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#### S1. Energy Minimization and ECD Calculations

The initial conformational distribution search was performed using MMFF94 method overlaid with key correlations observed in the NOESY spectra of **1**. The corresponding minimum geometries were preoptimized at HF/6-31G level in Gaussian 03 program package [1,2], which was further checked by frequency calculation and resulted in no imaginary frequencies. And their minimum geometries were further optimized by DFT calculation B3LYP at 6-31 + g(d) level in the gas phase. The stable conformers obtained were submitted to ECD calculation by TDDFT [b3lyp/aug-cc-pvdz] method under Self-Consistent Reaction Field model of solvent (MeOH). The overall predicted ECD spectra of **1** were subsequently compared with the experimental one.

#### S1.1. Energy Minimization of Four Possible Relative Structures of 1 (1A–1D)



Formula:  $\Delta E = (E - E_{1A}) \times 627.51 \text{ kcal/mol} [2]$ 



# E(RHF/6-31G(d)) = -551.3563 a.u. $\Delta E = 0 \text{ kcal/mol}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstron X Y Z					
1	6	0	-3.102171	-0.099256	-0.930399			
2	6	0	-1.798273	-0.426787	-0.255432			
3	6	0	-1.277377	0.601481	0.733570			
4	8	0	-0.319261	0.057862	1.582865			
5	6	0	0.741647	-0.526112	0.850402			
6	6	0	0.227165	-1.795318	0.176444			
7	6	0	-1.099086	-1.523185	-0.483627			
8	7	0	-0.733857	1.744730	0.013558			
9	6	0	1.291673	0.513891	-0.102040			
10	6	0	2.637915	0.374606	-0.644413			
11	6	0	0.573753	1.606699	-0.376782			
12	8	0	3.356972	-0.558984	-0.440264			
13	1	0	2.976650	1.204636	-1.275062			
14	1	0	1.504967	-0.769485	1.574830			
15	1	0	-2.083543	0.956218	1.360713			
16	1	0	-3.029737	0.834941	-1.479812			
17	1	0	-3.903737	0.013643	-0.203414			
18	1	0	-3.388959	-0.878972	-1.625918			
19	1	0	0.953011	-2.147325	-0.548555			
20	1	0	0.116056	-2.581577	0.920072			
21	1	0	-1.473031	-2.264134	-1.171138			
22	1	Õ	-0.988967	2.647504	0.353125			
23	1	0	0.981117	2.424296	-0.946894			

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E(RHF/6-31G(d)) = -551.2413 a.u.
$\Delta E = 72.2 \text{ kcal/mol}$
Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Туре	X	Y	Z	
1	6	0	3.473705	-0.218837	-0.438751	
2	6	0	2.084722	0.233903	-0.080757	
3	6	0	1.135059	-0.792785	0.600811	
4	8	0	0.189380	-0.016980	1.182020	
5	6	0	-0.450188	0.544816	0.013426	
6	6	0	0.173358	1.929571	-0.012140	
7	6	0	1.657201	1.497217	-0.198855	
8	7	0	0.327975	-1.765557	-0.230878	
9	6	0	-1.625824	-0.380148	-0.157152	
10	6	0	-3.057186	-0.151050	-0.195651	
11	6	0	-1.054412	-1.604168	-0.268576	
12	8	0	-3.583063	0.918178	-0.104642	
13	1	0	-3.660977	-1.056224	-0.332393	
14	1	0	0.066627	0.187292	-0.854753	
15	1	0	1.679276	-1.364427	1.344142	
16	1	0	3.440492	-0.992517	-1.202957	
17	1	0	3.988639	-0.640250	0.421801	
18	1	0	4.073142	0.598762	-0.820566	
19	1	0	-0.134072	2.527461	-0.863597	
20	1	0	0.018954	2.501589	0.894354	
21	1	0	2.345761	2.252628	-0.539983	
22	1	0	0.641932	-2.710380	-0.215747	
23	1	0	-1.624747	-2.505729	-0.407308	





E(RHF/6-31G(d)) = -551.2345 a.u.  $\Delta E = 70.9$  kcal/mol Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)				
Number	Number	Туре	X	Y	Z		
1	6	0	-3.589795	0.245618	-0.204881		
2	6	0	-2.165260	-0.210188	-0.202053		
3	6	0	-0.907013	0.619393	-0.007103		
4	8	0	-0.348234	0.090703	1.187403		
5	6	0	0.651525	-0.691763	0.626756		
6	6	0	-0.164112	-1.771791	-0.219065		
7	6	0	-1.690721	-1.453934	-0.301720		
8	7	0	-0.351136	1.936015	-0.158793		
9	6	0 1.537007		0.401717	-0.038906		
10	6	0	2.956043	0.153922	-0.299352		
11	6	0	1.039860	1.650345	-0.195034		
12	8	0	3.478952	-0.912519	-0.172552		
13	1	0	3.537994	1.020699	-0.630466		
14	1	0	1.226537	-1.174355	1.404237		
15	1	0	-0.397099	0.208240	-0.848281		
16	1	0	-3.764042	0.978754	-0.987595		
17	1	0	-3.846337	0.715106	0.741247		
18	1	0	-4.263334	-0.588229	-0.364557		
19	1	0	0.245380	-1.878972	-1.220162		
20	1	0	-0.051057	-2.739291	0.257694		
21	1	0	-2.352507	-2.299270	-0.385857		
22	1	0	-0.605149	2.636377	0.511627		
23	1	0	1.676621	2.483443	-0.436992		



Energetically could not exist

S1.2. Standard Orientation of Two Enantiomers of 1A for ECD Calculation

Optimized structure of 1a



1a (4S, 24*R*)

Cartesian coordinate of **1a** optimized: Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)					
Number	Number	Туре	X	Y	Z			
1	6	0	3.149957	-0.092595	0.900662			
2	6	0	1.831941	-0.418435	0.251470			
3	6	0	1.289853	0.607391	-0.737823			
4	8	0	0.318826	0.053978	-1.602059			
5	6	0	-0.750079	-0.544368	-0.830420			
6	6	0	-0.213168	-1.805750	-0.140902			
7	6	0	1.123753	-1.528448	0.495959			
8	7	0	0.709516	1.752775	-0.012310			
9	6	0	-1.317427	0.503220	0.107874			
10	6	0	-2.661483	0.379048	0.629509			
11	6	0	-0.589665	1.626778	0.376800			
12	8	0	-3.413888	-0.569962	0.421567			
13	1	0	-3.002564	1.229117	1.262961			
14	1	0	-1.514927	-0.811558	-1.563754			
15	1	0	2.091837	0.989067	-1.377028			
16	1	0	3.092828	0.845144	1.470528			
17	1	0	3.946859	0.032966	0.153304			
18	1	0	3.457226	-0.885290	1.590639			
19	1	0	-0.938695	-2.149436	0.606426			
20	1	0	-0.117369 -2.616906		-0.878655			
21	1	0	1.520930	-2.277754	1.180550			
22	1	0	1.090493	2.678056	-0.160992			
23	1	0	-1.014826	2.463982	0.927344			

Optimized structure of the enantiomer 1b



1b (4*R*, 24*S*)

Cartesian coordinate of the enantiomer **1b** optimized: Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)					
Number	Number	Туре	X	Y	Z			
1	6	0	-3.149957	-0.092595	-0.900662			
2	6	0	-1.831941	-0.418435	-0.251470			
3	6	0	-1.289853	0.607391	0.737823			
4	8	0	-0.318826	0.053978	1.602059			
5	6	0	0.750079	-0.544368	0.830420			
6	6	0	0.21316	-1.805750	0.140902			
7	6	0	-1.123753	-1.528448	-0.495959			
8	7	0	-0.709516	1.752775	0.012310			
9	6	0	1.317427	0.503220	-0.107874			
10	6	0	2.661483	0.379048	-0.629509			
11	6	0	0.589665	1.626778	-0.376800			
12	8	0	3.413888	-0.569962	-0.421567			
13	1	0	3.002564	1.229117	-1.262961			
14	1	0	1.514927	-0.811558	1.563754			
15	1	0	-2.091837	0.989067	1.377028			
16	1	0	-3.092828	0.845144	-1.470528			
17	1	0	-3.946859	0.032966	-0.153304			
18	1	0	-3.457226	-0.885290	-1.590639			
19	1	0	0.938695	-2.149436	-0.606426			
20	1	0	0.117369	-2.616906	0.878655			
21	1	0	-1.520930	-2.277754	-1.180550			
22	1	0	-1.090493	2.678056	0.160992			
23	1	0	1.014826	2.463982	-0.927344			

#### Figure S1. HRESIMS spectrum of compound 1.

#### **Elemental Composition Report**

Page 1

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0 Selected filters: None

Monoisotopic Mass, Even Electron Ions 50 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass) **Elements Used:** C: 5-50 H: 5-100 N: 1-1 O: 1-18 Na: 1-1 12-May-2010,14:30:05 Q-Tof micro SIPI 0.00000000 YA019 PSJ-B6 M.W=369 TOF MS ES+ WQ10180H3 25 (0.880) AM (Med,6, Ar,5000.0,403.13,0.70); Sm (SG, 2x3.00); Cm (23:64) 7.70e4 392.2567 100 % 393.2690 395.1739 393.4765 394.2568 394.6560 390.3648 391.2214 391.9143 392.5368 393.0116 389.5371 0-┍┶╼┼┲╼┲╼┲╼ 395.00 394.00 392.00 393.00 391.00 390.00 -1.5 Minimum: 30.00 50.0 10.0 5.0 100.00 Maximum: Formula i-FIT DBE Calc. Mass mDa PPM RA Mass C24 H35 N O2 Na 7.5 451.4 0.2 0.5 100.00 392.2565 392.2567



Figure S2. IR spectrum of compound 1.



**Figure S4.** <sup>13</sup>C NMR spectrum of compound **1** in CDCl<sub>3</sub>.



Figure S5. DEPT spectrum of compound 1 in CDCl<sub>3</sub>.



Figure S6. HSQC spectrum of compound 1 in CDCl<sub>3</sub>.



**Figure S7.**  $^{1}H^{-1}H$  COSY spectrum of compound 1 in CDCl<sub>3</sub>.









#### Figure S10. HRESIMS spectrum of compound 2.

#### **Elemental Composition Report**

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0 Selected filters: None

Monoisoto 34 formula	pic Mass a(e) evalu	, Even E ated wit	Electron I h 1 resul	ons ts within lin	nits (up to s	50 closest r	esults for each	n mass)				
Elements	Used:											
C: 5-30	H: 5-42	N: 0-1	O: 1-6	Na: 1-1								
SIPI					Q-	Tof micro				10-N	lay-201	0,15:32:08
PSJ-B84 M	.W=415					YA019					0	.00000000
WQ10172H	30 (1.057)	AM (Cen,	5, 80.00, Ai	r,5000.0,447.0	03,0.70); Sm	(SG, 2x3.00);	Cm (25:42)				101	- MS ES+
100					438.	2619						9.1164
-												
-												
-												
%												
						420 2	703					
1				107.0	000	435.2	.705					
	131 3851	125 2	010 126	437.2	128 0617	439.0775	440.2774	441 2761	442	2879	443.1	778
0		435.5	430.		430.0017	1 + + + + + + + + + + + + + + + + + + +	- <del> </del>					m/z
4	34.0	435.0	436.0	437.0	438.0	439.0	440.0	441.0	442.0		443.0	
Minimum.	25 00					1	5					
Maximum:	100 0	0		5 0	10	0 50.	0					
Maximum.	100.0	0		0.0	10.							
Mass	RA	Ca	lc. Mas	s mDa	PPN	1 DBE	i-FIT	Form	nula			
438.2619	100.0	0 43	8.2620	-0.	1 -0.	.2 7.5	487.0	C25	Н37	Ν	04 1	la

Page 1



Figure S11. IR spectrum of compound 2.

Figure S12. <sup>1</sup>H NMR spectrum of compound 2 in CDCl<sub>3</sub>.



Figure S13. <sup>1</sup>H NMR spectrum of compound 2 in DMSO.



**Figure S14.** <sup>13</sup>C NMR and DEPT spectrum of compound **2** in CDCl<sub>3</sub>.



Figure S15. HSQC spectrum of compound 2 in CDCl<sub>3</sub>.



**Figure S16.**  $^{1}H^{-1}H$  COSY spectrum of compound **2** in CDCl<sub>3</sub>.



Figure S17. HMBC spectrum of compound 2 in CDCl<sub>3</sub>.



Figure S18. NOESY spectrum of compound 2 in CDCl<sub>3</sub>.





Figure S19. Partial NOESY spectrum of compound 2 in CDCl<sub>3</sub>.

# Figure S20. HRESIMS spectrum of compound 3.

#### Elemental Composition Report

Page 1

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0 Selected filters: None

Monoisotopi 20 formula(e	c Mass, Ev e) evaluate sed:	ven Electron lo d with 1 results	ns ; within limits (u	p to 50 d	closest resu	Its for each r	mass)			
C: 5-27 H	10-50 N	· 1-3 O· 3-4	Na: 1-1							
SIPI	10 00 11			Q-Tof	micro			04	-Oct-2010,	11:47:44
PSJ-B10 M.W	=415			YAC	19				0.0	0000000
WQ10348H1 4	(0.138) AM	(Cen,6, 80.00, Ar,5	5000.0,447.03,1.00	); Sm (SG	, 2x3.00); Cm	(1:22)			TOFI	1 63e4
100			4	38.2622						1.0004
-										
				2						
_										
%-										
-										
-				439	2706					
430 2275	431.2220	101 1001	437.209	9	440 2819	441.2874 444.	.0306 445	.2032	448.0	439
0		434.4024			440.2013	$\cdot$	+++++++++++++++++++++++++++++++++++++++	+++++++++++++++++++++++++++++++++++++++		m/z
430.0	432.0	434.0	436.0 4	38.0	440.0	442.0	444.0	446.0	448.	0
Mimimum	F0 00		vet		-1 5					
Minimum:	100 00		5.0	20.0	50.0					
Max Indin.	100.00		0.0	10.0	0010					
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Form	ula		
438.2622	100.00	438.2620	0.2	0.5	7.5	464.9	C25	H37 N	O4 Na	



Figure S21. IR spectrum of compound 3.



8

6.0

7.0

8.0

9.0

94

5.0

8

8

4.0

5.0

3.0

14.8

2.0

# Figure S22. <sup>1</sup>H NMR spectrum of compound 3 in CDCl<sub>3</sub>.

ppm

1.0



**Figure S24.** <sup>13</sup>C NMR spectrum of compound **3** in CDCl<sub>3</sub>.



Figure S25. DEPT spectrum of compound 3 in CDCl<sub>3</sub>.



Figure S26. HSQC spectrum of compound 3 in CDCl<sub>3</sub>.





Figure S28. HMBC spectrum of compound 3 in CDCl<sub>3</sub>.





9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5

Figure S29. NOESY spectrum of compound 3 in CDCl<sub>3</sub>.

1.5 1.0

2.0

ppm

#### Figure S30. HRESIMS spectrum of compound 4.

# **Elemental Composition Report**

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0 Selected filters: None Monoisotopic Mass, Even Electron Ions 7 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass) Elements Used: C: 5-27 H: 10-50 O: 3-4 Na: 1-1 04-Oct-2010,13:56:02 Q-Tof micro SIPI 0.00000000 YA019 PSJ-B11 M.W=370 WQ10350H2 46 (1.589) AM (Cen,6, 80.00, Ar,5000.0,384.16,1.00); Sm (SG, 2x3.00); Cm (29:46) TOF MS ES+ 9.00e4 393.2404 100-%-394.2528 395.2503 388.4164 389.4276 390.3991 391.2592 392.2385 393.7303 396.2611 397.2505 398.2496 m/z 0-390.0 393.0 394.0 395.0 397.0 398.0 399.0 389.0 391.0 392.0 396.0 388.0 8. vet, -1.5 50.00 Minimum: 5.0 10.0 50.0 Maximum: 100.00 DBE i-FIT Formula PPM Mass RA Calc. Mass mDa 393.2404 100.00 393.2406 -0.2 -0.5 7.5 2754.3 C24 H34 O3 Na

Page 1

![](_page_37_Figure_1.jpeg)

Figure S31. IR spectrum of compound 4.

Figure S32. <sup>1</sup>H NMR spectrum of compound 4 in CDCl<sub>3</sub>.

![](_page_38_Figure_2.jpeg)

Figure S33. <sup>13</sup>C NMR spectrum of compound 4 in CDCl<sub>3</sub>.

![](_page_39_Figure_2.jpeg)

Figure S34. DEPT spectrum of compound 4 in CDCl<sub>3</sub>.

![](_page_40_Figure_2.jpeg)

Figure S35. HSQC spectrum of compound 4 in CDCl<sub>3</sub>.

![](_page_41_Figure_2.jpeg)

**Figure S36.** <sup>1</sup>H–<sup>1</sup>H COSY spectrum of compound **4** in CDCl<sub>3</sub>.

![](_page_42_Figure_2.jpeg)

Figure S37. HMBC spectrum of compound 4 in CDCl<sub>3</sub>.

![](_page_43_Figure_2.jpeg)

Figure S38. NOESY spectrum of compound 4 in CDCl<sub>3</sub>.

![](_page_44_Figure_2.jpeg)

### Figure S39. HRESIMS spectrum of compound 5.

# Elemental Composition Report

![](_page_45_Picture_3.jpeg)

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0 Selected filters: None

Monoisotopic Mass, Even Electron Ions 42 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass) Elements Used:										
C: 5-30 H:	5-45 N: 0	)-1 0: 1-6	Na: 1-1							
SIPI	260			Q-Tof micro	0			1	3-May-20	010,13:10:28
WQ10182H1 6	3 (2.176) AM	(Cen,6, 80.00, A	r,5000.0,385.24,0.70	)); Sm (SG, 2)	x3.00); Cm (	49:66)			Т	OF MS ES+
100-			3	92.2564						2.53e4
0/										
%										
						393.2681				
3	90.7656	4 0004 301 364	7	000 54	393	.1644	00 5400 394.0	)149	394.2675	
0-1		1.2231 <u>391.304</u>	4 50 000 00	392.51	21		93.5492		 د	
390	.50 39	91.00 391	1.50 392.00	392.50	) 39.	3.00 35	93.50	394.00	3	94.50
Minimum:	30.00		-		-1.5					
Maximum:	100.00		5.0	10.0	50.0					
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formu	la		
392.2564	100.00	392.2565	-0.1	-0.3	7.5	57.9	C24 1	H35 1	N 02	Na

![](_page_46_Figure_1.jpeg)

Figure S40. IR spectrum of compound 5.

Figure S41. <sup>1</sup>H NMR spectrum of compound 5 in CDCl<sub>3</sub>.

![](_page_47_Figure_2.jpeg)

![](_page_48_Figure_1.jpeg)

**Figure S42.** <sup>1</sup>H NMR spectrum of compound **5** in DMSO-d<sub>6</sub>.

Figure S43. <sup>13</sup>C NMR spectrum of compound 5 in CDCl<sub>3</sub>.

![](_page_49_Figure_2.jpeg)

Figure S44. DEPT spectrum of compound 5 in CDCl<sub>3</sub>.

![](_page_50_Figure_2.jpeg)

Figure S45. HSQC spectrum of compound 5 in CDCl<sub>3</sub>.

![](_page_51_Figure_2.jpeg)

**Figure S46.** <sup>1</sup>H–<sup>1</sup>H COSY spectrum of compound **5** in CDCl<sub>3</sub>.

![](_page_52_Figure_2.jpeg)

Figure S47. HMBC spectrum of compound 5 in CDCl<sub>3</sub>.

![](_page_53_Figure_2.jpeg)

Figure S48. NOESY spectrum of compound 5 in CDCl<sub>3</sub>.

![](_page_54_Figure_2.jpeg)

# Figure S49. <sup>1</sup>H NMR data of MTPA esters (2*S*, 2*R*, 3*S*, 3*R*).

<sup>1</sup>H NMR data of **2S** (500 MHz, CDCl<sub>3</sub>): δ 2.893 (1H, m, H-2a), 2.769 (1H, m, H-2b), 3.858 (1H, m, H-4), 2.313 (1H, m, H-5a), 2.163 (1H, m, H-5b), 5.462 (1H, br s, H-6).

<sup>1</sup>H NMR data of **2***R* (500 MHz, CDCl<sub>3</sub>): δ 2.901 (1H, m, H-2a), 2.782 (1H, m, H-2b), 3.860 (1H, m, H-4), 2.231 (1H, m, H-5a), 2.143 (1H, m, H-5b), 5.457 (1H, br s, H-6).

<sup>1</sup>H NMR data of **3S** (500 MHz, CDCl<sub>3</sub>): δ 2.733 (1H, m, H-2), 4.141 (1H, m, H-4), 2.419 (1H, m, H-5a), 2.208 (1H, m, H-5b), 5.381 (1H, br s, H-6).

<sup>1</sup>H NMR data of **3***R* (500 MHz, CDCl<sub>3</sub>): δ 2.735 (1H, m, H-2), 4.145 (1H, m, H-4), 2.385 (1H, m, H-5a), 2.194 (1H, m, H-5b), 5.363 (1H, br s, H-6).

#### References

- 1. Frisch, M.J.; Trucks, G.W.; Schlegel, H.B.; Scuseria, G.E.; Robb, M.A.; Cheeseman, J.R.; Montgomery, J.A., Jr.; Vreven, T.; Kudin, K.N.; Burant, J.C.; *et al. Gaussian 03*, revision D.01; Gaussian, Inc.: Wallingford, CT, USA, 2013.
- 2. Available online: http://www.gaussian.com (accessed on 11 December 2013).

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