Supporting Information for

Back electron transfer rates determine the photoreactivity of donor-acceptor stilbene complexes in a macrocyclic host

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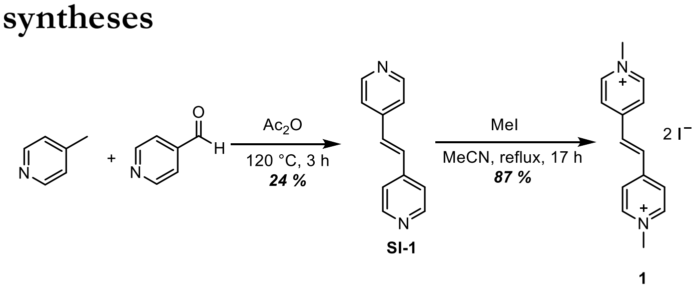
I. General experimental notes

Unless otherwise noted, reactions were performed under N_2 atmosphere in oven-dried (150 ºC) glassware. Reaction progress was monitored by thin layer chromatography (EMD 250 µm silica gel 60-F254 plates) or by liquid chromatography-mass spectrometry using a Agilent 6120 Quadrupole LC/MS. Automated column chromatography was performed using SiliCycle SiliaFlash F60 (40-63 µm, 60 Å) in SNAP cartridges on a Biotage Isolera One. Organic solvents were removed in vacuo using a rotary evaporator (Büchi Rotovapor R-100, ~20–200 torr) and residual solvent was removed under high vacuum (<0.1 torr). Commercial reagents and solvents were purchased from Sigma-Aldrich, Acros, Alfa Aesar, TCI, or Oakwood and used as received. Cucurbit[8]uril was purchases from Strem Chemicals and used as received. DMF and dichlormethane were purified and dried using a solvent-purification system that contained activated alumina then degassed with N_2 sparging prior to use. Proton nuclear magnetic resonance (^{1}H NMR) spectra, carbon nuclear magnetic resonance (^{13}C NMR), and phosphorous nuclear magnetic resonance (^{31}P NMR) spectra were recorded on Bruker AVANCE-500 spectrometers at 500 MHz and 125 MHz, and referenced to the solvent residual peaks. NMR data are represented as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constant in Hertz (Hz), integration. UV-vis spectra were collected on a Cary 5000 or Cary 3500 UV-vis-NIR spectrophotometer with an Hg lamp; cuvettes were 10-mm or 2-mm path length quartz cells (Starna 23-Q-10 or 23-Q-2). High-resolution mass spectra were recorded on an Agilent 6210A LC-TOF mass spectrometer. Red (626 nm, 6.6 W), amber (605 nm, 2.4 W), green (525 nm, 5.7 W), and violet (400 nm, power = 6.1 W) LEDs were purchased from superbrightleds.com. See Figures S1-S5 for emission profiles of the LEDs. 350 nm irradiation was provided by ten Rayonet RPR-3500A lamps (power = 8 W). Semi-prep HPLC was performed using a Shimadzu LC-6A with a C18 column and a water/acetronitrile mobile phase with 0.1% trifluoroacetic acid. LCMS was performed on an Agilent 6120 Quadrupole LC/MS using a 2.1 X 50 mm "Poroshell 120" C18 column with a water/acetonitrile mobile phase with 0.1% formic acid.

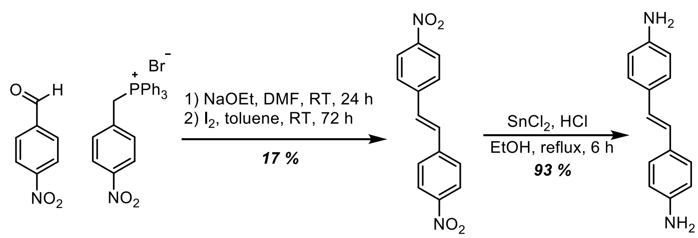
II. Starting material syntheses



Scheme S1. Synthesis of **1**.

(*E*)-1,2-di(pyridin-4-yl)ethene: Based on a literature procedure,[1] 4-methylpyridine (4.89 mL, 50.3 mmol), 4-pyridinecarboxaldehyde (4.73 mL, 50.3 mmol), and acetic anhydride (4.81 mL, 50.9 mmol) were combined in a non-dried 100 mL round bottom flask with a magnetic stir bar. The reaction was heated to 120 °C and stirred for 3 hours under nitrogen. The reaction was then cooled to 23 ºC an aqueous solution of NaOH (4.0 g in 40 mL water) was added to the brown mixture. A dark red solid was collected via vacuum filtration. The solid was recrystallized from an ethanol/water mixture (9 mL ethanol, 35 mL water) and dried in a vacuum desiccator to yield the product as an orange solid (2.18 g, 24% yield). ^{1}H NMR matched the literature report.[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (d, *J* = 6.2 Hz, 3H), 7.39 (d, *J* = 6.2 Hz, 3H), 7.21 (s, 2H).

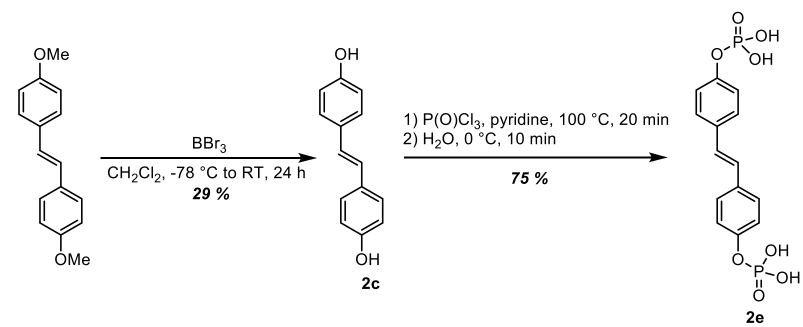
(*E*)-4,4'-(ethene-1,2-diyl)bis(1-methylpyridin-1-ium) iodide (1): Following a literature procedure,[2] **(*E*)-1,2-di(pyridin-4-yl)ethene** (218 mg, 1.20 mmol) was dissolved in 3 mL of acetonitrile in a non-dried 10 mL round bottom flask fitted with a reflux condenser and a magnetic stir bar. Methyl iodide (2.21 g, 0.968 mL, 15.6 mmol) was added and the reaction was heated to reflux under nitrogen for 17 hours. The resulting orange mixture was then cooled and an orange solid was recovered by vacuum filtration. Washing with acetonitrile yielded the product as a chalky orange solid (485 mg, 87% yield). ^{1}H NMR in D_2O matched the literature report.[2] ^{1}H NMR (500 MHz, D_2O) δ 8.79 (d, *J* = 6.8 Hz, 4H), 8.24 (d, *J* = 6.9 Hz, 4H), 7.89 (s, 2H), 4.39 (s, 6H).



Scheme S2. Synthesis of **2a**.

(*E*)-1,2-bis(4-nitrophenyl)ethene: Following a literature procedure,[3] (4-nitrobenzyl)triphenylphosphonium bromide (5.00 g, 10.5 mmol), 4-nitrobenaldehyde (1.58 g, 10.5 mmol) and sodium ethoxide (925 mg, 13.6 mmol) were added to an oven-dried 250 mL round bottom flask with a magnetic stir bar. Dry DMF was added and the red solution was stirred at 23 ºC under nitrogen. After 24 hours, the reaction mixture was filtered and the filtrate was collected. Solvent was removed *in vacuo* to provide a bright yellow solid, which was recrystallized twice from ethanol. Comparison to the literature ^{1}H NMR revealed that we had produced the undesired *Z*-isomer.[3] ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.9 Hz, 4H), 7.35 (d, *J* = 8.8 Hz, 4H), 6.84 (s, 2H). We produced the desired *E*-isomer via iodine-catalyzed isomerization. The Z-isomer was suspended in 20 mL of toluene and two crystals of iodine were added. The mixture was stirred at 23 ºC under nitrogen. Isomerization was monitored using ^{1}H NMR. After 72 hours, the isomerization was complete. The reaction mixture was diluted in 100 mL of ethyl acetate and washed with 100 mL of aqueous sodium thiosulfate (10 wt%). The aqueous layer was removed and the yellow solid suspended in the organic layer was collected via vacuum filtration. This solid was washed with hexanes and dried on high vacuum to provide the desired product (485 mg, 17% yield). ^{1}H NMR matched the literature report.[3] ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.9 Hz, 4H), 7.69 (d, *J* = 8.9 Hz, 1H), 7.30 (s, 1H).

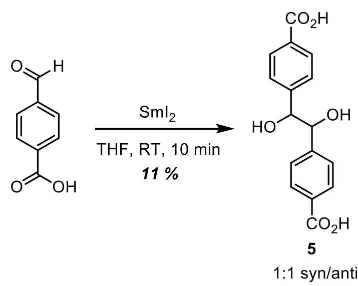
(*E*)-4,4'-(ethene-1,2-diyl)dianiline (2a): Following a literature procedure,[3] **(*E*)-1,2-bis(4-nitrophenyl)ethene** (200 mg, 0.740 mmol) and $SnCl_2$ (1.67 g, 7.40 mmol) were suspended in a mixture of ethanol (10 mL) and hydrochloric acid (3 mL) in a round bottom flask equipped with a magnetic stir bar. The reaction was stirred under N_2 for one hour then heated to reflux for six hours. The reaction mixture was then poured onto ice and the pH was adjusted to ~8 using a sodium hydroxide solution. The resulting mixture was extracted with ethyl acetate (3 X 20 mL), and the combined organic layers were dried of $MgSO_4$. Filtration and removal of the solvent *in vacuo* provided the product as a light orange solid (145 mg, 93% yield). ^{1}H NMR matched the literature report.[3] ^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 7.26 – 7.02 (m, 4H), 6.71 (s, 2H), 6.57 – 6.47 (m, 4H), 5.13 (s, 4H).



Scheme S3. Synthesis of the **2c** and **2e.**

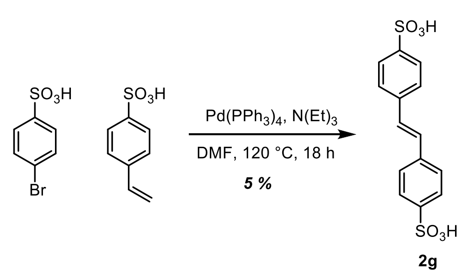
(*E*)-4,4'-(ethene-1,2-diyl)diphenol (2c): (*E*)-1,2-bis(4-methoxyphenyl)ethene (2.40 g, 9.99 mmol) was dissolved in 100 mL of dry dichloromethane in a flame-dried 200 mL Schlenk flask. The resultant yellow slurry was cooled to -78 °C in a dry ice/acetone bath. Tribromoborane (2.84 mL, 30.0 mmol) was added over five minutes, causing an immediate darkening and precipitation of a white solid. The reaction was stirred under nitrogen while the bath slowly warmed overnight. After 24 hours, the reaction was quenched by slow addition of 100 mL of ice-cold water. 200 mL of ethyl acetate were added and the oraganic layer was separated and washed with brine. The solvent was removed *in vacuo* and the residue was purified via column chromatography (hexanes/ethyl acetate; 2 to 45% linear gradient) to provide the produce as a white solid (624 mg, 29% yield). ^{1}H NMR matched the literature report.[4] ^{1}H NMR (500 MHz, Acetone-*d*$_6$) δ 7.44 – 7.36 (m, 4H), 6.96 (s, 2H), 6.86 – 6.79 (m, 4H).

(*E*)-4-(4-(phosphonooxy)styryl)phenyl dihydrogen phosphate (2e): **(*E*)-4,4'-(ethene-1,2-diyl)diphenol** (255 mg, 1.20 mmol) was dissolved in 1 mL of pyridine to produce a yellow solution. Addition of this solution to phosphoryl trichloride (1.12 mL, 12.0 mmol) led to an exothermic reaction and a white precipitate. The reaction was heated to 100 °C and stirred under nitrogen for 20 minutes. The reaction mixture was then cooled to 0 °C in an ice bath and water (300 uL) was slowly added to hydrolyze the phosphoryl chlorides. The resultant white slurry was basified with 1 M NaOH to a pH of ~10. The aqueous solution was washed with 5x10 mL of ethyl acetate, then acidified with concentrated HCl to produce a white precipitate, which was collected via vacuum filtration, washed with water, and dried under high vacuum to provide the product (333 mg, 75% yield). ^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 7.34 (d, *J* = 8.3 Hz, 4H), 7.05 – 6.98 (m, 6H). ^{13}C{^{1}H} NMR (126 MHz, DMSO) δ 151.49 (d, *J* = 6.4 Hz), 132.90, 127.57, 127.08, 120.46 (d, *J* = 5.0 Hz). ^{31}P NMR (202 MHz, DMSO) δ -5.16 HRMS (ESI-ToF): *m/z* = -392.9911 (calc'd for [M-2H+Na]$^-$: -392.9911).



Scheme S4. Synthesis of **5**.

4,4'-(1,2-dihydroxyethane-1,2-diyl)dibenzoic acid (5): Following a literature procedure,[5] 4-Carboxybenzaldehyde (212 mg, 1.41 mmol) was dissolved in 5 mL of dry THF then dropwise added to 14.1 mL of a 0.1 M THF solution of samarium diiodide (1.41 mmol) in a round bottom flask with a stir bar. The solution immediately turned yellow and was stirred under N_2 for an additional 10 minutes. Then, about 30 mL of 0.1 M HCl were added followed by 30 mL of ethyl acetate. The organic layer was separated and the aqueous layer was extracted with a further 20 mL of ethyl acetate. The combined organic layers were washed with aqueous sodium thiosulfate and brine before being dried over Na_2SO_4. Filtration and removal of the solvent *in vacuo* provided a crude product that contained some of the starting material. The desired diol was purified via column chromatography (20% methanol in dichloromethane), yielding a white solid that contained a 1:1 mixture of the *syn* and *anti* diastereomers (23 mg, 11% yield). ^{1}H NMR matched a literature report.[6] ^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 7.86 – 7.80 (m, 2H), 7.85 – 7.79 (m, 2H), 7.78 – 7.72 (m, 2H), 7.34 (d, *J* = 8.3 Hz, 2H), 7.22 (d, *J* = 8.2 Hz, 2H), 5.58 (s, 1H), 5.48 (s, 1H), 4.73 (d, *J* = 2.2 Hz, 1H), 4.66 (d, *J* = 2.4 Hz, 1H).



Scheme S5. Synthesis of **2g**.

(E)-4,4'-(ethene-1,2-diyl)dibenzenesulfonic acid (2g): Following a modified literature proecedure,[7] *p*-bromosulfonic acid hydrate (510 mg, 2.00 mmol), sodium *p*-vinylbenzenesulfonate (412 mg, 2.00 mmol), tetrakis(triphenylphosphine)palladium(0) (231 mg, 0.200 mmol), and triethylamine (697 μL, 5.00 mmol) were dissolved in dry, N_2-sparged dimethylformamide. The mixture was sparged with N_2 for 5 minutes before heating to 120 °C under N_2 overnight. After 18 hours, the mixture was cooled and filtered. The residue was collected and dissolved in 5 mL of hot 1:1 water/ethanol, then this mixture was hot filtered and the filtrate was collected. Solvent was removed *in vacuo* to yield a grey powder. This powder was suspended in 5 mL of DMF then re-subjected to the purification above to yield 33 mg (5%) of the final lightly grey product. ^{1}H NMR matched the literature report.[7] ^{1}H NMR (500 MHz, DMSO) δ 7.60 – 7.54 (m, 8H), 7.27 (s, 2H).

III. Figures S1-S5: Emission profiles of LEDs

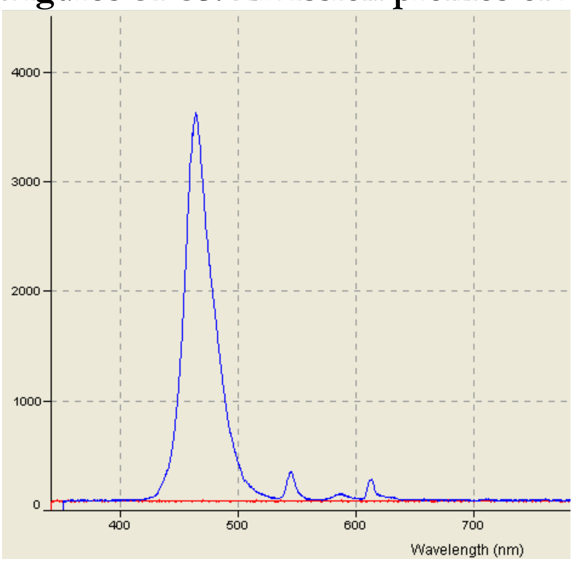


Figure S1. Emission of blue LEDs centered at 470 nm.

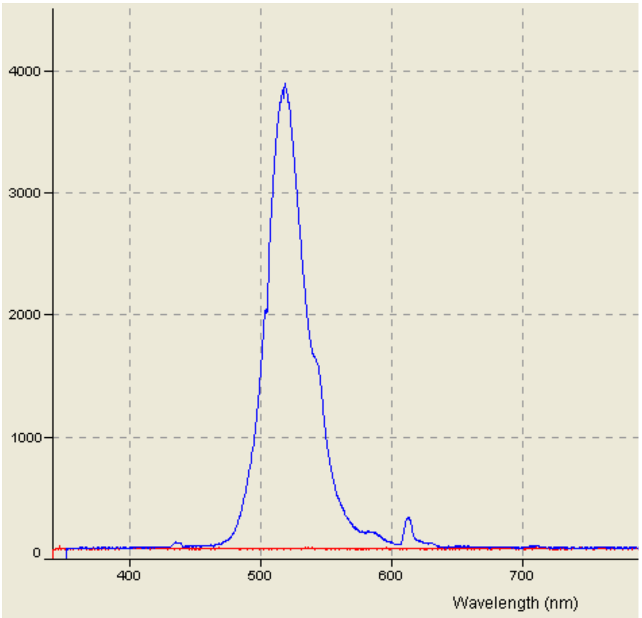


Figure S2. Emission of green LEDs centered at 525 nm.

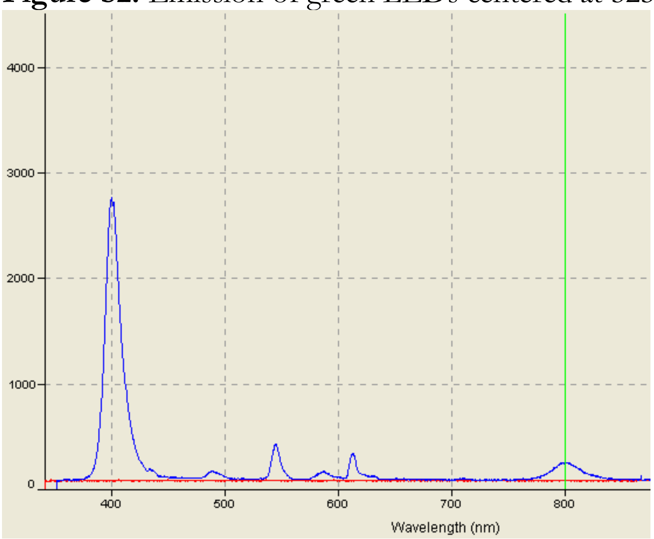


Figure S3. Emission of violet LEDs centered at 400 nm.

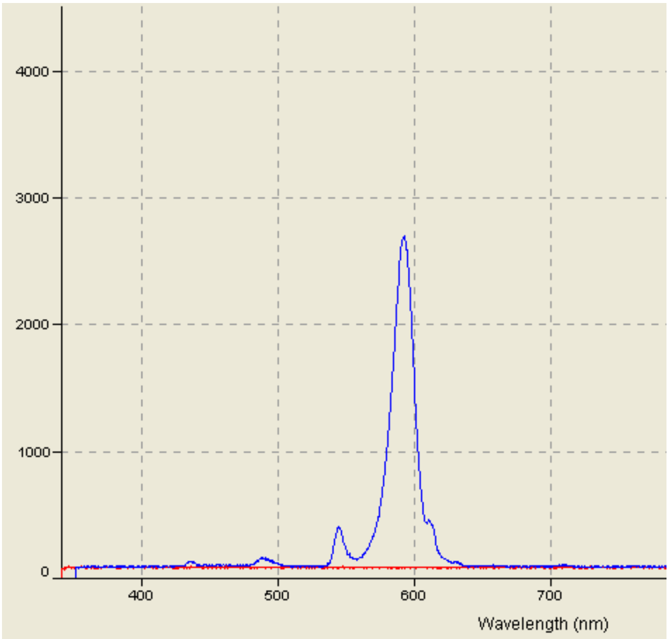


Figure S4. Emission of amber LEDs centered at 605 nm.

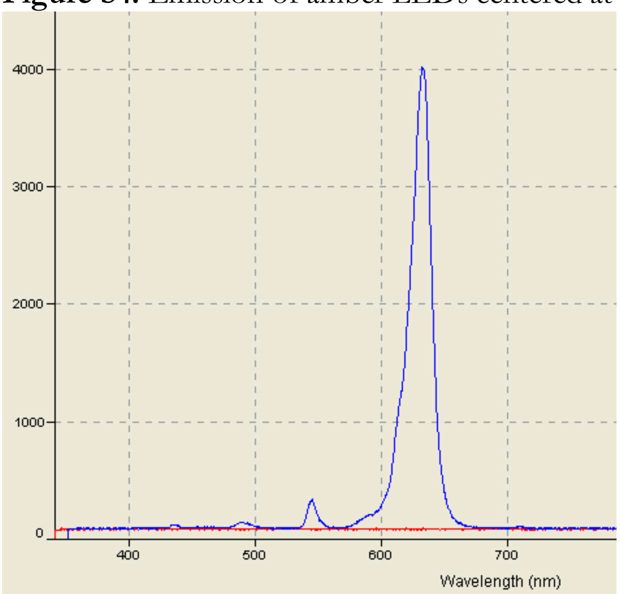
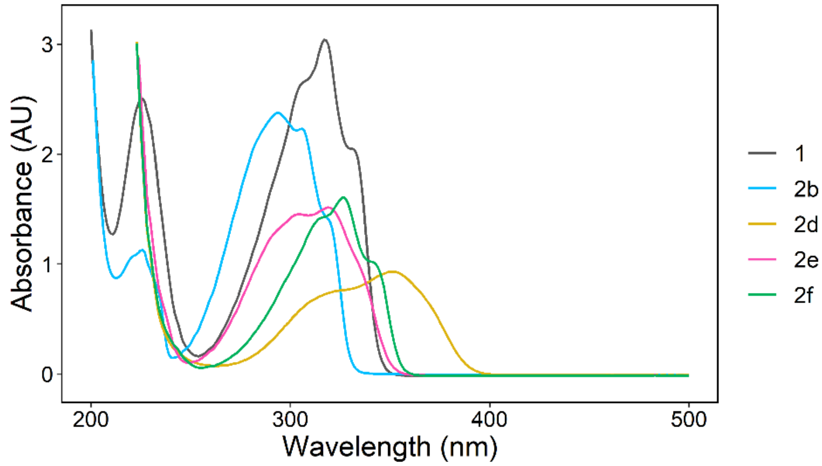


Figure S5. Emission of red LEDs centered at 626 nm.

IV. Figure S6: UV-Vis of free stilbenes



Figures S6. UV-Vis of aqueous solutions of the indicated stilbenes. **1** was measured in H_2O. **2b** was measured in 0.1 M HCl. All others were measured in 0.1 M Na_2CO_3. All at 25 μM in standard 1 cm quartz cuvettes.

V. Figure S7. UV-Vis spectra of product 3f

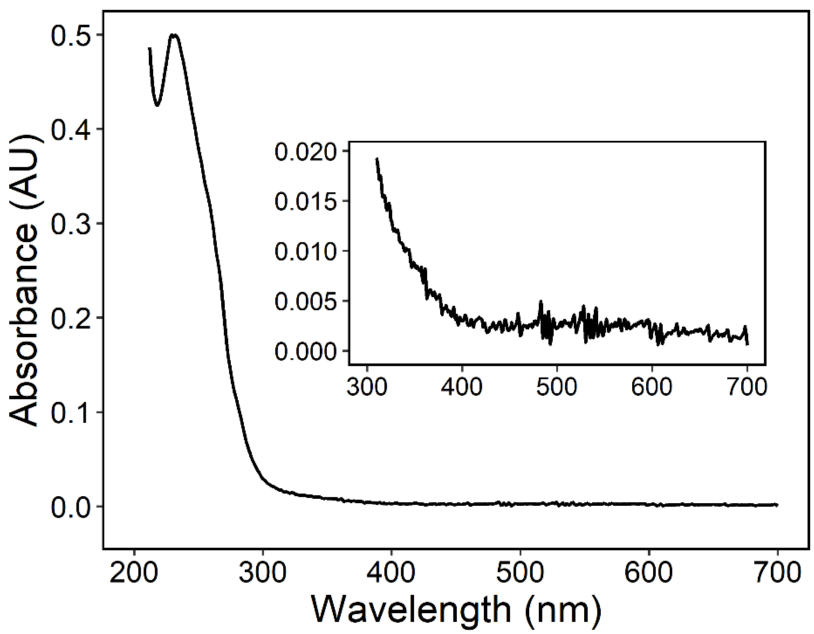


Figure S7. UV-Vis of **3f** in H_2O. The inset is zoomed in to show a small amount of absorbance at 400 nm.

VI. Figures S8-S14: NMRs of host-guest complexes

Samples were prepared at a volume of 1 mL with the reagents, solvents, and concentrations indicated in the figure captions below. All samples were sonicated in vials for twenty minutes following addition of all of the components. All spectra in this section are ^1H NMR measured at 400 MHz in D_2O. Up-field shifts of the signals from **1**, which are indicated with dotted lines, or other stilbenes are indicative of supramolecular interactions.[8] In all cases, integration of the stilbene and **CB[8]** signals reveals 1:1:1 stoichiometry, which is further confirmed by the titrations in the next section.

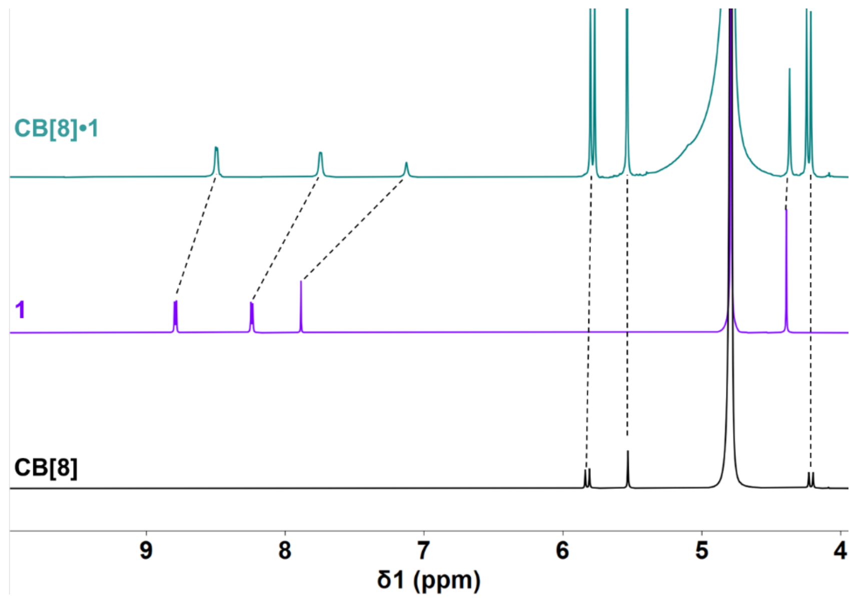


Figure S8. 1 and **CB[8]**. Measured at 1 mM in D_2O.

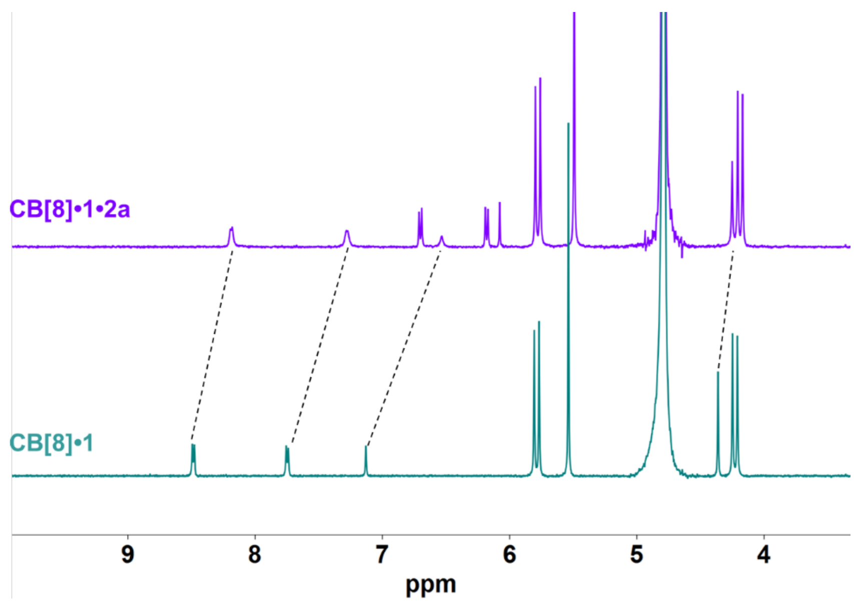


Figure S9. 1, **2a**, and **CB[8]**. Measured at 0.5 mM in D_2O.

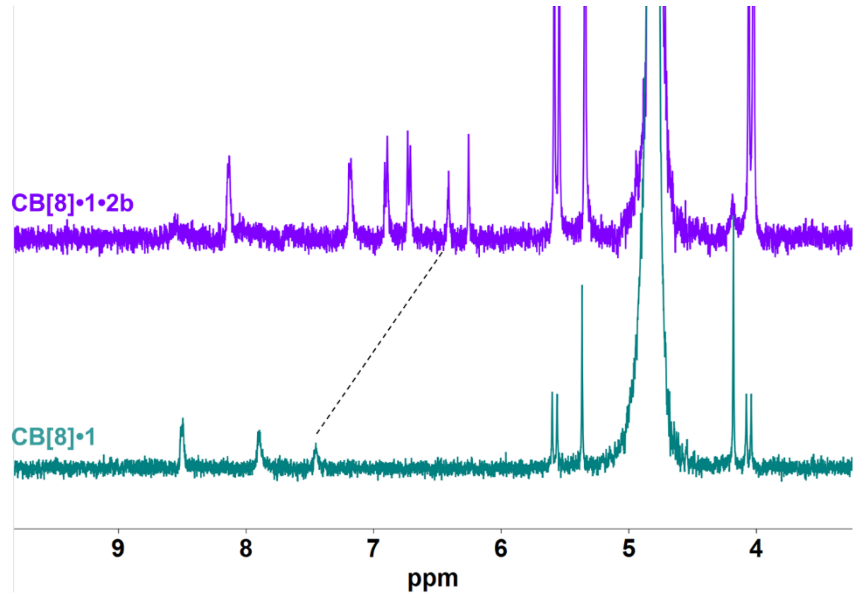


Figure S10. 1, **2b**, and **CB[8]**. Measured at 0.5 mM in 10 mM D_2SO_4.

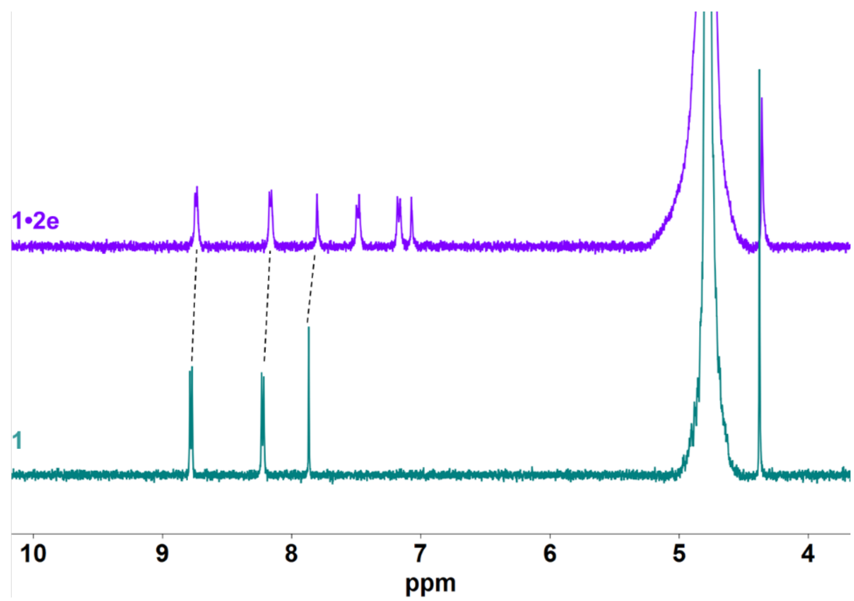


Figure S11. 1 and **2e**. Measured at 0.5 mM in 10 mM Na_2CO_3 in D_2O.

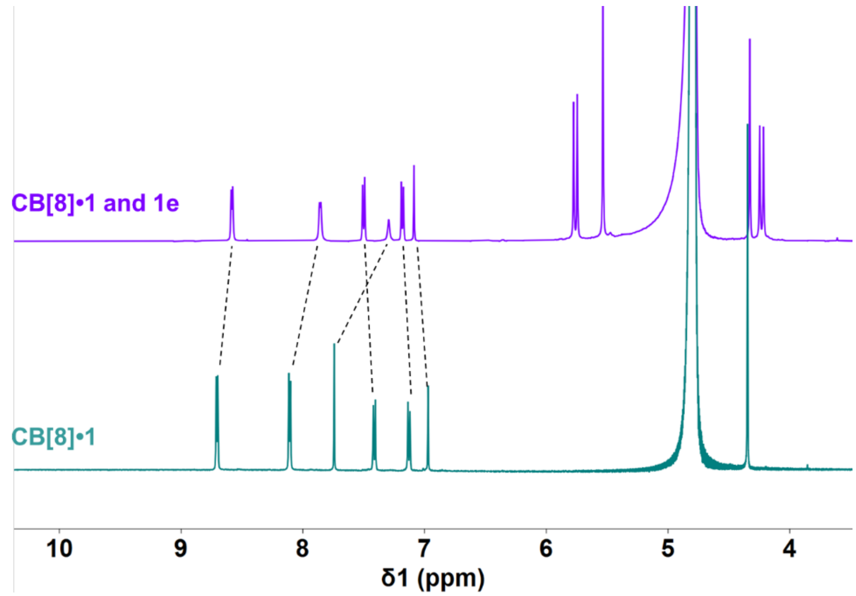


Figure S12. 1, **2e**, and **CB[8]**. Measured at 1.5 mM in 10 mM Na_2CO_3 in D_2O. Down-field shifts of the signals from **2e** indicate that **2e** is not binding in the **CB[8]**, but is instead competing with **CB[8]** for **1**.

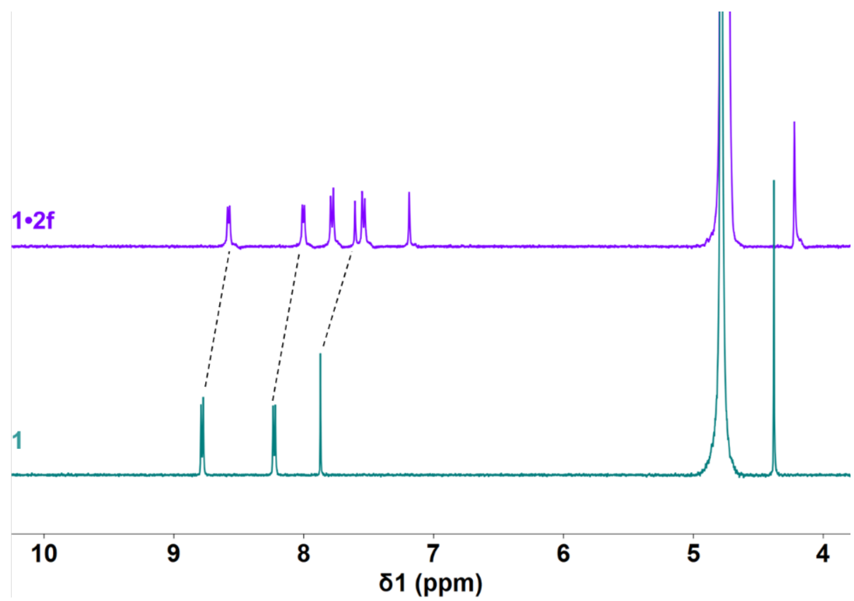


Figure S13. 1 and **2f**. Measured at 1 mM in 10 mM Na_2CO_3 in D_2O.

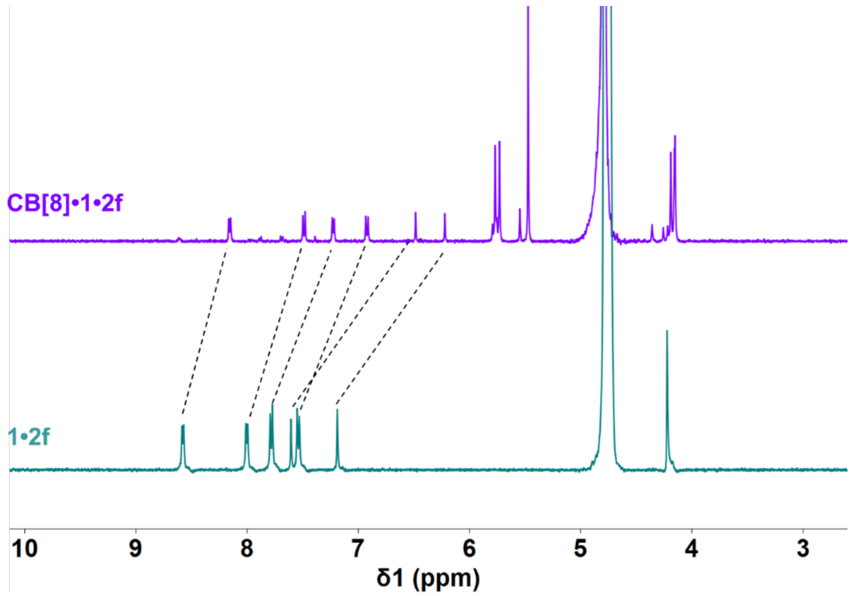


Figure S14. 1, **2f**, and **CB[8]**. Measured at 1 mM in 10 mM Na_2CO_3 in D_2O. Up-field shifts of the signals from **2f** indicate that **2f** is binding in the **CB[8]** to form a ternary complex.

VII. Supramolecular interaction titrations

To determine the strength of the various host-guest interactions relevant to this work, we used ^{1}H NMR titrations (Figure S15-S22). We prepared solutions of **1** and **CB[8]•1** in D_2O at concentrations of 1.0 or 0.5 mM. For each experiment, we split a sample into two parts and added an excess (~5 times) of the second substrate (the "guest") to one of the portions. We then iteratively added small amounts of this second portion to the first and measured ^{1}H NMR after each addition. For some samples, this led to a gradual shifting of **1** peaks, which we could then track (indicated by "Chemical Shift" y-axes). For others, exchange between bound and unbound states was slow on the NMR time scale so new sets of peaks emerged upon addition of the "guest", which we could integrate to determine the concentration of bounds species (indicated by "Conc. complex" y-axes). In all cases, we fit the experimental data to a 1:1 binding model using supramolecular.org.[8] For some of the interactions, the data appear linear, which precludes accurate fitting. Based on the concentrations at which we performed these experiments, we estimate that these samples exhibit binding constants of a greater order of magnitude than 10^5 M^{-1}. For **2a** and **2c**, analysis is further complicated by the insolubility of these molecules in D_2O, such that we can only observe the bound "guest" in our experiments. This observation indicates that the binding constant of these stilbenes is also $>10^5$ M^{-1}. Using the same titration experiment, **3f** exhibited a binding constant with **CB[8]** of greater than 10^5 M^{-1}.

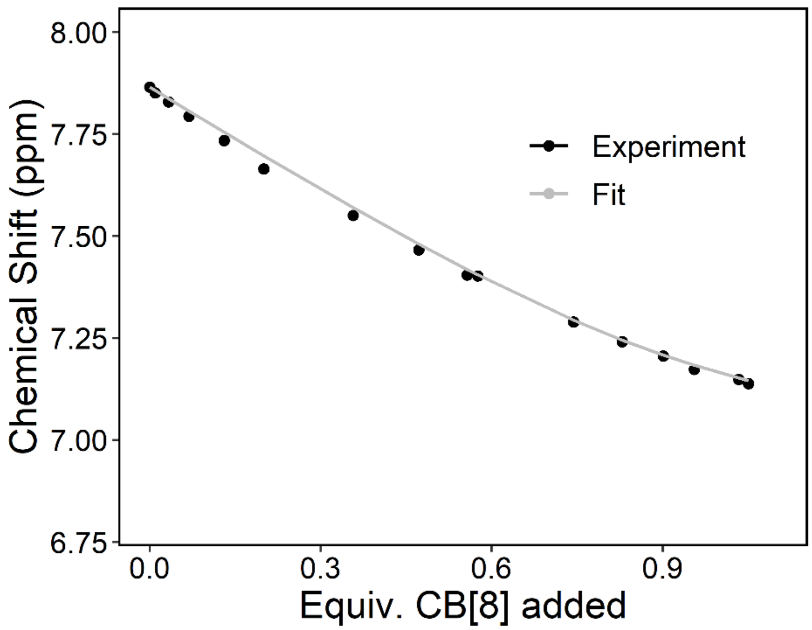


Figure S15. Titration of **CB[8]** into a D_2O solution of **1** (1.0 mM). Fit to a 1:1 binding model on supramolecular.org.[8]

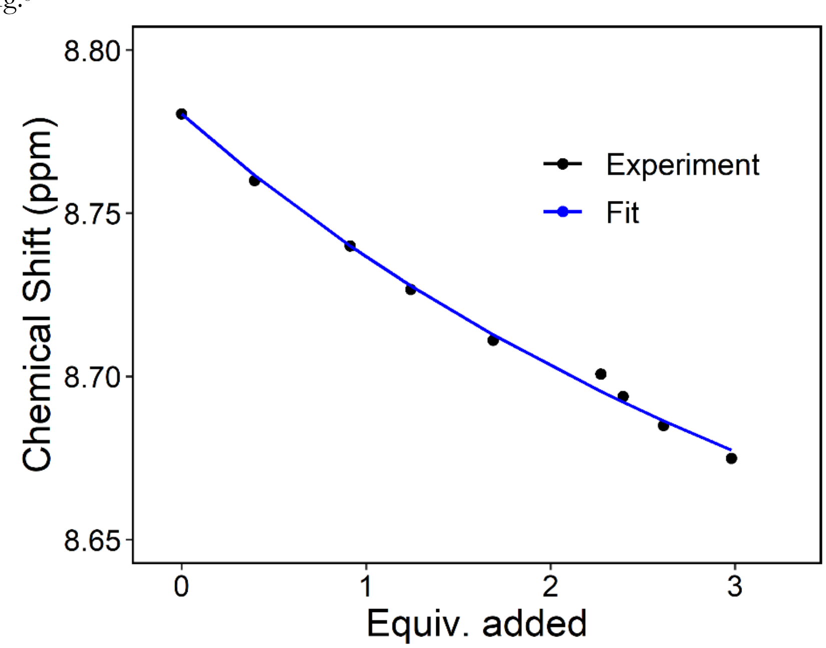


Figure S16. Titration of **2e** into a 10 mM Na_2CO_3, D_2O solution of **1** (0.5 mM). Fit to a 1:1 binding done on supramolecular.org.[8]

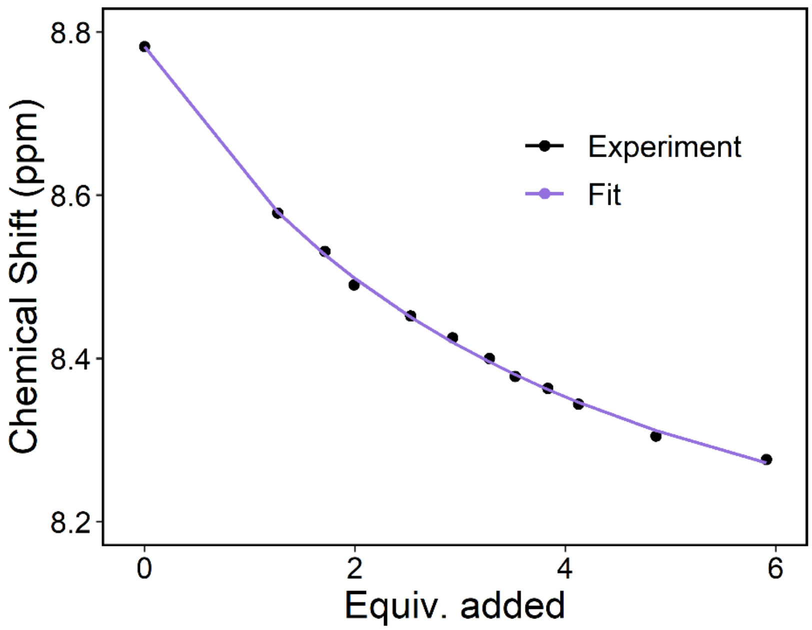


Figure S17. Titration of **2f** into a 10 mM Na_2CO_3, D_2O solution of **1** (1.0 mM). Fit to a 1:1 binding done on supramolecular.org.[8]

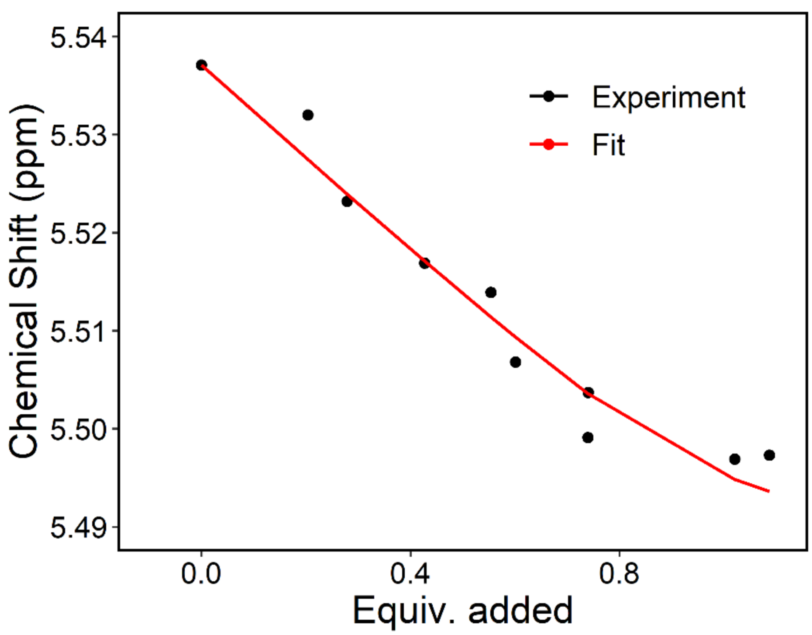


Figure S18. Titration of **2a** into a D_2O solution of **CB[8]•1** (0.5 mM). Fit to a 1:1 binding done on supramolecular.org.[8]

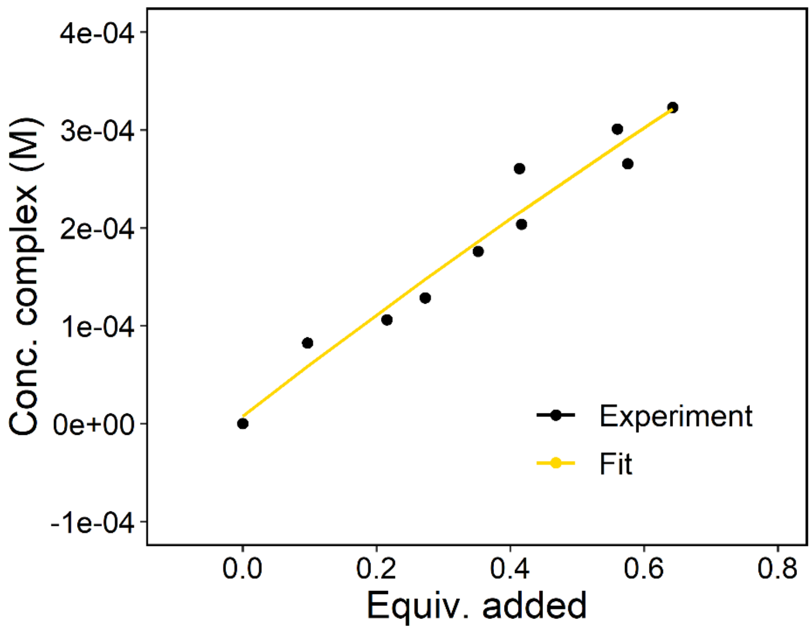


Figure S19. Titration of **2b** into a 10 mM D_2SO_4, D_2O solution of **CB[8]•1** (0.5 mM). Fit to a 1:1 binding done on supramolecular.org.[8]

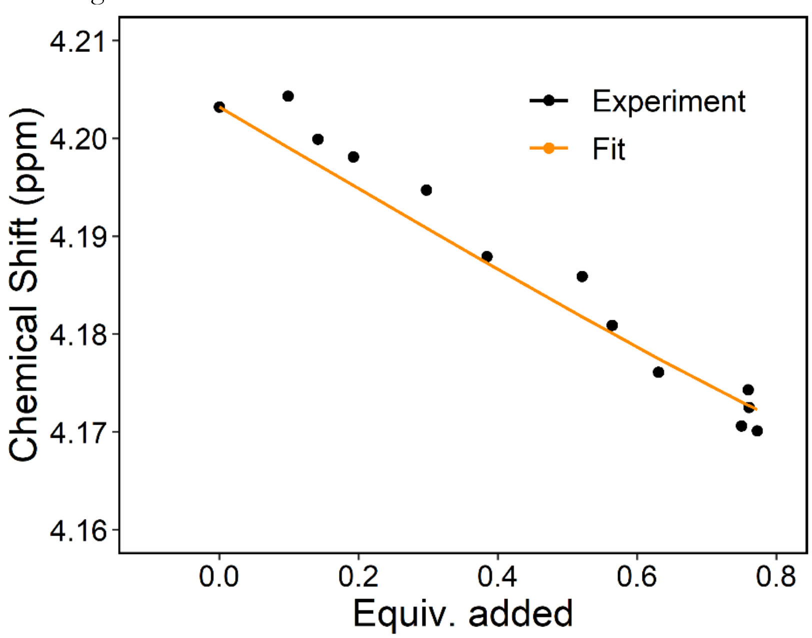


Figure S20. Titration of **2c** into a D_2O solution of **CB[8]•1** (0.5 mM). Fit to a 1:1 binding done on supramolecular.org.[8]

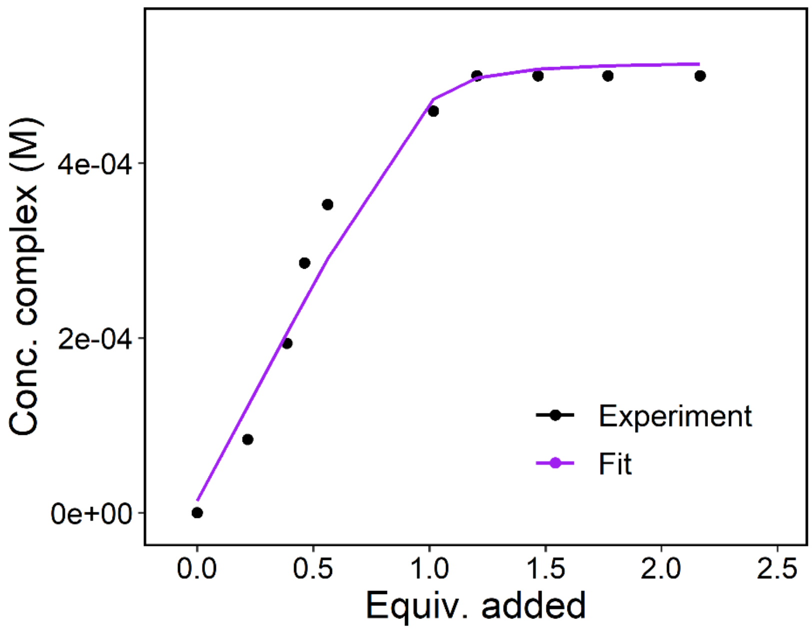


Figure S21. Titration of **2f** into a 10 mM Na_2CO_3, D_2O solution of **CB[8]•1** (0.5 mM). Fit to a 1:1 binding done on supramolecular.org.[8]

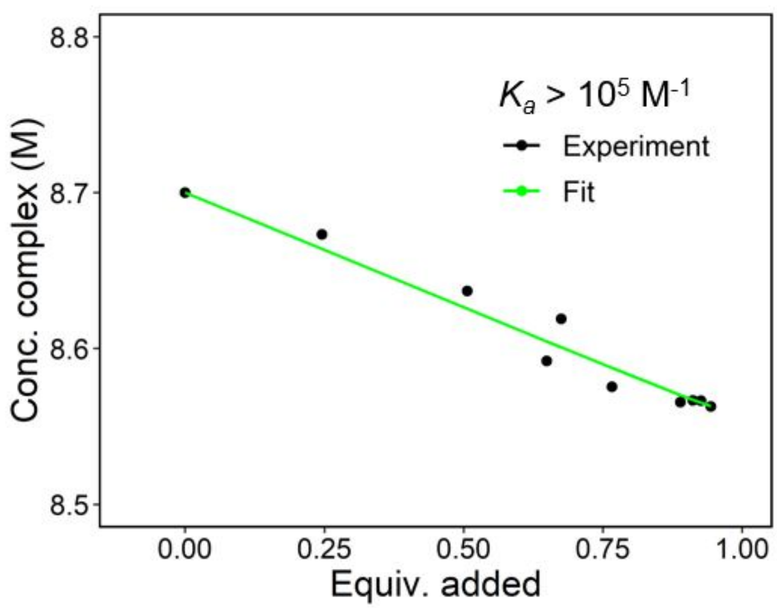


Figure S22. Titration of **CB[8]** into a solution of **3f** in D_2O at 0.5 mM.

VIII. Irradiation experiments

General procedure for irradiation experiments. In general, reaction components were weighed, added to water, then sonicated for 15 min. Reaction solutions were filtered through a Kimwipe inserted into the end of pipette and degassed with nitrogen bubbling for 20 min before being irradiated for 3 days. Since the **CB[8]** contains residual salts from recrystallization, we determined the amount of **CB[8]** to add based on the NMR titrations above. In our initial screenings, we verified the appropriate 1:1:1 stoichiometry using NMR prior to irradiation. All reactions were analyzed using a Agilent 6120 Quadrupole LC/MS.

Rigorous oxygen exclusion. The reaction between **1** and **2f** was set up as usual (see Main Text, Experimental Section), except that prior to irradiation, the reaction solution was subjected to three freeze-pump-thaw cycles under Ar, and the irradiation at 400 nm was conducted under an Ar atmosphere. After three days, the reaction mixture was subjected to LCMS. The relative yield of **3f** and **4** was the same as was observed under the standard conditions, about 7:2, indicating that exogenous oxygen is probably not responsible for the formation of **4**.

Alternative polar solvents. 1 (464 μg), **2f** (318 μg), **CB[8]** (as applicable 2 mg), and triethylamine (as applicable 0.5 μL) were added to either dimethyl sulfoxide, acetonitrile, or nitromethane (all 1 mL). The reaction mixtures were degassed with N_2 sparging before being irradiated by 400 nm LEDs for 3 days before being analyzed by LCMS. The results are summarized in **Table S1.** "Degradation" indicates that no peaks appeared in the LCMS beyond the solvent front.

IX. Table S1: Polar organic solvent screen.

Solvent	**CB[8] Present?**	**Triethylamine present?**	**Result**
Acetonitrile	Yes	No	Degradation
Acetonitrile	No	No	Only **3g** observed
Dimethyl sulfoxide	Yes	No	n.r.
Dimethyl sulfoxide	No	No	n.r.
Nitromethane	Yes	No	Degradation
Nitromethane	No	No	Degradation
Acetonitrile	Yes	Yes	Degradation
Acetonitrile	No	Yes	Only **4** observed
Dimethyl sulfoxide	Yes	Yes	n.r.
Dimethyl sulfoxide	No	Yes	n.r.
Nitromethane	Yes	Yes	Degradation
Nitromethane	No	Yes	Degradation

Table S1. Results of the photoreaction between **1** and **2f** conducted in various polar organic solvents in the prescence or absence of **CB[8]** and/or triethylamine. Results determined by LCMS.

X. Isolation and characterization of product 3f

Product **3f** was isolated by acidification of the reaction solution with a few drops of trifluoroacetic acid (TFA), followed by purification *via* semi-prep HPLC (water/acetonitrile 0.1% TFA). Product-containing fractions were combined and lyophilized to yield pure **3f** (2.1 mg, 25 % yield). The ^{1}H NMR of **3f** is shown in Figure S28. ^{1}H NMR (500 MHz, D2O) δ 8.70 (d, J = 6.3 Hz, 4H), 7.97 (d, J = 6.3 Hz, 4H), 7.91 (d, J = 7.9 Hz, 4H), 7.50 (d, J = 7.9 Hz, 4H), 4.42 (d, J = 9.1 Hz, 2H), 4.35 (s, 6H), 4.10 (d, J = 9.2 Hz, 2H). ^{13}C{^{1}H} NMR (126 MHz, D_2O) δ 162.46, 144.89, 129.48, 129.45, 127.18, 126.13, 124.62, 117.41, 115.10, 51.31, 48.27, 47.20. HRMS (ESI-ToF): *m/z* = +479.1974 (calc'd for [M-H]: +479.1965). Important NOE contacts are provided in Table S3.

XI. Determination of side products

The reaction between **1** and **3f** was set up as usual ("General procedure for irradiation experiments" above) on a 10 mL scale at a 1.5 mM concentration without **CB[8]**. After 10 days of 400 nm irradiation, the crude reaction mixture was subjected to semi-prep HPLC (water/acetonitrile, 0.1% TFA) to isolate the various products. In most cases, an insufficient quantity of material was obtained for ^{13}C NMR, so these assignments should not be considered as robust, synthetically valuable syntheses. However, we are confident in our use of these experiments as aids to mechanistic hypothesis.

4-formylbenzoic acid (4): ^{1}H NMR (500 MHz, D_2O) δ 10.02 (s, 1H), 8.05 – 8.00 (m, 4H). 13C NMR (126 MHz, D2O) δ 214.96, 163.31, 129.59, 129.10, 116.92, 114.61. LRMS (ESI): *m/z* = -149.1 (calc'd for $[M-H]^-$: -149.0)

3g: ^{1}H NMR of major isomer (500 MHz, D_2O) δ 7.58 (d, *J* = 8.3 Hz, 8H), 7.25 (d, *J* = 8.3 Hz, 8H), 3.94 (p, *J* = 6.2 Hz, 8H). LRMS (ESI): *m/z* = -535.1 (calc'd for $[M-H]^-$: -535.1)

3h: LRMS (ESI): *m/z* = 508.2 (calc'd for [M]: 508.2). ^{1}H NMR of this side product was very complicated due to residual impurities and multiple isomers. However, the presence of a complicated set of overlapping doublets is consistent with the assigned structure.

XII. Yield determination by LCMS

After completion of the reaction, a 100 µL aliquot was diluted with 900 µL of a 1.0 mg/mL solution of the internal standard 2,6-ditertbutyl-4-methylphenol in 9:1 acetonitrile/water with 0.1% formic acid. The resulting solution was subjected to LCMS and the relative peak areas of **3f**, **4**, and the internal standard on the 254 nm chromatogram trace were determined. To convert these values to yields, we constructed a calibration curve for **4**. Lacking adequate quantities of **3f** for a calibration curve, we instead subjected a sample prepared as above to ^{1}H NMR to determine the molar ratio of **3f** and the internal standard. This then provided a conversion factor between LCMS peak ratios and molar ratios.

XIII. Transient absorption

The setup for transient absorption (TA) measurements is described elsewhere.[9] For these experiments, the pump was tuned to the desired wavelength for each sample (see Table S2) with an OPA and focused onto the sample. The probe beam was generated using an 800 nm (100 fs) pulse routed through a delay stage and a 3-mm sapphire window to monitor the visible spectral region. The probe wavelength for kinetic analysis was taken from the peak of the excited state absorption. All kinetic traces were fit with mono-exponential decay functions convoluted with an instrument response function of 300 fs. See Table S2 for time constants and wavelengths used for fitting.

Sample	Solvent	λ_{pump} (nm)	λ_{probe} (nm)	Lifetime (ps)
CB[8]•1•2a	H_2O	540	600	<300 fs
CB[8]•1•2c	H_2O	490	550	0.66 ± 0.01
CB[8]•1•2d	0.1 M Na_2CO_3	540	540	<300 fs
1•2e	H_2O	440	490	0.82 ± 0.01
1•2f	0.1 M Na_2CO_3	440	480	32.6 ± 0.6
1•2f	0.1 M Cs_2CO_3	440	480	29.7 ± 0.3
CB[8]•1•2b	0.1 M HCl	450	535	10.0 ± 0.2
CB[8]•1•2e	0.1 M Na_2CO_3	450	490	0.73 ± 0.01
CB[8]•1•2f	0.1 M Na_2CO_3	450	485	42.0 ± 0.4
CB[8]•1•2f	0.1 M Cs_2CO_3	450	485	40.3 ± 0.4

Table S2. Pump and probe wavelengths for samples and time constants extracted from mono-exponential fits to kinetic traces.

XIV. Full Marcus theory treatment

Eq. 1 relates the rate of electron transfer, k_{BET}, to the associated free energy change:

$$k_{\mathrm{BET}} = \frac{k_B T}{h} e^{-\frac{\Delta G^\ddagger}{RT}} \qquad (1)$$

where k_B is Bolzmann's constant, T is temperature, h is Planck's constant, R is the gas constant and $\Delta G^\ddagger$ is the free energy of activation given by Eq. 2.

$$\Delta G^\ddagger = \frac{\lambda}{4}\left(1 + \frac{\Delta G_{\mathrm{BET}}}{\lambda}\right)^2 \qquad (2)$$

In Eq. 2, λ is the reorganization energy and ΔG_{BET} is the free energy change of the back electron transfer. ΔG_{BET} represents a combination of the energy difference between the LUMO of one molecule and the HOMO of the other, ΔE_{CT}, and the Coulombic work associated with charge separation and recombination, w_p and w_r

$$\Delta G_{\text{BET}} = \Delta E_{\text{CT}} + w_p - w_r \qquad (3)$$

The work terms in Eq. 3 are then defined by Coulomb's Law in Eq. 4:

$$w = \frac{e z_A z_B}{4\pi\epsilon_s\epsilon_0 a} \qquad (4)$$

where ϵ_0 is the permittivity of free space, ϵ_s is the dielectric constant of the solvent, and the two molecules have charges z_A and z_B and are separated by distance a.[10]

XV. Computational modeling

All calculations were carried out with the ORCA 4.2.1 program.[11,12] Avogadro was used to visualize orbitals.[13] Ternary complexes were modeled using a B3LYP functional, 6-31G(d) basis set, and a CPCM solvent model in water. [14,15] The ternary complexes are shown in Figure 3a. In all ternary complexes, the potentially reactive double bonds are nearly parallel and well within the 4.2 Å distance of the Schmidt criterion for [2+2] reaction.[16] Geometry optimizations for individual stilbenes were performed using a B3LYP functional, 6-31G(d) basis set, and a CPCM solvent model in water.[14,17–19] We confirmed that all of the computed stilbene structures contained no imaginary frequencies. The stilbene frontier molecular orbital energies are shown in Table S4. To predict BET rates with **1**, we used Eqs. 1-4, which are reproduced here.

$$k_{\text{BET}} = \frac{k_B T}{h} e^{-\frac{\Delta G^{\ddagger}}{RT}} \qquad (1)$$

$$\Delta G^{\ddagger} = \frac{\lambda}{4}\left(1 + \frac{\Delta G_{\text{BET}}}{\lambda}\right)^2 \qquad (2)$$

$$\Delta G_{\text{BET}} = \Delta E_{\text{ET}} + w_p - w_r \qquad (3)$$

$$w = \frac{e z_A z_B}{4\pi\epsilon_s\epsilon_0 a} \qquad (4)$$

where k_B is Bolzmann's constant, T is temperature, h is Planck's constant, R is the gas constant, ϵ_0 is the permittivity of free space, ϵ_s is the dielectric constant of the solvent, $\Delta G^{\ddagger}$ is the free energy of activation, λ is the reorganization energy, ΔG_{BET} is the free energy change of the back electron transfer, ΔE_{ET} is the energy of the charge separated state as measured by UV-Vis, and w_p and w_r are the Coloumbic work terms associated with separation of products or reactants, respectively, of charges z_A and z_B by distance a in solvent of dielectric ϵ_s.[10] We used the DFT-calculated frontier MO energies to determine ΔE_{ET}. We estimated the dielectric within the **CB[8]** cavity to be 10 based on the previously estimated dielectric with cucurbit[7]uril.[20] We estimated the reorganization energy to be 1.6

eV based on measurements of single molecule conductance through **CB[8]**-viologen complexes.[21] Lastly, we estimated the distance between the substrates to be 3.4 Å based on the distance between substrates in the DFT-calculated structures of ternary complexes above. The frontier molecular energies, CT gaps with **1** (i.e. difference between LUMO energy of **1** and HOMO energy of the donor stilbene), and predicted BET rate are shown in Table S4. XYZ coordinates are in Table S5.

XVI. References

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XVII. Figure S23: ^{1}H NMR of diol 5

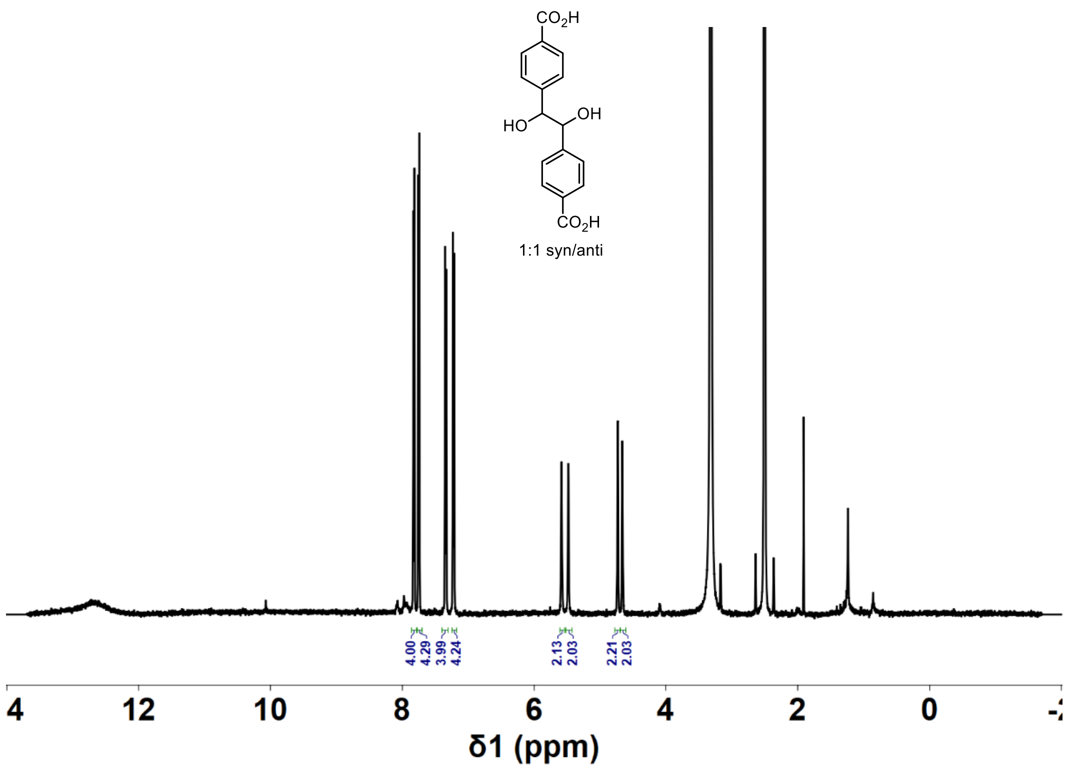


Figure S23. ^{1}H NMR (500 MHz) of **5** in DMSO-d_6 showing 1:1 mixture of *syn* and *anti* diastereomers.

XVIII. Figures S24-S31: NMR and mass spectra for newly synthesized compounds

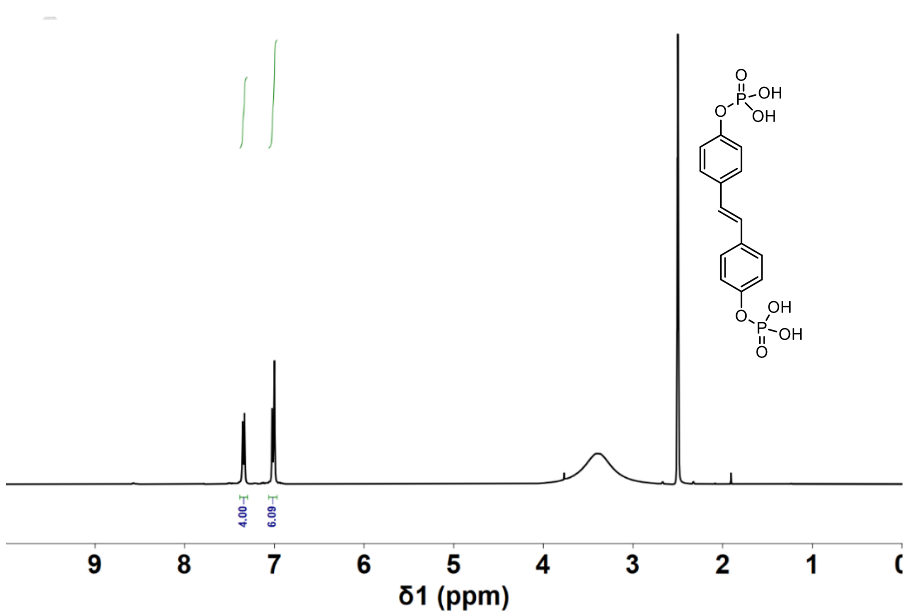


Figure S24. ^{1}H NMR (400 MHz) of **2e** in DMSO-d_6.

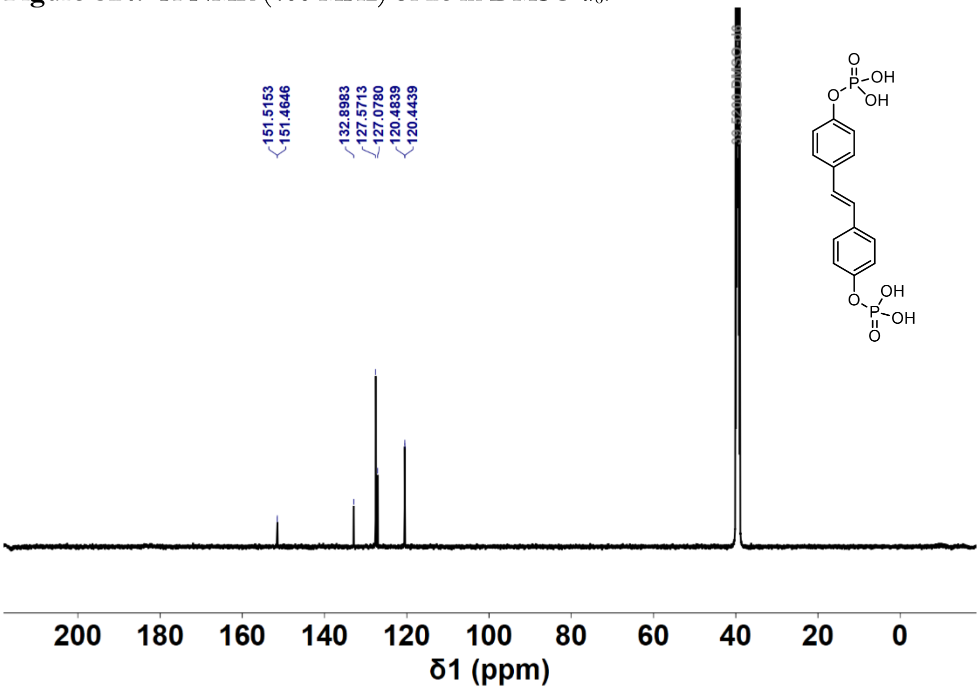


Figure S25. ^{13}C{^{1}H} NMR (126 MHz) of **2e** in DMSO-d_6.

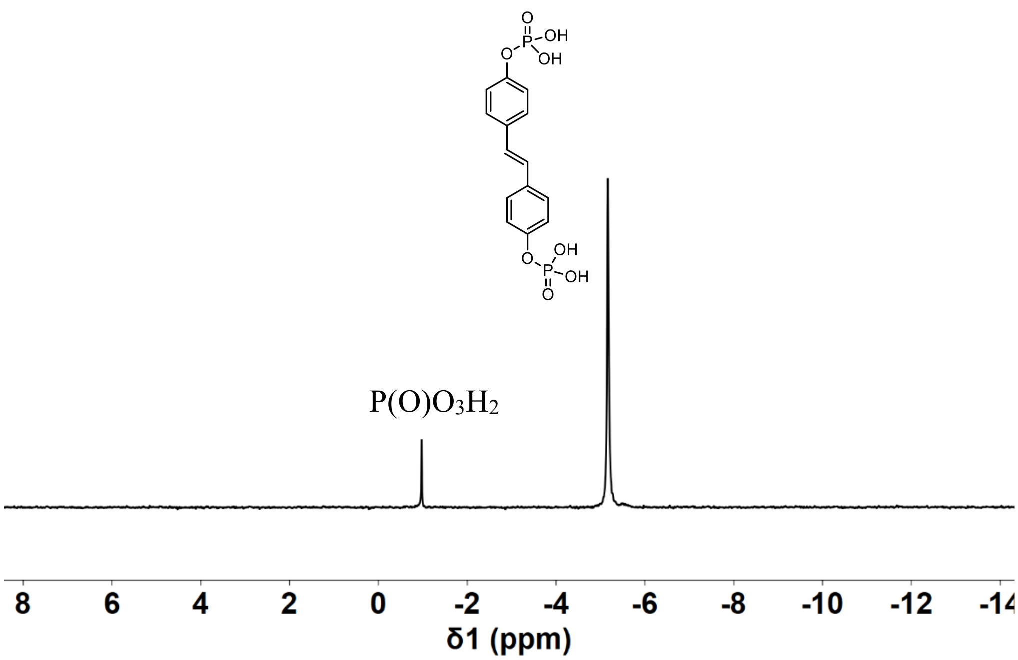


Figure S26. ^{35}P NMR (202 MHz) of **2e** in DMSO-d_6.

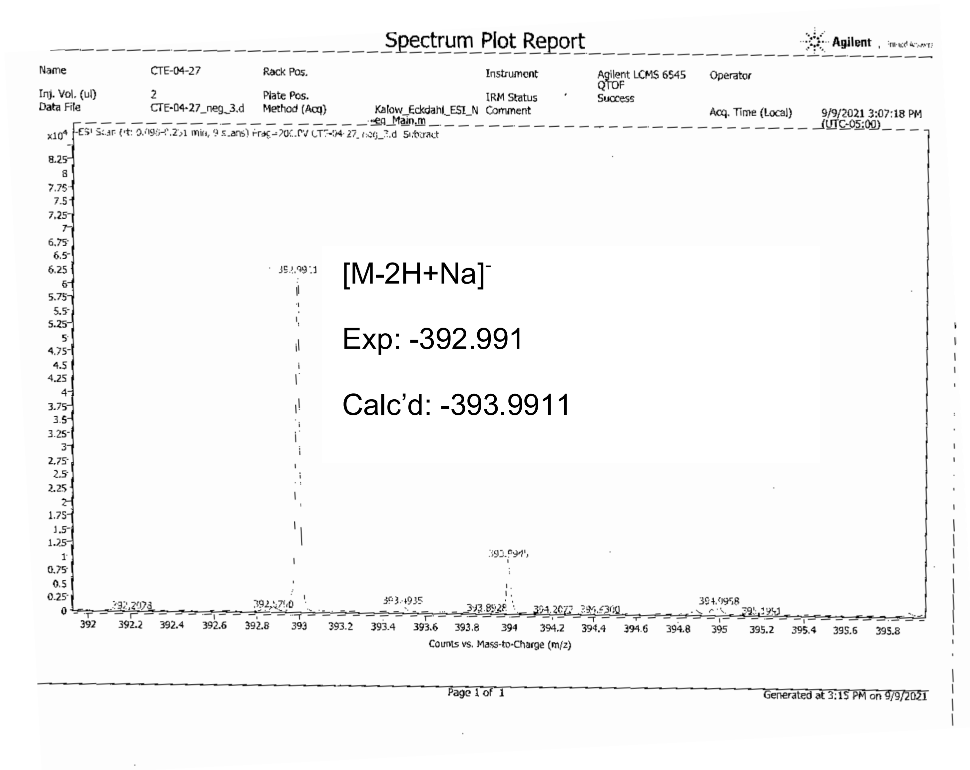


Figure S27. HRMS (ESI, negative) of **2e**.

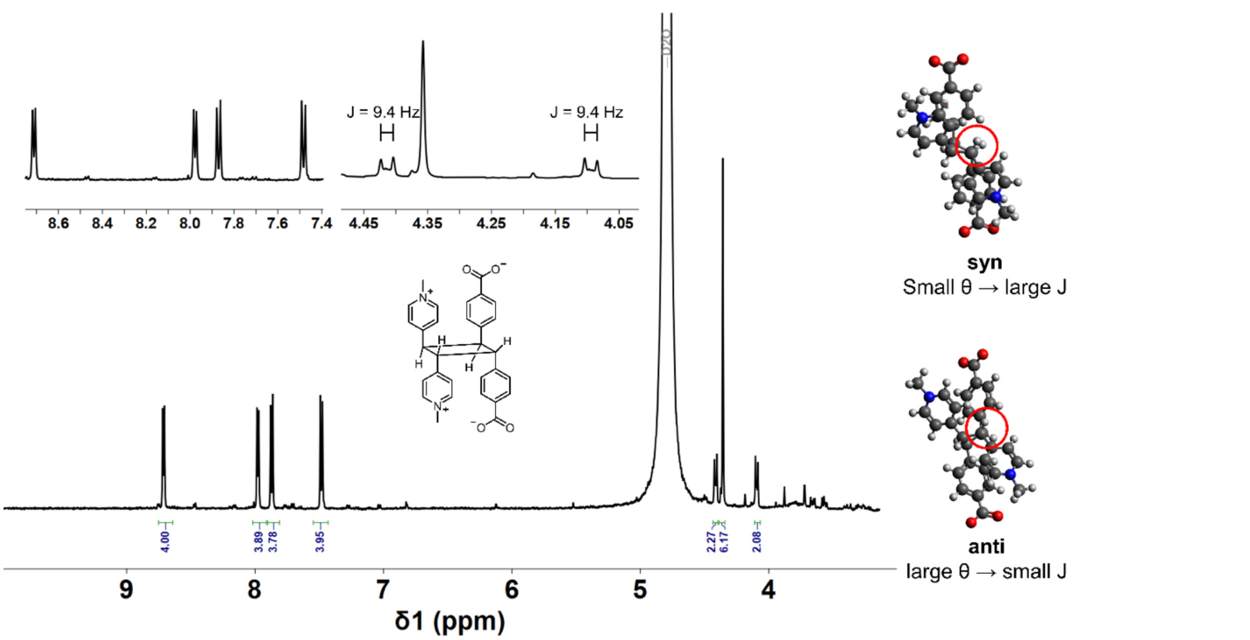


Figure S28. [1]H NMR (500 MHz, D_2O) of the cyclobutane product **3f**. The coupling strength of the cyclobutane protons is large, indicating a small dihedral angle between them and thus supporting the as-drawn syn, as opposed to the anti, structure.

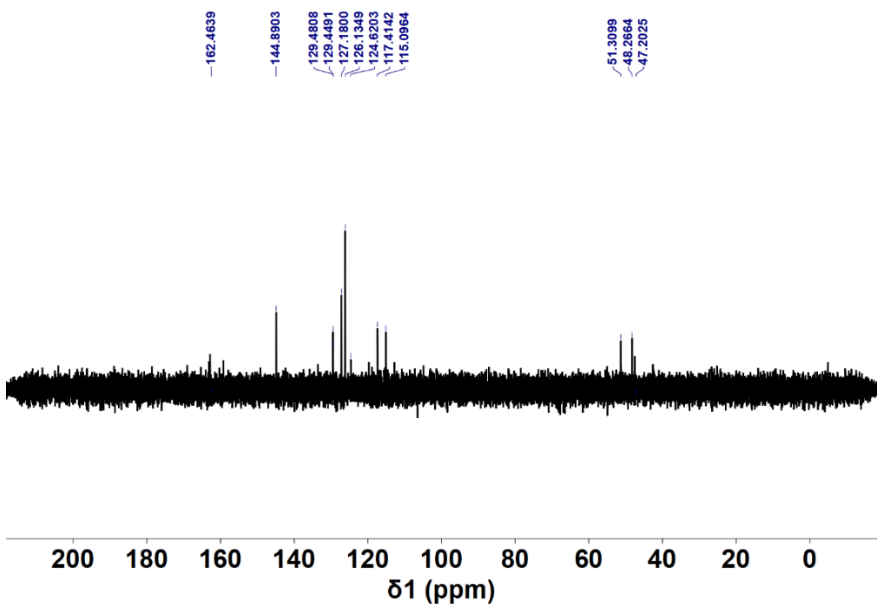


Figure S29. $^{13}C\{^{1}H\}$ NMR (126 MHz, D_2O) of product **3f**.

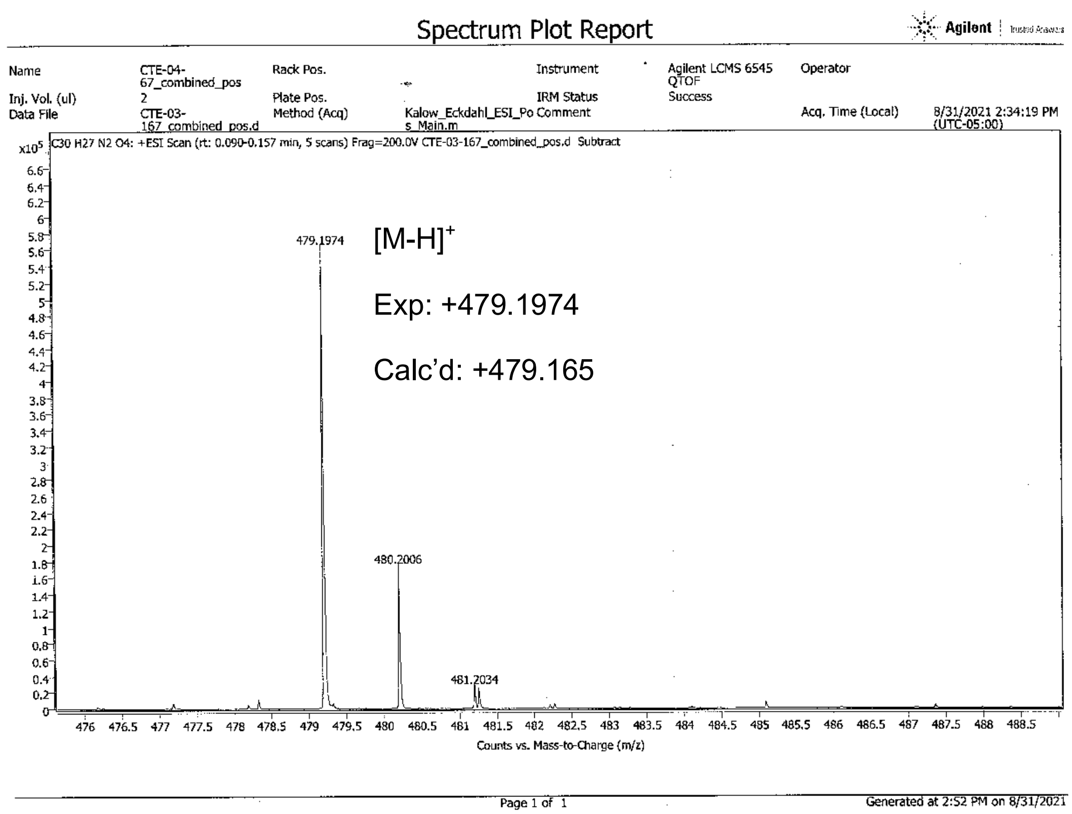


Figure S30. HRMS (ESI, positive) of product **3f**.

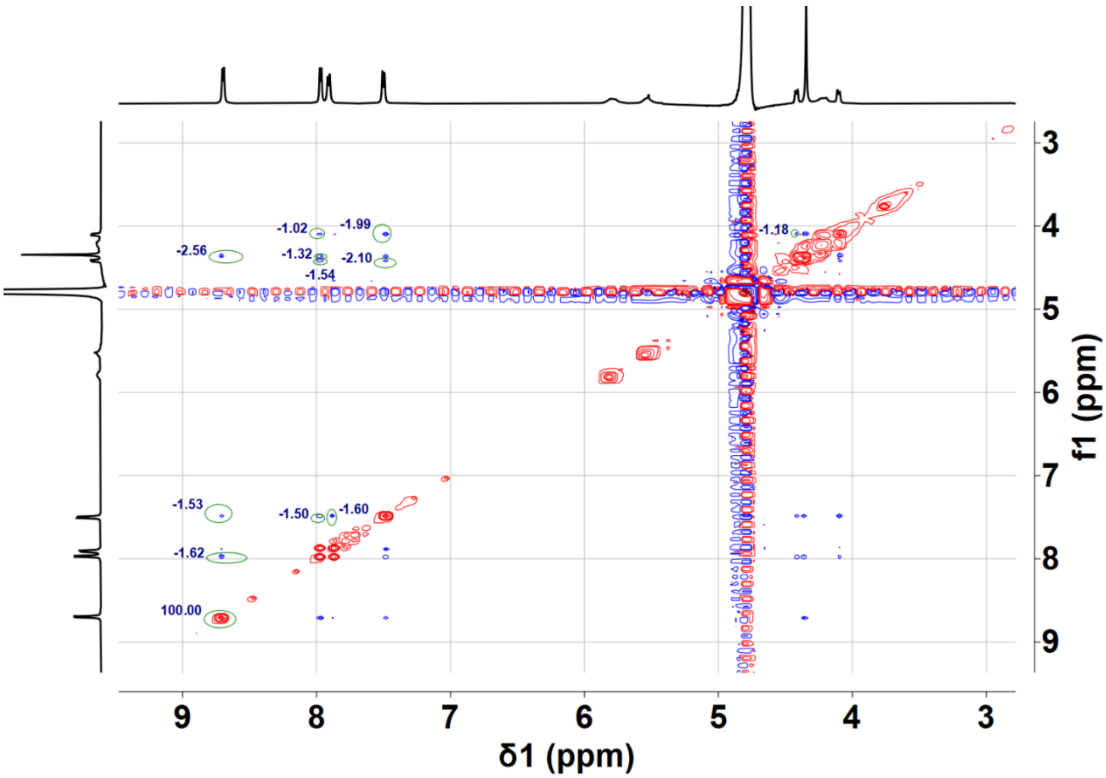
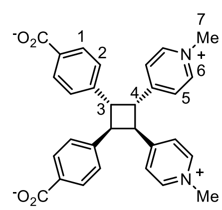


Figure S31. 2D NOESY of **3f**. Measured at 500 MHz in D_2O with a 0.3 s mixing time.

XIX. Table S3: NOE values for product 3f



Protons	NOE value (vs. 100 for diagonal)
1 and 2	-1.60
2 and 5	-1.50
2 and 6	-1.53
2 and 3	-1.99
3 and 4	-1.18
3 and 5	-1.02
4 and 5	-1.54
4 and 6	-2.56
5 and 6	-1.62
5 and 7	-1.32
6 and 7	-2.56

Table S3. NOE values for product **3f**.

XX. Figures S32-S38: NMR and mass spectra of side products

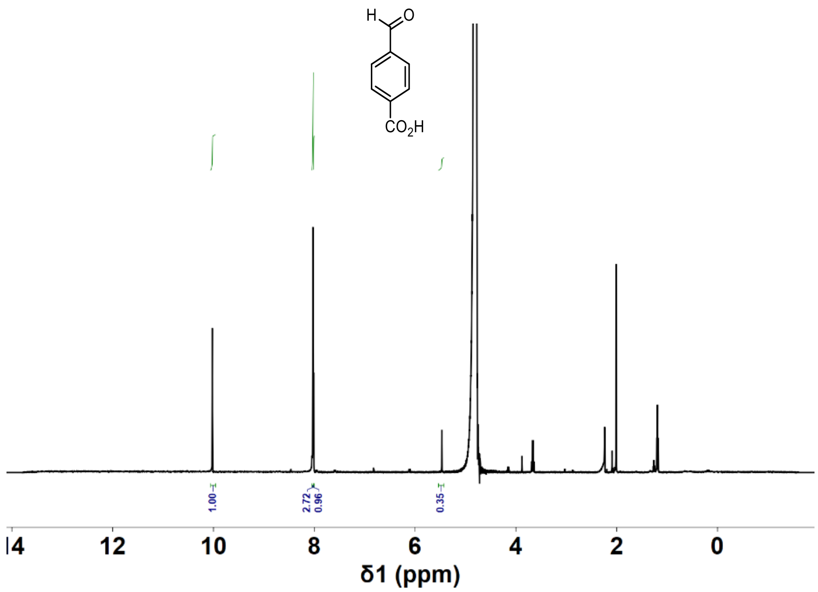


Figure S32. ^{1}H NMR (500 MHz) of **4** in D_2O.

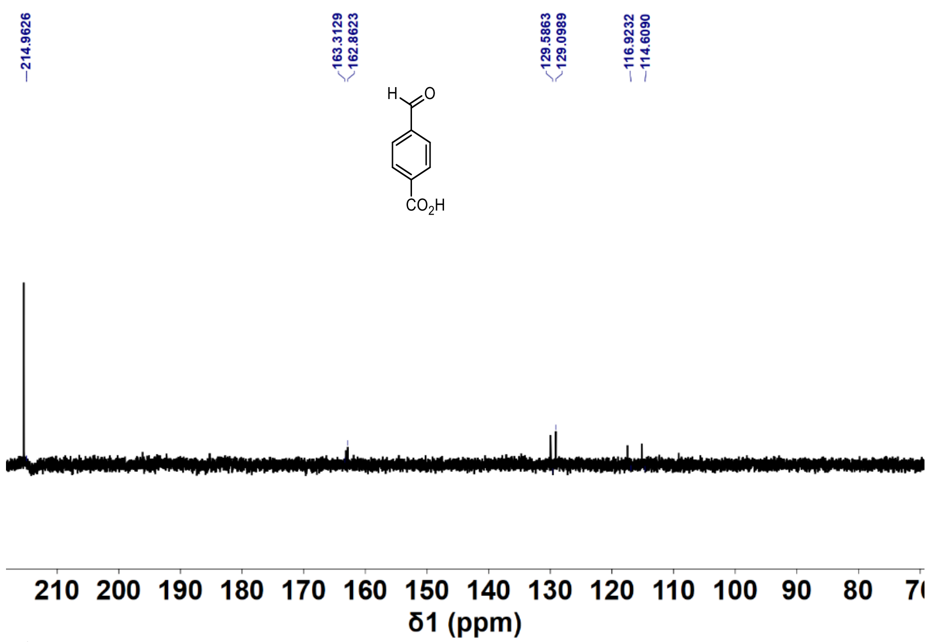


Figure S33. $^{13}C\{^{1}H\}$ NMR (126 MHz) of **4** in D_2O.

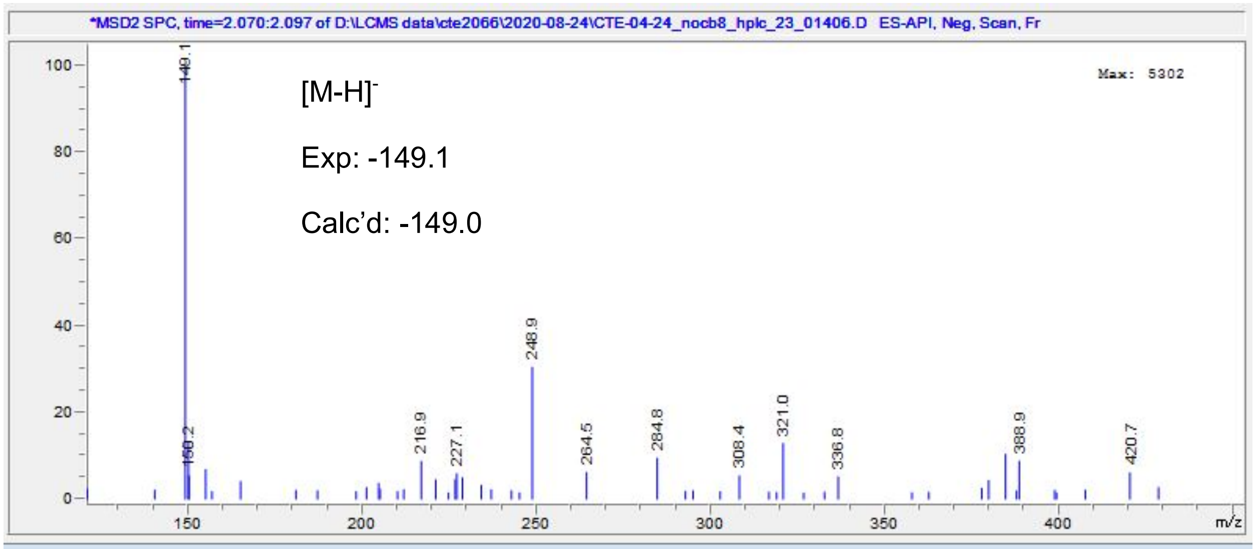


Figure S34. LRMS (ESI, negative) of **4**.

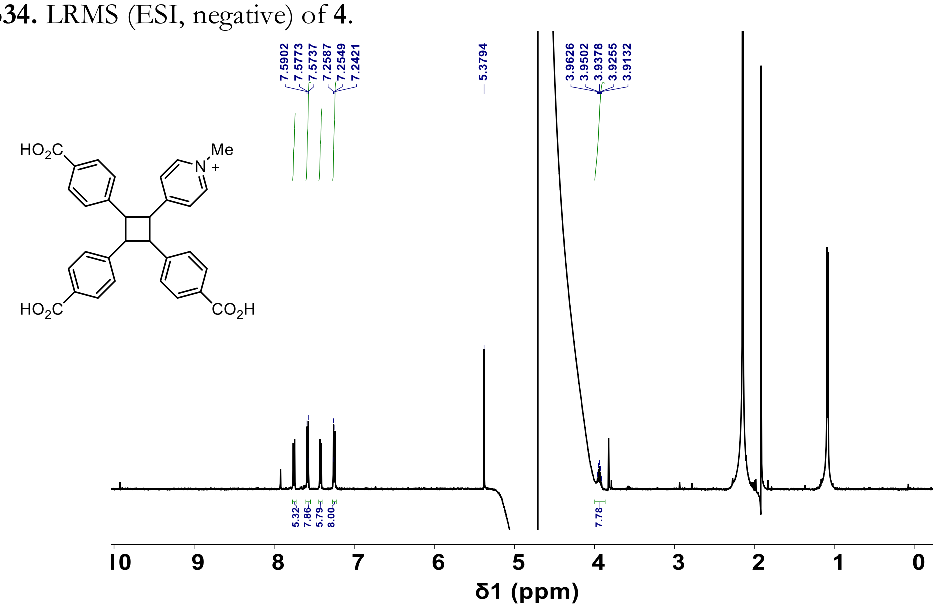


Figure S35. ¹H NMR (500 MHz) of **3g** in D_2O.

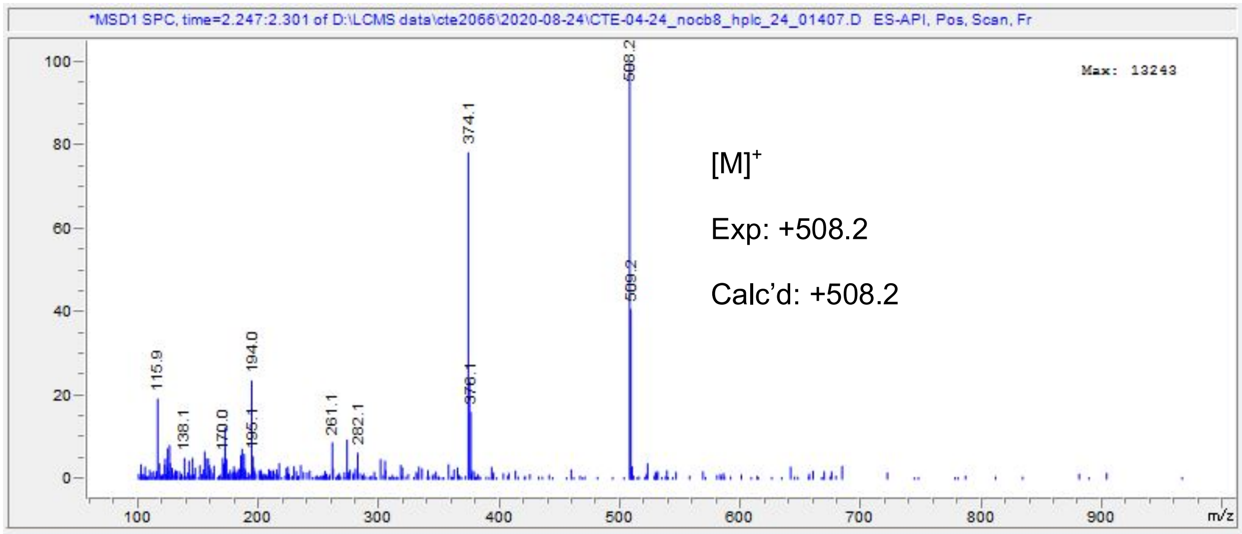


Figure S36. LRMS (ESI, negative) of **3g**.

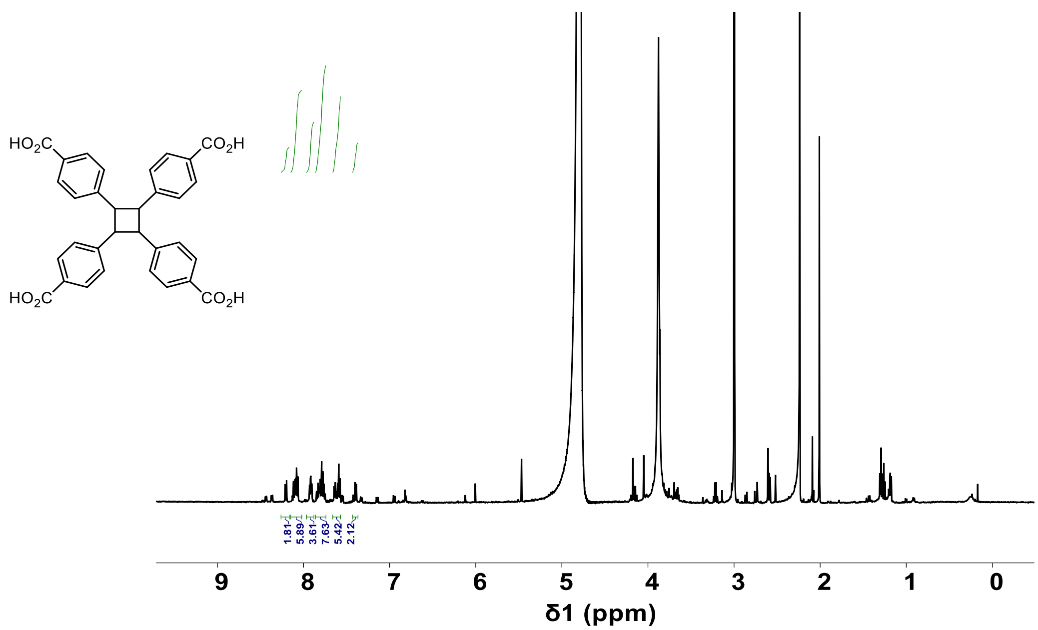


Figure S37. ^{1}H NMR (500 MHz) of **3h** in D_2O.

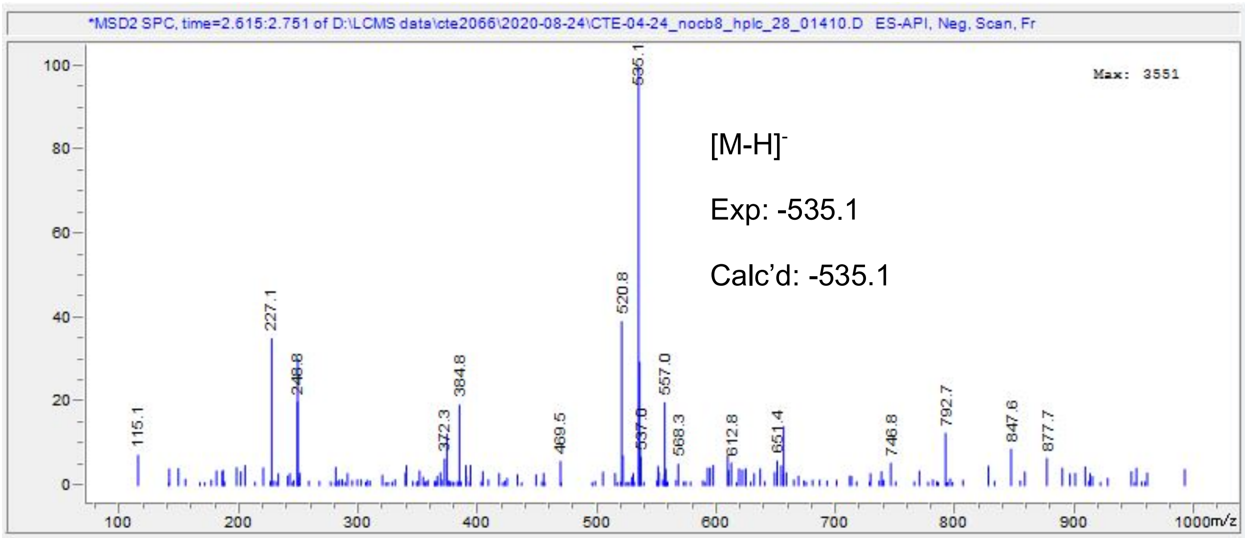
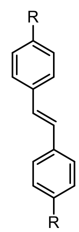


Figure S38. LRMS (ESI, positive) of **3h**.

XXI. Table S4. DFT energies of *para*-substituted stilbenes



R =	HOMO (eV)	CT gap with **1** (eV) (LUMO of **1** = 3.5067 eV)	Calculated BET rate with **1** (s^{-1})
CO_2^-	-5.6531	2.1464	8.3 X 10^{3}
CO_2H	-6.3458	2.8391	2.3 X 10^{5}
OH	-5.3021	1.7954	5.7 X 10^{11}
O^-	-3.9973	0.4906	5.2 X 10^{12}
NH_2	-4.8853	1.3786	4.7 X 10^{12}
NH_3^+	-6.1981	2.6914	3.9 X 10^{11}
N(Me)Me	-4.6683	1.1616	6.1 X 10^{12}
C(O)Me	-6.0625	2.5558	4.7 X 10^{7}
CN	-6.1770	2.6703	6.2 X 10^{6}
Cl	-5.8045	2.2978	2.6 X 10^{9}
OMe	-5.2510	1.7443	8.3 X 10^{11}
Me	-5.5159	2.0092	8.4 X 10^{10}
NO_2	-6.4217	2.9150	4.6 X 10^{4}
SH	-5.3683	1.8616	3.4 X 10^{11}
SMe	-5.2274	1.7207	9.8 X 10^{11}

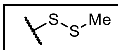
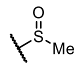
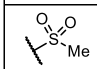
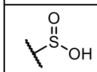
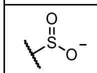
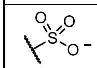
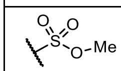
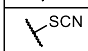
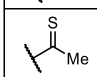
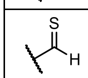
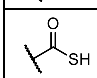
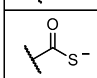
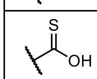
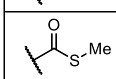
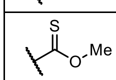
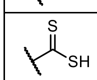
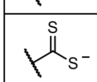
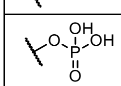
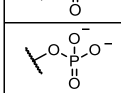
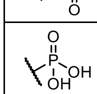
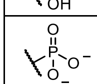
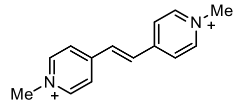
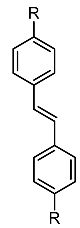
	-5.9357	2.4290	3.7 X 10^8
	-5.9310	2.4243	4.0 X 10^8
	-6.2630	2.7563	1.2 X 10^6
	-6.1307	2.6240	1.4 X 10^7
	-5.4893	1.9826	2.8 X 10^5
	-5.8637	2.3570	55 (yielded an insoluble complex with **1** and **CB[8]**)
	-6.3457	2.8480	1.9 X 10^5
	-6.1533	2.6466	9.5 X 10^6
	-5.9887	2.4820	1.6 X 10^8
	-6.0535	2.5468	5.5 X 10^7
	-6.1609	2.6542	8.3 X 10^6
	-5.4537	1.9470	5.7 X 10^5
	-6.0758	2.5691	3.8 X 10^7
	-6.0704	2.5637	4.1 X 10^7
	-5.9850	2.4783	1.7 X 10^8
	-6.0088	2.5021	1.2 X 10^8
	-5.0777	1.5710	4.4 X 10^8
	-5.8345	2.3278	1.7 X 10^9
	-4.9089	1.4022	7.7 X 10^2
	-6.1194	2.6127	1.8 X 10^7
	-5.2857	1.7790	4.1 X 10^{-2}

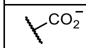
Table S4. DFT-calculated HOMO energies, CT gaps with **1**, and predicted BET rates with **1** of various *para*-substituted symmetric stilbenes.

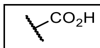
XXII. XYZ-coordinates of DFT-optimized stilbene structures

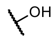


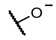
N	-4.82485643474470	3.40424019844862	0.00404089383726
C	-5.94504753192825	2.64770164377947	-0.00423110244284
C	-3.60029436663616	2.81851208028469	-0.00237227468745
C	-5.86495843787266	1.26648577819474	-0.01592684332103
C	-4.61292713969962	0.62356462909991	-0.01865800765770
C	-3.46600058971985	1.44655065478630	-0.01364486432654
C	-4.57078612285339	-0.83774393595581	-0.02272352277701
C	-3.44462401740265	-1.58415053792492	-0.02116946742158
C	-3.40439635619883	-3.04584701928760	-0.01614211466835
C	-4.55001335922354	-3.86621162791873	-0.00788761249744
C	-2.15085464969658	-3.69127288766828	-0.01584229708202
C	-4.41859898017348	-5.24106123984503	0.00353266100300
N	-3.19708891266779	-5.82690293216332	0.00640261513127
C	-2.07388446875490	-5.07002828697301	-0.00458039335966
H	-5.54514557633301	-1.31906781669247	-0.02537477702443
H	-2.47013477793169	-1.10332485465839	-0.01930921673505
H	-5.55174905771456	-3.45503787690194	-0.00796245583224
H	-5.27485273213780	-5.90337429453897	0.01159267831132
H	-1.22956204480159	-3.11909937401218	-0.02313449521275
H	-1.13156400733338	-5.60462551947431	-0.00294938642030
H	-6.89059804504676	3.17516498241413	0.00040114012142
H	-6.78604436834822	0.69410469637074	-0.02121885985438
H	-2.74823103861023	3.48708451343876	0.00429920293244
H	-2.46415947405367	1.03560401117115	-0.01700981005974
C	-4.90977296486187	4.88238888643012	0.02627146979598
H	-5.95727065665554	5.17671498523669	0.01216961722748
H	-4.39802798242454	5.27651299833814	-0.85326863769914
H	-4.42968945812733	5.24699975909425	0.93615445864325
C	-3.06837770842347	-7.30209634134159	0.02395209894661
H	-4.06271288148144	-7.74449496385454	0.03254057623215
H	-2.52055910421871	-7.59569876432600	0.92124187627459
H	-2.52638675392378	-7.61781154355064	-0.86920314937711



R =	XYZ coordinates
	C -4.08096331785862 4.31060938726136 0.00098981382511
	C -5.20289375990829 3.46836707795963 0.00232304927384
	C -2.80570082293412 3.71778600888752 0.00081198770991
	C -5.05457344364221 2.08117993613489 0.00277217033228
	C -3.77813753501274 1.47928955928016 0.00143211660011
	C -2.65258595329295 2.33387139375407 0.00063616834310
	C -3.69125646836266 0.01530641488813 0.00074838573480
	C -2.56148242675625 -0.72834206353731 -0.00283368823086
	H -4.65578984703918 -0.49030217272998 0.00404780406887
	C -2.47482312319440 -2.19234718651465 -0.00298281703838
	H -1.59693667225489 -0.22279815665021 -0.00595056124679
	C -3.60055476212131 -3.04669125758652 -0.00284187297718
	C -1.19851323675466 -2.79450915312991 -0.00265685163806
	C -3.44773466898193 -4.43062262427079 -0.00184688691121
	C -2.17261192598093 -5.02373681982202 -0.00015365201267
	C -1.05048975961904 -4.18174796921113 -0.00100852933702
	H -6.19367003567355 3.91173776096367 0.00274605179049
	H -5.93916515426299 1.44783998529334 0.00359203040899
	H -1.93115675537363 4.36073576549167 0.00133805528455
	H -1.64971614618108 1.91706300457570 0.00032691147241
	H -4.60334178130822 -2.62969140738346 -0.00397302208965
	H -4.32236101520518 -5.07344357557575 -0.00285796376070
	H -0.31378730966065 -2.16134175789218 -0.00292288396601
	H -0.05979363833726 -4.62530886155480 -0.00004326884934
	C -4.23744784325320 5.82731114412580 -0.00087699284891
	O -5.41760801189218 6.29154415711876 -0.00838526663702
	O -3.17659895972995 6.52287244839664 0.00467081013506
	C -2.01669870834810 -6.54050469248459 0.00324400050505
	O -3.07786815014654 -7.23557917417807 -0.00281912569713
	O -0.83675876691324 -7.00524717160997 0.01247402775639

	H	-2.21213783648516	4.17365864730496	0.59630579715640
	O	-0.11243004869788	-8.83847193834671	-0.56882769358758
	H	-5.86416228250069	1.84736502827546	-0.21485181869528
	C	-4.86090377772913	1.44170482311260	-0.13831581966495
	C	-4.64148136895485	0.07522701796226	-0.27501233415578
	H	-5.48489219592777	-0.58437703570729	-0.46013163801115
	O	-3.06676831839164	4.62140387311070	0.50057279623727
	C	-3.78667869114112	2.31419243506337	0.10299546049692
	C	-4.08977912186329	3.76717661041650	0.24943623143028
	C	-3.18171660223154	-1.92125136578079	-0.31608645515245
	C	-3.34432716782099	-0.47231655038848	-0.17371750233454
	C	-2.66243323323553	-6.28478738157863	-0.90036704437643
	C	-1.06792636726493	-8.24292131751687	-1.04381048377582
	C	-2.89801839992607	-4.93179184097238	-0.68985989715336
	C	-1.36058272173544	-6.80653029284193	-0.79370100407688
	C	-1.83901094563784	-4.04998000876873	-0.38392296206265
	C	-2.01893053425999	-2.60452287384223	-0.22288013283216
	H	-4.10577792546922	-2.46061042065080	-0.51369985191478
	C	-0.30315314615400	-5.94976850136396	-0.44712635442450
	C	-0.53908862970310	-4.59171589692633	-0.25506769558370
	H	-3.50682730426537	-6.93040747713198	-1.12489699397919
	H	-3.91369619736223	-4.56208048152924	-0.77852126353642
	C	-2.48832261249409	1.77911710477274	0.19707248650609
	O	-5.21285580839042	4.23332603038947	0.15104616065753
	C	-2.27023990268146	0.41396779083014	0.06050130132039
	H	0.70025731762957	-6.35187110465112	-0.35086013701147
	H	0.29091105751894	-3.93515579481596	-0.00919275835151
	H	-1.10046415871441	-2.05999540550529	-0.01304893945158
	O	-1.91918148344211	-8.92516556775046	-1.84687920485306
	H	-1.62346204653738	2.41351331500649	0.37459445352633
	H	-1.25519831710029	0.03910637394720	0.13724625804064
	H	-2.55159122903057	-8.33322779412276	-2.28574296038660

	C	-3.85606706250975	2.29856151683432	0.21846308623512
	C	-4.92042987450746	1.42807806321435	-0.02861597131820
	C	-4.67126382326943	0.06736113857099	-0.21568472928634
	C	-3.36934527455461	-0.46838692637288	-0.16324380579541
	C	-2.30999516310033	0.43391863607750	0.09401199744603
	C	-2.54631983768388	1.79725982554633	0.28177439874380
	H	-5.94122878621892	1.79628550356365	-0.10247439896013
	H	-5.50776203922027	-0.60089454368840	-0.40756734479043
	H	-1.28406051085668	0.07670295706135	0.14195205268872
	H	-1.71356827019038	2.47099710936253	0.45984192252084
	C	-3.17721253677050	-1.91253753227914	-0.35853952666734
	C	-2.02166370588377	-2.60262314448832	-0.22501651056181
	H	-4.08483123309395	-2.45077360493563	-0.63031719260104
	C	-1.83125156419613	-4.04966341206493	-0.41975875840031
	H	-1.11566643982623	-2.06484310687778	0.05214384459105
	C	-2.88794743537511	-4.95936638941456	-0.62996163762215
	C	-0.52021445598365	-4.57081983038413	-0.41361371169537
	C	-2.65064570591420	-6.32249982036120	-0.81302569610033
	C	-0.26505968778534	-5.92840718590260	-0.62048723398762
	C	-1.33477292034439	-6.80711664533528	-0.83701184234919
	H	-3.91779003850508	-4.61556370912227	-0.64383262295741
	H	-3.48883783993236	-6.99097879789446	-0.98649178812132
	H	0.32265605989946	-3.89584267437443	-0.27927472438738
	H	0.75050304304315	-6.30817570529486	-0.62538443401825
	O	-4.02232744756581	3.64587770146069	0.42063272684292
	H	-4.94108592518707	3.89946187847705	0.24409177568316
	O	-1.04122278067937	-8.12455899704931	-1.06988358217198
	H	-1.85424074378787	-8.65119030432858	-1.07032529295959

	C	-3.86535716501617	2.38540840534144	0.16187798030002
	C	-4.92279886095790	1.44156915423173	-0.04330317943873
	C	-4.67551357512779	0.08020671448110	-0.20951336198945
	C	-3.37007944050201	-0.46399099453180	-0.18193620158464
	C	-2.31404841318547	0.46039853032410	0.01170879635401
	C	-2.54461838518509	1.82143278852541	0.17725269542244
	H	-5.94550998482361	1.81592078359504	-0.06749899788894
	H	-5.51934740732916	-0.59273137718385	-0.36341238688587
	H	-1.28510853364882	0.10532219401926	0.02692092859594
	H	-1.70496899726646	2.50017390635492	0.32065226334438
	C	-3.17720070188726	-1.90447832193328	-0.36651971401703
	C	-2.02107918949778	-2.60779672272444	-0.24794564589351
	H	-4.09077257344210	-2.44972888307988	-0.60936089263896
	C	-1.82563217562213	-4.04781719774198	-0.43197748120275
	H	-1.10851307537119	-2.06214083948247	-0.00232633885133
	C	-2.87730707763661	-4.97038542083463	-0.65632107508067
	C	-0.52204861973284	-4.59380709387669	-0.37096448920351
	C	-2.64470563738242	-6.33211635325565	-0.81324639003425
	C	-0.27281252979134	-5.95591953727150	-0.52777841730102
	C	-1.32629289908198	-6.89896134740287	-0.75613271183275
	H	-3.90438147423659	-4.61301958425307	-0.70495531545243
	H	-3.48109496484945	-7.00884394057757	-0.98266748582226
	H	0.31869280243437	-3.92224993519050	-0.19559158619641
	H	0.74810316223909	-6.33209422196555	-0.47442739353456
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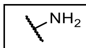
	O	-1.11156266764662	-8.17557235025165	-0.89771773287455

	C	-3.85100664957311	2.33564071969346	0.10523894463047
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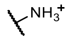	C	-3.82117662801507	2.25124293391957	0.16307976097043
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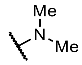	C	-3.96816226794050	2.18620463176381	0.26924347442386
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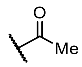	C	-3.89391031968434	2.00055664305440	0.61728833947962
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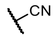	301850535746	1.98777332059518	0.60210021414419
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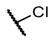	C	-10.32099250145456	-11.68740087355710	0.00358998559773
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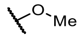	C	-3.73132844927921	1.91490039814776	0.98328305400120
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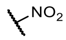	C	-3.60014110740318	1.85984783975706	0.94872111905798
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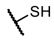	C	-4.11132465982039	4.74545821883876	-0.00772230490064
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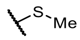	C	-4.32944384159392	4.58576297446412	0.19616800223095
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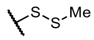	C	-4.16963568938771	1.44525369683948	1.60783829484957
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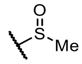	C	-3.81586727897573	3.57007245840820	-0.58911100710711
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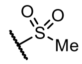	C	-3.76203694011702	1.54045151227577	1.39762034702986
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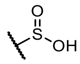	C	-3.76329569371208	3.66289941545300	-0.26579504644634
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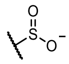	C	-3.35960203197280	1.70333970889196	1.20764424153076
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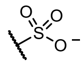	C	-4.00303030718453	3.59375663775312	-0.11562178236560
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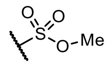	C	-3.86772959340207	0.94752800550952	1.87522734824119
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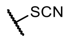	C	-4.11453628734904	3.55658672754338	-0.61670332784731
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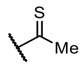	C	-4.03826077789635	3.57666992762053	0.19770135839019
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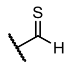	C	-3.96049241018912	3.56963872621335	-0.02362906969967
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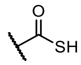	O	-4.79741923185689	5.03188413779200	-1.05757493448392
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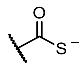	C	-5.28777989917729	3.01451455479881	-2.22203462809862
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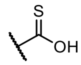	C	-5.28261764578582	2.98922202676692	-2.16356083932676
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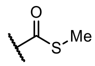	C	-3.69740994547898	3.66138454249629	0.00487814310041
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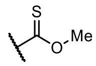	C	-3.89858880698503	3.62260864845501	0.04823608163149
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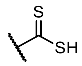	C	-3.79843613212310	3.62279002529220	-0.02504938124576
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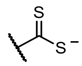	C	-3.74898646472591	3.65046062066144	-0.08036058448700
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	S	-2.54499415247422	6.11105513053314	0.14920056061699
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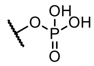	C	-3.53141271350463	3.42148310498401	0.84890841564566
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	H	-1.00988566625557	-0.98319738305620	0.07388822454251
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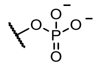	C	-3.23543056309204	3.59366117381685	0.21264249746049
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	H	-3.92158480051164	-5.74582581958754	-0.66809750960360
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	O	-1.93426298958085	-7.20857204612060	-0.01277398708964
	P	-4.55169556928910	6.01264427711258	-0.00519410556904
	O	-5.60991859340524	5.61002252365166	1.03713046430262
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	P	-0.64780167124531	-8.27818088874701	0.47752086179758
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	O	-0.44396352436128	-7.99164838949865	1.97591483893874
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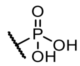	C	-3.55335303412110	3.61413527378825	0.05685155566626
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	H	0.17434451611955	-2.85889428151290	0.51035723267712
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	P	-3.76048981197030	5.39778493635279	0.12389661461490
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	H	-2.10740319683078	6.80808948061827	-0.10418804750413
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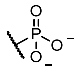	C	-3.55765722750855	3.65209533376224	0.08181765415511
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	O	-0.09081407760307	-7.89301500686847	0.04787932725508
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XXIII. XYZ-coordinates of DFT-optimized ternary complexes

Complex	Coordinates
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	N	-5.048668	-5.274936	-0.558180
	C	-4.673147	-6.172143	0.500308
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	H	1.032162	1.412471	-6.237809
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	H	4.443275	2.317225	4.379965
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	H	-7.018651	-4.800889	0.021839
	H	-5.593700	-6.623445	0.939675
	H	-4.047555	-6.967905	0.047521
	H	-6.233285	-4.791023	-4.535993
	H	-4.589723	-5.546745	-4.343243
	H	-1.803063	-1.833297	-7.390281
	H	-1.113102	-3.105340	-6.288491
	H	3.055360	0.078476	-5.896777
	H	2.933544	-1.417699	-4.878117
	H	6.561431	-0.501781	-2.151019
	H	6.947142	1.275983	-2.222949
	H	7.133273	-2.182978	2.104418
	H	7.651694	-0.900879	3.285529
	H	3.616654	-4.786668	3.657778
	H	3.689187	-4.574669	5.460980
	H	-0.570138	-6.666292	3.135818
	H	-1.428967	-6.507375	4.728189
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	C	-2.474432	4.194297	0.277779
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	C	-2.395663	1.828780	0.897888
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	C	-2.028028	-0.178622	-0.602686

	C	-1.745042	-1.587688	-0.774103
	C	-1.750435	-2.184135	-2.066836
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	C	-1.150232	-4.365203	-1.142535
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	C	-1.400003	-2.429907	0.324755
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	N	-0.833252	-5.694191	-1.312752
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	N	-0.241861	4.898272	3.877951
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	C	0.426403	3.566731	1.996202
	C	0.433770	2.391721	2.799667
	C	0.793020	1.090266	2.290615
	C	0.939229	0.790267	0.958884
	C	1.343961	-0.491709	0.425662
	C	1.247985	-0.740209	-0.971640
	C	1.584376	-1.975958	-1.501469
	N	2.032462	-2.981922	-0.695271
	C	2.165822	-2.780100	0.650773
	C	1.829359	-1.566900	1.225360
	C	2.366592	-4.292447	-1.281338
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	H	0.733525	1.570986	0.210661
	H	0.888588	0.041159	-1.655300
	H	1.492851	-2.217284	-2.570749
	H	2.544239	-3.631379	1.233882
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	H	-1.292476	2.877970	5.046825
	N	-0.734570	4.135817	3.492866
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	H	-1.368680	5.215780	5.181896
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	C	-6.066619	-3.650308	-1.629890
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	N	-5.063353	-1.032589	-3.356719
	C	-4.610219	-1.924638	-4.405750
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	C	-1.269355	-1.642010	-6.088640
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	N	1.645111	0.422713	-5.651654
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	C	4.639299	0.139243	-3.880869
	O	4.835829	-1.047848	-4.125152
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	C	6.115645	-1.039574	-0.186518
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	N	6.110676	-0.867051	1.187978
	C	6.314706	-1.987108	2.087916
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	C	4.432485	-3.351719	2.957163
	O	4.429202	-4.188405	2.055834
	N	3.648298	-3.390401	4.096115

	C	2.960153	-4.600477	4.495476
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	H	-7.046788	-1.650113	-3.206807
	H	-5.458941	-2.268541	-5.008781
	H	-3.887185	-0.869612	-6.241343
	H	-3.343793	2.226292	-4.393518
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	H	0.998514	2.225129	-6.514905
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	H	1.739250	3.883875	-4.879441
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	H	5.798628	2.898376	-3.208118
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	H	-1.551708	-1.797285	-2.074469
	H	-0.813921	-4.143461	-1.881864
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	H	-4.420364	6.578355	0.223009
	H	0.152578	-5.682162	1.245601
	H	-0.002585	-5.894014	-0.404798
	C	1.339575	0.668721	0.346475
	C	1.885438	-0.513103	-0.318690
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	C	3.649387	-3.776220	-2.415009
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	H	2.289433	-1.846409	-3.449893
	H	3.580870	-3.436715	0.170288
	H	2.633846	-1.542169	1.443814
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	N	-6.017946	-2.373605	-1.866234
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	C	-5.108696	-2.326689	-5.089023
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	O	-4.738053	0.766711	-3.399952
	N	-3.920650	-0.288930	-5.314025
	C	-4.086563	-1.547250	-6.002045
	C	-3.283763	0.887524	-5.845715
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	C	0.917696	2.610652	-4.111202
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	O	2.452444	1.272510	5.242273
	N	3.182414	-0.837001	5.922911
	C	4.345898	-1.680919	5.743015
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