

## Supporting Information

### **Diaryl-pyrano-chromenes atropisomers: stereodynamics and conformational studies**

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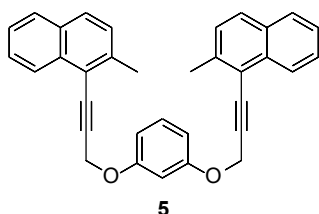
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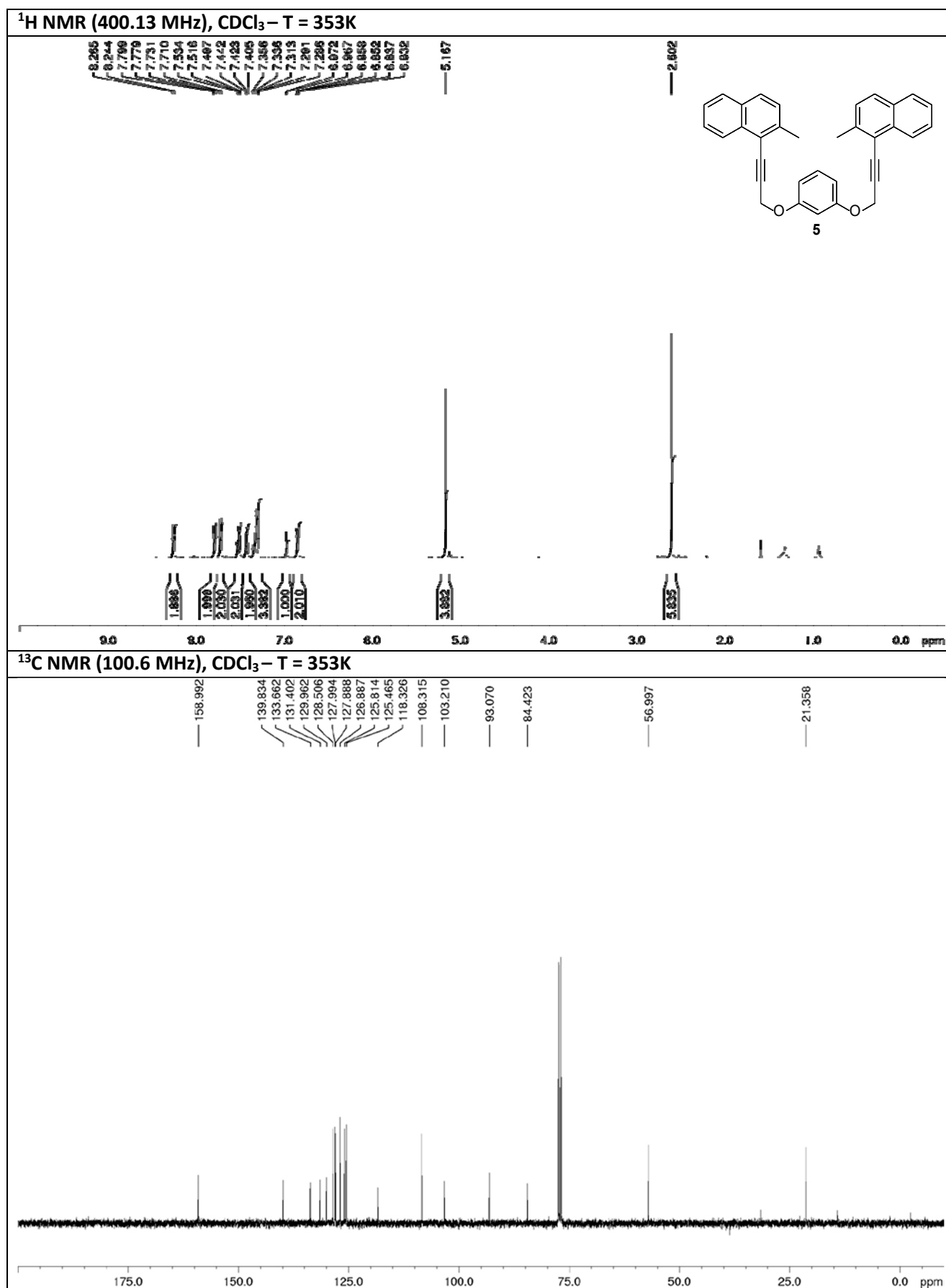
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### 1. Synthesis of 1,3-bis((3-(2-methylnaphthalen-1-yl)prop-2-yn-1-yl)oxy)benzene (5)

In a 50 ml round bottom flask equipped with a magnetic stirring bar, resorcinol (144.8 mg, 1.3 mmol., 1 equiv.) was dissolved in DMF (6 mL) at room temperature. Then  $K_2CO_3$  (545 mg, 3.95 mmol., 3 equiv.) was added and after 15 minutes 1-(3-bromoprop-1-yn-1-yl)-2-methylnaphthalene (750 mg, 2.89 mmol., 2.2 equiv.) was added to the mixture. Reaction was monitored by TLC until disappearance of the starting material, then diluted with  $Et_2O$  and washed with  $NaHSO_4$  (x2) and brine (x2). The organic extract was dried over  $Na_2SO_4$  and concentrated under reduced pressure. The residue was purified by chromatography on  $SiO_2$  (25-40  $\mu m$ ), eluting with a 98/2 (v/v) *n*-hexane/ $AcOEt$  mixture to obtain 589.0 mg (97% yield) of 1,3-bis((3-(2-methylnaphthalen-1-yl)prop-2-yn-1-yl)oxy)benzene **5**.



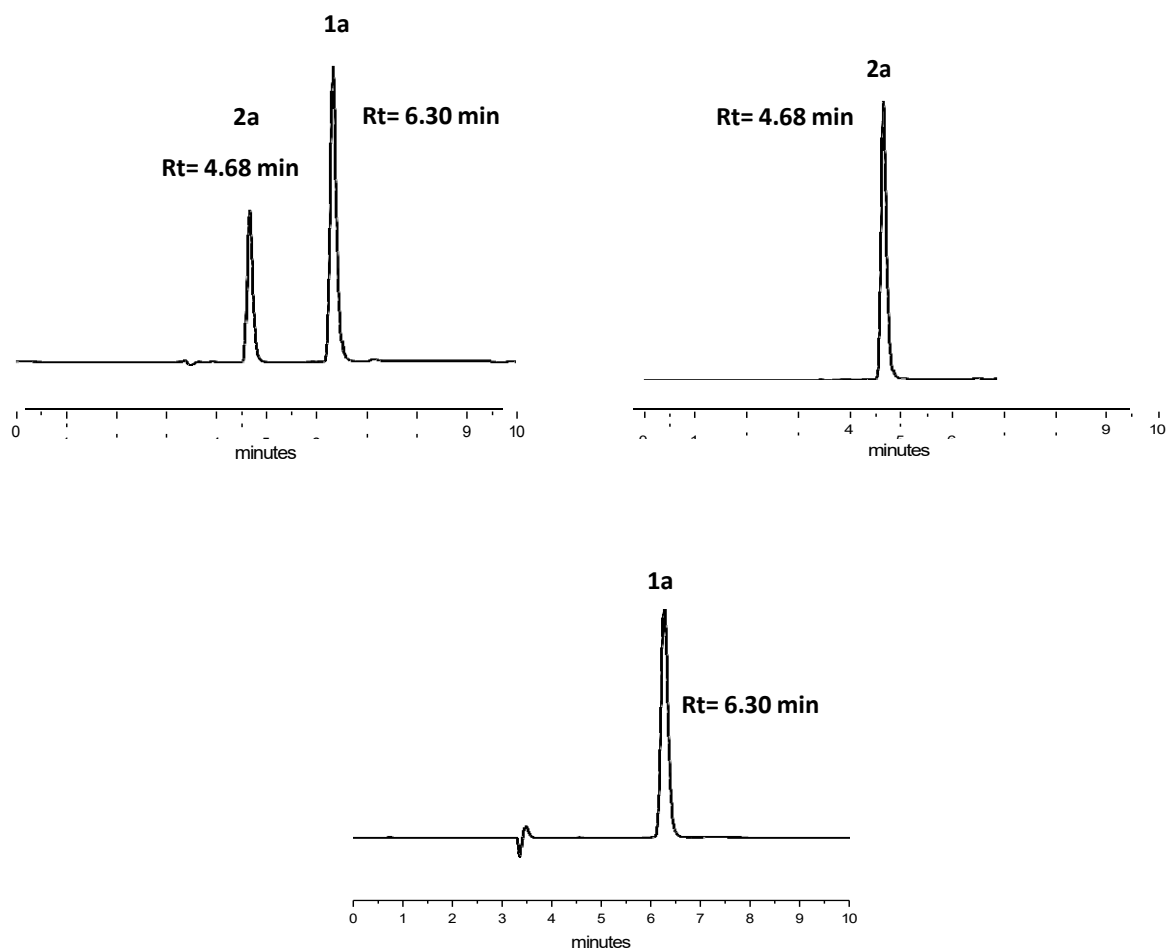
**5**: pale yellow solid; 97% yield;  $^1H$  NMR (400 MHz) ( $CDCl_3$ )  $\delta$  (ppm) 8.25 (d,  $J$  = 8.4 Hz, 2H), 7.79 (d,  $J$  = 8.1 Hz, 2H), 7.52 (t,  $J$  = 7.3 Hz, 2H), 7.42 (t,  $J$  = 7.5 Hz, 2H), 7.36 – 7.28 (m, 3H), 6.97 (m, 1H), 6.84 (dd,  $J_1$  = 8.2 Hz,  $J_2$  = 2.2 Hz, 2H), 5.17 (s, 4H), 2.60 (s, 6H);  $^{13}C\{^1H\}$  NMR (100.6 MHz) ( $CDCl_3$ )  $\delta$  (ppm) 159.0, 139.8, 133.7, 131.4, 130.0, 128.5, 128.0, 127.9, 126.9, 125.8, 125.5, 118.3, 108.3, 103.2, 57.0, 21.3.



**Figure S1.**  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra of compound **5** at +25 °C.

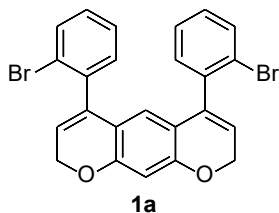
## 2. Separation of compounds **1a**/**2a**

Linear and angulated **1a**/**2a** were separated by semipreparative HPLC on silica (a). Column: Silica Adamas (250\*10 mm ID), eluent *n*-Hex/DCM 50/50, flow: 4.0 ml/min, Detector: UV 254 nm. Analytical controls of purified fraction are in Figure S2.



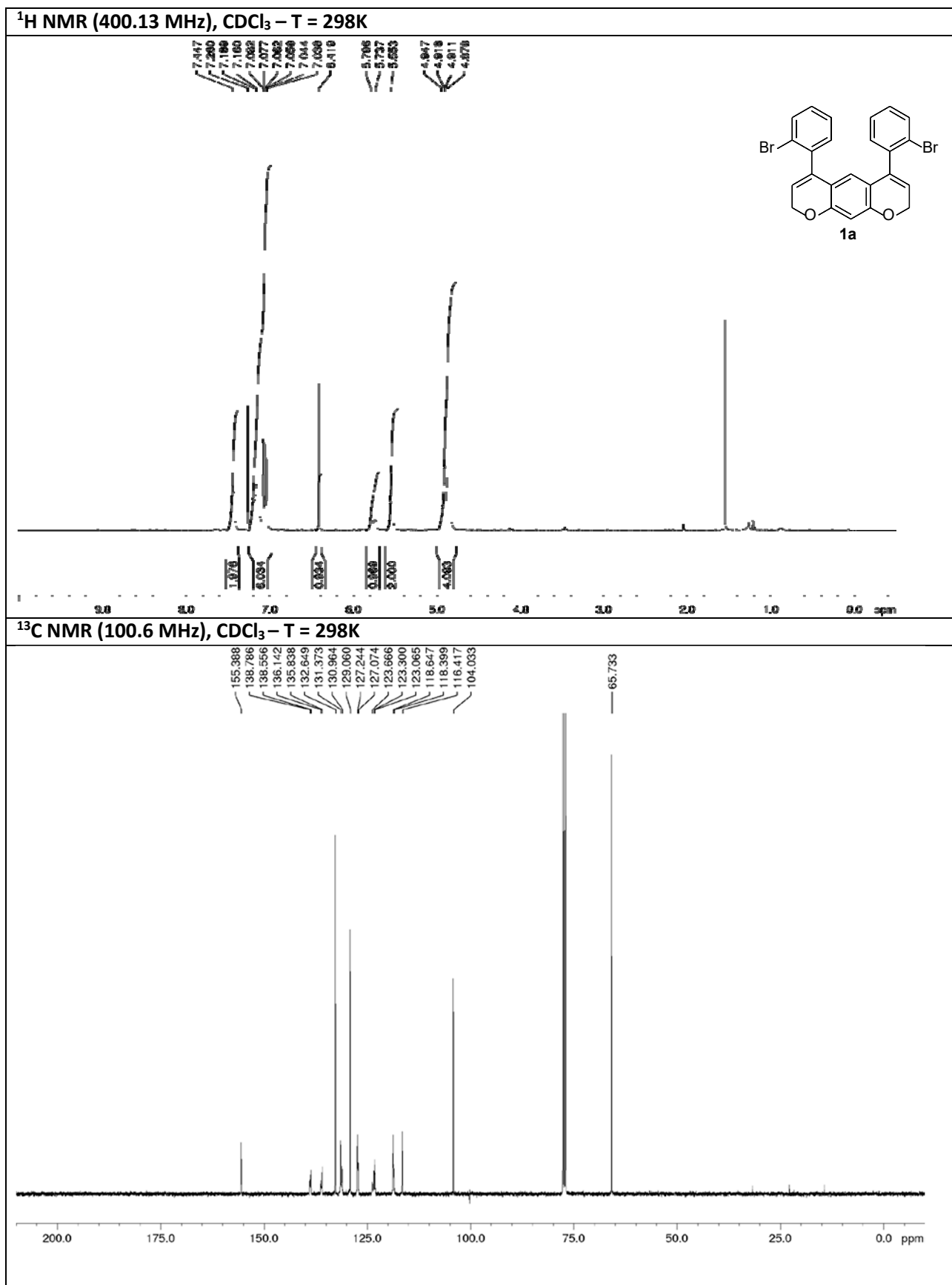
**Figure S2.** Column: Silica Adamas (250\*4.6 mm ID), eluent *n*-Hex/DCM 50/50, flow: 1 ml/min, Detector: UV 254 nm. Isolated product purity: **1a** 99.9 % (c) and **2a** 99.9% (b).

### 3. Characterization of compound 1a

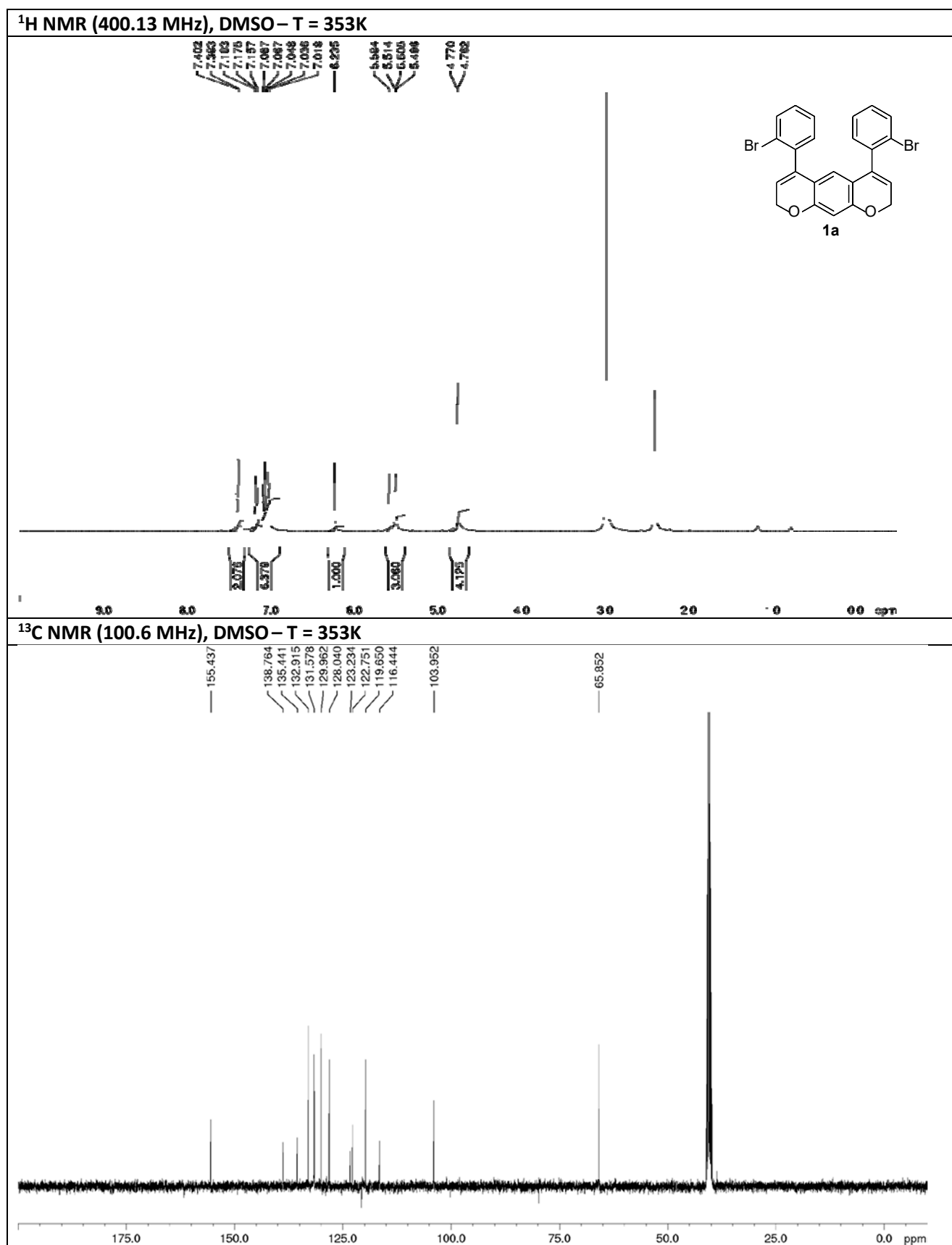


**1a (mixture of stereoisomers):** white solid; mp = 159 - 161 °C; IR (neat): 2925, 2837, 1676, 1576, 1488, 1427  $\text{cm}^{-1}$ ;  $^1\text{H}$ -NMR (400.13 MHz,  $\text{CDCl}_3$ , +25 °C):  $\delta$  7.45 (m, 2 H), 7.19 - 7.16 (m, 3H), 7.06 (dt,  $J_1 = 7.6$  Hz,  $J_2 = 1.8$  Hz, 3H), 6.42 (s, 1H), 5.80 - 5.74 (m, 1H), 5.55 (s, 2H), 4.95 - 4.88 (m, 4H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100.6 MHz,  $\text{DMSO-d}_6$ , +80 °C):  $\delta$  155.4, 138.7, 136.0, 132.6, 131.2, 129.1, 127.2, 123.7, 123.2, 118.5, 116.4, 104.0, 65.7; HRMS:  $m/z$   $[\text{M} + \text{H}]^+$  calcd for  $\text{C}_{24}\text{H}_{17}\text{Br}_2\text{O}_2$ : 496.9569; found: 496.9565.

Additional  $^1\text{H}$ -NMR e  $^{13}\text{C}$ -NMR at 80 °C in  $\text{DMSO-d}_6$  were recorded to obtain mediated signals for a good quality of spectra considering the faster interconversion of *syn/anti* stereoisomers.

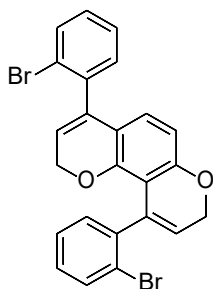


**Figure S3.** <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound **1a** at +25 °C.



**Figure S4.** <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound **1a** at +80 °C.

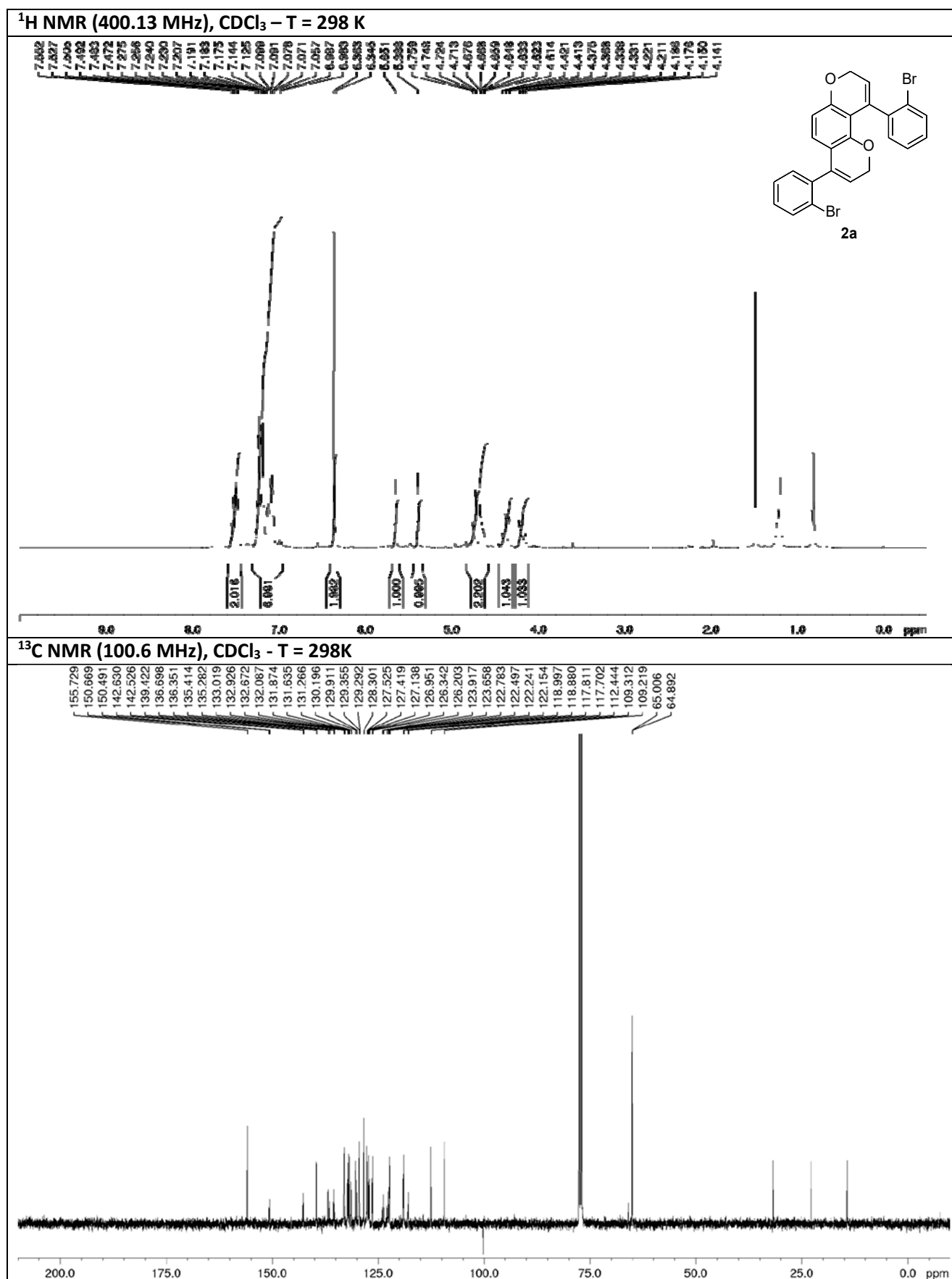
#### 4. Full characterization of compound 2a



**2a**

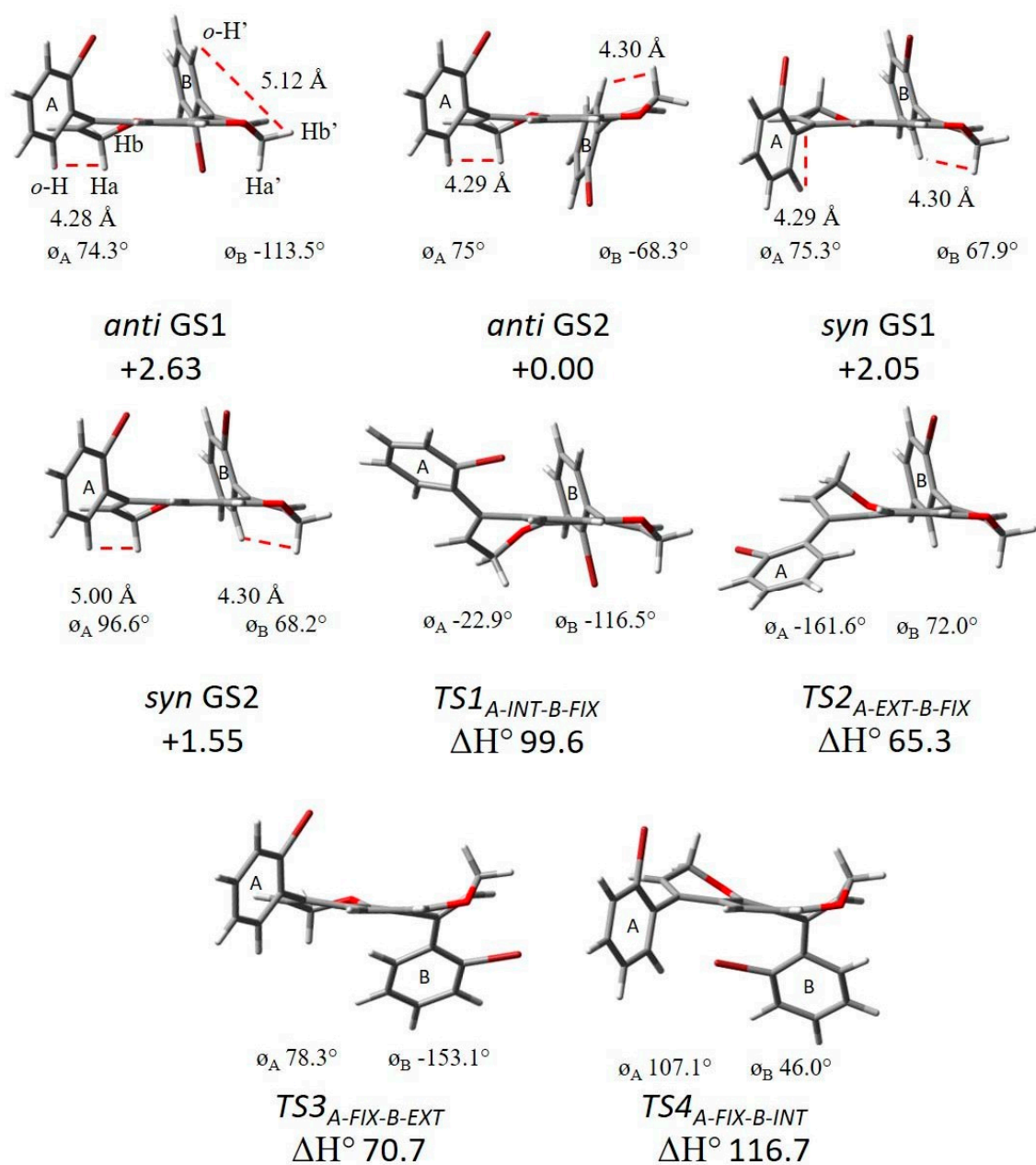
**2a (mixture of stereoisomers):** yellow oil; IR (neat): 2930, 2835, 1676, 1575, 1490, 1427  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400.13 MHz) ( $\text{CDCl}_3$ ): 7.55-7.47 (m, 2H), 7.27-6.98 (m, 6H), 6.36 (s, 2H), 5.65 (bs, 1H), 5.39 (bs, 1H), 4.76 - 4.61 (m, 2H), 4.42 - 4.33 (m, 1H), 4.22 - 4.14 (m, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100.6 MHz) ( $\text{CDCl}_3$ ):  $\delta$  155.7, 150.6, 142.6, 139.4, 136.5, 135.3, 133.0, 132.0, 131.4, 130.0, 129.3, 128.3, 127.5, 127.0, 126.3, 123.8, 122.6, 122.2, 118.9, 117.8, 112.4, 109.3, 65.0, 64.9; HRMS:  $m/z$   $[\text{M} + \text{H}]^+$  calcd for  $\text{C}_{24}\text{H}_{17}\text{Br}_2\text{O}_2$ : 496.9569; found: 496.9565.





**Figure S5.** <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound **2a** at +25 °C.

#### 4.1 DFT Calculations of *syn/anti* for compounds **2a**

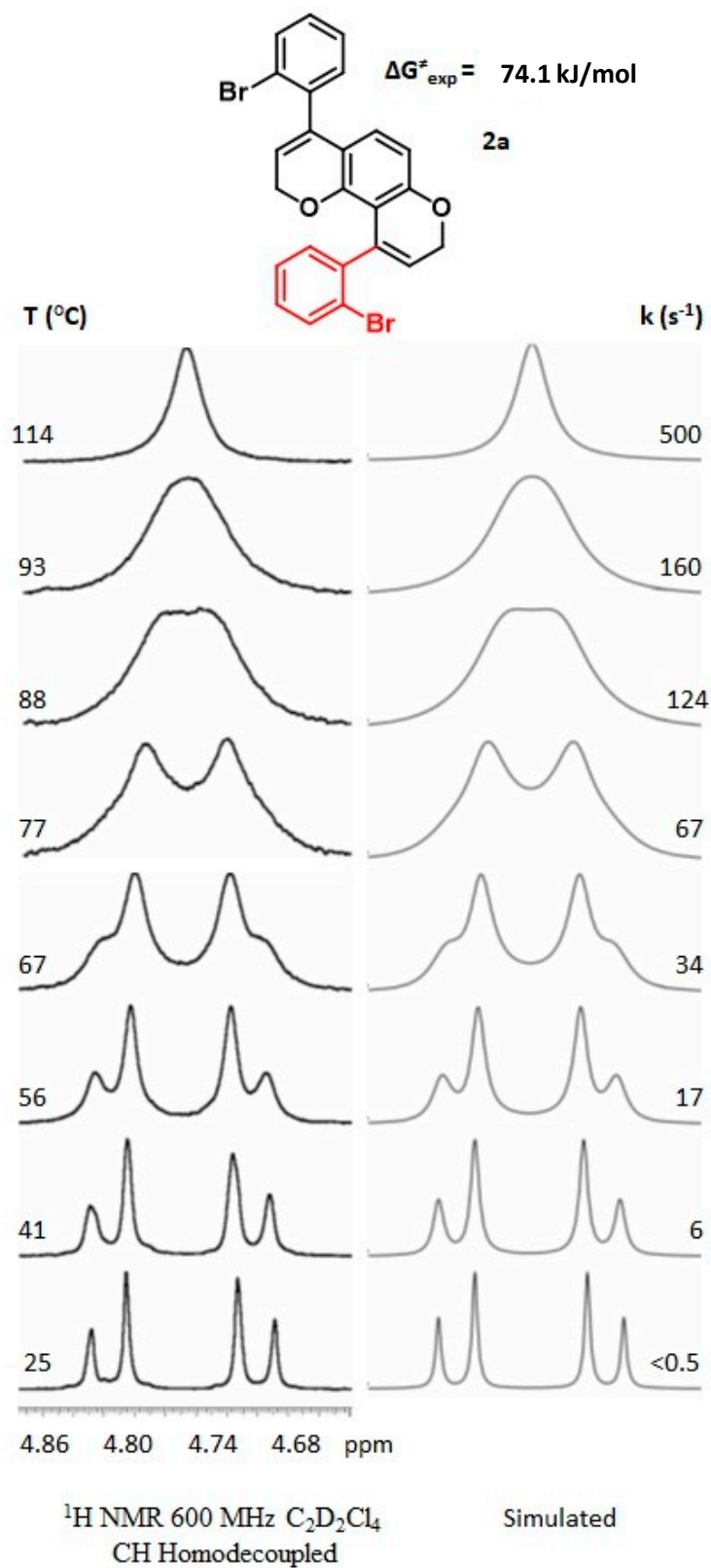


**Figure S6.** Predicted DFT (6-311++G(d,p), PCM=chloroform) conformations of *syn/anti* for compounds **2a** are shown. The relative Enthalpy energies are reported in kJ/mol.

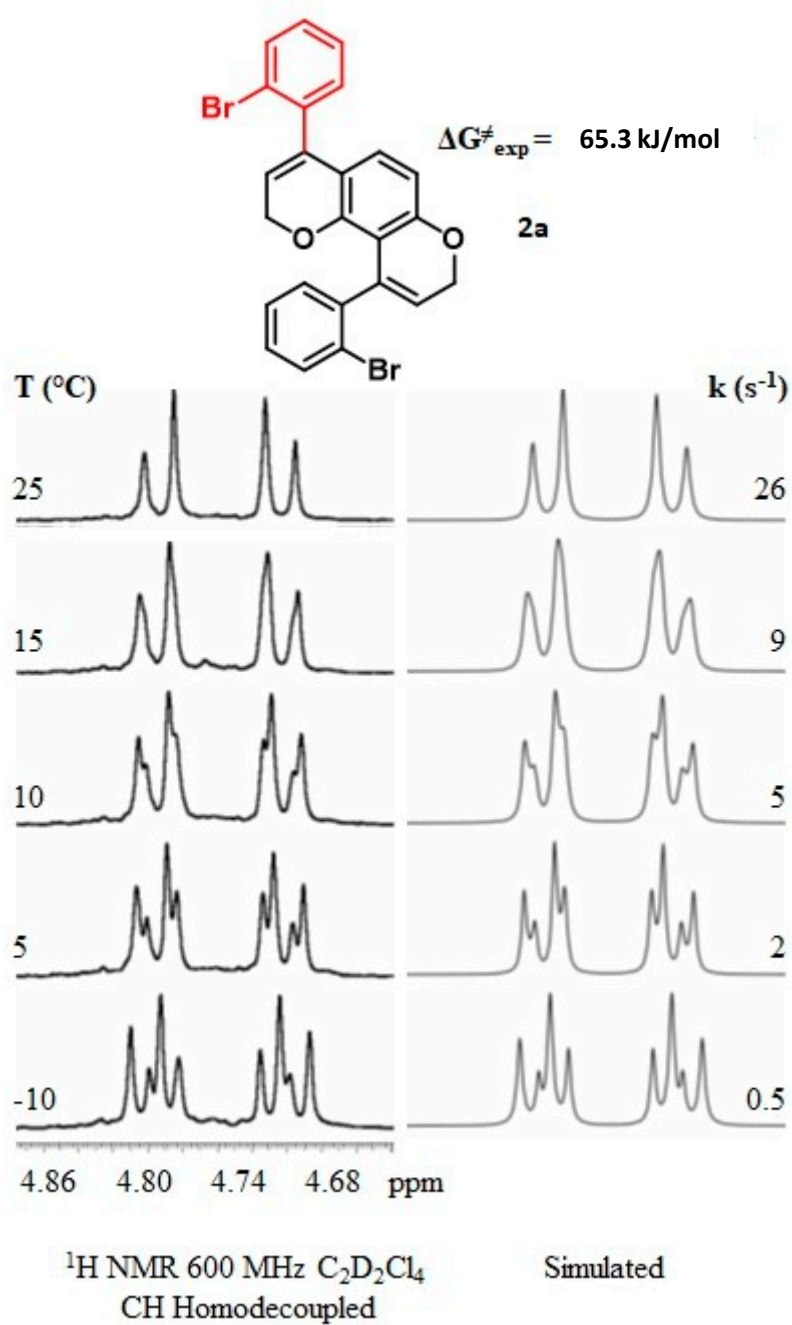
**Table S1.** Descriptors are shown:  $r$  = atom distance;  $\phi$  = dihedral angle

2a	$r(\text{H}_a - \text{oH})$	$r(\text{H}_b - \text{oH})$	$r(\text{H}_a' - \text{oH}')$	$r(\text{H}_b' - \text{oH}')$	$\phi_A$	$\phi_B$	% <i>pop</i>
GS1 <i>anti</i>	4.28	5.09	5.40	5.12	74.30	-113.50	15.74
GS2 <i>anti</i>	4.29	5.11	4.30	4.99	75.00	-68.30	43.71
GS1 <i>syn</i>	4.29	5.11	4.30	4.99	75.30	67.90	16.16
GS2 <i>syn</i>	5.41	5.00	4.30	4.99	96.60	68.20	24.37
avg. <i>anti</i> vs <i>syn</i>	4.29 vs 4.96	5.10 vs 5.04	4.59 vs 4.29	5.02 vs 4.99	74.8 vs 88.1	-80.3 vs 68.1	59.5/40.5

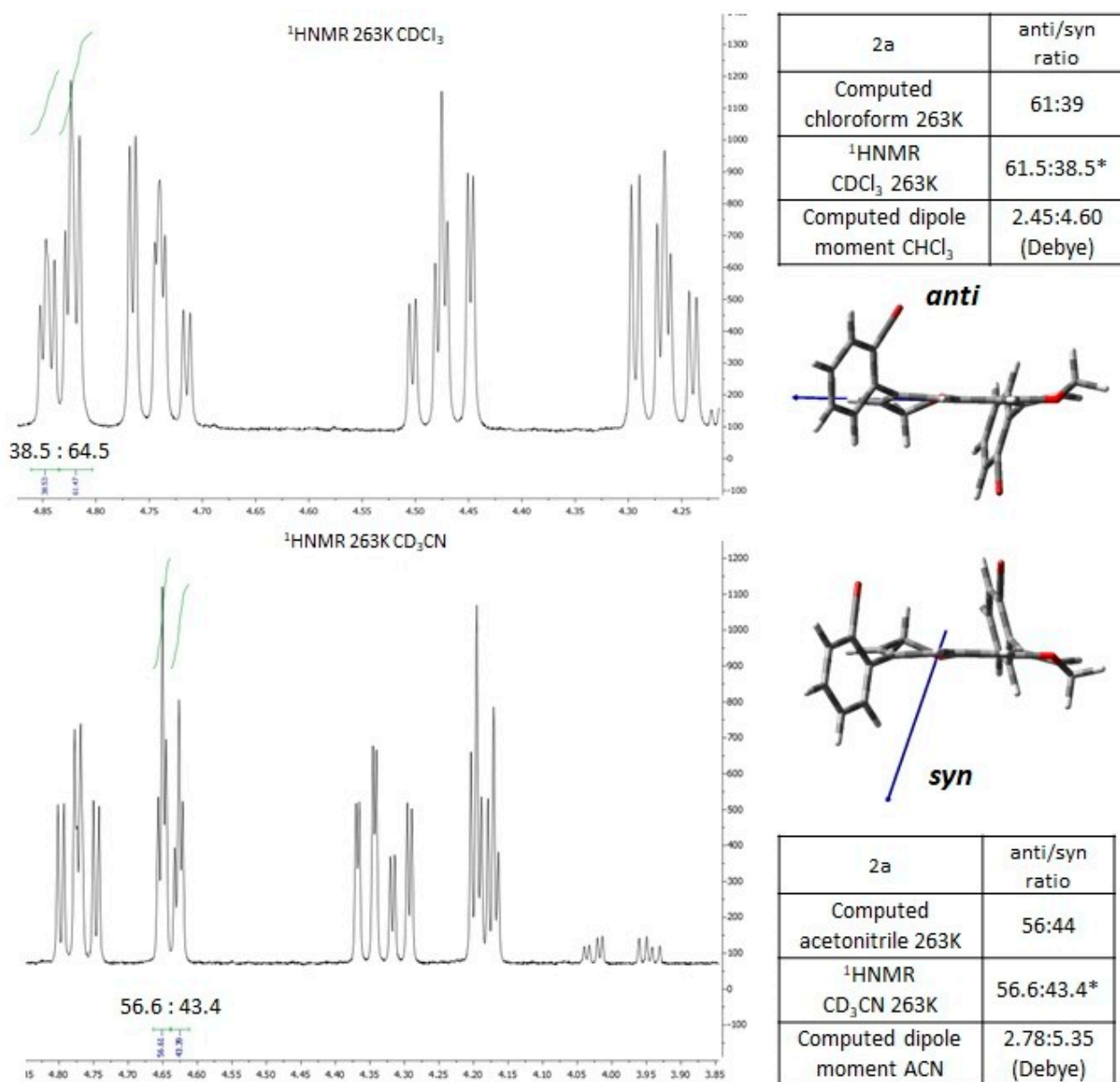
#### 4.2 DNMR experiment of compound 2a.



**Figure S7.** Simulated and experimental dynamic  $^1\text{H NMR}$  (600 MHz) spectra in  $\text{C}_2\text{D}_2\text{Cl}_4$  of compound **2a** for the enantiomerization process. For each temperature (left column) correspond a kinetic constant (right column). The vinylic  $^1\text{H NMR}$  signal at 5.77 ppm was homo-decoupled to simplify the spin system of adjacent  $\text{CH}_2$  from ABX to AB system.



**Figure S8.** Simulated and experimental dynamic <sup>1</sup>H NMR (600 MHz) spectra in C<sub>2</sub>D<sub>2</sub>Cl<sub>4</sub> of compound **2a** for the diastereomerization process. For each temperature (left column) correspond a kinetic constant (right column). The vinylic <sup>1</sup>H NMR signal at 5.77 ppm was homo-decoupled to simplify the spin system of adjacent CH<sub>2</sub> from ABX to AB system.

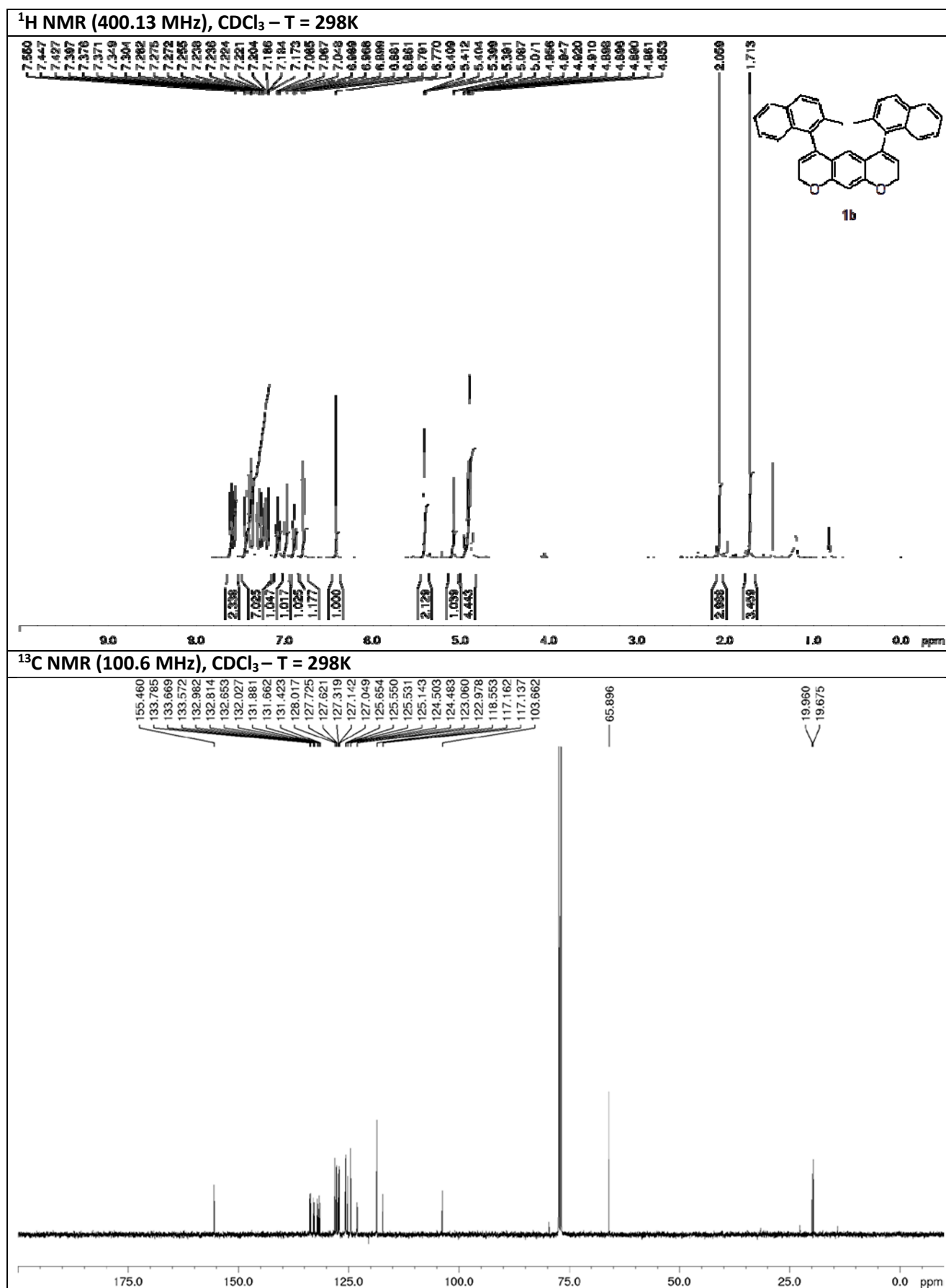


**Figure S9.** top: recorded <sup>1</sup>H NMR spectra of **2a** at -10 °C (263 K) in CDCl<sub>3</sub>, CH<sub>2</sub> signals (ABX system region).  
bottom: recorded <sup>1</sup>H NMR spectra of **2a** at -10 °C (263 K) in CD<sub>3</sub>CN, CH<sub>2</sub> signals (ABX system region).

\* Computed dipole moments were averaged using the Boltzmann population of the single GSs.

**5. Synthesis of 4,6-bis(2-methylnaphthalen-1-yl)-2*H*,8*H*-pyrano[3,2-*g*]chromene (**1b**) and 4,10-bis(2-methylnaphthalen-1-yl)-2*H*,8*H*-pyrano[2,3-*f*]chromene (**2b**):**

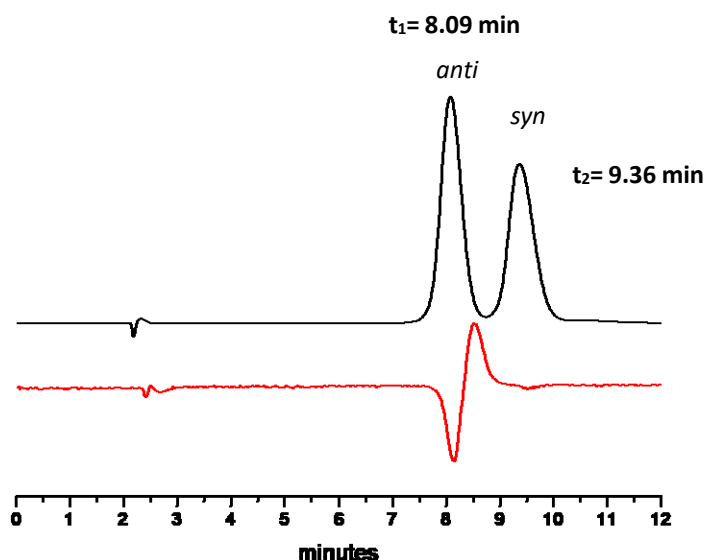
In a 50 mL Carousel Tube Reactor (Radely Discovery Technology) containing a magnetic stirring bar 1,3-bis((3-(2-methylnaphthalen-1-yl)prop-2-yn-1-yl)oxy)benzene (121 mg, 0.26 mmol, 1 equiv.) was dissolved in CH<sub>2</sub>Cl<sub>2</sub> (2 mL) at room temperature. Then [tris(2,4-di-*tert*-butylphenyl)phosphite]gold(I) chloride (9.1 mg, 0.01 mmol., 0.04 equiv.) was added followed by AgSbF<sub>6</sub> (3.6 mg, 0.01 mmol., 0.04 equiv.). The mixture was allowed to stir for an hour and then CH<sub>2</sub>Cl<sub>2</sub> was evaporated under reduced pressure. The residue was purified by chromatography on SiO<sub>2</sub> (25-40 μm), eluting with a 97/3 (v/v) *n*-hexane/AcOEt mixture to obtain a mixture of 4,6-bis(2-methylnaphthalen-1-yl)-2*H*,8*H*-pyrano[3,2-*g*]chromene **1b** and 4,10-bis(2-methylnaphthalen-1-yl)-2*H*,8*H*-pyrano[2,3-*f*]chromene **2b** in a ratio of 87/13. For product characterization see following sections.



**Figure S10.**  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra of compound **1b** mixture of isomers at +25 °C.

## 6. Full characterization of *syn/anti* 1b

*Syn/Anti* stereoisomers were separated by semipreparative HPLC on (*S,S*)-Whelk-O2 10 micron (250\*10 mm L\*ID) by using hexane/dichloromethane 95/5 + 0.1% ethanol at flow rate of 4.0 ml/min. Detector UV 254 nm. In the analytical version, geometry of column was 150\*4.6 mm L\*ID (chromatographic trace in **figure S11** (black trace). *Anti* and *syn* stereoisomers were assigned based on CD signal (see red trace on the same figure). After separation, <sup>1</sup>H-NMR spectra of two stereoisomer were acquired.

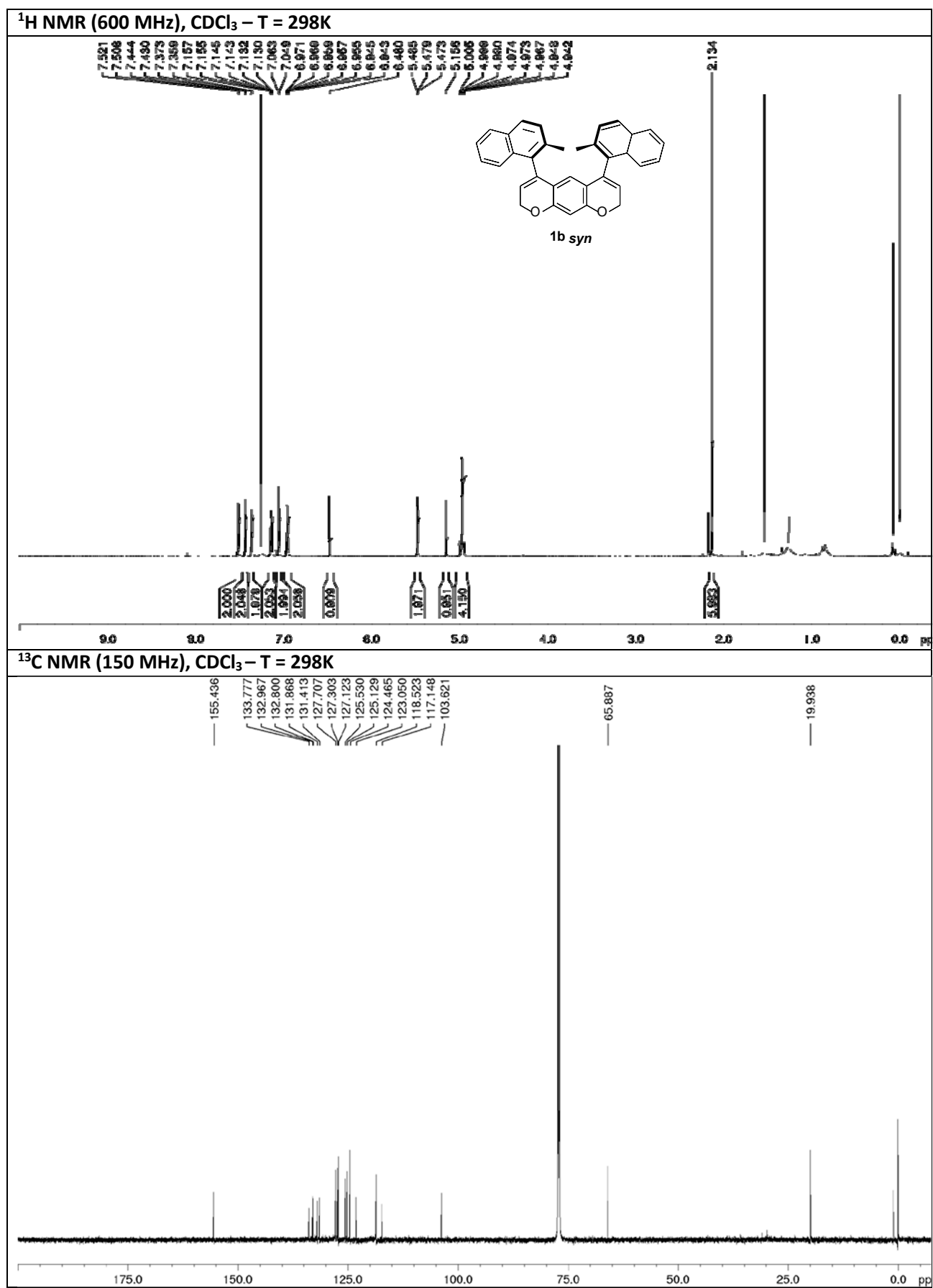


**Figure S11.** HPLC separation on (*S,S*)-Whelk-O2 10 micron (250\*10 mm L\*ID) by using *n*-hexane/dichloromethane 95/5 + 0.1% ethanol at flow rate of 4.0 ml/min. Detector UV 254 nm. In the analytical version, geometry of column was 150\*4.6 mm L\*ID (chromatographic black trace). *Anti* and *syn* stereoisomers were assigned based on CD signal (red trace).

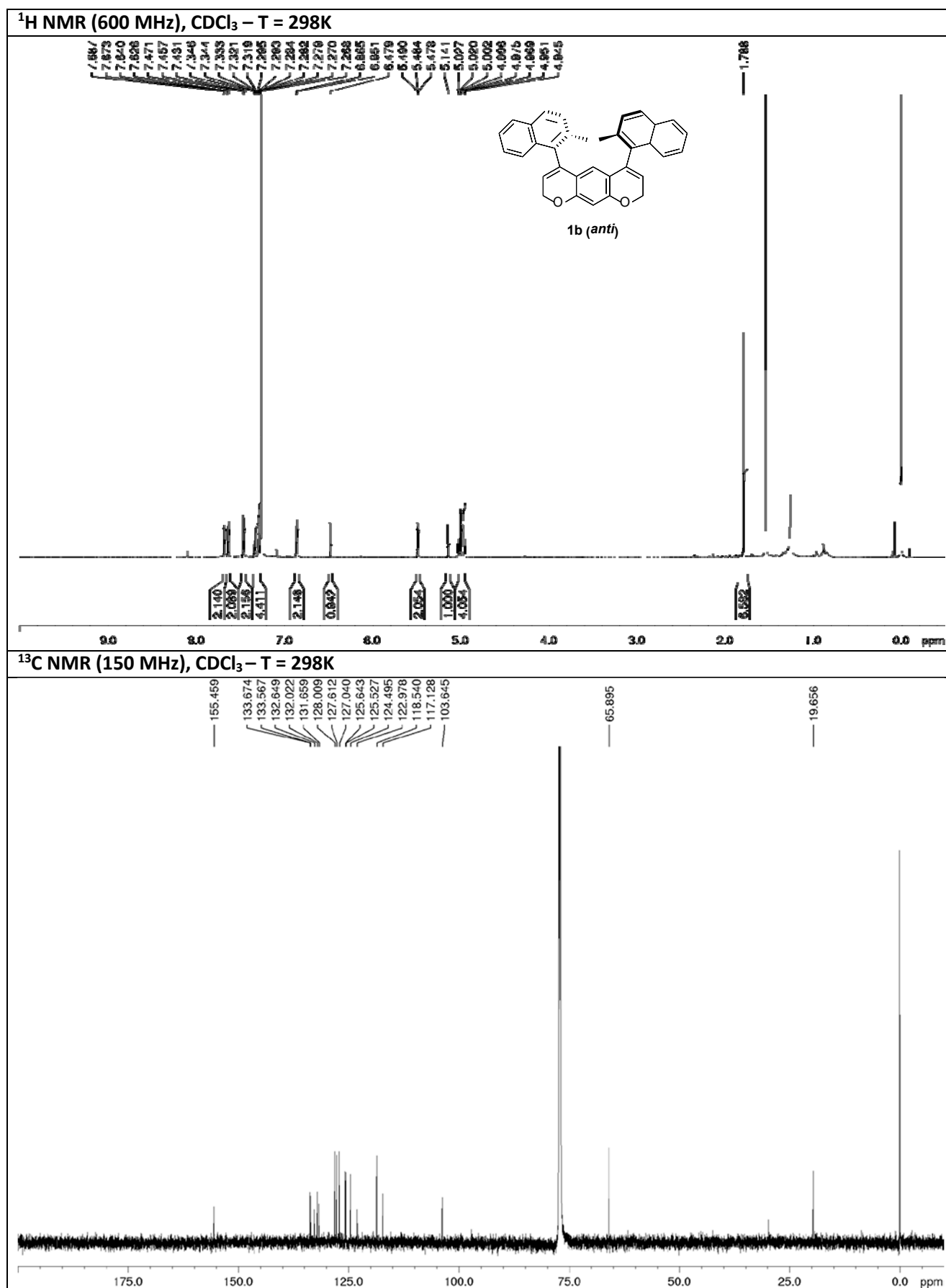
**1b (*syn*):** <sup>1</sup>H NMR (600 MHz) (CDCl<sub>3</sub>): d (ppm) 7.51 (d, *J* = 5.4 Hz, 2H), 7.44 (d, *J* = 5.5 Hz, 2H), 7.37 (d, *J* = 5.6 Hz, 2H), 7.16 – 7.13 (m, 2H), 7.06 (d, *J* = 5.6 Hz, 2H), 6.97 – 6.94 (m, 2H), 6.48 (s, 1H), 5.48 (t, *J* = 2.4 Hz, 2H), 5.16 (s, 1H), 5.00 – 4.94 (m, 4H), 2.13 (s, 6H); <sup>13</sup>C{<sup>1</sup>H} NMR (150 MHz) (CDCl<sub>3</sub>): d (ppm) 155.4, 133.8, 133.0, 132.8, 131.9, 131.4, 127.7, 127.3, 127.1, 125.5, 125.1, 124.5, 123.0, 118.5, 117.1, 103.6, 65.9, 19.9.

**1b (*anti*):** <sup>1</sup>H NMR (600 MHz) (CDCl<sub>3</sub>): d (ppm) 7.68 (d, *J* = 5.3 Hz, 2H), 7.63 (d, *J* = 5.5 Hz, 2H), 7.46 (d, *J* = 5.6 Hz, 2H), 7.35 – 7.27 (m, 4H), 6.86 (d, *J* = 5.6 Hz, 2H), 6.48 (s, 1H), 5.48 (t, *J* = 2.4 Hz, 2H), 5.14 (s, 1H), 5.03 – 4.94 (m, 4H), 1.79 (s, 6H); <sup>13</sup>C{<sup>1</sup>H} NMR (150 MHz) (CDCl<sub>3</sub>): d (ppm) 155.5, 133.7, 133.6, 132.6, 132.0, 131.7, 128.0, 127.6, 127.0, 125.6, 125.5, 124.5, 123.0, 118.5, 117.1, 103.6, 65.9, 19.6.



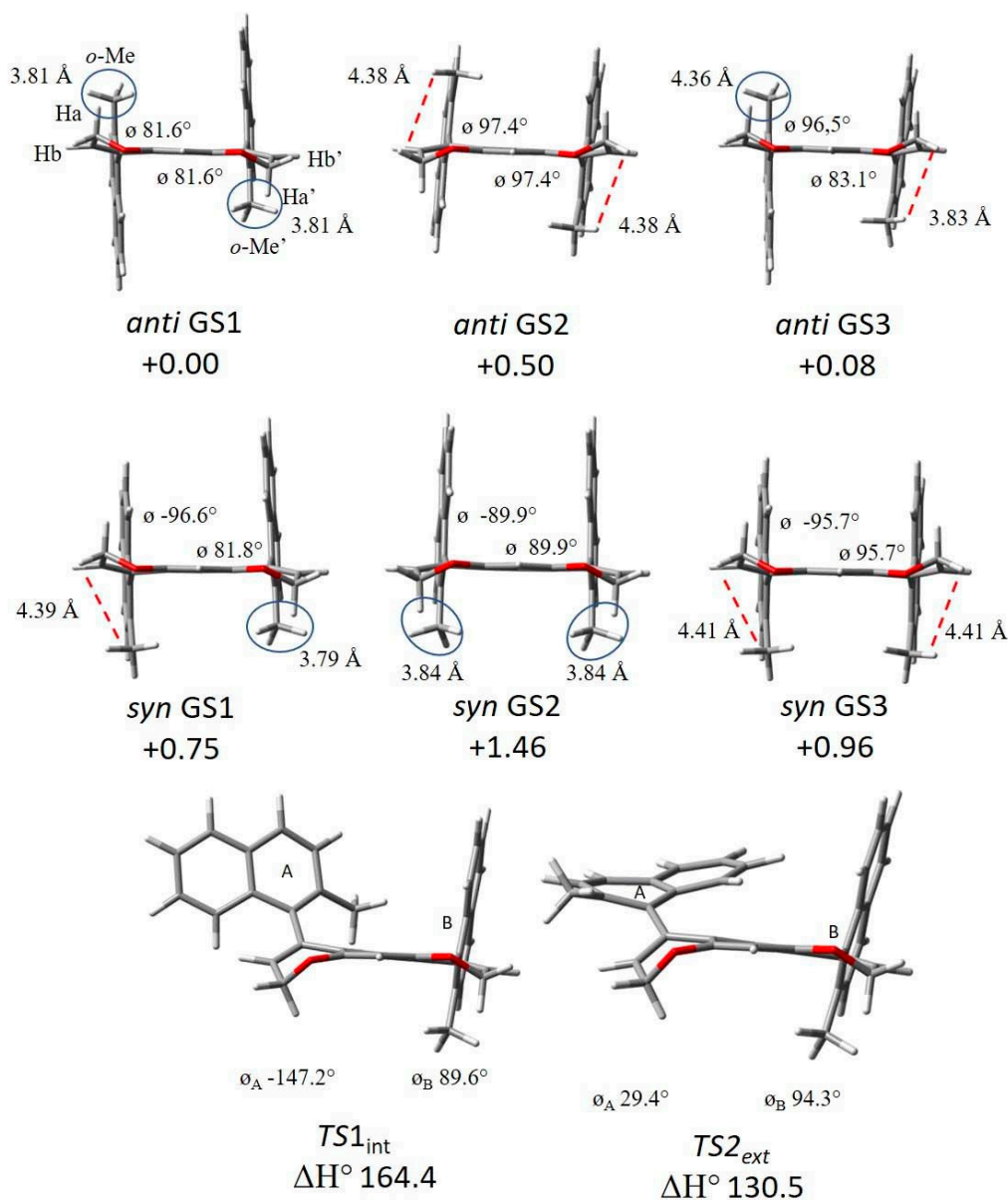


**Figure S12.** <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound **1b (syn)** at +25 °C.



**Figure S13.** <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound **1b (anti)** at +25 °C.

## 6.1 DFT Calculations of *syn/anti* for compounds **1b**

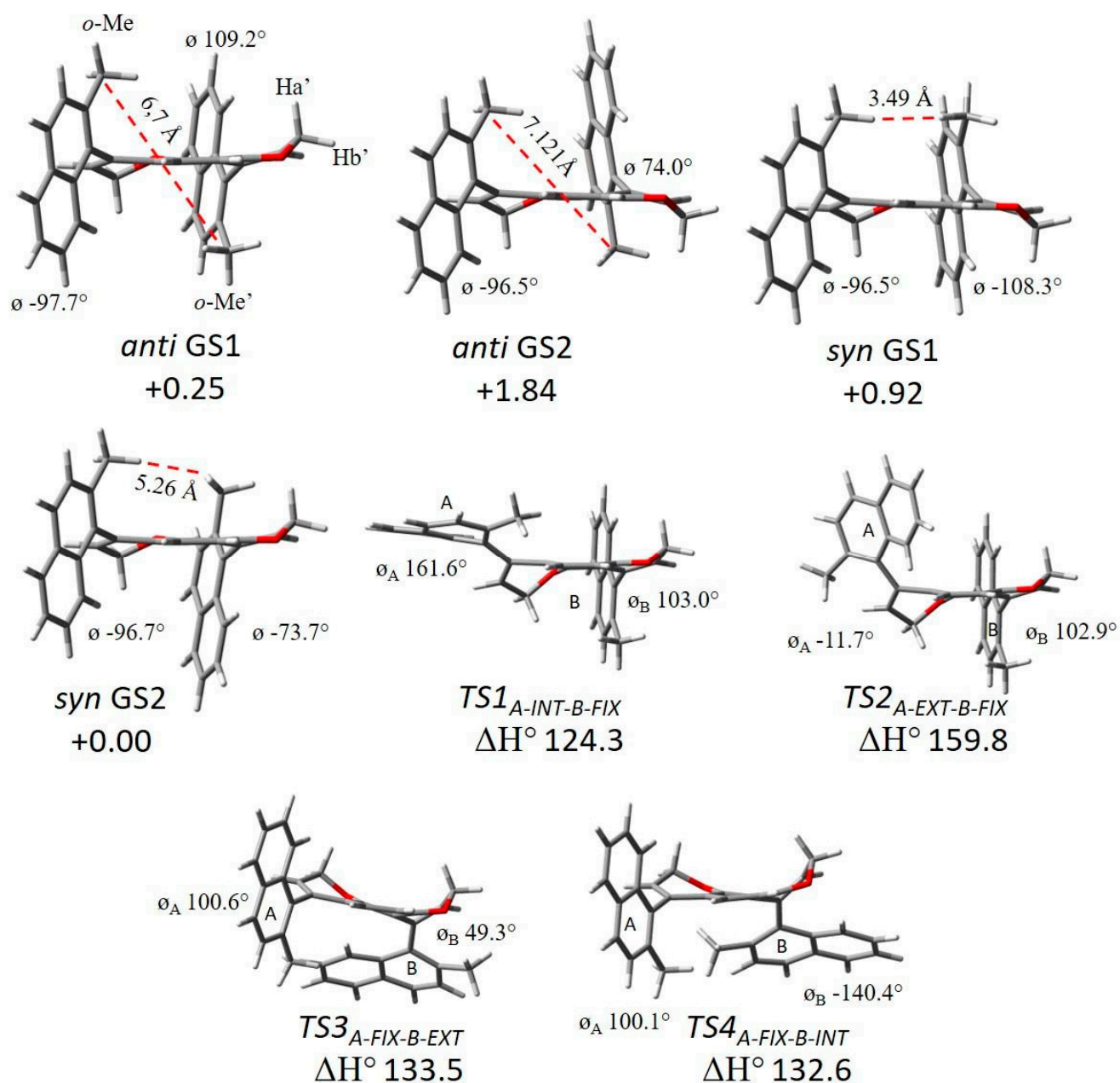


**Figure S14.** Predicted DFT (6-31+G(d,p), PCM=chloroform) conformations of *syn/anti* for compounds **1b** are shown. The relative Enthalpy energies are reported in kJ/mol.

**Table S2.** Descriptors are shown: *r* = atom distance;  $\phi$  = dihedral angle

<b>1b</b>	<b><i>r</i> (H<sub>a</sub> - <i>o</i>Me)</b>	<b><i>r</i> (H<sub>b</sub> - <i>o</i>Me)</b>	<b><i>r</i> (H<sub>a</sub>' - <i>o</i>Me')</b>	<b><i>r</i> (H<sub>b</sub>' - <i>o</i>Me')</b>	<b><math>\phi_A</math></b>	<b><math>\phi_B</math></b>	<b>% <i>pop</i></b>
GS1 <i>anti</i>	3.81	5.03	3.81	5.03	81.60	81.60	20.10
GS2 <i>anti</i>	5.17	4.38	5.17	4.38	97.40	97.40	17.02
GS3 <i>anti</i>	4.36	5.16	5.00	3.83	96.50	83.10	19.31
GS1 <i>syn</i>	5.19	4.39	3.79	5.01	-96.60	81.80	15.80
GS2 <i>syn</i>	3.84	5.00	3.84	5.00	-89.90	89.90	12.90
GS3 <i>syn</i>	5.22	4.41	5.22	4.41	-95.74	95.71	14.80
avg. <i>anti</i> vs <i>syn</i>	4.40 vs 4.80	4.87 vs 4.58	4.63 vs 4.29	4.42 vs 4.80	91.5 vs -94.3	86.9 vs 88.1	56/44

## 6.2 DFT Calculations of *syn/anti* for compounds **2b**

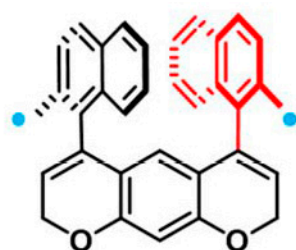
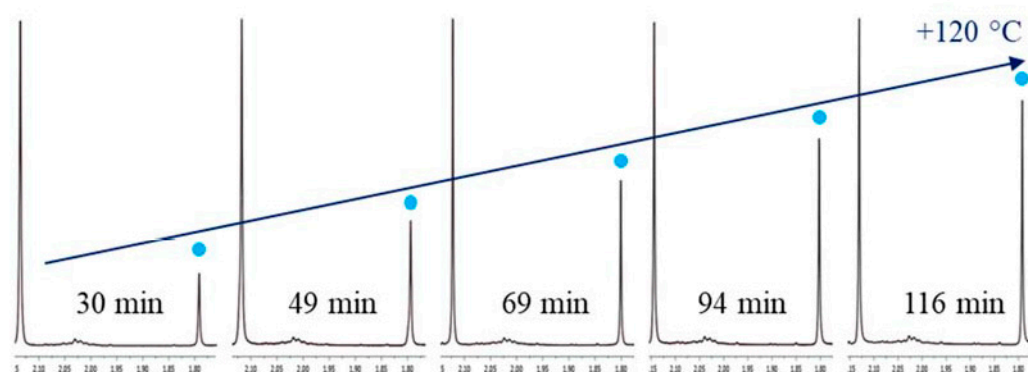


**Figure S15.** Predicted DFT (6-31+G(d,p), PCM=chloroform) conformations of *syn/anti* for compounds **2b** are shown. The relative Enthalpy energies are reported in kJ/mol.

**Table S3.** Descriptors are shown: *r* = atom distance;  $\phi$  = dihedral angle

<b>2b</b>	<b>r (oMe - oMe)</b>	<b><math>\phi_A</math></b>	<b><math>\phi_B</math></b>	<b>% <i>pop</i></b>
GS1 <i>anti</i>	6.70	-97.70	109.20	28.96
GS2 <i>anti</i>	7.11	-96.50	74.00	14.65
GS1 <i>syn</i>	3.49	-96.50	-108.30	22.55
GS2 <i>syn</i>	5.26	-96.70	-73.70	33.83
avg. <i>anti</i> vs <i>syn</i>	7.17 vs 4.53	-96.8 vs -96.2	97.0 vs -87.8	44/56

### 6.3 Kinetic Study at 120 °C – $^1\text{H}$ NMR

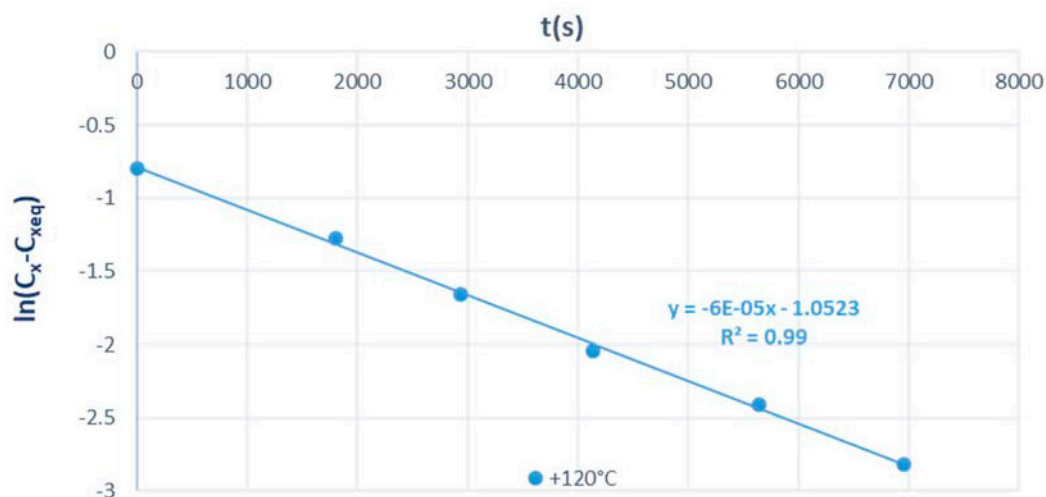


**1b anti**

120 °C

t (s)	ln (Cx - Cxeq)
0	-0.7985077
1800	-1.27296568
2940	-1.66073121
4140	-2.04022083
5640	-2.40794561
6960	-2.81341072

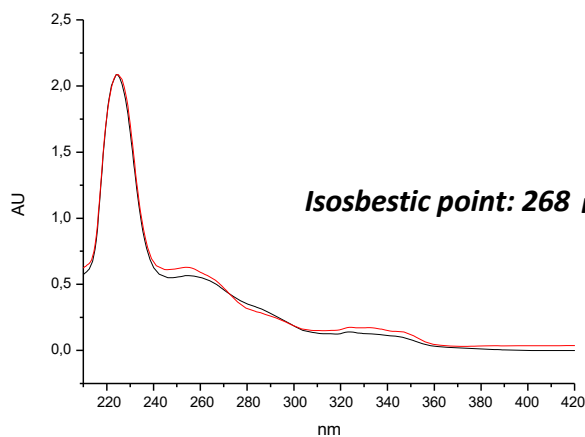
$$\Delta G^\ddagger_{120^\circ\text{C}} = 129.3 \text{ kJ/mol}$$



**Figure S16.** Kinetic studies of reversible first-order diastereomerization of **1b**. A sample of the first eluted atropisomer was heated in tube NMR at +120 °C (bath oil) constant temperature in 1,1,2,2-tetrachloroethane- $d_2$ . After cooling at room temperature,  $^1\text{H}$  NMR was acquired at different times and analyzed the integrals of methyl signals to measure the atropisomeric diastereomerization. Xa molar fraction of first eluted atropisomer. Xaeq molar fraction at equilibrium.

#### 6.4 Kinetic off-column of *syn/anti* interconversion of **1b**

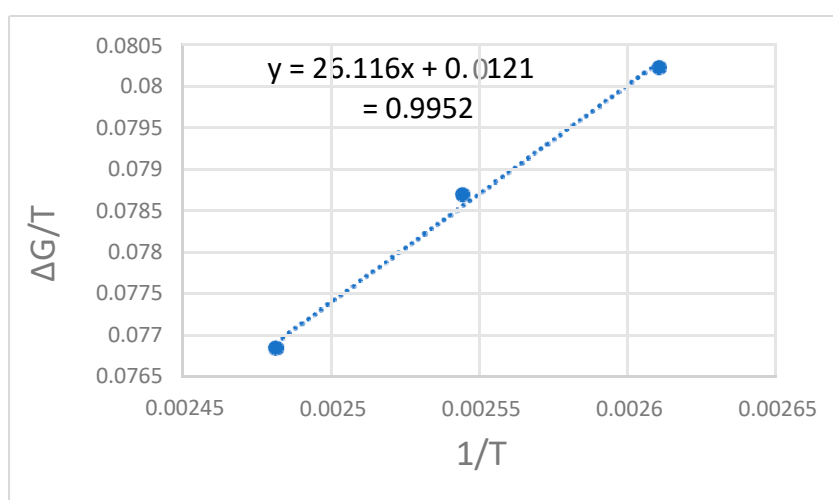
Analytical conditions: (S,S)-Whelk-O2 10 micron (250\*4.6 mm L\*ID) by using *n*-hexane/dichloromethane 95/5 + 0.1% ethanol at flow rate of 1.0 mL/min. Detector UV 268 nm.



**Figure S17.** Overlapped UV spectra of two *syn/anti* isomers after separation at the same concentration.

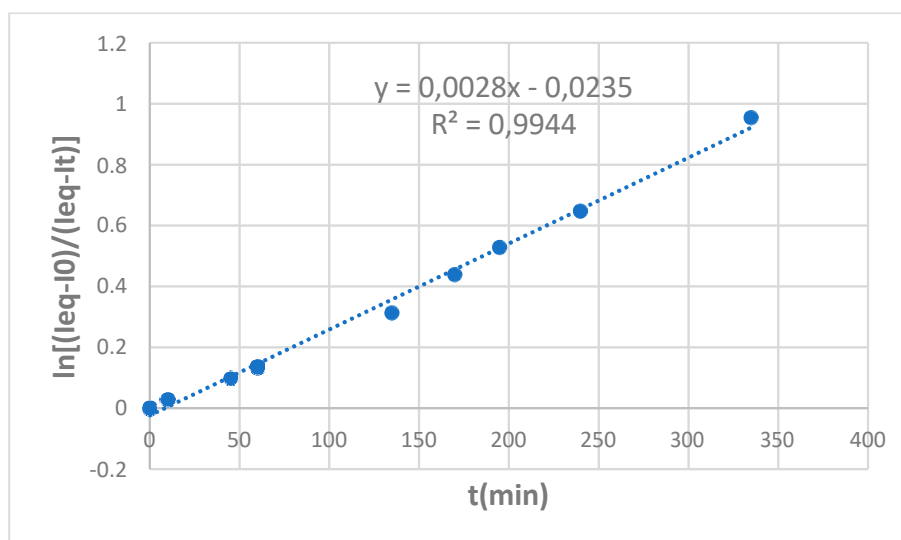
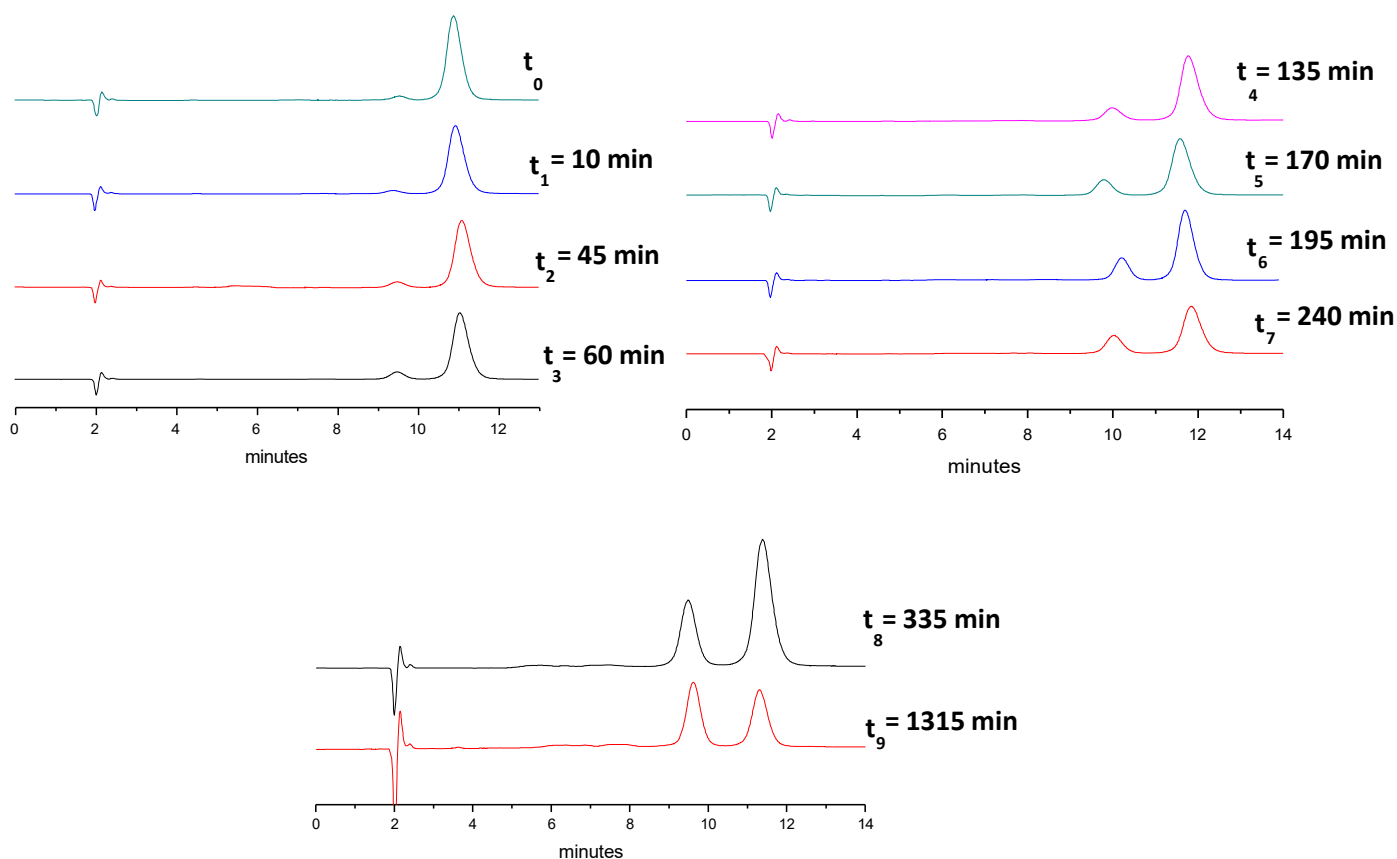
**Table S4.** Data related to kinetic at different temperatures.

T (°C)	K <sub>eq</sub>	k (min <sup>-1</sup> )	k <sub>-1</sub> (min <sup>-1</sup> )	ΔG (Kcal/mol)	ΔG (KJ/mol)
110	0,996	0,00139	0,00140	30,74	128,61
120	0,996	0,00309	0,00310	30,94	129,45
130	0,996	0,00808	0,00811	30,98	129,61



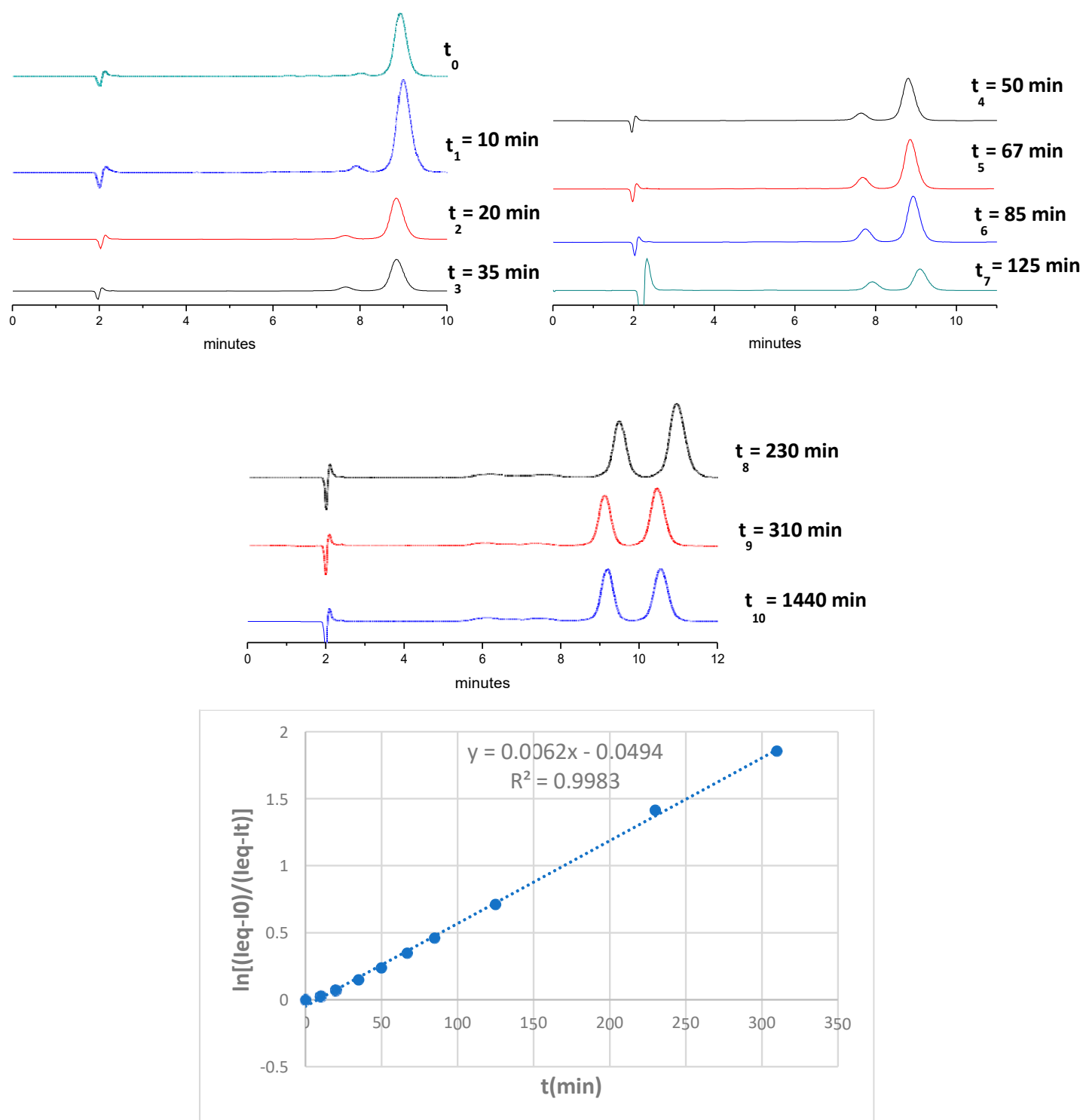
**Figure S18:** Eyring plot of Kinetic off-column of *syn/anti* interconversion of **1b**.

#### 6.4.1 Kinetic study at 110 °C



**Figure S19.** Kinetic studies of reversible first-order diastereomerization of **1b**. A sample of the second eluted atropisomer was heated in tube NMR at +110 °C (bath oil) constant temperature in cis/trans decaline. After the time reported the sample was cooled at room temperature and analyzed by HPLC.

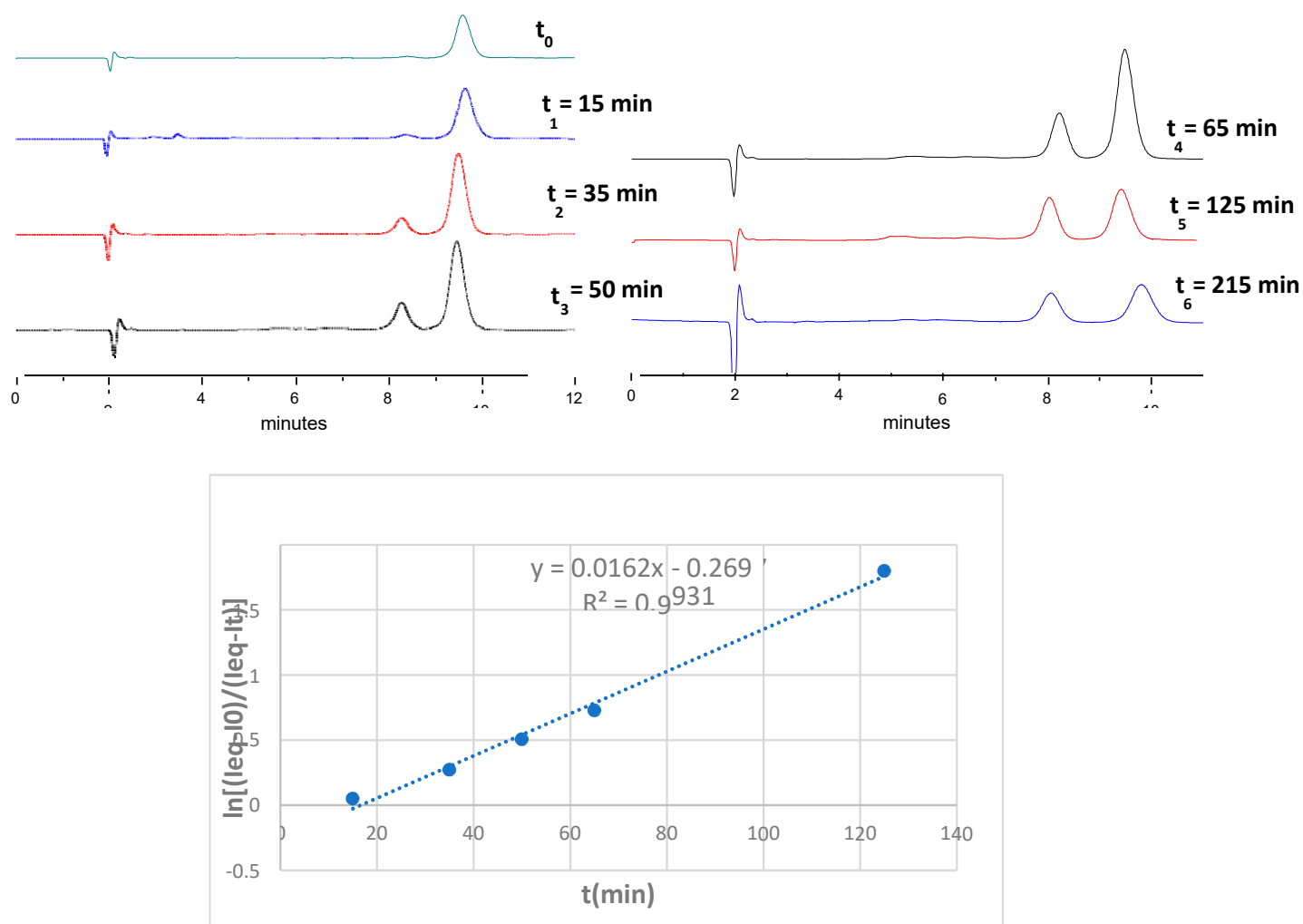
# Kinetic study at 120 °C



**Figure S20.** Kinetic studies of reversible first-order diastereomerization of **1b**. A sample of the second eluted atropisomer was heated in tube NMR at +120 °C (bath oil) constant temperature in cis/trans decaline. After the time reported the sample was cooled at room temperature and analyzed by HPLC.

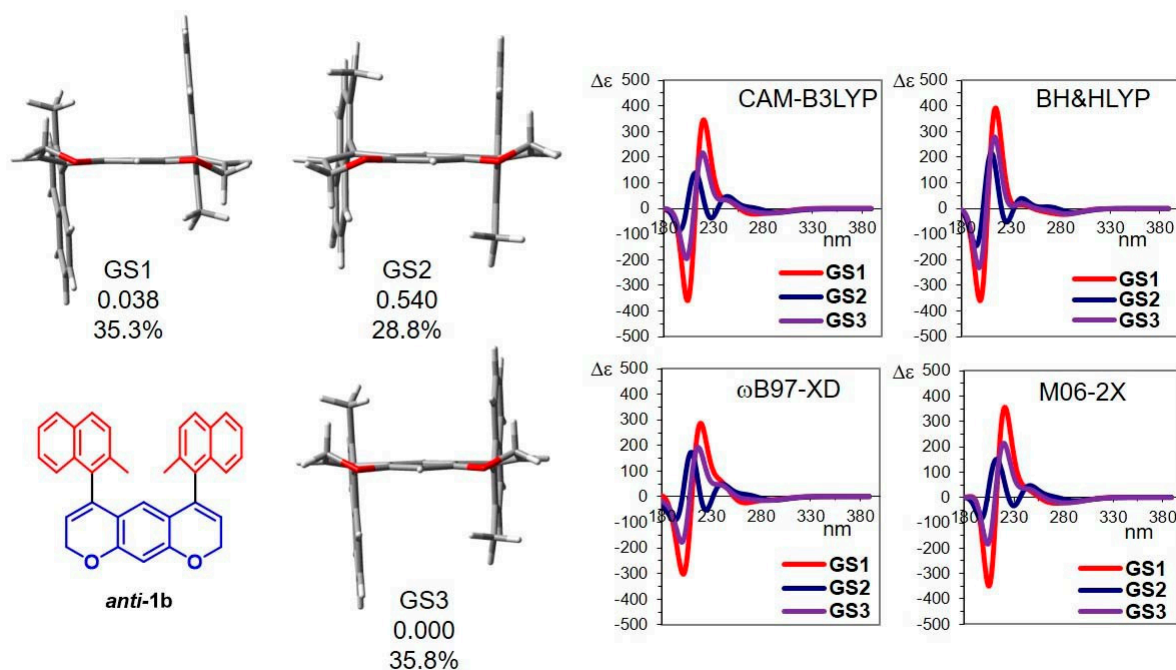


#### 6.4.2 Kinetic study at 130 °C



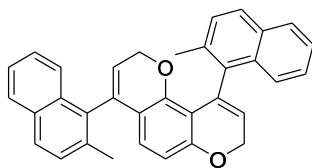
**Figure S21.** Kinetic studies of reversible first-order diastereomerization of **1b**. A sample of the second eluted atropisomer was heated in tube NMR at +110 °C (bath oil) constant temperature in cis/trans decaline. After the time reported the sample was cooled at room temperature and analyzed by HPLC.

## 6.5 ECD of 1b:



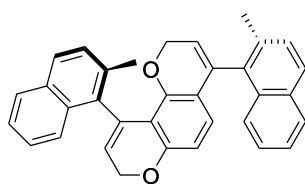
**Figure S22.** ECD studies of compound **anti-1b**. In the Figure was reported all the simulated ECD spectra of GSs with the different functionals and same basis set 6-311++G(2d,p), PCM=acetonitrile. The sum of spectra was reported in the main text.

## 7. Characterization of 2b



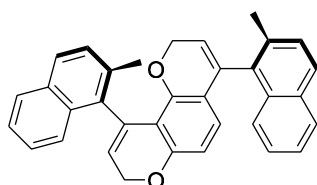
**2b**

*Syn/Anti* stereoisomers were separated by semipreparative CSP-HPLC on Chiralpak IB-N5 (250\*10 mm L\*ID) by using *n*-hexane/chloroform 85/15 at flow rate of 5.0 ml/min. Detector UV 254 nm. *Anti* and *syn* stereoisomers were assigned based on  $^1\text{H}$  NMR and NOE effect.



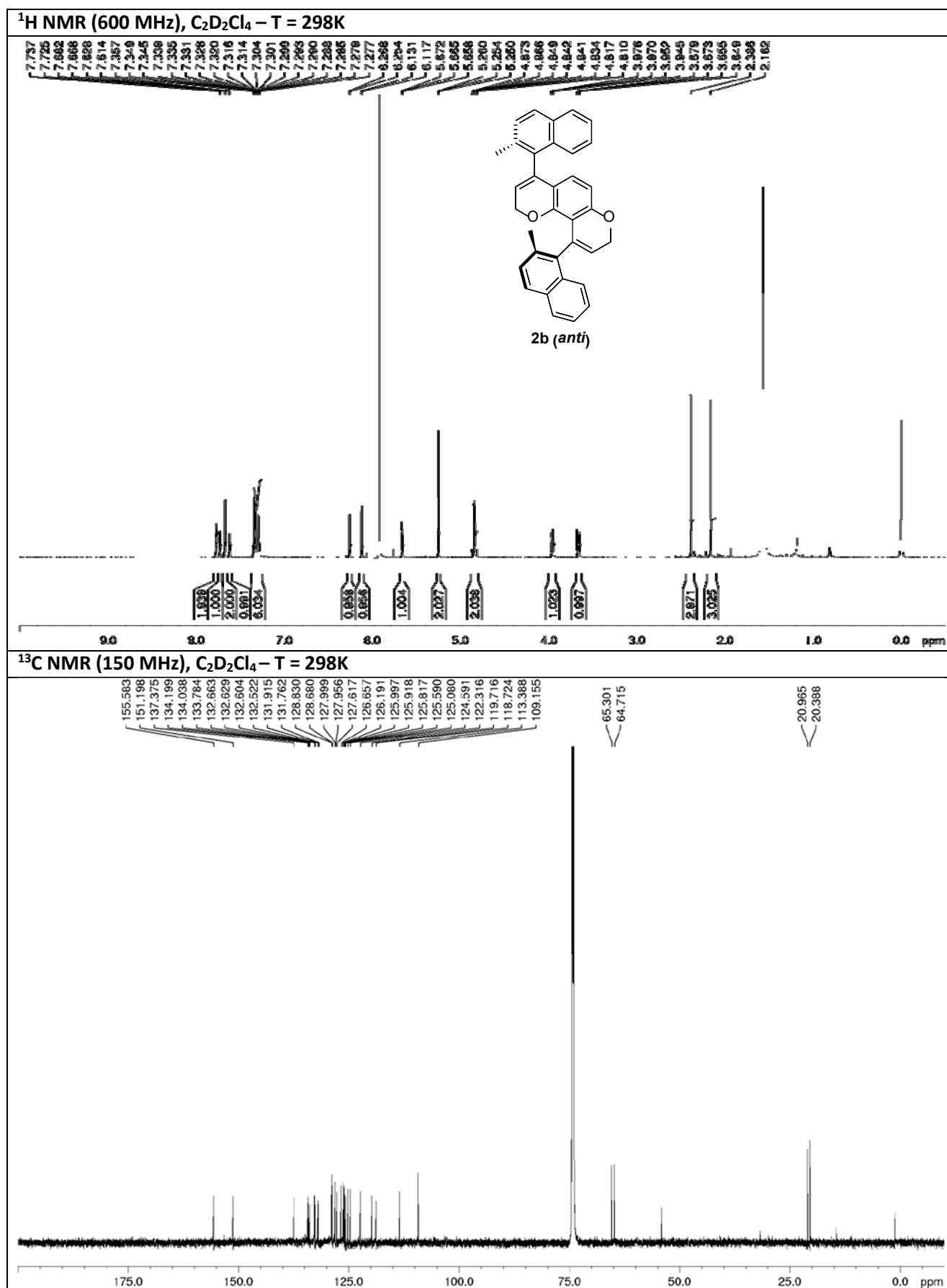
**2b (*anti*)**

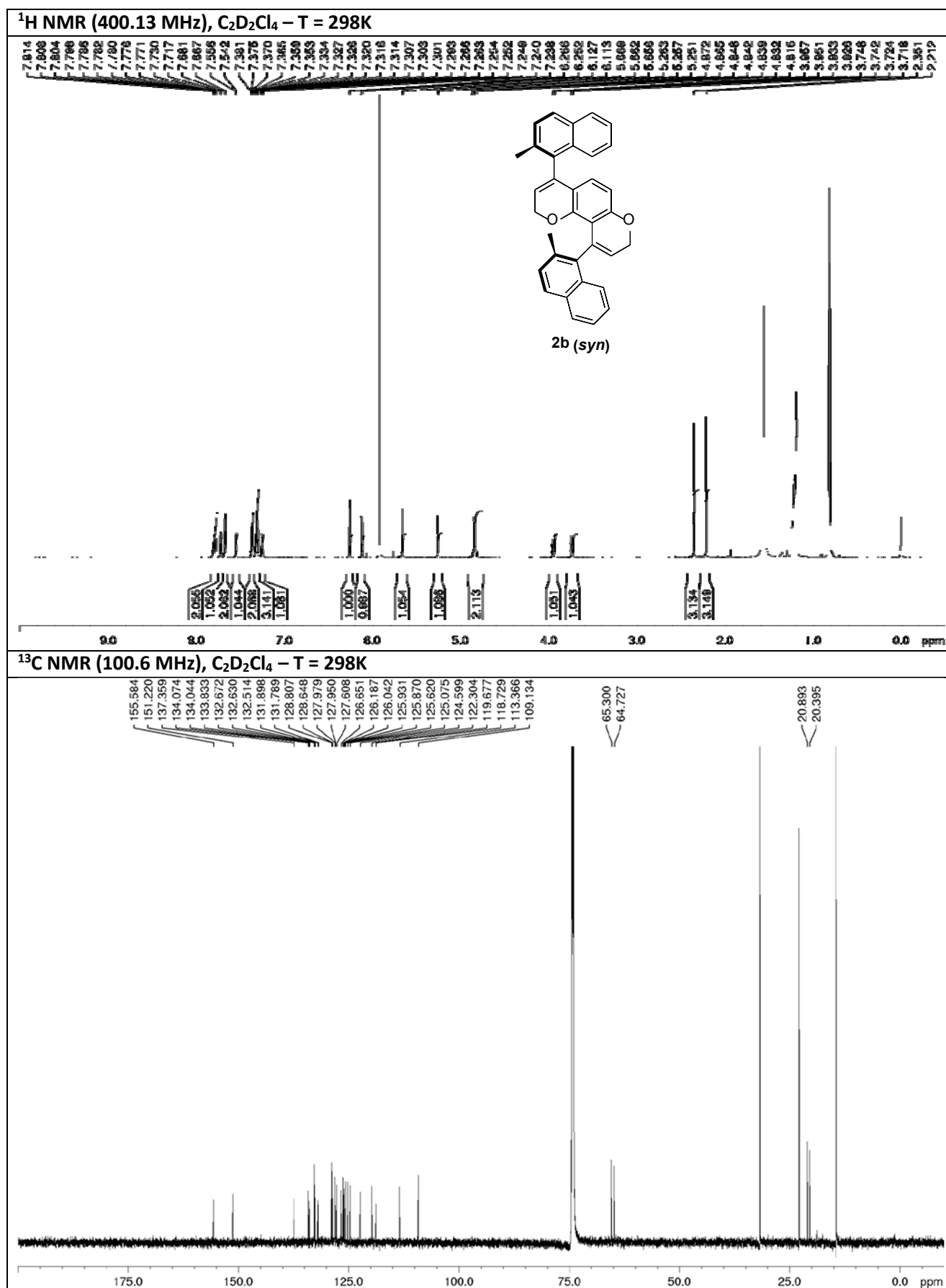
**2b (*anti*):**  $^1\text{H}$  NMR (600 MHz) ( $\text{C}_2\text{D}_2\text{Cl}_4$ ):  $\delta$  (ppm) 7.78 – 7.76 (m, 2 H), 7.73 (d,  $J$  = 5.0 Hz, 1 H), 7.67 (d,  $J$  = 5.6 Hz, 2 H), 7.62 (d,  $J$  = 5.5 Hz, 1 H), 7.36 – 7.28 (m, 6 H), 7.26 – 7.24 (m, 2 H), 6.26 (d,  $J$  = 5.6 Hz, 1 H), 6.12 (d,  $J$  = 5.6 Hz, 1 H), 5.66 (t,  $J$  = 2.7 Hz, 1 H), 5.25 (, t,  $J$  = 2.5 Hz, 1 H), 5.25 (s, 1 H), 4.87 – 4.81 (m, 2 H), 3.96 (dd,  $J_1$  = 9.8 Hz,  $J_2$  = 2.6 Hz, 1 H), 3.66 (dd,  $J_1$  = 9.8 Hz,  $J_2$  = 2.4 Hz, 1 H), 2.39 (s, 3 H), 2.16 (s, 3 H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (150 MHz) ( $\text{C}_2\text{D}_2\text{Cl}_4$ ):  $\delta$  (ppm) 155.6, 151.2, 137.4, 134.2, 134.0, 133.8, 132.7, 132.63, 132.60, 132.5, 131.9, 131.8, 128.8, 128.7, 128.0, 127.9, 127.6, 126.6, 126.2, 126.0, 125.9, 125.8, 125.6, 125.1, 124.6, 122.3, 119.7, 118.7, 113.4, 109.1, 65.3, 64.7, 21.0, 20.4.



**2b (*syn*)**

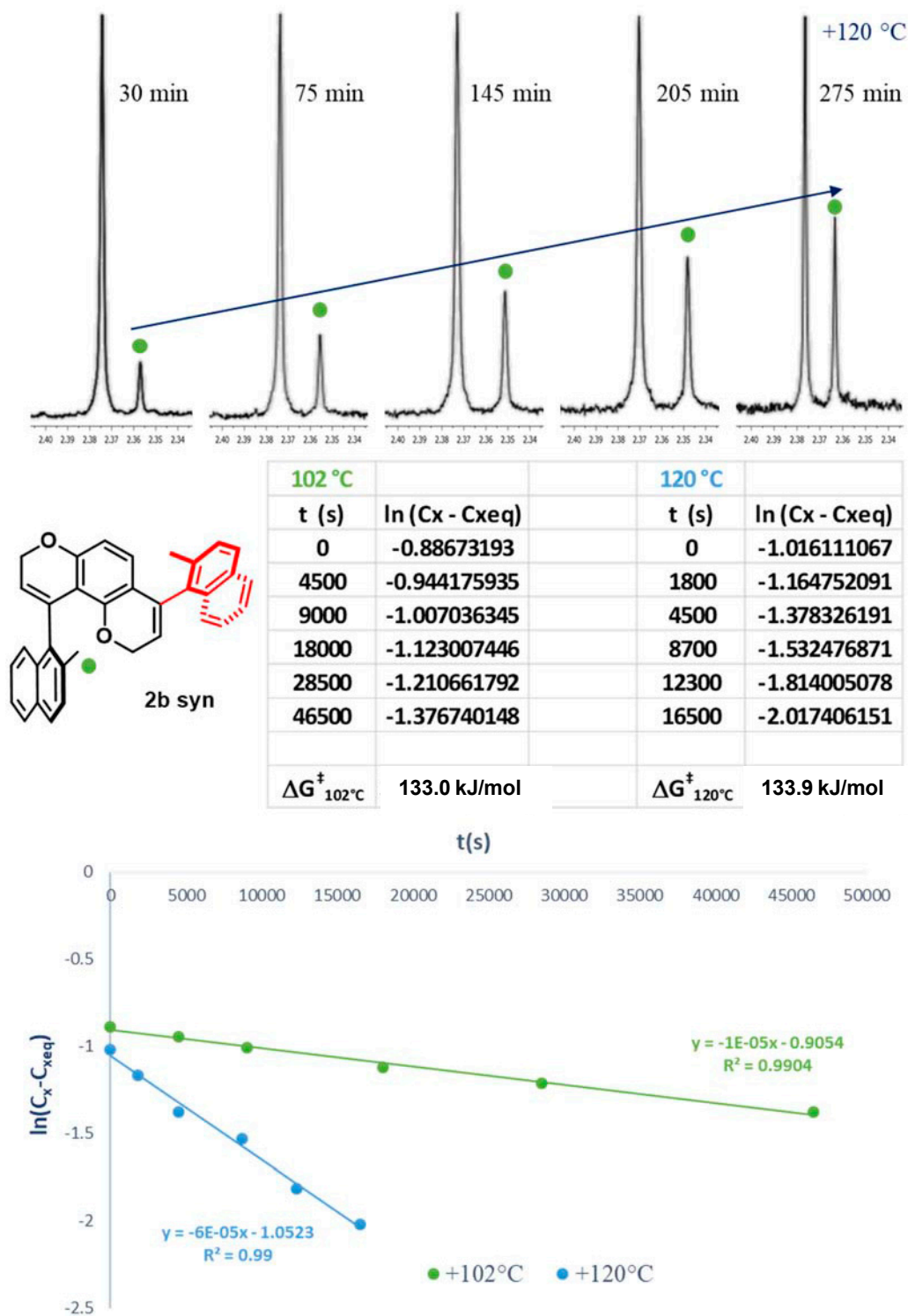
**2b (*syn*):**  $^1\text{H}$  NMR (600 MHz) ( $\text{C}_2\text{D}_2\text{Cl}_4$ ):  $\delta$  (ppm) 7.81 – 7.76 (m, 2 H), 7.72 (d,  $J$  = 5.3 Hz, 1 H), 7.67 (d,  $J$  = 5.5 Hz, 2 H), 7.55 (d,  $J$  = 5.6 Hz, 1 H), 7.38 – 7.35 (m, 2 H), 7.33 – 7.29 (m, 3 H), 7.26 – 7.24 (m, 2 H), 6.26 (d,  $J$  = 5.6 Hz, 1 H), 6.12 (d,  $J$  = 5.6 Hz, 1 H), 5.66 (t,  $J$  = 2.7 Hz, 1 H), 5.26 (, t,  $J$  = 2.5 Hz, 1 H), 4.87 – 4.81 (m, 2 H), 3.94 (dd,  $J_1$  = 9.8 Hz,  $J_2$  = 2.6 Hz, 1 H), 3.73 (dd,  $J_1$  = 9.8 Hz,  $J_2$  = 2.5 Hz, 1 H), 2.35 (s, 3 H), 2.21 (s, 3 H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (150 MHz) ( $\text{C}_2\text{D}_2\text{Cl}_4$ ):  $\delta$  (ppm) 155.6, 151.2, 137.4, 134.1, 134.0, 133.8, 132.7, 132.6, 132.5, 131.9, 131.8, 128.8, 128.6, 128.0, 127.9, 127.6, 126.6, 126.2, 126.0, 125.9, 125.6, 125.1, 124.6, 122.3, 119.7, 118.7, 113.4, 109.1, 65.3, 64.7, 20.9, 20.4.





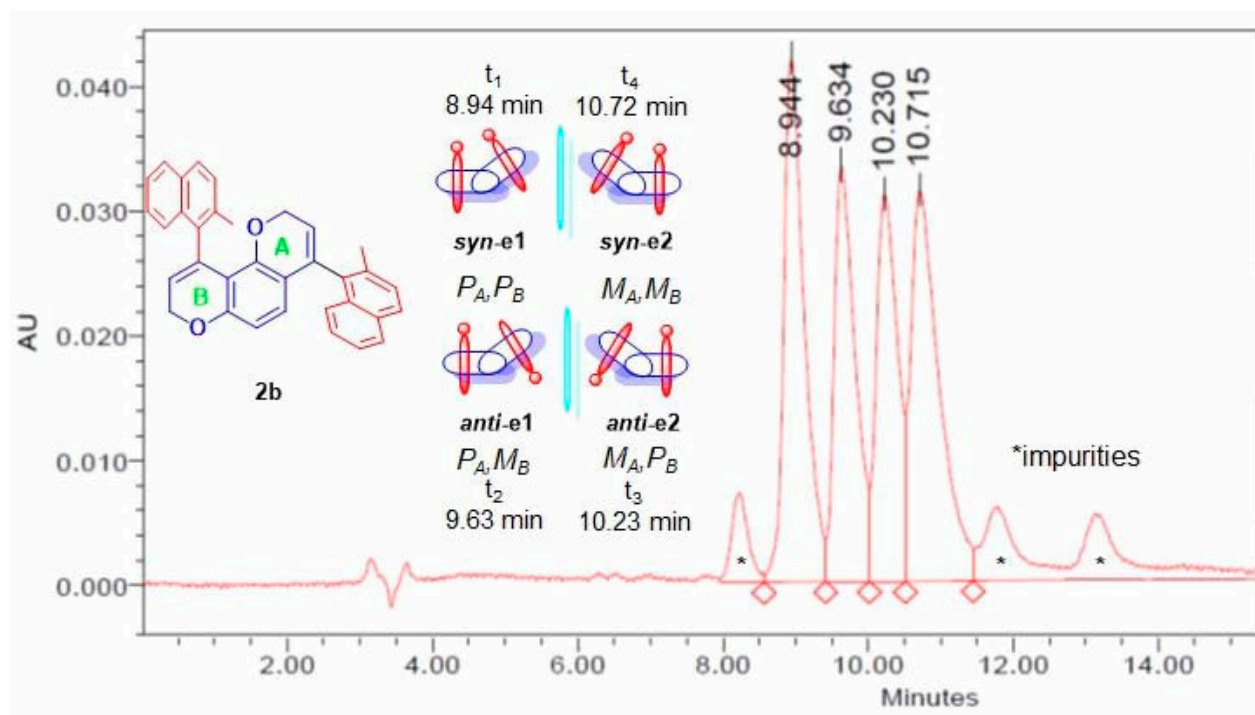
**Figure S24.** <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound **2b (syn)** at +25 °C.

## 7.1 Kinetic Study at 102 °C and 120 °C - <sup>1</sup>H NMR

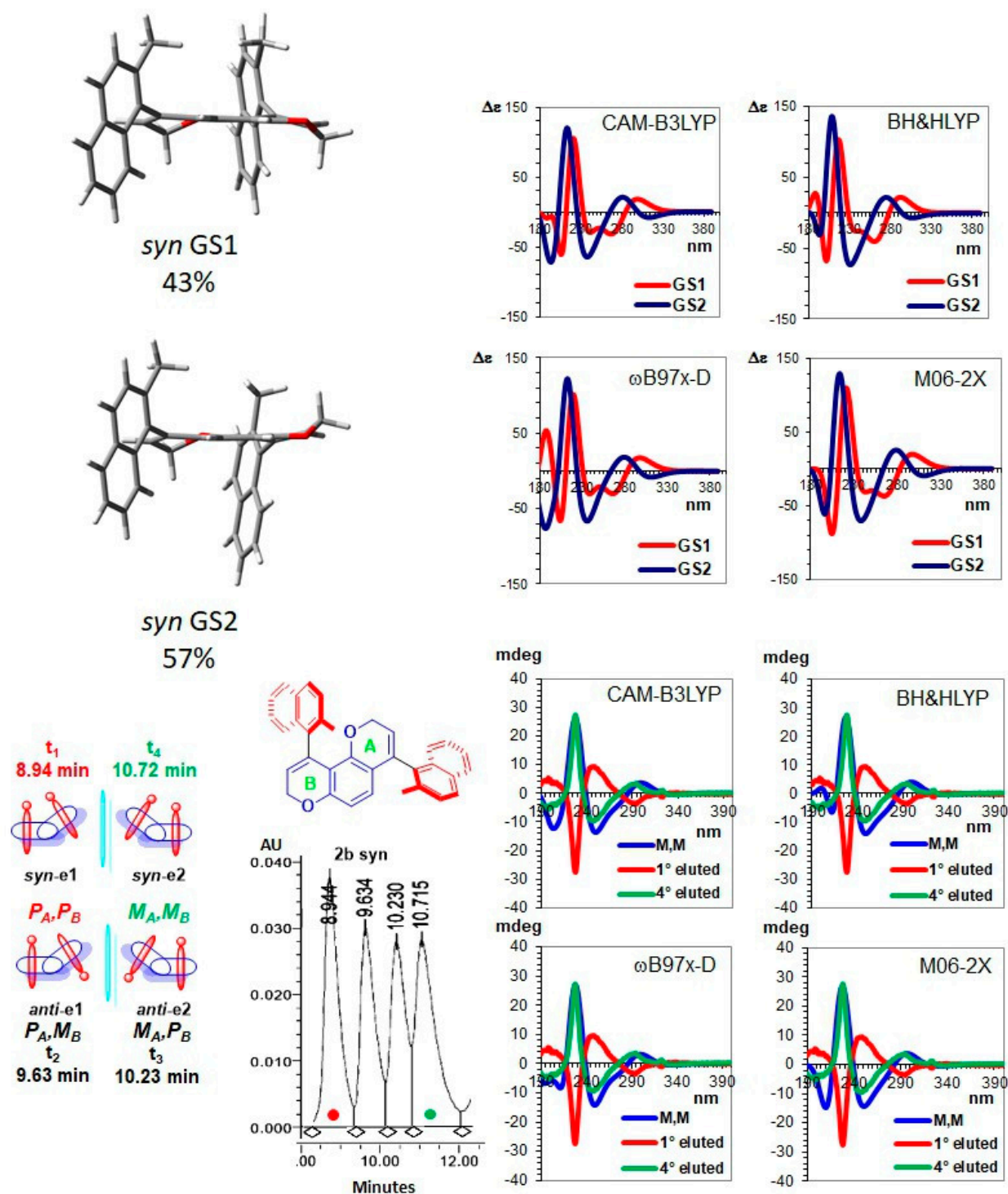


**Figure S25.** Kinetic studies of reversible first-order diastereomerization of **2b**. A sample of the first eluted atropisomer was heated in tube NMR at +102 °C and +120°C (bath oil) constant temperature in 1,1,2,2-tetrachloroethane-d<sub>2</sub>. After cooling at room temperature, <sup>1</sup>H NMR was acquired at different times and analyzed the integrals of methyl signals to measure the atropisomeric diastereomerization. X<sub>a</sub> molar fraction of first eluted atropisomer. X<sub>aeq</sub> molar fraction at equilibrium.

## 7.2 CSP separation and ECD of 2b:

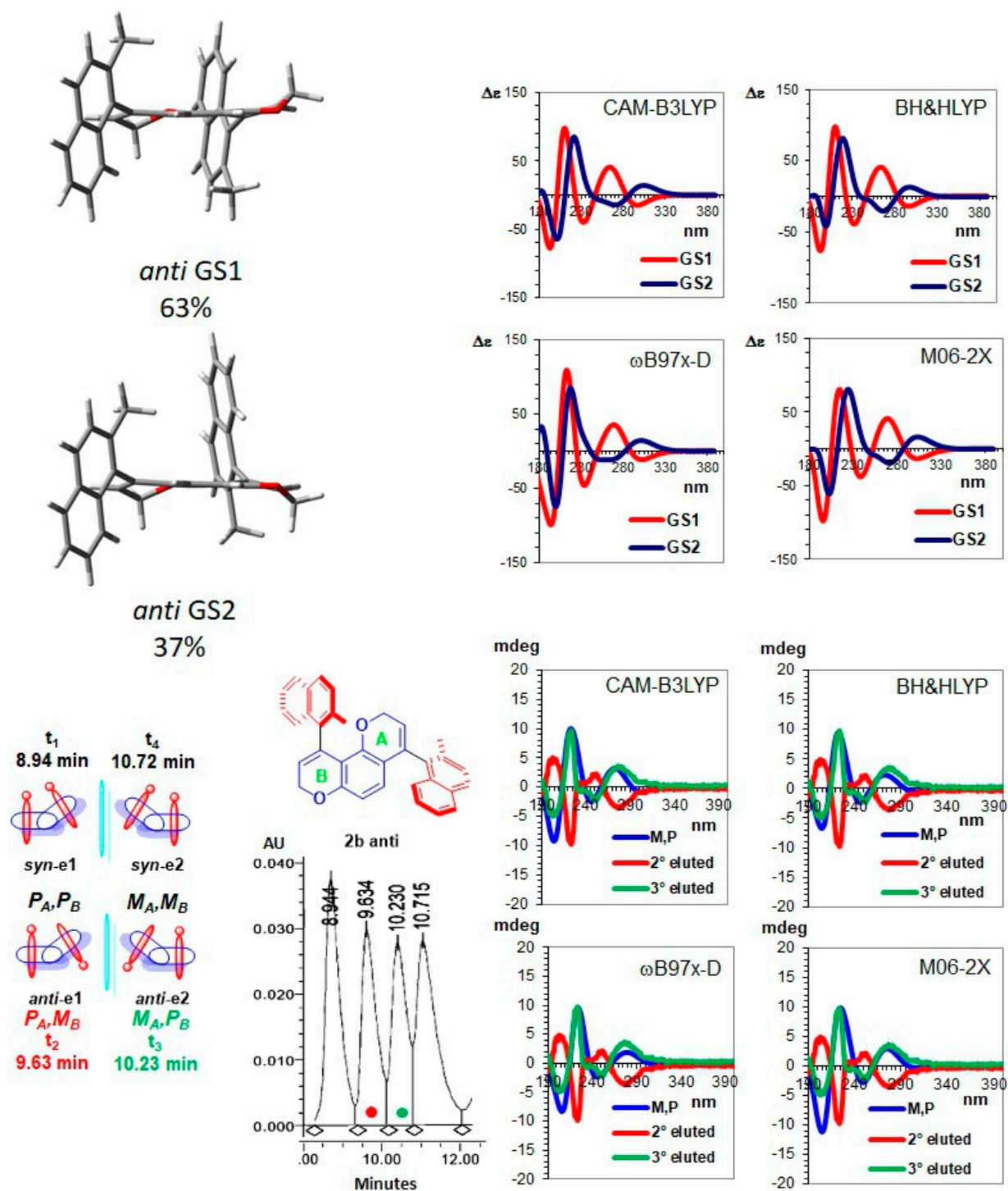


**Figure S26.** CSP-HPLC separation of compound **2b**. Chiralpak IB-N5 column: 5 mm 10 mm I.D. x 250 mm L; eluent 85:15 *n*-hexane/chloroform.

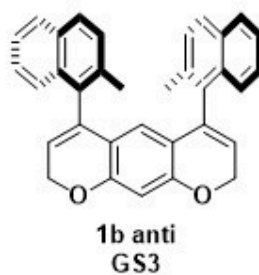
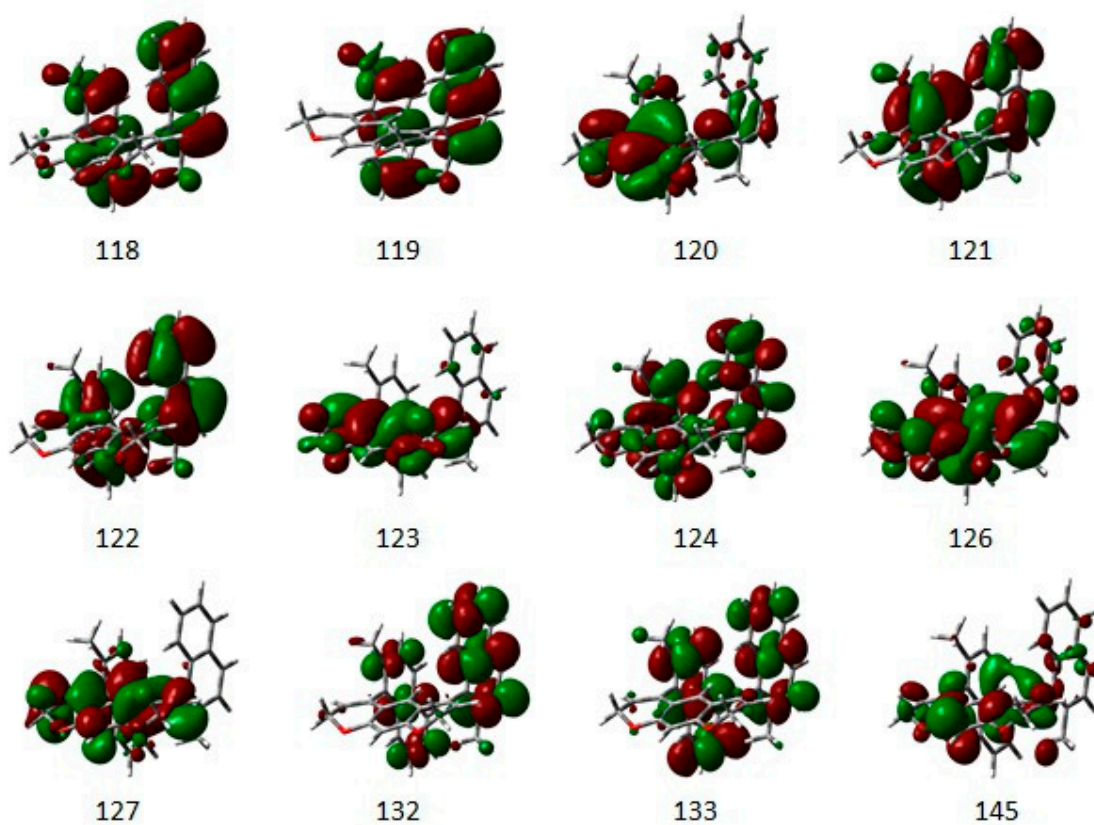


**Figure S27.** ECD studies of compound **syn-2b**. In the Figure was reported all the simulated ECD spectra of GSs with the different functionals and same basis set 6-311++G(2d,p) PCM=acetonitrile. Four different functionals and 6-311++G(2d,p) basis set were used. To obtain a better overlap, the calculated spectra were red-shifted by 11 nm for CAM-B3LYP, 15 nm for BH&HLYP and 12 nm for  $\omega$ B97x-D, and 10 nm for M06-2X while they were multiplied by a factor of 0.28 for all the functionals.



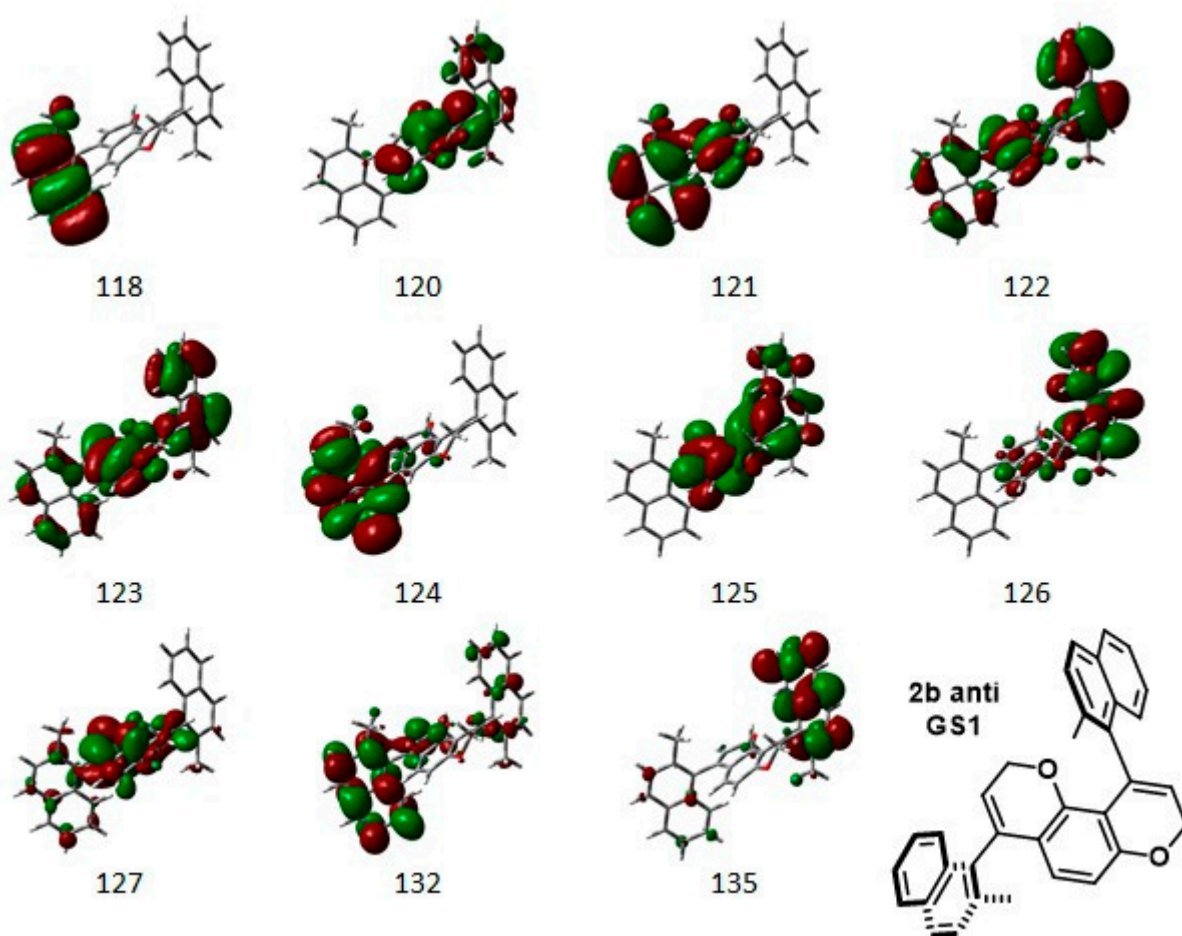


**Figure S28.** ECD studies of compound **anti-2b**. In the Figure was reported all the simulated ECD spectra of GSs with the different functionals and same basis set 6-311++G(2d,p) PCM=acetonitrile. Four different functionals and 6-311++G(2d,p) basis set were used. To obtain a better overlap, the calculated spectra were red-shifted by 10 nm for CAM-B3LYP, 11 nm for BH&HLYP, 9 nm for ωB97x-D, and 7 nm for M06-2X while they were multiplied by a factor of 0.15 for CAM-B3LYP and M06-2X, 0.12 for BH&HLYP and 0.10 for ωB97x-D.



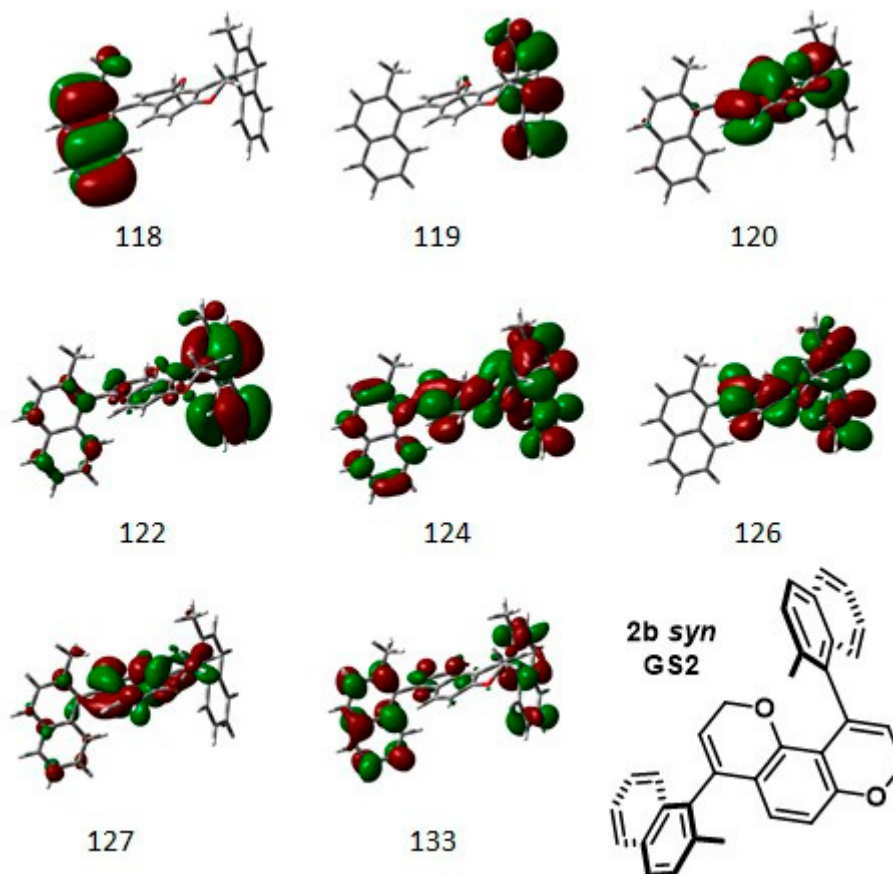
Excited State	Wavelength (nm)	HOMO	MO	LUMO	%
9	243.37	123	->	127	12.3
		120	->	126	17.7
14	217.65	122	->	126	23.5
		123	->	145	15.3
20	211.34	120	->	126	13.4
		122	->	124	12.1
		123	->	133	17.0
24	206.53	121	->	126	10.8
33	200.42	119	->	133	20.7
		119	->	126	16.8
		118	->	132	13.6

**Figure S29.** Homo-Lumo orbitals of best calculated GS3 *anti* conformation of compound **1b**.



Excited State	Wavelength (nm)	HOMO	MO	LUMO	%
7	266.38	120	->	125	14.1
		123	->	127	14.8
13	233.6	120	->	127	19.6
		122	->	127	27.6
31	208.82	121	->	126	37.3
33	208.16	118	->	124	14.8
		121	->	126	16.2
		121	->	132	14.7
42	201.49	120	->	134	11.8
		120	->	135	16.5

**Figure S30.** Homo-Lumo orbitals of best calculated GS1 *anti* conformation of compound **2b**.



Excited State	Wavelength (nm)	HOMO	MO	LUMO	%
2	282.49	122	->	124	30.9
		122	->	125	17.3
		122	->	126	10.5
14	229.63	120	->	127	16.9
		122	->	127	19.0
36	206.93	119	->	126	20.2
47	198.77	118	->	129	12.2
61	192.9	120	->	133	13.1

**Figure S31.** Homo-Lumo orbitals of best calculated GS1 *syn* conformation of compound **2b**.

## 8. DFT calculations

**Table S4.** Summarizing tables for experimental and calculated populations:

<b>1a</b>	<b>anti/syn ratio</b>	<b>2a</b>	<b>anti/syn ratio</b>	<b>1b</b>	<b>anti/syn ratio</b>	<b>2b</b>	<b>anti/syn ratio</b>
PCM CHCl <sub>3</sub>	<b>62:38</b>	PCM CHCl <sub>3</sub>	<b>59:41</b>	PCM CHCl <sub>3</sub>	<b>56:44</b>	PCM CHCl <sub>3</sub>	<b>44:56</b>
<b>C<sub>2</sub>D<sub>2</sub>Cl<sub>4</sub></b>	<b>60:40</b>	C <sub>2</sub> D <sub>2</sub> Cl <sub>4</sub>	<b>59:41*</b>	C <sub>2</sub> D <sub>2</sub> Cl <sub>4</sub>	<b>56:44</b>	C <sub>2</sub> D <sub>2</sub> Cl <sub>4</sub>	<b>51:49</b>

**Table S5.** Summarizing tables for experimental and calculated energy barriers (*kJ/mol*):

<b>1a</b>	<b>Energy barrier</b>	<b>2a</b>	<b>Energy barrier</b>	<b>1b</b>	<b>Energy barrier</b>	<b>2b</b>	<b>Energy barrier</b>
PCM CHCl <sub>3</sub>	<b>TS<sub>1EXT</sub> 66.5</b>	PCM CHCl <sub>3</sub>	<b>TS<sub>2A-EXT-B-UP</sub> 66.5</b> <b>TS<sub>3A-UP-B-EXT</sub> 70.7</b>	PCM CHCl <sub>3</sub>	<b>TS<sub>2EXT</sub> 130.5</b>	PCM CHCl <sub>3</sub>	<b>TS<sub>1A-INT-B-DO</sub> 124.3</b> <b>TS<sub>4A-DO-B-INT</sub> 131.4</b>
D-NMR C <sub>2</sub> D <sub>2</sub> Cl <sub>4</sub>	<b>TS<sub>1EXT</sub> 65.7</b>	D-NMR C <sub>2</sub> D <sub>2</sub> Cl <sub>4</sub>	<b>TS<sub>2A-EXT-B-UP</sub> 15.6</b> <b>TS<sub>3A-UP-B-EXT</sub> 74.1</b>	Kinetic <sup>1</sup> HNMR C <sub>2</sub> D <sub>2</sub> Cl <sub>4</sub>	<b>TS<sub>2EXT</sub> 129.3</b>	Kinetic <sup>1</sup> HNMR C <sub>2</sub> D <sub>2</sub> Cl <sub>4</sub>	<b>TS<sub>A-EXT-B-UP</sub> 133.9</b> <b>/</b>
D-HPLC	<b>/</b>	D-HPLC	<b>/</b> <b>TS<sub>3A-UP-B-EXT</sub> 70.7</b>	Kinetic HPLC cis/trans-decalin	<b>TS<sub>2EXT</sub> 129.3</b>	Kinetic HPLC cis/trans-decalin	<b>/</b> <b>/</b>

**Table S6.** Comparison for calculated **H**, **G** and **qh-G** (free energy after frequency cut-off at 100 *cm*<sup>-1</sup>) in *kJ/mol* at 298K for compound **1a/2a**, PCM (chloroform):

<b>1a</b>	<b>H</b>	<b>G</b>	<b>qh-G(T)</b>	<b>2a</b>	<b>H</b>	<b>G</b>	<b>qh-G(T)</b>
PCM CHCl <sub>3</sub>	<b>TS<sub>1EXT</sub> 66.5</b>	<b>TS<sub>1EXT</sub> 77.0</b>	<b>TS<sub>1EXT</sub> 72.8</b>	PCM CHCl <sub>3</sub>	<b>TS<sub>2A-EXT-B-UP</sub> 65.3</b> <b>TS<sub>3A-UP-B-EXT</sub> 70.7</b>	<b>TS<sub>2A-EXT-B-UP</sub> 87.1</b> <b>TS<sub>3A-UP-B-EXT</sub> 80.7</b>	<b>TS<sub>2A-EXT-B-UP</sub> 72.0</b> <b>TS<sub>3A-UP-B-EXT</sub> 77.0</b>
<b>1a</b>	<b>anti/syn ratio</b>	<b>anti/syn ratio</b>	<b>anti/syn ratio</b>	<b>2a</b>	<b>anti/syn ratio</b>	<b>anti/syn ratio</b>	<b>anti/syn ratio</b>
PCM CHCl <sub>3</sub>	<b>62:38</b>	<b>54:46</b>	<b>59:41</b>	PCM CHCl <sub>3</sub>	<b>59:41</b>	<b>51:49</b>	<b>56:44</b>

**Table S7.** Comparison for calculated **H** and **G** in *kJ/mol* at 298K for compound **1a**, with or without empirical dispersion **GD3**, PCM (chloroform):

<b>1a</b>	<b>H</b>	<b>G</b>	<b>1a</b>	<b>H (GD3)</b>	<b>G (GD3)</b>
PCM CHCl <sub>3</sub>	<b>TS<sub>1EXT</sub></b> <b>76.5</b>	<b>TS<sub>1EXT</sub></b> <b>77.0</b>	PCM CHCl <sub>3</sub>	<b>TS<sub>1EXT</sub></b> <b>71.5</b>	<b>TS<sub>1EXT</sub></b> <b>80.3</b>

# Compound 1a

1a-anti-GS1

Method: opt freq b3lyp/6-311++g(d,p) scrf(solvent=Chloroform)

SCF Done: E(RB3LYP) = -6223.16714758 A.U. after 1 cycles

Lowest frequency = 9.0786

Zero-point correction= 0.329884  
(Hartree/Particle)  
Thermal correction to Energy= 0.353132  
Thermal correction to Enthalpy= 0.354077  
Thermal correction to Gibbs Free Energy= 0.272168  
Sum of electronic and zero-point Energies= -6222.837263  
Sum of electronic and thermal Energies= -6222.814015  
Sum of electronic and thermal Enthalpies= -6222.813071  
Sum of electronic and thermal Free Energies= -6222.894980

## Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.169093	-3.023733	-0.274260
2	6	0	-1.186404	-1.613035	-0.301008
3	6	0	-2.437070	-0.947400	-0.698145
4	6	0	-3.560492	-1.676107	-0.763889
5	6	0	-0.000024	-3.725182	0.000005
6	6	0	-0.000011	-0.938320	-0.000002
7	6	0	1.186375	-1.613044	0.301008
8	6	0	1.169051	-3.023742	0.274266
9	6	0	3.560464	-1.676135	0.763879
10	6	0	2.437048	-0.947419	0.698140
11	1	0	-0.000029	-4.807782	0.000007
12	1	0	-4.505682	-1.239106	-1.064938
13	1	0	-0.000006	0.144979	-0.000005
14	1	0	4.505659	-1.239142	1.064925
15	8	0	2.275995	-3.750505	0.601793
16	8	0	-2.276042	-3.750488	-0.601784
17	6	0	3.549875	-3.118784	0.357010
18	1	0	4.272669	-3.704595	0.924596
19	1	0	3.790308	-3.226778	-0.711883
20	6	0	-3.549919	-3.118755	-0.357015
21	1	0	-4.272713	-3.704560	-0.924606
22	1	0	-3.790363	-3.226743	0.711875
23	6	0	2.422761	0.498405	1.071830
24	6	0	2.005510	0.872617	2.358397
25	6	0	2.809909	1.523842	0.201270
26	6	0	1.991588	2.203546	2.762202
27	1	0	1.694153	0.094349	3.045861
28	6	0	2.800777	2.863021	0.587913
29	6	0	2.391138	3.201267	1.874557
30	1	0	1.670528	2.460020	3.764901
31	1	0	3.109527	3.630304	-0.110073
32	1	0	2.384692	4.242092	2.176711
33	6	0	-2.422771	0.498424	-1.071838
34	6	0	-2.809886	1.523866	-0.201270

35	6	0	-2.005539	0.872629	-2.358412
36	6	0	-2.800740	2.863045	-0.587912
37	6	0	-1.991605	2.203559	-2.762217
38	1	0	-1.694209	0.094356	-3.045883
39	6	0	-2.391121	3.201285	-1.874564
40	1	0	-3.109466	3.630333	0.110080
41	1	0	-1.670561	2.460028	-3.764922
42	1	0	-2.384664	4.242110	-2.176717
43	35	0	3.369943	1.124771	-1.599338
44	35	0	-3.369897	1.124800	1.599346

-----  
1a-anti-GS2

Method: opt freq b3lyp/6-311++g(d,p) scrf(solvent=Chloroform)  
 SCF Done: E(RB3LYP) = -6223.16804199 A.U. after 1 cycles  
 Lowest frequency = 14.9143

Zero-point correction= 0.329951  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.353111  
 Thermal correction to Enthalpy= 0.354055  
 Thermal correction to Gibbs Free Energy= 0.273376  
 Sum of electronic and zero-point Energies= -6222.838091  
 Sum of electronic and thermal Energies= -6222.814931  
 Sum of electronic and thermal Enthalpies= -6222.813987  
 Sum of electronic and thermal Free Energies= -6222.894666

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.036926	2.675414	0.604372
2	6	0	1.071880	1.265473	0.588527
3	6	0	2.254591	0.600835	1.159110
4	6	0	3.087411	1.322691	1.924111
5	6	0	0.000011	3.377796	-0.000010
6	6	0	-0.000003	0.590178	0.000015
7	6	0	-1.071878	1.265473	-0.588508
8	6	0	-1.036913	2.675413	-0.604377
9	6	0	-3.087418	1.322688	-1.924082
10	6	0	-2.254589	0.600834	-1.159092
11	1	0	0.000015	4.460375	-0.000018
12	1	0	3.978708	0.888062	2.362071
13	1	0	-0.000008	-0.493366	0.000023
14	1	0	-3.978706	0.888049	-2.362053
15	8	0	-2.063069	3.398707	-1.139188
16	8	0	2.063091	3.398701	1.139178
17	6	0	-2.789074	2.764142	-2.211830
18	1	0	-3.701361	3.349486	-2.324663
19	1	0	-2.201880	2.869443	-3.137110
20	6	0	2.789029	2.764137	2.211867
21	1	0	3.701297	3.349496	2.324775
22	1	0	2.201761	2.869414	3.137101
23	6	0	-2.499575	-0.849395	-0.909393
24	6	0	-2.281014	-1.768952	-1.946442
25	6	0	-2.951196	-1.361616	0.314433
26	6	0	-2.499320	-3.132800	-1.771691
27	1	0	-1.927069	-1.393993	-2.899794
28	6	0	-3.175984	-2.722299	0.506412



29	6	0	-2.944811	-3.610661	-0.541694
30	1	0	-2.320285	-3.817322	-2.592507
31	1	0	-3.534600	-3.082187	1.462072
32	1	0	-3.118573	-4.669924	-0.391953
33	6	0	2.499593	-0.849387	0.909396
34	6	0	2.951192	-1.361600	-0.314442
35	6	0	2.281074	-1.768952	1.946448
36	6	0	3.175995	-2.722279	-0.506430
37	6	0	2.499395	-3.132796	1.771688
38	1	0	1.927147	-1.394000	2.899810
39	6	0	2.944860	-3.610647	0.541679
40	1	0	3.534595	-3.082159	-1.462099
41	1	0	2.320391	-3.817322	2.592507
42	1	0	3.118634	-4.669907	0.391930
43	35	0	-3.335373	-0.180520	1.785634
44	35	0	3.335335	-0.180495	-1.785646

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1a-anti-GS3

Method: opt freq b3lyp/6-311++g(d,p) scrf(solvent=Chloroform)  
SCF Done: E(RB3LYP) = -6223.16765424 A.U. after 1 cycles  
Lowest frequency = 12.5752

Zero-point correction= 0.329927  
(Hartree/Particle)  
Thermal correction to Energy= 0.353124  
Thermal correction to Enthalpy= 0.354068  
Thermal correction to Gibbs Free Energy= 0.273025  
Sum of electronic and zero-point Energies= -6222.837727  
Sum of electronic and thermal Energies= -6222.814530  
Sum of electronic and thermal Enthalpies= -6222.813586  
Sum of electronic and thermal Free Energies= -6222.894629

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.400465	2.781356	-0.358276
2	6	0	1.260627	1.390724	-0.547058
3	6	0	2.422864	0.646501	-1.058583
4	6	0	3.437451	1.337689	-1.599572
5	6	0	0.374296	3.541269	0.192422
6	6	0	0.046112	0.800422	-0.189385
7	6	0	-1.014481	1.538797	0.342306
8	6	0	-0.827688	2.925450	0.524852
9	6	0	-3.296081	1.771123	1.114792
10	6	0	-2.285506	0.950727	0.793597
11	1	0	0.503287	4.605195	0.345105
12	1	0	4.322767	0.842901	-1.982380
13	1	0	-0.069912	-0.270123	-0.308613
14	1	0	-4.247917	1.390480	1.467229
15	8	0	-1.792835	3.699679	1.099051
16	8	0	2.572823	3.416387	-0.647453
17	6	0	-3.154314	3.252285	0.932103
18	1	0	-3.499736	3.559477	-0.067033
19	1	0	-3.730377	3.808013	1.671817
20	6	0	3.361444	2.831921	-1.704652
21	1	0	4.345132	3.292316	-1.615293
22	1	0	2.929333	3.139728	-2.669305

23	6	0	-2.411289	-0.530334	0.942051
24	6	0	-2.022452	-1.138433	2.145125
25	6	0	-2.908825	-1.364856	-0.065505
26	6	0	-2.137786	-2.511472	2.338004
27	1	0	-1.627400	-0.510782	2.935682
28	6	0	-3.030010	-2.742163	0.108936
29	6	0	-2.642877	-3.315017	1.317404
30	1	0	-1.834676	-2.951093	3.280961
31	1	0	-3.423339	-3.357015	-0.690145
32	1	0	-2.737830	-4.385831	1.455355
33	6	0	2.452599	-0.843866	-0.995512
34	6	0	2.679273	-1.566248	0.183701
35	6	0	2.254204	-1.583263	-2.171312
36	6	0	2.708039	-2.958284	0.201499
37	6	0	2.278445	-2.975262	-2.171605
38	1	0	2.072658	-1.043746	-3.093689
39	6	0	2.503167	-3.664045	-0.982104
40	1	0	2.895323	-3.483935	1.128839
41	1	0	2.120916	-3.517430	-3.096592
42	1	0	2.524315	-4.747562	-0.968185
43	35	0	-3.457665	-0.630776	-1.760868
44	35	0	3.015707	-0.647774	1.841842

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1a-syn-GS1

Method: opt freq b3lyp/6-311++g(d,p) scrf(solvent=Chloroform)

SCF Done: E(RB3LYP) = -6223.16728046 A.U. after 1 cycles

Lowest frequency = 7.8333

Zero-point correction= 0.329911  
(Hartree/Particle)  
Thermal correction to Energy= 0.353119  
Thermal correction to Enthalpy= 0.354063  
Thermal correction to Gibbs Free Energy= 0.272494  
Sum of electronic and zero-point Energies= -6222.837369  
Sum of electronic and thermal Energies= -6222.814162  
Sum of electronic and thermal Enthalpies= -6222.813218  
Sum of electronic and thermal Free Energies= -6222.894786

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.774108	2.668183	0.401340
2	6	0	1.521173	1.298693	0.624990
3	6	0	2.676225	0.414261	0.849166
4	6	0	3.864545	0.971261	1.127000
5	6	0	0.744633	3.550701	0.093400
6	6	0	0.194441	0.862589	0.584842
7	6	0	-0.866349	1.728447	0.304600
8	6	0	-0.562360	3.079311	0.032241
9	6	0	-3.196402	2.185179	-0.159546
10	6	0	-2.283852	1.334446	0.331685
11	1	0	0.958171	4.595115	-0.095336
12	1	0	4.750709	0.368867	1.291205
13	1	0	-0.019293	-0.182163	0.776221
14	1	0	-4.255276	1.953892	-0.148314
15	8	0	-1.548980	3.989483	-0.211060
16	8	0	3.047686	3.157823	0.399346

17	6	0	-2.761087	3.470185	-0.797131
18	1	0	-3.501903	4.258593	-0.666109
19	1	0	-2.594014	3.336676	-1.876953
20	6	0	3.993310	2.461487	1.236722
21	1	0	4.973575	2.805879	0.907814
22	1	0	3.847793	2.795987	2.275528
23	6	0	-2.681767	0.038312	0.957615
24	6	0	-2.744933	-0.056470	2.356675
25	6	0	-3.005228	-1.108956	0.223577
26	6	0	-3.128690	-1.232547	2.992098
27	1	0	-2.492664	0.819255	2.943955
28	6	0	-3.389839	-2.296932	0.843789
29	6	0	-3.452772	-2.355975	2.232942
30	1	0	-3.176057	-1.271200	4.074063
31	1	0	-3.635461	-3.164613	0.245418
32	1	0	-3.753448	-3.278805	2.715303
33	6	0	2.513540	-1.067631	0.791487
34	6	0	2.367319	-1.785321	-0.403304
35	6	0	2.512250	-1.804013	1.985694
36	6	0	2.223620	-3.170260	-0.417869
37	6	0	2.368774	-3.188873	1.989508
38	1	0	2.620808	-1.267356	2.921181
39	6	0	2.220966	-3.872795	0.785254
40	1	0	2.121303	-3.693717	-1.359593
41	1	0	2.371219	-3.729038	2.928977
42	1	0	2.107681	-4.950604	0.773865
43	35	0	-2.918304	-1.103973	-1.701274
44	35	0	2.411945	-0.876453	-2.099131

1a-syn-GS2

Method: opt freq b3lyp/6-311++g(d,p) scrf(solvent=Chloroform)

SCF Done: E(RB3LYP) = -6223.16717319 A.U. after 1 cycles

Lowest frequency = 15.9570

Zero-point correction= 0.329950  
(Hartree/Particle)  
Thermal correction to Energy= 0.353082  
Thermal correction to Enthalpy= 0.354026  
Thermal correction to Gibbs Free Energy= 0.274115  
Sum of electronic and zero-point Energies= -6222.837223  
Sum of electronic and thermal Energies= -6222.814092  
Sum of electronic and thermal Enthalpies= -6222.813147  
Sum of electronic and thermal Free Energies= -6222.893058

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.202702	2.877117	-0.141439
2	6	0	-1.225297	1.534812	-0.573754
3	6	0	-2.537645	0.888638	-0.739050
4	6	0	-3.633936	1.660982	-0.760466
5	6	0	-0.002742	3.540023	0.092154
6	6	0	-0.001499	0.892014	-0.778598
7	6	0	1.221698	1.536149	-0.574359
8	6	0	1.197839	2.878372	-0.141817
9	6	0	3.630160	1.664958	-0.761933
10	6	0	2.534683	0.891488	-0.740547
11	1	0	-0.003216	4.567916	0.431787

12	1	0	-4.625618	1.237635	-0.872676
13	1	0	-0.001019	-0.145396	-1.091432
14	1	0	4.622212	1.242682	-0.874915
15	8	0	2.353774	3.554401	0.120487
16	8	0	-2.359298	3.551971	0.121022
17	6	0	3.507076	3.155329	-0.648103
18	1	0	3.440205	3.623953	-1.642197
19	1	0	4.360920	3.590721	-0.129268
20	6	0	-3.512205	3.151534	-0.647454
21	1	0	-4.366464	3.586446	-0.128907
22	1	0	-3.445642	3.619700	-1.641784
23	6	0	2.631853	-0.588265	-0.908830
24	6	0	2.836749	-1.121612	-2.190024
25	6	0	2.537738	-1.494601	0.155390
26	6	0	2.940749	-2.493901	-2.401052
27	1	0	2.910419	-0.436928	-3.027207
28	6	0	2.640989	-2.870015	-0.037481
29	6	0	2.840036	-3.369653	-1.322578
30	1	0	3.099547	-2.875551	-3.402834
31	1	0	2.572681	-3.541654	0.808472
32	1	0	2.919611	-4.440068	-1.472827
33	6	0	-2.633405	-0.591306	-0.906202
34	6	0	-2.535092	-1.496890	0.158303
35	6	0	-2.841342	-1.125706	-2.186473
36	6	0	-2.637082	-2.872549	-0.033449
37	6	0	-2.944168	-2.498255	-2.396367
38	1	0	-2.918245	-0.441624	-3.023854
39	6	0	-2.839173	-3.373226	-1.317669
40	1	0	-2.565514	-3.543580	0.812716
41	1	0	-3.105354	-2.880726	-3.397455
42	1	0	-2.917770	-4.443835	-1.467051
43	35	0	2.303878	-0.859885	1.956156
44	35	0	-2.297371	-0.860780	1.958077

1a-syn-GS3

Method: opt freq b3lyp/6-311++g(d,p) scrf(solvent=Chloroform) iop(1/8=1, 1/9  
SCF Done: E(RB3LYP) = -6223.16710227 A.U. after 2 cycles  
Lowest frequency = 8.5585

Zero-point correction= 0.329843  
(Hartree/Particle)  
Thermal correction to Energy= 0.353096  
Thermal correction to Enthalpy= 0.354040  
Thermal correction to Gibbs Free Energy= 0.272021  
Sum of electronic and zero-point Energies= -6222.837259  
Sum of electronic and thermal Energies= -6222.814006  
Sum of electronic and thermal Enthalpies= -6222.813062  
Sum of electronic and thermal Free Energies= -6222.895081

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.200266	3.035759	0.309381
2	6	0	1.223895	1.626116	0.369683
3	6	0	2.534435	0.964294	0.468085
4	6	0	3.639079	1.687193	0.234055
5	6	0	-0.000567	3.737166	0.298154

6	6	0	-0.000176	0.952394	0.403053
7	6	0	-1.224435	1.625779	0.369951
8	6	0	-1.201200	3.035431	0.309709
9	6	0	-3.639673	1.686206	0.234896
10	6	0	-2.534771	0.963573	0.468513
11	1	0	-0.000720	4.819252	0.264774
12	1	0	4.629652	1.253368	0.308670
13	1	0	-0.000020	-0.128431	0.476864
14	1	0	-4.630099	1.252055	0.309584
15	8	0	-2.354634	3.762936	0.335514
16	8	0	2.353511	3.763563	0.334794
17	6	0	-3.527597	3.116032	-0.201192
18	1	0	-4.368932	3.713448	0.149459
19	1	0	-3.492364	3.190701	-1.298881
20	6	0	3.526433	3.116893	-0.202304
21	1	0	3.490667	3.191329	-1.299990
22	1	0	4.367749	3.714623	0.147851
23	6	0	-2.616058	-0.469551	0.881349
24	6	0	-2.596495	-0.795334	2.245989
25	6	0	-2.717820	-1.528249	-0.028611
26	6	0	-2.688599	-2.113124	2.682132
27	1	0	-2.513055	0.010102	2.966852
28	6	0	-2.808603	-2.854628	0.390019
29	6	0	-2.794812	-3.145247	1.751398
30	1	0	-2.678388	-2.332528	3.743324
31	1	0	-2.889606	-3.648765	-0.340784
32	1	0	-2.866999	-4.176097	2.078195
33	6	0	2.616240	-0.468692	0.881303
34	6	0	2.718349	-1.527622	-0.028331
35	6	0	2.596874	-0.794069	2.246051
36	6	0	2.809686	-2.853842	0.390696
37	6	0	2.689517	-2.111687	2.682589
38	1	0	2.513164	0.011557	2.966669
39	6	0	2.796091	-3.144053	1.752160
40	1	0	2.890954	-3.648166	-0.339873
41	1	0	2.679451	-2.330778	3.743847
42	1	0	2.868707	-4.174774	2.079269
43	35	0	-2.734286	-1.191073	-1.925382
44	35	0	2.734528	-1.191022	-1.925208

1a-TS1-ext

Method: opt(ts,calcfc,noeigen) freq b3lyp/6-311++g(d,p) scrf(solvent=Chlorof  
SCF Done: E(RB3LYP) = -6223.14216740 A.U. after 1 cycles  
Lowest frequency = -39.4369

Zero-point correction= 0.330516  
(Hartree/Particle)  
Thermal correction to Energy= 0.352591  
Thermal correction to Enthalpy= 0.353535  
Thermal correction to Gibbs Free Energy= 0.276413  
Sum of electronic and zero-point Energies= -6222.811651  
Sum of electronic and thermal Energies= -6222.789576  
Sum of electronic and thermal Enthalpies= -6222.788632  
Sum of electronic and thermal Free Energies= -6222.865754

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	-0.718656	2.691531	-0.327435
2	6	0	-0.727685	1.296371	-0.089889
3	6	0	-2.046323	0.694713	0.308122
4	6	0	-2.837422	1.532474	1.011950
5	6	0	0.396476	3.356563	-0.827545
6	6	0	0.520536	0.661222	-0.174713
7	6	0	1.677824	1.306368	-0.622442
8	6	0	1.586923	2.662845	-0.989218
9	6	0	4.056110	1.379014	-1.068253
10	6	0	2.976953	0.633873	-0.789471
11	1	0	0.346183	4.418629	-1.030584
12	1	0	-3.786730	1.233244	1.418504
13	1	0	0.631248	-0.362484	0.147253
14	1	0	5.032344	0.930651	-1.213987
15	8	0	2.649780	3.328902	-1.526104
16	8	0	-1.819506	3.444404	-0.032199
17	6	0	3.958175	2.874037	-1.123087
18	1	0	4.646112	3.296132	-1.855723
19	1	0	4.193995	3.317621	-0.143553
20	6	0	-2.458597	2.969520	1.171438
21	1	0	-1.779396	3.141600	2.019824
22	1	0	-3.340672	3.594817	1.303644
23	6	0	3.066067	-0.855259	-0.708646
24	6	0	2.885131	-1.621490	-1.870157
25	6	0	3.331124	-1.546299	0.479687
26	6	0	2.975213	-3.010016	-1.848421
27	1	0	2.675260	-1.105787	-2.800338
28	6	0	3.422659	-2.936342	0.520812
29	6	0	3.244040	-3.668661	-0.649837
30	1	0	2.838674	-3.573951	-2.763696
31	1	0	3.633803	-3.437955	1.456271
32	1	0	3.317564	-4.749537	-0.619728
33	6	0	-2.495723	-0.673537	-0.119838
34	6	0	-3.824968	-1.179158	-0.091525
35	6	0	-1.559103	-1.581907	-0.661851
36	6	0	-4.136899	-2.487108	-0.463802
37	6	0	-1.859480	-2.880495	-1.050228
38	1	0	-0.547144	-1.255590	-0.809677
39	6	0	-3.157688	-3.355568	-0.928143
40	1	0	-5.165575	-2.816909	-0.407569
41	1	0	-1.072786	-3.509505	-1.449707
42	1	0	-3.420223	-4.367477	-1.212624
43	35	0	-5.434035	-0.171020	0.324577
44	35	0	3.591378	-0.586582	2.129796

1a-TS2-int

Method: opt(ts,calcfc,noeigen) freq b3lyp/6-311++g(d,p) scrf(solvent=Chlorof  
SCF Done: E(RB3LYP) = -6223.12825759 A.U. after 1 cycles  
Lowest frequency = -35.7809

Zero-point correction=	0.330310
(Hartree/Particle)	
Thermal correction to Energy=	0.352312
Thermal correction to Enthalpy=	0.353256
Thermal correction to Gibbs Free Energy=	0.277027
Sum of electronic and zero-point Energies=	-6222.797947
Sum of electronic and thermal Energies=	-6222.775946
Sum of electronic and thermal Enthalpies=	-6222.775002

Sum of electronic and thermal Free Energies= -6222.851231

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.030044	2.958870	-0.358474
2	6	0	-1.144740	1.593487	-0.005806
3	6	0	-2.463581	1.167658	0.577767
4	6	0	-3.023621	2.131274	1.347766
5	6	0	0.096076	3.473335	-0.991136
6	6	0	0.037104	0.848259	-0.083387
7	6	0	1.217671	1.347783	-0.645185
8	6	0	1.210501	2.662694	-1.151165
9	6	0	3.573349	1.197293	-1.194083
10	6	0	2.460313	0.568429	-0.787948
11	1	0	0.127070	4.515651	-1.281254
12	1	0	-3.923564	1.976277	1.924132
13	1	0	0.057586	-0.149858	0.319297
14	1	0	4.508727	0.664101	-1.321413
15	8	0	2.286522	3.182214	-1.812151
16	8	0	-2.019901	3.836772	-0.006884
17	6	0	3.579206	2.678595	-1.420650
18	1	0	4.253966	2.959547	-2.229613
19	1	0	3.901061	3.212121	-0.512830
20	6	0	-2.484315	3.525187	1.324701
21	1	0	-1.656294	3.683416	2.031338
22	1	0	-3.269048	4.248439	1.543978
23	6	0	2.474041	-0.904994	-0.542117
24	6	0	2.352018	-1.785411	-1.627900
25	6	0	2.632757	-1.473772	0.726965
26	6	0	2.388279	-3.165957	-1.455259
27	1	0	2.227746	-1.365313	-2.619362
28	6	0	2.667319	-2.853353	0.919633
29	6	0	2.543401	-3.700960	-0.177943
30	1	0	2.295368	-3.819719	-2.314523
31	1	0	2.795513	-3.258204	1.915118
32	1	0	2.571265	-4.774185	-0.029759
33	6	0	-3.283600	-0.081055	0.303089
34	6	0	-2.937959	-1.347362	-0.229240
35	6	0	-4.670745	0.034221	0.599714
36	6	0	-3.851447	-2.407877	-0.298659
37	6	0	-5.584432	-1.002339	0.527106
38	1	0	-5.060351	1.001392	0.872766
39	6	0	-5.168776	-2.258557	0.099357
40	1	0	-3.513179	-3.357209	-0.691362
41	1	0	-6.620945	-0.815894	0.782494
42	1	0	-5.856746	-3.092909	0.033841
43	35	0	-1.258019	-1.848018	-1.040017
44	35	0	2.843625	-0.352332	2.279633

**Compound 2a:**

2a-anti-GS1

Method: opt freq b3lyp/6-311++g(d,p) scrf(solvent=Chloroform)

SCF Done: E(RB3LYP) = -6223.16229827 A.U. after 1 cycles  
 Lowest frequency = 13.7385

Zero-point correction= 0.330013  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.353144  
 Thermal correction to Enthalpy= 0.354089  
 Thermal correction to Gibbs Free Energy= 0.273471  
 Sum of electronic and zero-point Energies= -6222.832285  
 Sum of electronic and thermal Energies= -6222.809154  
 Sum of electronic and thermal Enthalpies= -6222.808210  
 Sum of electronic and thermal Free Energies= -6222.888827

## Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.856689	2.862704	0.630366
2	6	0	-0.483472	2.526379	0.794031
3	6	0	-0.997551	1.280124	0.367558
4	6	0	-0.119222	0.426098	-0.322928
5	6	0	1.245434	0.743254	-0.491191
6	6	0	1.710720	1.966053	0.001580
7	8	0	-0.604308	-0.764888	-0.773497
8	6	0	0.044673	-1.317311	-1.935650
9	6	0	1.537930	-1.254326	-1.827752
10	6	0	2.111328	-0.254882	-1.141910
11	8	0	-1.286162	3.425057	1.435671
12	6	0	-2.676873	3.383239	1.057883
13	6	0	-3.197450	1.979899	1.079785
14	6	0	-2.396853	0.964705	0.720468
15	6	0	-2.884551	-0.443577	0.830220
16	6	0	-3.823583	-1.016670	-0.033496
17	6	0	-4.291663	-2.317275	0.142543
18	6	0	-3.815599	-3.079892	1.205510
19	6	0	-2.874781	-2.538516	2.080113
20	6	0	-2.419888	-1.238852	1.888353
21	6	0	3.595721	-0.129173	-1.058873
22	6	0	4.311796	0.287663	-2.191324
23	6	0	5.697761	0.418992	-2.172325
24	6	0	6.404319	0.133364	-1.006558
25	6	0	5.722772	-0.288625	0.132981
26	6	0	4.336393	-0.413571	0.096418
27	35	0	-4.488614	-0.042971	-1.560070
28	35	0	3.458606	-1.046567	1.688248
29	1	0	1.208504	3.821230	0.990319
30	1	0	2.756435	2.222532	-0.119369
31	1	0	-0.314180	-2.344153	-1.999288
32	1	0	-0.314632	-0.775721	-2.824035
33	1	0	2.125176	-2.021142	-2.319768
34	1	0	-3.191023	4.018521	1.777899
35	1	0	-2.781417	3.837838	0.060963
36	1	0	-4.220169	1.809026	1.394876
37	1	0	-5.017070	-2.729294	-0.546995
38	1	0	-4.179804	-4.091328	1.343623
39	1	0	-2.498591	-3.124996	2.910224



40	1	0	-1.689469	-0.815920	2.568903
41	1	0	3.757810	0.516204	-3.094488
42	1	0	6.221201	0.744223	-3.063728
43	1	0	7.483218	0.231978	-0.977567
44	1	0	6.263739	-0.525320	1.040016

2a-anti-GS2

Method: opt freq b3lyp/6-311++g(d,p) scrf(solvent=Chloroform)  
 SCF Done: E(RB3LYP) = -6223.16326195 A.U. after 1 cycles  
 Lowest frequency = 17.3605

Zero-point correction=	0.330103
(Hartree/Particle)	
Thermal correction to Energy=	0.353174
Thermal correction to Enthalpy=	0.354118
Thermal correction to Gibbs Free Energy=	0.274094
Sum of electronic and zero-point Energies=	-6222.833159
Sum of electronic and thermal Energies=	-6222.810088
Sum of electronic and thermal Enthalpies=	-6222.809144
Sum of electronic and thermal Free Energies=	-6222.889168

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.580965	2.062561	-1.753930
2	6	0	-0.653837	2.172154	-1.122514
3	6	0	-1.116524	1.191343	-0.215179
4	6	0	-0.237810	0.141329	0.096621
5	6	0	1.040238	0.039312	-0.490426
6	6	0	1.416551	1.000298	-1.433461
7	8	0	-0.622630	-0.752478	1.052271
8	6	0	-0.083927	-2.084196	0.933531
9	6	0	1.387500	-2.069413	0.648767
10	6	0	1.921505	-1.053110	-0.044129
11	8	0	-1.445302	3.231208	-1.461912
12	6	0	-2.335483	3.680515	-0.421855
13	6	0	-3.087738	2.531389	0.175290
14	6	0	-2.500539	1.328275	0.284597
15	6	0	-3.279674	0.191727	0.860420
16	6	0	-3.729790	-0.902408	0.111397
17	6	0	-4.492027	-1.921603	0.675697
18	6	0	-4.828232	-1.860641	2.026374
19	6	0	-4.408367	-0.777657	2.795285
20	6	0	-3.647262	0.231568	2.213415
21	6	0	3.373146	-1.034092	-0.388495
22	6	0	3.853213	-1.897688	-1.384690
23	6	0	5.198370	-1.923510	-1.743135
24	6	0	6.101170	-1.075805	-1.105803
25	6	0	5.656443	-0.210558	-0.108384
26	6	0	4.307489	-0.197403	0.236704
27	35	0	-3.347728	-1.024818	-1.773640
28	35	0	3.762408	0.986714	1.653345
29	1	0	0.879868	2.821866	-2.465407
30	1	0	2.392513	0.932294	-1.899122
31	1	0	-0.306788	-2.566142	1.885138
32	1	0	-0.637790	-2.616059	0.145260

33	1	0	1.990606	-2.895822	1.007158
34	1	0	-1.744108	4.215889	0.336429
35	1	0	-3.003075	4.395741	-0.900691
36	1	0	-4.113297	2.688142	0.489034
37	1	0	-4.827758	-2.748542	0.063251
38	1	0	-5.420977	-2.654079	2.466607
39	1	0	-4.669941	-0.718234	3.845378
40	1	0	-3.308505	1.068218	2.813115
41	1	0	3.146239	-2.550397	-1.883699
42	1	0	5.537484	-2.601574	-2.517477
43	1	0	7.150797	-1.085059	-1.375642
44	1	0	6.352092	0.443230	0.401536

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2a-syn-GS1

Method: opt freq b3lyp/6-311++g(d,p) scrf(solvent=Chloroform)  
SCF Done: E(RB3LYP) = -6223.16232288 A.U. after 1 cycles  
Lowest frequency = 14.8887

Zero-point correction= 0.330032  
(Hartree/Particle)  
Thermal correction to Energy= 0.353121  
Thermal correction to Enthalpy= 0.354065  
Thermal correction to Gibbs Free Energy= 0.274093  
Sum of electronic and zero-point Energies= -6222.832290  
Sum of electronic and thermal Energies= -6222.809202  
Sum of electronic and thermal Enthalpies= -6222.808258  
Sum of electronic and thermal Free Energies= -6222.888230

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.530463	2.760394	-1.075000
2	6	0	0.824497	2.527932	-0.863244
3	6	0	1.281112	1.528444	0.025894
4	6	0	0.306855	0.835355	0.765075
5	6	0	-1.072997	1.051527	0.562865
6	6	0	-1.466565	2.014815	-0.370319
7	8	0	0.726160	-0.118623	1.643690
8	6	0	-0.131562	-0.368270	2.773635
9	6	0	-1.572033	-0.475227	2.375252
10	6	0	-2.022326	0.216887	1.318952
11	8	0	1.712143	3.270061	-1.589039
12	6	0	2.977682	3.510331	-0.945429
13	6	0	3.551285	2.243229	-0.391036
14	6	0	2.738368	1.285498	0.084797
15	6	0	3.338053	0.022407	0.608594
16	6	0	3.217766	-1.218213	-0.029646
17	6	0	3.826525	-2.366560	0.468396
18	6	0	4.585890	-2.291945	1.634077
19	6	0	4.738155	-1.069054	2.283526
20	6	0	4.121765	0.068514	1.770921
21	6	0	-3.462259	0.176010	0.929140
22	6	0	-4.403345	0.860273	1.713266
23	6	0	-5.759854	0.852605	1.399586
24	6	0	-6.207814	0.152724	0.281789
25	6	0	-5.298646	-0.541452	-0.513538
26	6	0	-3.945266	-0.522459	-0.185780

27	35	0	2.230686	-1.381426	-1.674798
28	35	0	-2.744857	-1.537533	-1.294914
29	1	0	-0.831057	3.524477	-1.780636
30	1	0	-2.522546	2.188920	-0.539077
31	1	0	0.237446	-1.296091	3.210094
32	1	0	0.019231	0.436752	3.509683
33	1	0	-2.224801	-1.109611	2.963841
34	1	0	3.617379	3.939767	-1.715595
35	1	0	2.832472	4.267142	-0.159187
36	1	0	4.627083	2.111580	-0.405120
37	1	0	3.715170	-3.307550	-0.054757
38	1	0	5.058867	-3.186416	2.022611
39	1	0	5.332992	-0.999676	3.186921
40	1	0	4.228983	1.018698	2.281166
41	1	0	-4.049997	1.409465	2.578395
42	1	0	-6.461532	1.391736	2.025192
43	1	0	-7.260829	0.138832	0.025651
44	1	0	-5.638233	-1.098511	-1.377129

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2a-syn-GS2

Method: opt freq b3lyp/6-311++g(d,p) scrf(solvent=Chloroform)

SCF Done: E(RB3LYP) = -6223.16271061 A.U. after 1 cycles

Lowest frequency = 9.6202

Zero-point correction= 0.330055  
(Hartree/Particle)  
Thermal correction to Energy= 0.353176  
Thermal correction to Enthalpy= 0.354120  
Thermal correction to Gibbs Free Energy= 0.273298  
Sum of electronic and zero-point Energies= -6222.832656  
Sum of electronic and thermal Energies= -6222.809534  
Sum of electronic and thermal Enthalpies= -6222.808590  
Sum of electronic and thermal Free Energies= -6222.889412

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.427017	2.566916	-1.276774
2	6	0	0.910693	2.452368	-0.912159
3	6	0	1.354888	1.456480	-0.012328
4	6	0	0.375727	0.635980	0.571080
5	6	0	-0.992061	0.761840	0.249074
6	6	0	-1.365233	1.724309	-0.694414
7	8	0	0.774306	-0.244736	1.532843
8	6	0	-0.028977	-1.431511	1.690807
9	6	0	-1.494210	-1.119203	1.691114
10	6	0	-1.954511	-0.087060	0.970769
11	8	0	1.802322	3.297131	-1.507271
12	6	0	2.962380	3.613533	-0.713465
13	6	0	3.585439	2.372711	-0.152181
14	6	0	2.812678	1.330662	0.195825
15	6	0	3.459796	0.094218	0.727917
16	6	0	3.521970	-1.115723	0.025667
17	6	0	4.173148	-2.234727	0.537700
18	6	0	4.790402	-2.160187	1.784456
19	6	0	4.759062	-0.966217	2.501280
20	6	0	4.103127	0.141657	1.973335
21	6	0	-3.410393	0.245671	0.931111

22	6	0	-3.922937	1.199673	1.823432
23	6	0	-5.273436	1.533273	1.838017
24	6	0	-6.148980	0.918008	0.944782
25	6	0	-5.669547	-0.026774	0.041730
26	6	0	-4.313466	-0.349542	0.042549
27	35	0	2.736883	-1.274793	-1.726573
28	35	0	-3.709761	-1.654292	-1.240277
29	1	0	-0.716733	3.326628	-1.991621
30	1	0	-2.411354	1.835013	-0.953349
31	1	0	0.226155	-2.136057	0.884947
32	1	0	0.293922	-1.868706	2.635353
33	1	0	-2.159026	-1.768388	2.249274
34	1	0	3.640115	4.136890	-1.386737
35	1	0	2.660846	4.311788	0.082160
36	1	0	4.664539	2.329012	-0.060580
37	1	0	4.205827	-3.151356	-0.037055
38	1	0	5.296997	-3.031245	2.183621
39	1	0	5.241620	-0.896456	3.469244
40	1	0	4.066605	1.067587	2.535288
41	1	0	-3.238970	1.677047	2.515974
42	1	0	-5.640172	2.269174	2.543937
43	1	0	-7.203334	1.168947	0.945808
44	1	0	-6.340576	-0.509195	-0.657041

2a-TS4-A-fix-DOWN-B-int

Method: opt(ts,calcfc,noeigen) freq b3lyp/6-311++g(d,p) scrf(solvent=Chlorof

SCF Done: E(RB3LYP) = -6223.11744317 A.U. after 1 cycles

Lowest frequency = -24.5883

Zero-point correction= 0.329931  
(Hartree/Particle)  
Thermal correction to Energy= 0.351879  
Thermal correction to Enthalpy= 0.352824  
Thermal correction to Gibbs Free Energy= 0.277053  
Sum of electronic and zero-point Energies= -6222.787512  
Sum of electronic and thermal Energies= -6222.765564  
Sum of electronic and thermal Enthalpies= -6222.764620  
Sum of electronic and thermal Free Energies= -6222.840390

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.400790	2.832566	-1.276656
2	6	0	-0.902976	2.618069	-0.841366
3	6	0	-1.244842	1.560894	0.038023
4	6	0	-0.174550	1.044224	0.787011
5	6	0	1.164077	1.219816	0.361656
6	6	0	1.421509	2.077121	-0.711567
7	8	0	-0.454603	0.392280	1.939787
8	6	0	0.598364	0.303663	2.922118
9	6	0	1.931010	0.005293	2.307389
10	6	0	2.209314	0.474482	1.082396
11	8	0	-1.879982	3.511291	-1.190475
12	6	0	-2.761061	3.745005	-0.054406
13	6	0	-3.436334	2.452268	0.282488
14	6	0	-2.716504	1.311368	0.192790
15	6	0	-3.477653	0.045866	-0.151942

16	6	0	-3.233900	-1.323403	0.105826
17	6	0	-4.143134	-2.322020	-0.262139
18	6	0	-5.313421	-2.022732	-0.942637
19	6	0	-5.553762	-0.700392	-1.295656
20	6	0	-4.649541	0.281553	-0.922818
21	6	0	3.549544	0.270392	0.460622
22	6	0	4.652734	0.972143	0.970364
23	6	0	5.927637	0.821355	0.431497
24	6	0	6.127654	-0.044280	-0.641066
25	6	0	5.053633	-0.760539	-1.165198
26	6	0	3.784878	-0.597089	-0.615111
27	35	0	-1.652250	-2.061081	0.910845
28	35	0	2.353930	-1.655008	-1.346434
29	1	0	0.602728	3.618588	-1.993174
30	1	0	2.441980	2.213337	-1.049516
31	1	0	0.620973	1.252854	3.478732
32	1	0	0.280777	-0.481533	3.608363
33	1	0	2.647399	-0.575603	2.876612
34	1	0	-2.160606	4.165765	0.762547
35	1	0	-3.479481	4.492330	-0.387285
36	1	0	-4.513820	2.449464	0.384375
37	1	0	-3.911789	-3.349633	-0.016198
38	1	0	-5.998690	-2.815365	-1.218793
39	1	0	-6.425254	-0.429081	-1.879815
40	1	0	-4.832961	1.286572	-1.270995
41	1	0	4.491406	1.650939	1.799843
42	1	0	6.758672	1.378999	0.847204
43	1	0	7.114501	-0.170614	-1.070956
44	1	0	5.201260	-1.446193	-1.989528

2a-TS2-B-fix-DOWN-A-ext

Method: opt (ts,calcfc,noeigen) freq b3lyp/6-311++g(d,p) scrf(solvent=Chlorof  
SCF Done: E(RB3LYP) = -6223.13721221 A.U. after 1 cycles  
Lowest frequency = -39.2377

Zero-point correction= 0.330575  
(Hartree/Particle)  
Thermal correction to Energy= 0.352562  
Thermal correction to Enthalpy= 0.353506  
Thermal correction to Gibbs Free Energy= 0.276839  
Sum of electronic and zero-point Energies= -6222.806637  
Sum of electronic and thermal Energies= -6222.784650  
Sum of electronic and thermal Enthalpies= -6222.783706  
Sum of electronic and thermal Free Energies= -6222.860373

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.092165	3.532975	-0.674255
2	6	0	1.308909	2.974945	-0.302168
3	6	0	1.485065	1.573943	-0.275914
4	6	0	0.344508	0.780700	-0.488895
5	6	0	-0.951025	1.323490	-0.668093
6	6	0	-1.013542	2.712017	-0.863164
7	8	0	0.506667	-0.572455	-0.545681
8	6	0	-0.327930	-1.156436	-1.565949

9	6	0	-1.760135	-0.844925	-1.276817
10	6	0	-2.089087	0.343905	-0.729365
11	8	0	2.358503	3.817977	-0.088712
12	6	0	3.389069	3.294387	0.774060
13	6	0	3.792020	1.917707	0.345264
14	6	0	2.868338	1.072432	-0.137555
15	6	0	3.290339	-0.271591	-0.639464
16	6	0	3.581305	-1.357089	0.192838
17	6	0	4.029575	-2.575203	-0.313552
18	6	0	4.197086	-2.727684	-1.687421
19	6	0	3.916115	-1.663244	-2.542393
20	6	0	3.469516	-0.454602	-2.018331
21	6	0	-3.446312	0.619626	-0.147408
22	6	0	-3.809025	1.940493	0.199173
23	6	0	-5.049646	2.306105	0.703904
24	6	0	-6.023892	1.339462	0.910747
25	6	0	-5.702798	0.013187	0.652633
26	6	0	-4.446660	-0.343095	0.160885
27	35	0	3.339119	-1.227480	2.099898
28	35	0	-4.243755	-2.274918	0.095341
29	1	0	0.017240	4.605791	-0.800455
30	1	0	-1.928436	3.180508	-1.193006
31	1	0	0.004248	-0.787548	-2.547926
32	1	0	-0.142188	-2.228722	-1.519927
33	1	0	-2.476558	-1.627887	-1.450369
34	1	0	4.214262	4.001438	0.702527
35	1	0	3.014223	3.303280	1.808454
36	1	0	4.832927	1.628429	0.430040
37	1	0	4.242922	-3.395302	0.359776
38	1	0	4.547430	-3.674502	-2.081815
39	1	0	4.049103	-1.771455	-3.612605
40	1	0	3.256026	0.376498	-2.681274
41	1	0	-3.080851	2.722241	0.090756
42	1	0	-5.242194	3.346872	0.936383
43	1	0	-7.004541	1.595918	1.293291
44	1	0	-6.426480	-0.764829	0.855355

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- 2a-TS3-A-fix-UP-B-ext

Method: opt(ts,calcfc,noeigen) freq b3lyp/6-311++g(d,p) scrf(solvent=Chlorof  
SCF Done: E(RB3LYP) = -6223.13541046 A.U. after 1 cycles  
Lowest frequency = -39.2879

Zero-point correction= 0.330318  
(Hartree/Particle)  
Thermal correction to Energy= 0.352304  
Thermal correction to Enthalpy= 0.353248  
Thermal correction to Gibbs Free Energy= 0.276776  
Sum of electronic and zero-point Energies= -6222.805092  
Sum of electronic and thermal Energies= -6222.783107  
Sum of electronic and thermal Enthalpies= -6222.782163  
Sum of electronic and thermal Free Energies= -6222.858634

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.713257	-1.704051	1.731598
2	6	0	-0.500517	-1.641829	1.057638

3	6	0	-0.857845	-0.542559	0.237070
4	6	0	0.201770	0.305749	-0.134330
5	6	0	1.472993	0.223541	0.474939
6	6	0	1.682117	-0.748740	1.457019
7	8	0	0.019085	1.135028	-1.209318
8	6	0	0.820671	2.331668	-1.280753
9	6	0	2.237417	2.103837	-0.857459
10	6	0	2.543839	1.109295	-0.014073
11	8	0	-1.355988	-2.701944	1.157935
12	6	0	-1.993442	-2.959537	-0.116898
13	6	0	-2.777076	-1.750400	-0.516915
14	6	0	-2.289334	-0.525421	-0.232003
15	6	0	-3.159084	0.694999	-0.177360
16	6	0	-4.576801	0.710174	-0.077155
17	6	0	-5.309885	1.896727	-0.036748
18	6	0	-4.674514	3.131780	-0.044792
19	6	0	-3.286391	3.162544	-0.062940
20	6	0	-2.569934	1.975313	-0.122084
21	6	0	3.948986	0.909591	0.450036
22	6	0	4.474278	1.761288	1.433139
23	6	0	5.780286	1.624085	1.895788
24	6	0	6.596053	0.620366	1.378916
25	6	0	6.104625	-0.238679	0.398357
26	6	0	4.795393	-0.087798	-0.051688
27	35	0	-5.727603	-0.839081	0.152606
28	35	0	4.183974	-1.281592	-1.432289
29	1	0	0.908270	-2.534622	2.398110
30	1	0	2.646391	-0.810984	1.946345
31	1	0	0.757262	2.649211	-2.321796
32	1	0	0.349616	3.115178	-0.665281
33	1	0	2.994312	2.777112	-1.243373
34	1	0	-1.217978	-3.242689	-0.842348
35	1	0	-2.647673	-3.814376	0.047696
36	1	0	-3.767286	-1.905697	-0.908175
37	1	0	-6.388544	1.846202	0.026532
38	1	0	-5.260309	4.042581	-0.008978
39	1	0	-2.753077	4.105461	-0.030895
40	1	0	-1.499960	2.036788	-0.140133
41	1	0	3.834633	2.537666	1.836990
42	1	0	6.156969	2.297868	2.656344
43	1	0	7.614504	0.502540	1.730276
44	1	0	6.733956	-1.015003	-0.017134

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- 2a-TS1-B-fix-UP-A-int

Method: opt(ts,calcfc,noeigen) freq b3lyp/6-311++g(d,p) scrf(solvent=Chlorof  
SCF Done: E(RB3LYP) = -6223.12446587 A.U. after 1 cycles  
Lowest frequency = -37.2478

Zero-point correction=	0.330357
(Hartree/Particle)	
Thermal correction to Energy=	0.352279
Thermal correction to Enthalpy=	0.353223
Thermal correction to Gibbs Free Energy=	0.277296
Sum of electronic and zero-point Energies=	-6222.794109
Sum of electronic and thermal Energies=	-6222.772187
Sum of electronic and thermal Enthalpies=	-6222.771243
Sum of electronic and thermal Free Energies=	-6222.847170

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.362569	2.855512	-0.713538
2	6	0	-0.979337	2.541783	-0.538674
3	6	0	-1.445912	1.221485	-0.693892
4	6	0	-0.496406	0.247462	-1.046596
5	6	0	0.895576	0.499880	-1.045748
6	6	0	1.279535	1.842047	-0.967023
7	8	0	-0.942605	-0.976990	-1.463288
8	6	0	-0.169337	-1.419589	-2.599469
9	6	0	1.265679	-1.544653	-2.201913
10	6	0	1.791308	-0.675874	-1.306882
11	8	0	-1.840869	3.553787	-0.217860
12	6	0	-3.174759	3.410747	-0.741812
13	6	0	-3.713498	2.032975	-0.504751
14	6	0	-2.887761	0.973334	-0.493615
15	6	0	-3.445783	-0.387451	-0.240938
16	6	0	-3.180536	-1.137648	0.911655
17	6	0	-3.745515	-2.392811	1.121444
18	6	0	-4.607905	-2.927454	0.167240
19	6	0	-4.905794	-2.198300	-0.981882
20	6	0	-4.330224	-0.946615	-1.175631
21	6	0	3.078733	-1.069374	-0.605632
22	6	0	3.397437	-2.454071	-0.684485
23	6	0	4.569051	-3.024542	-0.219135
24	6	0	5.517194	-2.229098	0.414468
25	6	0	5.219945	-0.891189	0.610793
26	6	0	4.024999	-0.327329	0.144314
27	35	0	-2.052148	-0.434760	2.305529
28	35	0	3.855956	1.494798	0.774790
29	1	0	0.676387	3.890495	-0.660560
30	1	0	2.305811	2.114656	-1.143265
31	1	0	-0.582380	-2.388326	-2.878823
32	1	0	-0.331452	-0.717288	-3.430426
33	1	0	1.802329	-2.401940	-2.581315
34	1	0	-3.768804	4.167719	-0.230663
35	1	0	-3.158271	3.657079	-1.814949
36	1	0	-4.776667	1.918873	-0.326467
37	1	0	-3.521068	-2.941651	2.026929
38	1	0	-5.046424	-3.905114	0.330304
39	1	0	-5.581089	-2.602836	-1.726915
40	1	0	-4.548594	-0.384079	-2.075903
41	1	0	2.666932	-3.124233	-1.108091
42	1	0	4.723168	-4.091109	-0.333043
43	1	0	6.446832	-2.641361	0.787978
44	1	0	5.912251	-0.261966	1.153420

2a-TS4-A-fix-UP-B-int

Method: opt(ts,calcfc,noeigen) freq b3lyp/6-311++g(d,p) scrf(solvent=Chlorof  
SCF Done: E(RB3LYP) = -6223.11744683 A.U. after 1 cycles  
Lowest frequency = -28.4483

Zero-point correction= 0.329895  
(Hartree/Particle)  
Thermal correction to Energy= 0.351921  
Thermal correction to Enthalpy= 0.352865  
Thermal correction to Gibbs Free Energy= 0.275906  
Sum of electronic and zero-point Energies= -6222.787552



Sum of electronic and thermal Energies= -6222.765526  
Sum of electronic and thermal Enthalpies= -6222.764582  
Sum of electronic and thermal Free Energies= -6222.841541

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.252815	2.443589	-1.551308
2	6	0	-0.993401	2.406113	-0.934224
3	6	0	-1.389998	1.337845	-0.092067
4	6	0	-0.333888	0.582663	0.444390
5	6	0	0.941579	0.574629	-0.170991
6	6	0	1.191671	1.477385	-1.208923
7	8	0	-0.564547	-0.122503	1.574845
8	6	0	0.579381	-0.527760	2.357164
9	6	0	1.723561	-0.983187	1.506719
10	6	0	1.922234	-0.410868	0.311380
11	8	0	-1.836675	3.476457	-1.062303
12	6	0	-2.497540	3.737033	0.209618
13	6	0	-3.336133	2.544592	0.549589
14	6	0	-2.846344	1.316263	0.268304
15	6	0	-3.856358	0.229451	-0.046084
16	6	0	-3.820506	-1.180165	0.066593
17	6	0	-4.931575	-1.978508	-0.229235
18	6	0	-6.116442	-1.429076	-0.694301
19	6	0	-6.171181	-0.056639	-0.904623
20	6	0	-5.066959	0.725276	-0.604663
21	6	0	3.062114	-0.801570	-0.569632
22	6	0	2.816850	-1.623057	-1.681539
23	6	0	3.842259	-2.035973	-2.525000
24	6	0	5.150804	-1.622741	-2.278565
25	6	0	5.424811	-0.797231	-1.192094
26	6	0	4.384583	-0.395137	-0.355176
27	35	0	-2.295698	-2.243466	0.560291
28	35	0	4.835063	0.776103	1.108569
29	1	0	0.488925	3.252005	-2.231507
30	1	0	2.161187	1.474736	-1.692489
31	1	0	0.871446	0.323207	2.990735
32	1	0	0.211345	-1.321672	3.007316
33	1	0	2.388751	-1.743705	1.898368
34	1	0	-1.725401	3.971237	0.953732
35	1	0	-3.112455	4.620573	0.046536
36	1	0	-4.372618	2.707305	0.815168
37	1	0	-4.849748	-3.049281	-0.100092
38	1	0	-6.960743	-2.070026	-0.918827
39	1	0	-7.056191	0.408194	-1.322977
40	1	0	-5.121080	1.776515	-0.842944
41	1	0	1.798132	-1.941851	-1.870899
42	1	0	3.621093	-2.677582	-3.369842
43	1	0	5.959424	-1.936394	-2.928491
44	1	0	6.435920	-0.464759	-0.996240

2a-TS1-B-fix-DOWN-A-int

Method: opt(ts,calcfc,noeigen) freq b3lyp/6-311++g(d,p) scrf(solvent=Chlorof  
SCF Done: E(RB3LYP) = -6223.12454746 A.U. after 1 cycles  
Lowest frequency = -37.0681

Zero-point correction= 0.330348  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.352311  
 Thermal correction to Enthalpy= 0.353256  
 Thermal correction to Gibbs Free Energy= 0.276848  
 Sum of electronic and zero-point Energies= -6222.794199  
 Sum of electronic and thermal Energies= -6222.772236  
 Sum of electronic and thermal Enthalpies= -6222.771292  
 Sum of electronic and thermal Free Energies= -6222.847699

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.750749	2.821300	-0.462131
2	6	0	-0.546574	2.576400	-0.029558
3	6	0	-1.059670	1.265075	0.028232
4	6	0	-0.207085	0.226759	-0.385736
5	6	0	1.168249	0.425752	-0.651009
6	6	0	1.587352	1.754613	-0.770253
7	8	0	-0.747276	-1.010999	-0.602132
8	6	0	-0.199293	-1.579065	-1.811702
9	6	0	1.280641	-1.723133	-1.662473
10	6	0	1.976963	-0.801369	-0.956930
11	8	0	-1.318102	3.644242	0.334280
12	6	0	-2.730024	3.494833	0.083585
13	6	0	-3.234413	2.168842	0.564016
14	6	0	-2.443696	1.085968	0.507386
15	6	0	-2.910141	-0.219981	1.061201
16	6	0	-3.914998	-1.004426	0.484356
17	6	0	-4.351296	-2.191807	1.068694
18	6	0	-3.775932	-2.622964	2.260782
19	6	0	-2.767378	-1.867200	2.856174
20	6	0	-2.345063	-0.685201	2.258455
21	6	0	3.360267	-1.180728	-0.461101
22	6	0	3.630451	-2.577933	-0.467552
23	6	0	4.854406	-3.148768	-0.166163
24	6	0	5.917235	-2.336962	0.214091
25	6	0	5.688213	-0.976941	0.336092
26	6	0	4.441037	-0.412000	0.038304
27	35	0	-4.722246	-0.508709	-1.196305
28	35	0	4.425439	1.463275	0.517731
29	1	0	1.091062	3.843983	-0.565935
30	1	0	2.571659	1.971417	-1.148059
31	1	0	-0.676670	-2.551882	-1.923506
32	1	0	-0.492646	-0.946087	-2.661732
33	1	0	1.722420	-2.628793	-2.051909
34	1	0	-3.205422	4.321992	0.609572
35	1	0	-2.909780	3.626151	-0.994626
36	1	0	-4.244004	2.111361	0.953805
37	1	0	-5.129096	-2.774788	0.592716
38	1	0	-4.115742	-3.546166	2.715710
39	1	0	-2.313264	-2.194919	3.784038
40	1	0	-1.562663	-0.095137	2.722479
41	1	0	2.822126	-3.254740	-0.693021
42	1	0	4.963490	-4.226105	-0.207587
43	1	0	6.890062	-2.749415	0.453193

44 1 0 6.479779 -0.329014 0.687203

- 2a-TS3-A-fix-DOWN-B-ext

Method: opt(ts,calcfc,noeigen) freq b3lyp/6-311++g(d,p) scrf(solvent=Chlorof  
SCF Done: E(RB3LYP) = -6223.13525737 A.U. after 1 cycles  
Lowest frequency = -39.5397

Zero-point correction= 0.330280  
(Hartree/Particle)  
Thermal correction to Energy= 0.352304  
Thermal correction to Enthalpy= 0.353248  
Thermal correction to Gibbs Free Energy= 0.276370  
Sum of electronic and zero-point Energies= -6222.804977  
Sum of electronic and thermal Energies= -6222.782953  
Sum of electronic and thermal Enthalpies= -6222.782009  
Sum of electronic and thermal Free Energies= -6222.858887

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.612676	-2.301828	-1.192385
2	6	0	0.662006	-2.062523	-0.692976
3	6	0	0.954450	-0.955201	0.141691
4	6	0	-0.161055	-0.313378	0.711046
5	6	0	-1.477529	-0.572700	0.270499
6	6	0	-1.670209	-1.531339	-0.728627
7	8	0	0.045907	0.471894	1.814040
8	6	0	-0.924043	1.495758	2.115292
9	6	0	-2.330091	1.055405	1.859252
10	6	0	-2.592937	0.100891	0.957679
11	8	0	1.653191	-2.957609	-0.980616
12	6	0	2.505222	-3.158043	0.173237
13	6	0	3.132978	-1.852077	0.543078
14	6	0	2.416805	-0.716581	0.411639
15	6	0	3.059103	0.635676	0.321709
16	6	0	4.424394	0.895850	0.024677
17	6	0	4.942270	2.190124	-0.034759
18	6	0	4.124504	3.297618	0.149253
19	6	0	2.768252	3.091511	0.364360
20	6	0	2.269499	1.798504	0.439996
21	6	0	-3.999214	-0.323033	0.682174
22	6	0	-4.585256	-1.325266	1.469519
23	6	0	-5.896582	-1.741896	1.261246
24	6	0	-6.655139	-1.162145	0.246028
25	6	0	-6.100109	-0.167387	-0.554819
26	6	0	-4.785886	0.238042	-0.330629
27	35	0	5.761435	-0.423912	-0.473496
28	35	0	-4.073086	1.621936	-1.465519
29	1	0	-0.768977	-3.126404	-1.876322
30	1	0	-2.673027	-1.735086	-1.083208
31	1	0	-0.759937	1.736461	3.166081
32	1	0	-0.686985	2.397158	1.527550
33	1	0	-3.122573	1.570502	2.390109
34	1	0	1.901945	-3.601099	0.978144
35	1	0	3.257879	-3.880989	-0.137794
36	1	0	4.181966	-1.853964	0.782769
37	1	0	5.992968	2.326408	-0.252759

38	1	0	4.543512	4.295376	0.095168
39	1	0	2.091094	3.930664	0.472832
40	1	0	1.218205	1.677515	0.611298
41	1	0	-3.991189	-1.775860	2.256402
42	1	0	-6.323363	-2.515171	1.889112
43	1	0	-7.677459	-1.477935	0.073584
44	1	0	-6.681602	0.291422	-1.343907

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- 2a-TS2-B-fix-UP-A-ext

Method: opt(ts,calcfc,noeigen) freq b3lyp/6-311++g(d,p) scrf(solvent=Chlorof  
SCF Done: E(RB3LYP) = -6223.13787337 A.U. after 1 cycles  
Lowest frequency = -38.2596

Zero-point correction= 0.330618  
(Hartree/Particle)  
Thermal correction to Energy= 0.352574  
Thermal correction to Enthalpy= 0.353519  
Thermal correction to Gibbs Free Energy= 0.277295  
Sum of electronic and zero-point Energies= -6222.807255  
Sum of electronic and thermal Energies= -6222.785299  
Sum of electronic and thermal Enthalpies= -6222.784355  
Sum of electronic and thermal Free Energies= -6222.860579

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.374523	3.251928	0.442056
2	6	0	-1.441135	2.702041	-0.257967
3	6	0	-1.499830	1.316271	-0.518913
4	6	0	-0.371510	0.552162	-0.176586
5	6	0	0.816239	1.121469	0.343076
6	6	0	0.730399	2.464110	0.742760
7	8	0	-0.439235	-0.801560	-0.335631
8	6	0	0.226273	-1.490099	0.744177
9	6	0	1.659741	-1.072948	0.792211
10	6	0	1.993838	0.200560	0.496403
11	8	0	-2.485343	3.519398	-0.576368
12	6	0	-3.244227	3.104659	-1.728918
13	6	0	-3.613245	1.656190	-1.633737
14	6	0	-2.772343	0.784838	-1.052906
15	6	0	-3.176786	-0.649539	-0.949121
16	6	0	-3.573389	-1.257022	0.248126
17	6	0	-3.991810	-2.583367	0.301430
18	6	0	-4.024448	-3.339595	-0.868535
19	6	0	-3.648857	-2.759957	-2.078094
20	6	0	-3.234654	-1.431560	-2.111263
21	6	0	3.411122	0.629343	0.242642
22	6	0	3.727451	2.004355	0.166437
23	6	0	5.008271	2.504761	-0.024924
24	6	0	6.077230	1.631355	-0.169689
25	6	0	5.818936	0.266790	-0.170773
26	6	0	4.524639	-0.223133	0.006589
27	35	0	-3.588866	-0.253529	1.893277
28	35	0	4.466430	-2.150134	-0.240794
29	1	0	-0.411051	4.294599	0.731755
30	1	0	1.521065	2.916851	1.321955
31	1	0	-0.314969	-1.283538	1.678708

32	1	0	0.132200	-2.551248	0.517145
33	1	0	2.387869	-1.838624	0.992104
34	1	0	-4.124177	3.746355	-1.743507
35	1	0	-2.650106	3.313751	-2.631393
36	1	0	-4.575018	1.338245	-2.019226
37	1	0	-4.296842	-3.017626	1.244849
38	1	0	-4.349157	-4.372870	-0.828638
39	1	0	-3.676854	-3.338920	-2.993856
40	1	0	-2.932627	-0.981704	-3.049828
41	1	0	2.932395	2.722561	0.239165
42	1	0	5.158748	3.577218	-0.063871
43	1	0	7.089065	1.992438	-0.309677
44	1	0	6.627037	-0.433658	-0.333497

### Compound 1b:

1b-anti-GS1

Method: opt freq b3lyp/6-31+g(d,p) scrf(solvent=Chloroform)

SCF Done: E(RB3LYP) = -1461.81839842 A.U. after 1 cycles

Lowest frequency = 14.0019

Zero-point correction= 0.499875  
(Hartree/Particle)  
Thermal correction to Energy= 0.528862  
Thermal correction to Enthalpy= 0.529806  
Thermal correction to Gibbs Free Energy= 0.438317  
Sum of electronic and zero-point Energies= -1461.318523  
Sum of electronic and thermal Energies= -1461.289537  
Sum of electronic and thermal Enthalpies= -1461.288592  
Sum of electronic and thermal Free Energies= -1461.380081

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.023082	3.039608	0.632382
2	6	0	1.057313	1.626073	0.622980
3	6	0	2.228538	0.954733	1.217919
4	6	0	3.060423	1.689030	1.980089
5	6	0	0.000000	3.744627	0.000000
6	6	0	0.000000	0.950656	0.000000
7	6	0	-1.057313	1.626073	-0.622980
8	6	0	-1.023082	3.039607	-0.632382
9	6	0	-3.060423	1.689030	-1.980089
10	6	0	-2.228538	0.954733	-1.217919
11	1	0	0.000000	4.829031	0.000000
12	1	0	3.948286	1.254617	2.430844
13	1	0	0.000000	-0.134723	0.000000
14	1	0	-3.948286	1.254617	-2.430844
15	8	0	-2.041510	3.766519	-1.183990
16	8	0	2.041510	3.766519	1.183990
17	6	0	-2.757150	3.131900	-2.266138
18	1	0	-3.667979	3.721269	-2.389120
19	1	0	-2.156936	3.238603	-3.185491
20	6	0	2.757150	3.131900	2.266138
21	1	0	3.667979	3.721269	2.389120
22	1	0	2.156935	3.238603	3.185491

23	6	0	-2.475777	-0.499122	-0.952897
24	6	0	-3.116264	-0.896506	0.269803
25	6	0	-2.084567	-1.456594	-1.884690
26	6	0	-3.536802	0.044345	1.254094
27	6	0	-3.355652	-2.288241	0.520946
28	6	0	-2.332855	-2.831685	-1.612044
29	6	0	-4.153150	-0.367305	2.417779
30	1	0	-3.371549	1.101875	1.078437
31	6	0	-3.995308	-2.680971	1.729732
32	6	0	-2.947317	-3.239353	-0.451588
33	6	0	-4.386369	-1.743864	2.661764
34	1	0	-4.464427	0.369345	3.152949
35	1	0	-4.172180	-3.739277	1.904632
36	1	0	-4.874622	-2.055509	3.580518
37	6	0	2.475777	-0.499122	0.952896
38	6	0	3.116264	-0.896506	-0.269803
39	6	0	2.084566	-1.456594	1.884690
40	6	0	3.536803	0.044345	-1.254094
41	6	0	3.355652	-2.288241	-0.520946
42	6	0	2.332854	-2.831685	1.612044
43	6	0	4.153151	-0.367305	-2.417778
44	1	0	3.371550	1.101875	-1.078437
45	6	0	3.995309	-2.680971	-1.729731
46	6	0	2.947317	-3.239353	0.451587
47	6	0	4.386371	-1.743863	-2.661763
48	1	0	4.464429	0.369345	-3.152948
49	1	0	4.172181	-3.739277	-1.904632
50	1	0	4.874624	-2.055509	-3.580517
51	1	0	3.123377	-4.295557	0.264202
52	1	0	2.019899	-3.571463	2.344220
53	1	0	-3.123377	-4.295557	-0.264202
54	1	0	-2.019900	-3.571463	-2.344220
55	6	0	1.409156	-1.085173	3.187205
56	1	0	0.880623	-1.946014	3.606209
57	1	0	2.140729	-0.751738	3.933342
58	1	0	0.689239	-0.272549	3.057880
59	6	0	-1.409157	-1.085173	-3.187206
60	1	0	-0.880621	-1.946013	-3.606208
61	1	0	-2.140732	-0.751743	-3.933343
62	1	0	-0.689244	-0.272546	-3.057882

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1b-anti-GS2

Method: opt freq b3lyp/6-31+g(d,p) scrf(solvent=Chloroform)  
 SCF Done: E(RB3LYP) = -1461.81815460 A.U. after 1 cycles  
 Lowest frequency = 12.7558

Zero-point correction= 0.499697  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.528776  
 Thermal correction to Enthalpy= 0.529720  
 Thermal correction to Gibbs Free Energy= 0.437218  
 Sum of electronic and zero-point Energies= -1461.318457  
 Sum of electronic and thermal Energies= -1461.289379  
 Sum of electronic and thermal Enthalpies= -1461.288435  
 Sum of electronic and thermal Free Energies= -1461.380936

Standard orientation:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.199526	3.277894	-0.088545
2	6	0	1.221955	1.864318	-0.114526
3	6	0	2.519904	1.193058	-0.316030
4	6	0	3.640419	1.928013	-0.185873
5	6	0	0.000000	3.982765	0.000000
6	6	0	0.000000	1.188622	0.000000
7	6	0	-1.221955	1.864318	0.114526
8	6	0	-1.199526	3.277894	0.088545
9	6	0	-3.640419	1.928013	0.185873
10	6	0	-2.519904	1.193058	0.316030
11	1	0	0.000000	5.067217	0.000000
12	1	0	4.624460	1.491315	-0.331809
13	1	0	0.000000	0.103306	0.000000
14	1	0	-4.624460	1.491314	0.331809
15	8	0	-2.347259	4.005278	0.240844
16	8	0	2.347259	4.005278	-0.240844
17	6	0	-3.563027	3.373370	-0.214707
18	1	0	-4.371502	3.960140	0.226090
19	1	0	-3.621016	3.486873	-1.310560
20	6	0	3.563027	3.373370	0.214707
21	1	0	4.371501	3.960141	-0.226090
22	1	0	3.621015	3.486874	1.310560
23	6	0	-2.566726	-0.259417	0.681707
24	6	0	-2.779266	-1.241613	-0.343085
25	6	0	-2.406291	-0.650597	2.009278
26	6	0	-2.927076	-0.897609	-1.719114
27	6	0	-2.839103	-2.630634	0.014182
28	6	0	-2.468331	-2.032708	2.337168
29	6	0	-3.130712	-1.866135	-2.679721
30	1	0	-2.878766	0.146343	-2.009253
31	6	0	-3.055184	-3.605201	-1.000300
32	6	0	-2.679846	-2.994752	1.376483
33	6	0	-3.199176	-3.235739	-2.319842
34	1	0	-3.238499	-1.578156	-3.721619
35	1	0	-3.102406	-4.652578	-0.712842
36	1	0	-3.362698	-3.988862	-3.085132
37	6	0	2.566726	-0.259417	-0.681707
38	6	0	2.779266	-1.241613	0.343085
39	6	0	2.406291	-0.650597	-2.009278
40	6	0	2.927076	-0.897609	1.719114
41	6	0	2.839103	-2.630634	-0.014182
42	6	0	2.468331	-2.032708	-2.337168
43	6	0	3.130712	-1.866134	2.679721
44	1	0	2.878766	0.146343	2.009253
45	6	0	3.055185	-3.605201	1.000300
46	6	0	2.679847	-2.994751	-1.376483
47	6	0	3.199176	-3.235739	2.319842
48	1	0	3.238499	-1.578156	3.721619
49	1	0	3.102406	-4.652577	0.712842
50	1	0	3.362699	-3.988861	3.085133
51	1	0	2.723902	-4.045550	-1.651126
52	1	0	2.346154	-2.326944	-3.376214
53	1	0	-2.723902	-4.045550	1.651126
54	1	0	-2.346154	-2.326944	3.376214
55	6	0	2.182265	0.358987	-3.112988
56	1	0	2.040565	-0.141551	-4.074384
57	1	0	1.298972	0.977375	-2.919982

58	1	0	3.033255	1.042542	-3.208425
59	6	0	-2.182265	0.358987	3.112988
60	1	0	-2.040566	-0.141551	4.074384
61	1	0	-1.298972	0.977374	2.919982
62	1	0	-3.033255	1.042542	3.208424

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1b-anti-GS3

Method: opt freq b3lyp/6-31+g(d,p) scrf(solvent=Chloroform)

SCF Done: E(RB3LYP) = -1461.81827116 A.U. after 1 cycles

Lowest frequency = 10.8279

Zero-point correction=	0.499717
(Hartree/Particle)	
Thermal correction to Energy=	0.528773
Thermal correction to Enthalpy=	0.529717
Thermal correction to Gibbs Free Energy=	0.437397
Sum of electronic and zero-point Energies=	-1461.318554
Sum of electronic and thermal Energies=	-1461.289498
Sum of electronic and thermal Enthalpies=	-1461.288554
Sum of electronic and thermal Free Energies=	-1461.380874

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.754183	3.279893	-0.466009
2	6	0	-0.986965	1.898407	-0.275330
3	6	0	-2.304478	1.355770	-0.656994
4	6	0	-3.301787	2.226544	-0.901263
5	6	0	0.490144	3.849641	-0.199693
6	6	0	0.071797	1.117415	0.205838
7	6	0	1.328735	1.659485	0.503812
8	6	0	1.514388	3.046184	0.299496
9	6	0	3.569239	1.517171	1.408251
10	6	0	2.486387	0.861376	0.950419
11	1	0	0.653956	4.909228	-0.361762
12	1	0	-4.291190	1.886873	-1.194697
13	1	0	-0.080207	0.050103	0.331537
14	1	0	4.458434	0.984812	1.734085
15	8	0	2.729698	3.634523	0.514846
16	8	0	-1.720962	4.093391	-0.988248
17	6	0	3.561493	3.014902	1.520053
18	1	0	3.203106	3.339376	2.511619
19	1	0	4.556190	3.438308	1.367248
20	6	0	-3.086410	3.702691	-0.727294
21	1	0	-3.688413	4.285447	-1.427485
22	1	0	-3.348258	4.025944	0.294553
23	6	0	2.444117	-0.634277	0.869462
24	6	0	2.760084	-1.285048	-0.371283
25	6	0	2.098563	-1.385698	1.989183
26	6	0	3.119784	-0.561582	-1.545264
27	6	0	2.723483	-2.716987	-0.445719
28	6	0	2.068065	-2.805436	1.889635
29	6	0	3.422697	-1.215473	-2.721748
30	1	0	3.159349	0.521707	-1.506611
31	6	0	3.042790	-3.361982	-1.673092
32	6	0	2.370186	-3.454139	0.715601
33	6	0	3.384911	-2.630691	-2.790171



34	1	0	3.693979	-0.641559	-3.603273
35	1	0	3.012592	-4.448000	-1.713074
36	1	0	3.627518	-3.134079	-3.721512
37	6	0	-2.498056	-0.124575	-0.786734
38	6	0	-3.045988	-0.865766	0.313498
39	6	0	-2.144300	-0.774822	-1.967047
40	6	0	-3.405010	-0.253210	1.550266
41	6	0	-3.237677	-2.282371	0.182761
42	6	0	-2.344575	-2.178684	-2.071777
43	6	0	-3.927593	-0.994403	2.589497
44	1	0	-3.263321	0.815490	1.669339
45	6	0	-3.783388	-3.017959	1.272166
46	6	0	-2.874374	-2.912740	-1.035659
47	6	0	-4.122973	-2.391912	2.451725
48	1	0	-4.191752	-0.504207	3.522263
49	1	0	-3.926377	-4.089347	1.155658
50	1	0	-4.538007	-2.964183	3.276264
51	1	0	-3.017841	-3.985292	-1.138803
52	1	0	-2.068818	-2.675708	-2.998047
53	1	0	2.337020	-4.539346	0.662446
54	1	0	1.792877	-3.382542	2.768567
55	6	0	-1.562599	-0.023741	-3.143789
56	1	0	-1.328745	-0.707536	-3.963834
57	1	0	-0.641384	0.501483	-2.869329
58	1	0	-2.260053	0.732718	-3.519963
59	6	0	1.763205	-0.743179	3.317843
60	1	0	1.199608	-1.435641	3.949413
61	1	0	1.169492	0.166703	3.194526
62	1	0	2.672079	-0.462892	3.864242

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1b-syn-GS1

Method: opt freq b3lyp/6-31+g(d,p) scrf(solvent=Chloroform)  
SCF Done: E(RB3LYP) = -1461.81811921 A.U. after 1 cycles  
Lowest frequency = 14.0986

Zero-point correction= 0.499764  
(Hartree/Particle)  
Thermal correction to Energy= 0.528809  
Thermal correction to Enthalpy= 0.529753  
Thermal correction to Gibbs Free Energy= 0.437825  
Sum of electronic and zero-point Energies= -1461.318355  
Sum of electronic and thermal Energies= -1461.289310  
Sum of electronic and thermal Enthalpies= -1461.288366  
Sum of electronic and thermal Free Energies= -1461.380294

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.514444	3.062890	-0.287893
2	6	0	1.358042	1.730093	0.158163
3	6	0	2.560104	1.001680	0.606786
4	6	0	3.681198	1.710292	0.837331
5	6	0	0.444545	3.779181	-0.822369
6	6	0	0.077465	1.165449	0.095222
7	6	0	-1.025994	1.865486	-0.409856
8	6	0	-0.810783	3.176878	-0.892984
9	6	0	-3.332265	2.004110	-1.130420

10	6	0	-2.404886	1.341281	-0.414010
11	1	0	0.586972	4.793334	-1.178992
12	1	0	4.601932	1.227596	1.152670
13	1	0	-0.063841	0.149158	0.448913
14	1	0	-4.366903	1.674234	-1.161946
15	8	0	-1.847331	3.934344	-1.363526
16	8	0	2.742072	3.665062	-0.295826
17	6	0	-2.947744	3.203947	-1.947850
18	1	0	-3.763797	3.925963	-2.017408
19	1	0	-2.662970	2.913827	-2.973364
20	6	0	3.677872	3.206192	0.703906
21	1	0	4.648854	3.586871	0.380826
22	1	0	3.424632	3.691752	1.661561
23	6	0	-2.749838	0.126054	0.392374
24	6	0	-2.771367	-1.162500	-0.239271
25	6	0	-3.050335	0.251192	1.747062
26	6	0	-2.452156	-1.348367	-1.616488
27	6	0	-3.117626	-2.320698	0.534840
28	6	0	-3.389264	-0.911331	2.492417
29	6	0	-2.481842	-2.600609	-2.193472
30	1	0	-2.180849	-0.485924	-2.215562
31	6	0	-3.143848	-3.598374	-0.091656
32	6	0	-3.425220	-2.157834	1.910678
33	6	0	-2.834250	-3.739850	-1.426763
34	1	0	-2.230362	-2.716491	-3.243814
35	1	0	-3.412399	-4.465288	0.506895
36	1	0	-2.855973	-4.720325	-1.893434
37	6	0	2.517407	-0.486425	0.776189
38	6	0	2.679235	-1.333752	-0.372368
39	6	0	2.320518	-1.042228	2.037132
40	6	0	2.886421	-0.814516	-1.683112
41	6	0	2.641195	-2.758099	-0.209081
42	6	0	2.286296	-2.459020	2.173263
43	6	0	3.042949	-1.653932	-2.766757
44	1	0	2.925711	0.260078	-1.825509
45	6	0	2.807103	-3.597270	-1.345927
46	6	0	2.440955	-3.292971	1.091271
47	6	0	3.003276	-3.060828	-2.600283
48	1	0	3.199359	-1.233767	-3.756227
49	1	0	2.776755	-4.674908	-1.205727
50	1	0	3.129179	-3.711351	-3.460871
51	1	0	2.406784	-4.371897	1.218953
52	1	0	2.127669	-2.882747	3.161553
53	1	0	-3.687880	-3.032394	2.500403
54	1	0	-3.626886	-0.802080	3.547370
55	6	0	-3.042839	1.594838	2.441784
56	1	0	-2.087236	2.113131	2.309313
57	1	0	-3.819815	2.255713	2.041121
58	1	0	-3.219584	1.478361	3.514303
59	6	0	2.150666	-0.190660	3.276824
60	1	0	1.650538	-0.757084	4.067605
61	1	0	3.121080	0.136682	3.669891
62	1	0	1.564503	0.710525	3.078204

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1b-syn-GS2

Method: opt freq b3lyp/6-31+g(d,p) scrf(solvent=Chloroform)

SCF Done: E(RB3LYP) = -1461.81785909 A.U. after 2 cycles

Lowest frequency = 9.2212

Zero-point correction= 0.499697  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.528740  
 Thermal correction to Enthalpy= 0.529685  
 Thermal correction to Gibbs Free Energy= 0.437623  
 Sum of electronic and zero-point Energies= -1461.318162  
 Sum of electronic and thermal Energies= -1461.289119  
 Sum of electronic and thermal Enthalpies= -1461.288175  
 Sum of electronic and thermal Free Energies= -1461.380236

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.202799	3.082684	-0.771864
2	6	0	1.227673	1.854057	-0.072525
3	6	0	2.539835	1.240633	0.208385
4	6	0	3.641685	1.994912	0.037776
5	6	0	0.000042	3.685418	-1.137517
6	6	0	0.000017	1.264993	0.256955
7	6	0	-1.227625	1.854094	-0.072505
8	6	0	-1.202728	3.082721	-0.771845
9	6	0	-3.641636	1.995008	0.037810
10	6	0	-2.539803	1.240709	0.208430
11	1	0	0.000052	4.622230	-1.683616
12	1	0	4.635568	1.593495	0.214864
13	1	0	0.000005	0.307010	0.767344
14	1	0	-4.635526	1.593621	0.214925
15	8	0	-2.359570	3.687266	-1.179102
16	8	0	2.359659	3.687187	-1.179141
17	6	0	-3.525164	3.437338	-0.363903
18	1	0	-3.474919	4.094974	0.520451
19	1	0	-4.372740	3.758271	-0.972871
20	6	0	3.525221	3.437256	-0.363894
21	1	0	4.372820	3.758226	-0.972808
22	1	0	3.474915	4.094860	0.520481
23	6	0	-2.624652	-0.186396	0.657714
24	6	0	-2.614750	-1.238930	-0.319243
25	6	0	-2.715364	-0.486950	2.013951
26	6	0	-2.525137	-0.983675	-1.718286
27	6	0	-2.705827	-2.603366	0.113617
28	6	0	-2.801540	-1.848930	2.418702
29	6	0	-2.525062	-2.016115	-2.633088
30	1	0	-2.459178	0.042040	-2.064794
31	6	0	-2.704324	-3.645862	-0.854614
32	6	0	-2.798366	-2.875786	1.504251
33	6	0	-2.615770	-3.362671	-2.200405
34	1	0	-2.453996	-1.796162	-3.694477
35	1	0	-2.774906	-4.674939	-0.511142
36	1	0	-2.615083	-4.166683	-2.930602
37	6	0	2.624671	-0.186491	0.657618
38	6	0	2.614640	-1.238986	-0.319391
39	6	0	2.715538	-0.487112	2.013824
40	6	0	2.524856	-0.983668	-1.718408
41	6	0	2.705769	-2.603440	0.113393
42	6	0	2.801771	-1.849118	2.418500
43	6	0	2.524658	-2.016066	-2.633260
44	1	0	2.458866	0.042064	-2.064863
45	6	0	2.704137	-3.645892	-0.854883

46	6	0	2.798490	-2.875927	1.504006
47	6	0	2.615411	-3.362640	-2.200651
48	1	0	2.453461	-1.796061	-3.694630
49	1	0	2.774760	-4.674984	-0.511466
50	1	0	2.614626	-4.166620	-2.930884
51	1	0	2.863099	-3.908826	1.836468
52	1	0	2.868405	-2.073201	3.480026
53	1	0	-2.862932	-3.908668	1.836772
54	1	0	-2.868053	-2.072966	3.480244
55	6	0	-2.739333	0.590048	3.077183
56	1	0	-2.044731	1.404062	2.852068
57	1	0	-3.737400	1.035694	3.168817
58	1	0	-2.474205	0.174164	4.053380
59	6	0	2.739670	0.589782	3.077155
60	1	0	2.473367	0.174065	4.053108
61	1	0	3.738119	1.034411	3.169650
62	1	0	2.046062	1.404496	2.851559

1b-syn-GS3

Method: opt freq b3lyp/6-31+g(d,p) scrf(solvent=Chloroform)  
 SCF Done: E(RB3LYP) = -1461.81801029 A.U. after 1 cycles  
 Lowest frequency = 14.0369

Zero-point correction= 0.499690  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.528762  
 Thermal correction to Enthalpy= 0.529707  
 Thermal correction to Gibbs Free Energy= 0.437517  
 Sum of electronic and zero-point Energies= -1461.318320  
 Sum of electronic and thermal Energies= -1461.289248  
 Sum of electronic and thermal Enthalpies= -1461.288304  
 Sum of electronic and thermal Free Energies= -1461.380494

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.203140	3.240139	-0.500628
2	6	0	1.227814	1.850967	-0.237869
3	6	0	2.539455	1.203700	-0.045346
4	6	0	3.642461	1.888230	-0.402179
5	6	0	0.000403	3.936195	-0.612967
6	6	0	0.000133	1.187872	-0.110345
7	6	0	-1.227419	1.851202	-0.237898
8	6	0	-1.202471	3.240368	-0.500665
9	6	0	-3.642052	1.888925	-0.402285
10	6	0	-2.539190	1.204193	-0.045393
11	1	0	0.000507	5.003802	-0.802961
12	1	0	4.636150	1.468079	-0.274082
13	1	0	0.000030	0.126279	0.115227
14	1	0	-4.635828	1.468978	-0.274193
15	8	0	-2.359103	3.964830	-0.580572
16	8	0	2.359910	3.964385	-0.580493
17	6	0	-3.525766	3.245600	-1.035783
18	1	0	-4.372650	3.886055	-0.781173
19	1	0	-3.476776	3.169805	-2.135266
20	6	0	3.526471	3.244949	-1.035636

21	1	0	3.477556	3.169202	-2.135126
22	1	0	4.373457	3.885236	-0.780939
23	6	0	-2.622322	-0.164484	0.559661
24	6	0	-2.698349	-1.313883	-0.296523
25	6	0	-2.629028	-0.316505	1.944320
26	6	0	-2.676991	-1.214889	-1.718788
27	6	0	-2.792865	-2.621870	0.286850
28	6	0	-2.723001	-1.622985	2.497969
29	6	0	-2.751596	-2.339281	-2.513976
30	1	0	-2.601146	-0.235029	-2.177650
31	6	0	-2.872089	-3.761890	-0.561392
32	6	0	-2.804246	-2.741583	1.700973
33	6	0	-2.853001	-3.628287	-1.932595
34	1	0	-2.730842	-2.237660	-3.595306
35	1	0	-2.946347	-4.745463	-0.104349
36	1	0	-2.912650	-4.505945	-2.569567
37	6	0	2.622303	-0.165021	0.559646
38	6	0	2.698051	-1.314397	-0.296595
39	6	0	2.629017	-0.317110	1.944297
40	6	0	2.676673	-1.215330	-1.718853
41	6	0	2.792302	-2.622432	0.286712
42	6	0	2.722718	-1.623637	2.497882
43	6	0	2.751013	-2.339699	-2.514098
44	1	0	2.601027	-0.235431	-2.177667
45	6	0	2.871254	-3.762428	-0.561586
46	6	0	2.803697	-2.742215	1.700830
47	6	0	2.852157	-3.628755	-1.932782
48	1	0	2.730251	-2.238022	-3.595423
49	1	0	2.945314	-4.746039	-0.104592
50	1	0	2.911600	-4.506396	-2.569798
51	1	0	2.874197	-3.731117	2.146646
52	1	0	2.731020	-1.731224	3.579358
53	1	0	-2.874951	-3.730448	2.146838
54	1	0	-2.731300	-1.730519	3.579450
55	6	0	-2.559140	0.873849	2.875105
56	1	0	-1.718562	1.531087	2.629963
57	1	0	-3.467790	1.483528	2.811089
58	1	0	-2.445011	0.549251	3.912801
59	6	0	2.559430	0.873214	2.875143
60	1	0	2.445022	0.548593	3.912803
61	1	0	3.468325	1.482549	2.811309
62	1	0	1.719141	1.530787	2.629913

1b-TS2-ext

Method: opt(ts,calcfc,noeigen) b3lyp/6-31+g(d,p) freq scrf(solvent=Chloroform)  
 SCF Done: E(RB3LYP) = -1461.76777077 A.U. after 1 cycles  
 Lowest frequency = -20.6403

Zero-point correction=	0.500613
(Hartree/Particle)	
Thermal correction to Energy=	0.528008
Thermal correction to Enthalpy=	0.528952
Thermal correction to Gibbs Free Energy=	0.443397
Sum of electronic and zero-point Energies=	-1461.267158
Sum of electronic and thermal Energies=	-1461.239763
Sum of electronic and thermal Enthalpies=	-1461.238819
Sum of electronic and thermal Free Energies=	-1461.324373

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.607940	2.922058	-0.502825
2	6	0	-1.458028	1.579572	-0.075487
3	6	0	-2.738761	0.832302	0.207821
4	6	0	-3.687221	1.634722	0.758670
5	6	0	-0.523987	3.721886	-0.860257
6	6	0	-0.141341	1.184521	0.224046
7	6	0	0.978817	1.987736	-0.045234
8	6	0	0.764715	3.247135	-0.648024
9	6	0	3.334419	2.534543	0.132735
10	6	0	2.372960	1.599400	0.254685
11	1	0	-0.687756	4.730666	-1.222295
12	1	0	-4.608651	1.234620	1.158704
13	1	0	0.034812	0.232981	0.707546
14	1	0	4.373706	2.299268	0.345718
15	8	0	1.808550	4.039963	-1.043577
16	8	0	-2.851914	3.503020	-0.498001
17	6	0	3.008417	3.948252	-0.249507
18	1	0	3.794808	4.390744	-0.865261
19	1	0	2.885202	4.582292	0.645254
20	6	0	-3.553849	3.123838	0.708646
21	1	0	-3.019341	3.548506	1.574270
22	1	0	-4.534872	3.599647	0.644108
23	6	0	2.726847	0.211350	0.698359
24	6	0	3.146813	-0.759522	-0.272372
25	6	0	2.703530	-0.113702	2.052197
26	6	0	3.170235	-0.484647	-1.670940
27	6	0	3.563824	-2.060376	0.166602
28	6	0	3.106607	-1.415779	2.460980
29	6	0	3.583809	-1.437462	-2.579028
30	1	0	2.857539	0.492933	-2.021612
31	6	0	3.993517	-3.018216	-0.794113
32	6	0	3.530656	-2.358535	1.554247
33	6	0	4.004264	-2.717859	-2.139308
34	1	0	3.588248	-1.205114	-3.640090
35	1	0	4.311700	-3.997612	-0.445545
36	1	0	4.332017	-3.457975	-2.863403
37	6	0	-3.135874	-0.598128	-0.053076
38	6	0	-2.233737	-1.744186	-0.093428
39	6	0	-4.511301	-0.890401	-0.204026
40	6	0	-0.886199	-1.682291	-0.542999
41	6	0	-2.739788	-3.058457	0.200494
42	6	0	-4.983028	-2.212717	0.034333
43	6	0	-0.063919	-2.793111	-0.561804
44	1	0	-0.509899	-0.761043	-0.958398
45	6	0	-1.858989	-4.173655	0.240751
46	6	0	-4.139221	-3.249489	0.334366
47	6	0	-0.534244	-4.047625	-0.115606
48	1	0	0.948257	-2.698693	-0.940686
49	1	0	-2.269811	-5.143546	0.509736
50	1	0	0.126822	-4.909145	-0.105082
51	1	0	-4.525373	-4.237058	0.571752
52	1	0	-6.055150	-2.386441	-0.014309
53	1	0	3.840543	-3.344747	1.890335
54	1	0	3.081939	-1.659370	3.519893
55	6	0	-5.587505	0.065813	-0.699342
56	1	0	-6.187908	-0.460868	-1.450227

57	1	0	-6.282109	0.383149	0.087535
58	1	0	-5.173864	0.962498	-1.161736
59	6	0	2.299609	0.889503	3.110759
60	1	0	2.071886	0.385683	4.054192
61	1	0	3.107840	1.605581	3.303835
62	1	0	1.421679	1.470343	2.814489

1b-TS1-int

Method: opt(ts,calcfc,noeigen) b3lyp/6-31+g(d,p) freq scrf(solvent=Chloroform)  
 SCF Done: E(RB3LYP) = -1461.75506826 A.U. after 1 cycles  
 Lowest frequency = -49.4085

Zero-point correction= 0.500591  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.528142  
 Thermal correction to Enthalpy= 0.529086  
 Thermal correction to Gibbs Free Energy= 0.442738  
 Sum of electronic and zero-point Energies= -1461.254477  
 Sum of electronic and thermal Energies= -1461.226927  
 Sum of electronic and thermal Enthalpies= -1461.225982  
 Sum of electronic and thermal Free Energies= -1461.312330

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.930627	2.806988	-0.534523
2	6	0	-0.843295	1.584193	0.190611
3	6	0	-2.158442	1.010901	0.694364
4	6	0	-3.053976	1.989583	0.999449
5	6	0	0.151512	3.360149	-1.219709
6	6	0	0.465652	1.102587	0.364465
7	6	0	1.595553	1.670246	-0.243710
8	6	0	1.409033	2.788669	-1.082983
9	6	0	3.988980	1.895922	-0.551389
10	6	0	2.969471	1.151759	-0.082494
11	1	0	0.018777	4.275434	-1.785437
12	1	0	-4.079734	1.790301	1.246595
13	1	0	0.645112	0.266991	1.015846
14	1	0	5.017900	1.557464	-0.465258
15	8	0	2.445185	3.338082	-1.786688
16	8	0	-2.086745	3.535893	-0.540279
17	6	0	3.747250	3.241326	-1.171798
18	1	0	4.458826	3.449287	-1.973877
19	1	0	3.838373	4.046623	-0.423151
20	6	0	-2.730372	3.427333	0.749824
21	1	0	-2.061018	3.868757	1.504816
22	1	0	-3.635279	4.032661	0.684305
23	6	0	3.224211	-0.170237	0.576879
24	6	0	3.250673	-1.365434	-0.218988
25	6	0	3.458269	-0.233696	1.947907
26	6	0	3.010416	-1.355209	-1.623994
27	6	0	3.526915	-2.625201	0.409546
28	6	0	3.725534	-1.496023	2.549073
29	6	0	3.042841	-2.520611	-2.361713
30	1	0	2.801331	-0.411870	-2.116697
31	6	0	3.557986	-3.808652	-0.379776

32	6	0	3.762624	-2.654924	1.809627
33	6	0	3.321110	-3.762060	-1.736774
34	1	0	2.854630	-2.487149	-3.430986
35	1	0	3.773073	-4.755035	0.110074
36	1	0	3.347710	-4.671990	-2.329127
37	6	0	-2.610797	-0.422681	0.442410
38	6	0	-4.042223	-0.727170	0.283540
39	6	0	-1.753770	-1.494250	0.130632
40	6	0	-5.082278	-0.175020	1.086951
41	6	0	-4.456311	-1.736215	-0.651313
42	6	0	-2.198414	-2.528395	-0.748349
43	6	0	-6.419798	-0.455017	0.864475
44	1	0	-4.835301	0.401806	1.967037
45	6	0	-5.835531	-1.960609	-0.907817
46	6	0	-3.475522	-2.584592	-1.232889
47	6	0	-6.813510	-1.311472	-0.184547
48	1	0	-7.168021	-0.030113	1.527620
49	1	0	-6.103423	-2.699490	-1.658767
50	1	0	-7.865063	-1.502926	-0.375487
51	1	0	-3.771423	-3.330380	-1.965227
52	1	0	-1.469009	-3.276011	-1.049964
53	1	0	3.969937	-3.607664	2.290244
54	1	0	3.905185	-1.534552	3.620366
55	6	0	-0.395351	-1.766375	0.739339
56	1	0	-0.363921	-2.831771	0.993865
57	1	0	0.440578	-1.584074	0.059889
58	1	0	-0.239688	-1.220341	1.669481
59	6	0	3.464303	1.003732	2.819200
60	1	0	3.338781	0.736083	3.872132
61	1	0	4.413064	1.546545	2.727317
62	1	0	2.668369	1.702335	2.546974

## Compound 2b:

2b-anti-GS1

Method: opt freq b3lyp/6-31+g(d,p) scrf(solvent=Chloroform)

SCF Done: E(RB3LYP) = -1461.81237347 A.U. after 2 cycles

Lowest frequency = 13.1670

Zero-point correction= 0.499907  
(Hartree/Particle)  
Thermal correction to Energy= 0.528815  
Thermal correction to Enthalpy= 0.529760  
Thermal correction to Gibbs Free Energy= 0.438488  
Sum of electronic and zero-point Energies= -1461.312466  
Sum of electronic and thermal Energies= -1461.283558  
Sum of electronic and thermal Enthalpies= -1461.282614  
Sum of electronic and thermal Free Energies= -1461.373886

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.837277	2.942034	0.106261
2	6	0	0.547728	2.777028	0.087890
3	6	0	1.150121	1.494826	0.034066
4	6	0	0.286209	0.388910	-0.089124



5	6	0	-1.120359	0.532935	-0.120907
6	6	0	-1.657943	1.822062	0.000144
7	8	0	0.848952	-0.842343	-0.266266
8	6	0	0.082673	-1.969446	0.204472
9	6	0	-1.357226	-1.877105	-0.208277
10	6	0	-1.942494	-0.672713	-0.343006
11	8	0	1.316851	3.902028	0.201523
12	6	0	2.614624	3.815000	-0.423151
13	6	0	3.320933	2.556880	-0.014694
14	6	0	2.621046	1.423065	0.188765
15	1	0	-1.250815	3.942018	0.178807
16	1	0	-2.735536	1.949452	-0.021292
17	1	0	0.574627	-2.844736	-0.224081
18	1	0	0.184735	-2.026975	1.301398
19	1	0	-1.909486	-2.799162	-0.366662
20	1	0	2.478069	3.872737	-1.515977
21	1	0	3.152004	4.707700	-0.098937
22	1	0	4.397528	2.584981	0.126540
23	6	0	-3.382788	-0.533305	-0.733549
24	6	0	-4.403003	-0.621643	0.272203
25	6	0	-3.725831	-0.316876	-2.066671
26	6	0	-4.106023	-0.820062	1.652862
27	6	0	-5.781412	-0.496704	-0.109174
28	6	0	-5.098200	-0.197196	-2.418985
29	6	0	-5.109833	-0.897417	2.595567
30	1	0	-3.070095	-0.912017	1.960513
31	6	0	-6.793840	-0.585872	0.887301
32	6	0	-6.096977	-0.284837	-1.476471
33	1	0	-5.355256	-0.034757	-3.462391
34	6	0	-6.469906	-0.782581	2.211993
35	1	0	-4.857289	-1.047083	3.641437
36	1	0	-7.833121	-0.493924	0.581828
37	1	0	-7.139459	-0.190982	-1.769728
38	1	0	-7.251376	-0.847976	2.963370
39	6	0	3.325804	0.189404	0.671303
40	6	0	4.119445	-0.584445	-0.240767
41	6	0	3.249254	-0.169914	2.014793
42	6	0	4.217764	-0.276696	-1.629273
43	6	0	4.834184	-1.730668	0.244500
44	6	0	3.963938	-1.312236	2.469680
45	6	0	4.986952	-1.042681	-2.480519
46	1	0	3.672171	0.574987	-2.019538
47	6	0	5.624475	-2.497224	-0.657489
48	6	0	4.733247	-2.071388	1.618853
49	1	0	3.902293	-1.578644	3.521830
50	6	0	5.704147	-2.163422	-1.992030
51	1	0	5.041222	-0.787318	-3.535051
52	1	0	6.165484	-3.357713	-0.271523
53	1	0	5.276139	-2.936654	1.990761
54	1	0	6.309631	-2.757168	-2.670703
55	6	0	2.426022	0.617536	3.010081
56	1	0	2.578339	1.695468	2.898940
57	1	0	1.352878	0.432670	2.879143
58	1	0	2.686637	0.339147	4.034911
59	6	0	-2.675777	-0.218608	-3.150849
60	1	0	-1.958101	0.583051	-2.944996
61	1	0	-2.098849	-1.146234	-3.233930
62	1	0	-3.136874	-0.018166	-4.121511

2b-anti-GS2

Method: opt freq b3lyp/6-31+g(d,p) scrf(solvent=Chloroform)

SCF Done: E(RB3LYP) = -1461.81168165 A.U. after 1 cycles

Lowest frequency = 10.3619

Zero-point correction= 0.499740  
(Hartree/Particle)  
Thermal correction to Energy= 0.528766  
Thermal correction to Enthalpy= 0.529710  
Thermal correction to Gibbs Free Energy= 0.437425  
Sum of electronic and zero-point Energies= -1461.311941  
Sum of electronic and thermal Energies= -1461.282915  
Sum of electronic and thermal Enthalpies= -1461.281971  
Sum of electronic and thermal Free Energies= -1461.374257

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.638866	-1.973951	-2.102445
2	6	0	-0.700507	-2.090960	-1.731758
3	6	0	-1.237256	-1.397725	-0.617674
4	6	0	-0.331688	-0.648586	0.162492
5	6	0	1.030563	-0.510871	-0.196017
6	6	0	1.489314	-1.178748	-1.339559
7	8	0	-0.821014	0.019820	1.247136
8	6	0	0.107842	0.267636	2.321593
9	6	0	1.427164	0.774943	1.819458
10	6	0	1.882278	0.379577	0.616749
11	8	0	-1.505145	-2.856608	-2.530907
12	6	0	-2.626842	-3.470557	-1.865062
13	6	0	-3.366195	-2.471508	-1.027262
14	6	0	-2.701278	-1.480977	-0.400579
15	1	0	0.995452	-2.510773	-2.974734
16	1	0	2.530381	-1.077479	-1.628779
17	1	0	0.229625	-0.666119	2.896970
18	1	0	-0.391406	0.995598	2.964071
19	1	0	2.004414	1.437469	2.458147
20	1	0	-2.254040	-4.314684	-1.260731
21	1	0	-3.251425	-3.874098	-2.663932
22	1	0	-4.445354	-2.561713	-0.942771
23	6	0	3.204421	0.840249	0.081732
24	6	0	4.402143	0.142915	0.454942
25	6	0	3.266875	1.938385	-0.773623
26	6	0	4.391953	-0.998231	1.310154
27	6	0	5.667282	0.593532	-0.052260
28	6	0	4.532209	2.365324	-1.262325
29	6	0	5.560708	-1.647923	1.648253
30	1	0	3.444939	-1.355489	1.699871
31	6	0	6.855639	-0.096203	0.319139
32	6	0	5.696825	1.719617	-0.915508
33	1	0	4.570658	3.226336	-1.924449
34	6	0	6.808371	-1.193235	1.151516
35	1	0	5.526071	-2.516113	2.300257
36	1	0	7.806305	0.260126	-0.069625
37	1	0	6.652712	2.064732	-1.301258
38	1	0	7.721986	-1.711771	1.427160
39	6	0	-3.466603	-0.473089	0.405161

40	6	0	-3.718076	0.826477	-0.149626
41	6	0	-3.966295	-0.809509	1.659379
42	6	0	-3.252312	1.212770	-1.440098
43	6	0	-4.475103	1.782517	0.606059
44	6	0	-4.717965	0.154033	2.387518
45	6	0	-3.508993	2.470216	-1.946618
46	1	0	-2.690050	0.501826	-2.035521
47	6	0	-4.723671	3.071154	0.056209
48	6	0	-4.965079	1.410609	1.885678
49	1	0	-5.096885	-0.116474	3.369899
50	6	0	-4.250762	3.413285	-1.192336
51	1	0	-3.142314	2.739270	-2.933173
52	1	0	-5.299504	3.783709	0.641653
53	1	0	-5.537797	2.131929	2.463134
54	1	0	-4.447656	4.399794	-1.601929
55	6	0	-3.717656	-2.162190	2.291497
56	1	0	-2.690851	-2.502423	2.128985
57	1	0	-4.379340	-2.931628	1.876186
58	1	0	-3.898162	-2.121637	3.369605
59	6	0	2.024257	2.696252	-1.184634
60	1	0	2.269036	3.484326	-1.901568
61	1	0	1.536791	3.162735	-0.321387
62	1	0	1.283124	2.035480	-1.646781

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2b-syn-GS1

Method: opt freq b3lyp/6-31+g(d,p) scrf(solvent=Chloroform)

SCF Done: E(RB3LYP) = -1461.81205939 A.U. after 1 cycles

Lowest frequency = 9.6479

Zero-point correction= 0.499738  
(Hartree/Particle)  
Thermal correction to Energy= 0.528737  
Thermal correction to Enthalpy= 0.529681  
Thermal correction to Gibbs Free Energy= 0.437627  
Sum of electronic and zero-point Energies= -1461.312322  
Sum of electronic and thermal Energies= -1461.283323  
Sum of electronic and thermal Enthalpies= -1461.282378  
Sum of electronic and thermal Free Energies= -1461.374432

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.850067	2.846092	-0.709467
2	6	0	-0.533112	2.671478	-0.738839
3	6	0	-1.142507	1.432275	-0.419043
4	6	0	-0.280555	0.348376	-0.153298
5	6	0	1.126236	0.500242	-0.117496
6	6	0	1.666450	1.764171	-0.390951
7	8	0	-0.842707	-0.856989	0.154506
8	6	0	-0.062311	-2.026965	-0.163304
9	6	0	1.368041	-1.880590	0.264935
10	6	0	1.946919	-0.665962	0.264174
11	8	0	-1.297104	3.768612	-1.030626
12	6	0	-2.558268	3.484506	-1.668916
13	6	0	-3.296093	2.399906	-0.943400
14	6	0	-2.621852	1.393980	-0.351481
15	1	0	1.265850	3.819642	-0.945089

16	1	0	2.743184	1.896485	-0.361122
17	1	0	-0.561756	-2.848484	0.353927
18	1	0	-0.140387	-2.212070	-1.248149
19	1	0	1.919593	-2.774507	0.542245
20	1	0	-3.107058	4.427860	-1.657208
21	1	0	-2.363680	3.213634	-2.720408
22	1	0	-4.380513	2.447503	-0.901839
23	6	0	3.380216	-0.474266	0.658463
24	6	0	4.415300	-0.667184	-0.317124
25	6	0	3.703086	-0.111353	1.964309
26	6	0	4.138894	-1.018080	-1.671427
27	6	0	5.787488	-0.494104	0.067458
28	6	0	5.069772	0.053973	2.320485
29	6	0	5.156613	-1.194337	-2.585504
30	1	0	3.107884	-1.149010	-1.981559
31	6	0	6.814614	-0.687763	-0.898646
32	6	0	6.082405	-0.131732	1.407531
33	1	0	5.311014	0.331707	3.343158
34	6	0	6.510546	-1.031009	-2.197958
35	1	0	4.919774	-1.460101	-3.611816
36	1	0	7.849032	-0.557640	-0.590525
37	1	0	7.120167	-0.000458	1.703129
38	1	0	7.303035	-1.175411	-2.926416
39	6	0	-3.374480	0.351264	0.421249
40	6	0	-4.096679	-0.672629	-0.279006
41	6	0	-3.407917	0.408060	1.812054
42	6	0	-4.077062	-0.796222	-1.699185
43	6	0	-4.857473	-1.634131	0.467219
44	6	0	-4.166723	-0.557782	2.528227
45	6	0	-4.778887	-1.795235	-2.341817
46	1	0	-3.496073	-0.089643	-2.281245
47	6	0	-5.576492	-2.648650	-0.225115
48	6	0	-4.871826	-1.547628	1.884017
49	1	0	-4.190577	-0.499077	3.613436
50	6	0	-5.542878	-2.730878	-1.600302
51	1	0	-4.744217	-1.867387	-3.425275
52	1	0	-6.154186	-3.363527	0.355680
53	1	0	-5.449958	-2.271862	2.452328
54	1	0	-6.094982	-3.510656	-2.116902
55	6	0	-2.651960	1.463007	2.588233
56	1	0	-1.575432	1.253155	2.600494
57	1	0	-2.778568	2.457896	2.150391
58	1	0	-2.993039	1.500031	3.626507
59	6	0	2.637411	0.097260	3.017145
60	1	0	3.080366	0.440793	3.955651
61	1	0	1.897174	0.839556	2.699946
62	1	0	2.089961	-0.829945	3.220298

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2b-syn-GS2

Method: opt freq b3lyp/6-31+g(d,p) scrf(solvent=Chloroform)

SCF Done: E(RB3LYP) = -1461.81252926 A.U. after 1 cycles

Lowest frequency = 9.6660

Zero-point correction=	0.499838
(Hartree/Particle)	
Thermal correction to Energy=	0.528825
Thermal correction to Enthalpy=	0.529769
Thermal correction to Gibbs Free Energy=	0.437685
Sum of electronic and zero-point Energies=	-1461.312691
Sum of electronic and thermal Energies=	-1461.283705

Sum of electronic and thermal Enthalpies= -1461.282761  
Sum of electronic and thermal Free Energies= -1461.374844

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.591220	-1.938409	2.169463
2	6	0	-0.763744	-2.000749	1.844151
3	6	0	-1.294957	-1.337222	0.709033
4	6	0	-0.376750	-0.672413	-0.127660
5	6	0	1.008026	-0.630639	0.157269
6	6	0	1.464279	-1.257634	1.324928
7	8	0	-0.848227	-0.127471	-1.287501
8	6	0	-0.129937	1.018163	-1.789481
9	6	0	1.354206	0.795892	-1.770438
10	6	0	1.904380	0.018850	-0.819241
11	8	0	-1.586466	-2.664384	2.711903
12	6	0	-2.767353	-3.238948	2.115280
13	6	0	-3.473024	-2.236680	1.251892
14	6	0	-2.767765	-1.330557	0.546662
15	1	0	0.944466	-2.439126	3.064314
16	1	0	2.524081	-1.234962	1.557712
17	1	0	-0.414171	1.897970	-1.188486
18	1	0	-0.507432	1.166877	-2.803004
19	1	0	1.962178	1.295728	-2.519306
20	1	0	-3.386414	-3.562621	2.953686
21	1	0	-2.467542	-4.132856	1.543099
22	1	0	-4.558484	-2.253246	1.216186
23	6	0	3.383290	-0.213492	-0.746830
24	6	0	4.218810	0.738332	-0.071475
25	6	0	3.940650	-1.348573	-1.332002
26	6	0	3.697487	1.904277	0.563033
27	6	0	5.636103	0.516895	-0.014901
28	6	0	5.347276	-1.545027	-1.262742
29	6	0	4.527246	2.798523	1.206562
30	1	0	2.628622	2.085957	0.534741
31	6	0	6.465539	1.461366	0.652850
32	6	0	6.172550	-0.644977	-0.628357
33	1	0	5.772701	-2.430417	-1.727840
34	6	0	5.927324	2.579609	1.251472
35	1	0	4.105256	3.678272	1.684021
36	1	0	7.537310	1.281855	0.683079
37	1	0	7.245341	-0.815842	-0.588916
38	1	0	6.570455	3.292650	1.758930
39	6	0	-3.491112	-0.312658	-0.285251
40	6	0	-3.627892	1.029050	0.205863
41	6	0	-4.062230	-0.676612	-1.500858
42	6	0	-3.085780	1.447649	1.456248
43	6	0	-4.343082	1.997644	-0.574762
44	6	0	-4.771805	0.299869	-2.253389
45	6	0	-3.232045	2.745446	1.901375
46	1	0	-2.553749	0.729410	2.070340
47	6	0	-4.476816	3.328351	-0.088374
48	6	0	-4.908892	1.595913	-1.813357
49	1	0	-5.207414	0.006646	-3.205215
50	6	0	-3.932539	3.699864	1.122152
51	1	0	-2.809834	3.037828	2.858641
52	1	0	-5.022778	4.049637	-0.691507

53	1	0	-5.451501	2.325723	-2.408936
54	1	0	-4.042644	4.718215	1.483464
55	6	0	-3.932925	-2.074496	-2.066286
56	1	0	-4.610423	-2.777951	-1.568007
57	1	0	-2.918818	-2.466298	-1.945511
58	1	0	-4.176962	-2.081786	-3.132444
59	6	0	3.088378	-2.370841	-2.050577
60	1	0	2.580537	-1.930323	-2.915687
61	1	0	2.307568	-2.775245	-1.397240
62	1	0	3.698491	-3.205833	-2.404862

2b-TS1-A-int-B-fix-down

Method: opt(ts,calcfc,noeigen) b3lyp/6-31+g(d,p) freq scrf(solvent=Chloroform)

SCF Done: E(RB3LYP) = -1461.76395522 A.U. after 1 cycles

Lowest frequency = -28.3606

Zero-point correction= 0.500654  
(Hartree/Particle)  
Thermal correction to Energy= 0.527990  
Thermal correction to Enthalpy= 0.528934  
Thermal correction to Gibbs Free Energy= 0.443339  
Sum of electronic and zero-point Energies= -1461.263301  
Sum of electronic and thermal Energies= -1461.235965  
Sum of electronic and thermal Enthalpies= -1461.235021  
Sum of electronic and thermal Free Energies= -1461.320616

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.015140	3.607293	-0.132594
2	6	0	-1.252285	3.064609	0.206850
3	6	0	-1.490973	1.671842	0.110513
4	6	0	-0.381003	0.859616	-0.193479
5	6	0	0.938823	1.364670	-0.310081
6	6	0	1.057967	2.758548	-0.397976
7	8	0	-0.588875	-0.471783	-0.437293
8	6	0	0.187259	-0.895886	-1.579464
9	6	0	2.038034	0.360208	-0.522053
10	8	0	-2.267723	3.931324	0.502211
11	6	0	-3.303154	3.380428	1.341919
12	6	0	-3.769586	2.056794	0.813351
13	6	0	-2.895230	1.214203	0.228443
14	1	0	0.101808	4.685248	-0.166891
15	1	0	2.001739	3.199983	-0.680168
16	1	0	-0.030982	-1.958376	-1.705569
17	1	0	-0.175292	-0.360646	-2.472545
18	1	0	-2.908998	3.295463	2.368465
19	1	0	-4.101911	4.123943	1.343410
20	1	0	-4.820780	1.799018	0.904963
21	6	0	3.452133	0.385351	-0.003996
22	6	0	4.191076	-0.886450	-0.002626
23	6	0	4.178164	1.507190	0.444012
24	6	0	3.571271	-2.161452	0.173411
25	6	0	5.625810	-0.888792	-0.042405
26	6	0	5.603859	1.465109	0.423423
27	6	0	4.293513	-3.339191	0.170363
28	1	0	2.506812	-2.211326	0.362662

29	6	0	6.343053	-2.115696	-0.113908
30	6	0	6.315649	0.343552	0.091145
31	1	0	6.133660	2.380292	0.676586
32	6	0	5.693081	-3.326718	-0.028344
33	1	0	3.777886	-4.280512	0.337481
34	1	0	7.426586	-2.073423	-0.190071
35	1	0	7.400315	0.363961	0.031760
36	1	0	6.250849	-4.257889	-0.063259
37	6	0	-3.388530	-0.081376	-0.346303
38	6	0	-3.608926	-1.205787	0.516275
39	6	0	-3.681452	-0.168282	-1.704635
40	6	0	-3.313231	-1.174465	1.910317
41	6	0	-4.131030	-2.424133	-0.033742
42	6	0	-4.196054	-1.386964	-2.226140
43	6	0	-3.532051	-2.274590	2.713187
44	1	0	-2.906782	-0.266553	2.342240
45	6	0	-4.351148	-3.540065	0.821849
46	6	0	-4.415807	-2.482535	-1.423153
47	1	0	-4.425215	-1.442805	-3.287322
48	6	0	-4.060672	-3.471282	2.167135
49	1	0	-3.295255	-2.225462	3.772271
50	1	0	-4.753712	-4.453539	0.391061
51	1	0	-4.813752	-3.402700	-1.843513
52	1	0	-4.231941	-4.330169	2.809576
53	6	0	-3.467124	0.998796	-2.643218
54	1	0	-2.404058	1.247983	-2.742379
55	1	0	-3.849897	0.770054	-3.641441
56	1	0	-3.970122	1.902561	-2.283828
57	6	0	3.631233	2.778930	1.067180
58	1	0	3.667946	3.644363	0.395596
59	1	0	2.617404	2.672817	1.444452
60	1	0	4.272288	3.024740	1.920664
61	6	0	1.641093	-0.677631	-1.305356
62	1	0	2.332452	-1.418408	-1.682931

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2b-TS4-A-fix-up-B-int

Method: opt(ts,calcfc,noeigen) b3lyp/6-31+g(d,p) freq scrf(solvent=Chloroform)  
SCF Done: E(RB3LYP) = -1461.76076505 A.U. after 1 cycles  
Lowest frequency = -29.3997

Zero-point correction= 0.500226  
(Hartree/Particle)  
Thermal correction to Energy= 0.527692  
Thermal correction to Enthalpy= 0.528637  
Thermal correction to Gibbs Free Energy= 0.442409  
Sum of electronic and zero-point Energies= -1461.260539  
Sum of electronic and thermal Energies= -1461.233073  
Sum of electronic and thermal Enthalpies= -1461.232128  
Sum of electronic and thermal Free Energies= -1461.318356

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.566958	-2.172266	-1.710893
2	6	0	0.708648	-2.009545	-1.172052
3	6	0	0.966547	-1.164596	-0.062047

4	6	0	-0.161244	-0.869216	0.727200
5	6	0	-1.477565	-1.008025	0.216196
6	6	0	-1.649302	-1.609486	-1.038180
7	8	0	0.041494	-0.436566	2.002140
8	6	0	-1.044998	-0.628148	2.934595
9	6	0	-2.372700	-0.265739	2.338767
10	6	0	-2.594265	-0.490122	1.030549
11	8	0	1.743938	-2.766642	-1.660655
12	6	0	2.555795	-3.251570	-0.551301
13	6	0	3.151452	-2.069144	0.151499
14	6	0	2.419639	-0.930244	0.250244
15	1	0	-0.700524	-2.781923	-2.597855
16	1	0	-2.650276	-1.705788	-1.446478
17	1	0	-1.026994	-1.680558	3.263481
18	1	0	-0.794761	-0.002350	3.793931
19	1	0	-3.141937	0.141205	2.988601
20	1	0	1.921567	-3.886792	0.084988
21	1	0	3.331513	-3.871431	-1.004308
22	1	0	4.209107	-2.092155	0.383212
23	6	0	-3.923204	-0.221737	0.392532
24	6	0	-4.118118	0.983592	-0.364482
25	6	0	-4.961243	-1.139594	0.530586
26	6	0	-3.090232	1.955746	-0.533390
27	6	0	-5.392417	1.237656	-0.971709
28	6	0	-6.216726	-0.864681	-0.082284
29	6	0	-3.307585	3.105700	-1.263884
30	1	0	-2.122068	1.785503	-0.075599
31	6	0	-5.586357	2.433725	-1.717502
32	6	0	-6.431034	0.282677	-0.808752
33	1	0	-7.019143	-1.589370	0.028744
34	6	0	-4.567761	3.350535	-1.864242
35	1	0	-2.506858	3.830490	-1.379654
36	1	0	-6.558230	2.612373	-2.170698
37	1	0	-7.397445	0.469229	-1.270107
38	1	0	-4.727249	4.259958	-2.436099
39	6	0	3.162653	0.375432	0.407797
40	6	0	4.515110	0.421746	-0.167247
41	6	0	2.722547	1.546273	1.050297
42	6	0	4.942542	-0.394374	-1.261075
43	6	0	5.455874	1.411958	0.276076
44	6	0	3.678989	2.525603	1.447807
45	6	0	6.219589	-0.323396	-1.780139
46	1	0	4.235400	-1.065935	-1.729709
47	6	0	6.787390	1.421972	-0.228485
48	6	0	5.014087	2.428875	1.158256
49	1	0	3.316144	3.375626	2.020122
50	6	0	7.176358	0.561088	-1.229040
51	1	0	6.484295	-0.947087	-2.629229
52	1	0	7.481083	2.158479	0.169038
53	1	0	5.720752	3.169895	1.522093
54	1	0	8.188876	0.588065	-1.620856
55	6	0	1.292373	1.945916	1.339134
56	1	0	0.586903	1.508667	0.636091
57	1	0	0.972768	1.680852	2.348844
58	1	0	1.219717	3.034036	1.242742
59	6	0	-4.806564	-2.424297	1.316217
60	1	0	-3.817469	-2.870370	1.182320
61	1	0	-4.938988	-2.251930	2.391286
62	1	0	-5.557571	-3.156916	1.006937



2b-TS2-A-ext-B-fix-up

Method: opt(ts,calcfc,noeigen) b3lyp/6-31+g(d,p) freq scrf(solvent=Chloroform)

SCF Done: E(RB3LYP) = -1461.75091465 A.U. after 2 cycles

Lowest frequency = -68.6439

Zero-point correction= 0.500548  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.528023  
 Thermal correction to Enthalpy= 0.528967  
 Thermal correction to Gibbs Free Energy= 0.442470  
 Sum of electronic and zero-point Energies= -1461.250366  
 Sum of electronic and thermal Energies= -1461.222892  
 Sum of electronic and thermal Enthalpies= -1461.221947  
 Sum of electronic and thermal Free Energies= -1461.308445

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.597488	2.575994	-1.520720
2	6	0	-0.439291	2.591231	-0.591539
3	6	0	-0.910207	1.388998	-0.011472
4	6	0	-0.175738	0.219807	-0.295574
5	6	0	1.051172	0.221590	-1.016098
6	6	0	1.317786	1.401639	-1.728240
7	8	0	-0.710753	-0.983313	0.069360
8	6	0	-0.494244	-1.940707	-0.997263
9	6	0	1.821640	-1.086170	-1.033698
10	8	0	-1.086319	3.775916	-0.381049
11	6	0	-1.763715	3.876913	0.888669
12	6	0	-2.609175	2.664266	1.138972
13	6	0	-2.194300	1.450165	0.726289
14	1	0	0.844908	3.484773	-2.058726
15	1	0	2.078629	1.417684	-2.492701
16	1	0	-0.992779	-2.856817	-0.677665
17	1	0	-0.991598	-1.563617	-1.903624
18	1	0	-1.004281	4.015457	1.676144
19	1	0	-2.362094	4.787342	0.826641
20	1	0	-3.557831	2.787016	1.653433
21	6	0	3.257270	-1.253679	-0.545966
22	6	0	4.128944	-0.118530	-0.239059
23	6	0	3.751399	-2.513789	-0.128689
24	6	0	4.188934	1.071426	-1.012353
25	6	0	5.098339	-0.210358	0.819984
26	6	0	4.784113	-2.584719	0.849017
27	6	0	4.987270	2.146811	-0.672363
28	1	0	3.666456	1.105353	-1.950220
29	6	0	5.864649	0.927433	1.197996
30	6	0	5.363950	-1.473288	1.401195
31	1	0	5.079448	-3.570982	1.196635
32	6	0	5.796010	2.103473	0.484646
33	1	0	5.009080	3.020197	-1.317925
34	1	0	6.548879	0.828046	2.036765
35	1	0	6.085476	-1.557048	2.209041
36	1	0	6.398557	2.961102	0.768512
37	6	0	-3.064042	0.252348	0.971990
38	6	0	-3.904424	-0.235533	-0.083485
39	6	0	-3.090539	-0.348429	2.226140

40	6	0	-3.927509	0.356095	-1.379996
41	6	0	-4.762261	-1.359455	0.159362
42	6	0	-3.952337	-1.459151	2.444075
43	6	0	-4.743707	-0.137465	-2.377198
44	1	0	-3.295062	1.213953	-1.581520
45	6	0	-5.593618	-1.844215	-0.888915
46	6	0	-4.761752	-1.954937	1.448512
47	1	0	-3.959909	-1.926366	3.425596
48	6	0	-5.586643	-1.250400	-2.132884
49	1	0	-4.743000	0.332195	-3.356788
50	1	0	-6.240225	-2.695004	-0.688295
51	1	0	-5.409093	-2.807530	1.637760
52	1	0	-6.226816	-1.628839	-2.924545
53	6	0	-2.216383	0.129591	3.365420
54	1	0	-1.197493	0.346492	3.031341
55	1	0	-2.608331	1.048889	3.816690
56	1	0	-2.162093	-0.627423	4.152889
57	6	0	3.290487	-3.878377	-0.603702
58	1	0	2.434367	-4.263275	-0.034641
59	1	0	3.032860	-3.892457	-1.665353
60	1	0	4.107285	-4.591023	-0.458595
61	6	0	0.979931	-2.151117	-1.143848
62	1	0	1.304252	-3.173701	-1.142567

2b-TS4-A-fix-down-B-int

Method: opt(ts,calcfc,noeigen) b3lyp/6-31+g(d,p) freq scrf(solvent=Chloroform)  
 SCF Done: E(RB3LYP) = -1461.76091893 A.U. after 1 cycles  
 Lowest frequency = -24.5050

Zero-point correction= 0.500289  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.527736  
 Thermal correction to Enthalpy= 0.528680  
 Thermal correction to Gibbs Free Energy= 0.442413  
 Sum of electronic and zero-point Energies= -1461.260630  
 Sum of electronic and thermal Energies= -1461.233183  
 Sum of electronic and thermal Enthalpies= -1461.232239  
 Sum of electronic and thermal Free Energies= -1461.318506

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.556135	2.229086	-1.225031
2	6	0	-0.704133	2.047317	-0.656686
3	6	0	-1.030908	0.913028	0.130199
4	6	0	0.077187	0.233297	0.670552
5	6	0	1.374447	0.375742	0.113977
6	6	0	1.575275	1.344360	-0.879221
7	8	0	-0.125633	-0.577092	1.745517
8	6	0	1.021141	-0.839653	2.584040
9	6	0	2.250011	-1.144851	1.780177
10	6	0	2.437286	-0.524872	0.600257
11	8	0	-1.640602	3.044124	-0.770988
12	6	0	-2.322854	3.217268	0.505566
13	6	0	-3.050421	1.947373	0.829405
14	6	0	-2.486642	0.763272	0.479390

15	1	0	0.736722	3.085119	-1.865986
16	1	0	2.560503	1.454401	-1.320865
17	1	0	1.173440	0.038506	3.233397
18	1	0	0.723911	-1.678889	3.216377
19	1	0	2.979832	-1.839885	2.185117
20	1	0	-1.575314	3.516689	1.255301
21	1	0	-3.020484	4.043141	0.355869
22	1	0	-4.081741	2.017534	1.152286
23	6	0	3.663622	-0.747836	-0.231361
24	6	0	4.872197	-0.040245	0.084885
25	6	0	3.628385	-1.635056	-1.305570
26	6	0	4.956570	0.898977	1.154825
27	6	0	6.048337	-0.265929	-0.707039
28	6	0	4.806797	-1.841107	-2.073897
29	6	0	6.132861	1.564374	1.430435
30	1	0	4.076445	1.088700	1.759335
31	6	0	7.248082	0.432595	-0.393065
32	6	0	5.980865	-1.182946	-1.787919
33	1	0	4.770550	-2.541373	-2.904242
34	6	0	7.294442	1.328589	0.652605
35	1	0	6.170213	2.276634	2.249785
36	1	0	8.131344	0.246325	-0.998828
37	1	0	6.869777	-1.358157	-2.388522
38	1	0	8.215476	1.856628	0.881534
39	6	0	-3.400778	-0.420090	0.266388
40	6	0	-4.772527	-0.107580	-0.161169
41	6	0	-3.102137	-1.782998	0.441810
42	6	0	-5.131818	1.075752	-0.879366
43	6	0	-5.822846	-1.070277	0.018055
44	6	0	-4.168734	-2.718261	0.582327
45	6	0	-6.429964	1.337307	-1.269036
46	1	0	-4.359747	1.777468	-1.166019
47	6	0	-7.165364	-0.750236	-0.332402
48	6	0	-5.488666	-2.371286	0.468863
49	1	0	-3.904038	-3.748828	0.805035
50	6	0	-7.475590	0.438853	-0.951584
51	1	0	-6.643875	2.238791	-1.836121
52	1	0	-7.937224	-1.489963	-0.135440
53	1	0	-6.275559	-3.102517	0.632806
54	1	0	-8.499642	0.667020	-1.232105
55	6	0	-1.732021	-2.424608	0.447420
56	1	0	-1.003018	-1.862277	-0.131630
57	1	0	-1.332234	-2.561436	1.454201
58	1	0	-1.821490	-3.414609	-0.011498
59	6	0	2.371274	-2.392464	-1.669991
60	1	0	1.992653	-2.972400	-0.821661
61	1	0	1.567581	-1.712370	-1.974140
62	1	0	2.558735	-3.081866	-2.497251

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2b-TS3-A-fix-down-B-ext

Method: opt(ts,calcfc,noeigen) b3lyp/6-31+g(d,p) freq scrf(solvent=Chloroform)  
 SCF Done: E(RB3LYP) = -1461.76050922 A.U. after 1 cycles  
 Lowest frequency = -31.3555

Zero-point correction=	0.500215
(Hartree/Particle)	
Thermal correction to Energy=	0.527713
Thermal correction to Enthalpy=	0.528657
Thermal correction to Gibbs Free Energy=	0.442196

Sum of electronic and zero-point Energies=	-1461.260294
Sum of electronic and thermal Energies=	-1461.232796
Sum of electronic and thermal Enthalpies=	-1461.231852
Sum of electronic and thermal Free Energies=	-1461.318313

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.585932	2.618711	-1.105778
2	6	0	-0.713707	2.521394	-0.610708
3	6	0	-1.194499	1.364744	0.058999
4	6	0	-0.185790	0.529556	0.578630
5	6	0	1.146001	0.583712	0.091918
6	6	0	1.493828	1.608120	-0.798591
7	8	0	-0.518857	-0.357177	1.560385
8	6	0	0.553009	-0.798847	2.422872
9	6	0	1.784495	-1.158450	1.646342
10	6	0	2.088543	-0.461671	0.535542
11	8	0	-1.535567	3.617629	-0.683710
12	6	0	-2.273854	3.759704	0.564504
13	6	0	-3.139655	2.549382	0.739278
14	6	0	-2.678239	1.344272	0.321609
15	1	0	0.882118	3.502662	-1.659991
16	1	0	2.506335	1.653195	-1.186546
17	1	0	0.755612	0.005637	3.149312
18	1	0	0.143402	-1.651794	2.967160
19	1	0	2.421131	-1.957622	2.014719
20	1	0	-1.547960	3.920135	1.375510
21	1	0	-2.876261	4.662329	0.448547
22	1	0	-4.178994	2.694507	1.008633
23	6	0	3.323683	-0.737784	-0.266503
24	6	0	4.583142	-0.198535	0.163103
25	6	0	3.247108	-1.509944	-1.424281
26	6	0	4.714500	0.620118	1.323526
27	6	0	5.765389	-0.473504	-0.603813
28	6	0	4.432689	-1.768233	-2.165311
29	6	0	5.939298	1.125573	1.706623
30	1	0	3.831577	0.845354	1.911470
31	6	0	7.015111	0.058611	-0.178476
32	6	0	5.653960	-1.270792	-1.772412
33	1	0	4.363094	-2.378444	-3.061951
34	6	0	7.105271	0.840972	0.952056
35	1	0	6.011964	1.748479	2.593612
36	1	0	7.901567	-0.163457	-0.767277
37	1	0	6.547161	-1.483051	-2.354397
38	1	0	8.064366	1.242613	1.265689
39	6	0	-3.734396	0.331421	-0.067494
40	6	0	-3.677308	-1.112836	0.119814
41	6	0	-4.931905	0.849273	-0.610741
42	6	0	-2.471912	-1.860763	0.184589
43	6	0	-4.895868	-1.878398	0.141492
44	6	0	-6.112086	0.051669	-0.621787
45	6	0	-2.460888	-3.228901	0.378973
46	1	0	-1.532902	-1.362740	0.034528
47	6	0	-4.862249	-3.277111	0.395209
48	6	0	-6.123236	-1.243591	-0.178539
49	1	0	-7.029835	0.504523	-0.988469
50	6	0	-3.666840	-3.948612	0.528761

51	1	0	-1.510499	-3.754883	0.400802
52	1	0	-5.806483	-3.813859	0.440178
53	1	0	-7.045638	-1.817457	-0.148557
54	1	0	-3.649994	-5.020184	0.704773
55	6	0	-5.097260	2.196675	-1.300112
56	1	0	-5.668471	2.916019	-0.701633
57	1	0	-4.146143	2.660028	-1.561364
58	1	0	-5.664978	2.039141	-2.224434
59	6	0	1.936494	-2.087114	-1.910002
60	1	0	1.442657	-2.674309	-1.128789
61	1	0	1.235969	-1.297536	-2.205145
62	1	0	2.094031	-2.735844	-2.775523

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2b-TS3-A-fix-up-B-ext

Method: opt(ts,calcfc,noeigen) b3lyp/6-31+g(d,p) freq scrf(solvent=Chloroform)  
SCF Done: E(RB3LYP) = -1461.76041610 A.U. after 1 cycles  
Lowest frequency = -34.2921

Zero-point correction= 0.500253  
(Hartree/Particle)  
Thermal correction to Energy= 0.527702  
Thermal correction to Enthalpy= 0.528646  
Thermal correction to Gibbs Free Energy= 0.442799  
Sum of electronic and zero-point Energies= -1461.260163  
Sum of electronic and thermal Energies= -1461.232715  
Sum of electronic and thermal Enthalpies= -1461.231770  
Sum of electronic and thermal Free Energies= -1461.317618

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.559892	-2.784175	-1.244822
2	6	0	0.768137	-2.583099	-0.871550
3	6	0	1.175403	-1.507817	-0.037742
4	6	0	0.141042	-0.943770	0.734855
5	6	0	-1.223415	-1.110313	0.382434
6	6	0	-1.544631	-1.994933	-0.655551
7	8	0	0.479600	-0.209742	1.833759
8	6	0	-0.522236	-0.091334	2.868127
9	6	0	-1.878599	0.208849	2.303708
10	6	0	-2.230645	-0.319958	1.117296
11	8	0	1.709690	-3.510295	-1.241179
12	6	0	2.612326	-3.762377	-0.125410
13	6	0	3.328414	-2.486590	0.198016
14	6	0	2.665034	-1.309999	0.074562
15	1	0	-0.806396	-3.585304	-1.933037
16	1	0	-2.583458	-2.118117	-0.944519
17	1	0	-0.525752	-1.031513	3.444346
18	1	0	-0.160262	0.705087	3.520991
19	1	0	-2.561119	0.824516	2.882202
20	1	0	2.022142	-4.175514	0.706124
21	1	0	3.307606	-4.526823	-0.476539
22	1	0	4.403501	-2.518588	0.328435
23	6	0	-3.594129	-0.117317	0.530289
24	6	0	-3.781949	0.856048	-0.509796
25	6	0	-4.671243	-0.871448	0.988716
26	6	0	-2.714453	1.655021	-1.012112

27	6	0	-5.088846	1.049645	-1.067842
28	6	0	-5.958863	-0.660385	0.418492
29	6	0	-2.925553	2.583669	-2.010295
30	1	0	-1.719901	1.528860	-0.598879
31	6	0	-5.275239	2.016390	-2.094944
32	6	0	-6.166675	0.266882	-0.574954
33	1	0	-6.791972	-1.256812	0.781325
34	6	0	-4.218390	2.768743	-2.560450
35	1	0	-2.094278	3.178674	-2.377431
36	1	0	-6.272096	2.151888	-2.506924
37	1	0	-7.158311	0.407962	-0.997322
38	1	0	-4.372472	3.503602	-3.345164
39	6	0	3.522872	-0.095119	-0.210046
40	6	0	3.302781	1.265834	0.262675
41	6	0	4.699123	-0.318478	-0.960977
42	6	0	2.028307	1.797993	0.592772
43	6	0	4.404098	2.191021	0.312884
44	6	0	5.754739	0.637487	-0.931801
45	6	0	1.863438	3.090881	1.051999
46	1	0	1.151368	1.197653	0.442208
47	6	0	4.220823	3.499529	0.838478
48	6	0	5.653272	1.818025	-0.245920
49	1	0	6.669772	0.402807	-1.469782
50	6	0	2.974642	3.946500	1.219296
51	1	0	0.863055	3.453653	1.271140
52	1	0	5.085058	4.156603	0.893904
53	1	0	6.489585	2.510191	-0.195562
54	1	0	2.840703	4.953669	1.602965
55	6	0	4.949047	-1.477838	-1.915695
56	1	0	5.678918	-2.199500	-1.530535
57	1	0	4.040244	-2.023854	-2.167689
58	1	0	5.370703	-1.071541	-2.842309
59	6	0	-4.526846	-1.911504	2.079136
60	1	0	-3.581291	-2.455090	2.005151
61	1	0	-4.556903	-1.451842	3.074550
62	1	0	-5.344117	-2.636752	2.028742

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2b-TS2-A-ext-B-fix-down

Method: opt(ts,calcfc,noeigen) b3lyp/6-31+g(d,p) freq scrf(solvent=Chloroform)  
SCF Done: E(RB3LYP) = -1461.75043526 A.U. after 1 cycles  
Lowest frequency = -67.9539

Zero-point correction= 0.500441  
(Hartree/Particle)  
Thermal correction to Energy= 0.527952  
Thermal correction to Enthalpy= 0.528896  
Thermal correction to Gibbs Free Energy= 0.442260  
Sum of electronic and zero-point Energies= -1461.249995  
Sum of electronic and thermal Energies= -1461.222483  
Sum of electronic and thermal Enthalpies= -1461.221539  
Sum of electronic and thermal Free Energies= -1461.308175

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.847962	3.086076	-0.795700
2	6	0	-0.350289	2.855109	-0.125457

3	6	0	-0.940849	1.568908	-0.120364
4	6	0	-0.178071	0.519786	-0.672144
5	6	0	1.167555	0.676538	-1.108162
6	6	0	1.581693	2.006676	-1.283069
7	8	0	-0.787930	-0.687127	-0.866216
8	6	0	-0.365516	-1.236552	-2.138370
9	6	0	1.916830	-0.599130	-1.446393
10	8	0	-1.009903	3.934177	0.390831
11	6	0	-1.912239	3.625214	1.473582
12	6	0	-2.809997	2.481642	1.106877
13	6	0	-2.343564	1.470921	0.346664
14	1	0	1.207599	4.102889	-0.911071
15	1	0	2.479022	2.230211	-1.837952
16	1	0	-0.925387	-2.164706	-2.260058
17	1	0	-0.663523	-0.535009	-2.932752
18	1	0	-1.311961	3.403436	2.371631
19	1	0	-2.473014	4.543538	1.655206
20	1	0	-3.837574	2.490429	1.458673
21	6	0	3.227905	-1.031605	-0.797364
22	6	0	4.029607	-0.141077	0.043226
23	6	0	3.622713	-2.391273	-0.768582
24	6	0	4.257461	1.231559	-0.241929
25	6	0	4.764151	-0.664525	1.163860
26	6	0	4.436791	-2.872788	0.295831
27	6	0	4.979948	2.060530	0.594943
28	1	0	3.938474	1.622234	-1.190595
29	6	0	5.447437	0.212533	2.051766
30	6	0	4.898119	-2.066890	1.302919
31	1	0	4.650873	-3.937816	0.321585
32	6	0	5.535402	1.562681	1.794215
33	1	0	5.141723	3.096343	0.310422
34	1	0	5.946796	-0.219791	2.915076
35	1	0	5.440372	-2.478174	2.149670
36	1	0	6.075303	2.222250	2.467003
37	6	0	-3.271927	0.361796	-0.053472
38	6	0	-3.549988	-0.700733	0.868466
39	6	0	-3.902036	0.399865	-1.294276
40	6	0	-2.921114	-0.795361	2.144260
41	6	0	-4.483575	-1.726802	0.500469
42	6	0	-4.820897	-0.629488	-1.636954
43	6	0	-3.207201	-1.832184	3.007823
44	1	0	-2.202846	-0.036732	2.435112
45	6	0	-4.762070	-2.780272	1.416193
46	6	0	-5.107224	-1.661557	-0.772891
47	1	0	-5.310443	-0.588094	-2.606713
48	6	0	-4.140821	-2.835400	2.644942
49	1	0	-2.711202	-1.882893	3.972986
50	1	0	-5.476960	-3.546049	1.125277
51	1	0	-5.816877	-2.435319	-1.054836
52	1	0	-4.360734	-3.645252	3.334564
53	6	0	-3.633587	1.506361	-2.290227
54	1	0	-3.798767	2.494793	-1.848760
55	1	0	-2.595793	1.488195	-2.643304
56	1	0	-4.284639	1.410328	-3.163284
57	6	0	3.263020	-3.468126	-1.774205
58	1	0	2.315350	-3.971455	-1.542866
59	1	0	3.212549	-3.091284	-2.798419
60	1	0	4.038905	-4.238622	-1.749587
61	6	0	1.106050	-1.497039	-2.071680

62 1 0 1.415335 -2.482201 -2.362717

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2b-TS1-A-int-B-fix-up-Chloroform-yoda-NM-M

Method: opt(ts,calcfc,noeigen) b3lyp/6-31+g(d,p) freq scrf(solvent=Chloroform)  
SCF Done: E(RB3LYP) = -1461.76441419 A.U. after 1 cycles  
Lowest frequency = -28.9342

Zero-point correction= 0.500750  
(Hartree/Particle)  
Thermal correction to Energy= 0.528046  
Thermal correction to Enthalpy= 0.528991  
Thermal correction to Gibbs Free Energy= 0.443462  
Sum of electronic and zero-point Energies= -1461.263664  
Sum of electronic and thermal Energies= -1461.236368  
Sum of electronic and thermal Enthalpies= -1461.235424  
Sum of electronic and thermal Free Energies= -1461.320952

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.202264	3.331918	-0.805523
2	6	0	-1.339134	2.910890	-0.119699
3	6	0	-1.491245	1.562239	0.286176
4	6	0	-0.382036	0.715424	0.092860
5	6	0	0.868661	1.175226	-0.391742
6	6	0	0.878149	2.462865	-0.945109
7	8	0	-0.529405	-0.625481	0.329874
8	6	0	0.089253	-1.385734	-0.732744
9	6	0	1.989188	0.173071	-0.447603
10	8	0	-2.362104	3.807196	0.021501
11	6	0	-3.241412	3.550896	1.135406
12	6	0	-3.677967	2.116521	1.151624
13	6	0	-2.830278	1.143241	0.764011
14	1	0	-0.166967	4.338335	-1.208880
15	1	0	1.738522	2.802037	-1.501745
16	1	0	-0.072559	-2.434926	-0.476742
17	1	0	-0.443378	-1.173674	-1.673855
18	1	0	-2.715223	3.828128	2.064259
19	1	0	-4.083209	4.232667	1.003480
20	1	0	-4.687463	1.882883	1.477313
21	6	0	3.459466	0.384875	-0.198921
22	6	0	4.270318	-0.806793	0.094288
23	6	0	4.169619	1.600786	-0.258153
24	6	0	3.764907	-1.962895	0.764376
25	6	0	5.681655	-0.803166	-0.167415
26	6	0	5.577115	1.572799	-0.487508
27	6	0	4.552520	-3.067468	1.025478
28	1	0	2.743913	-1.962866	1.123462
29	6	0	6.457754	-1.976543	0.046694
30	6	0	6.303639	0.413696	-0.547548
31	1	0	6.078367	2.527092	-0.630230
32	6	0	5.905343	-3.101853	0.616545
33	1	0	4.127213	-3.909762	1.563605
34	1	0	7.514047	-1.947277	-0.208348
35	1	0	7.364904	0.427703	-0.779801
36	1	0	6.510344	-3.985980	0.794584
37	6	0	-3.294073	-0.283760	0.769149



38	6	0	-3.722301	-0.888943	-0.459264
39	6	0	-3.353797	-0.996881	1.961927
40	6	0	-3.700649	-0.194686	-1.703988
41	6	0	-4.197627	-2.242522	-0.451456
42	6	0	-3.832558	-2.336395	1.945095
43	6	0	-4.115830	-0.803969	-2.870419
44	1	0	-3.357058	0.833786	-1.730687
45	6	0	-4.620043	-2.842651	-1.670635
46	6	0	-4.240047	-2.945976	0.781287
47	1	0	-3.867584	-2.887601	2.881406
48	6	0	-4.579789	-2.143127	-2.857697
49	1	0	-4.089997	-0.252351	-3.805926
50	1	0	-4.979948	-3.868355	-1.647585
51	1	0	-4.598340	-3.972258	0.792772
52	1	0	-4.906204	-2.611833	-3.781542
53	6	0	-2.904975	-0.401370	3.278954
54	1	0	-3.649891	0.294663	3.682681
55	1	0	-2.750392	-1.187161	4.023767
56	1	0	-1.969863	0.156572	3.173789
57	6	0	3.637300	2.999803	-0.005421
58	1	0	3.513488	3.590955	-0.920029
59	1	0	2.700862	3.011088	0.546412
60	1	0	4.380419	3.526476	0.602937
61	6	0	1.549905	-1.068159	-0.786094
62	1	0	2.225473	-1.880221	-1.017698

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