Chemical Science

Controlling Dynamic Stereoisomerism in Transition-Metal Folded Baskets

Sandra Stojanovic, Daniel A Turner, Christopher M Hadad and Jovica D Badjic*

The Ohio State University, 100 W. 18th Avenue, Columbus OH 43210, USA.

E-mail: badjic@chemistry.ohio-state.edu

SUPPLEMENTARY INFORMATION

General

All chemicals were purchased from commercial sources, and used as received unless stated otherwise. All solvents were dried prior to use according to standard literature protocols. Chromatography purifications were performed using silica gel 60 (Sorbent Technologies 40-75μm, 200 x 400 mesh). Thin-layer chromatography (TLC) was performed on silica-gel plate w/UV254 (200μm). ^{1}H and ^{13}C NMR spectra were recorded, at 400 MHz and 100 MHz respectively, on a Bruker DPX-400 spectrometer unless otherwise noted. The NMR spectra were referenced using solvent residual signal as an internal standard. NMR samples were prepared with $CDCl_3$ and CD_3CN solvents that were purchased from Cambridge Isotope Laboratories. The chemical shift values are expressed as δ values (ppm) and the couple constants (J) are given in Hertz (Hz). The following abbreviations were used for signal multiplicities: s, singlet; d, doublet; t, triplet; m, multiplet; and br, broad. MALDI-TOF mass spectra were measured with 2,5-dihydroxybenzoic acid as matrix.

Synthesis

The preparation of baskets (*R*/*S*)-**1** and model compounds (*R*/*S*)-**2** was completed in accord with Scheme 1. Note that the synthesis of compounds (*R*/*S*)-**7** was already reported (see G. Chelucci and coworkers *Tetrahedron Asymmetry* **2006**, *17*, 3163-3169) and we followed these protocols. Compound **8** was made in accord with our previously published procedure (Badjic and coworkers *Org. Lett.* **2007**, *9*, 2301).

We hereby report a full characterization of new compounds (*R*/*S*)-**1** and (*R*/*S*)-**2** while only the ^{1}H NMR characterization of the known compounds (see G. Chelucci and coworkers *Tetrahedron Asymmetry* **2006**, *17*, 3163-3169).

Chiral basket (R_3)-1: Compound (*R*)-**7** (1.9 mg, 0.0158 mmol) was added to a solution of *tris*-anhydride **8** (2.0 mg, 0.00317 mmol) in 2 mL of toluene. The solution was heated to reflux and stirred for 1 h upon which 200 μL of neat pyridine was added. The resulting mixture was stirred for additional 12 h and then cooled down to room temperature. The mixture was concentrated under reduced pressure and the residue purified with thin-layer chromatography (SiO_2, acetone:benzene=3:1) to yield 1.64 mg of basket (R_3)-**1** (55%) as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$, 300 K): δ = 8.60 (d, J=1.8 Hz, 3H), 8.46 (dd, J=4.8, 1.8 3H), 7.78 (dt, J=7.9, 1.8, 1.8 3H), 7.47 (d, J=5.6 6H), 7.20 (dd, J=7.9, 4.8 3H), 5.44 (q, J=7.4 Hz, 3H), 4.49 (s, 6H), 2.58 (s, 6H), 1.79 (d, J=7.4 Hz, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, 300 K): δ = 167.80, 167.78, 156.93, 156.89, 149.33, 149.09, 137.99, 135.95, 135.17, 130.55, 130.43, 123.38, 116.18, 116.14, 65.98, 49.26, 47.31, 17.44 ppm; HRMS MALDI-TOF: m/z calcd for $C_{60}H_{42}N_6O_6$: 943.327 $[M + H]^+$, found: 943.373.

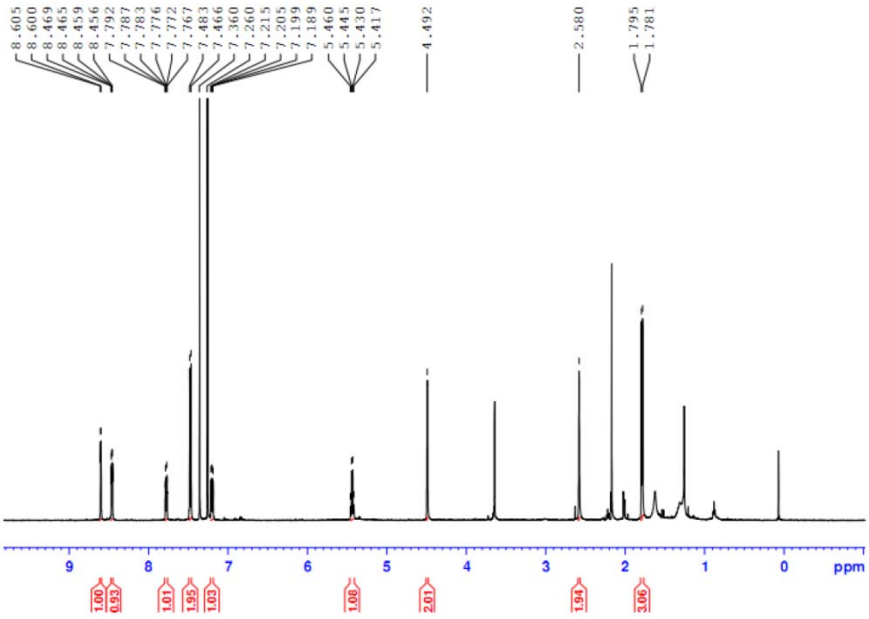


Figure S1: ^{1}H NMR spectrum (500 MHz) of basket (R_3)-**1** (4.24 mM) in $CDCl_3$ at 300 K.

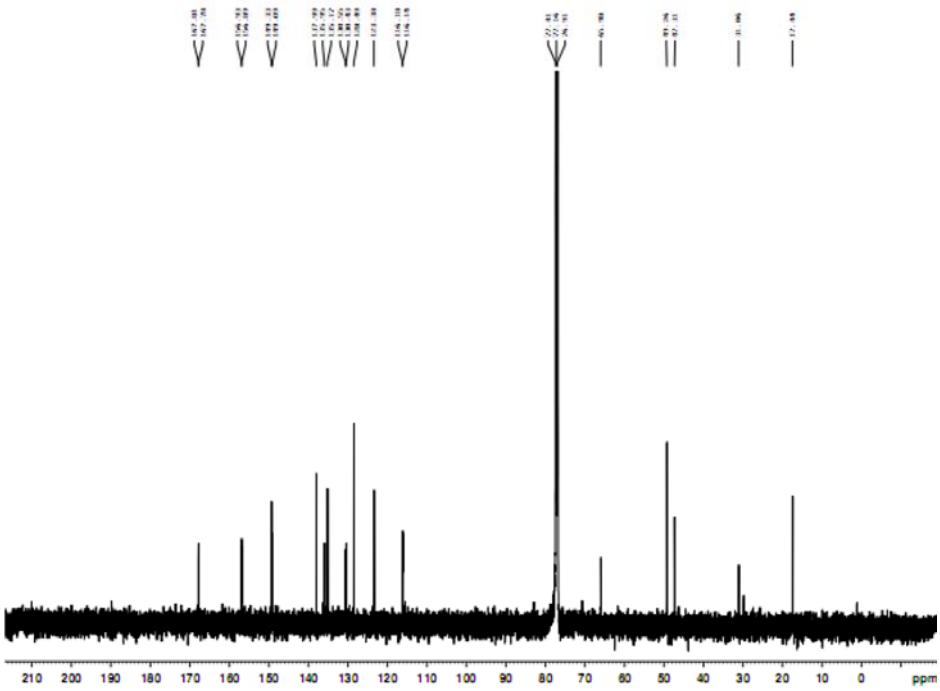


Figure S2: ^{13}C NMR spectrum (125 MHz) of chiral basket (R_3)-**1** (4.24 mM) in $CDCl_3$ at 300 K.

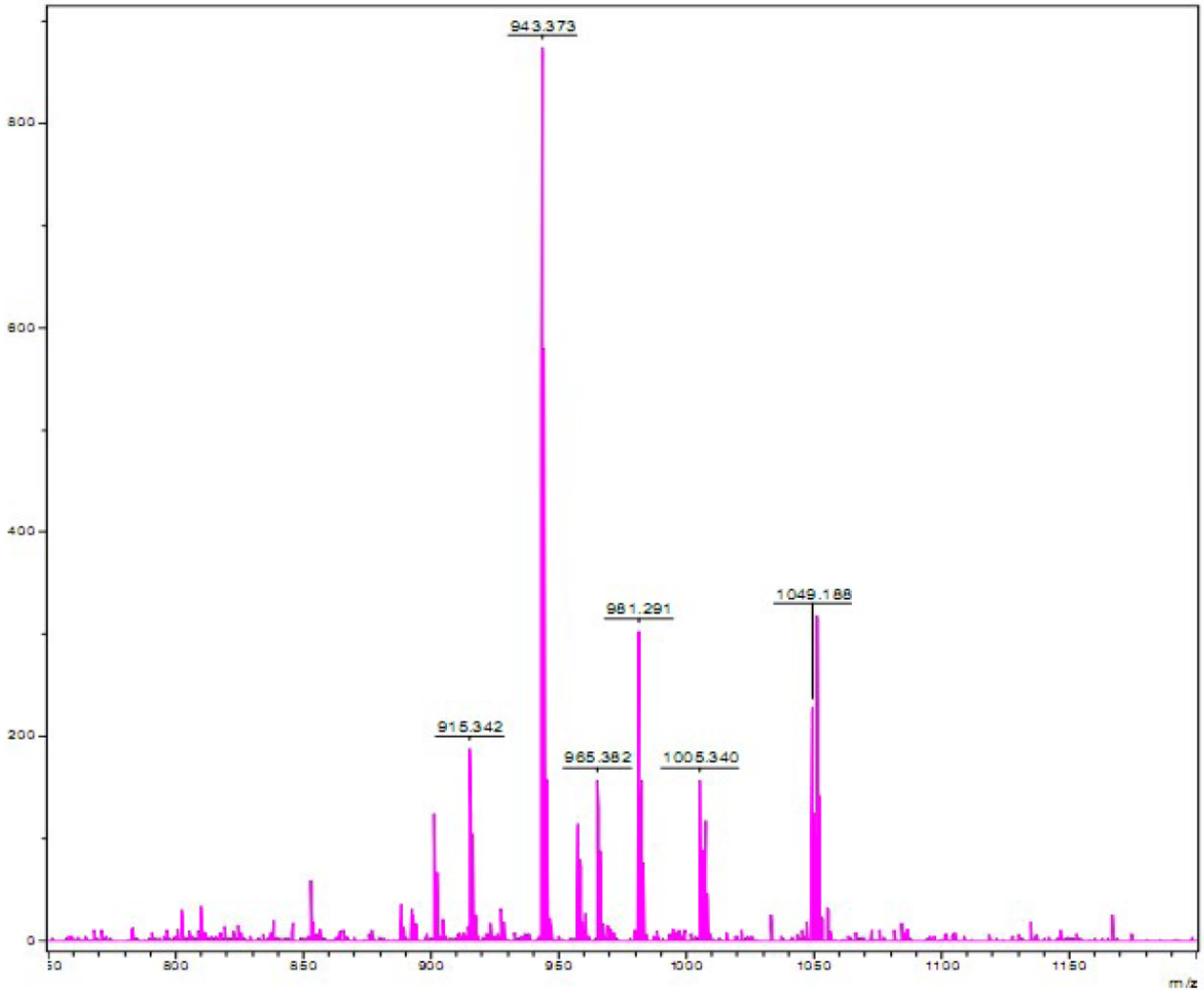


Figure S3: High resolution MS (MALDI-TOF) spectrum of chiral basket (R_3)-**1** showing a strong signal at 943.373 corresponding to its $(M+H)^+$ ion.

Chiral basket (S_3)-1: Compound (*S*)-**7** (13.5 mg, 0.111 mmol) was added to a solution of *tris*-anhydride **8** (14 mg, 0.022 mmol) in 7 mL of toluene. The resulting solution was heated to reflux for 1 h upon which 700 µL of neat pyridine was added. The resulting mixture was stirred for 12 h and cooled down to room temperature. The mixture was concentrated under reduced pressure and the residue purified with thin-layer chromatography (SiO_2, acetone:benzene=3:1) to yield 17.6 mg of basket (S_3)-**1** (84 %) as a colorless oil.
^{1}H NMR (500 MHz, $CDCl_3$, 300 K): δ = 8.60 (d, *J*=1.8 Hz, 3H), 8.46 (dd, *J*=4.8, 1.8 3H), 7.78 (dt, *J*=7.9, 1.8, 1.8 3H), 7.47 (d, *J*=5.6 6H), 7.20 (dd, *J*=7.9, 4.8 3H), 5.44 (q, *J*=7.4 Hz, 3H), 4.49 (s, 6H), 2.58 (s, 6H), 1.79 (d, *J*=7.4 Hz, 9H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 300 K): δ = 167.80, 167.76, 156.93, 156. 89, 149.30, 149.07, 137.97, 135.95, 135.16, 130.53, 130.41, 123.37, 116.17, 116.13, 65.96, 49.24, 47.29, 17.43 ppm; HRMS MALDI-TOF: *m*/*z* calcd for $C_{60}H_{42}N_6O_6$: 943.327 $[M + H]^+$, found: 943.347.

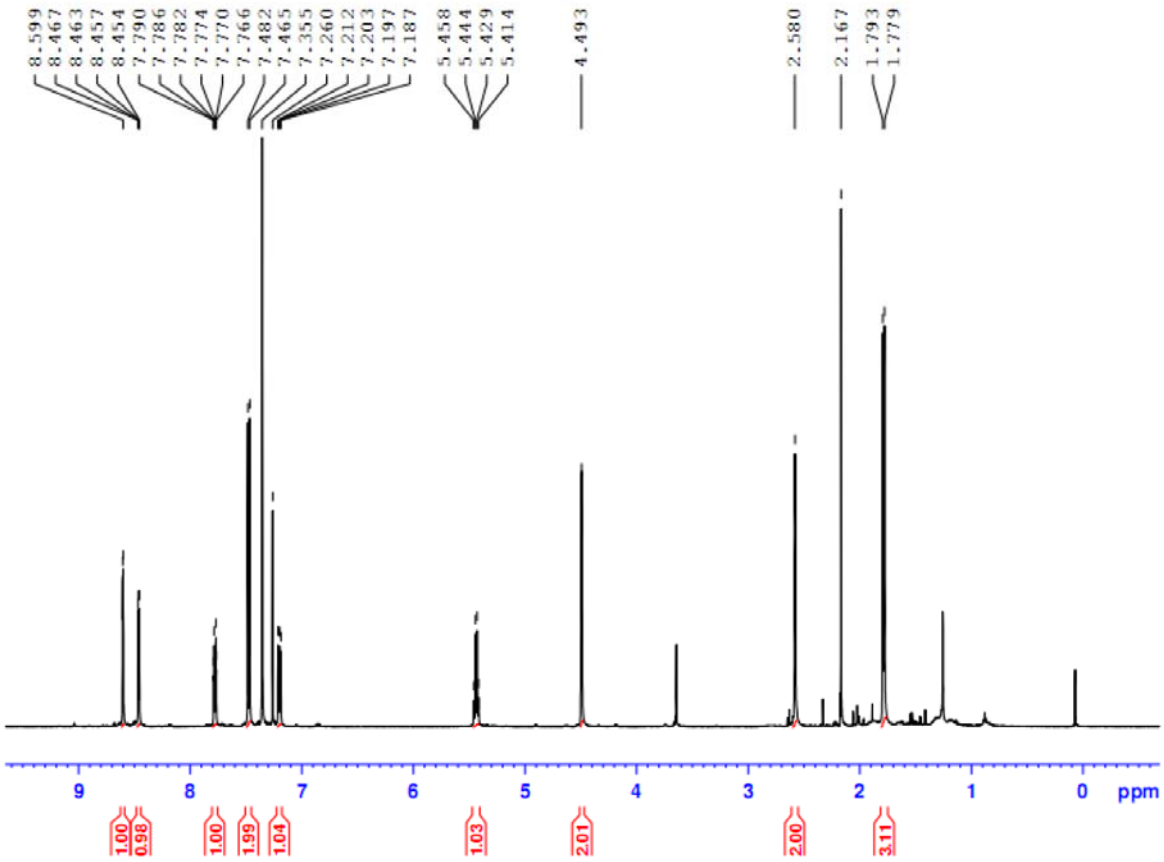


Figure S4: ^{1}H NMR spectrum (500 MHz) of chiral basket (S_3)-**1** (27.57 mM) in $CDCl_3$ at 300 K.

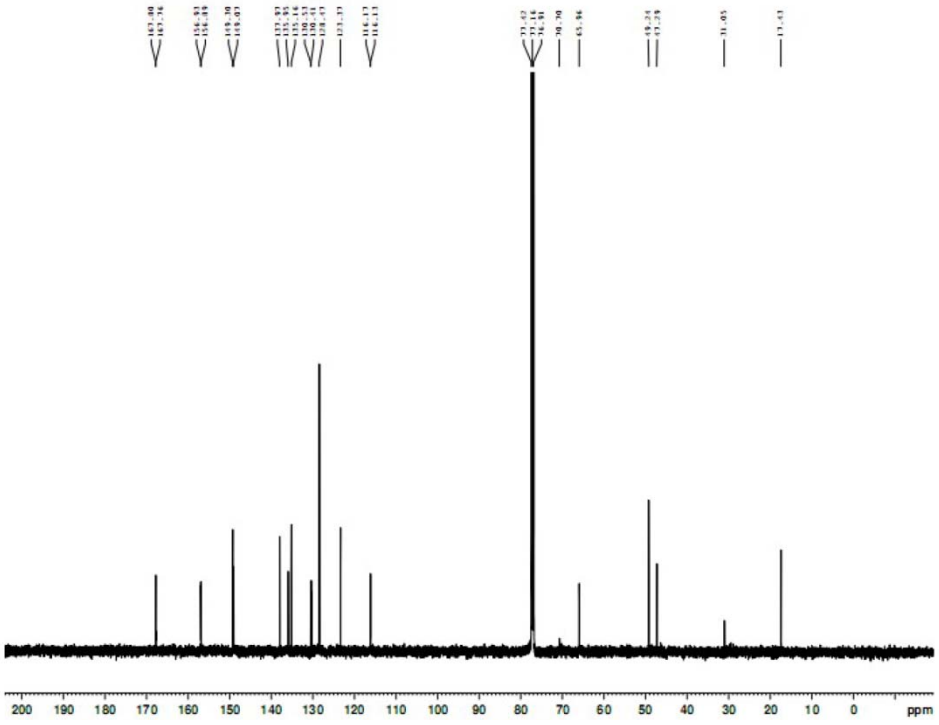


Figure S5: ^{13}C NMR spectrum (125 MHz) of chiral basket (*S*$_3$)-**1** (27.57 mM) in $CDCl_3$ at 300 K.

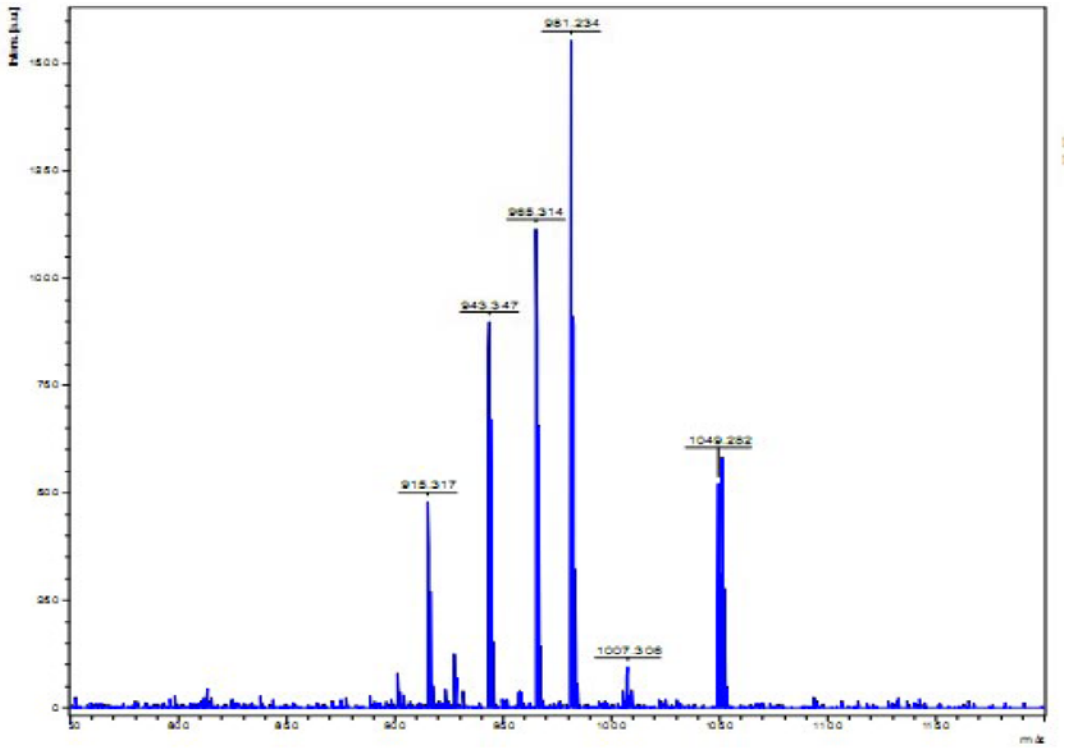


Figure S6: High resolution MS spectrum (MALDI-TOF) of chiral basket (S_3)-**1** showing a strong signal at 943.347 corresponding to its $(M+H)^+$ ion.

Model compound (*R*)-2: Compound (*R*)-**7** (48 mg, 0.394 mmol) was added to a solution of phthalic anhydride (70 mg, 0.473 mmol) in 8 mL of toluene. The resulting solution was heated to reflux for 1 h upon which 800 µL of neat pyridine was added. The resulting mixture was stirred for additional 12 h and then cooled down to room temperature. The mixture was concentrated under reduced pressure and the residue purified via flash chromatography (SiO2, ethyl acetate:hexanes=1:1) to yield 96.6 mg of compound (*R*)-**2** (81%) as a colorless oil.
^{1}H NMR (500 MHz, $CDCl_3$, 300 K): δ = 8.70 (d, *J*=2.3 Hz, 1H), 8.50 (dd, *J*=4.8, 1.8, 1H), 7.87 (dt, *J*=7.9, 1.8, 1.8, 1H), 7.80 (dd, *J*=5.5, 3.0, 2H), 7.68 (dd, *J*=5.5, 3.0, 2H), 7.25 (dd, *J*=7.9, 4.8, 1H), 5.58 (q, *J*=7.4 Hz, 1H), 1.92 (d, *J*=7.4 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 300 K): δ = 168.0 , 149.4, 149.2, 135.8, 135.2, 134.2, 131.9, 123.44, 123.42, 47.5, 17.4 ppm; HRMS ESI: *m*/*z* calcd for$C_{15}H_{12}N_2O_2$: 253.0999 $[M + H]^+$, found: 253.0968.

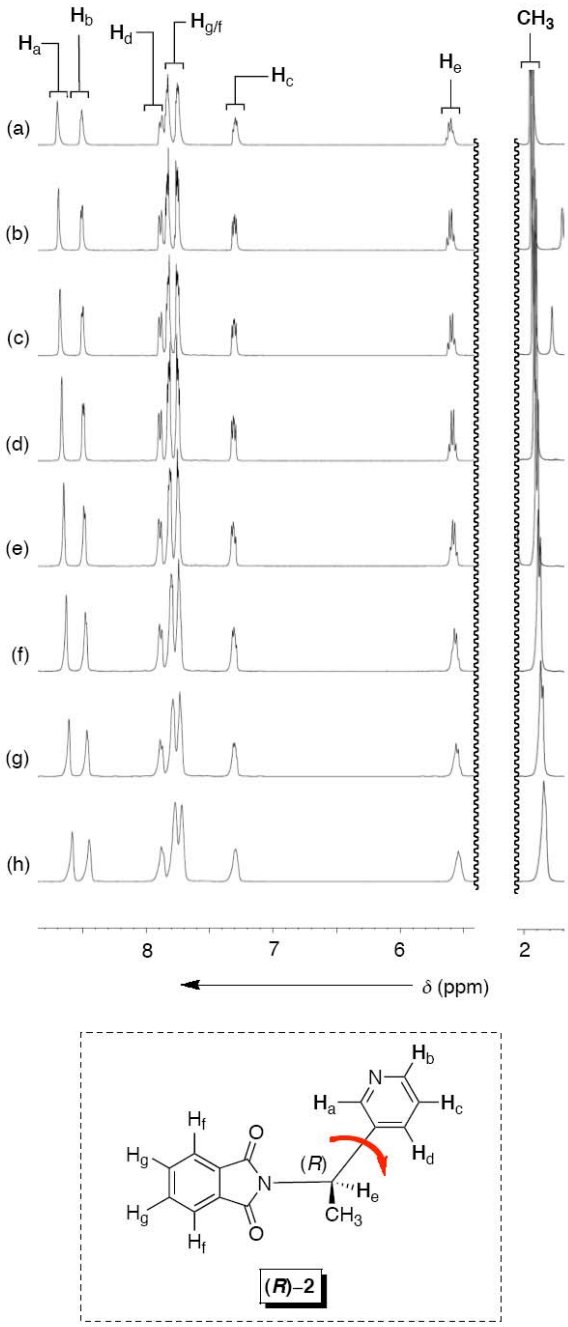


Figure *S*7: Variable temperature ^{1}H NMR spectrum (500 MHz) of model compound (*R*)-**2** (0.158 M) in $CDCl_3$ at (a) 298.0, (b) 283.0, (c) 268, (d) 253.0, (e) 238.0, (f) 223.0, (g) 208.0 and (h) 193.0 K.

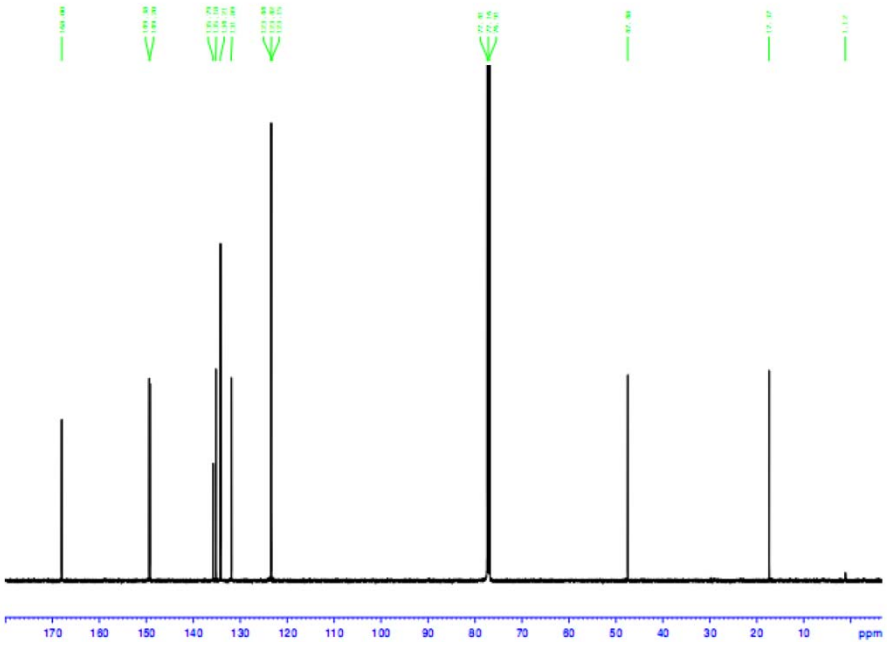


Figure *S*8: ^{13}C NMR spectrum (125 MHz) of model compound (*R*)-**2** (0.158 M) in $CDCl_3$ at 300 K.

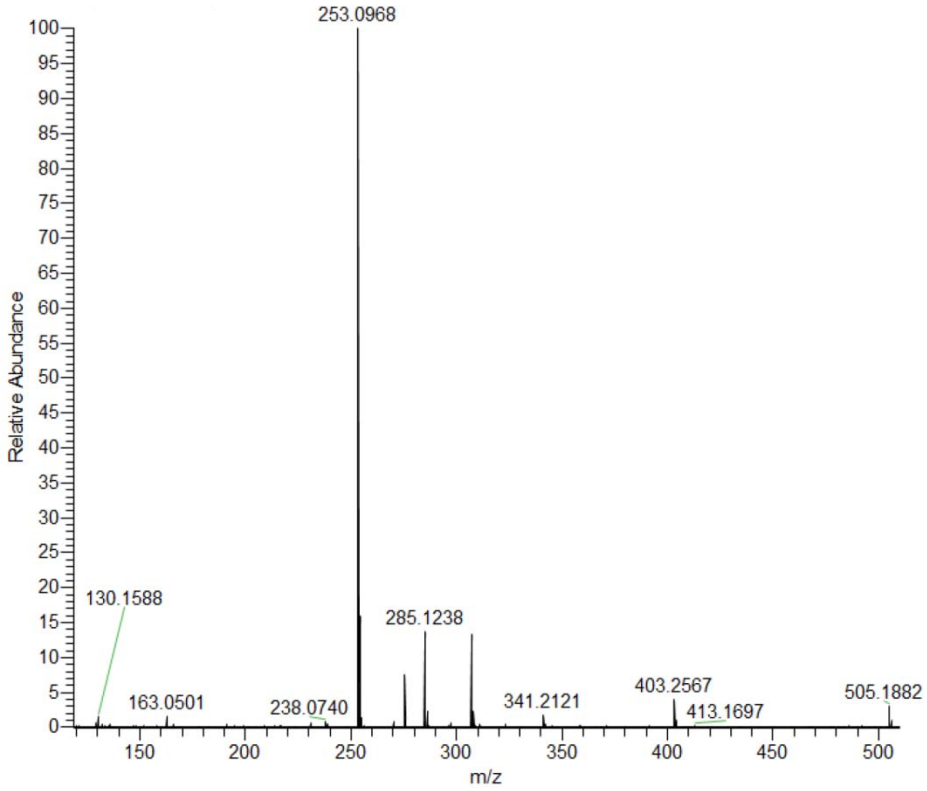


Figure *S*9: High resolution MS (ESI) spectrum of model compound (*R*)-**2** showing a strong signal at 253.0968 corresponding to its $(M+H)^+$ ion.

Model compound (S)-2: Compound (*S*)-**7** (48 mg, 0.394 mmol) was added to a solution of phthalic anhydride (70 mg, 0.473 mmol) in 8 mL of toluene. The resulting solution was heated to reflux and stirred for 1h upon which 800 µL of neat pyridine was added. The resulting mixture was stirred for 12 h and then cooled down to room temperature. The mixture was concentrated under reduced pressure and the residue purified via flash chromatography (SiO_2, ethyl acetate:hexane=1:1) to yield 75 mg of model compound (*S*)-**2** (63%) as a colorless oil.
^{1}H NMR (500 MHz, $CDCl_3$, 300 K): δ = 8.71 (d, *J*=2.3 Hz, 1H), 8.51 (dd, *J*=4.8, 1.8, 1H), 7.88 (dt, *J*=7.9, 1.8, 1.8, 1H), 7.81 (dd, *J*=5.5, 3.0, 2H), 7.69 (dd, *J*=5.5, 3.0, 2H), 7.26 (dd, *J*=7.9, 4.8, 1H), 5.59 (q, *J*=7.4 Hz, 1H), 1.93 (d, *J*=7.4 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 300 K): δ = 168.0 , 149.4, 149.2, 135.8, 135.2, 134.2, 131.9, 123.4, 123.4, 47.5, 17.4 ppm; HRMS ESI: *m*/*z* calcd for$C_{15}H_{12}N_2O_2$: 253.0999 $[M + H]^+$, found: 253.0970.

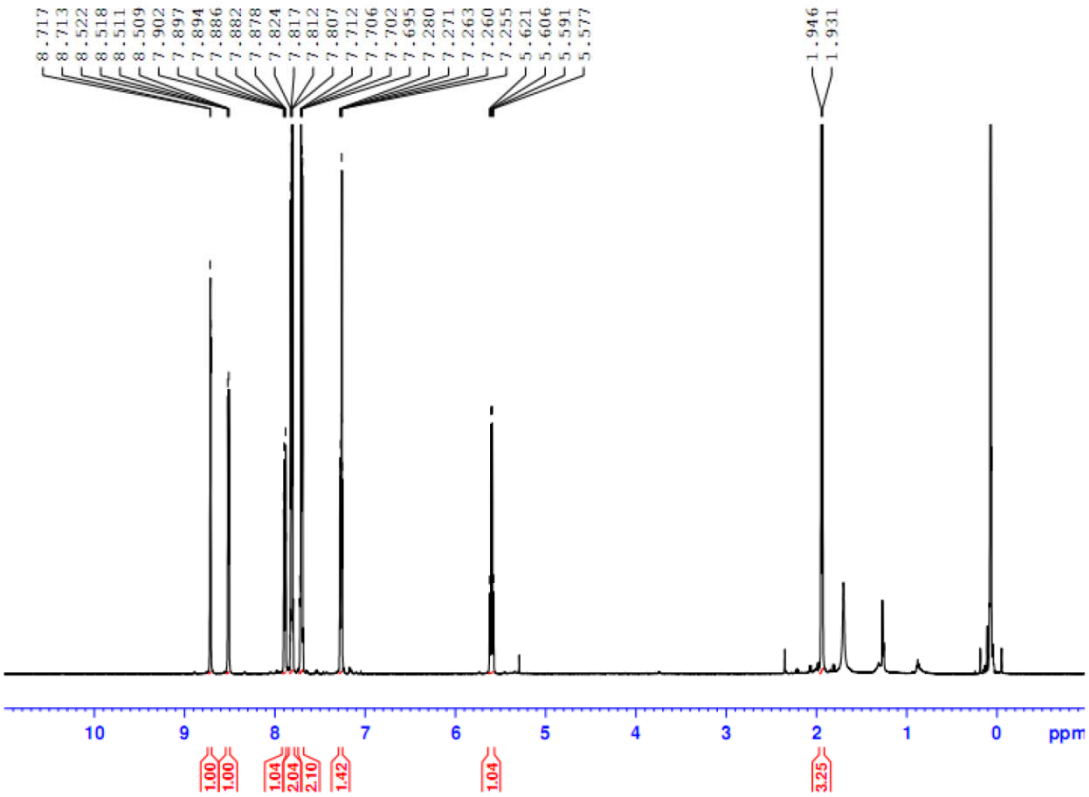


Figure *S*10: ^{1}H NMR spectrum (500 MHz) of model compound (*S*)-**2** (0.238 M) in $CDCl_3$ at 300 K.

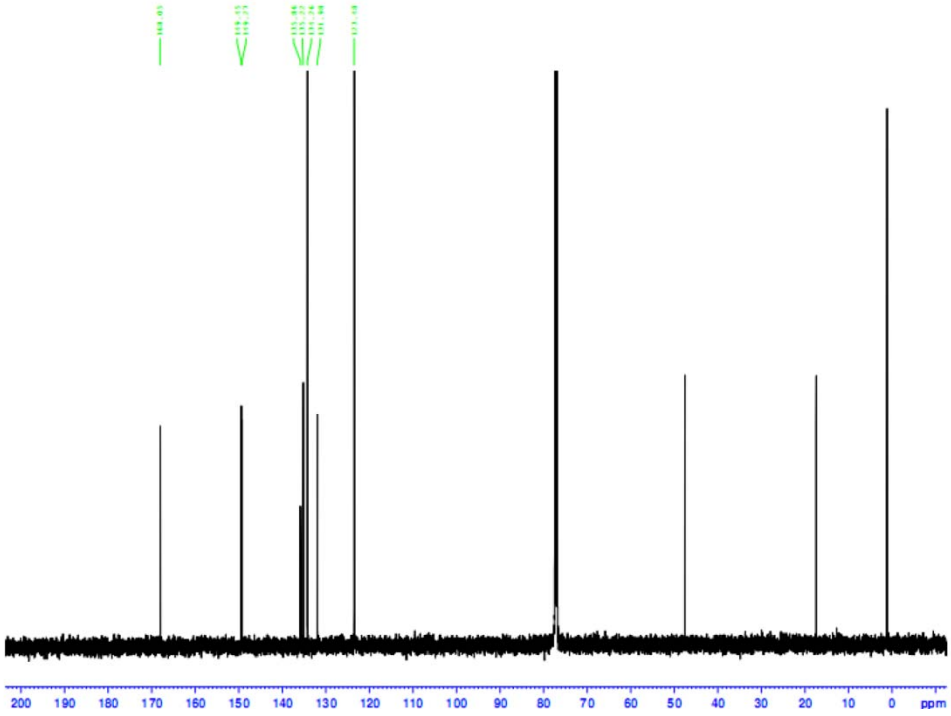


Figure *S*11: ^{13}C NMR spectrum (125 MHz) of model compound (*S*)-**2** (0.238 M) in $CDCl_3$ at 300 K.

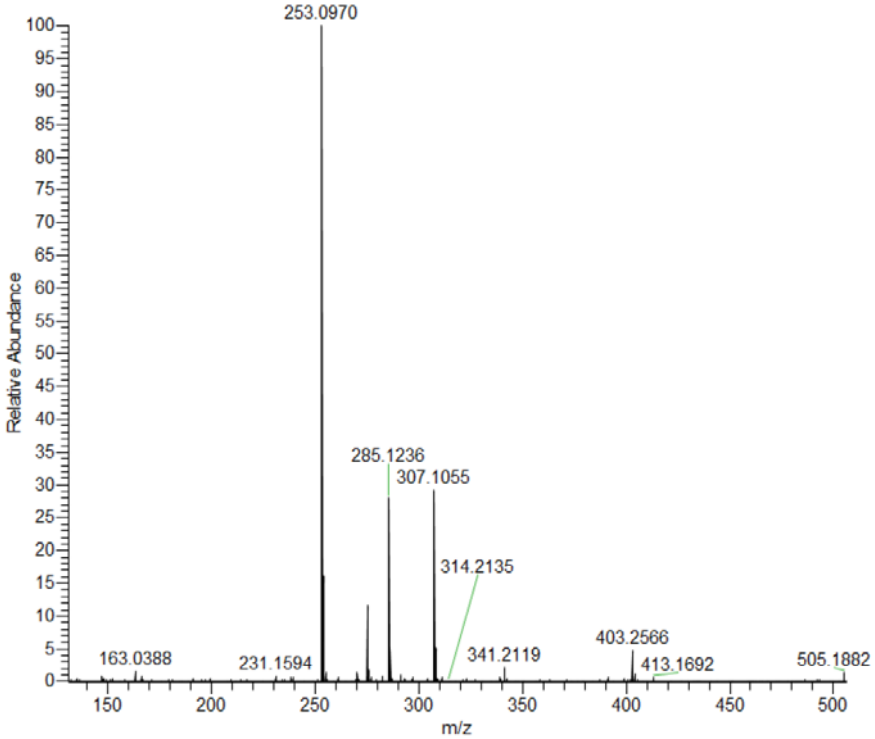


Figure *S*12: High resolution MS (ESI) spectrum of model compound (*S*)-**2** showing a strong signal at 253.0970 corresponding to its $(M+H)^+$ ion.

Compound (R_A)-5: $Ti(OEt)_4$ (1.74 mL, 7.42 mmol) was added to a solution of 3-acetylpyridine **3** (494 mg, 4.08 mmol) and compound (R_A)-**4** (501 mg, 4.12 mmol) in dry dichloromethane (16 mL). The resulting solution was stirred at reflux for 60 h. After cooling to room temperature, the solvent was removed under vacuum and the residue extracted with ethyl acetate (80 mL). Upon a slow addition of brine (16 mL), the mixture was filtered through a pad of Celite. The organic phase was dried over $MgSO_4$ and the solvent evaporated in vacuum to give a solid residue. The residue was purified with flash chromatography (SiO_2, ethyl acetate: hexanes=4:1)] to give 694 mg of (R_A)-**5** (75 %) as a yellow oil. ^{1}H NMR (250 MHz, $CDCl_3$, 300 K): δ = 9.09 (s, 1H), 8.71 (d, *J*=4.8, 1H), 8.15 (dt, *J*=8.1, 1.8, 1.8, 1H), 7.37 (dd, *J*=8.1, 4.8, 1H), 2.80 (s, 3H), 1.33 (s, 9H) ppm.

Compound (R_A, *S*)-6: 2.22 mL of 1.0 M solution of *L*-Selectride (2.22 mmol) in THF was added dropwise at -78^0 C to a solution of compound (R_A)-**5** (500 mg, 2.22 mmol) in dry THF (20 mL). After 6 h, the reaction mixture was quenched with saturated solution of NH_4Cl (30 mL) and extracted with 30 mL of ethyl acetate. The organic phase was dried over $MgSO_4$ and the solvent evaporated under reduced pressure. The solid residue was purified with flash chromatography (SiO_2, dichloromethane:methanol=9:1) to give 323 mg of (R_A, *S*)-**6** (64 %) as a yellow oil.^{1}H NMR (250 MHz, $CDCl_3$, 300 K): δ = 8.54 (s, 1H), 8.47 (d, *J*=4.8, 1H), 7.60 (td, *J*=7.9, 1.8, 1.8, 1H), 7.22 (dd, *J*=7.9, 4.8, 1H), 4.56 (q, *J*=6.7, 1H), 1.51 (d, *J*=6.7, 3H), 1.15 (s, 9H) ppm.

Compound (R_A, *R*)-6: 5.0 mL of 1.0 M solution of DIBAL (5 mmol) in THF was added dropwise, at -78^0 C, to a solution of compound (R_A)-**5** (500 mg, 2.22 mmol) in dry THF (20 ml). After 6 h the reaction mixture was quenched with methanol (10 ml) at -78^0 C and then warmed up to room temperature. The solvent was evaporated under reduced pressure, upon which 2 M NaOH (20 ml) was added and the crude mixture extracted with 30 mL of ethyl acetate. The organic phase was dried with $MgSO_4$ and the solvent evaporated under reduced pressure. The solid residue was purified with flash chromatography (SiO_2, dichloromethane:methanol=9:1) to give 404 mg of (R_A, *R*)-**6** (80%) as a yellow oil. ^{1}H NMR (250 MHz, $CDCl_3$, 300 K): δ = 8.63 (s, 1H), 8.56 (d, *J*=4.8, 1H), 7.71 (dt, *J*=7.9, 1.8, 1.8, 1H), 7.31 (dd, *J*=7.9, 4.8, 1H), 4.60 (q, *J*=6.7, 1H), 1.56 (d, *J*=6.7, 3H), 1.24 (s, 9H) ppm.

Compound (*S*)-7: Compound (R_A, *S*)-**6** (318 mg, 1.4 mmol) was dissolved in 28 mL of methanol upon which 28 ml of 6 M HCl (in methanol) was added. The reaction mixture was stirred at room temperature for one hour. Methanol was evaporated under reduced pressure and 10 ml of H_2O was added. Upon the extraction of aqueous solution with diethyl ether (3 X 20 mL), 2 M NaOH was added dropwise until pH~12. The organic layer was extracted with dichloromethane (3 X 20 mL) and dried with $MgSO_4$. The solvent was evaporated under reduced pressure to give 95 mg of (*S*)-**7** as a colorless oil (yield 55%). ^{1}H NMR (250 MHz, $CDCl_3$, 300 K): δ = 8.59 (d, *J*=1.8, 1H), 8.49 (dd, *J*=4.8, 1.8, 1H), 7.71 (td, *J*=7.9, 1.8, 1.8, 1H), 7.25 (dd, *J*=7.9, 4.8, 1H), 4.18 (q, *J*=6.7, 1H), 1.41 (d, *J*=6.7, 3H) ppm.

Compound (*R*)-7: Compound (R_A, *R*)-**6** (230 mg, 1.02 mmol) was dissolved in 20 mL of methanol upon which 20 ml of 6 M HCl (in methanol) was added. The reaction mixture was stirred at room temperature for one hour. Methanol was evaporated under reduced pressure and 10 ml of H_2O was added. Upon the extraction of aqueous solution with diethyl ether (3 X 20 mL), 2 M NaOH was added dropwise until pH~12. The organic layer was extracted with dichloromethane (3 X 20 mL) and dried with $MgSO_4$. The

solvent was evaporated under reduced pressure to give 68 mg of (*R*)-**7** (55%) as a colorless oil. NMR (250 MHz, $CDCl_3$, 300 K): δ = 8.55 (d, *J*=1.8, 1H), 8.44 (dd, *J*=4.8, 1.8, 1H), 7.67 (td, *J*=7.9, 1.8, 1.8, 1H), 7.22 (dd, *J*=7.9, 4.8, 1H), 4.14 (q, *J*=6.7, 1H), 1.37 (d, *J*=6.7, 3H) ppm.

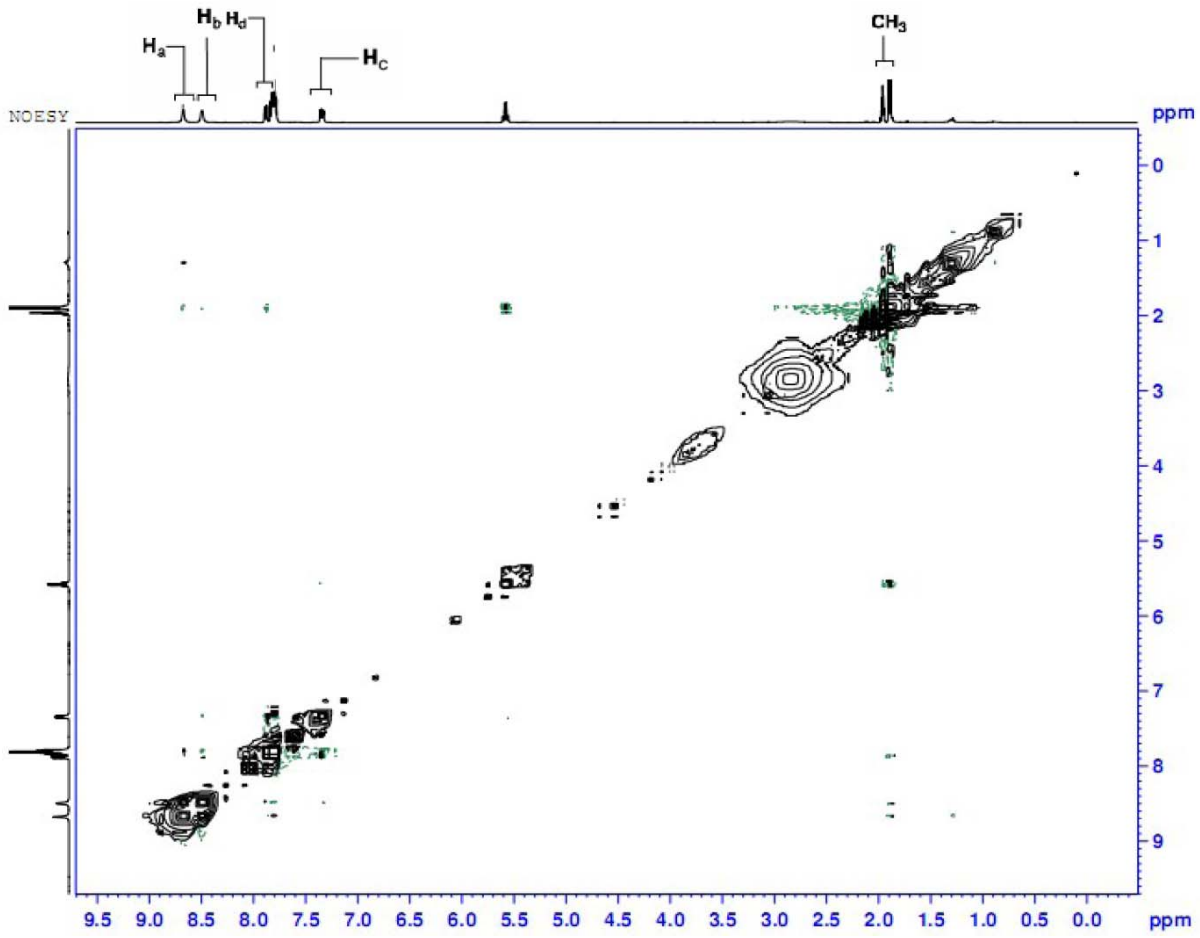


Figure S13: 2-D ^{1}H-^{1}H NOESY Spectrum (400 MHz, 298 K) of 0.16 M solution of (*R*)-**2** in CD_3CN; mixing time 400 ms.

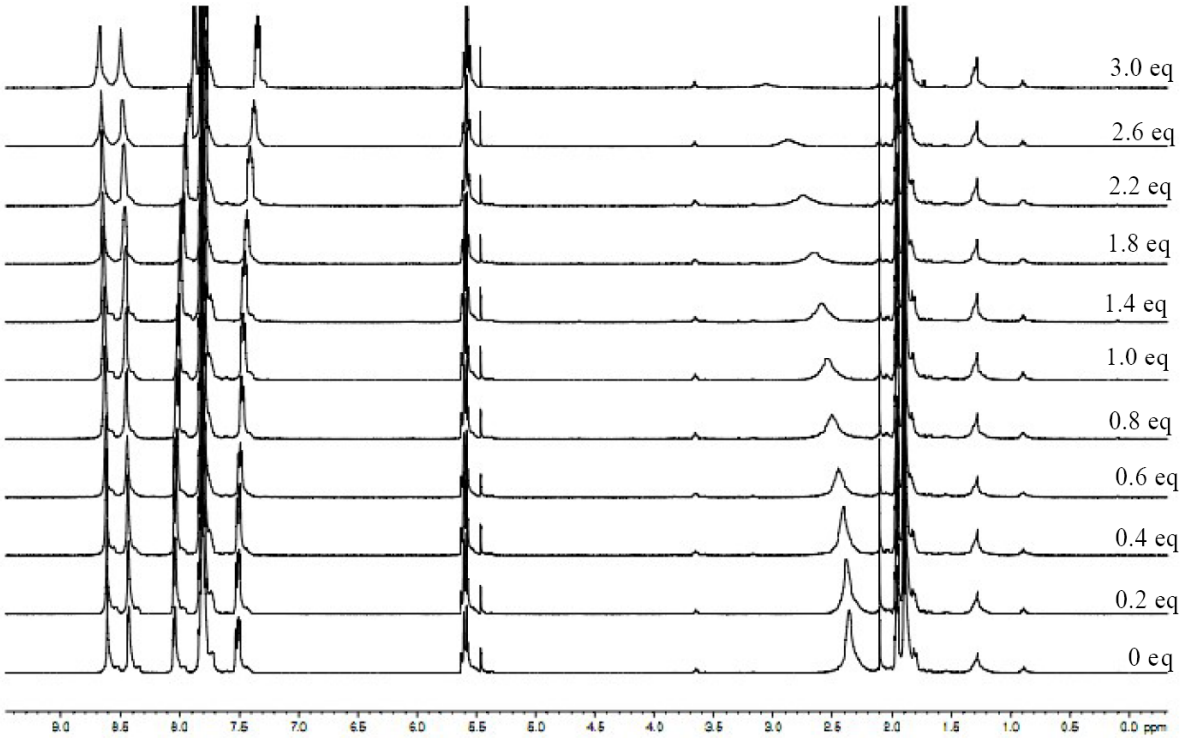


Figure S14: A series of ^{1}H NMR spectra (400 MHz, CD_3CN, 298 K) recorded on addition of 1.60 M standard solution of $AgBF_4$ to 80.0 mM solution of (*R*)-**2**.

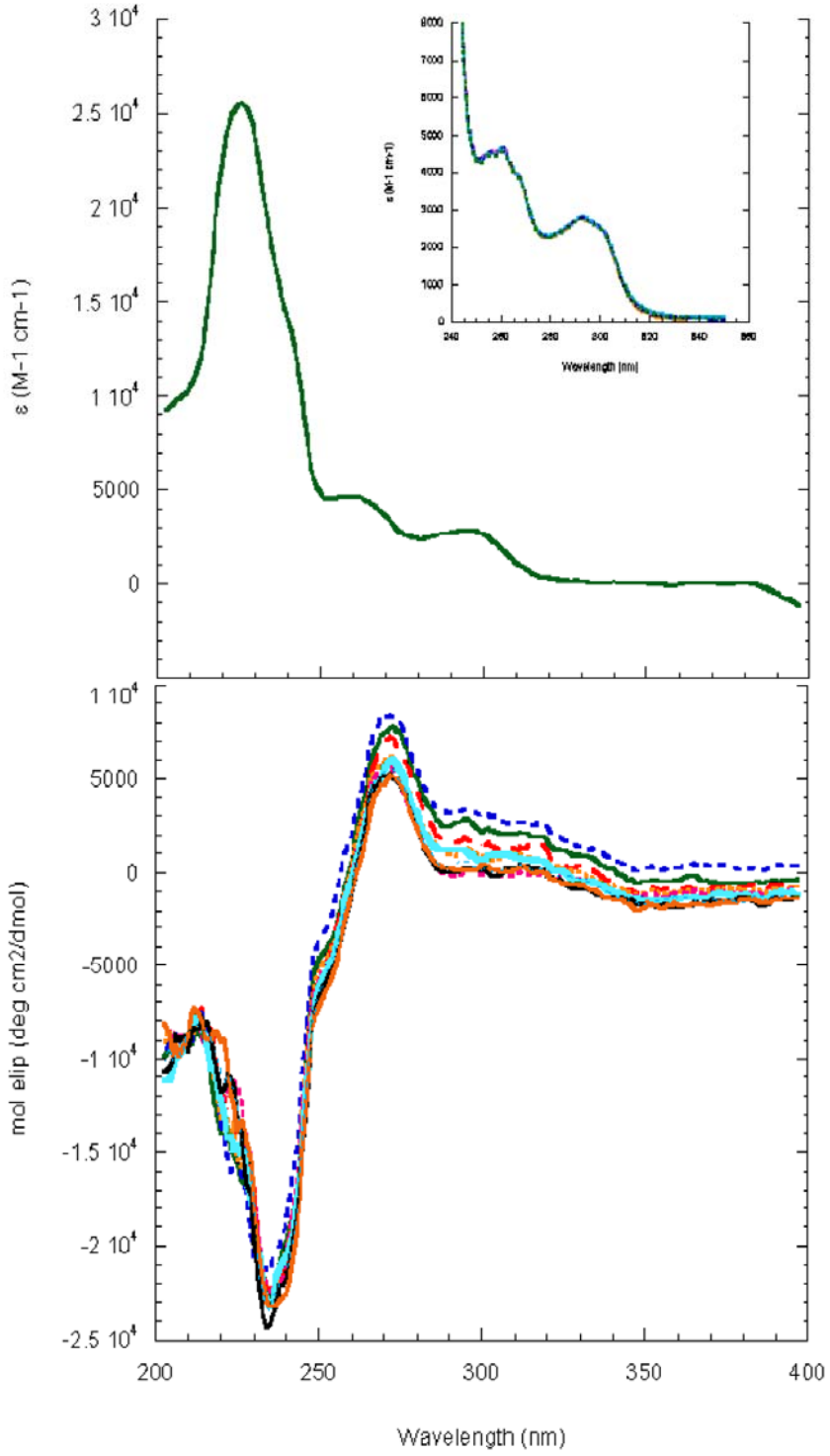


Figure S15: UV-Vis and CD titration of 0.0635 mM (*R*)-**2** solution recorded upon incremental addition of 0.0, 0.2, 0.4, 0.6, 0.8, 1.0 molar equivalents of 0.292 mM solution of $AgBF_4$ in CH_3CN.

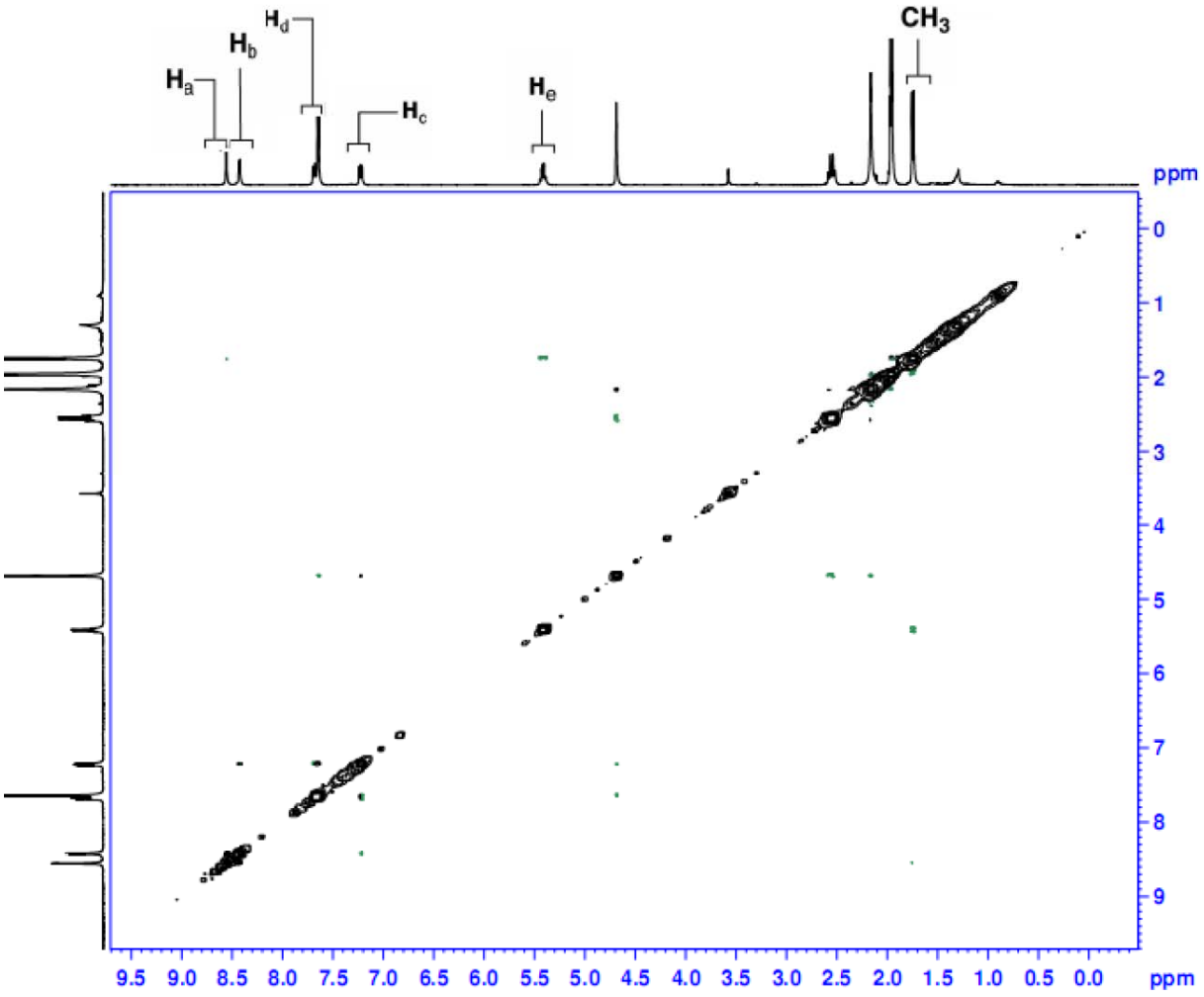


Figure S16: 2-D ^{1}H-^{1}H NOESY Spectrum (400 MHz, 298 K) of 2.12 mM solution of (*R*)-**1** in CD_3CN.

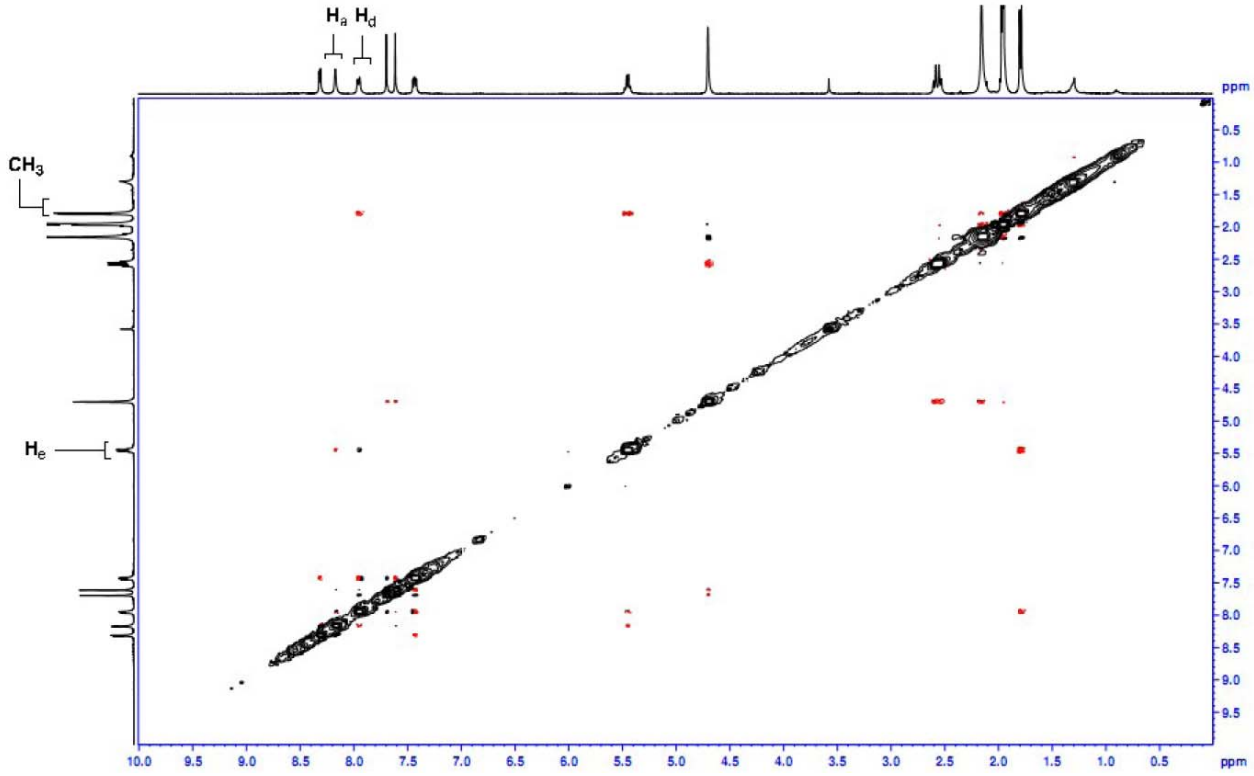


Figure S17: 2-D ^{1}H-^{1}H NOESY Spectrum (400 MHz, 298 K) of 2.12 mM solution of (*R*)-**1** in CD_3CN after the addition of 1 molar equivalent of 10.6 mM $AgBF_4$.

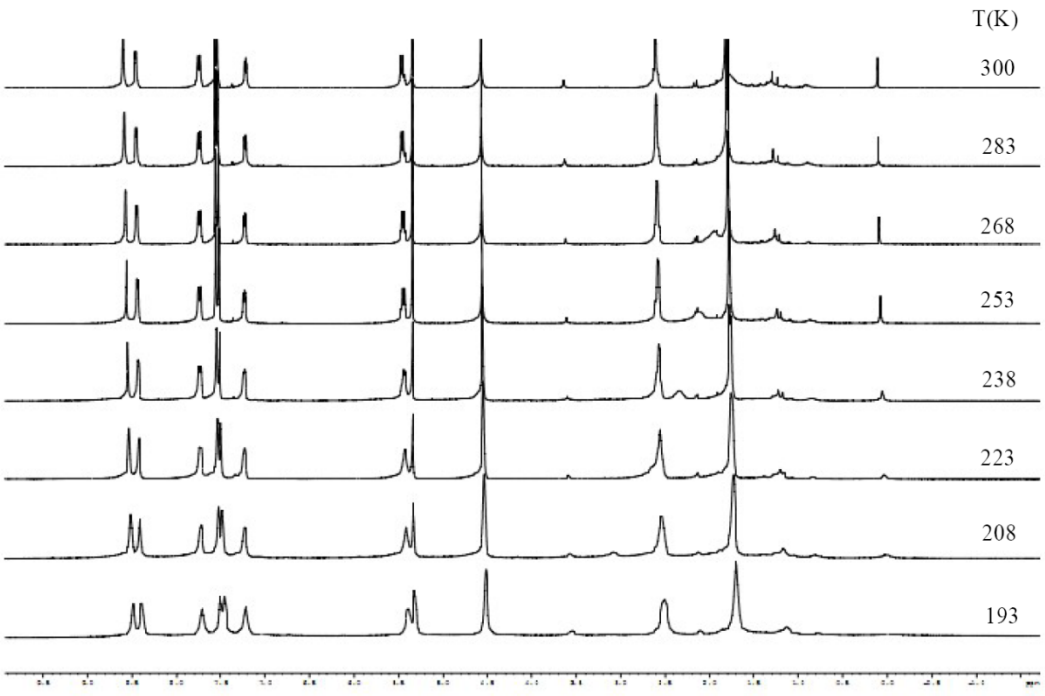


Figure S18: Variable temperature ^{1}H NMR (400 MHz) spectra of 13.6 mM solution of (*R*)-**1** in CD_2Cl_2**.**

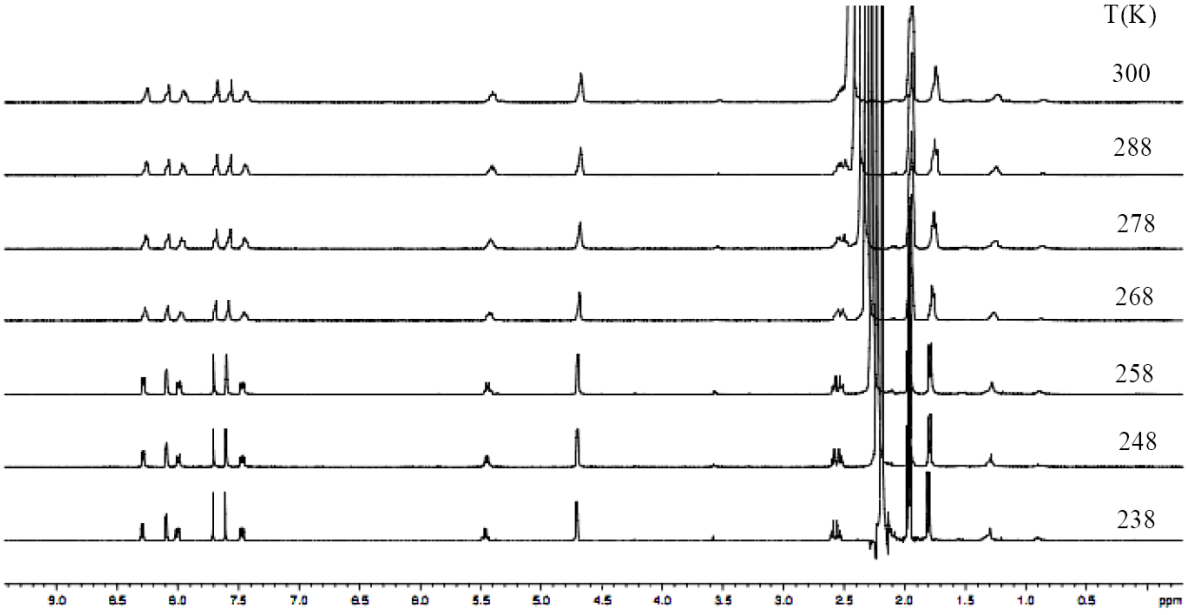


Figure *S*19: Variable temperature ^{1}H NMR (400 MHz) spectra of 3.39 mM solution of (*R*)-**1** upon the addition of 3.0 molar equivalents of 0.169 M $AgBF_4$ in CD_3CN.

Computational Studies

The Monte Carlo/Molecular Mechanics (MC/MM) calculations were performed using MacroModel v9.7 from the Schrödinger '09 software suite (using the Maestro v9.0 interface). The Monte Carlo multiple minimum search protocol was used for the conformational search, generating 5,000 starting structures for (*R*)-**2** and 10,000 for (R_3)-**1**. The MM3 force field, as implemented in MacroModel, was used to optimize the conformations. The GB/SA model as implemented in MacroModel was utilized for the calculation of the aqueous solvent. Structures within 20 kcal/mol of the lowest energy conformation were retained in the final results. Six unique conformations were found for the search of (*R*)-**2**. The top two conformations are presented in the paper; DFT optimization of the bottom four conformations caused the geometries to adopt either the 1st or 2nd best conformation. 207 conformations were found for (R_3)-**1** when no solvent was included and 247 conformations when water was used as a solvent. The lowest energy values of the four distinct conformations of (R_3)-**1** (three in, two in, one in and none in) were included in the paper. The energies of all conformations are included in the supporting information as a table.

Density functional theory (DFT) calculations were performed using the Turbomole 5.10 software package. Geometry optimizations were performed using the B3LYP and BHLYP functionals in conjunction with the resolution-of-the-identity (RI) approximation, decreasing the time required for the calculations with a minimal loss of accuracy. For (*R*)-**2**, all atoms were treated using the TZVP basis set, whereas for Ag(I)-(R_3)-**1**, only the silver atom was treated with TZVP and all other atoms were treated with the SV(P) basis set. Optimizations were performed using the jobex module implemented in Turbomole. The analytical second derivative was calculated for each structure to verify that no imaginary frequencies were present, thus confirming the structure as a minimum. These calculations were done using the aoforce module available in Turbomole. Thermodynamic corrections were calculated using the freeh module available in Turbomole.

Excited state calculations were performed using the escf package in Turbomole. The first 50 excitations were evaluated for the (*R*)-**2** and Ag(I)-(R_3)-**1** systems using time-dependent density functional theory (TD-DFT) with the functionals used in optimization (TD-B3LYP and TD-BHLYP). The excitation values, oscillator strengths and rotatory strengths are included in this document for all calculations. A uniform 0.3 eV Gaussian line broadening was applied to the oscillator and rotatory values, in order to simulate UV and CD spectra, respectively. Previous work on organic systems using TD-DFT calculations suggests a uniform phase shift to the energy of excitations. For (*R*)-**2** and Ag(I)-(R_3)-**1**, a shift of -0.85 eV was applied to the TD-BHLYP results and -0.15 eV for the TD-B3LYP calculations. The phase shift values were chosen to align the UV spectra with the experimental peak at 220 nm. While the BHLYP results required a more significant shift than the B3LYP system, the theoretical CD spectrum of Ag(I)-(R_3)-**1** calculated using B3LYP only went out to 265 nm, whereas the BHLYP calculation provided information through 215 nm. Thus, we have decided to only include the BHLYP results in the paper and have put the B3LYP results in the supporting information. Due to hardware limitations, calculation of additional excited states for B3LYP is unfeasible, as the escf module in Turbomole is limited to one processor and the excited state

calculations performed for this paper were on the order of 275 hours, 25 hours short of the time limit for the hardware.

Figure S20. Comparison of relative bottom-of-the-well energy (E_{bw}) and free energy (G at 298 K) values (in kcal/mol) from a variety of DFT methods for the optimization of (*R*)-**2**.

Conformer	**RI-BP86/TZVP**		**RI-B3LYP/TZVP**		**RI-BHLYP/TZVP**	
	$\mathbf{E_{bw}}$	$\boldsymbol{G_{298}}$	$\mathbf{E_{bw}}$	$\boldsymbol{G_{298}}$	$\mathbf{E_{bw}}$	$\boldsymbol{G_{298}}$
A	0.0	0.0	0.0	0.0	0.0	0.0
B	0.7	0.3	0.7	0.4	0.7	0.5

Figure **S21**. Comparison of relative bottom-of-the-well energy (E_{bw}) and free energy (G at 298 K) values (in kcal/mol) from a variety of DFT methods for the optimization of Ag(I)-(R_3)-**1**.

Helical Sense	**RI-BP86/TZVP**		**RI-B3LYP/SV(P),TZVP**		**RI-BHLYP/SV(P),TZVP**	
	$\boldsymbol{E_{bw}}$	$\boldsymbol{G_{298}}$	$\boldsymbol{E_{bw}}$	$\boldsymbol{G_{298}}$	$\boldsymbol{E_{bw}}$	$\boldsymbol{G_{298}}$
P	0.0	0.0	0.0	0.0	0.0	0.0
M	5.7	5.2	6.5	6.0	6.6	5.7

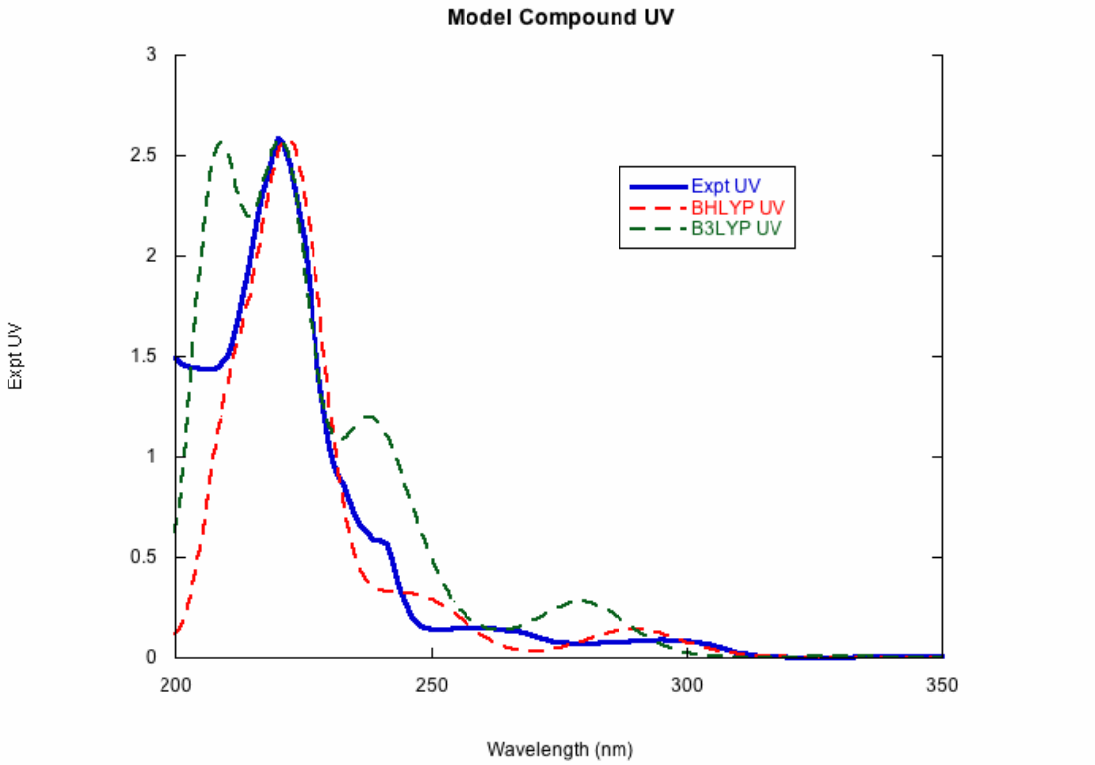


Figure S22. Calculated UV-Vis spectra of (*R*)-**2**(Conformer A) using the TD-B3LYP and TD-BHLYP functionals with a TZVP basis set. The B3LYP spectra was shifted by -0.15 eV and the BHLYP spectra was shifted by -0.85 eV. A 0.3 eV Gaussian line-broadening was applied to each excitation and the spectra were normalized to the experimental peak at 220 nm.

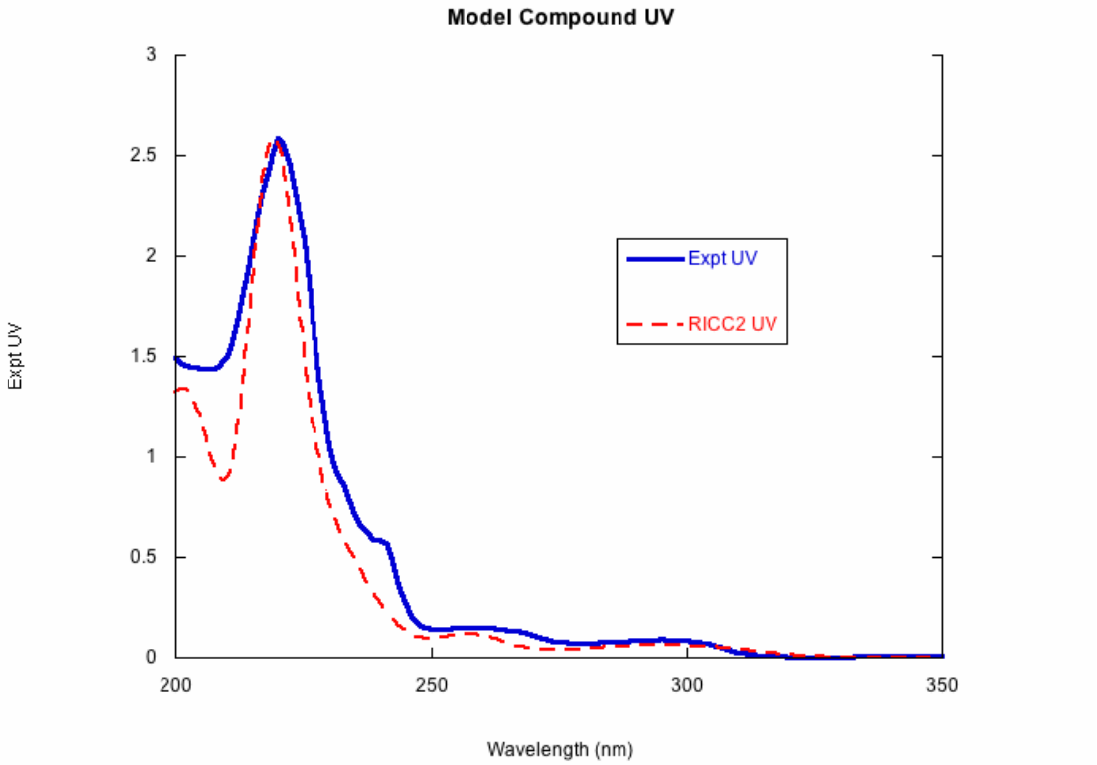


Figure S23. Calculated UV-Vis spectra of (*R*)-**2**(Conformer A) using the second-order approximate coupled-cluster model (RI-CC2/TZVP//RI-BHLYP/TZVP). The spectrum was shifted by -0.6 eV. A 0.3 eV Gaussian line-broadening was applied to each excitation and the spectrum was normalized to the experimental peak at 220 nm.

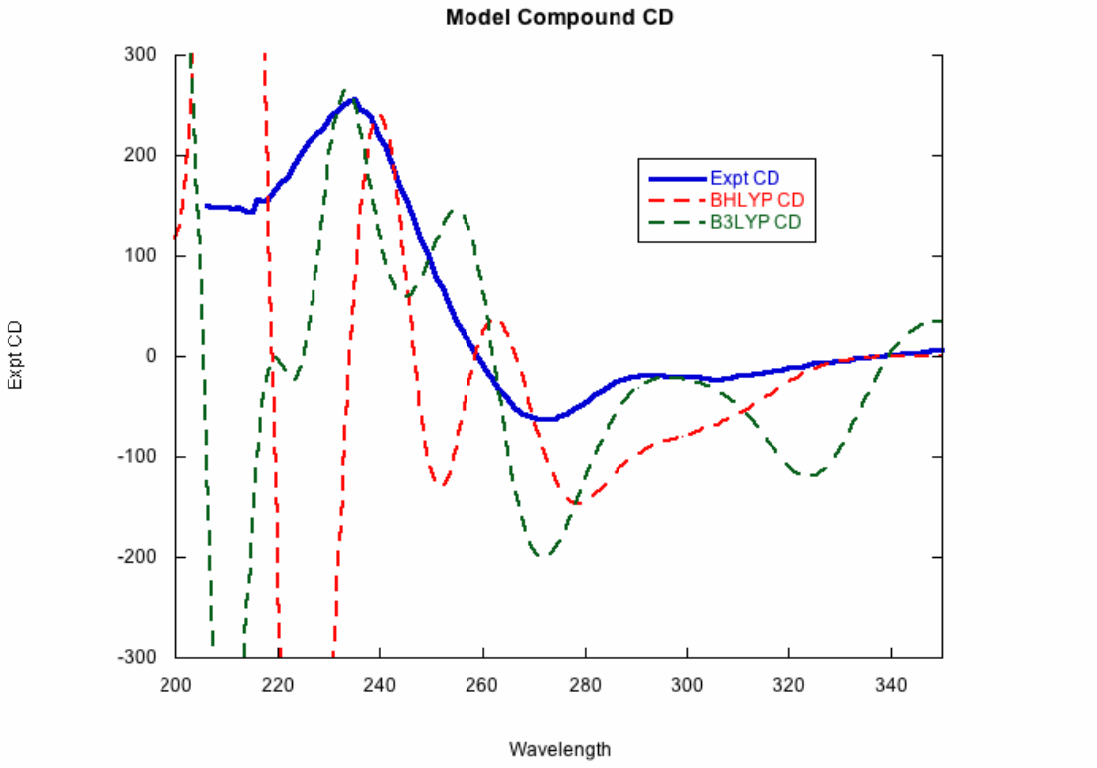


Figure S24. Calculated CD spectra of (*R*)-**2**(Conformer A) using the TD-B3LYP and TD-BHLYP functionals with a TZVP basis set. The B3LYP spectra was shifted by -0.15 eV and the BHLYP spectra was shifted by -0.85 eV. A 0.3 eV Gaussian line-broadening was applied to each excitation and the spectra were normalized to the experimental peak at 235 nm.

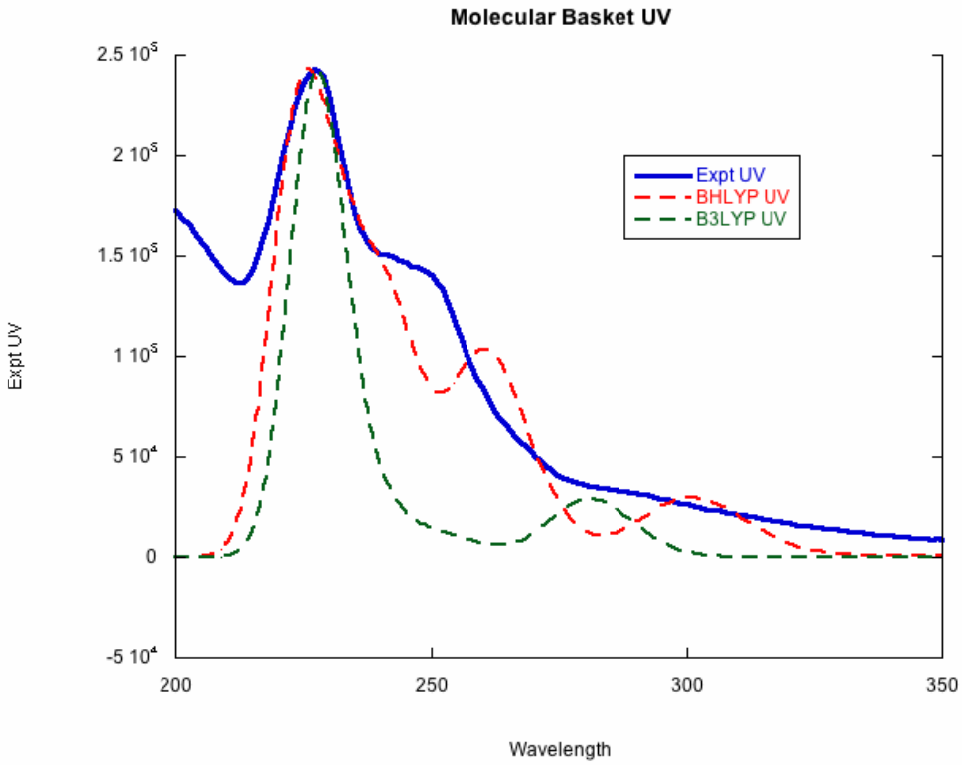


Figure S25. Calculated UV-Vis spectra of Ag(I)-(R_3)-**1**(P) using the TD-B3LYP and TD-BHLYP functionals with a TZVP basis set. The B3LYP spectra was shifted by -0.15 eV and the BHLYP spectra was shifted by -0.85 eV. A 0.3 eV Gaussian line-broadening was applied to each excitation and the spectra were normalized to the experimental peak at 220 nm.

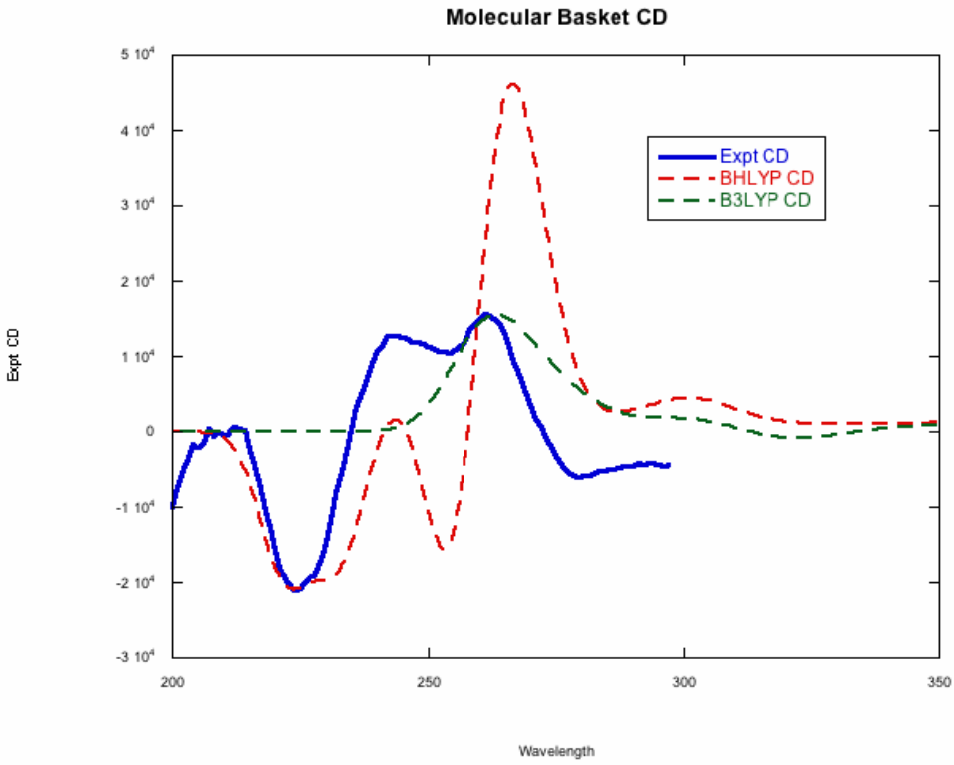


Figure S26. Calculated CD spectra of Ag(I)-(R_3)-**1**(P) using the TD-B3LYP and TD-BHLYP functionals with a TZVP basis set. The B3LYP spectra was shifted by -0.15 eV and the BHLYP spectra was shifted by -0.85 eV and a 0.3 eV Gaussian line-broadening was applied to each excitation. The B3LYP spectrum was normalized to the experimental peak at 260 nm and the BHLYP spectrum was normalized to 220 nm.

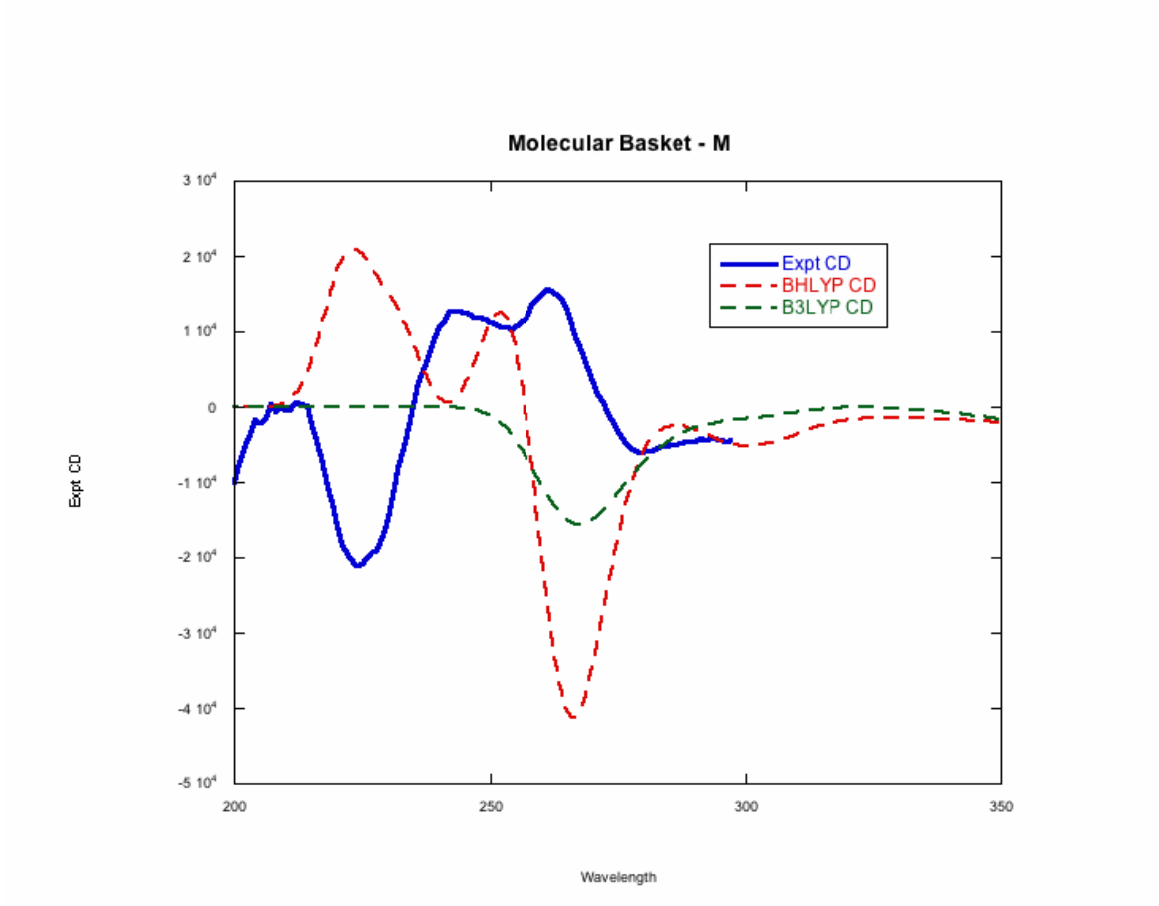


Figure S27. Calculated CD spectra of Ag(I)-(R_3)-**1**(*M*) using the TD-B3LYP and TD-BHLYP functionals with a TZVP basis set. The B3LYP spectra was shifted by -0.15 eV and the BHLYP spectra was shifted by -0.85 eV and a 0.3 eV Gaussian line-broadening was applied to each excitation. The B3LYP spectrum was normalized to the experimental peak at 260 nm and the BHLYP spectrum was normalized to 220 nm.

Figure S28. Electron density difference plots of (*R*)-**2**(Conformer A) as calculated by TD-BHLYP/TZVP. The contour values are ±0.002 au. Excitation energies in wavelengths are provided for each excited state before and after (in parentheses) a -0.85 eV shift was applied. Excited states with large oscillator or rotatory strengths were chosen for presenting these plots.

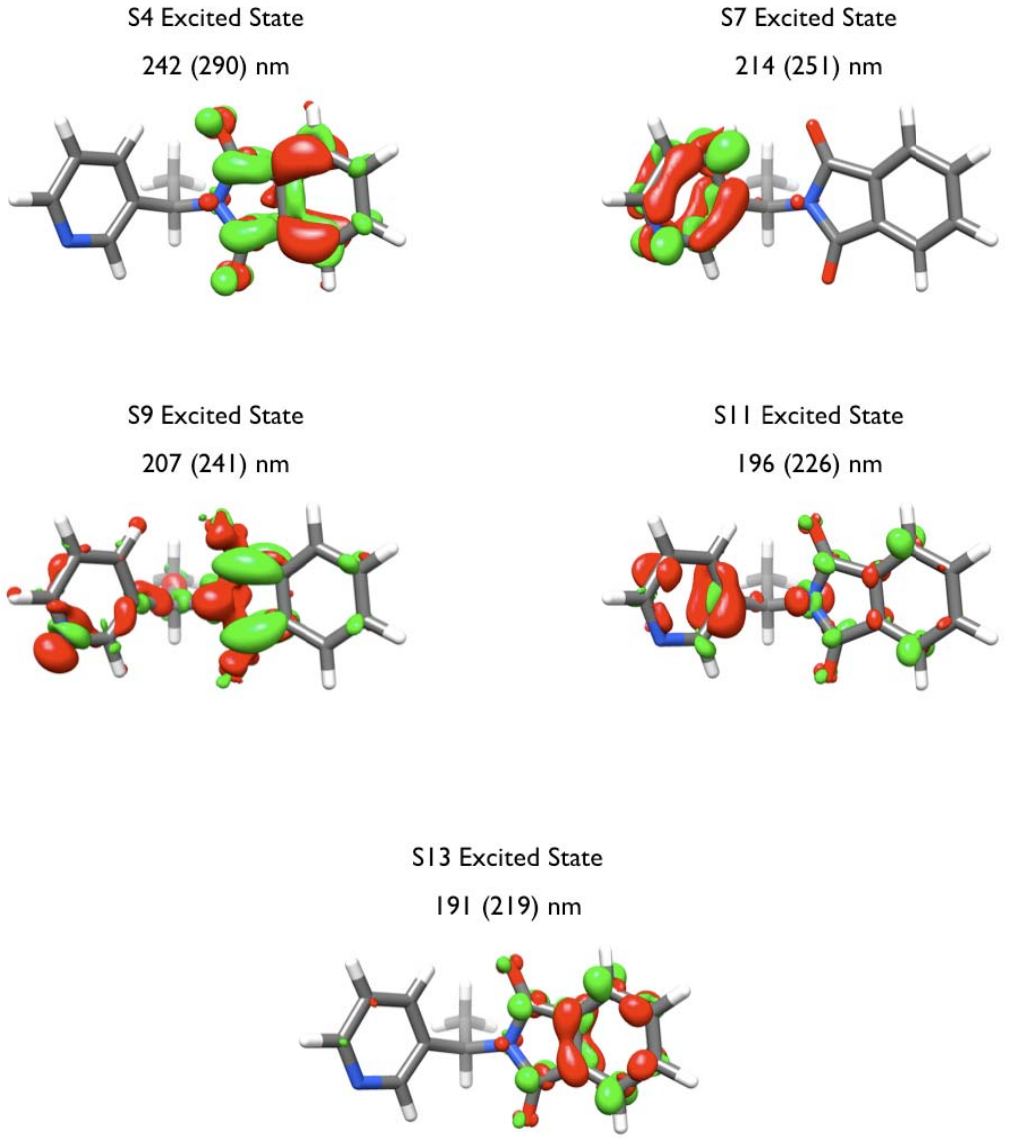


Figure S29. Electron density difference plots of (*R*)-**2**(Conformer A) as calculated by TD-B3LYP/TZVP. The contour values are ±0.002 au. Excitation energies in wavelengths are provided for each excited state before and after (in parentheses) a -0.15 eV shift was applied. Excited states with large oscillator or rotatory strengths were chosen for presenting these plots.

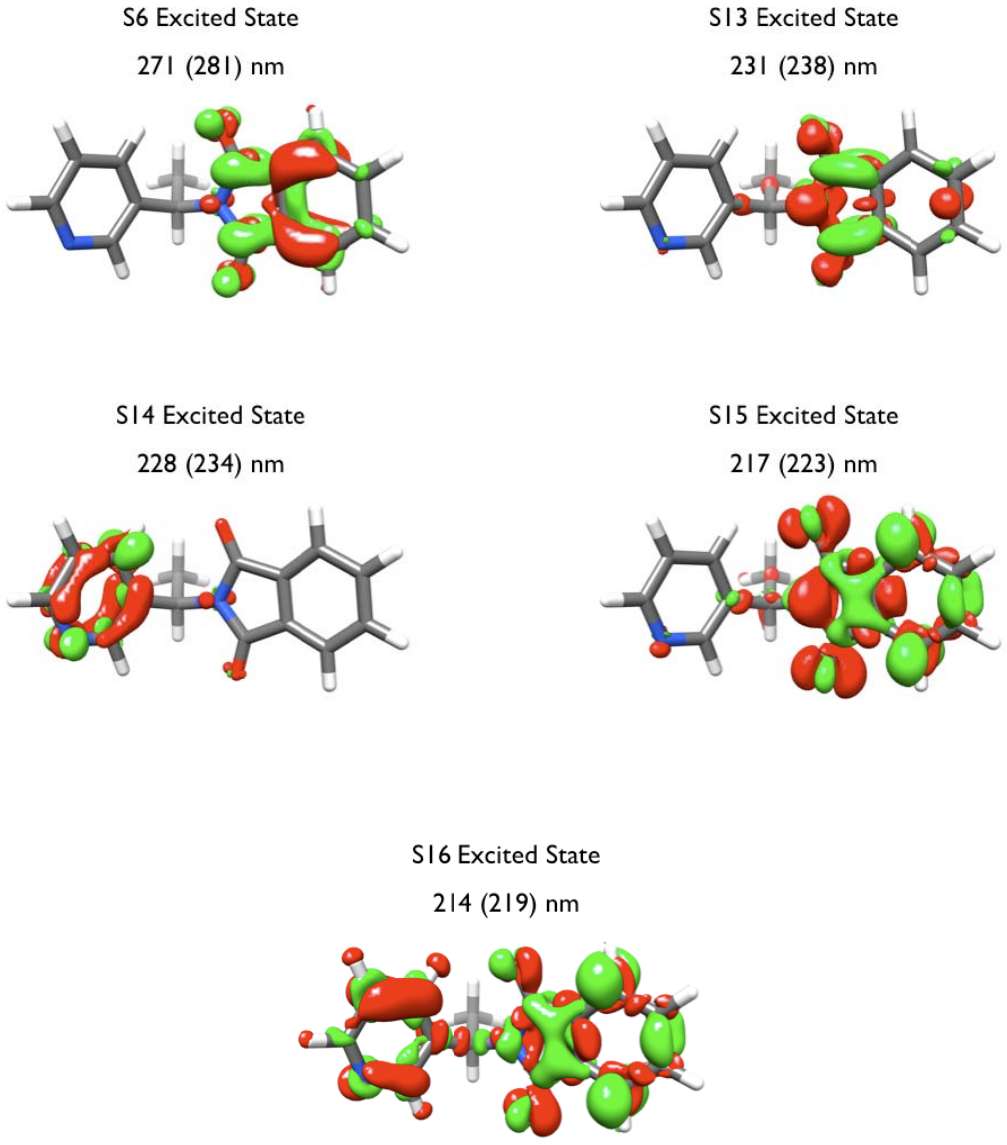


Figure S30. Electron density difference plots of (*R*)-**2**(Conformer A) as calculated by RI-CC2/TZVP. The contour values are ±0.002 au. Excitation energies in wavelengths are provided for each excited state before and after (in parentheses) a -0.6 eV shift was applied. Excited states with large oscillator or rotatory strengths were chosen for presenting these plots.

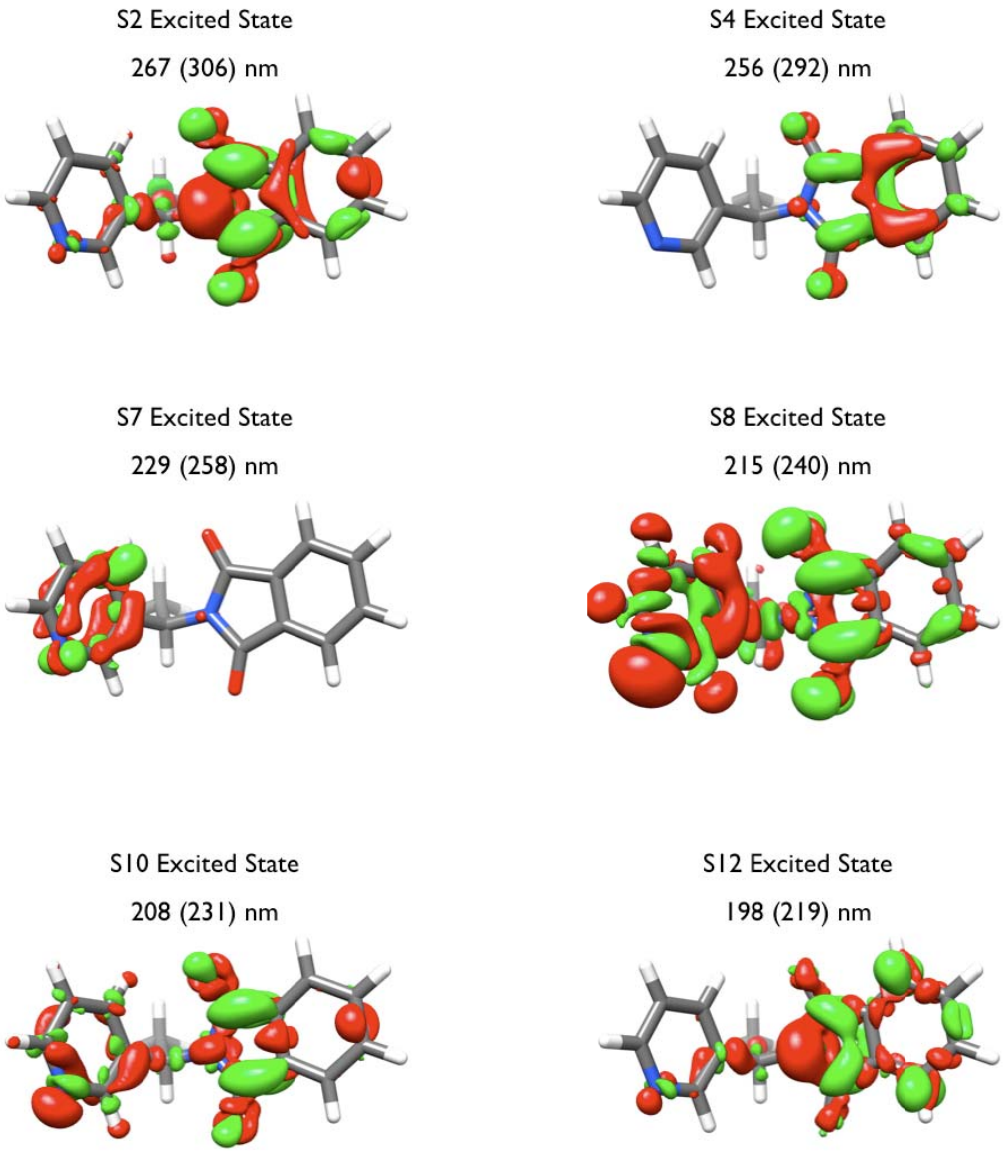
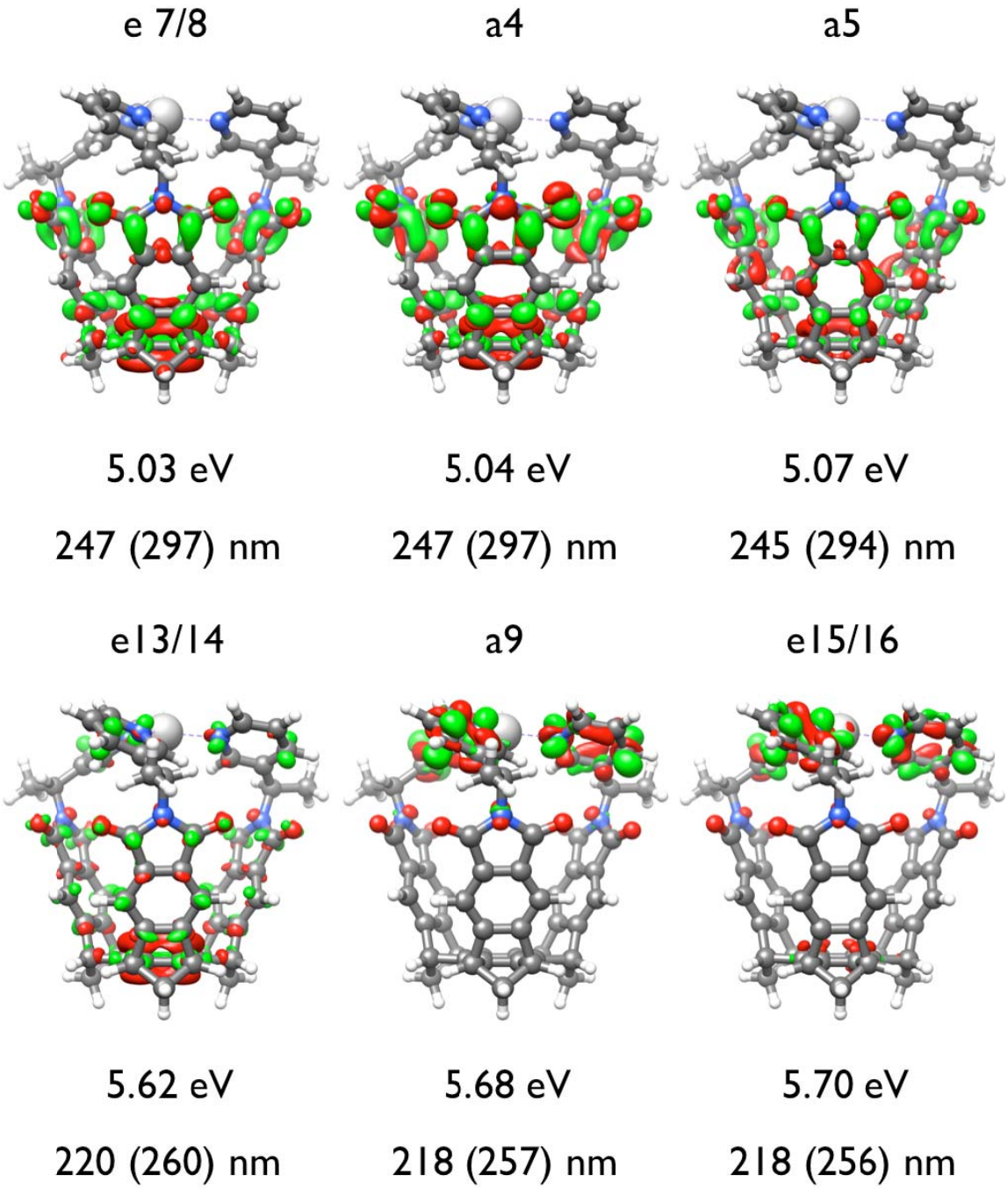
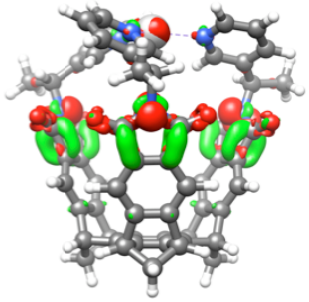


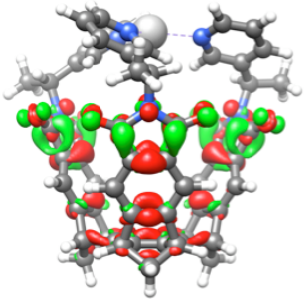
Figure S31. Electron density difference plots of Ag(I)-(R_3)-**1**(*P*) as calculated by TD-BHLYP/TZVP. The contour values are ±0.002 au. Excitation energies in wavelengths are provided for each excited state before and after (in parentheses) a -0.85 eV shift was applied. Excited states with large oscillator or rotatory strengths chosen for presenting these plots.



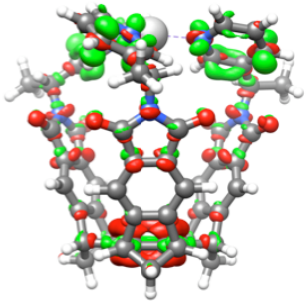
e23/24
6.01 eV
206 (240) nm



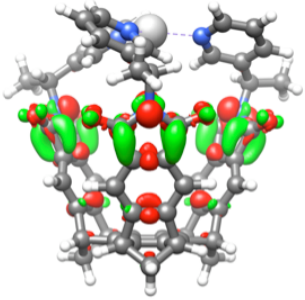
a12
6.03 eV
206 (240) nm



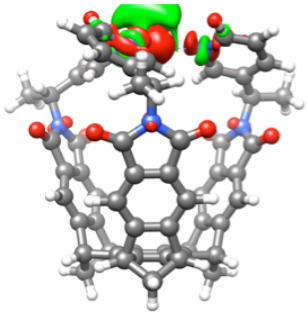
e27/28
6.08 eV
204 (237) nm



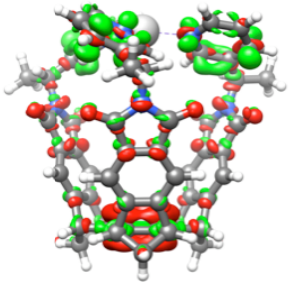
a11
6.01 eV
206 (240) nm



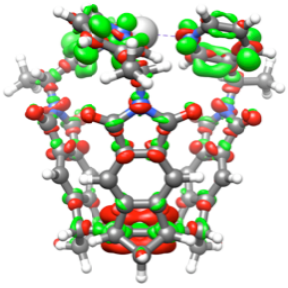
e25/26
6.04 eV
205 (239) nm



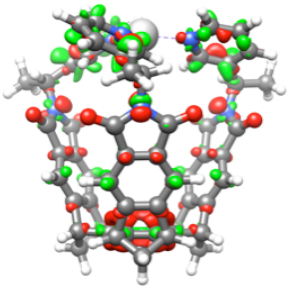
e31/32
6.21 eV
200 (232) nm



a15
6.23 eV
199 (231) nm



e33/34
6.22 eV
199 (231) nm



a16
6.24 eV
199 (230) nm

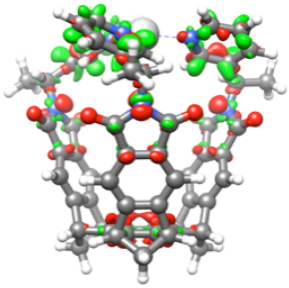
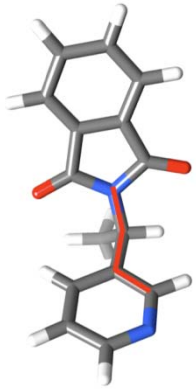
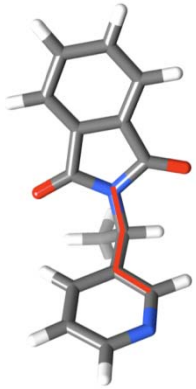


Figure S32. DFT (RI-BP86/TZVP) calculations for relaxed potential energy scan along the N-C-C-C dihedral angle (shown in red).



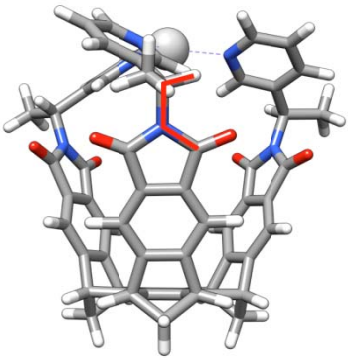
N-C-C-C Dihedral Angle (in degrees)	**RI-BP86/TZVP energies** (in hartrees)	E_{bw} **Relative Energies** (in kcal/mol)
-105 (Conformer A)	-839.1309967	0.00
-75	-839.1300471	0.60
-45	-839.1287398	1.42
-15	-839.127563	2.15
0	-839.1275033	2.19
15	-839.127659	2.09
45	-839.1286508	1.47
79 (Conformer B)	-839.1299215	0.67

Figure S33. Monte Carlo/Molecular Mechanics (MC/MM) conformational search on (*R*)-**2** using the MM3 force field. Bolded entries are the starting geometries for DFT optimization of conformations A and B, respectively. Dihedral angle is measured along the N-C-C-C torsion depicted (in red) on the structure below.



Entry ID	Potential Energy (kJ/mol)	Times Found	Relative PE (kJ/mol)	Dihedral 13-14-19-22
1	**24.57**	**1979**	**0.00**	**-92.95**
2	**25.11**	**1954**	**0.54**	**99.63**
3	32.86	3	8.29	169.91
4	33.34	8	8.76	-14.02
5	40.60	3	16.02	-117.00
6	43.07	4	18.50	68.51

Figure S34. Monte Carlo/Molecular Mechanics (MC/MM) conformational search on Ag(I)-(R_3)-**1** using the MM3 force field. The first table is the gas phase calculation and the second table is the calculation with water included as an implicit solvent. Bolded entries are the starting geometries for DFT optimization of $\mathbf{1}_{\text{three in}}$, $\mathbf{1}_{\text{two in}}$, $\mathbf{1}_{\text{one in}}$ and $\mathbf{1}_{\text{none in}}$ respectively. Dihedral is measured along the C-N-C-H torsion for each 'arm' as depicted (in red) on the structure below.



Entry ID	Potential Energy (kJ/mol)	Times Found	Relative PE (kJ/mol)	Dihedral 28-96-32-63	Dihedral 25-95-31-62	Dihedral 30-94-33-64
1	**542.23**	**145**	**0.00**	**-14.43**	**-14.51**	**-14.48**
2	**546.08**	**46**	**3.84**	**-19.24**	**-6.90**	**152.96**
3	546.21	2	3.98	-15.53	-15.13	-14.91
4	546.44	209	4.21	-9.76	-4.28	4.62
5	546.62	19	4.39	-13.37	-15.29	-15.23
6	546.68	55	4.45	-19.44	-6.93	154.68
7	547.04	4	4.80	21.29	32.36	-14.66
8	548.01	367	5.78	156.42	-13.20	2.44
9	549.02	32	6.79	163.46	-13.12	1.68
10	549.16	94	6.93	8.53	-19.45	-18.06
11	549.18	124	6.95	-6.91	5.11	7.10
12	549.44	304	7.21	0.48	173.97	-14.81
13	549.49	51	7.26	-11.92	8.04	6.27
14	550.34	20	8.10	11.05	-11.82	156.83
15	550.40	125	8.17	-18.32	-18.54	-18.21
16	550.78	270	8.55	9.47	-179.56	-7.74
17	550.80	32	8.57	11.17	-12.13	161.48
18	550.88	4	8.64	-1.20	-9.99	-1.61
19	550.94	6	8.71	22.18	22.23	22.19
20	551.63	74	9.40	2.44	-22.47	4.03
21	551.83	270	9.60	-7.34	9.37	176.37
22	553.42	267	11.18	-1.90	-178.46	5.10
23	553.43	82	11.20	-4.30	179.90	-14.62
24	553.80	26	11.56	-12.15	11.41	-23.19
25	553.96	6	11.73	3.58	-17.08	-21.60

26	554.48	66	12.25	-7.13	-22.65	-2.91
27	554.50	1	12.27	-4.60	173.28	-14.23
28	555.41	10	13.17	-3.59	-29.80	-3.01
29	555.41	81	13.18	165.78	-67.71	-12.78
30	555.47	53	13.23	-12.61	161.51	-67.82
31	555.47	1	13.24	-26.45	-16.07	7.22
32	555.62	66	13.38	15.68	-14.39	-13.88
33	555.65	1	13.42	11.66	-2.12	-18.19
34	555.68	275	13.45	-3.41	174.29	6.07
35	555.92	180	13.68	-18.47	-178.43	-28.85
36	555.99	36	13.76	-17.16	-179.14	-0.17
37	556.04	82	13.80	-18.79	-178.74	-28.63
38	556.04	129	13.80	-26.04	-28.68	-40.94
39	556.10	48	13.87	-28.47	-18.54	-178.62
40	556.13	17	13.89	13.25	-26.38	-4.80
41	556.14	9	13.91	26.58	-31.94	-5.33
42	556.31	9	14.08	-15.40	-4.96	-4.79
43	556.59	31	14.36	-19.30	-179.42	-26.81
44	556.76	11	14.53	5.87	-32.96	-5.10
45	556.78	15	14.55	-21.69	-8.24	150.18
46	557.09	1	14.85	-16.69	-0.23	177.10
47	557.25	9	15.02	-15.71	5.26	-177.88
48	557.41	1	15.17	-15.81	5.72	-177.37
49	**557.49**	**32**	**15.25**	**153.55**	**-9.98**	**-178.59**
50	557.56	19	15.33	-18.38	173.85	0.19
51	557.61	25	15.38	20.14	-24.81	1.41
52	557.62	26	15.39	-177.62	-33.97	-7.63
53	557.69	61	15.46	153.23	-15.55	-22.35
54	557.71	6	15.48	-21.05	-8.09	153.66
55	557.85	45	15.62	-179.55	-6.98	-179.19
56	557.89	21	15.66	-178.69	-12.33	-16.66
57	557.99	13	15.76	-178.83	157.40	-9.04
58	558.05	114	15.82	-177.31	-33.92	-17.02
59	558.07	137	15.83	-19.85	175.71	-27.80
60	558.08	3	15.84	-17.26	179.83	-23.64
61	558.18	36	15.94	176.14	-27.36	-20.31
62	558.27	2	16.04	-177.64	-33.71	-19.43
63	558.32	33	16.09	178.80	13.62	20.57
64	558.34	8	16.10	28.22	-36.55	-6.07
65	558.36	31	16.12	153.56	-9.54	176.30
66	558.44	115	16.21	0.56	179.73	179.77
67	558.50	9	16.27	-21.76	179.44	-20.79
68	558.55	17	16.32	2.95	-178.35	-15.63

69	558.55	13	16.32	179.56	179.89	0.61
70	558.59	23	16.36	177.35	-34.34	-7.62
71	558.60	41	16.37	-179.74	-23.28	-22.45
72	558.61	14	16.37	0.23	-30.16	4.25
73	558.80	25	16.57	167.38	-9.53	-179.55
74	558.83	44	16.59	-179.29	-6.55	175.37
75	558.90	52	16.67	179.58	1.17	179.25
76	558.91	5	16.68	176.06	159.42	-9.05
77	558.97	137	16.73	-18.42	172.64	-25.30
78	559.00	1	16.77	16.52	179.06	5.24
79	559.01	10	16.77	-15.96	4.76	173.44
80	559.02	4	16.78	-27.61	-26.68	-10.20
81	559.05	1	16.82	-15.95	-9.24	-25.38
82	559.06	9	16.82	125.91	-36.68	-7.50
83	559.09	92	16.86	172.45	-34.52	-18.72
84	559.19	1	16.96	-15.72	5.68	174.16
85	559.22	14	16.99	-179.20	173.88	-7.53
86	559.23	2	17.00	-19.88	172.81	-34.42
87	559.24	5	17.01	-23.14	-17.48	172.51
88	559.37	204	17.13	-178.56	-179.90	-21.81
89	559.42	38	17.19	13.33	19.54	174.92
90	559.48	19	17.25	165.64	-9.28	175.19
91	559.59	151	17.36	174.50	179.74	1.78
92	559.62	7	17.39	-8.77	-178.69	-2.51
93	559.70	1	17.46	172.15	-29.68	-21.14
94	559.74	6	17.51	-13.72	-41.10	-17.27
95	559.77	27	17.54	-0.24	179.06	179.51
96	559.83	107	17.60	0.94	179.58	171.71
97	559.95	27	17.71	-178.52	-15.88	157.99
98	559.99	96	17.76	0.15	179.63	179.58
99	560.05	8	17.82	-0.38	179.48	179.51
100	560.07	1	17.84	-0.33	179.32	179.49
101	560.11	19	17.88	-7.62	175.06	173.32
102	560.13	12	17.89	-0.41	179.14	179.41
103	560.14	1	17.91	14.12	-31.18	2.74
104	560.17	2	17.93	16.47	174.46	5.99
105	560.30	7	18.07	0.03	178.92	179.31
106	560.35	136	18.12	1.18	173.27	179.21
107	560.36	57	18.13	13.58	-37.32	-37.21
108	560.40	1	18.16	0.17	179.55	178.82
109	560.42	41	18.19	-178.78	-17.83	166.55
110	**560.48**	**120**	**18.25**	**179.50**	**179.67**	**179.72**
111	560.52	21	18.28	0.93	173.63	178.96

112	560.55	15	18.32	122.43	-36.58	-7.34
113	560.65	8	18.41	7.81	-33.82	2.64
114	560.72	162	18.48	-178.89	173.63	-21.62
115	560.72	114	18.49	171.88	0.92	174.19
116	560.76	24	18.53	173.20	-20.80	-179.05
117	560.78	10	18.55	-15.56	1.95	174.57
118	560.79	88	18.56	1.16	179.55	171.50
119	560.82	23	18.59	-39.94	-13.49	-34.24
120	560.91	148	18.68	179.87	-22.75	175.58
121	561.02	42	18.79	-18.70	-179.84	179.58
122	561.07	120	18.84	171.47	-0.23	179.32
123	561.13	54	18.90	179.83	179.30	-18.27
124	561.14	11	18.91	20.31	-13.60	148.34
125	561.16	7	18.93	-6.48	-7.77	-179.10
126	561.30	188	19.07	172.27	179.51	179.46
127	561.35	104	19.12	0.90	173.09	171.79
128	561.39	16	19.15	175.41	-16.28	158.14
129	561.43	26	19.20	179.57	179.17	171.90
130	561.43	14	19.20	179.43	179.40	171.65
131	561.46	24	19.22	172.03	179.68	179.90
132	561.47	1	19.24	138.98	-36.40	-7.85
133	561.49	37	19.26	179.70	-21.67	174.37
134	561.54	1	19.31	-1.45	-10.50	176.12
135	561.56	21	19.32	179.06	179.27	171.61
136	561.56	1	19.33	179.35	171.68	179.18
137	561.57	24	19.33	0.20	172.44	171.99
138	561.57	29	19.33	0.35	172.29	170.82
139	561.57	12	19.34	179.65	179.70	171.57
140	561.57	1	19.34	179.39	179.64	171.69
141	561.60	72	19.37	-17.17	179.22	179.39
142	561.72	31	19.49	-30.07	-32.02	-44.75
143	561.73	9	19.49	30.28	-37.46	-1.09
144	561.73	5	19.50	-44.55	-26.43	-22.49
145	561.78	11	19.55	19.82	-13.67	149.84
146	561.78	20	19.55	175.81	-18.44	168.10
147	561.97	12	19.73	29.56	-5.08	-2.31
148	561.98	8	19.74	-14.81	179.08	179.49
149	562.14	199	19.90	171.85	179.05	171.55
150	562.15	15	19.91	-179.54	-40.30	-36.24
151	562.16	59	19.92	179.73	172.21	171.62
152	562.28	16	20.04	179.32	171.67	171.75
153	562.28	5	20.05	179.21	172.02	172.05
154	562.28	3	20.05	179.20	171.73	171.68

155	562.29	71	20.06	-17.81	-179.95	171.43
156	562.32	101	20.09	-20.28	172.67	179.63
157	562.38	132	20.15	-22.18	175.53	173.30
158	562.40	5	20.16	-21.93	175.21	172.65
159	562.44	9	20.20	12.95	-34.15	-7.74
160	562.46	3	20.23	-21.11	-23.81	173.09
161	562.47	4	20.24	46.80	-36.91	-5.75
162	562.56	32	20.33	179.30	-18.49	172.07
163	562.63	2	20.39	173.14	-22.23	175.36
164	562.64	17	20.40	175.78	172.15	-21.62
165	562.65	55	20.41	-16.49	179.85	171.74
166	562.73	13	20.50	-6.07	-8.63	174.58
167	562.94	46	20.71	-39.43	179.08	-35.94
168	562.98	73	20.75	171.71	172.08	172.46
169	563.38	12	21.15	172.11	-20.31	172.74
170	563.49	19	21.26	-17.84	-10.26	-69.33
171	563.49	15	21.26	-36.40	173.99	-40.05
172	563.55	102	21.32	170.74	-17.44	172.31
173	563.55	7	21.32	-9.90	-32.54	-10.90
174	563.61	1	21.38	-15.79	172.36	171.56
175	563.69	2	21.46	-16.89	-4.89	-71.86
176	563.79	25	21.55	-38.53	-37.51	173.18
177	563.82	1	21.59	28.42	-36.74	-7.56
178	563.87	5	21.64	173.06	-36.95	-38.68
179	563.93	11	21.70	-14.75	13.21	-86.90
180	564.07	1	21.84	-6.38	-34.31	-12.41
181	564.82	21	22.58	-16.53	1.28	-66.64
182	565.11	3	22.88	1.48	-29.44	175.73
183	565.39	2	23.16	48.98	-37.10	-1.93
184	565.57	7	23.34	10.47	-13.78	-67.33
185	565.88	2	23.64	-2.84	-28.64	141.41
186	566.59	1	24.36	-1.13	-19.04	-61.82
187	566.70	5	24.47	-3.56	-28.50	141.55
188	567.06	1	24.83	178.88	-26.39	175.32
189	567.23	1	24.99	-71.30	-57.34	-30.94
190	567.38	1	25.15	34.34	-11.26	-16.09
191	567.72	9	25.49	29.84	-10.21	-20.51
192	567.75	13	25.52	13.67	-7.83	-67.84
193	568.00	1	25.77	22.09	-52.15	-24.42
194	569.87	8	27.63	19.61	1.78	-77.24
195	570.12	3	27.89	-14.84	-35.44	-13.95
196	570.15	8	27.92	-0.45	-36.10	-3.13
197	570.86	9	28.63	-18.75	-33.25	-14.99

198	572.48	7	30.25	-22.08	-16.19	-80.17
199	572.64	13	30.40	-178.34	-21.02	-61.77
200	573.74	10	31.50	175.90	-21.59	-60.36
201	574.41	4	32.18	-176.79	-30.23	-55.09
202	574.63	5	32.40	17.64	-9.88	-72.60
203	574.90	1	32.67	1.40	-30.02	-41.91
204	577.08	1	34.85	-9.35	-12.80	-76.94
205	577.66	2	35.43	2.63	-37.24	-66.28
206	577.84	19	35.60	-13.53	-16.05	-80.55
207	580.30	1	38.07	6.87	-27.67	-62.29

Entry ID	Potential Energy (kJ/mol)	Times Found	Relative PE (kJ/mol)	Dihedral 28-96-32-63	Dihedral 25-95-31-62	Dihedral 30-94-33-64
1	**463.34**	**108**	**0.00**	**2.79**	**2.38**	**4.51**
2	463.36	279	0.02	7.74	6.98	2.40
3	**465.02**	**264**	**1.68**	**7.96**	**-171.55**	**-1.04**
4	465.04	10	1.70	-171.54	-1.46	8.14
5	465.04	17	1.71	-171.60	-1.17	8.10
6	465.07	7	1.73	-171.71	-0.92	8.18
7	465.11	349	1.77	10.84	-171.96	-3.87
8	465.13	1	1.79	-3.68	10.93	-172.16
9	465.23	1	1.89	10.46	-172.76	-3.79
10	465.30	72	1.96	6.86	-172.68	-0.04
11	465.43	379	2.09	9.20	-172.38	1.50
12	465.46	23	2.12	9.11	-172.81	1.31
13	465.78	19	2.45	-173.45	-1.77	8.47
14	465.79	148	2.45	7.65	-173.99	-1.36
15	465.81	98	2.47	-174.52	-0.88	8.50
16	465.81	1	2.47	-174.13	-1.66	8.22
17	465.81	16	2.48	-0.74	8.03	-173.67
18	465.83	7	2.49	-0.96	7.72	-174.23
19	465.90	335	2.57	10.85	-174.27	-3.84
20	466.01	4	2.67	-174.86	-3.64	10.27
21	466.07	146	2.73	-8.36	3.41	5.41
22	466.10	62	2.76	5.46	-9.36	3.68
23	466.11	25	2.77	-6.99	3.52	4.94
24	466.12	4	2.79	3.34	4.52	-5.89
25	466.13	5	2.79	4.70	4.62	-5.14
26	466.14	1	2.80	3.36	5.17	-6.87
27	466.15	328	2.81	0.43	9.49	-174.98
28	466.17	3	2.83	3.29	4.34	-5.50
29	466.18	3	2.84	-175.33	0.85	9.30

30	466.21	1	2.87	-175.19	0.73	9.05
31	466.23	5	2.89	-11.99	-11.66	-11.64
32	466.28	52	2.94	2.75	2.96	-15.36
33	466.46	72	3.12	-17.29	2.75	3.96
34	466.89	2	3.55	2.78	8.71	-24.31
35	467.14	54	3.80	-20.80	5.02	-0.85
36	467.14	1	3.81	7.00	-26.26	3.11
37	467.30	184	3.96	7.74	-171.90	-18.41
38	467.32	23	3.98	7.79	-172.05	-17.73
39	467.36	26	4.02	-20.33	4.88	-2.57
40	467.56	46	4.22	-15.03	-17.70	3.33
41	467.73	8	4.39	-15.77	2.90	-12.37
42	467.95	45	4.61	-15.98	5.82	2.19
43	468.03	149	4.69	8.25	-173.98	-17.89
44	468.05	33	4.71	8.34	-175.01	-17.71
45	468.12	19	4.78	7.93	-174.45	-16.67
46	468.13	64	4.79	5.07	-173.98	-16.59
47	468.26	3	4.93	-15.47	7.72	-11.67
48	468.44	17	5.10	11.59	-169.79	-27.79
49	468.44	27	5.11	-15.64	6.59	-175.06
50	468.48	3	5.14	2.48	3.33	-174.40
51	468.60	48	5.26	-12.13	-172.88	0.25
52	**468.75**	**19**	**5.42**	**-172.70**	**-172.60**	**-3.85**
53	468.89	15	5.55	6.60	-171.31	-36.45
54	469.09	44	5.75	-10.96	3.97	-174.23
55	469.09	102	5.75	-172.84	-173.31	-0.12
56	469.15	1	5.81	-176.79	2.49	3.19
57	469.24	70	5.90	0.85	-173.28	-172.65
58	469.32	47	5.98	-12.56	-175.26	0.52
59	469.35	13	6.01	11.08	-173.27	-29.69
60	469.40	17	6.06	-172.70	-175.12	-4.57
61	469.40	14	6.06	6.98	-23.59	-15.22
62	469.46	33	6.12	-11.72	5.28	-176.44
63	469.47	49	6.13	4.46	-172.91	-172.86
64	469.50	13	6.17	-173.16	-2.78	-174.97
65	469.51	103	6.18	3.54	-173.57	-173.18
66	469.53	124	6.19	-10.82	-10.28	-8.58
67	469.57	47	6.23	-8.96	-172.64	-39.67
68	469.69	10	6.35	-35.98	7.25	-173.73
69	469.71	2	6.37	20.82	20.63	21.34
70	469.74	23	6.40	-2.54	-174.64	-171.97
71	469.77	24	6.43	-173.50	8.19	13.60
72	469.78	1	6.44	1.11	-171.85	-37.68

73	469.80	69	6.46	-1.18	-173.80	-175.06
74	469.83	27	6.49	-173.78	4.18	-173.85
75	469.87	47	6.53	8.28	-173.00	-0.04
76	469.87	22	6.53	11.72	-174.42	5.89
77	469.88	108	6.54	0.90	-175.01	-172.90
78	469.93	31	6.59	2.95	-174.43	-173.14
79	469.93	59	6.59	-173.03	2.81	-175.02
80	469.97	80	6.63	0.94	-173.37	-174.96
81	470.01	26	6.67	-176.15	-172.70	1.72
82	470.02	82	6.68	-175.22	3.43	-173.02
83	470.08	42	6.74	-174.94	-173.91	5.38
84	470.08	17	6.74	-174.56	-173.93	5.86
85	470.10	36	6.76	3.94	-176.52	-10.01
86	470.10	72	6.76	-174.41	5.56	-174.25
87	470.15	54	6.81	-173.56	8.39	-172.99
88	470.17	22	6.83	-11.14	-16.89	-0.35
89	470.17	43	6.83	-9.06	-175.00	-39.62
90	470.17	15	6.83	-173.69	8.03	-173.38
91	470.18	73	6.84	3.19	-176.54	-173.12
92	470.20	16	6.86	-174.66	-175.05	-3.79
93	470.20	13	6.86	-173.20	-173.59	7.72
94	470.27	44	6.93	-173.51	-174.91	4.39
95	470.28	58	6.94	1.96	-174.43	-7.74
96	470.38	30	7.04	-12.75	-173.05	-0.16
97	470.41	8	7.07	-173.31	-0.15	-12.71
98	470.42	14	7.08	5.25	-174.63	-173.94
99	470.42	10	7.08	3.25	12.55	-175.28
100	470.42	8	7.09	0.06	-13.34	-173.16
101	470.44	8	7.10	-174.75	-173.82	-2.57
102	470.45	3	7.11	1.66	-174.32	-38.62
103	470.45	19	7.11	13.05	-175.98	6.42
104	470.56	33	7.22	-26.52	-16.26	0.78
105	470.59	72	7.25	-174.52	2.28	-174.70
106	470.61	3	7.27	-8.98	4.96	-176.50
107	470.61	107	7.27	-176.01	-175.55	2.19
108	470.61	83	7.28	-176.62	5.31	-173.41
109	470.62	7	7.29	-173.88	5.83	-175.03
110	470.69	1	7.35	-176.32	-9.06	2.94
111	470.70	8	7.36	-20.44	-9.28	0.56
112	470.75	34	7.42	-173.72	5.58	-174.33
113	470.82	61	7.48	5.56	-177.24	-173.70
114	470.82	49	7.48	-176.18	7.48	-173.53
115	470.83	78	7.49	7.24	-176.17	-173.82

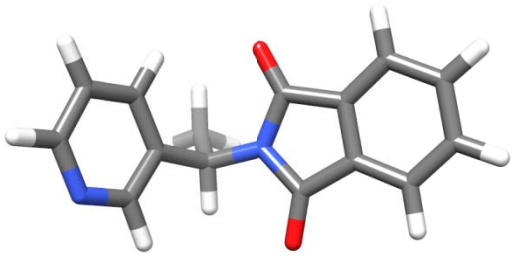
116	470.84	30	7.50	-174.52	-176.22	5.38
117	470.85	42	7.51	-173.80	6.19	-174.25
118	470.88	30	7.54	1.34	-176.14	-174.96
119	470.88	10	7.54	-4.46	3.65	-22.14
120	470.90	5	7.56	-173.77	5.61	-174.71
121	470.97	3	7.63	-11.58	-172.49	-11.78
122	470.97	30	7.63	8.18	-174.63	6.10
123	470.99	9	7.65	-176.40	8.09	-173.88
124	470.99	10	7.65	-174.05	5.16	-174.03
125	471.02	38	7.68	-175.90	7.54	-173.94
126	471.06	9	7.72	8.65	163.09	-0.52
127	471.07	65	7.73	-173.70	6.42	-176.63
128	471.09	14	7.75	-173.91	6.36	-173.92
129	471.09	29	7.75	-13.13	-174.61	-0.03
130	471.09	4	7.75	-175.56	3.97	-176.56
131	471.09	64	7.76	-175.95	3.17	-176.46
132	471.10	12	7.76	-177.21	6.49	9.02
133	471.12	15	7.78	5.78	-173.75	-1.70
134	471.12	3	7.78	5.78	-174.32	-173.77
135	471.16	1	7.82	-174.34	-173.83	5.60
136	471.16	25	7.82	-11.46	-172.96	-25.01
137	471.16	6	7.82	0.46	-14.36	-174.88
138	471.18	11	7.84	-173.90	5.02	-174.17
139	471.24	9	7.90	10.31	162.99	-2.77
140	471.24	54	7.90	4.81	-176.87	-174.58
141	471.26	1	7.92	-174.16	6.57	-174.11
142	471.26	6	7.92	-7.09	1.42	-175.91
143	471.26	3	7.93	0.73	-19.03	-19.64
144	471.31	1	7.97	-174.15	-173.88	6.37
145	471.35	10	8.01	8.91	161.31	1.74
146	471.36	7	8.02	5.73	-174.28	-176.90
147	471.43	4	8.09	-174.39	-175.87	6.59
148	471.44	26	8.10	-173.70	4.21	-176.67
149	471.44	13	8.10	-177.09	5.24	-176.70
150	471.44	8	8.10	-12.33	-12.62	-174.67
151	471.46	67	8.12	-174.28	6.94	-176.48
152	471.46	4	8.12	-173.63	-6.10	-18.68
153	471.49	1	8.15	-176.10	5.32	-26.41
154	471.51	120	8.17	-174.31	-176.46	5.19
155	471.58	21	8.25	3.96	8.03	-173.79
156	471.60	64	8.26	-176.56	5.73	-177.33
157	471.67	66	8.33	-173.55	5.24	-174.13
158	471.67	1	8.34	-173.91	5.17	-174.09

159	471.68	68	8.34	-177.14	-173.85	5.40
160	471.68	11	8.34	-174.27	-173.60	5.29
161	471.75	23	8.41	-173.90	-176.06	6.38
162	471.82	1	8.49	-173.46	5.38	-174.30
163	471.88	26	8.54	-11.64	-174.99	-24.82
164	471.90	1	8.56	-174.06	6.53	-174.29
165	471.90	60	8.56	6.34	-176.81	1.05
166	471.90	51	8.56	-173.92	4.76	-176.77
167	471.94	4	8.60	-173.67	4.89	-174.14
168	471.96	2	8.62	3.08	-25.07	-26.80
169	471.99	7	8.65	-173.98	6.06	-176.85
170	471.99	2	8.65	4.41	8.21	-174.22
171	472.02	7	8.69	-175.40	-6.36	-18.62
172	472.07	69	8.73	5.49	-174.35	-176.42
173	472.15	10	8.81	-0.46	-21.18	-173.69
174	472.18	11	8.84	-176.33	5.29	-176.87
175	**472.18**	**132**	**8.84**	**-173.75**	**-173.95**	**-173.69**
176	472.20	23	8.86	-176.61	5.12	8.31
177	472.20	49	8.86	5.38	-174.11	-176.56
178	472.27	46	8.93	-176.41	5.42	-177.03
179	472.34	54	9.00	-176.70	4.70	-175.64
180	472.34	2	9.00	5.79	-174.61	-176.31
181	472.40	23	9.06	-174.21	5.43	-176.49
182	472.40	7	9.07	-176.05	5.87	-176.72
183	472.42	25	9.08	6.22	-28.82	-38.04
184	472.50	4	9.16	-177.07	3.95	7.27
185	472.58	2	9.25	5.60	-174.43	-175.80
186	472.60	13	9.27	-176.36	-2.79	-17.97
187	472.63	4	9.29	-176.28	6.34	-177.03
188	472.67	8	9.33	-176.27	6.44	-177.08
189	472.68	10	9.35	-12.48	-15.86	-172.92
190	472.81	1	9.47	6.60	-23.15	-29.95
191	472.82	9	9.48	-176.43	4.54	-176.64
192	472.83	192	9.49	-173.78	-176.75	-173.78
193	472.83	57	9.49	-173.79	-176.32	-173.50
194	472.85	3	9.51	-15.14	-12.99	-17.64
195	472.85	34	9.51	-173.61	-176.14	-174.16
196	472.85	1	9.51	-13.82	-173.00	-20.23
197	472.85	19	9.51	-5.40	-18.11	-31.53
198	472.86	3	9.52	-173.69	-176.07	-173.80
199	472.87	24	9.53	-176.40	-173.66	-173.68
200	472.87	7	9.53	-173.59	-176.63	-174.15
201	472.91	2	9.57	14.50	14.60	14.40

202	472.94	1	9.60	6.44	-174.28	-176.85
203	472.94	33	9.60	5.79	-176.85	-176.22
204	472.99	1	9.65	-176.42	5.93	-176.45
205	473.04	12	9.70	-176.61	5.80	-176.56
206	473.15	30	9.81	3.06	1.00	1.06
207	473.16	4	9.82	8.87	162.47	-16.49
208	473.39	11	10.05	-174.64	-11.95	-15.91
209	473.42	9	10.08	6.77	6.73	7.03
210	473.47	124	10.13	-176.07	-173.97	-176.35
211	473.49	136	10.15	-173.72	-176.09	-176.27
212	473.50	16	10.17	-176.55	-173.05	-176.42
213	473.51	20	10.17	-174.27	-176.41	-176.22
214	473.51	6	10.17	-173.91	-176.46	-176.37
215	473.58	1	10.24	-13.92	-175.05	-19.45
216	473.61	1	10.27	-28.40	-172.96	-15.24
217	473.70	5	10.37	-13.93	6.86	159.18
218	473.86	22	10.53	-173.35	-44.38	-33.71
219	473.91	3	10.57	-39.42	-33.86	-172.06
220	474.12	1	10.78	-172.77	160.38	-7.46
221	474.14	79	10.80	-176.33	-175.86	-175.95
222	474.54	1	11.20	-175.50	-15.59	-25.63
223	474.55	28	11.22	-175.97	-44.41	-33.55
224	474.68	25	11.34	-20.13	-41.74	-32.40
225	474.75	9	11.41	-173.90	-37.51	-33.85
226	474.88	4	11.54	7.92	163.62	-39.64
227	474.97	6	11.63	-173.57	-20.82	-173.50
228	475.07	4	11.73	-32.66	-34.74	-172.30
229	475.22	1	11.89	10.19	162.66	-39.64
230	475.26	1	11.93	167.73	-63.88	-14.32
231	475.38	2	12.04	4.17	157.27	-173.80
232	475.40	3	12.06	175.01	-60.83	-17.29
233	475.64	4	12.30	-30.98	-36.91	-172.71
234	475.65	9	12.31	-19.33	-175.41	-173.72
235	475.68	6	12.34	-173.64	-176.44	-18.40
236	475.89	1	12.55	-173.39	-45.96	-13.65
237	476.08	1	12.74	-174.65	-32.92	-35.96
238	476.16	3	12.82	-175.37	4.46	160.60
239	476.37	7	13.03	-176.21	-19.88	-175.50
240	476.63	2	13.29	-175.30	-46.55	-13.01
241	476.85	6	13.51	-175.03	-26.17	-37.81
242	476.92	9	13.58	-173.53	-23.95	-39.52
243	477.40	2	14.06	160.17	-25.65	-12.54
244	477.72	2	14.38	-24.91	-40.04	-176.22

245	482.08	1	18.74	-52.23	-51.46	-51.34
246	488.54	1	25.20	-176.69	-100.36	-176.22
247	491.46	18	28.12	-62.32	-62.10	-62.37

(*R*)-2 Conformer A



BHLYP/TZVP

Cartesian Coordinates

H	2.310333	3.517727	0.736446
C	1.244333	3.415727	0.648446
C	-1.549666	3.121727	0.410446
C	0.679333	2.264727	0.158446
C	0.381333	4.434727	1.025446
C	-0.991666	4.289727	0.908446
C	-0.686666	2.121727	0.039446
H	0.782333	5.351727	1.416446
H	-1.633666	5.097727	1.209446
H	-2.613666	2.999727	0.315446
C	1.315333	1.015727	-0.327553
C	-0.966666	0.772727	-0.515553
C	0.165333	-2.241272	-0.231553
C	-0.259666	-4.212272	1.587446
C	-1.135666	-2.628272	0.049446
C	1.181333	-2.899272	0.442446
N	0.986333	-3.860272	1.329446
C	-1.350666	-3.626272	0.974446
H	-1.963666	-2.144272	-0.434553
H	2.209333	-2.631272	0.254446
H	-2.346666	-3.948272	1.219446
H	-0.392666	-4.996272	2.313446
N	0.270333	0.176727	-0.712553
O	2.476333	0.747727	-0.395553
O	-2.030666	0.280727	-0.750553
C	0.517333	-1.169272	-1.235553
H	1.591333	-1.193272	-1.359553
C	-0.124666	-1.366272	-2.599553
H	0.222333	-0.605272	-3.288553
H	-1.202666	-1.318272	-2.549553

H 0.161333 -2.336272 -2.990553

Excited State Data (before shifting)

Excitation Energy (in eV)	**Oscillator Strength**	**Rotatory Strength**
4.6791	0.0001	0.2012
4.8547	0.0018	-1.1109
5.0837	0.0003	-3.6322
5.1271	0.0426	1.6752
5.3232	0.0069	-6.3887
5.6550	0.0096	5.9661
5.7944	0.0622	-15.2421
5.9561	0.0037	0.8772
6.0053	0.0725	15.1353
6.3298	0.0048	0.0418
6.3449	0.4465	-59.6907
6.4039	0.0195	-12.7558
6.5061	0.5008	57.9120
6.7478	0.3287	32.4555
6.8082	0.0250	-2.5257
6.9720	0.0001	0.1299
7.1638	0.0147	4.1275
7.3571	0.0237	26.5557
7.4636	0.1666	32.0666
7.5483	0.3759	-9.6242
7.5696	0.1881	-75.9366
7.6671	0.2950	-1.0240
7.7408	0.0400	33.4744
7.8323	0.0008	0.2833
7.9217	0.0263	-11.1293
8.0972	0.0015	1.7164
8.1764	0.0052	2.4097
8.2033	0.0023	2.3471
8.2432	0.0194	-11.3434
8.2665	0.0915	14.4903
8.2813	0.0006	1.5094
8.3981	0.0309	11.2030
8.4572	0.0030	5.8995
8.5262	0.1040	14.3298
8.5554	0.0121	-6.0990
8.5884	0.0843	-27.4202
8.6018	0.0264	4.1249
8.6044	0.0039	-7.6869
8.6259	0.0315	11.3622

8.6314	0.0098	7.4081
8.6555	0.0024	6.7562
8.6782	0.0129	-13.8524
8.7221	0.0017	-1.9604
8.7352	0.0005	1.2856
8.8820	0.0022	0.4754
8.8940	0.0031	-5.8743
8.9054	0.0061	0.7177
8.9675	0.0020	10.8179
9.0600	0.0023	-3.7342
9.0763	0.0011	0.5964

Energies and Thermochemistry

E_{bw}	-838.5863034
ZPE (kJ/mol)	657.6
ln(qtrans)	18.9
ln(qrot)	15.26
ln(qvib)	11.67
chem. pot. (kJ/mol)	543.94
energy (kJ/mol)	695.95
entropy (kJ/mol/K)	0.51815
Cv (kJ/mol-K)	0.2375339
Cp (kJ/mol-K)	0.2458482
E_{bw} + ZPE	-838.335837
H_{298}	-838.320286
G_{298}	-838.3791267

B3LYP/TZVP

Cartesian Coordinates

H	2.331257	3.542848	0.726696
C	1.256257	3.441848	0.645696
C	-1.557742	3.149848	0.421696
C	0.685257	2.281848	0.155696
C	0.392257	4.469848	1.028696
C	-0.991742	4.326848	0.918696
C	-0.693742	2.138848	0.043696
H	0.800257	5.394848	1.419696
H	-1.635742	5.141848	1.224696
H	-2.629742	3.028848	0.332696
C	1.323257	1.025848	-0.334303
C	-0.983742	0.782848	-0.510303
C	0.164257	-2.260151	-0.234303
C	-0.251742	-4.249151	1.598696

C	-1.143742	-2.658151	0.047696
C	1.193257	-2.915151	0.445696
N	1.005257	-3.886151	1.340696
C	-1.353742	-3.666151	0.979696
H	-1.980742	-2.177151	-0.440303
H	2.227257	-2.638151	0.255696
H	-2.355742	-3.997151	1.224696
H	-0.383742	-5.040151	2.329696
N	0.264257	0.177848	-0.716303
O	2.498257	0.753848	-0.410303
O	-2.063742	0.286848	-0.741303
C	0.512257	-1.179151	-1.245303
H	1.595257	-1.199151	-1.370303
C	-0.131742	-1.378151	-2.621303
H	0.215257	-0.609151	-3.313303
H	-1.218742	-1.333151	-2.573303
H	0.159257	-2.352151	-3.017303

Excited State Data (before shifting)

Excitation Energy (in eV)	**Oscillator Strength**	**Rotatory Strength**
3.8323	0.0004	6.5092
3.9309	0.0005	-11.2603
4.0474	0.0000	0.6910
4.2687	0.0005	-0.3470
4.4721	0.0012	3.0959
4.5719	0.0386	-2.7396
4.7419	0.0103	-10.7812
4.8462	0.0006	-2.5955
4.9633	0.0124	11.5851
5.1479	0.0240	-0.2025
5.2365	0.0495	-0.1290
5.3388	0.0023	4.0363
5.3628	0.1034	-16.6283
5.4516	0.0564	26.5045
5.7284	0.2210	-18.6737
5.8069	0.1867	14.9286
6.0431	0.0108	-0.1958
6.0648	0.1373	-20.7843
6.0746	0.0618	-7.4431
6.0986	0.0749	7.0068
6.1816	0.1085	-59.6589
6.2072	0.0334	77.7830
6.4075	0.0012	0.2422
6.4579	0.0010	1.0572

6.4644	0.0052	-6.3067
6.5017	0.0007	2.4155
6.5892	0.0075	-1.9350
6.6621	0.0155	14.2629
6.7711	0.0000	-0.0627
6.8115	0.0039	3.7600
6.8696	0.0209	29.7762
6.9226	0.0739	11.6117
6.9744	0.0611	-14.7727
7.0053	0.0220	5.7380
7.0461	0.0027	-14.2232
7.1165	0.0016	1.5384
7.1940	0.2285	-46.7765
7.2449	0.0778	76.8140
7.2823	0.2610	71.8557
7.3018	0.1489	-80.3253
7.3883	0.0581	-10.6017
7.4439	0.1461	-72.2161
7.5453	0.0552	33.0623
7.5495	0.0059	8.3038
7.5535	0.0801	-50.3610
7.5616	0.2019	12.4857
7.6183	0.0753	18.4543
7.6578	0.0078	-5.2710
7.6811	0.0073	-1.8462
7.7340	0.0003	-2.1825

Energies and Thermochemistry

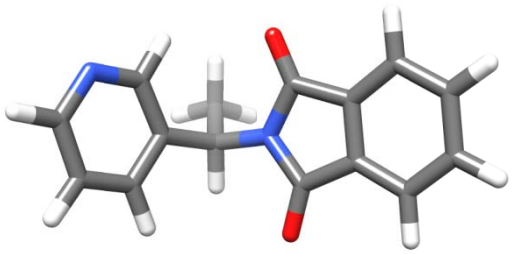
E_{bw}	-838.5946339
ZPE (kJ/mol)	632.4
ln(qtrans)	18.9
ln(qrot)	15.29
ln(qvib)	12.26
chem. pot. (kJ/mol)	517.27
energy (kJ/mol)	672.23
entropy (kJ/mol/K)	0.52807
Cv (kJ/mol-K)	0.2476201
Cp (kJ/mol-K)	0.2559344
E_{bw} + ZPE	-838.3537655
H_{298}	-838.3376509
G_{298}	-838.3976182

RI-CC2/TZVP//BHLYP/TZVP

Excited State Data (before shifting)

Excitation Energy (in eV)	Oscillator Strength
4.2566	0.0001
4.6555	0.0113
4.8262	0.0002
4.8559	0.0128
5.0604	0.0079
5.3087	0.0007
5.4175	0.0340
5.7692	0.0360
5.8681	0.0013
5.9668	0.1380
6.1508	0.0221
6.2645	0.7359
6.3604	0.0044
6.6547	0.2680
6.8261	0.0484
6.8548	0.0444
6.8708	0.1899
7.1015	0.0027
7.1697	0.0046
7.3602	0.0288

(*R*)-2 Conformer B



BHLYP/TZVP

Cartesian Coordinates

H	2.324348	3.493075	0.640734
C	1.255348	3.394075	0.597734
C	-1.546651	3.106075	0.477734
C	0.668348	2.249075	0.119734
C	0.412348	4.409075	1.022734
C	-0.965651	4.268075	0.963734
C	-0.701651	2.109075	0.058734

H	0.831348	5.322075	1.405734
H	-1.592651	5.073075	1.301734
H	-2.613651	2.986075	0.428734
C	1.280348	1.003075	-0.404265
C	-1.008651	0.766075	-0.496265
C	0.196348	-2.232924	-0.242265
C	-0.268651	-4.145924	1.625734
C	1.267348	-2.806924	0.417734
C	-1.073651	-2.676924	0.097734
N	-1.305651	-3.607924	1.006734
C	1.036348	-3.779924	1.368734
H	2.271348	-2.492924	0.190734
H	-1.940651	-2.253924	-0.376265
H	1.848348	-4.244924	1.896734
H	-0.490651	-4.902924	2.358734
N	0.220348	0.176075	-0.763265
O	2.437348	0.729075	-0.512265
O	-2.080651	0.274075	-0.684265
C	0.439348	-1.171924	-1.293265
H	1.498348	-1.182924	-1.510265
C	-0.312651	-1.395924	-2.596265
H	-0.036651	-0.634924	-3.317265
H	-1.383651	-1.364924	-2.459265
H	-0.041651	-2.363924	-3.000265

Excited State Data (before shifting)

Excitation Energy (in eV)	**Oscillator Strength**	**Rotatory Strength**
4.6718	0.0001	-0.2719
4.8570	0.0019	-2.3399
5.0714	0.0001	-0.3767
5.1288	0.0423	-0.7528
5.3051	0.0059	0.7341
5.6641	0.0080	1.3574
5.7926	0.0795	8.0458
5.8788	0.0006	-1.2913
6.0420	0.0581	-6.2410
6.1918	0.0122	-5.0125
6.3185	0.3714	109.2764
6.4808	0.0515	-9.9552
6.4984	0.5292	-121.9388
6.7432	0.3329	14.8310
6.7841	0.0383	11.9812
6.9700	0.0007	1.0861
7.1805	0.0195	-8.7771

7.4053	0.0491	-47.2203
7.4089	0.0500	1.7193
7.4990	0.1292	1.3487
7.5863	0.3341	24.4121
7.6047	0.3763	54.2687
7.7596	0.0766	-16.3913
7.7997	0.0646	-18.1591
7.8408	0.0056	-1.8508
8.1187	0.0015	0.1492
8.1647	0.0108	2.4425
8.1988	0.0053	1.6341
8.2440	0.0521	-20.8467
8.2748	0.0333	1.8638
8.3036	0.0205	4.3781
8.4370	0.0013	-4.7783
8.4590	0.0019	-1.6436
8.4664	0.0082	7.0236
8.5147	0.0170	-18.1101
8.5368	0.0522	11.3544
8.5459	0.0897	17.0591
8.5781	0.1341	15.7424
8.6132	0.0028	-11.5488
8.6170	0.0038	5.8798
8.6821	0.0056	2.7819
8.7041	0.0014	6.0514
8.7396	0.0037	-5.7398
8.7546	0.0026	-4.6742
8.8129	0.0003	0.0952
8.8546	0.0062	-7.3468
8.9257	0.0069	11.7115
8.9278	0.0050	18.6458
8.9506	0.0039	-2.6812
8.9798	0.0017	-10.7731

Energies and Thermochemistry

E_{bw}	-838.5852293
ZPE (kJ/mol)	657.4
ln(qtrans)	18.9
ln(qrot)	15.26
ln(qvib)	11.97
chem. pot. (kJ/mol)	543.05
energy (kJ/mol)	695.89
entropy (kJ/mol/K)	0.52094
Cv (kJ/mol-K)	0.2377038
Cp (kJ/mol-K)	0.2460181
E_{bw} + ZPE	-838.3348389

H_{298}	-838.3192347
G_{298}	-838.3783923

B3LYP/TZVP

Cartesian Coordinates

H	2.343098	3.521287	0.639924
C	1.265098	3.422287	0.598924
C	-1.555901	3.137287	0.481924
C	0.674098	2.267287	0.119924
C	0.419098	4.448287	1.024924
C	-0.968901	4.308287	0.967924
C	-0.708901	2.128287	0.060924
H	0.844098	5.368287	1.407924
H	-1.598901	5.121287	1.305924
H	-2.630901	3.018287	0.433924
C	1.289098	1.014287	-0.402075
C	-1.023901	0.777287	-0.493075
C	0.197098	-2.252712	-0.244075
C	-0.265901	-4.188712	1.631924
C	1.277098	-2.831712	0.418924
C	-1.081901	-2.704712	0.096924
N	-1.316901	-3.648712	1.009924
C	1.047098	-3.814712	1.372924
H	2.288098	-2.511712	0.191924
H	-1.956901	-2.277712	-0.379075
H	1.867098	-4.283712	1.902924
H	-0.487901	-4.955712	2.367924
N	0.217098	0.176287	-0.762075
O	2.461098	0.735287	-0.515075
O	-2.109901	0.281287	-0.681075
C	0.439098	-1.180712	-1.299075
H	1.509098	-1.186712	-1.512075
C	-0.308901	-1.404712	-2.616075
H	-0.028901	-0.636712	-3.340075
H	-1.388901	-1.377712	-2.485075
H	-0.030901	-2.376712	-3.025075

Excited State Data (before shifting)

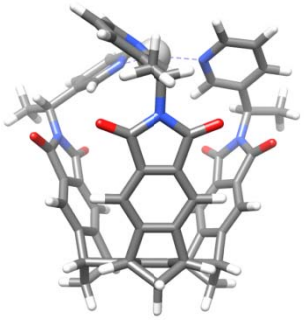
Excitation Energy (in eV)	**Oscillator Strength**	**Rotatory Strength**
3.8409	0.0002	-2.2656
3.9189	0.0004	5.4205
3.9975	0.0001	-0.6847
4.2505	0.0004	-2.4362

4.5002	0.0018	-10.1803
4.5760	0.0373	4.2494
4.7334	0.0081	7.8141
4.8943	0.0020	1.5792
4.9027	0.0029	-8.0447
5.1197	0.0139	-4.7664
5.2022	0.0630	8.5248
5.3254	0.0135	-12.1954
5.3441	0.1081	26.2470
5.4531	0.0440	-20.8498
5.7002	0.3163	14.0336
5.8380	0.0483	-1.1407
6.0275	0.0016	-0.3425
6.0557	0.2978	15.7533
6.1058	0.0137	-3.8290
6.1243	0.0140	0.5531
6.1571	0.0264	-56.9425
6.1809	0.1210	29.7604
6.3025	0.0016	7.1855
6.3766	0.0038	3.1396
6.4822	0.0076	6.5778
6.6032	0.0006	3.1482
6.6614	0.0155	-12.8370
6.6812	0.0001	-0.3584
6.7387	0.0025	-3.5045
6.7851	0.0028	-0.0093
6.8429	0.0049	-9.4774
6.8584	0.0009	-2.7347
6.8781	0.0099	13.8335
6.9041	0.0883	-14.9590
6.9908	0.0071	2.8833
7.0363	0.0116	19.9759
7.2069	0.3131	38.2750
7.2393	0.1705	-98.1432
7.2666	0.2176	41.8918
7.3085	0.0177	-14.1664
7.3574	0.0624	-28.4062
7.4382	0.1978	13.5262
7.4719	0.0110	11.6014
7.5441	0.1295	53.7354
7.5778	0.2564	-18.5048
7.6484	0.0058	-2.0090
7.6846	0.0006	-1.5164
7.7017	0.0031	3.5814
7.7155	0.0186	9.4703
7.7426	0.0043	4.5843

Energies and Thermochemistry

E_{bw}	-838.5935767
ZPE (kJ/mol)	632.3
ln(qtrans)	18.9
ln(qrot)	15.28
ln(qvib)	12.62
chem. pot. (kJ/mol)	516.24
energy (kJ/mol)	672.2
entropy (kJ/mol/K)	0.5314
Cv (kJ/mol-K)	0.2477837
Cp (kJ/mol-K)	0.256098
E_{bw} + ZPE	-838.3527464
H_{298}	-838.3366052
G_{298}	-838.3969506

Ag(I)-(R_3)-1(P)



BHLYP/SV(P),TZVP

Cartesian Coordinates

Ag	0.000033	-0.006074	-4.197660
C	0.049033	1.396925	4.923339
C	2.221033	-1.845074	4.924339
C	0.202033	-2.878074	4.883339
C	-2.719966	-0.997074	4.917339
C	2.108033	-2.507074	3.561339
C	0.848033	-3.135074	3.527339
C	2.290033	2.307925	3.521339
C	1.116033	3.084925	3.551339
C	-3.145966	0.835925	3.518339
C	-3.231966	-0.569074	3.553339
C	2.973033	-2.541074	2.485339

C	-1.164966	0.772925	4.916339
C	0.397033	-3.795074	2.399339
C	3.088033	2.243925	2.394339
C	0.714033	3.848925	2.472339
C	-3.489966	1.556925	2.389339
C	-3.691966	-1.301074	2.475339
C	2.518033	-3.221074	1.363339
C	1.269033	-3.816074	1.317339
C	-4.050966	-0.567074	1.352339
C	-3.941966	0.811925	1.306339
C	2.672033	3.005925	1.309339
C	-1.235966	-0.645074	4.925339
C	1.532033	3.790925	1.351339
C	1.090033	-4.409074	-0.033660
C	3.192033	-3.450074	0.058339
C	-4.582966	-1.036074	0.046339
C	-4.363966	1.262925	-0.044660
C	1.395033	4.483925	0.044339
C	3.277033	3.144925	-0.041660
C	2.515033	-4.589074	-2.088660
C	-5.229966	0.119925	-2.101660
C	2.724033	4.462925	-2.100660
C	-0.089966	-1.384074	4.920339
C	1.777033	2.739925	5.763339
C	-3.263966	0.181925	5.762339
C	1.471033	-2.904074	5.772339
C	-0.502966	3.143925	-4.539660
C	-0.396966	4.503925	-4.311660
C	0.643033	4.970925	-3.521660
C	1.560033	4.068925	-2.995660
C	1.367033	2.724925	-3.292660
C	-2.474966	-2.018074	-4.537660
C	-3.704966	-2.605074	-4.309660
C	1.174033	-0.737074	4.928339
C	-4.629966	-1.936074	-3.519660
C	-4.306966	-0.692074	-2.994660
C	-3.045966	-0.187074	-3.291660
C	2.986033	-1.133074	-4.524660
C	1.686033	-2.549074	-3.284660
C	2.755033	-3.384074	-2.982660
C	3.996033	-3.036074	-3.501660
C	4.112033	-1.901074	-4.290660
C	1.241033	0.625925	4.919339
C	-2.603966	1.267925	4.875339
C	0.485033	2.856925	4.914339
C	2.389033	1.624925	4.879339

H	-2.767966	2.311925	5.140339
H	3.953033	-2.075074	2.500339
H	3.991033	1.643925	2.344339
H	-0.178966	4.463925	2.484339
H	1.564033	-5.034074	-2.389660
H	-5.138966	1.165925	-2.401660
H	3.584033	3.858925	-2.399660
H	2.369033	3.658925	5.768339
H	1.586033	2.411925	6.789339
H	-4.355966	0.235925	5.766339
H	-2.884966	0.182925	6.788339
H	-0.260966	3.588925	5.222339
H	1.970033	-3.877074	5.778339
H	1.279033	-2.574074	6.796339
H	0.731033	6.029925	-3.313660
H	2.061033	1.982925	-2.903660
H	-5.590966	-2.390074	-3.312660
H	-2.749966	0.784925	-2.903660
H	0.696033	-2.783074	-2.900660
H	4.871033	-3.638074	-3.289660
C	3.122033	5.929925	-2.178660
C	3.589033	-5.665074	-2.163660
H	3.374033	1.244925	5.148339
C	-6.699966	-0.271074	-2.176660
H	5.067033	-1.606074	-4.710660
H	-3.929966	-3.577074	-4.732660
H	-1.125966	5.184925	-4.735660
H	-1.724966	-2.517074	-5.143660
H	3.043033	-0.234074	-5.129660
H	-1.309966	2.744925	-5.146660
H	3.226033	-1.564074	5.235339
H	-0.619966	-3.542074	5.149339
H	-2.978966	-2.008074	5.226339
H	-3.421966	2.637925	2.337339
H	-3.778966	-2.382074	2.490339
H	-0.573966	-4.277074	2.346339
N	2.466033	4.047925	-0.730660
N	2.281033	-4.159074	-0.719660
N	-4.740966	0.106925	-0.731660
N	0.363033	2.266925	-4.034660
N	-2.147966	-0.829074	-4.032660
N	1.791033	-1.450074	-4.025660
O	0.141033	-4.967074	-0.494660
O	4.281033	-3.109074	-0.295660
O	-4.832966	-2.150074	-0.307660
O	-4.372966	2.364925	-0.505660

O	0.555033	5.255925	-0.314660
O	4.237033	2.600925	-0.498660
H	-7.055966	-0.226074	-3.210660
H	-7.293966	0.430925	-1.584660
H	-6.870966	-1.277074	-1.786660
H	3.341033	6.213925	-3.212660
H	4.026033	6.093925	-1.584660
H	2.336033	6.582925	-1.790660
H	4.546033	-5.309074	-1.773660
H	3.279033	-6.531074	-1.571660
H	3.730033	-5.996074	-3.198660

Excited State Data (before shifting)

Excitation Energy (in eV)	**Oscillator Strength**	**Rotatory Strength**
4.3762	0.0001	9.9833
4.4414	0.0020	0.2213
4.4414	0.0020	0.2213
4.6495	0.0000	0.4076
4.6593	0.0023	4.2083
4.6593	0.0023	4.2083
4.7433	0.0008	-0.5843
4.9356	0.0305	1.2942
4.9356	0.0305	1.2942
5.0309	0.0651	18.4551
5.0309	0.0651	18.4551
5.0354	0.0004	19.1920
5.0686	0.0342	-21.0550
5.0890	0.0079	0.1286
5.0890	0.0079	0.1286
5.1662	0.0000	-0.1237
5.2264	0.0077	5.6400
5.2264	0.0077	5.6400
5.4935	0.0975	-10.2460
5.6183	0.0001	-7.1868
5.6295	0.1983	584.0910
5.6295	0.1983	584.0910
5.6828	0.1239	-305.9565
5.7025	0.0956	-364.4254
5.7025	0.0956	-364.4254
5.7839	0.0414	49.8696
5.7839	0.0414	49.8696
5.7995	0.0002	-0.2879
5.9477	0.0023	2.4403
5.9477	0.0023	2.4403

5.9816	0.0007	12.2224
5.9816	0.0007	12.2224
6.0112	0.0665	122.0159
6.0112	0.0665	122.0159
6.0145	0.0023	-54.3806
6.0250	0.4259	-77.4145
6.0408	0.0002	14.7519
6.0419	0.1210	-83.4479
6.0419	0.1210	-83.4479
6.0830	0.0166	44.1534
6.0830	0.0166	44.1534
6.1249	0.0019	-0.7506
6.1249	0.0019	-0.7506
6.1428	0.0262	6.9094
6.2088	0.0025	-22.8105
6.2088	0.0025	-22.8105
6.2281	0.0382	71.0401
6.2281	0.0382	71.0401
6.2322	0.0333	-48.2129
6.2423	0.4583	-281.1990
6.3293	0.4308	-26.0374
6.3481	0.0733	72.7614
6.3481	0.0733	72.7614
6.3932	0.0000	-4.4527
6.4378	0.0279	6.3739
6.4378	0.0279	6.3739
6.4439	0.0037	-7.3252
6.4508	0.0094	-4.1224
6.4508	0.0094	-4.1224
6.4658	0.9811	-203.6669
6.4698	0.0011	-0.7213
6.4698	0.0011	-0.7213
6.4746	0.1054	-7.4133
6.4987	0.0558	-15.7859
6.5077	0.0035	5.0178
6.5077	0.0035	5.0178
6.5367	0.0038	1.6491
6.5367	0.0038	1.6491
6.6021	0.0091	0.7134
6.6021	0.0040	-5.3750
6.6021	0.0040	-5.3750
6.6122	0.0010	0.8135
6.6282	0.0156	13.9648
6.6282	0.0156	13.9648
6.6374	0.0062	-26.5652

Energies and Thermochemistry

E_{bw}	-3234.227051
ZPE (kJ/mol)	2448
ln(qtrans)	21.04
ln(qrot)	18.02
ln(qvib)	55.5
chem. pot. (kJ/mol)	2213.85
energy (kJ/mol)	2589.78
entropy (kJ/mol/K)	1.26922
Cv (kJ/mol-K)	0.9064513
Cp (kJ/mol-K)	0.9147656
E_{bw} + ZPE	-3233.294657
H_{298}	-3233.239712
G_{298}	-3233.383844

B3LYP/SV(P),TZVP

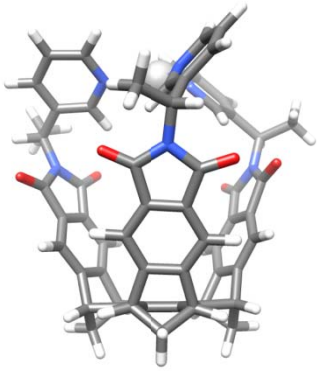
Excited State Data (before shifting)

Excitation Energy (in eV)	**Oscillator Strength**	**Rotatory Strength**
3.5104	0.0001	6.6562
3.5383	0.0005	0.4423
3.5383	0.0005	0.4423
3.5587	0.0007	-0.0861
3.6092	0.0202	3.2457
3.6092	0.0202	3.2457
3.8561	0.0000	-0.2366
3.8566	0.0001	2.9159
3.8566	0.0001	2.9159
4.0342	0.0039	-6.4180
4.0342	0.0039	-6.4180
4.0374	0.0001	-3.0680
4.2271	0.0014	9.2833
4.2271	0.0014	9.2833
4.2944	0.0000	0.0888
4.2944	0.0000	0.0888
4.2985	0.0025	-6.6998
4.3199	0.0001	2.7843
4.3231	0.0003	0.4895
4.3231	0.0003	0.4895
4.3315	0.0049	-4.4827
4.3383	0.0042	3.6037
4.3383	0.0042	3.6037

4.3466	0.0099	-12.3038
4.3492	0.0019	14.8866
4.3598	0.0007	0.1361
4.3598	0.0007	0.1361
4.4138	0.0018	-1.2088
4.4489	0.0057	1.8884
4.4489	0.0057	1.8884
4.5845	0.0004	-8.3956
4.6073	0.0061	3.0759
4.6073	0.0061	3.0759
4.6397	0.1192	4.6317
4.6428	0.0612	26.9915
4.6428	0.0612	26.9915
4.6894	0.0039	5.4985
4.6894	0.0039	5.4985
4.7038	0.0169	-36.4101
4.7214	0.0001	0.2758
4.7214	0.0001	0.2758
4.7261	0.0220	-23.0864
4.7309	0.0001	0.3606
4.7473	0.0002	-0.8966
4.7473	0.0002	-0.8966
4.7496	0.0166	3.8061
4.7555	0.0568	11.8881
4.7555	0.0568	11.8881
4.7579	0.0034	9.9848
4.7607	0.0002	-1.0533
4.7607	0.0002	-1.0533
4.7760	0.0000	-0.5478
4.7807	0.0024	-0.5313
4.7807	0.0024	-0.5313
4.7807	0.0001	-2.0815
4.7873	0.0053	-3.1758
4.7917	0.0186	2.9616
4.7917	0.0186	2.9616
4.7967	0.0050	13.4898
4.7967	0.0050	13.4898
4.8006	0.0015	-1.2179
4.8160	0.0003	-3.5559
4.8160	0.0003	-3.5559
4.8161	0.0022	0.1314
4.8403	0.0060	41.4604
4.8403	0.0060	41.4604
4.9158	0.0015	2.2557
4.9158	0.0015	2.2557
4.9202	0.0021	1.6957

4.9202	0.0021	1.6957
4.9418	0.0033	-0.5054
4.9511	0.0073	31.5838
4.9511	0.0073	31.5838
4.9705	0.0061	-8.7455
5.0085	0.0012	2.5166

Ag(I)-(R_3)-1(M)



BHLYP/SV(P),TZVP

Cartesian Coordinates

Ag	-0.025625	-0.058064	3.963031
C	0.927374	-0.928064	-4.958968
C	-2.909625	-0.211064	-4.933968
C	-2.231625	1.948935	-4.793968
C	1.154374	2.725935	-4.891968
C	-3.319625	0.270935	-3.556968
C	-2.866625	1.600935	-3.448968
C	0.065374	-3.181064	-3.573968
C	1.444374	-2.906064	-3.662968
C	2.745374	1.737935	-3.484968
C	1.817374	2.795935	-3.530968
C	-3.990625	-0.362064	-2.529968
C	1.331374	0.374935	-4.914968
C	-3.007625	2.318935	-2.275968
C	-0.493625	-3.695064	-2.417968
C	2.321374	-3.201064	-2.637968
C	3.470374	1.462935	-2.338968
C	1.631374	3.658935	-2.468968
C	-4.160625	0.382935	-1.370968
C	-3.662625	1.665935	-1.235968
C	2.392374	3.395935	-1.337968
C	3.260374	2.321935	-1.263968
C	0.391374	-3.966064	-1.379968

C	0.369374	1.418935	-4.897968
C	1.753374	-3.752064	-1.497968
C	-3.941625	2.129935	0.151031
C	-4.858625	0.025935	-0.112968
C	2.463374	4.133935	-0.055968
C	3.841374	2.286935	0.107031
C	2.400374	-4.204064	-0.244968
C	0.119374	-4.470064	-0.004968
C	-5.283625	1.072935	2.078031
C	3.642374	3.912935	2.096031
C	1.692374	-5.119064	1.930031
C	-0.961625	1.115935	-4.878968
C	0.647374	-3.085064	-5.843968
C	2.381374	2.291935	-5.733968
C	-3.136625	1.101935	-5.724968
C	2.568374	-1.825064	4.469031
C	3.524374	-2.814064	4.333031
C	3.248374	-3.891064	3.504031
C	2.023374	-3.962064	2.854031
C	1.126374	-2.921064	3.066031
C	0.423374	3.000935	4.719031
C	0.867374	4.308935	4.661031
C	-1.384625	-0.238064	-4.922968
C	1.911374	4.615935	3.802031
C	2.496374	3.609935	3.043031
C	1.984374	2.325935	3.183031
C	-2.864625	-1.297064	4.648031
C	-3.079625	0.440935	3.171031
C	-4.442625	0.218935	3.008031
C	-5.007625	-0.828064	3.725031
C	-4.212625	-1.593064	4.565031
C	-0.457625	-1.240064	-4.936968
C	2.689374	1.055935	-4.849968
C	1.666374	-2.262064	-5.016968
C	-0.544625	-2.758064	-4.908968
H	3.553374	0.446935	-5.109968
H	-4.371625	-1.374064	-2.608968
H	-1.555625	-3.889064	-2.312968
H	3.388374	-3.022064	-2.704968
C	-5.599625	2.444935	2.663031
C	4.991374	3.459935	2.644031
C	0.649374	-6.065064	2.514031
H	0.889374	-4.151064	-5.876968
H	0.508374	-2.701064	-6.858968
H	3.184374	3.034935	-5.730968
H	2.123374	2.023935	-6.761968

H	2.697374	-2.229064	-5.365968
H	-4.181625	1.425935	-5.720968
H	-2.763625	1.054935	-6.750968
H	3.990374	-4.668064	3.349031
H	0.156374	-2.930064	2.576031
H	2.263374	5.638935	3.711031
H	2.407374	1.504935	2.610031
H	-2.592625	1.249935	2.632031
H	-6.063625	-1.054064	3.615031
H	2.618374	-5.682064	1.801031
H	-6.227625	0.540935	1.947031
H	-1.513625	-3.196064	-5.145968
H	3.672374	4.998935	1.993031
H	-4.625625	-2.417064	5.135031
H	0.390374	5.072935	5.264031
H	4.472374	-2.731064	4.851031
H	-0.403625	2.723935	5.366031
H	-2.207625	-1.884064	5.282031
H	2.753374	-0.958064	5.096031
H	-3.406625	-1.113064	-5.289968
H	-2.132625	3.011935	-5.008968
H	0.612374	3.617935	-5.204968
H	4.171374	0.638935	-2.267968
H	0.943374	4.495935	-2.501968
H	-2.644625	3.333935	-2.157968
N	1.369374	-4.637064	0.593031
N	-4.703625	1.120935	0.743031
N	3.357374	3.425935	0.753031
N	1.393374	-1.875064	3.844031
N	0.968374	2.027935	3.990031
N	-2.307625	-0.302064	3.960031
O	-3.562625	3.130935	0.681031
O	-5.447625	-0.973064	0.169031
O	1.898374	5.131935	0.276031
O	4.540374	1.444935	0.586031
O	3.558374	-4.216064	0.048031
O	-0.942625	-4.653064	0.512031
H	1.042374	-6.483064	3.446031
H	0.451374	-6.891064	1.824031
H	-0.297625	-5.565064	2.721031
H	5.027374	2.384935	2.823031
H	5.794374	3.714935	1.947031
H	5.176374	3.984935	3.587031
H	-4.700625	3.023935	2.874031
H	-6.161625	2.305935	3.592031
H	-6.220625	3.021935	1.971031

Excited State Data (before shifting)

Excitation Energy (in eV)	**Oscillator Strength**	**Rotatory Strength**
4.3863	0.0008	-26.4657
4.4518	0.0021	2.1136
4.4518	0.0021	2.1136
4.6443	0.0002	-0.9313
4.6524	0.0017	-6.4704
4.6524	0.0017	-6.4704
4.7467	0.0010	0.1151
4.9398	0.0287	-6.5408
4.9398	0.0287	-6.5408
5.0438	0.0805	-21.9113
5.0438	0.0805	-21.9113
5.0689	0.0323	-2.2162
5.0866	0.0000	1.5539
5.1228	0.0011	-4.8262
5.1228	0.0011	-4.8262
5.1306	0.0004	3.2431
5.2014	0.0041	0.8275
5.2014	0.0041	0.8275
5.4904	0.0984	-9.7499
5.6145	0.0008	-16.5696
5.6265	0.1918	-538.9832
5.6265	0.1918	-538.9832
5.6810	0.1459	335.5542
5.6891	0.0714	222.2581
5.6891	0.0714	222.2581
5.7620	0.0880	19.4836
5.7620	0.0880	19.4836
5.7634	0.0097	12.9507
5.9476	0.0007	-2.4812
5.9476	0.0007	-2.4812
5.9995	0.0006	-6.7580
5.9995	0.0006	-6.7580
6.0314	0.0524	-62.8456
6.0314	0.0524	-62.8456
6.0356	0.0069	97.8210
6.0412	0.4300	137.6886
6.0416	0.0189	13.8708
6.0416	0.0189	13.8708
6.0597	0.0079	-103.7200
6.0635	0.1293	-33.1971
6.0635	0.1293	-33.1971

6.1059	0.0000	-0.2393
6.1434	0.0016	0.4463
6.1434	0.0016	0.4463
6.1669	0.0002	-1.0390
6.1669	0.0002	-1.0390
6.1945	0.0005	1.6656
6.2615	0.0180	-51.9768
6.2615	0.0180	-51.9768
6.2655	0.6740	339.5721
6.3328	0.1656	-47.9523
6.3559	0.1006	-104.2995
6.3559	0.1006	-104.2995
6.3876	0.0103	124.4234
6.4418	0.0024	-22.6777
6.4438	0.0024	-0.7916
6.4438	0.0024	-0.7916
6.4503	0.0303	-1.5503
6.4503	0.0303	-1.5503
6.4665	1.1402	253.1483
6.4692	0.0028	2.9598
6.4692	0.0028	2.9598
6.4817	0.0001	1.9586
6.5115	0.0221	13.5326
6.5178	0.0028	-3.4450
6.5178	0.0028	-3.4450
6.5642	0.0010	0.6551
6.5642	0.0010	0.6551
6.5675	0.0186	-26.5277
6.5697	0.0028	1.0737
6.5697	0.0028	1.0737
6.5891	0.0089	29.4646
6.6245	0.0020	-5.5937
6.6245	0.0020	-5.5937
6.6323	0.0001	1.4545

Energies and Thermochemistry

E_{bw}	-3234.216515
ZPE (kJ/mol)	2448
ln(qtrans)	21.04
ln(qrot)	18.01
ln(qvib)	56.79
chem. pot. (kJ/mol)	2210.1
energy (kJ/mol)	2589.74
entropy (kJ/mol/K)	1.28164
Cv (kJ/mol-K)	0.9071422
Cp (kJ/mol-K)	0.9154565

E_{bw} + ZPE	-3233.284122
H_{298}	-3233.229191
G_{298}	-3233.374734

B3LYP/SV(P),TZVP

Excited State Data (before shifting)

Excitation Energy (in eV)	**Oscillator Strength**	**Rotatory Strength**
3.5141	0.0006	-16.2691
3.5415	0.0005	-0.5969
3.5415	0.0005	-0.5969
3.5634	0.0005	1.2878
3.6126	0.0200	-3.9640
3.6126	0.0200	-3.9640
3.8539	0.0003	-1.4837
3.8542	0.0001	-1.0707
3.8542	0.0001	-1.0707
4.0609	0.0050	1.9293
4.0609	0.0050	1.9293
4.0642	0.0002	2.4445
4.1864	0.0009	-6.2144
4.1864	0.0009	-6.2144
4.2562	0.0056	8.2774
4.2771	0.0007	-0.0586
4.2771	0.0007	-0.0586
4.2909	0.0000	0.0064
4.3120	0.0003	-1.2604
4.3120	0.0003	-1.2604
4.3356	0.0022	-11.7008
4.3470	0.0085	7.9955
4.3513	0.0002	-3.6182
4.3513	0.0002	-3.6182
4.3606	0.0001	1.8341
4.3675	0.0014	1.2774
4.3675	0.0014	1.2774
4.4154	0.0000	-0.0616
4.4532	0.0092	-4.9210
4.4532	0.0092	-4.9210
4.5645	0.0020	19.1652
4.6057	0.0009	-3.1931

4.6057	0.0009	-3.1931
4.6310	0.0726	-17.7062
4.6310	0.0726	-17.7062
4.6326	0.1154	-35.1182
4.6576	0.0033	-7.1334
4.6576	0.0033	-7.1334
4.6803	0.0438	60.1170
4.7200	0.0029	-3.4520
4.7231	0.0000	-0.0496
4.7231	0.0000	-0.0496
4.7352	0.0000	0.0473
4.7426	0.0001	1.3253
4.7426	0.0001	1.3253
4.7444	0.0069	-17.4040
4.7468	0.0000	0.0557
4.7566	0.0044	4.5254
4.7566	0.0044	4.5254
4.7591	0.0456	-18.7204
4.7591	0.0456	-18.7204
4.7699	0.0051	14.8230
4.7765	0.0004	-1.7159
4.7807	0.0002	2.1853
4.7807	0.0002	2.1853
4.7883	0.0020	-8.4028
4.7950	0.0108	-16.0605
4.7950	0.0108	-16.0605
4.7969	0.0002	-1.0686
4.7971	0.0009	-8.2060
4.7971	0.0009	-8.2060
4.8060	0.0131	-9.0762
4.8060	0.0131	-9.0762
4.8075	0.0002	0.0996
4.8234	0.0021	-8.3690
4.8234	0.0021	-8.3690
4.8903	0.0075	-7.3115
4.8903	0.0075	-7.3115
4.9223	0.0017	0.9080
4.9223	0.0017	0.9080
4.9308	0.0130	-9.3534
4.9308	0.0130	-9.3534
4.9318	0.0076	5.2957
4.9392	0.0019	4.0220
4.9810	0.0034	2.2313