Supporting Information

Oxazine-based Molecular Switches with Finely Tunable pH and Temperature Sensitivity via Substituent Engineering

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Material and Methods

Chemicals were purchased from commercial sources and used as received. H_2O (18.2 MΩ-cm) was purified with a Barnstead International NANOpure DIamond Analytical system. NMR spectra were recorded with a Zhongke Niujin QUANTUM-I-400MHz. Absorption spectra were recorded with Cary 5000 UV-Vis-NIR Spectrophotometer and emission spectra were recorded with Horiba FluoroMax-4 spectrometer. HRMS was done with a Thermo Scientific Q Exactive Orbitrap.

Molar extinction coefficients (ε). ε were determined by measuring the UV-vis absorption spectra of solutions with different concentrations (1 to 10 μM) of each molecular switch in MeCN with TFA or TEA at room temperature. The absorbance at the maximum wavelength (λ_{max}) corresponding to the SP/MC was recorded using a UV-vis spectrophotometer. The molar extinction coefficient was calculated using the Beer-Lambert law:

$$A=\varepsilon \times c \times l$$

where A is the measured absorbance, ε is the molar extinction coefficient, c is the concentration of the solution, and l is the path length of the cuvette (1 cm). The extinction coefficient was determined by fitting the absorbance data at λ_{max} to the Beer-Lambert law and calculating ε from the slope of the linear absorbance vs. concentration plot.

Quantum yield (*Φ*). *Φ* was determined by measuring the fluorescence emission spectra of each molecular switch in MeCN with TFA or TEA at room temperature. The fluorescence intensity at the emission maximum was recorded using a fluorometer. For the SP form, 7-amino-4-methylcoumarin (7-AMC) was used as the standard, and for the MC form, Crystal Violet was used as the standard. The quantum yield was calculated using the following equation:

$$\Phi_s = \Phi_r \times \frac{A_s}{A_r} \times \frac{F_r}{F_s} \times \left(\frac{n_s}{n_r}\right)^2,$$

where Φ is the quantum yield, A is the absorbance at the excitation wavelength, F is the integrated fluorescence intensity, n is the refractive index of the solvent, and the subscripts s and r refer to the sample and reference, respectively.

pH-Dependent Behavior: pH-dependent behavior was investigated by preparing 10 μM solutions of each molecular switch in aqueous buffers ranging from pH 3 to 9. UV-vis absorption spectra were recorded at each pH value, with a particular focus on the transition from the SP form to the MC form, as evidenced by a bathochromic shift in the absorption maxima. Fluorescence spectra were also measured to track changes in emission upon pH variation. The excitation wavelength used was where the corresponding SP/MC absorption peaks locates. All measurements were conducted at room temperature.

DFT Calculations: DFT calculations were performed using Gaussian 09 (Revision A.01) to investigate the electronic structure and energy profiles of the molecular switches. The geometry of the spiro (SP) and merocyanine (MC) forms, along with their protonated intermediates, was optimized in the gas phase using the B3LYP functional with the 6-31G(d) basis set, without symmetry constraints. Protonation was applied at the relevant nitrogen atoms of the oxazine ring and coumarin moiety to model the pH-induced ring-opening process, with transition states located via a saddle-point search. The total electronic energies of the optimized structures were computed, and the impact of substituents on the SP-to-MC equilibrium was examined by evaluating the energy differences for systems with electron-withdrawing and electron-donating groups. Thermodynamic calculations for the protonated species included Gibbs free energy (ΔG) corrections based on optimized geometries at 298 K. For solvent effects, the SMD solvation model was applied in some cases.

Temperature-Dependent Kinetics: Temperature-dependent kinetics were investigated by heating 10 μM solutions of each molecular switch in 70% DMSO with different amount of acid/base to the desired temperature using an oven. The samples were placed in a pre-heated oven at a temperature of 333 K for a specified duration, ensuring the solution reached thermal equilibrium. Following this, the samples were removed from the oven and allowed to cool back to room temperature (298 K). Absorption spectra were recorded continuously during the cooling process using a UV-vis spectrophotometer. The changes in absorbance, particularly at the characteristic wavelengths corresponding to the SP and MC forms, were monitored to determine the kinetics of the SP-to-MC transition.

Absorption Spectra at Different Temperatures: Absorption spectra at different temperatures were recorded by preparing 10 μM solutions of each molecular switch in 70% DMSO with

different amount of acid/base. The samples were placed in a temperature-controlled oven, and the temperature was incrementally varied from 298 K to 333 K. At each temperature, the samples were equilibrated for 1 hour to ensure uniform temperature distribution and the equilibrium of the SP-to-MC form. Absorption spectra were then measured using a UV-vis spectrophotometer at each temperature point. The absorbance at the characteristic λ_{max} for both forms was recorded to track the temperature-dependent shifts in the equilibrium between the SP and MC states. The temperature-dependent absorption data were analyzed to calculate the temperature sensitivity.

Table S1. Photophysical Properties properties of the switches

Dye	Solvent	λ_{Abs} (nm)	λ_{em} (nm)	ε ($\times 10^4$ M^{-1} cm^{-1})	Φ_{FL}	Brigtness ($\times 10^4$ M^{-1} cm^{-1})
3-a	MeCN+TFA	608	676	7.53	0.047	0.35
	MeCN+TEA	409	474	3.43	0.306	1.05
3-b	MeCN+TFA	602	678	6.73	0.069	0.46
	MeCN+TEA	409	474	3.29	0.470	1.55
3-c	MeCN+TFA	594	675	8.42	0.106	0.89
	MeCN+TEA	409	474	3.15	0.329	1.04
3-d	MeCN+TFA	594	684	7.56	0.114	0.86
	MeCN+TEA	409	474	3.49	0.235	0.82
3'-d	MeCN+TFA	594	680	7.47	0.110	0.82
	MeCN+TEA	409	474	3.44	0.034	0.12
3-e	MeCN+TFA	577	662	9.44	0.265	2.50
	MeCN+TEA	409	474	3.03	0.533	1.61
3-f	MeCN+TFA	577	657	8.70	0.078	0.68

MeCN+TEA	**409**	**474**	**3.07**	**0.093**	**0.29**

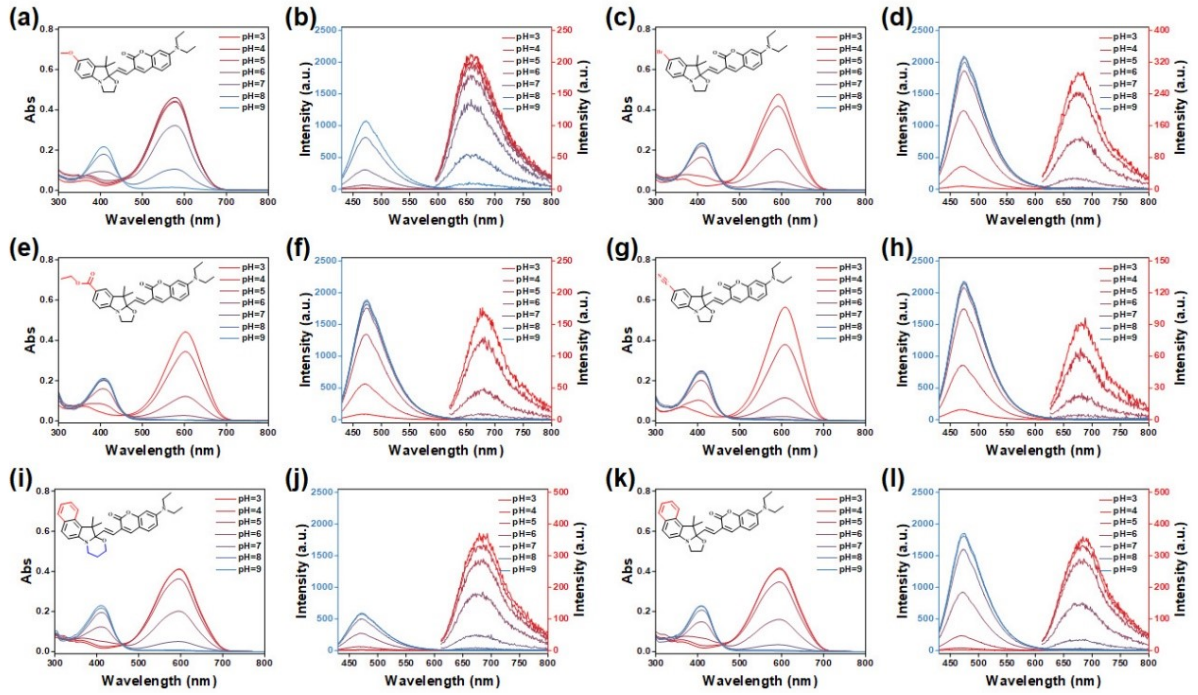


Figure S1. The absorption and emission spectra of **3-f** (a, b), **3-c** (c, d), **3-b** (e, f), **3-a** (g, h), **3'-d** (i, j) and **3-d** (k, l) in water (10% DMSO, 10 μM) at various pH, recorded at room temperature.

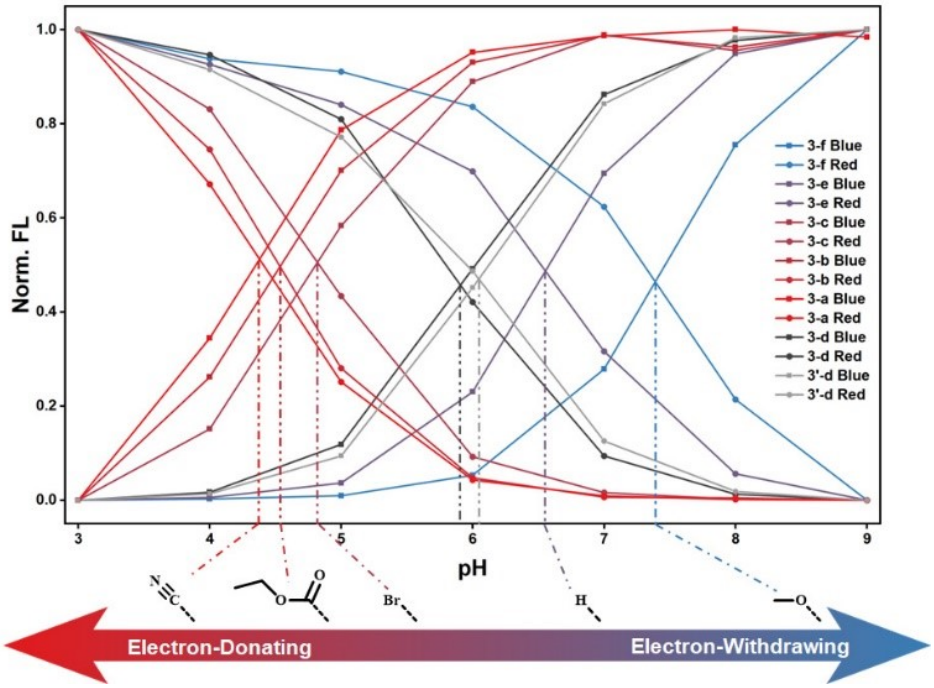


Figure S2. Normalized bimodal fluorescence intensity of the synthesized switches as a function of pH in the water (10% DMSO, 10 μM).

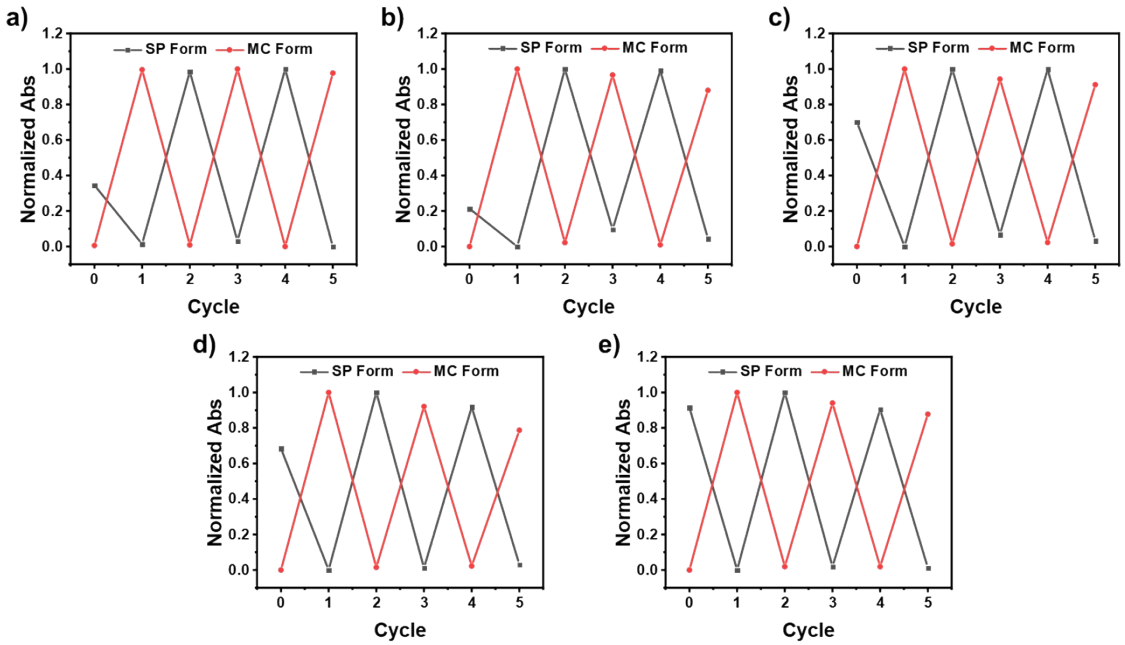


Figure S3. The normalized absorbance of (a) 3-c, (b) 3-d, (c) 3'-d, (d) 3-e, and (e) 3-f in water adjusting pH between 2 and 9.

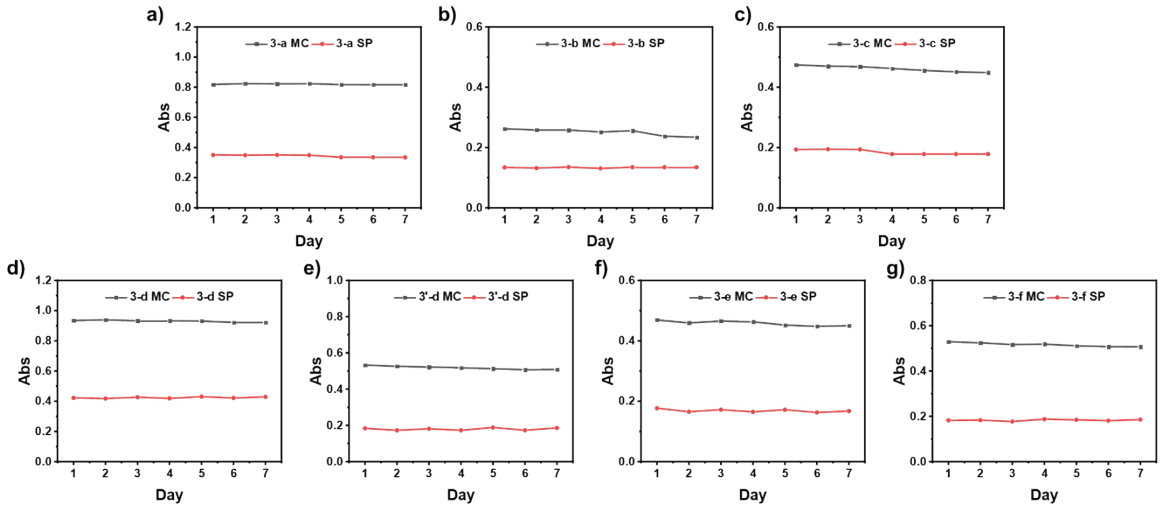


Figure S4. Stability test of 3-a – 3-f (a-f) under the condition of pH 2 or 9 for a week continuously. The absorption peak of the MC (black) or SP (red) form were plotted.

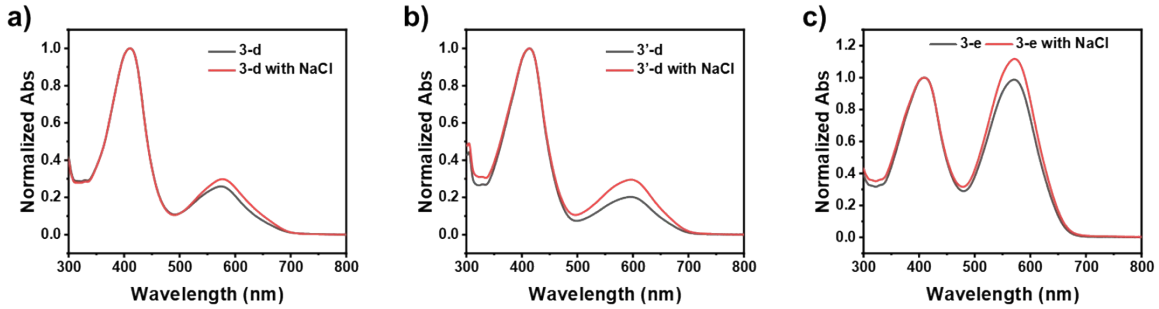


Figure S5. Normalized absorption spectra of 3-d, 3'-d and 3-e with or without NaCl (50mM).

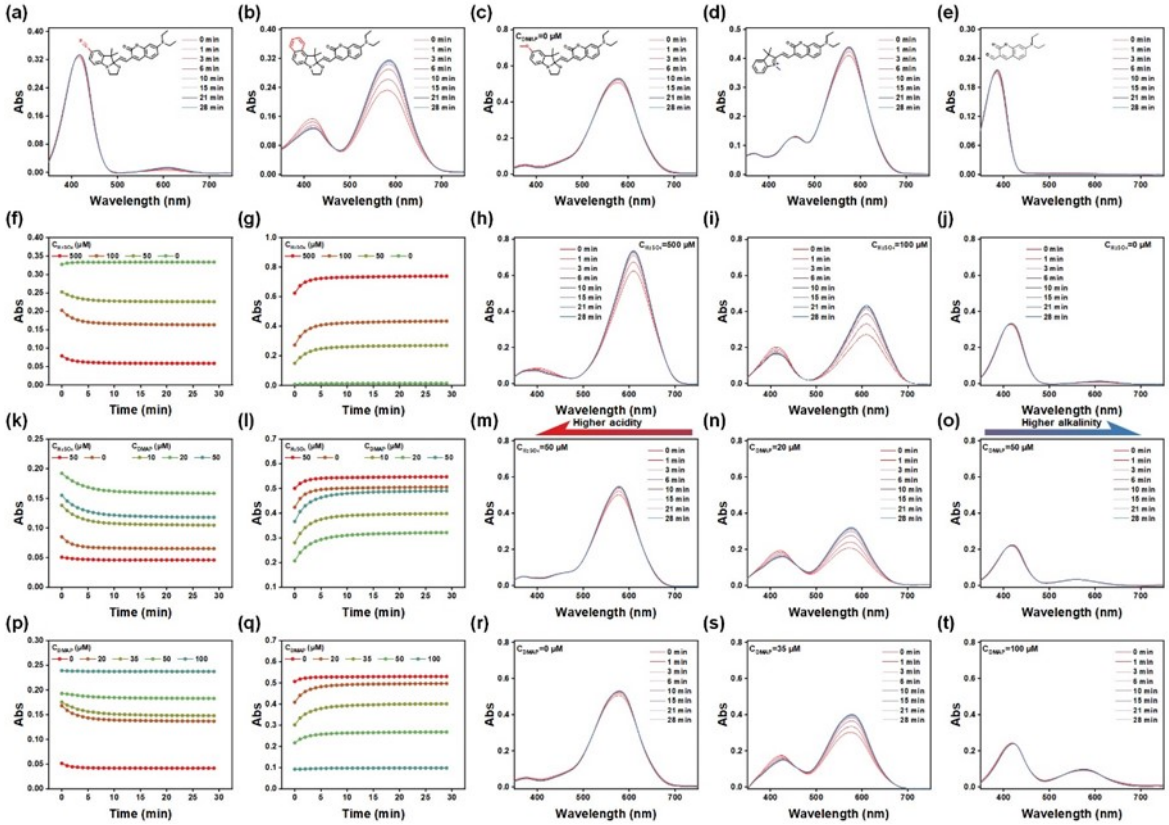


Figure S6. The time-resolved cooling absorption spectra (60 °C to 25 °C) of switches **3-a** (a), **3-d** (b), **3-f** (c), the hemicyanine template (d) and the aldehyde coumarin (e) in 70% DMSO. The time-resolved cooling response dynamic curve (60 °C to 25 °C) of switches **3-a** absorbed in 415 nm (f) and 610 nm (g) after adjusting different pH, and representative absorption spectra in 500 μM (h), 100 μM (i), 0 (j) H_2SO_4. Similarly, for switches **3-e** (k, l, m, n, o) and **3-f** (p, q, r, s, t), the only difference is the pH they adjust.

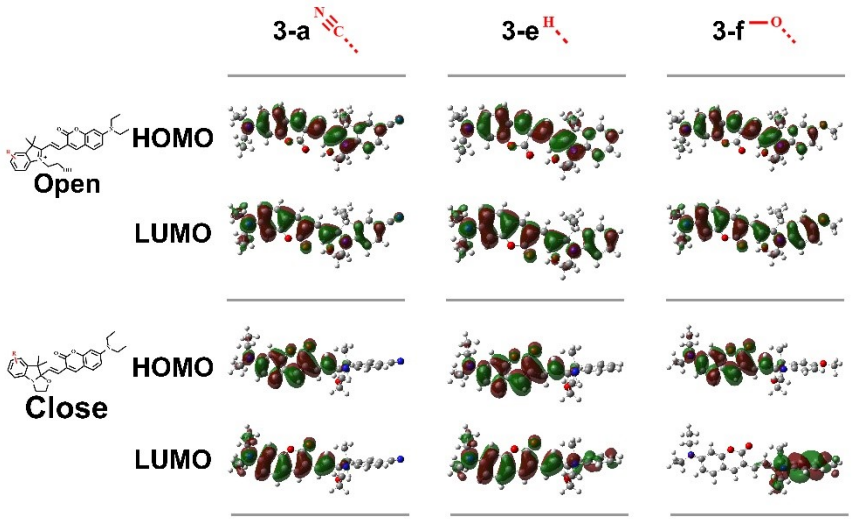


Figure S7. Schematic representation of contour surface of HOMO & LUMO of representative switches in the state of open/close.

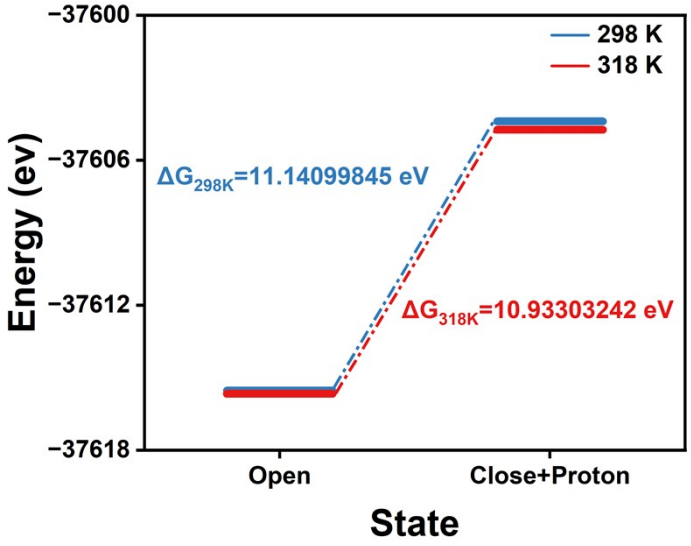


Figure S8. Temperature dependent schematic diagram of potential energy surface of **3-e** calculated by DFT.

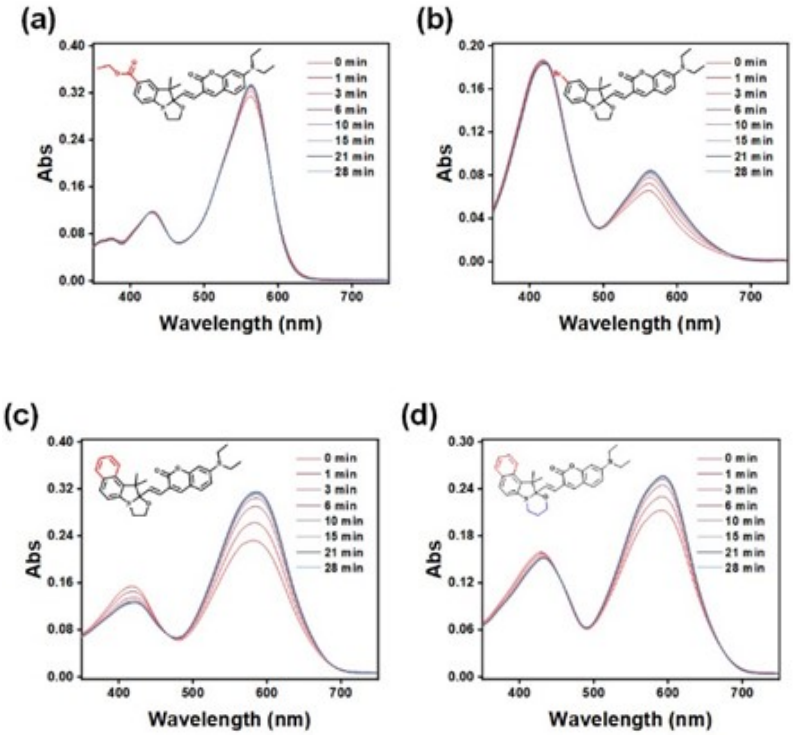


Figure S9. The time-resolved cooling absorption spectra (333 K to 298 K) of switches **3-b** (a), **3-c** (b), **3-d** (c), and **3'-d** (d) in 70% DMSO.

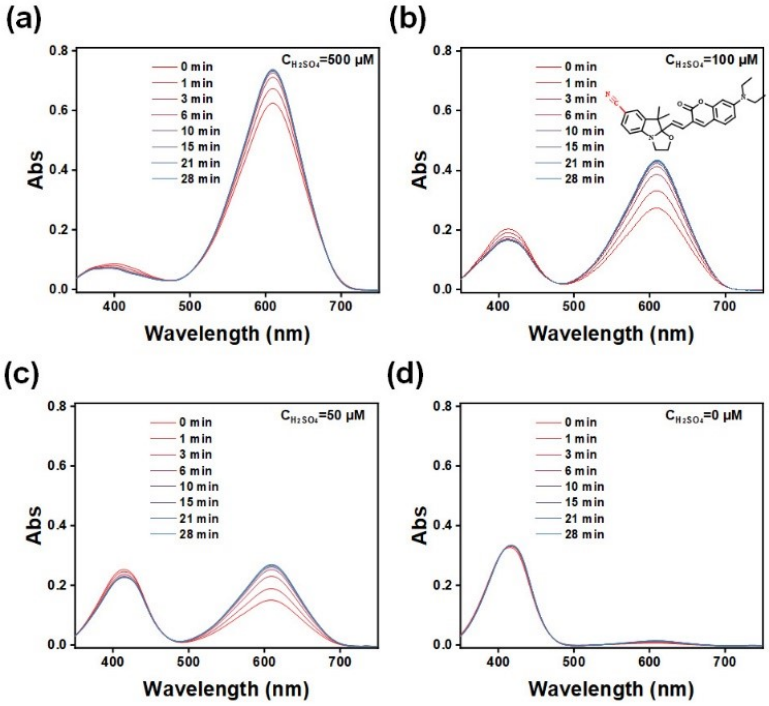


Figure S10. The time-resolved cooling absorption spectra (333 K to 298 K) of switches **3-a** in 70% DMSO with (a) 500 μM, (b) 100 μM, (c) 50 μM and (d) 0 μM H_2SO_4.

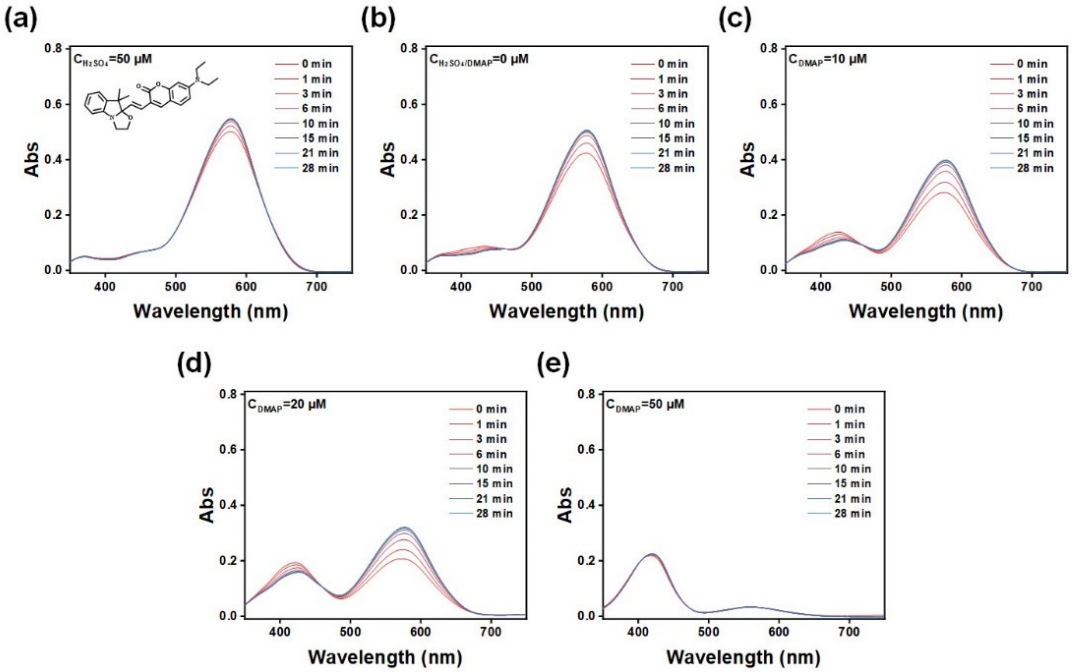


Figure S11. The time-resolved cooling absorption spectra (333 K to 298 K) of switches **3-e** in 70% DMSO with (a) 50 μM H_2SO_4, (b) no H_2SO_4 or DMAP, (c) 10 μM DMAP, (d) 20 μM DMAP and (e) 50 μM DMAP.

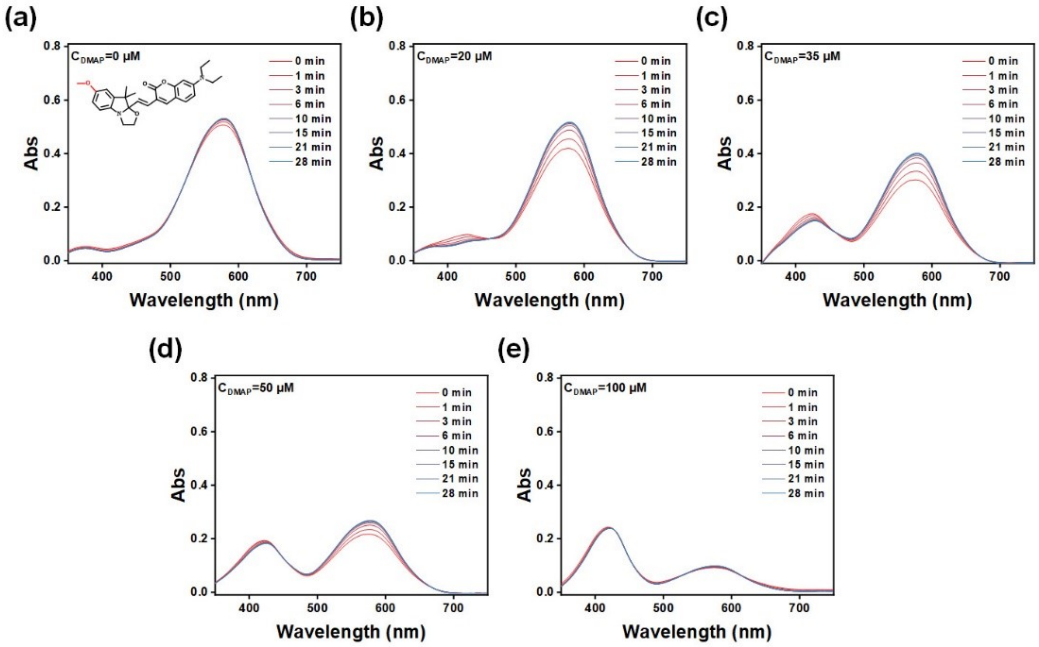
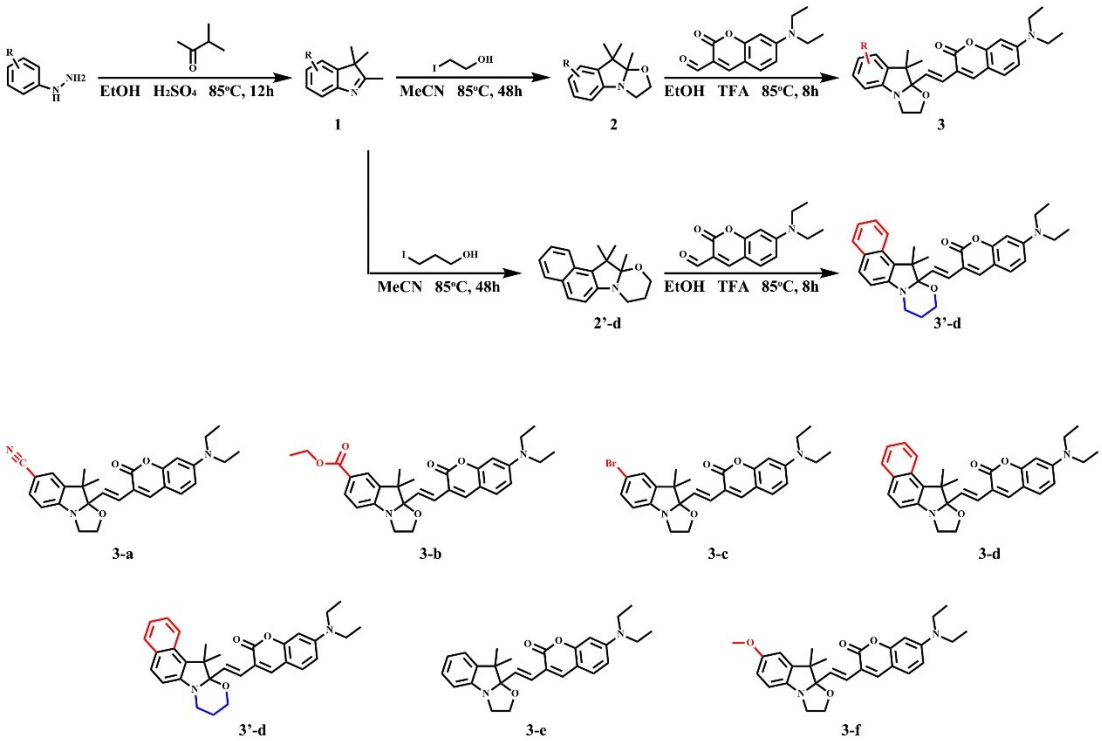


Figure S12. The time-resolved cooling absorption spectra (333 K to 298 K) of switches **3-f** in 70% DMSO with (a) 0 μM, (b) 20 μM, (c) 35 μM, (d) 50 μM and (e) 100 μM DMAP.



Scheme S1. Synthetic routes of the oxazine-based molecular switches.

3-a. 2-a (25.1 mg, 0.11 mmol, 1.1 equiv) and 3-aldehyde-7-diethylamino coumarin (24.5 mg, 0.1 mmol, 1equiv) were dissolved in 20 mL ethanol, and then 200 μL TFA was added as the catalytic agent. The reaction was stirred and heated to 85°C for 8 hours. After the reaction was

completed, the product was obtained by flash column chromatography [SiO_2, EtOAc/ PE (1:10, v/v) and triethylamine (5%, v%)] as a blue powder (39.6 mg, 86.9 % yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (s, 1H), 7.46 (dd, J = 8.1, 1.6 Hz, 1H), 7.30 (s, 1H), 7.26 (s, 1H), 6.79 (d, J = 2.2 Hz, 1H), 6.77 (d, J = 9.7 Hz, 1H), 6.63 (d, J = 15.8 Hz, 1H), 6.59 (dd, J = 8.8, 2.4 Hz, 1H), 6.50 (d, J = 2.5 Hz, 1H), 3.85-3.76 (m, 1H), 3.64 (td, J = 10.3, 7.3 Hz, 2H), 3.50 (dt, J = 10.7, 8.3 Hz, 1H), 3.42 (q, J = 7.1 Hz, 4H), 1.44 (s, 3H), 1.22 (t, J = 7.0 Hz, 6H), 1.17 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.14, 155.93, 155.25, 150.80, 141.10, 140.09, 132.90, 129.00, 127.60, 126.50, 126.36, 120.10, 116.40, 112.26, 109.91, 109.16, 108.74, 104.10, 97.13, 63.58, 49.62, 47.62, 44.92, 28.31, 20.33, 12.55. HRMS (m/z): $[M+H]^+$ calcd. for $C_{28}H_{29}N_3O_3$, 456.22817; found, 456.22722.

3-b. 3-b was synthesized referring to 3-a, in which 2-b (60.6 mg, 0.22 mmol, 1 equiv) and 3-aldehyde-7-diethylamino coumarin (49.1 mg, 0.2 mmol, 1equiv) were reacted as raw agents. The product was saved as a brown solid (53.2 mg, 51.7 % yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.75 (s, 1H), 7.59 (s, 1H), 7.27 (d, *J* = 8.8 Hz, 1H), 6.80 (d, *J* = 9.3 Hz, 1H), 6.77 (s, 1H), 6.66 (d, *J* = 15.9 Hz, 1H), 6.58 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.50 (d, *J* = 2.4 Hz, 1H), 4.35 (q, *J* = 7.1 Hz, 2H), 3.84-3.76 (m, 1H), 3.73 – 3.58 (m, 2H), 3.55-3.46 (m, 1H), 3.42 (q, *J* = 7.1 Hz, 4H), 1.47 (s, 3H), 1.38 (t, *J* = 7.1 Hz, 3H), 1.22 (t, *J* = 7.0 Hz, 6H), 1.19 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.86, 161.17, 155.89, 155.44, 150.70, 140.04, 139.79, 130.43, 128.96, 127.25, 127.14, 124.12, 123.82, 116.68, 111.31, 110.22, 109.10, 108.80, 97.14, 63.59, 60.58, 49.74, 47.59, 44.90, 28.42, 20.48, 14.53, 12.55. HRMS (m/z): $[M+H]^+$ calcd. for $C_{30}H_{34}N_2O_5$, 503.25405; found, 503.25349.

3-c. 3-c was synthesized referring to 3-a, in which 2-b (60.6 mg, 0.22 mmol, 1.1 equiv) and 3-aldehyde-7-diethylamino coumarin (49.1 mg, 0.2 mmol, 1equiv) were reacted as raw agents. The product was saved as a brown solid (53.2 mg, 51.7 % yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (s, 1H), 7.26 (s, 1H), 7.25-7.23 (m, 1H), 7.15 (d, *J* = 2.0 Hz, 1H), 6.78 (d, *J* = 15.8 Hz, 1H), 6.66 (d, *J* = 2.0 Hz, 1H), 6.63 (d, *J* = 9.5 Hz, 1H), 6.58 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.50 (d, *J* = 2.4 Hz, 1H), 3.78 (dd, *J* = 8.0, 4.2 Hz, 1H), 3.67-3.55 (m, 2H), 3.50-3.44 (m, 1H), 3.45-3.39 (m, 4H), 1.41 (s, 3H), 1.22 (t, *J* = 7.0 Hz, 6H), 1.16 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.16, 155.88, 150.67, 150.09, 142.33, 139.71, 130.31, 128.93, 127.37, 127.16, 125.70, 116.77, 113.68, 113.61, 110.29, 109.08, 108.81, 97.16, 63.58, 50.18, 48.08, 44.91, 28.43, 20.32, 12.55. HRMS (m/z): $[M+H]^+$ calcd. for $C_{27}H_{29}BrN_2O_3$, 509.14343; found, 509.14330.

3-d. 3-d was synthesized referring to 3-a, in which 2-d (83.6 mg, 0.33 mmol, 1.1 equiv) and 3-aldehyde-7-diethylamino coumarin (73.6 mg, 0.3 mmol, 1equiv) were reacted as raw agents. The product was saved as a green powder (103.1 mg, 71.6 % yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.5 Hz, 1H), 7.81 (d, *J* = 8.2 Hz, 1H), 7.72 (d, *J* = 8.6 Hz, 1H), 7.62 (s, 1H), 7.47-7.40 (m, 1H), 7.28 (s, 2H), 7.12 (d, *J* = 8.7 Hz, 1H), 6.87 (d, *J* = 15.8 Hz, 1H), 6.76 (d, *J* = 15.8 Hz, 1H), 6.58 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.50 (d, *J* = 2.5 Hz, 1H), 3.88-3.78 (m, 2H), 3.65-3.49 (m, 2H), 3.42 (q, *J* = 7.1 Hz, 4H), 1.80 (s, 3H), 1.39 (s, 3H), 1.22 (t, *J* = 7.0 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.24, 155.88, 150.62, 147.80, 139.54, 130.81, 130.38, 130.01, 129.42, 129.03, 128.92, 127.90, 127.13, 126.25, 122.70, 122.24, 117.03, 114.10, 110.60, 109.06, 108.89, 97.19, 63.42, 50.24, 49.62, 44.90, 26.59, 21.70, 12.56. HRMS (m/z): $[M+H]^+$ calcd. for $C_{31}H_{32}N_2O_3$, 481.24857; found, 481.24727.

3'-d. 3'-d was synthesized referring to 3-a, in which 2'-d (88.2 mg, 0.33 mmol, 1.1 equiv) and 3-aldehyde-7-diethylamino coumarin (73.6 mg, 0.3 mmol, 1equiv) were reacted as raw agents.

The product was saved as a green powder (111.5 mg, 75.1 % yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.6 Hz, 1H), 7.77 (d, *J* = 8.2 Hz, 1H), 7.72 (d, *J* = 8.6 Hz, 1H), 7.66 (s, 1H), 7.37 (dd, *J* = 8.5, 6.8 Hz, 1H), 7.28 (d, *J* = 18.1 Hz, 2H), 7.20 (t, *J* = 7.5 Hz, 1H), 6.85 (d, *J* = 16.4 Hz, 1H), 6.69 (d, *J* = 16.4 Hz, 1H), 6.59 (dd, *J* = 8.8, 2.5 Hz, 1H), 6.53 (d, *J* = 2.4 Hz, 1H), 4.11 (td, *J* = 11.8, 2.3 Hz, 1H), 3.86-3.70 (m, 2H), 3.61 (td, *J* = 13.6, 2.9 Hz, 1H), 3.43 (q, *J* = 7.1 Hz, 4H), 2.06-1.93 (m, 2H), 1.68 (s, 3H), 1.23 (t, *J* = 7.0 Hz, 6H), 1.18 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.28, 155.92, 150.68, 145.71, 139.32, 130.77, 129.74, 129.57, 129.42, 128.96, 128.69, 128.57, 128.27, 126.03, 121.91, 121.66, 117.08, 111.50, 109.12, 108.88, 102.09, 97.21, 62.55, 51.21, 44.92, 40.50, 25.37, 22.99, 20.23, 12.57. HRMS (m/z): $[M+H]^+$ calcd. for $C_{32}H_{34}N_2O_3$, 495.26422; found, 495.26289.

3-e. 3-e was synthesized referring to 3-a, in which 2-e (22.4 mg, 0.11 mmol, 1.1 equiv) and 3-aldehyde-7-diethylamino coumarin (24.5 mg, 0.1 mmol, 1equiv) were reacted as raw agents. The product was saved as a light green powder (22.3 mg, 51.8 % yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (s, 1H), 7.25 (d, *J* = 3.4 Hz, 1H), 7.16 (t, *J* = 7.6 Hz, 1H), 7.07 (d, *J* = 7.3 Hz, 1H), 6.93 (t, *J* = 7.4 Hz, 1H), 6.85-6.76 (m, 2H), 6.67 (d, *J* = 15.9 Hz, 1H), 6.58 (dd, *J* = 8.8, 2.5 Hz, 1H), 6.50 (d, *J* = 2.5 Hz, 1H), 3.82-3.76 (m, 1H), 3.63 (td, *J* = 12.9, 5.3 Hz, 2H), 3.50-3.45 (m, 1H), 3.42 (q, *J* = 7.2 Hz, 4H), 1.44 (s, 3H), 1.22 (t, *J* = 7.1 Hz, 6H), 1.17 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.21, 155.86, 150.82, 150.60, 139.90, 139.45, 128.89, 128.06, 127.56, 126.78, 122.41, 121.58, 117.02, 112.05, 110.18, 109.04, 108.87, 97.18, 63.57, 50.23, 47.95, 44.90, 28.59, 20.48, 12.56. HRMS (m/z): $[M+H]^+$ calcd. for $C_{27}H_{30}N_2O_3$, 431.23292; found, 431.23189.

3-f. 3-f was synthesized referring to 3-a, in which 2-f (25.7 mg, 0.11 mmol, 1.1 equiv) and 3-aldehyde-7-diethylamino coumarin (24.5 mg, 0.1 mmol, 1equiv) were reacted as raw agents. The product was saved as a dark blue solid (20.2 mg, 43.9% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (s, 1H), 7.26 (s, 1H), 6.81 (d, *J* = 15.8 Hz, 1H), 6.68 (d, *J* = 10.5 Hz, 4H), 6.57 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.48 (d, *J* = 2.4 Hz, 1H), 3.77 (s, 4H), 3.64-3.56 (m, 2H), 3.40 (q, *J* = 7.0 Hz, 5H), 1.43 (s, 3H), 1.20 (t, *J* = 7.2 Hz, 6H), 1.17 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.19, 155.84, 155.41, 150.60, 144.34, 141.27, 139.54, 128.94, 128.08, 126.83, 116.94, 112.41, 112.30, 110.76, 109.08, 108.85, 97.10, 63.62, 55.83, 50.64, 48.24, 44.89, 28.53, 20.36, 12.56. HRMS (m/z): $[M+H]^+$ calcd. for $C_{28}H_{32}N_2O_4$, 461.24348; found, 461.24233.

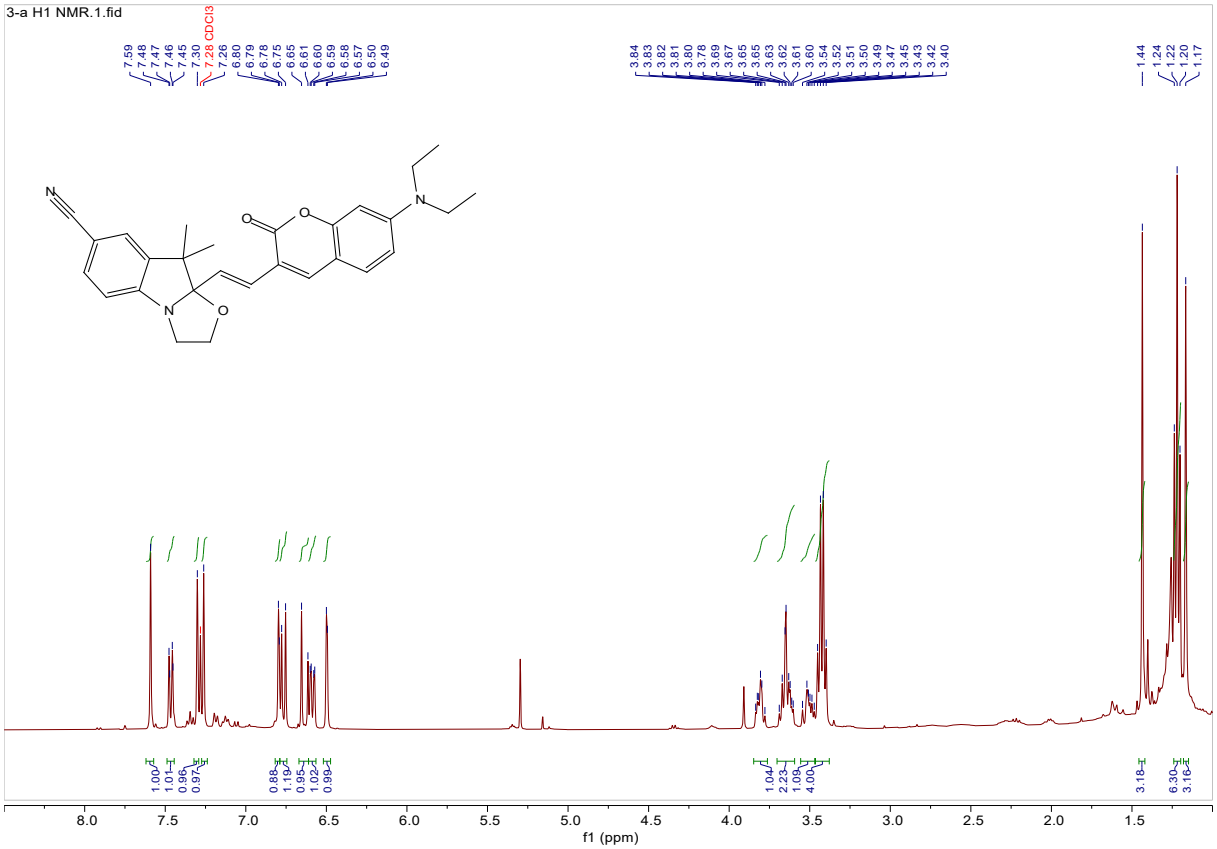


Figure S13. ^{1}H NMR of 3-a.

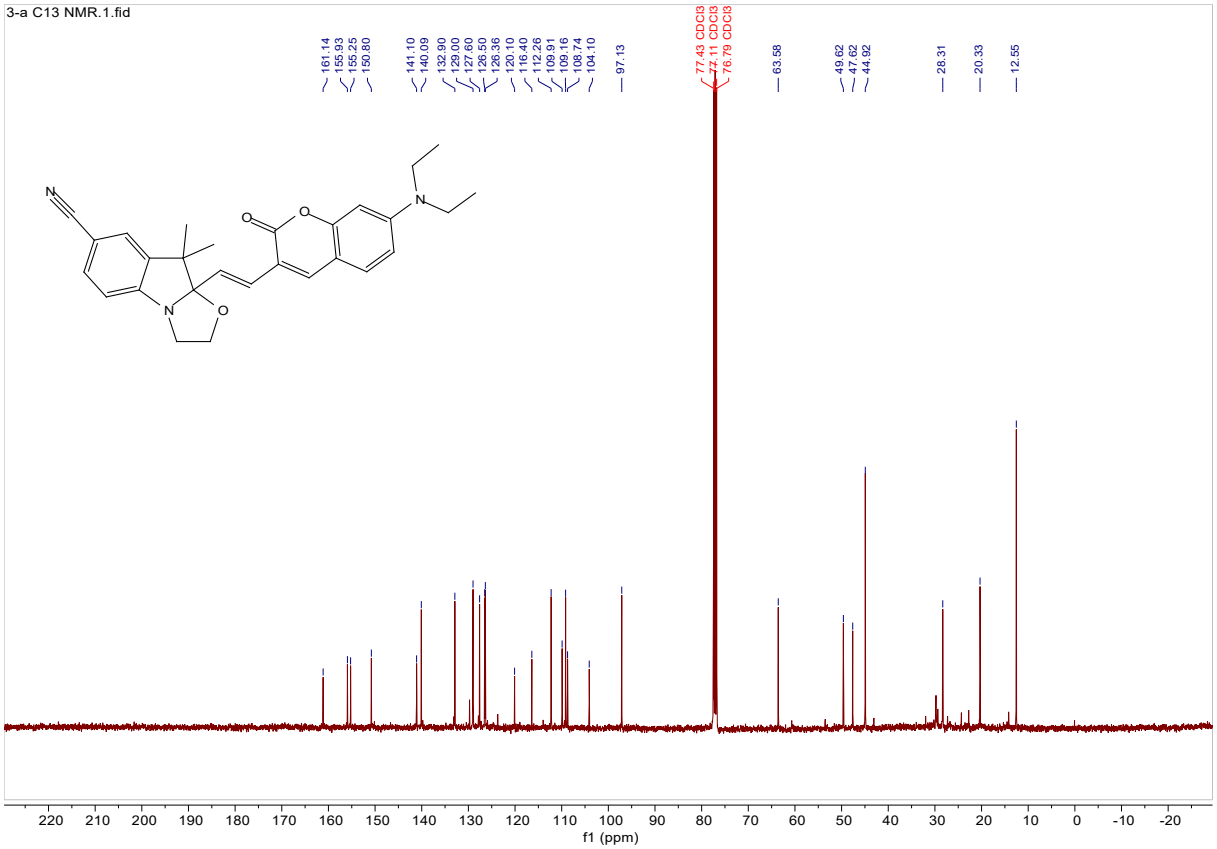


Figure S14. ^{13}C NMR of 3-a.

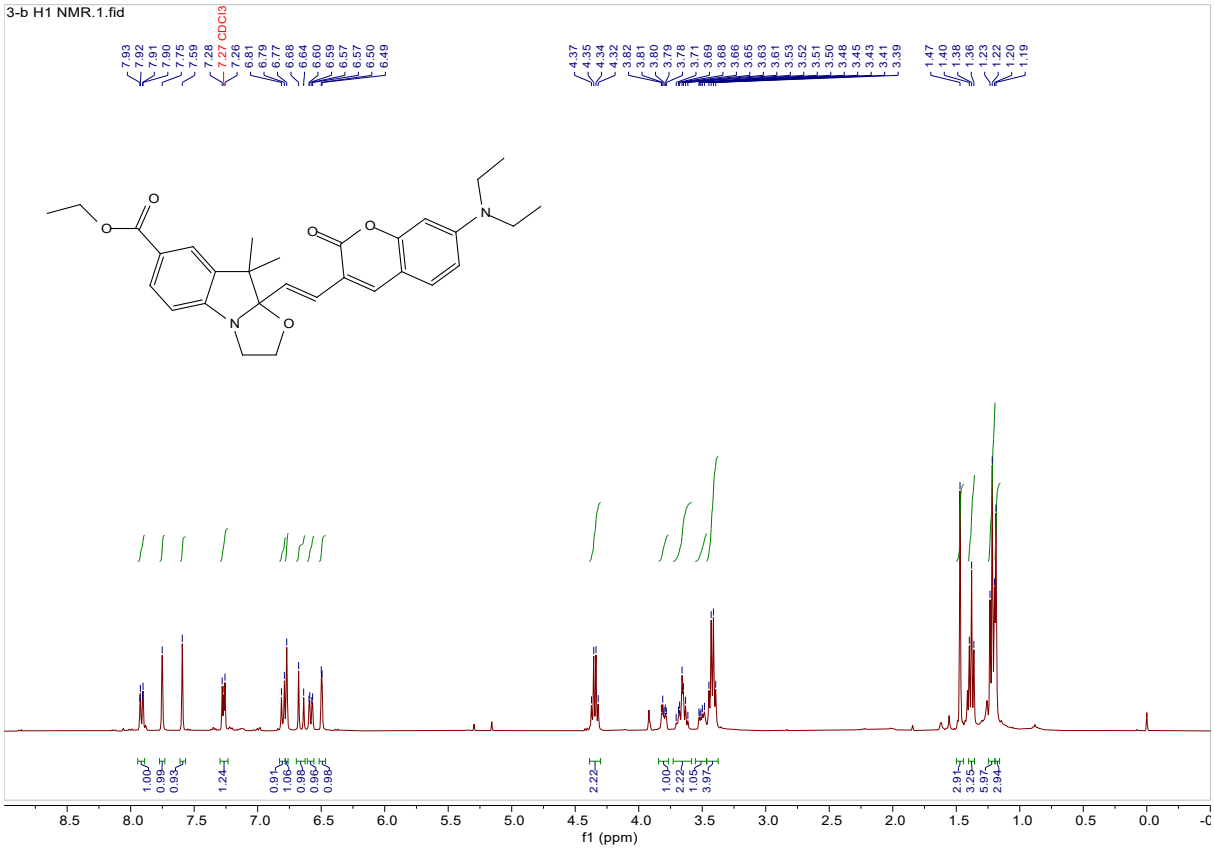


Figure S15. ^{1}H NMR of 3-b.

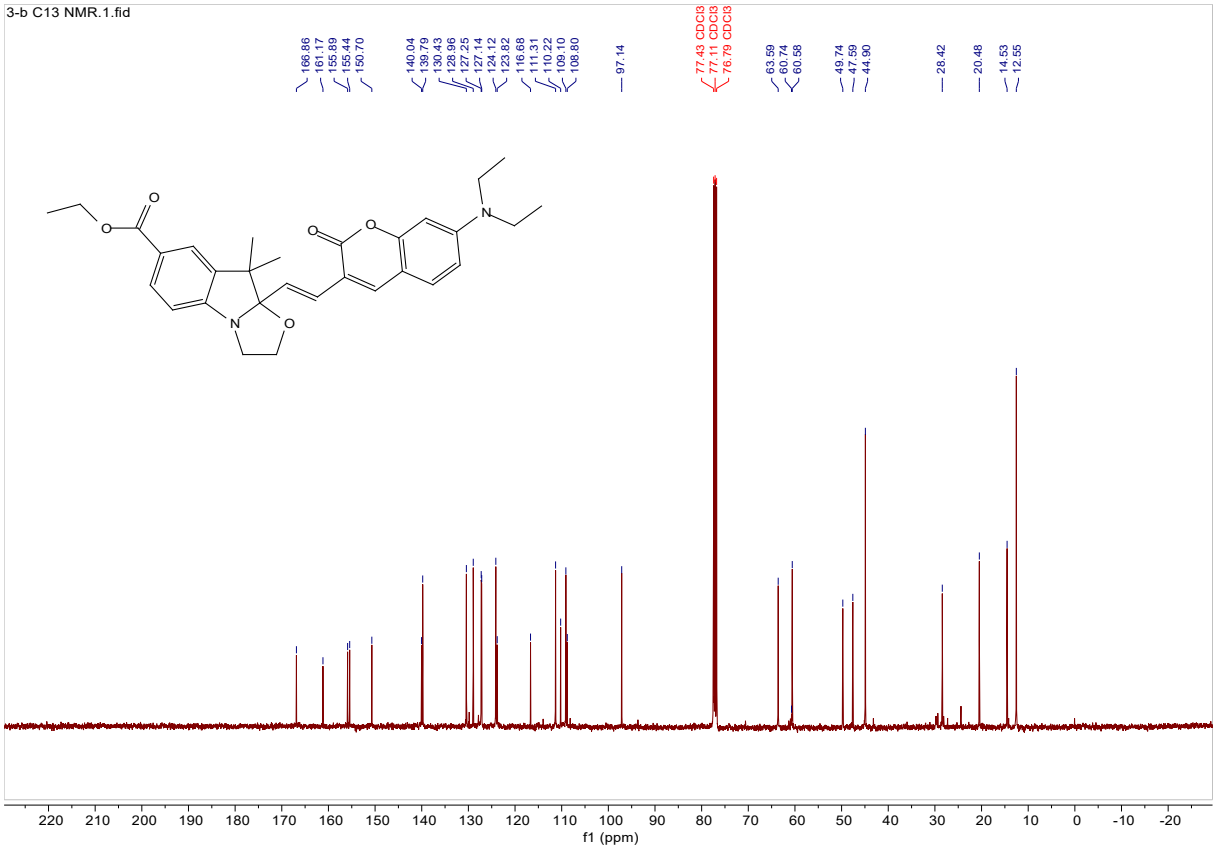


Figure S16. ^{13}C NMR of 3-b.

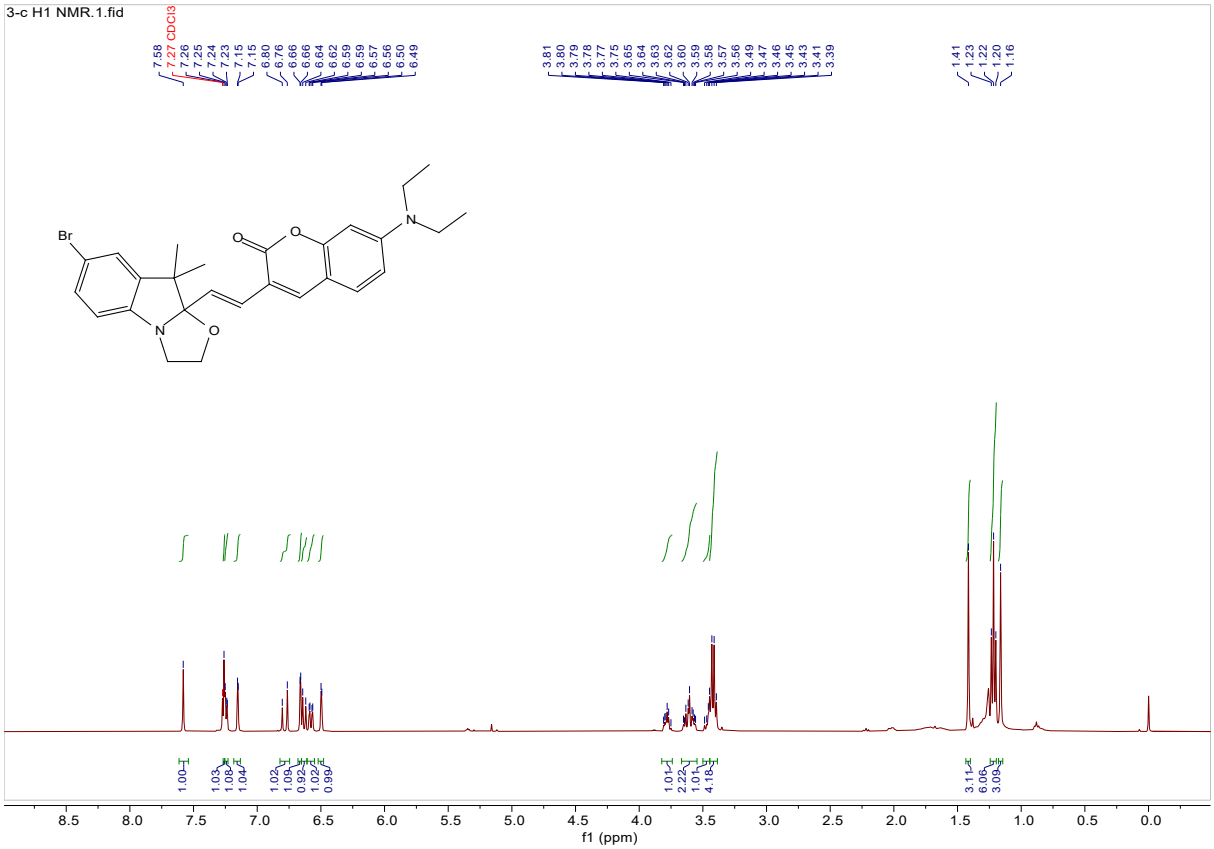


Figure S17. ^{1}H NMR of 3-c.

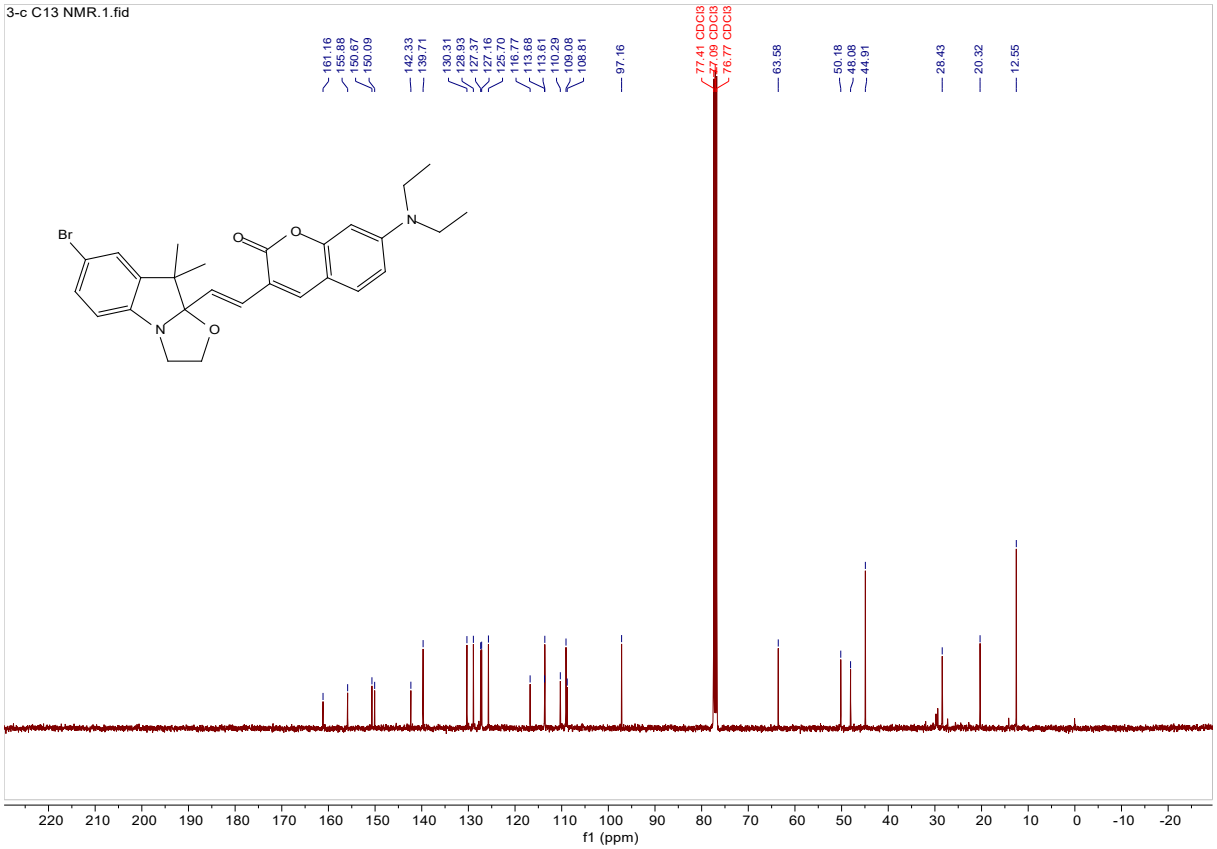


Figure S18. ^{13}C NMR of 3-c.

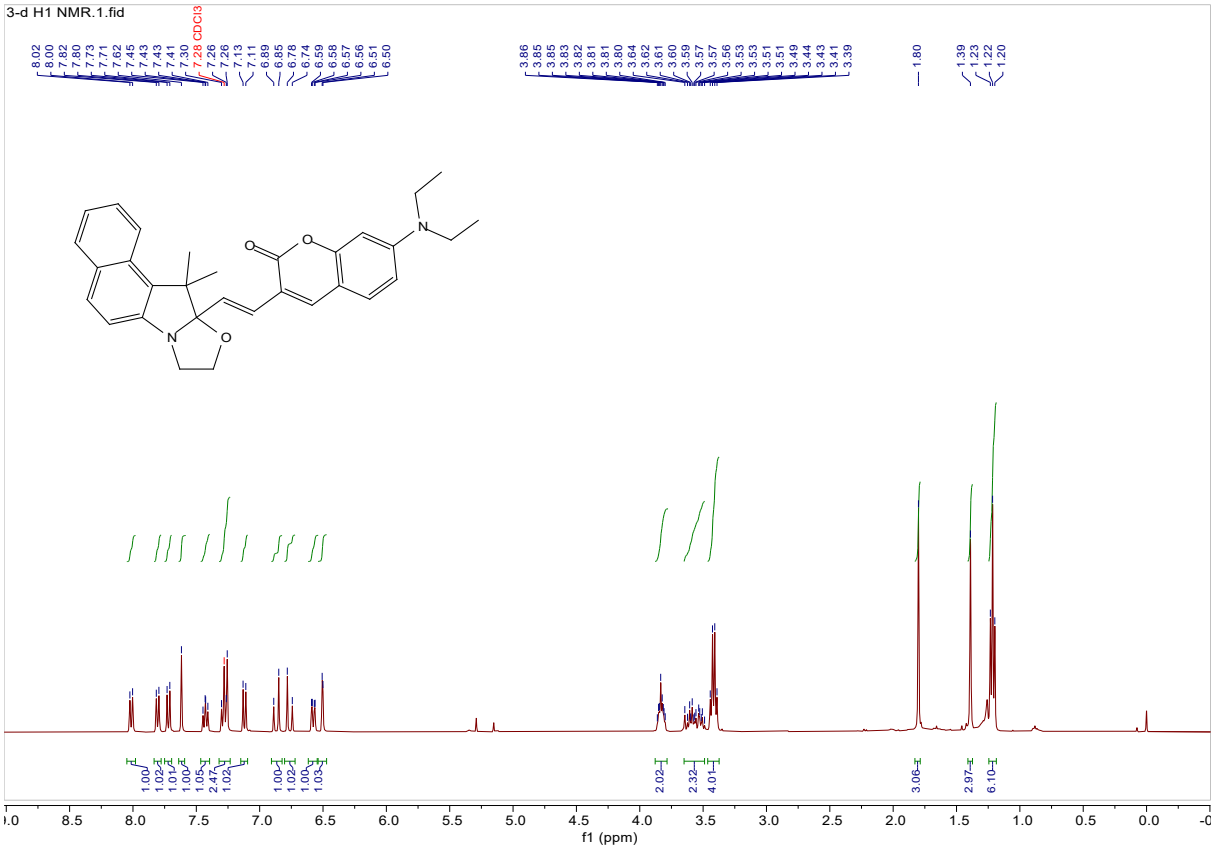


Figure S19. ^{1}H NMR of 3-d.

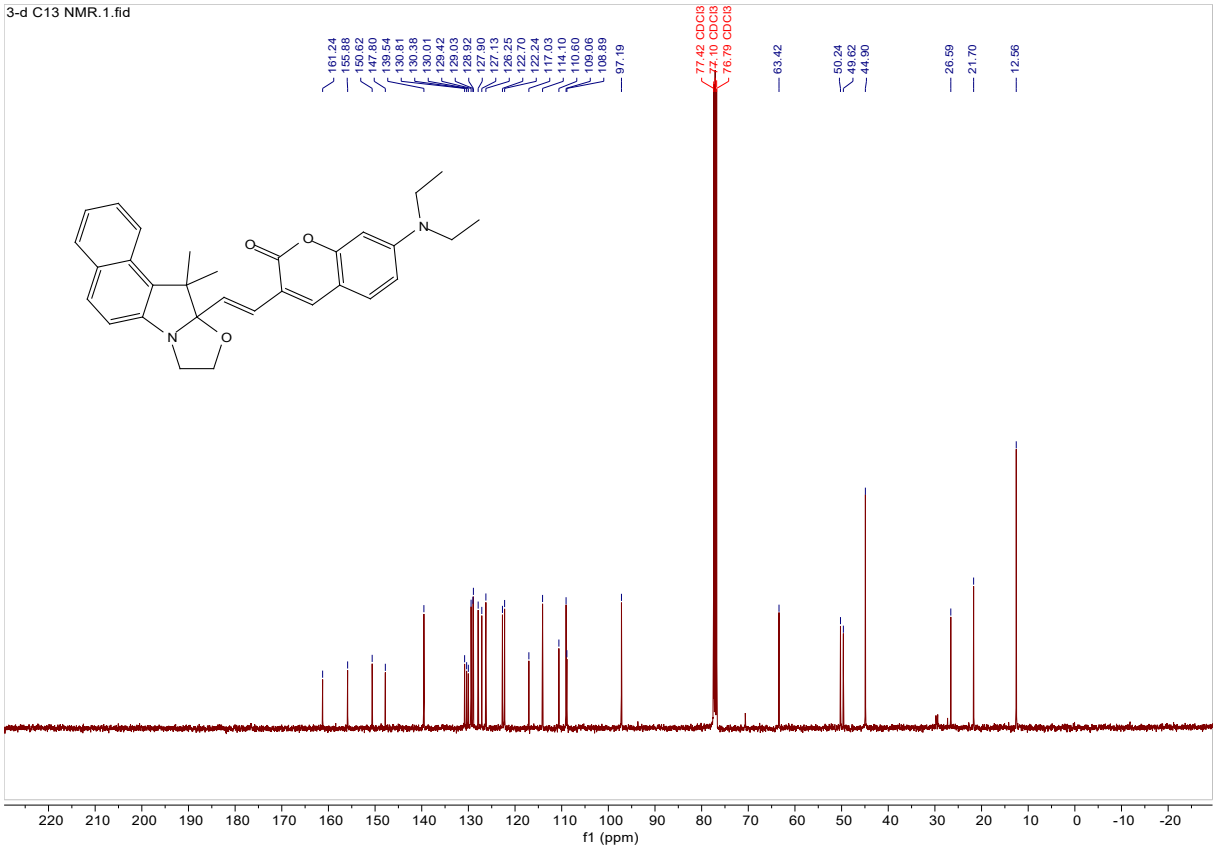


Figure S20. ^{13}C NMR of 3-d.

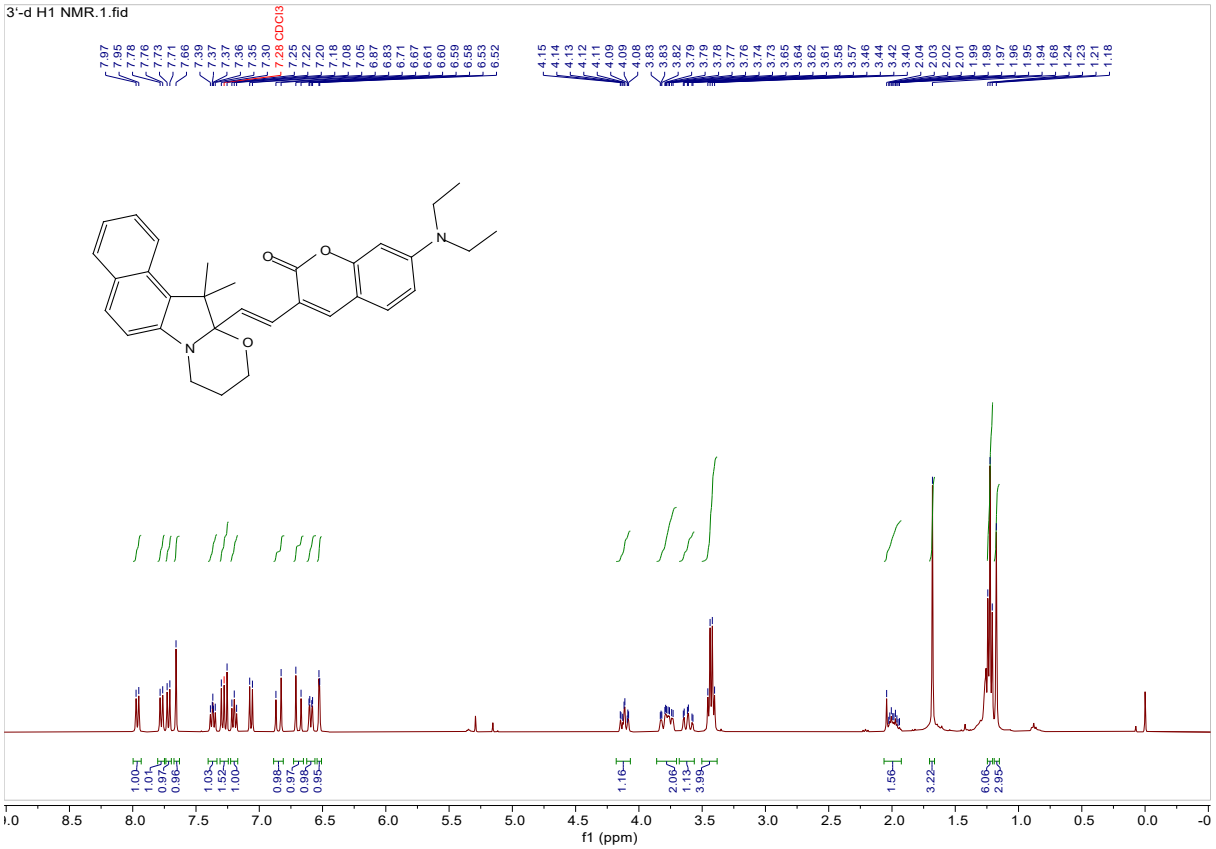


Figure S21. ^{1}H NMR of 3'-d.

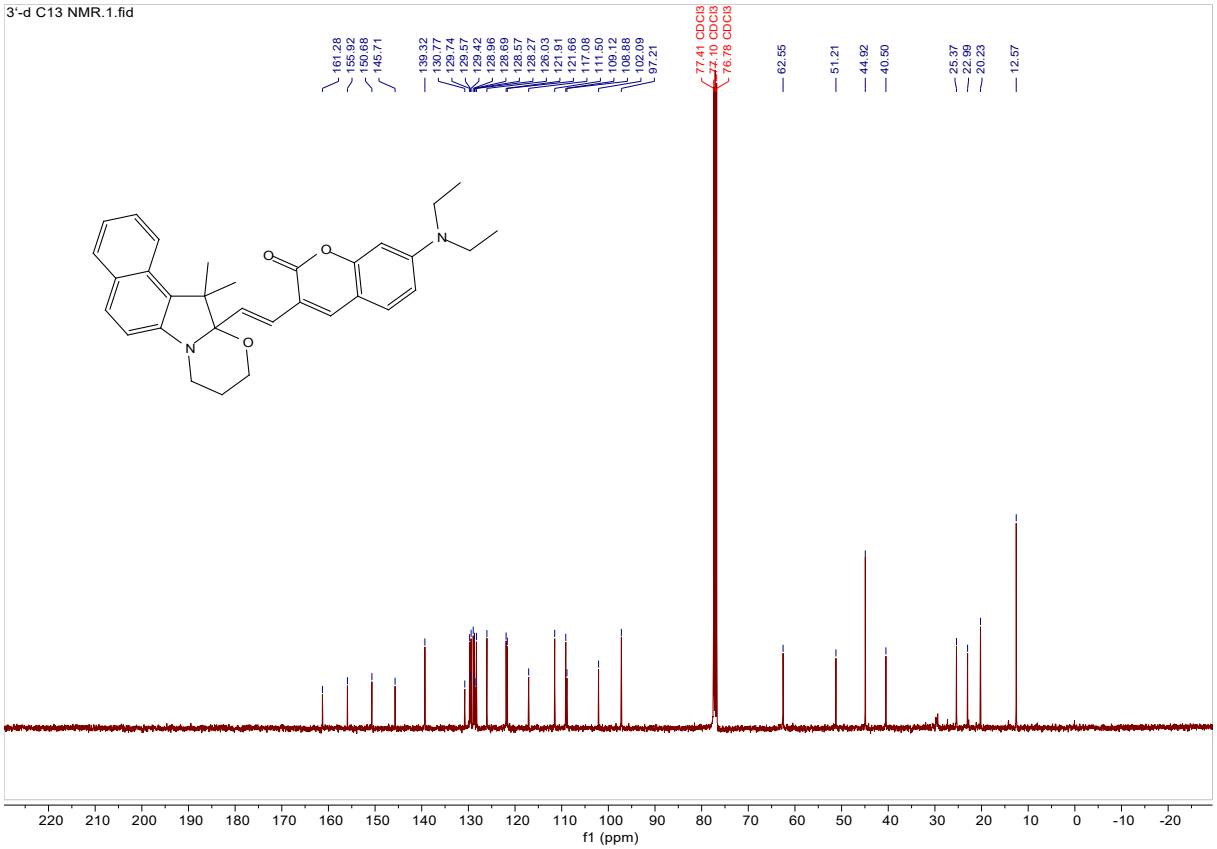


Figure S22. ^{1}H NMR of 3'-d.

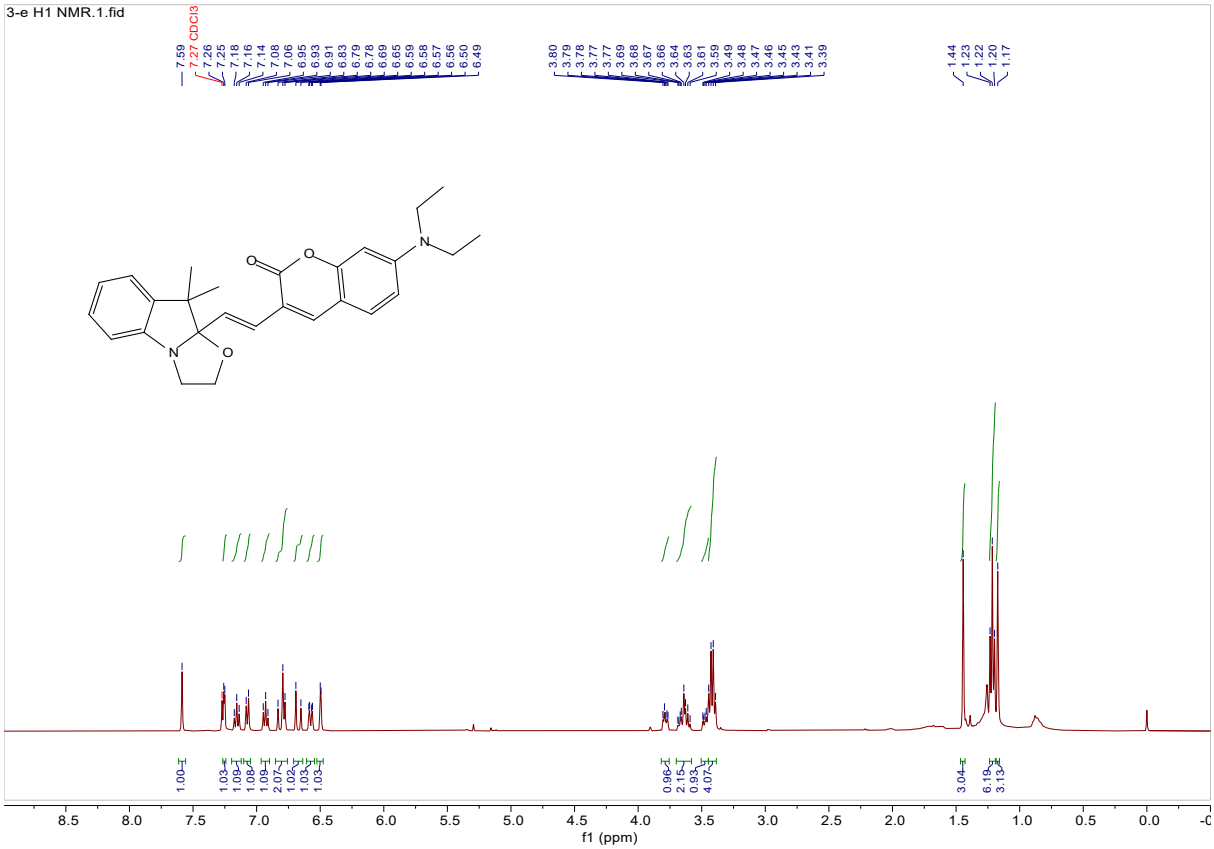


Figure S23. ^{1}H NMR of 3-e.

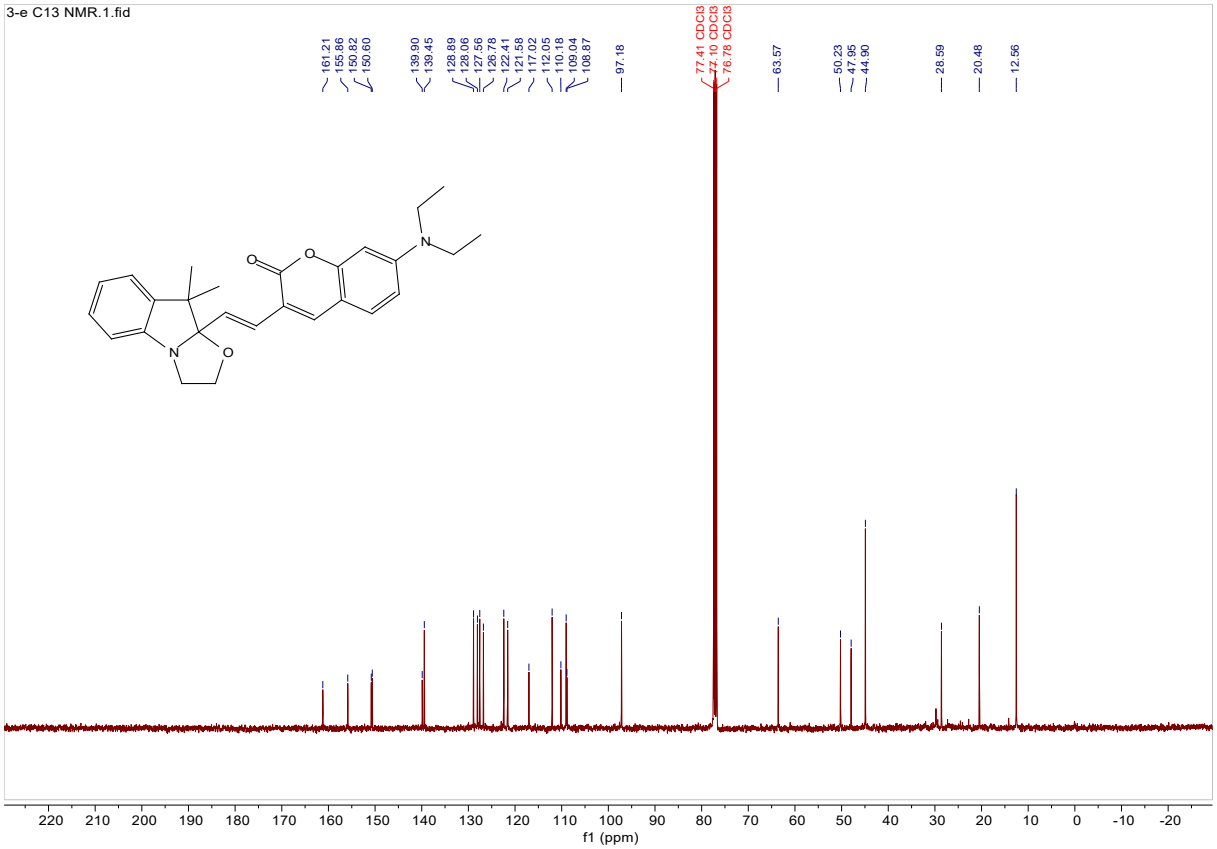


Figure S24. ^{13}C NMR of 3-e.

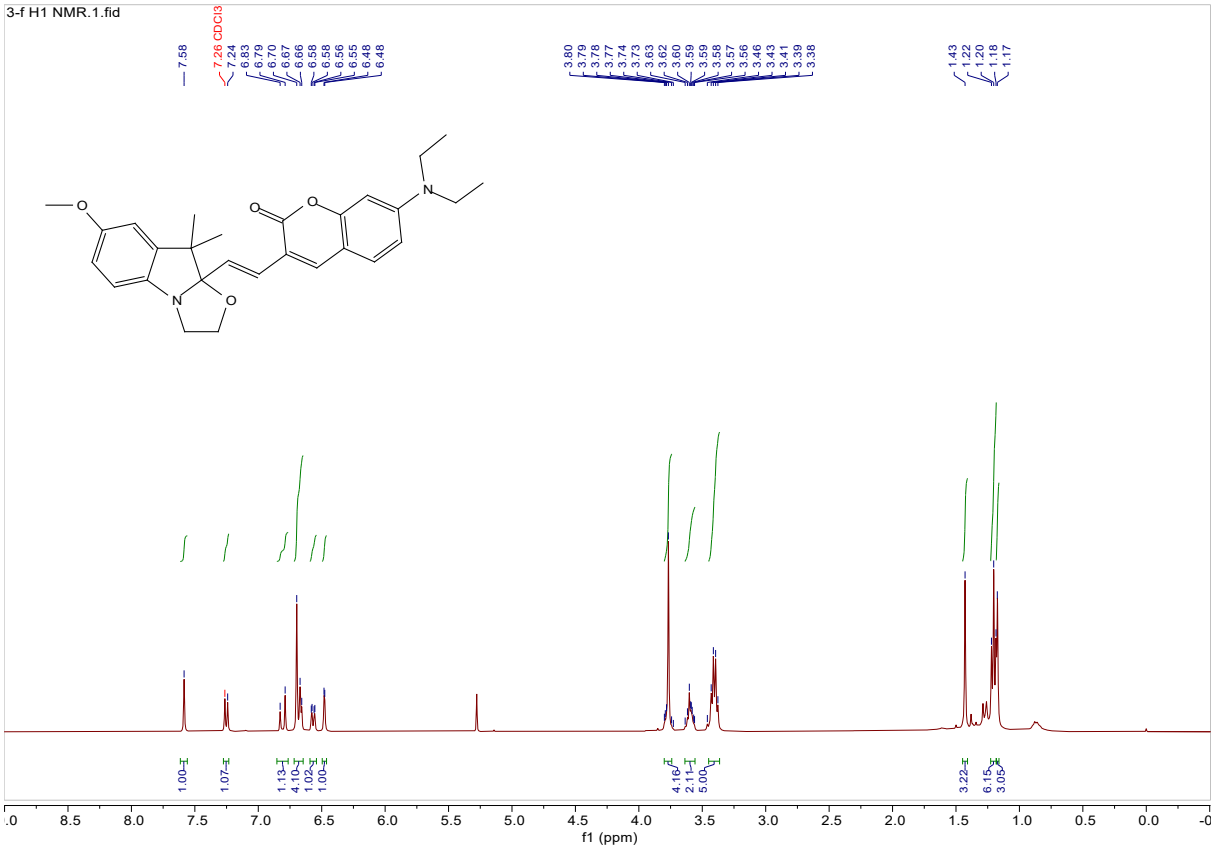


Figure S25. ^{1}H NMR of 3-f.

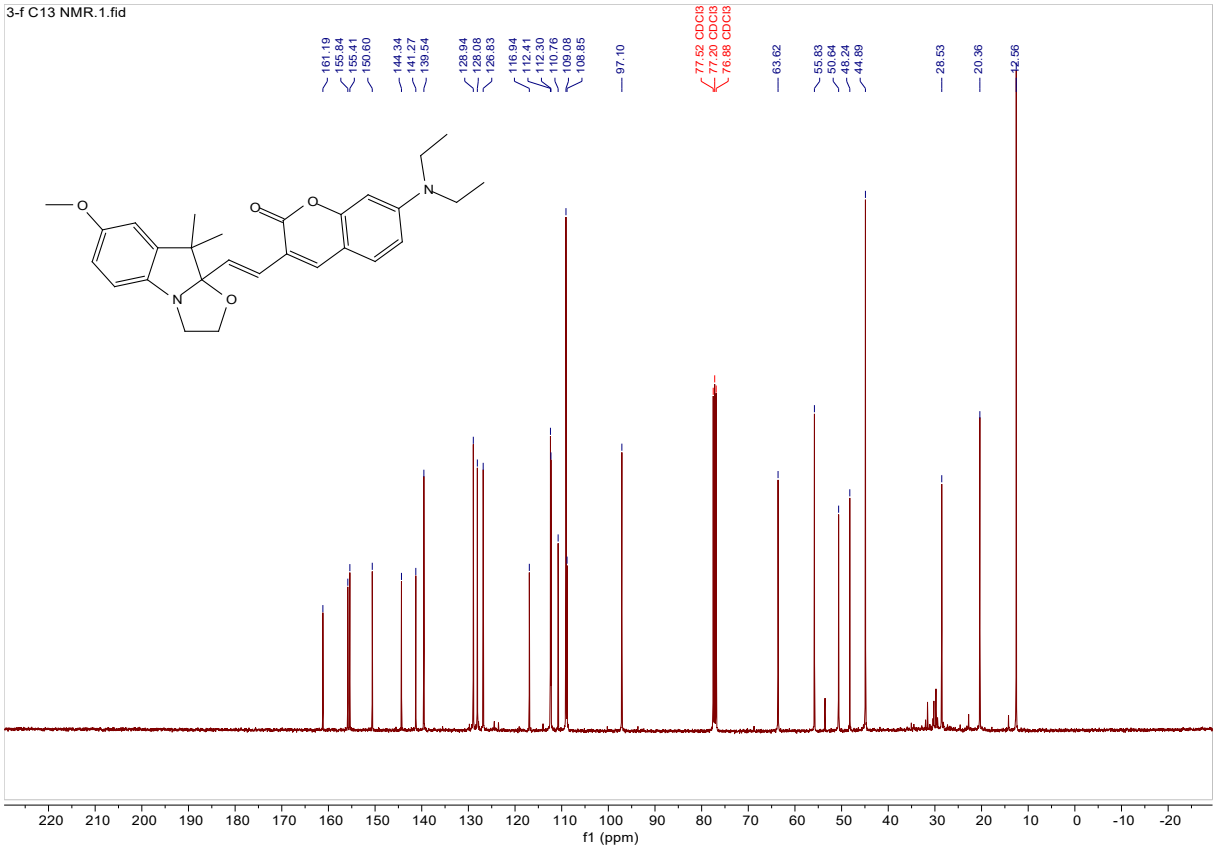


Figure S26. ^{13}C NMR of 3-f.

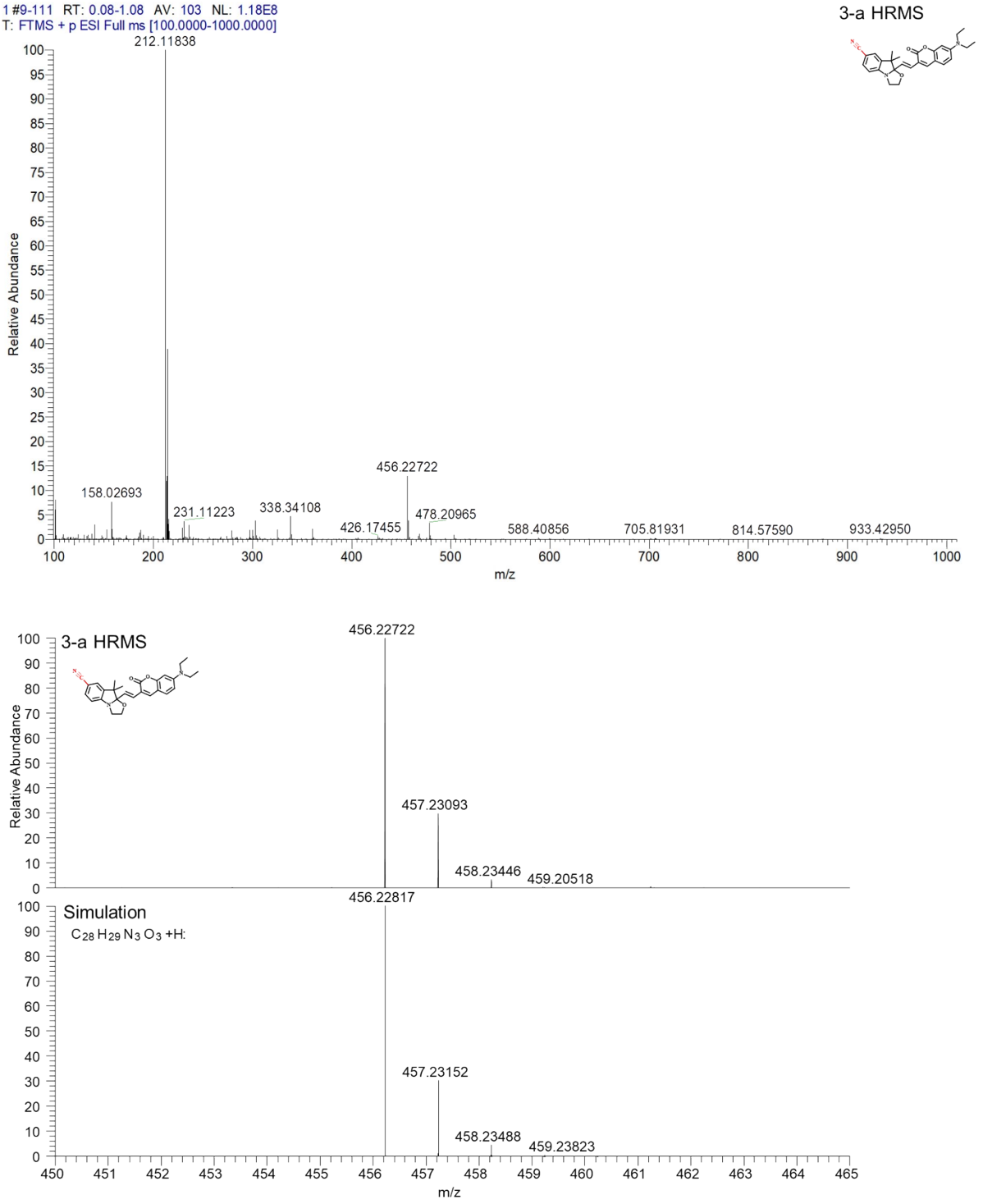


Figure S27. HRMS of 3-a.

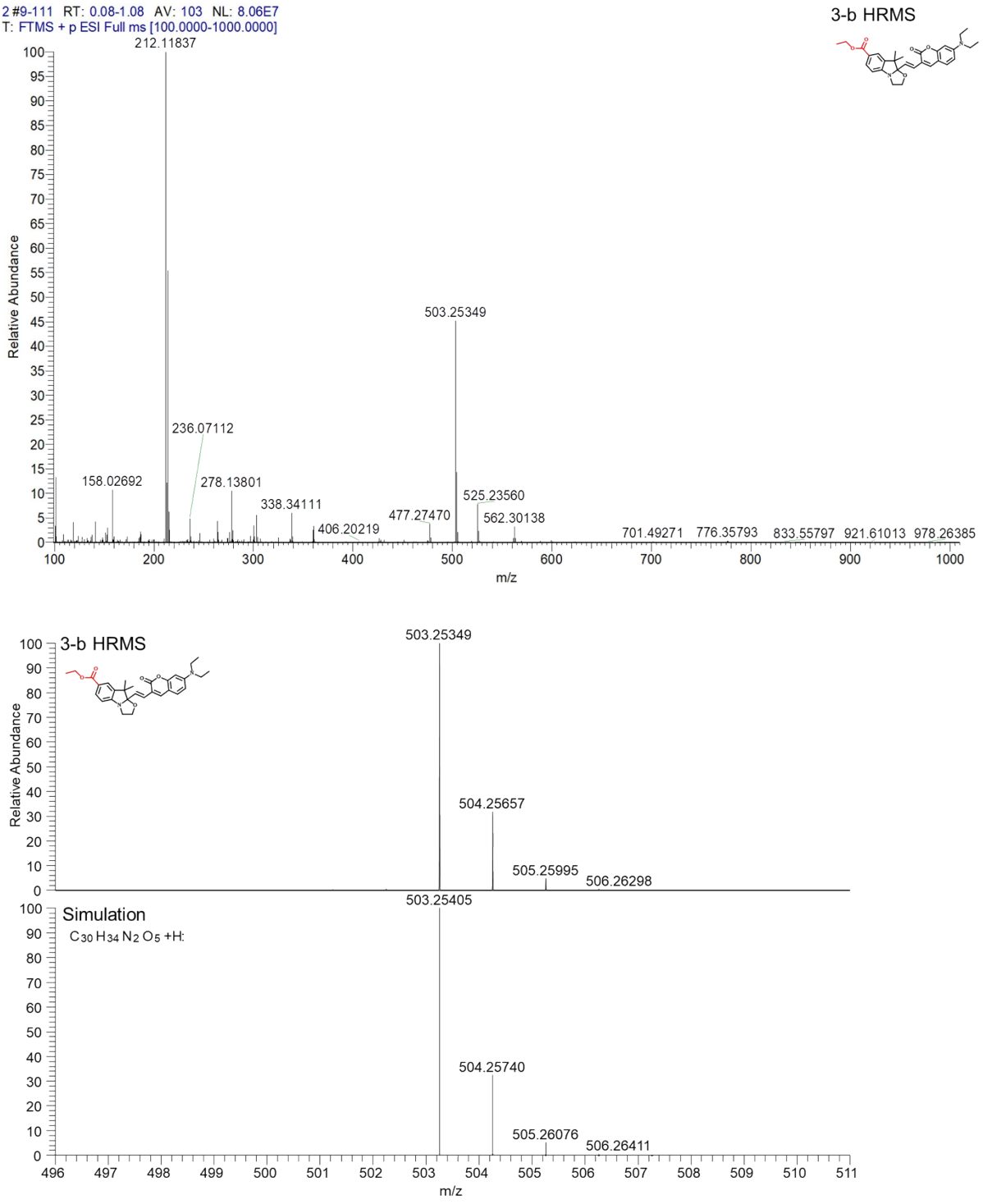


Figure S28. HRMS of 3-b.

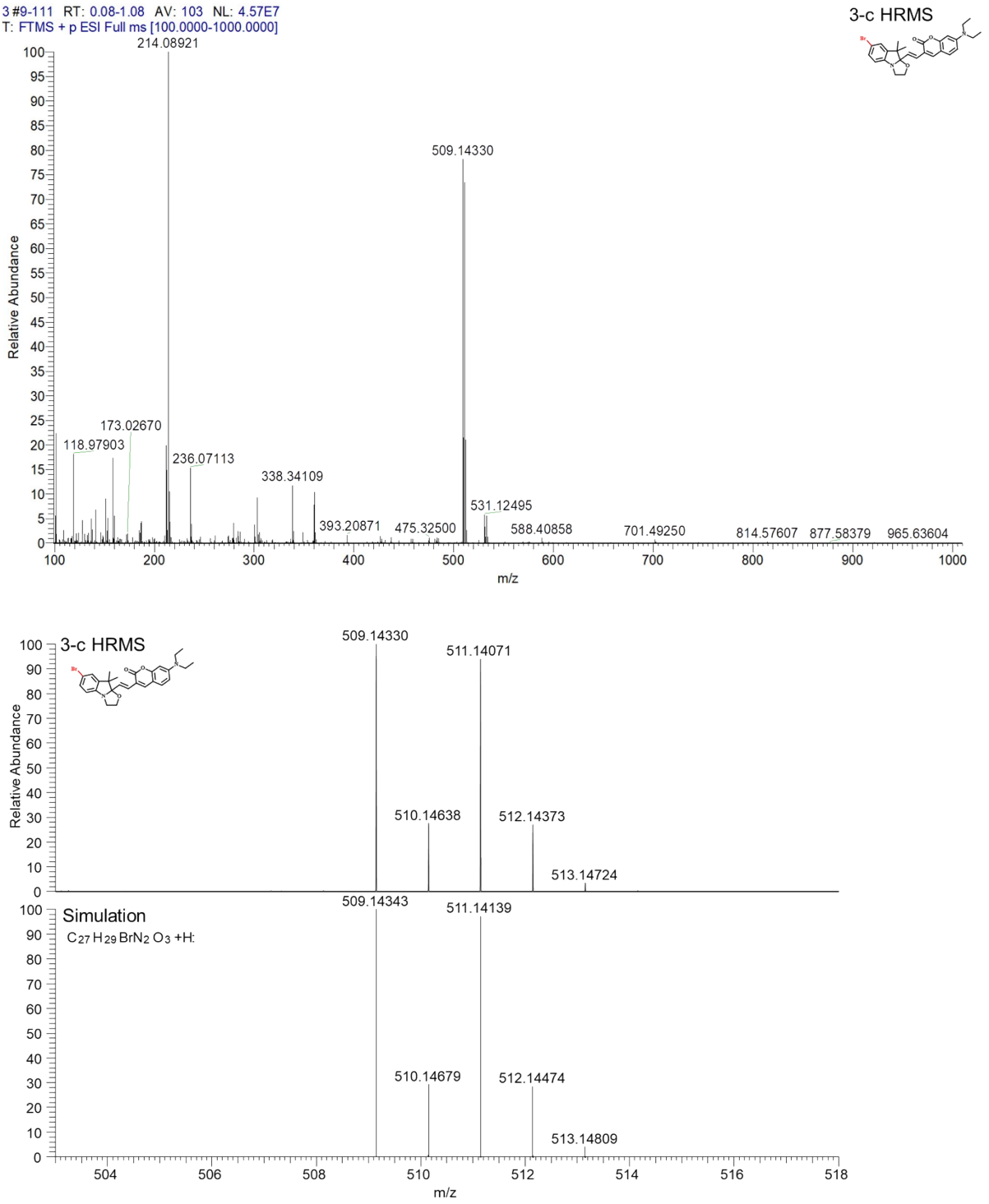


Figure S29. HRMS of 3-c.

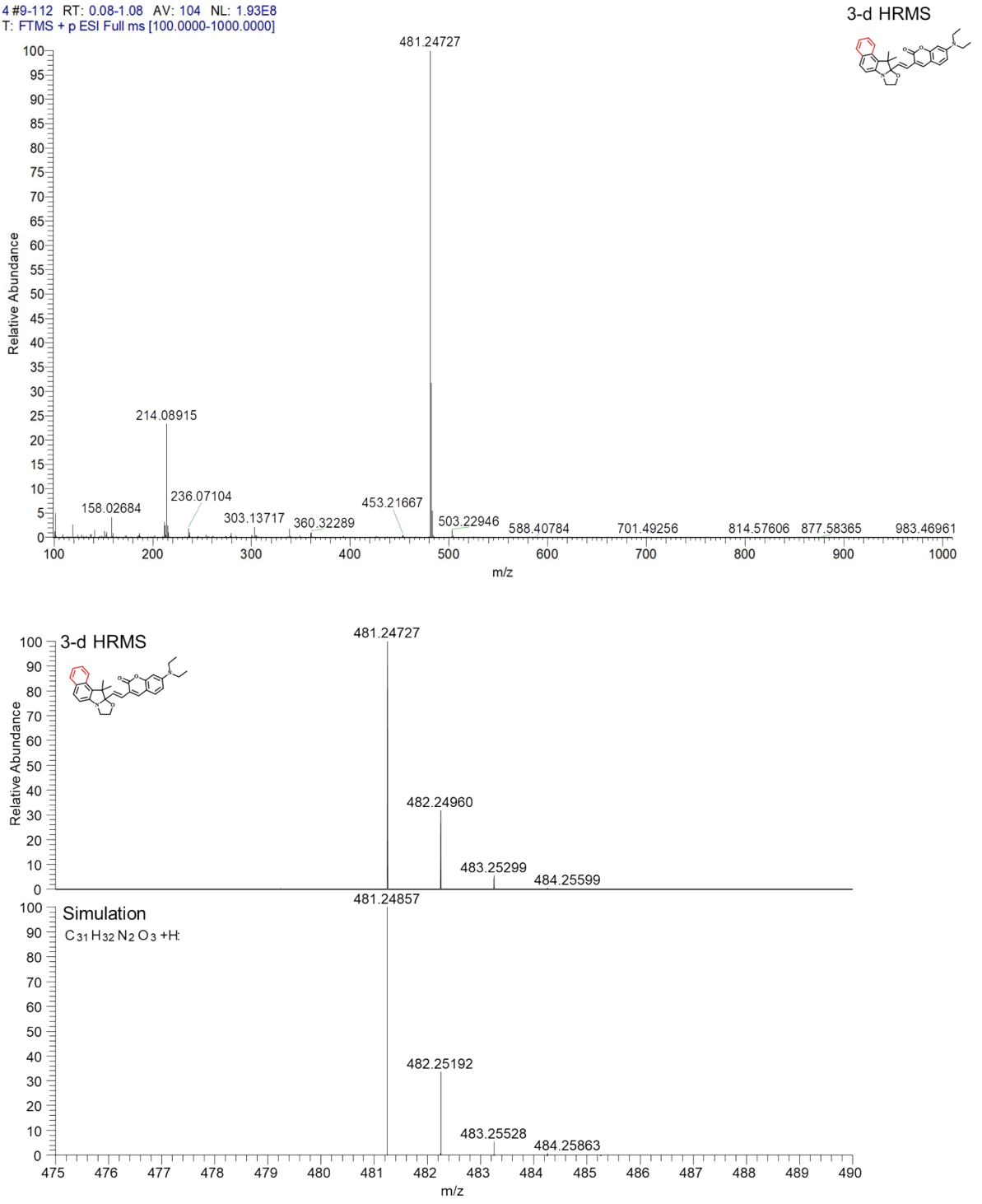


Figure S30. HRMS of 3-d.

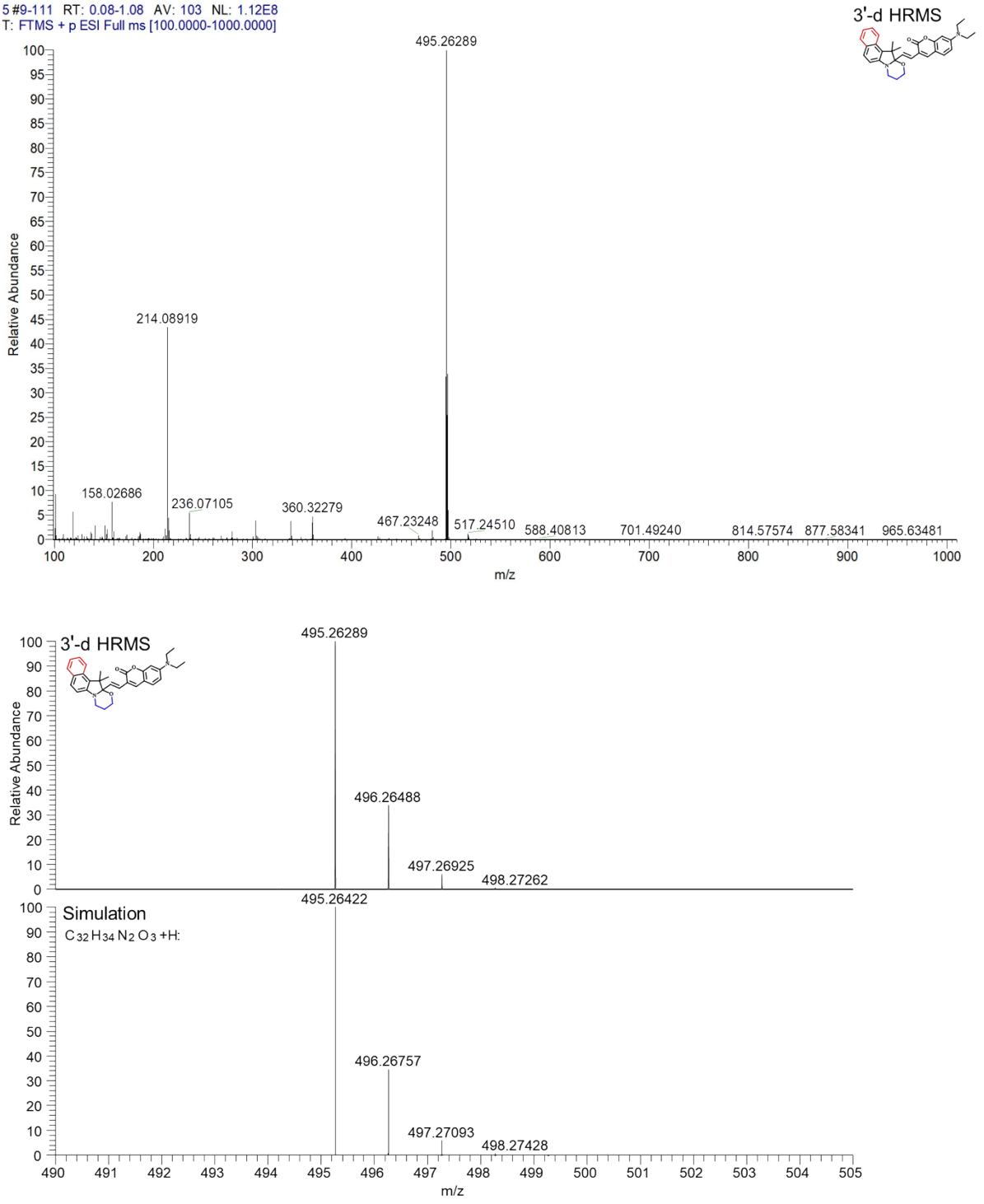


Figure S31. HRMS of 3’-d.

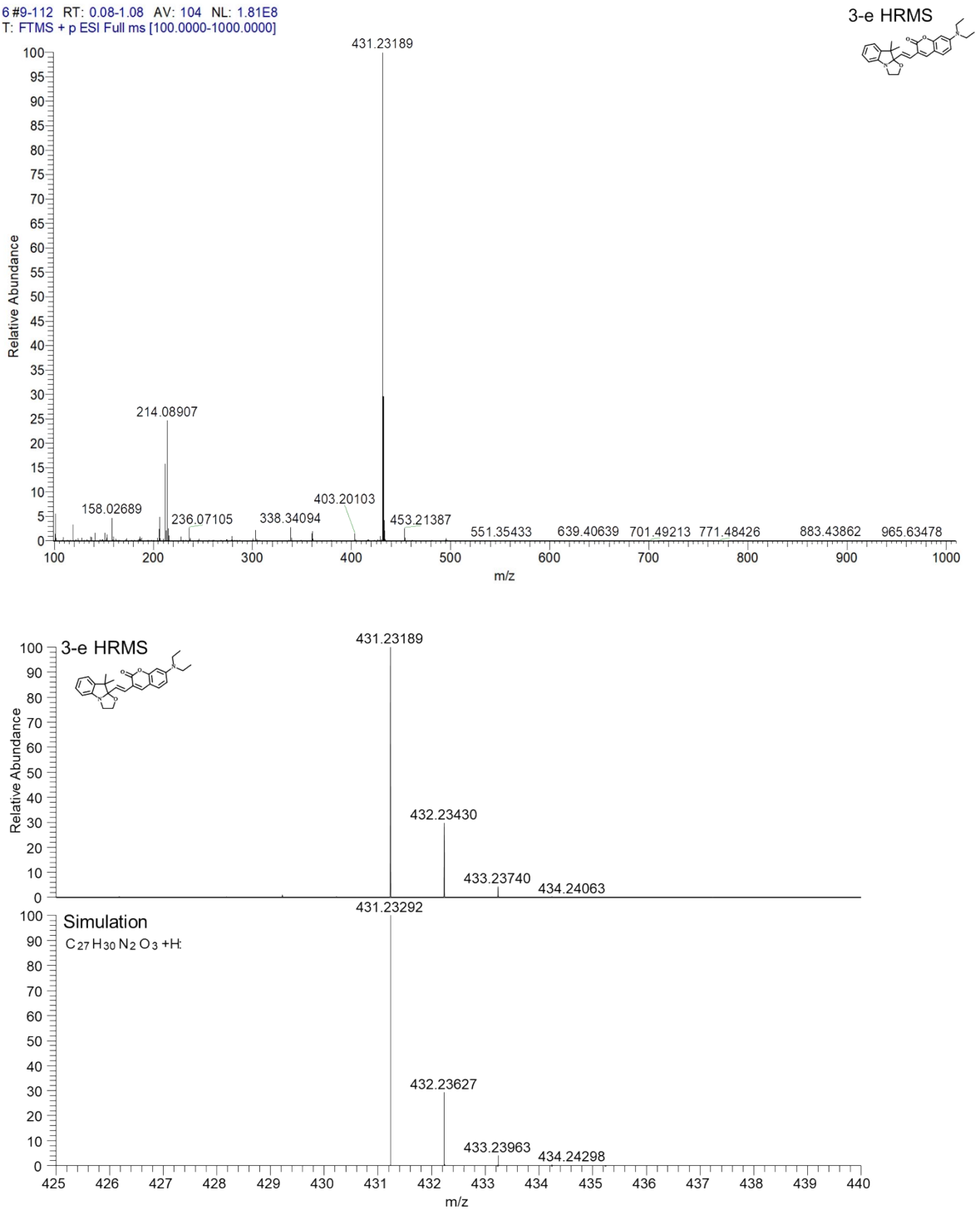


Figure S32. HRMS of 3-e.

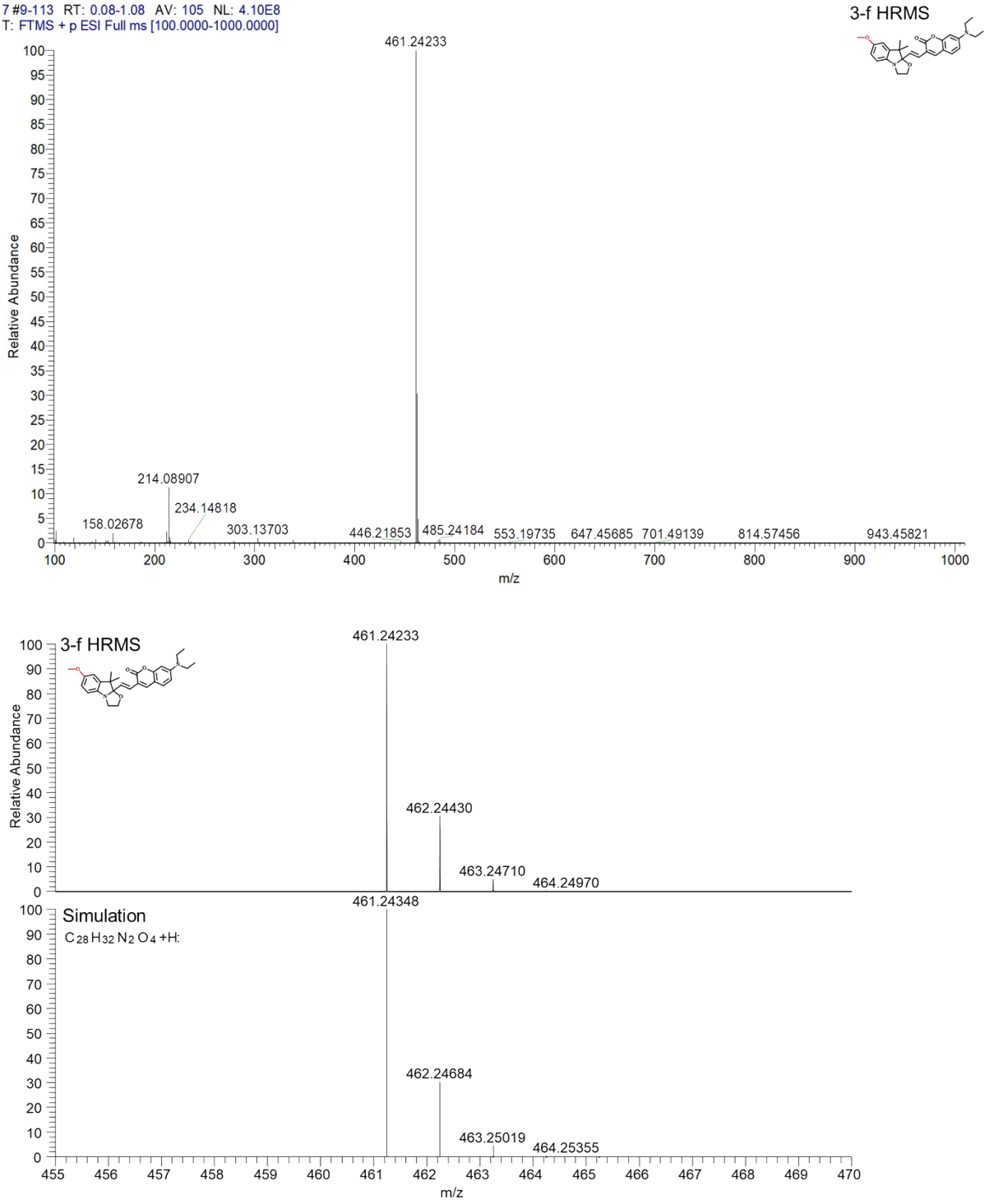


Figure S33. HRMS of 3-f.

Computational results

3-a close

C	5.07971600	-0.39800900	0.39271600
C	5.07971600	-0.39800900	0.39271600
C	6.30180300	-0.78272300	0.90470700

C	7.46854400	-0.56449000	0.14385000
C	7.37575300	0.03164200	-1.12262800
C	6.14408600	0.41915400	-1.63966800
H	6.38190400	-1.24126900	1.88326000
H	8.27814200	0.18944200	-1.70032300
H	6.08459900	0.86816300	-2.62367900
N	3.67069200	0.49629300	-1.21319900
C	3.68223300	-0.56766800	0.96591700
C	2.86744200	0.40313500	0.02648900
C	3.55811100	-0.17412900	2.44290000
H	2.51858800	-0.25112700	2.77282100
H	4.15240600	-0.85198600	3.06171400
H	3.89776000	0.84679200	2.60945500
C	3.24118200	-2.03670500	0.77572000
H	3.89998800	-2.69002300	1.35291400
H	2.21732600	-2.18860200	1.12467100
H	3.29741600	-2.34496800	-0.27048300
C	1.45247100	-0.02515500	-0.26848100
H	1.33339500	-0.92211300	-0.85956400
C	0.38008500	0.64414800	0.17757900
H	0.56253400	1.54014100	0.76570900
C	3.35280300	1.81516000	-1.76693100
H	2.45342200	1.74116100	-2.37967600
H	4.16740300	2.18791700	-2.38590800
C	3.10763200	2.67505900	-0.50182100
H	3.97545600	3.28957300	-0.24852600
H	2.23247300	3.32260600	-0.61091300
O	2.90214600	1.74038800	0.56616900
C	-1.03115700	0.32759600	-0.01878100
C	-1.44495900	-0.88207000	-0.74259600
C	-1.99720200	1.15841600	0.48242800
C	-3.38711900	0.90556200	0.32520800
H	-1.69196800	2.05061100	1.02239700
C	-3.76780100	-0.25611600	-0.36878700
O	-2.82132200	-1.09797800	-0.86777400
O	-0.72911500	-1.71247100	-1.23919500
C	-5.09305600	-0.60256500	-0.57372900
H	-5.28554000	-1.52033200	-1.10761100
C	-4.42517700	1.72064300	0.81527600
H	-4.17007400	2.62177200	1.36291500
C	-6.12945100	0.22653900	-0.09434100
C	-5.75003800	1.40041300	0.62216300
H	-6.50331500	2.05730100	1.03034400

N	-7.45362500	-0.07855200	-0.31943500
C	-7.83421700	-1.30055200	-1.03125000
C	-7.84151600	-2.57183300	-0.17228200
H	-7.17147800	-1.43197500	-1.89109600
H	-8.83145800	-1.13433200	-1.44445400
H	-8.10034600	-3.43813700	-0.78789000
H	-6.86390400	-2.75601000	0.27735700
H	-8.57482300	-2.49880400	0.63372300
C	-8.52804000	0.78446800	0.17408400
C	-8.91059000	0.56744600	1.64405400
H	-9.39999600	0.60345800	-0.45832600
H	-8.25147900	1.82928700	0.00785300
H	-9.69546900	1.27174000	1.93529200
H	-9.28739300	-0.44420600	1.80905300
H	-8.05537600	0.71887700	2.30585500
C	8.74242500	-0.94949400	0.66127300
N	9.77337900	-1.26085200	1.08239400

EE + Thermal Free Energy Correction = -1474.268646 Hartree

3-a close +H state1

C	5.03533600	0.04512000	-0.89502800
C	5.05703100	-0.35939100	0.43239600
C	6.28362400	-0.64534100	1.01695100
C	7.45208000	-0.52847300	0.24792100
C	7.39285900	-0.13333100	-1.09774100
C	6.16670000	0.16116700	-1.68612500
H	6.35273900	-0.95591400	2.05163900
H	8.30563200	-0.05663500	-1.67367000
H	6.11879300	0.46580900	-2.72477300
N	3.65290200	0.31132000	-1.33304900
C	3.66324100	-0.48878000	1.02582700
C	2.80916200	0.38496700	0.04611900
C	3.54759400	0.04514200	2.46203500
H	2.50757900	0.01269000	2.79421500
H	4.12620900	-0.58679100	3.13897500
H	3.90730900	1.06966100	2.54177900
C	3.23226800	-1.97230200	0.98163100
H	3.89983500	-2.56147200	1.61301200
H	2.21415000	-2.09103000	1.35532400
H	3.27813500	-2.39725800	-0.02506200
C	1.40862400	-0.02748800	-0.23779600
H	1.25178400	-0.97927500	-0.72968100
C	0.34227600	0.69493400	0.16338800

H	0.53112800	1.62079800	0.70295800
C	3.37633400	1.63634600	-1.99214300
H	2.59541200	1.48643500	-2.73476200
H	4.28108200	1.99234900	-2.47811200
C	2.90979200	2.53945600	-0.82407700
H	3.56606600	3.39315400	-0.66567900
H	1.89015400	2.88942000	-0.99284400
O	2.99283800	1.73137500	0.35381100
C	-1.05717600	0.37683700	-0.01658100
C	-1.45861400	-0.82691100	-0.74778800
C	-2.03352200	1.20690600	0.49580100
C	-3.40616800	0.93812200	0.34351700
H	-1.73557300	2.09997000	1.03886900
C	-3.77876900	-0.22951300	-0.35973200
O	-2.82189000	-1.05708200	-0.87032400
O	-0.72242300	-1.63732700	-1.25739700
C	-5.09402300	-0.59001200	-0.56079300
H	-5.28133600	-1.50645800	-1.09800500
C	-4.45624900	1.74122400	0.84730100
H	-4.20889700	2.64107400	1.39988400
C	-6.14207500	0.22714300	-0.06852400
C	-5.77081100	1.40613000	0.65881800
H	-6.53190100	2.04843500	1.07422200
N	-7.45034500	-0.08689900	-0.28603300
C	-7.82774200	-1.30329100	-1.02171800
C	-7.83224600	-2.58362700	-0.17900200
H	-7.16320200	-1.41430200	-1.88182900
H	-8.82354000	-1.12984700	-1.43238700
H	-8.09272400	-3.43882900	-0.80805300
H	-6.85442800	-2.77655700	0.26679600
H	-8.56539700	-2.52397400	0.62747700
C	-8.54043500	0.75367800	0.23273800
C	-8.89810400	0.50434400	1.70202500
H	-9.41217400	0.56119800	-0.39433500
H	-8.28485500	1.80397900	0.07396600
H	-9.69939400	1.18238500	2.00750500
H	-9.24638300	-0.51842500	1.85749000
H	-8.04281400	0.67240200	2.35978900
H	3.29641500	-0.45114200	-1.91259200
C	8.72120400	-0.81741600	0.84410200
N	9.74299100	-1.05033800	1.32737200

EE + Thermal Free Energy Correction = -1474.629814 Hartree

3-a close +H state2

C	-4.94603300	0.33067600	0.86837600
C	-5.02037900	-0.51240600	-0.24561100
C	-6.22936600	-1.06392200	-0.62292400
C	-7.38237600	-0.76880200	0.12932200
C	-7.29327300	0.06941300	1.25059400
C	-6.07521000	0.62375200	1.63024000
H	-6.30847200	-1.71214600	-1.48741500
H	-8.18668100	0.28303900	1.82381300
H	-6.01616500	1.26077400	2.50430300
N	-3.62461300	0.77471700	1.09147700
C	-3.63296000	-0.71889200	-0.83067800
C	-2.85339200	0.46603400	-0.12687200
C	-3.57254300	-0.61481600	-2.35956700
H	-2.54187600	-0.71073800	-2.71296100
H	-4.15000200	-1.42634300	-2.80963500
H	-3.96952000	0.33615500	-2.70987000
C	-3.10502400	-2.10004100	-0.37903000
H	-3.74396800	-2.88251300	-0.79397400
H	-2.08688900	-2.27390700	-0.73722100
H	-3.11628600	-2.20628200	0.70795900
C	-1.41853300	0.14296600	0.21542300
H	-1.26813200	-0.60900700	0.97661200
C	-0.37776800	0.73572700	-0.38980000
H	-0.60212600	1.48554100	-1.14281200
C	-3.40780700	2.20947800	1.31806100
H	-2.47140200	2.35059700	1.86122300
H	-4.21636800	2.64192300	1.90440500
C	-3.32492500	2.77173400	-0.11402200
H	-4.29706700	3.12371500	-0.46931400
H	-2.59609400	3.58019700	-0.21023200
O	-2.91709800	1.65884000	-0.92975800
C	1.04148400	0.49213200	-0.17409200
C	1.49921900	-0.49973300	0.82668300
C	1.97300800	1.17344100	-0.90191200
C	3.38268000	0.96814700	-0.73784100
H	1.64033900	1.89801000	-1.63769900
C	3.79601300	0.02678200	0.22147900
O	2.89714200	-0.65856800	0.95566200
O	0.82762300	-1.18095400	1.53948200
C	5.14392200	-0.24333700	0.45500300
H	5.39287200	-0.98101000	1.20259100
C	4.37261400	1.64608400	-1.46756100

H	4.07804500	2.38059300	-2.20743800
C	6.08790700	0.44991500	-0.28609000
C	5.71796100	1.39318200	-1.24800700
H	6.46738900	1.93303100	-1.81791100
N	7.54551100	0.21532800	-0.10032400
C	8.04498100	0.17530600	1.35964700
C	8.07760900	-1.17611200	2.05373800
H	7.41414500	0.88709700	1.89148800
H	9.05587300	0.58467900	1.31060000
H	8.46731600	-1.00464600	3.06006600
H	7.09701400	-1.63626100	2.16331600
H	8.75125400	-1.88083200	1.56569600
C	8.13136800	-0.87913900	-1.02006100
C	7.35957200	-2.18568700	-1.06255900
H	9.16072000	-1.01709900	-0.68542200
H	8.15429000	-0.42500300	-2.01164900
H	7.89028100	-2.85397900	-1.74483100
H	7.30013400	-2.68274200	-0.09563200
H	6.35172000	-2.04802600	-1.45365500
C	-8.64186700	-1.32687600	-0.24976700
N	-9.65837400	-1.78049000	-0.56059300
H	7.96936700	1.07373400	-0.45443800

EE + Thermal Free Energy Correction = -1474.609848 Hartree

3-a open

C	5.04235000	0.61305600	-0.32130900
C	5.02933800	-0.76096000	-0.08056800
C	6.21803800	-1.44593100	0.07730400
C	7.42575700	-0.72836400	-0.00637000
C	7.41815100	0.65514200	-0.24345400
C	6.22093700	1.34585900	-0.40412400
H	6.24177900	-2.51262700	0.26306500
H	8.35879600	1.18740200	-0.29996700
H	6.23180100	2.41301400	-0.58105100
N	3.70870500	1.06283100	-0.45755600
C	3.59301900	-1.24884200	-0.03884300
C	2.83004200	0.05477500	-0.29249400
C	3.26018600	-1.82942100	1.35794300
H	2.22876800	-2.17996600	1.40940900
H	3.91653900	-2.67695100	1.56450700
H	3.40788400	-1.08362100	2.14093300
C	3.33446200	-2.28478400	-1.16000000
H	3.97323900	-3.15601100	-1.00239100

H	2.29815300	-2.62430000	-1.16275600
H	3.56330100	-1.87033700	-2.14353600
C	1.44675500	0.28899600	-0.33625100
H	1.13630700	1.31205800	-0.43725900
C	0.43383200	-0.62599800	-0.17310500
H	0.66796100	-1.68138600	-0.08455200
C	3.36854600	2.46960400	-0.71930400
H	2.48826000	2.49333600	-1.36200500
H	4.19024900	2.90380100	-1.29106100
C	3.13666600	3.29009500	0.56338800
H	4.04138100	3.27382800	1.17514400
H	2.95964000	4.32912200	0.25798900
O	2.10171300	2.78126100	1.37562400
C	-0.95441800	-0.31844500	-0.09294400
C	-1.43389900	1.07326700	-0.06612500
C	-1.89143300	-1.34791900	0.00223300
C	-3.26159000	-1.10842300	0.09452200
H	-1.53851300	-2.37540500	0.00190100
C	-3.70738100	0.23880900	0.09312300
O	-2.80498400	1.25638200	0.01188100
O	-0.76272300	2.07745400	-0.09573600
C	-5.03483900	0.58201900	0.17510700
H	-5.28088300	1.63197900	0.16088100
C	-4.26243800	-2.11338600	0.18395400
H	-3.95926600	-3.15432200	0.17656400
C	-6.02926000	-0.42779400	0.28637900
C	-5.58721800	-1.79737900	0.27105000
H	-6.30817500	-2.59837900	0.32181600
N	-7.34078100	-0.11367300	0.41385800
C	-7.79833600	1.28810900	0.37529300
C	-7.91166000	1.87888600	-1.03389200
H	-7.13139900	1.89246300	0.99463600
H	-8.77142900	1.31422600	0.86583500
H	-8.23435100	2.92082000	-0.96772800
H	-6.95706800	1.85370700	-1.56272900
H	-8.64499000	1.33699200	-1.63339700
C	-8.37627400	-1.15113400	0.57712900
C	-8.90196400	-1.73645400	-0.73711800
H	-9.19558000	-0.69123600	1.13114400
H	-7.98488900	-1.93971100	1.22174200
H	-9.64639300	-2.50725500	-0.52266300
H	-9.38040200	-0.97120800	-1.35082400
H	-8.10225100	-2.19118400	-1.32557100

H	1.24121600	3.00919800	1.00150300
C	8.66881700	-1.41628600	0.15364300
N	9.66938300	-1.97792800	0.28302200

EE + Thermal Free Energy Correction = -1474.670023 Hartree

3-b close

C	3.97012100	1.18594800	-0.71673200
C	4.12346700	-0.07580600	-0.12603800
C	5.37885800	-0.63712800	0.00132500
C	6.50220700	0.06963300	-0.46506900
C	6.33380800	1.32743500	-1.05645000
C	5.07263800	1.89741400	-1.19102900
H	5.51538000	-1.60753400	0.46095100
H	7.21481800	1.84816400	-1.41043800
H	4.95591300	2.86598200	-1.66270300
N	2.61681500	1.55973000	-0.77719300
C	2.75786400	-0.64030700	0.23142500
C	1.87392500	0.66257900	0.13330300
C	2.68647800	-1.27787200	1.62404400
H	1.66543400	-1.60056300	1.84645300
H	3.32926000	-2.16173400	1.66240400
H	3.00280100	-0.57781400	2.39558000
C	2.35033500	-1.67766700	-0.83916900
H	3.05346800	-2.51388200	-0.81688100
H	1.34749400	-2.06808800	-0.65047700
H	2.37028500	-1.25113300	-1.84440800
C	0.45832500	0.44643700	-0.34121800
H	0.33425100	0.15227300	-1.37394700
C	-0.60566100	0.58930500	0.46143700
H	-0.41401000	0.88702000	1.48937500
C	2.23682700	2.91328200	-0.36500900
H	1.32295300	3.20723500	-0.88352100
H	3.02064000	3.62948700	-0.60665000
C	1.99968700	2.76457000	1.15972800
H	2.84134100	3.14136400	1.74646500
H	1.08552900	3.27367300	1.48055800
O	1.89303400	1.35531700	1.39911600
C	-2.01673200	0.39126700	0.14549100
C	-2.44574800	-0.02867900	-1.19558100
C	-2.96847200	0.58921500	1.10918400
C	-4.35824100	0.41128000	0.86771100
H	-2.65165900	0.89486500	2.10262500
C	-4.75438700	0.01429100	-0.42096100

O	-3.82238000	-0.19101800	-1.39181000
O	-1.74337800	-0.25061200	-2.14710600
C	-6.08102500	-0.19090700	-0.76353200
H	-6.28612400	-0.50661700	-1.77487700
C	-5.38022100	0.59093000	1.81875000
H	-5.11166600	0.88853900	2.82692000
C	-7.10267300	0.00750600	0.18938300
C	-6.70586900	0.39311400	1.50383800
H	-7.44535700	0.53498700	2.27741700
N	-8.43105000	-0.15282600	-0.14010900
C	-8.82894800	-0.54686700	-1.49313400
C	-8.74321900	-2.05133100	-1.78258400
H	-8.22486800	0.00840200	-2.21638200
H	-9.85686100	-0.20708300	-1.63747000
H	-9.02481900	-2.24833200	-2.82107700
H	-7.73150900	-2.43130600	-1.62860300
H	-9.41812000	-2.61719600	-1.13663400
C	-9.48966200	0.04122800	0.85184500
C	-9.74749000	-1.16282200	1.76719300
H	-10.40295500	0.28103300	0.30302400
H	-9.26136700	0.92693300	1.45136800
H	-10.53183500	-0.92263900	2.49109600
H	-10.07343300	-2.03212800	1.19214500
H	-8.84901400	-1.44425800	2.32031900
C	7.87971100	-0.46898600	-0.36094200
O	8.87581000	0.10595900	-0.74211700
O	7.90975700	-1.69863800	0.21217000
C	9.20876200	-2.31792700	0.35600500
H	8.99851100	-3.38810000	0.35942800
H	9.81472300	-2.06857100	-0.51584600
C	9.89417400	-1.88212000	1.64133700
H	10.83417600	-2.42808000	1.76461700
H	10.11933300	-0.81492700	1.61327100
H	9.26116400	-2.08844100	2.50769800

EE + Thermal Free Energy Correction = -1649.207511 Hartree

3-b close +H state1

C	4.01572500	-1.38754300	0.45935700
C	4.13424700	-0.05252500	0.10389300
C	5.40645900	0.50701100	0.05546100
C	6.51466800	-0.28480400	0.37437300
C	6.35517100	-1.62476700	0.74475800
C	5.08858300	-2.19907600	0.79207200

H	5.55520700	1.54147400	-0.22357400
H	7.23769700	-2.20133500	0.99003900
H	4.96284100	-3.23613300	1.08015300
N	2.59924400	-1.80335300	0.44895200
C	2.78383600	0.61243900	-0.11451400
C	1.84507700	-0.62212700	-0.33979500
C	2.74429000	1.54932400	-1.33125300
H	1.73179200	1.92924100	-1.48608400
H	3.39361300	2.40907700	-1.15352500
H	3.07095700	1.04384900	-2.23848600
C	2.39072500	1.39219900	1.16012100
H	3.11522700	2.19045700	1.33088500
H	1.40267200	1.84231300	1.05212400
H	2.38429900	0.76343000	2.05495400
C	0.44182500	-0.54544500	0.15628400
H	0.28604200	-0.48036100	1.22585300
C	-0.61811300	-0.47266100	-0.67301800
H	-0.42561700	-0.48840200	-1.74378700
C	2.25014600	-3.04426700	-0.33118700
H	1.44719100	-3.55980100	0.19171200
H	3.12440000	-3.68752600	-0.38740300
C	1.79935500	-2.49770900	-1.70773400
H	2.41484100	-2.86537800	-2.52654200
H	0.75336500	-2.74553800	-1.89599900
O	1.99291500	-1.08179400	-1.64836700
C	-2.01540200	-0.35364500	-0.31244000
C	-2.42481500	-0.35824700	1.09372700
C	-2.98070100	-0.23962100	-1.29061600
C	-4.35121500	-0.12534100	-0.98806400
H	-2.67648800	-0.23482100	-2.33404800
C	-4.73161700	-0.13232100	0.37198900
O	-3.78527700	-0.24497700	1.34805100
O	-1.69880600	-0.45477100	2.05388200
C	-6.04480400	-0.02293100	0.77871200
H	-6.23736300	-0.02266800	1.84015600
C	-5.38925600	0.00410500	-1.93971500
H	-5.13491100	0.01947900	-2.99395000
C	-7.08196000	0.09211100	-0.17948400
C	-6.70149300	0.11427100	-1.56141600
H	-7.45307900	0.21878300	-2.32859400
N	-8.39140400	0.16754300	0.19453500
C	-8.78122400	0.12407800	1.61147900
C	-8.69704500	1.46882000	2.34212500

H	-8.17069000	-0.62541000	2.12054500
H	-9.80583800	-0.24960000	1.64745600
H	-8.98014900	1.33787200	3.38989300
H	-7.68647700	1.88137700	2.31408200
H	-9.37433300	2.20263200	1.90093400
C	-9.46619200	0.32835400	-0.79657100
C	-9.66534600	1.76234500	-1.29989700
H	-10.38450900	-0.02349100	-0.32445400
H	-9.28311300	-0.34900900	-1.63440300
H	-10.47127600	1.78585800	-2.03820400
H	-9.93720200	2.43401100	-0.48355700
H	-8.76225200	2.15460300	-1.77203900
H	2.22993100	-1.87142900	1.39930700
C	7.91781100	0.25394600	0.33919200
O	8.88568200	-0.41366300	0.60817600
O	7.95483000	1.54253600	-0.02092800
C	9.27686900	2.15767600	-0.08481600
H	9.73955400	2.07007500	0.89991100
H	9.88160200	1.58883900	-0.79344900
C	9.09115100	3.59759400	-0.50967600
H	8.47786200	4.14406200	0.20986700
H	10.06547300	4.08841200	-0.56860100
H	8.61856300	3.65963300	-1.49216800

EE + Thermal Free Energy Correction = -1649.578612 Hartree

3-b close +H state2

C	-3.91939800	-1.29560700	-0.68677300
C	-4.11091100	-0.06334300	-0.05545400
C	-5.37456200	0.49528700	0.01487000
C	-6.46022200	-0.19003800	-0.55356600
C	-6.25205800	-1.42010600	-1.18796300
C	-4.98338900	-1.98493800	-1.26538400
H	-5.54380800	1.44594400	0.50403700
H	-7.10750000	-1.92323300	-1.62097800
H	-4.83435900	-2.93127300	-1.77156000
N	-2.55821200	-1.67995800	-0.66890400
C	-2.77435800	0.49327700	0.40843100
C	-1.87479900	-0.80629900	0.30113300
C	-2.79122500	1.06040100	1.83296400
H	-1.79193400	1.38938700	2.13289400
H	-3.45097600	1.93081300	1.87561100
H	-3.13983000	0.32047100	2.55106000
C	-2.32064700	1.58835900	-0.58387800

H	-3.03775200	2.41174700	-0.55997000
H	-1.33905400	1.98986000	-0.31714800
H	-2.27960200	1.21667600	-1.61014600
C	-0.45438600	-0.53862500	-0.13546000
H	-0.32897900	-0.17814000	-1.14615000
C	0.60369500	-0.72446100	0.66935800
H	0.40768800	-1.09258700	1.67218900
C	-2.23654900	-3.04542200	-0.23608700
H	-1.26353100	-3.33277600	-0.63986300
H	-2.98221200	-3.75483500	-0.58992600
C	-2.19785700	-2.91497700	1.29724400
H	-3.17008800	-3.13522200	1.74660400
H	-1.43789000	-3.54941300	1.75974700
O	-1.88033500	-1.53411600	1.54489700
C	2.00786200	-0.48655300	0.36951000
C	2.42645800	0.02709600	-0.95587300
C	2.96271600	-0.73031900	1.31376900
C	4.35946600	-0.51334100	1.07452100
H	2.65849800	-1.10316700	2.28614800
C	4.73610400	-0.03244100	-0.19204600
O	3.81455400	0.21905200	-1.14255400
O	1.73217500	0.29993100	-1.88663500
C	6.06943500	0.20809700	-0.52188500
H	6.28910400	0.58124800	-1.51055700
C	5.37258100	-0.75592300	2.01656600
H	5.10682500	-1.13412500	2.99637000
C	7.03686000	-0.04699900	0.43702200
C	6.70420400	-0.52653800	1.70643900
H	7.47212900	-0.72759400	2.44643700
N	8.48122200	0.19064900	0.16516600
C	9.00088700	-0.27977300	-1.20893200
C	8.96799800	0.72115000	-2.35221500
H	8.42144100	-1.17372800	-1.43810000
H	10.03265700	-0.58170600	-1.01906000
H	9.37974000	0.21337800	-3.22775100
H	7.96547600	1.05413900	-2.61568800
H	9.59551800	1.59261300	-2.16361300
C	8.98113100	1.58420400	0.60694300
C	8.12102300	2.75640500	0.17098900
H	10.00349500	1.65847100	0.23299400
H	9.02085800	1.53282200	1.69586000
H	8.59089900	3.66507200	0.55471400
H	8.04589800	2.85673100	-0.91054100

H	7.11772100	2.70013000	0.59267500
C	-7.84876100	0.34412700	-0.51623300
O	-8.81084700	-0.22305900	-0.98036400
O	-7.92243600	1.54601100	0.09697400
C	-9.24219200	2.13900000	0.17620100
H	-9.64682400	2.22654500	-0.83443400
H	-9.89427000	1.46515400	0.73670600
C	-9.09786200	3.48642800	0.85249500
H	-8.43997600	4.14287300	0.27855500
H	-10.07637300	3.96680900	0.93201900
H	-8.68734000	3.37742100	1.85884400
H	8.95092700	-0.44666500	0.80942600

EE + Thermal Free Energy Correction = -1649.552403 Hartree

3-b open

C	3.97439300	1.19190800	-0.36316300
C	3.99987800	-0.19433900	-0.22336200
C	5.20984300	-0.86476900	-0.20766700
C	6.39172900	-0.12029400	-0.33204000
C	6.34246100	1.27320800	-0.45983200
C	5.13069800	1.95698000	-0.47665800
H	5.26730600	-1.94031800	-0.10366300
H	7.27789600	1.81168900	-0.54247600
H	5.10195600	3.03591100	-0.53252100
N	2.62262900	1.62166400	-0.37069500
C	2.57914600	-0.71478200	-0.10975400
C	1.77408000	0.58921600	-0.20759600
C	2.37011600	-1.41675500	1.25345300
H	1.34966200	-1.78320100	1.37082100
H	3.04681800	-2.27037600	1.32678500
H	2.58904900	-0.74182500	2.08314900
C	2.26106700	-1.66596200	-1.29048500
H	2.94868600	-2.51352700	-1.26306200
H	1.24371200	-2.05524700	-1.23817600
H	2.38667700	-1.16059700	-2.24980800
C	0.38116000	0.78534600	-0.14261100
H	0.01087700	1.79813600	-0.18544700
C	-0.56620800	-0.20754700	-0.01890000
H	-0.24025400	-1.24024400	0.03146100
C	2.24087300	3.02924200	-0.57263400
H	1.28107000	3.05727000	-1.08794500
H	2.98389200	3.47010600	-1.23776200
C	2.17214500	3.84481400	0.72443900

H	1.78777200	4.83398600	0.46304900
H	1.46357400	3.38787000	1.42385900
O	3.45026200	4.03253000	1.30760100
C	-1.97699100	-0.04407100	0.04793900
C	-2.60038000	1.28852200	-0.00386300
C	-2.80048700	-1.16427100	0.16079800
C	-4.19006200	-1.06910700	0.22139700
H	-2.34192600	-2.14831600	0.20146000
C	-4.77713800	0.22235700	0.16346000
O	-3.99000100	1.32713900	0.05625900
O	-2.03538400	2.34699000	-0.09208000
C	-6.13637700	0.42032600	0.20650800
H	-6.49328200	1.43624300	0.14456400
C	-5.07836600	-2.17288400	0.32833900
H	-4.66412300	-3.17407700	0.36954400
C	-7.01869000	-0.68749300	0.32486600
C	-6.43139800	-2.00049600	0.37388900
H	-7.06261300	-2.87257600	0.44377500
N	-8.36103600	-0.51645900	0.39817600
C	-8.96579700	0.82649400	0.32370900
C	-9.12216400	1.37361400	-1.09888400
H	-8.37550500	1.51048000	0.93718700
H	-9.94286500	0.75854300	0.80291600
H	-9.54784000	2.37928400	-1.05876800
H	-8.16352000	1.43234600	-1.61774300
H	-9.79144800	0.74921400	-1.69319700
C	-9.28350200	-1.66146500	0.51413000
C	-9.62257300	-2.34167700	-0.81591100
H	-10.19483000	-1.28283200	0.97795900
H	-8.86506800	-2.38147600	1.22003900
H	-10.29186300	-3.18646900	-0.63479400
H	-10.12723500	-1.65444700	-1.49707900
H	-8.72866100	-2.71871300	-1.31696300
H	3.60866700	3.35153600	1.96718400
C	7.74265200	-0.76701600	-0.32869600
O	8.77467200	-0.14931600	-0.43138600
O	7.66096700	-2.10294300	-0.20438400
C	8.91777600	-2.84232900	-0.19334600
H	8.64500100	-3.82883000	-0.56679100
H	9.60343000	-2.36297100	-0.89188200
C	9.50493800	-2.91086700	1.20506900
H	10.40261800	-3.53482300	1.19346000
H	9.78718900	-1.91780400	1.55788800

H	8.79297200	-3.35099800	1.90698200

EE + Thermal Free Energy Correction = -1649.615701 Hartree

3-c close

C	4.22737700	0.46937000	-0.98278600
C	4.32919900	-0.23106900	0.22364000
C	5.56543100	-0.63553000	0.70148700
C	6.70063200	-0.32418500	-0.04977700
C	6.61048900	0.36446300	-1.25400300
C	5.36117200	0.76655400	-1.73313100
H	5.65922500	-1.17392400	1.63630500
H	7.50550500	0.58804800	-1.81983700
H	5.29067400	1.29270900	-2.67781100
N	2.88057900	0.75730900	-1.29760900
C	2.93965800	-0.48618300	0.78491700
C	2.09844000	0.54661100	-0.06121200
C	2.81358000	-0.23354200	2.29178500
H	1.77822500	-0.36819000	2.61702800
H	3.42924600	-0.94938800	2.84359100
H	3.12807000	0.77625800	2.54996500
C	2.53161700	-1.94151200	0.46179200
H	3.21012700	-2.62982300	0.97173000
H	1.51423900	-2.14933400	0.80106900
H	2.58665200	-2.14838300	-0.60907600
C	0.68596400	0.11992700	-0.37353900
H	0.57500100	-0.71189800	-1.05466200
C	-0.39054700	0.71417300	0.15975100
H	-0.21346700	1.54637400	0.83633400
C	2.54485100	2.12125400	-1.71734600
H	1.63025000	2.09837300	-2.31208800
H	3.34140200	2.55391400	-2.32092800
C	2.32804900	2.86127100	-0.37572300
H	3.21018700	3.43408600	-0.07650300
H	1.46361200	3.53127900	-0.41048700
O	2.11464700	1.83197300	0.59854600
C	-1.79944100	0.38989100	-0.04189200
C	-2.20809100	-0.72156300	-0.91187300
C	-2.76857700	1.12097200	0.59072600
C	-4.15719600	0.85558400	0.43789000
H	-2.46726000	1.93998400	1.23812300
C	-4.53295900	-0.20725300	-0.40126000
O	-3.58361200	-0.94775600	-1.03664400
O	-1.48984700	-1.46264000	-1.53076300

C	-5.85618300	-0.55576900	-0.61746700
H	-6.04450400	-1.39494000	-1.26926300
C	-5.19747900	1.56516600	1.06702400
H	-4.94591200	2.38712600	1.72896700
C	-6.89538100	0.16869700	0.00388800
C	-6.52044100	1.23897500	0.86868800
H	-7.27509300	1.81119500	1.38698300
N	-8.21916800	-0.13788000	-0.22535900
C	-8.59339100	-1.24911500	-1.10254700
C	-8.53927000	-2.63683300	-0.45043900
H	-7.95814900	-1.22819900	-1.99273600
H	-9.60843100	-1.05232700	-1.45448800
H	-8.79901900	-3.40506300	-1.18455100
H	-7.54217100	-2.85987700	-0.06611000
H	-9.24495600	-2.71109000	0.37987100
C	-9.29725700	0.60643100	0.42736200
C	-9.61917300	0.15889500	1.85925900
H	-10.18697000	0.49387600	-0.19617800
H	-9.05615200	1.67293700	0.41215000
H	-10.41588300	0.78165400	2.27684200
H	-9.95611800	-0.87968300	1.88110500
H	-8.74626900	0.24217100	2.51007200
Br	8.42891800	-0.86487300	0.59871300

EE + Thermal Free Energy Correction = -3955.558991 Hartree

3-c close +H state1

C	4.26430700	0.43360800	-0.99964100
C	4.31343200	-0.23421200	0.21444000
C	5.55110400	-0.63134100	0.70892000
C	6.69327700	-0.35259700	-0.04302200
C	6.62155300	0.30590700	-1.27263500
C	5.38351100	0.71129700	-1.76710500
H	5.63597100	-1.14783300	1.65590400
H	7.52266500	0.50263000	-1.83737500
H	5.32066100	1.22213900	-2.72074400
N	2.87361200	0.77881800	-1.34872700
C	2.93063800	-0.49421600	0.79150500
C	2.05194100	0.54854300	0.01786400
C	2.83607000	-0.26028800	2.30685500
H	1.80375000	-0.37737400	2.64436200
H	3.43822300	-1.00416900	2.83281700
H	3.18411400	0.73363100	2.58273400
C	2.50949500	-1.94309700	0.45745500

H	3.19502800	-2.63948700	0.94355100
H	1.50013500	-2.14607300	0.81843100
H	2.53802800	-2.15423600	-0.61511000
C	0.65354400	0.17138900	-0.33178200
H	0.50930800	-0.64797000	-1.02484500
C	-0.41961500	0.75064800	0.24267500
H	-0.23992300	1.53541100	0.97463200
C	2.59026400	2.21486000	-1.70888900
H	1.83155700	2.22823000	-2.48872600
H	3.50328400	2.67539800	-2.07686700
C	2.08353700	2.83474000	-0.38370500
H	2.69990600	3.66651100	-0.04807900
H	1.04779100	3.16348300	-0.48376100
O	2.20734800	1.80514700	0.60097400
C	-1.81595800	0.44033900	0.02091900
C	-2.20707300	-0.57237300	-0.96214200
C	-2.79800800	1.09827600	0.73164600
C	-4.16806900	0.83016800	0.54968900
H	-2.50788400	1.84964000	1.46135200
C	-4.53049300	-0.15172300	-0.39877500
O	-3.56754800	-0.80787800	-1.10827500
O	-1.46531200	-1.22042000	-1.66075700
C	-5.84174700	-0.49568300	-0.65121700
H	-6.02113300	-1.26553700	-1.38526400
C	-5.22318200	1.46009200	1.24996400
H	-4.98332600	2.21285600	1.99302300
C	-6.89553800	0.15069500	0.04110900
C	-6.53399000	1.13717200	1.01665600
H	-7.29908400	1.63930600	1.58828300
N	-8.20167500	-0.14472100	-0.21648500
C	-8.56816500	-1.17238300	-1.20232800
C	-8.50422300	-2.61254100	-0.68111900
H	-7.93256500	-1.05755200	-2.08388300
H	-9.58311100	-0.94687400	-1.53282900
H	-8.76297800	-3.30714400	-1.48461700
H	-7.50548400	-2.86830300	-0.32181400
H	-9.20842400	-2.76917400	0.13815100
C	-9.29827100	0.52491100	0.49894600
C	-9.62920700	-0.07476700	1.86997500
H	-10.17620400	0.46993000	-0.14672400
H	-9.06395000	1.58768100	0.59282700
H	-10.43283600	0.49801800	2.34039400
H	-9.96365200	-1.10998200	1.77977000

H	-8.76467400	-0.05754900	2.53696500
H	2.50859900	0.15752400	-2.07314600
Br	8.39462700	-0.88574800	0.62411400

EE + Thermal Free Energy Correction = -3955.923254 Hartree

3-c close +H state2

C	-4.17027400	0.61946100	0.90956100
C	-4.29378000	-0.25086900	-0.17450100
C	-5.53120200	-0.77117900	-0.52318200
C	-6.64261200	-0.40263100	0.23672900
C	-6.52562300	0.45650600	1.32524900
C	-5.27682400	0.97458400	1.67377200
H	-5.64426200	-1.44340600	-1.36437700
H	-7.40168500	0.72158200	1.90237800
H	-5.18641700	1.63339900	2.52932400
N	-2.82151400	1.01940100	1.10540900
C	-2.92363400	-0.53815000	-0.76627400
C	-2.08717800	0.63831800	-0.11502800
C	-2.87532000	-0.49516300	-2.29832800
H	-1.85360600	-0.64836100	-2.65798100
H	-3.49202700	-1.29753900	-2.71138200
H	-3.23507200	0.45803900	-2.68131000
C	-2.44916100	-1.92254900	-0.26753900
H	-3.12626100	-2.69200600	-0.64464300
H	-1.44373400	-2.15351900	-0.62966100
H	-2.45179600	-1.98553700	0.82280700
C	-0.66129600	0.26928300	0.21693800
H	-0.53137300	-0.47517000	0.98899700
C	0.39563700	0.81689400	-0.40337300
H	0.19176200	1.56298600	-1.16575900
C	-2.56249300	2.45742600	1.25849700
H	-1.60621500	2.59850800	1.76664200
H	-3.34161300	2.93566100	1.84927700
C	-2.50957000	2.95287200	-0.19699600
H	-3.49062600	3.28533100	-0.54747200
H	-1.78492000	3.75656300	-0.34854300
O	-2.11170500	1.80308900	-0.96348500
C	1.80654400	0.53214200	-0.18826800
C	2.23626500	-0.47243500	0.81248400
C	2.75769900	1.18594600	-0.91665300
C	4.16085900	0.94424700	-0.74950600
H	2.44545500	1.91861400	-1.65332300
C	4.54785100	-0.00674900	0.21151200

O	3.62991900	-0.66926100	0.94281800
O	1.54652800	-1.13786900	1.52262700
C	5.88783600	-0.30941800	0.45001400
H	6.11594700	-1.05245800	1.19892600
C	5.16999800	1.59751000	-1.47568600
H	4.89602800	2.33896700	-2.21654000
C	6.85128100	0.36123000	-0.28699400
C	6.50806600	1.31268500	-1.25064400
H	7.27260600	1.83449600	-1.81729200
N	8.30235800	0.09271000	-0.09407200
C	8.79054800	0.02527000	1.36845400
C	8.79148300	-1.33506500	2.04574100
H	8.16990800	0.74264200	1.90468900
H	9.80959200	0.41527200	1.33186800
H	9.17336300	-1.18352400	3.05823700
H	7.80167900	-1.77861300	2.13869500
H	9.45737700	-2.04576100	1.55575900
C	8.86967700	-1.00440500	-1.02171200
C	8.06979700	-2.29335700	-1.08154500
H	9.89408700	-1.16813000	-0.68355000
H	8.90753200	-0.54092600	-2.00848800
H	8.58801100	-2.96539000	-1.76971400
H	7.99611800	-2.79985700	-0.12049000
H	7.06653100	-2.12902900	-1.47409100
Br	-8.36671000	-1.10271800	-0.22767100
H	8.74715000	0.94545800	-0.43586400

EE + Thermal Free Energy Correction = -3955.896243 Hartree

3-c open

C	4.26480500	0.90122800	-0.35331700
C	4.30676800	-0.47149700	-0.11853700
C	5.52331900	-1.11556800	0.02941400
C	6.68807200	-0.34744500	-0.06036600
C	6.64109500	1.02809600	-0.29020400
C	5.41513500	1.67507700	-0.44077700
H	5.58630000	-2.18090600	0.21041100
H	7.55983600	1.59572300	-0.35063000
H	5.38887000	2.74296200	-0.61378700
N	2.91038700	1.29903900	-0.47827300
C	2.88998900	-1.01428200	-0.06893800
C	2.07525100	0.25980900	-0.31251100
C	2.58853200	-1.61121400	1.32774200
H	1.57154600	-2.00104100	1.38513100

H	3.27879800	-2.43315800	1.52702100
H	2.71323400	-0.86234100	2.11178600
C	2.66240300	-2.05506900	-1.19193200
H	3.33559100	-2.90147400	-1.04248600
H	1.63974600	-2.43402600	-1.18868500
H	2.86814200	-1.62827600	-2.17529900
C	0.68033500	0.44035000	-0.34561100
H	0.33184100	1.45144200	-0.44237900
C	-0.29501600	-0.50998100	-0.17836300
H	-0.02272500	-1.55644900	-0.09215400
C	2.51513700	2.69280700	-0.72819700
H	1.63022900	2.68846100	-1.36488500
H	3.31651200	3.16161700	-1.30142600
C	2.26141600	3.49552000	0.56174300
H	3.17012200	3.50777300	1.16750400
H	2.04489200	4.52943100	0.26404100
O	1.25115500	2.94515200	1.37774100
C	-1.69608700	-0.25224100	-0.08991000
C	-2.22331000	1.12116600	-0.05006400
C	-2.59482300	-1.31290900	-0.00006400
C	-3.97431100	-1.12242900	0.09742200
H	-2.20698000	-2.32766700	-0.00980100
C	-4.46609000	0.20735800	0.10817300
O	-3.59931100	1.25640300	0.03488900
O	-1.58747700	2.14891300	-0.07421300
C	-5.80523500	0.50448900	0.19365600
H	-6.08654500	1.54567600	0.18825300
C	-4.93918600	-2.16117300	0.17930800
H	-4.60062100	-3.19110700	0.16400700
C	-6.76398300	-0.53911800	0.29430100
C	-6.27491300	-1.89149400	0.26882500
H	-6.96772300	-2.71738900	0.31398500
N	-8.08737700	-0.27129700	0.42104600
C	-8.59205800	1.11373700	0.39402600
C	-8.72123000	1.71485000	-1.00952000
H	-7.94834200	1.73478700	1.02150300
H	-9.56728700	1.10240500	0.88112300
H	-9.07876800	2.74481200	-0.93444300
H	-7.76479500	1.72671400	-1.53549500
H	-9.43425300	1.15458800	-1.61669400
C	-9.08635800	-1.34540600	0.56742600
C	-9.57937000	-1.94013700	-0.75533800
H	-9.92680100	-0.91914900	1.11679900

H	-8.67354900	-2.12457100	1.21040400
H	-10.29824200	-2.73821000	-0.55341100
H	-10.07843800	-1.18766500	-1.36847900
H	-8.75871800	-2.36235700	-1.33922300
H	0.38054600	3.13329900	1.00454600
Br	8.38056800	-1.20111400	0.13959100

EE + Thermal Free Energy Correction = -3955.968240 Hartree

3'-d close

C	-5.40200500	1.09937000	1.85894900
C	-6.67847300	0.62731400	1.67803000
C	-6.98519100	-0.31609900	0.66526000
C	-5.93586400	-0.79618400	-0.19714600
C	-4.62877200	-0.27789500	-0.01099500
C	-4.37957000	0.63325900	1.00285500
H	-9.08361700	-0.42641700	1.15302000
H	-5.18601200	1.81179000	2.64567000
H	-7.47945400	0.97538000	2.32203900
C	-8.30651800	-0.80274500	0.49499000
C	-6.28819500	-1.76411300	-1.18160900
C	-7.57927800	-2.21495100	-1.31313900
C	-8.60591800	-1.73055100	-0.47141700
H	-5.52540200	-2.15538000	-1.83928200
H	-7.81377600	-2.95355700	-2.07210400
H	-9.62007200	-2.09492700	-0.58875100
C	-3.30413200	-0.63103000	-0.69138200
N	-3.02510100	0.98199300	1.07614500
O	-2.27108000	1.62088400	-1.10239400
C	-2.35536400	0.53650500	-0.15043500
C	-0.94529800	0.08621700	0.14634000
H	-0.84641500	-0.67174200	0.90900400
C	0.14296200	0.57285800	-0.46633700
H	-0.00912300	1.34311700	-1.21609700
C	1.53929900	0.20118400	-0.25510800
C	2.52889400	0.83360300	-0.95801600
C	1.91501100	-0.85179200	0.69903800
C	3.90757200	0.51880600	-0.80387900
C	4.25098700	-0.49061800	0.11109800
O	1.17773400	-1.50354600	1.39171700
O	3.28153800	-1.13291000	0.81856900
C	5.56219800	-0.87476100	0.34187300
C	4.96794300	1.14165100	-1.48836600
C	6.27964900	0.77900600	-1.27670700

H	7.05270000	1.29955100	-1.82159700
C	6.61969200	-0.25799900	-0.35907100
N	7.92856100	-0.65061500	-0.17408200
C	8.26861000	-1.71286000	0.77382200
H	9.22611000	-2.13250800	0.45716700
H	7.53960000	-2.52213300	0.67559700
C	9.02605200	0.00178700	-0.88904900
H	9.85763600	-0.70589800	-0.91350700
H	8.73401300	0.15449200	-1.93197200
C	8.36547400	-1.26724300	2.23890000
H	7.43225400	-0.81613200	2.58157200
H	8.58102200	-2.12804000	2.87861600
H	9.16442900	-0.53539200	2.37727200
C	9.50278900	1.32553700	-0.27626300
H	9.89248100	1.17533600	0.73283700
H	10.30215300	1.75554400	-0.88710500
H	8.69097000	2.05328800	-0.21734000
H	5.72690000	-1.65287700	1.07126200
H	4.74225400	1.93136000	-2.19727300
H	2.25240400	1.61078000	-1.66520400
C	-2.84487500	-2.01718400	-0.17982600
H	-1.87829300	-2.29678400	-0.60578400
H	-2.75988500	-2.03647500	0.90851800
H	-3.57754700	-2.77411300	-0.46833800
C	-3.29778700	-0.62647200	-2.22961200
H	-3.74825100	-1.53795400	-2.62572400
H	-3.83256900	0.22965100	-2.64022400
H	-2.26862000	-0.58415400	-2.59424900
C	-2.60301000	2.30198000	1.53842300
H	-1.53180700	2.23936800	1.73768100
H	-3.08754100	2.52195900	2.48999100
C	-3.15474800	2.72080200	-0.87972400
H	-2.97098200	3.40839100	-1.70667700
H	-4.19777100	2.39386100	-0.94455200
C	-2.88666600	3.39488500	0.47387900
H	-2.02693100	4.06683100	0.39926000
H	-3.75341500	4.00509000	0.74645400

EE + Thermal Free Energy Correction = -1574.917054 Hartree

3'-d close +H state1

C	5.61023000	1.72049000	-1.14494400
C	6.80217900	1.05523400	-1.26650900
C	6.94690600	-0.28193500	-0.81112100

C	5.83338000	-0.97211800	-0.21740300
C	4.59908200	-0.26016200	-0.08373500
C	4.54360500	1.02757300	-0.54500700
H	9.01991600	-0.42002100	-1.39640400
H	5.50141400	2.73793300	-1.49942500
H	7.65405700	1.54697400	-1.72120300
C	8.18772200	-0.95425200	-0.95198000
C	6.02702200	-2.31998400	0.18422400
C	7.24303700	-2.94167800	0.02647400
C	8.33674200	-2.25505000	-0.54136000
H	5.21195000	-2.87602700	0.62075100
H	7.36296700	-3.97146600	0.34165800
H	9.28907600	-2.75872200	-0.65549500
C	3.23357700	-0.75493300	0.39319600
N	3.21498100	1.63117100	-0.34996800
O	2.53314500	1.03274300	1.85965400
C	2.39329900	0.58572400	0.55544400
C	0.99030300	0.54205300	0.02916900
H	0.83787700	0.69827100	-1.03204700
C	-0.07257900	0.22012800	0.78997500
H	0.09237900	0.01468900	1.84558000
C	-1.45530300	0.09721400	0.36776500
C	-2.42653000	-0.29398200	1.26358800
C	-1.84219100	0.39700600	-1.01244800
C	-3.78104600	-0.42917300	0.89833600
C	-4.13749600	-0.14368500	-0.43722300
O	-1.11027800	0.76246000	-1.90175200
O	-3.18556300	0.25340700	-1.33050100
C	-5.43343300	-0.23899200	-0.90011000
C	-4.82532400	-0.82483600	1.76523000
C	-6.12090400	-0.92827700	1.32991100
H	-6.88056100	-1.22584600	2.03626800
C	-6.47347300	-0.64982700	-0.03095100
N	-7.75759900	-0.78674500	-0.47247800
C	-8.11308400	-0.50503700	-1.87075900
H	-9.01773000	-1.07437900	-2.08998800
H	-7.33583000	-0.91516300	-2.52019900
C	-8.84367200	-1.18854600	0.43334500
H	-9.63234800	-1.61418700	-0.18891000
H	-8.49320000	-2.00484500	1.06971600
C	-8.34747900	0.97620500	-2.18800400
H	-7.46782900	1.58163200	-1.96053600
H	-8.57452800	1.09466400	-3.25082400

H	-9.18908300	1.37530600	-1.61865600
C	-9.41955500	-0.05331300	1.28702000
H	-9.85191100	0.73087800	0.66274300
H	-10.20959900	-0.44164000	1.93533300
H	-8.65592500	0.40337400	1.92019900
H	-5.61124700	0.01411500	-1.93356400
H	-4.59119800	-1.04839100	2.80041800
H	-2.14189700	-0.51178400	2.28965300
C	2.63377200	-1.65768000	-0.71206600
H	1.65147700	-2.03202800	-0.42143600
H	2.53041600	-1.13565100	-1.66627000
H	3.29181600	-2.51156300	-0.87855500
C	3.21705800	-1.50959900	1.73698100
H	3.55603200	-2.53613300	1.60715900
H	3.83471000	-1.02290800	2.48943300
H	2.19527500	-1.56119700	2.11821800
C	3.26632000	3.02113800	0.26813600
H	3.41483600	3.73265200	-0.54341400
H	4.14465300	3.03351100	0.91197300
C	1.89187100	2.28859100	2.20448000
H	0.85407400	2.11663800	2.49183800
H	2.44735400	2.62464400	3.08012100
C	1.99736100	3.29742400	1.05955700
H	1.12408200	3.24897300	0.40514100
H	2.04737600	4.31358200	1.45714400
H	2.72264800	1.69994200	-1.24377100

EE + Thermal Free Energy Correction = -1575.295204 Hartree

3'-d close +H state2

C	5.42927900	1.53666000	-1.47057500
C	6.69167200	0.99804400	-1.47172500
C	6.98605400	-0.20873800	-0.78732600
C	5.94142100	-0.89309800	-0.07163200
C	4.64773800	-0.30552900	-0.06212500
C	4.41268800	0.86723200	-0.75579000
H	9.06813400	-0.22721200	-1.35243400
H	5.22135200	2.45156200	-2.01145800
H	7.49057100	1.49647600	-2.01020500
C	8.29323900	-0.75873900	-0.80973900
C	6.27989400	-2.11564600	0.57429900
C	7.55746400	-2.61991000	0.52672100
C	8.58047000	-1.93749200	-0.16781900
H	5.52102900	-2.66466500	1.11311300

H	7.78329600	-3.55457900	1.02797500
H	9.58316800	-2.34754700	-0.19442000
C	3.32957400	-0.81291000	0.52631000
N	3.06577400	1.26970500	-0.68143000
O	2.28893400	1.23221900	1.57917300
C	2.39997900	0.48348800	0.35909500
C	0.99391300	0.15395800	-0.08346900
H	0.91431100	-0.35890200	-1.02963300
C	-0.10620100	0.48402600	0.61277200
H	0.03445800	1.01401600	1.54893500
C	-1.49275900	0.21522700	0.26450300
C	-2.50084700	0.64317300	1.08043400
C	-1.83896600	-0.53103400	-0.96792700
C	-3.88385300	0.40020300	0.79445400
C	-4.18921800	-0.31556700	-0.37682700
O	-1.09641600	-0.97282200	-1.78997600
O	-3.21765100	-0.75045400	-1.20089800
C	-5.50743200	-0.60301700	-0.72988500
C	-4.94842900	0.82646800	1.60770600
C	-6.26622600	0.55235300	1.27391300
H	-7.06529000	0.88845900	1.92242300
C	-6.52392800	-0.16192900	0.10272100
N	-7.92268500	-0.49777800	-0.27039700
C	-8.57446700	-1.45221200	0.73603800
H	-8.86126900	-0.84467000	1.59425300
H	-7.78063000	-2.13052200	1.04653500
C	-8.78166100	0.73114500	-0.56433100
H	-9.79211900	0.36214800	-0.73551400
H	-8.78026000	1.32639200	0.34805800
C	-9.75101700	-2.21503800	0.14760300
H	-9.45719200	-2.79629900	-0.73121600
H	-10.10784100	-2.92416100	0.89722400
H	-10.59260000	-1.57310400	-0.11589200
C	-8.27089000	1.51599800	-1.76000100
H	-8.27158000	0.91239300	-2.67192400
H	-8.93886400	2.36255500	-1.92954300
H	-7.26659000	1.90699300	-1.59512400
H	-5.69133500	-1.15944500	-1.64239200
H	-4.73076400	1.37788100	2.51460500
H	-2.24957000	1.18861000	1.98391300
C	2.82738800	-1.99437800	-0.33719300
H	1.86290100	-2.36964900	0.01712800
H	2.72917200	-1.71490200	-1.38822100

H	3.54562400	-2.81448200	-0.28463300
C	3.35747800	-1.23740300	2.00509100
H	3.82146900	-2.21764500	2.11872100
H	3.90259500	-0.52805000	2.62717900
H	2.33905400	-1.30915100	2.39477300
C	2.71737100	2.69147600	-0.65629500
H	1.63629900	2.75810500	-0.79395100
H	3.17066500	3.18791300	-1.51412000
C	3.26450500	2.26793600	1.75987100
H	3.07668400	2.66602200	2.75721000
H	4.27195300	1.84198100	1.75384500
C	3.12849500	3.35499300	0.68176400
H	2.37585400	4.09398000	0.97092000
H	4.08097200	3.88363900	0.58617200
H	-7.86059000	-1.01760200	-1.14972300

EE + Thermal Free Energy Correction = -1575.274785 Hartree

3'-d open

C	5.70599100	1.40383600	-0.72408000
C	6.89385800	0.73673500	-0.56145500
C	6.94054400	-0.63268300	-0.18728500
C	5.71982800	-1.36241000	0.03258700
C	4.50142800	-0.65512100	-0.14215100
C	4.52078800	0.67559200	-0.50533700
H	9.09625000	-0.73730000	-0.19640500
H	5.69633800	2.44684300	-1.00860400
H	7.82926400	1.26052000	-0.72128000
C	8.18285300	-1.29676300	-0.02754800
C	5.81789100	-2.73152600	0.40405400
C	7.04126500	-3.34021400	0.54911900
C	8.23660300	-2.62044900	0.33222500
H	4.92199900	-3.31126800	0.57712600
H	7.09069400	-4.38487900	0.83311700
H	9.19245500	-3.11633200	0.45045000
C	3.05100600	-1.10243700	-0.00784400
N	3.18993100	1.15248700	-0.62347800
C	2.29872900	0.18826500	-0.35244200
C	0.91004200	0.43306500	-0.41694400
H	0.59255200	1.42799700	-0.68854100
C	-0.08913300	-0.47738800	-0.16313100
H	0.17698100	-1.48715200	0.12808300
C	-1.49445800	-0.25210900	-0.23421300
C	-2.37747600	-1.28724000	0.06264400

C	-2.04496400	1.05771100	-0.61846700
C	-3.76396000	-1.13122500	0.00482600
C	-4.27938100	0.13507600	-0.37347100
O	-1.42321700	2.04869100	-0.89879900
O	-3.43243400	1.15978400	-0.66270300
C	-5.62793800	0.38990900	-0.46035100
C	-4.71168500	-2.14601000	0.30087800
C	-6.05565500	-1.91610200	0.22187900
H	-6.73382000	-2.71898400	0.46576000
C	-6.57036300	-0.63409700	-0.17790000
N	-7.90507900	-0.41681700	-0.29058300
C	-8.43299600	0.89343800	-0.71067700
H	-9.41537900	0.71172800	-1.14821400
H	-7.80907000	1.27834300	-1.51996200
C	-8.88972800	-1.46534900	0.03123500
H	-9.80406500	-1.21106600	-0.50575500
H	-8.54870400	-2.41323600	-0.39033700
C	-8.54997000	1.92409700	0.41718200
H	-7.58540300	2.11668300	0.89096800
H	-8.92307000	2.86834900	0.01272800
H	-9.24633400	1.59117400	1.18884800
C	-9.19338400	-1.61584500	1.52539200
H	-9.61588700	-0.69837400	1.93863800
H	-9.92126500	-2.41774100	1.67282600
H	-8.29719400	-1.86230700	2.09847100
H	-5.92853700	1.38651700	-0.74265100
H	-4.35268400	-3.12468500	0.59936300
H	-1.97239800	-2.25381600	0.34936200
C	2.73247500	-1.53583200	1.44621300
H	2.94926800	-0.72867500	2.14852300
H	1.68454900	-1.81338900	1.56211100
H	3.34258700	-2.39414400	1.72650100
C	2.71340700	-2.20609800	-1.04322000
H	1.66592900	-2.50298400	-0.98578300
H	2.91348800	-1.85940700	-2.05887300
H	3.32652600	-3.08930700	-0.86615400
C	2.85476700	2.54040400	-1.00397900
H	2.02629800	2.49795600	-1.71107000
H	3.71075800	2.93550200	-1.54998000
C	2.49036400	3.44163400	0.18099900
H	1.66176300	3.00723300	0.74546600
H	2.12623400	4.38952100	-0.22539000
C	3.63383600	3.74043000	1.14339300

H	4.03332200	2.80994500	1.57205000
H	4.45350100	4.24016000	0.60563900
O	3.09196400	4.57727000	2.15264500
H	3.79109600	4.81316900	2.76947700

EE + Thermal Free Energy Correction = -1575.335467 Hartree

3-d close

C	-5.57546700	1.59825900	1.53316900
C	-6.85882000	1.15169400	1.34118500
C	-7.13824800	0.04238000	0.50215100
C	-6.05692700	-0.63403100	-0.16532700
C	-4.74049400	-0.13421300	0.02133800
C	-4.52308500	0.94431600	0.85805100
H	-9.26951200	0.10199700	0.83206800
H	-5.37187300	2.42711300	2.20101400
H	-7.68502000	1.64167500	1.84572700
C	-8.46643300	-0.42258200	0.32393000
C	-6.38337800	-1.76392700	-0.96735400
C	-7.68235100	-2.18800700	-1.11254500
C	-8.74053500	-1.51164900	-0.46566400
H	-5.59442800	-2.30303500	-1.47177300
H	-7.89797500	-3.05331000	-1.72991200
H	-9.76059500	-1.85653000	-0.59086100
C	-3.39061800	-0.66044100	-0.47150000
N	-3.15044400	1.25388100	0.99662000
C	-2.73884200	2.65446000	0.86204600
H	-1.79018300	2.79929900	1.38182300
H	-3.47794700	3.32667300	1.29519200
C	-2.57702700	2.83047400	-0.66544700
H	-3.45854500	3.29212600	-1.11985300
H	-1.69387900	3.42450400	-0.92057000
O	-2.44484300	1.50423400	-1.18839400
C	-2.45432900	0.55435000	-0.09562900
C	-1.04548600	0.18343700	0.29518800
H	-0.92979300	-0.35642900	1.22419700
C	0.02327800	0.48740700	-0.45468700
H	-0.15816500	1.03416000	-1.37644900
C	1.42773700	0.17950500	-0.20208200
C	2.38849600	0.58483500	-1.08874000
C	1.84064000	-0.56897800	0.99349700
C	3.77269100	0.31611300	-0.90218400
C	4.15294100	-0.39514700	0.24855300
O	1.12970100	-1.00118300	1.86264500

O	3.21222700	-0.80762900	1.14176300
C	5.47338500	-0.70366300	0.53312700
C	4.80514600	0.71193500	-1.77301300
C	6.12505500	0.41660200	-1.51381200
H	6.87512300	0.75542000	-2.21264700
C	6.50280900	-0.31662400	-0.35055200
N	7.81915900	-0.64502100	-0.10614800
C	8.19960700	-1.37729500	1.10313200
H	9.15444200	-1.86555300	0.89610100
H	7.48058700	-2.18425300	1.27088600
C	8.88690800	-0.24089600	-1.02157500
H	9.71499600	-0.93817300	-0.87585000
H	8.55021900	-0.38975500	-2.05123800
C	8.32964000	-0.51672200	2.36673400
H	7.39924700	0.00888200	2.58990700
H	8.57712900	-1.14758100	3.22543300
H	9.11985300	0.22928900	2.25680400
C	9.39230000	1.19593600	-0.83513500
H	9.82906700	1.33502400	0.15613400
H	10.16240100	1.42243800	-1.57855100
H	8.58427900	1.92127700	-0.95057700
H	5.66675300	-1.24378000	1.44713100
H	4.55073800	1.26853500	-2.66888900
H	2.08397200	1.13562400	-1.97450100
C	-3.01607700	-1.92131600	0.34145000
H	-2.03181700	-2.29869400	0.05335300
H	-3.00680000	-1.71932300	1.41463100
H	-3.75084900	-2.70819800	0.15743900
C	-3.27310200	-0.95788400	-1.97628300
H	-3.76534500	-1.89703000	-2.23310100
H	-3.70108400	-0.15710900	-2.57707600
H	-2.21913900	-1.06064600	-2.24954300

EE + Thermal Free Energy Correction = -1535.624527 Hartree

3-d close +H state1

C	-5.63275700	2.08339000	0.68520900
C	-6.90143100	1.56167100	0.68964300
C	-7.13314900	0.18913700	0.40895300
C	-6.03187500	-0.69052600	0.11840000
C	-4.71804200	-0.13075800	0.09934900
C	-4.58144400	1.20584900	0.37624000
H	-9.27435700	0.33989300	0.64093900
H	-5.45669300	3.12707700	0.91621900

H	-7.74826200	2.19790800	0.91825800
C	-8.45187300	-0.33315600	0.42647000
C	-6.31771900	-2.06123900	-0.11608100
C	-7.60846000	-2.53224900	-0.08407600
C	-8.68753700	-1.66301500	0.18392800
H	-5.51384200	-2.75084700	-0.32305900
H	-7.80053300	-3.58298600	-0.26613500
H	-9.69913400	-2.05027800	0.20208500
C	-3.35727600	-0.81040600	-0.08836000
N	-3.16301500	1.61750300	0.35783200
C	-2.80311300	2.82455100	-0.47029900
H	-1.98374000	3.34122700	0.02551600
H	-3.66588300	3.48181700	-0.53792900
C	-2.37981600	2.21815100	-1.82812600
H	-3.02390100	2.53401600	-2.64692400
H	-1.34413800	2.47552600	-2.05884400
O	-2.54337400	0.80403300	-1.69311700
C	-2.41627300	0.41753200	-0.35495300
C	-1.01396200	0.35028900	0.15113400
H	-0.86376400	0.32289600	1.22317400
C	0.04834400	0.24060900	-0.67014000
H	-0.14026800	0.22498000	-1.74151800
C	1.44356500	0.11402200	-0.30121900
C	2.40879700	-0.04371400	-1.27244000
C	1.84928700	0.14917500	1.10560200
C	3.77567800	-0.18494100	-0.96223300
C	4.15169100	-0.15750700	0.39843000
O	1.12353100	0.29083200	2.06012900
O	3.20629700	0.00980100	1.36760200
C	5.46077600	-0.29093400	0.81217100
C	4.81375100	-0.35266400	-1.90722300
C	6.12175800	-0.48850800	-1.52180900
H	6.87538700	-0.60023000	-2.28590800
C	6.49450700	-0.47919200	-0.13794100
N	7.79122000	-0.65663400	0.24814900
C	8.17399100	-0.60922400	1.66679500
H	9.11614800	-1.15130100	1.75930500
H	7.44269200	-1.17571200	2.24918700
C	8.86367600	-0.87673700	-0.73312100
H	9.65176500	-1.43159800	-0.22125000
H	8.49458000	-1.53997200	-1.51844300
C	8.33453200	0.80386700	2.23908500
H	7.41515500	1.38462900	2.14324900

H	8.58931900	0.74565100	3.30056200
H	9.13236200	1.34848900	1.73059500
C	9.44783600	0.40246900	-1.34267300
H	9.91039800	1.03028300	-0.57869700
H	10.21633700	0.14546300	-2.07656600
H	8.68118100	0.99460300	-1.84678600
H	5.65324300	-0.24959700	1.87274100
H	4.56422500	-0.36950400	-2.96259900
H	2.10769800	-0.06748500	-2.31651100
C	-2.96814300	-1.53717800	1.21915100
H	-1.98180300	-1.99553100	1.12987400
H	-2.95723600	-0.86812000	2.08409400
H	-3.69423700	-2.32367200	1.42912600
C	-3.22769600	-1.77745200	-1.28139700
H	-3.65604700	-2.74996300	-1.04326200
H	-3.70625200	-1.38604200	-2.17731300
H	-2.17026700	-1.94349000	-1.50130600
H	-2.80493000	1.73057400	1.30853400

EE + Thermal Free Energy Correction = -1536.000812 Hartree

3-d close +H state2

C	5.58964200	1.78021600	-1.25979000
C	6.85271400	1.24569300	-1.23514600
C	7.11199600	-0.01568700	-0.63849100
C	6.03284100	-0.75920500	-0.04484900
C	4.73731700	-0.17086700	-0.05439800
C	4.54192600	1.05611900	-0.65369900
H	9.22249300	0.01189700	-1.08587100
H	5.39854300	2.72936500	-1.74615400
H	7.67769300	1.78372700	-1.68937400
C	8.42007800	-0.56390400	-0.63657700
C	6.33727600	-2.03449700	0.50674200
C	7.61717800	-2.53543000	0.48646700
C	8.67443100	-1.79541100	-0.08617700
H	5.55105600	-2.62769500	0.95099500
H	7.81767000	-3.51139300	0.91428300
H	9.67857300	-2.20283200	-0.09264800
C	3.38923100	-0.72785800	0.40790200
N	3.18108400	1.46377200	-0.63790600
C	2.88947600	2.82177100	-0.15845500
H	1.91500000	3.13560800	-0.53927800
H	3.64033400	3.53062800	-0.50229800
C	2.86742900	2.64541100	1.36751100

H	3.85798500	2.79917300	1.80607700
H	2.14988800	3.30154800	1.86591600
O	2.47431900	1.27890300	1.56854800
C	2.49121200	0.57619900	0.30689200
C	1.07548200	0.31686700	-0.14907400
H	0.96372500	-0.04104200	-1.16200900
C	0.00483800	0.51312100	0.63696500
H	0.18679800	0.88012100	1.64271600
C	-1.39549400	0.28806000	0.31259900
C	-2.36413200	0.53515100	1.24215700
C	-1.79676200	-0.21627500	-1.02177800
C	-3.75839000	0.32833900	0.98119800
C	-4.11823600	-0.14709000	-0.29421700
O	-1.09097800	-0.48822100	-1.94379600
O	-3.18373700	-0.39892300	-1.23087000
C	-5.44772200	-0.37838600	-0.64101600
C	-4.78169300	0.56802900	1.91229300
C	-6.11184800	0.34356400	1.58644400
H	-6.88937100	0.53465200	2.31848500
C	-6.42408300	-0.12590300	0.31121900
N	-7.84940200	-0.38486400	-0.01852400
C	-8.37416700	0.48333200	-1.16167100
H	-9.39205900	0.14823600	-1.35566900
H	-7.76047600	0.24471100	-2.02948400
C	-8.12829600	-1.87785600	-0.22792100
H	-7.73679000	-2.12618100	-1.21431400
H	-7.52276200	-2.39087000	0.51853100
C	-8.33663200	1.96344100	-0.82348800
H	-7.32086200	2.31984900	-0.65089000
H	-8.75047500	2.52113600	-1.66573100
H	-8.94854300	2.19506500	0.05291700
C	-9.59945200	-2.23223300	-0.08104100
H	-10.22795800	-1.79577500	-0.85807600
H	-9.69746200	-3.31696200	-0.15810900
H	-9.99050000	-1.94271700	0.89863600
H	-5.66254800	-0.74756400	-1.63551400
H	-4.52521600	0.93420000	2.89911300
H	-2.07250300	0.90155200	2.22080500
C	2.92486800	-1.81328500	-0.59123400
H	1.94129600	-2.20896600	-0.32197100
H	2.87988700	-1.43050000	-1.61315800
H	3.63278600	-2.64393900	-0.58384400
C	3.33342700	-1.28345700	1.84148100

H	3.81413200	-2.26015700	1.90029600
H	3.81314100	-0.61152200	2.55077000
H	2.29282900	-1.41563400	2.15191200
H	-8.38164600	-0.11195300	0.81180300

EE + Thermal Free Energy Correction = -1535.982253 Hartree

3-d open

C	5.77211800	1.70719600	-0.32184500
C	6.96725600	1.04337500	-0.21764300
C	7.03353300	-0.36618600	-0.04534400
C	5.82441000	-1.14144100	0.03811400
C	4.59688900	-0.43737100	-0.07582400
C	4.60087400	0.92951300	-0.25758300
H	9.18994600	-0.43054600	-0.00517400
H	5.73373200	2.78382300	-0.39716700
H	7.89535700	1.60206000	-0.25515600
C	8.28465600	-1.02403400	0.05864700
C	5.94152600	-2.54617800	0.22576000
C	7.17346600	-3.14758800	0.32171300
C	8.35768000	-2.38357900	0.23734700
H	5.05402200	-3.15992700	0.29499900
H	7.23814300	-4.21998100	0.46406800
H	9.32080400	-2.87350200	0.31501800
C	3.15292000	-0.92086400	-0.03373200
N	3.26304300	1.39094500	-0.36895100
C	2.38406500	0.39043600	-0.22792300
C	0.99073500	0.62359800	-0.26078100
H	0.65846600	1.64550200	-0.35960400
C	0.00350000	-0.32724100	-0.16420400
H	0.28246800	-1.36942800	-0.05974900
C	-1.40558600	-0.10750200	-0.18989400
C	-2.27675700	-1.18904500	-0.09626900
C	-1.97039900	1.24506300	-0.31486400
C	-3.66540500	-1.03994400	-0.12855700
C	-4.19454800	0.26884600	-0.26139100
O	-1.35903600	2.27955600	-0.39300200
O	-3.35790600	1.33962000	-0.34375000
C	-5.54586900	0.52114000	-0.30655500
C	-4.60164300	-2.10278000	-0.03695200
C	-5.94810800	-1.87681300	-0.08017500
H	-6.61725100	-2.71883500	0.00369000
C	-6.47682600	-0.54865600	-0.23305200
N	-7.81393900	-0.32947800	-0.31468800

C	-8.35621800	1.03119200	-0.47499700
H	-9.33726600	0.92708200	-0.93993500
H	-7.73736900	1.57156400	-1.19461300
C	-8.78666000	-1.43240500	-0.21711800
H	-9.69613000	-1.09236600	-0.71353900
H	-8.42338600	-2.27808200	-0.80471600
C	-8.48330100	1.82516300	0.82936300
H	-7.52030700	1.93746000	1.33134000
H	-8.87064200	2.82397400	0.61307500
H	-9.17265300	1.34121300	1.52346800
C	-9.11193700	-1.86936900	1.21491200
H	-9.55902900	-1.05436900	1.78674700
H	-9.82654700	-2.69605900	1.19289600
H	-8.22036800	-2.20614300	1.74788000
H	-5.85750800	1.54985800	-0.39565400
H	-4.23216800	-3.11631500	0.07260100
H	-1.86152400	-2.18820300	0.00224700
C	2.81418900	-1.54009400	1.34607100
H	3.00544400	-0.82493700	2.14843300
H	1.76894300	-1.84568700	1.40357500
H	3.43497500	-2.41692800	1.52747100
C	2.85539000	-1.88837600	-1.20888800
H	1.81370300	-2.21012200	-1.21360900
H	3.06940700	-1.41184700	-2.16749200
H	3.48288700	-2.77575900	-1.13176000
C	2.92129600	2.79530400	-0.65193600
H	2.03161700	2.81468300	-1.28033300
H	3.74213900	3.21567300	-1.23230100
C	2.69784500	3.63483500	0.59978100
H	1.90045300	3.19353700	1.21059100
H	2.36717100	4.62946300	0.27303500
O	3.92881500	3.68932900	1.30157500
H	3.80920800	4.19767200	2.10948600

EE + Thermal Free Energy Correction = -1536.040669 Hartree

3-e close

C	-5.51372100	0.13668100	-0.69721900
C	-5.54158100	0.47106800	0.66043400
C	-6.74584600	0.76919500	1.27912200
C	-7.92988300	0.72859600	0.53454800
C	-7.89132400	0.40094100	-0.81914900
C	-6.68229700	0.10342200	-1.45308800
H	-6.77565500	1.02608000	2.33291300

H	-8.87699100	0.95524700	1.01035300
H	-8.81109900	0.37633600	-1.39323900
H	-6.66056800	-0.13831000	-2.50958200
N	-4.19024600	-0.10003600	-1.14154900
C	-4.12322400	0.50551000	1.20584600
C	-3.36113700	-0.27754000	0.06781300
C	-3.95727700	-0.16534900	2.57455900
H	-2.90574200	-0.16931000	2.87569700
H	-4.51655400	0.39088900	3.33217100
H	-4.31465800	-1.19357400	2.55558800
C	-3.65455800	1.97639000	1.28680500
H	-4.28400400	2.51684000	1.99831300
H	-2.61815600	2.04442700	1.62641400
H	-3.73422500	2.47962500	0.32079000
C	-1.93958500	0.16481000	-0.17324600
H	-1.80928500	1.15374500	-0.58927300
C	-0.87711300	-0.59996600	0.11400400
H	-1.07374800	-1.58533500	0.52841900
C	-3.93842800	-1.30399800	-1.93812400
H	-3.03611900	-1.15739000	-2.53442200
H	-4.76999600	-1.51184500	-2.60983000
C	-3.73327900	-2.39993500	-0.86644100
H	-4.64521500	-2.97916700	-0.69522900
H	-2.92031700	-3.08496100	-1.12617400
O	-3.41651700	-1.69703600	0.34145300
C	0.53888300	-0.28574700	-0.05198600
C	0.97375200	1.01369600	-0.58347600
C	1.49093200	-1.20490100	0.29740800
C	2.88567400	-0.96047000	0.16197800
H	1.17077200	-2.16361600	0.69624500
C	3.28592400	0.28334200	-0.35495300
O	2.35437200	1.21185200	-0.70557700
O	0.27420700	1.93071100	-0.92621500
C	4.61717200	0.62769400	-0.52496100
H	4.82509100	1.61149200	-0.91673400
C	3.90956400	-1.86011000	0.51301000
H	3.63950200	-2.82748900	0.92333000
C	5.63888500	-0.28433000	-0.18644800
C	5.24013000	-1.54200300	0.35443200
H	5.98186200	-2.26822600	0.65143900
N	6.96843600	0.02324700	-0.38252000
C	7.36755600	1.31518700	-0.94354500
C	7.42169900	2.47181900	0.06319900

H	6.69356500	1.56704800	-1.76723600
H	8.35323500	1.17906700	-1.39433700
H	7.69377100	3.39998900	-0.44782200
H	6.45643400	2.62409500	0.54985100
H	8.16535800	2.28451500	0.84101300
C	8.02940800	-0.90954800	-0.00093400
C	8.40177800	-0.89246200	1.48751500
H	8.90841400	-0.65579300	-0.59753700
H	7.74509500	-1.92080100	-0.30550900
H	9.17797400	-1.63662900	1.68935100
H	8.78530300	0.08540400	1.78637700
H	7.53952400	-1.12099400	2.11722200

EE + Thermal Free Energy Correction = -1381.996317 Hartree

3-e close +H state1

C	-5.54524000	0.28299100	-0.63864500
C	-5.51370700	0.35573300	0.74611300
C	-6.71953200	0.50764400	1.42456300
C	-7.90658300	0.59154900	0.69605300
C	-7.90216800	0.53028700	-0.69825800
C	-6.70306900	0.37259300	-1.39339200
H	-6.74089900	0.56047600	2.50639600
H	-8.84735800	0.70726900	1.22062200
H	-8.83252900	0.60340800	-1.24727700
H	-6.69297300	0.32679100	-2.47610300
N	-4.17947300	0.12068600	-1.17830700
C	-4.09598300	0.32089200	1.29611900
C	-3.29870200	-0.29712500	0.09729700
C	-3.93900400	-0.54817300	2.55309800
H	-2.88848100	-0.60507700	2.84737900
H	-4.48764000	-0.09747300	3.38286400
H	-4.31190900	-1.55840500	2.39281900
C	-3.63093800	1.76346900	1.59592400
H	-4.26176200	2.19058900	2.37746500
H	-2.59714400	1.77432900	1.94497000
H	-3.70515500	2.42081600	0.72496300
C	-1.89519100	0.14937100	-0.12816800
H	-1.72971300	1.18780300	-0.38652100
C	-0.83738000	-0.66527500	0.05583700
H	-1.03531200	-1.68944900	0.36493500
C	-3.94762800	-0.99881900	-2.15619500
H	-3.16607500	-0.68553100	-2.84542600
H	-4.86527400	-1.19449600	-2.70470700

C	-3.50015000	-2.17891900	-1.26131700
H	-4.20140400	-3.01125300	-1.28370800
H	-2.50907400	-2.52984200	-1.55491100
O	-3.49601900	-1.67860100	0.07943500
C	0.56605900	-0.33768100	-0.08441000
C	0.97932600	0.99264200	-0.53640600
C	1.53329000	-1.27637400	0.20665400
C	2.90967900	-1.00186600	0.09134000
H	1.22678000	-2.26354800	0.54247900
C	3.29380200	0.28606700	-0.34232200
O	2.34539600	1.22061500	-0.63911200
O	0.25182600	1.90971400	-0.83274100
C	4.61323800	0.66294300	-0.48039500
H	4.80976200	1.67342100	-0.80296300
C	3.95109000	-1.91132600	0.38811600
H	3.69487800	-2.90784200	0.73111500
C	5.65233400	-0.25695600	-0.19567200
C	5.26946900	-1.56144500	0.25865400
H	6.02404000	-2.29104500	0.50890500
N	6.96433800	0.07916200	-0.35746900
C	7.35382000	1.41575300	-0.83012700
C	7.39639100	2.49432500	0.25814200
H	6.67879900	1.71395800	-1.63602200
H	8.33980500	1.31611100	-1.28668700
H	7.66720200	3.45592200	-0.18576400
H	6.42884100	2.60975900	0.75064500
H	8.13840400	2.25682400	1.02277500
C	8.04588200	-0.86329000	-0.03325900
C	8.40202300	-0.94222600	1.45540000
H	8.92099100	-0.54594500	-0.60215000
H	7.78383800	-1.85235400	-0.41688000
H	9.20243100	-1.67151500	1.60606800
H	8.75040700	0.02193500	1.83030700
H	7.54598500	-1.24894600	2.05999300
H	-3.82989600	0.99985500	-1.56426600

EE + Thermal Free Energy Correction = -1382.371700 Hartree

3-e close +H state2

C	5.42562600	-0.09115300	-0.81314000
C	5.50038500	-0.67402600	0.45273300
C	6.71151800	-1.15932000	0.92531700
C	7.85008900	-1.05631600	0.12099400
C	7.76230100	-0.48122600	-1.14574500

C	6.54686100	0.00550700	-1.63146100
H	6.78104200	-1.61088500	1.90918100
H	8.80181300	-1.42837300	0.48107800
H	8.64787900	-0.41075100	-1.76690900
H	6.48535100	0.43857100	-2.62313700
N	4.09970800	0.32460300	-1.11762300
C	4.11755100	-0.72706600	1.08078800
C	3.34475300	0.29255200	0.14722300
C	4.07885500	-0.29622900	2.55236600
H	3.05274500	-0.29489900	2.93190900
H	4.65278200	-1.00158700	3.15897200
H	4.49522600	0.70073800	2.68428900
C	3.56282100	-2.16348600	0.94408300
H	4.20040000	-2.84888300	1.50668900
H	2.54862400	-2.24247800	1.34565800
H	3.55456700	-2.49969200	-0.09512500
C	1.90336000	-0.07510200	-0.11115500
H	1.73983300	-0.98852000	-0.66426200
C	0.87193400	0.67436600	0.30930900
H	1.10897000	1.58299600	0.85491200
C	3.92399100	1.69281400	-1.62055100
H	2.97885800	1.76015300	-2.16382900
H	4.73180400	1.96751300	-2.29627500
C	3.89545800	2.53125900	-0.33109000
H	4.89386600	2.88131600	-0.05375200
H	3.22145000	3.38923500	-0.39375200
O	3.42232100	1.62935900	0.68350100
C	-0.54953500	0.42603900	0.12468000
C	-1.02572900	-0.79108900	-0.57355500
C	-1.46944300	1.31520600	0.60082300
C	-2.88135800	1.12601400	0.44307200
H	-1.12344400	2.20430700	1.11732500
C	-3.31224300	-0.03012300	-0.23183400
O	-2.42703600	-0.92867200	-0.70594900
O	-0.36931200	-1.67181300	-1.03820200
C	-4.66438900	-0.30014200	-0.44021200
H	-4.92734000	-1.20669700	-0.96371400
C	-3.85805200	2.02230700	0.90761100
H	-3.54876600	2.92365800	1.42292200
C	-5.59374400	0.61298100	0.03184500
C	-5.20689500	1.77391200	0.70599200
H	-5.94533900	2.48356900	1.06481500
N	-7.05604700	0.39779200	-0.14859700

C	-7.50140200	-0.13565100	-1.52525400
C	-7.60397700	-1.64265000	-1.69486800
H	-6.80393700	0.30454300	-2.23737900
H	-8.48225400	0.31589200	-1.68599300
H	-7.93949800	-1.82281900	-2.71900100
H	-6.65666100	-2.16470800	-1.56996300
H	-8.34629300	-2.08840500	-1.03230900
C	-7.74394800	-0.27090500	1.06164200
C	-7.04849900	-1.50395900	1.60968800
H	-8.76495000	-0.47924300	0.73836300
H	-7.78216400	0.50755400	1.82475300
H	-7.63947800	-1.86144200	2.45619300
H	-6.98111500	-2.31704000	0.88864900
H	-6.04908000	-1.27361400	1.97834700
H	-7.43604600	1.34515100	-0.14571800

EE + Thermal Free Energy Correction = -1382.341847 Hartree

3-e open

C	5.54675400	0.30766200	-0.28635500
C	5.48189300	-1.05898500	-0.02271200
C	6.65126300	-1.78008300	0.15948900
C	7.87423800	-1.10809900	0.07623500
C	7.91948300	0.26219200	-0.18381500
C	6.74909000	0.99873500	-0.37078600
H	6.62821900	-2.84430000	0.36418000
H	8.79768400	-1.65622400	0.21705100
H	8.87645000	0.76614500	-0.24103000
H	6.79616500	2.06188600	-0.56718200
N	4.22482300	0.80144000	-0.44295800
C	4.02842700	-1.49323200	0.01256600
C	3.31410100	-0.16881800	-0.27106000
C	3.65956600	-2.03624300	1.41514100
H	2.61565100	-2.34876200	1.46286200
H	4.28399600	-2.90224500	1.64337900
H	3.82691400	-1.28190000	2.18591200
C	3.74055500	-2.53786300	-1.09288100
H	4.34725500	-3.42795700	-0.91511300
H	2.69260000	-2.84026400	-1.09997000
H	3.99317400	-2.14828500	-2.08078900
C	1.93536300	0.11300500	-0.33267600
H	1.66315800	1.14410500	-0.45855700
C	0.89154200	-0.75838500	-0.15810300
H	1.08399900	-1.81974700	-0.04441500

C	3.93679700	2.21576100	-0.72135600
H	3.06484200	2.26619000	-1.37375100
H	4.78043000	2.61527100	-1.28612400
C	3.72101400	3.05503100	0.55242000
H	4.61988500	3.01380300	1.17135600
H	3.58108400	4.09653900	0.23581200
O	2.66347000	2.58951900	1.36131900
C	-0.48859800	-0.39575600	-0.09145500
C	-0.91315700	1.01286600	-0.08121300
C	-1.46296100	-1.38489100	0.01086000
C	-2.82585400	-1.09207800	0.09613000
H	-1.15035700	-2.42533700	0.02279200
C	-3.21829100	0.26979600	0.08043900
O	-2.27630500	1.25060700	-0.00930600
O	-0.20324700	1.99067500	-0.11899700
C	-4.53258800	0.66567800	0.15676700
H	-4.73721800	1.72429000	0.13143500
C	-3.86400400	-2.05555600	0.19194000
H	-3.60183000	-3.10765000	0.19485900
C	-5.56500100	-0.30273900	0.27578400
C	-5.17679500	-1.68738200	0.27281600
H	-5.92790900	-2.45979600	0.32899500
N	-6.86537000	0.06373600	0.40026900
C	-7.26596100	1.48156900	0.35823200
C	-7.36421300	2.07195100	-1.05238300
H	-6.57122200	2.06139900	0.97056800
H	-8.23420700	1.54980600	0.85477700
H	-7.64232900	3.12690700	-0.98881000
H	-6.41509000	2.00423900	-1.58736900
H	-8.12362400	1.55891500	-1.64490400
C	-7.93935400	-0.93207800	0.56492300
C	-8.47634800	-1.51223600	-0.74730400
H	-8.74611500	-0.43671400	1.10683300
H	-7.58352800	-1.72836500	1.22102200
H	-9.24962900	-2.25380600	-0.53139900
H	-8.92206000	-0.73648000	-1.37247400
H	-7.68898600	-2.00096800	-1.32498900
H	1.81331400	2.82773300	0.96987100

EE + Thermal Free Energy Correction = -1382.415762 Hartree

3-f close

C	4.86078700	0.15630200	-0.83070500
C	4.92759700	-0.37734300	0.46446000

C	6.14634900	-0.71946300	1.02307400
C	7.32425700	-0.52135700	0.28037000
C	7.25682500	0.00558400	-1.01280600
C	6.01677400	0.34386500	-1.57681500
H	6.22676100	-1.13166800	2.02413600
H	8.15625200	0.15904300	-1.59686400
H	5.97807500	0.74252300	-2.58617500
N	3.51381900	0.40535800	-1.21884900
C	3.52037200	-0.54896400	1.01491000
C	2.71346000	0.37614000	0.02374100
C	3.35350300	-0.10805600	2.47489100
H	2.30404400	-0.17996400	2.77942100
H	3.93593500	-0.76130500	3.13297300
H	3.68328700	0.92145800	2.61772500
C	3.10306200	-2.03059600	0.86618600
H	3.76303000	-2.65683600	1.47437100
H	2.07422500	-2.18886200	1.20340400
H	3.18216100	-2.36922500	-0.17067000
C	1.29531600	-0.06205600	-0.24869300
H	1.17243600	-0.99297200	-0.78701700
C	0.22183100	0.63938000	0.15225800
H	0.40674700	1.57045300	0.68497200
C	3.21727100	1.71752500	-1.80099200
H	2.28340400	1.65469200	-2.36649800
H	4.01185400	2.03979600	-2.47560600
C	3.06088800	2.62565700	-0.56126800
H	3.99638800	3.14461500	-0.31919600
H	2.26692500	3.37130800	-0.68601900
O	2.73768900	1.73921400	0.51446500
C	-1.19135100	0.31849300	-0.03316600
C	-1.61234600	-0.92988800	-0.68805900
C	-2.15684600	1.18370700	0.41351500
C	-3.55012400	0.92853000	0.26276500
H	-1.84987200	2.10611300	0.90271300
C	-3.93373400	-0.27078800	-0.36650100
O	-2.98796100	-1.14653400	-0.81061200
O	-0.89526800	-1.79808400	-1.13335800
C	-5.26205400	-0.62372400	-0.56130100
H	-5.45737800	-1.57074800	-1.04404500
C	-4.58844400	1.77535600	0.69897500
H	-4.33173800	2.70700200	1.19606300
C	-6.29754400	0.23809500	-0.13599300
C	-5.91687800	1.44982100	0.51546100

H	-6.67009500	2.13466600	0.88031900
N	-7.62589100	-0.07149400	-0.35695700
C	-8.00711000	-1.33573900	-0.98838400
C	-8.00841800	-2.55261800	-0.05286700
H	-7.34613100	-1.51959600	-1.84253100
H	-9.00776400	-1.19751900	-1.40885700
H	-8.26775700	-3.45732600	-0.61294400
H	-7.02696200	-2.70587200	0.40365500
H	-8.73929000	-2.43169100	0.75188600
C	-8.69722000	0.80880400	0.10943800
C	-9.05760300	0.66208400	1.59420400
H	-9.57908100	0.59445200	-0.50182000
H	-8.42793700	1.84752300	-0.11109500
H	-9.84035900	1.37881100	1.86516300
H	-9.42900500	-0.34298200	1.81321200
H	-8.19062000	0.84604900	2.23458000
O	8.48646600	-0.87937200	0.91643700
C	9.70563300	-0.70840300	0.21802000
H	9.88572500	0.34471700	-0.03721300
H	10.49251900	-1.05161800	0.89192200
H	9.73579800	-1.30594500	-0.70308700

EE + Thermal Free Energy Correction = -1496.187449 Hartree

3-f close +H state1

C	4.89898100	-0.04358600	-0.83424200
C	4.89226800	-0.29018200	0.53740500
C	6.09501000	-0.52746500	1.18092000
C	7.29231800	-0.52124000	0.43754100
C	7.26861500	-0.28416500	-0.94902100
C	6.05526700	-0.04136800	-1.59655500
H	6.15065000	-0.72039400	2.24654500
H	8.18337200	-0.28482900	-1.52707600
H	6.04071600	0.13923100	-2.66714700
N	3.52994500	0.19357900	-1.33015200
C	3.48093500	-0.33149700	1.10527100
C	2.66294800	0.42809200	0.00498600
C	3.33277700	0.36888100	2.46561400
H	2.28262400	0.38486200	2.77182200
H	3.88904600	-0.18483400	3.22690700
H	3.70491100	1.39324000	2.43502200
C	3.02613000	-1.80467200	1.22462600
H	3.67345800	-2.32472600	1.93512900
H	1.99649900	-1.86781200	1.58480000

H	3.08977000	-2.34258000	0.27288200
C	1.26074900	-0.00554200	-0.26192700
H	1.10290200	-0.99172200	-0.68486400
C	0.19191900	0.74282700	0.08591500
H	0.37825300	1.70890300	0.55445700
C	3.30241600	1.44499900	-2.14034800
H	2.57672700	1.22303000	-2.92278900
H	4.24580200	1.74999800	-2.58979600
C	2.76012300	2.46123100	-1.10287400
H	3.37337600	3.36066900	-1.03505700
H	1.72968900	2.73936200	-1.33981000
O	2.84348400	1.80364600	0.16321800
C	-1.20972200	0.40665400	-0.07372200
C	-1.60750200	-0.84624700	-0.72277500
C	-2.19034300	1.26437600	0.38308200
C	-3.56549800	0.97503900	0.25376100
H	-1.89742000	2.19597400	0.86410700
C	-3.93125900	-0.24152100	-0.36795900
O	-2.96859900	-1.09521200	-0.82663000
O	-0.86320800	-1.68850000	-1.18408500
C	-5.24700500	-0.62859900	-0.53893600
H	-5.42913700	-1.58252000	-1.01220700
C	-4.62159100	1.80080100	0.70773600
H	-4.37992500	2.74001600	1.19726300
C	-6.30055000	0.21109600	-0.09556200
C	-5.93735500	1.44039400	0.54899600
H	-6.70310800	2.10446900	0.92420800
N	-7.61136500	-0.12930800	-0.28659900
C	-7.97840400	-1.39538100	-0.93666600
C	-7.95677400	-2.61931000	-0.01299100
H	-7.31918000	-1.55344700	-1.79604300
H	-8.98197000	-1.26319200	-1.34914000
H	-8.21216000	-3.51844600	-0.58249900
H	-6.97030100	-2.76944300	0.43403400
H	-8.68292300	-2.51647900	0.79777400
C	-8.70437300	0.72074200	0.20688800
C	-9.02186700	0.55380800	1.69759700
H	-9.58904400	0.47587300	-0.38624800
H	-8.47323700	1.76612800	-0.02059200
H	-9.82735100	1.23701600	1.98491000
H	-9.34829600	-0.46520000	1.92145100
H	-8.15134600	0.77291200	2.32206500
H	3.16633200	-0.61964600	-1.83473200

O	8.41203100	-0.75605800	1.15166900
C	9.67542000	-0.77228400	0.48491100
H	9.89203800	0.19688600	0.02177000
H	10.41352500	-0.97661500	1.25951700
H	9.71418900	-1.56287000	-0.27279400

EE + Thermal Free Energy Correction = -1496.574835 Hartree

3-f close +H state2

C	4.80188800	0.23597300	-0.84246500
C	4.88722800	-0.46440600	0.36628100
C	6.10420100	-0.94302500	0.81987100
C	7.26092700	-0.71486400	0.05267600
C	7.17119600	-0.02295300	-1.16099900
C	5.93334000	0.45217100	-1.61739900
H	6.20052700	-1.48860300	1.75324300
H	8.05358400	0.15371600	-1.76359600
H	5.87700300	0.97782700	-2.56565500
N	3.45566200	0.62258300	-1.12971100
C	3.49687800	-0.64197300	0.95550900
C	2.70064600	0.44393900	0.12320000
C	3.41241900	-0.38276500	2.46555600
H	2.37781200	-0.46086300	2.81680100
H	4.00078200	-1.13228900	3.00395500
H	3.78887000	0.60801700	2.72045200
C	3.00327000	-2.07433300	0.64373000
H	3.65974500	-2.79731600	1.13608500
H	1.98548600	-2.23761800	1.01376000
H	3.02340700	-2.28612700	-0.42912700
C	1.26726000	0.06765200	-0.17241800
H	1.12035000	-0.78954100	-0.81622700
C	0.21927500	0.74729800	0.32946200
H	0.44161200	1.60156000	0.96458900
C	3.23816800	2.03095600	-1.48574300
H	2.28514500	2.12714900	-2.01504900
H	4.03239100	2.39895800	-2.13605000
C	3.19376900	2.73182400	-0.11619700
H	4.18759900	3.07489100	0.19421600
H	2.50280400	3.58106300	-0.09046500
O	2.74105700	1.72070000	0.79675000
C	-1.19833600	0.48219800	0.13596400
C	-1.65744500	-0.65520300	-0.69732600
C	-2.13508700	1.28269800	0.73112300
C	-3.54466500	1.06587200	0.57910300

H	-1.80460600	2.11593700	1.34518800
C	-3.95605200	-0.01824500	-0.22198300
O	-3.05241600	-0.82399700	-0.82063100
O	-0.97911800	-1.45515800	-1.28251500
C	-5.30463800	-0.31238000	-0.43238700
H	-5.55384300	-1.16205100	-1.05243600
C	-4.53991800	1.86395500	1.17210300
H	-4.24635700	2.70756700	1.78821000
C	-6.25344800	0.50478100	0.17047900
C	-5.88709700	1.59132700	0.97309500
H	-6.64015400	2.22449700	1.43585300
N	-7.71119400	0.25727500	-0.00215000
C	-8.18459900	-0.01064200	-1.44655600
C	-8.23423600	-1.45697900	-1.91485200
H	-7.52654600	0.59433300	-2.07249300
H	-9.18893700	0.41959300	-1.48778500
H	-8.60171900	-1.44098300	-2.94521500
H	-7.26129000	-1.94917300	-1.92788900
H	-8.93407600	-2.06173700	-1.33465900
C	-8.32392000	-0.67022600	1.07112800
C	-7.56872200	-1.96233900	1.32955900
H	-9.35330500	-0.84696600	0.74963500
H	-8.34952900	-0.06245000	1.97860400
H	-8.11041700	-2.50383300	2.11061300
H	-7.51393400	-2.61188700	0.45556700
H	-6.55850700	-1.77366800	1.69616400
O	8.41886000	-1.21360800	0.57972600
C	9.62308900	-1.02933100	-0.14802300
H	9.85873900	0.03471600	-0.27882100
H	10.40836600	-1.49948000	0.44520500
H	9.57884400	-1.51062400	-1.13347300
H	-8.13051800	1.16698600	0.20223500

EE + Thermal Free Energy Correction = -1496.539572 Hartree

3-f open

C	4.89597800	0.58568000	-0.32297300
C	4.89132400	-0.79084200	-0.07027100
C	6.07989100	-1.47116300	0.09817200
C	7.29167400	-0.75322100	0.01516700
C	7.28159400	0.63038400	-0.23303400
C	6.07525900	1.31483900	-0.40527600
H	6.12273300	-2.53730900	0.29407200
H	8.20943100	1.18435400	-0.29262300

H	6.08762200	2.38301100	-0.59077000
N	3.55473100	1.02268100	-0.46731100
C	3.45465100	-1.28375600	-0.02881700
C	2.68459300	0.01389500	-0.29711400
C	3.11902400	-1.85495300	1.37157200
H	2.08564000	-2.20431100	1.42621200
H	3.77658900	-2.70237300	1.58300800
H	3.26881100	-1.10342700	2.15065600
C	3.19938400	-2.33098000	-1.14062300
H	3.83941900	-3.20102100	-0.97135600
H	2.16123600	-2.67080700	-1.14458000
H	3.43304900	-1.92581700	-2.12854400
C	1.29227400	0.24088500	-0.34946000
H	0.97610500	1.26115400	-0.47430800
C	0.28260400	-0.66974700	-0.16675500
H	0.51217200	-1.72576700	-0.05455600
C	3.20496400	2.42544500	-0.73036900
H	2.33901900	2.44518900	-1.39518100
H	4.03740600	2.87236400	-1.27886900
C	2.93350600	3.23553600	0.55410100
H	3.83397700	3.23448800	1.17650800
H	2.74615600	4.27495600	0.24711900
O	1.90062000	2.70707300	1.35177200
C	-1.11186100	-0.34955400	-0.08953500
C	-1.58062100	1.04574800	-0.06161300
C	-2.05605200	-1.36883700	0.00694300
C	-3.43072600	-1.11635700	0.09980600
H	-1.71303800	-2.40157900	0.00671300
C	-3.86244600	0.23483100	0.09900800
O	-2.94754700	1.24468700	0.01800900
O	-0.89717000	2.05274400	-0.09184800
C	-5.19002800	0.59599400	0.18088000
H	-5.42485900	1.65019600	0.16646000
C	-4.44216300	-2.10957300	0.18786300
H	-4.15047900	-3.15568800	0.18045500
C	-6.19501500	-0.40365300	0.29005800
C	-5.76818400	-1.77747400	0.27421400
H	-6.49829900	-2.57264400	0.32368200
N	-7.50953700	-0.07445800	0.41877100
C	-7.94905000	1.33098300	0.37831500
C	-8.04804600	1.92451200	-1.03161900
H	-7.27630400	1.92846600	1.00172200
H	-8.92568800	1.37149900	0.86557700

H	-8.35472000	2.97299600	-0.96847200
H	-7.09022700	1.88242700	-1.55685800
H	-8.78786300	1.39217000	-1.63483000
C	-8.55338300	-1.10391400	0.56094900
C	-9.05182300	-1.69152900	-0.76383200
H	-9.38530000	-0.63864200	1.09525400
H	-8.18135100	-1.89479700	1.21805500
H	-9.80667000	-2.45885000	-0.56641300
H	-9.51007900	-0.92330200	-1.39207100
H	-8.23893300	-2.15208000	-1.33225400
H	1.03730600	2.89389400	0.95157300
O	8.40966700	-1.49235700	0.19181600
C	9.68314100	-0.85132600	0.12867000
H	9.78247400	-0.08640600	0.90728500
H	10.41778500	-1.63780900	0.29823400
H	9.85318400	-0.40039000	-0.85570500

EE + Thermal Free Energy Correction = -1496.609105 Hartree

3-6 close temp=333.15K

C	-5.51372100	0.13668100	-0.69721900
C	-5.54158100	0.47106800	0.66043400
C	-6.74584600	0.76919500	1.27912200
C	-7.92988300	0.72859600	0.53454800
C	-7.89132400	0.40094100	-0.81914900
C	-6.68229700	0.10342200	-1.45308800
H	-6.77565500	1.02608000	2.33291300
H	-8.87699100	0.95524700	1.01035300
H	-8.81109900	0.37633600	-1.39323900
H	-6.66056800	-0.13831000	-2.50958200
N	-4.19024600	-0.10003600	-1.14154900
C	-4.12322400	0.50551000	1.20584600
C	-3.36113700	-0.27754000	0.06781300
C	-3.95727700	-0.16534900	2.57455900
H	-2.90574200	-0.16931000	2.87569700
H	-4.51655400	0.39088900	3.33217100
H	-4.31465800	-1.19357400	2.55558800
C	-3.65455800	1.97639000	1.28680500
H	-4.28400400	2.51684000	1.99831300
H	-2.61815600	2.04442700	1.62641400
H	-3.73422500	2.47962500	0.32079000
C	-1.93958500	0.16481000	-0.17324600
H	-1.80928500	1.15374500	-0.58927300
C	-0.87711300	-0.59996600	0.11400400

H	-1.07374800	-1.58533500	0.52841900
C	-3.93842800	-1.30399800	-1.93812400
H	-3.03611900	-1.15739000	-2.53442200
H	-4.76999600	-1.51184500	-2.60983000
C	-3.73327900	-2.39993500	-0.86644100
H	-4.64521500	-2.97916700	-0.69522900
H	-2.92031700	-3.08496100	-1.12617400
O	-3.41651700	-1.69703600	0.34145300
C	0.53888300	-0.28574700	-0.05198600
C	0.97375200	1.01369600	-0.58347600
C	1.49093200	-1.20490100	0.29740800
C	2.88567400	-0.96047000	0.16197800
H	1.17077200	-2.16361600	0.69624500
C	3.28592400	0.28334200	-0.35495300
O	2.35437200	1.21185200	-0.70557700
O	0.27420700	1.93071100	-0.92621500
C	4.61717200	0.62769400	-0.52496100
H	4.82509100	1.61149200	-0.91673400
C	3.90956400	-1.86011000	0.51301000
H	3.63950200	-2.82748900	0.92333000
C	5.63888500	-0.28433000	-0.18644800
C	5.24013000	-1.54200300	0.35443200
H	5.98186200	-2.26822600	0.65143900
N	6.96843600	0.02324700	-0.38252000
C	7.36755600	1.31518700	-0.94354500
C	7.42169900	2.47181900	0.06319900
H	6.69356500	1.56704800	-1.76723600
H	8.35323500	1.17906700	-1.39433700
H	7.69377100	3.39998900	-0.44782200
H	6.45643400	2.62409500	0.54985100
H	8.16535800	2.28451500	0.84101300
C	8.02940800	-0.90954800	-0.00093400
C	8.40177800	-0.89246200	1.48751500
H	8.90841400	-0.65579300	-0.59753700
H	7.74509500	-1.92080100	-0.30550900
H	9.17797400	-1.63662900	1.68935100
H	8.78530300	0.08540400	1.78637700
H	7.53952400	-1.12099400	2.11722200

EE + Thermal Free Energy Correction = -1382.007435 Hartree

3-6 open temp=333.15K

C	5.54675400	0.30766200	-0.28635500
C	5.48189300	-1.05898500	-0.02271200

C	6.65126300	-1.78008300	0.15948900
C	7.87423800	-1.10809900	0.07623500
C	7.91948300	0.26219200	-0.18381500
C	6.74909000	0.99873500	-0.37078600
H	6.62821900	-2.84430000	0.36418000
H	8.79768400	-1.65622400	0.21705100
H	8.87645000	0.76614500	-0.24103000
H	6.79616500	2.06188600	-0.56718200
N	4.22482300	0.80144000	-0.44295800
C	4.02842700	-1.49323200	0.01256600
C	3.31410100	-0.16881800	-0.27106000
C	3.65956600	-2.03624300	1.41514100
H	2.61565100	-2.34876200	1.46286200
H	4.28399600	-2.90224500	1.64337900
H	3.82691400	-1.28190000	2.18591200
C	3.74055500	-2.53786300	-1.09288100
H	4.34725500	-3.42795700	-0.91511300
H	2.69260000	-2.84026400	-1.09997000
H	3.99317400	-2.14828500	-2.08078900
C	1.93536300	0.11300500	-0.33267600
H	1.66315800	1.14410500	-0.45855700
C	0.89154200	-0.75838500	-0.15810300
H	1.08399900	-1.81974700	-0.04441500
C	3.93679700	2.21576100	-0.72135600
H	3.06484200	2.26619000	-1.37375100
H	4.78043000	2.61527100	-1.28612400
C	3.72101400	3.05503100	0.55242000
H	4.61988500	3.01380300	1.17135600
H	3.58108400	4.09653900	0.23581200
O	2.66347000	2.58951900	1.36131900
C	-0.48859800	-0.39575600	-0.09145500
C	-0.91315700	1.01286600	-0.08121300
C	-1.46296100	-1.38489100	0.01086000
C	-2.82585400	-1.09207800	0.09613000
H	-1.15035700	-2.42533700	0.02279200
C	-3.21829100	0.26979600	0.08043900
O	-2.27630500	1.25060700	-0.00930600
O	-0.20324700	1.99067500	-0.11899700
C	-4.53258800	0.66567800	0.15676700
H	-4.73721800	1.72429000	0.13143500
C	-3.86400400	-2.05555600	0.19194000
H	-3.60183000	-3.10765000	0.19485900
C	-5.56500100	-0.30273900	0.27578400

C	-5.17679500	-1.68738200	0.27281600
H	-5.92790900	-2.45979600	0.32899500
N	-6.86537000	0.06373600	0.40026900
C	-7.26596100	1.48156900	0.35823200
C	-7.36421300	2.07195100	-1.05238300
H	-6.57122200	2.06139900	0.97056800
H	-8.23420700	1.54980600	0.85477700
H	-7.64232900	3.12690700	-0.98881000
H	-6.41509000	2.00423900	-1.58736900
H	-8.12362400	1.55891500	-1.64490400
C	-7.93935400	-0.93207800	0.56492300
C	-8.47634800	-1.51223600	-0.74730400
H	-8.74611500	-0.43671400	1.10683300
H	-7.58352800	-1.72836500	1.22102200
H	-9.24962900	-2.25380600	-0.53139900
H	-8.92206000	-0.73648000	-1.37247400
H	-7.68898600	-2.00096800	-1.32498900
H	1.81331400	2.82773300	0.96987100

EE + Thermal Free Energy Correction = -1382.420703 Hartree

proton

H	0.00000000	0.00000000	0.00000000

EE + Thermal Free Energy Correction = -0.010000 Hartree

proton temp=333.15K

H	0.00000000	0.00000000	0.00000000

EE + Thermal Free Energy Correction = -0.011466 Hartree