Electronic Supplementary Material (ESI) for ChemComm.

Supporting information:

Improving the kinetics and dark equilibrium of donor-acceptor Stenhouse adduct by triene backbone design

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1. General Procedures

General Information

All reagents were purchased from commercial sources and used without further purification. Samples for NMR were dissolved in 1 g ampules of deuterated solvents purchased from Cambridge Isotope Laboratories. ^{1}H and ^{13}C NMR spectroscopy measurements were taken on either a Varian 600 MHz or Bruker 500 MHz spectrometer. Chemical shifts are reported relative to residual solvent peaks. Mass spectral data was collected on a Micromass QTOF2 Quadrupole/Time of Flight Tandem mass spectrometer (ESI-MS).

Time-dependent UV-Vis setup

The photoinduced optical absorption kinetics were measured on a pump-probe setup. The pump beam was generated by a 617 nm (240 mW/cm^2) light emitting diode (LED) source (Thorlabs) coupled into a multimode optical fiber terminated with an output collimator. The LED intensity was controlled through a digital-to-analog converter (National Instruments USB-6009) using LabVIEW. The probe beam was produced by High Power MINI Deuterium Tungsten Halogen Source w/shutter 200–2000 nm (Ocean Optics DH-MINI) coupled into a multimode fiber with an output collimator for the light delivery. The probe light was modulated by a shutter (Thorlabs SHB05T optical shutter connected to a SHM05 mounting adapter) which could be controlled manually or through a digital output port (National Instruments USB-6009) using LabVIEW. Pump and probe beams were overlapped using steering and focusing optics at a 90° angle inside a sample holder, which allowed for a 10x10 mm rectangular spectrophotometer cell that was connected to a circulating bath for temperature control. Additionally, the solutions were stirred during the measurements by a miniature stirring plate inserted into the sample holder (Starna Cells SCS 1.11). Both pump and probe beams were nearly collimated inside the cell with a diameter of about 2 mm. The pump beam was blocked after passing through the sample and the probe beam was directed by a system of lenses into the detector (Ocean Optics Flame-S1-XR spectrometer), which acquired spectra of the probe light. The detector was connected to a PC via USB port. The experiment was controlled by a National Instrument LabVIEW program which collected the probe light spectra, determined sample optical absorption spectra, controlled pump and probe light sources, and stored the data on the computer S3 hard drive according to the experimental protocol.

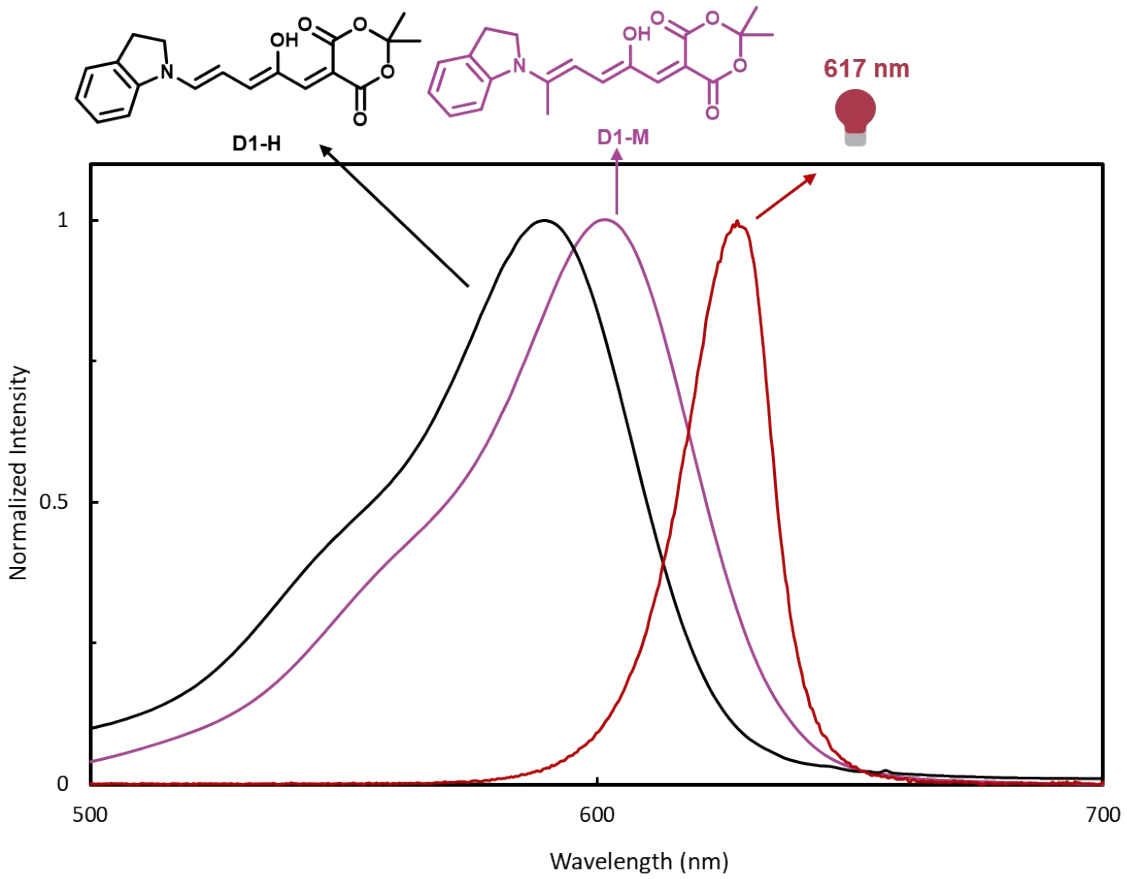
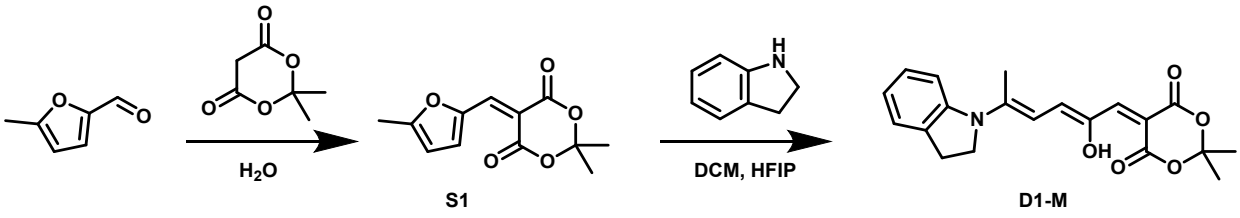


*Figure S1. Emission profile of the 240 mW/cm² Thorlabs 617 nm LED (intensity at the center of the focused beam was measured using an Ocean Optics hand-held spectrometer model USB 2000) used for irradiation of samples for time-dependent UV-Vis measurements overlayed with the unsubstituted DASA derivative **D1-H** and the DASA derivative substituted with a methyl on the triene next to the donor **D1-M** dissolved in toluene with 5% DCM, showing that the 617 nm light hits the absorbance band of both of the shoulders, but there is a better overlap with **D1-M**.*

General Synthesis Information:

D1-H,[1], and **S2**[2] were prepared and purified as previously reported.



S1: The synthesis of this compound was adapted from a previously reported synthesis.[3] To a solution of 2,2-dimethyl-1,3-dioxane-4,6-dione (1.0 g, 0.007 mol, 1 eq) stirring in water was added 5-methyl-2-furfural (1.0 mL, 0.01 mol, 1.4 eq). The solution was stirred at room temperature overnight after which a yellow precipitate had formed. The precipitate was filtered via vacuum filtration and washed with water. It was then redissolved in ethyl acetate, dried over sodium sulfate to remove the residual water and the

solvent was removed under vacuum. The crude product was run through a short silica gel plug and eluted off with dichloromethane. The yellow fractions were combined, and the solvent was removed under vacuum to give 1.7 g of **S1** as a bright yellow solid (73% yield). Characterization matches previously reported data.[3]

D1-M: To a solution of **S1** (250 mg, 1.06 mmol, 1.1 eq) stirring at room temperature in 2 mL dichloromethane in a scintillation vial was added 200 µL HFIP followed by indoline (120 µL, 0.95 mmol, 1 eq). The solution was stirred for two hours before it was rotavapped down. 2 mL of diethyl ether was added to the dark blue crude mixture, sonicated for 15 minutes and filtered. The process was repeated two more times on the precipitate. The final solid was dried under vacuum to give 37 mg of **D1-M** as a dark blue powder (11% yield). ^{1}H NMR (600 MHz, CD_2Cl_2) δ 11.44 (s, 1 H), 7.41 (d, *J* = 8.2 Hz, 1H), 7.33 (d, *J* = 7.4 Hz, 1H), 7.26 (t, *J* = 8.1 Hz, 1H), 7.17 (s, 1H), 7.14 (t, *J* = 7.4 Hz, 1H), 7.01 (d, *J* = 12.8 Hz, 1H), 6.39 (d, *J* = 12.8 Hz, 1H), 4.25 (t, *J* = 7.9 Hz, 2H), 3.23 (t, *J* = 7.9 Hz, 2H), 2.60 (s, 3H). ^{13}C NMR (126 MHz, CD_2Cl_2) δ 167.49, 164.98, 158.61, 146.85, 144.65, 141.01, 136.13, 128.24, 126.62, 125.93, 117.27, 107.08, 104.01, 93.28, 28.28, 27.13, 18.21. HRMS (ESI+) *m/z* for $[C_{20}H_{21}NO_5 + H]^+$ calc = 356.1498, found = 356.1848.

2. General mechanism of donor-acceptor Stenhouse adducts

Donor-acceptor Stenhouse adducts undergo an initial light-triggered Z/E isomerization followed by a bond rotation. The M1 isomers (below) are colored but short-lived. Then, the molecule undergoes a 4-π electrocyclization to form a cyclic α,β-unsaturated ketone colorless closed form. This closed form undergoes rotation of the carbon acid, and finally a proton transfer to a more stabilized keto or zwitterionic closed form. Below is a scheme of the proposed productive isomerization pathway from the open to closed forms. However, it should be noted that there has still been little investigation of how differing donors and acceptors influence the proposed mechanistic steps.

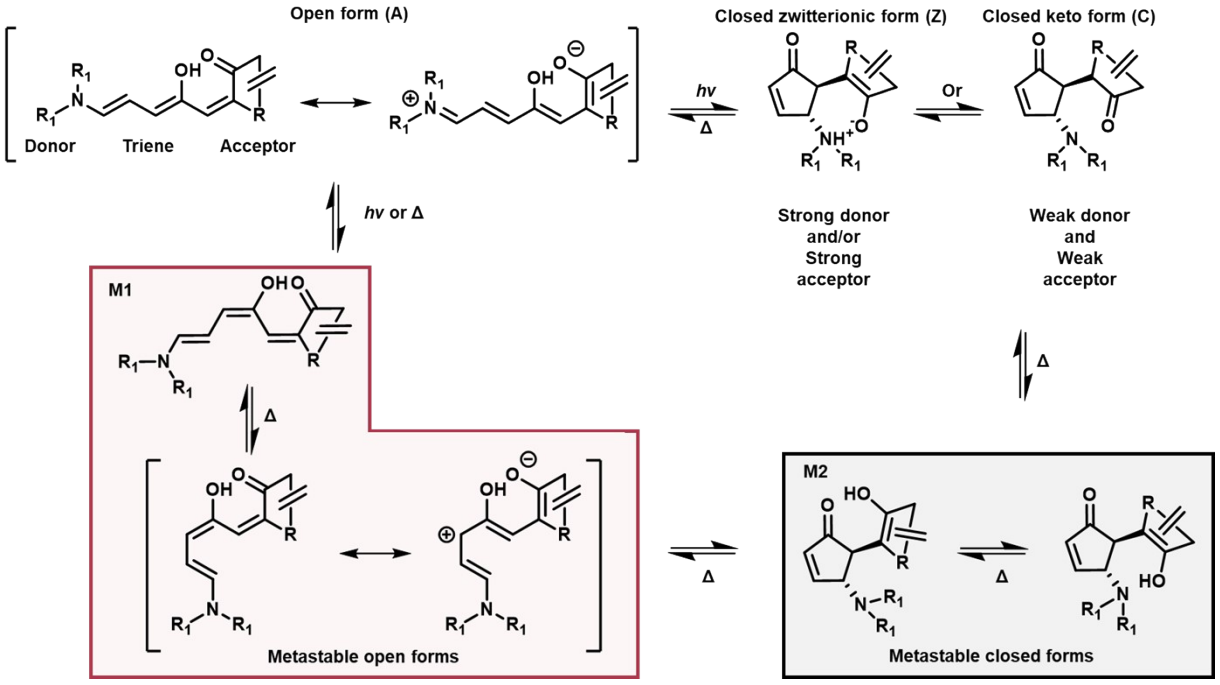


Figure S2. Scheme of the proposed productive isomerization pathway of donor-acceptor Stenhouse adducts

3. Measuring switching kinetics of D1-H and D1-M via time-dependent UV-Vis spectroscopy

10 µM solutions of **D1-M** and **D1-H** in toluene with 5% DCM were prepared by making a 1 mM stock solution in dichloromethane, transferring 100 µL of the solution to empty scintillation vials and drying under high vacuum overnight. The residue was then redissolved in 0.5 mL dichloromethane and diluted to 10 mL with toluene. **D1-H** was stored in complete darkness for one week in the dark prior to the study due to its slow equilibration in toluene. **D1-M** was initially equilibrated by irradiating the compound on the pump probe setup and monitoring for 1.5 hours, after which recovery was complete. For the study, 25 measurements were taken prior to irradiation at 1 s intervals, the samples were irradiated with a 617 nm Thorlabs LED for 95 s total with measurements taken at 1 s intervals. Recovery was subsequently monitored in complete darkness for a total of 1,000 s with the measurement interval increased to 10 s. Absorbance is reported as a boxcar average of 5 absorbances around the λ_{max} and averaging every 5 time points for clarity. Spectra were baselined by subtracting the average absorbance between 400–450 nm, where the compound does not absorb, and normalized by dividing by the maximum absorbance prior irradiation.

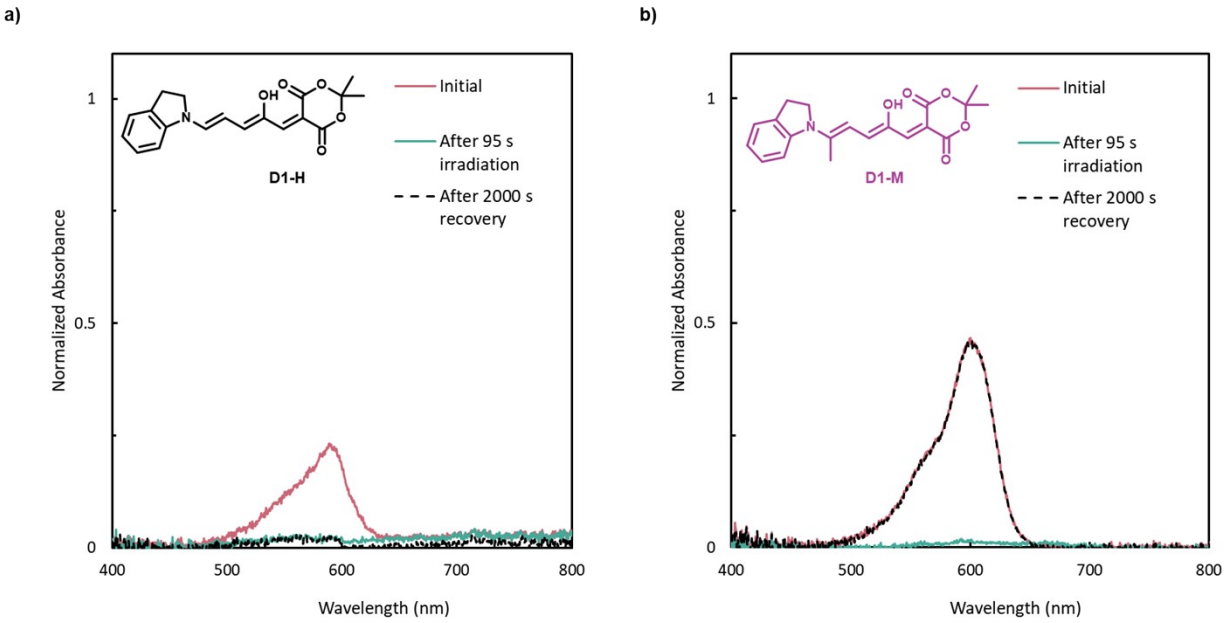


Figure S3. Example absorbance spectra (not normalized) from a pump probe run of **D1-H** (a) and **D1-M** (b) in toluene at 10 µM, showing initial absorbance (pink), absorbance after 95 s of irradiation with 617 nm light (blue), and absorbance after monitoring recovery for 2,000 s (dotted black line). **D1-M** fully recovers within 2,000 s while **D1-H** shows no recovery over the same amount of time.

4. Equillibrium Studies of D1-H and D1-M by NMR in CD_2Cl_2

Approximately 1 mM solutions of the DASAs were prepared by dissolving the appropriate amount of the DASA in a 1 g ampule of CD_2Cl_2 from Cambridge Isotopes Laboratory. The solutions were sonicated for 15 minutes and filtered through a cotton plug into fresh NMR tubes. The initial NMR of **D1-M** was taken after approximately 1 h after being dissolved and again at 10 h and 24 h to determine the thermodynamic equilibrium. **D1-M** thermally reverts to the starting materials over time, however there was no closed form visible after longer periods of time (see Figure S10). Instead, there was a small amount of the EZZ isomer present and **D1-M** was present in 96%. **D1-H** is sensitive to ambient light and has very slow thermal recovery. Therefore, the solution was immediately covered in foil, placed in a box, and kept in a drawer. The box was transported to the NMR room and the NMR tube was exposed to less than 1 minute of ambient light before being inserted into the instrument. We took NMRs initially after one day in solution and again after one week. The initial NMR shows **D1-H** as 70% open while the NMR after sitting for a week shows 28% open which roughly matches our group's previously reported value of 29%. It should be noted that while it was sealed, the NMR after 7 days appeared to have more water content which may contribute to a higher percentage of closed form. However, since this value closely matches the previously reported value, we will compare the equilibrium of **D1-M** to the previously reported value of 29% open form for **D1-H** in deuterated dichloromethane

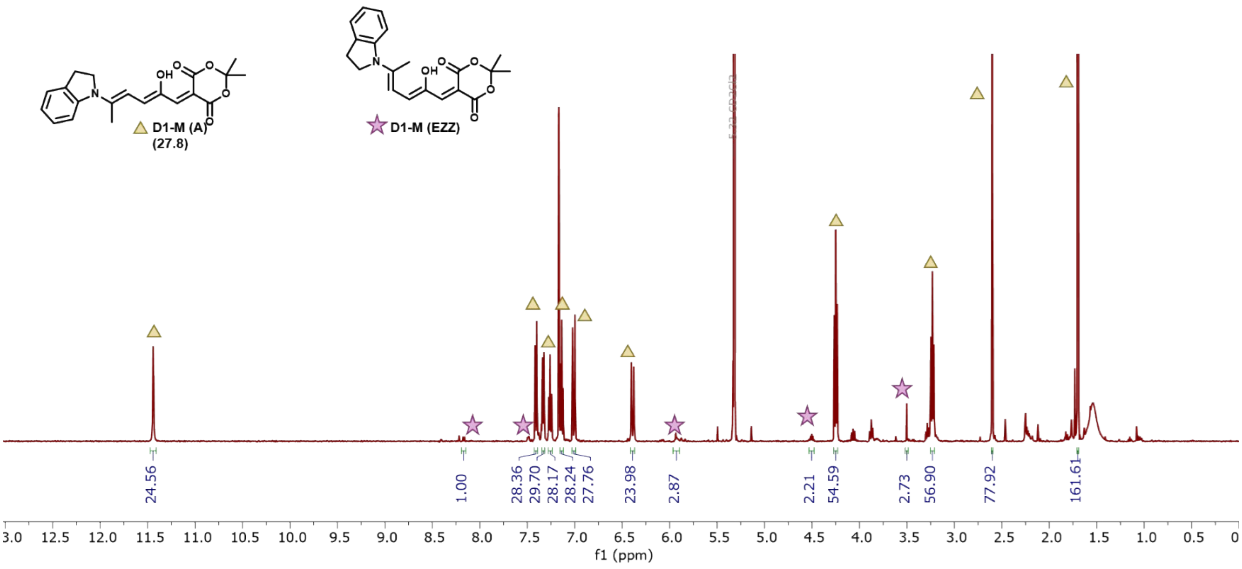


*Figure S4. ^{1}H NMR data of **D1-M** after being dissolved in deuterated dichloromethane for 1 h. The integrations of (~25:1) give an equilibrium of 96% open with approximately 4% of the EZZ isomer present, however the closed form is not visible by ^{1}H NMR in deuterated dichloromethane. Additional small peaks around 2.5 and 8.5 ppm correspond to **S1** growing in over time. See below for more details.*

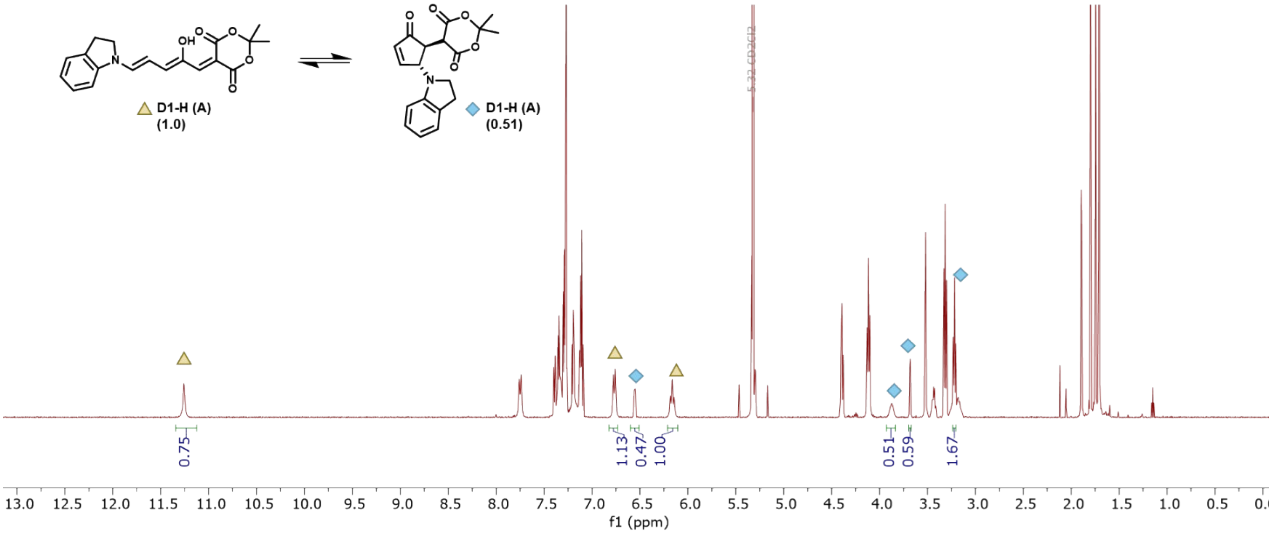


*Figure S5. [1]H NMR of **D-H** dissolved in deuterated dichloromethane after sitting overnight in the dark. The integration of the open and closed forms (1.0:0.42) correspond to about 70% open.*

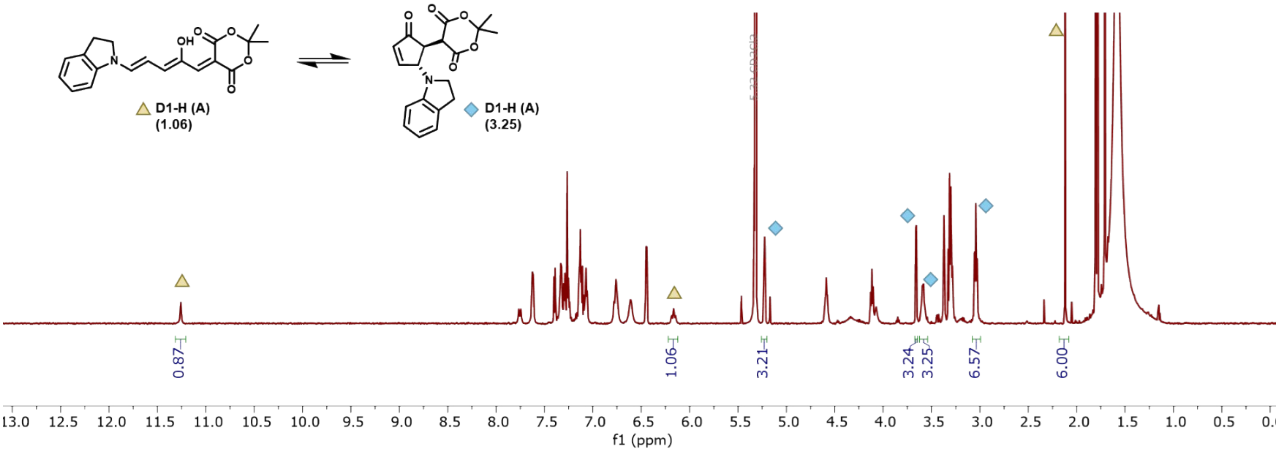


*Figure S6. [1]H NMR of **D1-H** dissolved in deuterated dichloromethane after sitting in the dark for 7 days. The sample clearly has a large water that was not present in the initial NMR ~ 1.56 ppm. This data matches the previously reported equilibrium more closely and gives integrations from the open to closed forms (0.38:1) at 28% open, close to the previously reported value of 29%.*

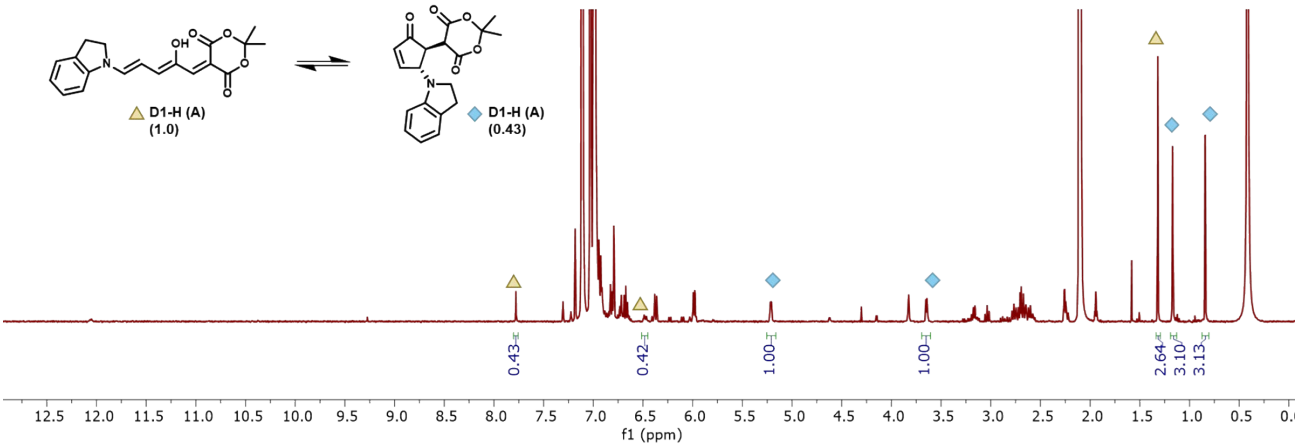


Figure S7. ^{1}H NMR of **D1-H** dissolved in deuterated toluene. The sample was initially irradiated until colorless then set in the dark covered in foil for 7 days. The ration of integrations of the open to closed forms (0.42:1) indicate that it is 29% open, similar to the ratio of the open to closed form dissolved in deuterated chloroform.

5. Reformation of S1 from D1-M over time

Initially, we dissolved a small amount of **D1-M** in methanol to see if the substitution increases the equilibrium in methanol, as it does in toluene and chloroform. After dissolving the DASA in methanol, the solution quickly becomes colorless. We followed the absorbance by UV-Vis and noticed a new species with a λ_{max} at 384 nm growing in. The absorbance of the compound after being dissolved in methanol for 8 minutes matches well with the absorbance of **S1** in methanol (yellow line **Figure S#**). While the compound appears to be almost fully decomposed in methanol in 10 minutes, it appears to be relatively stable in toluene (**Figure S#**b), losing only about 5% of its initial absorbance while sitting in the dark in toluene over 7 hours. We also notice the activated furan growing in by NMR when a solution of **D1-M** sits in the dark dissolved in deuterated dichloromethane over time (**Figure S#**).

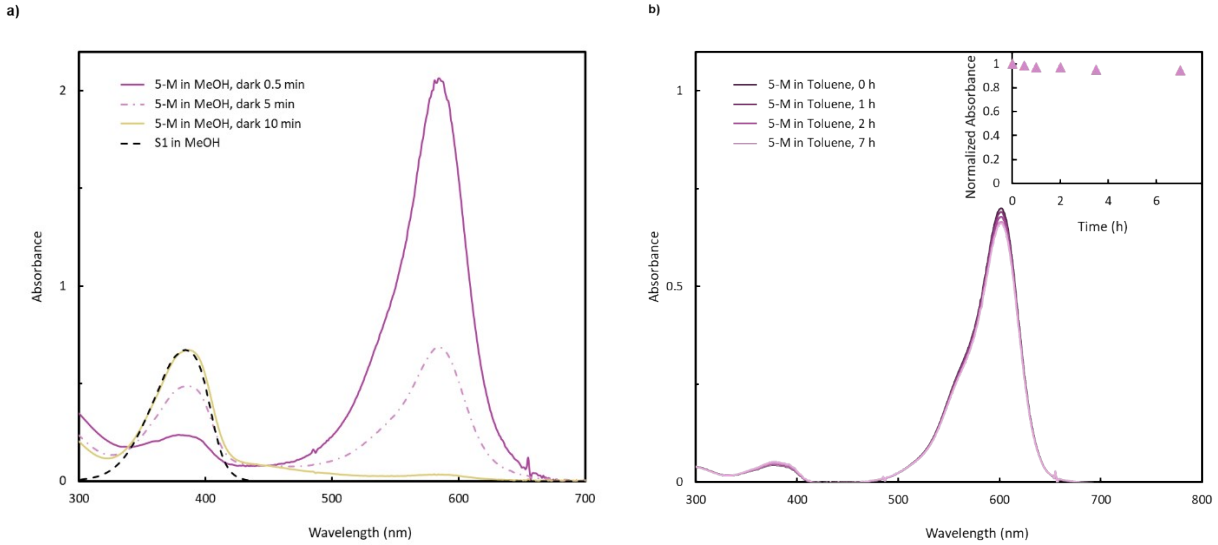


*Figure S8. a) UV-Vis data of compound **D1-M** in solution dissolved in methanol sitting in the dark over time dissolved in a) methanol or b) toluene sitting in the dark over time and the UV-Vis absorbance of the activated furan **S-1** dissolved in methanol, normalized to have the same absorbance of the solution of **D1-M** after 8 minutes showing that the compounds have a similar absorbance profile.*

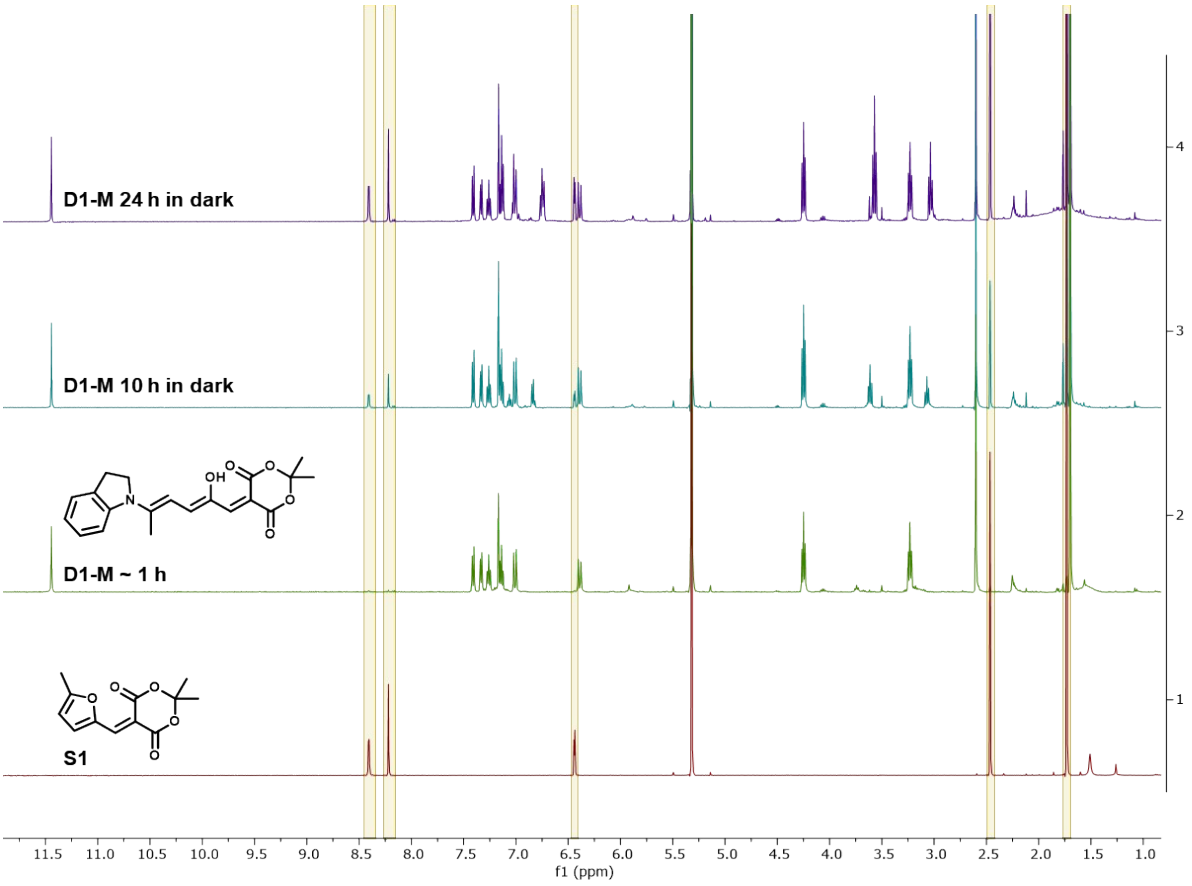


*Figure S9. ^{1}H NMRs of compound **D1-M** after 1 h, 10 h, and 24 h being dissolved in the dark in deuterated dichloromethane. New peaks grow in corresponding to the activated furan **S1**, showing reversion to the starting material over time.*

6. Slow Recovery of D1-H on time-dependent UV-Vis spectroscopy

D1-H was monitored in complete darkness. However, every spectrum taken exposes the sample to a small amount of light. We monitored the sample after irradiation in toluene for 3.5 hours. It should be noted that initially we were monitoring the recovery at 10 s intervals and did not observe any increase in absorbance. After 15 minutes of probing the sample every 10 s the interval of measurements was increased to 120 s. By increasing this interval we decrease the amount of light the sample is exposed to and because of this recovery becomes observable. The recovery is clearly not complete, but the sample recovered ~8% over the 3.5 h of our measurement.

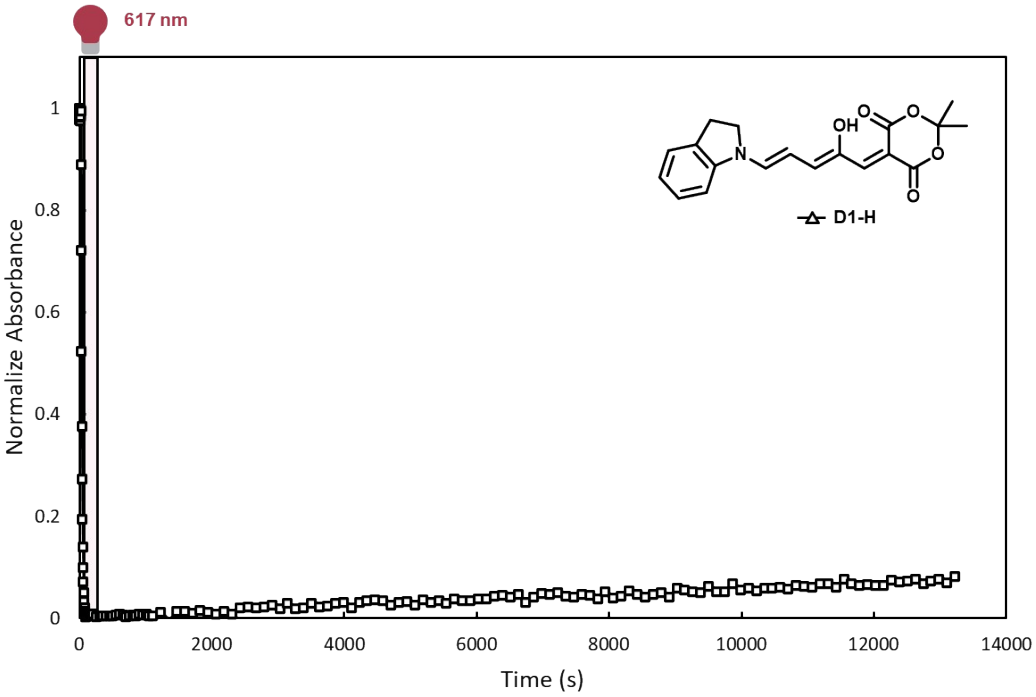


Figure S10. ***Time-dependent pump probe UV-Vis spectroscopy*** *of a 10 µM solution of* ***D1-H*** *in toluene after irradiation for 95 s with 617 nm light. Compound is monitored at 10 s intervals for 1,000 s and then monitored at 120 s intervals for the remaining time.*

7. Solvatochromic Studies:

Small amounts of **D1-M** were dissolved in various solvents, ensuring that the absorbance is below one to compare with previously reported DASA derivatives **D1-H** and **D2**.[2]. **D1-M** has a solvatochromic slope of -24 nm compared to **D1-H** with a slope of -7 nm and **D2** with a slope of -57 nm. This indicates that **D1-M** has a slightly more polar ground state than **D1-H**, but significantly less polar than **D2**.

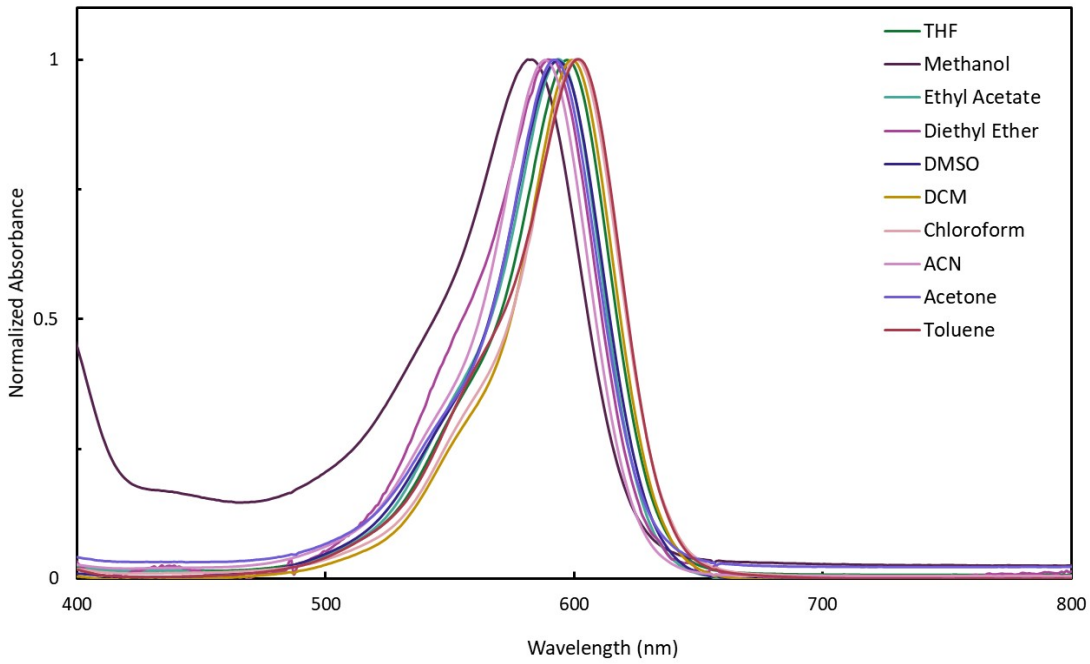


*Figure S11. UV-Vis data of **D1-M** in different solvents to generate solvatochromic slope. **D1-M** is not stable in methanol so the absorbance was taken within a minute of dissolving the solution, however there is already significant decomposition present, evident with the high absorbance below 400 nm.*

*Table S1. Values of the λ_{max} for compounds **D1-M**, **D1-H**, and **D-2** dissolved in different solvents*

Solvent (E_N^T)	λ_{max} D1-M (nm)	λ_{max} D1-H (nm)	λ_{max} D-2 (nm)
Toluene (0.099)	602	588	655
Diethyl Ether (0.117)	590	578	643
THF (0.207)	597	587	645
Ethyl Acetate (0.228)	593	581	639
Chloroform (0.259)	601	590	650
DCM (0.309)	599	590	644
Acetone (0.355)	592	584	632
DMSO (0.444)	593	589	624
ACN (0.46)	588	582	626
Methanol (0.762)	581	578	616

8. Determination of equilibrium of D1-M in toluene by UV-Vis

A 1 mM solution of **D1-M** in DCM was freshly prepared in dichloromethane in which **D1-M** has an equilibrium of 96%. 20 µM of this solution was injected into 2 mL of toluene and a UV-Vis was taken after mixing the solution within 10 seconds of the injection. The solution was irradiated for 30 seconds to close the DASA and allowed to recover incomplete darkness. The absorbance was taken again at 1 h, after which the solution should be fully recovered. The recovered solution had 99% of the initial absorbance of the solution in dichloromethane. Given that the equilibrium of the initial solution in dichloromethane was determined to be 96% in DCM, the equilibrium is determined to be 95% in

toluene. Determination in this manner may not be entirely accurate due to the instability of the compound over long periods of time as well as the possibility for the UV-Vis light to influence the equilibrium of the compound. In general, determination of equilibrium by ^{1}H NMR is more reliable and should be used whenever possible. The data below is normalized based on the maximum absorbance of the initial UV-Vis.

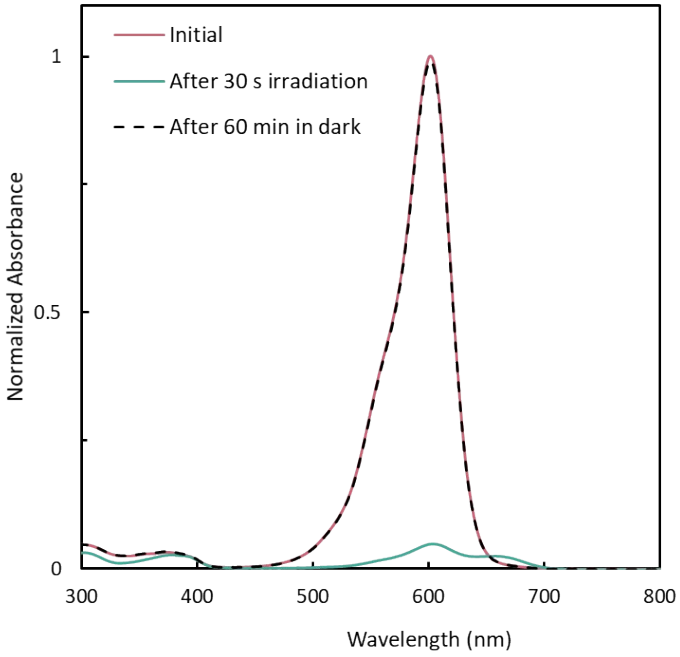


*Figure S12. UV-Vis data of **D1-M** in toluene with approximately 1% dichloromethane after dissolving in toluene (red), after irradiation with a white light for 30 s (teal), and after sitting in the dark for 60 minutes to thermally recover (black dotted).*

9. Determination of the extinction coefficient of D1-M in dichloromethane

A fresh 1 mM solution of **D1-M** was prepared in dichloromethane. Concentrations of 1.5, 2.5, 3.5, 5, 7.5, and 10 µM were prepared by diluting aliquots of the 1 mM stock solution with dichloromethane. The absorbance of these solutions was taken immediately after dilution using a 1 cm pathlength cuvette. The absorbance at the λ_{max} (599 nm in DCM) was plotted against the concentration, corrected for the equilibrium (96% in DCM). The data gives an extinction coefficient of ~130,000 $M^{-1}cm^{-1}$, consistent with the extinction coefficient of other DASA derivatives.

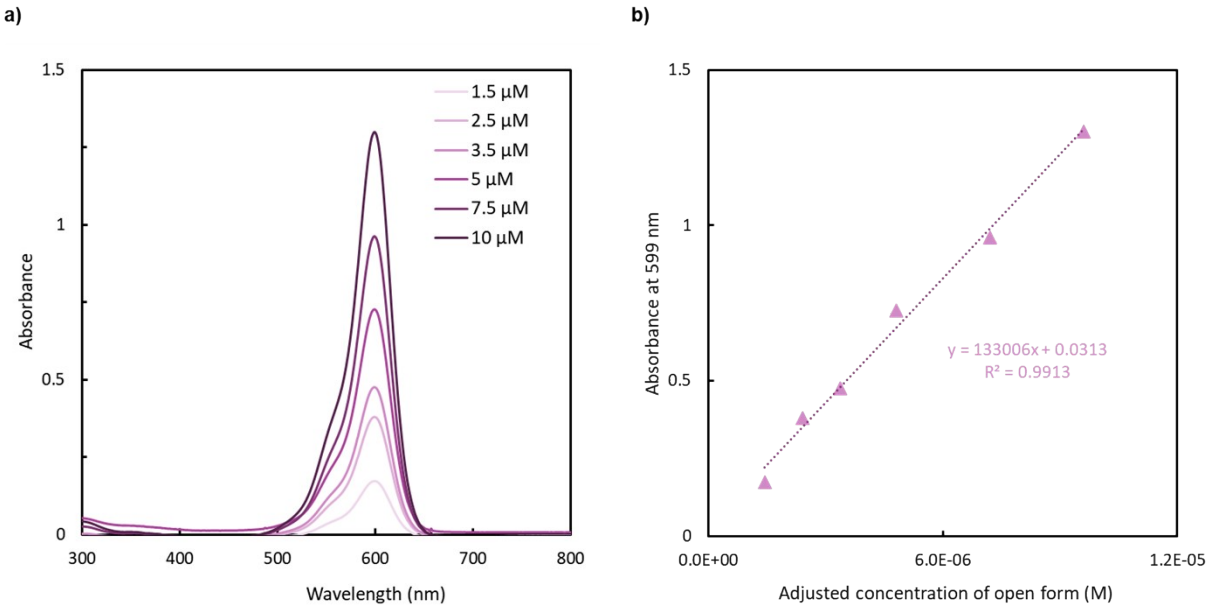
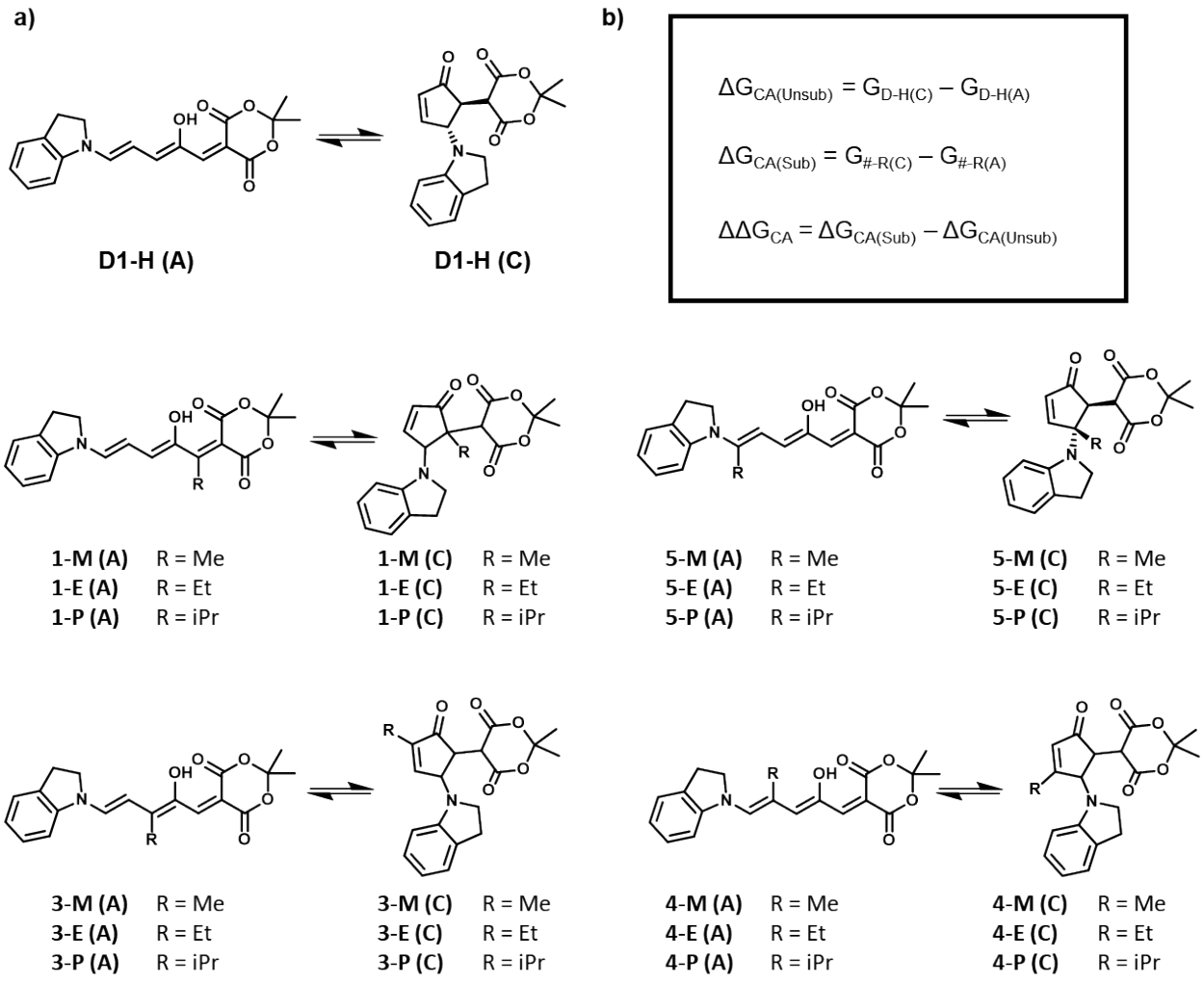


*Figure S13. a) UV-Vis spectra of **D1-M** dissolved in dichloromethane at concentrations ranging from 1.5 to 10 µM. b) absorbance at 599 nm plotted against the concentration of the open form, adjusted for being 96% open in dichloromethane.*

10. DFT Calculations

Optimizations and frequencies were calculated using M06-2x/6-31+G(d,p) in toluene with an SMD solvent model in the gaussian 16 software[4] on the center for scientific computing cluster at University of California, Santa Barbara. Initial searches for the lowest energy conformation of the A and C isomers were done on **D1-H**. From there, substituents (methyl, ethyl, isopropyl) were added on the 1,3,4 and 5-positions of the triene. Different rotamers of the substituents were calculated to find the lowest energy conformations. Geometries, electronic energies, and free energies of the final optimized structures are listed below. The energies reported in the paper are the electronic energy + thermal free energy correction.



Scheme S1. a) Structures investigated computationally in the study. b) calculation used to find the plotted values of $\Delta\Delta G_{CA}$

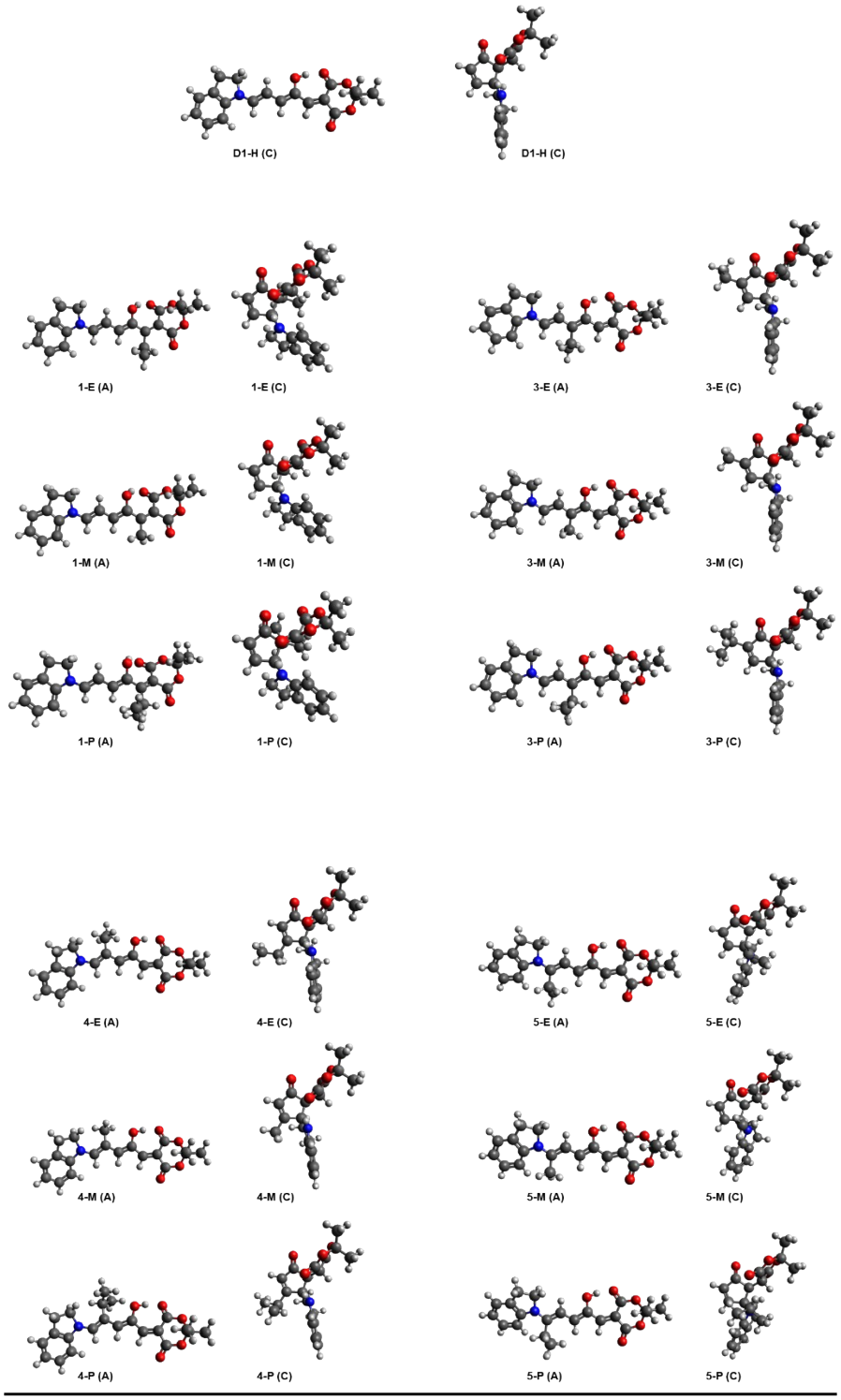


*Figure S14. Optimized geometries of the structures listed in **Figure S#** calculated with M06-2x/6-31+G(d,p) in toluene with an SMD solvent model.*

While substitution on the 5-position results in higher zwitterionic character compared to the unsubstituted derivative, it appears that steric strain between the substitution and the donor is the main driving force of the relative destabilization of the closed form. We looked at bond length alternation of the optimized geometries of **D1-H**, **5-M**, and **5-P** in toluene, which have increasing destabilization of the closed form. Values in Figure S15a are calculated by taking the average length of the C–C single bonds (2,4, and 6) subtracted by the average length of the C–C double bonds (3,5). Increasingly negative values indicate more hybrid to zwitterionic character. While **5-M** has a smaller BLA value than **D1-H**, **5-P** has a value in between the two, even though the closed form is more destabilized, giving evidence that the relative destabilization of the closed form is not due to the zwitterionic nature of the open form.

Instead, it appears that the destabilization of the closed form is due to steric strain between the donor and the substitution on the 5-position (i.e., hydrogen (S15b) vs methyl (S15c) or isopropy (S15d). The steric strain between the donor and the substitution causes the donor to rotate out of its preferred geometry (**Figure S15**).

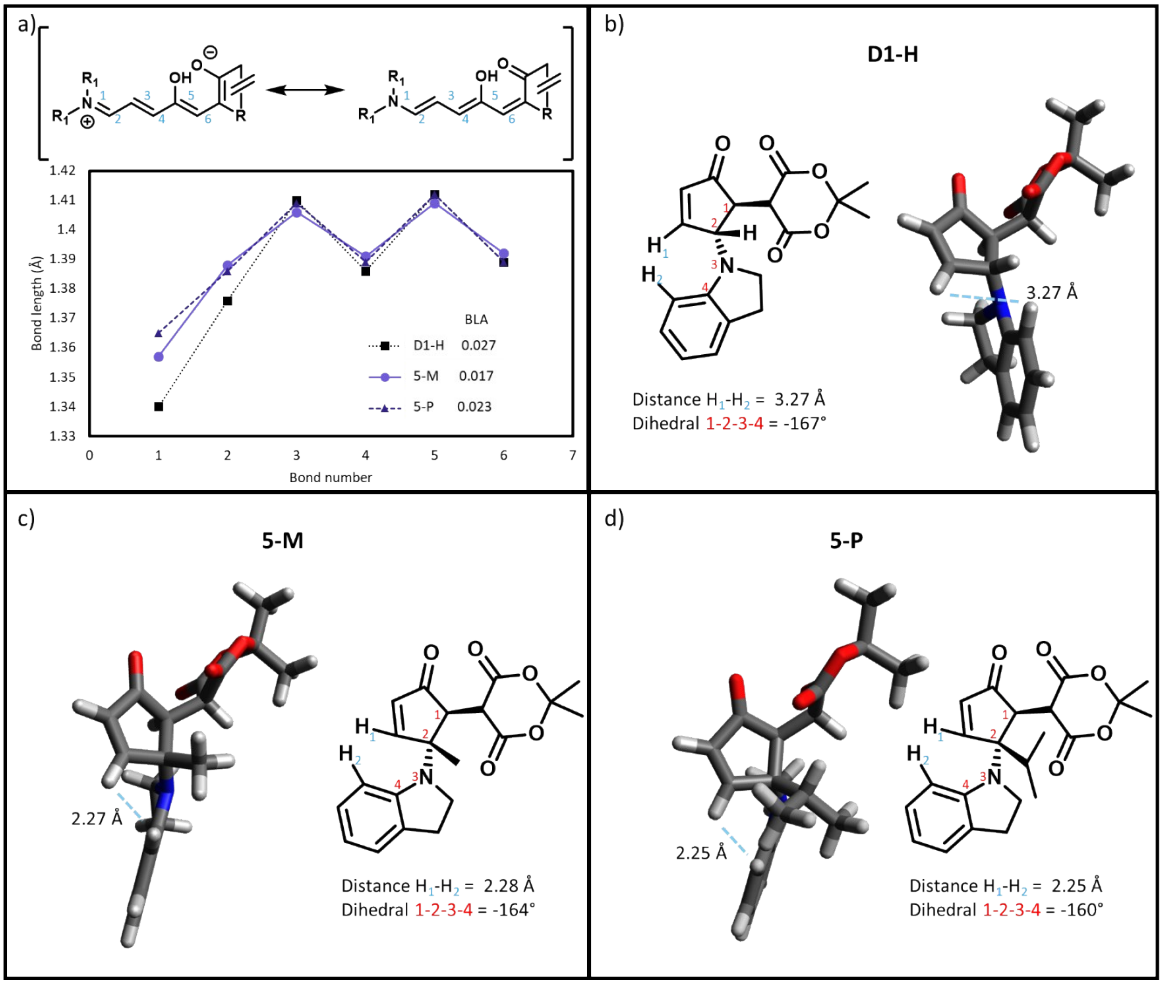
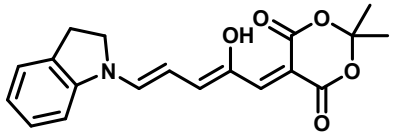


Figure S15. a) Bond length alternation of optimized geometries of **D1-H**, **5-M**, and **5-P** in toluene showing that while **5-M** has a less positive bond length alternation compared to **D1-H**, **5-P** has a bond length alternation between the two. b-d) Optimized geometries of the closed forms of **D1-H**, **5-M**, and **5-P** in toluene, showing that steric demand in the 5-position causes the donor to rotate out of its preferred geometry.

Cartesian coordinates of optimized geometry of D1-H(A)



D1-H (A)

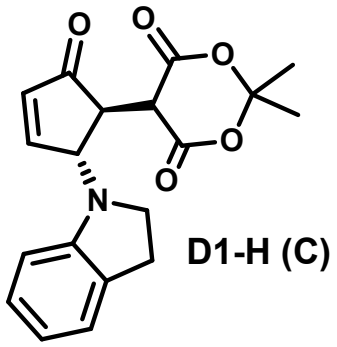
C	5.21755	0.32728	0.04058
C	6.24346	-0.61940	0.10597
C	5.66371	-2.01239	0.16039
H	5.91486	-2.50539	1.10378
C	4.14210	-1.78509	0.03587
H	3.58074	-2.20850	0.87368
H	3.73198	-2.19212	-0.89418
H	6.04115	-2.63933	-0.65128
C	7.56655	-0.20534	0.12356
H	8.36875	-0.93622	0.17463
C	7.85470	1.16245	0.07482
H	8.88589	1.49952	0.08671
C	6.81958	2.09558	0.00878
H	7.05149	3.15519	-0.03143
N	3.96950	-0.32178	0.03202
C	2.76488	0.26375	-0.00713
H	2.77206	1.35118	-0.00063
C	1.56308	-0.40496	-0.05128
H	1.52219	-1.48865	-0.06311
C	0.34903	0.31176	-0.09209
H	0.37915	1.39842	-0.08271
C	-0.89698	-0.29391	-0.13901
O	-0.93738	-1.64463	-0.10668
H	-1.85440	-1.94675	-0.32420
C	-2.02723	0.55041	-0.18700
H	-1.78063	1.60915	-0.17265
C	-3.39464	0.31195	-0.23591
C	-4.25268	1.50851	-0.26140
O	-5.59455	1.29010	-0.22575
C	-6.06667	0.05424	0.29563
C	-5.88810	0.00602	1.80522
H	-6.44217	0.83026	2.25998
H	-6.27518	-0.94130	2.18754
H	-4.83512	0.09452	2.08672
C	-7.50831	-0.07397	-0.13651
H	-8.09074	0.74701	0.28692
H	-7.91490	-1.02451	0.21535
H	-7.56923	-0.03533	-1.22610
O	-5.36781	-1.03593	-0.31555
O	-3.85705	2.64863	-0.35847
C	-4.02299	-0.99293	-0.37660
O	-3.44602	-2.04972	-0.60663
C	5.48268	1.69344	-0.01056
H	4.69164	2.43339	-0.06845

Electronic energy = -1205.237467 Hartree

Electronic energy + thermal free energy correction = -1204.911271 Hartree

Cartesian coordinates of optimized geometry of D1-H(C)

O	-3.31246300	-0.97088300	-1.05139500
C	-1.46760000	-0.09192900	0.29050000
C	-2.53082700	0.33556200	1.29483400
O	-3.76987700	-0.15232000	1.10805300
C	-4.00481900	-1.21357100	0.17936200
C	-3.57827000	-2.54583800	0.77238600
C	-5.47689100	-1.15774800	-0.15508100
C	-2.05801700	-0.49728100	-1.05165200
H	-2.51170800	-2.57058100	1.01006100
H	-3.79253200	-3.34353500	0.05773600
H	-4.14149500	-2.72774200	1.69038000
H	-5.71875900	-0.17878800	-0.57359900
H	-6.06404000	-1.32035100	0.75096600
H	-5.71526700	-1.93388900	-0.88521000
O	-2.30759400	1.06904200	2.21984600
O	-1.45215400	-0.40360200	-2.08780700
C	-0.41514900	0.99962000	0.12669000
C	-0.90805500	2.14523000	-0.75314600
H	-0.23792600	1.43623400	1.11572500
O	-2.06836400	2.49064100	-0.83801300
C	0.26988400	2.68387100	-1.46681900
H	0.24365900	3.59248900	-2.05675200
C	1.29856900	1.84044100	-1.30722300
H	2.29033100	1.96133600	-1.73527400
C	0.93627400	0.60917700	-0.49073700
H	-0.97990600	-0.98304700	0.71382500
N	1.92649700	0.17977700	0.47855400
C	3.08528100	-0.46294900	0.00814500
C	2.35822800	1.13329100	1.51958400
C	4.13726800	-0.31148300	0.92608300
C	3.26495700	-1.18666200	-1.16983800
C	3.62924300	0.49125000	2.09949400
H	2.59326500	2.11029500	1.06717700
H	1.57990000	1.27439300	2.27193900
C	5.36871800	-0.89640400	0.68732800
C	4.51625200	-1.77046900	-1.40075900
H	2.47125000	-1.29878000	-1.90160600
H	4.34037900	1.23458700	2.46620600
H	3.37421100	-0.17627400	2.93170600
C	5.56077700	-1.63334200	-0.48957000
H	6.17958800	-0.77922600	1.40158100
H	4.67180300	-2.33359500	-2.31623400
H	6.52400100	-2.08918300	-0.69432600
H	0.77643600	-0.22040100	-1.18715400



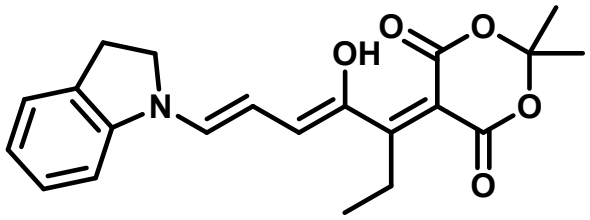
D1-H (C)

Electronic energy = -1165.960675 Hartree

Electronic energy + thermal free energy correction = -1165.655754 Hartree

Cartesian coordinates of optimized geometry of 5-E(A)

C	-3.63634	-1.00638	-0.82756
C	-4.42658	1.23244	-0.05798
C	-3.29140	0.34700	-0.39096
C	-1.96822	0.83212	-0.41724
O	-2.91297	-1.74686	-1.48729
C	-0.82182	-0.01792	-0.27314
C	0.47425	0.46753	-0.31111
C	1.61283	-0.33996	-0.09600
C	2.86821	0.22141	-0.13803
O	-0.93763	-1.33492	0.06541
H	-1.57065	-1.75395	-0.55982
C	5.31324	0.09492	0.00888
C	4.06020	-1.89730	0.29619
C	6.25480	-0.91558	0.22018
C	5.69118	1.42020	-0.18985
C	5.56114	-2.24471	0.39890
H	3.51525	-2.10849	1.22164
C	7.60679	-0.60812	0.23581
C	7.05586	1.71484	-0.17151
H	4.96496	2.20927	-0.35213
H	5.80057	-2.69443	1.36597
C	8.00819	0.71702	0.03842
H	8.34412	-1.38912	0.39899
H	7.37556	2.74096	-0.32319
H	9.06312	0.97042	0.04879
N	4.01586	-0.44774	0.03570
H	5.85833	-2.95396	-0.37829
O	-4.40878	2.43746	0.06220
O	-5.63319	0.62096	0.12028
O	-4.88700	-1.45196	-0.59128
C	-5.67178	-0.77159	0.38604
C	-7.10048	-1.21397	0.16953
H	-7.17983	-2.29212	0.32486
H	-7.75432	-0.69861	0.87631
H	-7.40842	-0.97157	-0.84972
C	-5.16308	-1.07650	1.78773
H	-4.12483	-0.75996	1.91757
H	-5.78488	-0.55250	2.51735
H	-5.22634	-2.15182	1.97059
H	3.56126	-2.42199	-0.52401
H	2.97342	1.28729	-0.32698
H	1.47268	-1.39710	0.09673
H	0.64786	1.52239	-0.49148
C	-1.71226	2.32636	-0.51477
H	-0.83928	2.49046	-1.14902
H	-2.55190	2.80320	-1.01289



1-E (A)

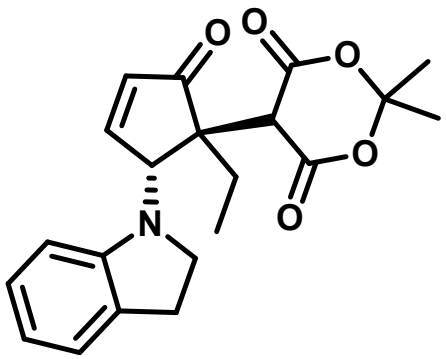
C	-1.49476	2.98398	0.85298
H	-2.37168	2.84532	1.48969
H	-0.62466	2.55896	1.36358
H	-1.33476	4.05942	0.73197

Electronic energy = -1244.533136 Hartree

Electronic energy + thermal free energy correction = -1244.179443 Hartree

Cartesian coordinates of optimized geometry of 5-E(C)

O	2.80862	1.07531	-1.23361
C	1.24096	-0.14358	0.18477
C	2.37248	-0.18553	1.21571
O	3.36697	0.70986	1.01033
C	3.29989	1.68166	-0.03061
C	2.44328	2.87129	0.37372
C	4.72998	2.07618	-0.32502
C	1.84466	0.14183	-1.18895
H	1.41860	2.59498	0.63046
H	2.41519	3.58750	-0.45067
H	2.89441	3.35134	1.24499
H	5.30092	1.19091	-0.61194
H	5.17649	2.52242	0.56598
H	4.75006	2.80071	-1.14179
O	2.43470	-0.90613	2.17008
O	1.50897	-0.40713	-2.20595
C	0.28944	-1.35335	0.16875
C	1.00801	-2.57953	-0.41381
O	2.18065	-2.83935	-0.24313
C	0.03198	-3.33045	-1.23075
H	0.22986	-4.31446	-1.63838
C	-1.04422	-2.56485	-1.43977
H	-1.90120	-2.83761	-2.04815
C	-0.93068	-1.19127	-0.81787
H	0.64785	0.74375	0.45138
N	-2.15956	-0.70428	-0.24059
C	-2.53627	0.62757	-0.30696
C	-3.35488	-1.52576	-0.00848
C	-3.83366	0.79149	0.21715
C	-1.81170	1.72715	-0.76902
C	-4.31586	-0.55725	0.70447
H	-3.79065	-1.85353	-0.96488
H	-3.11760	-2.41178	0.58587
C	-4.41384	2.04397	0.27402
C	-2.41664	2.99013	-0.70974
H	-0.81384	1.62039	-1.18546
H	-5.36197	-0.76345	0.46885
H	-4.19034	-0.62580	1.79257
C	-3.69999	3.15748	-0.19914
H	-5.41399	2.16689	0.68170
H	-1.86838	3.85236	-1.07845
H	-4.14843	4.14483	-0.16622
H	-0.64706	-0.51439	-1.63234
C	-0.23454	-1.73905	1.58120
H	-1.08117	-2.41672	1.43084
H	0.54224	-2.30582	2.09756



1-E (C)

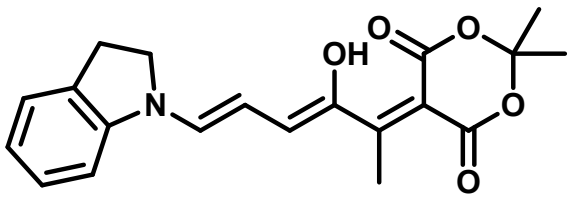
C	-0.66664	-0.57261	2.47245
H	-1.14611	-0.96559	3.37453
H	0.19209	0.01743	2.80432
H	-1.37966	0.09197	1.97892

Electronic energy = -1244.542120 Hartree

Electronic energy + thermal free energy correction= -1244.181749 Hartree

Cartesian coordinates of optimized geometry of 5-M(A)

C	-3.59028	-0.81498	-0.77827
C	-4.50511	1.40187	-0.13006
C	-3.32162	0.51634	-0.21967
C	-2.03990	0.99133	0.06529
O	-2.78587	-1.51396	-1.37955
C	-0.88423	0.13362	0.19634
C	0.40298	0.61435	0.11355
C	1.55352	-0.21458	0.17368
C	2.80377	0.33569	0.05225
O	-1.01557	-1.20388	0.44979
H	-1.54305	-1.60364	-0.27382
C	5.25297	0.18298	-0.01398
C	4.00645	-1.81442	0.24763
C	6.19867	-0.84504	0.04539
C	5.63034	1.51703	-0.14682
C	5.50535	-2.18003	0.17964
H	3.55336	-2.07764	1.20922
C	7.55046	-0.54724	-0.02830
C	6.99565	1.80175	-0.22055
H	4.90273	2.32028	-0.19068
H	5.82718	-2.71227	1.07846
C	7.95063	0.78674	-0.16209
H	8.28955	-1.34234	0.01722
H	7.31344	2.83458	-0.32370
H	9.00581	1.03266	-0.22017
N	3.95826	-0.35279	0.08031
H	5.71841	-2.82269	-0.67912
O	-4.50502	2.61134	-0.15305
O	-5.71467	0.78216	-0.06047
O	-4.85809	-1.26880	-0.71274
C	-5.76523	-0.61781	0.17836
C	-7.15045	-1.07100	-0.22104
H	-7.23491	-2.15252	-0.09478
H	-7.89240	-0.57516	0.40851
H	-7.33354	-0.81284	-1.26608
C	-5.43080	-0.94668	1.62580
H	-4.42149	-0.62521	1.89381
H	-6.14626	-0.44474	2.28125
H	-5.50563	-2.02622	1.77672
H	3.42057	-2.28538	-0.54751
H	2.90753	1.41010	-0.07952
H	1.41589	-1.28071	0.31257
H	0.56982	1.67554	-0.03595
C	-1.84204	2.46410	0.33775
H	-2.02626	3.06169	-0.55841
H	-2.57008	2.80225	1.07782



1-M (A)

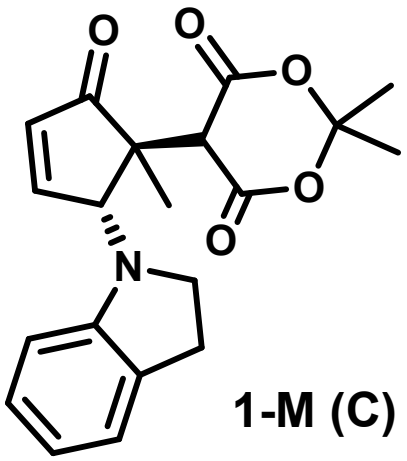
H	-0.85155	2.67462	0.73080

Electronic energy = -1205.237467 Hartree

Electronic energy + thermal free energy correction = -1204.911271 Hartree

Cartesian coordinates of optimized geometry of 5-M(C)

O	-2.69655	1.10187	1.14902
C	-1.20694	-0.19317	-0.29240
C	-2.33897	-0.15600	-1.31928
O	-3.27608	0.79519	-1.10058
C	-3.16344	1.74601	-0.04333
C	-2.25386	2.90219	-0.42730
C	-4.57457	2.19887	0.25826
C	-1.77093	0.13229	1.08970
H	-1.22957	2.59002	-0.64142
H	-2.22985	3.62256	0.39368
H	-2.65742	3.39138	-1.31658
H	-5.18641	1.33470	0.52435
H	-4.99810	2.68507	-0.62305
H	-4.56315	2.90532	1.09078
O	-2.44681	-0.85626	-2.28512
O	-1.42967	-0.42013	2.10314
C	-0.31366	-1.44491	-0.26938
C	-1.01878	-2.63936	0.37967
O	-2.19988	-2.89268	0.26883
C	0.00118	-3.38491	1.15164
H	-0.17952	-4.35971	1.58859
C	1.10565	-2.63708	1.26480
H	2.00047	-2.91903	1.81107
C	0.95302	-1.26737	0.64149
H	-0.55927	0.65307	-0.57049
N	2.11900	-0.73670	-0.02524
C	2.51783	0.58555	0.14274
C	3.30725	-1.54138	-0.34588
C	3.79968	0.77879	-0.40676
C	1.83031	1.64721	0.73253
C	4.24943	-0.52879	-1.01901
H	3.76879	-1.92900	0.57533
H	3.05155	-2.38556	-0.99027
C	4.39828	2.02364	-0.37169
C	2.45241	2.90256	0.76427
H	0.84623	1.51903	1.17582
H	5.30184	-0.76003	-0.84211
H	4.07949	-0.51107	-2.10291
C	3.71930	3.09919	0.22350
H	5.38742	2.16811	-0.79865
H	1.93184	3.73390	1.23096
H	4.18262	4.07935	0.26407
H	0.70590	-0.59464	1.47010
C	0.15194	-1.87848	-1.67171
H	0.60839	-1.03492	-2.19815
H	0.90468	-2.66529	-1.57535



1-M (C)

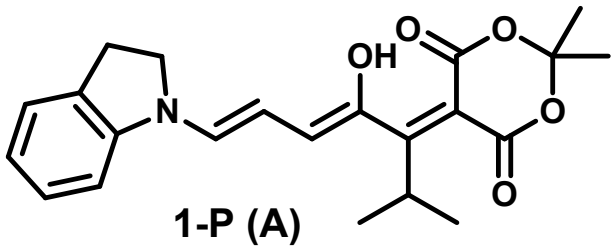
H	-0.67783	-2.25936	-2.26252

Electronic energy = -1205.247508 Hartree

Electronic energy + thermal free energy correction = -1204.914418 Hartree

Cartesian coordinates of optimized geometry of 5-P(A)

C	-3.34607	-1.12070	-0.78089
C	-4.44825	1.05748	-0.33860
C	-3.20148	0.25280	-0.25569
C	-1.98159	0.78039	0.14165
O	-2.46718	-1.77185	-1.31813
C	-0.81327	-0.06464	0.34565
C	0.45757	0.40016	0.15817
C	1.62978	-0.40384	0.26937
C	2.86075	0.13549	0.01752
O	-0.95686	-1.36663	0.76067
H	-1.30515	-1.88928	0.01523
C	5.31070	0.00531	-0.10524
C	4.10850	-1.96043	0.42874
C	6.27417	-1.00167	0.01720
C	5.66522	1.32640	-0.36731
C	5.60068	-2.32848	0.27832
H	3.74709	-2.09563	1.45459
C	7.61820	-0.69568	-0.12441
C	7.02379	1.61946	-0.50915
H	4.92476	2.11414	-0.45603
H	5.98637	-2.81310	1.17857
C	7.99516	0.62595	-0.38960
H	8.37001	-1.47461	-0.03084
H	7.32288	2.64304	-0.71246
H	9.04449	0.87842	-0.50099
N	4.02961	-0.53492	0.07740
H	5.75574	-3.01488	-0.55940
O	-4.52829	2.25240	-0.50638
O	-5.61156	0.35872	-0.27924
O	-4.58061	-1.66305	-0.74333
C	-5.57994	-1.02457	0.05380
C	-6.90560	-1.59899	-0.38944
H	-6.92488	-2.67321	-0.19375
H	-7.71530	-1.11711	0.16266
H	-7.04282	-1.42295	-1.45830
C	-5.31221	-1.23494	1.53639
H	-4.34305	-0.83173	1.83865
H	-6.09629	-0.74028	2.11443
H	-5.32925	-2.30495	1.75658
H	3.46091	-2.53395	-0.24086
H	2.94332	1.18370	-0.26042
H	1.51688	-1.44302	0.55671
H	0.59394	1.43697	-0.12896
C	-1.86826	2.27230	0.46841
C	-1.51215	3.10376	-0.77495
H	-1.58013	4.16833	-0.52884



1-P (A)

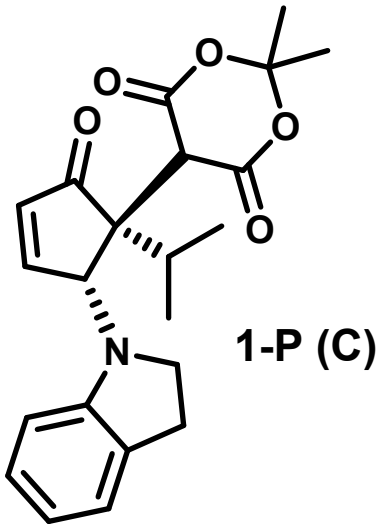
H	-0.49618	2.90361	-1.12927
H	-2.21009	2.89992	-1.59018
C	-0.98734	2.62373	1.67590
H	-1.15585	1.93443	2.50889
H	0.08303	2.63209	1.46078
H	-1.25684	3.62960	2.01386
H	-2.87501	2.58235	0.74370

Electronic energy = -1283.822078 Hartree

Electronic energy + thermal free energy correction = -1283.441322 Hartree

Cartesian coordinates of optimized geometry of 5-P(C)

O	2.59284	1.48418	-1.19286
C	1.22276	-0.07004	0.09864
C	2.40397	-0.12674	1.06672
O	3.26169	0.91745	0.97512
C	3.04934	1.99548	0.06582
C	2.07813	3.02228	0.62814
C	4.41558	2.58703	-0.20230
C	1.75186	0.43741	-1.24564
H	1.09053	2.61011	0.84415
H	1.96329	3.83414	-0.09392
H	2.48951	3.42852	1.55484
H	5.07407	1.81614	-0.60725
H	4.83670	2.97049	0.72935
H	4.32689	3.40343	-0.92213
O	2.61574	-0.96898	1.89027
O	1.46135	-0.02759	-2.31627
C	0.32939	-1.31697	-0.05660
C	1.06108	-2.40933	-0.84423
O	2.24990	-2.63952	-0.77718
C	0.06200	-3.07851	-1.70654
H	0.26144	-3.99608	-2.24720
C	-1.04032	-2.32278	-1.76825
H	-1.91742	-2.54200	-2.36942
C	-0.91706	-1.03089	-0.99223
H	0.58733	0.73526	0.49490
N	-2.12870	-0.60394	-0.32898
C	-2.49825	0.73459	-0.25350
C	-3.35247	-1.41689	-0.25805
C	-3.80042	0.84588	0.27340
C	-1.77501	1.87695	-0.59866
C	-4.29767	-0.54750	0.58599
H	-3.77632	-1.56403	-1.26387
H	-3.15515	-2.39727	0.18272
C	-4.37815	2.08585	0.46551
C	-2.37597	3.12809	-0.40136
H	-0.78513	1.82075	-1.04134
H	-5.34803	-0.70919	0.33548
H	-4.15970	-0.76159	1.65380
C	-3.65867	3.24281	0.12392
H	-5.38241	2.16512	0.87378
H	-1.82559	4.02285	-0.67816
H	-4.10486	4.22186	0.26328
H	-0.64924	-0.26429	-1.72764
C	-0.22744	-1.93853	1.28267
H	-1.20998	-2.32707	1.00178
C	-0.48223	-0.89144	2.37204



1-P (C)

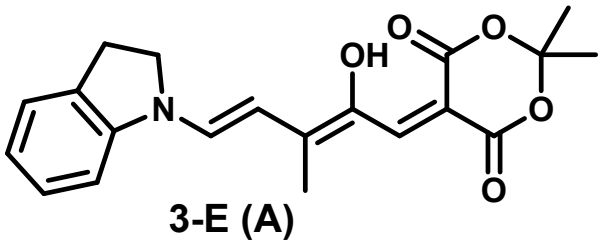
H	-1.10596	-1.33415	3.15569
H	0.44666	-0.56222	2.84515
H	-1.01827	-0.01893	1.98464
C	0.54027	-3.14925	1.82766
H	1.58620	-2.92700	2.03145
H	0.06409	-3.47288	2.75973
H	0.49574	-3.99363	1.13152

Electronic energy = -1283.831946 Hartree

Electronic energy + thermal free energy correction = -1283.443773 Hartree

Cartesian coordinates of optimized geometry of 3-E(A)

C	-6.10067	-0.39036	0.21715
C	-5.98222	-0.59504	1.71977
H	-6.64626	0.10464	2.23243
H	-4.95930	-0.42608	2.06725
H	-6.27432	-1.61711	1.97163
O	-5.74543	0.93998	-0.13793
C	-4.43461	1.29774	-0.07455
O	-4.16335	2.47762	-0.03033
C	-3.45226	0.20199	-0.12248
C	-2.12238	0.58374	0.03988
H	-2.02317	1.65728	0.15327
C	-0.91439	-0.13472	0.08932
C	0.31084	0.54036	0.19875
C	0.40375	2.04441	0.32504
H	1.27955	2.29485	0.92993
H	-0.44632	2.44061	0.88277
C	0.50076	2.74663	-1.03616
H	0.62352	3.82516	-0.90151
H	1.35154	2.37201	-1.61352
H	-0.40444	2.57726	-1.62618
C	1.49697	-0.24279	0.13057
C	2.76828	0.28011	0.17454
H	2.93582	1.34671	0.28615
N	3.88813	-0.45423	0.08072
C	5.20723	0.03213	0.09912
C	5.64112	1.35187	0.19866
H	4.94775	2.18260	0.27517
C	7.01772	1.58490	0.19354
H	7.37979	2.60536	0.26928
C	7.92871	0.53322	0.09061
H	8.99396	0.73928	0.08741
C	7.47213	-0.78503	-0.00969
H	8.17714	-1.60774	-0.09020
C	6.10775	-1.03153	-0.00537
C	5.35910	-2.33982	-0.08921
H	5.59288	-2.98248	0.76417
H	5.61297	-2.89164	-0.99786
C	3.87409	-1.91849	-0.08221
H	3.31243	-2.36461	0.74367
H	3.36237	-2.16616	-1.01788
H	1.36817	-1.31092	0.00793
O	-0.85947	-1.48997	0.03767
H	-1.71469	-1.84034	-0.31817
C	-3.92784	-1.13024	-0.45675
O	-3.23099	-2.08300	-0.79060
C	-7.50026	-0.61736	-0.30383



3-E (A)

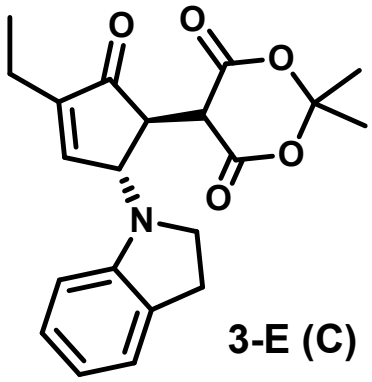
H	-8.18701	0.08358	0.17541
H	-7.81400	-1.63959	-0.08194
H	-7.51921	-0.45946	-1.38420
O	-5.26188	-1.32136	-0.47385

Electronic energy = -1244.544114 Hartree

Electronic energy + thermal free energy correction = -1244.189862 Hartree

Cartesian coordinates of optimized geometry of 3-E(C)

C	0.92978	0.30986	-0.27482
C	1.28673	1.71649	-0.72517
N	1.92490	-0.36288	0.54194
C	2.37458	0.29156	1.78621
H	1.60090	0.24925	2.55542
C	3.63967	-0.49045	2.17481
H	3.38015	-1.34598	2.81051
H	4.36136	0.12705	2.71395
C	4.13255	-0.97217	0.83142
C	5.35600	-1.48891	0.44216
H	6.17195	-1.56432	1.15632
C	5.53338	-1.90589	-0.88445
H	6.49021	-2.30406	-1.20608
C	4.48183	-1.79853	-1.79152
C	3.23860	-1.28024	-1.41013
H	2.43952	-1.19763	-2.13998
H	4.62538	-2.11413	-2.82072
H	2.62103	1.34785	1.59209
C	3.07333	-0.87507	-0.08614
C	-0.41771	0.51192	0.43499
H	-0.23503	0.64380	1.50713
C	-1.47417	-0.57845	0.28330
C	-2.52722	-0.46268	1.37810
O	-2.29517	-0.02681	2.47352
O	-3.76720	-0.88399	1.07305
C	-4.01877	-1.61034	-0.13274
C	-3.58922	-3.06008	0.01523
H	-4.12665	-3.51274	0.85132
H	-2.51618	-3.15680	0.19857
H	-3.83233	-3.60214	-0.90132
C	-5.49543	-1.45565	-0.41147
H	-6.06945	-1.88821	0.41057
H	-5.73948	-0.39567	-0.50582
H	-5.74890	-1.97069	-1.34030
O	-3.34182	-1.00265	-1.23873
H	-0.98658	-1.55477	0.42626
C	-2.07681	-0.57312	-1.11409
O	-1.47419	-0.19442	-2.08488
C	-0.90353	1.86003	-0.08062
O	-2.06139	2.22701	-0.06288
H	0.76716	-0.30626	-1.16464
C	0.26844	2.58685	-0.63332
C	0.18966	4.02657	-1.03106
C	0.02999	4.94694	0.18421
H	0.89249	4.86242	0.85258
H	-0.86976	4.69091	0.75099



3-E (C)

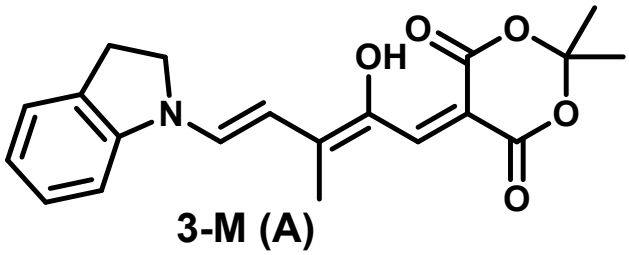
H	-0.05537	5.99028	-0.13198
H	1.08463	4.29719	-1.59970
H	-0.67374	4.15284	-1.69482
H	2.27244	1.94707	-1.12407

Electronic energy = -1244.560494 Hartree

Electronic energy + thermal free energy correction = -1244.202816 Hartree

Cartesian coordinates of optimized geometry of 3-M(A)

C	-3.44288	0.29505	-0.23513
C	-2.11286	0.70264	-0.19090
C	-0.89478	-0.00111	-0.11457
O	-0.84066	-1.35346	-0.01519
H	-1.70891	-1.74219	-0.29156
C	0.33588	0.66939	-0.10219
C	1.51562	-0.12770	-0.05897
C	2.78270	0.40376	-0.03712
N	3.90939	-0.32735	-0.01246
C	5.22273	0.16881	0.05073
C	5.64449	1.49499	0.10731
C	7.01826	1.73748	0.16791
H	7.37085	2.76306	0.21344
C	7.93821	0.68866	0.17315
H	9.00092	0.90199	0.22217
C	7.49373	-0.63641	0.11585
H	8.20562	-1.45717	0.11884
H	4.94397	2.32326	0.10656
C	6.13254	-0.89233	0.05450
C	5.39567	-2.20774	-0.02598
H	5.64128	-2.86029	0.81565
H	5.64835	-2.74403	-0.94501
C	3.90671	-1.80023	-0.00729
H	3.38713	-2.15063	0.89067
H	3.35827	-2.16034	-0.88261
H	2.93978	1.47791	-0.03846
H	1.38509	-1.20216	-0.04945
C	0.48129	2.16865	-0.12686
H	1.06166	2.50296	0.73943
H	-0.46028	2.71036	-0.11094
H	1.02140	2.47844	-1.02767
H	-2.02674	1.78160	-0.20453
C	-4.43481	1.38470	-0.26242
O	-5.74262	1.01629	-0.21022
C	-6.06525	-0.26466	0.31609
C	-5.86724	-0.29164	1.82391
H	-6.51001	0.46202	2.28451
H	-6.13768	-1.27764	2.20871
H	-4.82944	-0.08078	2.09623
C	-7.48744	-0.55711	-0.10081
H	-8.15591	0.19183	0.32903
H	-7.77877	-1.54771	0.25483
H	-7.56378	-0.52666	-1.18969
O	-5.25387	-1.26645	-0.30558
O	-4.17419	2.56230	-0.37262
C	-3.92380	-1.06983	-0.38614



3-M (A)

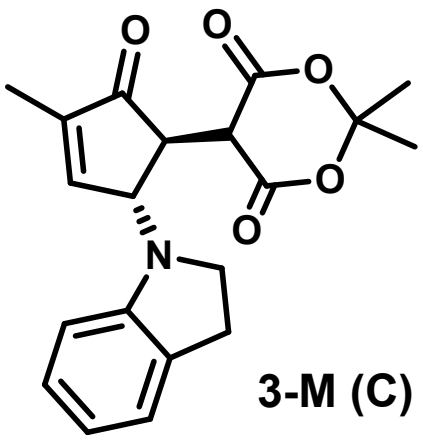
O	-3.23758	-2.05176	-0.64880

Electronic energy = -1205.248042 Hartree

Electronic energy + thermal free energy correction= -1204.920626 Hartree

Cartesian coordinates of optimized geometry of 3-M(C)

O	-1.47222	0.16254	-2.06627
C	-2.07024	-0.28898	-1.12413
C	-1.47299	-0.37376	0.27279
C	-2.53226	-0.32258	1.36661
O	-2.30759	0.05035	2.48642
O	-3.76992	-0.72603	1.02868
C	-4.00452	-1.40095	-0.20968
C	-3.56200	-2.85166	-0.11959
H	-4.11001	-3.34504	0.68609
H	-2.49178	-2.94657	0.08027
H	-3.78337	-3.35557	-1.06305
C	-5.48021	-1.24922	-0.49502
H	-6.05693	-1.72450	0.30113
H	-5.73497	-0.18873	-0.54445
H	-5.71904	-1.72487	-1.44846
C	-0.41918	0.70630	0.49536
H	-0.23900	0.76843	1.57419
C	-0.90392	2.08502	0.06781
O	-2.05940	2.45592	0.11576
C	0.26885	2.84579	-0.43169
C	1.29038	1.98593	-0.57189
H	2.27919	2.24413	-0.94496
C	0.18028	4.29800	-0.76123
H	-0.10792	4.87744	0.12152
H	1.13215	4.67725	-1.13888
H	-0.59212	4.46359	-1.51908
C	0.93005	0.55158	-0.22236
N	1.91986	-0.18204	0.54619
C	2.36569	0.37397	1.83868
H	1.58773	0.27711	2.59852
C	3.62479	-0.44216	2.17275
H	4.34621	0.12808	2.76195
H	3.35731	-1.34282	2.73908
C	4.12325	-0.82137	0.79895
C	5.34668	-1.31218	0.37734
H	6.15840	-1.44592	1.08777
C	5.52962	-1.62606	-0.97663
H	6.48665	-2.00233	-1.32309
C	4.48341	-1.44455	-1.87808
C	3.24008	-0.95195	-1.46422
H	2.44536	-0.81004	-2.18960
H	4.63157	-1.67998	-2.92790
H	2.61852	1.44063	1.72666
C	3.06933	-0.64962	-0.11375
H	0.76869	0.00132	-1.15468
H	-0.98386	-1.35565	0.36011



3-M (C)

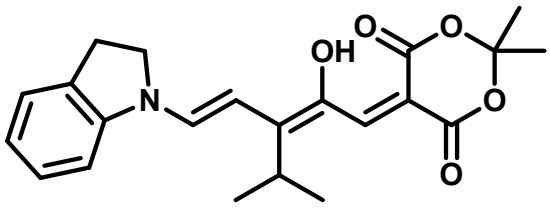
O	-3.32518	-0.73665	-1.28190

Electronic energy = -1205.264722 Hartree

Electronic energy + thermal free energy correction = -1204.934016 Hartree

Cartesian coordinates of optimized geometry of 3-P(A)

C	0.25845	0.61742	-0.08338
C	1.42629	-0.19806	-0.04648
C	2.72803	0.24468	-0.01837
H	2.97806	1.29745	-0.00558
N	3.79577	-0.56911	-0.00786
C	5.13885	-0.16134	0.06718
C	5.64173	1.13352	0.16504
C	7.02777	1.28767	0.22980
H	7.44413	2.28703	0.30774
C	7.87964	0.18289	0.20012
H	8.95358	0.32761	0.25388
C	7.35338	-1.10951	0.10293
H	8.01287	-1.97262	0.07959
H	4.99225	2.00229	0.19491
C	5.97859	-1.27763	0.03656
C	5.15793	-2.53913	-0.08532
H	5.36825	-3.23940	0.72686
H	5.36731	-3.05295	-1.02788
C	3.69801	-2.03888	-0.03454
H	3.17039	-2.37569	0.86388
H	3.11544	-2.34347	-0.90857
H	1.25520	-1.26660	-0.04808
C	0.33803	2.13741	-0.09028
C	0.96302	2.71435	1.19165
H	0.49347	2.28373	2.08111
H	2.03972	2.54572	1.26806
H	0.79990	3.79652	1.21398
H	-0.67660	2.53006	-0.10499
C	0.99731	2.69317	-1.36317
H	0.88839	3.78225	-1.38051
H	2.06394	2.46600	-1.43239
H	0.51214	2.29041	-2.25723
C	-0.96854	-0.07707	-0.10459
O	-0.89026	-1.43022	-0.01397
H	-1.74345	-1.83743	-0.31353
C	-2.20996	0.58267	-0.17650
H	-2.17586	1.66375	-0.17874
C	-3.52610	0.12398	-0.22508
C	-4.55545	1.17793	-0.22919
O	-5.85004	0.76353	-0.18266
C	-6.12596	-0.53812	0.31812
C	-5.92161	-0.58939	1.82464
H	-6.58835	0.13195	2.30268
H	-6.15667	-1.59184	2.18969
H	-4.89069	-0.34875	2.09804
C	-7.53908	-0.87111	-0.09954



3-P (A)

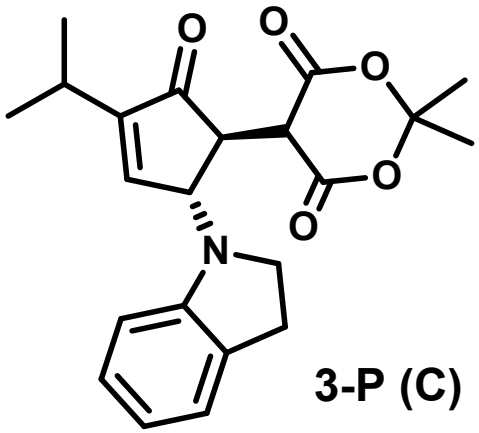
H	-8.23096	-0.15452	0.34809
H	-7.79444	-1.87831	0.23668
H	-7.62124	-0.82101	-1.18728
O	-5.28287	-1.49723	-0.32728
O	-4.33769	2.36662	-0.31531
C	-3.96048	-1.25128	-0.40743
O	-3.24241	-2.20312	-0.69808

Electronic energy = -1283.834224 Hartree

Electronic energy + thermal free energy correction = -1283.454867 Hartree

Cartesian coordinates of optimized geometry of 3-P(C)

C	-0.44262	0.19430	0.68426
H	-0.26550	0.01832	1.75075
C	-0.87526	1.64978	0.56136
O	-2.01362	2.04092	0.72638
C	0.31990	2.45548	0.20131
C	0.27393	3.95535	0.14308
H	-0.24091	4.29720	1.05085
C	1.66742	4.57722	0.09472
H	2.27965	4.26509	0.94705
H	1.59521	5.66883	0.10949
H	2.19094	4.29306	-0.82535
C	-0.56845	4.39521	-1.06452
H	-1.56926	3.95734	-1.03180
H	-0.66855	5.48526	-1.07893
H	-0.08517	4.08161	-1.99644
C	1.31175	1.60500	-0.11179
H	2.31378	1.89143	-0.42327
C	-1.53951	-0.76966	0.24086
C	-2.59333	-0.92198	1.33061
O	-2.34808	-0.83104	2.50315
O	-3.85143	-1.17104	0.92470
C	-4.11860	-1.54978	-0.42725
C	-3.75073	-3.00603	-0.65511
H	-4.33720	-3.63415	0.01911
H	-2.69062	-3.19801	-0.47180
H	-3.97966	-3.27870	-1.68765
C	-5.58418	-1.26599	-0.65949
H	-6.18605	-1.86997	0.02258
H	-5.78369	-0.20778	-0.47944
H	-5.84596	-1.51463	-1.69006
O	-3.40476	-0.70525	-1.33893
H	-1.09037	-1.76472	0.10141
C	-2.13368	-0.35273	-1.09617
O	-1.51730	0.27357	-1.91926
C	0.90024	0.14328	-0.05814
N	1.86624	-0.76342	0.53743
C	2.32584	-0.50220	1.91570
H	1.54753	-0.73994	2.64337
C	3.56557	-1.39924	2.06414
H	4.30048	-0.98211	2.75605
H	3.27673	-2.39200	2.43076
C	4.05427	-1.49331	0.63882
C	5.26565	-1.91167	0.11646
H	6.07449	-2.21109	0.77795
C	5.44073	-1.93611	-1.27424
H	6.38846	-2.25283	-1.69732



3-P (C)

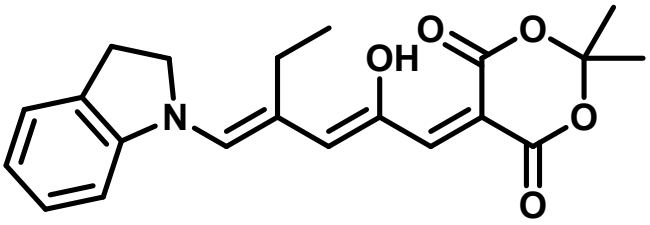
C	4.39942	-1.54275	-2.11149
C	3.16838	-1.11997	-1.59609
H	2.37723	-0.80649	-2.26980
H	4.54223	-1.55315	-3.18804
H	2.60339	0.55825	2.02897
C	3.00473	-1.10816	-0.21146
H	0.72187	-0.20041	-1.08223

Electronic energy = -1283.858392 Hartree

Electronic energy + thermal free energy correction= -1283.474646 Hartree

Cartesian coordinates of optimized geometry of 4-E(A)

C	3.42196	-0.36915	-0.19737
C	2.03502	-0.41090	-0.16586
C	1.03520	0.58566	-0.04986
O	1.30289	1.90088	0.11268
H	2.25190	2.07118	-0.11538
C	-0.27704	0.13351	-0.06145
C	-1.50005	0.86766	-0.00290
C	-2.61689	0.05402	0.04993
N	-3.92601	0.35022	0.19154
C	-4.51954	1.62331	0.64789
H	-3.90851	2.04180	1.44857
C	-5.93824	1.24560	1.12136
H	-5.98265	1.18600	2.21401
H	-6.67763	1.98009	0.79525
C	-6.15855	-0.11632	0.51176
C	-7.30443	-0.89160	0.43148
H	-8.24729	-0.51953	0.82241
C	-7.23060	-2.15943	-0.15674
H	-8.12125	-2.77491	-0.22911
C	-6.01786	-2.63031	-0.65892
C	-4.85691	-1.85570	-0.59142
H	-3.92817	-2.22192	-1.01547
H	-5.97192	-3.60925	-1.12559
H	-4.55695	2.33191	-0.18627
C	-4.94862	-0.60335	0.00959
H	-2.44619	-1.01853	-0.01931
C	-1.51259	2.37498	-0.15417
H	-0.77069	2.81719	0.51215
H	-2.47997	2.78838	0.12374
C	-1.20006	2.78300	-1.59854
H	-1.18624	3.87308	-1.69614
H	-0.22088	2.40541	-1.90505
H	-1.95405	2.38592	-2.28708
H	-0.37603	-0.94735	-0.10789
H	1.64426	-1.42311	-0.22952
C	4.23839	0.83489	-0.25257
O	5.57235	0.67679	-0.16608
C	6.09020	-0.54283	0.37798
C	5.88291	-0.57227	1.88440
H	6.39071	0.28151	2.33873
H	6.30377	-1.49631	2.28737
H	4.82148	-0.52883	2.14382
C	7.54538	-0.59768	-0.02278
H	8.07628	0.25643	0.40295
H	7.99196	-1.52224	0.34903
H	7.62744	-0.56919	-1.11128



4-E (A)

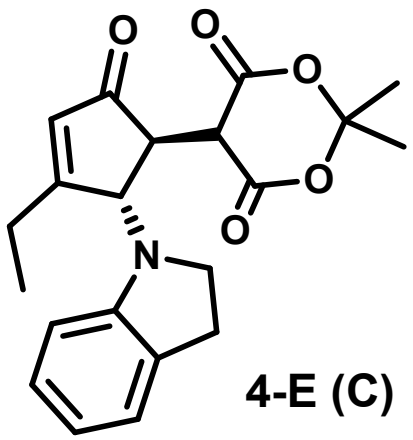
O	5.45611	-1.65720	-0.23713
O	3.82676	1.97528	-0.43403
C	4.09802	-1.67462	-0.30129
O	3.54295	-2.73453	-0.48467

Electronic energy = -1244.536336 Hartree

Electronic energy + thermal free energy correction = -1244.181605 Hartree

Cartesian coordinates of optimized geometry of 4-E(C)

N	1.68770	-0.36927	0.61350
C	2.17383	0.00318	1.95394
H	1.37303	-0.05927	2.69362
C	3.30843	-0.99985	2.22713
H	4.10351	-0.56928	2.83981
H	2.92055	-1.88404	2.74733
C	3.75023	-1.37226	0.83138
C	4.88115	-2.03206	0.38295
H	5.65473	-2.33244	1.08500
C	5.02071	-2.30423	-0.98517
H	5.90653	-2.81281	-1.35125
C	4.02111	-1.91473	-1.87393
C	2.87148	-1.24885	-1.43389
H	2.11266	-0.94532	-2.14840
H	4.13379	-2.12225	-2.93404
H	2.56055	1.03488	1.95020
C	2.74521	-0.98399	-0.07049
C	0.76811	0.51220	-0.07753
C	-0.58460	0.65311	0.63535
H	-0.42696	0.55589	1.71493
C	-0.98341	2.10407	0.39300
O	-2.12272	2.51941	0.48201
C	0.23372	2.83455	0.00944
H	0.26198	3.91218	-0.10540
C	-1.69454	-0.32099	0.25182
C	-2.77153	-0.35614	1.32875
O	-2.54486	-0.17389	2.49448
O	-4.02770	-0.61112	0.92133
C	-4.28371	-1.08519	-0.40249
C	-3.95253	-2.56388	-0.51246
H	-4.55772	-3.12292	0.20457
H	-2.89805	-2.76710	-0.30891
H	-4.18330	-2.91045	-1.52218
C	-5.73667	-0.78033	-0.68192
H	-6.36642	-1.31392	0.03294
H	-5.90839	0.29357	-0.58572
H	-5.98909	-1.09901	-1.69534
O	-3.53159	-0.33475	-1.36335
H	-1.26707	-1.33439	0.20941
C	-2.25114	-0.01061	-1.12934
O	-1.59667	0.50912	-1.99606
C	1.22646	1.96337	-0.25185
C	2.60735	2.26934	-0.73773
H	3.32931	1.76881	-0.07827
C	2.92503	3.75624	-0.84604
H	2.82306	4.25403	0.12342



4-E (C)

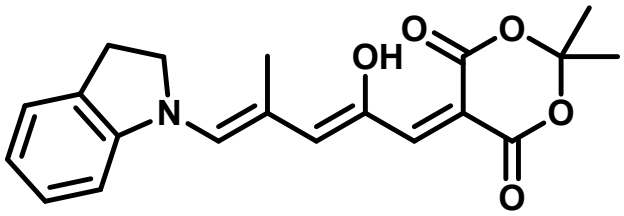
H	3.95092	3.90193	-1.19341
H	2.25622	4.25265	-1.55555
H	2.73452	1.77765	-1.71214
H	0.60184	0.09862	-1.07793

Electronic energy = -1244.563469 Hartree

Electronic energy + thermal free energy correction = -1244.204420 Hartree

Cartesian coordinates of optimized geometry of 4-M(A)

C	-2.00415	0.38630	-0.29878
C	-3.39003	0.31675	-0.25846
C	-4.09389	1.61034	-0.21299
O	-5.44593	1.55686	-0.07759
C	-6.02470	0.37901	0.47042
C	-5.73534	0.28324	1.96053
H	-6.15197	1.15830	2.46452
H	-6.20035	-0.61876	2.36483
H	-4.66056	0.24397	2.15836
C	-7.50056	0.43528	0.15423
H	-7.94277	1.31362	0.62906
H	-7.99187	-0.46441	0.53076
H	-7.64195	0.49929	-0.92666
O	-5.51588	-0.77693	-0.20488
O	-3.56899	2.69458	-0.33285
C	-4.18533	-0.89674	-0.37427
O	-3.76310	-2.00761	-0.67484
H	-1.63363	1.40818	-0.30296
C	-0.98378	-0.59429	-0.31583
O	-1.21264	-1.92487	-0.23844
H	-2.16634	-2.10179	-0.43544
C	0.32009	-0.12148	-0.34394
H	0.41835	0.95937	-0.28808
C	1.53593	-0.85989	-0.40117
C	2.66668	-0.08846	-0.22193
N	3.95124	-0.47400	-0.07160
C	4.44370	-1.81228	0.31903
C	5.77039	-1.52797	1.05042
H	5.62308	-1.50835	2.13603
H	6.52308	-2.28604	0.82476
C	6.14360	-0.15303	0.55112
C	7.32550	0.56180	0.66256
H	8.19276	0.11870	1.14399
C	7.38519	1.86371	0.15075
H	8.30638	2.43214	0.22645
C	6.26909	2.43074	-0.46383
C	5.07320	1.71834	-0.58938
H	4.22018	2.15479	-1.09828
H	6.32967	3.43647	-0.86766
H	3.70088	-2.30741	0.94478
H	4.62229	-2.41476	-0.57716
C	5.03255	0.42984	-0.06629
H	2.53904	0.99150	-0.16720
C	1.55926	-2.33947	-0.70924
H	1.35081	-2.95894	0.16836
H	2.52159	-2.63338	-1.12925



4-M (A)

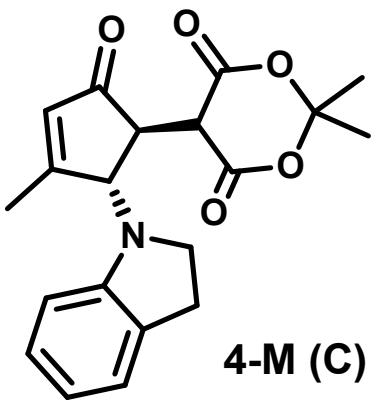
H	0.79051	-2.57129	-1.44679

Electronic energy = -1205.241499 Hartree

Electronic energy + thermal free energy correction = -1204.912714 Hartree

Cartesian coordinates of optimized geometry of 4-M(C)

C	0.84645	0.67175	-0.27101
N	1.83487	0.02174	0.56657
C	2.31082	0.71002	1.78031
H	1.52959	0.74766	2.54235
C	3.52740	-0.12109	2.22382
H	3.22067	-0.90045	2.93183
H	4.29374	0.49018	2.70547
C	3.97689	-0.74869	0.92550
C	5.15208	-1.39872	0.59087
H	5.95865	-1.47975	1.31508
C	5.29325	-1.94591	-0.69204
H	6.21283	-2.44998	-0.97069
C	4.25104	-1.83589	-1.60982
C	3.05639	-1.18352	-1.28397
H	2.26389	-1.10353	-2.02150
H	4.36443	-2.25661	-2.60465
H	2.61259	1.74282	1.54323
C	2.92941	-0.64235	-0.00492
C	-0.50445	0.87773	0.42995
H	-0.32780	1.02038	1.50145
C	-1.55747	-0.21825	0.28733
C	-2.61608	-0.08400	1.37484
O	-2.38318	0.34894	2.47123
O	-3.86131	-0.48457	1.06343
C	-4.11624	-1.22251	-0.13381
C	-3.71357	-2.67715	0.03907
H	-4.26796	-3.10909	0.87508
H	-2.64432	-2.78816	0.23688
H	-3.95479	-3.22798	-0.87272
C	-5.58737	-1.04495	-0.42750
H	-6.17615	-1.45314	0.39659
H	-5.81042	0.01782	-0.54081
H	-5.84300	-1.57008	-1.35007
O	-3.41877	-0.64510	-1.24336
H	-1.06981	-1.19167	0.44956
C	-2.14821	-0.23497	-1.11477
O	-1.52904	0.10978	-2.08826
C	-1.00002	2.21781	-0.10296
O	-2.16326	2.57074	-0.07520
C	0.16245	2.92160	-0.66366
H	0.12790	3.94982	-1.00694
C	1.20501	2.07673	-0.76027
C	2.54986	2.36496	-1.33600
H	3.34624	2.08629	-0.63703
H	2.65400	3.42120	-1.59315
H	2.70786	1.76386	-2.23903



4-M (C)

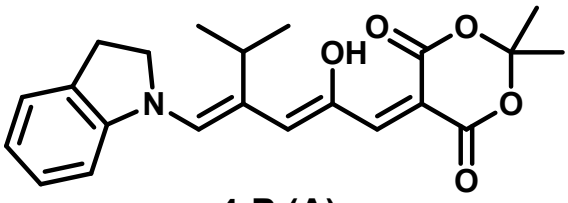
H	0.69638	0.04434	-1.15550

Electronic energy = -1205.266864 Hartree

Electronic energy + thermal free energy correction = -1204.935479 Hartree

Cartesian coordinates of optimized geometry of 4-P(A)

C	1.07955	0.56329	-0.19361
O	1.38982	1.86439	-0.00438
H	2.35317	2.00344	-0.19791
C	-0.24195	0.14332	-0.26399
C	-1.48964	0.84282	-0.25815
C	-2.56628	-0.02105	-0.14900
N	-3.88144	0.22640	0.03206
C	-4.51681	1.45398	0.55719
C	-5.79745	0.95136	1.25173
H	-5.63804	0.83334	2.32941
H	-6.62967	1.64303	1.10630
C	-6.02371	-0.39494	0.60845
C	-7.12074	-1.24115	0.63937
H	-8.02611	-0.94862	1.16377
C	-7.04448	-2.47926	-0.00967
H	-7.89816	-3.14903	0.00224
C	-5.87974	-2.85231	-0.67964
C	-4.76859	-2.00558	-0.72433
H	-3.87990	-2.29068	-1.27792
H	-5.83549	-3.80871	-1.19103
H	-3.82975	1.96199	1.23419
H	-4.76831	2.12216	-0.27259
C	-4.86153	-0.78451	-0.06391
H	-2.35707	-1.08850	-0.19387
C	-1.66157	2.34131	-0.46344
C	-1.27618	3.19306	0.75307
H	-1.80772	2.86762	1.65390
H	-0.20507	3.12782	0.95018
H	-1.53133	4.24274	0.56946
H	-2.72704	2.49958	-0.64661
C	-0.95861	2.81848	-1.74262
H	0.12614	2.74133	-1.65660
H	-1.21137	3.86772	-1.93069
H	-1.28655	2.23215	-2.60718
H	-0.33987	-0.93836	-0.29937
C	2.05368	-0.46350	-0.26606
C	3.44140	-0.46174	-0.23188
C	4.29512	0.71695	-0.25776
O	5.61902	0.52026	-0.11677
C	6.07787	-0.70967	0.45618
C	5.80876	-0.72036	1.95302
H	6.32414	0.12105	2.42167
H	6.18386	-1.65357	2.37933
H	4.73953	-0.64185	2.16869
C	7.54577	-0.81096	0.11544
H	8.08465	0.02977	0.55748



4-P (A)

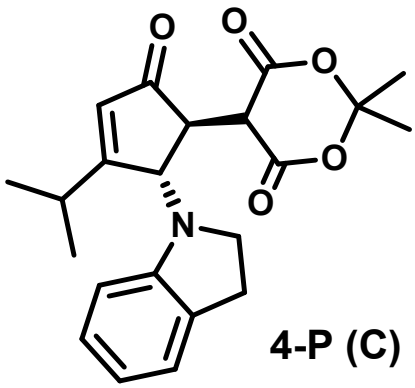
H	7.94835	-1.74604	0.51054
H	7.67278	-0.79267	-0.96897
O	5.43639	-1.80978	-0.17664
O	3.92575	1.86847	-0.46099
C	4.08254	-1.78741	-0.29906
O	3.50459	-2.83194	-0.49927
H	1.63993	-1.46449	-0.35248

Electronic energy = -1283.829100 Hartree

Electronic energy + thermal free energy correction = -1283.445958 Hartree

Cartesian coordinates of optimized geometry of 4-P(C)

N	1.58120	-0.47381	0.70453
C	2.12616	-0.10521	2.02315
H	1.34281	-0.10389	2.78442
C	3.20971	-1.16498	2.28730
H	4.04823	-0.76529	2.86180
H	2.79069	-2.01199	2.84384
C	3.58193	-1.59956	0.88914
C	4.65338	-2.34338	0.42701
H	5.43100	-2.66827	1.11355
C	4.72673	-2.67168	-0.93410
H	5.56650	-3.24605	-1.31118
C	3.71717	-2.25860	-1.80022
C	2.62596	-1.50906	-1.34568
H	1.85243	-1.20197	-2.04216
H	3.77387	-2.51592	-2.85387
H	2.57202	0.90175	1.98643
C	0.68568	0.44724	0.03353
C	-0.67389	0.57590	0.73785
H	-0.52970	0.40152	1.80974
C	-1.03671	2.04773	0.58689
O	-2.16731	2.48406	0.68600
C	0.20236	2.77178	0.26649
H	0.25808	3.85416	0.23288
C	-1.79825	-0.34641	0.27797
C	-2.89690	-0.42021	1.33110
O	-2.69107	-0.30739	2.50924
O	-4.14910	-0.62815	0.88538
C	-4.38410	-1.02407	-0.46743
C	-4.07380	-2.50019	-0.65309
H	-4.71135	-3.08754	0.01141
H	-3.03049	-2.73741	-0.42876
H	-4.27921	-2.78378	-1.68770
C	-5.82639	-0.68157	-0.75894
H	-6.47841	-1.24392	-0.08743
H	-5.98453	0.38794	-0.60672
H	-6.06221	-0.93993	-1.79337
O	-3.60153	-0.23185	-1.36929
H	-1.39199	-1.36465	0.18262
C	-2.32106	0.05613	-1.09232
O	-1.64060	0.61471	-1.91389
C	1.17440	1.89737	-0.05504
C	2.55661	2.20986	-0.55337
C	3.05591	3.57695	-0.08832
H	3.02425	3.66784	1.00205
H	4.08867	3.73110	-0.41449
H	2.44974	4.38256	-0.51631



4-P (C)

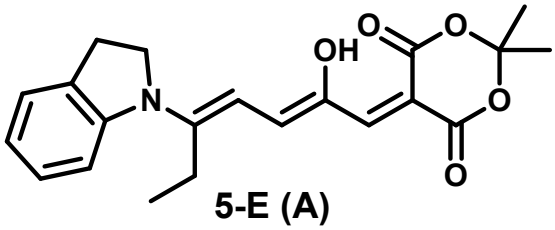
H	3.23296	1.43350	-0.17028
C	2.57288	2.11828	-2.08920
H	2.22235	1.14516	-2.44386
H	3.59162	2.26460	-2.46072
H	1.92901	2.89177	-2.52076
H	0.52884	0.08247	-0.98673
C	2.57109	-1.17767	0.00800

Electronic energy = -1283.860164 Hartree

Electronic energy + thermal free energy correction = -1283.475534 Hartree

Cartesian coordinates of optimized geometry of 5-E(A)

C	-1.12013	-0.23885	-0.13578
C	0.10009	0.38164	0.11391
H	0.05733	1.42288	0.41628
C	1.33277	-0.28376	-0.00364
C	2.56553	0.32784	0.19651
C	2.66218	1.80257	0.49725
H	1.87202	2.04951	1.21081
H	3.60053	2.01376	1.01177
C	2.50162	2.67498	-0.75523
H	2.67426	3.72705	-0.51158
H	1.49228	2.57936	-1.16427
H	3.19857	2.38456	-1.54672
N	3.70163	-0.41081	0.13531
C	3.65161	-1.88929	0.10237
H	2.86686	-2.23886	0.77399
C	5.05261	-2.33582	0.53884
H	5.06754	-2.58515	1.60559
C	5.88873	-1.11288	0.27158
C	7.26741	-0.98689	0.22741
H	7.89851	-1.85424	0.39969
C	7.83195	0.26144	-0.04969
H	8.91014	0.37503	-0.09195
C	7.00454	1.35510	-0.29254
C	5.61245	1.24110	-0.25296
H	5.00897	2.10705	-0.48533
H	7.44115	2.31941	-0.53282
H	5.39348	-3.21113	-0.01763
H	3.41917	-2.21894	-0.91728
C	5.05780	-0.00298	0.05617
H	1.28594	-1.32417	-0.29961
C	-2.28305	0.54085	0.01383
H	-2.08542	1.56527	0.31919
C	-3.64122	0.27182	-0.13500
C	-4.54821	1.39742	0.13412
O	-4.20177	2.53630	0.35896
O	-5.88091	1.12978	0.06803
C	-6.30934	-0.21664	0.22508
C	-6.16173	-0.66028	1.67266
H	-6.76283	-0.00981	2.31220
H	-5.12010	-0.60984	2.00152
H	-6.51342	-1.68939	1.77594
C	-7.73464	-0.27709	-0.27183
H	-8.36153	0.37861	0.33617
H	-8.10654	-1.30133	-0.19946
H	-7.77394	0.04965	-1.31305
O	-5.55101	-1.07758	-0.63097



5-E (A)

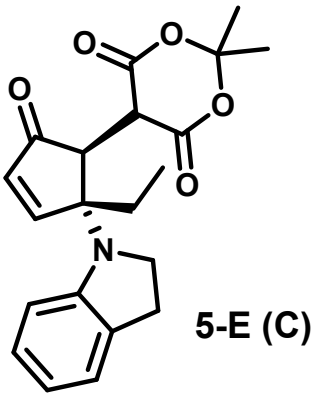
C	-4.20740	-0.96913	-0.63419
O	-3.58037	-1.90790	-1.11467
O	-1.09998	-1.54628	-0.47653
H	-2.00327	-1.81498	-0.78237

Electronic energy = -1244.543575 Hartree

Electronic energy + thermal free energy correction = -1244.186557 Hartree

Cartesian coordinates of optimized geometry of 5-E(C)

C	-0.67362	1.24944	1.33645
C	-0.80929	0.25040	2.48556
H	-0.48035	0.71761	3.41878
H	-1.84450	-0.07486	2.61601
H	-0.21468	-0.65565	2.33271
H	-1.36892	2.07668	1.50101
H	0.31082	1.72031	1.34480
C	-0.89476	0.65741	-0.08323
N	-1.89589	-0.43579	-0.03837
C	-3.24643	-0.16847	0.26843
C	-3.82101	0.89515	0.97087
H	-3.23333	1.71510	1.36100
C	-5.20704	0.90590	1.16835
H	-5.64846	1.73779	1.70938
C	-6.02133	-0.11243	0.68353
H	-7.09393	-0.07963	0.84401
C	-5.44317	-1.17751	-0.01815
H	-6.06083	-1.98358	-0.40585
C	-4.07505	-1.19565	-0.22135
C	-3.21032	-2.23001	-0.88870
H	-3.04334	-3.07637	-0.21111
H	-3.62526	-2.61799	-1.82152
C	-1.90371	-1.45992	-1.10852
H	-1.03678	-2.11749	-1.03205
H	-1.90163	-0.97991	-2.10129
C	0.43418	0.18725	-0.75322
C	1.68591	-0.13602	0.07386
H	1.38076	-0.47865	1.07151
C	2.60120	1.06441	0.30209
O	3.90192	0.80158	0.51401
C	4.36620	-0.53829	0.69138
C	4.09713	-1.01480	2.10912
H	4.60714	-0.35236	2.81206
H	3.03170	-1.02103	2.35224
H	4.48573	-2.02853	2.22799
C	5.83703	-0.51965	0.34534
H	6.36436	0.15147	1.02630
H	6.24811	-1.52682	0.43931
H	5.96578	-0.16929	-0.68066
O	3.74901	-1.41007	-0.26052
O	2.21972	2.20414	0.30794
C	2.43918	-1.31618	-0.53884
O	1.91816	-2.14910	-1.23202
H	0.23532	-0.72050	-1.32252
C	0.73613	1.21413	-1.84500



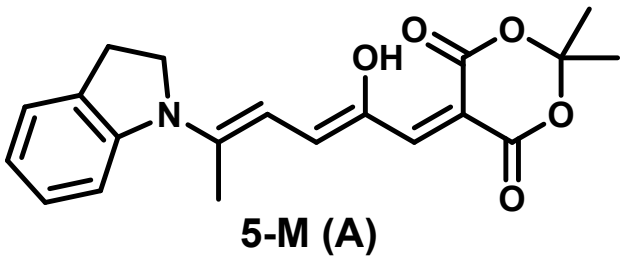
5-E (C)

C	-0.45793	2.06279	-2.00017
H	-0.55639	2.81524	-2.77369
O	1.77611	1.24529	-2.46884
C	-1.34224	1.75570	-1.04459
H	-2.31587	2.22248	-0.92354

Electronic energy = -1244.539496 Hartree
Electronic energy + thermal free energy correction = -1244. 178871 Hartree

Cartesian coordinates of optimized geometry of 5-M(A)

C	-2.18352	0.62847	-0.04745
H	-2.00217	1.67989	0.16062
C	-1.00913	-0.14778	-0.10333
C	0.19973	0.50815	0.10342
H	0.14361	1.57333	0.30037
C	1.44058	-0.15160	0.05393
C	2.66752	0.48039	0.20464
C	2.77454	1.95721	0.46603
H	3.66188	2.18808	1.05694
H	1.90506	2.29566	1.02869
H	2.81070	2.53032	-0.46589
N	3.80994	-0.25008	0.15885
C	3.79613	-1.72670	0.22237
H	3.04210	-2.05223	0.93988
C	5.22467	-2.10306	0.64151
H	5.28300	-2.26220	1.72402
C	6.01768	-0.88594	0.24221
C	7.38736	-0.72544	0.11341
H	8.05569	-1.55672	0.31972
C	7.89517	0.51161	-0.29612
H	8.96567	0.65087	-0.40559
C	7.02271	1.55784	-0.58762
C	5.63880	1.40864	-0.46419
H	4.98907	2.22804	-0.73875
H	7.41664	2.50812	-0.93410
H	5.56802	-3.01349	0.14638
H	3.54501	-2.13038	-0.76599
C	5.14592	0.18153	-0.01812
H	1.40798	-1.21169	-0.16538
O	-0.97069	-1.48187	-0.31434
H	-1.86376	-1.78829	-0.61427
C	-3.53511	0.32829	-0.18920
C	-4.46080	1.46105	-0.03669
O	-4.13230	2.62029	0.08747
O	-5.78858	1.16878	-0.09563
C	-6.20071	-0.16324	0.18244
C	-6.06530	-0.46759	1.66664
H	-6.68460	0.22948	2.23582
H	-5.02899	-0.36954	2.00172
H	-6.40215	-1.48834	1.86120
C	-7.61848	-0.29090	-0.32283
H	-8.26198	0.41015	0.21288
H	-7.97776	-1.30904	-0.15865
H	-7.64856	-0.06450	-1.39069
O	-5.41989	-1.08922	-0.58079
C	-4.07831	-0.96148	-0.58002



5-M (A)

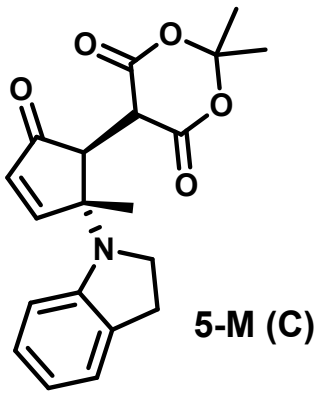
O	-3.43238	-1.92969	-0.96759

Electronic energy = -1205.248368 Hartree

Electronic energy + thermal free energy correction = -1204.919367 Hartree

Cartesian coordinates of optimized geometry of 5-M(C)

C	0.70814	1.10399	-1.59960
C	0.93624	0.78012	-0.11362
C	-0.39715	0.50763	0.63843
H	-0.16866	-0.15117	1.47971
C	-0.73870	1.81144	1.35077
O	-1.82404	2.06499	1.82855
C	0.50544	2.60384	1.40182
H	0.60780	3.51459	1.98005
C	-1.59114	-0.13163	-0.07006
C	-2.35576	-1.04678	0.88532
O	-1.85942	-1.55931	1.85345
O	-3.64314	-1.28615	0.59311
C	-4.21652	-0.82892	-0.63682
C	-5.70658	-0.75733	-0.39770
H	-5.91031	-0.08255	0.43605
H	-6.08739	-1.75288	-0.16048
H	-6.20316	-0.38424	-1.29567
O	-3.79487	0.50665	-0.91571
C	-3.84370	-1.75829	-1.77969
H	-4.17520	-2.77189	-1.54399
H	-2.76697	-1.77720	-1.96426
H	-4.34256	-1.42221	-2.69140
C	-2.51195	0.87818	-0.74957
O	-2.15638	1.95950	-1.13101
H	-1.21793	-0.79782	-0.86257
C	1.43271	2.01990	0.63305
H	2.44688	2.38449	0.50495
N	1.86245	-0.36490	-0.02190
C	1.77353	-1.32604	1.09819
H	1.86915	-0.80576	2.06600
H	0.82609	-1.86724	1.08234
C	2.97234	-2.25309	0.87515
H	3.34851	-2.67891	1.80765
H	2.69539	-3.07817	0.20674
C	3.94670	-1.33283	0.18844
C	5.31090	-1.45810	0.00149
H	5.83891	-2.31668	0.40839
C	6.00312	-0.46628	-0.70544
H	7.07490	-0.54618	-0.85431
C	5.30491	0.62865	-1.20303
C	3.92287	0.76488	-1.02171
H	3.43489	1.64893	-1.41167
H	5.83734	1.40902	-1.73894
C	3.23221	-0.23411	-0.32827
H	0.09098	1.99487	-1.71304
H	0.21069	0.26094	-2.08955



5-M (C)

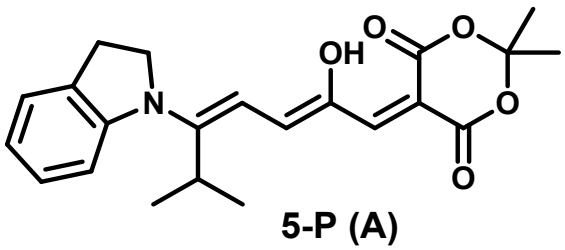
H	1.65058	1.25745	-2.12278

Electronic energy = -1205.245536 Hartree

Electronic energy + thermal free energy correction = -1204.912206 Hartree

Cartesian coordinates of optimized geometry of 5-P(A)

C	4.95464	-0.17058	-0.10450
C	5.77666	-1.23872	0.28369
C	4.93069	-2.31718	0.91077
H	5.00397	-2.27799	2.00379
H	5.20908	-3.32148	0.58579
C	3.51809	-1.93222	0.44838
H	2.74819	-2.12989	1.19511
H	3.25244	-2.44543	-0.48469
C	7.14210	-1.19588	0.05549
H	7.77306	-2.02596	0.36073
C	7.69303	-0.08160	-0.58626
H	8.76034	-0.03654	-0.77645
C	6.86538	0.95633	-1.00968
H	7.29042	1.80290	-1.53980
N	3.60869	-0.47724	0.20815
C	2.50683	0.32874	0.18826
C	2.73138	1.81062	0.45447
C	2.09520	2.24276	1.78722
H	2.40918	1.58174	2.60053
H	2.42931	3.25693	2.02789
H	1.00414	2.24906	1.75983
H	3.80380	1.93925	0.60498
C	2.31357	2.71803	-0.70886
H	2.66279	3.73823	-0.52116
H	1.22890	2.75709	-0.83430
H	2.73862	2.38021	-1.65889
C	1.26372	-0.26293	0.03182
C	0.01825	0.39663	0.04309
H	-0.05045	1.46502	0.20050
C	-1.18308	-0.27357	-0.14982
C	-2.36289	0.50135	-0.13179
H	-2.18513	1.56135	0.03107
C	-3.71097	0.19103	-0.26122
C	-4.64209	1.32697	-0.15873
O	-4.31720	2.49157	-0.09441
O	-5.96809	1.02570	-0.19408
C	-6.37094	-0.29356	0.15147
C	-6.21934	-0.52613	1.64688
H	-6.83836	0.19290	2.18832
H	-5.18086	-0.40532	1.96755
H	-6.54706	-1.53878	1.89272
C	-7.79269	-0.45256	-0.33292
H	-8.43495	0.26915	0.17621
H	-8.14385	-1.46389	-0.11729
H	-7.83502	-0.27665	-1.40982
O	-5.59196	-1.25086	-0.57488



5-P (A)

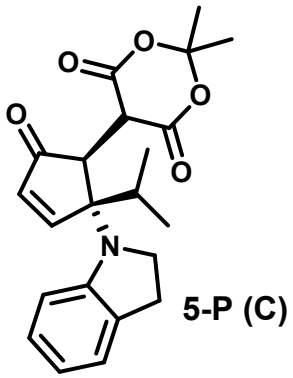
C	-4.25162	-1.11880	-0.58994
O	-3.60337	-2.09958	-0.93787
O	-1.14169	-1.61428	-0.30615
H	-2.03250	-1.93572	-0.59552
H	1.21888	-1.32928	-0.15756
C	5.48591	0.92329	-0.78869
H	4.86177	1.72129	-1.17244

Electronic energy = -1283.834427 Hartree

Electronic energy + thermal free energy correction = -1283.834427 Hartree

Cartesian coordinates of optimized geometry of 5-P(C)

O	-2.26825	2.14047	0.02649
C	-2.64307	1.00928	-0.12865
C	-1.71621	-0.20457	-0.07209
C	-0.47957	0.01676	0.80521
C	-0.79022	0.84424	2.04846
O	-1.85381	0.81528	2.63162
C	0.44581	1.55826	2.40745
H	0.56908	2.11249	3.33039
C	1.34336	1.40661	1.42670
H	2.34542	1.82196	1.44889
H	-0.26866	-0.95796	1.24548
C	0.86051	0.58512	0.22960
N	1.81200	-0.51674	-0.06257
C	1.64222	-1.85563	0.54587
H	1.61869	-1.78362	1.64607
H	0.72090	-2.33197	0.20633
C	2.88700	-2.62953	0.10126
H	3.18233	-3.39023	0.82704
C	3.89296	-1.52385	-0.07280
C	5.27043	-1.57710	-0.18536
H	5.78659	-2.52962	-0.09652
C	5.99020	-0.39680	-0.41225
H	7.07182	-0.42172	-0.49413
C	5.30409	0.80764	-0.53344
C	3.91016	0.86993	-0.42484
H	3.41459	1.82472	-0.53442
H	5.85441	1.72661	-0.71321
H	2.70450	-3.12548	-0.86046
C	3.19576	-0.30587	-0.18579
C	0.61095	1.48613	-1.05439
C	1.00069	2.96229	-0.90581
H	0.48775	3.42440	-0.05820
H	2.07469	3.12935	-0.78661
H	0.69027	3.50030	-1.80717
H	-0.46964	1.52910	-1.17815
C	1.15363	0.88304	-2.35280
H	2.24539	0.88754	-2.40031
H	0.82399	-0.15115	-2.48918
H	0.78063	1.47392	-3.19606
C	-2.45896	-1.46781	0.36258
O	-1.92643	-2.39110	0.91975
O	-3.77083	-1.52759	0.08712
C	-4.39939	-0.53667	-0.73162
C	-5.86808	-0.57634	-0.37893
H	-5.99294	-0.37077	0.68603
H	-6.27331	-1.56410	-0.60785



5-P (C)

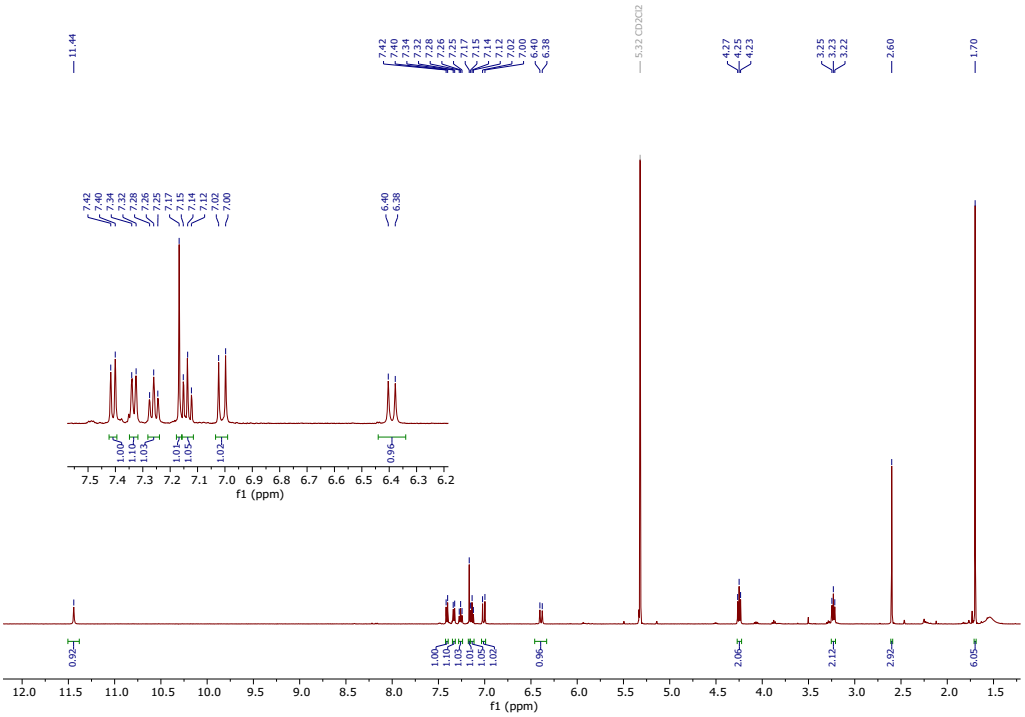
H	-6.40362	0.17819	-0.95872
C	-4.13711	-0.81503	-2.20225
H	-3.07280	-0.79402	-2.44932
H	-4.53020	-1.80194	-2.45578
H	-4.64767	-0.06193	-2.80654
H	-1.39260	-0.39746	-1.10598
O	-3.94252	0.76916	-0.37378

Electronic Energy = -1283.828179 Hartree

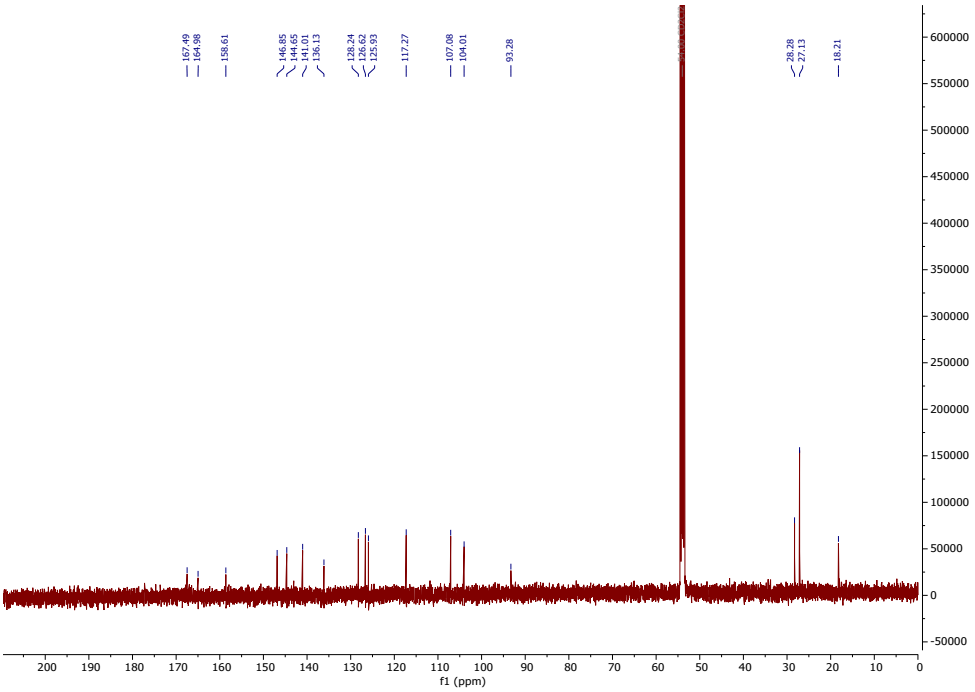
Electronic energy + thermal free energy correction = -1283.439542 Hartree

11. Characterization data for **D1-M**

^{1}H NMR of **D1-M** in CD_2Cl_2 (600 MHz)



^{13}C NMR of **D1-M** in CD_2Cl_2 (125 MHz)



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