

Synthesis, Properties, and Design Principles of Donor-Acceptor Nanohoops

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General Experimental Details:

Moisture sensitive reactions were carried out under an inert atmosphere of nitrogen using standard Schlenk technique. 2,5-dibromopyridine was purchased from Oakwood Scientific. All other starting materials were purchased from TCI America, Alfa Aesar, and Sigma Aldrich.

^1H NMR spectra were recorded at 400 MHz or 500 MHz on a Varian VNMR spectrometer or at 600 MHz on a Bruker Avance-III-HD NMR spectrometer. ^{13}C NMR spectra were recorded at 100 MHz or 125 MHz on a Varian VNMR Spectrometer or at 150 MHz on a Bruker Avance-III-HD NMR spectrometer. Deuterated chloroform (CDCl_3) was used as the NMR solvent for compounds **1-4** and **6-12d** while deuterated dimethyl sulfoxide ($\text{DMSO}-d_6$) was used for compound **5** due to poor solubility. All the compounds and all spectra were referenced to tetramethylsilane (TMS).

Absorbance spectra for **1-5** were obtained using dichloromethane as the solvent in a 1 cm quartz cuvette on an Agilent Cary 60 UV-Vis spectrophotometer. Emission spectra for **1-5** were collected using dichloromethane as the solvent in a 1 cm quartz cuvette using a Horiba Jobin Yvon FluoroMax-4 spectrophotometer.

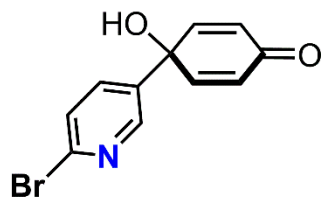
THF, dichloromethane and DMF were dried by filtration through alumina according to the methods described by Grubbs.¹ Silica column chromatography was conducted with Zeochem Zeoprep 60 Eco 40-63 μm silica gel. Thin Layer Chromatography (TLC) was performed using Sorbent Technologies Silica Gel XHT TLC plates. Developed plates were visualized using UV light at wavelengths of 254 and 265 nm. All glassware was oven or flame dried and cooled under an inert atmosphere of nitrogen unless otherwise noted.

Cyclic voltammetry was conducted utilizing a platinum working electrode, platinum counter electrode, and a silver wire pseudoreference that was separated from the solution via a glass frit. Experiments were performed using a custom designed potentiostat at a scan rate of 50 mV/s. Analyte solutions were freeze-pump-thaw degassed three times and all experiments were conducted under airfree conditions. Analyte solutions were prepared using 0.1M tetrabutylammonium tetrafluoroborate in THF, with analyte concentrations 1-5mM. The Ag pseudoreference was calibrated versus the ferrocene/ferrocinium redox couple following the CV of each compound.

Diffraction intensities were collected at 173 (**1**) and 200(2) (**5**) on a Bruker Apex2 CCD diffractometer using an Incoatec $I\mu\text{S}$ micro-focus source with $\text{CuK}\alpha$ radiation, $\lambda = 1.54178 \text{ \AA}$. Space groups were determined based on systematic absences. Absorption corrections were applied by SADABS². Structures were solved by direct methods and Fourier techniques and refined on F^2 using full matrix least-squares procedures. All non-H atoms were refined with anisotropic thermal parameters. H atoms in both structures were refined in calculated positions in a rigid group model. Crystals of **1** were very small and even with using a strong Incoatec Cu $I\mu\text{S}$ micro-focus source provided non-zero reflections only up to $2\theta_{\text{max}} = 106.6^\circ$. Only such reflections were involved in the final refinement. The molecule of **1** has C_2 symmetry. The structure of **1** has additionally solvent molecule Me_2SO located inside the main molecule. It was found that the crystal structure of **5** has six solvent CHCl_3 molecules. One of them is located inside the cation and others fill out empty spaces in the crystal packing. Four of these molecules are highly disordered and were treated by SQUEEZE³. The correction of the X-ray data by SQUEEZE is 938 electron/cell; the required value is 928 electron/cell for 16 solvent molecules CHCl_3 in the full unit cell. All calculations were performed by the SHELXL-2013 packages⁴.

Compounds **7a**, **7b**, **8a**, **8b**, **9a**, **10a**, **11a**, **12a**, and **[8]CPP** were prepared in accordance with Jasti *et. al.* All spectra matched previously reported.

Experimental Details

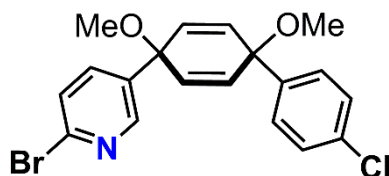


7c

nButyllithium (2.50 M in hexanes , 45.0 mL, 112 mmol, 1.15 eq) was diluted into a flask of THF (550 mL) and cooled to $-78\text{ }^{\circ}\text{C}$. This solution was allowed to cool for another 30 minutes with stirring.³ To this solution was added dropwise a solution of 2,5-dibromopyridine (25.0 g, 107 mmol, 1.10 eq) in THF (100 mL). The reaction was stirred for 30 minutes at $-78\text{ }^{\circ}\text{C}$ to give the lithiated species as a deep red solution.

In a separate flask, 4,4-dimethoxycyclohexa-2,5-dienone **6** (15.0 g, 97.4 mmol, 1.00 eq) was dissolved in THF (200 mL) and cooled to $-78\text{ }^{\circ}\text{C}$. To this was added the solution of lithiated 2-bromo-pyridine dropwise by cannula. The reaction was stirred for 3 hours at $-78\text{ }^{\circ}\text{C}$ after completion of the transfer. After 3 hours, the reaction was quenched with MeOH and allowed to warm to room temperature. The mixture was extracted with ether. After separation of the phases, the aqueous layer was washed with ether (3 x 200 mL). The combined organic layers were washed with brine and dried over sodium sulfate before being filtered and concentrated down to a yellowish-brown semi-solid. The solid was carried on crude.

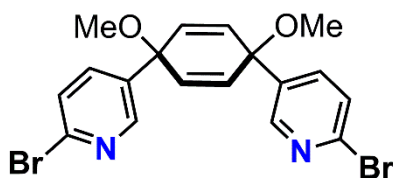
The solid from above was dissolved in acetone (250 mL). An equal volume of 10% AcOH (250 mL) was added. The solution was stirred at room temperature for 4 hours. The acetone was removed by rotary evaporation. The remaining aqueous layer was extracted with dichloromethane (3 x 100 mL). The combined organic layers were washed with brine and dried over sodium sulfate before being concentrated down to a brown solid. The solid was then purified by recrystallization with absolute ethanol to yield a pale tan solid (10.7 g, 42% yield). mp $145\text{--}147\text{ }^{\circ}\text{C}$. ^1H NMR (400 MHz, CDCl_3): δ 6.30 (d, $J = 10\text{ Hz}$, 2H), 6.85 (d, $J = 10\text{ Hz}$, 2H), 7.50 (d, $J = 8.4\text{ Hz}$, 1H), 7.61 (dd, $J = 8.4\text{ Hz}$, 2.8 Hz, 1H), 8.50 (d, $J = 2.8\text{ Hz}$, 1 H); ^{13}C NMR (125 MHz, CDCl_3): δ 185.14, 149.62, 148.10, 142.38, 136.35, 134.58, 128.44, 127.98, 69.82; HRMS (Q-TOF, ES+) (m/z): $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{11}\text{H}_8\text{BrNO}_2$, 265.9817; found: 265.9722. IR (neat): 3396, 3097, 3067, 3045, 2964, 1662, 1616, 1441, 1388, 1237, 1175, 1093, 1016, 921, 861 cm^{-1} .



8c

To a solution of 4-bromo-1-chlorobenzene (14.9 g, 77.8 mmol, 2.40 eq) in THF (225 mL) at -78°C . Was added nBuLi (2.5 M in hexanes, 31.0 mL, 77.5 mmol, 2.00 eq). The solution was stirred for 30 minutes at -78°C and generated a cloudy white suspension.

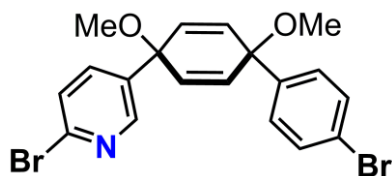
In a separate flask, NaH (1.60 g, 60% suspension in mineral oil, 40.0 mmol, 1.20 eq) was suspended in THF (150 mL) and cooled to -78°C . Pyridyl quinol **7c** (9.10 g, 34.3 mmol, 1.00 eq) was dissolved in THF (50 mL) and added drop wise via cannula to the NaH suspension. The mixture was stirred for 2 hours at -78°C . At this time, lithiated chlorobenzene was transferred dropwise via cannula into the NaH/Quinol mixture. The reaction was stirred for 3 hours at -78°C , during which the reaction turned a yellow-brown color. Next, MeI (10.6 mL, 170 mmol, 5.00 eq) and DMF (75 mL) were added and the reaction was allowed to warm to room temperature and stir for 18 hours. Water (100 mL) and ether (250 mL) were added and the phases allowed to separate. The aqueous layer was washed with ether (3 X 250 mL). The combined organic phases were washed with brine before being dried over sodium sulfate. Solvent was removed under reduced pressure to give a brown solid. The crude material was purified by washing with hexanes and recrystallization from hot ethanol (7.00 g, 51%) mp $107\text{--}109^{\circ}\text{C}$. ^1H NMR (500 MHz, CDCl_3): δ 3.41 (s, 3H), 3.42 (s, 3H), 6.03 (d, $J = 8$ Hz, 2H), 6.17 (d, $J = 8$ Hz, 2H), 7.30 (bs, 4H), 7.41 (d, $J = 8.4$ Hz, 1H), 7.53 (dd, $J = 8.4, 2.6$ Hz, 1H), 8.31 (d, $J = 2.6$ Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3): δ 148.63, 141.64, 141.54, 138.77, 136.67, 134.53, 134.08, 132.80, 129.08, 127.95, 127.50, 74.38, 73.52, 52.40, 52.28. HRMS (Q-TOF, ES+) (m/z): $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{19}\text{H}_{17}\text{BrClNO}_2$, 406.0208; found 406.0208. IR (neat): 2992, 2924, 2854, 2820, 1572, 1486, 1449, 1398, 1361, 1171, 1070, 1015, 947, 832, 732 cm^{-1} .



8d

nButyllithium (2.5 M in hexanes, 1.79 mL, 4.48 mmol, 2.40 eq) was diluted in THF (25 mL) at -78°C . This solution was allowed to cool for another 30 minutes with stirring.³ To this was added via cannula a solution of 2,5-dibromopyridine (1.10 g, 4.48 mmol, 2.40 eq) in THF (5 mL). The deep red solution was stirred for 30 minutes at -78°C .

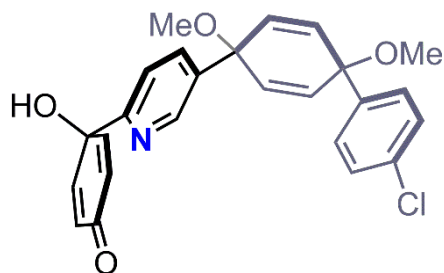
In a separate flask, NaH (100 g, 2.26 mmol, 1.20 eq) was suspended in THF (7 mL) and cooled to -78°C . Quinol **7c** (0.500 g, 1.87 mmol, 1.00 eq) was dissolved in THF (5 mL), and transferred into the NaH solution by cannula. After stirring at -78°C for 2 hours, the lithiated 2-bromopyridine was transferred by cannula to this solution. The reaction was stirred for 3 hours at -78°C . After this time, methyl iodide (0.700 mL, 11.2 mmol, 6.00 eq) and DMF (15 mL) were added. The flask was raised out of the bath and allowed to warm to room temperature over 20 hours. Water (50 mL) and ether (50 mL) were added and the phases allowed to separate. The aqueous layer was washed with ether (3 X 100 mL). The combined organic phases were washed with brine before being dried over sodium sulfate. Solvent was removed under reduced pressure to give a brown solid. The crude material was re-crystallized with hot ethanol yielding a light tan solid (0.350 g, 43%) mp $197\text{--}198^{\circ}\text{C}$. ^1H NMR (400 MHz, CDCl_3): δ 3.42 (s, 6H), 6.13 (s, 4H), 7.44 (d, $J = 8.2$ Hz, 2H), 7.51 (dd, $J = 8.2$ Hz, 2.2 Hz, 2H), 8.35 (d, $J = 2.2$ Hz, 2H); ^{13}C NMR (125 MHz, CDCl_3): δ 148.47, 141.84, 138.35, 136.45, 133.73, 128.17, 73.29, 52.41. HRMS (Q-TOF, ES+) (m/z): $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{18}\text{H}_{16}\text{Br}_2\text{N}_2\text{O}_2$, 450.9657; found, 450.9650. IR (neat): 3063, 3008, 2994, 2938, 2896, 2822, 1574, 1556, 1446, 1403, 1359, 1289, 1276, 1233, 1180, 1080, 1054, 1025, 1008, 952, 901, 833 cm^{-1} .



8e

To a solution of 1,4-dibromobenzene (10.5 g, 44.5 mmol, 2.40 eq) in THF (225 mL) at $-78\text{ }^{\circ}\text{C}$ was added nBuLi (2.5 M in hexanes, 19 mL, 46.3 mmol, 2.50 eq). The solution was stirred for 30 minutes at $-78\text{ }^{\circ}\text{C}$ and generated a cloudy white suspension.

In a separate flask, NaH (0.890 g, 60% suspension in mineral oil, 22.3 mmol, 1.20 eq) was suspended in THF (80 mL) and cooled to $-78\text{ }^{\circ}\text{C}$. Pyridyl quinol **7c** (5.00 g, 18.5 mmol, 1.00 eq) was dissolved in THF (15 mL) and added drop wise via cannula to the NaH suspension. The mixture was stirred for 2 hours at $-78\text{ }^{\circ}\text{C}$. At this time, lithiated bromobenzene was transferred dropwise via cannula into the NaH/Ketone mixture. The reaction was stirred for 3 hours at $-78\text{ }^{\circ}\text{C}$, during which the reaction turned a yellowy-brown color. Next, MeI (5.76 mL, 92.5 mmol, 5.00 eq) and DMF (45 mL) were added and the reaction was allowed to warm to room temperature and stir for 18 hours. Water (100 mL) and ether (250 mL) were added and the phases allowed to separate. The aqueous layer was washed with ether (3 X 100 mL). The combined organic phases were washed with brine before being dried over sodium sulfate. Solvent was removed under reduced pressure to give a brown solid. The crude material was purified by column chromatography (silica gel, 30% Ethyl Acetate in Hexanes eluent) to recover a pale yellow solid which was then recrystallized from hot ethanol to give a light tan solid (4.20 g, 50%) mp $124\text{--}125\text{ }^{\circ}\text{C}$. ^1H NMR (500 MHz, CDCl_3): δ 3.40 (s, 3H), 3.42 (s, 3H), 6.03 (d, $J = 10\text{ Hz}$, 2H), 6.16 (d, $J = 10\text{ Hz}$, 2H), 7.24 (d, $J = 8.8\text{ Hz}$, 2H), 7.41 (d, $J = 9.3\text{ Hz}$, 1H), 7.46 (d, $J = 8.8\text{ Hz}$, 2H) 7.54 (dd, $J = 9.3, 3\text{ Hz}$, 1H), 8.31 (d, $J = 3\text{ Hz}$, 1H). ^{13}C NMR (125 MHz, CDCl_3): δ 148.75, 141.75, 141.67, 138.89, 136.79, 134.65, 134.22, 132.92, 129.21, 128.08, 127.62, 74.51, 73.65, 52.52, 52.40. HRMS (Q-TOF, ES+) (m/z): $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{19}\text{H}_{17}\text{Br}_2\text{NO}_2$, 449.9704 found 449.9720. IR: 2973, 2939, 2894, 2818, 1570, 1554, 1482, 1447, 1393, 1360, 1288, 1175, 1065, 1029, 1018, 1004, 992, 946, 836 cm^{-1}



9b

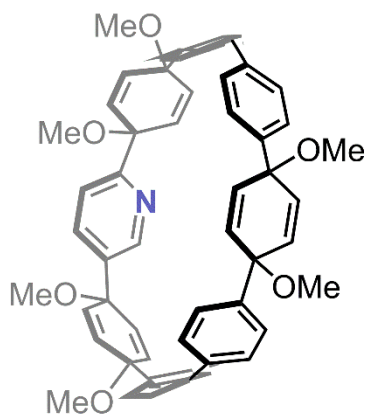
8e (5.80 g, 14.3 mmol, 1.00 eq) was added to a dry flask and dissolved in dry THF (200 mL). The solution was cooled to -78°C . $n\text{BuLi}$ (2.5 M in hexanes, 6.30 mL, 15.7 mmol, 1.10 eq) was added dropwise over 5 minutes resulting in a deep reddish-purple solution. After stirring at -78°C for 10 minutes, 4,4-dimethoxycyclohexa-2,5-dienone **6** (2.80 g, 18.5 mmol, 1.30 eq) was added neat. The solution then turned yellow-orange. The reaction was stirred for 1 hour before being quenched with H_2O . The aqueous layer was then washed with diethyl ether (3 X 100 mL). The combined organic layers were washed with brine and dried over Na_2SO_4 , and concentrated down to a yellow oil. The oil was dissolved in acetone (50 mL) and 5% $\text{AcOH}/\text{H}_2\text{O}$ was added (50 mL). The solution was stirred at room temperature for 2 hours. The solution was neutralized with sodium bicarbonate and extracted with diethyl ether (3 X 100 mL). The combined organic layers were washed with brine and dried over Na_2SO_4 . The solution was concentrated under reduced pressure to yield a yellow solid. The solid was purified by column chromatography to give a light tan solid (silica gel, 30% EtOAc/DCM eluent), (4.00 g, 65%). mp $156\text{--}159^{\circ}\text{C}$. ^1H NMR (400 MHz, CDCl_3): δ 3.42 (s, 3H), 3.45 (s, 3H), 6.05 (d, $J = 11$ Hz, 2H), 6.20 (d, $J = 11$ Hz, 2H), 6.28 (d, $J = 10.2$ Hz, 2H), 6.75 (d, $J = 10.2$ Hz, 2H), 7.20 (d, $J = 8.4$ Hz, 1H), 7.32 (s, 4H), 7.69 (dd, $J = 8.4, 1.6$ Hz, 1H), 8.56 (d, $J = 1.6$ Hz, 1H). ^{13}C NMR (100 MHz, CDCl_3): δ 185.86, 154.71, 150.75, 146.40, 141.62, 139.70, 135.93, 134.53, 134.05, 132.81, 129.00, 128.20, 127.40, 120.40, 74.27, 73.58, 70.97, 52.36, 52.27. HRMS (Q-TOF, ES+) (m/z) calculated for $\text{C}_{25}\text{H}_{22}\text{ClNO}_4$: 436.1316; found, 436.1303. IR: 2938, 2902, 2820, 2106, 1667, 1627, 1481, 1401, 1075, 954, 857, 726 cm^{-1} .



8

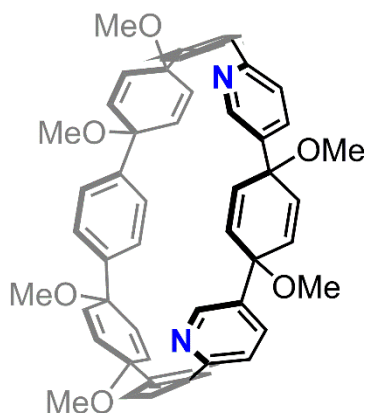


9



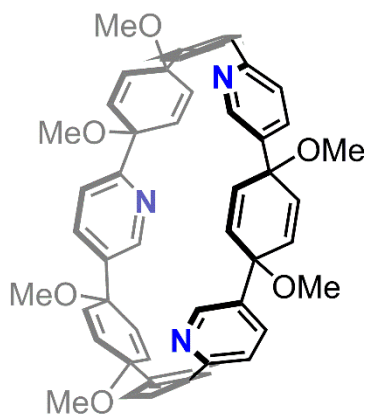
12b

Dibromide **8a** (0.585 g, 1.30 mmol, 1.00 eq), diboronate **11b** (1.00 g, 1.30 mmol, 1.00 eq), $n\text{Bu}_4\text{Br}$ (0.084 g, 0.260 mmol, 0.200 eq) and $\text{Pd}(\text{PPh}_3)_4$ (0.150 g, 0.130 mmol, 0.100 eq,) NaHCO_3 (1.10 g, 13.0 mmol, 10.0 eq) were charged to a dried flask, which was then purged with argon. Degassed toluene (225 mL), methanol (25 mL), and water 13 mL (to make base 1 M) were added. The mixture was heated to 90 °C and stirred for 24 hours. The reaction was cooled to room temperature and washed with water. The organic layer was washed with brine and dried over sodium sulfate. The organic layer was concentrated down under reduced pressure to a yellow solid. The solid was purified by column chromatography (silica gel, 30% ethyl acetate in DCM eluent) to recover a white solid. Material was further purified by washes with cold ethyl acetate (0.257 mg, 25%) mp 285 °C dec. ^1H NMR (500 MHz, CDCl_3): δ 3.40-3.48 (m, 18H), 6.02-6.17 (m, 8H), 6.22 (d, J = 10 Hz, 2H), 6.32 (d, J = 10.0 Hz, 2H), 7.13 (d, J = 8.6 Hz, 2H), 7.39 (d, J = 8.6 Hz, 2H), 7.50 (m, 12H), 7.93 (m, 2H), 8.26 (m, 1H). ^{13}C NMR (125 MHz, CDCl_3): δ 52.11, 52.39, 52.41, 52.43, 52.50, 74.29, 74.41, 74.92, 75.01, 76.13, 119.73, 126.49, 126.52, 126.53, 127.04, 127.13, 132.91, 133.06, 133.10, 133.61, 133.87, 134.65, 135.18, 135.83, 143.10, 143.58, 148.57, 156.25. MALDI-TOF (m/z): $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{53}\text{H}_{50}\text{NO}_6$, 796.36; found, 796.45 and 767.27 (loss of methoxy). IR (neat): 2982, 2926, 2896, 2823, 1589, 1490, 1081, 1069, 1014, 978, 852 cm^{-1} .



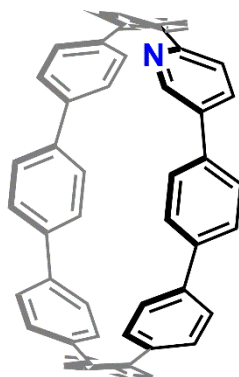
12c

Dibromide **8d** (0.415 g, 0.920 mmol, 1.00 eq), diboronate **11a** (0.700 g, 0.920 mmol, 1.00 eq), $^t\text{Bu}_4\text{NBr}$ (0.323 g, 0.184 mmol, 0.200 eq) and $\text{Pd}(\text{PPh}_3)_4$ (0.106 g, 0.0920 mmol, 0.100 eq), and NaHCO_3 (0.865 g, 10.0 mmol, 10.0 eq) were charged to a dried flask, which was then evacuated and backfilled with N_2 three times. Degassed toluene (118 mL), methanol (13 mL) and H_2O (10 mL to make base 1M) were added. The mixture was heated to 90 °C and stirred for 24 hours. The reaction was cooled to room temperature and extracted between washed with H_2O . The organic layer was washed with brine and dried over sodium sulfate. The organic layer was concentrated down under reduced pressure to a yellow solid. The solid was purified by column chromatography (silica gel, 30% ethyl acetate in DCM eluent) to give a white solid (140 mg, 20%) mp 290 °C dec. ^1H NMR (500 MHz, CDCl_3): δ 3.40 (s, 6H), 3.46 (s, 6H), 3.48 (s, 6H), 6.05 (d, J = 10 Hz, 4H), 6.13 (d, J = 10 Hz, 4H), 6.28 (s, 4H), 7.51-7.57 (m, 12H), 7.92 (d, J = 8.5 Hz, 4H), 8.29 (dd, J = 2 Hz, 1 Hz, 2H). ^{13}C NMR (125 MHz, CDCl_3): δ 52.11, 52.41, 52.49, 74.33, 74.85, 74.93, 119.99, 126.45, 126.52, 127.20, 133.09, 133.66, 133.79, 134.93, 135.42, 138.28, 143.57, 144.79, 148.12, 156.64. MALDI-TOF (m/z): $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{52}\text{H}_{49}\text{N}_2\text{O}_6$, 797.36; found 797.52. IR (neat): 3022, 2983, 2920, 2850, 2821, 1589, 1471, 1390, 1229, 1081, 1068, 101, 102, 978, 829, 662, 610, 543 cm^{-1} .



12d

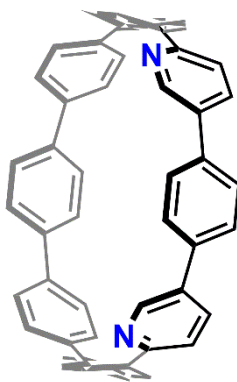
Dibromide **8d** (0.178 g, 0.395 mmol, 1.00 eq), diboronate **11b** (0.300 g, 0.395 mmol, 1.00 eq), $n\text{Bu}_4\text{Br}$ (0.0250 g, 0.0790 mmol, 0.200 eq) and $\text{Pd}(\text{PPh}_3)_4$ (0.0500 g, 0.0400 mmol, 0.100 eq), and NaHCO_3 (0.336 g, 4.00 mmol, 10.0 eq) were charged to a dried flask, which was then evacuated and backfilled with N_2 three times. Degassed toluene (180 mL), methanol (20 mL), and H_2O (4 mL to make base 1M) were added. The mixture was heated to 90 °C and stirred for 24 hours. The reaction was cooled to room temperature and washed with H_2O . The organic layer was washed with brine and dried over sodium sulfate. The organic layer was concentrated down under reduced pressure to a yellow solid. The solid was purified by column chromatography (silica gel, 40% ethyl acetate in DCM eluent) to recover a white solid (16.0 mg, 16%) mp 290 °C dec. ^1H NMR (500 MHz, CDCl_3): δ 3.42-3.51 (m, 18H), 6.09-6.29 (m, 12H), 7.40 (dd, J = 8.3, 2.3 Hz, 1H), 7.49-7.61 (m, 8H), 7.84 (dd, J = 8.3, 2.3 Hz, 1H), 7.88-7.95 (m, 4H), 8.30 (s, 1H), 8.32 (s, 1H), 8.80 (d, J = 2.3 Hz, 1H). ^{13}C NMR (125 MHz, CDCl_3) δ 161.47, 156.55, 156.28, 148.04, 147.92, 144.44, 144.18, 134.85, 134.73, 134.70, 134.67, 134.48, 133.68, 133.57, 131.99, 131.70, 127.06, 126.41, 126.22, 120.83, 119.78, 119.72, 75.39, 74.90, 74.80, 74.72, 74.52, 72.96, 52.36, 52.34, 52.32, 52.7, 51.95. MALDI-TOF (m/z): $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{51}\text{H}_{48}\text{N}_3\text{O}_6$, 798.35; found, 799.56. IR: 3023, 2935, 2896, 2822, 1590, 1556, 1470, 1393, 1227, 1175, 1114, 1074, 1014, 948, 825, 771, 753, 730, 662, 645, 610, 573, 543 cm^{-1} .



1 Aza[8]CPP

To a dry flask charged with 15 mL of THF was added sodium metal (0.200 g, 8.30 mmol) and naphthalene (1.20 g, 9.36 mmol). The solution was stirred for 15 hours at room temperature during which time a dark green solution of sodium naphthalide formed.

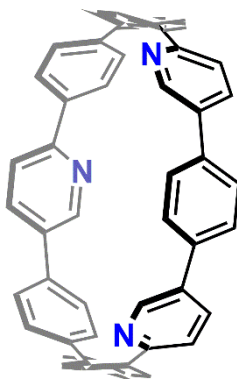
Macrocyclic **12b** (0.200 g, 0.250 mmol, 1.00 eq) was dissolved in dry THF (20 mL) and cooled to -78°C . To this solution, sodium naphthalide was added dropwise until the solution sustained a dark purple color (approximately 3 eq. per OMe, 3 mL naphthalide). The reaction was stirred for an additional 30 mins at -78°C . The reaction was quenched with a solution of I_2 in THF (1 mL of 1 M solution). The solution was warmed to room temperature. The mixture was extracted with DCM and was washed with saturated sodium thiosulfate to quench excess iodine. The aqueous layer was extracted with DCM (3 X 10 mL). The combined organic layers were washed with brine and dried over sodium sulfate. The solvent was removed under reduced pressure to yield an orange solid. The solid was purified by column (5% ether/DCM eluent) followed by preparative TLC with the same solvent system (silica, 5% ether/DCM eluent). The pure product was received as an yellow solid (0.0860 g, 56%) mp 250°C dec. ^1H NMR (400 MHz, CDCl_3): δ 7.43-7.61 (m, 28H), 7.81-7.84 (m, 2H), 8.76 (s, 1H). ^{13}C NMR (125 MHz, CDCl_3): δ 153.99, 140.85, 137.62, 17.60, 137.47, 137.45, 137.43, 137.42, 134.67, 132.45, 130.16, 128.25, 127.6, 127.51, 127.47, 119.04. MALDI-TOF (m/z): $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{47}\text{H}_{32}\text{N}$, 610.25; found, 609.92. IR (neat): 3023, 2923, 2853, 1567, 1479, 1467, 1390, 1364, 1261, 1224, 1055, 996, 816, 760, 741 cm^{-1} .



2 1,15-Diaza[8]CPP

To a dry flask charged with 15 mL of THF was added sodium metal (0.200 g, 8.30 mmol) and naphthalene (1.20 g, 9.36 mmol). The solution was stirred for 15 hours at room temperature during which time a dark green solution of sodium naphthalide formed.

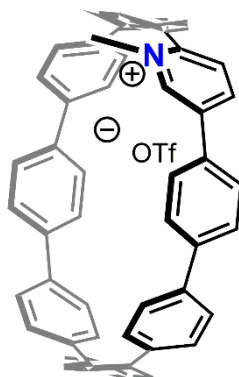
Macrocyclic **12c** (0.174 g, 219 μ mol, 1.00 eq) was dissolved in dry THF (20 mL) and cooled to -78°C . To this solution, sodium naphthalide was added dropwise until the solution sustained a dark purple color (approximately 2 mL of 1 M sodium naphthalide). The reaction was stirred for an additional 3 hours at -78°C . The reaction was quenched with a solution of I_2 in THF (1 mL of 1 M solution). The solution was warmed to room temperature. The reaction was extracted with DCM and was washed with saturated sodium thiosulfate to quench excess iodine. The aqueous layer was extracted with DCM (3 X 10 mL). The combined organic layers were washed with brine and dried over sodium sulfate. The solvent was removed under reduced pressure to yield an orange solid. The solid was washed with hexanes to remove excess naphthalene. The solid was then purified by preparatory TLC (silica, 5% MeOH/DCM eluent). The pure product was received as a yellow solid (0.0720 g, 55%) mp 236°C dec. ^1H NMR (500 MHz, CDCl_3): δ 7.26-7.86 (m, 28H), 8.75 (s, 2H). ^{13}C NMR (125 MHz, CDCl_3): δ 154.24, 146.86, 138.86, 137.91, 137.64, 137.04, 136.94, 135.31, 132.72, 130.13, 128.28, 127.66, 127.52, 127.47, 127.41, 127.02, 119.07. MALDI-TOF (m/z): $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{46}\text{H}_{31}\text{N}_2$, 611.25; found, 611.26. IR (neat): 2967, 2879, 1472, 880, 830, 739, 556 cm^{-1} .



3 1,15,31-Triaza[8]CPP

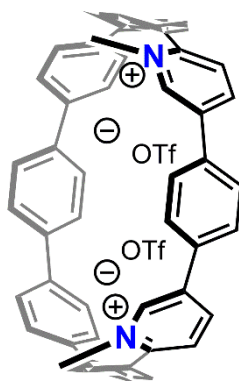
To a dry flask charged with 15 mL of THF was added sodium metal (0.200 g, 8.30 mmol) and naphthalene (1.20 g, 9.36 mmol). The solution was stirred for 15 hours at room temperature during which time a dark green solution of sodium naphthalide formed.

Macrocyclic **12d** (0.0500 g, 0.0630 mmol, 1.00 eq) was dissolved in dry THF (15 mL) and cooled to -78°C . To this solution, sodium naphthalide was added dropwise until the solution sustained a dark purple color (approximately 3 eq per OMe). The reaction was stirred for an additional 30 mins at -78°C . The reaction was quenched with a solution of I_2 in THF (1 mL of 1 M solution). The solution was warmed to room temperature. The mixture was extracted with DCM and washed with saturated sodium thiosulfate to quench excess iodine. The aqueous layer was extracted with DCM (3 X 10 mL). The combined organic layers were washed with brine and dried over sodium sulfate. The solvent was removed under reduced pressure to yield an orange solid. The solid was washed with a small amount of hexanes to remove most of the excess naphthalene. The residue was then purified by preparatory TLC (silica, 20% ether/DCM eluent). The pure product was received as an yellow solid (0.0190 g, 50%) mp 230°C dec. ^1H NMR (500 MHz, CDCl_3): δ 7.51-7.61 (m, 17H), 7.79-7.86 (m, 9H), 8.75-8.77 (m, 3H). ^{13}C NMR (125 MHz, CDCl_3): δ 154.13, 154.11, 153.94, 146.89, 138.83, 138.48, 138.40, 137.79, 137.30, 137.23, 135.26, 135.23, 135.02, 132.67, 132.65, 132.59, 130.22, 130.09, 128.29, 128.23, 127.77, 127.76, 127.47, 127.17, 127.02, 119.20, 119.15, 119.06. MALDI-TOF (m/z): $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{45}\text{H}_{30}\text{N}_3$, 612.24; found, 612.32. IR (neat): 3026, 2924, 2853, 1733, 1567, 1463, 1363, 1263, 1228, 1174, 1153, 1114, 1077, 1015, 948, 911, 819, 740, 699, 664, 650 cm^{-1} .



4 *N*-methylaza[8]CPP Triflate

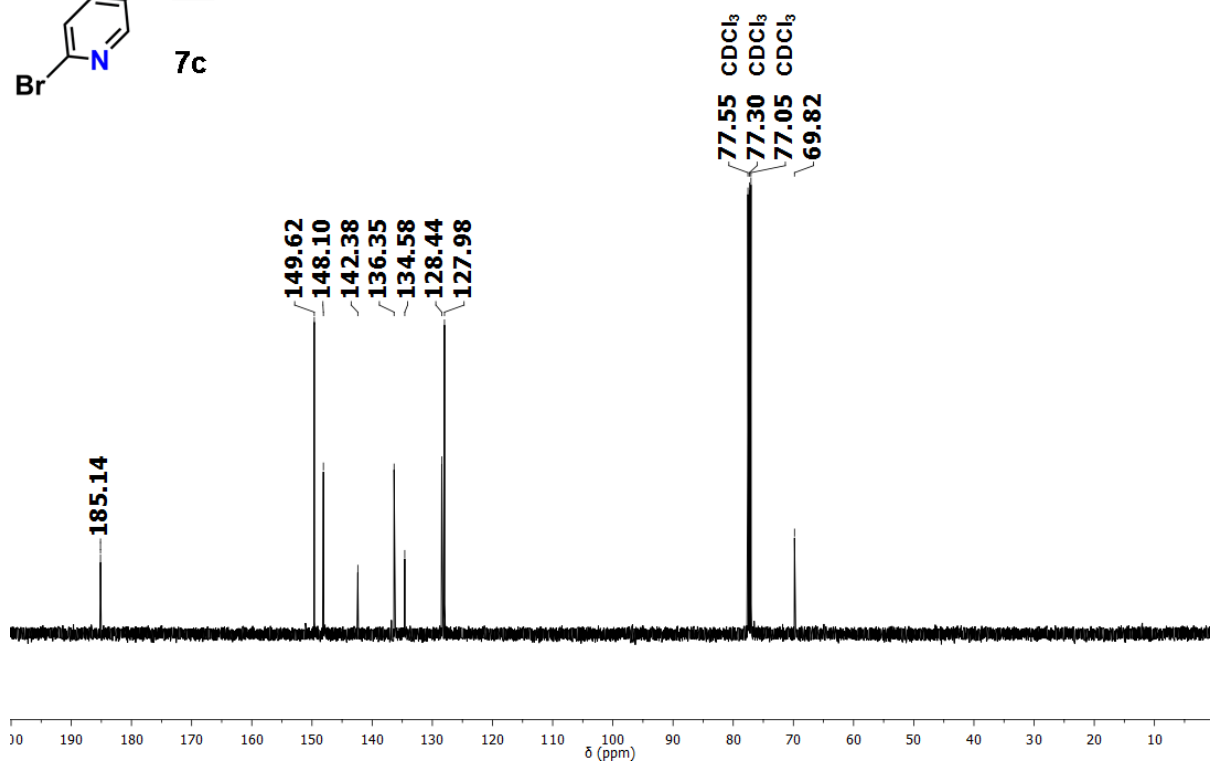
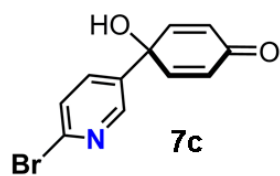
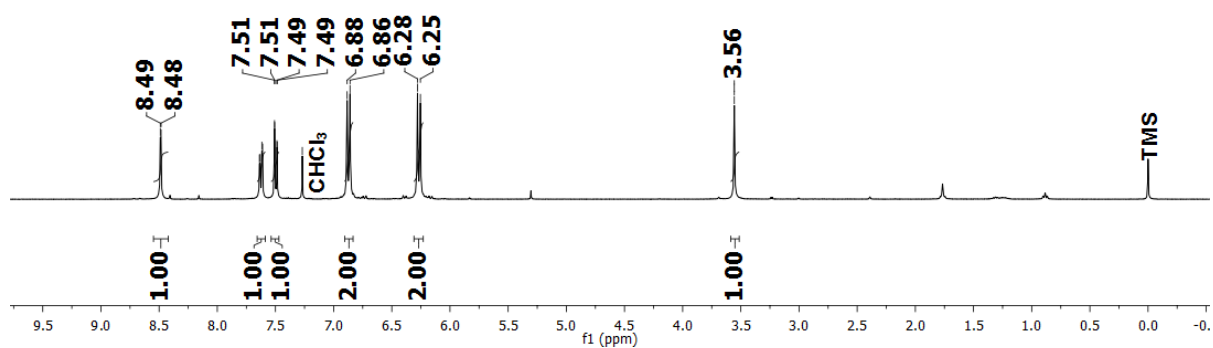
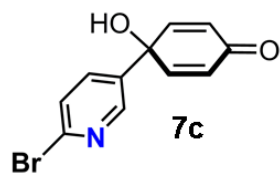
Aza[8]CPP **1** (0.0230 g, 0.0377 mmol, 1 equiv) was added to a flame dry flask charged under nitrogen. 20 mL of dry dichloromethane was added. Once all solids had dissolved methyl triflate (0.0200 mL, 0.189 mmol, 5 equiv) was added dropwise. This was allowed to stir for 18 hours during which the color turned from a bright fluorescent yellow to a dull orange. The reaction was quenched by addition of saturated ammonium chloride (20 mL). The aqueous layer was extracted with DCM (3 X 10 mL). The combined organic layers were washed with brine and dried over sodium sulfate. The solvent was removed under reduced pressure to yield a red/ orange solid (0.0290 g, 99%). Single crystal was grown by slow liquid diffusion by layering toluene onto a concentrated dichloromethane solution of **4**. mp 230 °C dec. ^1H NMR (600 MHz, CDCl_3): δ 9.29 (s, 1H), 7.91 (d, $J = 9$ Hz, 1H), 7.70 (d, $J = 9$ Hz, 1H), 7.64-7.26 (m, 19H), 4.76 (s, 3H). ^{13}C NMR (150 MHz, CDCl_3): δ 151.90, 145.48, 142.88, 141.61, 141.40, 139.48, 138.87, 138.23, 137.95, 137.82, 137.60, 137.50, 137.22, 136.81, 136.64, 136.30, 131.06, 130.24, 129.54, 129.37, 128.46, 127.92, 127.70, 127.57, 121.58 (q, $J_{\text{C-F}} = 318$ Hz), 47.96. ESI-MS (m/z): $[\text{M}+\text{Na}]^+$ calculated for $\text{C}_{49}\text{H}_{34}\text{NF}_3\text{NNaO}_3\text{S}^+$, 796.2109; found, 796.2096. IR (neat): 3025, 2923, 1585, 1486, 1260, 1165, 1029, 822, 730, 638 cm^{-1} .

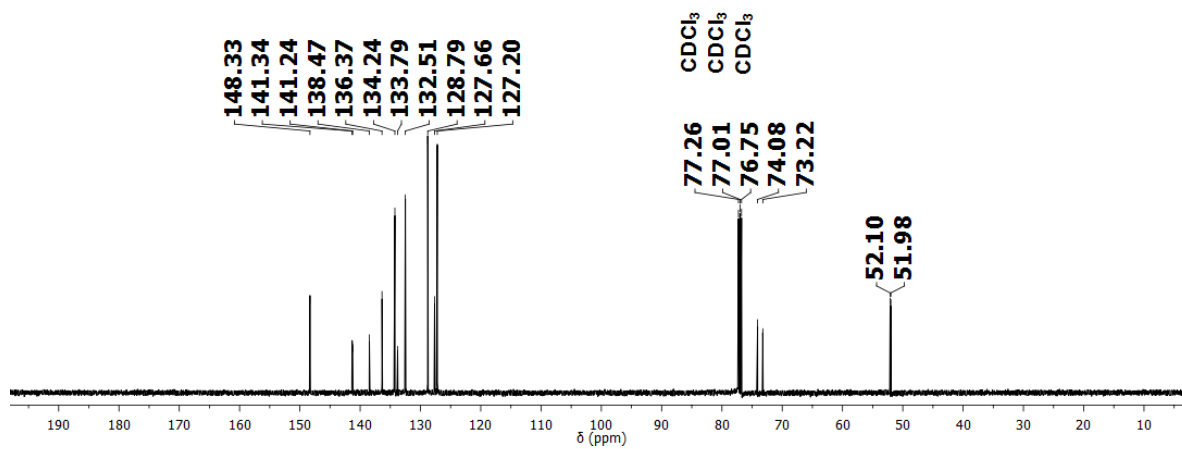
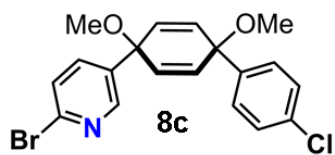
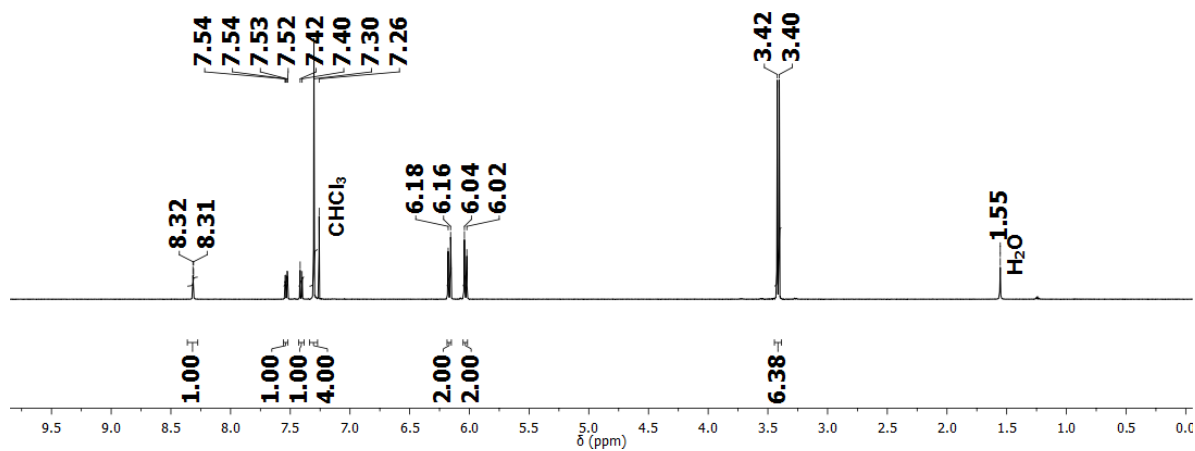
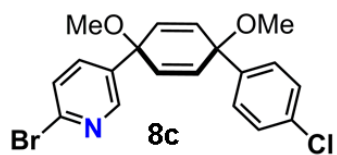


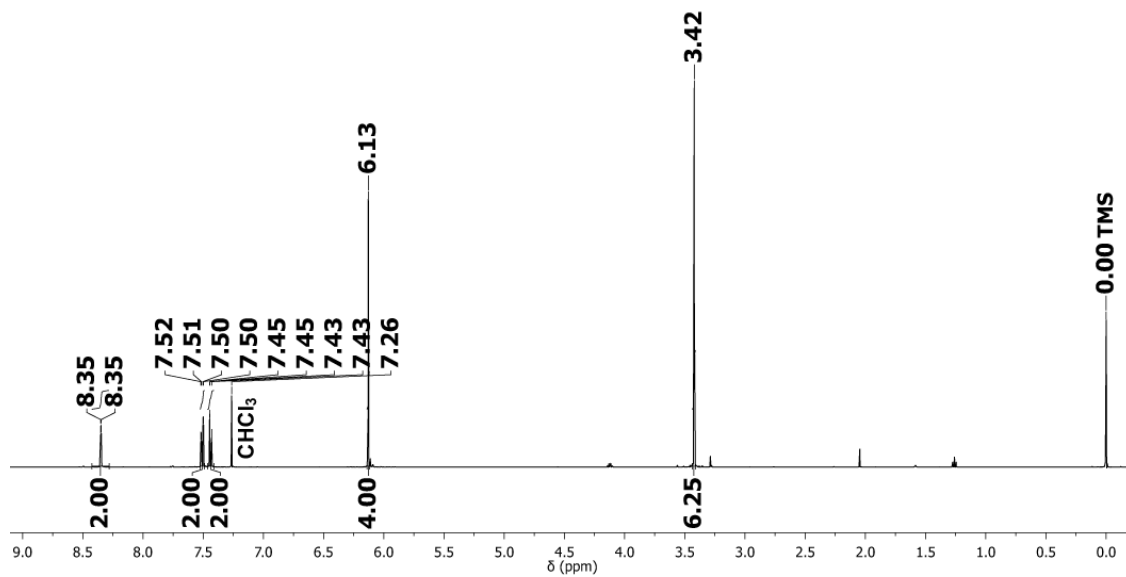
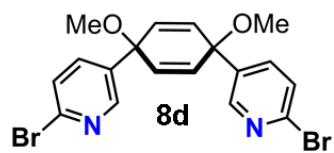
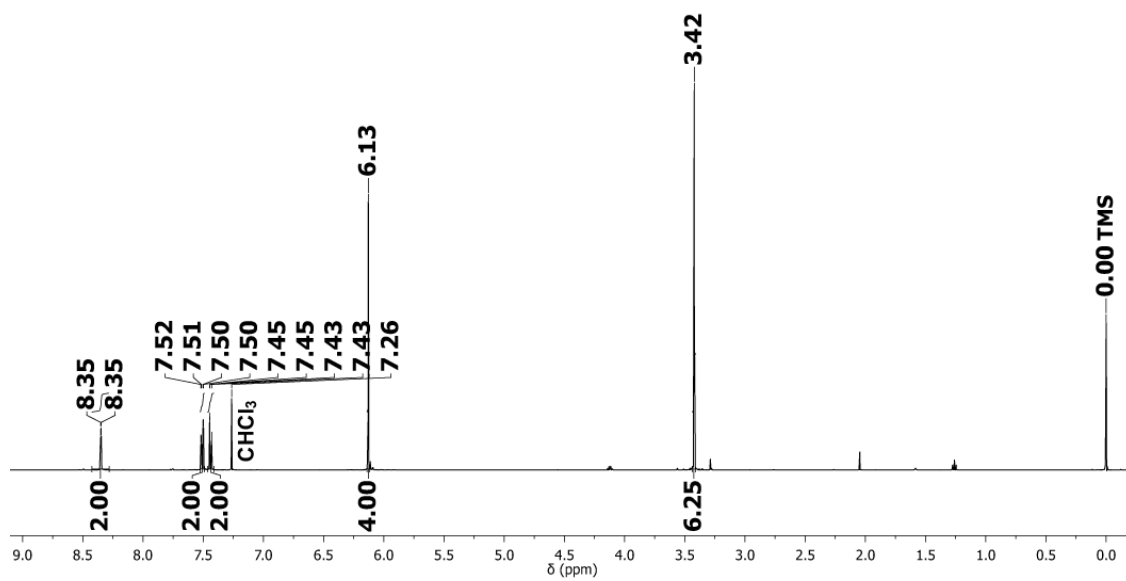
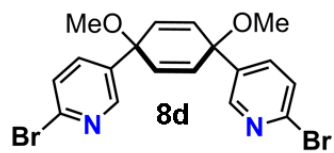
5 *N,N*-dimethyl-1,15-diaza[8]CPP Ditriflate

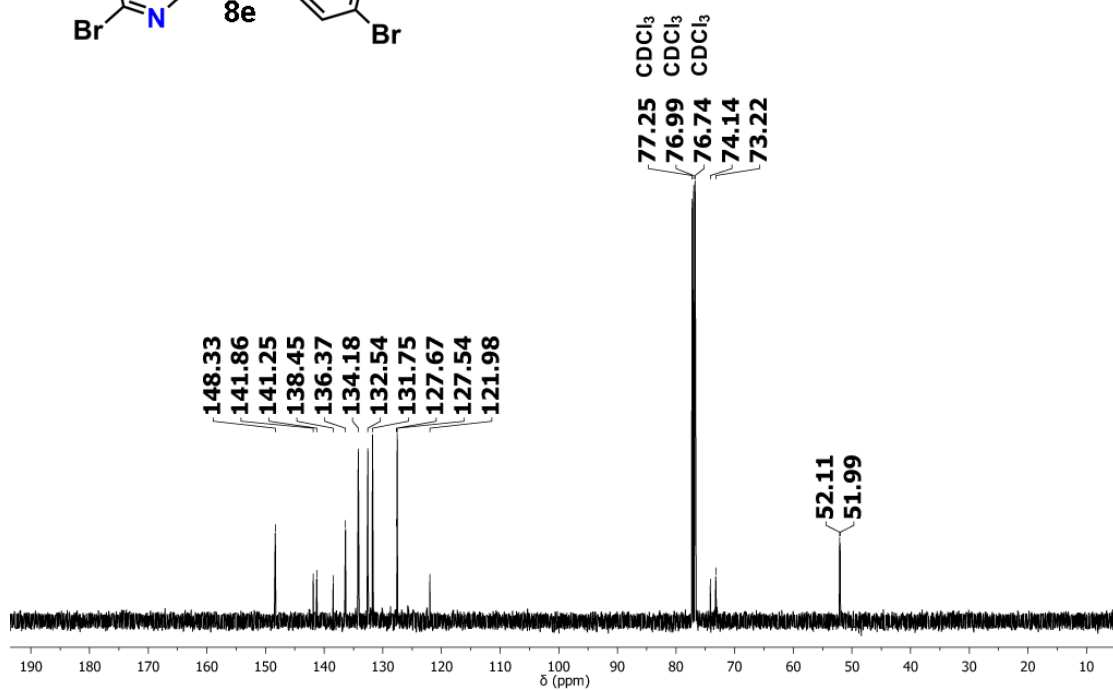
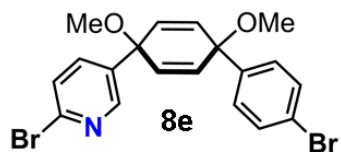
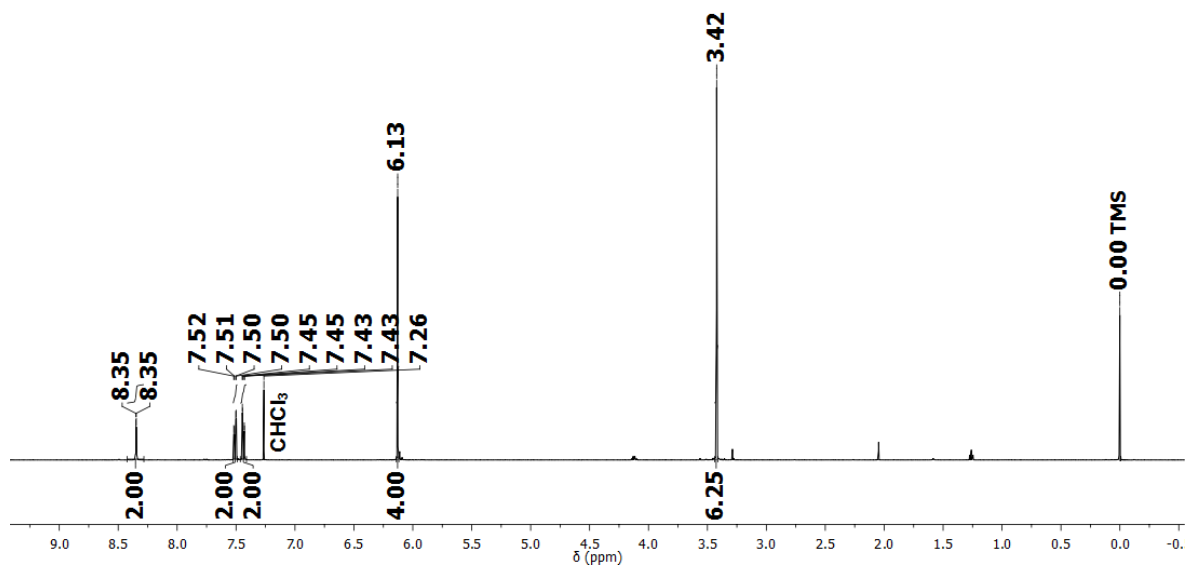
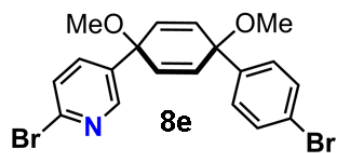
1,15-diaza[8]CPP2N **2** (0.0170 g, 0.0383 mmol, 1 equiv) was added to a flame dry flask charged under nitrogen. 20 mL of dry dichloromethane was added. Once all solids had dissolved methyl triflate (0.0280 mL, 0.283 mmol, 10 equiv) was added dropwise. This was allowed to stir for 18 hours during which the color turned from a bright fluorescent yellow to a dull orange. The reaction was quenched by addition of saturated ammonium chloride (20 mL). The aqueous layer was extracted with DCM (3 X 10 mL). The combined organic layers were washed with brine and dried over sodium sulfate. The solvent was removed under reduced pressure to yield a red/ orange solid (0.0263 g, 99%). Single crystals were grown by slow evaporation of CDCl_3 . mp 230 °C dec. ^1H NMR (600 MHz, DMSO d_6): δ 9.63 (s, 2H), 8.40 (d, $J = 9$ Hz, 2H), 8.05 (s, 4H), 7.82-7.62 (m, 24H), 4.58 (s, 6H). ^{13}C NMR (150 MHz, DMSO): δ 151.89, 144.09, 143.03, 141.14, 137.80, 136.32, 136.09, 133.76, 133.54, 131.27, 129.93, 129.61, 129.39, 128.46, 128.08, 127.26, 127.16, 120.68 (q, $J_{\text{C-F}} = 320$ Hz), 47.57. ESI-MS (m/z): $[\text{M}+\text{Na}]^+$ calculated for $\text{C}_{50}\text{H}_{36}\text{F}_6\text{N}_2\text{NaO}_6\text{S}_2$, 961.1816; found, 961.1819. IR (neat): 3058, 2925, 2854, 1590, 1523, 1435, 1258, 1166, 1030, 825, 734, 638, 574 cm^{-1} .

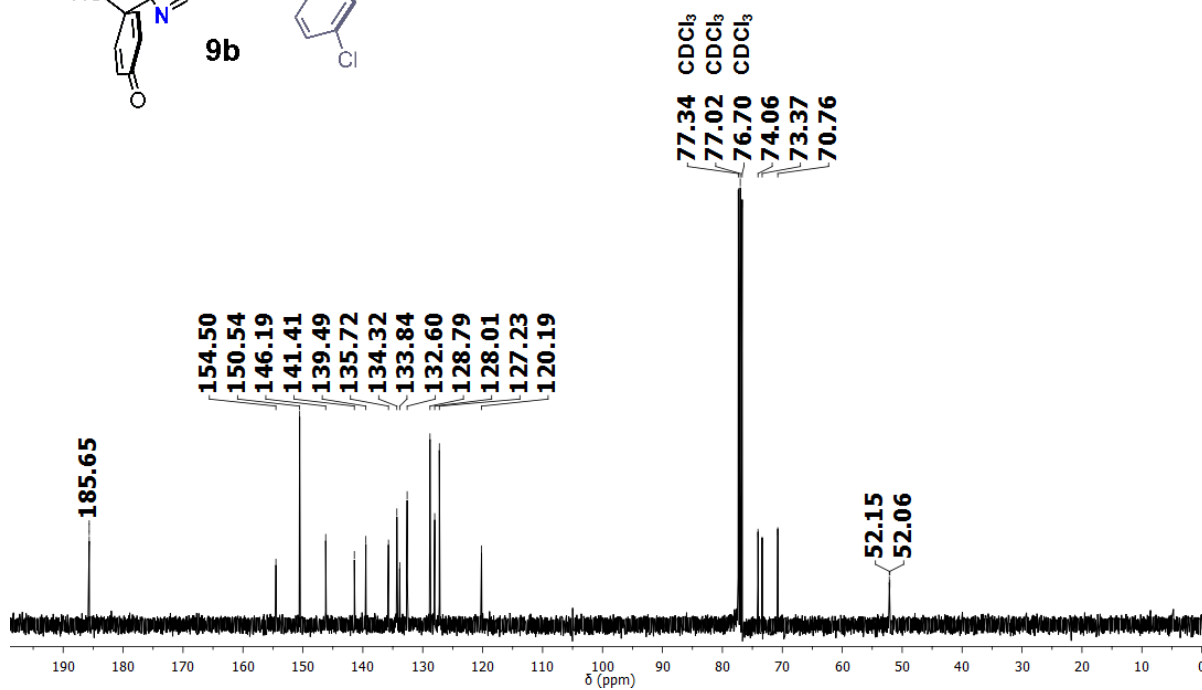
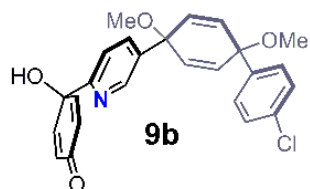
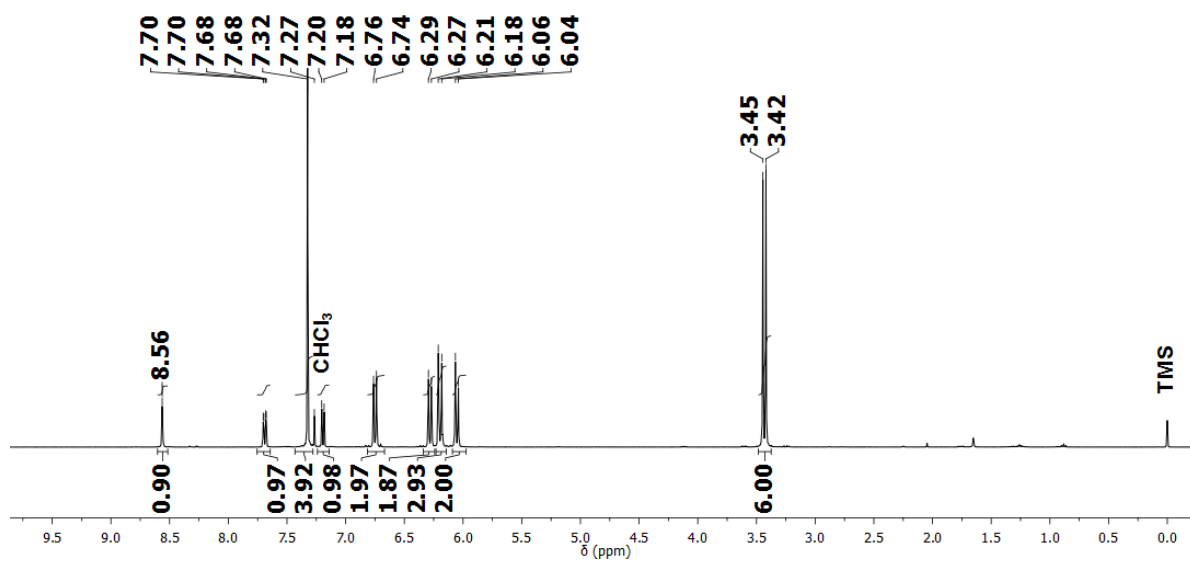
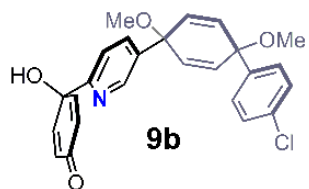
NMR Spectra

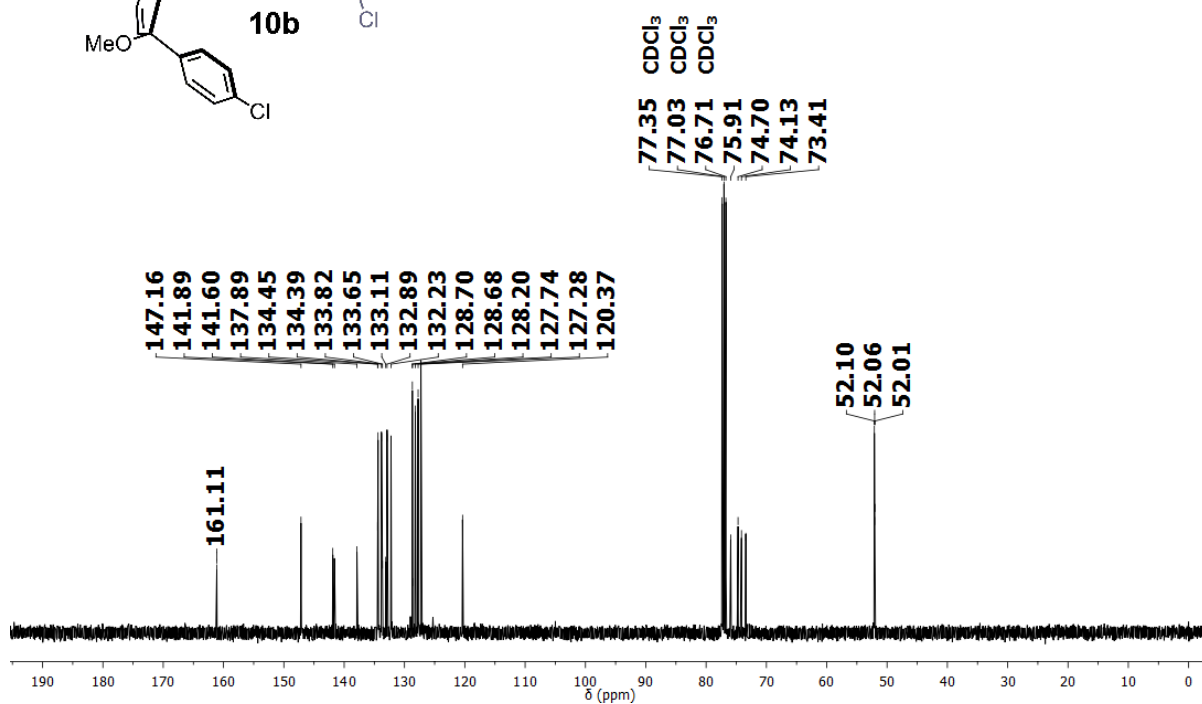
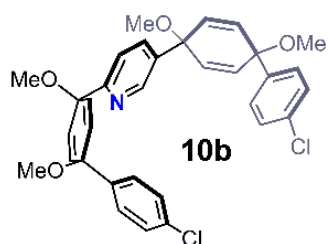
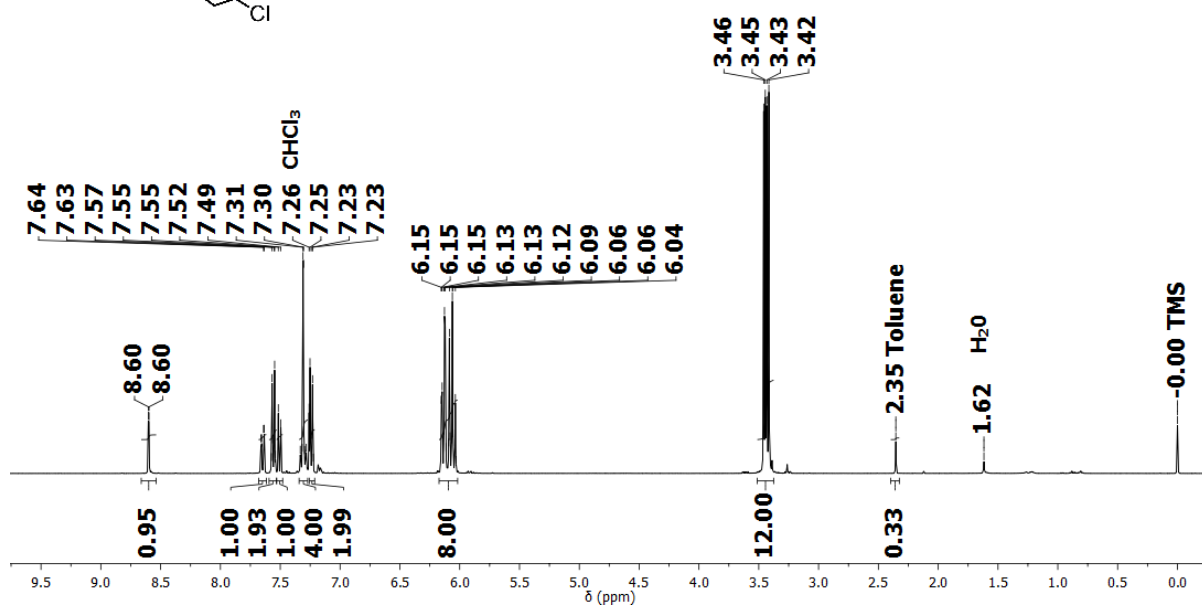
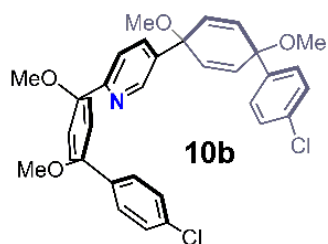


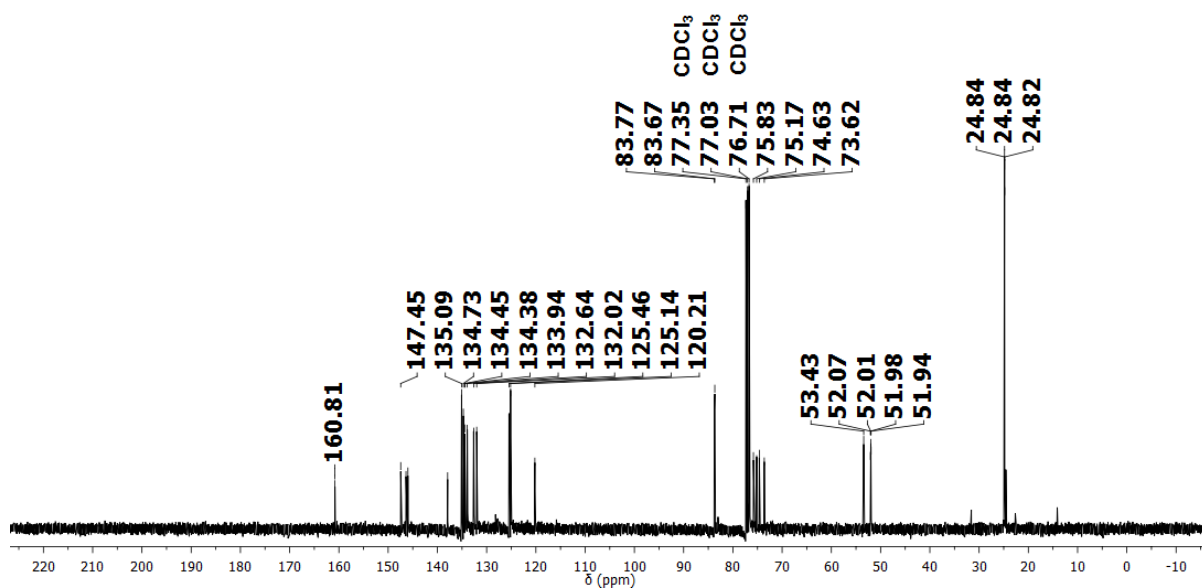
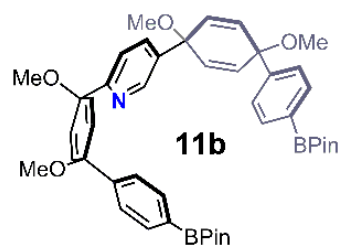
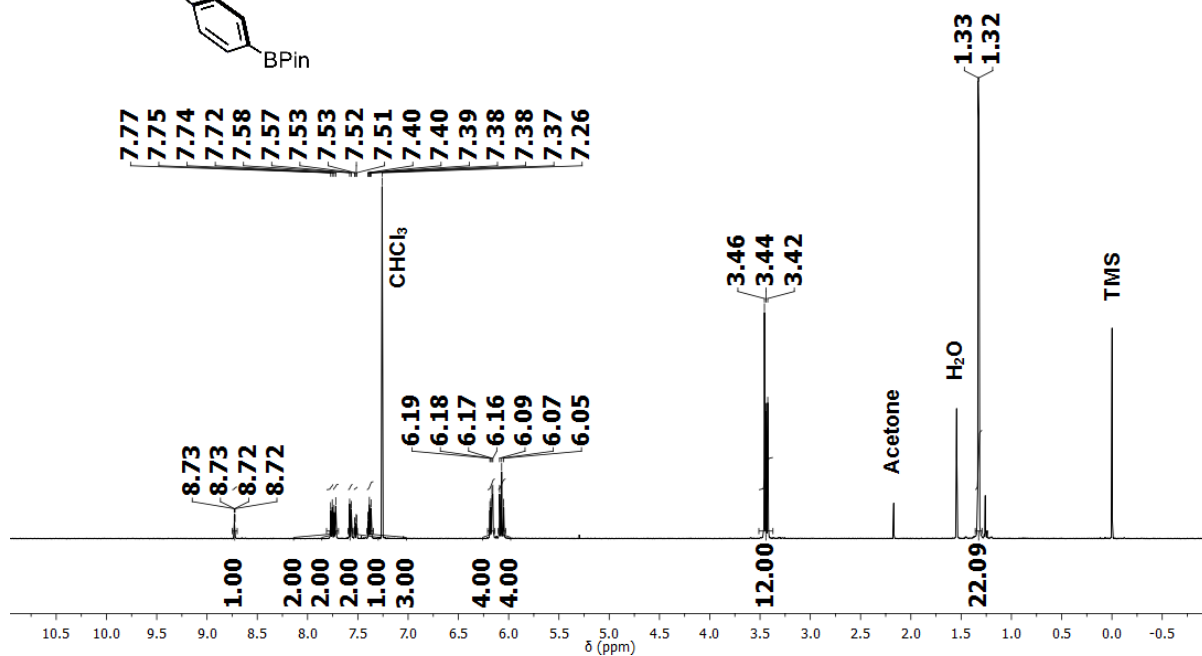
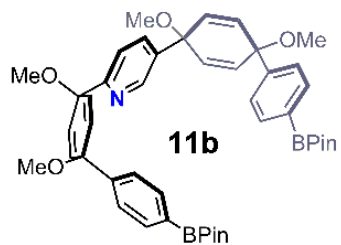


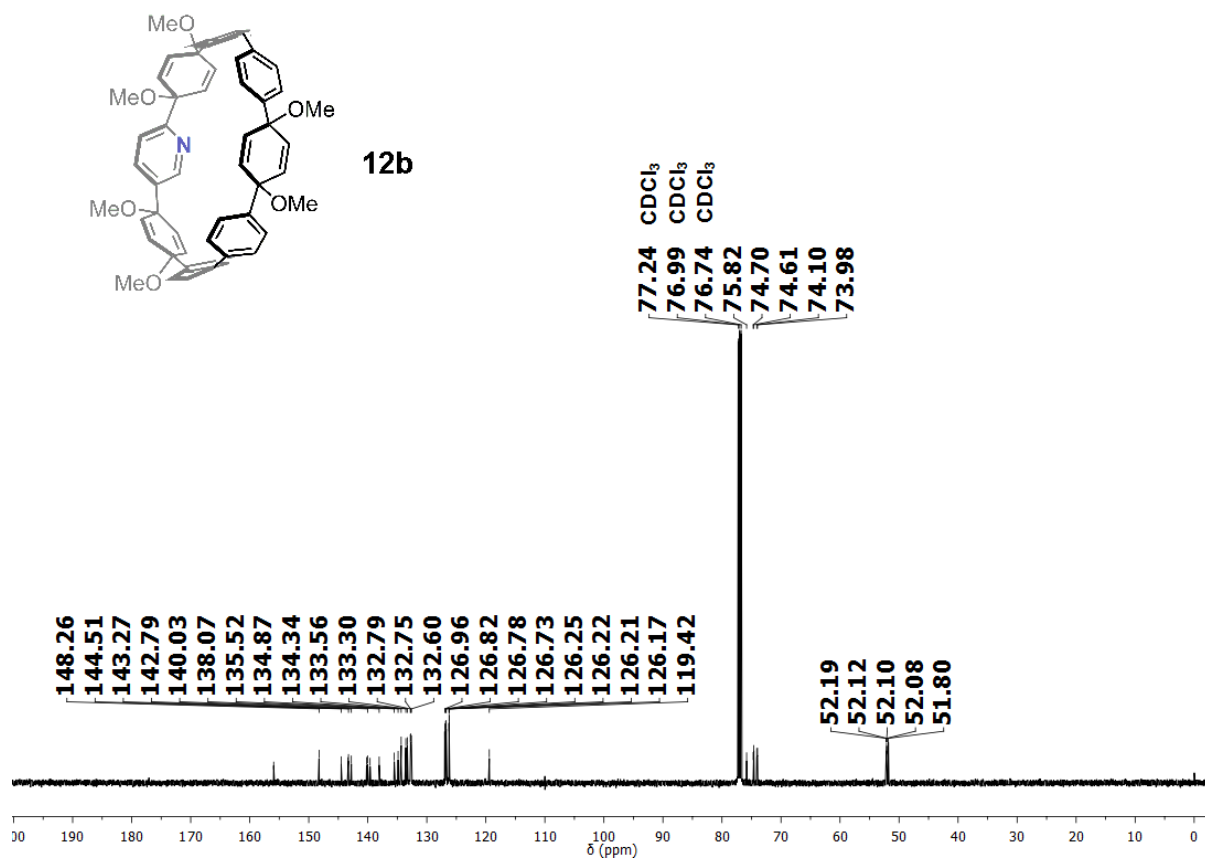
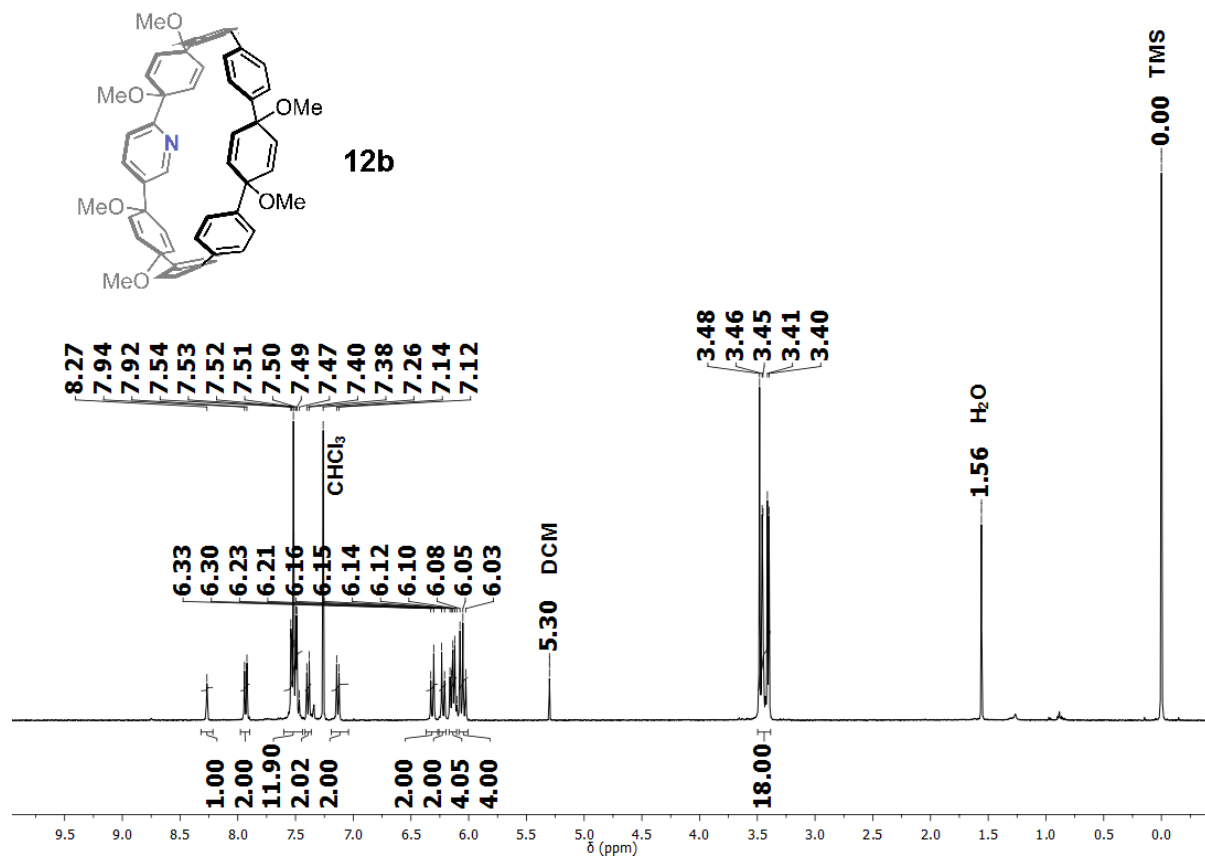


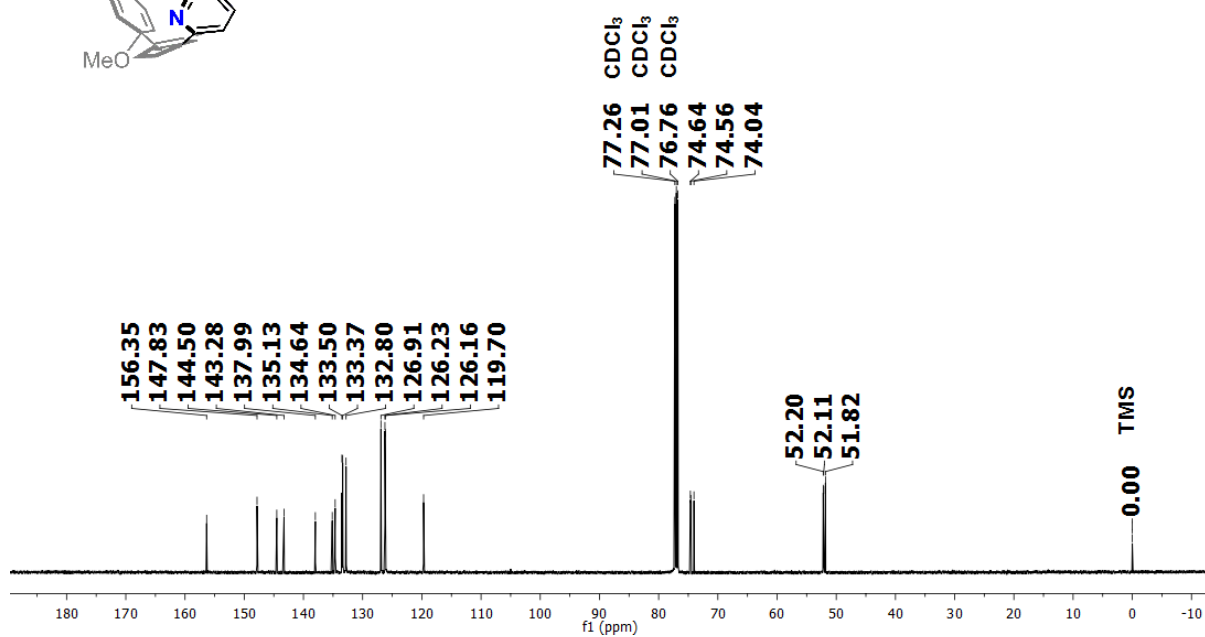
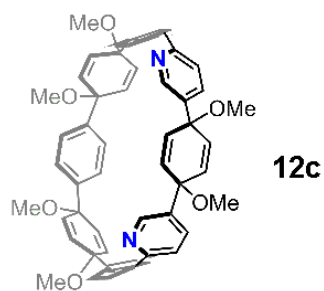
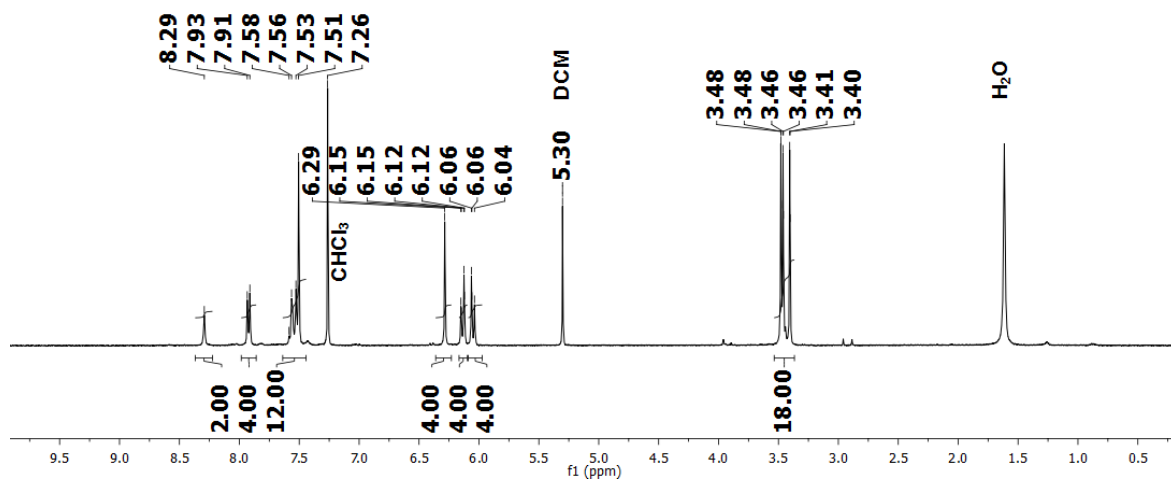
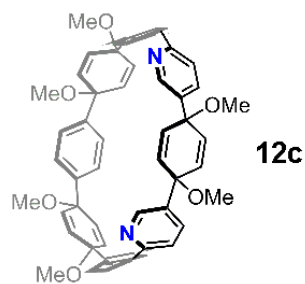


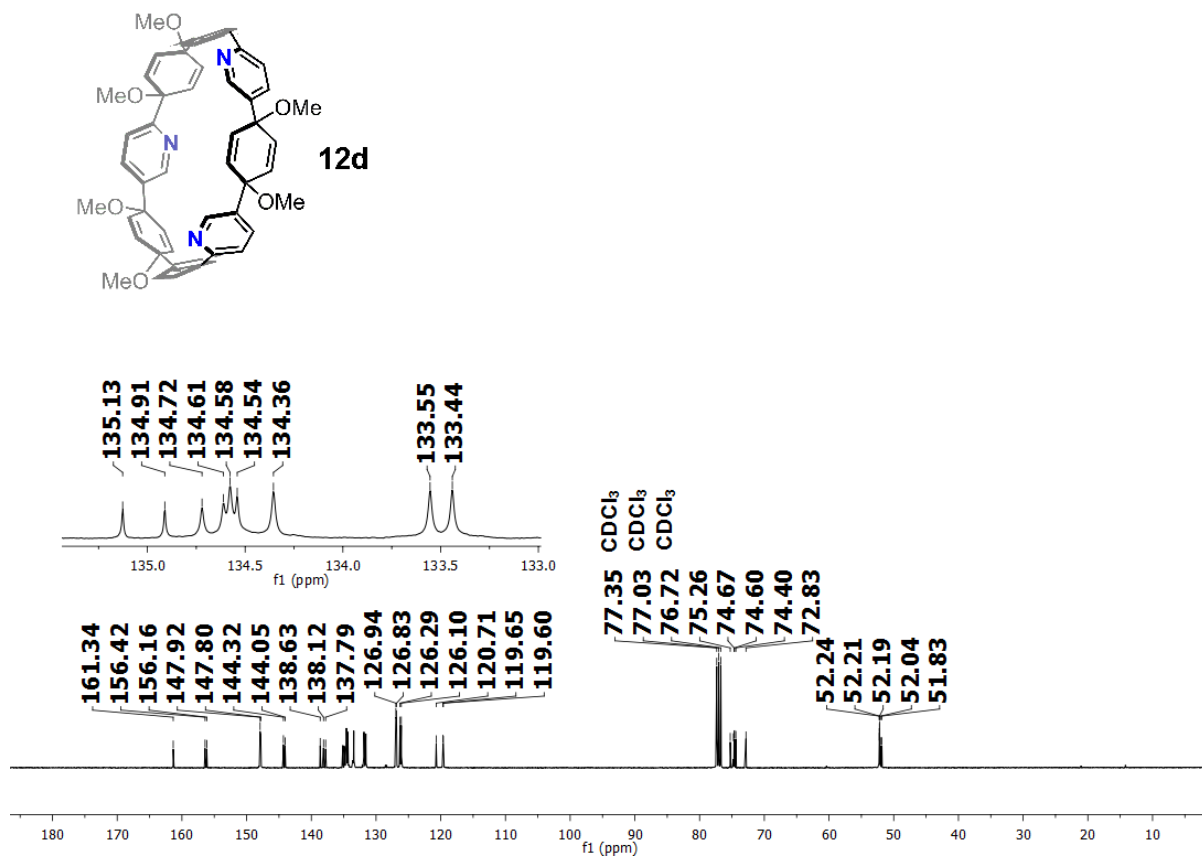
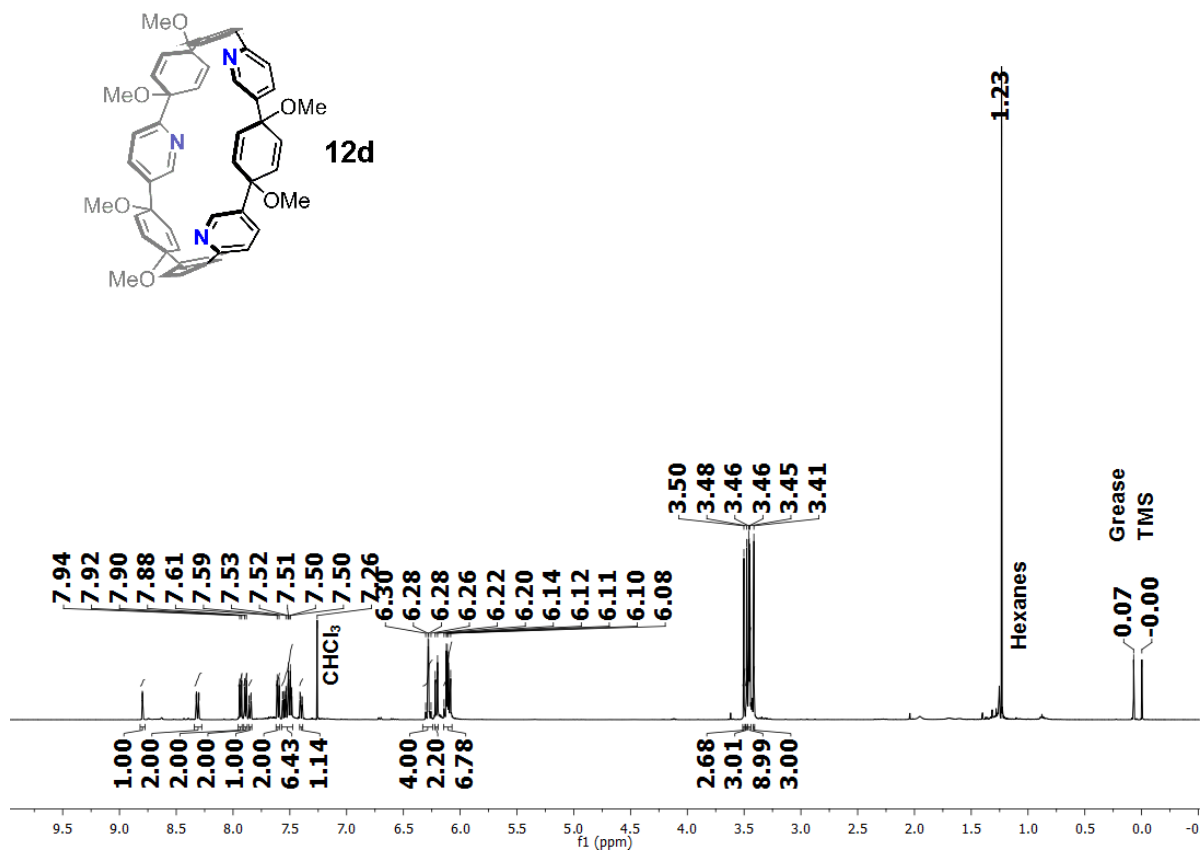


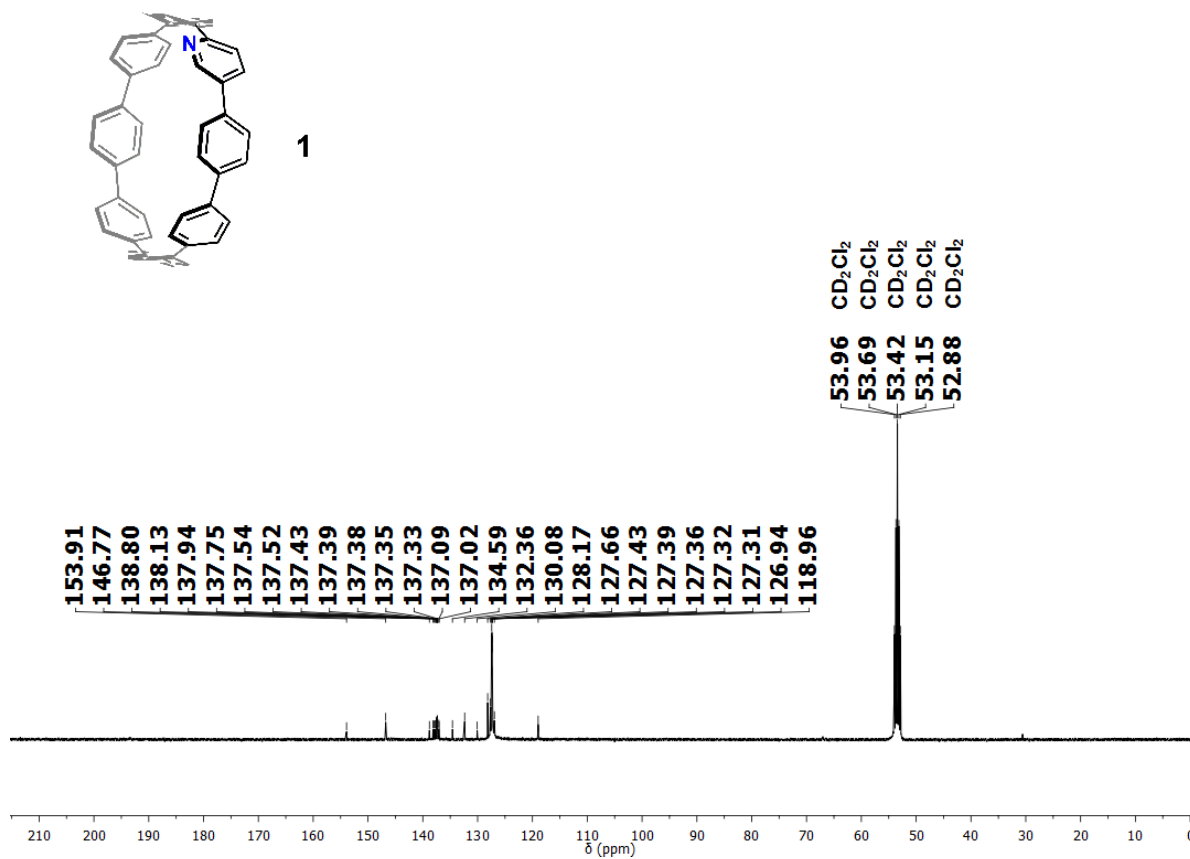


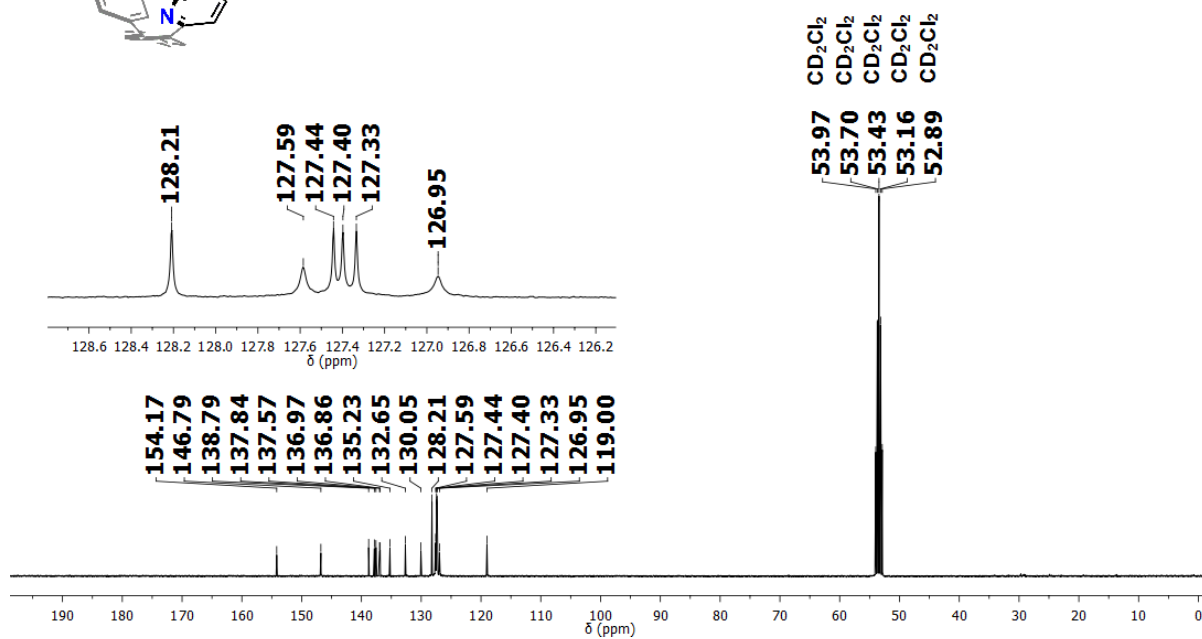
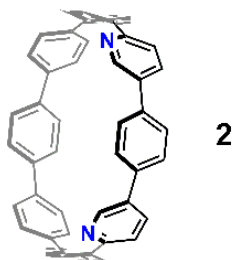
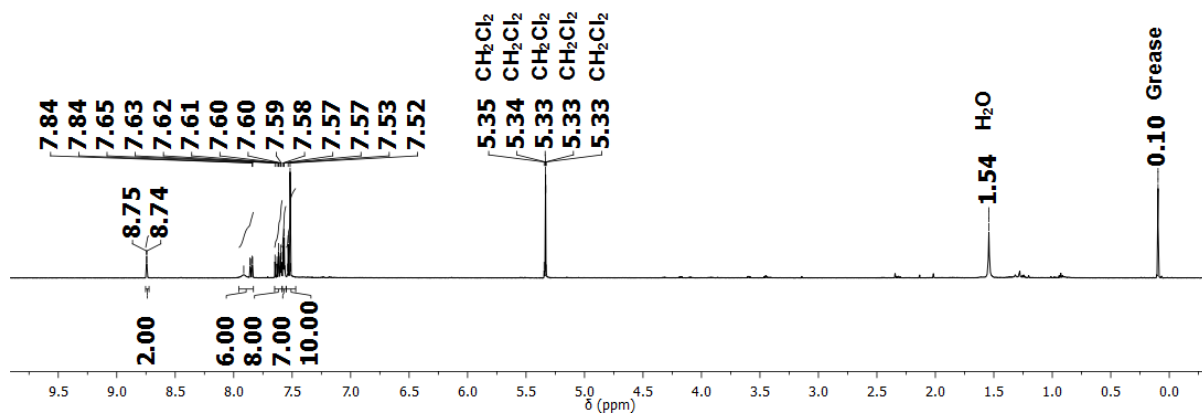
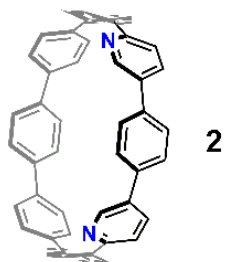


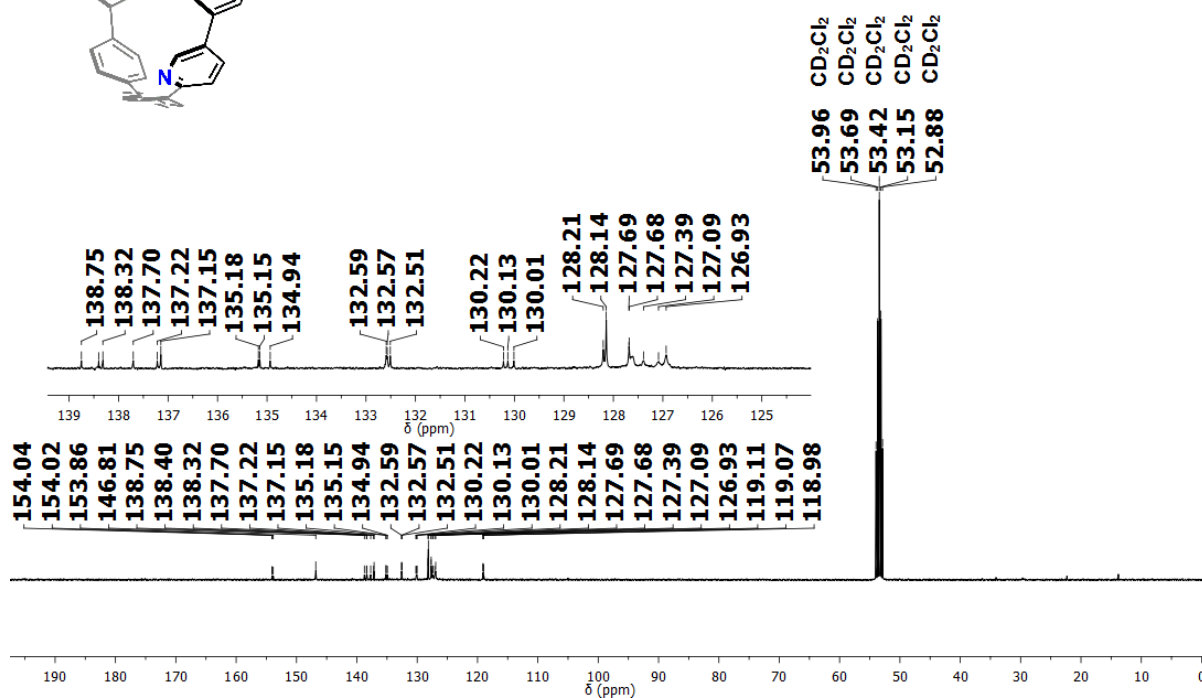
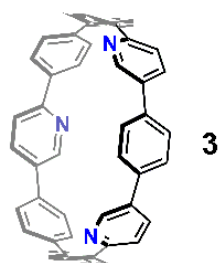
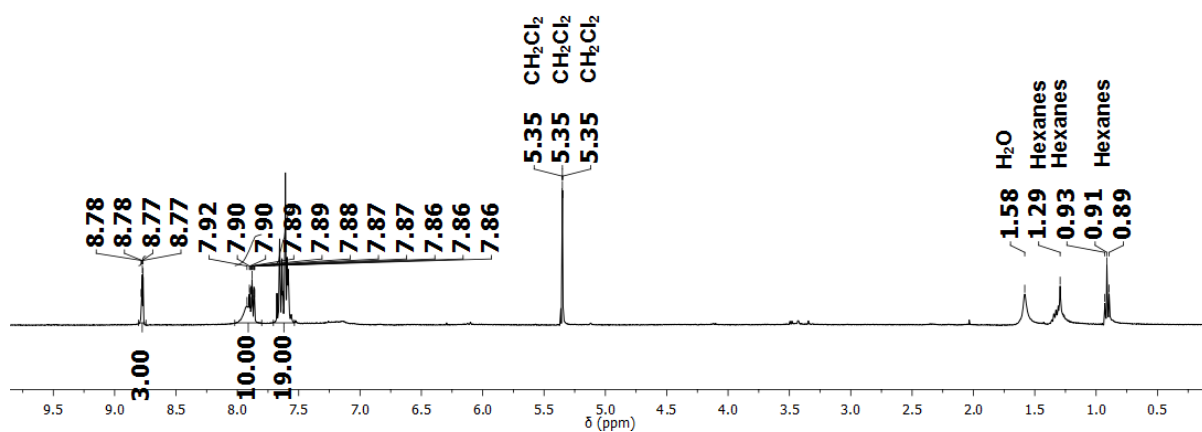
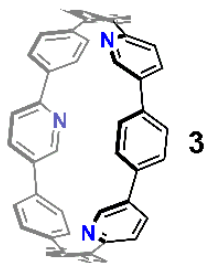


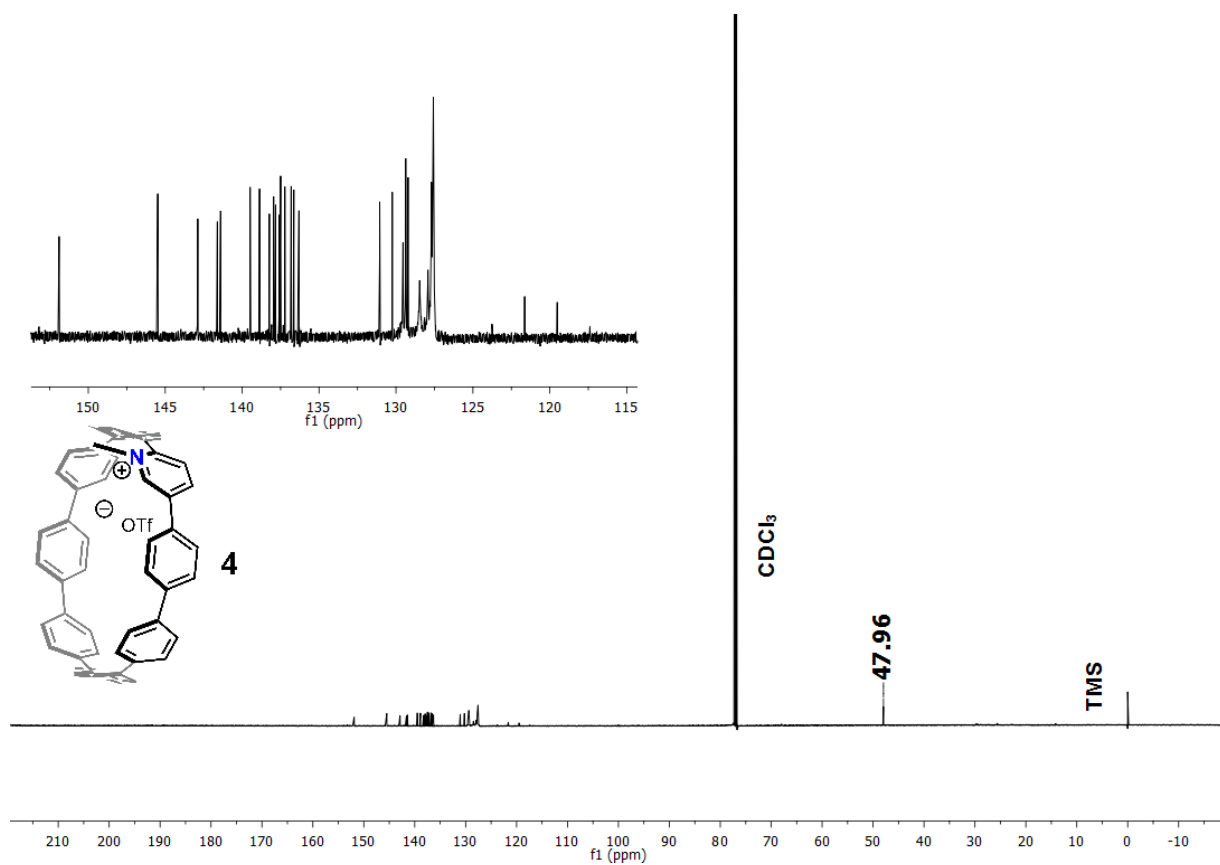
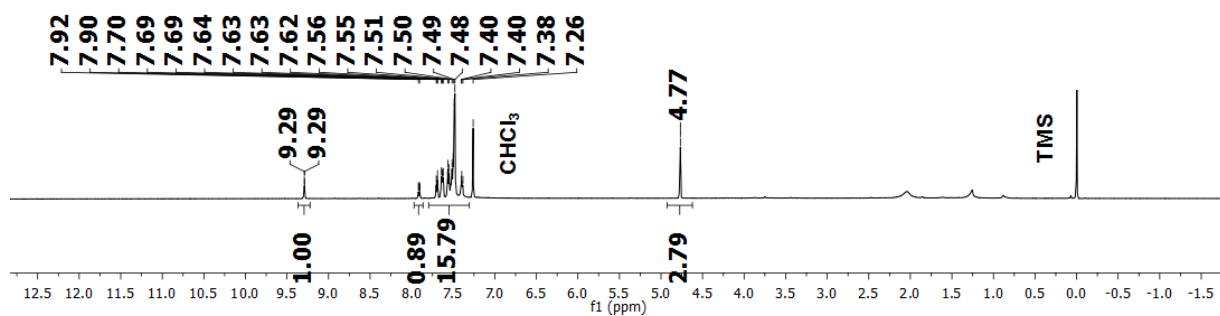
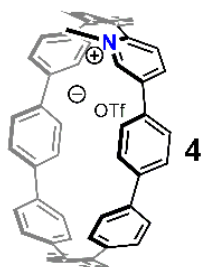


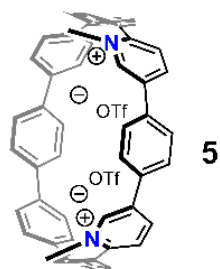




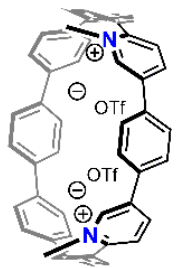
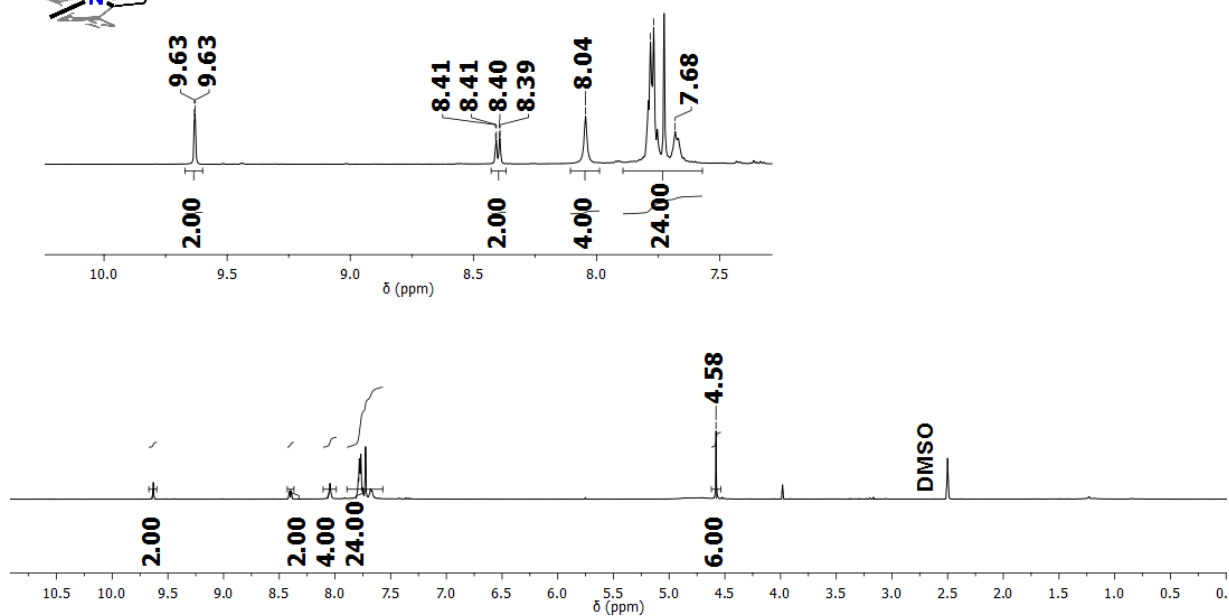




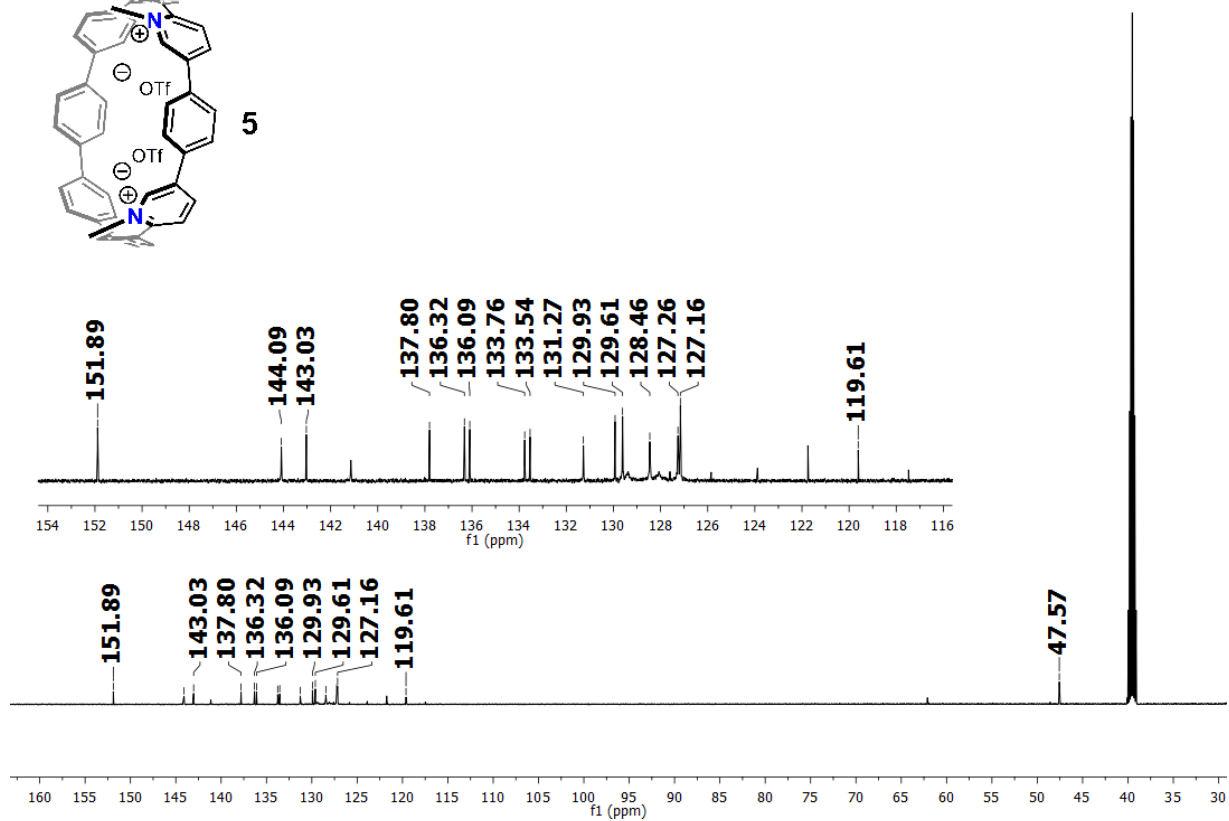




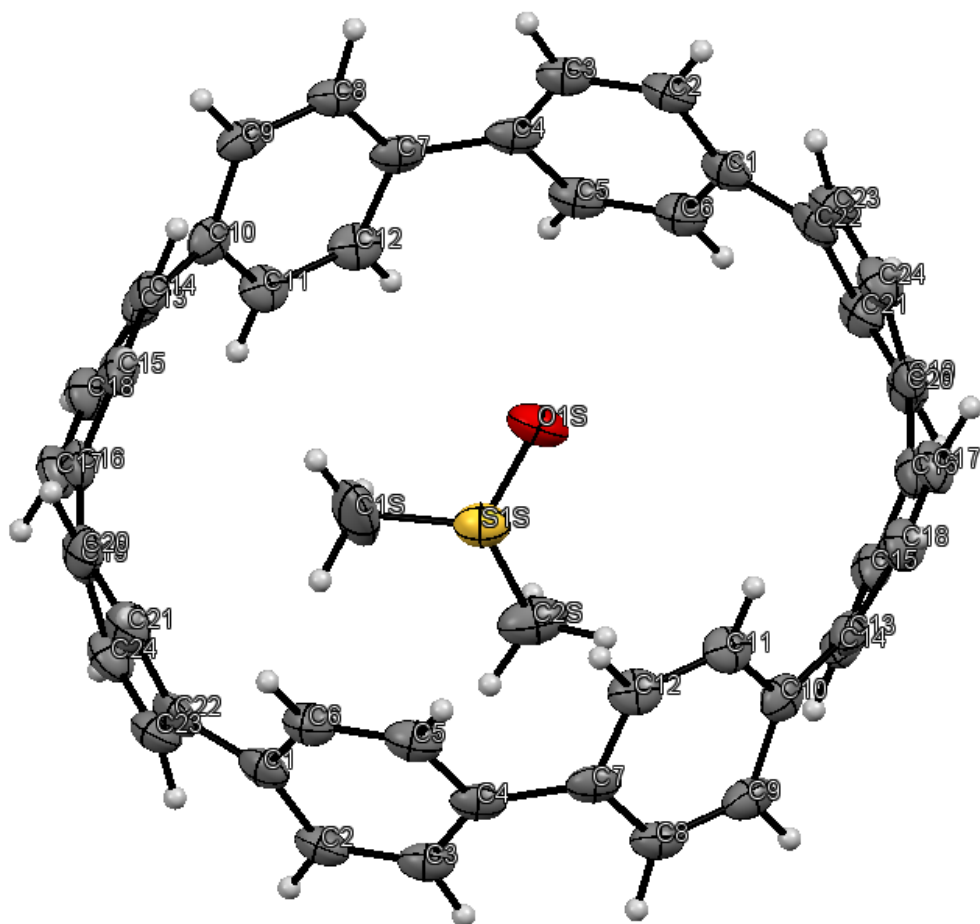
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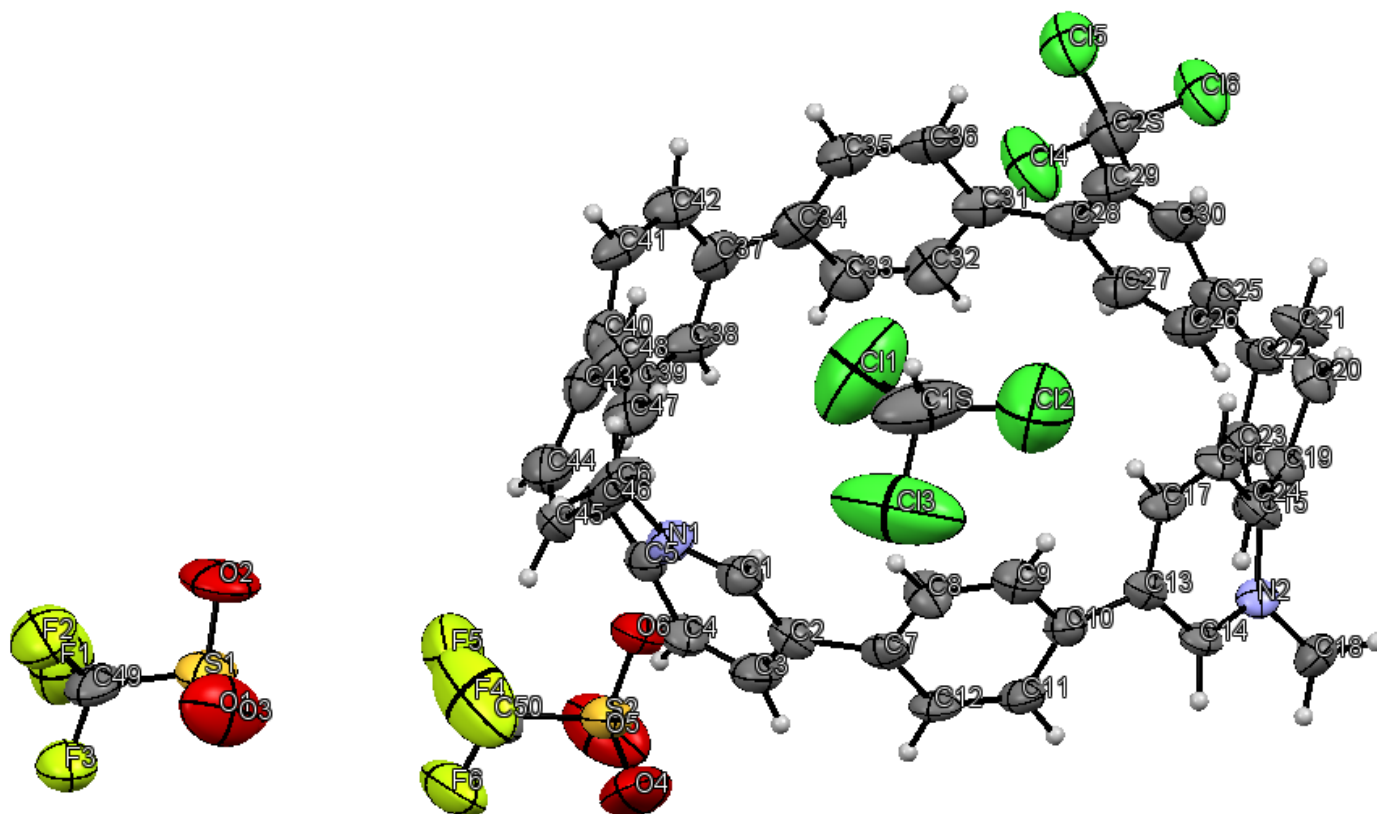
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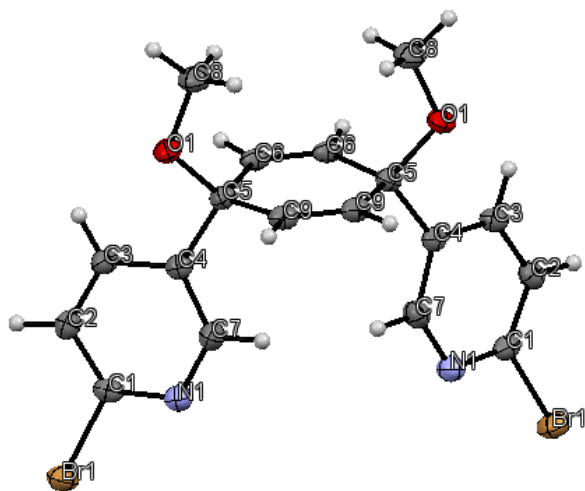


Crystallographic Data for **1**: C₅₂H₄₄O₂S₂, M = 6764.99, 0.05 x 0.04 x 0.02 mm, T = 173(2) K, Monoclinic, space group *P*2₁/*c*, *a* = 13.3179(5) Å, *b* = 9.3373(4) Å, *c* = 16.7050(8) Å, β = 105.759(2)°, *V* = 1999.24(15) Å³, *Z* = 2, *D*_c = 1.271 Mg/m³, μ(Mo) = 1.526 mm⁻¹, *F*(000) = 808, 2θ_{max} = 106.6°, 17195 reflections, 2315 independent reflections [*R*_{int} = 0.0592], *R*1 = 0.0468, *wR*2 = 0.1139 and GOF = 1.078 for 2317 reflections (253 parameters) with *I* > 2σ(*I*), *R*1 = 0.0625, *wR*2 = 0.1228 and GOF = 1.078 for all reflections, max/min residual electron density +0.332/-0.402 eÅ⁻³.



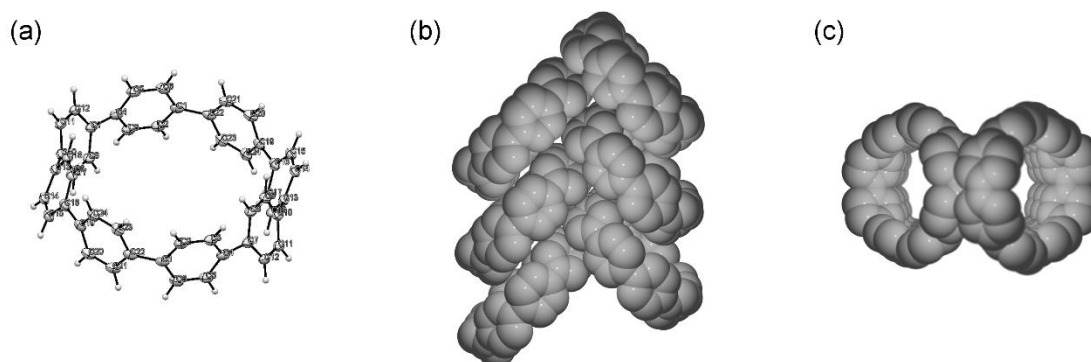
Supplementary Figure 2. ORTEP representation of X-ray crystallographic structure *N,N*-dimethyl-1,15-diaza[8]CPP ditriflate **5** (CCDC Registry #).

Crystallographic Data for **5**: $C_{56}H_{42}Cl_{18}F_6N_2O_6S_2$, $M = 1655.13$, $0.13 \times 0.08 \times 0.03$ mm, $T = 200(2)$ K, Monoclinic, space group $P2_1/c$, $a = 24.745(12)$ Å, $b = 10.384(5)$ Å, $c = 27.866(13)$ Å, $\beta = 96.257(11)^\circ$, $V = 7117(6)$ Å³, $Z = 4$, $D_c = 1.545$ Mg/m³, $\mu(\text{Mo}) = 7.445$ mm⁻¹, $F(000) = 3328$, $2\theta_{\text{max}} = 135.3^\circ$, 29341 reflections, 7210 independent reflections [$R_{\text{int}} = 0.0828$], $R1 = 0.1035$, $wR2 = 0.3177$ and $\text{GOF} = 1.036$ for 7210 reflections (667 parameters) with $I > 2\sigma(I)$, $R1 = 0.1285$, $wR2 = 0.3387$ and $\text{GOF} = 1.036$ for all reflections, max/min residual electron density $+0.649/-0.497$ eÅ⁻³.



Supplementary Figure 3. ORTEP representation of X-ray crystallographic structure **8d** (CCDC Registry #).

Crystallographic Data for **8d**: $C_{18}H_{16}Br_2N_2O_2$, $M = 452.15$, $0.22 \times 0.08 \times 0.03$ mm, $T = 100$ K, Orthorhombic, space group $Pnma$, $a = 12.562$ (10) Å, $b = 20.755$ (17) Å, $c = 6.453$ (5) Å, $V = 1682.4$ (2) Å³, $Z = 4$, $D_c = 1.785$ Mg/m³, $\mu(Cu) = 6.23$ mm⁻¹, $F(000) = 896$, $2\theta_{max} = 131.68^\circ$, 16796 reflections, 1497 independent reflections [$R_{int} = 0.0468$], $R1 = 0.0308$, $wR2 = 0.0806$ and $GOF = 0.930$ for 1497 reflections (110 parameters) with $I > 2\sigma(I)$, $R1 = 0.0333$, $wR2 = 0.0806$ and $GOF = 0.930$ for all reflections, max/min residual electron density $+0.89/-0.39$ eÅ³.

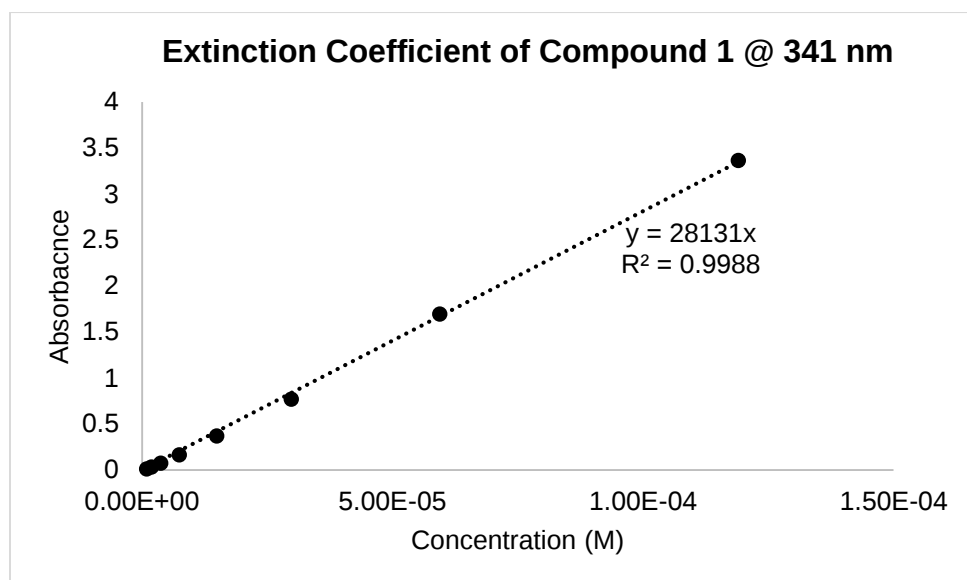


Supplementary Figure 4. Published crystallographic information for [8]CPP. (a) ORTEP representation of X-ray crystallographic structure [8]CPP (CCDC Registry 871414)⁵ (b) side-on packing (c) and top-down packing.

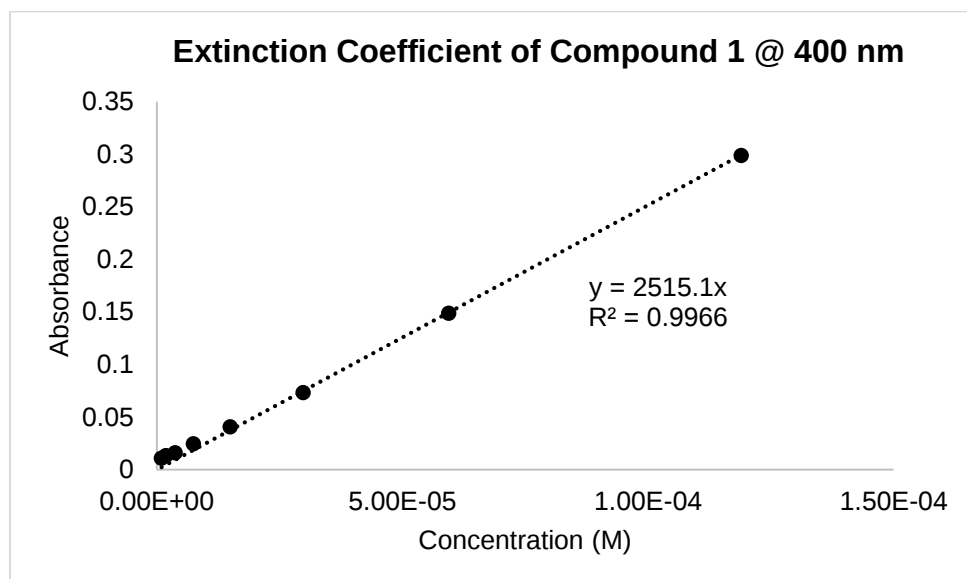
Cyclic Voltammetry Data

Cyclic voltammetry was conducted utilizing a platinum working electrode, platinum counter electrode, and a silver wire pseudoreference that was separated from the solution via a glass frit. Experiments were performed using a custom designed potentiostat at a scan rate of 50 mV/s. Analyte solutions were freeze-pump-thaw degassed three times and all experiments were conducted under airfree conditions. Analyte solutions were prepared using 0.1M tetrabutylammonium tetrafluoroborate in THF, with analyte concentrations 1-5mM. The Ag pseudoreference was calibrated versus the ferrocene/ferrocinium redox couple following the CV of each compound.

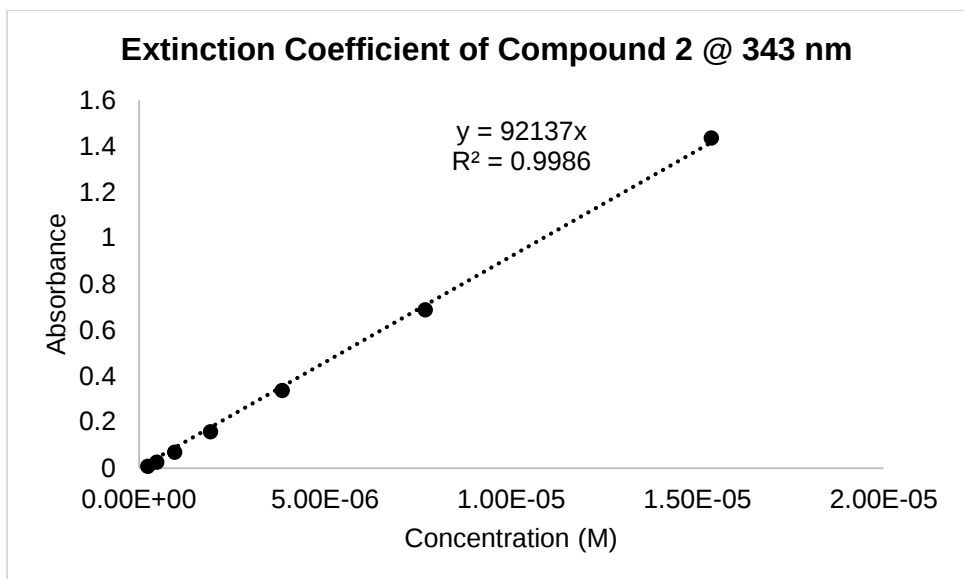
Photophysical Data:



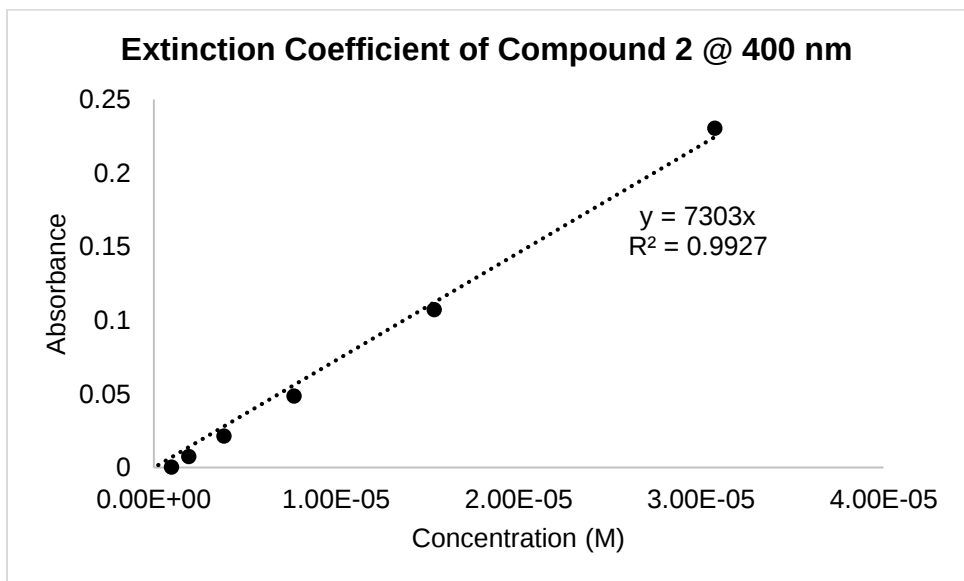
Supplementary Figure 5. Beer-Lambert plot of **1** at 341 nm. ($\epsilon = 2.8 \times 10^4 \text{ M}^{-1} \text{ cm}^{-1}$)



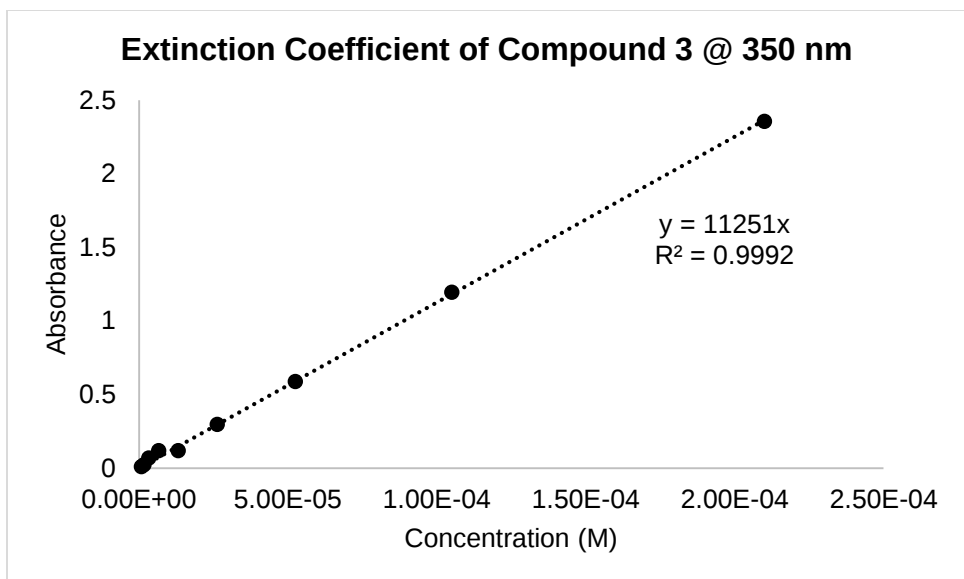
Supplementary Figure 6. Beer-Lambert plot of **1** at 400 nm. ($\epsilon = 0.25 \times 10^4 \text{ M}^{-1} \text{ cm}^{-1}$)



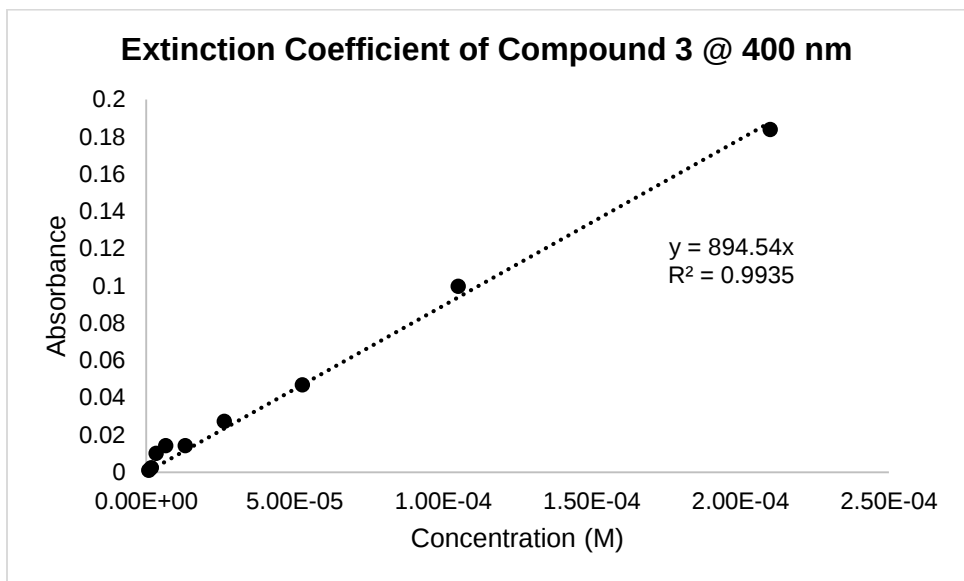
Supplementary Figure 7. Beer-Lambert plot of **2** at 343 nm. ($\epsilon = 9.2 \times 10^4 \text{ M}^{-1} \text{ cm}^{-1}$)



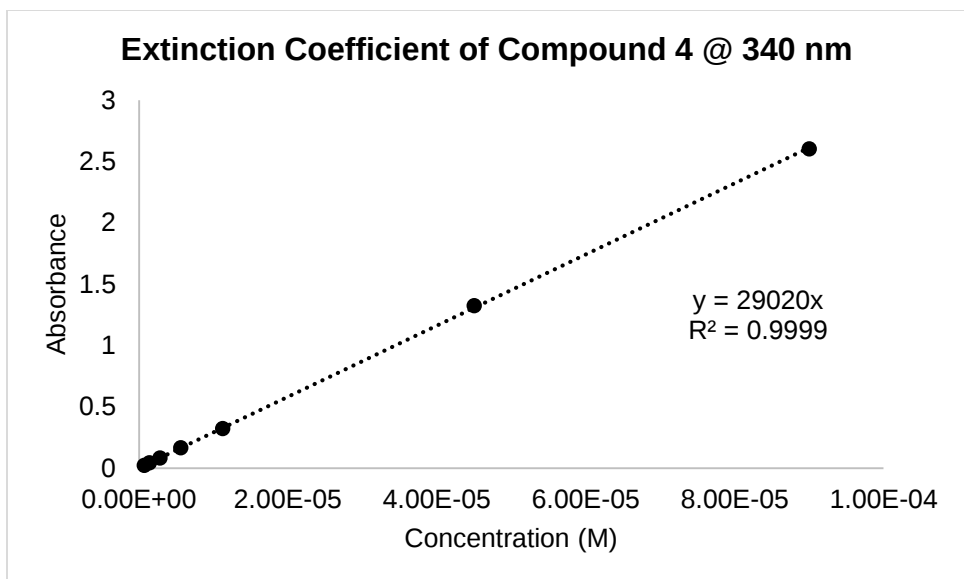
Supplementary Figure 8. Beer-Lambert plot of **2** at 400 nm. ($\epsilon = 0.73 \times 10^4 \text{ M}^{-1} \text{ cm}^{-1}$)



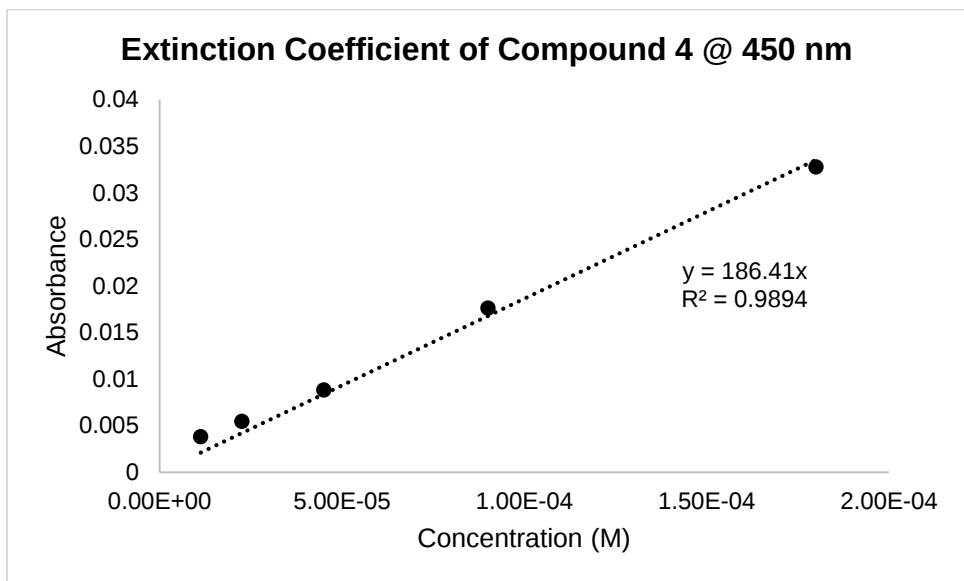
Supplementary Figure 9. Beer-Lambert plot of **3** at 350 nm. ($\epsilon = 1.1 \times 10^4 \text{ M}^{-1} \text{ cm}^{-1}$)



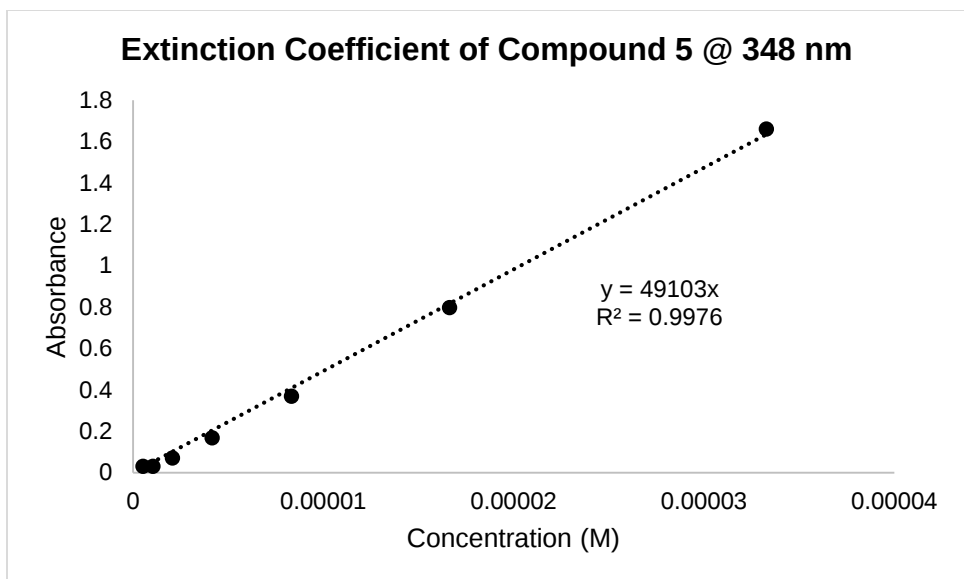
Supplementary Figure 10. Beer-Lambert plot of **3** at 400 nm. ($\epsilon = 0.089 \times 10^4 \text{ M}^{-1} \text{ cm}^{-1}$)



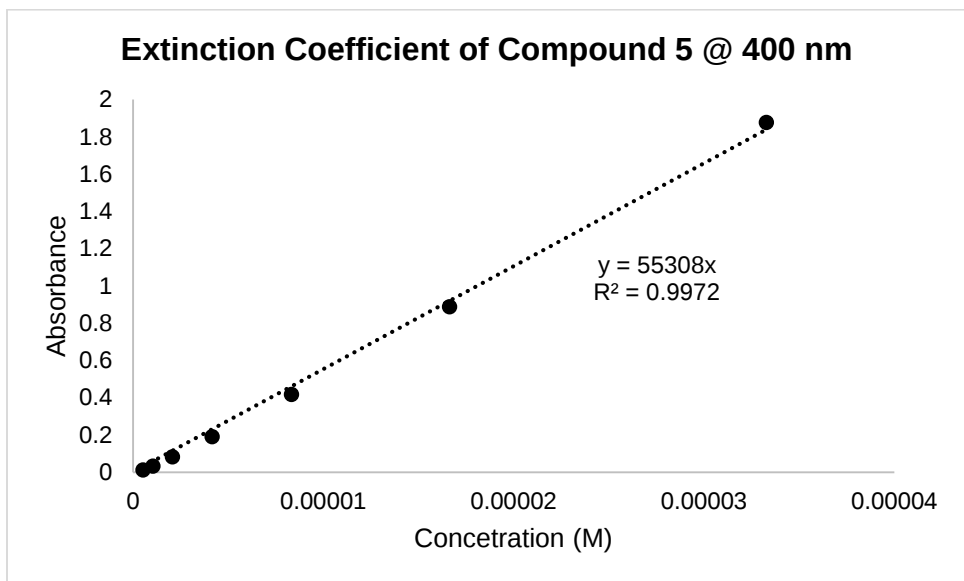
Supplementary Figure 11. Beer-Lambert plot of **4** at 340 nm. ($\epsilon = 2.9 \times 10^4 \text{ M}^{-1} \text{ cm}^{-1}$)



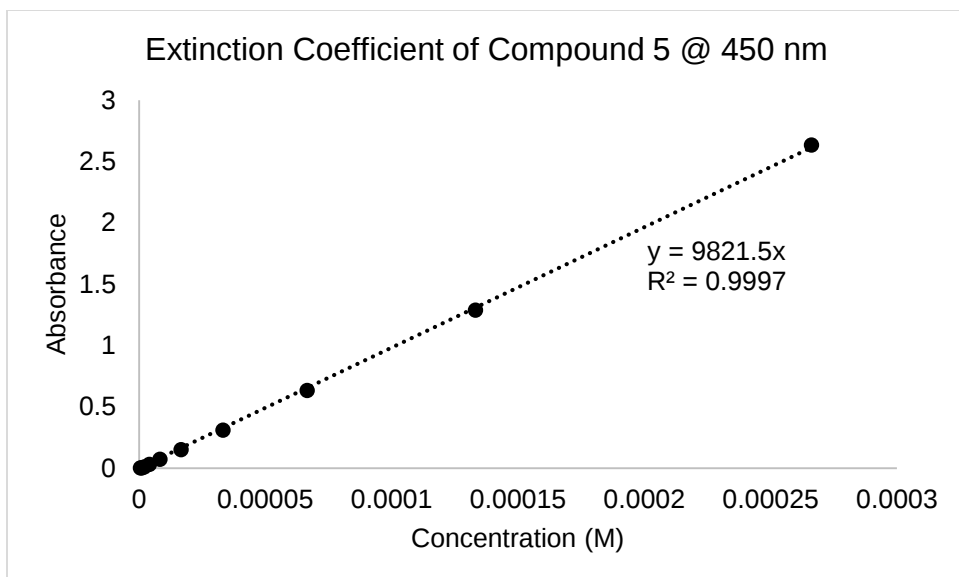
Supplementary Figure 12. Beer-Lambert plot of **4** at 450 nm. ($\epsilon = 0.019 \times 10^4 \text{ M}^{-1} \text{ cm}^{-1}$)



Supplementary Figure 13. Beer-Lambert plot of 5 at 348 nm. ($\epsilon = 4.9 \times 10^4 \text{ M}^{-1} \text{ cm}^{-1}$)



Supplementary Figure 14. Beer-Lambert plot of 5 at 400 nm. ($\epsilon = 5.5 \times 10^4 \text{ M}^{-1} \text{ cm}^{-1}$)



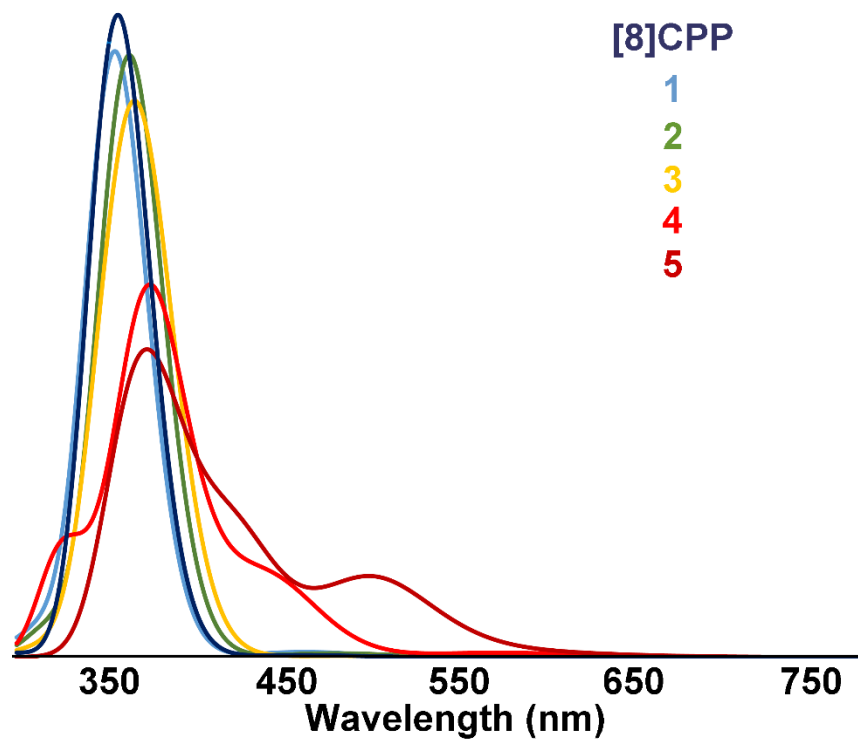
Supplementary Figure 15. Beer-Lambert plot of **5** at 450 nm. ($\epsilon = 0.98 \times 10^4 \text{ M}^{-1} \text{ cm}^{-1}$)

Computation details:

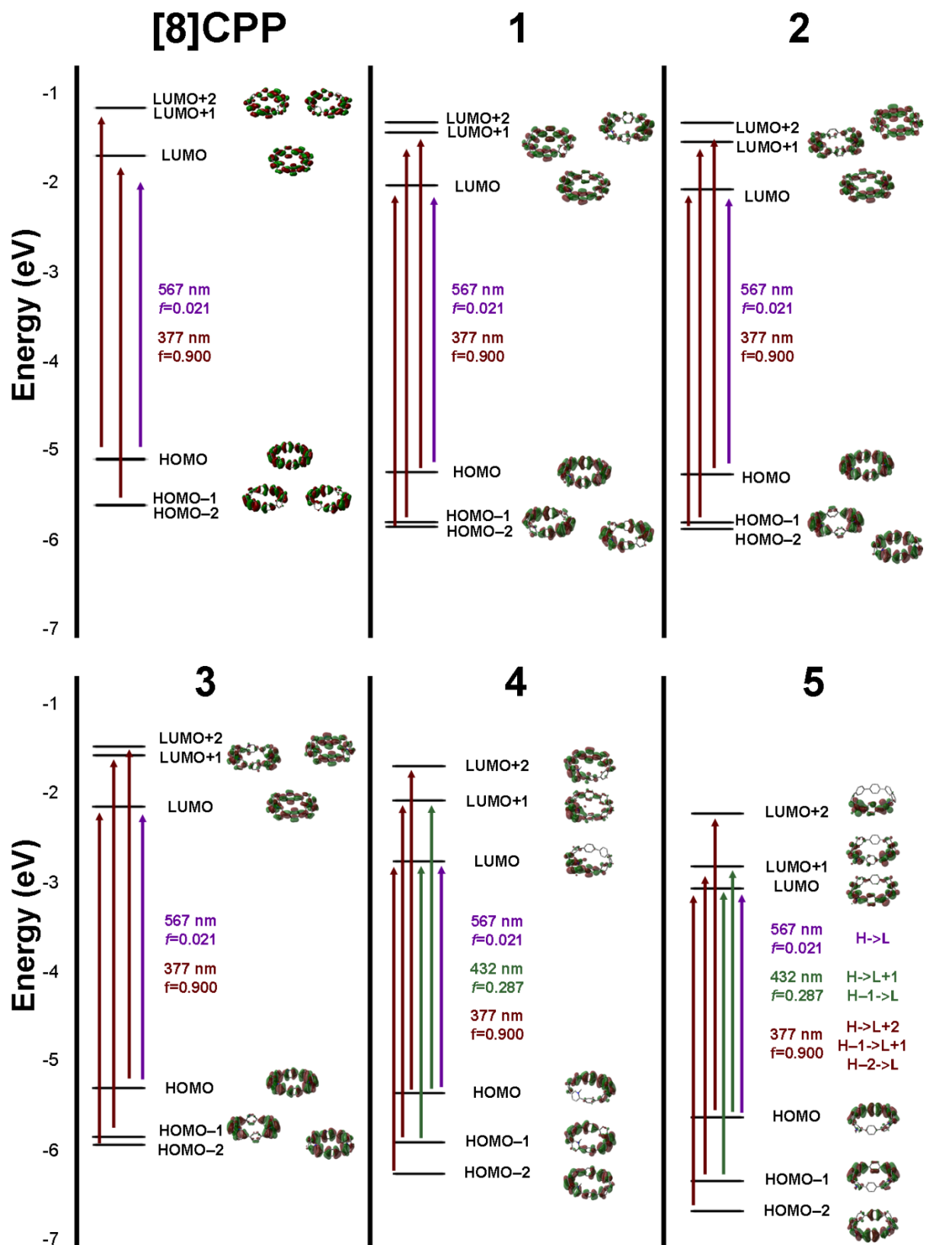
All calculations were carried out with Gaussian 09 package at B3LYP/6-31g* level of theory.⁶ Geometries were first optimized in the gas phase. Once optimized a single point calculation was carried out using the CPCM solvation model with acetonitrile as the solvent continuum to account for charged species.⁷ All excited state calculations (TD-DFT) were performed on fully optimized structures. The fully optimized structures were confirmed to be true minima by vibrational analysis. Structures were minimized with no symmetry restrictions.

Calculated Optical Transitions using TD-DFT B3LYP/6-31g*

TD-DFT Absorbance (B3LYP/6-31g*)



Supplementary Figure 16. TD-DFT (B3LYP/6-31g*) plot for compounds 1-5 and [8]CPP.



Supplementary Figure 17. TD-DFT (B3LYP/6-31g*) major transitions and orbital densities for compounds **1-5** and **[8]CPP**.

Energy (cm ⁻¹)	Wavelength (nm)	Osc. Strength	Major contributions
21813	458	0.0252	HOMO->LUMO (97%)
27563	363	0.2349	H-1->LUMO (76%), HOMO->L+1 (22%)
27841	359	0.4107	H-2->LUMO (37%), H-1->LUMO (14%), HOMO->L+1 (44%)
28068	356	1.4312	H-2->LUMO (60%), HOMO->L+1 (32%)
28800	347	1.092	HOMO->L+2 (96%)
31438	318	0.0443	HOMO->L+3 (81%)
31728	315	0.0577	H-2->L+1 (14%), H-2->L+2 (17%), H-1->L+1 (59%)
32008	312	0.0296	H-2->L+1 (44%), H-1->L+1 (17%), H-1->L+2 (26%)
33290	300	0.0036	H-5->LUMO (12%), HOMO->L+4 (58%)
33354	300	0.0187	H-3->LUMO (36%), H-1->L+2 (13%)
33876	295	0.0021	H-2->L+1 (33%), H-1->L+2 (48%)
33996	294	0.0146	H-2->L+2 (65%), H-1->L+1 (17%)

Supplementary Table 1: Major electronic transitions for Aza[8]CPP **1** determined by TD-DFT method using B3LYP/6-31g*

Energy (cm ⁻¹)	Wavelength (nm)	Osc. Strength	Major contributions
21813	458	0.0252	HOMO->LUMO (97%)
27563	363	0.2349	H-1->LUMO (76%), HOMO->L+1 (22%)
27841	359	0.4107	H-2->LUMO (37%), H-1->LUMO (14%), HOMO->L+1 (44%)
28068	356	1.4312	H-2->LUMO (60%), HOMO->L+1 (32%)
28800	347	1.092	HOMO->L+2 (96%)
31438	318	0.0443	HOMO->L+3 (81%)
31728	315	0.0577	H-2->L+1 (14%), H-2->L+2 (17%), H-1->L+1 (59%)
32008	312	0.0296	H-2->L+1 (44%), H-1->L+1 (17%), H-1->L+2 (26%)
33290	300	0.0036	H-5->LUMO (12%), HOMO->L+4 (58%)
33354	300	0.0187	H-3->LUMO (36%), H-1->L+2 (13%)
33876	295	0.0021	H-2->L+1 (33%), H-1->L+2 (48%)
33996	294	0.0146	H-2->L+2 (65%), H-1->L+1 (17%)

Supplementary Table 2: Major electronic transitions for 1,15-diaza[8]CPP **2** determined by TD-DFT method using B3LYP/6-31g*

Energy (cm ⁻¹)	Wavelength (nm)	Osc. Strength	Major contributions
20895	479	0.0056	HOMO->LUMO (97%)
26474	378	0.3135	H-1->LUMO (10%), HOMO->L+1 (88%)
26966	371	1.2147	H-1->LUMO (87%)
27332	366	0.6758	H-2->LUMO (95%)

28522	351	1.0314	HOMO->L+2 (97%)
30548	327	0.0113	H-1->L+1 (84%)
30865	324	0.018	H-2->L+1 (77%), H-1->L+2 (19%)
31323	319	0.0111	HOMO->L+3 (78%)
31671	316	0.0148	HOMO->L+4 (77%)
32907	304	0.0029	HOMO->L+5 (61%)
32973	303	0.011	H-5->LUMO (10%), H-3->LUMO (30%), HOMO->L+5 (13%)
33348	300	0.007	H-2->L+1 (14%), H-1->L+2 (63%)

Supplementary Table 3: Major electronic transitions for 1,15,31-triaza[8]CPP **3** determined by TD-DFT method using B3LYP/6-31g*

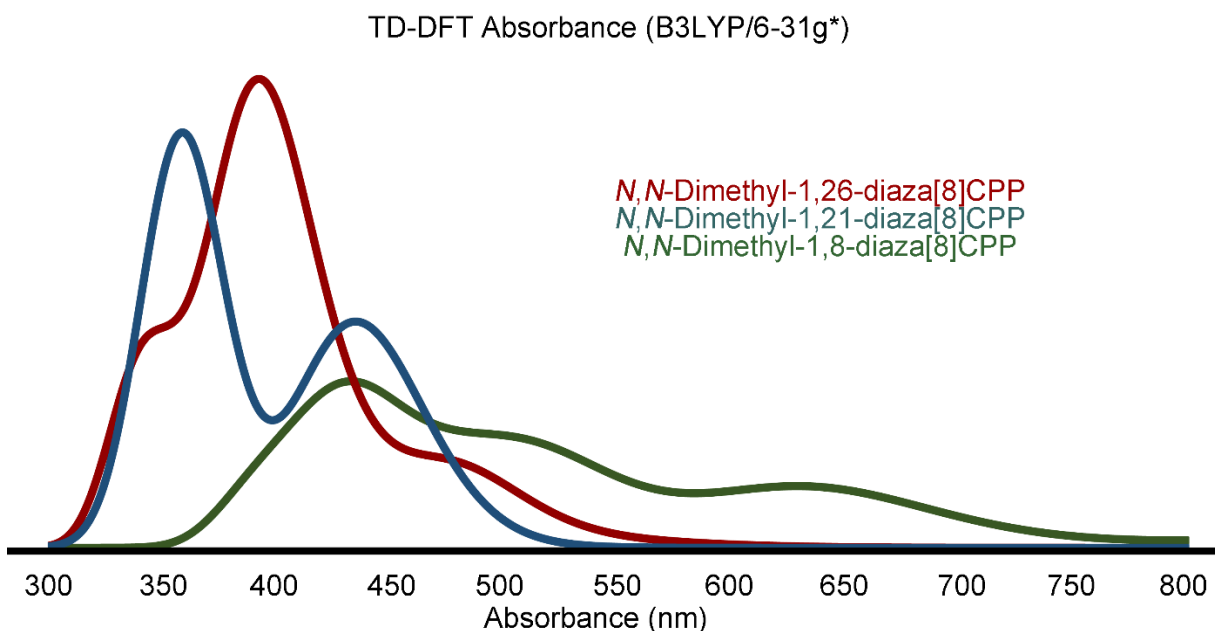
Energy (cm-1)	Wavelength (nm)	Osc. Strength	Major contributions
17642	567	0.0211	HOMO->LUMO (97%)
22549	443	0.2872	H-1->LUMO (96%)
23135	432	0.0754	HOMO->L+1 (91%)
24872	402	0.2284	H-2->LUMO (86%)
26530	377	0.9003	HOMO->L+2 (81%)
26958	371	0.6285	HOMO->L+3 (92%)
27713	361	0.3411	H-1->L+1 (96%)
30261	330	0.1507	H-2->L+1 (90%)
30575	327	0.0542	H-3->LUMO (81%)
30753	325	0.0062	H-4->LUMO (76%)
30829	324	0.3272	H-1->L+2 (80%)
31115	321	0.0277	H-1->L+3 (80%)

Supplementary Table 4: Major electronic transitions for *N*-methylaza[8]CPP Triflate **4** determined by TD-DFT method using B3LYP/6-31g*

Energy (cm-1)	Wavelength (nm)	Osc. Strength	Major contributions
17128.11	583.8356	0.021	HOMO->LUMO (97%)
20140.61	496.5093	0.3892	HOMO->L+1 (100%)
23722.54	421.54	0.5499	H-1->LUMO (96%)
24537.17	407.545	0.027	HOMO->L+2 (86%)
24910.61	401.4354	0.026	H-2->LUMO (24%), H-1->L+1 (49%), HOMO->L+3 (11%)
25917.19	385.8443	0.1648	H-2->LUMO (57%), H-1->L+1 (39%)

26478.56	377.6641	0.7374	HOMO->L+3 (84%)
27597.26	362.3549	0.5307	HOMO->L+4 (91%)
27845.68	359.1222	0.2789	H-2->L+1 (94%)
29147.47	343.083	0.0067	H-3->LUMO (89%)
29804.01	335.5254	0.0012	H-4->LUMO (79%)
30058.07	332.6893	0.0075	H-1->L+2 (95%)

Supplementary Table 5: Major electronic transitions for *N,N*-dimethylaza[8]CPP Ditriflate **5** determined by TD-DFT method using B3LYP/6-31g*



Supplementary Figure 18: TD-DFT (B3LYP/6-31g*) plots for theoretical structures *N,N*-Dimethyl-1,26-diaza[8]CPP, *N,N*-Dimethyl-1,21-diaza[8]CPP, and *N,N*-Dimethyl-1,8-diaza[8]CPP.

Energy (cm-1)	Wavelength (nm)	Osc. Strength	Major contribs
20050.28	498.7463	0.0006	HOMO->LUMO (96%)
22248.15	449.4756	0.3873	HOMO->L+1 (98%)
23544.29	424.7314	0.4828	H-1->LUMO (97%)
24300.04	411.522	0.001	H-1->L+1 (95%)
26658.42	375.116	0.0032	HOMO->L+2 (92%)
27455.3	364.2284	0.3974	H-2->LUMO (89%)
27720.66	360.7418	0.7907	HOMO->L+3 (91%)
28378.81	352.3755	0.0047	H-2->L+1 (87%)
29091.81	343.7393	0.3808	H-1->L+2 (95%)

29895.15	334.5025	0.0001	H-1->L+3 (87%)
30956.58	323.0331	0.0001	H-3->LUMO (86%)
31111.44	321.4252	0.0129	H-4->LUMO (85%)

Supplementary Table 5: Major electronic transitions for *N,N*-Dimethyl-1,26-diaza[8]CPP determined by TD-DFT method using B3LYP/6-31g*

Energy (cm-1)	Wavelength (nm)	Osc. Strength	Major contribs
18031.46	554.5864	0.0182	HOMO->LUMO (96%)
20902	478.4231	0.2643	HOMO->L+1 (98%)
23527.36	425.0371	0.1906	H-1->LUMO (74%), HOMO->L+2 (19%)
24769.46	403.723	0.587	H-1->LUMO (21%), HOMO->L+2 (72%)
25784.92	387.8236	0.5172	H-2->LUMO (79%)
25867.19	386.5902	0.146	H-1->L+1 (30%), HOMO->L+3 (64%)
26030.92	384.1586	0.389	H-2->LUMO (16%), H-1->L+1 (57%), HOMO->L+3 (25%)
27589.19	362.4608	0.0975	H-2->L+1 (86%)
29068.42	344.0159	0.5039	HOMO->L+4 (90%)
29570.91	338.1702	0.0016	H-3->LUMO (91%)
29945.96	333.9349	0.1504	H-1->L+2 (94%)
30617.02	326.6157	0.0021	H-4->LUMO (70%), H-3->L+1 (14%)

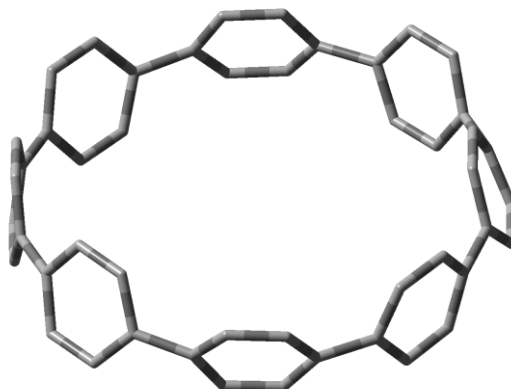
Supplementary Table 6: Major electronic transitions for *N,N*-Dimethyl-1,21-diaza[8]CPP determined by TD-DFT method using B3LYP/6-31g*

Energy (cm-1)	Wavelength (nm)	Osc. Strength	Major contribs
10786.93	927.0475	0.0437	HOMO->LUMO (99%)
15746.47	635.0629	0.2011	H-1->LUMO (99%)
19117.09	523.0923	0.2372	H-2->LUMO (91%)
20606.8	485.2767	0.0869	HOMO->L+1 (98%)
20860.87	479.3664	0.114	HOMO->L+2 (88%)
23061.16	433.6295	0.4661	HOMO->L+3 (98%)
23502.35	425.4893	0.002	H-3->LUMO (95%)
23957.25	417.4101	0.0031	H-6->LUMO (11%), H-4->LUMO (87%)
24416.18	409.5644	0.0037	H-5->LUMO (91%)
24540.39	407.4914	0.0351	H-1->L+1 (95%)
24807.37	403.1061	0.0026	H-6->LUMO (80%), H-4->LUMO (12%)
25446.16	392.9866	0.189	H-7->LUMO (45%), H-1->L+2 (49%)

Supplementary Table 7: Major electronic transitions for *N,N*-Dimethyl-1,8-diaza[8]CPP determined by TD-DFT method using B3LYP/6-31g*

Minimized Geometries

Dipole moments are shown pictorially and numerically



[8]CPP

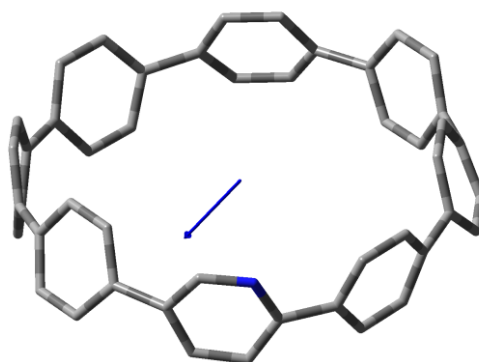
Calculated Dipole: 0.0085 D

C	-5.24779	1.26112	-0.58206
C	-4.72856	2.5419	-0.75326
C	-4.42158	3.36301	0.3514
C	-4.89724	2.92482	1.60214
C	-5.42765	1.65228	1.77292
C	-5.50345	0.74429	0.70221
H	-5.38101	0.62585	-1.45418
H	-4.48099	2.86906	-1.75906
H	-4.7186	3.52101	2.49031
H	-5.63686	1.30775	2.78132
C	-3.41314	4.49746	-0.09638
C	-2.69183	4.4503	1.11261
C	-2.86142	5.3042	-1.11094
C	-1.38914	4.92951	1.19652
H	-3.10504	3.93465	1.97404
C	-1.57149	5.81381	-1.01439
H	-3.39374	5.43877	-2.04725

C	-0.7477	5.51544	0.08822
H	-0.82689	4.72681	2.10284
H	-1.16903	6.36108	-1.86158
C	-5.52744	-0.72669	-0.09491
C	-5.02433	-1.65834	0.83285
C	-5.70961	-1.18475	-1.41157
C	-4.52412	-2.89009	0.41825
H	-4.94927	-1.38569	1.88258
C	-5.19827	-2.40814	-1.82592
H	-6.11489	-0.51069	-2.1604
C	-4.48476	-3.24449	-0.94614
H	-4.08127	-3.5453	1.16292
H	-5.23096	-2.63653	-2.88563
C	5.68517	1.57218	-0.92697
C	5.14918	2.85702	-0.94803
C	4.43162	3.36486	0.15263
C	4.4871	2.61854	1.34317
C	5.02058	1.33457	1.36334
C	5.52606	0.7357	0.19511
H	6.16064	1.18521	-1.82456
H	5.21757	3.44176	-1.86181
H	3.96452	2.9779	2.22471
H	4.89534	0.73631	2.26071
C	5.52539	-0.74798	0.09942
C	5.65755	-1.58477	1.22476
C	5.04469	-1.34572	-1.07978
C	5.11828	-2.86838	1.23386
H	6.1138	-1.19883	2.13271
C	4.50792	-2.62846	-1.07151
H	4.94084	-0.74721	-1.97972

C	4.42423	-3.3746	0.1175
H	5.16498	-3.45323	2.14894
H	4.00426	-2.98664	-1.96446
C	3.36401	-4.40945	0.23364
C	2.88995	-5.15874	-0.8602
C	2.56793	-4.41557	1.39264
C	1.60219	-5.68999	-0.86721
H	3.50665	-5.26317	-1.74935
C	1.28095	-4.93711	1.38136
H	2.89629	-3.86703	2.27017
C	0.71984	-5.48764	0.21358
H	1.25579	-6.1997	-1.76204
H	0.65971	-4.77305	2.25518
C	-3.38892	-4.4211	-0.2003
C	-2.27984	-4.44627	-1.06833
C	-1.07209	-5.01698	-0.68194
C	-0.91578	-5.6264	0.57793
C	-2.10002	-5.84653	1.30767
C	-3.29827	-5.24615	0.93794
H	-2.31762	-3.91844	-2.01631
H	-0.20864	-4.87048	-1.32352
H	-2.06947	-6.40538	2.23824
H	-4.13978	-5.3262	1.61883
C	0.73511	5.48629	-0.02597
C	1.32082	4.93435	-1.18095
C	2.60652	4.40987	-1.16353
C	3.37661	4.4021	0.01289
C	2.87999	5.15253	1.09589
C	1.5936	5.68671	1.0742
H	0.71877	4.77165	-2.06835

H	2.9531	3.86047	-2.0335
H	3.47694	5.25561	1.99857
H	1.2285	6.19726	1.96109



Aza[8]CPP 1

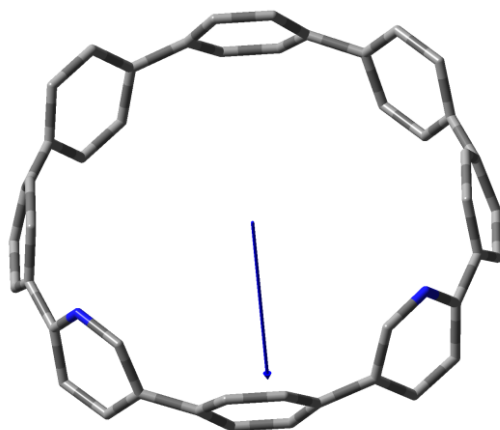
Dipole: 2.9265 D

C	5.52888	2.15328	1.06614
H	5.6616	2.76786	1.95132
C	4.91116	2.70047	-0.07999
C	4.00676	3.88246	-0.01544
C	3.26745	4.10505	1.16538
H	3.55752	3.60164	2.08117
C	2.05889	4.79839	1.1408
H	1.44927	4.81269	2.0379
C	1.53022	5.30134	-0.06618
C	0.05691	5.48691	-0.17715
C	-0.75786	5.81577	0.92801
H	-0.31432	6.2804	1.80354
C	-2.10968	5.46802	0.95662
H	-2.68606	5.67405	1.85331
C	-2.708	4.7713	-0.11653
C	3.91301	-3.95993	0.25618
C	4.04774	-3.15308	1.40673
H	3.4603	-3.3685	2.29129

C	4.7767	-1.96722	1.3808
H	4.72541	-1.30763	2.2403
C	5.40617	-1.52114	0.20023
C	5.63045	-0.05896	0.03047
C	5.24122	0.54538	-1.1831
H	5.0599	-0.07498	-2.0543
C	4.88875	1.89267	-1.23642
H	4.44428	2.27612	-2.1484
C	3.59345	4.58753	-1.16703
H	4.18486	4.52779	-2.07564
C	2.38145	5.27994	-1.19248
H	2.05751	5.7421	-2.12007
C	4.74333	-3.6325	-0.83989
H	4.76277	-4.27296	-1.71574
C	5.46738	-2.43895	-0.87034
H	6.02205	-2.1823	-1.76798
C	-0.59788	5.00038	-1.32778
H	-0.01577	4.75004	-2.20804
C	-1.94575	4.65006	-1.29768
H	-2.36598	4.13876	-2.1564
C	5.87861	0.803	1.12096
H	6.27285	0.39705	2.04778
C	-5.38672	-1.85806	-1.10595
H	-5.44122	-2.25688	-2.11411
C	-4.92091	-2.65389	-0.03304
C	-3.97834	-3.78053	-0.24113
C	-3.15327	-3.76073	-1.38593
H	-3.37714	-3.07874	-2.19827
C	-1.50595	-5.22041	-0.32181
C	-0.04799	-5.49111	-0.18557

C	0.81948	-5.43669	-1.298
H	0.42116	-5.54894	-2.30094
C	2.16568	-5.10923	-1.14813
H	2.75402	-4.93676	-2.04244
C	2.72293	-4.84879	0.12347
C	-3.90705	3.90495	0.05479
C	-5.3552	2.20838	-0.94677
H	-5.79651	1.76323	-1.83022
C	-5.40473	1.48899	0.26634
C	-5.65617	0.02701	0.25262
C	-5.55225	-0.7875	1.39881
H	-5.66158	-0.37107	2.39306
C	-5.14756	-2.11343	1.24979
H	-4.89918	-2.69121	2.13391
C	-3.63577	-4.70366	0.77133
H	-4.28328	-4.82536	1.63452
C	-2.42975	-5.40721	0.73079
H	-2.17554	-6.05534	1.56365
C	-4.14519	3.30011	1.30755
H	-3.63318	3.67107	2.18866
C	-4.88029	2.12102	1.41228
H	-4.92463	1.62984	2.37796
C	0.56447	-5.47849	1.08629
H	-0.04394	-5.57645	1.97914
C	1.91881	-5.18194	1.23565
H	2.32155	-5.10502	2.23978
C	-1.95284	-4.46166	-1.42485
H	-1.29242	-4.29625	-2.26769
H	-4.55457	3.88269	-2.01309
C	-4.63157	3.39539	-1.04624

N -5.7064 -0.56331 -0.97307



1,15-Diaza[8]CPP 2

Dipole: 4.6799 D

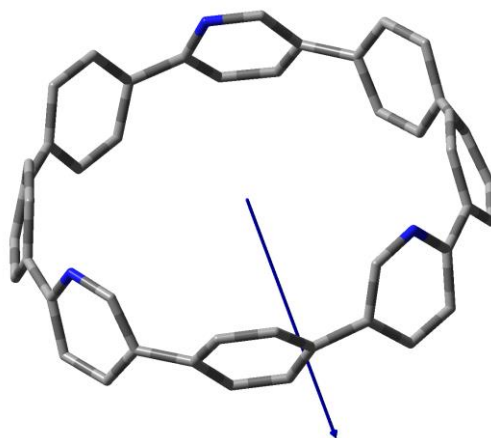
C	-0.6875	5.82207	1.115
H	-1.21399	6.09464	2.02609
C	-1.41573	5.37544	-0.00493
C	-2.78114	4.79804	0.10262
C	-3.11413	4.08497	1.26822
H	-2.49701	4.19085	2.15521
C	-4.09044	3.09609	1.25433
H	-4.19864	2.46667	2.13202
C	-4.78517	2.77131	0.07493
C	-5.35489	1.40571	-0.06315
C	-5.75175	0.63605	1.04766
H	-5.97627	1.12546	1.99147
C	-5.74714	-0.75503	0.99747
H	-5.95104	-1.30324	1.91277
C	-5.36078	-1.43712	-0.17166
C	4.7935	2.7573	0.07481

C	4.0997	3.08404	1.25421
H	4.20608	2.45428	2.13188
C	3.12624	4.07573	1.26812
H	2.50944	4.18338	2.15511
C	2.79532	4.78978	0.10255
C	1.43161	5.37119	-0.00496
C	0.70284	5.15932	-1.18909
H	1.22064	4.83042	-2.08509
C	-0.68761	5.16141	-1.18908
H	-1.20639	4.83403	-2.08507
C	-3.63384	4.63203	-1.00603
H	-3.47695	5.22936	-1.90054
C	-4.61383	3.64279	-1.01897
H	-5.19878	3.4954	-1.92294
C	4.62465	3.62929	-1.01908
H	5.20914	3.4802	-1.92308
C	3.6475	4.62133	-1.00612
H	3.49232	5.21913	-1.90062
C	-5.19711	0.72027	-1.28313
H	-4.9216	1.27214	-2.17668
C	-5.20151	-0.66699	-1.33798
H	-4.93854	-1.17186	-2.26012
C	0.70473	5.81998	1.11499
H	1.23204	6.091	2.02606
C	0.68773	-5.78844	-0.95345
H	1.21243	-6.11729	-1.84639
C	1.41635	-5.28594	0.14237
C	2.79889	-4.76397	0.02076
C	3.20291	-4.14692	-1.18119
H	2.66632	-4.35027	-2.10621

C	4.7896	-2.82724	-0.14126
C	5.35639	-1.45282	-0.1717
C	5.19903	-0.68228	-1.338
H	4.93425	-1.18641	-2.26003
C	5.19887	0.70499	-1.28323
H	4.92473	1.25766	-2.17672
C	5.35912	1.39001	-0.06335
C	-4.79802	-2.81318	-0.14143
C	-3.21493	-4.13712	-1.18137
H	-2.67867	-4.34174	-2.10631
C	-2.81296	-4.75567	0.0205
C	-1.43199	-5.28172	0.14222
C	-0.70209	-4.98608	1.30795
H	-1.22027	-4.60664	2.18367
C	0.68721	-4.98813	1.30802
H	1.20641	-4.61021	2.18379
C	3.65254	-4.5436	1.11479
H	3.48245	-5.06342	2.05432
C	4.66432	-3.59183	1.03357
H	5.27553	-3.38453	1.90597
C	-4.67524	-3.57847	1.03321
H	-5.28609	-3.36968	1.9055
C	-3.66619	-4.53315	1.11441
H	-3.49781	-5.05374	2.05383
C	5.74522	-0.77185	0.99725
H	5.94789	-1.32063	1.91248
C	5.75404	0.61923	1.04738
H	5.98037	1.10801	1.99108
C	-0.70474	-5.78636	-0.95353
H	-1.23033	-6.11365	-1.84651

N -4.15236 -3.20132 -1.26099

N 4.14307 -3.21384 -1.26085



1,15,31-Triaza[8]CPP 3

Dipole: 6.8770 D

C 1.83155 -5.48384 0.92901

H 2.41205 -5.62526 1.83609

C 2.43041 -4.94301 -0.2243

C 3.69001 -4.15393 -0.17423

C 4.4118 -3.91767 1.01045

H 4.30486 -4.56779 1.87272

C 5.17206 -2.75697 1.11684

H 5.64436 -2.51279 2.06508

C 5.24923 -1.86082 0.03783

C 5.50996 -0.40859 0.18603

C 5.05763 0.23573 1.35189

H 4.76584 -0.35735 2.21357

C 4.7925 1.59941 1.36402

H 4.30227 2.0244 2.23477

C 4.96765 2.38668 0.21144

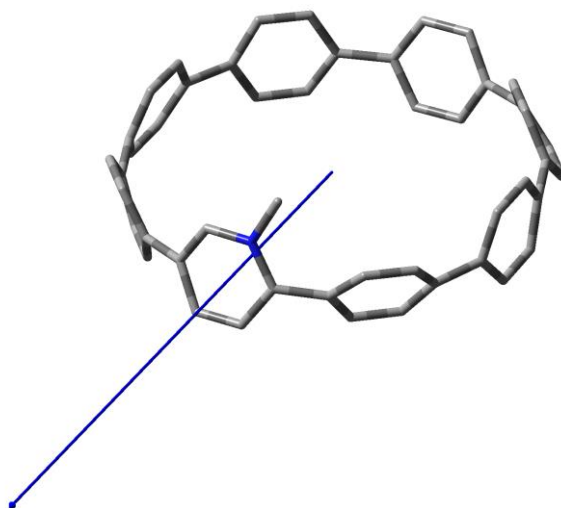
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C -3.4126 -3.77639 1.28311

H -3.62628 -3.21547 2.18804

C	-2.25136	-4.5371	1.23493
H	-1.60098	-4.54256	2.10387
C	-1.81447	-5.12815	0.03548
C	-0.36912	-5.43547	-0.12053
C	0.27141	-5.11396	-1.33225
H	-0.32485	-4.90532	-2.21533
C	1.63836	-4.87594	-1.38491
H	2.08575	-4.49589	-2.29582
C	-3.87942	-4.33914	-1.00034
H	-4.50762	-4.28436	-1.88543
C	-2.71435	-5.10058	-1.04818
H	-2.46479	-5.6201	-1.96946
C	5.89086	0.41592	-0.89054
H	6.33024	-0.02599	-1.78081
C	5.62691	1.78303	-0.87749
H	5.86819	2.37245	-1.75786
C	0.46258	-5.73101	0.97694
H	0.02384	-6.07276	1.91049
C	-1.62315	4.82382	-1.35243
H	-2.0774	4.40604	-2.24489
C	-2.36907	4.90435	-0.16054
C	-3.61889	4.10924	-0.03415
C	-4.34732	3.67225	-1.16048
H	-4.21717	4.17373	-2.11516
C	-5.27622	1.80167	0.08647
C	-5.61075	0.35565	0.06255
C	-5.08841	-1.57547	-1.0869
H	-4.79128	-2.00417	-2.04217
C	-5.06158	-2.3641	0.08253
C	4.18396	3.63932	0.08454

C	1.88444	5.1908	-0.12897
C	0.4241	5.46002	-0.20349
C	-0.35762	5.75509	0.92934
H	0.10954	6.10967	1.84375
C	-1.72467	5.49169	0.94642
H	-2.27766	5.6661	1.86519
C	-3.92623	3.4956	1.19419
H	-3.40653	3.80321	2.09599
C	-4.74117	2.36999	1.2548
H	-4.83134	1.84737	2.20252
C	3.75403	4.40902	1.17861
H	4.26293	4.33091	2.13606
C	2.61624	5.20312	1.07297
H	2.25326	5.73613	1.94576
C	-5.9135	-0.39601	1.21217
H	-6.28968	0.08594	2.10957
C	-5.6161	-1.75516	1.22146
H	-5.74897	-2.32648	2.13672
C	-0.26324	5.09818	-1.37603
H	0.31178	4.90064	-2.27294
C	-5.14194	2.53355	-1.10757
H	-5.58254	2.13997	-2.01729
N	-5.33663	-0.2702	-1.10045
N	3.96985	-3.4341	-1.28063
N	2.43683	4.66086	-1.24033
C	4.72459	-2.34772	-1.17743
H	4.84101	-1.7697	-2.09245
C	3.53969	3.93108	-1.13561
H	3.88178	3.46629	-2.05852



***N*-methylaza[8]CPP Triflate 4**

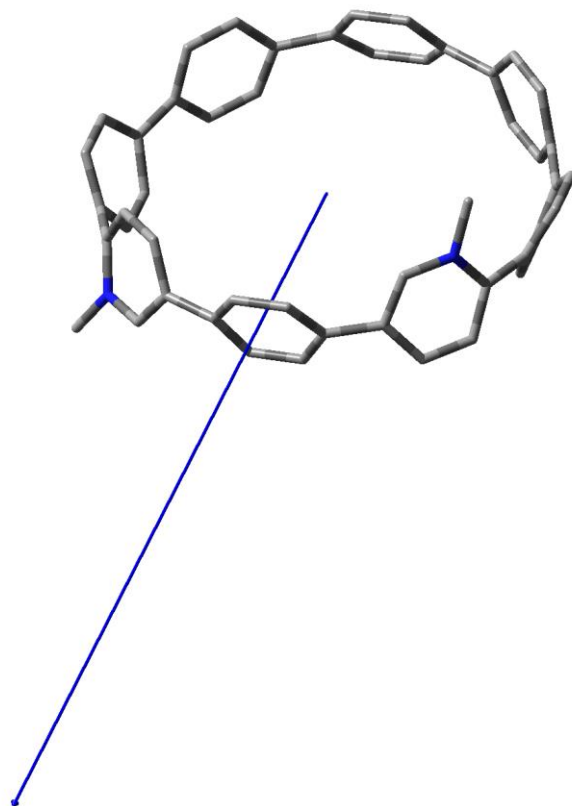
Dipole: 20.8018 D

C	3.94474	-4.60472	-0.85084
H	3.85266	-5.2555	-1.7157
C	3.03932	-4.72389	0.22397
C	1.68951	-5.32334	0.06904
C	1.1072	-5.42779	-1.21209
H	1.73231	-5.36841	-2.09671
C	-0.26958	-5.4413	-1.38041
H	-0.66932	-5.4368	-2.39033
C	-1.13819	-5.34622	-0.27428
C	-2.48119	-4.74136	-0.40009
C	-2.72612	-3.8493	-1.46416
H	-2.03125	-3.79543	-2.29402
C	-3.73048	-2.90016	-1.39511
H	-3.77628	-2.14546	-2.17312
C	-4.56104	-2.79017	-0.25584
C	5.4637	1.54744	-0.15828
C	5.24553	0.74245	-1.29243
H	4.89516	1.1874	-2.21705
C	5.29225	-0.64382	-1.21806

H	4.9741	-1.22103	-2.08106
C	5.55153	-1.29886	-0.00141
C	5.01368	-2.67097	0.17982
C	4.27964	-2.94931	1.34657
H	4.35328	-2.27916	2.19752
C	3.31315	-3.94681	1.36581
H	2.66987	-4.01434	2.23673
C	0.82324	-5.51454	1.165
H	1.22396	-5.56121	2.17256
C	-0.55712	-5.50754	0.9994
H	-1.18335	-5.50514	1.88693
C	5.96289	0.89146	0.98635
H	6.25526	1.46615	1.86003
C	5.99651	-0.49775	1.06725
H	6.30402	-0.96374	1.99981
C	-3.46395	-4.7877	0.615
H	-3.40412	-5.54568	1.39003
C	-4.47104	-3.83155	0.69538
H	-5.17738	-3.89214	1.51641
C	4.90759	-3.60048	-0.8736
H	5.53245	-3.48861	-1.75548
C	-3.64626	4.54906	0.99255
H	-3.50115	5.1098	1.91089
C	-2.78891	4.77431	-0.10791
C	-1.43664	5.35813	0.04498
C	-0.74158	5.11269	1.24366
H	-1.27963	4.76282	2.11939
C	1.41516	5.39043	0.13753
C	2.80826	4.87956	0.05999
C	3.50482	4.4514	1.2071

H	3.20686	4.80165	2.1906
C	4.50039	3.4853	1.12726
H	4.90505	3.093	2.05447
C	4.87416	2.91299	-0.10504
C	-5.20145	-1.46937	-0.10284
C	-5.09649	0.62947	1.02701
H	-4.8553	1.11169	1.96463
C	-5.29362	1.37023	-0.13293
C	-4.78419	2.75475	-0.19253
C	-4.10582	3.15139	-1.36086
H	-4.22504	2.58501	-2.28004
C	-3.13466	4.14371	-1.31891
H	-2.53325	4.31792	-2.20496
C	-0.67807	5.84195	-1.0395
H	-1.17509	6.14433	-1.9576
C	0.7116	5.87142	-0.98809
H	1.25526	6.20006	-1.86846
C	-5.68698	-0.761	-1.2208
H	-5.94847	-1.3315	-2.1045
C	-5.73627	0.62095	-1.24812
H	-6.0557	1.12856	-2.15302
C	3.35806	4.49459	-1.17823
H	2.91224	4.84329	-2.10441
C	4.37608	3.55133	-1.25799
H	4.70865	3.23876	-2.24262
C	-4.61128	3.55117	0.9581
H	-5.20159	3.35914	1.85121
N	-5.06312	-0.72864	1.05296
C	0.64538	5.12743	1.28734
H	1.12796	4.78993	2.1975

C	-4.73219	-1.36035	2.3497
H	-5.5715	-1.96851	2.68969
H	-3.84444	-1.98341	2.23989
H	-4.54201	-0.57502	3.07938



***N,N*-Dimethyl-1,15-diaza[8]CPP Ditriflate 5**

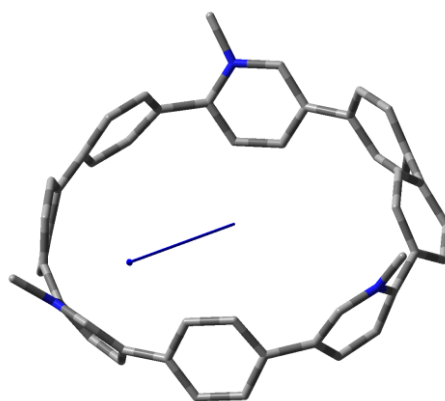
Dipole: 24.5243 D

C	1.71094	5.80444	-0.81505
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C	3.6499	4.35151	-0.02986
C	3.99491	3.92573	-1.32975
H	3.52341	4.38481	-2.19252
C	4.80873	2.82037	-1.53095
H	4.98049	2.48278	-2.54846

C	5.31389	2.08157	-0.44
C	5.60582	0.63915	-0.55534
C	5.02949	-0.09881	-1.61148
H	4.60658	0.41665	-2.46539
C	4.81544	-1.46028	-1.50715
H	4.23035	-1.94192	-2.28276
C	5.17092	-2.17617	-0.33573
C	-4.24241	3.68538	-0.00078
C	-3.62435	4.24578	-1.13979
H	-3.99512	4.01857	-2.1343
C	-2.47265	5.01084	-1.02726
H	-1.96157	5.31183	-1.93587
C	-1.88314	5.26416	0.22899
C	-0.43017	5.54572	0.32783
C	0.27941	5.03169	1.42944
H	-0.25646	4.67223	2.30107
C	1.64682	4.80803	1.36579
H	2.11707	4.28364	2.19046
C	4.38372	3.7871	1.0335
H	4.25287	4.16233	2.04346
C	5.18489	2.66976	0.83588
H	5.61783	2.18686	1.70653
C	-3.79871	4.15991	1.25253
H	-4.28137	3.82972	2.16658
C	-2.65743	4.94226	1.36286
H	-2.31535	5.22627	2.35285
C	6.21192	-0.12172	0.47385
H	6.81544	0.3723	1.22851
C	5.98984	-1.48669	0.59364
H	6.45492	-2.01215	1.41951

C	0.33905	6.02869	-0.75131
H	-0.14493	6.53442	-1.58173
C	-1.54376	-5.25337	1.21267
H	-2.06546	-5.44885	2.14519
C	-2.23313	-4.69748	0.11791
C	-3.5076	-3.95361	0.27745
C	-3.75379	-3.20609	1.45683
H	-3.1653	-3.39544	2.34857
C	-5.26845	-1.74701	0.24767
C	-5.62046	-0.34652	0.02534
C	-5.953	0.51184	1.10135
H	-6.38205	0.10071	2.01127
C	-5.6896	1.8698	1.0355
H	-5.92823	2.48562	1.89603
C	-5.03059	2.44024	-0.08357
C	4.39679	-3.40666	-0.13113
C	2.61075	-4.40099	1.10207
H	2.1331	-4.44368	2.07199
C	2.0137	-4.9394	-0.02573
C	0.55219	-5.20235	-0.0248
C	-0.17523	-4.83965	-1.17167
H	0.34128	-4.6211	-2.10087
C	-1.54047	-4.58907	-1.1001
H	-2.03559	-4.18021	-1.97564
C	-4.38863	-3.72481	-0.76769
H	-4.40766	-4.34032	-1.6601
C	3.98243	-4.20101	-1.22684
H	4.56619	-4.15173	-2.13838
C	2.82123	-4.94523	-1.18855
H	2.50661	-5.4939	-2.07121

C	-5.2032	0.26569	-1.17989
H	-4.95074	-0.33512	-2.0469
C	-4.92348	1.61936	-1.22891
H	-4.48024	2.01107	-2.13644
C	-0.17596	-5.50327	1.14203
H	0.33106	-5.89142	2.02118
N	3.77409	-3.69374	1.06918
C	-4.61678	-2.13212	1.43697
H	-4.67417	-1.46754	2.2907
C	4.25473	-3.13846	2.35407
H	5.25092	-3.52545	2.57147
H	4.28138	-2.04937	2.30074
H	3.57437	-3.45291	3.14388
C	-6.23282	-2.60274	-1.89126
H	-6.96597	-1.82679	-1.68162
H	-5.71426	-2.38019	-2.82662
H	-6.73796	-3.56754	-1.97326
N	-5.26953	-2.68099	-0.76411



***N,N,N*-Trimethyl-1,15,31-triaza[8]CPP**

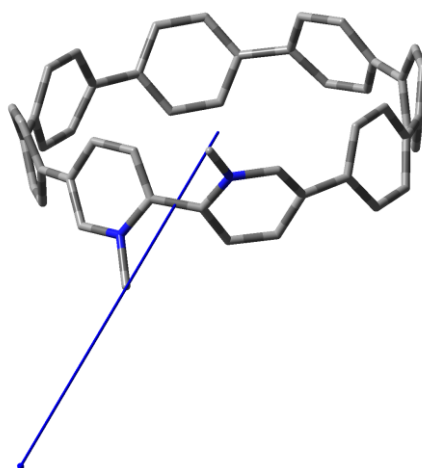
Dipole: 6.4829 D

C	4.01873	-3.09359	-1.6274
H	3.43252	-3.27269	-2.52147
C	3.87978	-3.94223	-0.50479

C	2.69185	-4.81689	-0.36005
C	1.87926	-5.12731	-1.46721
H	2.27039	-5.06057	-2.47765
C	0.53333	-5.43226	-1.29858
H	-0.08178	-5.54691	-2.18496
C	-0.0543	-5.45578	-0.01839
C	-1.51517	-5.225	0.13373
C	-2.44765	-5.45902	-0.90115
H	-2.19172	-6.11329	-1.72847
C	-3.6734	-4.80299	-0.92652
H	-4.33486	-4.95127	-1.77567
C	-4.03316	-3.90942	0.10506
C	4.76516	2.55971	0.22089
C	5.51166	2.13005	-0.8986
H	5.7333	2.81611	-1.70917
C	5.90844	0.80377	-1.03695
H	6.41142	0.49537	-1.94917
C	5.60222	-0.14532	-0.04108
C	5.41699	-1.57757	-0.35722
C	4.78909	-3.70086	0.52563
H	4.92753	-4.38529	1.35461
C	2.15967	-5.07289	0.91942
H	2.76102	-4.91674	1.81003
C	0.82026	-5.40244	1.08526
H	0.44104	-5.53889	2.0928
C	4.65555	1.65173	1.29248
H	4.14292	1.93134	2.20461
C	5.06136	0.33107	1.16917
H	4.82891	-0.35297	1.9786
C	-1.96894	-4.49251	1.24775

H	-1.30715	-4.31256	2.08701
C	-3.19658	-3.84806	1.2386
H	-3.43255	-3.18671	2.06554
C	4.76987	-1.93638	-1.54835
H	4.73463	-1.21355	-2.35491
C	-3.99143	3.15137	0.94302
H	-3.44204	3.45216	1.83025
C	-3.82852	3.85399	-0.26325
C	-2.6404	4.733	-0.41317
C	-2.11513	5.52218	0.60325
H	-2.70538	5.84596	1.45358
C	0.07585	5.50314	-0.34706
C	1.51603	5.31399	-0.09195
C	1.95451	4.87539	1.17574
H	1.33571	5.00348	2.0564
C	3.12329	4.13888	1.30992
H	3.38432	3.78394	2.30005
C	3.88728	3.7626	0.18666
C	-4.94129	-2.77223	-0.12989
C	-5.87459	-0.80443	0.84308
H	-6.33244	-0.39246	1.73561
C	-5.54885	-0.02347	-0.26056
C	-5.3004	1.43949	-0.18607
C	-5.31885	2.25625	-1.33353
H	-5.85543	1.94066	-2.22357
C	-4.5916	3.442	-1.37272
H	-4.57567	4.01938	-2.2928
C	-1.82219	4.59488	-1.55683
H	-2.20124	4.07817	-2.43244
C	-0.49278	4.9625	-1.51353

H	0.16182	4.69609	-2.33368
C	-4.89513	-2.08834	-1.35558
H	-4.46327	-2.59298	-2.21185
C	-5.19358	-0.74109	-1.42601
H	-5.02408	-0.21173	-2.35782
C	2.41563	5.16201	-1.16983
H	2.18081	5.58187	-2.14338
C	3.56991	4.403	-1.03122
H	4.17632	4.23721	-1.91458
C	-4.71351	1.96267	0.97973
H	-4.69909	1.37954	1.89556
N	-5.60472	-2.13974	0.89246
N	-0.8112	5.92615	0.61332
N	5.53599	-2.5638	0.58779
C	6.50367	-2.44481	1.71314
H	7.11346	-1.55562	1.57021
H	5.97216	-2.38698	2.66528
H	7.14525	-3.32831	1.70203
C	-6.07648	-2.88698	2.09098
H	-5.9046	-3.95053	1.94155
H	-7.14761	-2.70532	2.20117
H	-5.55038	-2.54417	2.98438
C	-0.4076	6.87479	1.68782
H	-1.11535	7.70609	1.68556
H	0.58975	7.25455	1.47742
H	-0.42652	6.3798	2.6612



N,N-Dimethyl-1,8-diaza[8]CPP

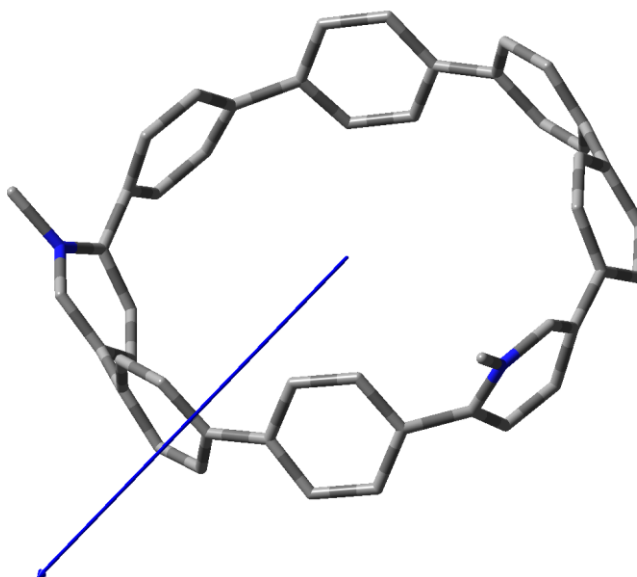
Dipole: 24.9785 D

C	0.12608	0.26867	-0.00586
C	1.35835	0.27645	-0.67305
C	2.03848	1.49503	-0.8086
C	1.33516	2.70374	-0.6987
C	0.09913	2.69585	-0.03379
C	-0.36899	1.48191	0.49097
H	-0.40214	-0.64801	0.15216
H	1.78746	-0.6331	-1.03961
H	1.7462	3.61366	-1.07993
H	-0.45439	3.6009	0.10216
C	3.56985	1.48969	-0.9773
C	4.28685	2.69365	-1.00425
C	4.255	0.26793	-1.01498
C	5.64092	2.67263	-0.62951
H	3.80755	3.61107	-1.26955
C	5.60616	0.2445	-0.64335
H	3.74993	-0.63345	-1.28822
C	6.21067	1.44595	-0.24936
H	6.21356	3.57725	-0.60124

H	6.1526	-0.67648	-0.62648
C	7.43904	1.41464	0.67986
C	7.95613	0.18734	1.11628
C	7.98228	2.61262	1.15968
C	8.66374	0.15727	2.32544
H	7.78293	-0.71012	0.56121
C	8.68601	2.58281	2.3712
H	7.8328	3.53284	0.63612
C	8.80299	1.35617	3.03591
H	9.05221	-0.76094	2.71236
H	9.08986	3.47938	2.79401
C	-1.34673	1.47723	1.68053
C	-1.7545	2.67761	2.26121
C	-1.75706	0.26479	2.24912
C	-2.14739	2.63199	3.59803
H	-1.73342	3.59737	1.71772
H	-1.73351	-0.64057	1.68056
C	-2.11436	1.38812	4.24342
H	-2.43002	3.52264	4.12287
C	-1.84156	0.08695	6.41897
C	-1.16228	0.04656	7.63628
C	-0.62639	1.24733	8.10167
C	-1.13917	2.46033	7.62848
C	-1.94195	1.32702	5.7713
H	-2.24	-0.80149	5.97916
H	-1.02578	-0.87169	8.16966
H	-0.97697	3.36904	8.17018
C	0.58637	1.23574	9.04711
C	1.19117	2.44011	9.43211
C	1.14098	0.01372	9.44699

C	2.53997	2.41054	9.80829
H	0.65119	3.36404	9.40518
C	2.49179	-0.01471	9.81633
H	0.55551	-0.88287	9.43707
C	3.21587	1.18371	9.77812
H	3.05324	3.31206	10.07891
H	2.96533	-0.9343	10.08747
C	4.74527	1.17395	9.6072
C	5.44312	-0.0349	9.46962
C	5.42705	2.39221	9.50217
C	6.68635	-0.01539	8.81679
H	5.02415	-0.95301	9.82258
C	6.66443	2.41289	8.84898
H	4.99523	3.29395	9.88134
C	7.165	1.21158	8.33037
H	7.23763	-0.91982	8.66487
H	7.19802	3.33254	8.72083
C	8.16355	1.24845	7.1587
C	8.56475	2.48273	6.62311
C	8.59708	0.05258	6.56839
C	8.99081	2.51913	5.28972
H	8.51229	3.38047	7.20472
C	9.01914	0.09013	5.23377
H	8.57356	-0.87057	7.10861
C	8.97657	1.32045	4.56318
H	9.28153	3.44111	4.82983
H	9.32803	-0.80214	4.72898
C	-2.32084	3.72958	5.91193
H	-3.18476	3.52598	5.31532
H	-2.58699	4.38459	6.71485

H	-1.56975	4.19439	5.30778
C	-2.53566	-1.01128	4.17582
H	-2.97613	-1.65651	3.44381
H	-1.67259	-1.4831	4.59687
H	-3.24562	-0.81092	4.95029
N	-1.80013	2.47021	6.45894
N	-2.13879	0.25063	3.53543



***N,N*-Dimethyl-1,21-diaza[8]CPP**

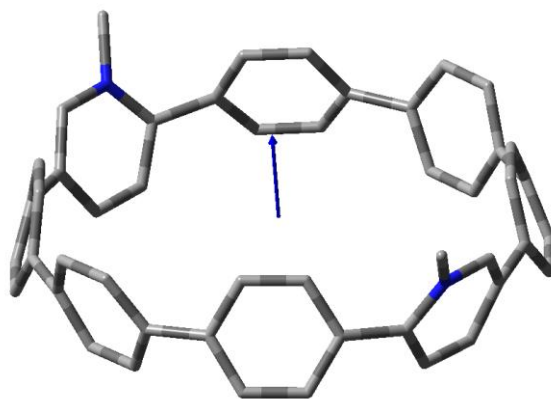
Dipole: 11.4715 D

C	-1.80455	1.70888	-0.45512
C	-0.57678	1.77839	0.21695
C	0.11643	2.99633	0.21007
C	-0.57142	4.19093	-0.04244
C	-1.79913	4.12139	-0.71461
C	-2.2755	2.86085	-1.09939
H	-2.35011	0.78976	-0.50513
H	-0.16291	0.91357	0.69204
H	-0.15355	5.13514	0.23822
H	-2.34058	5.01127	-0.95927
C	1.64706	3.01115	0.3792

C	2.34515	1.80664	0.53956
C	3.69652	4.17466	-0.10694
C	3.69115	1.76208	0.152
H	1.85409	0.93299	0.91437
C	4.26945	2.92431	-0.37592
H	4.26121	5.07527	-0.22913
H	4.25185	0.8536	0.22401
C	-3.23779	2.73429	-2.29505
C	-3.63608	3.87979	-2.99731
C	-3.64158	1.46732	-2.73738
C	-4.02626	3.73645	-4.33566
H	-3.60874	4.8445	-2.53525
C	-4.03176	1.32399	-4.07571
H	-3.61836	0.62308	-2.0804
C	-3.99795	2.45506	-4.90241
H	-4.30378	4.58916	-4.91942
H	-4.31343	0.36776	-4.46453
C	5.47208	2.81875	-1.33206
C	5.98685	1.56064	-1.67277
C	5.99238	3.97311	-1.93265
C	6.66291	1.4276	-2.89306
H	5.83657	0.71472	-1.03502
C	6.66846	3.84007	-3.15298
H	5.84624	4.93614	-1.4898
C	6.7892	2.55957	-3.7095
H	7.04092	0.47772	-3.20886
H	7.05063	4.69915	-3.6637
C	-0.73521	0.67555	-10.02679
C	0.61081	0.631	-10.41443
C	1.31427	1.83906	-10.51294

C	0.61616	3.04357	-10.6733
C	-0.72985	3.08813	-10.28574
C	-1.30816	1.9259	-9.7578
H	-1.29991	-0.22506	-9.90461
H	1.09786	-0.30442	-10.59521
H	1.1072	3.91722	-11.04813
H	-1.29056	3.9966	-10.35777
C	2.84492	1.85388	-10.34379
C	3.53814	3.07182	-10.35067
C	3.53278	0.65929	-10.09128
H	3.12429	3.93665	-10.82576
C	4.7605	0.72883	-9.41908
H	3.11494	-0.28492	-10.37195
C	5.23686	1.98937	-9.0343
H	5.30194	-0.16104	-9.17442
C	6.19914	2.11593	-7.8386
C	6.59742	0.97044	-7.13633
C	6.60293	3.38291	-7.39626
C	6.98757	1.11377	-5.79797
H	6.57009	0.00573	-7.59839
C	6.99309	3.52623	-6.05793
H	6.57971	4.22715	-8.05323
C	6.95927	2.39516	-5.23123
H	7.26508	0.26106	-5.21421
H	7.27474	4.48246	-5.66909
C	-2.5108	2.03146	-8.80163
C	-3.02558	3.28957	-8.46091
C	-3.0311	0.8771	-8.20102
C	-3.70163	3.42261	-7.24061
H	-2.87533	4.13549	-9.09866

C	-3.70717	1.01015	-6.98068
H	-2.88498	-0.08593	-8.64387
C	-3.82791	2.29065	-6.42415
H	-4.07964	4.37249	-6.9248
H	-4.08934	0.15107	-6.46995
N	4.76591	3.14134	-9.67858
N	2.3505	4.21922	0.28069
C	5.51541	4.40405	-9.60986
H	5.27061	4.91518	-8.70228
H	6.56505	4.19737	-9.63083
H	5.25614	5.01869	-10.44645
C	1.68137	5.50432	0.52903
H	1.17882	5.82251	-0.36041
H	0.96917	5.38879	1.31918
H	2.40906	6.23708	0.80908



***N,N*-Dimethyl-1,26-diaza[8]CPP**

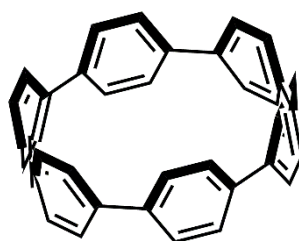
Dipole: 1.9950 D

C	-2.89847	-0.32846	-6.2934
C	-2.51334	-0.25031	-4.94752
C	-2.11318	0.99421	-4.44197
C	-2.51104	2.17187	-5.08918
C	-2.89697	2.09372	-6.43454

C	-2.86335	0.84201	-7.06379
H	-3.17725	-1.26477	-6.72983
H	-2.49112	-1.12564	-4.33228
H	-2.48669	3.11276	-4.58007
H	-3.17524	2.97335	-6.97667
C	-1.15538	1.06435	-3.23739
C	-0.68079	2.3056	-2.79206
C	-0.68659	-0.11613	-2.64513
C	0.54417	2.34405	-2.11176
H	-1.22157	3.20575	-2.99746
C	0.53843	-0.07774	-1.9648
H	-1.23166	-1.03188	-2.7402
C	1.23176	1.13913	-1.91194
H	0.96026	3.2743	-1.78572
H	0.95028	-0.96361	-1.52838
C	2.76218	1.14662	-1.73539
C	3.46154	-0.06343	-1.62816
C	4.80936	-0.08864	-2.01248
H	2.97041	-0.95402	-1.29554
C	4.8126	2.33295	-2.15841
C	5.38822	1.09748	-2.48323
H	5.3709	-0.99887	-1.98098
H	5.37689	3.23884	-2.23622
C	6.595	1.03931	-3.43818
C	7.1159	2.2224	-3.97926
C	7.11319	-0.19991	-3.83776
C	7.79748	2.15059	-5.20174
H	6.96624	3.16223	-3.4901
C	7.7949	-0.27191	-5.06045
H	6.96138	-1.07637	-3.24265

C	7.92303	0.89927	-5.82028
H	8.18033	3.03451	-5.66778
H	8.176	-1.20456	-5.42056
C	0.42424	-0.68056	-12.25335
C	1.77176	-0.70595	-12.63745
C	2.47471	0.50572	-12.67644
C	0.42756	1.74103	-12.39916
C	-0.1514	0.5549	-11.92857
H	-0.14011	-1.58643	-12.17564
H	2.26001	-1.6315	-12.8601
H	-0.134	2.65128	-12.43067
C	-1.35814	0.61308	-10.97351
C	-1.87623	1.85231	-10.57386
C	-1.87901	-0.57004	-10.43245
C	-2.55795	1.92427	-9.3512
H	-1.72448	2.72878	-11.16896
C	-2.56057	-0.49824	-9.20998
H	-1.72943	-1.50984	-10.92166
C	-2.68614	0.75306	-8.59142
H	-2.93904	2.85691	-8.99104
H	-2.94346	-1.38216	-8.74395
C	4.00516	0.51319	-12.49986
C	4.69849	1.73007	-12.44694
C	4.69276	-0.69173	-12.30005
C	5.9235	1.76844	-11.76662
H	4.28664	2.61593	-12.88335
C	5.91773	-0.65328	-11.61977
H	4.2767	-1.62197	-12.62616
C	6.39244	0.58795	-11.17447
H	6.46861	2.68419	-11.67159

H	6.45857	-1.55344	-11.41447
C	7.35017	0.65809	-9.96977
C	7.74813	-0.51957	-9.32258
C	7.75035	1.90262	-9.46423
C	8.13403	-0.4414	-7.9772
H	7.72384	-1.46044	-9.83169
C	8.13545	1.98077	-8.11833
H	7.72813	2.77795	-10.07946
C	8.10036	0.8103	-7.3479
H	8.41234	-1.32102	-7.43506
H	8.41421	2.9171	-7.68188
N	1.77535	1.7158	-12.78353
N	3.46506	2.35832	-1.77436
C	2.45005	2.93927	-13.24047
H	2.9502	3.40043	-12.41458
H	3.16497	2.69105	-13.9969
H	1.72611	3.61688	-13.64252
C	2.79413	3.63003	-1.46856
H	2.29568	3.98992	-2.3443
H	2.07823	3.47697	-0.6882
H	3.52013	4.34887	-1.15059

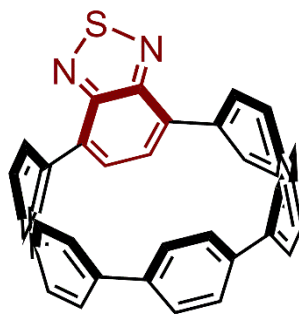


[6]CPP

C	2.58501	3.67073	1.03622
C	1.33524	4.28618	1.03614
C	0.46814	4.17027	-0.07039

C	1.04529	3.69396	-1.26264
C	2.29245	3.07967	-1.26249
C	3.02174	2.91268	-0.07025
H	3.17278	3.68195	1.95068
H	0.98571	4.759	1.95053
H	0.44053	3.62206	-2.16131
H	2.60413	2.55603	-2.16087
C	-1.01193	4.07254	0.07015
C	-1.88673	4.07354	-1.03636
C	-1.52156	3.52496	1.26249
C	-3.0449	3.2994	-1.03633
H	-1.60223	4.588	-1.95081
C	-2.67745	2.75246	1.26255
H	-0.91251	3.53303	2.16106
C	-3.37835	2.49072	0.07029
H	-3.62902	3.23326	-1.95082
H	-2.9177	2.19267	2.16106
C	-1.04528	-3.6941	1.26255
C	-2.29244	-3.07981	1.26247
C	-3.02173	-2.91269	0.07024
C	-2.58501	-3.67062	-1.03631
C	-1.33523	-4.28606	-1.0363
C	-0.46813	-4.17027	0.07024
H	-0.44052	-3.62229	2.16122
H	-2.60412	-2.55627	2.1609
H	-3.17278	-3.68176	-1.95077
H	-0.98571	-4.75877	-1.95075
C	1.01193	-4.07253	-0.07029
C	1.52157	-3.52484	-1.26258
C	1.88672	-4.07363	1.03623

C	2.67745	-2.75234	-1.26257
H	0.91253	-3.53282	-2.16115
C	3.04489	-3.29949	1.03627
H	1.60221	-4.58817	1.95063
C	3.37835	-2.49071	-0.07027
H	2.91771	-2.19247	-2.16102
H	3.62899	-3.23342	1.95078
C	4.03415	-1.1602	0.0702
C	3.81515	-0.44508	1.26258
C	4.47241	-0.40307	-1.03633
C	3.72369	0.94221	1.26261
H	3.51786	-0.9766	2.16116
C	4.38065	0.98699	-1.03635
H	4.77585	-0.90655	-1.95081
C	3.84681	1.68002	0.07023
H	3.35942	1.43003	2.16137
H	4.61538	1.52596	-1.95082
C	-4.03416	1.1602	-0.07005
C	-4.47223	0.40307	1.03656
C	-4.38045	-0.98699	1.03657
C	-3.84681	-1.68003	-0.0701
C	-3.72388	-0.94222	-1.2625
C	-3.81535	0.44507	-1.26246
H	-4.77551	0.90655	1.95109
H	-4.61503	-1.52596	1.95108
H	-3.35976	-1.43004	-2.16132
H	-3.51822	0.97659	-2.16109

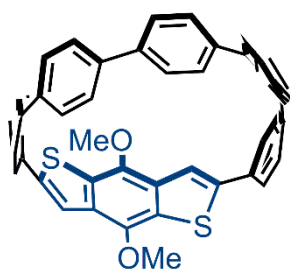


1,4-BT[6]CPP

C	-3.29365	-1.81557	0.01828
C	-2.96459	-2.34063	1.2751
C	-2.80266	-2.4239	-1.14405
C	-1.73638	-3.00842	1.37969
H	-3.59617	-2.1966	2.12668
C	-1.57749	-3.09383	-1.03972
H	-3.31434	-2.33983	-2.08004
C	-0.95775	-3.09059	0.21672
H	-1.3892	-3.39424	2.31537
H	-1.11396	-3.54446	-1.89233
C	-3.36081	3.73053	-0.28665
C	-2.88371	4.22142	-1.50883
C	-3.04611	4.39646	0.90537
C	-1.67523	4.92829	-1.47958
H	-3.39236	4.02423	-2.42934
C	-1.83435	5.10078	0.9352
H	-3.67511	4.33057	1.76839
C	-1.05668	5.07548	-0.23109
H	-1.22213	5.29551	-2.37665
H	-1.49741	5.59361	1.82318
C	3.92882	1.7017	-0.95086
C	3.94593	0.30251	-0.87405
C	3.59196	-0.27578	0.35247

C	3.80062	0.4328	1.54402
C	3.78365	1.83316	1.46716
C	3.55944	2.4019	0.2055
H	4.14319	2.21055	-1.86732
H	4.17403	-0.29822	-1.72961
H	3.92075	-0.07121	2.48019
H	3.89041	2.43935	2.34237
C	2.85374	-1.62828	0.37738
C	2.393	-2.15664	1.59174
C	2.53611	-2.26971	-0.82748
C	1.20226	-2.89645	1.55549
H	2.90095	-1.96482	2.51374
C	1.34539	-3.00715	-0.86363
H	3.15065	-2.16268	-1.69682
C	0.57855	-3.03852	0.30844
H	0.76559	-3.29306	2.44824
H	1.01394	-3.48504	-1.76178
C	2.78877	3.73074	0.08337
C	2.31354	4.37678	1.23344
C	2.45771	4.22945	-1.18385
C	1.10539	5.07927	1.11823
H	2.82455	4.29869	2.17025
C	1.24987	4.93016	-1.2988
H	3.07597	4.04301	-2.03703
C	0.48045	5.07023	-0.13622
H	0.65785	5.55973	1.96309
H	0.90878	5.2999	-2.24323
C	-4.10846	2.38612	-0.24226
C	-4.53749	1.76803	1.08811
C	-4.2851	1.66048	-1.38634

C	-4.52124	0.25304	1.17541
C	-4.26582	0.09913	-1.29961
H	-4.38695	2.15003	-2.33237
C	-4.07438	-0.49317	-0.08241
H	-4.35327	-0.4937	-2.18601
N	-4.86586	2.34089	2.19478
N	-4.83925	-0.22334	2.34314
S	-5.13658	1.01904	3.2355

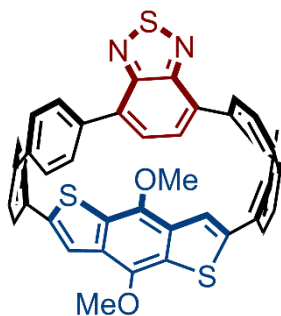


2,6-BDT[6]CPP

C	-5.36504	-0.17325	-1.49856
C	-5.07181	-1.17614	-0.56431
C	-5.22322	-0.9578	0.81535
C	-5.47641	0.31417	1.344
C	-5.35627	1.35899	0.42259
C	-5.398	1.12411	-0.96279
S	-4.95801	-2.45848	1.70131
S	-5.40222	2.6609	-1.83199
C	-4.0415	-3.0089	0.29011
C	-4.51819	-2.4491	-0.85897
C	-4.68946	3.37425	-0.37433
C	-5.09246	2.71301	0.74683
O	-5.76867	0.52947	2.7272
O	-5.55391	-0.43986	-2.89245
C	-4.54762	0.7175	3.44963
H	-4.03154	1.57067	3.06121

H	-4.76502	0.87392	4.48609
H	-3.93222	-0.15117	3.34227
C	-4.29503	-0.39559	-3.57018
H	-3.64236	-1.13719	-3.159
H	-4.44433	-0.59007	-4.61187
H	-3.85663	0.57276	-3.44753
C	-2.76751	-3.8706	0.32406
C	-2.19571	-4.23226	1.55094
C	-2.12092	-4.19808	-0.8745
C	-0.80332	-4.40683	1.58932
H	-2.78967	-4.32774	2.4356
C	-0.73558	-4.38663	-0.83569
H	-2.66067	-4.26044	-1.79682
C	-0.09175	-4.22013	0.39502
H	-0.29978	-4.63362	2.50526
H	-0.18248	-4.60706	-1.72504
C	-3.622	4.48161	-0.32733
C	-3.05235	4.9719	-1.51034
C	-3.14047	4.91853	0.91336
C	-1.72259	5.42127	-1.44683
H	-3.5914	4.96227	-2.43418
C	-1.82301	5.38212	0.97676
H	-3.7469	4.86065	1.7929
C	-1.07201	5.36427	-0.2032
H	-1.211	5.7569	-2.325
H	-1.39202	5.69755	1.90362
C	3.87189	1.66707	-0.9979
C	4.01121	0.27432	-0.91901
C	3.78121	-0.34252	0.31855
C	3.91359	0.39667	1.50017

C	3.77045	1.78946	1.42251
C	3.50526	2.35523	0.1662
H	4.00198	2.18172	-1.9275
H	4.2474	-0.3038	-1.78698
H	4.07863	-0.08905	2.43858
H	3.82266	2.3964	2.30188
C	3.27326	-1.79707	0.37555
C	2.96483	-2.38998	1.60869
C	3.02145	-2.49253	-0.81366
C	1.97849	-3.38733	1.62885
H	3.43692	-2.06377	2.51133
C	2.03202	-3.48224	-0.79388
H	3.53794	-2.24798	-1.7177
C	1.36228	-3.71563	0.41423
H	1.67859	-3.84887	2.54668
H	1.76758	-4.0137	-1.68391
C	2.71151	3.67351	0.06586
C	2.23854	4.29048	1.23175
C	2.37264	4.20229	-1.18914
C	1.06948	5.057	1.13795
H	2.7303	4.14753	2.17139
C	1.20543	4.97611	-1.28303
H	2.96342	3.98911	-2.055
C	0.45248	5.16233	-0.116
H	0.64047	5.51374	2.00455
H	0.88078	5.3749	-2.22164
H	-5.1362	3.13174	1.73143
H	-4.42735	-2.87112	-1.83644

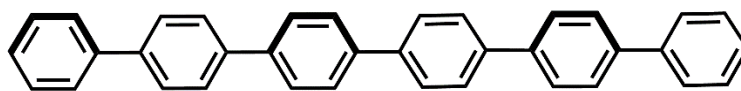


2,6-BDT-1,4-BT[6]CPP

C	3.89375	-0.19491	1.42277
C	3.82313	-1.29564	0.54354
C	3.85308	-1.08011	-0.86344
C	3.89446	0.19452	-1.42214
C	3.82358	1.29526	-0.54294
C	3.85284	1.07973	0.86404
S	3.4701	-2.56813	-1.73152
S	3.46959	2.56777	1.73196
C	2.98604	-3.36746	-0.21094
C	3.36732	-2.61714	0.8718
C	2.98633	3.36718	0.21115
C	3.36807	2.61682	-0.87141
O	3.85908	0.39036	-2.78482
O	3.85766	-0.39071	2.78543
C	2.55123	0.37966	-3.37647
H	1.91629	1.16371	-2.94664
H	2.70271	0.57367	-4.44046
H	2.06107	-0.59108	-3.24744
C	2.54949	-0.37993	3.3764
H	1.9147	-1.16387	2.94615
H	2.70039	-0.57405	4.44044
H	2.05952	0.59088	3.24718

C	1.88875	-4.35119	-0.20075
C	1.05216	-4.48269	-1.32602
C	1.39113	-4.87345	1.0143
C	-0.29533	-4.79528	-1.18082
H	1.40449	-4.16863	-2.30327
C	0.04484	-5.18751	1.15452
H	2.03572	-4.9192	1.88776
C	-0.86322	-5.00121	0.08911
H	-0.93906	-4.69967	-2.04978
H	-0.32366	-5.47895	2.13453
C	1.88919	4.35106	0.20055
C	1.05259	4.4832	1.32575
C	1.39166	4.87284	-1.01474
C	-0.29486	4.79592	1.18037
H	1.40484	4.16958	2.30316
C	0.04542	5.18703	-1.15515
H	2.03627	4.91809	-1.88821
C	-0.86268	5.00133	-0.08967
H	-0.93862	4.70083	2.04936
H	-0.32302	5.47806	-2.1353
C	-5.22788	0.85204	1.08733
C	-5.24596	-0.52548	1.27807
C	-5.08872	-1.41477	0.19659
C	-5.22835	-0.85149	-1.08724
C	-5.24628	0.52603	-1.27798
C	-5.08858	1.41528	-0.19656
H	-5.18685	-1.48828	-1.96557
H	-5.26311	0.90389	-2.29592
C	-4.44473	-2.74657	0.36428
C	-4.29948	-3.66914	-0.69296

C	-3.64247	-2.97622	1.49814
C	-3.24314	-4.57684	-0.7221
H	-4.96297	-3.61942	-1.55197
C	-2.59159	-3.88349	1.47178
H	-3.72696	-2.32683	2.3627
C	-2.28125	-4.61109	0.3079
H	-3.11507	-5.20062	-1.60303
H	-1.90482	-3.89544	2.31214
C	-4.44441	2.74698	-0.36434
C	-3.64209	2.97626	-1.49823
C	-4.29908	3.66971	0.69274
C	-2.59112	3.88342	-1.47205
H	-3.72664	2.32663	-2.36259
C	-3.24262	4.5773	0.72169
H	-4.96259	3.62022	1.55175
C	-2.28075	4.61126	-0.30832
H	-1.90431	3.89511	-2.31239
H	-3.11446	5.20124	1.60251
H	3.13709	2.89895	-1.89086
H	3.13576	-2.89924	1.89113
N	-5.17111	1.71427	2.27654
N	-5.26837	-1.03692	2.65605
S	-5.32477	1.09397	3.69537

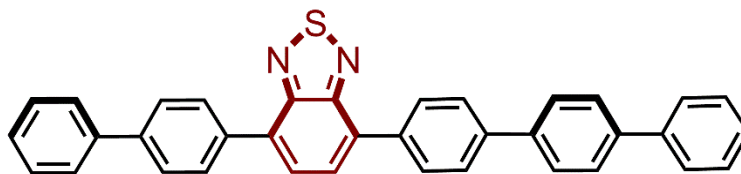


p-Sexiphenyl

C	-3.87745	1.64065	0.77739
C	-2.48229	1.6406	0.77769
C	-1.78457	2.61781	0.06814
C	-2.48203	3.59498	-0.64312

C	-3.87686	3.59468	-0.64376
C	-4.57465	2.61769	0.06686
H	-4.42736	0.87038	1.33724
H	-1.93293	0.87064	1.33859
H	-1.93168	4.36534	-1.20255
H	-4.42683	4.36467	-1.20423
C	-0.24457	2.61836	0.06912
C	0.45262	3.82632	0.06902
C	0.45344	1.41006	0.06972
C	1.84778	3.82672	0.07071
H	-0.09716	4.77867	0.06891
C	1.84826	1.41054	0.07094
H	-0.09649	0.45776	0.06975
C	2.54551	2.61895	0.07183
H	2.39727	4.7792	0.07108
H	2.39866	0.45842	0.07141
C	-6.11465	2.61781	0.06617
C	-6.81218	3.82556	0.065
C	-6.8123	1.4093	0.06712
C	-8.20734	3.82556	0.06358
H	-6.26267	4.77807	0.06388
C	-8.20713	1.40938	0.06618
H	-6.26211	0.45716	0.06811
C	-8.90472	2.61759	0.06401
H	-8.7571	4.77788	0.0622
H	-8.75725	0.4571	0.06693
C	4.08551	2.61913	0.07345
C	4.78251	1.64263	0.78468
C	4.78371	3.59674	-0.6365
C	6.17767	1.64241	0.78544

H	4.23258	0.87189	1.34394
C	6.17853	3.59674	-0.63531
H	4.23393	4.36661	-1.19716
C	6.87559	2.61928	0.07538
H	6.727	0.87216	1.34588
H	6.72908	4.36708	-1.19473
C	8.41559	2.61939	0.07627
C	9.11313	3.82714	0.0766
C	9.11325	1.41088	0.07635
C	10.50829	3.82714	0.07821
H	8.56362	4.77965	0.07691
C	10.50807	1.41096	0.07748
H	8.56305	0.45874	0.07603
C	11.20567	2.61916	0.0788
H	11.05805	4.77946	0.07892
H	11.05819	0.45868	0.07753
H	12.30527	2.61898	0.07989
C	-10.44472	2.61733	0.06269
C	-11.1428	1.64054	0.77247
C	-11.14184	3.59436	-0.64912
C	-12.53796	1.64087	0.77186
H	-10.59371	0.8707	1.33379
C	-12.53667	3.59434	-0.65007
H	-10.59122	4.36439	-1.20873
C	-13.2348	2.61777	0.06079
H	-13.08814	0.87093	1.3319
H	-13.08636	4.36421	-1.21096
H	-14.33441	2.61806	0.06006

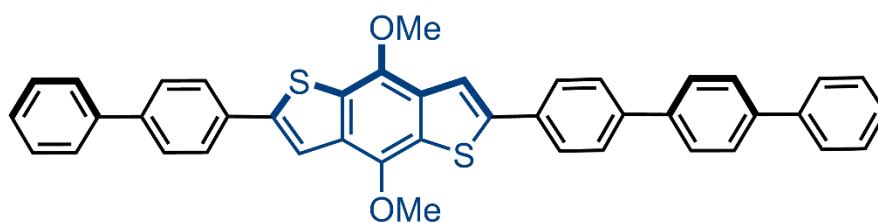


BT-*p*-sexiphenyl

C	-3.04673	-4.5979	0.29701
C	-2.53808	-5.3634	1.35498
C	-3.72367	-5.22369	-0.75847
C	-2.70661	-6.75465	1.35753
H	-2.02108	-4.88562	2.16081
C	-3.8921	-6.61491	-0.75595
H	-4.11194	-4.63925	-1.5663
C	-3.38369	-7.38039	0.30208
H	-2.31833	-7.33912	2.16532
H	-4.40891	-7.0927	-1.56187
C	-1.32481	2.17459	0.51598
C	-1.03971	3.08051	-0.51456
C	-1.06323	2.52349	1.84781
C	-0.49417	4.33577	-0.21317
H	-1.23863	2.81384	-1.53153
C	-0.51778	3.77873	2.14922
H	-1.28006	1.8315	2.63461
C	-0.23374	4.68512	1.1188
H	-0.27658	5.02744	-1.00004
H	-0.31826	4.04514	3.16614
C	2.33078	10.86456	1.35395
C	2.87326	12.12107	1.65548
C	3.13281	12.47089	2.98747
C	2.84986	11.56425	4.01792
C	2.30741	10.30776	3.71641

C	2.04775	9.95794	2.38444
H	2.1327	10.59745	0.33696
H	3.08925	12.81333	0.86871
H	3.04798	11.83138	5.03492
H	2.0915	9.61546	4.50318
C	-3.90631	-11.69163	0.30915
C	-3.95911	-10.97748	1.51379
C	-3.68499	-11.01454	-0.89768
C	-3.79054	-9.58624	1.51158
H	-4.12814	-11.49446	2.43525
C	-3.51647	-9.62333	-0.89989
H	-3.64469	-11.55979	-1.81744
C	-3.56913	-8.90918	0.30473
H	-3.83086	-9.04098	2.43134
H	-3.34755	-9.10636	-1.82136
C	1.4513	8.57725	2.05334
C	0.51285	7.99449	2.91565
C	1.84682	7.90363	0.88983
C	-0.0306	6.73844	2.61418
H	0.21121	8.50861	3.80423
C	1.30344	6.64748	0.58836
H	2.56364	8.34843	0.23163
C	0.36439	6.06504	1.45037
H	-0.74717	6.29356	3.27258
H	1.60549	6.13317	-0.29998
C	-2.86189	-3.06904	0.29421
C	-2.63854	-2.39553	-0.90651
C	-2.91748	-2.35747	1.49329
C	-2.47189	-1.01036	-0.90904
H	-2.59504	-2.95596	-1.85164

C	-2.75039	-0.97269	1.49074
C	-2.52796	-0.29902	0.28945
H	-2.29625	-0.4795	-1.85587
N	-3.15283	-3.06763	2.75867
N	-2.80888	-0.22272	2.75368
S	-1.49621	-1.43638	5.50446
H	3.54704	13.43022	3.21769
H	-4.03499	-12.75386	0.31082

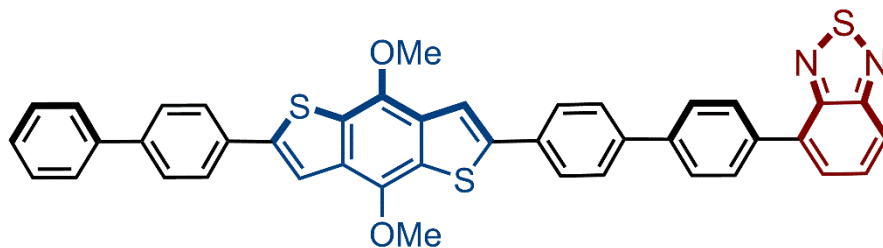


2,6-BDT-*p*-sexiphenyl

C	-2.6729	-1.3573	-1.3
C	-2.97984	-2.34304	-0.35256
C	-2.98435	-2.04579	1.01648
C	-2.57984	-0.80034	1.51521
C	-2.22411	0.17036	0.56916
C	-2.32507	-0.09411	-0.80295
S	-3.54957	-3.43385	1.9404
S	-1.95445	1.35448	-1.73247
C	-3.5123	-4.4497	0.48796
C	-3.29172	-3.69889	-0.6374
C	-1.42424	2.19398	-0.26375
C	-1.7269	1.46863	0.85928
O	-2.5324	-0.53346	2.91927
O	-2.7127	-1.62707	-2.70377
C	-1.23957	-0.87524	3.4259
H	-0.49499	-0.2911	2.92663
H	-1.20406	-0.67582	4.47655

H	-1.05227	-1.91454	3.25362
C	-1.43054	-2.08879	-3.13709
H	-1.17665	-2.98403	-2.60888
H	-1.46047	-2.29071	-4.18744
H	-0.69516	-1.33717	-2.93918
C	-3.69715	-5.97858	0.49076
C	-3.18849	-6.74408	1.54873
C	-4.37409	-6.60437	-0.56471
C	-3.35702	-8.13533	1.55129
H	-2.6715	-6.2663	2.35456
C	-4.54251	-7.99559	-0.56219
H	-4.76236	-6.01993	-1.37254
C	-4.03411	-8.76107	0.49584
H	-2.96875	-8.7198	2.35907
H	-5.05933	-8.47339	-1.36812
C	-0.71032	3.55856	-0.25139
C	-1.06118	4.54155	-1.1866
C	0.29007	3.81743	0.69527
C	-0.41252	5.78381	-1.17438
H	-1.8244	4.34364	-1.90995
C	0.93866	5.05968	0.70756
H	0.55861	3.06663	1.40877
C	0.58702	6.04309	-0.22691
H	-0.6805	6.53432	-1.88841
H	1.70233	5.25734	1.43051
C	2.95088	12.24476	-1.10387
C	3.59717	13.48819	-1.08965
C	4.59602	13.74793	-0.14162
C	4.94856	12.76428	0.79222
C	4.3023	11.52086	0.77799

C	3.30337	11.26112	-0.16996
H	2.18832	12.04643	-1.82776
H	3.32797	14.23925	-1.80263
H	5.71115	12.96262	1.51609
H	4.57157	10.76978	1.49092
C	-4.55673	-13.07231	0.5029
C	-4.60953	-12.35816	1.70755
C	-4.33541	-12.39522	-0.70393
C	-4.44096	-10.96692	1.70533
H	-4.77856	-12.87514	2.629
C	-4.16689	-11.00401	-0.70614
H	-4.29511	-12.94047	-1.62369
C	-4.21955	-10.28987	0.49848
H	-4.48128	-10.42166	2.62509
H	-3.99796	-10.48704	-1.6276
C	2.59305	9.89478	-0.18518
C	2.32383	9.23174	1.01971
C	2.21582	9.31449	-1.40375
C	1.67679	7.98874	1.00614
H	2.61225	9.6746	1.95007
C	1.56883	8.07139	-1.41736
H	2.42172	9.82058	-2.32374
C	1.29896	7.40867	-0.21234
H	1.4712	7.48256	1.92614
H	1.28088	7.62833	-2.34778
H	-1.58958	1.83809	1.85403
H	-3.33647	-4.09712	-1.62951
H	5.08951	14.69728	-0.13079
H	-4.68541	-14.13454	0.50458



2,6-BDT-1,4-BT-*p*-sexiphenyl

C	-1.99966	-1.43916	0.12796
C	-3.12517	-0.59866	0.05457
C	-2.9421	0.81245	-0.01148
C	-1.68265	1.40296	-0.01432
C	-0.55658	0.56098	0.02816
C	-0.73966	-0.84986	0.09842
S	-4.48317	1.64819	-0.11137
S	0.80294	-1.68849	0.12728
C	-5.36475	0.10692	-0.04418
C	-4.51217	-0.95981	0.03379
C	1.68427	-0.14829	0.037
C	0.83077	0.91974	-0.0097
O	-1.54092	2.77037	-0.10439
O	-2.14337	-2.80833	0.17658
C	-1.46518	3.43936	1.15988
H	-0.59535	3.09929	1.73607
H	-1.36251	4.50348	0.93638
H	-2.37512	3.27563	1.75009
C	-2.21571	-3.34726	1.50219
H	-3.0826	-2.94865	2.0441
H	-2.32191	-4.42807	1.38642
H	-1.30308	-3.12832	2.06982
C	-6.82974	0.08894	-0.09308
C	-7.59843	1.19592	0.30831

C	-7.51759	-1.05288	-0.54597
C	-8.98775	1.16028	0.26516
H	-7.10326	2.08637	0.68601
C	-8.90576	-1.08742	-0.58037
H	-6.95487	-1.90976	-0.90414
C	-9.67591	0.0181	-0.17683
H	-9.54988	2.02259	0.61208
H	-9.4036	-1.97343	-0.96413
C	3.14957	-0.13263	0.0129
C	3.89743	-1.24297	-0.41814
C	3.85975	1.01147	0.4238
C	5.28699	-1.20781	-0.44343
H	3.38435	-2.13498	-0.76703
C	5.2477	1.04569	0.39012
H	3.31536	1.87192	0.80124
C	5.99711	-0.06316	-0.04317
H	5.83065	-2.07246	-0.81311
H	5.76353	1.93431	0.74273
C	12.55157	-1.01781	-0.61477
C	13.94479	-0.98282	-0.64173
C	14.62846	0.15607	-0.21199
C	13.90515	1.25914	0.24535
C	12.51198	1.22304	0.27317
C	11.80911	0.08422	-0.15659
H	12.02974	-1.89895	-0.97776
H	14.49709	-1.84429	-1.00808
C	-13.97649	-0.09402	-0.30567
C	-13.29347	1.08154	-0.62301
C	-13.25307	-1.23266	0.05391
C	-11.9007	1.11791	-0.58158

H	-13.84584	1.97155	-0.91303
C	-11.86035	-1.19558	0.09599
H	-13.77435	-2.15102	0.31124
C	-11.15814	-0.01992	-0.22117
H	-11.37943	2.03005	-0.85842
H	-11.30926	-2.07978	0.40408
C	10.32585	0.04651	-0.12754
C	9.56146	1.18544	-0.43246
C	9.63281	-1.12956	0.2057
C	8.17115	1.15036	-0.40499
H	10.06347	2.10176	-0.7302
C	8.24251	-1.16539	0.23265
H	10.19198	-2.01895	0.48246
C	7.478	-0.02605	-0.07191
H	7.61273	2.03992	-0.68282
H	7.74127	-2.08205	0.53068
H	1.16527	1.94452	-0.11897
H	-4.8485	-1.98837	0.0868
H	15.71453	0.18371	-0.23336
H	-15.06223	-0.12256	-0.33849
N	11.76597	2.37829	0.79257
N	14.61069	2.46133	0.71209
S	13.02015	4.32578	-0.03079

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