.170575	
22	1	0	-0.062200	-0.514195	_0 /0/920	
24	1	0	-0.003200	-1.382019	1 590206	
25	1	0	1 400519	0.021940	1.360290	
25	1	0	-1.400518	-0.025244	-1.000015	
27	1	0	-3.727041	1 5/2022	1 200200	
20	1	0	-2.05035	1.343833	1.000390	
20	1	0	-5.93/131	2.001/24	0.750140	
39	1	0	-5.100470	0.549802	0.048318	
40	1	0	-5.U82/43	1.390035	1 022550	
41	1	0	-5.0490/9	-1./0/010	1.033559	
42	1	0	-2.229322	-2.0/4048		
43	1	0		-3.249895	0.303150	
44	1	0	-3.021412		-2.350992	
45	1	0	-1.9010U1		1 170120	
40	1	0	-2.014451	-3.41004/	-1.1/9130	
4/	1	0	-1./93528	2.201011	-1.924472	
40	L 1	U	-0.1120/2	2.333339	-0.0400/4	

Table S11. DFT Coordinates of the optimized conformers of (10*S*, 11*R*, 12*S*, 15*R*)-**1** at M06-2X/6-31G(d,p) theory level.

49	1	0	-1.193557	3.593751	0.619672			
50	1	0	-0.883958	2.104294	1.530158			
		<u> </u>	Conformer (10S, 11R	, 12 <i>S</i> , 15 <i>R</i>)- 1-b				
Center	Atomic	Atomic		Coordinates (Angstroms)				
Number	Number	Type	Х	γ	Z			
1	6	0	4.488302	1.125670	-2.043699			
2	6	0	3.562738	1.063472	-0.979671			
3	6	0	4.081288	0.191392	-0.034106			
4	7	0	5.283814	-0.264244	-0.510762			
5	6	0	5.543284	0.289891	-1.719045			
6	6	0	3.629180	-0.288567	1.272097			
7	6	0	2.297582	0.218648	1.802557			
8	8	0	4.310242	-1.084922	1.898772			
9	6	0	1.125246	-0.248865	0.965031			
10	6	0	1.076971	-1.732936	0.713117			
11	6	0	0.224923	0.624430	0.506139			
12	6	0	-0.985394	0.291436	-0.342553			
13	6	0	-2.054731	-0.589254	0.344388			
14	6	0	-3.214320	0.391898	0.687756			
15	6	0	-2.710237	1.772203	0.200578			
16	8	0	-1.675773	1.469467	-0.744100			
17	6	0	-2.693700	-1.711947	-0.513161			
18	6	0	-4.154740	-1.697597	-0.037047			
19	6	0	-4.478652	-0.206653	0.035759			
20	6	0	-3.730160	2.623769	-0.542957			
21	6	0	-2.149452	2.565572	1.386702			
22	8	0	-2.028407	-2.926576	-0.188752			
23	6	0	-2.609799	-1.459705	-2.020865			
24	1	0	4.401130	1.708043	-2.949335			
25	1	0	2.615071	1.578040	-0.905823			
26	1	0	5.851758	-0.913859	0.016015			
27	1	0	6.447382	0.056877	-2.261984			
28	1	0	2.214513	-0.172113	2.823105			
29	1	0	2.317496	1.313601	1.846308			
30	1	0	1.947072	-2.037118	0.116908			
31	1	0	0.174907	-2.058167	0.190398			
32	1	0	1.139529	-2.284810	1.658911			
33	1	0	0.369921	1.687080	0.695662			
34	1	0	-0.630246	-0.172337	-1.268987			
35	1	0	-1.650356	-1.066555	1.241350			
36	1	0	-3.370209	0.426138	1.770952			
37	1	0	-4.188572	-2.148257	0.962345			
38	1	0	-4.822546	-2.266932	-0.693941			
39	1	0	-4.631475	0.185579	-0.974373			
40	1	0	-5.384371	0.014093	0.607461			
41	1	0	-4.019516	2.152418	-1.484870			
42	1	0	-4.625513	2.778760	0.067653			
43	1	0	-3.295838	3.600657	-0.775442			
44	1	0	-2.970012	2.922878	2.018353			
45	1	0	-1.583640	3.430163	1.026115			
46	1	0	-1.492207	1.949318	2.007739			
47	1	0	-2.383965	-3.622387	-0.761193			
48	1	0	-1.598778	-1.668166	-2.381203			
49	1	0	-3.303182	-2.120533	-2.554867			

50	1	0	-2.853527	-0.423595	-2.275401		
Conformer (10S. 11R. 12S. 15R)- 1-c							
Center	Atomic	Atomic		Coordinates (Angstroms)			
Number	Number	Туре	Х	Ŷ	Z		
1	6	0	-6.616097	0.904552	-0.489955		
2	6	0	-5.325613	1.272205	-0.051606		
3	6	0	-4.515896	0.153445	-0.169575		
4	7	0	-5.289684	-0.863453	-0.664821		
5	6	0	-6.557036	-0.427092	-0.862852		
6	6	0	-3.105316	-0.112482	0.114054		
7	6	0	-2.263795	1.056719	0.610704		
8	8	0	-2.644360	-1.228533	-0.065090		
9	6	0	-0.900366	0.623406	1.083149		
10	6	0	-0.911691	-0.187490	2.352111		
11	6	0	0.181597	0.937634	0.366201		
12	6	0	1.593561	0.489930	0.600222		
13	6	0	2.104167	-0.403757	-0.557887		
14	6	0	3.531300	0.116784	-0.819785		
15	6	0	3.434885	1.590653	-0.379928		
16	8	0	2.486409	1.598114	0.691953		
17	6	0	2.273738	-1.877147	-0.189592		
18	6	0	3.541914	-1.857268	0.676367		
19	6	0	4.463231	-0.843320	-0.026412		
20	6	0	4.716747	2.212268	0.157188		
21	6	0	2.891412	2.440703	-1.534313		
22	8	0	2.561134	-2.511410	-1.437149		
23	6	0	1.057466	-2.524265	0.459929		
24	1	0	-7.493864	1.532766	-0.529427		
25	1	0	-5.014345	2.242398	0.310469		
26	1	0	-4.911205	-1.785254	-0.836116		
27	1	0	-7.322672	-1.083255	-1.249660		
28	1	0	-2.820847	1.559445	1.413477		
29	1	0	-2.186747	1.776553	-0.214197		
30	1	0	-1.546131	0.300117	3.101845		
31	1	0	0.080910	-0.311567	2.788526		
32	1	0	-1.335124	-1.179858	2.160939		
33	1	0	0.051744	1.542911	-0.532960		
34	1	0	1.661412	-0.046831	1.553250		
35	1	0	1.448262	-0.319871	-1.430455		
36	1	0	3.777052	0.066466	-1.883906		
37	1	0	3.295433	-1.525827	1.691764		
38	1	0	3.985935	-2.855971	0.762656		
39	1	0	5.107505	-0.323701	0.686245		
40	1	0	5.117242	-1.363515	-0.730379		
41	1	0	4.554583	3.274211	0.365030		
42	1	0	5.527137	2.121368	-0.573487		
43	1	0	5.020230	1.731037	1.089095		
44	1	0	2.007219	1.977562	-1.985739		
45	1	0	2.608423	3.428440	-1.158936		
46	1	0	3.645773	2.564707	-2.318572		
47	1	0	2.728157	-3.447734	-1.253819		
48	1	0	0.873689	-2.122148	1.460070		
49	1	0	0.159026	-2.362174	-0.144159		
50	1	0	1.218284	-3.604337	0.566358		

Atomic Coordinates (Angstroms) Number Type X Y Z 1 6 0 -3.629674 -0.104428 -0.373959 2 6 0 -3.62281 -3.32281 0.332951 3 6 0 -3.632281 -2.332501 0.038199 4 6 0 -4.243933 -0.763267 -1.412068 6 6 0 -3.84778 1.357453 -0.406809 7 8 0 -4.224069 1.967431 -1.270052 8 6 0 -2.838803 2.103600 0.643744 9 6 0 -1.548653 1.950190 1.028813 10 6 0 -0.994470 2.834891 2.12267 12 6 0 0.616779 0.713533 0.787342 14 6 0 3.034935 -0.040273 0.225135 15 6		Conformer (11 <i>S</i> , 12 <i>S</i> , 15 <i>R</i>)- 3-a					
Number Type x Y Z 1 6 0 -3.629674 -0.104428 -0.373959 2 6 0 -3.241972 -1.074944 0.550792 3 6 0 -4.249133 -2.132501 0.038199 4 6 0 -4.249333 -0.763267 -1.412068 5 7 0 -4.24069 1.967431 -1.270052 8 6 0 -2.538803 2.103600 0.643744 9 6 0 -1.548653 1.950190 1.028813 10 6 0 -0.534885 1.00297 0.380670 11 6 0 0.034935 -0.040273 0.225135 13 6 0 1.546611 -0.291302 0.114262 14 6 0 3.682088 -1.465581 0.20806 15 6 0 1.257273 -1.848260 2.17785 15 6	Center	Atomic	Atomic	Co	pordinates (Angstroms)	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Number	Number	Туре	Х	Ŷ	Z	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1	6	0	-3.629674	-0.104428	-0.373959	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	2	6	0	-3.241972	-1.074944	0.550792	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	3	6	0	-3.632281	-2.332501	0.038199	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	6	0	-4.254133	-2.102777	-1.182938	
6 6 0 -3.584778 1.357453 -0.406809 7 8 0 -4.224069 1.967431 -1.270052 8 6 0 -2.838803 2.103600 0.643744 9 6 0 -1.548653 1.950190 1.028813 10 6 0 -0.634885 1.002997 0.380670 11 6 0 -0.994470 2.834891 2.122267 12 6 0 0.616779 0.713533 0.787337 13 6 0 1.504601 -0.291302 0.114262 14 6 0 3.632088 -1.46581 0.208806 15 6 0 2.522888 -2.467346 0.060978 16 0 1.2567273 -1.848260 2.17785 17 6 0 1.257273 -1.848260 2.17785 18 8 0 3.144844 0.212771	5	7	0	-4.249393	-0.763267	-1.412068	
7 8 0 -4.224069 1.967431 -1.270052 8 6 0 -2.83803 2.103600 0.643744 9 6 0 -1.548653 1.950190 1.022813 10 6 0 -0.634885 1.002997 0.380670 11 6 0 -0.634885 1.002997 0.380670 11 6 0 0.616779 0.713533 0.787337 13 6 0 1.504601 -0.291302 0.114262 14 6 0 3.034935 -0.040273 0.225135 15 6 0 3.562088 -1.46584 0.208006 16 0 1.285902 -1.756576 0.645914 18 8 0 0.128046 -2.351571 0.096097 19 6 0 1.27573 -1.84260 2.177885 20 6 0 3.614598 0.901355	6	6	0	-3.584778	1.357453	-0.406809	
8 6 0 -2.838203 2.103600 0.643744 9 6 0 -1.548653 1.950190 1.028813 10 6 0 -0.634885 1.002997 0.380670 11 6 0 -0.634885 1.002997 0.380670 11 6 0 0.616779 0.7135333 0.787337 13 6 0 1.504601 -0.291302 0.114262 14 6 0 3.632088 -2.467346 0.060978 15 6 0 2.522888 -2.467346 0.060978 17 6 0 1.257273 -1.848260 2.177885 20 6 0 3.614598 0.901355 -0.635499 21 6 0 2.893176 2.257731 -0.396547 23 8 0 3.414844 0.212771 -2.109177 24 1 0 -2.761886	7	8	0	-4.224069	1.967431	-1.270052	
9 6 0 -1.548653 1.950190 1.028813 10 6 0 -0.634885 1.002997 0.380670 11 6 0 -0.994470 2.834891 2.12267 12 6 0 0.616779 0.713533 0.787337 13 6 0 1.504601 -0.291302 0.114262 14 6 0 3.034935 -0.040273 0.225135 15 6 0 3.682088 -1.466581 0.208806 16 6 0 2.522888 -2.467346 0.060978 17 6 0 1.296902 -1.756576 0.645914 18 8 0 0.1287273 -1.848260 2.177885 20 6 0 3.614598 0.901355 -0.862547 21 6 0 2.893176 2.257731 -0.906547 23 8 0 3.414884	8	6	0	-2.838803	2.103600	0.643744	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	9	6	0	-1.548653	1.950190	1.028813	
11 6 0 -0.994470 2.834891 2.122267 12 6 0 0.616779 0.713533 0.787337 13 6 0 1.504601 -0.291302 0.114262 14 6 0 3.034935 -0.040273 0.225135 15 6 0 3.682088 -1.466581 0.208806 16 6 0 2.522888 -2.467346 0.060978 17 6 0 1.286902 -1.756576 0.645914 18 8 0 0.128046 -2.351571 0.096097 19 6 0 1.54252 -0.862547 21 6 0 5.119023 1.134283 -0.635499 22 6 0 2.893176 2.257731 -2.109177 23 8 0 3.414884 0.212711 -2.109177 24 1 0 -2.761886 -0.875895	10	6	0	-0.634885	1.002997	0.380670	
12 6 0 0.616779 0.713533 0.787337 13 6 0 1.504601 -0.291302 0.114262 14 6 0 3.034935 -0.040273 0.225135 15 6 0 3.682088 -1.466581 0.208806 16 6 0 2.522888 -2.467346 0.060978 17 6 0 1.257273 -1.848260 2.177885 20 6 0 3.614598 0.901355 -0.862547 21 6 0 5.119023 1.134283 -0.635499 22 6 0 2.893176 2.257731 -0.906547 23 8 0 3.44484 0.2127171 -2.109177 24 1 0 1.243245 -0.351806 -0.948208 25 1 0 -2.761886 -0.277373 -2.1893619 28 1 0 -4.650265	11	6	0	-0.994470	2.834891	2.122267	
13 6 0 1.504601 -0.291302 0.114262 14 6 0 3.34935 -0.040273 0.225135 15 6 0 3.682088 -1.466581 0.208806 16 6 0 2.522888 -2.467346 0.060978 17 6 0 1.252723 -1.848260 2.177855 20 6 0 3.614598 0.901355 -0.862547 21 6 0 5.119023 1.134283 -0.633499 22 6 0 2.177855 -0.806547 23 8 0 3.414884 0.212771 -2.109177 24 1 0 1.243245 -0.351806 -0.948208 25 1 0 -2.761886 -0.87595 1.498066 26 1 0 -4.650265 -0.257373 -2.189336 29 1 0 -4.650265 -0.257373 -2.18936 <td>12</td> <td>6</td> <td>0</td> <td>0.616779</td> <td>0.713533</td> <td>0.787337</td>	12	6	0	0.616779	0.713533	0.787337	
1011111111111460 3.034935 -0.040273 0.225135 1560 3.682088 -1.466581 0.208806 1660 2.522888 -2.467346 0.060978 1760 1.266902 -1.756576 0.645914 1880 0.128046 -2.351571 0.096097 1960 1.27273 -1.848260 2.177885 2060 3.644598 0.901355 -0.862547 2160 2.893176 2.257731 -0.906547 2380 3.414884 0.212771 -2.109177 2410 1.243245 -0.351806 -0.948208 2510 -2.761886 -0.875895 1.498066 2610 -3.433525 -3.298693 0.498466 2710 -4.650265 -0.257373 -2.189336 2910 -3.415363 2.923090 1.067390 3010 -1.74992 3.533598 2.487509 3210 -0.650806 2.236087 2.974176 3310 -0.131659 3.409969 1.76813 3410 1.005778 1.179841 1.692106 3510 3.24422 0.441003 1.189813 3610 4.238140 -1.641899 1.35802	13	6	0	1,504601	-0.291302	0.114262	
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3710 4.337003 -1.373343 -0.010341 38 10 2.316201 -2.659874 -0.996500 39 10 2.716089 -3.430704 0.543676 40 10 -0.643810 -1.847512 0.393830 41 10 0.400096 -1.300597 2.584126 42 10 1.163012 -2.896612 2.475580 43 10 2.162489 -1.439896 2.640215 44 10 5.527793 1.770944 -1.429348 45 10 5.674435 0.193838 -0.641005 46 10 5.302798 1.639801 0.318591 47 10 3.349059 2.901390 -1.669279 48 10 1.836198 2.137577 -1.149493 49 10 2.969762 2.783468 0.051180 50 10 3.736983 0.786506 -2.817087	27	1	0	4.23014U	-1 572512	_0 6165/1	
3910 2.310201 -2.033074 -0.990300 39 10 2.716089 -3.430704 0.543676 40 10 -0.643810 -1.847512 0.393830 41 10 0.400096 -1.300597 2.584126 42 10 1.163012 -2.896612 2.475580 43 10 2.162489 -1.439896 2.640215 44 10 5.527793 1.770944 -1.429348 45 10 5.674435 0.193838 -0.641005 46 10 5.302798 1.639801 0.318591 47 10 3.349059 2.901390 -1.669279 48 10 1.836198 2.137577 -1.149493 49 10 2.969762 2.783468 0.051180 50 10 3.736983 0.786506 -2.817087	20	1	0	2 316201	-2 650824	-0.010341	
3510 2.710005 -3.430704 0.343076 40 10 -0.643810 -1.847512 0.393830 41 10 0.400096 -1.300597 2.584126 42 10 1.163012 -2.896612 2.475580 43 10 2.162489 -1.439896 2.640215 44 10 5.527793 1.770944 -1.429348 45 10 5.674435 0.193838 -0.641005 46 10 5.302798 1.639801 0.318591 47 10 3.349059 2.901390 -1.669279 48 10 1.836198 2.137577 -1.149493 49 10 2.969762 2.783468 0.051180 50 10 3.736983 0.786506 -2.817087	20	1	0	2.310201	-2.039074	0.530300	
4010 -0.043010 -1.847312 0.393830 4110 0.400096 -1.300597 2.584126 4210 1.163012 -2.896612 2.475580 4310 2.162489 -1.439896 2.640215 4410 5.527793 1.770944 -1.429348 4510 5.674435 0.193838 -0.641005 4610 5.302798 1.639801 0.318591 4710 3.349059 2.901390 -1.669279 4810 1.836198 2.137577 -1.149493 4910 2.969762 2.783468 0.051180 5010 3.736983 0.786506 -2.817087	23	1	0	2./10009	-3.430704	0.0400/0	
41 0 0.400050 -1.300597 2.384120 42 1 0 1.163012 -2.896612 2.475580 43 1 0 2.162489 -1.439896 2.640215 44 1 0 5.527793 1.770944 -1.429348 45 1 0 5.674435 0.193838 -0.641005 46 1 0 5.302798 1.639801 0.318591 47 1 0 3.349059 2.901390 -1.669279 48 1 0 1.836198 2.137577 -1.149493 49 1 0 3.736983 0.786506 -2.817087	40	1	0	0.043010	-1 200507	0.33303U 2 50/176	
42101.103012 -2.890012 2.475380 4310 2.162489 -1.439896 2.640215 4410 5.527793 1.770944 -1.429348 4510 5.674435 0.193838 -0.641005 4610 5.302798 1.639801 0.318591 4710 3.349059 2.901390 -1.669279 4810 1.836198 2.137577 -1.149493 4910 2.969762 2.783468 0.051180 5010 3.736983 0.786506 -2.817087	41	1	0	1 162012	-7 805613	2.304120	
4.5 1 0 2.102405 -1.439896 2.040215 44 1 0 5.527793 1.770944 -1.429348 45 1 0 5.674435 0.193838 -0.641005 46 1 0 5.302798 1.639801 0.318591 47 1 0 3.349059 2.901390 -1.669279 48 1 0 1.836198 2.137577 -1.149493 49 1 0 2.969762 2.783468 0.051180 50 1 0 3.736983 0.786506 -2.817087	42	1	0	2 162/00	-2.030012	2.475560	
44 1 0 5.527795 1.770944 -1.429348 45 1 0 5.674435 0.193838 -0.641005 46 1 0 5.302798 1.639801 0.318591 47 1 0 3.349059 2.901390 -1.669279 48 1 0 1.836198 2.137577 -1.149493 49 1 0 2.969762 2.783468 0.051180 50 1 0 3.736983 0.786506 -2.817087	45	1	0	2.102469 5 507700	-1.433030 1.7700//	2.040215 _1 /20270	
4.5 1 0 3.674435 0.193838 -0.641005 46 1 0 5.302798 1.639801 0.318591 47 1 0 3.349059 2.901390 -1.669279 48 1 0 1.836198 2.137577 -1.149493 49 1 0 2.969762 2.783468 0.051180 50 1 0 3.736983 0.786506 -2.817087	44 1E	1	0	5.527755	1.770544 0 102020	-1.423340 _0 6/1005	
40 1 0 5.502796 1.639801 0.318591 47 1 0 3.349059 2.901390 -1.669279 48 1 0 1.836198 2.137577 -1.149493 49 1 0 2.969762 2.783468 0.051180 50 1 0 3.736983 0.786506 -2.817087	45	1	0	5.0/4433	1 620001	0.041005	
47 1 0 3.349039 2.901390 -1.669279 48 1 0 1.836198 2.137577 -1.149493 49 1 0 2.969762 2.783468 0.051180 50 1 0 3.736983 0.786506 -2.817087	40	1	0	2 240050	2 001200	_1 660270	
40 1 0 1.830198 2.137577 -1.149493 49 1 0 2.969762 2.783468 0.051180 50 1 0 3.736983 0.786506 -2.817087	47	1	0	3.343039	2.301330	-1.0092/9	
45 1 0 2.909762 2.783468 0.051180 50 1 0 3.736983 0.786506 -2.817087	40	1	0	1.030130	2.13/3//	-1.149493	
<u> </u>	49	1	0	2.303/02	2./03400		
	50		U	5./30383	15 P) 2 h	-2.01/08/	

Table S12. DFT Coordinate	es of the optimized	d conformers of (115	, 12 <i>S</i> , 15 <i>R</i>)- 3 at B	3LYP/6-31G(d,p) theory
level.				

Center	Atomic	Atomic	Co	oordinates (Angstroms)
Number	Number	Туре	Х	Ŷ	Z
1	6	0	3.579920	0.249300	-0.429173
2	6	0	2.917542	1.312110	0.189068
3	6	0	3.327517	2.500168	-0.455876
4	6	0	4.235684	2.143418	-1.445307
5	7	0	4.375440	0.793538	-1.416936
6	6	0	3.691766	-1.197631	-0.225231
7	8	0	4.535939	-1.821711	-0.883220
8	6	0	2.911618	-1.939265	0.800027
9	6	0	1.599248	-1.881891	1.138110
10	6	0	0.641324	-0.987214	0.489903
11	6	0	1.081580	-2.813587	2.210661
12	6	0	-0.632550	-0.783176	0.873305
13	6	0	-1.529979	0.235988	0.241470
14	6	0	-3.034270	-0.138718	0.109822
15	6	0	-3.808397	1.219179	0.240568
16	6	0	-2.736759	2.314264	0.363665
17	6	0	-1.524009	1.613116	1.000899
18	8	0	-0.299549	2.318526	0.823004
19	6	0	-1.678530	1.476566	2.516819
20	6	0	-3.391301	-0.911196	-1.186523
21	6	0	-4.882185	-1.292356	-1.201311
22	6	0	-2.544417	-2.180561	-1.367589
23	8	0	-3.115110	0.005683	-2.261824
24	1	0	-1.157711	0.461939	-0.767132
25	1	0	2.205054	1.242446	0.996870
26	1	0	3.007302	3.505753	-0.222477
27	1	0	4.779756	2.752624	-2.152412
28	1	0	4.985845	0.206391	-1.968107
29	1	0	3.519356	-2.716359	1.258394
30	1	0	1.006909	-0.434157	-0.369635
31	1	0	1.873244	-3.464383	2.587200
32	1	0	0.678448	-2.247289	3.058673
33	1	0	0.268099	-3.442023	1.830722
34	1	0	-1.032756	-1.315755	1.734958
35	1	0	-3.308379	-0.795247	0.945645
36	1	0	-4.454025	1.204889	1.124638
37	1	0	-4.448023	1.399317	-0.624607
38	1	0	-2.448918	2.665126	-0.635592
39	1	0	-3.063141	3.186659	0.938395
40	1	0	-0.132215	2.396448	-0.126709
41	1	0	-0.822977	0.947233	2.943177
42	1	0	-1.719963	2.472368	2.967424
43	1	0	-2.592769	0.938834	2.784544
44	1	0	-5.134241	-1.798477	-2.140821
45	1	0	-5.523383	-0.412754	-1.112221
46	1	0	-5.122242	-1.979834	-0.383234
47	1	0	-2.846632	-2.705186	-2.282643
48	1	0	-1.482159	-1.944641	-1.444399
49	1	0	-2.680547	-2.876015	-0.532758
50	1	0	-3.295046	-0.453739	-3.092879
			Conformer (11S, 12S,	15 <i>R</i>)- 3-c	
Center	Atomic	Atomic	Co	pordinates (Angstroms	
Number	Number	Туре	Х	Y	Z
1	6	0	-3.550694	0.568604	-0.243609
2	6	0	-2.820676	1.595421	0.354280

3	6	0	-3.086627	2.781358	-0.365095
4	6	0	-3.976229	2.456052	-1.381517
5	7	0	-4 246186	1 127449	-1 293719
6	6	0	-3 788426	-0.843372	0.056123
7	8	0	-4 677700	-1 447022	-0 555540
8	6	0	-3 051198	-1 535356	1 147654
9	6	0	_1 717315	-1 613725	1 378586
10	6	0	_0.715200	_0.006225	0.506251
10	6	0	-0.715288	-0.330223	2 5/0221
12	6	0	-1.229100	-2.437320	2.349551
12	6	0	1 626297	-1.021728	0.708232
13	6	0	1.020567	-0.446566	-0.241001
14	6	0	2.001005	0.220008	0.429667
15	0	0	4.071000	-0.077570	-0.517508
10	0	0	3.4/1111		-1./530/9
1/	0	0	2.221/3/	-1.497154	-1.235533
18	8 C	0	1.238085	-1.701301	-2.250298
19	6	0	2.5/0///	-2.839587	-0.579627
20	6	0	2.684463	1.740952	0./11333
21	6	0	3.900098	2.298492	1.4/3449
22	6	0	1.405380	2.045187	1.50/143
23	8	0	2.601009	2.361865	-0.583400
24	1	0	1.138568	0.287686	-0.890150
25	1	0	-2.182757	1.486512	1.218779
26	1	0	-2.683726	3.765119	-0.170578
27	1	0	-4.422843	3.073588	-2.147074
28	1	0	-4.879989	0.573253	-1.852071
29	1	0	-3.714626	-2.140463	1.762106
30	1	0	-1.085269	-0.499798	-0.385500
31	1	0	-2.063778	-2.864860	3.108896
32	1	0	-0.582190	-3.256846	2.215772
33	1	0	-0.637627	-1.825038	3.240048
34	1	0	1.014369	-1.515296	1.593677
35	1	0	3.037378	-0.247279	1.404739
36	1	0	4.790795	-0.733615	-0.016419
37	1	0	4.603597	0.832658	-0.797567
38	1	0	3.136271	-0.012095	-2.475836
39	1	0	4.175743	-1.432293	-2.262356
40	1	0	1.554000	-2.406867	-2.830573
41	1	0	1.667450	-3.328598	-0.206255
42	1	0	3.042543	-3.505067	-1.313470
43	1	0	3.273557	-2.724950	0.252291
44	1	0	3.790353	3.379469	1.621545
45	1	0	4.829558	2.128655	0.925189
46	1	0	3.993195	1.838783	2.463225
47	1	0	1.342979	3.120415	1.717655
48	1	0	0.513623	1.754219	0.949753
49	1	0	1.396546	1.522425	2.469089
50	1	0	2.432843	3.303807	-0.447546
			Conformer (11S, 12S,	15 <i>R</i>)- 3-d	
Center	Atomic	Atomic	()	pordinates (Angstroms)
Number	Number	Туре	X	Y	Z
1	6	0	3.628803	0.248448	-0.423554
2	6	0	2.930459	1.346031	0.085430
3	6	0	3,390229	2.494053	-0.595685
4	6	0	4,362168	2.081197	-1.497978
5	7	0	4,492989	0.735306	-1.383817
6	, 6	0	3,723189	-1.185800	-0.141316
	, ~	ı ~	0.7 20 200		01212020

7	8	0	4.596915	-1.842544	-0.726741
8	6	0	2.901567	-1.886583	0.879896
9	6	0	1.583938	-1.811914	1.193878
10	6	0	0.637188	-0.921879	0.522174
11	6	0	1.047256	-2.726374	2.273155
12	6	0	-0.641941	-0.723953	0.890806
13	6	0	-1.559316	0.267706	0.238525
14	6	0	-3.043190	-0.181219	0.074834
15	6	0	-3.889880	1.129512	0.212968
16	6	0	-2.875020	2.274932	0.359768
17	6	0	-1.637158	1.627095	1.003528
18	8	0	-0.427055	2.334574	0.719112
19	6	0	-1.794573	1.474340	2.522229
20	6	0	-3.338290	-0.952720	-1.237666
21	6	0	-4.802294	-1.427413	-1.270670
22	6	0	-2.410826	-2.162263	-1.431066
23	8	0	-3.114229	-0.003624	-2.295273
24	1	0	-1.166575	0.530033	-0.750148
25	1	0	2.158561	1.323570	0.839473
26	1	0	3.049456	3.509622	-0.453820
27	1	0	4.954189	2.648469	-2.201450
28	1	0	5.132494	0.115310	-1.860867
29	1	0	3.490077	-2.661228	1.366642
30	1	0	1.010922	-0.371320	-0.335172
31	1	0	1.831405	-3.373412	2.671228
32	1	0	0.632054	-2.147527	3.106773
33	1	0	0.238447	-3.359045	1.890211
34	1	0	-1.044480	-1.259092	1.750162
35	1	0	-3.296859	-0.864596	0.895851
36	1	0	-4.544488	1.069920	1.088826
37	1	0	-4.527164	1.288421	-0.658068
38	1	0	-2.578656	2.646449	-0.626530
39	1	0	-3.259922	3.122257	0.939488
40	1	0	-0.449181	3.164020	1.215256
41	1	0	-0.911426	0.998042	2.955286
42	1	0	-1.913601	2.460721	2.987693
43	1	0	-2.675851	0.882267	2.789488
44	1	0	-5.014186	-1.934288	-2.219605
45	1	0	-5.498069	-0.590692	-1.175437
46	1	0	-5.005744	-2.140464	-0.464522
47	1	0	-2.679069	-2.696465	-2.351283
48	1	0	-1.366797	-1.855722	-1.506410
49	1	0	-2.499111	-2.873495	-0.603174
50	1	0	-3.236256	-0.465318	-3.135486
			Conformer (11S, 12S,	15 <i>R</i>)- 3-e	
Center	Atomic	Atomic	Co	pordinates (Angstroms	
Number	Number	Туре	Х	Y	Z
1	6	0	-3.614745	-0.120902	-0.373832
2	6	0	-3.214114	-1.080372	0.556968
3	6	0	-3.584683	-2.346659	0.050345
4	6	0	-4.207364	-2.132824	-1.173287
5	7	0	-4.222573	-0.794594	-1.409141
6	6	0	-3.592810	1.341922	-0.414996
7	8	0	-4.245712	1.935939	-1.278876
8	6	0	-2.853429	2.106149	0.626759
9	6	0	-1.561577	1.969199	1.012371
10	6	0	-0 639355	1 023870	0 373334

11	6	0	-1.015069	2.869674	2.096674
12	6	0	0.609645	0.739765	0.790586
13	6	0	1.504432	-0.266467	0.127995
14	6	0	3.032942	-0.009336	0.252479
15	6	0	3.676413	-1.436886	0.312700
16	6	0	2.530723	-2.439953	0.103500
17	6	0	1.283784	-1.733929	0.649173
18	8	0	0.139314	-2.334855	0.057436
19	6	0	1.193341	-1.831783	2.178472
20	6	0	3.614841	0.890207	-0.880254
21	6	0	5,118985	1,135838	-0.669048
22	6	0	2,892387	2,238571	-0.967631
23	8	0	3 398916	0 277137	-2 162178
24	1	0	1,259387	-0.322591	-0.939126
25	1	0	-2 740343	-0.868857	1 504712
26	1	0	-3 423629	-3 308001	0 516659
20	1	0	-4 628682	-2 835369	-1 877169
27	1	0	-4 629064	-0.298816	-2 190101
20	1	0	-3 /37509	2 924446	1 0/2201
29	1	0	-0.006350	0.527012	_0 520226
21	1	0	-0.330330	2 567264	2 / 52681
22	1	0	-1.773000	2.207204	2.432001
32	1	0	-0.009274	2.202001	2.950105
24	1	0	-0.155429	5.440076	1.757269
34	1	0	0.991604	1.211101	1.095021
35	1	0	3.234599	0.509188	1.199384
36	1	0	4.157201	-1.591679	1.283907
37	1	0	4.466579	-1.580756	-0.431729
38	1	0	2.361596	-2.620676	-0.963446
39	1	0	2.708276	-3.409183	0.580077
40	1	0	-0.648273	-1.843119	0.334447
41	1	0	0.319273	-1.290091	2.554909
42	1	0	1.095351	-2.881404	2.470538
43	1	0	2.0/8341	-1.41/318	2.6/3363
44	1	0	5.509700	1.750949	-1.484/64
45	1	0	5.689434	0.201227	-0.649928
46	1	0	5.306599	1.656702	0.275786
47	1	0	3.348930	2.849504	-1.751666
48	1	0	1.837256	2.106526	-1.211951
49	1	0	2.963430	2.781423	-0.019858
50	1	0	3.948651	-0.516661	-2.208700
	r		Conformer (11S, 12S,	, 15 <i>R</i>)- 3 -f	
Center	Atomic	Atomic	Co	pordinates (Angstroms)
Number	Number	Туре	Х	Ŷ	Z
1	6	0	3.568826	0.261973	-0.431287
2	6	0	2.906177	1.315583	0.201940
3	6	0	3.298069	2.510910	-0.440894
4	6	0	4.196059	2.167257	-1.444234
5	7	0	4.347307	0.818440	-1.425518
6	6	0	3.692579	-1.185250	-0.236647
7	8	0	4.536456	-1.799822	-0.903311
8	6	0	2.922385	-1.937357	0.788831
9	6	0	1.610886	-1.890531	1.131542
10	6	0	0.645586	-0.998317	0.490485
11	6	0	1.102134	-2.830871	2.200658
12	6	0	-0.627227	-0.801118	0.880058
13	6	0	-1.530540	0.217160	0.254204
14	6	0	-3.032581	-0.165227	0.120707

15	6	0	-3.811404	1.184940	0.300333
16	6	0	-2.746676	2.288876	0.391065
17	6	0	-1.521257	1.594074	1.012668
18	8	0	-0.305423	2,308660	0.818328
19	6	0	-1 655963	1 460323	2 530939
20	6	0	-3 378767	_0.903070	_1 207915
20	6	0	_4 962757		_1 2/2716
21	6	0	-4.803737	-1.301038	-1.245710
22	0	0	-2.518217	-2.153537	-1.415018
23	8	0	-3.074278	-0.058516	-2.333049
24	1	0	-1.165153	0.444195	-0.757490
25	1	0	2.206168	1.234510	1.019415
26	1	0	2.973324	3.512512	-0.196860
27	1	0	4.725621	2.784925	-2.154977
28	1	0	4.954122	0.239794	-1.989524
29	1	0	3.537128	-2.712362	1.241359
30	1	0	1.004484	-0.442218	-0.369878
31	1	0	1.899008	-3.478556	2.571494
32	1	0	0.697863	-2.271768	3.052945
33	1	0	0.291743	-3.462479	1.819458
34	1	0	-1.022593	-1.337923	1.741191
35	1	0	-3.303227	-0.844073	0.939904
36	1	0	-4.413980	1.154593	1.213356
37	1	0	-4.517892	1.380402	-0.512874
38	1	0	-2.473546	2.633732	-0.614862
39	1	0	-3.068145	3.164615	0.963111
40	1	0	-0.119791	2.341196	-0.130641
41	1	0	-0.792933	0.933862	2.945104
42	1	0	-1.693320	2.456705	2.980738
43	1	0	-2.564113	0.919754	2.813247
44	1	0	-5.092190	-1.788126	-2.196421
45	1	0	-5.526305	-0.435832	-1.139550
46	1	0	-5.104143	-1.999518	-0.434951
47	1	0	-2.825330	-2.661448	-2.333720
48	1	0	-1.461818	-1.897483	-1.505880
49	1	0	-2.631183	-2.849980	-0.578394
50	1	0	-3,736861	0.644346	-2,364739
	-		Conformer (115, 125	15R)- 3 -g	21001700
Center	Atomic	Atomic	C(pordinates (Angstroms)
Number	Number	Type	X	γ	7
1	6	0	3.626243	0.260044	-0.425006
2	6	0	2,925807	1.352664	0.091339
3	6	0	3 376523	2 505089	-0 588379
4	6	0	4 345153	2.099481	-1 497494
5	7	0	4 482947	0 753941	-1 388130
6	6	0	3 728704	-1 174548	-0 147193
7	8	0	4 604627	-1 82/953	-0 735870
8	6	0	2 911991	-1 882825	0.735070
9	6	0	1 59/311	-1 8171/0	1 18830/
10	6	0	0.6/1609	_0 020021	0 522003
11	6	0	1 064026	-2 740063	2 263634
12	6	0	-0 628212	-0 7/2/26	0.803/1/2
12	6	0	-1 56/001	0.742420	0.055442
1/	6	0	-3 0/13330	_0 216270	0.245465
15	6	0	-3 003003	1 076805	0.003020
16	6	0	_2 003092	2 222821	0.293400
17	6	0	-1 6/0700	1 60/15/	1 0102/5
10	Q	0		220071	0 7070/1
10	0	U	0.4510/0	2.3233/1	0.707041

19	6	0	-1.764242	1.448768	2.540891
20	6	0	-3.329165	-0.936644	-1.268765
21	6	0	-4.784620	-1.431768	-1.327050
22	6	0	-2.385348	-2.120748	-1.500955
23	8	0	-3.074636	-0.046024	-2.368483
24	1	0	-1.178456	0.515164	-0.740950
25	1	0	2,158820	1.323172	0.850013
26	1	0	3 032306	3 518784	-0 441471
27	1	0	4 930137	2 671538	-2 202931
28	1	0	5 121750	0 138249	-1 871685
29	1	0	3 505172	-2 656130	1 356215
30	1	0	1 010593	-0.372068	-0 333218
31	1	0	1.010555	-3 383619	2 658353
22	1	0	0.645260	-2 162124	2.000000
32	1	0	0.045200	-2.100104	1 277722
24	1	0	_1 026294		1.0///50
25	1	0	2 294520	-1.203073	1.749555
35	1	0	-3.284539	-0.934555	0.878493
30	1	0	-4.500461	0.990198	1.206617
37	1	0	-4.622747	1.248424	-0.513815
38	1	0	-2.632020	2.608698	-0.589757
39	1	0	-3.285080	3.083983	0.987765
40	1	0	-0.455521	3.142599	1.230773
41	1	0	-0.864484	0.984542	2.951918
42	1	0	-1.887132	2.432724	3.010656
43	1	0	-2.629113	0.842112	2.828185
44	1	0	-4.972694	-1.909615	-2.292819
45	1	0	-5.503304	-0.613393	-1.210414
46	1	0	-4.985733	-2.162482	-0.536651
47	1	0	-2.655527	-2.627707	-2.431764
48	1	0	-1.349450	-1.789635	-1.583863
49	1	0	-2.450694	-2.841631	-0.680209
50	1	0	-3.767191	0.627984	-2.372870
			Conformer (11S, 12S,	15 <i>R</i>)- 3-h	
Center	Atomic	Atomic	Co	pordinates (Angstroms)
Number	Number	Туре	Х	Y	Z
1	6	0	-3.634878	-0.086475	-0.352892
2	6	0	-3.256151	-1.029644	0.603633
3	6	0	-3.661402	-2.299322	0.134035
4	6	0	-4.282756	-2.103788	-1.093373
5	7	0	-4.263402	-0.772943	-1.367487
6	6	0	-3.573152	1.372876	-0.434366
7	8	0	-4.203880	1.961850	-1.317790
8	6	0	-2.817434	2.142687	0.592554
9	6	0	-1.526788	1.987940	0.974396
10	6	0	-0.627150	1.016164	0.342643
11	6	0	-0.956148	2.893702	2.041529
12	6	0	0.622382	0.719506	0.749716
13	6	0	1 498180	-0 304547	0.088907
14	6	0	3,031255	-0.094345	0.223989
15	6	0	3 642400	-1 532000	0 146062
16	6	0	2.042400	-2 508881	0.1240002
17	6	0	1 247645	-1 770326	0.010007
19	Q	0	0.062102	-2 325875	0.003222
10	6	0	1 105270	_1 072000	0.033370 2 122270
20	6	0	7.1222/0	-1.0/2200	2.1333/0
20	e e	0	5.000209	1.064100	-0.00/022
21	0	0	2.000667	1.004109	-0.52/89/
L 22	U D	0	2.99000/	2.204500	-0./999/5

23	8	0	3.599512	0.330339	-2.131655
24	1	0	1.231003	-0.364491	-0.975567
25	1	0	-2.773653	-0.803986	1.543706
26	1	0	-3.524431	-3.251073	0.626922
27	1	0	-4.725418	-2.814729	-1.775394
28	1	0	-4.660956	-0.289232	-2.160506
29	1	0	-3.385608	2.976956	0.998269
30	1	0	-1.003626	0.519633	-0.547890
31	1	0	-1.701650	3.610048	2.392753
32	1	0	-0.614785	2.313069	2.906853
33	1	0	-0.088987	3.449578	1.668056
34	1	0	1.021794	1.194879	1.644625
35	1	0	3.227216	0.330321	1.218187
36	1	0	4.237497	-1.744155	1.040005
37	1	0	4.305660	-1.623893	-0.715803
38	1	0	2.238435	-2.713157	-1.034534
39	1	0	2.632979	-3.471601	0.509028
40	1	0	-0.699086	-1.839614	0.373122
41	1	0	0.355822	-1.300404	2.540866
42	1	0	1.063415	-2.921350	2.419760
43	1	0	2.112276	-1.502727	2.603310
44	1	0	5.608337	1.722789	-1.272081
45	1	0	5.691743	0.097695	-0.583247
46	1	0	5.330407	1.482241	0.466040
47	1	0	3.488923	2.922559	-1.518119
48	1	0	1.933316	2.197223	-1.074117
49	1	0	3.044494	2.732163	0.188952
50	1	0	2.678113	0.367699	-2.421557

Atomic Atomic Coordinates (Angstroms) Number Number Type X Y Z 1 7 0 -5.344521 0.165452 -1.397021 2 6 0 -4.649558 0.016348 -0.212347 3 6 0 -5.61013 0.000491 0.795908 4 6 0 -6.879292 0.144946 0.200258 5 6 0 -3.198772 -0.087906 -0.210698 7 6 0 -2.500298 -0.240413 1.110041 8 8 0 -2.575599 -0.024721 -1.267800 9 6 0 -1.183134 -0.38806 0.356125 11 6 0 -1.184939 -0.533897 -0.538578 14 6 0 3.294719 0.571617 -0.447510 15 6 0 4.282795 2.029378 -0.151384 16 6 0	Conformer (11 <i>S</i> , 12 <i>S</i> , 15 <i>S</i>)- 4-a					
Number Number Type X Y Z 1 7 0 -5.344521 0.165452 -1.397021 2 6 0 -4.649558 0.016348 -0.212347 3 6 0 -5.601013 0.000491 0.795908 4 6 0 -5.601013 0.000491 0.795908 5 6 0 -5.601013 0.000491 0.20258 5 6 0 -3.198772 -0.087906 -0.210698 7 6 0 -2.575599 -0.042711 -1.267800 9 6 0 -1.183154 -0.33280 2.817026 11 6 0 -0.748123 -0.503280 2.817026 12 6 0 1.184939 -0.532876 0.353778 14 6 0 2.209389 -0.533761 1.44642 15 6 0 4.324170 -0.003249 0.54642 16	Center Atomic Atomic Coordinates (Angstroms)					
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Number	Number	Туре	Х	Y	Z
2 6 0 -4.649558 0.016348 -0.21347 3 6 0 -5.601013 0.000491 0.795908 4 6 0 -6.879292 0.144946 0.200258 5 6 0 -3.198772 -0.087906 -0.2106951 6 6 0 -2.500298 -0.240413 1.110041 8 8 0 -2.575599 -0.042721 -1.267800 9 6 0 -0.748123 -0.503280 2.817026 11 6 0 -0.748123 -0.503280 0.356125 12 6 0 1.184939 -0.53327 -0.533761 13 6 0 2.209389 -0.533781 -0.533761 14 6 0 3.086424 -1.820508 -0.513384 15 6 0 4.324170 -0.003249 0.545614 17 7 0 0 2.351131 -1.185887 <td< td=""><td>1</td><td>7</td><td>0</td><td>-5.344521</td><td>0.165452</td><td>-1.397021</td></td<>	1	7	0	-5.344521	0.165452	-1.397021
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	2	6	0	-4.649558	0.016348	-0.212347
4 6 0 -6.879292 0.144946 0.20258 5 6 0 -3.198772 -0.087906 -0.210698 7 6 0 -3.198772 -0.087906 -0.210698 7 6 0 -2.575599 -0.042721 -1.267800 9 6 0 -1.183154 -0.385760 1.372003 10 6 0 -0.748123 -0.503280 2.817026 11 6 0 -0.138133 -0.438950 0.356125 12 6 0 1.184939 -0.533897 -0.533578 14 6 0 3.2042170 -0.03249 0.554642 15 6 0 4.364395 -1.529589 0.516462 16 6 0 2.852295 2.029378 -0.151384 19 6 0 1.836197 2.531813 -1.185887 21 8 0 2.279214 2.143328 1.15237	3	6	0	-5.601013	0.000491	0.795908
5 6 0 -6.688477 0.244434 -1.156951 6 6 0 -3.198772 -0.087906 -0.210698 7 6 0 -2.575599 -0.042721 -1.67800 9 6 0 -1.183154 -0.385760 1.372003 10 6 0 -0.748123 -0.50280 2.817026 11 6 0 -0.748123 -0.538570 0.356125 12 6 0 1.184939 -0.533827 -0.538578 13 6 0 2.209389 -0.538678 -0.533761 14 6 0 3.294719 0.571617 -0.447510 15 6 0 4.324170 -0.003249 0.545614 17 6 0 2.327214 2.143328 -0.151384 19 6 0 1.38667 2.531813 -1.185877 20 6 0 2.351104	4	6	0	-6.879292	0.144946	0.200258
6 6 0 -3.198772 -0.087906 -0.210698 7 6 0 -2.500298 -0.240413 1.110041 8 8 0 -2.575599 -0.042721 -1.267800 9 6 0 -1.183154 -0.385760 1.372003 10 6 0 -0.748123 -0.503280 2.817026 11 6 0 -0.138133 -0.438950 0.356125 12 6 0 1.184939 -0.523222 0.576666 13 6 0 2.209389 -0.533857 -0.533761 15 6 0 4.164395 -1.529589 0.516462 16 6 0 2.83295 2.029378 -0.151384 17 6 0 2.85295 2.029378 -0.15910 21 8 0 2.77214 2.14328 1.15237 22 8 0 2.379214	5	6	0	-6.688457	0.244434	-1.156951
7 6 0 -2.50599 -0.240413 1.110041 8 8 0 -2.575599 -0.042721 -1.267800 9 6 0 -1.183154 -0.385760 1.372003 10 6 0 -0.748123 -0.503280 2.817026 11 6 0 -0.138133 -0.438950 0.356125 12 6 0 1.184939 -0.532222 0.576666 13 6 0 2.209378 -0.533761 14 6 0 3.294719 0.571617 -0.447510 15 6 0 4.324170 -0.003249 0.545614 17 6 0 2.32714 2.143328 -0.151384 19 6 0 1.836197 2.531813 -1.185887 20 6 0 4.065049 2.971522 -0.151334 18 0 2.379144 2.143328 1.153237	6	6	0	-3.198772	-0.087906	-0.210698
8 8 0 -2.575599 -0.042721 -1.267800 9 6 0 -1.183154 -0.385760 1.372003 10 6 0 -0.748123 -0.503280 2.817026 11 6 0 -0.138133 -0.438950 0.356125 12 6 0 1.184939 -0.532897 -0.538578 14 6 0 3.086424 -1.820508 -0.533761 15 6 0 4.164395 -1.529589 0.516462 16 6 0 3.294719 0.571617 -0.447510 18 6 0 2.852295 2.029378 -0.151384 19 6 0 1.836197 2.531813 -1.185887 20 6 0 4.065049 2.971522 -0.156910 21 8 0 3.738592 -1.94260 -1.807148 23 6 0 2.351104 -3.131333 1.57131	7	6	0	-2.500298	-0.240413	1.110041
960 -1.183154 -0.385760 1.372003 1060 -0.748123 -0.503280 2.817026 1160 -0.138133 -0.438950 0.356125 1260 1.184939 -0.523222 0.576666 1360 2.209389 -0.53897 -0.538578 1460 3.086424 -1.820508 -0.533761 1560 4.164395 -1.529589 0.516462 1660 4.324170 -0.003249 0.545614 1760 2.29255 2.029378 -0.151384 1960 1.836197 2.531813 -1.185887 2060 4.065049 2.971522 -0.156910 2180 2.279214 2.143328 1.153237 2280 3.738592 -1.944260 -1.807148 2360 2.351104 -3.131935 -0.271908 2410 -4.896302 0.208743 -2.305012 2510 -7.340777 0.364339 -1.971321 2810 -3.177258 -0.218846 1.957350 2910 -0.466347 -0.398511 -0.682749 3110 1.592506 -0.477294 3.511298 3310 1.52322 -0.567267 1.588284 3410 1.704194 -0.445826 <	8	8	0	-2.575599	-0.042721	-1.267800
10 6 0 -0.748123 -0.503280 2.817026 11 6 0 -0.138133 -0.438950 0.356125 12 6 0 1.184399 -0.523222 0.576666 13 6 0 2.209389 -0.539897 -0.538578 14 6 0 3.086424 -1.820508 -0.533761 15 6 0 4.164395 -1.529589 0.516462 16 0 3.294719 0.571617 -0.447510 18 6 0 2.852295 2.029378 -0.151384 19 6 0 4.065049 2.971522 -0.156910 21 8 0 2.779214 2.143328 1.153237 22 8 0 3.738592 -1.94260 -1.807148 23 6 0 2.351104 -3.131935 -0.271908 24 1 0 -7.834853 0.173	9	6	0	-1.183154	-0.385760	1.372003
1160 -0.138133 -0.438950 0.356125 1260 1.184939 -0.523222 0.576666 1360 2.209389 -0.5338578 1460 3.086424 -1.820508 -0.533761 1560 4.164395 -1.529589 0.516462 1660 4.324170 -0.003249 0.545614 1760 3.294719 0.571617 -0.447510 1860 2.852295 2.029378 -0.151384 1960 1.836197 2.531813 -1.185887 2060 4.065049 2.971522 -0.156910 2180 2.729214 2.143328 1.153237 2280 3.738592 -1.9442600 -1.807148 2360 2.351104 -3.131935 -0.271908 2410 -4.886302 0.208743 -2.305012 2510 -7.3390777 0.364339 -1.971321 2810 -7.390777 0.364339 -1.971321 2810 -0.224628 -1.450321 2.989068 3010 -0.28617 -0.882749 3110 -0.24628 -1.450321 2.989068 3310 1.582328 -0.567267 1.588284 3410 1.704194 -0.482826 -1.509078 <t< td=""><td>10</td><td>6</td><td>0</td><td>-0.748123</td><td>-0.503280</td><td>2.817026</td></t<>	10	6	0	-0.748123	-0.503280	2.817026
12601.184939 -0.523222 0.57666613602.09389 -0.5338578 -0.533761 14603.086424 -1.820508 -0.533761 15604.164395 -1.529589 0.516462 16604.324170 -0.003249 0.545614 1760 3.294719 0.571617 -0.447510 1860 2.852295 2.029378 -0.151384 1960 1.836197 2.531813 -1.185887 2060 4.065049 2.971522 -0.56910 2180 2.279214 2.143328 1.153237 2280 3.738592 -1.944260 -1.807148 2360 2.351104 -3.131935 -0.271908 2410 -4.896302 0.208743 -2.305012 2510 -7.834853 0.173026 0.708622 2710 -7.390777 0.364339 -1.971321 2810 -3.17258 -0.218846 1.957350 2910 -0.224628 -1.450321 2.989068 3010 -1.595606 -0.477294 3.511298 3110 0.224628 -1.450321 2.989068 3010 1.52328 -0.567267 1.588284 3410 1.704194 -0.445826 -1.50	11	6	0	-0.138133	-0.438950	0.356125
13 6 0 2.209389 -0.539897 -0.538578 14 6 0 3.086424 -1.820508 -0.533761 15 6 0 4.164395 -1.529589 0.516462 16 6 0 4.324170 -0.003249 0.545614 17 6 0 3.294719 0.571617 -0.447510 18 6 0 2.852295 2.029378 -0.151384 19 6 0 1.836197 2.531813 -1.185887 20 6 0 4.065049 2.971522 -0.156910 21 8 0 2.79214 2.143328 1.153237 22 8 0 3.738592 -1.944260 -1.807148 23 6 0 2.351104 -3.131935 -0.271908 24 1 0 -7.390777 0.364339 -1.971321 25 1 0 -7.390777 0	12	6	0	1.184939	-0.523222	0.576666
14 6 0 3.086424 -1.820508 -0.533761 15 6 0 4.164395 -1.529589 0.545614 16 6 0 3.294719 0.571617 -0.447510 18 6 0 2.852295 2.029378 -0.151384 19 6 0 1.836197 2.531813 -1.185887 20 6 0 4.065049 2.971522 -0.156910 21 8 0 2.279214 2.143328 1.153237 22 8 0 3.738592 -1.944260 -1.807148 23 6 0 2.351104 -3.131935 -0.271908 24 1 0 -5.417621 -0.102333 1.857181 26 1 0 -7.390777 0.364339 -1.971321 28 1 0 -3.177258 -0.218846 1.957350 29 1 0 -0.24628	13	6	0	2.209389	-0.539897	-0.538578
1560 4.164395 -1.529589 0.516462 1660 4.324170 -0.003249 0.545614 1760 3.294719 0.571617 -0.447510 1860 2.852295 2.029378 -0.151384 1960 1.836197 2.531813 -1.185887 2060 4.065049 2.971522 -0.156910 2180 2.279214 2.143328 1.153237 2280 3.738592 -1.944260 -1.807148 2360 2.351104 -3.131935 -0.271908 2410 -4.896302 0.208743 -2.305012 2510 -5.417621 -0.102333 1.857181 2610 -7.834853 0.173026 0.708622 2710 -7.390777 0.364339 -1.971321 2810 -3.177258 -0.218846 1.957350 2910 -0.224628 -1.450321 2.989068 3010 -1.595606 -0.477294 3.511298 3110 -0.086139 0.325711 3.090712 3210 1.582328 -0.567267 1.588284 3410 1.704194 -0.445826 -1.509078 3510 5.341408 0.283633 0.255774 3910 3.75502 4.02769 <td>14</td> <td>6</td> <td>0</td> <td>3.086424</td> <td>-1.820508</td> <td>-0.533761</td>	14	6	0	3.086424	-1.820508	-0.533761
1660 4.324170 -0.003249 0.545614 1760 3.294719 0.571617 -0.447510 1860 2.852295 2.029378 -0.151384 1960 1.836197 2.531813 -1.185887 2060 4.065049 2.971522 -0.156910 2180 2.779214 2.143328 1.153237 2280 3.738592 -1.944260 -1.807148 2360 2.351104 -3.131935 -0.271908 2410 -4.896302 0.208743 -2.305012 2510 -5.417621 -0.102333 1.857181 2610 -7.390777 0.364339 -1.971321 2810 -3.177258 -0.218846 1.957350 2910 -0.224628 -1.450321 2.989068 3010 -1.595606 -0.477294 3.511298 3110 -0.086639 0.325711 3.090712 3210 1.582328 -0.567267 1.588284 3410 1.704194 -0.445826 -1.509078 3510 5.117818 -2.012607 0.276164 3610 3.855905 -1.870853 1.511941 3710 4.160766 0.363112 1.565080 3810 3.752502 4.007095 </td <td>15</td> <td>6</td> <td>0</td> <td>4.164395</td> <td>-1.529589</td> <td>0.516462</td>	15	6	0	4.164395	-1.529589	0.516462
1760 3.294719 0.571617 -0.447510 1860 2.852295 2.029378 -0.151384 1960 1.836197 2.531813 -1.185887 2060 4.065049 2.971522 -0.156910 2180 2.279214 2.143328 1.153237 2280 3.738592 -1.944260 -1.807148 2360 2.351104 -3.131935 -0.271908 2410 -5.417621 -0.102333 1.857181 2610 -7.834853 0.173026 0.708622 2710 -7.390777 0.364339 -1.971321 2810 -3.177258 -0.218846 1.957350 2910 -0.224628 -1.450321 2.989068 3010 -1.595606 -0.477294 3.511298 3110 -0.086139 0.325711 3.090712 3210 1.704194 -0.445826 -1.509078 3310 1.582328 -0.567267 1.588284 3410 1.704194 -0.445826 -1.509078 3510 5.341408 0.283633 0.255774 3910 3.755905 -1.870853 1.511941 3710 4.160766 0.363112 1.565080 3810 5.341408 0.283633 <td>16</td> <td>6</td> <td>0</td> <td>4.324170</td> <td>-0.003249</td> <td>0.545614</td>	16	6	0	4.324170	-0.003249	0.545614
1860 2.852295 2.029378 -0.151384 1960 1.836197 2.531813 -1.185887 2060 4.065049 2.971522 -0.156910 2180 2.279214 2.143328 1.153237 2280 3.738592 -1.944260 -1.807148 2360 2.351104 -3.131935 -0.271908 2410 -4.896302 0.208743 -2.305012 2510 -7.834853 0.173026 0.708622 2710 -7.390777 0.364339 -1.971321 2810 -3.177258 -0.218846 1.957350 2910 -0.224628 -1.450321 2.989068 3010 -1.595606 -0.477294 3.511298 3110 -0.086139 0.325711 3.090712 3210 -0.456847 -0.398511 -0.682749 3310 1.582328 -0.567267 1.588284 3410 1.704194 -0.45833 1.511941 3710 4.160766 0.363112 1.565080 3810 5.341408 0.283633 0.255774 3910 3.752502 4.007095 0.023049 4410 4.765399 2.726328 0.649104 4510 4.52599 -2.156296 <	17	6	0	3.294719	0.571617	-0.447510
19601.8361972.531813-1.18588720604.0650492.971522-0.15691021802.2792142.1433281.15323722803.738592-1.944260-1.80714823602.351104-3.131935-0.2719082410-4.8963020.208743-2.3050122510-5.417621-0.1023331.8571812610-7.3907770.364339-1.9713212810-3.177258-0.2188461.9573502910-0.224628-1.4503212.9890683010-1.595606-0.4772943.5112983110-0.0861390.3257113.0907123210-0.456847-0.398511-0.68274933101.582328-0.5672671.58828434103.855905-1.8708531.51194137104.1607660.3631121.56508038105.3414080.2836330.25577439103.752522.522669-2.19723841100.9240641.927798-1.48103043103.057086-2.156296-2.46853544104.7653992.7263280.64910445103.057086-2.156296-2.468535 <t< td=""><td>18</td><td>6</td><td>0</td><td>2.852295</td><td>2.029378</td><td>-0.151384</td></t<>	18	6	0	2.852295	2.029378	-0.151384
20604.0650492.971522-0.15691021802.2792142.1433281.15323722803.738592-1.944260-1.80714823602.351104-3.131935-0.2719082410-4.8963020.208743-2.3050122510-5.417621-0.1023331.8571812610-7.3907770.364339-1.9713212810-3.177258-0.2188461.9573502910-0.224628-1.4503212.9890683010-1.595606-0.4772943.5112983110-0.0861390.3257113.0907123210-0.456847-0.398511-0.68274933101.704194-0.445826-1.50907835105.117818-2.0126070.27616436103.855905-1.8708531.51194137104.1607660.3631121.56508038103.7903970.598762-1.43103040102.2552552.522669-2.19723841104.7653992.7263280.64910445101.3386251.9017681.09099044104.7653992.7263280.64910445101.3386251.9017681.000119	19	6	0	1.836197	2.531813	-1.185887
21802.792142.1433281.1532372280 3.738592 -1.944260 -1.807148 2360 2.351104 -3.131935 -0.271908 2410 -4.896302 0.208743 -2.305012 2510 -5.417621 -0.102333 1.857181 2610 -7.834853 0.173026 0.708622 2710 -7.390777 0.364339 -1.971321 2810 -3.177258 -0.218846 1.957350 2910 -0.224628 -1.450321 2.989068 3010 -1.595606 -0.477294 3.511298 3110 -0.086139 0.325711 3.090712 3210 -0.456847 -0.398511 -0.682749 3310 1.582328 -0.567267 1.588284 3410 1.704194 -0.445826 -1.509078 3510 5.117818 -2.012607 0.276164 3610 3.790397 0.598762 -1.431030 4010 2.255255 2.522669 -2.197238 4110 4.765399 2.726328 0.649104 4310 3.752502 4.007095 0.023049 4410 4.765399 2.726328 0.649104 4510 1.338625 1.901768	20	6	0	4.065049	2.971522	-0.156910
2280 3.738592 -1.944260 -1.807148 2360 2.351104 -3.131935 -0.271908 2410 -4.896302 0.208743 -2.305012 2510 -5.417621 -0.102333 1.857181 2610 -7.390777 0.364339 -1.971321 2810 -7.390777 0.364339 -1.971321 2810 -3.177258 -0.218846 1.957350 2910 -0.224628 -1.450321 2.989068 3010 -1.595606 -0.477294 3.511298 3110 -0.086139 0.325711 3.090712 3210 -0.456847 -0.398511 -0.682749 3310 1.582328 -0.567267 1.588284 3410 1.704194 -0.445826 -1.509078 3510 5.117818 -2.012607 0.276164 3610 3.855905 -1.870853 1.511941 3710 4.160766 0.363112 1.565080 3810 5.341408 0.283633 0.255774 3910 3.752502 4.007095 0.023049 4410 4.755399 2.726328 0.649104 4510 1.338625 1.901768 1.090990 4710 3.057086 -2.156296 <	21	8	0	2,279214	2.143328	1,153237
23602.351104-1.311935-1.0711032410-4.8963020.208743-2.3050122510-5.417621-0.1023331.8571812610-7.8348530.1730260.7086222710-7.3907770.364399-1.9713212810-3.17258-0.2188461.9573502910-0.224628-1.4503212.9890683010-1.595606-0.4772943.5112983110-0.0861390.3257113.0907123210-0.456847-0.398511-0.68274933101.582328-0.5672671.58828434101.704194-0.445826-1.50907835105.117818-2.0126070.27616436103.855905-1.8708531.51194137104.1607660.3631121.56508038105.3414080.2836330.25577439103.7525024.0070950.02304944104.6015812.935468-1.1050445104.6015812.935468-1.10050445103.057086-2.156296-2.46853548101.920979-3.1775080.73346249101.544941-3.275482-1.000119 <t< td=""><td>22</td><td>8</td><td>0</td><td>3 738592</td><td>-1 944260</td><td>-1 807148</td></t<>	22	8	0	3 738592	-1 944260	-1 807148
2410 -1.896302 0.208743 -2.305012 2510 -5.417621 -0.102333 1.857181 2610 -7.834853 0.173026 0.708622 2710 -7.390777 0.364339 -1.971321 2810 -3.177258 -0.218846 1.957350 2910 -0.224628 -1.450321 2.989068 3010 -1.595606 -0.477294 3.511298 3110 -0.086139 0.325711 3.090712 3210 -0.456847 -0.398511 -0.682749 3310 1.582328 -0.567267 1.588284 3410 1.704194 -0.445826 -1.509078 3510 5.3117818 -2.012607 0.276164 3610 3.855905 -1.870853 1.511941 3710 4.160766 0.363112 1.565080 3810 3.790397 0.598762 -1.431030 4010 2.255255 2.522669 -2.197238 4110 4.601581 2.935468 -1.110504 4510 1.338625 1.901768 1.090990 4710 3.057086 -2.156296 -2.468535 4810 1.920979 -3.177508 0.733462 4910 1.544941 -3.275482	23	6	0	2 351104	-3 131935	-0.271908
2510-5.417621-0.1023331.8571812610-7.8348530.1730260.7086222710-7.3907770.364339-1.9713212810-3.177258-0.2188461.9573502910-0.224628-1.4503212.9890683010-1.595606-0.4772943.5112983110-0.0861390.3257113.0907123210-0.456847-0.398511-0.68274933101.582328-0.5672671.58828434101.704194-0.445826-1.50907835105.117818-2.0126070.27616436103.855905-1.8708531.51194137104.1607660.3631121.56508038105.3414080.2836330.25577439103.7903970.598762-1.43103040102.255252.522669-2.19723841104.7653992.7263280.64910445101.3386251.9017681.09099047103.057086-2.156296-2.46853548101.920979-3.1775080.73346249101.544941-3.275482-1.00011950103.031089-3.383989-0.387099 <td>24</td> <td>1</td> <td>0</td> <td>-4 896302</td> <td>0 208743</td> <td>-2 305012</td>	24	1	0	-4 896302	0 208743	-2 305012
2510 3.7834853 0.173026 1.057451 26 10 -7.834853 0.173026 0.708622 27 10 -7.390777 0.364339 -1.971321 28 10 -3.177258 -0.218846 1.957350 29 10 -0.224628 -1.450321 2.989068 30 10 -1.595606 -0.477294 3.511298 31 10 -0.086139 0.325711 3.090712 32 10 -0.456847 -0.398511 -0.682749 33 10 1.582328 -0.567267 1.588284 34 10 1.70267 0.276164 36 10 5.117818 -2.012607 0.276164 36 10 3.855905 -1.870853 1.511941 37 10 4.160766 0.363112 1.565080 38 10 5.341408 0.283633 0.255774 39 10 3.790397 0.598762 -1.431030 40 10 2.255255 2.522669 -2.197238 41 10 4.765399 2.726328 0.649104 45 10 4.38625 1.901768 1.090990 47 10 3.057086 -2.156296 -2.468535 48 10 1.544941 -3.275482 -1.000119 50 10 3.051089 <td>25</td> <td>1</td> <td>0</td> <td>-5 417621</td> <td>-0 102333</td> <td>1 857181</td>	25	1	0	-5 417621	-0 102333	1 857181
10 1 0 -7.390777 0.364339 -1.971321 28 1 0 -3.177258 -0.218846 1.957350 29 1 0 -0.224628 -1.450321 2.989068 30 1 0 -1.595606 -0.477294 3.511298 31 1 0 -0.086139 0.325711 3.090712 32 1 0 -0.456847 -0.398511 -0.682749 33 1 0 1.582328 -0.567267 1.588284 34 1 0 1.704194 -0.445826 -1.509078 35 1 0 5.117818 -2.012607 0.276164 36 1 0 3.855905 -1.870853 1.511941 37 1 0 4.160766 0.363112 1.565080 38 1 0 5.341408 0.283633 0.255774 39 1 0 3.790397 0.598762 -1.431030 40 1 0 2.255255 2.522669 -2.197238 41 1 0 4.765399 2.726328 0.649104 43 1 0 4.765399 2.726328 0.649104 45 1 0 1.338625 1.901768 1.090990 47 1 0 3.057086 -2.156296 -2.468535 48 1 0 1.544941 -3.275482 -1.000119 50 1 0 3.031089 </td <td>26</td> <td>1</td> <td>0</td> <td>-7 834853</td> <td>0.173026</td> <td>0 708622</td>	26	1	0	-7 834853	0.173026	0 708622
2810 -3.077258 -0.218846 1.957350 29 10 -0.224628 -1.450321 2.989068 30 10 -1.595606 -0.477294 3.511298 31 10 -0.086139 0.325711 3.090712 32 10 -0.456847 -0.398511 -0.682749 33 10 1.582328 -0.567267 1.588284 34 10 1.704194 -0.445826 -1.509078 35 10 5.117818 -2.012607 0.276164 36 10 3.855905 -1.870853 1.511941 37 10 4.160766 0.363112 1.565080 38 10 5.341408 0.283633 0.255774 39 10 3.790397 0.598762 -1.431030 40 10 0.2255255 2.522669 -2.197238 41 10 0.924064 1.927798 -1.186253 42 10 1.518407 3.554610 -0.951331 43 10 3.752502 4.007095 0.023049 44 10 4.601581 2.935468 -1.110504 45 10 1.338625 1.901768 1.090990 47 10 3.057086 -2.156296 -2.468535 48 10 1.920979 -3.177508 0.733462 49 10<	20	1	0	-7.390777	0.364339	-1.971321
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10^{-1} 10^{-1} 1.4301^{-1} 1.43031^{-1} 1.53030^{-1} 30^{-1} 0^{-1} -1.595606 -0.477294 3.511298 31^{-1} 0^{-0} -0.086139 0.325711 3.090712 32^{-1} 0^{-0} -0.456847 -0.398511 -0.682749 33^{-1} 0^{-1} 1.582328 -0.567267 1.588284 34^{-1} 0^{-1} 1.704194 -0.445826 -1.509078 35^{-1} 0^{-5} 5.117818 -2.012607 0.276164 36^{-1} 0^{-5} 3.855905 -1.870853 1.511941 37^{-1} 0^{-4} 4.160766 0.363112 1.565080 38^{-1} 0^{-5} 3.790397 0.598762 -1.431030 40^{-1} $0^{-2.255255}$ 2.522669 -2.197238 41^{-1} 0^{-1} 0.2255255 2.522669 -2.197238 41^{-1} 0^{-1} 0.5924064 1.927798 -1.186253 42^{-1} 0^{-1} 1.518407 3.554610^{-1} -0.951331 43^{-1} 0^{-1} 0.752502^{-1} 4.007095^{-1} 0.023049 44^{-1} 0^{-1} 4.601581^{-2} 2.935468^{-1} -1.10504^{-1} 45^{-1} 0^{-1} 4.601581^{-2} 2.935468^{-2} -1.10504^{-1} 45^{-1} 0^{-1} 1.920979^{-3} -3.177508^{-2} -2.468535^{-1} 48^{-1} 0^{-1} 1.920979^{-3} -3.177508^{-2} -0.387099^{-2} 48^{-1} <td>20</td> <td>1</td> <td>0</td> <td>-0 224628</td> <td>-1 450321</td> <td>2 989068</td>	20	1	0	-0 224628	-1 450321	2 989068
3010-1.0360300.31719743.1911903110-0.0861390.3257113.0907123210-0.456847-0.398511-0.68274933101.582328-0.5672671.58828434101.704194-0.445826-1.50907835105.117818-2.0126070.27616436103.855905-1.8708531.51194137104.1607660.3631121.56508038105.3414080.2836330.25577439103.7903970.598762-1.43103040102.2552552.522669-2.19723841100.9240641.927798-1.18625342101.5184073.554610-0.95133143103.7525024.0070950.02304944104.6015812.935468-1.11050445101.3386251.9017681.09099047103.057086-2.156296-2.46853548101.920979-3.1775080.73346249101.544941-3.275482-1.00011950103.031089-3.983898-0.387099	30	1	0	-1 595606	-0.477294	3 511298
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3210 1.580311 0.50311 33 10 1.582328 -0.567267 1.588284 34 10 1.704194 -0.445826 -1.509078 35 10 5.117818 -2.012607 0.276164 36 10 3.855905 -1.870853 1.511941 37 10 4.160766 0.363112 1.565080 38 10 5.341408 0.283633 0.255774 39 10 3.790397 0.598762 -1.431030 40 10 2.255255 2.522669 -2.197238 41 10 0.924064 1.927798 -1.186253 42 10 1.518407 3.554610 -0.951331 43 10 3.752502 4.007095 0.023049 44 10 4.765399 2.726328 0.649104 45 10 1.338625 1.901768 1.090990 47 10 3.057086 -2.156296 -2.468535 48 10 1.920979 -3.177508 0.733462 49 10 1.544941 -3.275482 -1.000119 50 10 3.031089 -3.983898 -0.387099	32	1	0	-0.456847	-0 398511	-0 682749
33 1 0 1.30210 0.507107 1.302104 34 1 0 1.704194 -0.445826 -1.509078 35 1 0 5.117818 -2.012607 0.276164 36 1 0 3.855905 -1.870853 1.511941 37 1 0 4.160766 0.363112 1.565080 38 1 0 5.341408 0.283633 0.255774 39 1 0 3.790397 0.598762 -1.431030 40 1 0 2.255255 2.522669 -2.197238 41 1 0 0.924064 1.927798 -1.186253 42 1 0 1.518407 3.554610 -0.951331 43 1 0 3.752502 4.007095 0.023049 44 1 0 4.765399 2.726328 0.649104 45 1 0 1.338625 1.901768 1.090990 4	32	1	0	1 582328	-0 567267	1 588284
3410 1.764134 0.445020 1.303070 35 10 5.117818 -2.012607 0.276164 36 10 3.855905 -1.870853 1.511941 37 10 4.160766 0.363112 1.565080 38 10 5.341408 0.283633 0.255774 39 10 3.790397 0.598762 -1.431030 40 10 2.255255 2.522669 -2.197238 41 10 0.924064 1.927798 -1.186253 42 10 1.518407 3.554610 -0.951331 43 10 3.752502 4.007095 0.023049 44 10 4.601581 2.935468 -1.110504 45 10 1.338625 1.901768 1.090990 47 10 3.057086 -2.156296 -2.468535 48 10 1.920979 -3.177508 0.733462 49 10 3.031089 -3.983898 -0.387099	34	1	0	1.302320	-0.445826	-1 509078
3610 3.117010 1.01017 1.01017 36 10 3.855905 -1.870853 1.511941 37 10 4.160766 0.363112 1.565080 38 10 5.341408 0.283633 0.255774 39 10 3.790397 0.598762 -1.431030 40 10 2.255255 2.522669 -2.197238 41 10 0.924064 1.927798 -1.186253 42 10 1.518407 3.554610 -0.951331 43 10 3.752502 4.007095 0.023049 44 10 4.765399 2.726328 0.649104 45 10 1.338625 1.901768 1.090990 47 10 3.057086 -2.156296 -2.468535 48 10 1.920979 -3.177508 0.733462 49 10 3.031089 -3.983898 -0.387099	35	1	0	5 117818	-2 012607	0 276164
3010 3.033303 1.010333 1.311341 37 10 4.160766 0.363112 1.565080 38 10 5.341408 0.283633 0.255774 39 10 3.790397 0.598762 -1.431030 40 10 2.255255 2.522669 -2.197238 41 10 0.924064 1.927798 -1.186253 42 10 1.518407 3.554610 -0.951331 43 10 3.752502 4.007095 0.023049 44 10 4.765399 2.726328 0.649104 45 10 1.338625 1.901768 1.090990 47 10 3.057086 -2.156296 -2.468535 48 10 1.920979 -3.177508 0.733462 49 10 1.544941 -3.275482 -1.000119 50 10 3.031089 -3.983898 -0.387099	36	1	0	3 855905	-1 870853	1 5119/1
37 1 0 4.100706 0.303112 1.303000 38 1 0 5.341408 0.283633 0.255774 39 1 0 3.790397 0.598762 -1.431030 40 1 0 2.255255 2.522669 -2.197238 41 1 0 0.924064 1.927798 -1.186253 42 1 0 1.518407 3.554610 -0.951331 43 1 0 3.752502 4.007095 0.023049 44 1 0 4.765399 2.726328 0.649104 45 1 0 4.601581 2.935468 -1.110504 46 1 0 1.338625 1.901768 1.090990 47 1 0 3.057086 -2.156296 -2.468535 48 1 0 1.920979 -3.177508 0.733462 49 1 0 3.031089 -3.983898 -0.387099	37	1	0	4 160766	0 363112	1.511541
39 1 0 3.790397 0.598762 -1.431030 40 1 0 2.255255 2.522669 -2.197238 41 1 0 0.924064 1.927798 -1.186253 42 1 0 1.518407 3.554610 -0.951331 43 1 0 3.752502 4.007095 0.023049 44 1 0 4.765399 2.726328 0.649104 45 1 0 4.601581 2.935468 -1.110504 46 1 0 1.338625 1.901768 1.090990 47 1 0 3.057086 -2.156296 -2.468535 48 1 0 1.920979 -3.177508 0.733462 49 1 0 3.031089 -3.983898 -0.387099	38	1	n	5,341408	0.283633	0.255774
40 1 0 2.255255 2.522669 -2.197238 41 1 0 0.924064 1.927798 -1.186253 42 1 0 1.518407 3.554610 -0.951331 43 1 0 3.752502 4.007095 0.023049 44 1 0 4.765399 2.726328 0.649104 45 1 0 4.601581 2.935468 -1.110504 46 1 0 1.338625 1.901768 1.090990 47 1 0 3.057086 -2.156296 -2.468535 48 1 0 1.920979 -3.177508 0.733462 49 1 0 3.031089 -3.983898 -0.387099	39	1	0	3,790397	0,598762	-1 431030
10 1 0 0.924064 1.927798 -1.186253 41 1 0 1.518407 3.554610 -0.951331 43 1 0 3.752502 4.007095 0.023049 44 1 0 4.765399 2.726328 0.649104 45 1 0 4.601581 2.935468 -1.110504 46 1 0 1.338625 1.901768 1.090990 47 1 0 3.057086 -2.156296 -2.468535 48 1 0 1.544941 -3.275482 -1.000119 50 1 0 3.031089 -3.983898 -0.387099	40	1	0	2 255255	2 522669	-2 197238
42 1 0 1.518407 3.554610 -0.951331 43 1 0 3.752502 4.007095 0.023049 44 1 0 4.765399 2.726328 0.649104 45 1 0 4.601581 2.935468 -1.110504 46 1 0 1.338625 1.901768 1.090990 47 1 0 3.057086 -2.156296 -2.468535 48 1 0 1.920979 -3.177508 0.733462 49 1 0 3.031089 -3.983898 -0.387099	41	1	0	0.924064	1,927798	-1,186253
12 13 0 1310407 131007 1310407	42	1	0	1 518407	3 554610	_0 951221
10 1 0 4.765399 2.726328 0.649104 45 1 0 4.601581 2.935468 -1.110504 46 1 0 1.338625 1.901768 1.090990 47 1 0 3.057086 -2.156296 -2.468535 48 1 0 1.920979 -3.177508 0.733462 49 1 0 1.544941 -3.275482 -1.000119 50 1 0 3.031089 -3.983898 -0.387099	42	1	0	3 752502	4 007095	0.0230/0
45 1 0 4.601581 2.935468 -1.110504 46 1 0 1.338625 1.901768 1.090990 47 1 0 3.057086 -2.156296 -2.468535 48 1 0 1.920979 -3.177508 0.733462 49 1 0 1.544941 -3.275482 -1.000119 50 1 0 3.031089 -3.983898 -0.387099	44	1	0	4 765399	2 726328	0 649104
46 1 0 1.338625 1.901768 1.090990 47 1 0 3.057086 -2.156296 -2.468535 48 1 0 1.920979 -3.177508 0.733462 49 1 0 1.544941 -3.275482 -1.000119 50 1 0 3.031089 -3.983898 -0.387099	45	1	0	4 601581	2.720020	-1 110504
47 1 0 3.057086 -2.156296 -2.468535 48 1 0 1.920979 -3.177508 0.733462 49 1 0 1.544941 -3.275482 -1.000119 50 1 0 3.031089 -3.983898 -0.387099	46	1	0	1 338625	1 901768	1 09090
48 1 0 1.920979 -3.177508 0.733462 49 1 0 1.544941 -3.275482 -1.000119 50 1 0 3.031089 -3.983898 -0.387099	40	1	0	3 057086	-2 156206	-2 /68525
49 1 0 1.526575 1.5177508 0.753402 49 1 0 1.544941 -3.275482 -1.000119 50 1 0 3.031089 -3.983898 -0.387099	18	1	0	1 920970	-3 177508	0 733/67
	40	1	0	1.520575 1 5//Q/1	-3 775/187	_1 000110
Conformer (115, 125, 155) -0.387033	50	1	0	3 031080	-3 983898	-0 387099
	50	<u> </u>	0	Conformer (115, 12)	5.565656 5.155)- 4-h	0.307033

Table S13. DFT Coordinates of the optimized conformers of (11*S*, 12*S*, 15*S*)-**4** at CAM-B3LYP/def2-TZVP theory level.

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	Х	Ŷ	Z	
1	7	0	-5.433687	0.178901	-1.381902	
2	6	0	-4.706810	0.035764	-0.216119	
3	6	0	-5.631918	0.023009	0.817377	
4	6	0	-6.926044	0.160798	0.256234	
5	6	0	-6.771310	0.254977	-1.105781	
6	6	0	-3.255064	-0.069075	-0.247780	
7	6	0	-2.533916	-0.205171	1.060371	
8	8	0	-2.651910	-0.043944	-1.316982	
9	6	0	-1.214682	-0.339222	1.312277	
10	6	0	-0.779677	-0.450062	2.759147	
11	6	0	-0.166910	-0.377260	0.295486	
12	6	0	1,148998	-0.509601	0.538186	
13	6	0	2.217653	-0.528698	-0.531905	
14	6	0	3.049333	-1.844329	-0.508657	
15	6	0	4,102769	-1.619151	0.592458	
16	6	0	4,214779	-0.096265	0.776984	
17	6	0	3 346724	0 517571	-0 333997	
18	6	0	3.003231	2 018866	-0 172368	
19	6	0	2 335803	2 558293	-1 444227	
20	6	0	2.555665	2.000200	1 042120	
20	8	0	4 244928	2.405002	-0.013801	
21	8	0	3 7/19151	_1 968893	-1 758254	
22	6	0	2 250578	_3 135131	_0.309533	
23	1	0	-5.010836	0 219305	-2 302020	
24	1	0	-5 /21125		1 87/021	
25	1	0	_7 867265	0.075257	0.700774	
20	1	0	-7 /96020	0.107502	-1 901007	
27	1	0	-3 20001/		1 916279	
20	1	0	-0.281816	_1 /08926	2 9/1273	
20	1	0	-1 623/172		2.541275	
31	1	0	-0.096338	0.352410	3.022898	
32	1	0	-0.474237	-0 277829	-0 742973	
32	1	0	1 507758	-0.615053	1 559065	
34	1	0	1 768565	-0 385186	-1 522793	
35	1	0	5 075540	-2 040526	0 315116	
36	1	0	3 799560	-2.070561	1 544275	
37	1	0	3 854211	0 174834	1 774604	
38	1	0	5 256157	0.234882	0 706668	
39	1	0	3 977883	0.470538	-1 237108	
40	1	0	1.353995	2,106005	-1.613871	
41	1	0	2.961062	2.368948	-2.324665	
42	1	0	2.211480	3.645923	-1.387861	
43	1	0	1,109160	2,116437	0.931581	
44	1	0	2.547771	1.970464	1.967134	
45	1	0	2.174799	3.490692	1.190627	
46	1	0	4 802010	2 537211	-0 787918	
47	1	0	3,088414	-2.146618	-2.450317	
48	1	0	1.768528	-3.180035	0.667173	
49	1	0	2,920093	-4.005811	-0.395177	
50	1	0	1.496045	-3.245753	-1.087790	
			Conformer (115, 12	S. 15S)- 4-c		
Center	Atomic	Atomic	(<u>110</u> , <u>12</u>	oordinates (Angstroms)		
Number	Number	Type	X	Υ	Z	
1	7	0	-5.400573	-0.064358	-1.408822	
2	6	0	-4.688628	0.007770	-0.227078	
_	-	-				

3	6	0	-5.624286	0.204621	0.777215
4	6	0	-6.910473	0.247194	0.182559
5	6	0	-6.740030	0.077077	-1.170224
6	6	0	-3.238845	-0.118549	-0.221881
7	6	0	-2.527392	-0.043583	1.098276
8	8	0	-2.627143	-0.283229	-1.273555
9	6	0	-1.207853	-0.131673	1.372932
10	6	0	-0.772484	-0.019535	2.818269
11	6	0	-0.160916	-0.323258	0.374517
12	6	0	1.159033	-0.419313	0.614732
13	6	0	2.186509	-0.604865	-0.478214
14	6	0	3.017996	-1.908819	-0.316924
15	6	0	4 096796	-1 518092	0.695237
16	6	0	4 437230	-0.058573	0.377432
17	6	0	3.307963	0.474236	-0.528609
18	6	0	2,954014	1,975996	-0.354557
19	6	0	4 166278	2 837816	-0 746899
20	6	0	2 494393	2 409560	1 043810
21	8	0	1 915003	2 310362	-1 282782
21	8	0	3 674986	-2 215399	-1 554470
22	6	0	2 242747	-3 152276	0 105931
23	1	0	-4 967013	-0.203986	-2 314282
25	1	0	-5 425773	0.205500	1 835465
26	1	0	-7 857274	0.387208	0.688736
20	1	0	-7 454083	0.045452	-1 982609
27	1	0	-3 200200	0.043432	1.982005
20	1	0	-1 618/02	0.101575	3 /00//8
30	1	0	-0.257708	-0.931326	3 1/0166
31	1	0	-0 103227	0.331320	2 956623
32	1	0	-0.477240	-0.392489	-0.664022
33	1	0	1 5//240	-0 372323	1 620801
34	1	0	1.544217	-0.612835	-1 454649
35	1	0	4 990254	-2 147429	0.624604
36	1	0	3 717097	-1 582/11	1 721987
37	1	0	4 559645	0 505120	1 305410
38	1	0	5 393524	-0.002087	-0 157084
39	1	0	3 693271	0.397725	-1 559714
40	1	0	3.0000271	3 903401	-0 737328
40	1	0	4 490960	2 615941	-1 769964
41	1	0	5 013363	2.613341	-0.070918
42	1	0	3 171871	2.004745	1 834241
45	1	0	1 484361	2.077620	1 275506
45	1	0	2 433204	3 503351	1 103303
46	1	0	1 094388	1 880081	-0.984389
40	1	0	2 986953	-2 398203	-2 218066
47	1	0	1 771375	-3 040642	1 087162
40	1	0	2 909011	-4 021752	0 151461
50	1	0	1 466197	-3 392752	-0.628471
	-	0	Conformer (115, 129	5.552752 5.155)- 4-d	0.020471
Center	Atomic	Atomic		oordinates (Angstroms)	
Number	Number	Type	X	V	7
1	7	0	-5 494402	-0 319635	-1 394579
2	,	0	5.757702	0.010000	1.554575
2	6	0	-4.775859	-0.009759	-0.256064
	6	0	-4.775859 -5 705413	-0.009759	-0.256064 0.691985
4	6 6 6	0 0 0	-4.775859 -5.705413 -6.994625	-0.009759 0.389987 0.314314	-0.256064 0.691985 0.107398
4 5	6 6 6	0 0 0	-4.775859 -5.705413 -6.994625 -6.832097	-0.009759 0.389987 0.314314 -0.128483	-0.256064 0.691985 0.107398 -1 183261

7	6	0	-2.606415	0.205688	1.037983
8	8	0	-2.724130	-0.508788	-1.237073
9	6	0	-1.286685	0.155218	1.320081
10	6	0	-0.833173	0.586822	2.698171
11	6	0	-0.253760	-0.286568	0.389083
12	6	0	1.073686	-0.250399	0.602927
13	6	0	2.098510	-0.684230	-0.415897
14	6	0	2.958139	-1.900186	0.035908
15	6	0	4.155162	-1.826203	-0.908152
16	6	0	4.476895	-0.343457	-0.954137
17	6	0	3.106692	0.377087	-0.978612
18	6	0	3.169080	1.809827	-0.377366
19	6	0	1.846272	2.578988	-0.514824
20	6	0	4.267480	2.636893	-1.072665
21	8	0	3.505428	1.725575	1.009638
22	8	0	2.262171	-3.124152	-0.203461
23	6	0	3.396116	-1.892731	1.503807
24	1	0	-5.065080	-0.643408	-2.253745
25	1	0	-5.500176	0.707164	1.705712
26	1	0	-7.938374	0.556672	0.579337
27	1	0	-7.550439	-0.323905	-1.968428
28	1	0	-3.268848	0.552633	1.823521
29	1	0	-0.182416	1.466009	2.633929
30	1	0	-1.672826	0.858318	3.347784
31	1	0	-0.291985	-0.222657	3.200524
32	1	0	-0.585986	-0.663298	-0.575539
33	1	0	1.476648	0.130086	1.538060
34	1	0	1.531406	-1.029771	-1.295878
35	1	0	5.006718	-2.424256	-0.567203
36	1	0	3.886918	-2.193447	-1.906966
37	1	0	5.059702	-0.065539	-0.068629
38	1	0	5.079167	-0.097177	-1.834929
39	1	0	2.843605	0.501275	-2.040835
40	1	0	1.404090	2.450014	-1.507620
41	1	0	1.116433	2.293733	0.245428
42	1	0	2.001802	3.653166	-0.356171
43	1	0	4.304872	3.655931	-0.669234
44	1	0	4.094839	2.702534	-2.152064
45	1	0	5.263715	2.217334	-0.899059
46	1	0	3.571478	2.633057	1.354760
47	1	0	1.407332	-3.059651	0.258936
48	1	0	2.541310	-2.045905	2.172149
49	1	0	4.080585	-2.726012	1.701888
50	1	0	3.897849	-0.964444	1.789916

Conformer (11 <i>S</i> . 12 <i>S</i>)- 5-a						
Center	Center Atomic Atomic Coordinates (Angstroms)					
Number	Number	Type	X	Y	Z	
1	7	0	-5.132756	0.550009	-1.302236	
2	6	0	-4.525131	0.097581	-0.155144	
3	6	0	-5.541406	-0.170801	0.767527	
4	6	0	-6.773581	0.133336	0.141532	
5	6	0	-6.481043	0.578749	-1.145008	
6	6	0	-3.056065	0.003228	-0.153256	
7	6	0	-2.429778	-0.484077	1.090493	
8	8	0	-2.447276	0.334182	-1.175775	
9	6	0	-1.101284	-0.668117	1.349834	
10	6	0	-0.691327	-1 172145	2 713111	
11	6	0	-0.057857	-0 397970	0 361527	
12	6	0	1 268228	-0 538723	0.501527	
12	6	0	2 32/018	-0.229629	-0 1/19920	
1/	6	0	2.324010	-1 //8198	-0.844882	
14	6	0	1 2/6/29	-1 /100556	0.044002	
15	6	0	4.240429	-1.499330	0.303813	
10	6	0		-0.022155	0.015262	
1/	6	0	3.354051	0.705732	0.104627	
18	6	0	3.224210	2.107741	0.120002	
19	6	0	2.009637	2.836256	-0.392871	
20	6	0	4.292261	3.013057	0.691184	
21	6	0	2.487810	-2.753977	-1.094650	
22	8	0	3.88/245	-1.135150	-2.069891	
23	1	0	-4.583/31	0.807822	-2.116056	
24	1	0	-5.407047	-0.544951	1.779945	
25	1	0	-7.768515	0.040909	0.572849	
26	1	0	-7.142030	0.908731	-1.944090	
27	1	0	-3.129756	-0.719643	1.895346	
28	1	0	-1.563419	-1.340711	3.359789	
29	1	0	-0.133903	-2.120428	2.635295	
30	1	0	-0.024913	-0.453052	3.218011	
31	1	0	-0.413708	-0.052536	-0.610709	
32	1	0	1.633220	-0.871714	1.553914	
33	1	0	1.833892	0.136536	-1.363834	
34	1	0	5.130603	-2.087995	0.022703	
35	1	0	3.792271	-1.989086	1.187120	
36	1	0	5.487051	0.296470	0.097564	
37	1	0	4.751309	0.146706	1.688670	
38	1	0	1.235283	2.170552	-0.792756	
39	1	0	2.294498	3.551311	-1.185627	
40	1	0	1.547267	3.437649	0.410331	
41	1	0	4.595857	3.770899	-0.052973	
42	1	0	3.904905	3.575938	1.559898	
43	1	0	5.193724	2.476571	1.015419	
44	1	0	1.967654	-3.105320	-0.191996	
45	1	0	1.745494	-2.626123	-1.897191	
46	1	0	3.204542	-3.526455	-1.413736	
47	1	0	4.214677	-0.226519	-2.016239	
		Conforme	r (11 <i>S</i> , 12 <i>S</i>)- 5 -b			
Center	Atomic	Atomic	Соог	rdinates (Angstro	oms)	
Number	Number	Туре	Х	Y	Z	
1	7	0	-4.740428	-1.239106	-0.324879	

Table S14. DFT Coordinates of the optimized conformers of (11*S*, 12*S*)-**5** at CAM-B3LYP/def2-TZVP theory level.

2	6	0	-4.238505	0.015701	-0.068725
3	6	0	-5.334043	0.865197	0.119525
4	6	0	-6.504479	0.085859	-0.029863
5	6	0	-6.097130	-1.217458	-0.306067
6	6	0	-2.782352	0.188740	-0.058279
7	6	0	-2.263668	1.529531	0.255102
8	8	0	-2.071407	-0.801667	-0.289755
9	6	0	-0.957235	1.910936	0.172266
10	6	0	-0.526992	3.267925	0.664695
11	6	0	0.062142	1.026229	-0.400251
12	6	0	1.313483	0.849172	0.067796
13	6	0	2.173702	-0.277248	-0.419055
14	6	0	1.705840	-1.665352	0.193836
15	6	0	2.931048	-2.541741	-0.101634
16	6	0	4.141464	-1.642867	0.186393
17	6	0	3.678653	-0.229393	-0.171555
18	6	0	4.494202	0.836860	-0.302383
19	6	0	4.043503	2.198895	-0.773826
20	6	0	5.976572	0.755077	-0.021896
21	6	0	1.422006	-1.588053	1.701063
22	8	0	0.587813	-2.182033	-0.486152
23	1	0	-4.124481	-2.026240	-0.501254
24	1	0	-5.288665	1.929980	0.337167
25	1	0	-7.534552	0.427091	0.052331
26	1	0	-6.684382	-2.115648	-0.486894
27	1	0	-2.991419	2.252512	0.630896
28	1	0	-1.364081	3.833278	1.098256
29	1	0	0.256294	3.171281	1.435501
30	1	0	-0.083741	3.858736	-0.154215
31	1	0	-0.270430	0.378186	-1.214884
32	1	0	1.667086	1.414900	0.937205
33	1	0	1.990967	-0.414199	-1.500713
34	1	0	2.889692	-2.813112	-1.168909
35	1	0	2.925771	-3.477391	0.478470
36	1	0	5.030341	-1.950403	-0.385836
37	1	0	4.425550	-1.703917	1.252872
38	1	0	2.992640	2.227055	-1.088944
39	1	0	4.659182	2.523935	-1.631994
40	1	0	4.186452	2.964446	0.010952
41	1	0	6.563008	0.909957	-0.946435
42	1	0	6.286371	-0.202677	0.416359
43	1	0	6.284211	1.556898	0.673160
44	1	0	2.269091	-1.169330	2.267432
45	1	0	1.212811	-2.599505	2.082483
46	1	0	0.539675	-0.961532	1.901580
47	1	0	-0.214915	-1.679018	-0.256030

Compounds	Xanthomonas oryzae RS105	methicillin-resistant Staphylococcus aureus (shhs A1)	Staphylococcus aureus (ATCC 6538)	Bacillus subtilis (ATCC 6633)
2	3.125	6.250	3.125	12.50
3	6.250	12.50	6.250	12.50
4	6.250	6.250	3.125	6.250
Acetone ^a	>50	>50	>50	>50
Kanamycin ^b	0.3906	-	12.50	6.250
Vancomycin ^{<i>b</i>}	_	1.5625	_	_

Table S15. MIC values ($\mu g/mL$) of the active compounds in the antibacterial bioassay.

^{*a*} Negative control; ^{*b*} positive controls



Figure S1. Chemical structures of previously reported pyrrolosesquiterpenes.



Figure S2. Key 2D NMR correlations of compounds 3–5.



Figure S3. View of the pack drawing of strepyrrolin A (1). Hydrogen-bonds are shown as dashed lines.



Figure S4. View of the pack drawing of compound **6**. Hydrogen-bonds are shown as dashed lines.



Figure S5. Calculated and experimental ECD spectra of compounds 1, 3, 4, and 5.



Figure S6. HR-ESI-MS spectrum of compound **3** fed with $[{}^{13}C_5, {}^{15}N]$ -L-Pro. (*m/z* 340.1885 [M + Na]⁺; *m/z* 356.1811 [M + K]⁺)



Figure S7. HR-ESI-MS spectrum (m/z [M + K]⁺) of compound **3** fed with [¹³C₅, ¹⁵N]-L-Glu.






Figure S9. The multiplicity analysis of labeled carbons of compound **3** fed with $[{}^{13}C_5, {}^{15}N]$ -L-Glu. Each pair of coupled carbons was shown in bold bonds. The weak splitting peaks of C-4 were thought to be caused by C-5. The splitting signals of C-5 were not detected because of its long relaxation lifetime, as well as the low involvement of labeled ${}^{13}C$.



Figure S10. ¹H-¹⁵N HMBC (800 MHz, CD₃OD) spectrum of compound **3** fed with [¹³C₅, ¹⁵N]-L-Glu.



Figure S11. HR-ESI-MS spectrum (m/z [M + Na]⁺) of compound **3** fed with ¹³C₂-Gly.



Figure S12. ¹³C NMR (200 MHz, CD₃OD) spectrum of compound **3** fed with ¹³C₂-Gly.



Figure S13. The multiplicity analysis of labeled carbons of compound **3** fed with ${}^{13}C_2$ -Gly. Each pair of coupled carbons was shown in bold bonds.



Figure S14. HR-ESI-MS spectrum (m/z [M + K]⁺) of compound **3** fed with ¹³C₂-sodium acetate.



Figure S15. ¹³C NMR (200 MHz, CD₃OD) spectrum of compound **3** fed with ¹³C₂-sodium acetate.



OH

OH

Figure S16. The multiplicity analysis of labeled carbons of compound **3** fed with ¹³C₂-sodium acetate. Each pair of coupled carbons was shown in bold bonds.



Figure S17. HR-ESI-MS spectrum (m/z [M + K]⁺) of compound **3** fed with ¹³C₆-glucose.



Figure S18. ¹³C NMR (200 MHz, CD₃OD) spectrum of compound **3** fed with ¹³C₆-glucose.









Figure S21. 1,n-ADEQUATE (800 MHz, CD₃OD) spectrum of compound 3 fed with ${}^{13}C_6$ -glucose.



Figure S22. The analyses of labeling pattern of isoprenic units and ${}^{13}C/{}^{13}C$ couplings in terpenoid moiety of **3** after incorporation of ${}^{13}C_6$ -glucose.

(A) Involvement of the oxidative pentose phosphate cycle in glucose breakdown. (B) Labeling patterns of terpene precursors, IPP (isopentenyl diphosphate) and DMAPP (dimethylallyl diphosphate), via MEP (methylerythritol phosphate) pathway.



Figure S23. HR-ESI-MS spectrum of compound **3** fed with $[{}^{13}C_3, {}^{15}N]$ -L-Ala. (*m/z* 340.1921 [M + Na]⁺, *m/z* 356.1861[M + K]⁺)



Figure S24. ¹³C NMR (200 MHz, CD₃OD) spectrum of compound **3** fed with [¹³C₃, ¹⁵N]-L-Ala.



Figure S25. The multiplicity analysis of labeled carbons of compound **3** fed with $[{}^{13}C_3, {}^{15}N]$ -L-Ala. Each pair of principally coupled carbons was shown in bold bonds.



Figure S26. ¹H-¹⁵N HMBC (800 MHz, CD₃OD) spectrum of compound **3** fed with [¹³C₃, ¹⁵N]-L-Ala.



Figure S27. HR-ESI-MS spectrum (m/z [M + K]⁺) of compound **3** fed with ¹³C₃-glycerol.



Figure S28. 13 C NMR (200 MHz, CD₃OD) spectrum of compound 3 fed with $^{13}C_3$ -glycerol.



Figure S29. The multiplicity analysis of labeled carbons of compound **3** fed with ${}^{13}C_{3}$ -glycerol. Each pair of the principally coupled carbons was shown in bold bonds.



14 133 132 131 130 129 128 127 126 125 124 123 122 121 120 119 118 117 116 115 114 113 112 111 110 109 108 107 106 105 104 f1 (ppm)

Figure S30. Selective gradient COSY (200 MHz) spectra targeting C-4 (**A**) and C-3 (**B**) of compound **3** fed with ${}^{13}C_{3}$ -glycerol.



Figure S31. 1,n-ADEQUATE (800 MHz, CD₃OD) spectrum of compound 3 fed with¹³C₃-glycerol.



Figure S32. HR-ESI-MS spectra (m/z [M + Na]⁺) of compound **3** fed with ¹⁵NH₄Cl.



Figure S34. 13 C NMR (125 MHz) spectrum of 1 in CD₃OD.



Figure S35. ¹H-¹H COSY (500 MHz) spectrum of 1 in CD₃OD.



Figure S36. HSQC (500 MHz) spectrum of 1 in CD₃OD.



Figure S37. HMBC (500 MHz) spectrum of 1 in CD₃OD.



Figure S38. ROESY (500 MHz) spectrum of 1 in CD₃OD.

User Spectra



--- End Of Report ---

Figure S39. HR-ESI-MS spectrum of 1.



Figure S40. IR spectrum of 1.



Figure S41. ¹H NMR (600 MHz) spectrum of 2 in CD₃OD.







Figure S43. ¹H-¹H COSY (600 MHz) spectrum of 2 in CD₃OD.



Figure S44. HSQC (600 MHz) spectrum of 2 in CD₃OD.



Figure S46. ROESY (600 MHz) spectrum of 2 in CD₃OD.

User Spectra



--- End Of Report ---

Figure S47. HR-ESI-MS spectrum of 2.



Figure S48. IR spectrum of 2.



Figure S49. ¹H NMR (600 MHz) spectrum of crystals obtained from 2.



Figure S50. ¹³C NMR (150 MHz) spectrum of crystals obtained from 2.



Figure S52. ¹³C NMR (150 MHz) spectrum of **3** in CD₃OD.



Figure S54. HSQC (600 MHz) spectrum of 3 in CD₃OD.



Figure S55. HMBC (600 MHz) spectrum of 3 in CD₃OD.



Figure S56. ROESY (600 MHz) spectrum of 3 in CD₃OD.

Use	r Spe	ctra

Fragmer	tor Vo 135	ltage		Collision E	nergy	Ionization ESI	Mod	e					
x10 5 + Sc	an (0.2	01 min) HWL15-2	27B.d Subtr	act								
1-						340.1882							
0.9-						(MI+INa)+							
0.8-													
0.7-													
0.6-													
0.4-													
0.3-													
0.2													
0.1-													
0 -	33	94	339.6	339.8	340	340.2	340	4 340	6 340.8	5	ц. Ц		
	00	0.1	000.0	000.0	Counts vs	Mass-to-Cha	rge (n	1/z)					
Peak List													
m/z	Z	Abu	nd	Formula		Ion							
282.1855	1	2298	2.51										
300.1958	1	6090	7.53										
318.2062	1	1590	9.82										
340.1882	1	9258	5.27	C19 H27	N O3	(M+	Na)+						
341.1918	1	1821	6.99	C19 H27 I	N O3	(M+	Na)+						
356.1625	1	2752	4.51										
657.3877	1	1288	37.84									ЮH	
658.3909	1	5162	2.02							/		\leftarrow	
Formula Ca	culate	or Ele	ement Lii	nits					~	1			
Element	Min		Мах	-								>	
С		3	60						∭_́́м́н	0			
Н		0	120								ÓH		
0		0	30						Chemica	al Eor	mula: C ₄₀ H	-NO	~
N		0	30						Evo	of Ma		1	3
Formula Ca	culate	or Re	sults						Exa		155. 517.199	· ·	
Formula		Calc	ulatedM	ass	Calculated	Mz	Mz		Diff. (mDa)		Diff. (ppm)		DBE
C19 H27 N O	3			317.1991		340.1883		340.1882		0.1		0.2	7.000

---- End Of Report ----

Figure S57. HR-ESI-MS spectrum of 3.



Figure S58. IR spectrum of 3.



Figure S60. $^{\rm 13}C$ NMR (150 MHz) spectrum of 4 in CD₃OD.



Figure S61. 1 H- 1 H COSY (600 MHz) spectrum of **4** in CD₃OD.



Figure S62. HSQC (600 MHz) spectrum of 4 in CD₃OD.



Figure S63. HMBC (600 MHz) spectrum of 4 in CD₃OD.



Figure S64. ROESY (600 MHz) spectrum of 4 in CD₃OD.

User Spectra



--- End Of Report ---

Figure S65. HR-ESI-MS spectrum of 4.



Figure S66. IR spectrum of 4.





Figure S68. $^{\rm 13}C$ NMR (150 MHz) spectrum of 5 in CD₃OD.



Figure S69. ¹H-¹H COSY (600 MHz) spectrum of 5 in CD₃OD.



Figure S70. HSQC (600 MHz) spectrum of 5 in CD₃OD.



Figure S71. HMBC (600 MHz) spectrum of 5 in CD₃OD.



Figure S72. ROESY (600 MHz) spectrum of 5 in CD₃OD.




--- End Of Report ---

Figure S73. HR-ESI-MS spectrum of 5.



Figure S74. IR spectrum of 5.