SUPPORTING INFORMATION

New butenolides and cyclopentenones from saline soil-derived fungus *Aspergillus sclerotiorum*

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Figure S2. ¹³C NMR spectrum (100 MHz) of 1 in DMSO- d_6 .



Figure S4. IR spectrum of 1.



Figure S5. UV spectrum of 1 in MeOH.



Figure S6. HRESIMS of 1.







DEPT135

Figure S10. HSQC spectrum of 2 in MeOH-d4.



Figure S12. IR spectrum of 2.







Figure S14. HRESIMS of 2.



Figure S16. ¹³C NMR spectrum (100 MHz) of **3** in acetone- d_6 .







Figure S19. UV spectrum of 3 in MeOH.



Figure S20. HRESIMS of 3.



Figure S22. ¹³C NMR spectrum (100 MHz) of 4 in acetone- d_6 .



Figure S24. HSQC spectrum of 4 in acetone-*d*₆.



Figure S26. HMBC spectrum of 4 in acetone-*d*₆.



Figure S28. UV spectrum of 4 in MeOH.



Figure S29. HRESIMS of 4.



Figure S30. ¹H NMR spectrum (400 MHz) of 5 in MeOH-d4.



Figure S31. ¹³C NMR spectrum (100 MHz) of 5 in MeOH-d₄.



Figure S32. HMBC spectrum of 5 in MeOH- d_4 .



Figure S33. NOE difference spectrum of 5 in MeOH-*d*₄.





Figure S35. UV spectrum of 5 in MeOH.



Figure S36. HRESIMS of 5.



Figure S38. ¹³C NMR spectrum (100 MHz) of 6 in DMSO-*d*₄.







Figure S42. ¹H NMR spectrum (400 MHz) of 6 in acetone-*d*₆.



Figure S44. ¹³C NMR spectrum (100 MHz) of 6 in MeOH-d₄.



Figure S46. HRESIMS of 6.



Figure S48. ¹³C NMR spectrum (100 MHz) of 6c in DMSO-d₆.



Figure S49. HMBC spectrum of 6c in DMSO-*d*₆.



Figure S50. HRESIMS of 6c.



Figure S52. ¹³C NMR spectrum (100 MHz) of 6d in DMSO- d_6 .







Figure S54. HRESIMS of 6d.

Attachment S1. Supporting information for the calculated ECD spectra of compounds 4, 5, and 6c.

1. Computational methods

1.1 Conformational analysis

Conformational analysis was initially performed using Confab [1] with systematic search at MMFF94 force field for undetermined relative configurations of compounds **4**, **5**, and **6c** (**Figure AS1**). Room-temperature equilibrium populations were calculated according to Boltzmann distribution law (1) and those with populations lower than 1% were filtered. The energies and populations of dominative conformers were provided in **Table AS1**.



Figure AS1. Chemical structure of all undetermined relative configurations of compounds 4, 5, and 6c.

$$\frac{N_{i}}{N} = \frac{g_{i}e^{-\frac{E_{i}}{k_{\rm B}T}}}{\sum g_{i}e^{-\frac{E_{i}}{k_{\rm B}T}}}$$
(1)

Where N_i is the number of conformer i with energy E_i and degeneracy g_i at temperature T, and k_B is Boltzmann constant.

1.2 ECD calculation

The theoretical calculations were carried out using Gaussian 09 [2]. At first, conformers were optimized at PM6 using semi-empirical theory method and again filtered by Boltzmann-based populations. The remaining structures were finally optimized at B3LYP/6-311G(d,p) in methanol using the IEFPCM model (**Error! Reference source not found.**). Vibrational frequency analysis confirmed the stable structures. Based on the optimized structures, the ECD calculation was conducted using Time-dependent Density functional theory (TD-DFT) in methanol at B3LYP/6-311G(d,p) for compounds **5** and **6c**, and at BP86/6-311G(d,p) for compound **4**. Rotatory strengths for a total of 30 excited states were calculated. The ECD spectrum was simulated in SpecDis [3] by overlapping Gaussian functions for each transition according to (2).

$$\Delta \varepsilon(E) = \frac{1}{2.297 \times 10^{-39}} \times \frac{1}{\sqrt{2\pi\sigma}} \sum_{i}^{A} \Delta E_{i} R_{i} e^{-\left(\frac{E-E_{i}}{2\sigma}\right)^{2}}$$
(2)

Where σ represents the width of the band at 1/e height, and ΔE_i and R_i are the excitation energies and rotatory strengths for transition *i*, respectively.

The σ values were 0.25 eV, 0.30 eV, and 0.32 eV for compounds 4, 5, and 6c and the UV-shift values were set -5 nm, 27 nm, and 4

1.3 References

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- 4. Lodewyk, M.W.; Siebert M.R.; Tantillo, D.J. Computational prediction of ¹H and ¹³C chemical shifts: a useful tool for natural product, mechanistic, and synthetic organic chemistry. *Chem. Rev.* **2012**, *112* (3), 1839–1862.

2. Energies and Coordinates

2.1 Energies at MMFF94 force field

Systematic conformational search was performed by Confab program at MMFF94 force field. Conformers for each configuration were obtained with filtration by RMSD threshold of 0.5 Å.

Configuration	Conformer	Energy (kcal/mol)	Population (%)
4 a	1	4.64	85.29
4 a	2	5.69	14.71
4 b	1	4.65	85.27
4 b	2	5.69	14.73
4 c	1	5.82	20.41
4 c	2	5.02	79.59
4d	1	5.82	20.43
4d	2	5.02	79.57
5a	1	7.11	99.78
5b	1	7.38	99.65
бса	1	-39.54	25.50
бса	2	-39.40	19.89
бса	3	-38.76	6.77
бса	4	-38.64	5.50
бса	5	-38.57	4.96
бса	6	-38.54	4.67
бса	7	-38.36	3.48
бса	8	-38.35	3.38
бса	9	-38.07	2.14
бса	10	-38.00	1.89
6са	11	-37.88	1.55
бса	12	-37.87	1.52
бса	13	-37.85	1.45
6са	14	-37.78	1.30
6са	15	-37.70	1.13
6са	16	-37.68	1.11
6са	17	-37.62	1.00
6cb	1	-39.51	19.18
6cb	2	-39.42	16.57
6cb	3	-39.40	16.04
6cb	4	-38.94	7.32
6cb	5	-38.84	6.25
6cb	6	-38.54	3.77
6cb	7	-38.42	3.09
6cb	8	-38.27	2.38
6cb	9	-38.26	2.33
6cb	10	-38.23	2.22
6cb	11	-38.10	1.80

Table AS1 Energies of compounds 4, 5, and 6c at MMFF94 force field.

6cb	12	-38.10	1.79
6cb	13	-37.89	1.24
6cb	14	-37.81	1.09
6cb	15	-37.80	1.07
6cb	16	-37.78	1.04

2.2 Energies at B3LYP theory level

Structures for ECD calculations were optimized at B3LYP/6-311G(d,p) in methanol.

Configuration	Conformer	Structure	E (Hartree)	E(kcal/mol)	Population (%)
4a	1		-957.58341493	-600892.66	100
4b	1	ی دی دی می دی می می دی می می دی دی دی دی دی دی دی دی دی دی دی دی دی	-957.58341493	-600892.66	100
4c	1		-957.58521469	-600893.79	100
4d	1	993 9999 9999999 9999999 999999 99999 99999	-957.58521469	-600893.79	100
5a	1	ა€3-0 ⁶ 3 ● 40-0 3-93 - 3 - 93 - 3	-498.54159321	-312839.57	100.00
5b	1		-498.54159322	-312839.57	100.00
бса	1	39 93 30 30 30 30 30 30 30 30 30 30 30 30 30	-993.76209792	-623595.13	34.12

бса	2	ిస్తో సంద్రాహని సర్పరించించింది సినియా సినియా	-993.76271899	-623595.52	65.88
6cb	1	ب رائی من م من م	-993.76209795	-623595.13	26.77
6cb	2	3 ⁴ 9 3 9 9 3 9	-993.76271900	-623595.52	51.68
6cb	4		-993.76189351	-623595.00	21.56

2.3 Coordinates at B3LYP theory level

Conformer 4a-1					
Center Atomic Atomic Coordinates (Angstroms)	Coordinates (Angstroms)				
Number Number Type X Y	Z				
1 6 0 -3.198983 -1.382865 -0.4	85884				
2 6 0 -3.663771 -0.204543 0.10	2471				
3 1 0 -4.719843 -0.118868 0.32	7582				
4 6 0 -2.784830 0.835834 0.38	9039				
5 6 0 -1.413206 0.711997 0.08	8582				
6 6 0 -0.974777 -0.482505 -0.48	85908				
7 6 0 -1.849646 -1.529082 -0.7	79880				
8 1 0 -1.452390 -2.431448 -1.23	31466				
9 6 0 -0.412981 1.804994 0.38	4467				
10 1 0 -0.847524 2.786885 0.17	7235				
11 1 0 -0.157715 1.798126 1.44	9312				
12 6 0 0.860096 1.653360 -0.4	57591				
13 1 0 1.658856 2.262785 -0.02	32818				
14 6 0 1.349237 0.196077 -0.4	19546				
15 8 0 0.339036 -0.720134 -0.82	28739				
16 6 0 -3.313284 2.100190 1.02	4158				
17 1 0 -4.379299 2.011810 1.23	7656				
18 1 0 -3.175301 2.967063 0.36	59234				
19 1 0 -2.799029 2.325046 1.96	3928				
20 8 0 -4.117915 -2.360834 -0.74	44581				
21 1 0 -3.675777 -3.107007 -1.10	52251				
22 6 0 0.632725 2.107836 -1.9	17807				
23 1 0 1.531992 1.970813 -2.5	17219				
24 1 0 0.363482 3.167141 -1.92	29187				
25 1 0 -0.179164 1.548539 -2.33	87520				
26 8 0 2.419544 0.013917 -1.32	29078				
27 6 0 3.533670 -0.524353 -0.68	88892				
28 6 0 3.204189 -0.694855 0.72	9624				
29 1 0 3.902617 -1.111870 1.43	6243				
30 6 0 1.943386 -0.274424 0.90	9414				
31 8 0 4.542948 -0.756550 -1.23	35403				
32 8 0 1.160945 -0.241495 1.98	1948				
33 6 0 1.704522 -0.784525 3.19	3207				
34 1 0 2.585507 -0.216059 3.50	3501				
35 1 0 1.969462 -1.835179 3.04	9638				
36 1 0 0.919585 -0.695817 3.94	0223				
Conformer 4b-1					
Center Atomic Atomic Coordinates (Angstroms))				
Number Number Type X Y	Z				
1 6 0 3.198983 -1.382865 -0.4	85884				
	2471				
2 6 0 3.663771 -0.204543 0.10					

4	6	0	2.784830	0.835834	0.389039
5	6	0	1.413206	0.711997	0.088582
6	6	0	0.974777	-0.482505	-0.485908
7	6	0	1.849646	-1.529082	-0.779880
8	1	0	1.452390	-2.431448	-1.231466
9	6	0	0.412981	1.804994	0.384467
10	1	0	0.847524	2.786885	0.177235
11	1	0	0.157715	1.798126	1.449312
12	6	0	-0.860096	1.653360	-0.467591
13	1	0	-1.658856	2.262785	-0.032818
14	6	0	-1.349237	0.196077	-0.419546
15	8	0	-0.339036	-0.720134	-0.828739
16	6	0	3.313284	2.100190	1.024158
17	1	0	4 379299	2.011810	1 237656
18	1	ů 0	3 175301	2.011010	0.369234
19	1	0	2 799029	2.307003	1 963928
20	8	0	A 117015	2.525040	0.744581
20	0	0	4.117913	2.300834	-0.744501
21	1	0	0.622725	-3.107007	-1.102231
22	0	0	-0.052725	2.10/000	-1.91/80/
25	1	0	-1.331992	2.167141	-2.31/219
24	1	0	-0.303482	5.10/141	-1.92918/
25	1	0	0.1/9164	1.548539	-2.38/520
26	8	0	-2.419544	0.013917	-1.329078
27	6	0	-3.533670	-0.524353	-0.688892
28	6	0	-3.204189	-0.694855	0.729624
29	I	0	-3.902617	-1.1118/0	1.436243
30	6	0	-1.943386	-0.274424	0.909414
31	8	0	-4.542948	-0.756550	-1.285403
32	8	0	-1.160945	-0.241495	1.981948
33	6	0	-1.704522	-0.784525	3.193207
34	1	0	-2.585507	-0.216059	3.503501
35	1	0	-1.969462	-1.835179	3.049638
36	1	0	-0.919585	-0.695817	3.940223
Со	onformer 4c	:-1			
Center	Atomic	Atomic	Coord	inates (Angs	troms)
Number	Number	Туре	Х	Y	Ζ
1	6	0	3.265586	1.443720	0.484805
2	6	0	3.800685	0.193387	0.166987
3	1	0	4.876182	0.043619	0.201840
4	6	0	2.969017	-0.867682	-0.191647
5	6	0	1.575815	-0.684968	-0.240563
6	6	0	1.070829	0.574152	0.100748
7	6	0	1.891031	1.639097	0.455564
8	1	0	1.459846	2.597073	0.712844
9	6	0	0.620543	-1.795420	-0.616880
10	1	0	1.039980	-2.406928	-1.420446
11	1	0	0.464001	-2.458847	0.239795
12	6	0	-0.737179	-1.234827	-1.082395
13	1	0	-1.474711	-2.042606	-1.069942
15					

	14	6	0	-1.184319	-0.215142	-0.018556
	15	8	0	-0.282784	0.861072	0.086871
	16	6	0	3.577168	-2.210311	-0.520979
	17	1	0	3.175715	-3.000657	0.120733
	18	1	0	4.660210	-2.191179	-0.390138
	19	1	0	3.372475	-2.503651	-1.556054
	20	8	0	4.046335	2.508617	0.837802
	21	1	0	4.968779	2.233863	0.839019
	22	6	0	-0.656339	-0.646350	-2.497873
	23	1	0	0.065226	0.171356	-2.550582
	24	1	0	-1.619195	-0.265201	-2.836648
	25	1	0	-0.333526	-1.424986	-3.194087
	26	8	0	-1.268948	-0.905844	1.236987
	27	6	0	-2.527657	-0.747376	1.800468
	28	6	0	-3.335115	0.070853	0.888363
	29	1	0	-4.353681	0.342235	1.111333
	30	6	0	-2.571989	0.397593	-0.165128
	31	8	0	-2.814199	-1.243721	2.850455
	32	8	0	-2.809504	1 148661	-1 233828
	33	6	0	-4 097508	1 774553	-1 302458
	34	1	0	-4 888395	1 019858	-1 332901
	35	1	0	-4 099731	2 355202	-2 221694
	36	1	0	-4 243783	2.333202	-0.442117
	C	nformer 4	I_ 1	1.213703	2.132901	0.112117
	00					
	Center	Atomic	Atomic	Coord	inates (Angs	troms)
	Center Number	Atomic Number	Atomic Type	Coord X	inates (Angs Y	troms) Z
	Center Number	Atomic Number	Atomic Type 0	Coord X -3.265586	inates (Angs Y 1.443720	troms) Z 0.484805
	Center Number 1 2	Atomic Number 6	Atomic Type 0 0	Coord X -3.265586 -3.800685	inates (Angs Y 1.443720 0.193387	troms) Z 0.484805 0.166987
	Center Number 1 2 3	Atomic Number 6 6	Atomic Type 0 0	Coord X -3.265586 -3.800685 -4 876182	inates (Angs Y 1.443720 0.193387 0.043619	troms) Z 0.484805 0.166987 0 201840
	Center Number 1 2 3 4	Atomic Number 6 6 1 6	Atomic Type 0 0 0 0	Coord X -3.265586 -3.800685 -4.876182 -2.969017	inates (Angs Y 1.443720 0.193387 0.043619 -0.867682	troms) Z 0.484805 0.166987 0.201840 -0.191647
	Center Number 1 2 3 4 5	Atomic Number 6 6 1 6 6	Atomic Type 0 0 0 0 0	Coord X -3.265586 -3.800685 -4.876182 -2.969017 -1.575815	inates (Angs Y 1.443720 0.193387 0.043619 -0.867682 -0.684968	troms) Z 0.484805 0.166987 0.201840 -0.191647 -0.240563
	Center Number 1 2 3 4 5 6	Atomic Number 6 6 1 6 6 6 6	Atomic Type 0 0 0 0 0 0 0	Coord X -3.265586 -3.800685 -4.876182 -2.969017 -1.575815 -1.070829	inates (Angs Y 1.443720 0.193387 0.043619 -0.867682 -0.684968 0 574152	troms) Z 0.484805 0.166987 0.201840 -0.191647 -0.240563 0 100748
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	Center Number 1 2 3 4 5 6 7 8 9	Atomic Number 6 6 1 6 6 6 6 1 6	Atomic Type 0 0 0 0 0 0 0 0 0 0 0	Coord X -3.265586 -3.800685 -4.876182 -2.969017 -1.575815 -1.070829 -1.891031 -1.459846 -0.620543	inates (Angs <u>Y</u> 1.443720 0.193387 0.043619 -0.867682 -0.684968 0.574152 1.639097 2.597073 -1.795420	troms) Z 0.484805 0.166987 0.201840 -0.191647 -0.240563 0.100748 0.455564 0.712844 -0.616880
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	Center Number 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17	Atomic Number 6 6 1 6 6 6 1 6 1 1 6 1 1 6 1 6 8 6 1	Atomic Type 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Coord X -3.265586 -3.800685 -4.876182 -2.969017 -1.575815 -1.070829 -1.891031 -1.459846 -0.620543 -1.039980 -0.464001 0.737179 1.474711 1.184319 0.282784 -3.577168 3 175715	inates (Angs Y 1.443720 0.193387 0.043619 -0.867682 -0.684968 0.574152 1.639097 2.597073 -1.795420 -2.406928 -2.458847 -1.234827 -2.042606 -0.215142 0.861072 -2.210311 3.000657	troms) Z 0.484805 0.166987 0.201840 -0.191647 -0.240563 0.100748 0.455564 0.712844 -0.616880 -1.420446 0.239795 -1.082395 -1.069942 -0.018556 0.086871 -0.520979 0.120723
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	Center Number 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18	Atomic Number 6 6 1 6 6 6 1 6 1 1 6 1 1 6 1 6 1 6 1	Atomic Type 0 0 0 0 0 0 0 0 0 0 0 0 0	Coord X -3.265586 -3.800685 -4.876182 -2.969017 -1.575815 -1.070829 -1.891031 -1.459846 -0.620543 -1.039980 -0.464001 0.737179 1.474711 1.184319 0.282784 -3.577168 -3.175715 -4.660210 2.272475	inates (Angs Y 1.443720 0.193387 0.043619 -0.867682 -0.684968 0.574152 1.639097 2.597073 -1.795420 -2.406928 -2.458847 -1.234827 -2.042606 -0.215142 0.861072 -2.210311 -3.000657 -2.191179 2.502651	troms) Z 0.484805 0.166987 0.201840 -0.191647 -0.240563 0.100748 0.455564 0.712844 -0.616880 -1.420446 0.239795 -1.082395 -1.069942 -0.018556 0.086871 -0.520979 0.120733 -0.390138
	Center Number 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20	Atomic Number 6 6 1 6 6 6 1 6 1 1 6 1 1 6 1 6 1 6 8 6 1 1 6 8 6 1 1 1 7 8	Atomic Type 0 0 0 0 0 0 0 0 0 0 0 0 0	Coord X -3.265586 -3.800685 -4.876182 -2.969017 -1.575815 -1.070829 -1.891031 -1.459846 -0.620543 -1.039980 -0.464001 0.737179 1.474711 1.184319 0.282784 -3.577168 -3.175715 -4.660210 -3.372475 4.046225	inates (Angs Y 1.443720 0.193387 0.043619 -0.867682 -0.684968 0.574152 1.639097 2.597073 -1.795420 -2.406928 -2.458847 -1.234827 -2.042606 -0.215142 0.861072 -2.210311 -3.000657 -2.191179 -2.503651 2.508(17)	troms) Z 0.484805 0.166987 0.201840 -0.191647 -0.240563 0.100748 0.455564 0.712844 -0.616880 -1.420446 0.239795 -1.082395 -1.069942 -0.018556 0.086871 -0.520979 0.120733 -0.390138 -1.556054 0.827802
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	Center Number 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22	Atomic Number 6 6 1 6 6 6 6 1 6 1 1 6 1 1 6 1 6 8 6 1 1 6 8 6 1 1 1 8 1 1 8 1	Atomic Type 0 0 0 0 0 0 0 0 0 0 0 0 0	Coord X -3.265586 -3.800685 -4.876182 -2.969017 -1.575815 -1.070829 -1.891031 -1.459846 -0.620543 -1.039980 -0.464001 0.737179 1.474711 1.184319 0.282784 -3.577168 -3.175715 -4.660210 -3.372475 -4.046335 -4.968779 0.656220	inates (Angs Y 1.443720 0.193387 0.043619 -0.867682 -0.684968 0.574152 1.639097 2.597073 -1.795420 -2.406928 -2.458847 -1.234827 -2.042606 -0.215142 0.861072 -2.210311 -3.000657 -2.191179 -2.503651 2.508617 2.233863 0.646255	troms) Z 0.484805 0.166987 0.201840 -0.191647 -0.240563 0.100748 0.455564 0.712844 -0.616880 -1.420446 0.239795 -1.082395 -1.069942 -0.018556 0.086871 -0.520979 0.120733 -0.390138 -1.556054 0.837802 0.839019 2.407072
	Center Number 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 22	Atomic Number 6 6 1 6 6 6 1 6 1 1 6 1 1 6 1 1 6 1 1 6 1 1 6 1 1 6 1 1 1 8 1 1 1 8 1 1 6	Atomic Type 0 0 0 0 0 0 0 0 0 0 0 0 0	Coord X -3.265586 -3.800685 -4.876182 -2.969017 -1.575815 -1.070829 -1.891031 -1.459846 -0.620543 -1.039980 -0.464001 0.737179 1.474711 1.184319 0.282784 -3.577168 -3.175715 -4.660210 -3.372475 -4.046335 -4.968779 0.656339	inates (Angs Y 1.443720 0.193387 0.043619 -0.867682 -0.684968 0.574152 1.639097 2.597073 -1.795420 -2.406928 -2.458847 -1.234827 -2.042606 -0.215142 0.861072 -2.210311 -3.000657 -2.191179 -2.503651 2.508617 2.233863 -0.646350 0.171255	troms) Z 0.484805 0.166987 0.201840 -0.191647 -0.240563 0.100748 0.455564 0.712844 -0.616880 -1.420446 0.239795 -1.082395 -1.069942 -0.018556 0.086871 -0.520979 0.120733 -0.390138 -1.556054 0.837802 0.839019 -2.497873 2 550502

25100.333526-1.424986-3.19408726801.268948-0.9058441.23698727602.527657-0.7473761.80046828603.3351150.0708530.88836329104.3536810.3422351.11133330602.5719890.397593-0.16512831802.8095041.148661-1.23382833604.0975081.774553-1.30245834104.8883951.019858-1.33290135104.097312.355202-2.2169436104.2437832.432901-0.442171Conterrer 5aVXYZ160-0.1230801.0616510.195321210-0.1706611.4177571.2360103600.907717-0.0447640.1072974600.371808-1.266847-0.0864095100.87829-2.221017-0.14212060-1.430700.369498-0.210449810-1.6018880.639034-1.2595239800.1618942.148097-0.671101010-2.26663820.7152020.6128711160-2.5107470.5043511.675250131<	24	1	0	1.619195	-0.265201	-2.836648
26801.268948-0.9058441.23697727602.527657-0.7473761.80046828603.3351150.0708530.88836329104.3536810.3422351.11133330602.5719890.397593-0.16512831802.8095041.148661-1.23382833604.0975081.774553-1.30245834104.8883951.019858-1.33290135104.0997312.355202-2.22169436104.2437832.432901-0.4421177510-0.1230801.0616510.195321210-0.1230801.0616510.195321210-0.1706611.4177571.2360103600.907717-0.0447640.1072974600.371808-1.266847-0.0864095100.878289-2.211017-0.142120660-1.4302700.369498-0.210449810-1.6018880.639034-1.2595239800.1618942.148097-0.6761101010-2.216631.7717820.5092901580-2.5107470.5043511.6752501680-1.899951-2.031033-0.2842611	25	1	0	0.333526	-1.424986	-3.194087
27602.527657 -0.747376 1.8004682860 3.335115 0.070853 0.888363 2910 4.353681 0.342235 1.111333 3060 2.571989 0.397593 -0.165128 3180 2.814199 -1.243721 2.850455 3280 2.809504 1.148661 -1.233828 3360 4.097508 1.774553 -1.302458 3410 4.888395 1.019858 -1.323901 3510 4.097508 1.774553 -1.302458 3410 4.888395 1.019858 -1.323901 3610 4.243783 2.432901 -0.442117 3610 4.243783 2.432901 -0.442117 3610 -0.123080 1.061651 0.195321 210 -0.123080 1.061651 0.195321 210 0.907717 -0.044764 0.107297 460 0.371808 -1.266847 -0.086409 510 0.878289 -2.21017 -0.142120 660 -1.601888 0.639034 -1.259523 980 0.161894 2.148097 -0.676110 1010 -2.2510747 0.504351 1.675250 1310 -2.510747 0.504351 1.67525	26	8	0	1.268948	-0.905844	1.236987
28603.3351150.0708530.88836329104.3536810.3422351.11133330602.5719890.397593-0.16512831802.8095041.148661-1.23382833604.0975081.774553-1.30245834104.8883951.019858-1.32390135104.0997312.355202-2.2169436104.2437832.432901-0.442177Center Atomic Atomic Coortinets (Angstrome StateNumber TypeXYZ160-0.1730801.0616510.195321210-0.1706611.4177571.2360103600.907717-0.0447640.1072974600.371808-1.266847-0.0864095100.878289-2.21017-0.14210660-1.6018880.639034-1.2595239800.1618942.148097-0.6761101010-2.5107470.5043511.6752501310-2.5107470.5043511.675250140-2.9256631.7717820.5092901580-1.89951-2.031033-0.2784291680-1.895250.434440.2604319103.18723-0.659095<	27	6	0	2.527657	-0.747376	1.800468
29104.3536810.3422351.11133330602.5719890.397593-0.16512831802.804199-1.2437212.85045532802.8095041.148661-1.23382833604.0975081.774553-1.30245834104.8883951.019858-1.33290135104.0997312.355202-2.2169436104.2437832.432901-0.442177Center SalAtomicCoordinates (Angstroms)NumberTypeXYZ160-0.1230801.0616510.195321210-0.1706611.417571.2360103600.907717-0.0447640.1072974600.371808-1.266847-0.0864095100.878289-2.21017-0.142120660-1.086779-1.135183-0.200705760-1.4302700.369498-0.210449810-1.6018880.639034-1.2595239800.1618942.148097-0.6761101010-2.5107470.5043511.6752501310-2.5107470.5043511.6752501410-2.9256631.7717820.5092901580-1.89951-2.0	28	6	0	3.335115	0.070853	0.888363
30602.5719890.397593-0.16512831802.814199-1.2437212.85045532802.8095041.148661-1.23382833604.0975081.774553-1.30245834104.8883951.019858-1.33290135104.0997312.355202-2.2164936104.2437832.432901-0.442117Conterrersa-VamberTypeXYZ160-0.1230801.0616510.195321210-0.1706611.4177571.2360103600.907717-0.0447640.1072974600.371808-1.266847-0.0864095100.878289-2.211017-0.142120660-1.086779-1.135183-0.20705760-1.6018880.639034-1.2595239801.618942.148097-0.6761101010-2.6668820.7152020.6128711160-2.816631.157650.2801711210-2.926631.717820.5092901580-1.89951-2.031033-0.2784921680-1.89951-2.031033-0.27849217603.188723-0.659050.145846 <td>29</td> <td>1</td> <td>0</td> <td>4.353681</td> <td>0.342235</td> <td>1.111333</td>	29	1	0	4.353681	0.342235	1.111333
31802.814199-1.2437212.85045532802.8095041.148661-1.23382833604.0975081.774553-1.30245834104.8883951.019858-1.33290135104.2437832.432901-0.442117Center Sa-TypeXYZ160-0.1230801.0616510.195321210-0.1706611.4177571.2360103600.907717-0.0447640.1072974600.371808-1.266847-0.0864095100.878289-2.221017-0.142120660-1.4302700.369498-0.210449810-1.6018880.639034-1.2595239800.1618942.148097-0.6761101010-2.2666820.7152020.6128711160-2.5107470.5043511.6752501310-2.5107470.5043511.6752501580-1.89951-2.031033-0.27849215802.1764040.3470550.2522561680-1.89951-0.31133-0.207849217603.188723-0.6590950.14584618103.141031-1.145590-0.813160<	30	6	0	2.571989	0.397593	-0.165128
32802.8095041.148661-1.23382833604.0975081.774553-1.30245834104.8883951.019858-1.33290135104.2437832.432901-0.44211736104.2437832.432901-0.442117Verture Satter Sa	31	8	0	2.814199	-1.243721	2.850455
33604.0975081.774553-1.30245834104.8883951.019858-1.33290135104.2437832.432901-0.44211736104.2437832.432901-0.442117Contruer 5a-1VumberNumberTypeXYZ160-0.1230801.0616510.195321210-0.1706611.4177571.2360103600.907717-0.0447640.1072974600.371808-1.266847-0.0864095100.878289-2.21017-0.142120660-1.086779-1.135183-0.200705760-1.4302700.369498-0.210449810-1.6018880.639034-1.2595239800.1618942.148097-0.6761101010-2.2666820.7152020.6128711210-2.2925631.7717820.50929015802.1764040.3470550.2522561680-1.899951-2.031033-0.27849217603.18723-0.6590950.14584618103.141031-1.14590-0.83136020103.07091-1.4045240.93653915800.1230801.061651<	32	8	0	2.809504	1.148661	-1.233828
34104.883951.019858-1.33290135104.0997312.355202-2.22169436104.2437832.432901-0.442117Conter sature	33	6	0	4.097508	1.774553	-1.302458
35104.0997312.355202-2.22169436104.2437832.432901-0.442117Center Sa-INumberNumberTypeXYZ160-0.1230801.0616510.195321210-0.1706611.4177571.2360103600.907717-0.0447640.1072974600.371808-1.266847-0.0864095100.878289-2.21017-0.142120660-1.4302700.369498-0.210449810-1.6018880.639034-1.2595239800.1618942.148097-0.67611010102.26668820.7152020.6128711210-2.25107470.5043511.6752501310-3.5158660.1157650.28017114102.9256631.7717820.5092901580-1.89951-2.031033-0.27849217603.18723-0.6590950.14584618103.141031-1.45990-0.83136020103.070991-1.4045240.9365391580-1.230801.0616510.1953212100.1706611.4177571.2360103600.1230801.0616510.195321 </td <td>34</td> <td>1</td> <td>0</td> <td>4.888395</td> <td>1.019858</td> <td>-1.332901</td>	34	1	0	4.888395	1.019858	-1.332901
36 1 0 4.243783 2.432901 -0.442117 Center Atomic Atomic Coordinates (Angstroms) Number Number Type X Y Z 1 6 0 -0.123080 1.061651 0.195321 2 1 0 -0.170661 1.417757 1.236010 3 6 0 0.907717 -0.044764 0.107297 4 6 0 0.371808 -1.266847 -0.086409 5 1 0 0.878289 -2.21017 -0.142120 6 6 0 -1.430270 0.369498 -0.210449 8 1 0 -1.601888 0.639034 -1.259523 9 8 0 0.161894 2.148097 -0.676110 10 1 0 -2.2510747 0.504351 1.675250 13 1 0 -2.510747 0.504351 1.675250 14 1	35	1	0	4.099731	2.355202	-2.221694
Conformer Sa-1 Center Atomic Atomic Coordinates (Angstroms) Number Number Type X Y Z 1 6 0 -0.123080 1.061651 0.195321 2 1 0 -0.170661 1.417757 1.236010 3 6 0 0.907717 -0.044764 0.107297 4 6 0 0.371808 -1.266847 -0.086409 5 1 0 0.878289 -2.221017 -0.142120 6 6 0 -1.430270 0.369498 -0.210449 8 1 0 -1.601888 0.639034 -1.259523 9 8 0 0.161894 2.148097 -0.676110 10 1 0 -2.2510747 0.504351 1.675250 13 1 0 -2.2510747 0.504351 1.675250 15 8 0 2.176404 0.347055 0.252256	36	1	0	4.243783	2.432901	-0.442117
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810-1.6018880.639034-1.2595239800.1618942.148097-0.67611010101.0207662.511057-0.4281611160-2.6668820.7152020.6128711210-2.5107470.5043511.6752501310-3.5158660.1157650.2801711410-2.9256631.7717820.50929015802.1764040.3470550.2522561680-1.899951-2.031033-0.27849217603.188723-0.6590950.14584618104.139550-0.1439440.26004319103.070991-1.4045240.936539Conformer 5b-1CenterAtomicCoordinates (Angstroms)NumberNumberTypeXYZ160-0.1230801.0616510.1953212100.1706611.4177571.236010360-0.907717-0.0447640.107297460-0.371808-1.266847-0.086409510-0.878289-2.21017-0.1421206601.086779-1.135183-0.200705	7	6	0	-1.430270	0.369498	-0.210449
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13 1 0 5.01000 0.110100 0.200111 14 1 0 -2.925663 1.771782 0.509290 15 8 0 2.176404 0.347055 0.252256 16 8 0 -1.899951 -2.031033 -0.278492 17 6 0 3.188723 -0.659095 0.145846 18 1 0 4.139550 -0.143944 0.260043 19 1 0 3.141031 -1.145990 -0.831360 20 1 0 3.070991 -1.404524 0.936539 Conformer 5b -1 1 6 0 0.123080 1.061651 0.195321 2 1 0 0.170661 1.417757 1.236010 3 6 0 -0.371808 -1.266847 -0.086409 5 1 0 -0.87	13	1	0	-3 515866	0.115765	0.280171
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10001.077512.051035 0.270172 1760 3.188723 -0.659095 0.145846 1810 4.139550 -0.143944 0.260043 1910 3.141031 -1.145990 -0.831360 2010 3.070991 -1.404524 0.936539 Conformer 5b -1Center Atomic Atomic Coordinates (Angstroms)NumberNumberTypeXYZ160 0.123080 1.061651 0.195321 210 0.170661 1.417757 1.236010 360 -0.907717 -0.044764 0.107297 460 -0.371808 -1.266847 -0.086409 510 -0.878289 -2.221017 -0.142120 660 1.086779 -1.135183 -0.200705	15	8	0	-1 899951	-2 031033	-0 278492
11 0 0 0.130723 0.03703 0.143040 18 1 0 4.139550 -0.143944 0.260043 19 1 0 3.141031 -1.145990 -0.831360 20 1 0 3.070991 -1.404524 0.936539 Conformer 5b -1 Center Atomic Atomic Coordinates (Angstroms) Number Type X Y Z 1 6 0 0.123080 1.061651 0.195321 2 1 0 0.170661 1.417757 1.236010 3 6 0 -0.371808 -1.266847 -0.086409 5 1 0 -0.878289 -2.221017 -0.142120 6 6 0 1.086779 -1.135183 -0.200705	17	6	0	3 188723	-0.659095	0.145846
10 1 0 4.133300 -0.143344 0.200043 19 1 0 3.141031 -1.145990 -0.831360 20 1 0 3.070991 -1.404524 0.936539 Conformer 5b-1 Conformer 5b-1 Center Atomic Atomic Coordinates (Angstroms) Number Number Type X Y Z 1 6 0 0.123080 1.061651 0.195321 2 1 0 0.170661 1.417757 1.236010 3 6 0 -0.371808 -1.266847 -0.086409 5 1 0 -0.878289 -2.221017 -0.142120 6 6 0 1.086779 -1.135183 -0.200705	18	1	0	A 139550	-0.037073	0.145040
10 1 0 3.141031 41.143330 40.031300 20 1 0 3.070991 -1.404524 0.936539 Conformer 5b -1 Center Atomic Atomic Coordinates (Angstroms) Number Number Type X Y Z 1 6 0 0.123080 1.061651 0.195321 2 1 0 0.170661 1.417757 1.236010 3 6 0 -0.907717 -0.044764 0.107297 4 6 0 -0.371808 -1.266847 -0.086409 5 1 0 -0.878289 -2.221017 -0.142120 6 6 0 1.086779 -1.135183 -0.200705	10	1	0	3 1/1031	-0.145990	-0.831360
Conformer 5b-1 Coordinates (Angstroms) Number Number Type X Y Z 1 6 0 0.123080 1.061651 0.195321 2 1 0 0.170661 1.417757 1.236010 3 6 0 -0.907717 -0.044764 0.107297 4 6 0 -0.371808 -1.266847 -0.086409 5 1 0 -0.878289 -2.221017 -0.142120 6 6 0 1.086779 -1.135183 -0.200705	20	1	0	3.070991	-1 404524	0.031500
Center Atomic Atomic Coordinates (Angstroms) Number Number Type X Y Z 1 6 0 0.123080 1.061651 0.195321 2 1 0 0.170661 1.417757 1.236010 3 6 0 -0.907717 -0.044764 0.107297 4 6 0 -0.371808 -1.266847 -0.086409 5 1 0 -0.878289 -2.221017 -0.142120 6 6 0 1.086779 -1.135183 -0.200705	Co	nformer 5 h	-1	5.070771	-1.404524	0.750557
Number Number Type X Y Z 1 6 0 0.123080 1.061651 0.195321 2 1 0 0.170661 1.417757 1.236010 3 6 0 -0.907717 -0.044764 0.107297 4 6 0 -0.371808 -1.266847 -0.086409 5 1 0 -0.878289 -2.221017 -0.142120 6 6 0 1.086779 -1.135183 -0.200705	Center	Atomic	Atomic	Coord	inates (Anos	troms)
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Number	Number	Type	X	Y	Z
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1	6	0	0.123080	1 061651	0 195321
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	2	1	0	0 170661	1.417757	1.236010
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	3	6	0	-0 907717	-0 044764	0 107297
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	4	6	0	-0 371808	-1.266847	-0.086409
6 6 0 1.086779 -1.135183 -0.200705	5	1	0	-0 878289	-2.221017	-0 142120
5 0 0 1.000777 -1.155105 -0.200705	6	6	0	1 086770	_1 135183	-0 200705
7 6 0 1 430270 0 360408 -0 210440	7	6	0	1 430270	0 360/08	-0.210//03
8 1 0 1 601888 0 63003/ 1 250523	، ۶	1	0	1 601888	0.507+90	-1 250522
9 8 0 _0 161894 2 148097 _0.676110	Q	8	0	-0 16180/	2 148097	-0 676110
10 1 0 -1 020766 2.11057 -0.070110	10	1	0	-1 020766	2.511057	-0 428161

11	6	0	2.666882	0.715202	0.612871
12	1	0	2.510747	0.504351	1.675250
13	1	0	3.515866	0.115765	0.280171
14	1	0	2.925663	1.771782	0.509290
15	8	0	-2.176404	0.347055	0.252256
16	8	0	1.899951	-2.031033	-0.278492
17	6	0	-3.188723	-0.659095	0.145846
18	1	0	-4.139550	-0.143944	0.260043
19	1	0	-3.141031	-1.145990	-0.831360
20	1	0	-3.070991	-1.404524	0.936539
Cor	nformer 6ca	a -1			
Center	Atomic	Atomic	Coord	inates (Angs	troms)
Number	Number	Type	X	Y	Z
1	6	0	0.833214	-1.086099	-0.381497
2	6	0	0.709146	0.217730	0.405306
3	8	0	1.463815	-0.036637	1.576316
4	6	0	1 878935	-1 376243	1 609282
5	6	0	1.070935	-2 018317	0.375250
6	1	0	1.429079	-3 049073	0.149936
0 7	8	0	2 487407	1 807677	2 5/1081
/ Q	6	0	2.407407	-1.807077	0.805361
0	1	0	-0.744400	0.250567	1 106112
9	I C	0	-1.10/333	-0.559507	1.190112
10	6	0	-1.585316	0.988/66	-0.409765
11	1	0	-1.460404	0.303833	-1.243325
12	l	0	-1.338261	2.001387	-0.724466
13	8	0	-2.98/95/	1.043146	-0.056257
14	8	0	0.332699	-1.112406	-1.608969
15	6	0	-0.783587	1.640714	1.903886
16	1	0	-0.312569	2.566795	1.566120
17	1	0	-0.266737	1.303797	2.801598
18	1	0	-1.820459	1.863392	2.162283
19	8	0	1.218165	1.376228	-0.262884
20	6	0	-3.690837	-0.107250	-0.185117
21	6	0	-5.127329	0.096919	0.226515
22	1	0	-5.710335	-0.783591	-0.035460
23	1	0	-5.543981	0.984037	-0.253511
24	1	0	-5.181757	0.256206	1.306770
25	6	0	2.463374	1.362274	-0.837070
26	6	0	2.812556	2.742899	-1.327407
27	1	0	2.017902	3.138958	-1.962692
28	1	0	3.749780	2.704897	-1.878446
29	1	0	2.917087	3.419204	-0.475358
30	8	0	-3.215139	-1.146396	-0.569461
31	8	0	3.152684	0.386568	-0.923829
32	6	0	0.405378	-2.364048	-2.305127
33	1	0	-0.168638	-3.123872	-1.770476
34	- 1	0	1.447497	-2.674884	-2.408209
35		0		r	2.100209
~~~	1	0	-0.032853	-2.186993	-3.283741

Center	Atomic	Atomic	Coord	inates (Angst	troms)
Number	Number	Туре	Х	Y	Z
1	6	0	-1.665154	-0.569139	0.758272
2	6	0	-0.578399	-0.096139	-0.196126
3	8	0	-1.015285	-0.568203	-1.458596
4	6	0	-2.188538	-1.326407	-1.313633
5	6	0	-2.550625	-1.333367	0.104505
6	1	0	-3.436531	-1.829714	0.467149
7	8	0	-2.708283	-1.841112	-2.257326
8	6	0	0.825487	-0.649419	0.140766
9	1	0	1.111829	-0.171012	1.082077
10	6	0	1.826314	-0.203923	-0.935863
11	1	0	1.817788	0.876740	-1.049118
12	1	0	1.607812	-0.681336	-1.889936
13	8	0	3.167067	-0.631168	-0.602484
14	8	0	-1.545244	-0.198546	2.026030
15	6	0	0.830669	-2.171634	0.312312
16	1	0	0.451497	-2.675366	-0.580312
17	1	0	0.228076	-2.489427	1.165252
18	1	0	1.851183	-2.517933	0.479043
19	8	0	-0.409852	1.324676	-0.238275
20	6	0	3.907255	0.207039	0.163456
21	6	0	5.282640	-0.366942	0.399111
22	1	0	5.898643	0.364990	0.917325
23	1	0	5.747443	-0.647377	-0.547978
24	1	0	5.209535	-1.273832	1.004941
25	6	0	-1.479932	2.173626	-0.333609
26	6	0	-0.987534	3.586505	-0.504810
27	1	0	-0.538158	3.697692	-1.495152
28	1	0	-0 215074	3 818091	0.230279
20 29	1	0	-1 823953	4 275820	-0.409633
30	8	0	3 505995	1.273626	0.591730
31	8	0	-2 625974	1.250044	-0.286227
31	6	0	-2.025974	-0 593244	2 908636
32	1	0	-2.003043	1 683064	2.908030
24	1	0	-2.070779	-1.065004	2.535554
24 25	1	0	-3.332003	-0.174017	2.304044
35		0	-2.345875	-0.189438	5.884510
0	onformer 6C	0-1	<u></u>	•••••	
Center	Atomic	Atomic	Coord	inates (Angsi	roms)
Number	Number	Туре	X	Y	L
1	6	0	-0.833214	-1.086099	-0.381497
2	6	0	-0.709146	0.217/30	0.405306
3	8	0	-1.463815	-0.036637	1.576316
4	6	0	-1.878935	-1.376243	1.609282
5	6	0	-1.429879	-2.018317	0.375250
6	1	0	-1.651841	-3.049073	0.149936
7	8	0	-2.487407	-1.807677	2.541981
8	6	0	0.744406	0.571464	0.805361
9	1	0	1.167553	-0.359567	1.196112

10	6	0	1.585316	0.988766	-0.409765
11	1	0	1.460404	0.303833	-1.243325
12	1	0	1.338261	2.001387	-0.724466
13	8	0	2.987957	1.043146	-0.056257
14	8	0	-0.332699	-1.112406	-1.608969
15	6	0	0.783587	1.640714	1.903886
16	1	0	0.312569	2.566795	1.566120
17	1	0	0.266737	1.303797	2.801598
18	1	0	1.820459	1.863392	2.162283
19	8	0	-1.218165	1.376228	-0.262884
20	6	0	3.690837	-0.107250	-0.185117
21	6	0	5.127329	0.096919	0.226515
22	1	0	5.710335	-0.783591	-0.035460
23	1	0	5.543981	0.984037	-0.253511
24	1	0	5.181757	0.256206	1.306770
25	6	0	-2.463374	1.362274	-0.837070
26	6	0	-2.812556	2.742899	-1.327407
27	1	0	-2.017902	3.138958	-1.962692
28	1	0	-3.749780	2.704897	-1.878446
29	1	0	-2.917087	3.419204	-0.475358
30	8	0	3.215139	-1.146396	-0.569461
31	8	0	-3.152684	0.386568	-0.923829
32	6	0	-0.405378	-2.364048	-2.305127
33	1	ů 0	0.168638	-3 123872	-1 770476
34	1	0	-1 447497	-2 674884	-2 408209
35	1	0	0.032853	-2 186993	-3 283741
C01	nformer <b>6cl</b>	<u> </u>	0.052055	2.100775	5.205711
Center	Atomic	Atomic	Coord	inates (Angs	troms)
Number	Number	Type	X	V	7
1	6	0	1 665154	0 560130	0.758272
2	6	0	0 578300	0.006130	0.196126
2	8	0	1.015285	0.568203	1 458596
3	6	0	2 199539	1 326407	1 313633
4	6	0	2.100550	1 222267	-1.515055
5	1	0	2.550025	1 920714	0.104303
0	1	0	2.420221	-1.029/14	0.407149
/	8	0	2.708283	-1.841112	-2.25/320
0	0	0	-0.823487	-0.049419	1.022077
9	I C	0	-1.111829	-0.1/1012	1.082077
10	0	0	-1.820314	-0.203923	-0.935803
11	1	0	-1.81//88	0.8/0/40	-1.049118
12	1	0	-1.60/812	-0.681336	-1.889936
13	ð	0	-3.10/00/	-0.031108	-0.002484
14	8	0	1.545244	-0.198546	2.020030
15	6	0	-0.830669	-2.171634	0.312312
10	1	0	-0.45149/	-2.0/3366	-0.580312
17	1	0	-0.228076	-2.489427	1.165252
18	4	0	1.051102	0 515000	0 4700 42
10	1	0	-1.851183	-2.517933	0.479043
19	1 8	0 0	-1.851183 0.409852	-2.517933 1.324676	0.479043 -0.238275

21	6	0	-5.282640	-0.366942	0.399111		
22	1	0	-5.898643	0.364990	0.917325		
23	1	0	-5.747443	-0.647377	-0.547978		
24	1	0	-5.209535	-1.273832	1.004941		
25	6	0	1.479932	2.173626	-0.333609		
26	6	0	0.987534	3.586505	-0.504810		
27	1	0	0.538158	3.697692	-1.495152		
28	1	0	0.215074	3.818091	0.230279		
29	1	0	1.823953	4.275820	-0.409633		
30	8	0	-3.505995	1.258844	0.591730		
31	8	0	2.625974	1.825266	-0.286227		
32	6	0	2.603643	-0.593244	2.908636		
33	1	0	2.670779	-1.683064	2.959994		
34	1	0	3.552065	-0.174617	2.564844		
35	1	0	2.345873	-0.189438	3.884310		
Cor	nformer <b>6c</b> l	<b>b</b> -4					
Center	Atomic	Atomic	Coord	Coordinates (Angstroms)			
Number	Number	Туре	Х	Y	Z		
1	6	0	-1.925587	-0.406188	-0.037205		
2	6	0	-0.456749	-0.124558	-0.325001		
3	8	0	0.183807	-0.451305	0.897198		
4	6	0	-0.745268	-0.943061	1.821212		
5	6	0	-2.065841	-0.929466	1.188307		
6	1	0	-2.956236	-1.237891	1.712489		
7	8	0	-0.398479	-1.300990	2.907323		
8	6	0	0.117162	-0.958542	-1.497592		
9	1	0	-0.471759	-0.662530	-2.374074		
10	6	0	1.569926	-0.581381	-1.823501		
11	1	0	1.883527	-1.121168	-2.719670		
12	1	0	1.681242	0.486789	-1.988142		
13	8	0	2.463803	-0.996696	-0.774531		
14	8	0	-2.786278	-0.126035	-1.008071		
15	6	0	-0.038949	-2.466478	-1.275116		
16	1	0	0.535299	-2.797408	-0.409509		
17	1	0	-1.081365	-2.754902	-1.127518		
18	1	0	0.331767	-3.010096	-2.147616		
19	8	0	-0.190215	1.230233	-0.679519		

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0

3.049335

3.732467

2.966886

4.226398

4.446272

-0.508681

0.194949

1.272846

-0.011675

-0.124406

3.000306

-1.230201

-0.033202

-0.648552

-0.874534

-1.583973

0.056389

2.264545

3.512535

3.360682

3.708196

4.355731

1.145031

2.154298

-0.015566

1.174961

1.922960

0.909726

1.597263

0.166520

-0.288758

-0.190969

-1.343107

0.320113

-0.262898

1.116812

32	6	0	-4.171716	-0.347571	-0.715211
33	1	0	-4.351923	-1.404817	-0.503794
34	1	0	-4.476910	0.261740	0.138476
35	1	0	-4.718203	-0.046960	-1.605429

#### 3. Experimental and calculated ECD spectra



Figure AS2 Calculated ECD spectra of compounds 4, 5, and 6c were compared with the experimental.