Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supporting Information

Structure-Property Relationships of Core-Substituted Diaryl Dihydrophenazine Organic Photoredox Catalysts and their Application in O-ATRP

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MATERIALS AND METHODS

Purchased Chemicals and Materials

Phenazine Reduction (Figure S3-a): Phenazine was purchased from Sigma Aldrich, sodium dithionite was purchased from VWR, reagent alcohol was purchased from Sigma Aldrich. All chemicals were used as received.

Buchwald-Hartwig Coupling (Figure S3-b): (This method was used for the synthesis of PC **5**): 2-bromonaphthalene, sodium t-butoxide, anhydrous Sure/Seal dioxane, dicyclohexylphospino-2,6-diisopropoxybiphennyl (RuPhos), and RuPhos Pd G4, were purchased from Sigma Aldrich and used as received unless noted otherwise in “Chemical preparation and Storage.”

Buchwald-Hartwig Coupling (Figure S3-b): (This method was used for the synthesis of PCs **3** and **4**): 4-bromoanisole, 2-bromonaphthalene, sodium t-butoxide, anhydrous Sure/Seal toluene, bis(dibenzylideneacetone) palladium(0) ($Pd(dba)_2$), and tritertbutylphosphine were purchased from Sigma Aldrich and used as received unless noted otherwise in “Chemical preparation and Storage.”

Bromination Method I (Figure S3-c&e): Molecular bromine, benzene, and methanol purchased from Sigma Aldrich and used as received. Copper wire was purchased from Fisher and used as received.

Bromination Method II (Figure S3-c&d)**:** Molecular bromine, benzene, and methanol purchased from Sigma Aldrich and used as received. Reagent grade Acetone was purchased form Fischer Scientific ad used as received.

Suzuki Coupling (Figure S3-f): Tetrakis(triphenyl phosphine) palladium (0) ($Pd(PPh_3)_4$), 4-(trifluoromethyl)phenylboronic acid, 2-naphthylboronic acid, 4-methoxyphenylboronic acid, and Sure/Seal tetrahydrafuran (THF) were purchased from Sigma Aldrich. Potassium carbonate was purchased from VWR. All chemicals were used as received unless noted otherwise in “Chemical preparation and Storage.”

Polymerizations: Monomers: methyl methacrylate (MMA), styrene, n-butyl acrylate (nBA), vinyl acetate (VA), and *N,N*-dimethylacrylamide (DMA), as well as solvents: anhydrous Sure/seal *N,N*-dimethylacetamide (DMAc), ethyl acetate (EtOAc), benzene, dichloromethane (DCM) and tetrahydrofuran (THF) and diethyl 2-bromo-2-methyl malonate (DBMM) were purchased from Sigma Aldrich.

Deuterated solvents for NMR: All deuterated solvents were purchased from Cambridge Isotope Laboratories Inc. and used without further purification.

Chemical Preparation and Storage

Cross coupling reactions: $Pd(dba)_2$ and $Pd(PPh_3)_4$ were used as received, but were transferred to a nitrogen-filled glovebox before use. Tetrakis(triphenyl phosphine) palladium(0) was stored in the dark at -10 °C. 4-bromoanisole was sparged with nitrogen while stirring for 20 minutes before use.

Monomers and initiators for polymerizations (add other monomers): MMA, styrene, nBA, VA, DMA, and DBMM, were dried by stirring over calcium hydride for 12-16 hours, distilled under vacuum, then degassed via three freeze-pump-thaw cycles before being transferred to amber vials in a nitrogen filled glovebox. Monomers and initiators were stored under nitrogen, in the dark, at -10 °C, but were allowed to warm to room temperature before use.

Solvents for polymerizations: Dimethylacetamide (DMAc), tetrahydrofuran (THF), dichloromethane (DCM), and ethyl acetate (EtOAc) were obtained from Sigma Aldrich in Sure/Seal bottles, then used without further purification. Benzene was obtained and purified using an mBraun MB-SPS-800 solvent purification system, kept under nitrogen atmosphere, and stored over 3Å molecular sieves.

Solvents for characterization: DMAc (99.8% anhydrous) was purchased form sigma Aldrich in Sure/Seal bottles and used without further purification. HPLC grade acetonitrile (MeCN) for cyclic voltammetry was purchased form Fischer Scientific and used without further purification.

Instrumentation for Characterization

Nuclear magnetic resonance (NMR) spectroscopy: NMR spectra were obtained using a Bruker 400 MHz NMR Spectrometer. All ^1H NMR experiments are reported in parts per million (ppm) and were measured relative to the signals for residual dimethyl sulfoxide (2.5 ppm), benzene (7.16 ppm), or chloroform (7.26) in deuterated dimethyl sulfoxide, deuterated benzene, or deuterated chloroform, respectively.

Mass Spectroscopy of Photocatalysts: Electrospray Ionization Mass Spectroscopy (ESI-MS) was performed at the Colorado State University Central Instrumentation Facility.

Ultraviolet-visible (UV-Vis) spectroscopy: UV-Vis spectroscopy was performed on a Cary 5000 spectrophotometer. DMAc was used as the solvent for all data presented in this work. All samples were analyzed in 1 cm pathlength quartz cuvettes.

Fluorescence spectroscopy: Emission Spectra: Emission spectra were obtained using an Edinburgh Instruments FS5 spectrofluorometer. DMAc was used as the solvent for all sample data presented in this work and all samples were measured in quartz cuvettes with a 1 cm pathlength.

Absolute fluorescence quantum yields: Absolute fluorescence quantum yields (AFQY) were measured using an FS5 Spectrofluorometer from Edinburg Instruments with an SC-30 Integrating Sphere accessory using a direct excitation method. All samples were dissolved in DMAc at a concentration where the absorption intensity (A) was between A=0.09 and A=0.1, those samples were sparged with argon gas for 20 minutes, then transferred to 1 cm pathlength quartz cuvettes in a nitrogen filled glovebox before quantum yield analysis. Measurement was made over the photocatalyst samples (S) and reference solvents (R) scattering (R_s and S_s) and emission (R_e and S_e). The equation for the calculation of AFQY using the direct excitation method is:

$$AFQY = \frac{S_e - R_e}{R_s - S_s}\, x\, 100$$

The scattering and emission spectral regions were measured separately. The AFQY values were calculated using the Fluoracle software via the equation above.

AFQY values were measured at the maximum wavelength of emission.

Cyclic voltammetry: Cyclic voltammograms were obtained using a Gamry electrochemical analyzer with an Ag/AgNO3 (0.01 M in acetonitrile (MeCN)) reference electrode and tetrabutylalammonium hexafluorophosphate ($TBAPF_6$) (0.1 M in DMAc) as the electrolyte for the working electrode. All samples were analyzed in DMAc at a concentration between 0.06 mM and 1 mM (depending on solubility) at a total volume of 25.0 mL and were sparged with nitrogen for 15 minutes before data collection. Platinum was used for the working and counter electrodes. Analysis was conducted at scan rates of 100 mV/s, 80 mV/s, 50 mV/s, and 20 mV/s with 7 cycles each. Data from the 6^{th} cycle was analyzed unless otherwise noted. All voltammograms were corrected using the $E_{1/2}$ of ferrocene as a reference.

Transient Absorption Spectroscopy: Transient absorption (TA) spectroscopy for determination of phenazine photocatalyst (PC) singlet and triplet excited state lifetimes was performed on an Edinburgh Instruments LP980KS spectrometer with a Minilite Nd:YAG Q-switched laser (Continuum Lasers) configured to deliver a 355 excitation pulse. Spectral absorption data was acquired from 300-800 nm with time delays as indicated in the spectra shown below with an iStar ICCD camera (Andor) as the detector. Kinetic data was recorded utilizing a photomultiplier tube (included in the LP980) interfaced with an MD03022 mixed domain oscilloscope (Tektronix) as the detector. Time zero was set on the instrument using the emission of $[Ru(bpy)_3]Cl_2$ to locate the pump pulse with a resolution of 1 ns. All kinetic traces shown were acquired with 50-75 averages and laser power between 3-15 mW/cm^2 at 1 Hz repetition rate. Time constants (excited state lifetimes) were calculated in the L900 software using an exponential tail fit. Spectral absorption data was offset corrected at all wavelengths using kinetic absorption data at the indicated wavelength to adjust ΔOD. Emission subtraction was done for spectra acquired at t = 0, while spectra acquired at t = 200 ns or t = 400 ns included a time delay to avoid emission signals and the emission subtraction step was omitted.

For each PC solution, the Beer-Lambert Law was used to calculate the concentration of PC needed for an absorbance intensity of 0.2 at the lambda max of absorbance. This resulted in solutions with an absorbance intensity of less than 0.2 at 355 nm (wavelength of the excitation pulse). To prepare the solutions, solid PC was weighed into a scintillation vial which was then brought into a N_2 filled glovebox. The appropriate amount of N,N-dimethylacetamide (DMAc) stored under N_2 was added to each vial, and 3 mL of the resulting solution was transferred to a quartz screw cap cuvette equipped with a Kontes valve and sidearm with a 1 cm path length. After completely sealing the cuvettes with caps, they were brought out of the glovebox. Each PC solution was analyzed by UV-vis on the instrument described herein both before and after TA spectroscopy to monitor if PC degradation occurred. None of the PC solutions analyzed in this work showed evidence of degradation after TA, indicated by no observable change in the UV-vis spectra before and after TA spectroscopy was performed (Figure S45).

Polymer Characterization: <u>Sample Prep for Analysis of Polymerization Kinetics and Molecular Weight Growth:</u> To evaluate the kinetics and growth of molecular weight relative to the conversion of monomer (into polymer), an 0.1 mL aliquot of reaction mixture was taken after 1 hour, 2 hours, 4 hours, 6 hours, and 8 hours then immediately injected into a GC vial containing 0.5 mL of a solution of deuterated chloroform containing 250 ppm of a radical inhibitor (butylated hydroxyl toluene (BHT)). The aliquot was then analyzed using ^{1}H NMR spectroscopy. Through ^{1}H NMR spectroscopy the ratio of polymer to monomer (% conversion) was determined. After ^{1}H NMR NMR analysis, the solvent was evaporated under air, then the sample was re-dissolved in HPCL-grade THF, filtered into a GPC vial using a 0.45 µm nylon filter, and finally analyzed by GPC with MALS. <u>Characterization Instrumentation:</u> Monomer conversion was determined using a Varian 400 MHz NMR Spectrometer. Molecular weights were determined by Gel Permeation Chromatography (GPC) coupled with multi-angle light scattering (MALS) using an Agilent HPLC fitted with one guard column, three PL-gel 5 µm MIXED-C gel permeation columns, a Wyatt Technology TrEX differential refractometer, and a Wyatt Technology miniDAWN TREOS light scattering detector (MALS). The dn/dc value used for MMA in THF was 0.084, A dn/dc value of 0.063 in THF was used for poly(n-butyl) acrylate analysis.

Polymerization Batch Reactor Supplies and Design

Light Beakers for Polymerizations (Materials): One sixteen-inch strip of double-density white LEDs was purchased from Creative Lighting Solutions (item no. CL-FRS1210-5M-12V-WH). Emission spectra of LEDs used is shown in Figure S2.

Light Beakers for Polymerizations (Setup): White light LED strip from Creative Lighting Solutions was wrapped inside a 400 mL beaker and used as the visible light source for the polymerizations described in this paper. The sides and bottom of the beaker were completely wrapped with tin foil and the led strips were coiled inside the bottommost portion of the beaker walls (Figure S1).

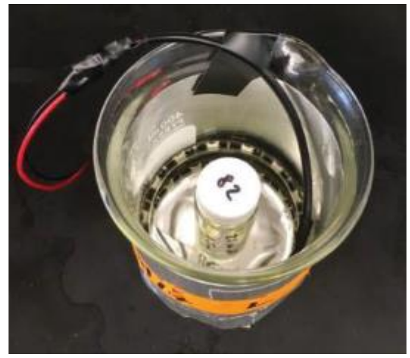


Figure S1. 400 mL white light LED beaker photoreactor for polymerizations.

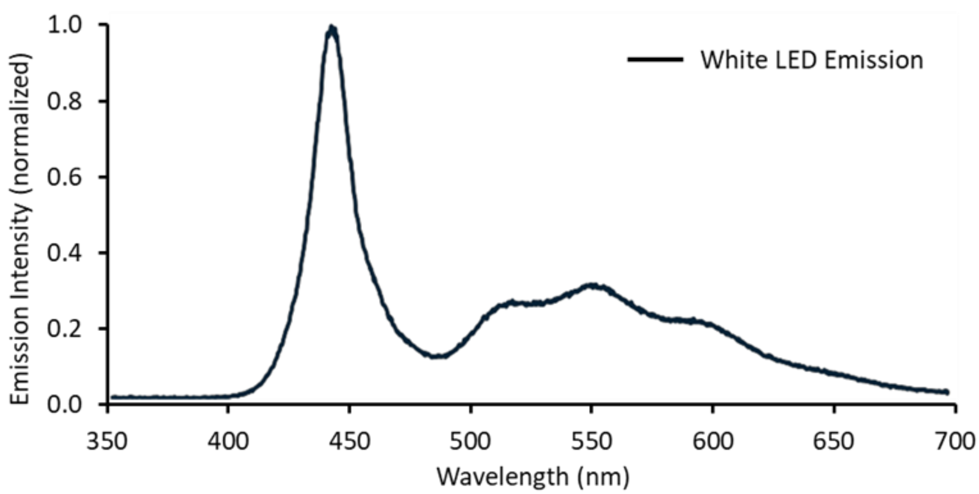


Figure S2. Normalized emission spectra of white light LEDs from creative lighting solutions.

PROCEDURES

Catalyst Synthesis

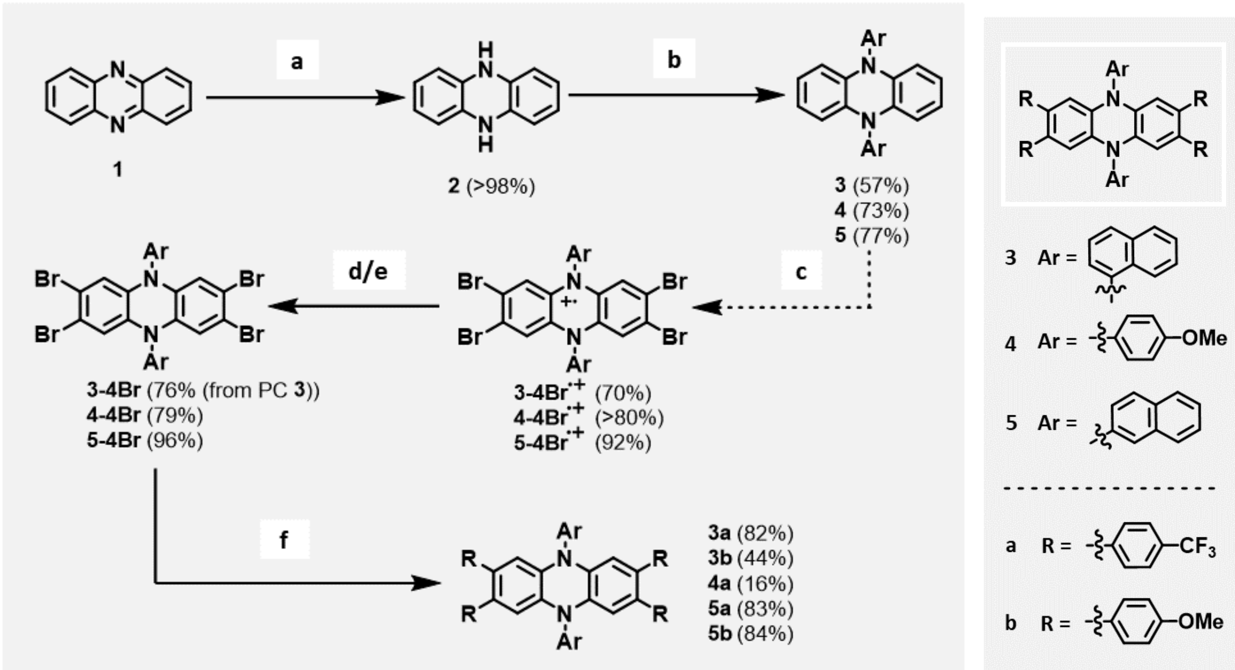


Figure S3. Synthetic scheme for synthesis of core-extended N,N-diaryl dihydrophenazines and structures. The mol percent yield from each step is noted adjacent to the labels of the final catalysts and catalyst intermediates.

Synthesis of *N,N*-diaryl dihydrophenazines (DHPs):

<u>Synthesis of **2** (5,10-dihydrophenazine) (a)[1]:</u> Phenazine (27.6 mmol) was dissolved in reagent alcohol (EtOH) (150 mL) that had been sparged with N_2 for 30 min. This mixture was brought to reflux under N_2 and a solution of sodium dithionite ($Na_2S_2O_4$) (555 mmol) dissolved in degassed water (~700 mL) was added to the solution of phenazine under N_2 via a canula transfer. The reaction was solution was refluxed for 3.5 hours and subsequently cooled to room temperature. The solid was collected using a swivel frit under N_2 and washed with sparged H_2O (3 x 100 mL). The solid was then dried overnight under vacuum before being brought into an N_2 filled glovebox. (yield: 94%)

<u>Synthesis of **3** (b)[2,3]:</u> 5,10-dihydrophenazine (1.098 mmol), NaOtBu (3.29 mmol), $P(tBu)_3$ (0.066 mmol), a stir bar, and 1-bromonaphthalene (4.39 mmol) were added to an oven dried Schlenk flask which was then cycled under reduced pressure and backfilled with N_2 three times. The Schlenk flask was then brought into in an N_2 filled glovebox and anhydrous 10 mL of Sure/Seal anhydrous toluene and $Pd(dba)_2$ (0.022 mmol) were added. The flask was then brought back out of the glovebox and the mixture was refluxed for 48 hours at 110°C then subsequently cooled to room temperature. The reaction mixture was then transferred to a separatory funnel and shaken in 100 mL of DI H_2O and 100 mL of DCM. The organic layer was recovered, washed with 100 mL

of brine three times, then dried over Mg_2SO_4. After filtering off the Mg_2SO_4, the DCM was removed via rotary evaporation. The solids extracted from the crude reaction mixture were then dissolved in a minimal amount of DCM and recrystallized in the freezer after layering x3 volume of methanol on top of the DCM. Dark yellow solids were recovered. (Yield: 57%). ^{1}H NMR (400 MHz, C_6D_6) δ 8.68 – 8.54 (m, 2H), 7.75 – 7.66 (m, 2H), 7.64 (d, *J* = 8.5 Hz, 2H), 7.46 (dd, *J* = 17.4, 7.1 Hz, 2H), 7.27 (dd, *J* = 15.5, 7.9 Hz, 7H), 6.07 (dd, *J* = 5.9, 3.4 Hz, 4H), 5.73 – 5.58 (m, 4H).

Synthesis of **4** (b) [2,3]: 5,10-dihydrophenazine (12.6 mmol), NaOtBu (37.9 mmol), $P(tBu)_3$ (0.756 mmol), and a stir bar were added to an oven dried Schlenk flask which was then cycled under reduced pressure and backfilled with N_2 three times. The Schlenk tube was then brought into in an N_2 filled glovebox and anhydrous Sure/Seal toluene, $Pd(dba)_2$ (0.025 mmol), and 4-bromoanisole (21.1 mmol) (which was sparged under N_2 for 40 minutes) were added. The flask was then brought back out of the glovebox and the mixture was refluxed for 31 hours at 110°C then subsequently cooled to room temperature. The reaction mixture was dissolved in DCM (~100 mL) then washed twice with 400 mL of water, then with 100 mL of brine three times. The organic layer was dried using Mg_2SO_4 then filtered. Next, the solvent was removed via rotary evaporation. The solids obtained were dissolved in hot DCM, then x3 volume of warm hexanes was layered onto of the DCM. Bright yellow crystals were recovered. (Yield: 73 %) ^{1}H NMR (400 MHz, DMSO) δ 7.34 – 7.27 (m, 4H), 7.24 – 7.17 (m, 4H), 6.24 (dd, *J* = 5.9, 3.4 Hz, 4H), 5.49 (dd, *J* = 5.8, 3.4 Hz, 4H), 3.84 (s, 6H).

Synthesis of **5** (b)[2,3]: 5,10-dihydrophenazine (27.4 mmol), NaOtBu (10.97 mmol), a stir bar, and 2-bromonaphthalene were added to an oven dried 250 mL Schlenk tube which was then cycled under reduced pressure and backfilled with N_2 three times. The Schlenk tube was then brought into in an N_2 filled glovebox and 50 mL of anhydrous Sure/Seal, RuPhos (1.09 mmol), and RuPhos Pd G4 (0.110 mmol) were added. The Schlenk tube was then brought back out of the glovebox and the mixture was refluxed for 48 hours at 110°C then subsequently cooled to room temperature. 600 mL of DCM and 300 mL of water were added to the crude reaction mixture. The product crashed out of solution over several minutes. Both aqueous and organic layers were filtered and the solid was collected. The product was then recrystallized from boiling DCM/MeOH in a 1:3 ratio to yield yellow crystals. (Yield: 77%) ^{1}H NMR (400 MHz, C_6D_6) δ 7.68 (dd, *J* = 5.3, 3.3 Hz, 4H), 7.64 – 7.57 (m, 2H), 7.57 – 7.49 (m, 2H), 7.32 (dd, *J* = 8.6, 2.0 Hz, 2H), 7.24 (dddd, *J* = 19.0, 8.2, 6.9, 1.4 Hz, 4H), 6.28 (dt, *J* = 7.5, 3.7 Hz, 4H), 5.86 (dd, *J* = 5.9, 3.4 Hz, 4H).

Synthesis of **3-4Br$^{•+}$** (c)[4]: PC **3** (0.460 mmol), benzene (200 mL), and bromine (9.20 mmol) were added to a round bottom flask containing a stir bar. The solution was refluxed at 60°C for 38.5 hours with a tube bubbling vapors from the reaction into a saturated aqueous solution of sodium dithionite. After 38.5 hours the reaction was cooled to room temperature and filtered. The reaction yielded 267 mg of dark blue solids. The filtrate (containing unreacted bromine) was neutralized using a solution of DI H_2O saturated with sodium thiosulfate. (Yield ~70%) (Not characterized by ^{1}H-NMR).

Synthesis of **4-4Br**$^{•+}$ (c)[4]: PC **4** (0.761 mmol), benzene (500 mL), and bromine (15.2 mmol) were added to a round bottom flask containing a stir bar. The solution was refluxed at 60°C for 24.5 hours with a tube bubbling vapors from the reaction into a saturated aqueous solution of sodium dithionite. After 24.5 hours the reaction was cooled to room temperature and filtered. The reaction yielded 267 mg of dark purple solids. The filtrate (containing unreacted bromine) was neutralized using a solution of DI H_2O saturated with sodium thiosulfate. (Yield >80%) (Not characterized by ^{1}H-NMR).

Synthesis of **5-4Br**$^{•+}$ (c)[4]: PC **5** (11.5 mmol), benzene (200 mL), and bromine (23.0 mmol) were added to a round bottom flask containing a stir bar. The solution was refluxed at 60°C for 12 hours hours with a tube bubbling vapors from the reaction into a saturated aqueous solution of sodium dithionite. After 12 hours the reaction was cooled to room temperature and filtered. The reaction yielded 882 mg of dark purple solids. The filtrate (containing unreacted bromine) was neutralized using a solution of DI H_2O saturated with sodium thiosulfate. (Yield ~92%) (Not characterized by ^{1}H-NMR).

Synthesis of **3-4Br** (d) (Method I)[4]: 160 mg of the solids obtained from the synthesis of **3-4Br**$^{•+}$ (~0.193 mmol) were added to a 1L round bottom flask. 500 mL of methanol was added along with a stir bar and 8g of copper wire cut into 1 inch pieces. The reaction mixture (a deep magenta color) was then stirred at ~60 °C for 30 minutes. After 30 minutes the reaction mixture had turned a creamy-orange color. The reaction mixture was subsequently cooled to room temperature and 86.4 mg of orange/yellow solids were collected via vacuum filtration and used without further purification. (Yield ~60%) (This sample was not used in synthesis, only the sample synthesized using Method II (see below) was used.

Synthesis of **3-4Br** (Method II) (c&e): Step 1): PC **3** (0.587 mmol), benzene (300 mL), and bromine (11.7 mmol) were added to a round bottom flask containing a stir bar. The solution was refluxed for 48.5 hours with a tube bubbling vapors from the reaction vessel into a saturated aqueous solution of sodium dithionite. After 48.5 hours the reaction was cooled to room temperature and filtered yielding shiny dark blue solids. The filtrate (containing unreacted bromine) was neutralized using a solution of DI H_2O saturated with sodium thiosulfate. Step 2): The recovered solids were dissolved in acetone (~500 mL) and allowed to stir for five hours at room temperature. The reaction mixture slowly changed from a deep magenta color to an opaque pale-yellow color. The reaction mixture was filtered and ~333 mg of solids were recovered. (Yield from

3 → 3-4Br: ~76%) ^1H NMR (400 MHz, C_6D_6) δ 8.36 (dd, *J* = 17.1, 8.4 Hz, 2H), 7.51 (dd, *J* = 8.3, 5.4 Hz, 2H), 7.45 (dd, *J* = 8.2, 4.5 Hz, 2H), 7.31 – 7.23 (m, 3H), 5.90 (d, *J* = 2.1 Hz, 4H).

Synthesis of **4-4Br** (d)[4]: 200 mg of the solids obtained from the synthesis of **4-4Br$^{•+}$** (~0.253 mmol) were added to a 1L round bottom flask. 500 mL of methanol was added along with a stir bar and 10g of copper wire cut into 1 inch pieces. The reaction mixture (a deep magenta color) was then stirred at ~80 °C for 3 hours. After 3 hours the reaction mixture had turned a light tan color. The reaction mixture was subsequently cooled to room temperature and 142 mg of light tan/yellow solids were collected via vacuum filtration. These solids were used without further purification. (Yield: 79%). ^1H NMR (400 MHz, C_6D_6) δ 6.78 (d, *J* = 8.5 Hz, 4H), 6.59 (d, *J* = 8.6 Hz, 4H), 6.06 (s, 4H), 3.15 (s, 6H).

Synthesis of **5-4Br** (d)[4]: 500 mL of methanol was added to **5-4Br$^{•+}$** solids in a round bottom flask with a stir bar. The solution was stirred at ~60 °C for 30 minutes. Then 7 ft of copper wire, cut into 1 inch pieces, was added to the round bottom flask. The solution was stirred at 60° C for 26 hours. The solution turned from a deep fusia color to a light orange color with a yellow solid precipitated. After 26 hours, the reaction mixture was cooled to room temperature and the solid was collected via vacuum filtration. (Yield: ~96%). ^1H NMR (400 MHz, C_6D_6) δ 7.57 – 7.41 (m, 9H), 7.01 (dd, *J* = 8.6, 2.1 Hz, 2H), 6.08 (s, 4H).

Synthesis of **3a** (e)[4]: **3-4Br** (0.173 mmol), 4-trifluoromethylphenyl boronic acid (1.39 mmol) n and a stir bar were added to a 100mL Schlenk tube. The Schlenk tube was then put under vacuum then backfilled with N_2 (three cycles) before transferring it to an N_2 filled glovebox. $Pd(PPh_3)_4$ (0.026 mmol) and 25.0 mL of anhydrous sure/seal THF was added. The storage tube was then taken out of the glove box and 4.50 mL of 2.00 M aqueous K_2CO_3 (that had been sparged with N_2 for >30 min) was added to the storage tube under N_2. The mixture was heated to 110 °C and stirred for 45 hours. After allowing the reaction mixture to cool, the reaction mixture was transferred to a round bottom flask using THF, then 100 mL of water was added. The THF was removed via rotary evaporation and yellow/green solids crashed out into the water. The solution was then filtered to recover the solids. The recovered solids were then dissolved in DCM, and the solution was washed with eqivolume of water three times then the organic layer was washed with brine. The solution was then dried with using Na_2SO_4 then filtered and concentrated via rotary evaporation. The recovered yellow solids were then dissolved in a minimal amount of warm toluene and any undissolved solids were filtered off. Small amounts of silver/grey solids were recovered from the solution during this step. Next, the toluene was removed by rotary evaporation then the recovered solids were redissolved in a minimal volume of DCM. Methanol (in three time the volume of DCM) was then layered on top of the DCM and the solution was put into the freezer to recrystallize. Bright yellow solids were recovered (Yield: 82%). ^1H NMR (400

MHz, C_6D_6) δ 8.85 (dd, *J* = 8.4, 4.5 Hz, 2H), 7.70 – 7.53 (m, 6H), 7.45 – 7.19 (m, 7H), 6.69 (dd, *J* = 8.5, 2.3 Hz, 9H), 6.57 (dd, *J* = 8.1, 5.9 Hz, 8H), 5.98 (d, *J* = 1.5 Hz, 4H). HRMS (ESI) calculated for (M^+) $C_{60}H_{34}F_{12}N_2$: 1010.2530; mass found: 1010.2480.

Synthesis of **4a** (e)[4]: **4-4Br** (0.446 mmol), 4-trifluoromethylphenyl boronic acid (3.57 mmol), and a stir bar were added to a 100mL Schlenk tube. The Schlenk tube was put under vacuum then backfilled with N_2 (three cycles) before transferring it to an N_2 filled glovebox. $Pd(PPh_3)_4$ (0.067 mmol) and 30.0 mL of THF were added. The storage tube was taken out of the glove box then 9.00 mL of 2.00 M aqueous K_2CO_3 that had been sparged with N_2 for >30 min was added to the storage tube under N_2. The mixture was heated to 100 °C and stirred for 48 hours. After allowing the reaction mixture to cool, the reaction mixture was transferred to a round bottom flask using THF and 100 mL of water, the THF was then removed via rotary evaporation and dark green/yellow solids crashed out into the water. The solids were recovered by vacuum filtration, then hot DCM was added until the solids were almost entirely dissolved ~400 mL). The solution was then filtered and small amounts of silver/grey solids were recovered. The filtrate was then rotovapped down to yield bright yellow solids (Yield: 80%). Although the 1H-NMR looked relatively clean, we attempted to further recrystallize the yellow powder. The bright yellow powder was then redissolved in warm DCM which was layered with methanol (x2 volume relative to DCM) and yellow solids started to crash out. The yellow solids were recovered via vacuum filtration then dissolved in ~300 mL of toluene. Warm hexanes in three times the volume of toluene was then layered on top of the solution. The solution was transferred to the freezer and allowed to recrystallize. Bright yellow solids were then recovered via vacuum filtration (Yield: 16 %) ^{1}H NMR (400 MHz, DMSO) δ 7.48 (dd, *J* = 8.6, 3.5 Hz, 13H), 7.20 (d, *J* = 8.9 Hz, 4H), 6.99 (d, *J* = 8.0 Hz, 8H), 5.57 (s, 4H), 3.80 (s, 6H). ^{1}H NMR (400 MHz, C_6D_6) δ 7.29 (d, *J* = 8.8 Hz, 4H), 6.94 – 6.78 (m, 20H), 6.12 (s, 4H), 3.11 (s, 6H). HRMS (ESI) calculated for (M^+) $C_{54}H_{34}F_{12}N_2O_2$: 970.2428; mass found: Not detected.

Synthesis of **5a** (e)[4]: **5-4Br** (0.533 mmol) and 4-trifluoromethylphenyl boronic acid (4.27 mmol) were added to a 100mL storage tube. The storage tube was put under vacuum then backfilled with N_2 (3 cycles) before transferring it to an N_2 filled glovebox. $Pd(PPh_3)_4$ (0.080 mmol) and 40.0 mL of THF was added. The storage tube was then taken out of the glove box then 12.0 mL of 2.00 M aqueous K_2CO_3 that had been sparged with N_2 for >30 min was added to the storage tube under N_2. The mixture was heated to 100 °C and refluxed for 24 hours. After allowing the reaction mixture to cool, the reaction mixture was transferred to a round bottom flask using THF, then THF was removed via rotary evaporation. DCM was added until the solids were almost entirely dissolved. The solution was then washed with eqivolume of water three times then the organic layer was washed with an equivolume of brine two times. The solution was then dried with sodium sulfate and concentrated via rotary evaporation. The recovered yellow/green solids were then stirred in ~300 mL of hot toluene until almost everything had dissolved, then, after allowing it to cool, the solution was filtered. Small amounts of silver/grey solids were recovered from the product solution during this step. Warm hexanes in three times the volume of toluene was then layered on top of the solution. The solution was transferred to the freezer and allowed to recrystallize. Bright yellow solids were recovered via vacuum filtration. (Yield: 83 %) ^{1}H NMR (400 MHz, C_6D_6) δ 7.97 (d, *J* = 2.0 Hz, 2H), 7.77 (d, *J* = 8.6 Hz, 2H), 7.58 (dt, *J* = 7.2, 3.6 Hz, 2H), 7.55 – 7.46 (m, 4H), 6.75 (q, *J* = 8.4 Hz, 16H), 6.18 (s, 4H). HRMS (ESI) calculated for (M^+) $C_{60}H_{34}F_{12}N_2$: 1010.2530; mass found: 1010.2517.

<u>Synthesis of **3b** (e)[4]:</u> **3-4Br** (0.175 mmol), 4-methoxyphenyl boronic acid (0.00140 mol), and a stir bar were added to a 100mL storage tube. The storage tube was put under vacuum then backfilled with N_2 (three cycles) before transferring it to an N_2 filled glovebox. $Pd(PPh_3)_4$ (0.026 mol) and 10 mL of anhydrous Sure/seal THF was added. The storage tube was then taken out of the glove box then 6 mL of 2M aqueous K_2CO_3 that had been sparged with N_2 for >30 min was added to the storage tube under N_2. The mixture was heated to 110 °C and stirred for 48 hours. After allowing the reaction mixture to cool, THF was used to transfer the mixture to a round bottom flask. 100 mL of DI H_2O was added to the round bottom flask and then the THF was then removed via rotary evaporation—yellow solids precipitated into the water. The solids were recovered by vacuum filtration, rinsed with ~100 mL of methanol, then dissolved in hot DCM until the solids were almost entirely dissolved ~400 mL). The solution was then filtered and small amounts of silver/grey solids were recovered. The filtrate was then layered with x2 volume of methanol and placed in the freezer to recrystallize. (Yield: 44%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.00 (dd, *J* = 8.8, 4.0 Hz, 2H), 7.76 (t, *J* = 6.7 Hz, 2H), 7.65 (dd, *J* = 13.4, 8.0 Hz, 3H), 7.59 (d, *J* = 8.3 Hz, 2H), 6.86 (dd, *J* = 8.4, 6.4 Hz, 9H), 6.37 – 6.24 (m, 9H), 6.19 (d, *J* = 1.7 Hz, 4H), 3.08 (s, 14H). HRMS (ESI) calculated for (M^+) $C_{60}H_{46}N_2O_4$: 858.3458; mass found: 858.3441.

<u>Synthesis of **5b** (e)[4]:</u> **5-4Br** (0.667 mmol) and 4-methoxyphenyl boronic acid (5.33 mmol) were added to a 250 mL storage tube along with a stir bar. The storage tube was put under vacuum then backfilled with N_2 (x3) before transferring it to an N_2 filled glovebox. $Pd(PPh_3)_4$ (0.099 mmol) and 50.0 mL of THF were added. The storage tube was then taken out of the glove box then 15.0 mL of a 2.00 M aqueous K_2CO_3 that had been sparged with N_2 for >30 min was added to the storage tube under N_2. The mixture was heated to 100 °C and stirred for 24 h. After allowing the reaction mixture to cool, it was transferred to a round bottom flask using 100 mL of THF and 100 mL of water. The THF was then removed via rotary evaporation and yellow/green solids crashed out. The solids were then filtered off and the filtrate disposed of. Hot DCM was added to the until the solids were almost entirely dissolved. The solution was then washed with eqivolume of water

three times then the organic layer was washed with brine. The solution was then dried with sodium sulfate, filtered, then concentrated via rotary evaporation. The solids were recrystallized by using hot dichloromethane to dissolve the solids, then adding three times that volume of methanol. The recovered yellow solids were then dissolved in warm toluene and filtered. Small amounts of silver/grey solids were recovered from the product solution during this step. The toluene was removed via rotary evaporation and the remaining solids were recrystallized again from hot DCM/MeOH in a ratio of 1:3 yielding bright yellow solids. (Yield: 84%) ^{1}H NMR (400 MHz, C_6D_6) δ 8.00 (s, 2H), 7.80 – 7.45 (m, 7H), 6.46 – 6.21 (m, 12H), 3.06 (d, *J* = 3.6 Hz, 12H). ^{1}H NMR (400 MHz, DMSO) δ 8.26 (d, *J* = 8.7 Hz, 2H), 8.19 (d, *J* = 1.9 Hz, 2H), 8.05 (t, *J* = 7.6 Hz, 4H), 7.72 – 7.65 (m, 2H), 7.61 (q, *J* = 6.9 Hz, 4H), 6.66 – 6.53 (m, 18H), 5.54 (s, 4H). HRMS (ESI) calculated for (M^+) $C_{60}H_{46}N_2O_4$: 858.3458; mass found: 858.3435.

<u>Polymer Synthesis:</u>

Approximately 15.0 mg of the catalyst was weighed into a 20 mL scintillation vial. Each catalyst was then dissolved in DMAc to a known concentration. A specific volume of the catalyst stock solution was then dispensed into a 20 mL scintillation vials such that when 1.00 mL of monomer was added to the reaction vial, the catalyst would either be at a 500 ppm, 100 ppm, 50 ppm, or 10 ppm catalyst loading relative to monomer. After the catalyst solutions were dispensed into scintillation vials, the DMAc was removed via rotary evaporation and the sample was dried on a high vac line for 24 hours. The scintillation vials containing catalyst were then equipped with a stir bar and brought into a nitrogen-filled glovebox. 1.00 mL of monomer and 1.00 mL of solvent was then added using Hamilton gas tight syringes and the solution stirred in the dark for 2 minutes. 17.8 µL of initiator (diethyl-2-bromo-2-methylmalonate) was then added using a Hamilton gas tight syringe and the reaction vessel was immediately placed in the center of an LED beaker, the latter of which had been turned on for at least 5 minutes. The initial time for the start of the polymerization was noted at the moment the reaction vessel was transferred to the LED beaker and the polymerizations were allowed to proceed for eight hours. Polymerizations were run according to previously described methods.[3,4]

CHARACTERIZATION OF CATALYST PROPERTIES

Table S1. Select experimentally determined and computationally predicted photophysical and electrochemical properties of PCs.

PC	$\lambda_{max,abs}$ (nm)[a]	ε_{max} ($M^{-1}s^{-1}$)[b]	$\lambda_{max,em}$ (nm)[c]	$E_{S1,exp}$ (eV)[d]	$E_{T1,comp}$ (eV)[e]	Stokes Shift (nm)	Φ_f (%) [f]	$E_{1/2}$ ($^2PC^{\bullet+}/^1PC$) (V vs SCE)[g]	$E^0_{ox,comp}$ ($^2PC^{\bullet+}/^1PC$) (V vs SCE)[e]	$E^{0*}_{S1,exp}$ ($^2PC^{\bullet+}/^1PC^*$) (V vs SCE)[h]	$E^{0*}_{T1,comp}$ ($^2PC^{\bullet+}/^3PC^*$) (V vs SCE)[e]

3	362	6,100	663	1.87	2.23	297	1.32	0.23	0.10	-1.64	-2.13
3a	385	21,900	586	2.12	1.91	201	9.00	0.34	0.24	-1.78	-1.67
3b	385	13,100	636	1.95	2.07	251	4.31	0.23	0.00	-1.72	-2.06
4	373	5,500	467	2.66	2.29	94.0	23.0	0.16	0.01	-2.50	-2.29
4a	392	21,000	599	2.07	1.82	207	36.0	0.34	0.16	-1.73	-1.66
5	343	5,900	654	1.90	2.19	311	0.72	0.21[i]	0.06	-1.69	-2.12
5a	373	27,400	587	2.11	1.89	214	35.0	0.38	0.15	-1.73	-1.75
5b	371	16,000	621	2.00	1.99	250	4.00	0.38	0.00	-1.62	-2.00

[a]Maximum wavelength of absorption was measured using UV-Vis in DMAc. [b]Molar absorptivity calculated at λ_{max} in DMAc. [c] Maximum wavelength of emission was measured using steady-state fluorescence spectroscopy in DMAc. [d]Singlet energies were calculated using the maximum wavelength of emission (E(eV)=1239.8 / λ (nm)). [e]DFT calculations were performed at the uM06/6-311+G(d,p)//uM06/6-31+G(d,p) level of theory with CPCM-described solvation in DMAc. [f]Quantum yield of fluorescence was measured in DMAc using absolute methods. [g]All measurements were performed in a 3-compartment electrochemical cell with an Ag/ AgNO3 reference electrode in MeCN (0.01 M) and 0.1 M NBu4PF6 electrolyte solution. DMAc was used to solvate the PCs and in the working electrode compartment, while platinum was used as both the working and counter electrodes. E (V vs SCE) = E (V vs Ag/AgNO3 [0.01 M]) + 0.298 V. [h]Singlet excited state reduction potentials were calculated using the singlet energies (estimated from the maximum wavelength of emission) and the $E_{1/2}$. [i]Values were taken from ref. 2.

Table S2. Experimentally determined singlet and triplet excited state lifetimes of PCs.

PC	τ_{S1} (ns)[a]	τ_{T1} (μs)[b]	$\lambda_{kinetic\ em}$ (nm)[c]	$\lambda_{kinetic\ abs}$ (nm)[d]
3	9	0.63	617	445
3a	17	144	569	440
3b	11	42	608	593
4	37	88	466	450
4a	13	NA[e]	585	NA[e]
5	NA[f]	3.5	600	450
5a	17	NA[e]	575	NA[e]
5b	11	108	598	550

[a]Singlet excited state lifetime determined by kinetic emission. [b]Triplet excited state lifetime determined by kinetic absorption. [c]Wavelength at which kinetic emission was measured. [d]Wavelength at which kinetic absorption was measured. [e]Excited state absorption signal was too weak to measure kinetic decay of excited state absorption, therefore a triplet excited state lifetime was not measured for this PC. [f]Kinetic emission measured at 600nm was determined to be 6.3 ns which is too close to the limit of detection for the instrument (6 ns) to be measured accurately, therefore this data is not included in the above table.

<u>Ultraviolet-Visible Spectroscopy</u>

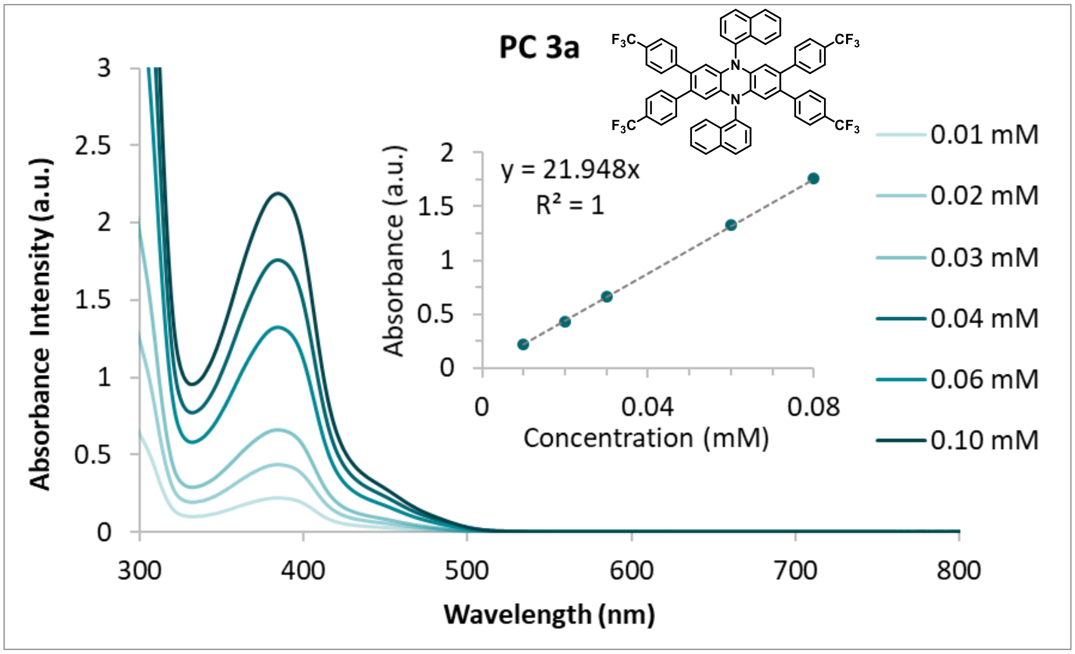


Figure S4. UV-Vis spectra of **3a** at varied concentrations in DMAc in a quartz cuvette with a pathlength of 1cm. Secondary graph demonstrates the Beer-Lambert law relationship between concentration and absorbance at 385 nm.

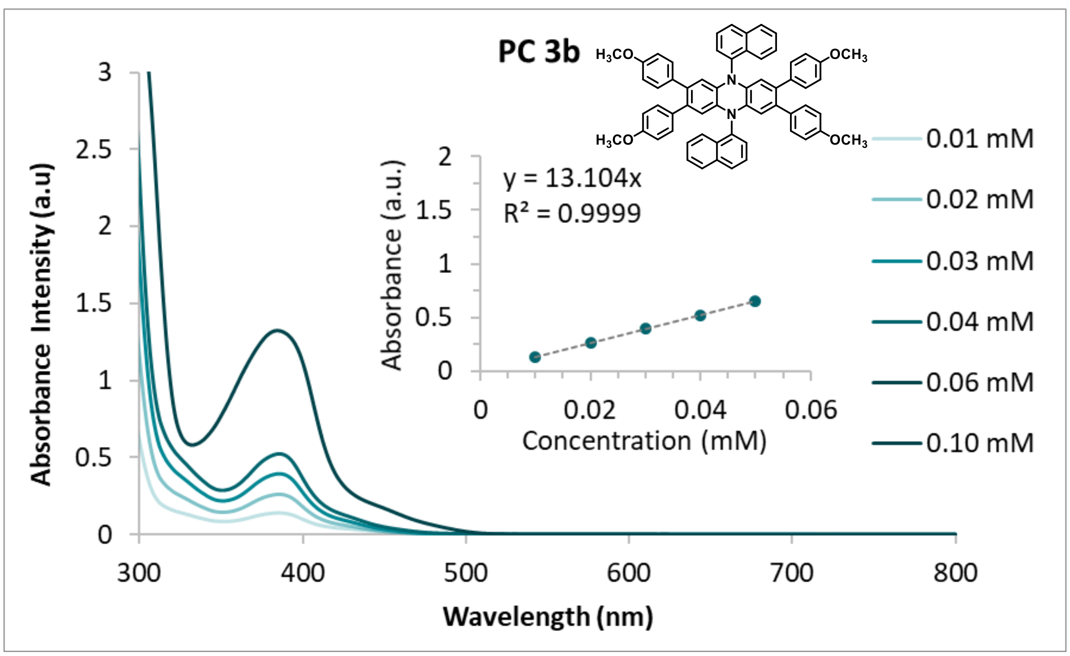


Figure S5. UV-Vis spectra of **3b** at varied concentrations in DMAc in a quartz cuvette with a pathlength of 1cm. Secondary graph demonstrates the Beer-Lambert law relationship between concentration and absorbance at 385 nm.

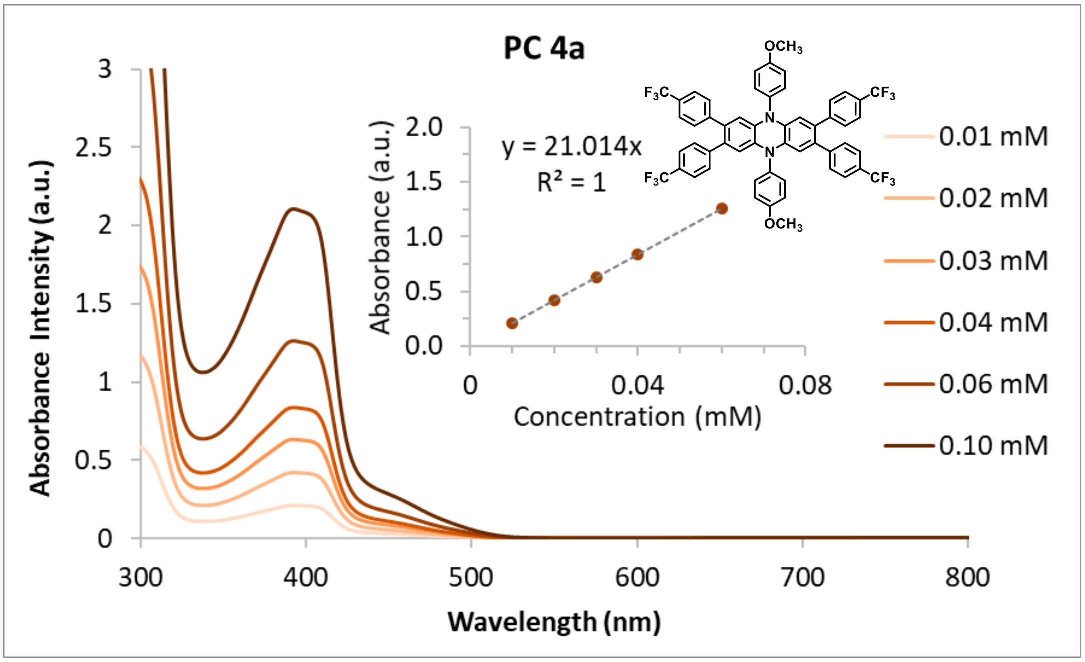


Figure S6. UV-Vis spectra of **4a** at varied concentrations in DMAc in a quartz cuvette with a pathlength of 1cm. Secondary graph demonstrates the Beer-Lambert law relationship between concentration and absorbance at 392 nm.

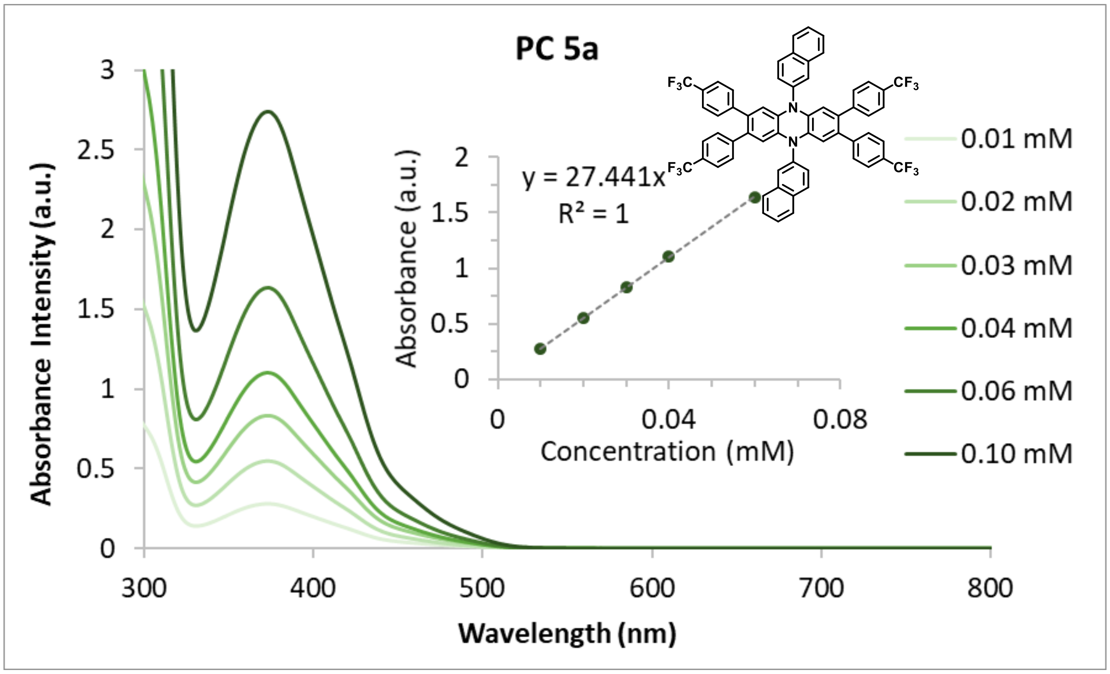


Figure S7. UV-Vis spectra of **5a** at varied concentrations in DMAc in a quartz cuvette with a pathlength of 1cm. Secondary graph demonstrates the Beer-Lambert law relationship between concentration and absorbance at 373 nm.

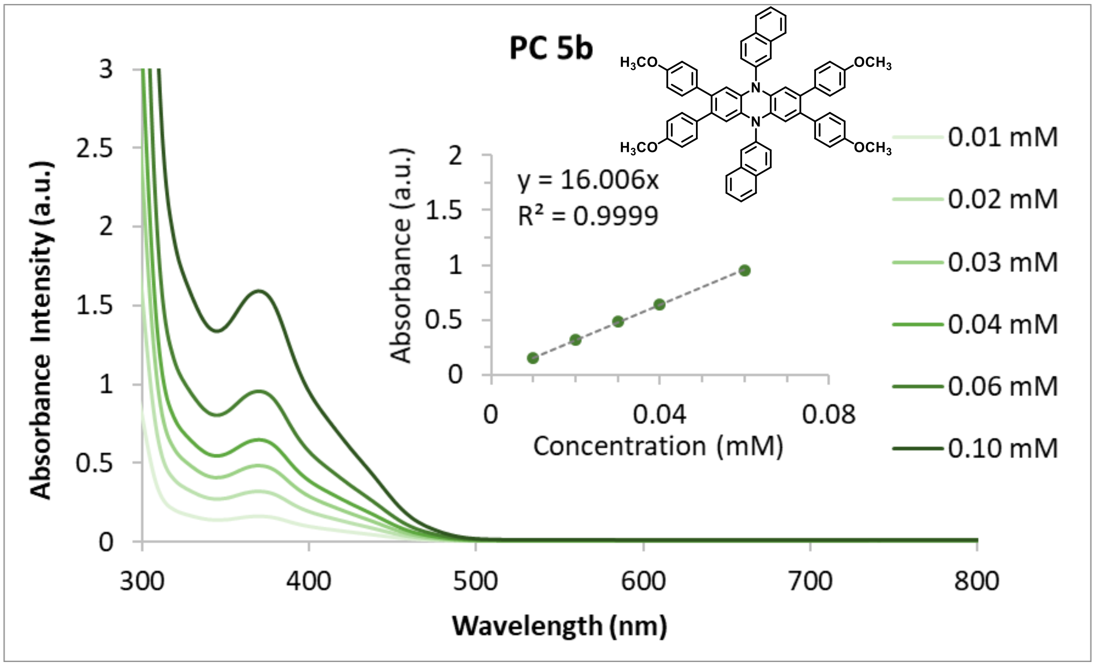


Figure S8. UV-Vis spectra of **5b** at varied concentrations in DMAc in a quartz cuvette with a pathlength of 1cm. Secondary graph demonstrates the Beer-Lambert law relationship between concentration and absorbance at 371 nm.

Fluorescence Spectroscopy

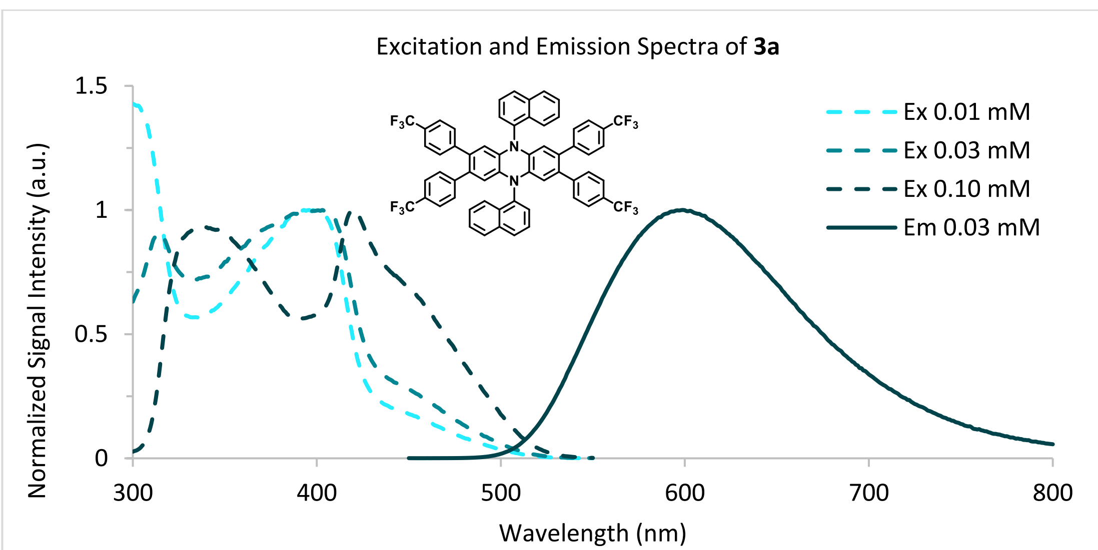


Figure S9. Fluorescence spectra of PC **3a.** Dashed lines are the excitation spectra at varying concentrations in DMAc and the solid line is the emission spectrum at 0.03 mM in DMAc. Emission spectra was collected using an excitation wavelength of 385 nm and is representative of emission profiles at all concentrations between 0.01 mM and 0.10 mM. Excitation spectra were collected for emission at 586 nm.

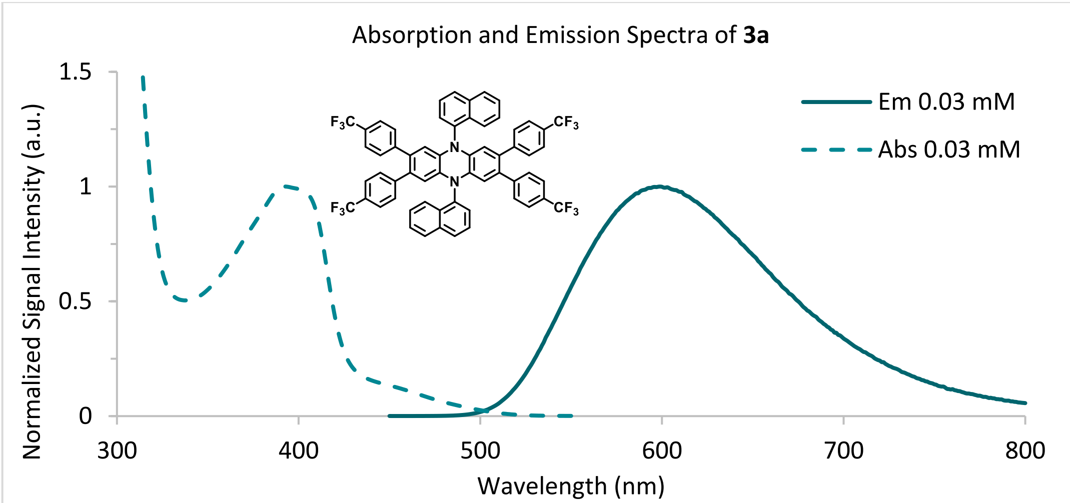


Figure S10. Emission spectra of PC **3a** (solid) and absorption spectra of **3a** (dashed) at 0.03 mM in DMAc. Absorption spectra was measured using UV-Vis and emission spectra was measured using fluorimetry. Emission spectra was collected using an excitation wavelength of 385 nm.

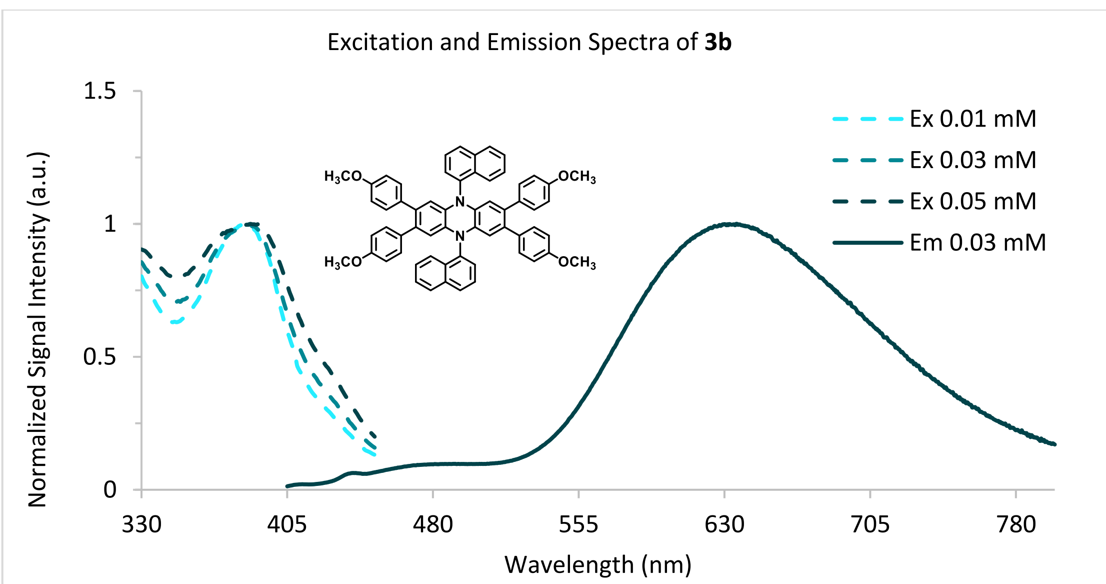


Figure S11. Fluorescence spectra of PC **3b.** Dashed lines are the excitation spectra at varying concentrations in DMAc and the solid line is the emission spectrum at 0.03 mM in DMAc. Emission spectra was collected using an excitation wavelength of 385 nm and is representative of emission profiles at all concentrations between 0.01 mM and 0.10 mM. Excitation spectra were collected for emission at 636 nm.

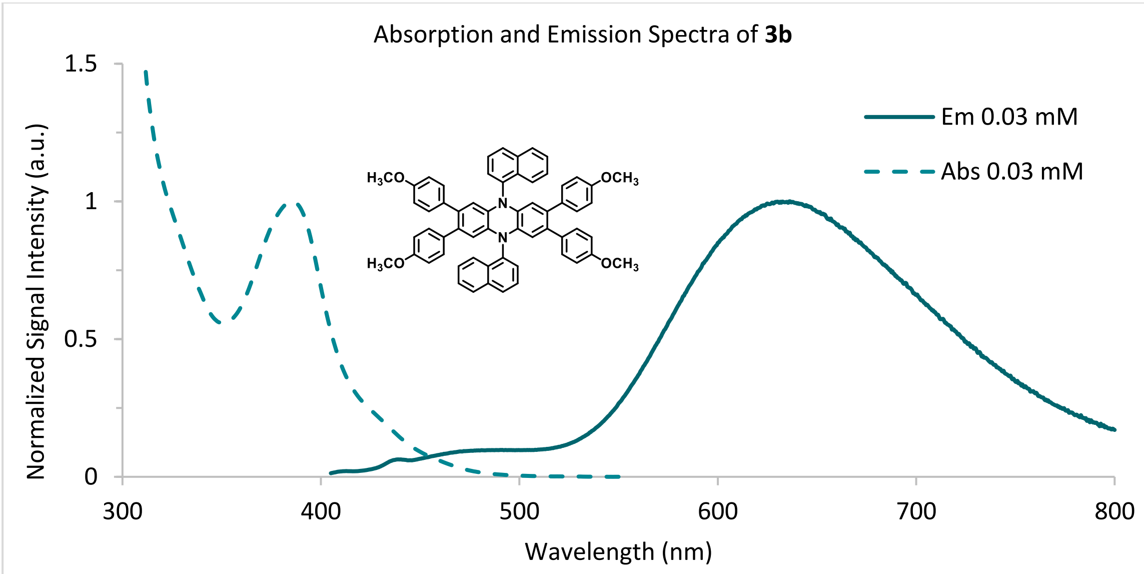


Figure S12. Emission spectra of PC **3b** (solid) and absorption spectra of **3b** (dashed) at 0.03 mM in DMAc. Absorption spectra was measured using UV-Vis and emission spectra was measured using fluorimetry. Emission spectra was collected using an excitation wavelength of 385 nm.

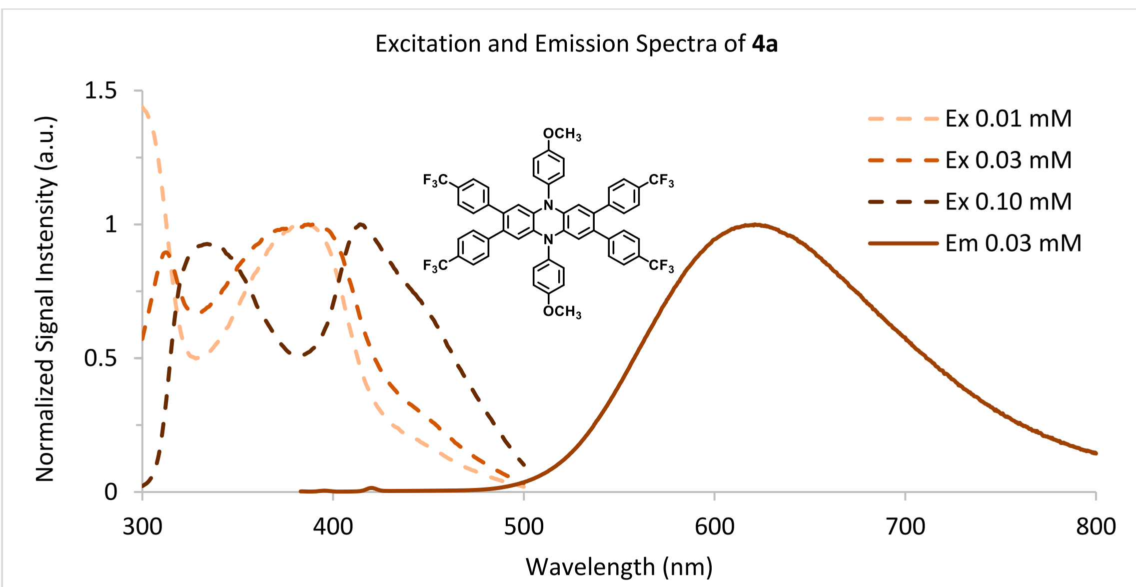


Figure S13. Fluorescence spectra of PC **4a.** Dashed lines are the excitation spectra at varying concentrations in DMAc and the solid line is the emission spectrum at 0.03 mM in DMAc. Emission spectra was collected using an excitation wavelength of 392 nm and is representative of emission profiles at all concentrations between 0.01 mM and 0.10 mM. Excitation spectra were collected for emission at 599 nm.

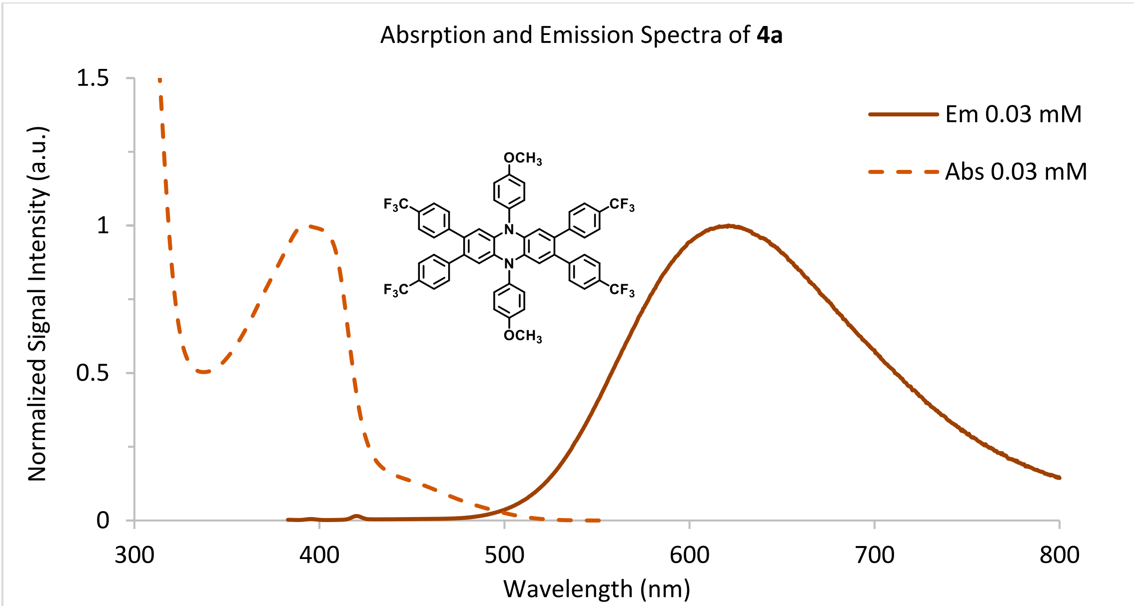


Figure S14. Emission spectra of PC **4a** (solid) and absorption spectra of **4a** (dashed) at 0.03 mM in DMAc. Absorption spectra was measured using UV-Vis and emission spectra was measured using fluorimetry. Emission spectra was collected using an excitation wavelength of 392 nm.

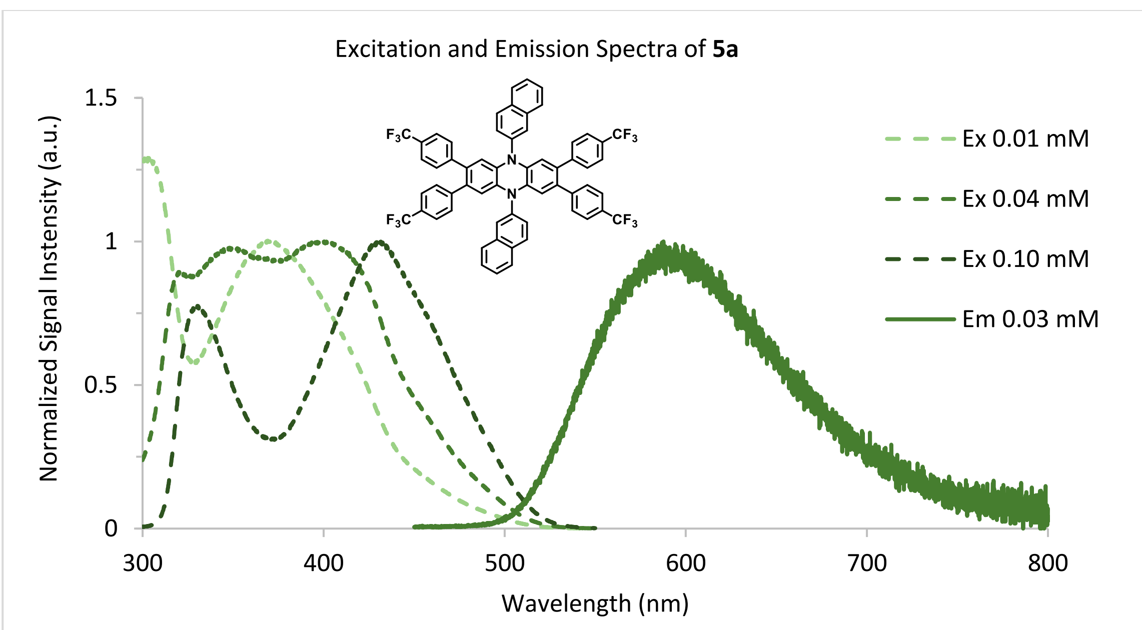


Figure S15. Fluorescence spectra of PC **5a.** Dashed lines are the excitation spectra at varying concentrations in DMAc and the solid line is the emission spectrum at 0.03 mM in DMAc. Emission spectra was collected using an excitation wavelength of 373 nm and is representative of emission profiles at all concentrations between 0.01 mM and 0.10 mM. Excitation spectra were collected for emission at 587 nm.

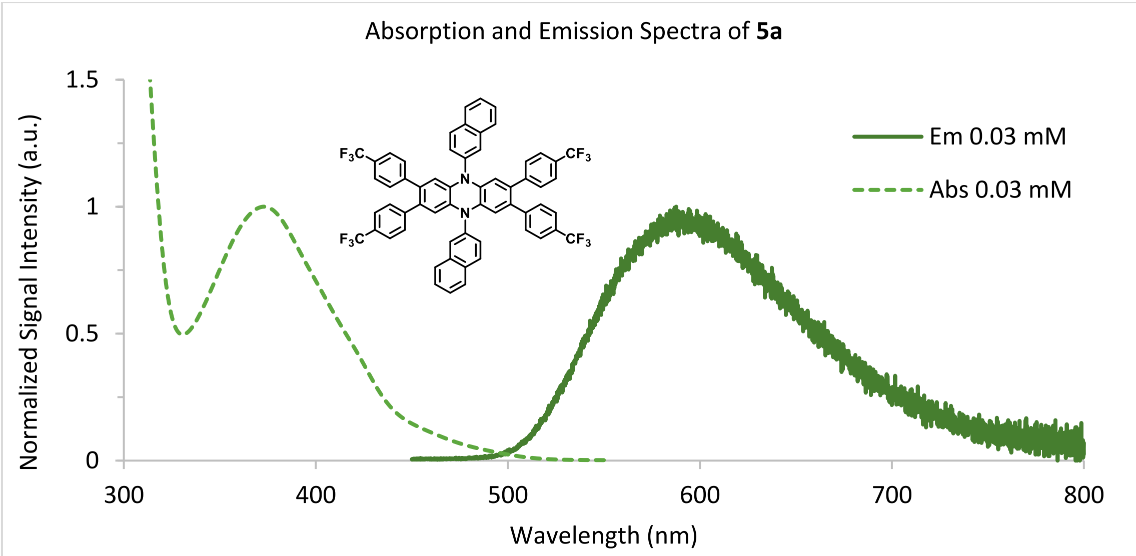


Figure S16. Emission spectra of PC **5a** (solid) and absorption spectra of **5a** (dashed) at 0.03 mM in DMAc. Absorption spectra was measured using UV-Vis and emission spectra was measured using fluorimetry. Emission spectra was collected using an excitation wavelength of 373 nm.

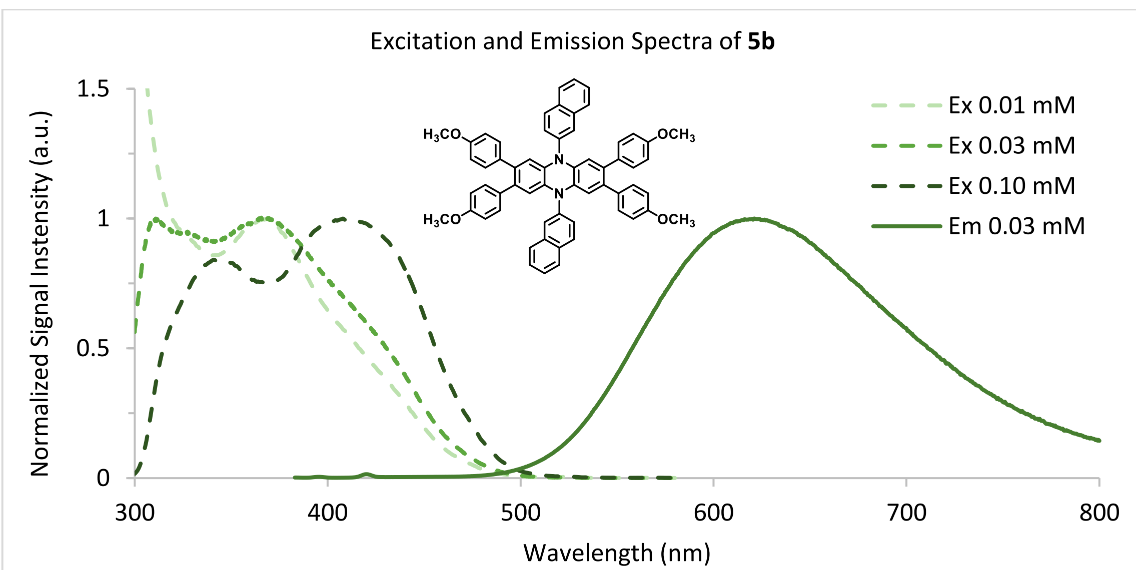


Figure S17. Fluorescence spectra of PC **5b.** Dashed lines are the excitation spectra at varying concentrations in DMAc and the solid line is the emission spectrum at 0.03 mM in DMAc. Emission spectra was collected using an excitation wavelength of 371 nm and is representative of emission profiles at all concentrations between 0.01 mM and 0.10 mM. Excitation spectra were collected for emission at 621 nm.

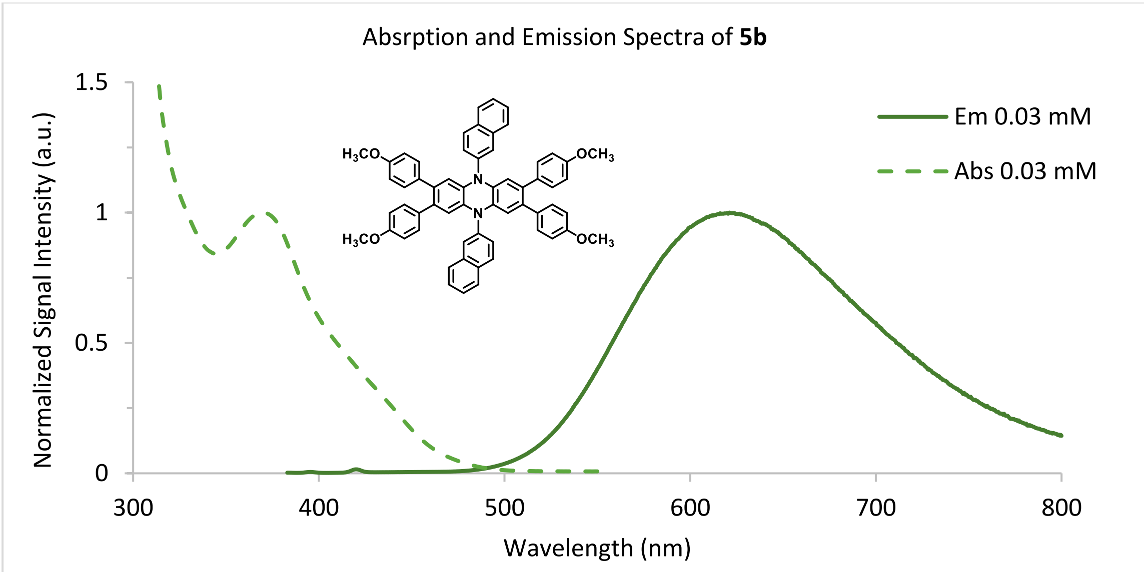


Figure S18. Emission spectra of PC **5b** (solid) and absorption spectra of **5b** (dashed) at 0.03 mM in DMAc. Absorption spectra was measured using UV-Vis and emission spectra was measured using fluorimetry. Emission spectra was collected using an excitation wavelength of 371 nm.

Transient Absorption Spectroscopy

Spectral Absorption Data

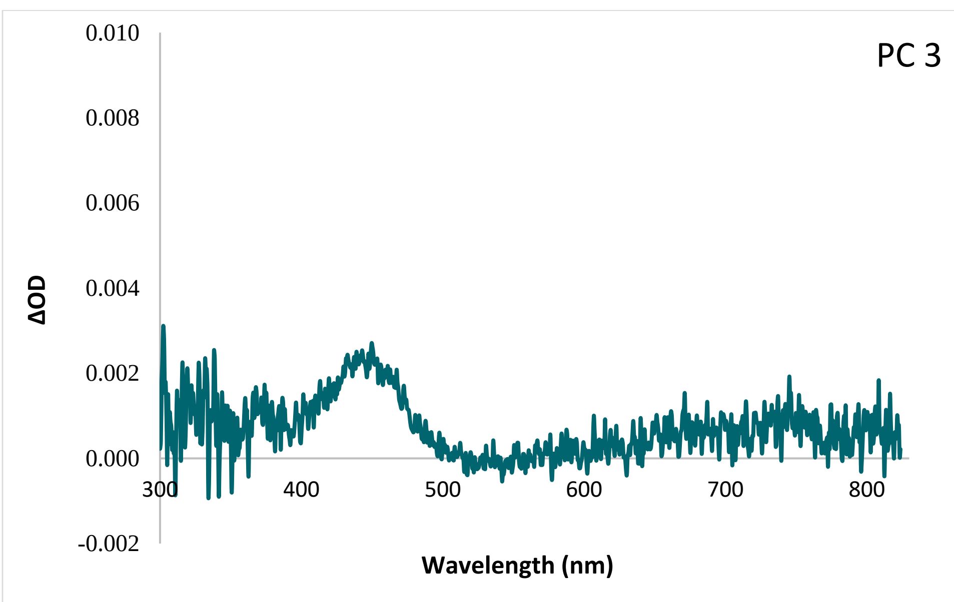


Figure S19. Spectral absorption of PC 3 in DMAc at a 200 ns time delay, with no emission subtraction. The excited state absorption (ESA) feature visible at λ = 445 nm was followed by kinetic absorption. The spectral absorption data was offset corrected using kinetic data acquired at λ = 445 nm.

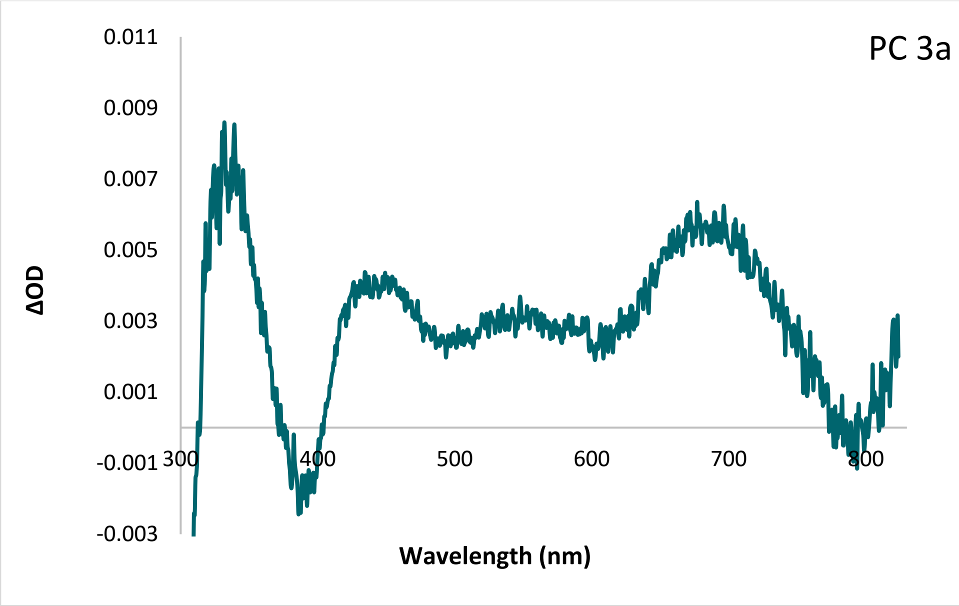


Figure S20. Spectral absorption of PC 3a in DMAc with no time delay (t = 0 ns) and with emission subtraction. The ESA feature visible at λ = 440 nm was followed by kinetic absorption. The spectral absorption data was offset corrected using kinetic data acquired at λ = 440 nm.

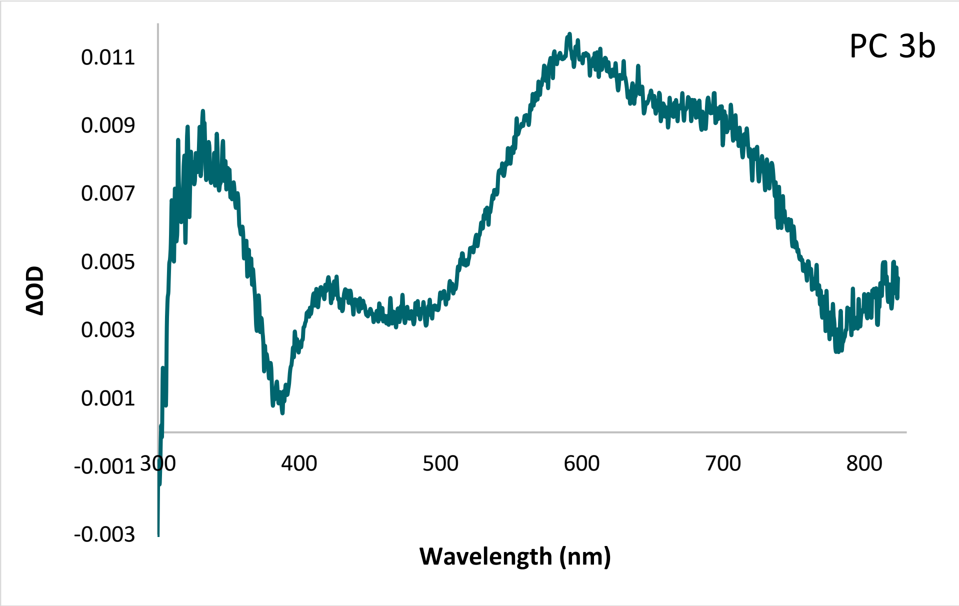


Figure S21. Spectral absorption of PC 3b in DMAc at a 200 ns time delay, with no emission subtraction. The ESA feature visible at λ = 593 nm was followed by kinetic absorption. The spectral absorption data was offset corrected using kinetic data acquired at λ = 593 nm.

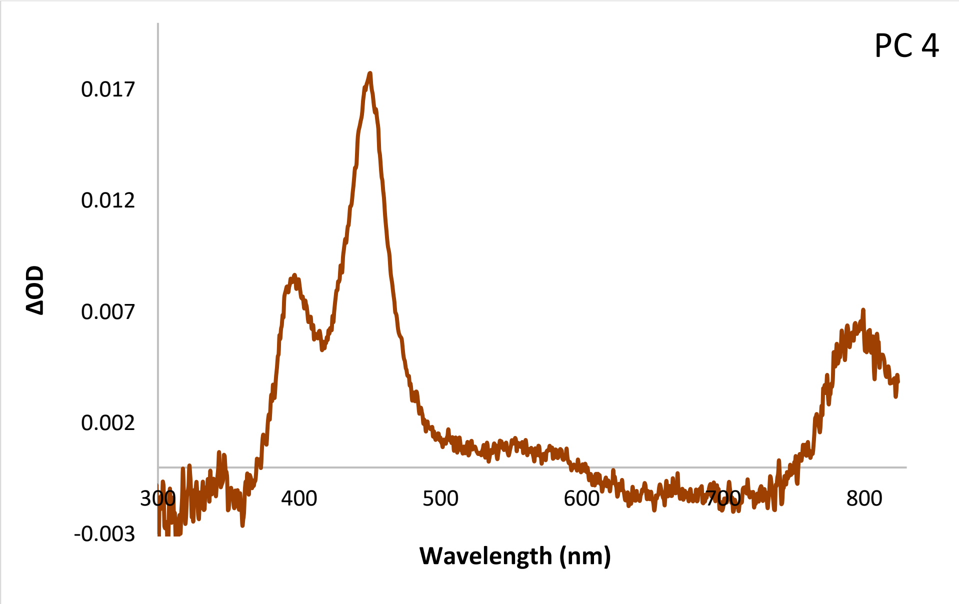


Figure S22. Spectral absorption of PC 4 in DMAc at a 400 ns time delay, with no emission subtraction. The ESA feature visible at λ = 450 nm was followed by kinetic absorption. The spectral absorption data was offset corrected using kinetic data acquired at λ = 450 nm.

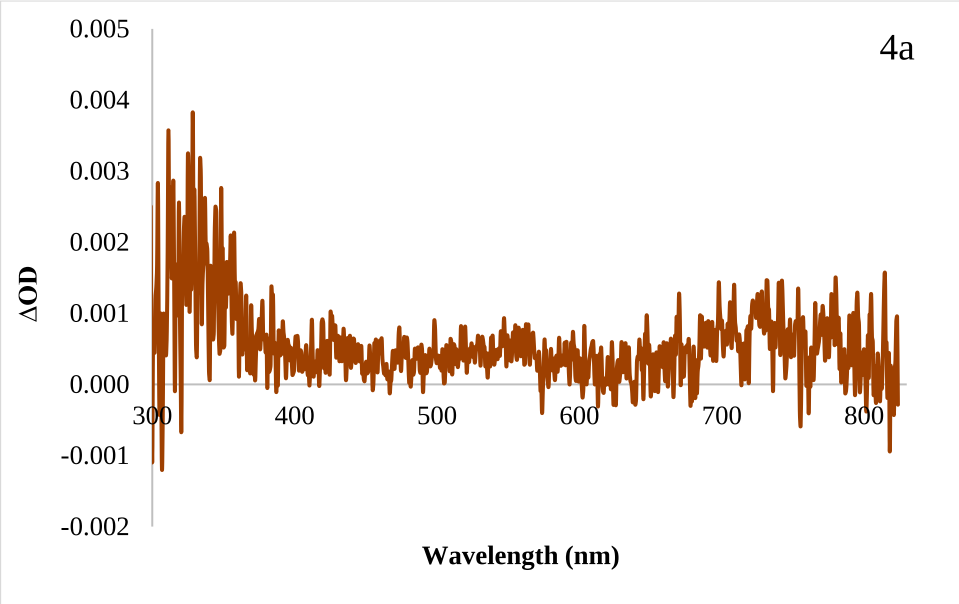


Figure S23. Spectral absorption of PC 4a in DMAc at a 200 ns time delay, with no emission subtraction. There are no distinguishable features that can be followed by kinetic absorption. The spectral absorption data was offset corrected using kinetic data acquired at λ = 450 nm.

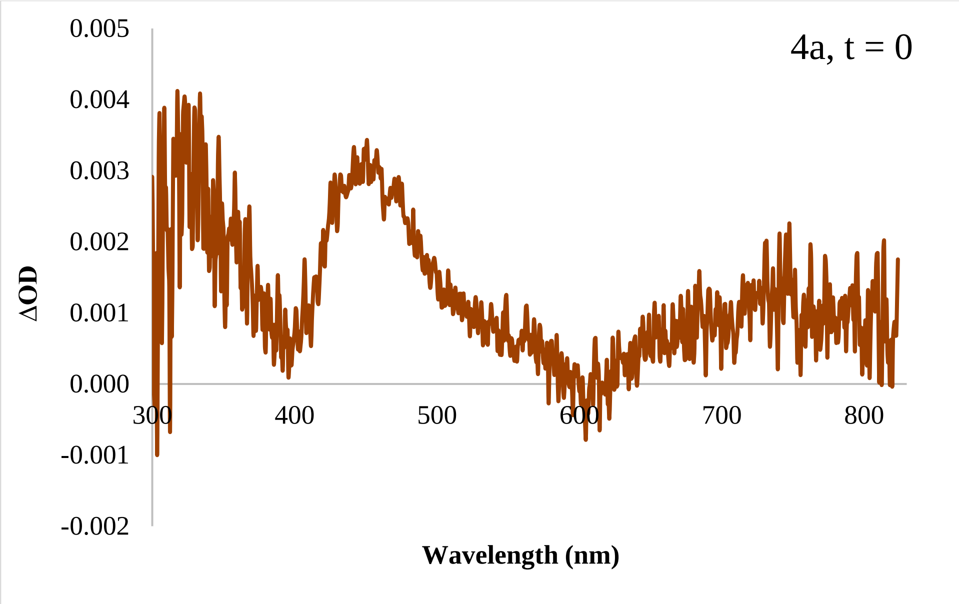


Figure S24. Spectral absorption of PC 4a in DMAc with a 0 ns time delay and with emission subtraction. The ESA feature at λ = 450 nm was followed by kinetic absorption and fit with an exponential tail fit, resulting in determination of $\boldsymbol{\tau_{S1}}$= 14 ns, in agreement with $\boldsymbol{\tau_{S1}}$ determined by kinetic emission (13 ns). The spectral absorption data was offset corrected using kinetic data acquired at λ = 450 nm.

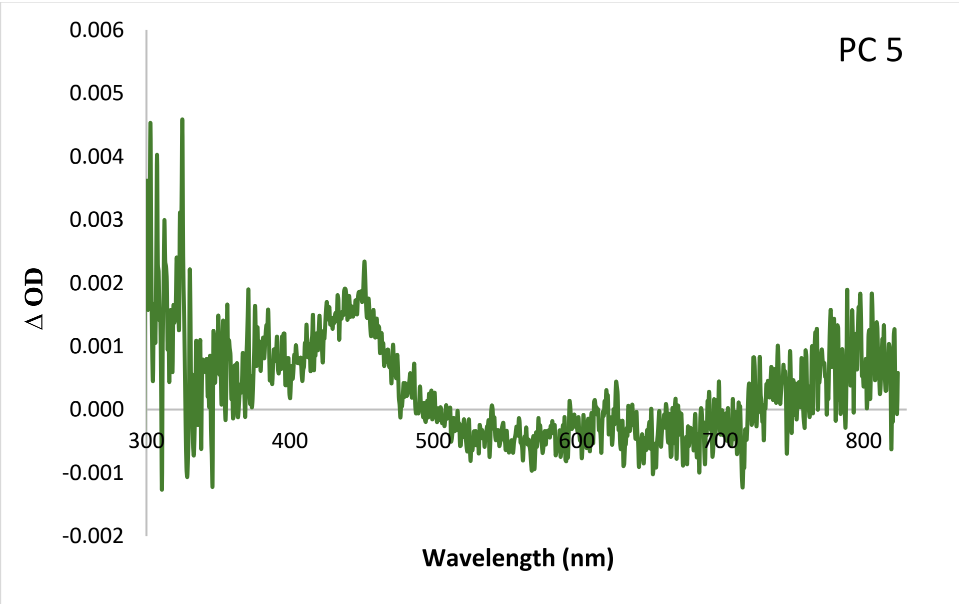


Figure S25. Spectral absorption of PC 5 in DMAc at a 200 ns time delay, with no emission subtraction. The ESA feature visible at λ = 450 nm was followed by kinetic absorption. The spectral absorption data was offset corrected using kinetic data acquired at λ = 450 nm.

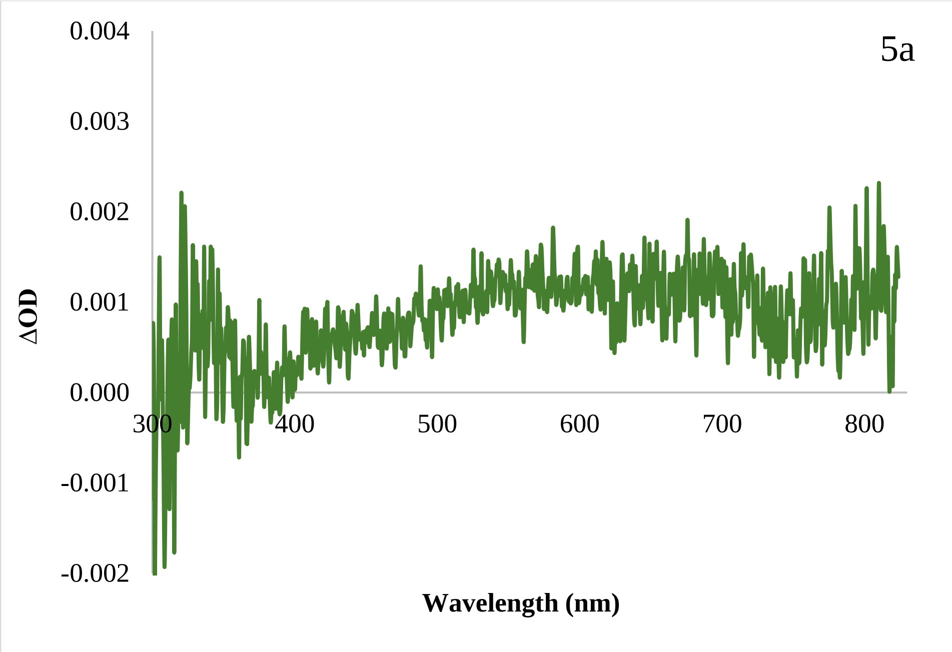


Figure S26. Spectral absorption of PC 5a in DMAc at a 200 ns time delay, with no emission subtraction. There are no features that can be followed by kinetic absorption – the weak ESA at 570 nm was followed but no triplet single was detected. The spectral absorption data was offset corrected using kinetic data acquired at λ = 570 nm.

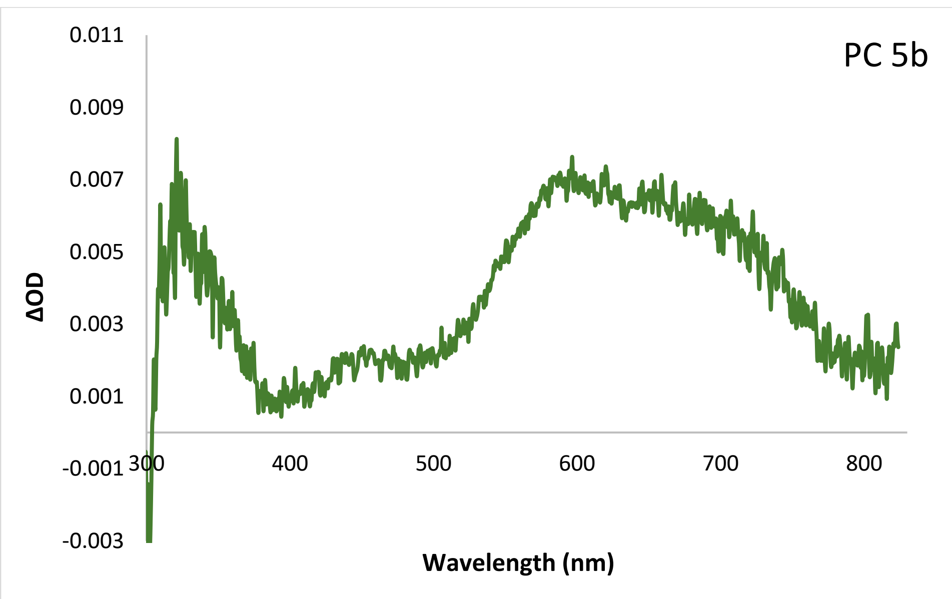


Figure S27. Spectral absorption of PC 5b in DMAc at a 200 ns time delay, with no emission subtraction. The ESA feature visible at λ = 550 nm was followed by kinetic absorption. The spectral absorption data was offset corrected using kinetic data acquired at λ = 550 nm.

Kinetic Emission Data

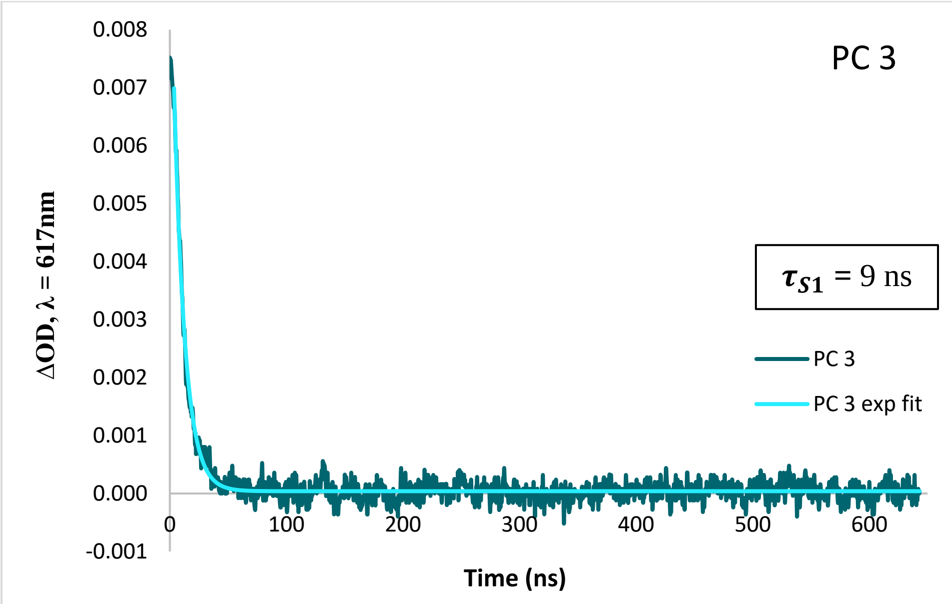


Figure S28. Kinetic emission trace for PC 3 in DMAc at 617 nm with an exponential tail fit for determination of τ_{S1}.

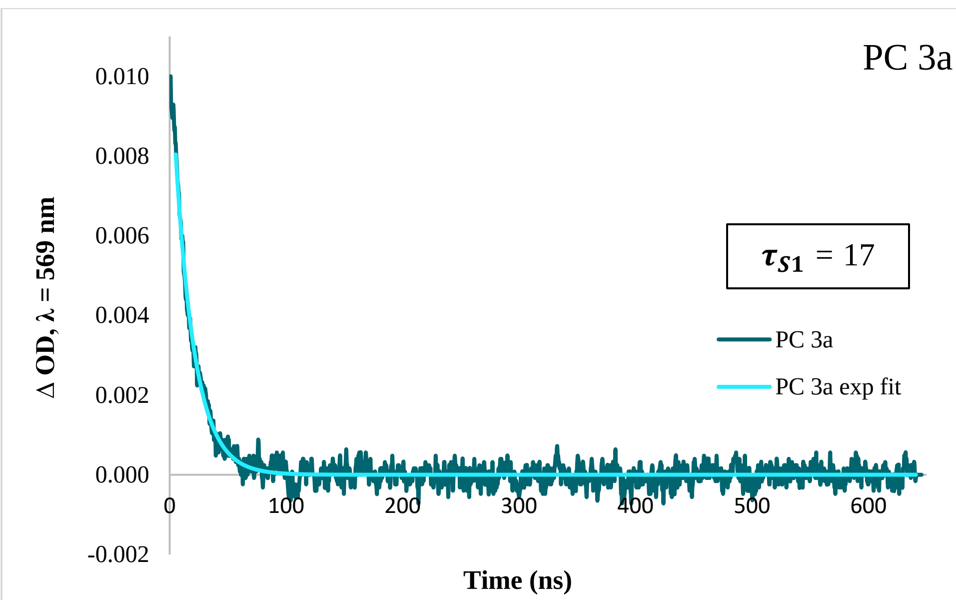


Figure S29. Kinetic emission trace for PC 3a in DMAc at 569 nm with an exponential tail fit for determination of τ_{S1}.

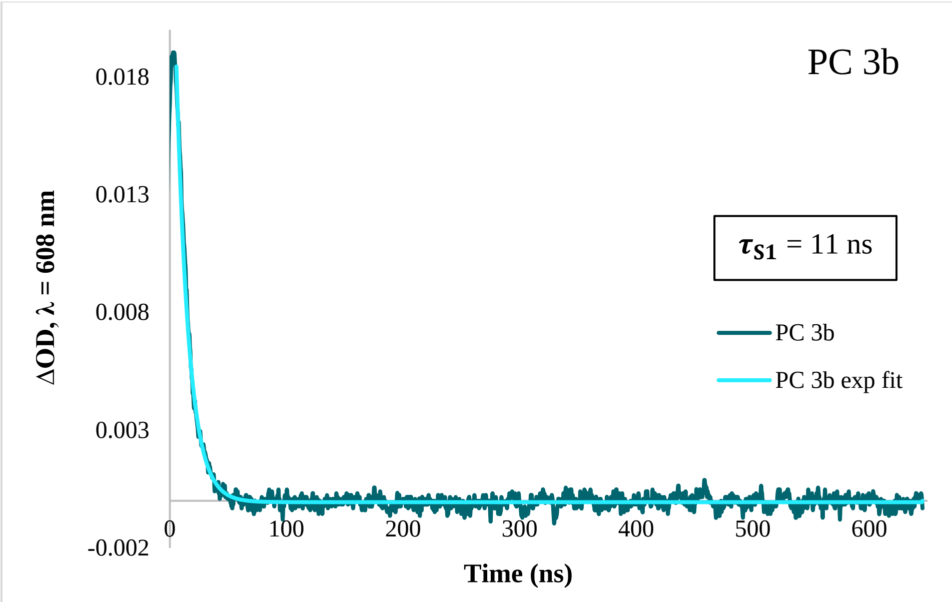


Figure S30. Kinetic emission trace for PC 3b in DMAc at 608 nm with an exponential tail fit for determination of τ_{S1}. Kinetic emission was also measured at 462 nm, but τ_{S1} was found to be less than the 6 ns duration of the instrument laser pulse (below limit of detection).

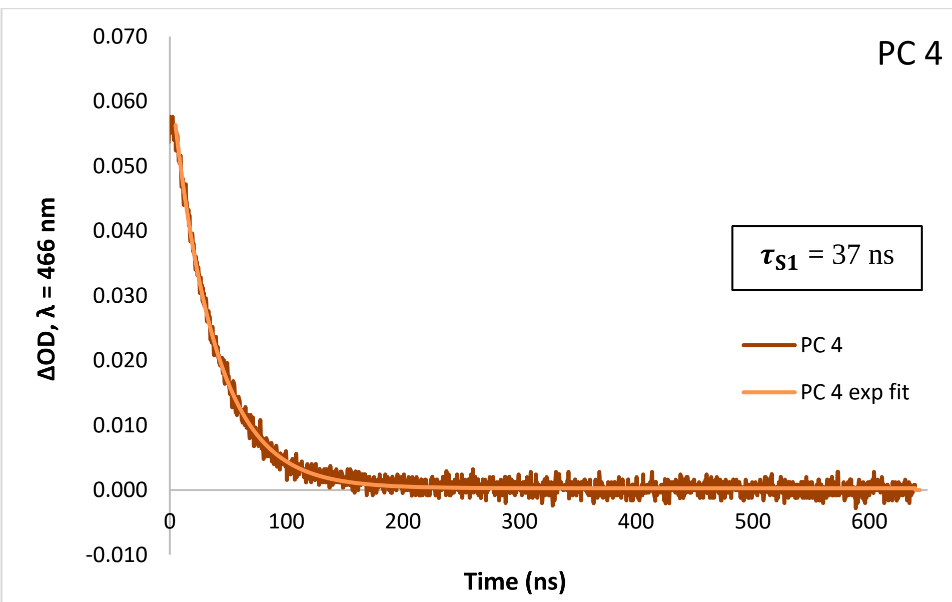


Figure S31. Kinetic emission trace for PC 4 in DMAc at 466 nm with an exponential tail fit for determination of τ_{S1}.

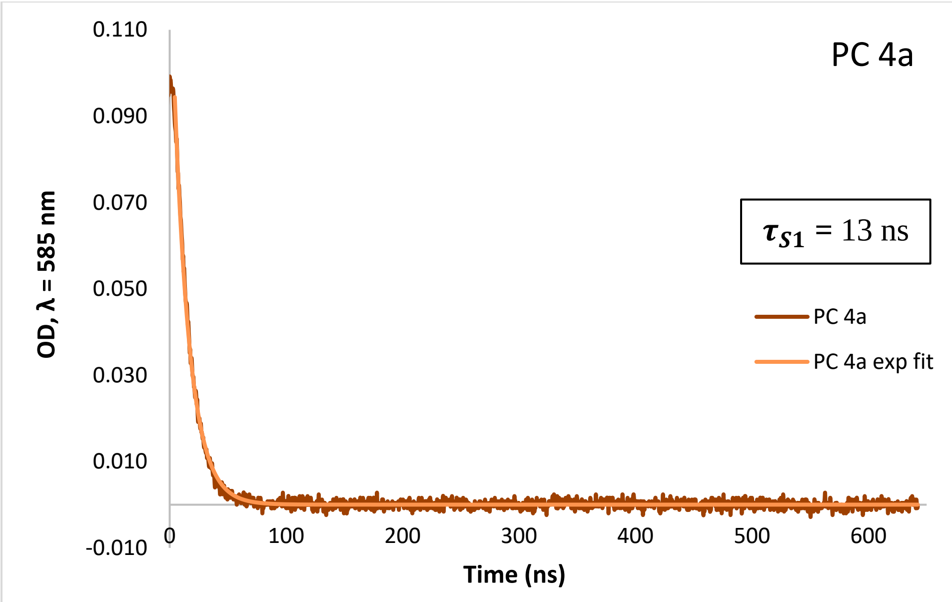


Figure S32. Kinetic emission trace for PC 4a in DMAc at 585 nm with an exponential tail fit for determination of τ_{S1}.

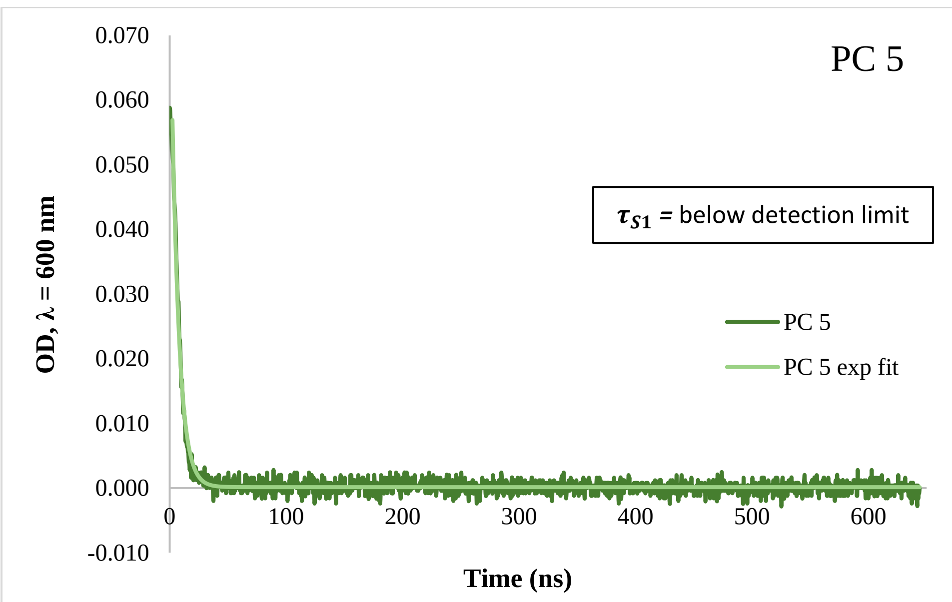


Figure S33. Kinetic emission trace for PC 5 in DMAc at 600 nm with an exponential tail fit for determination of τ_{S1} is shown above, however τ_{S1} was not reported because it was found to be less than the 6 ns duration of the instrument laser pulse (below limit of detection).

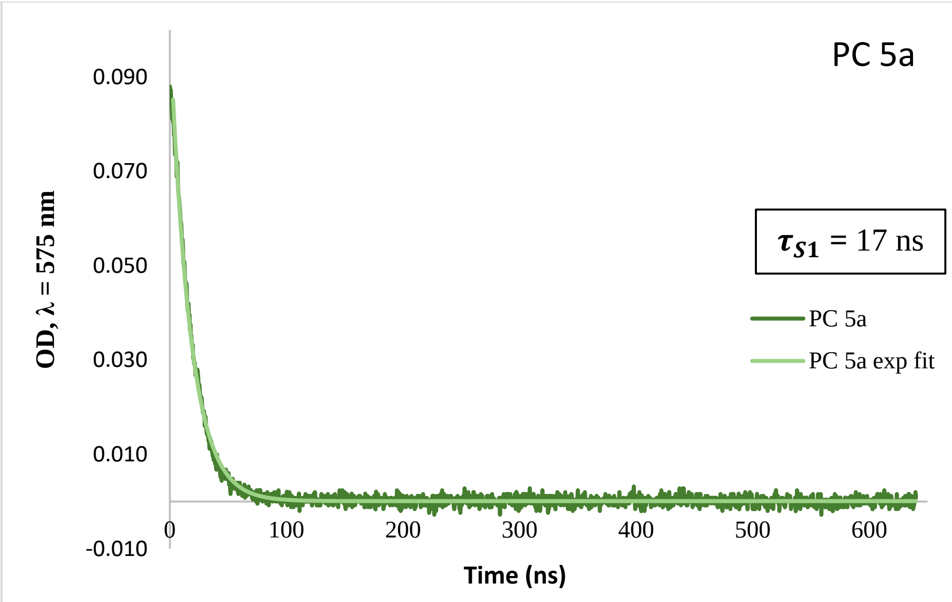


Figure S34. Kinetic emission trace for PC 5a in DMAc at 575 nm with an exponential tail fit for determination of τ_{S1}.

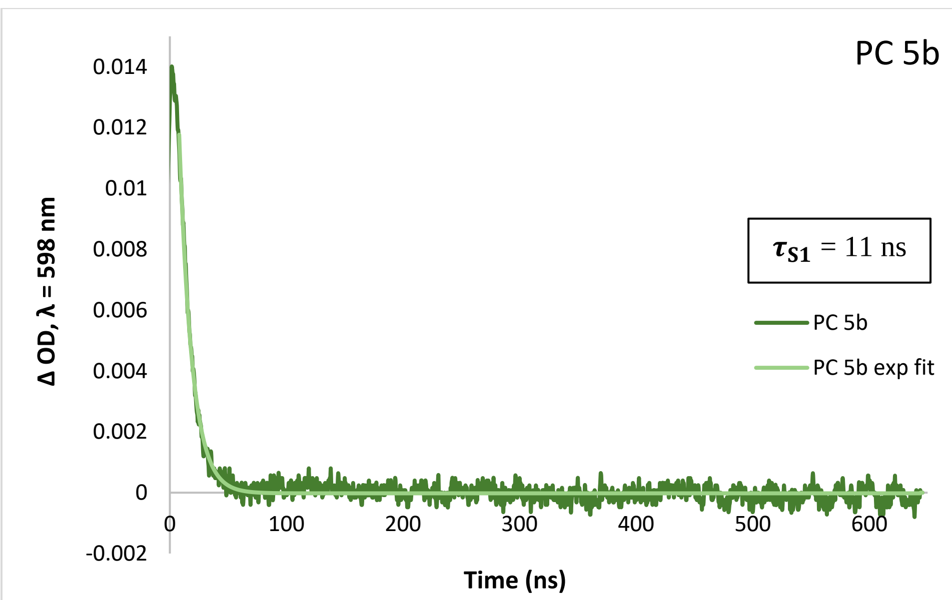


Figure S35. Kinetic emission trace for PC 5b in DMAc at 598 nm with an exponential tail fit for determination of τ_{S1}. Kinetic emission was also measured at 457 nm, but τ_{S1} was found to be less than the 6 ns duration of the instrument laser pulse (below limit of detection).

Kinetic Absorption Data

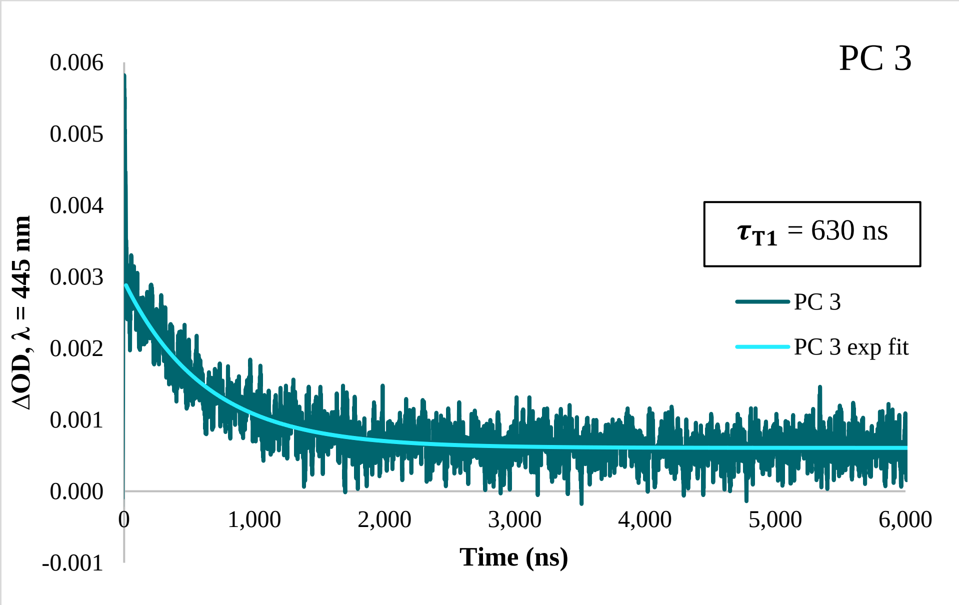


Figure S36. Kinetic absorption trace for PC 3 in DMAc at 445 nm with an exponential tail fit for determination of τ_{T1}.

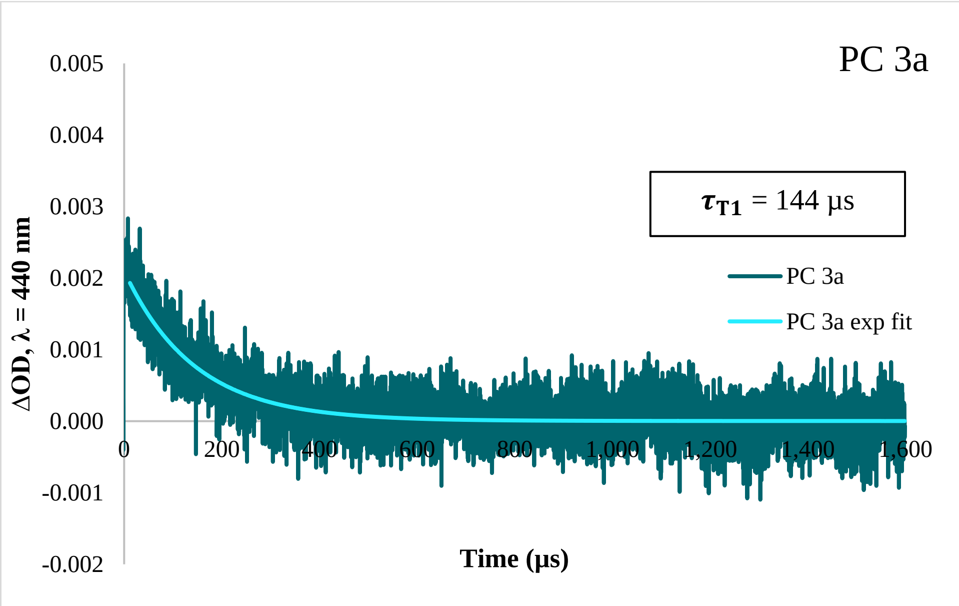


Figure S37. Kinetic absorption trace for PC 3a in DMAc at 440 nm with an exponential tail fit for determination of τ_{T1}.

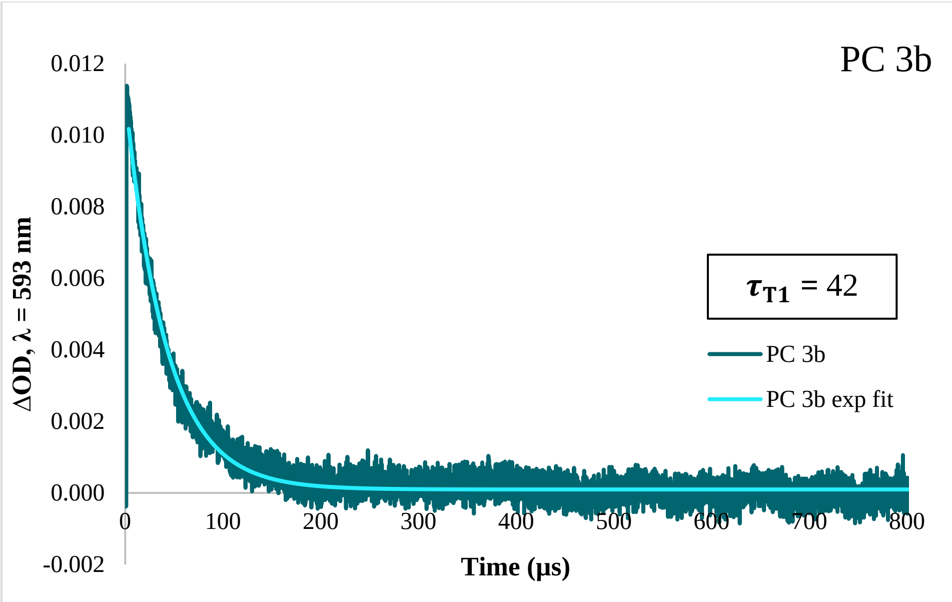


Figure S38. Kinetic absorption trace for PC 3b in DMAc at 593 nm with an exponential tail fit for determination of τ_{T1}.

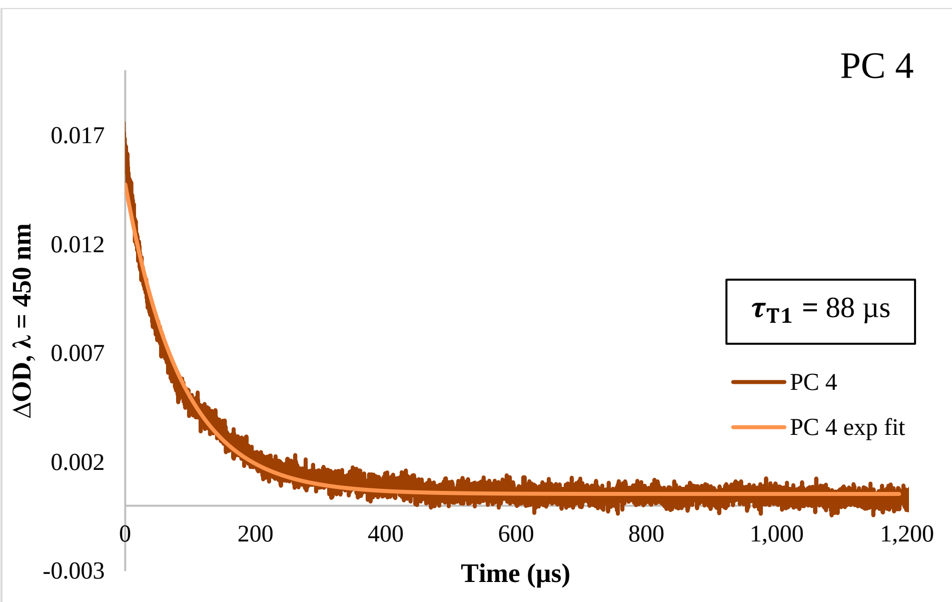


Figure S39. Kinetic absorption trace for PC 4 in DMAc at 450 nm with an exponential tail fit for determination of τ_{T1}.

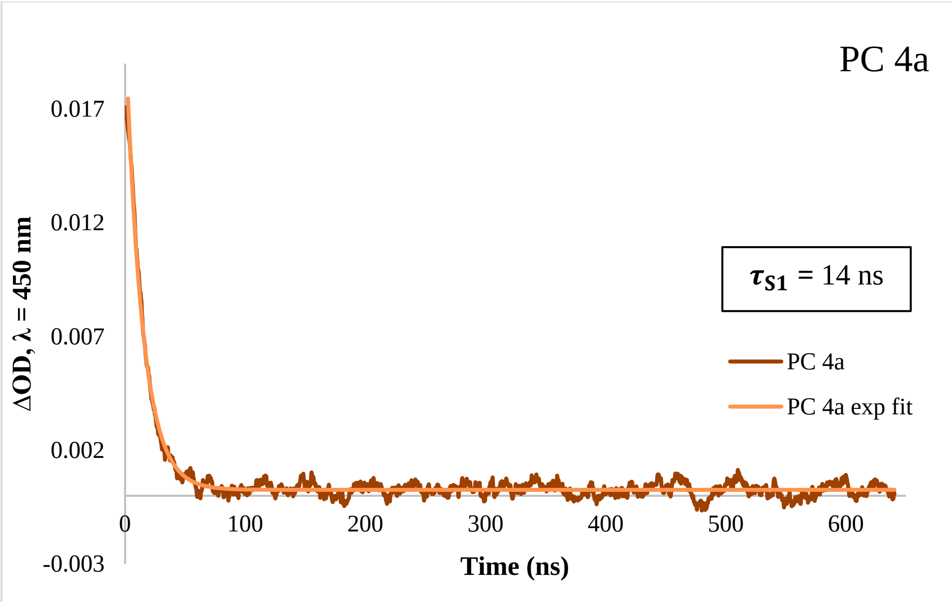


Figure S40. Kinetic absorption trace for PC 4a in DMAc at 450 nm with an exponential tail fit for determination of τ_{S1}. By kinetic absorption τ_{S1}= 14 ns, in good agreement with τ_{S1} determined by kinetic emission (τ_{S1}=13 ns).

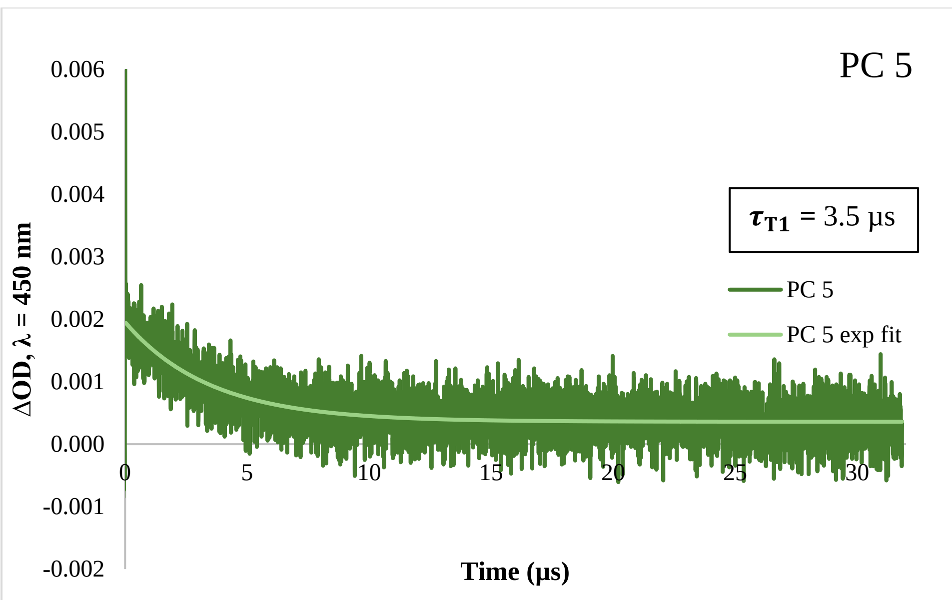


Figure S41. Kinetic absorption trace for PC 5 in DMAc at 450 nm with an exponential tail fit for determination of τ_{T1}.

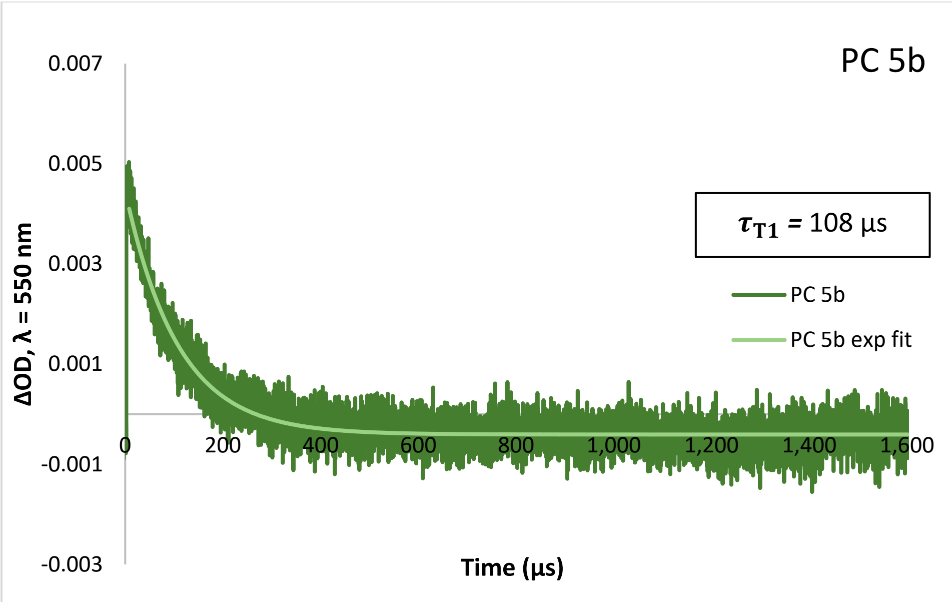


Figure S42. Kinetic absorption trace for PC 5b in DMAc at 550 nm with an exponential tail fit for determination of τ_{T1}.

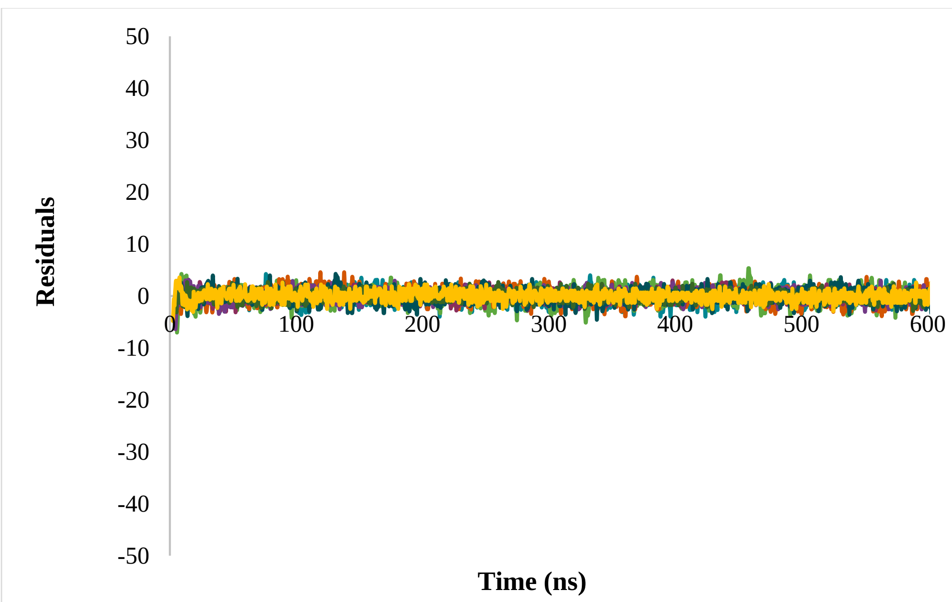


Figure S43. Overlayed residuals for exponential tail fits of the kinetic emission traces included in this work.

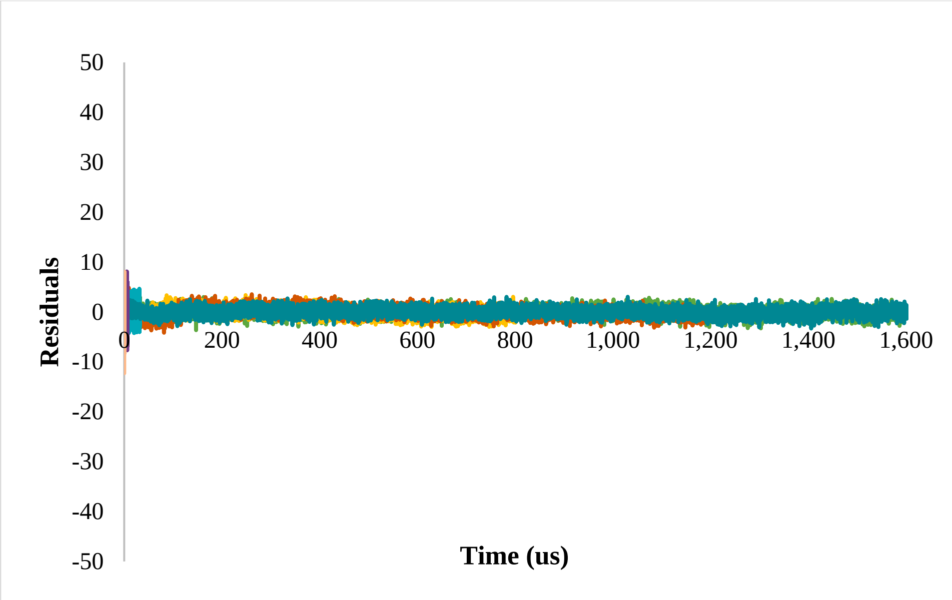


Figure S44. Overlayed residuals for exponential tail fits of the kinetic absorption traces included in this work.

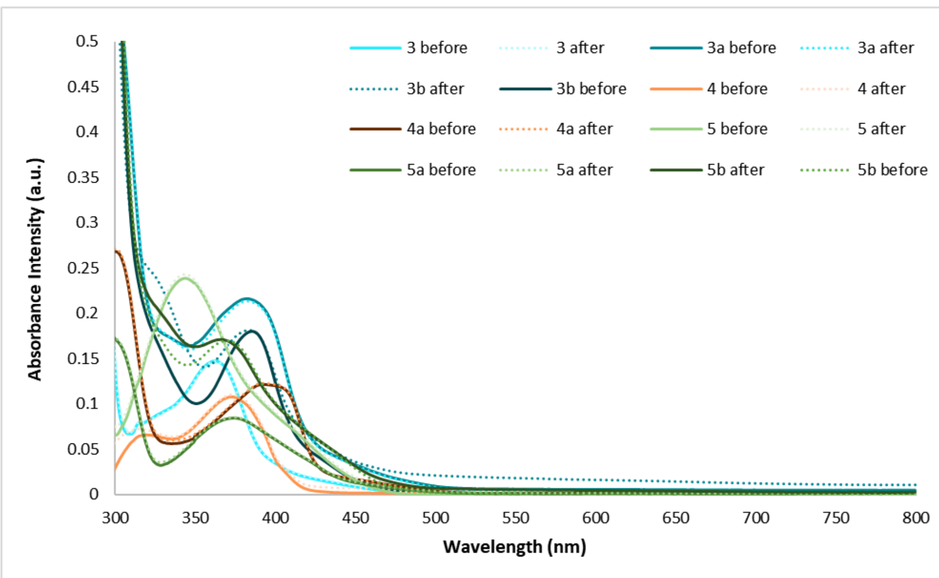
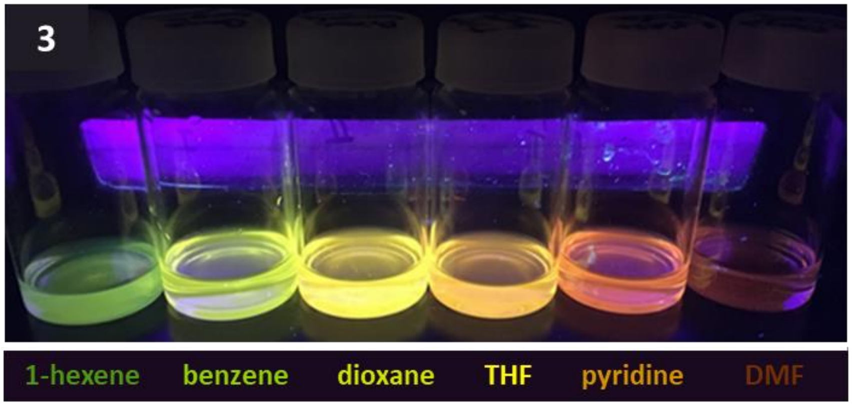


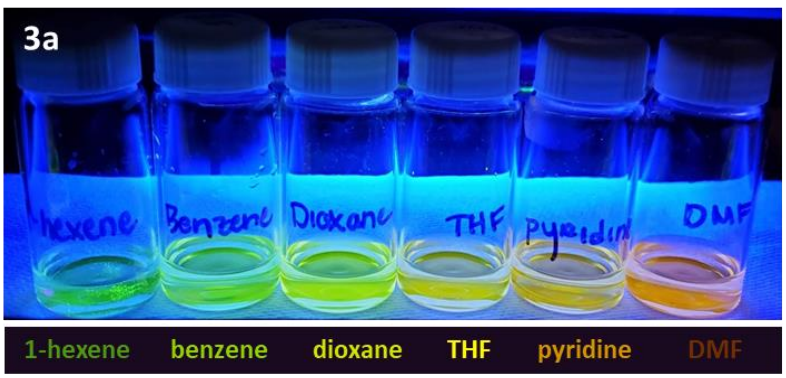
Figure S45. Overlaid UV-vis spectra of PC solutions used for TA spectroscopy, taken before and after TA spectroscopy was performed to monitor if PC degradation occurred. The PC solutions analyzed in this work did not show evidence of degradation after TA, indicated by no significant observable change in the UV-vis spectra before and after TA spectroscopy was performed.

Solvatochromism



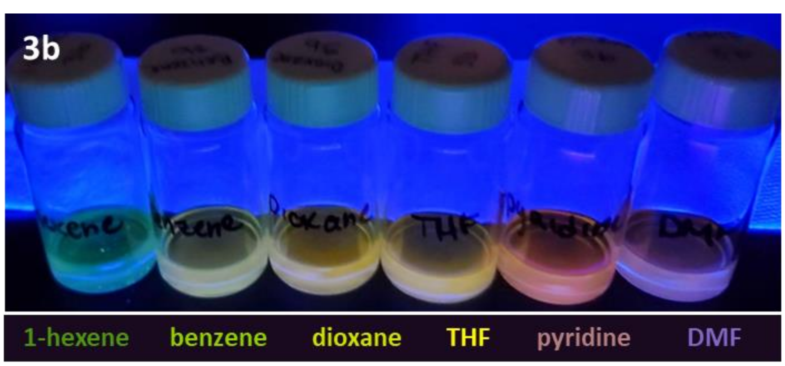
ε = 2.07 2.27 2.21 7.43 13.0 37.2

Figure S46. Previously reported photograph of PC **3** dissolved in solvents of increasing polarity (from left to right) while under irradiation with 365 nm light. (*J. Am. Chem. Soc.* **2017**, *139*, 348−355)



ε = 2.07 2.27 2.21 7.43 13.0 37.2

Figure S47. Photograph of PC **3a** dissolved in solvents of increasing polarity (from left to right) while under irradiation with 365 nm light.



ε = 2.07 2.27 2.21 7.43 13.0 37.2

Figure S48. Photograph of PC **3b** dissolved in solvents of increasing polarity (from left to right) while under irradiation with 365 nm light.

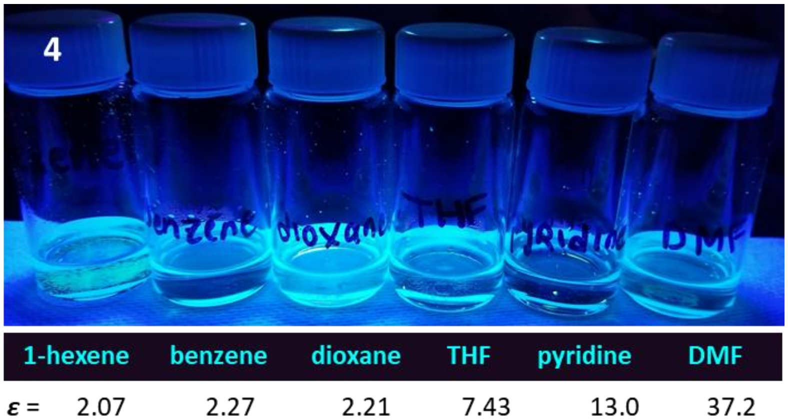


Figure S49. Photograph of PC **4** dissolved in solvents of increasing polarity (from left to right) while under irradiation with 365 nm light.

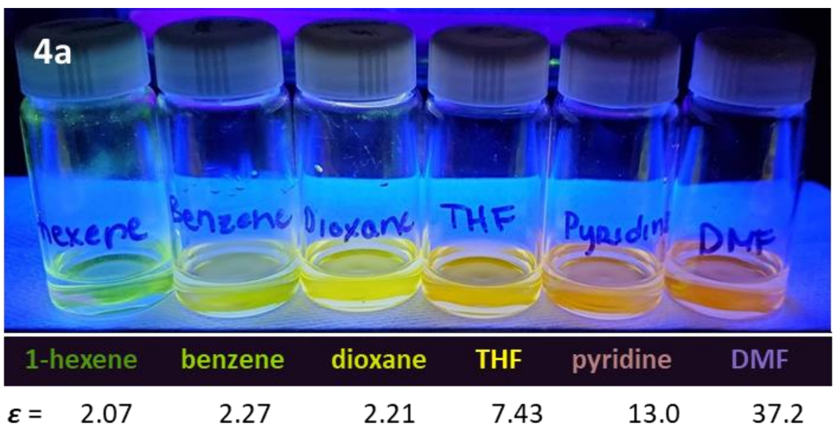


Figure S50. Photograph of PC **4** dissolved in solvents of increasing polarity (from left to right) while under irradiation with 365 nm light.

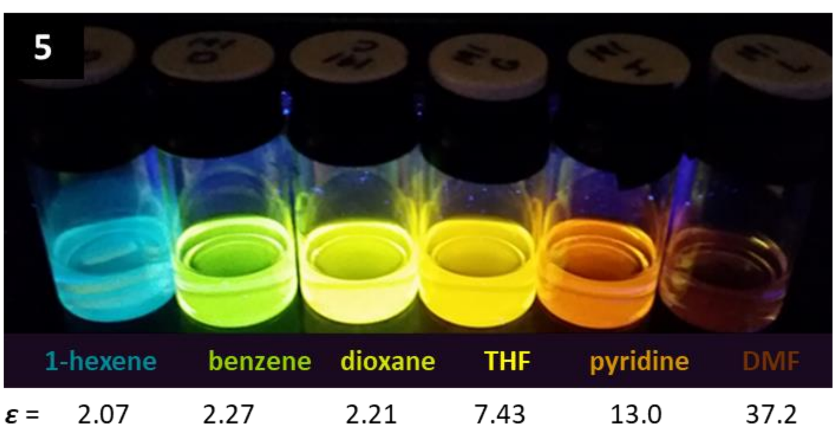
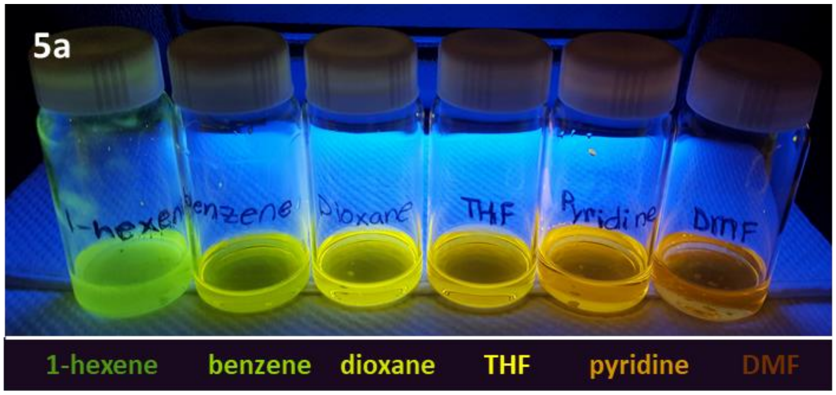
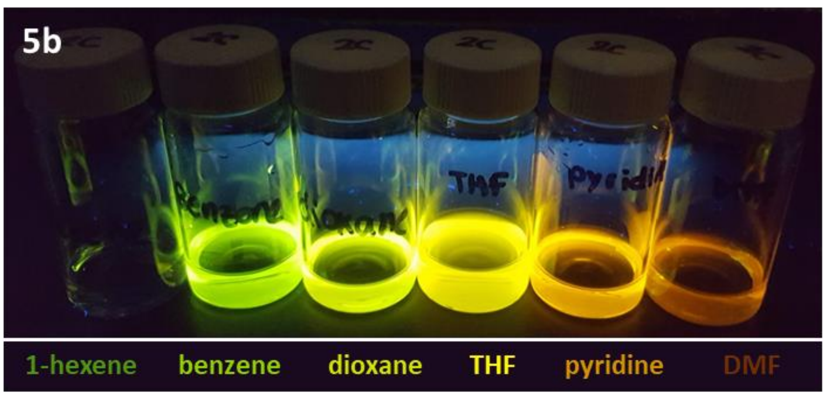


Figure S51. Previously reported Photograph of PC **5** dissolved in solvents of increasing polarity (from left to right) while under irradiation with 365 nm light. (*J. Am. Chem. Soc.* **2017**, *139*, 348−355)



ε = 2.07 2.27 2.21 7.43 13.0 37.2

. **Figure S52.** Photograph of PC **5a** dissolved in solvents of increasing polarity (from left to right) while under irradiation with 365 nm light.



ε = 2.07 2.27 2.21 7.43 13.0 37.2

Figure S53. Photograph of PC **5b** dissolved in solvents of increasing polarity (from left to right) while under irradiation with 365 nm light.

Cyclic Voltammetry

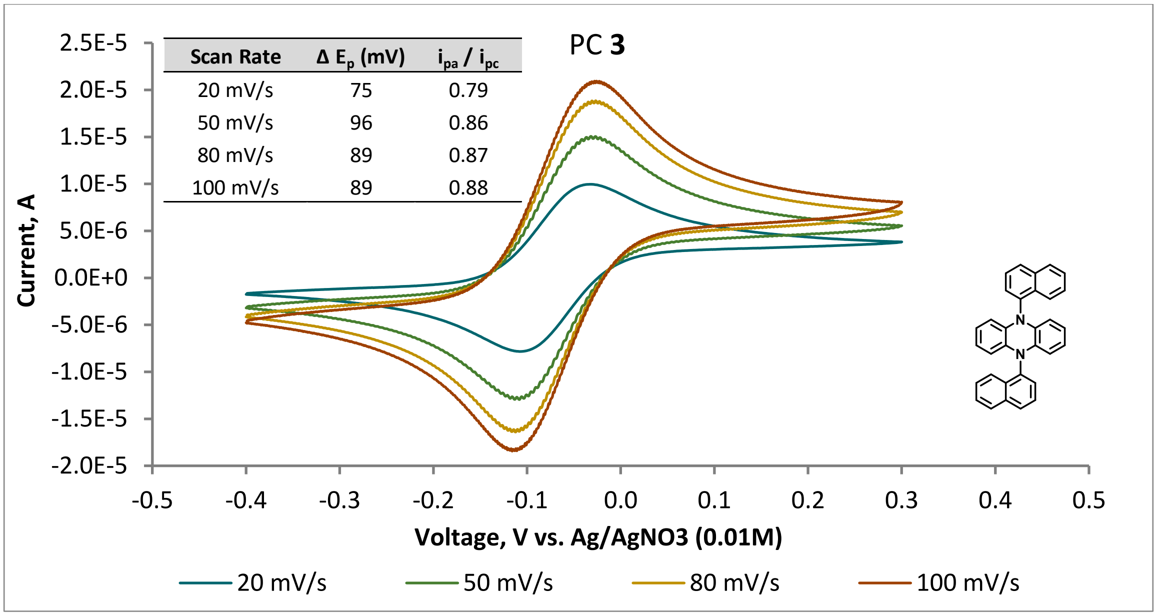


Figure S54. Cyclic voltammogram of PC **3** in DMAc at 20 mV/s, 50 mV/s, 80 mV/s, and 100 mV/s scan rates. Inserted into the graph is a chart showing the ratios of peak anodic current to peak cathodic current (i_{pa}/i_{pc}) and the difference between peak anodic and peak cathodic current (ΔE_p) at each scan rate.

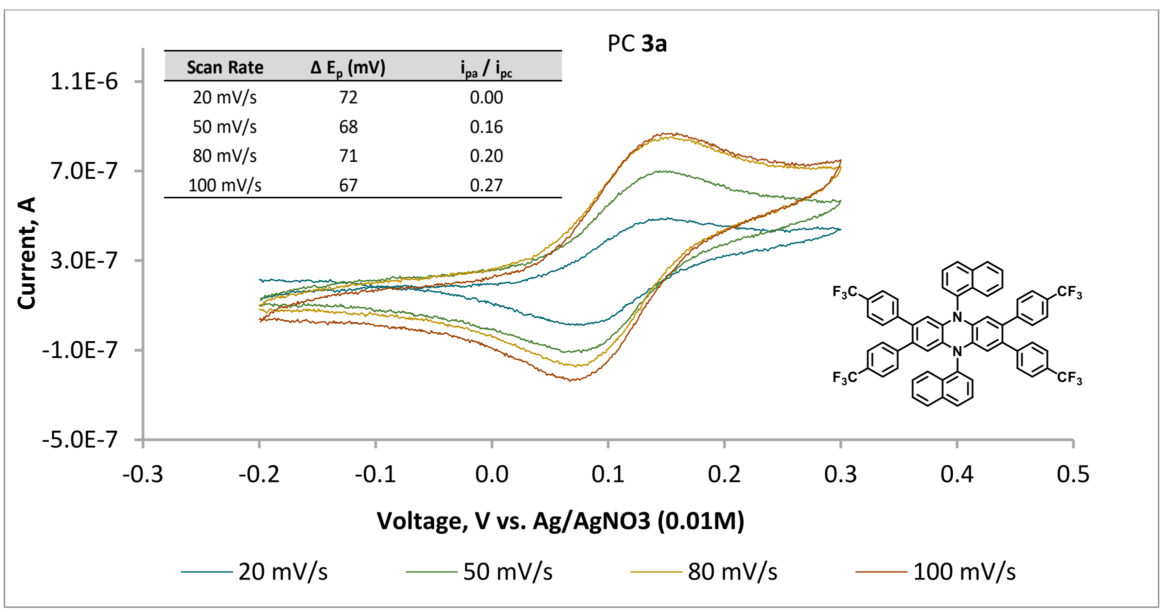


Figure S55. Cyclic voltammogram of PC **3a** in DMAc at 20 mV/s, 50 mV/s, 80 mV/s, and 100 mV/s scan rates. Inserted into the graph is a chart showing the ratios of peak anodic current to peak cathodic current (i_{pa}/i_{pc}) and the difference between peak anodic and peak cathodic current (ΔE_p) at each scan rate.

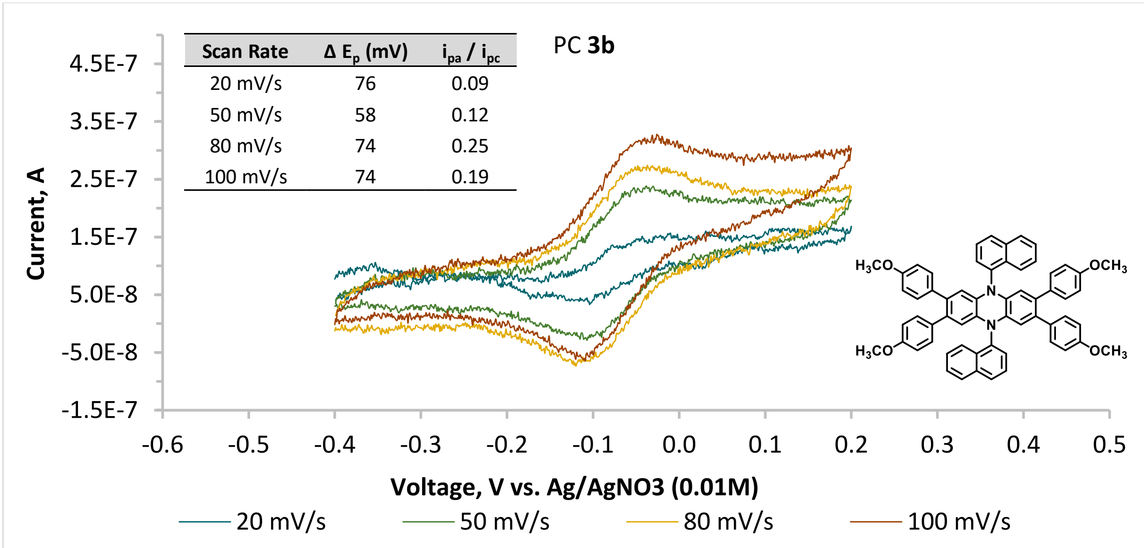


Figure S56. Cyclic voltammogram of PC **3b** in DMAc at 20 mV/s, 50 mV/s, 80 mV/s, and 100 mV/s scan rates. Inserted into the graph is a chart showing the ratios of peak anodic current to peak cathodic current (i_{pa}/i_{pc}) and the difference between peak anodic and peak cathodic current (ΔE_p) at each scan rate.

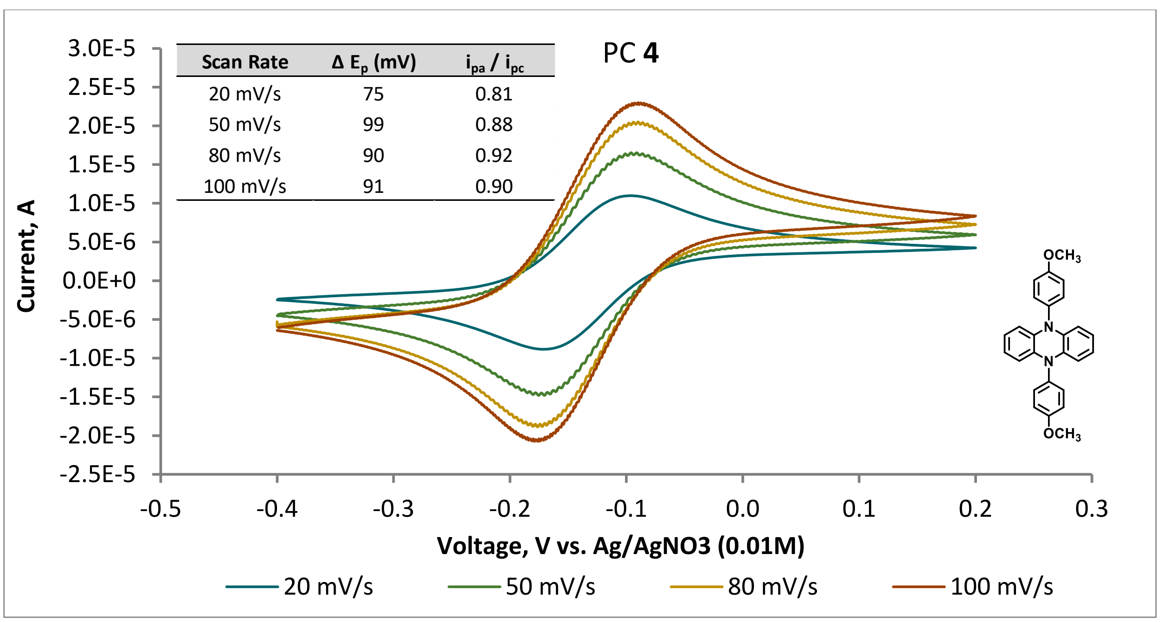


Figure S57. Cyclic voltammogram of PC **4** in DMAc at 20 mV/s, 50 mV/s, 80 mV/s, and 100 mV/s scan rates. Inserted into the graph is a chart showing the ratios of peak anodic current to peak cathodic current (i_{pa}/i_{pc}) and the difference between peak anodic and peak cathodic current (ΔE_p) at each scan rate.

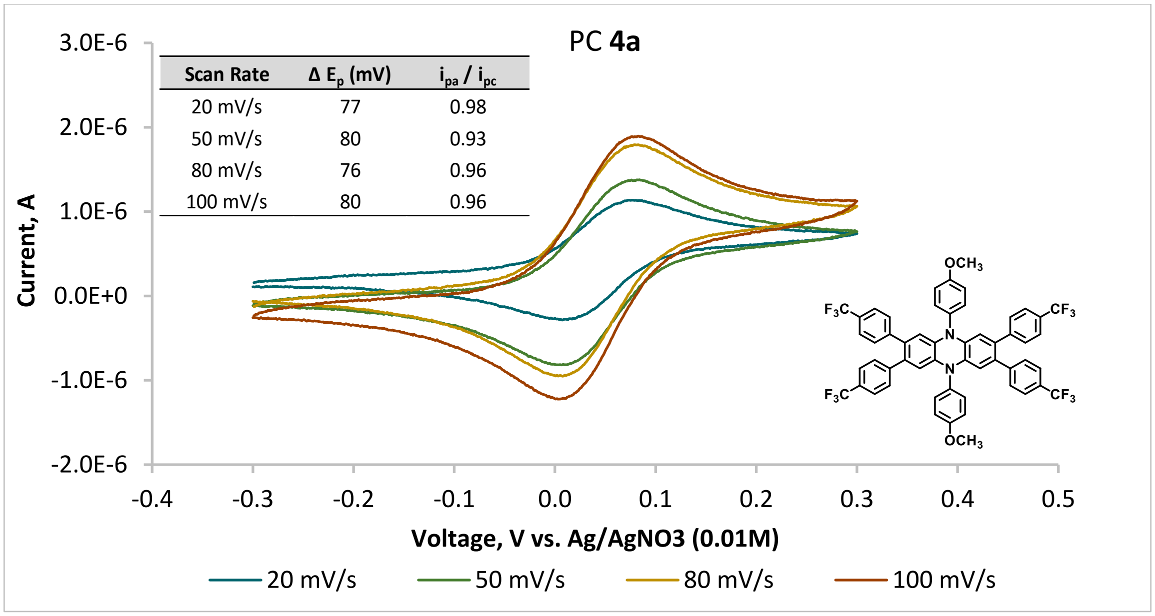


Figure S58. Cyclic voltammogram of PC **4a** in DMAc at 20 mV/s, 50 mV/s, 80 mV/s, and 100 mV/s scan rates. Inserted into the graph is a chart showing the ratios of peak anodic current to peak cathodic current (i_{pa}/i_{pc}) and the difference between peak anodic and peak cathodic current (ΔE_p) at each scan rate.

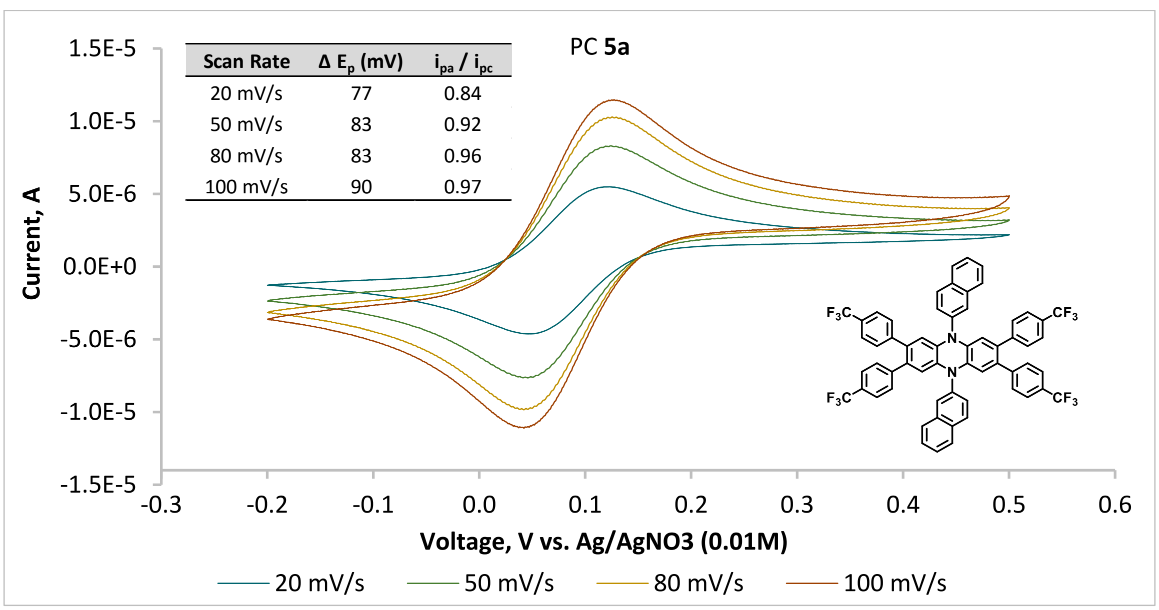
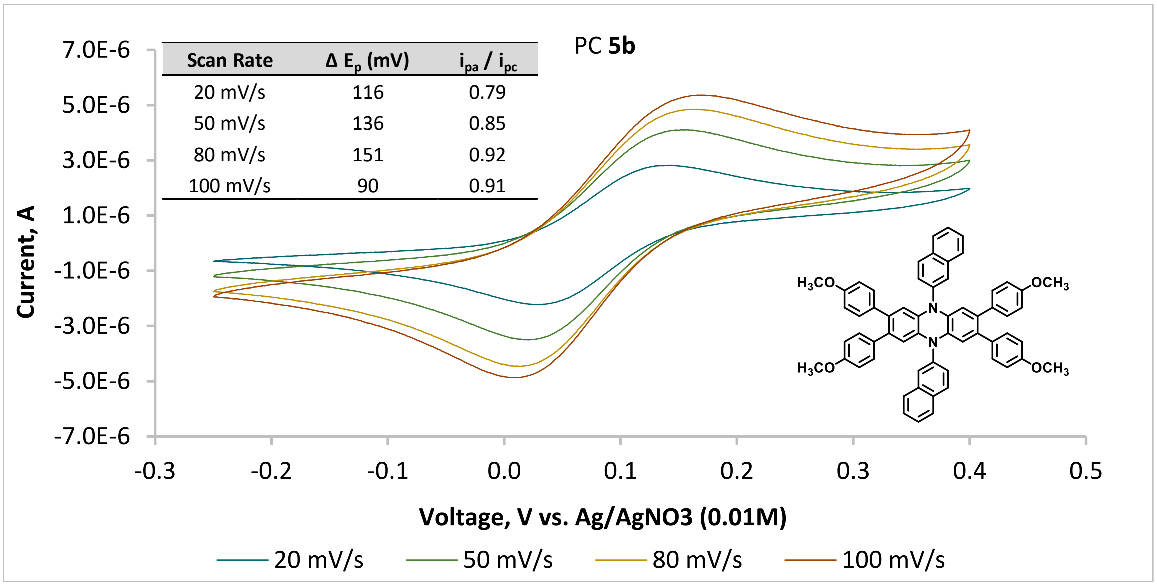


Figure S59. Cyclic voltammogram of PC **5a** in DMAc at 20 mV/s, 50 mV/s, 80 mV/s, and 100 mV/s scan rates. Inserted into the graph is a chart showing the ratios of peak anodic current to peak cathodic current (i_{pa}/i_{pc}) and the difference between peak anodic and peak cathodic current (ΔE_p) at each scan rate.



Scan Rate	Δ E_p (mV)	i_{pa} / i_{pc}
20 mV/s	116	0.79
50 mV/s	136	0.85
80 mV/s	151	0.92
100 mV/s	90	0.91

Figure S60. Cyclic voltammogram of PC **5b** in DMAc at 20 mV/s, 50 mV/s, 80 mV/s, and 100 mV/s scan rates. Inserted into the graph is a chart showing the ratios of peak anodic current to peak cathodic current (i_{pa}/i_{pc}) and the difference between peak anodic and peak cathodic current (ΔE_p) at each scan rate.

COMPUTATIONAL MODELING OF PCs

Excited State Calculations (TD-DFT)

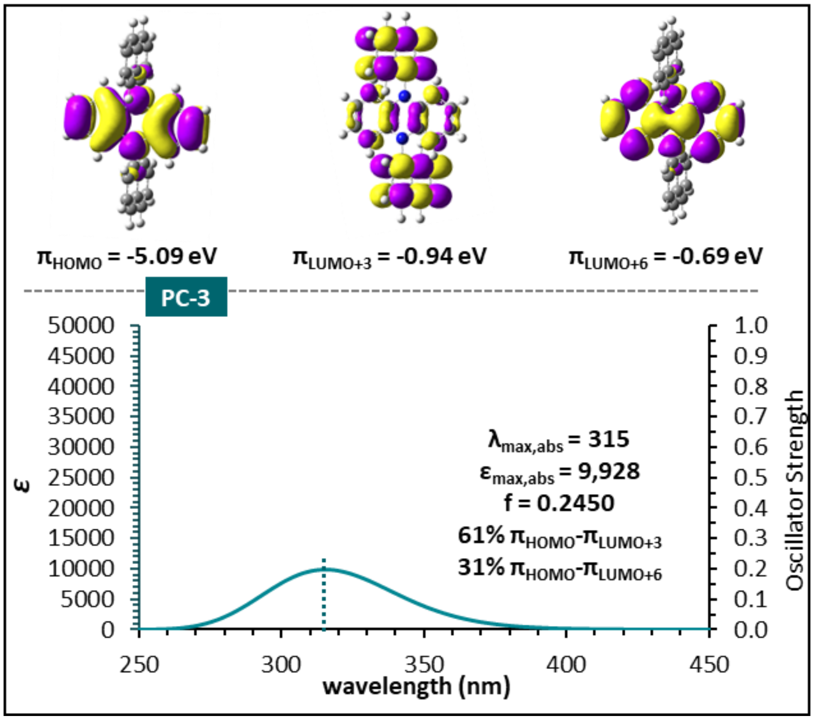


Figure S61: Computationally modeled molecular orbitals predicted to be involved in absorption transitions for PC **3** detailed below (top). Computationally predicted UV–vis spectrum of PCs **3** along with theoretically assigned percentage contributions (>15%) of various orbitals to the predicted absorption peaks. $\lambda_{max,abs}$ is the absorption maximum wavelength and is reported in units of nm, $\varepsilon_{max,abs}$ is the predicted molar extinction coefficient at $\lambda_{max,abs}$ and is reported in units of M^{-1} cm^{-1}, and ƒ is the predicted oscillator strength; all of these values were predicted at the TD-DFT CAM-B3LYP/6-31+G(d,p)/CPCM-DMA level of theory (bottom).

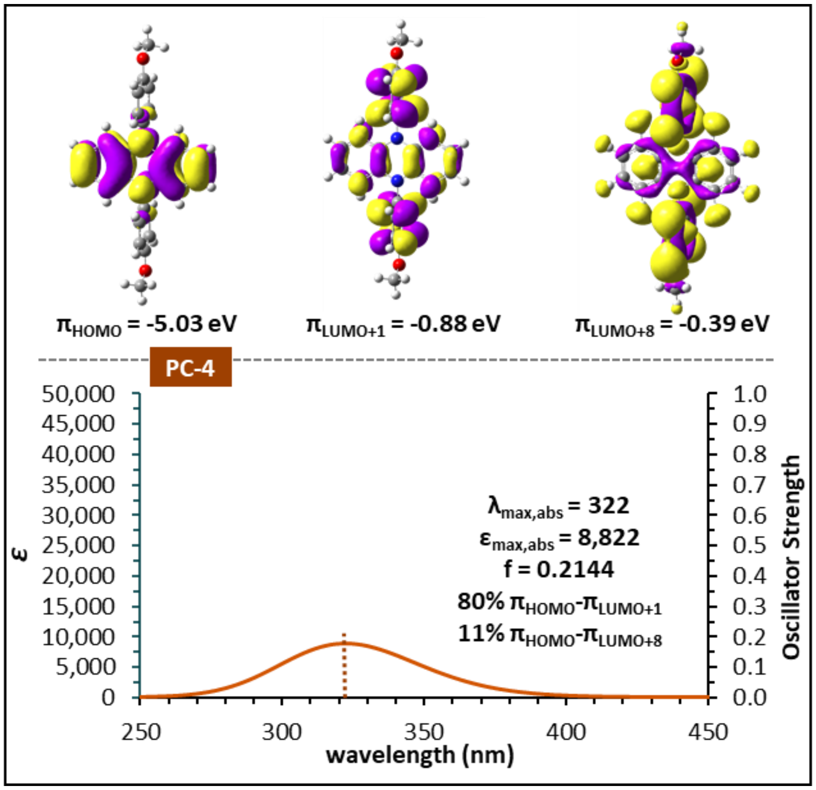


Figure S62: Computationally modeled molecular orbitals predicted to be involved in absorption transitions for PC **4** detailed below (top). Computationally predicted UV–vis spectrum of PCs **4** along with theoretically assigned percentage contributions (>15%) of various orbitals to the predicted absorption peaks. $\lambda_{max,abs}$ is the absorption maximum wavelength and is reported in units of nm, $\varepsilon_{max,abs}$ is the predicted molar extinction coefficient at $\lambda_{max,abs}$ and is reported in units of M^{-1} cm^{-1}, and ƒ is the predicted oscillator strength; all of these values were predicted at the TD-DFT CAM-B3LYP/6-31+G(d,p)/CPCM-DMA level of theory (bottom).

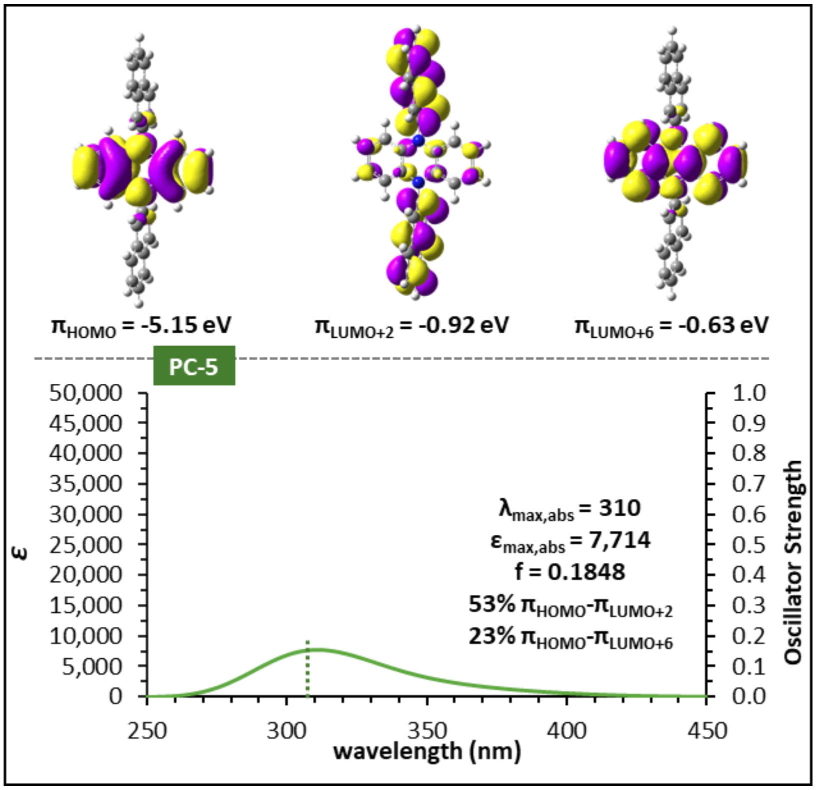


Figure S63: Computationally modeled molecular orbitals predicted to be involved in absorption transitions for PC **5** detailed below (top). Computationally predicted UV−vis spectrum of PCs **5** along with theoretically assigned percentage contributions (>15%) of various orbitals to the predicted absorption peaks. $\lambda_{max,abs}$ is the absorption maximum wavelength and is reported in units of nm, $\varepsilon_{max,abs}$ is the predicted molar extinction coefficient at $\lambda_{max,abs}$ and is reported in units of M^{-1} cm^{-1}, and ƒ is the predicted oscillator strength; all of these values were predicted at the TD-DFT CAM-B3LYP/6-31+G(d,p)/CPCM-DMA level of theory (bottom).

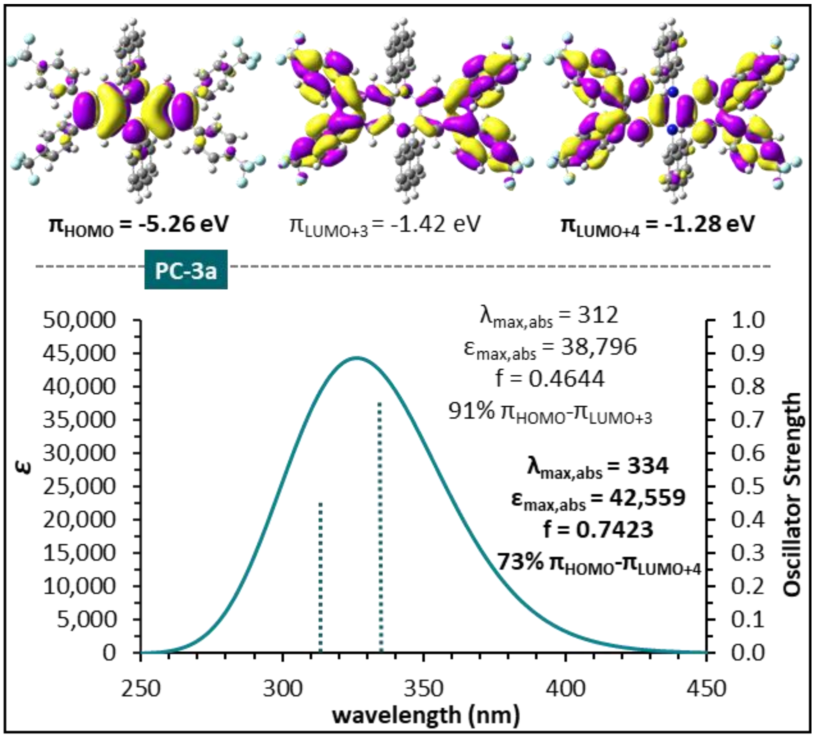


Figure S64: Computationally modeled molecular orbitals predicted to be involved in absorption transitions for PC **3a** detailed below (top). Computationally predicted UV−vis spectrum of PCs **3a** along with theoretically assigned percentage contributions (>15%) of various orbitals to the predicted absorption peaks. $\lambda_{max,abs}$ is the predicted absorption maximum wavelength and is reported in units of nm, $\varepsilon_{max,abs}$ is the predicted molar extinction coefficient at the predicted $\lambda_{max,abs}$ and is reported in units of M^{-1} cm^{-1}, and ƒ is the predicted oscillator strength; all of these values were predicted at the TD-DFT CAM-B3LYP/6-31+G(d,p)/CPCM-DMA level of theory (bottom).

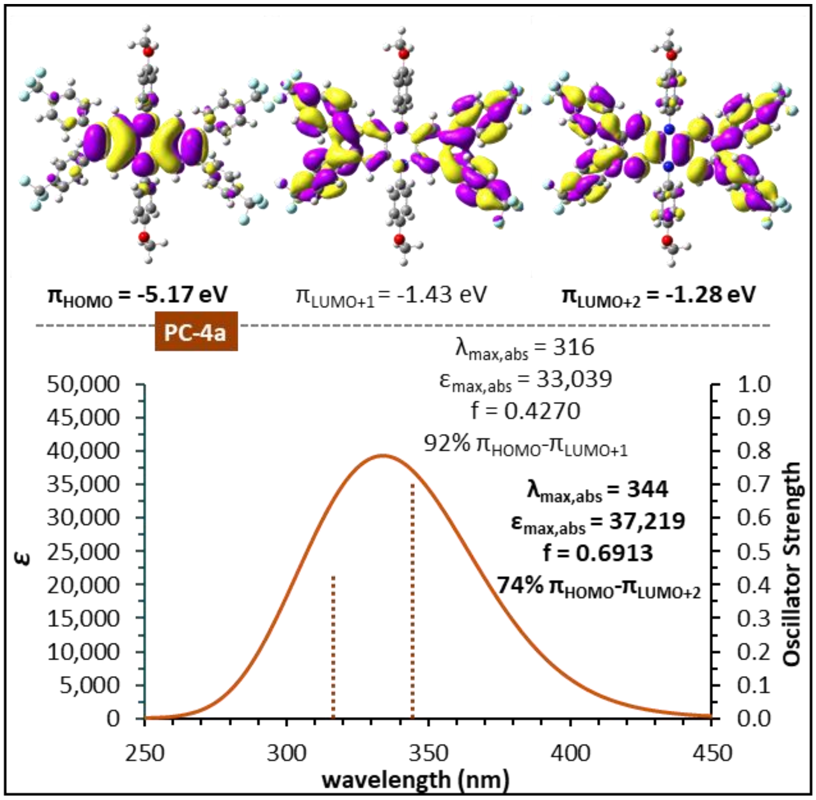


Figure S65: Computationally modeled molecular orbitals predicted to be involved in absorption transitions for PC **4a** detailed below (top). Computationally predicted UV−vis spectrum of PCs **4a** along with theoretically assigned percentage contributions (>15%) of various orbitals to the predicted absorption peaks. $\lambda_{max,abs}$ is the predicted absorption maximum wavelength and is reported in units of nm, $\varepsilon_{max,abs}$ is the predicted molar extinction coefficient at the predicted $\lambda_{max,abs}$ and is reported in units of M^{-1} cm^{-1}, and ƒ is the predicted oscillator strength; all of these values were predicted at the TD-DFT CAM-B3LYP/6-31+G(d,p)/CPCM-DMA level of theory (bottom).

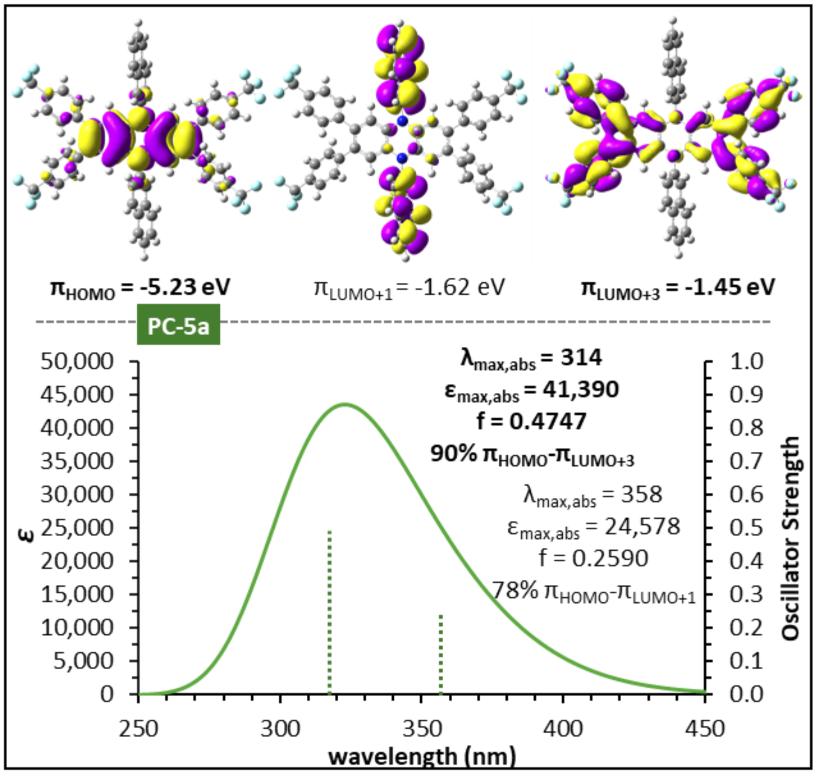


Figure S66: Computationally modeled molecular orbitals predicted to be involved in absorption transitions for PC **5a** detailed below (top). Computationally predicted UV−vis spectrum of PCs **5a** along with theoretically assigned percentage contributions (>15%) of various orbitals to the predicted absorption peaks. $\lambda_{max,abs}$ is the predicted absorption maximum wavelength and is reported in units of nm, $\varepsilon_{max,abs}$ is the predicted molar extinction coefficient at the predicted $\lambda_{max,abs}$ and is reported in units of M^{-1} cm^{-1}, and ƒ is the predicted oscillator strength; all of these values were predicted at the TD-DFT CAM-B3LYP/6-31+G(d,p)/CPCM-DMA level of theory (bottom).

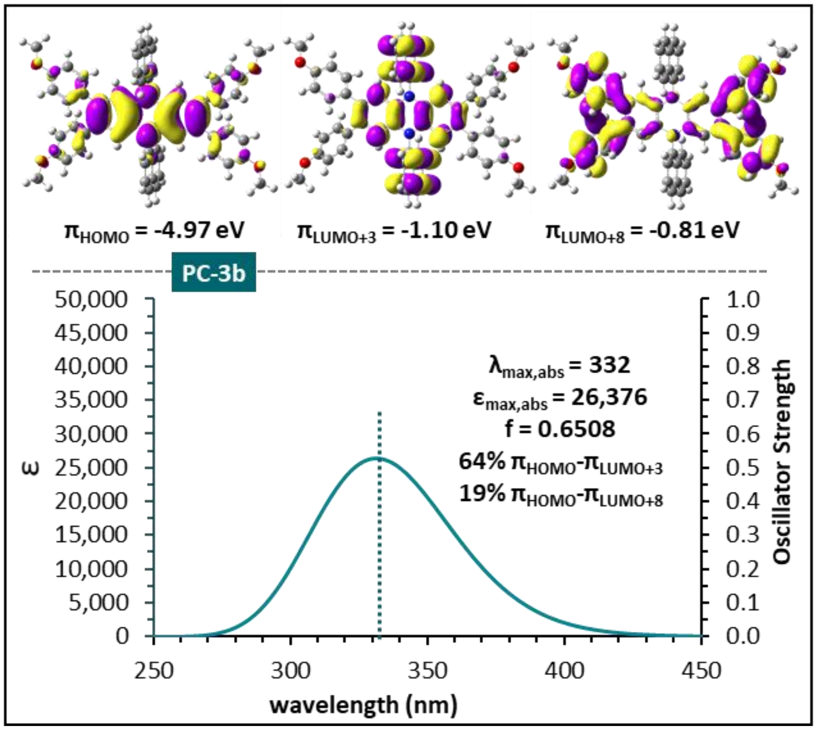


Figure S67: Computationally modeled molecular orbitals predicted to be involved in absorption transitions for PC **3b** detailed below (top). Computationally predicted UV−vis spectrum of PCs **3b** along with theoretically assigned percentage contributions (>15%) of various orbitals to the predicted absorption peaks. $\lambda_{max,abs}$ is the predicted absorption maximum wavelength and is reported in units of nm, $\varepsilon_{max,abs}$ is the predicted molar extinction coefficient at the predicted $\lambda_{max,abs}$ and is reported in units of M^{-1} cm^{-1}, and ƒ is the predicted oscillator strength; all of these values were predicted at the TD-DFT CAM-B3LYP/6-31+G(d,p)/CPCM-DMA level of theory (bottom).

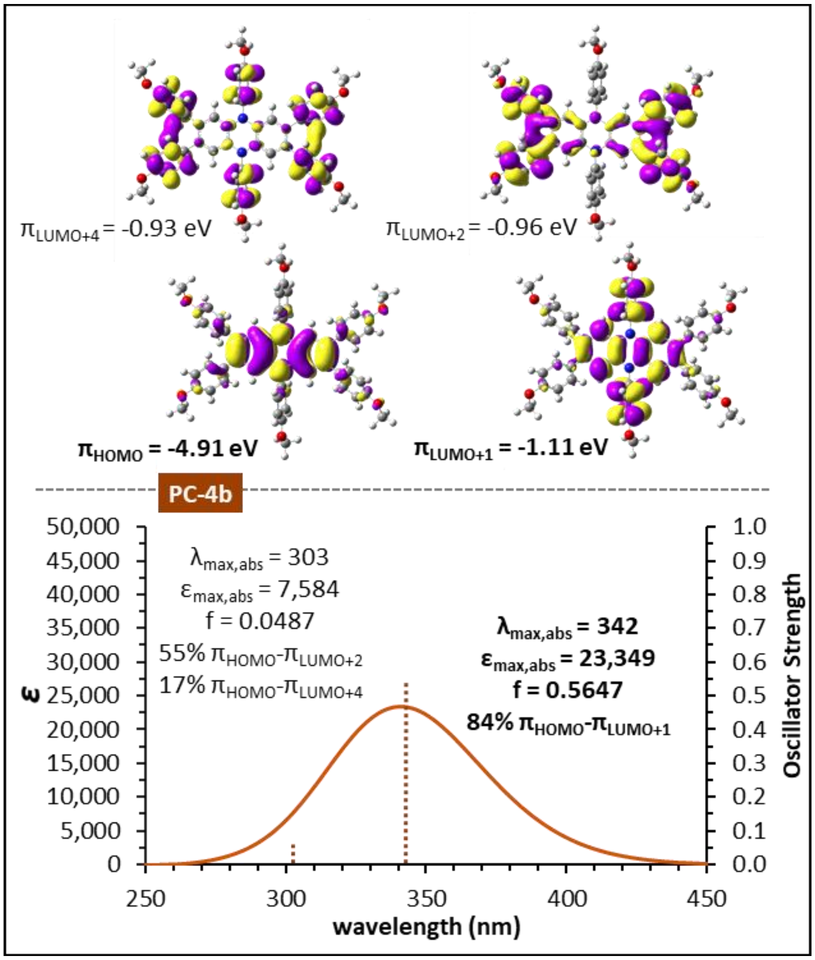


Figure S68: Computationally modeled molecular orbitals predicted to be involved in absorption transitions for PC **4b** detailed below (top). Computationally predicted UV−vis spectrum of PCs **4b** along with theoretically assigned percentage contributions (>15%) of various orbitals to the predicted absorption peaks. $\lambda_{max,abs}$ is the predicted absorption maximum wavelength and is reported in units of nm, $\varepsilon_{max,abs}$ is the predicted molar extinction coefficient at the predicted $\lambda_{max,abs}$ and is reported in units of M^{-1} cm^{-1}, and ƒ is the predicted oscillator strength; all of these values were predicted at the TD-DFT CAM-B3LYP/6-31+G(d,p)/CPCM-DMA level of theory (bottom).

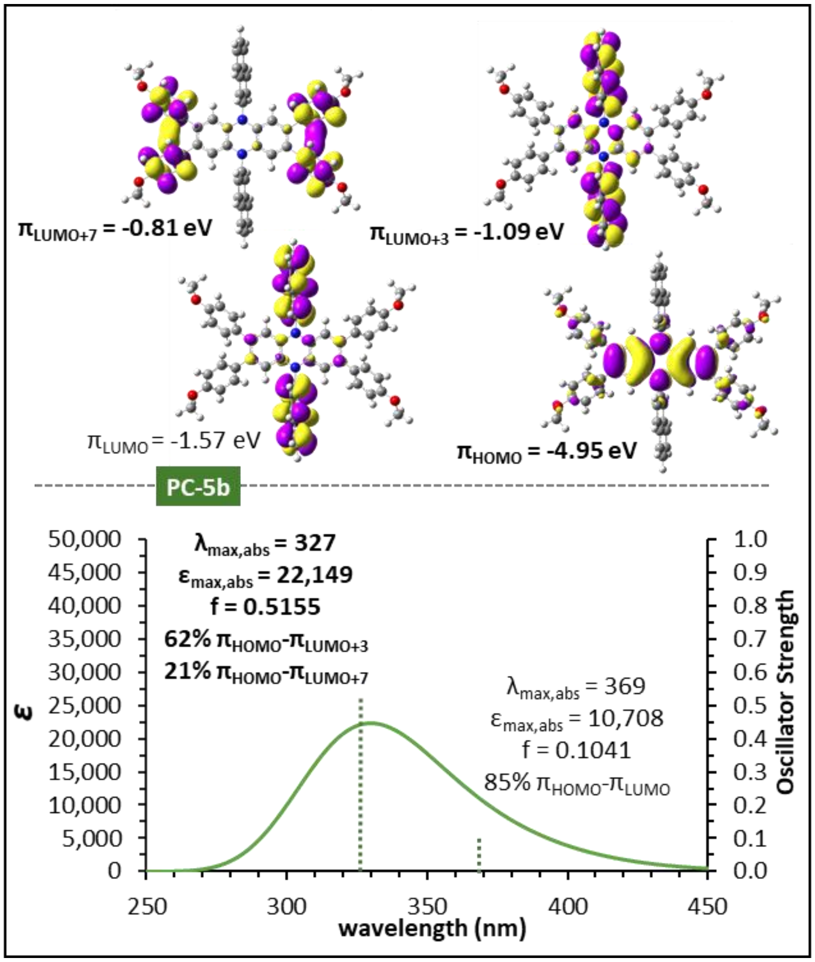


Figure S69: Computationally modeled molecular orbitals predicted to be involved in absorption transitions for PC **5b** detailed below (top). Computationally predicted UV−vis spectrum of PCs **5b** along with theoretically assigned percentage contributions (>15%) of various orbitals to the predicted absorption peaks. $\lambda_{max,abs}$ is the predicted absorption maximum wavelength and is reported in units of nm, $\varepsilon_{max,abs}$ is the predicted molar extinction coefficient at the predicted $\lambda_{max,abs}$ and is reported in units of M^{-1} cm^{-1}, and ƒ is the predicted oscillator strength; all of these values were predicted at the TD-DFT CAM-B3LYP/6-31+G(d,p)/CPCM-DMA level of theory (bottom).

Computationally Modeled Singly Occupied Molecular Orbitals (SOMOs) of PCs

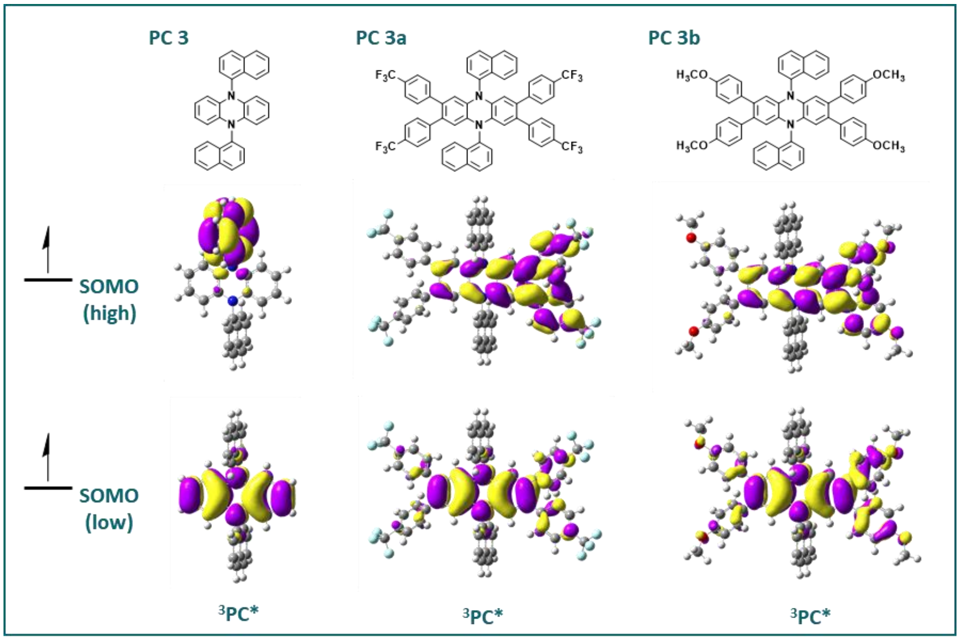


Figure S70. Computational modeling of the singularly occupied molecular orbitals (SOMOs) for PCs **3**, **3a**, and **3b** (from left to right); the lower lying SOMO (bottom row) and higher lying SOMO (top row) for each PC in the triplet excited state are shown.

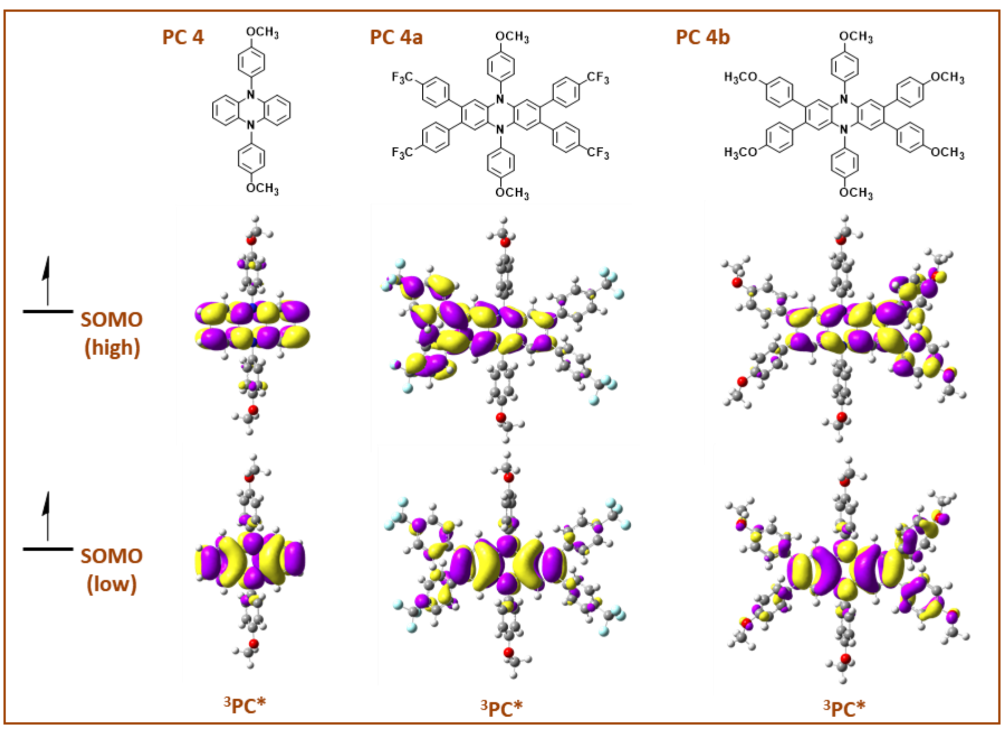


Figure S71. Computational modeling of the singularly occupied molecular orbitals (SOMOs) for PCs **4**, **4a**, and **4b** (from left to right); the lower lying SOMO (bottom row) and higher lying SOMO (top row) for each PC in the triplet excited state are shown.

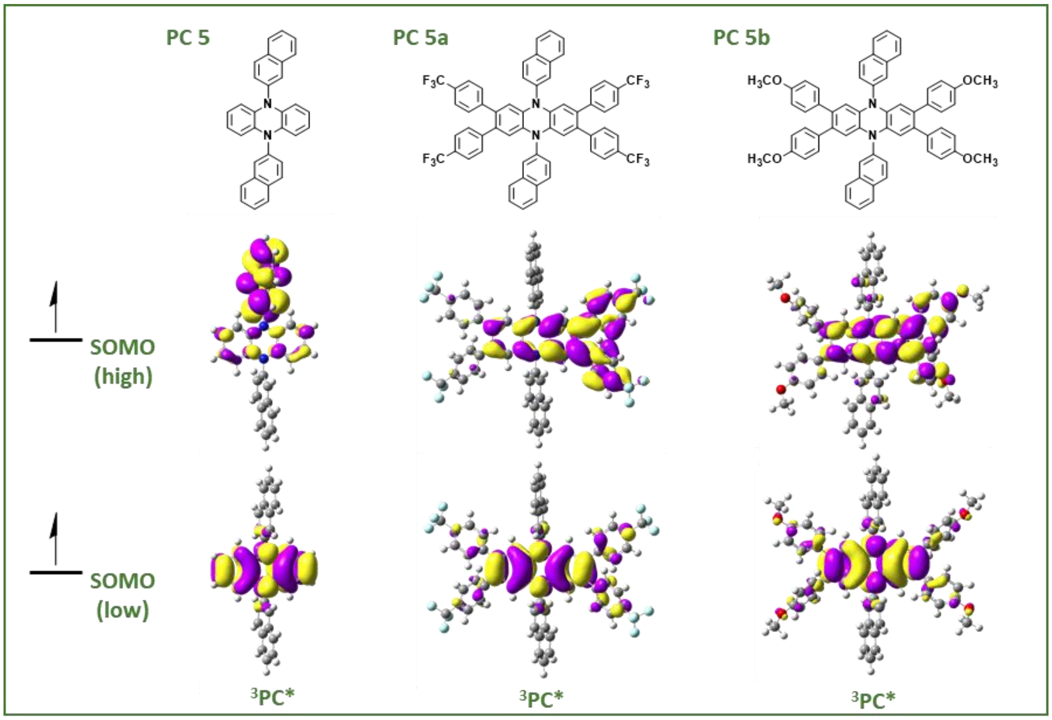


Figure S72. Computational modeling of the singularly occupied molecular orbitals (SOMOs) for PCs **5**, **5a**, and **5b** (from left to right); the lower lying SOMO (bottom row) and higher lying SOMO (top row) for each PC in the triplet excited state are shown.

Computationally Modeled Electrostatic Potential (ESP) Maps of PCs

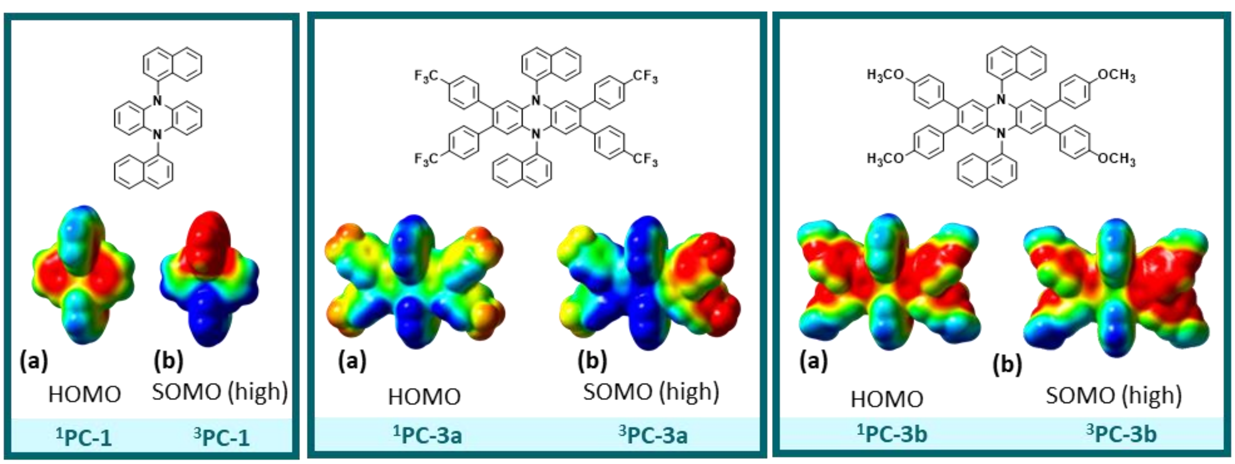


Figure S73. Electrostatic potential (ESP) mapped electron density for PCs **3**, **3a**, and **3b** (from left to right) in the ground state (a) and triplet excited state (b) are shown. Red color represents electron rich regions and blue color represents electron deficient regions.

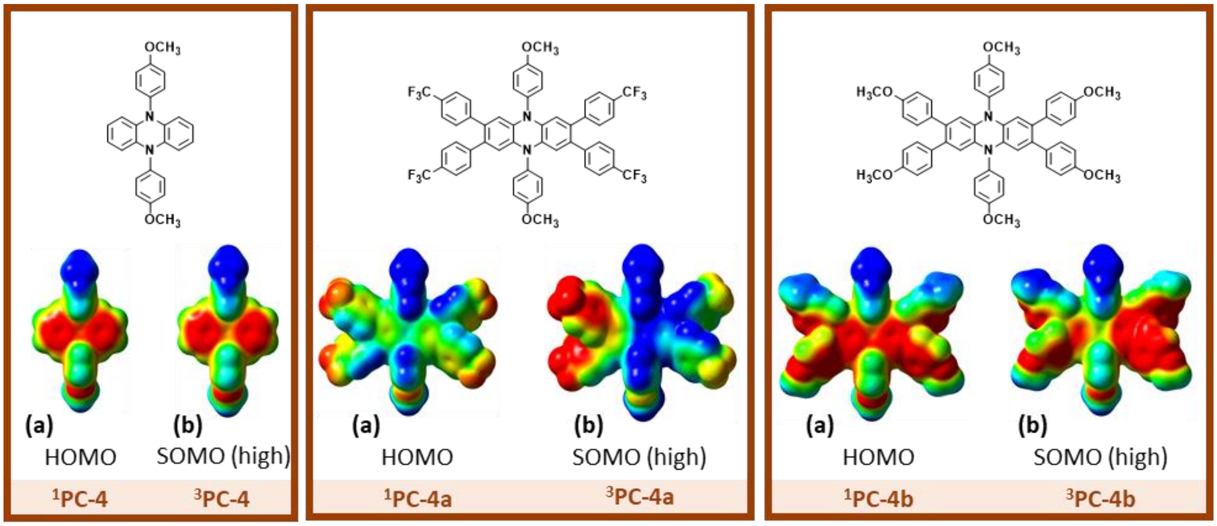


Figure S74. Electrostatic potential (ESP) mapped electron density for PCs **4**, **4a**, and **4b** (from left to right) in the ground state (a) and triplet excited state (b) are shown. Red color represents electron rich regions and blue color represents electron deficient regions.

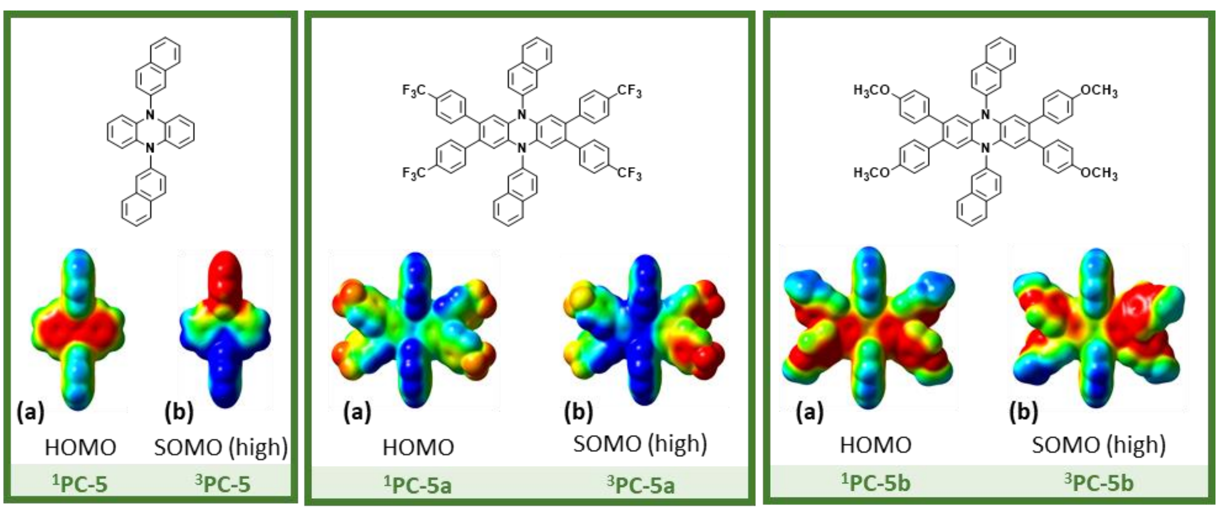


Figure S75. Electrostatic potential (ESP) mapped electron density for PCs **5**, **5a**, and **5b** (from left to right) in the ground state (a) and triplet excited state (b) are shown. Red color represents electron rich regions and blue color represents electron deficient regions.

POLYMERIZATION DATA

Table S3. O-ATRP Results from Employing CE-DHP PCs for the Polymerization of MMA at Varied Catalyst Loadings[a]

Run	PC	PC Loading (ppm)[b]	Conv. [c]	M_n (kDa)[d]	M_w (kDa)[d]	$Đ$ (M_w/M_n) [d]	I^*[e]
1	**3**	500	42.9%	5.71	6.37	1.12	79.5%
2	**3**	100	67.5%	8.97	9.63	1.07	78.1%
3	**3**	50	84.6%	8.26	9.87	1.19	105%
4	**3a**	500	67.7%	7.53	7.76	1.07	93.4%
5	**3a**	100	64.5%	7.71	8.93	1.16	87.0%
6	**3a**	50	85.8%	8.80	9.46	1.07	91.9%
7	**3a**	10	66.8%	7.17	10.7	1.49	96.8%
8	**3b**	100	51.2%	5.32	8.33	1.57	101%
10	**4a**	100	65.4%	7.57	8.70	1.15	89.8%
11	**4a**	50	75.5%	7.53	9.55	1.27	104%
12	**4a**	10	66.8%	7.17	10.7	1.49	96.8%
13	**5**	500	84.3%	10.2	11.7	1.15	85.6%
14	**5**	100	77.1%	8.74	10.4	1.18	91.2%
15	**5**	50	86.6%	12.8	15.3	1.20	69.9%
16	**5**	10	62.4%	7.43	13.3	1.79	87.5%
17	**5a**	500	60.5%	9.00	9.76	1.08	70.1%
18	**5a**	100	72.7%	8.08	8.87	1.09	93.2%
19	**5a**	50	79.5%	7.34	9.42	1.28	112%
20	**5a**	10	69.9%	7.54	10.71	1.42	96.1%
21	**5b**	500	52.4%	5.45	9.20	1.69	101%
22	**5b**	100	73.3%	8.25	12.7	1.54	92.1%

[a]All polymerizations were conducted using MMA as the monomer and DBMM as the initiator in a ratio of [1000]:[10] with DMAc as the solvent. [b]PC loading is relative to mols of monomer. [c]Conversion was determined by ^{1}H-NMR spectroscopy. [d]Measured using GPC. [e]Initiator efficiency (I^*) calculated by ((theoretical M_n/observed M_n)*100).

Table S4. Summary of results of O-ATRP of MMA in varied solvents using 50 ppm of **3a**, O-ATRP of varied monomers in benzene using 50ppm of **3a**, O-ATRP with **4a** using conditions optimized for PC **3a**, and O-ATRP of MMA with a phenoxazine PC at varied PC loadings. [a]

Run	PC	PC Loading (ppm)[b]	Monomer	Solvent	Conv. [c]	M_n (kDa)[d]	M_w (kDa)[d]	$Đ$ (M_w/M_n)[d]	I^*[e]
6	**3a**	50	MMA	DMAc	85.8%	8.80	9.46	1.07	91.9%
23	**3a**	50	MMA	THF	77.7%	9.88	11.5	1.17	81.0%
24	**3a**	50	MMA	EtOAc	86.9%	8.79	10.8	1.23	102%
25	**3a**	50	MMA	Benz	89.2%	10.0	10.6	1.06	92.0%
26	**3a**	50	MMA	DCM	94.1%	8.88	11.0	1.24	109%
27	**3a**	10	MMA	Benz	83.2%	7.24	10.9	1.51	119%
28	**3a**	50	nBA	Benz	93.3%	14.4	24.4	1.69	85.0%
29[f]	**3a**	50	DMA	Benz	85.8%	na	na	na	na
30[g]	**3a**	50	VA	Benz	0.00%	na	na	na	na
31[g]	**3a**	50	styrene	Benz	0.00%	na	na	na	na
32	**4a**	50	nBA	Benz	87.3%	11.9	28.8	2.41	96.0%
33	**4a**	10	MMA	Benz	51.9%	5.34	7.11	1.33	102%
34	**PhenO[h]**	50	MMA	DMAc	56.3%	6.77	12.2	1.81	87.0%
35	**PhenO[h]**	100	MMA	DMAc	60.8%	9.43	1.68	1.78	67.2%
36	**PhenO[h]**	500	MMA	DMAc	69.7%	6.73	9.37	1.39	107%

[a]All polymerizations were conducted using DBMM as the initiator in a ratio of [1000]:[10] for [monomer]:[DBMM]. [b]PC loading is relative to mols of monomer. [c]Conversion was determined by ^{1}H-NMR spectroscopy. [d]Measured using GPC. [e]Initiator efficiency (I^*) calculated by ((theoretical M_n/observed M_n)*100). [f]Molecular weight data was not obtained for this polymer. [g]Molecular weight data was not obtained as there was no conversion observed. **[h]PhenO** (3,7-Di([1,1'-biphenyl]-4-yl)-10-(naphthalen-1-yl)-10*H*-phenoxazine).

Polymerization Kinetics

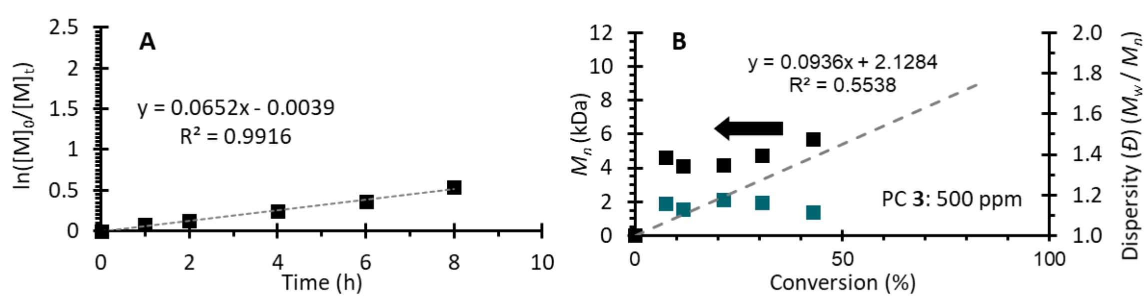


Figure S76. Polymerization data from Run 1 (Table S3). [MMA]:[DMAc]:[DBMM]:[**3**] = [1000]:[1000]:[10]:[0.5]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (blue squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

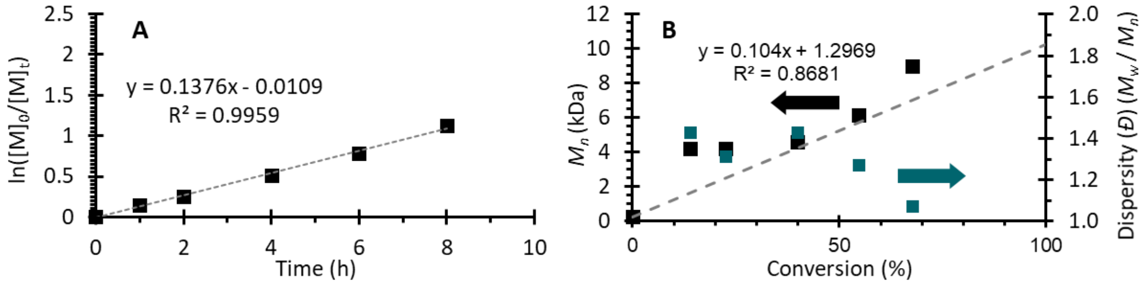


Figure S77. Polymerization data from Run 2 (Table S3). [MMA]:[DMAc]:[DBMM]:[**3**] = [1000]:[1000]:[10]:[0.1]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (blue squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

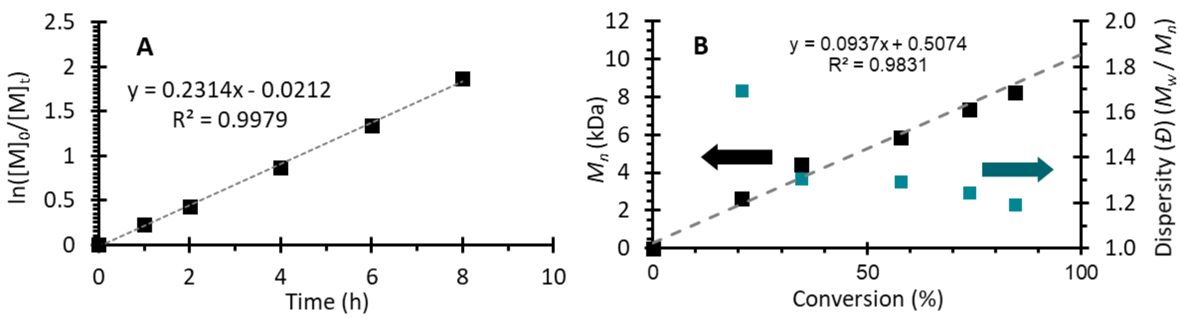


Figure S78. Polymerization data from Run 3 (Table S3). [MMA]:[DMAc]:[DBMM]:[**3**] = [1000]:[1000]:[10]:[0.05]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (blue squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

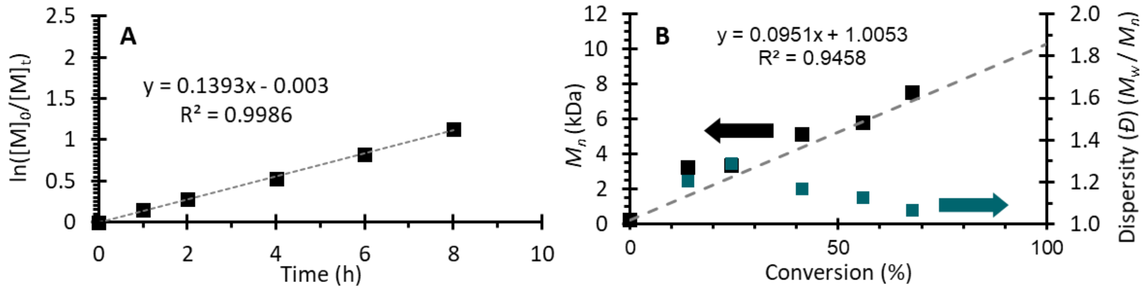


Figure S79. Polymerization data from Run 4 (Table S3). [MMA]:[DMAc]:[DBMM]:[**3a**] = [1000]:[1000]:[10]:[0.5]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (blue squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

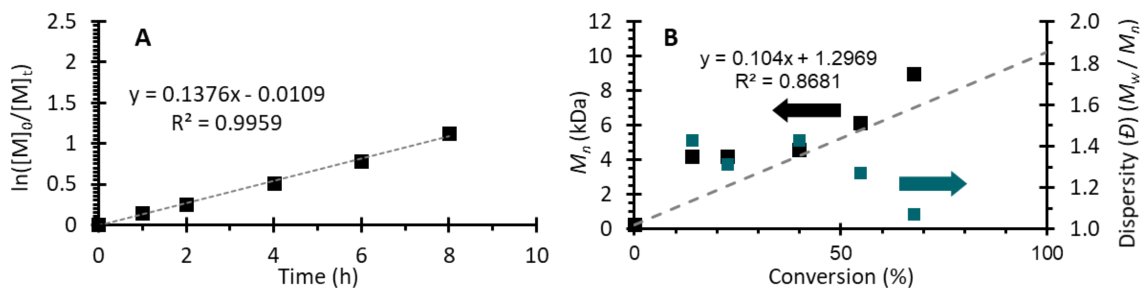


Figure S80. Polymerization data from Run 5 (Table S3). [MMA]:[DMAc]:[DBMM]:[**3a**] = [1000]:[1000]:[10]:[0.1]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (blue squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

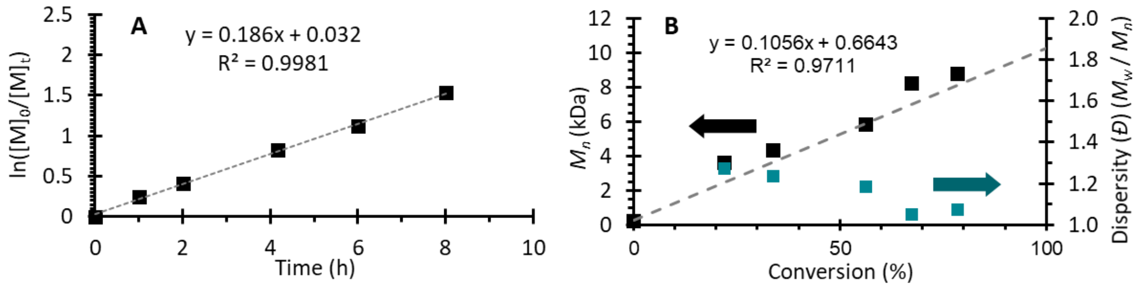


Figure S81. Polymerization data from Run 6 (Table S3). [MMA]:[DMAc]:[DBMM]:[**3a**] = [1000]:[1000]:[10]:[0.05]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (blue squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

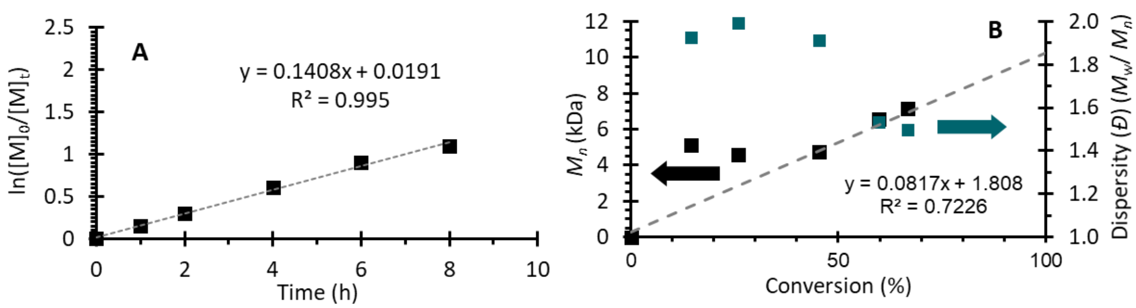


Figure S82. Polymerization data from Run 7 (Table S3). [MMA]:[DMAc]:[DBMM]:[**3a**] = [1000]:[1000]:[10]:[0.01]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (blue squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

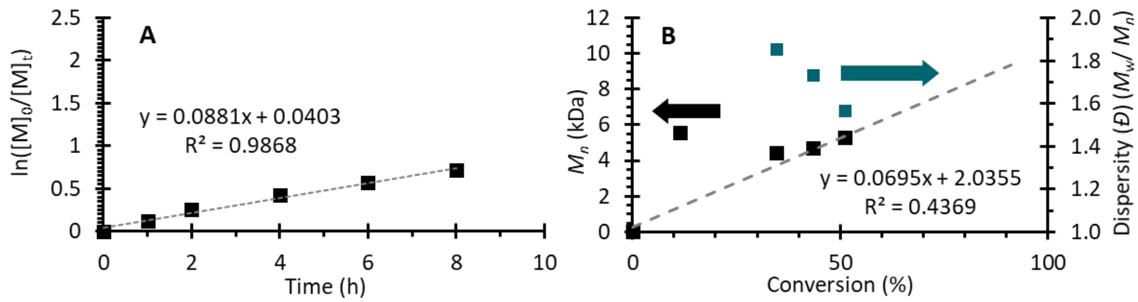


Figure S83. Polymerization data from Run 8 (Table S3). [MMA]:[DMAc]:[DBMM]:[**3b**] = [1000]:[1000]:[10]:[0.1]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (blue squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

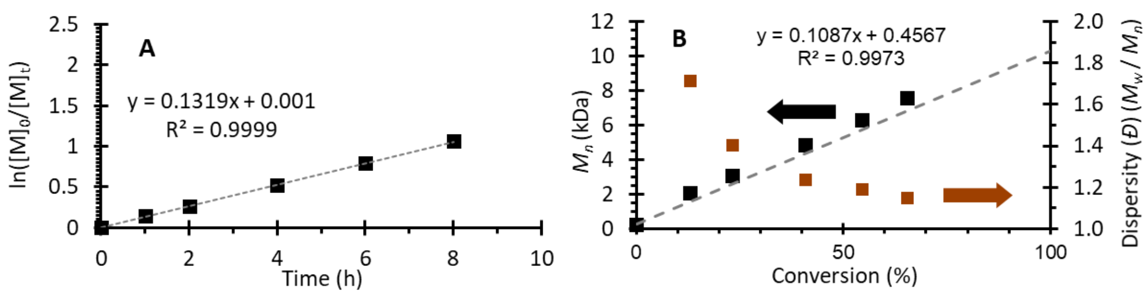


Figure S84. Polymerization data from Run 10 (Table S3). [MMA]:[DMAc]:[DBMM]:[**4a**] = [1000]:[1000]:[10]:[0.1]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (orange squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

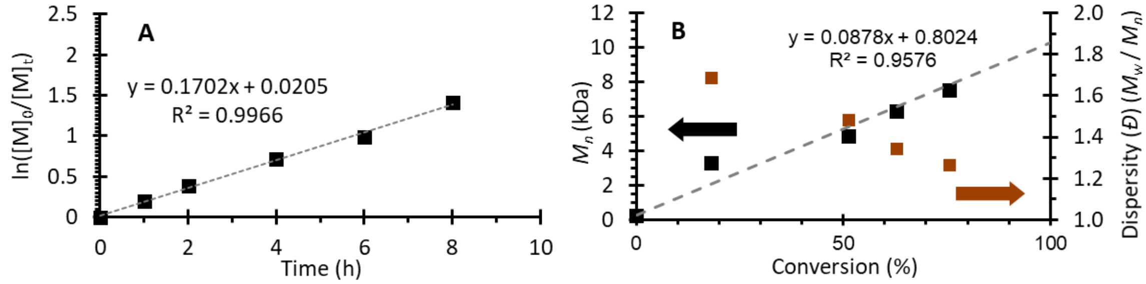


Figure S85. Polymerization data from Run 11 (Table S3). [MMA]:[DMAc]:[DBMM]:[**4a**] = [1000]:[1000]:[10]:[0.05]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (orange squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

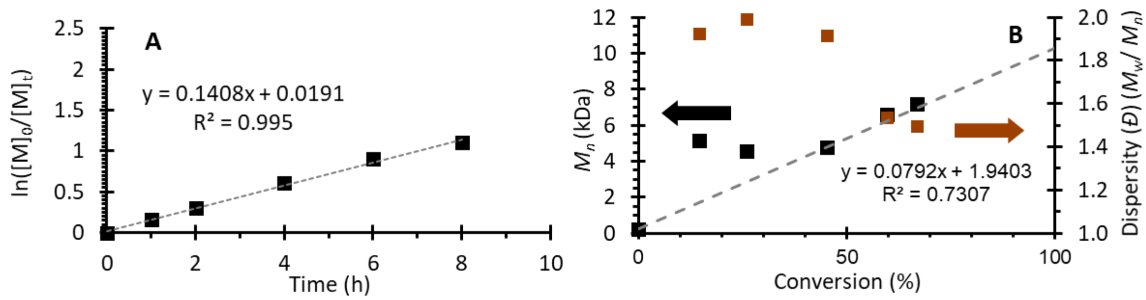


Figure S86. Polymerization data from Run 12 (Table S3). [MMA]:[DMAc]:[DBMM]:[**4a**] = [1000]:[1000]:[10]:[0.01]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (orange squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

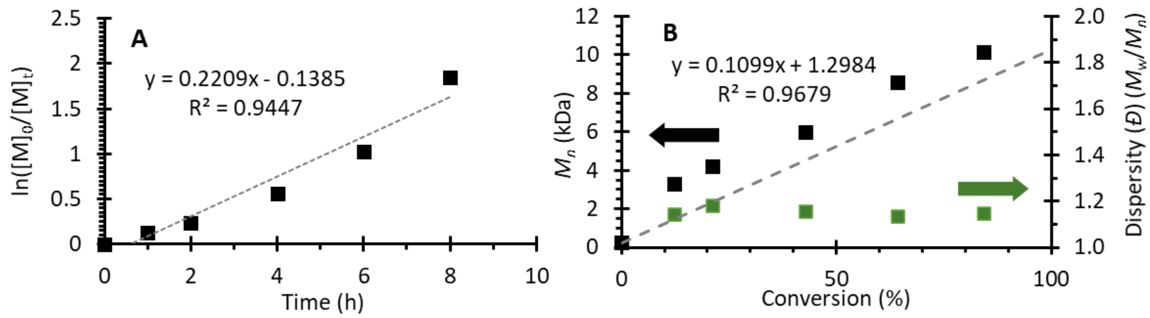


Figure S87. Polymerization data from Run 13 (Table S3). [MMA]:[DMAc]:[DBMM]:[**5**] = [1000]:[1000]:[10]:[0.5]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (green squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

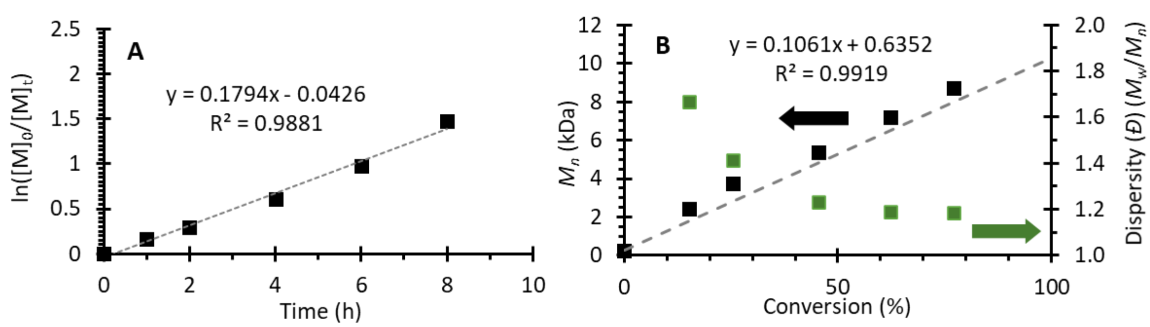


Figure S88. Polymerization data from Run 14 (Table S3). [MMA]:[DMAc]:[DBMM]:[**5**] = [1000]:[1000]:[10]:[0.1]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (green squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

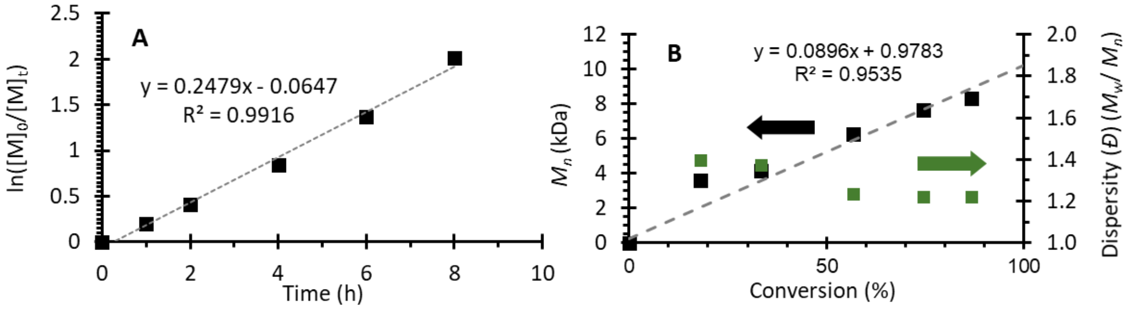


Figure S89. Polymerization data from Run 15 (Table S3). [MMA]:[DMAc]:[DBMM]:[**5**] = [1000]:[1000]:[10]:[0.05]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (green squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

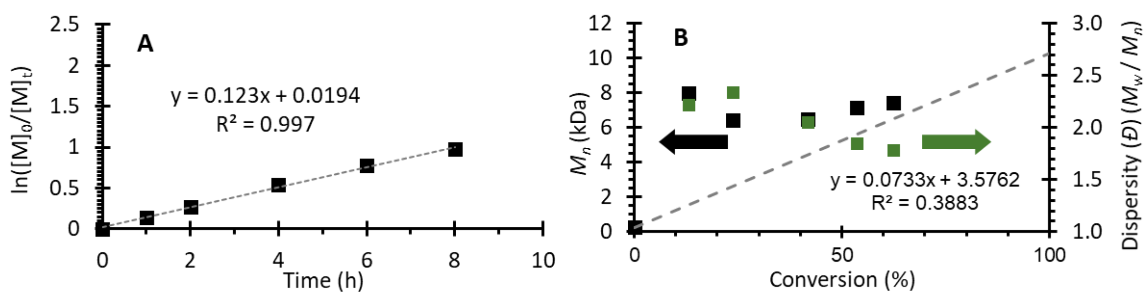


Figure S90. Polymerization data from Run 16 (Table S3). [MMA]:[DMAc]:[DBMM]:[**5**] = [1000]:[1000]:[10]:[0.01]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (green squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

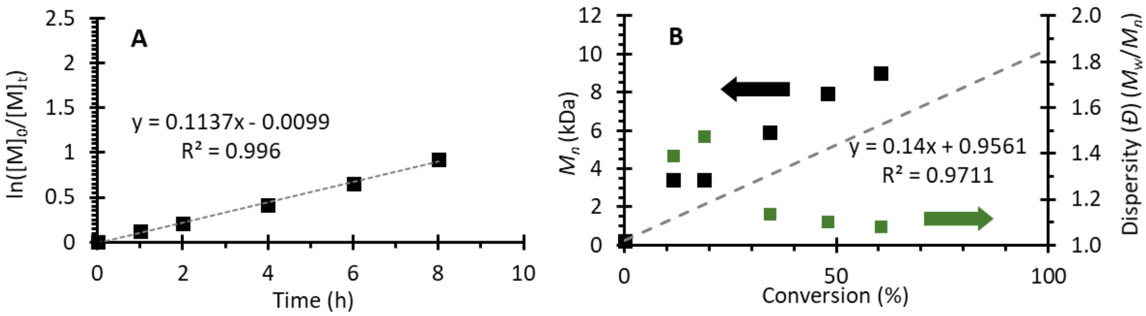


Figure S91. Polymerization data from Run 17 (Table S3). [MMA]:[DMAc]:[DBMM]:[**5a**] = [1000]:[1000]:[10]:[0.5]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (green squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

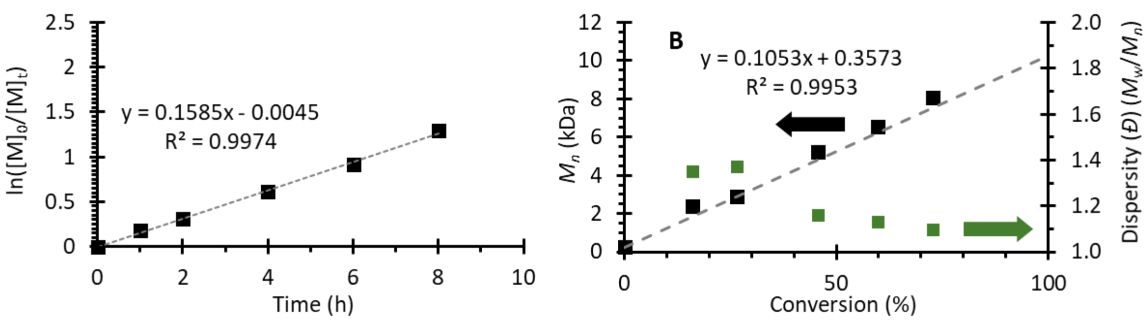


Figure S92. Polymerization data from Run 18 (Table S3). [MMA]:[DMAc]:[DBMM]:[**5a**] = [1000]:[1000]:[10]:[0.1]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (green squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

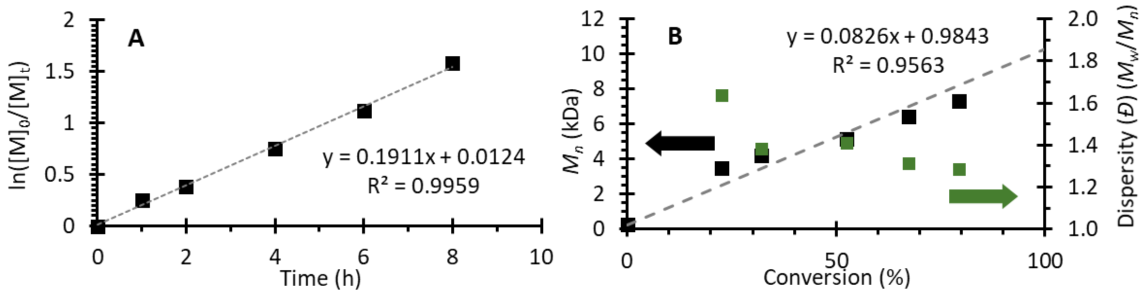


Figure S93. Polymerization data from Run 19 (Table S3). [MMA]:[DMAc]:[DBMM]:[**5a**] = [1000]:[1000]:[10]:[0.05]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (green squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

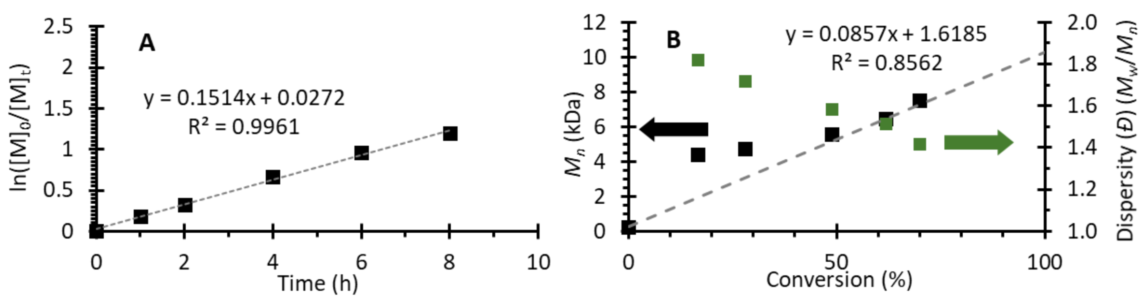


Figure S94. Polymerization data from Run 20 (Table S3). [MMA]:[DMAc]:[DBMM]:[**5a**] = [1000]:[1000}:[10]:[0.01]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (green squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

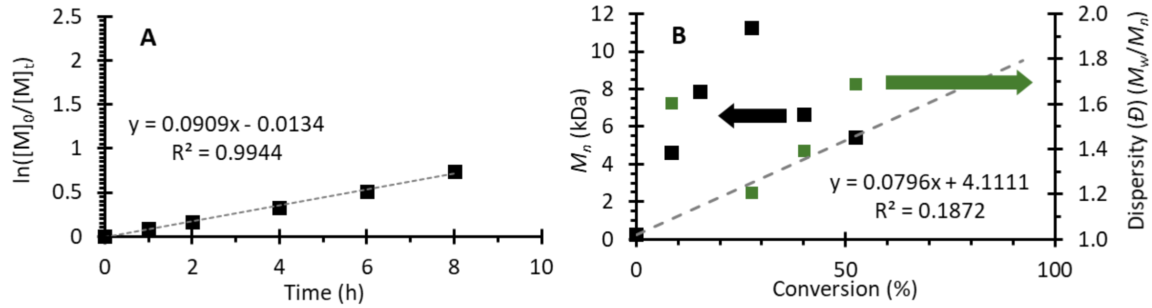


Figure S95. Polymerization data from Run 21 (Table S3). [MMA]:[DMAc]:[DBMM]:[**5b**] = [1000]:[1000]:[10]:[0.5]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (green squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

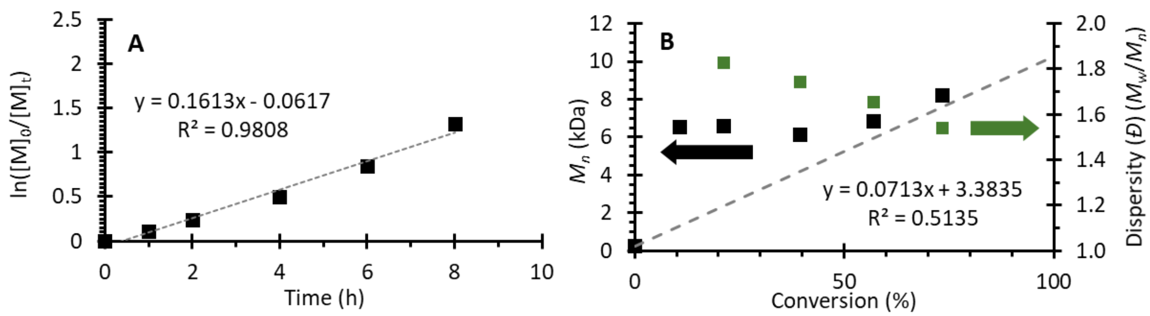


Figure S96. Polymerization data from Run 22 (Table S3). [MMA]:[DMAc]:[DBMM]:[**5b**] = [1000]:[1000]:[10]:[0.1]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (green squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

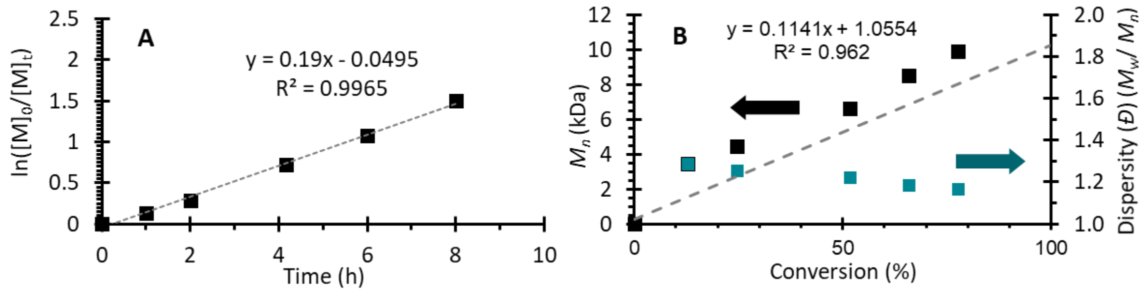


Figure S97. Polymerization data from Run 23 (Table S4). [MMA]:[THF]:[DBMM]:[**3a**] = [1000]:[1000]:[10]:[0.05]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (blue squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

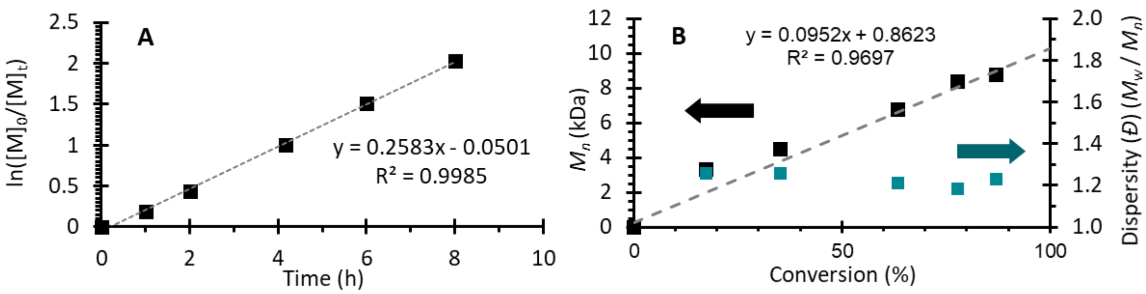


Figure S98. Polymerization data from Run 24 (Table S4). [MMA]:[EtOAc]:[DBMM]:[**3a**] = [1000]:[1000]:[10]:[0.05]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (blue squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

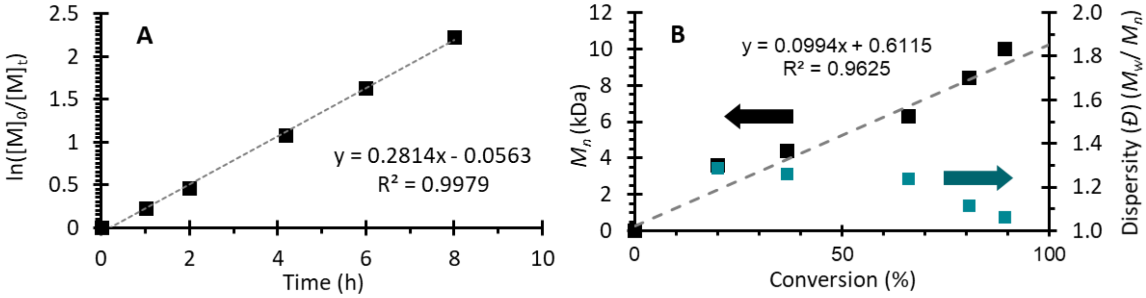


Figure S99. Polymerization data from Run 25 (Table S4). [MMA]:[Benz]:[DBMM]:[**3a**] = [1000]:[1000]:[10]:[0.05]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (blue squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

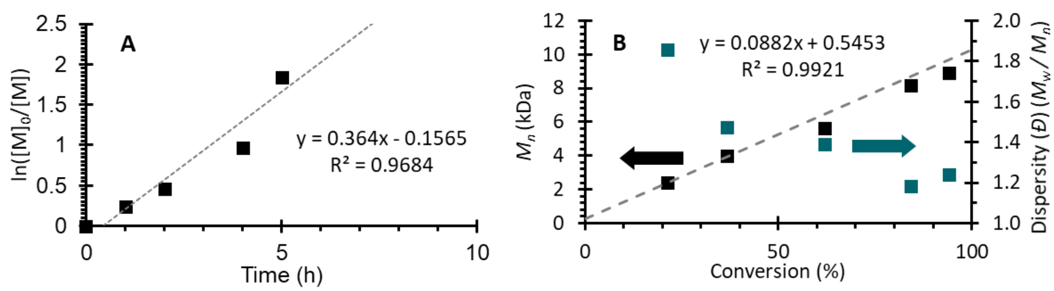


Figure S100. Polymerization data from Run 26 (Table S4). [MMA]:[DCM]:[DBMM]:[**3a**] = [1000]:[1000]:[10]:[0.05]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (blue squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

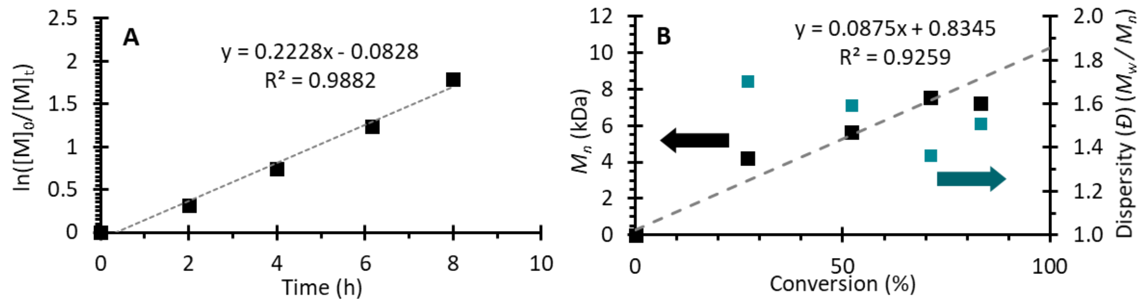


Figure S101. Polymerization data from Run 27 (Table S4). [MMA]:[Benz]:[DBMM]:[**3a**] = [1000]:[1000]:[10]:[0.01]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (blue squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

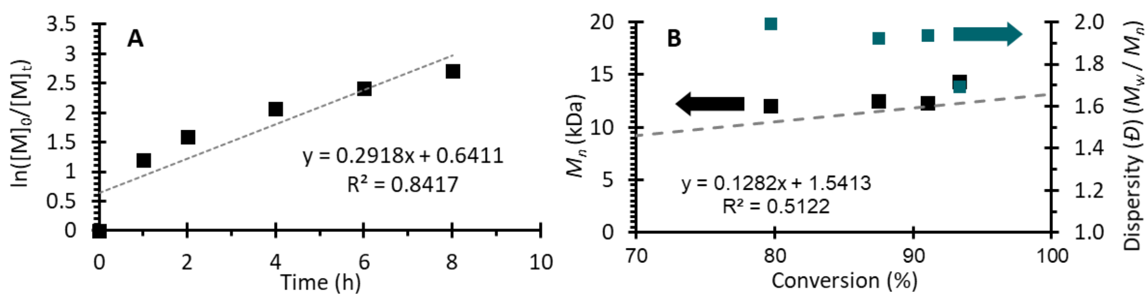


Figure S102. Polymerization data from Run 28 (Table S4). [nBA]:[Benz]:[DBMM]:[**3a**] = [1000]:[1000]:[10]:[0.05]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (blue squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

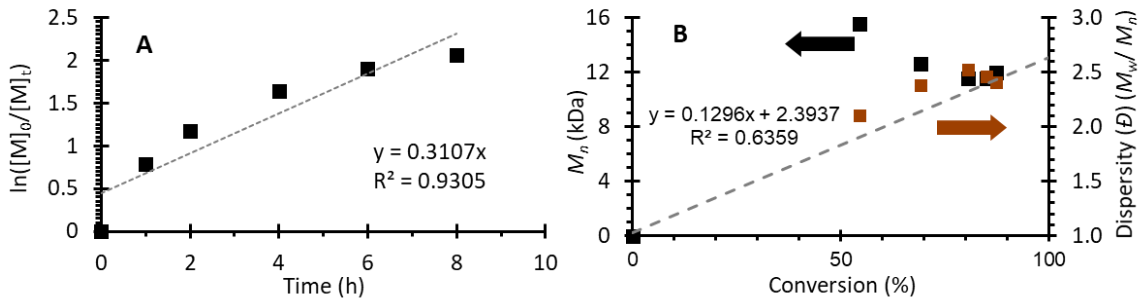


Figure S103. Polymerization data from Run 32 (Table S4). [nBA]:[Benz]:[DBMM]:[**4a**] = [1000]:[1000]:[10]:[0.05]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (orange squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

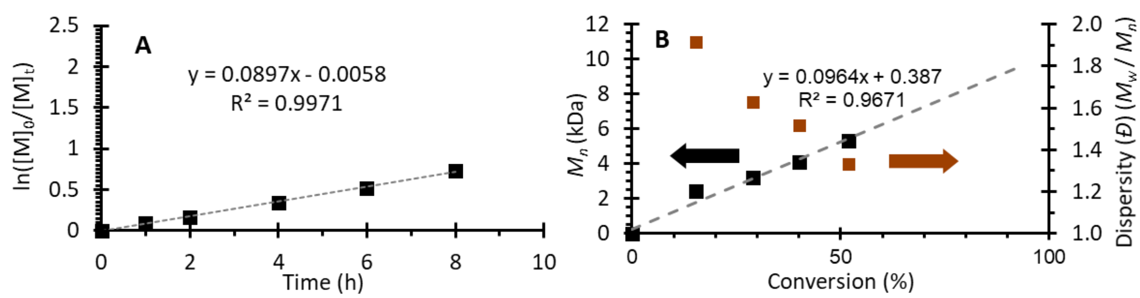


Figure S104. Polymerization data from Run 33 (Table S4). [MMA]:[Benz]:[DBMM]:[**4a**] = [1000]:[1000]:[10]:[0.01]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (orange squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion.

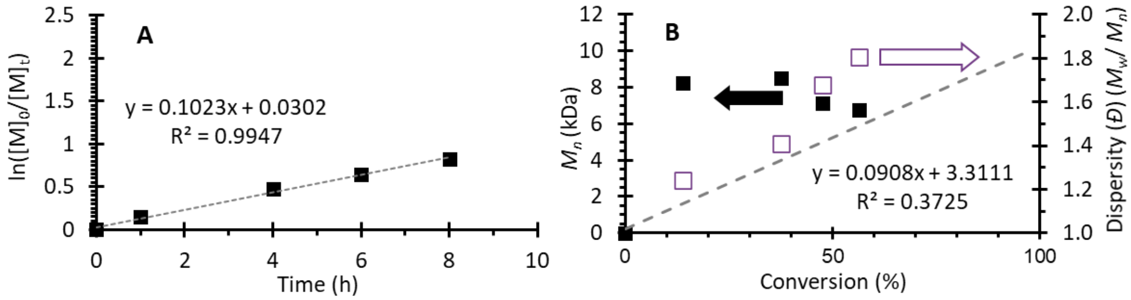


Figure S105. Polymerization data from Run 34 (Table S4). [MMA]:[DMAc]:[DBMM]:[**PhenO***] = [1000]:[1000]:[10]:[0.05]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (orange squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion. *(**PhenO**: 3,7-Di([1,1'-biphenyl]-4-yl)-10-(naphthalen-1-yl)-10*H*-phenoxazine).

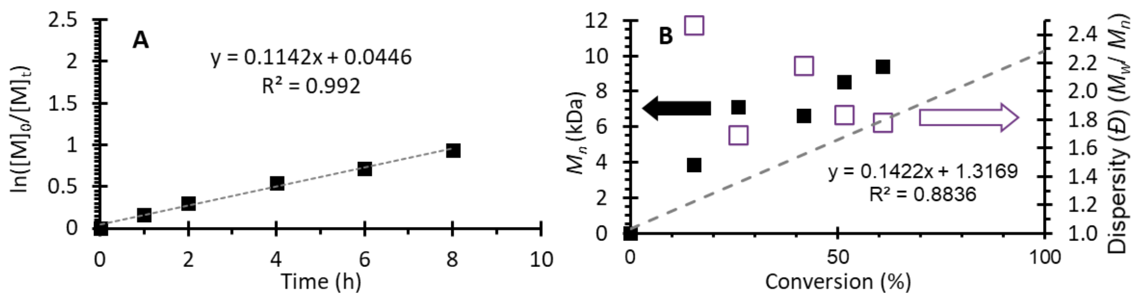


Figure S106. Polymerization data from Run 35 (Table S4). [MMA]:[DMAc]:[DBMM]:[**PhenO***] = [1000]:[1000]:[10]:[0.1]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (orange squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion. *(**PhenO**: 3,7-Di([1,1'-biphenyl]-4-yl)-10-(naphthalen-1-yl)-10*H*-phenoxazine).

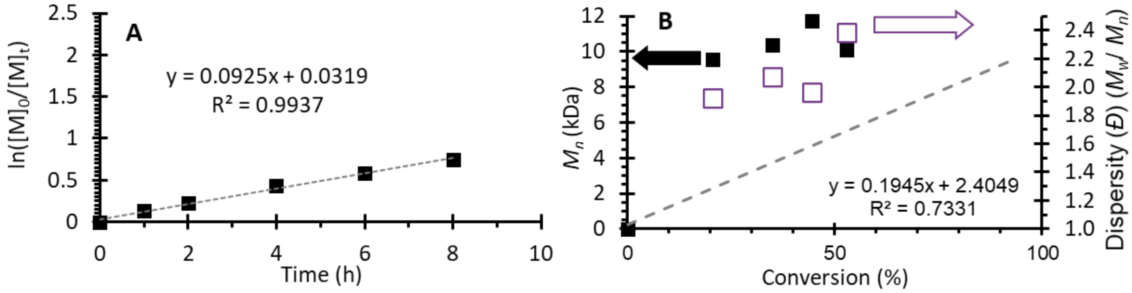
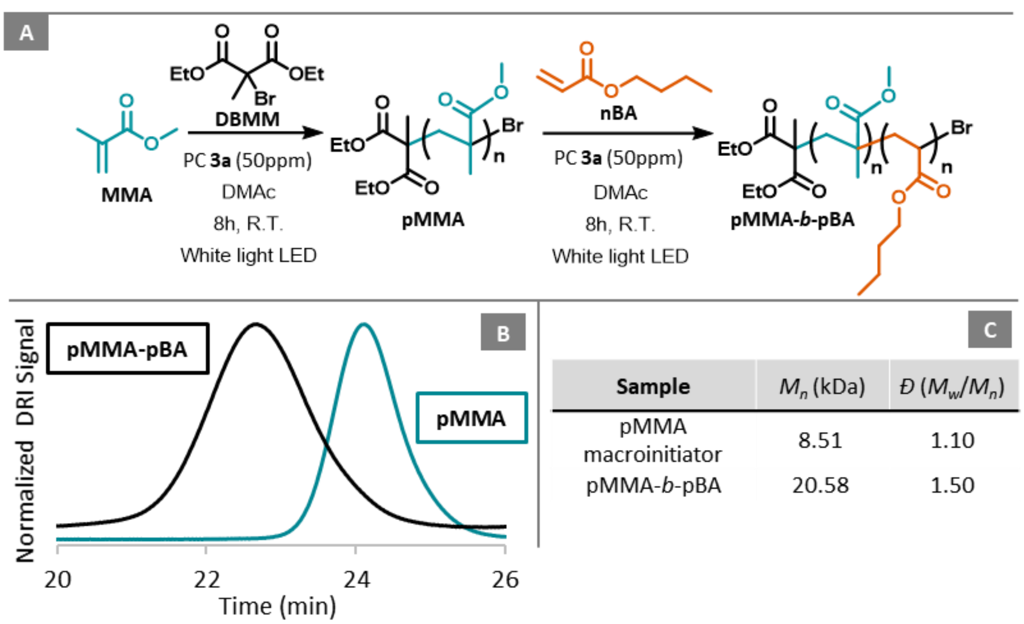


Figure S107. Polymerization data from Run 36 (Table S4). [MMA]:[DMAc]:[DBMM]:[**PhenO***] = [1000]:[1000]:[10]:[0.5]. (A) First order kinetic plot of the natural log of monomer consumption as a function of time. (B) Plot of molecular weight (M_n) growth as a function of monomer conversion (black squares), theoretical M_n growth as a function of monomer conversion (dashed grey line), and dispersity as a function of monomer conversion (orange squares). Equation on chart (B) represents the trendline for the measured M_n growth as a function of conversion. *(**PhenO**: 3,7-Di([1,1'-biphenyl]-4-yl)-10-(naphthalen-1-yl)-10*H*-phenoxazine).

__Chain Extension Experiment__



Sample	M_n (kDa)	$Đ$ (M_w/M_n)
pMMA macroinitiator	8.51	1.10
pMMA-*b*-pBA	20.58	1.50

Figure S108. (**A**) Reaction scheme for chain extension of pMMA macroinitiator with nBA to form pMMA-*b*-pBA. The polymerization of the macromonomer was run in DMAc using DBMM as the initiator and MMA as the monomer in a ratio of [MMA]:[DBMM]:[**3a**] = [1000]:[10]:[0.05]. (**B**) Overlaid GPC traces of the isolated pMMA macroinitator and the isolated pMMA-*b*-pBA block copolymer. (**C**) Molecular weight data (obtained using GPC) for the isolated pMMA macroinitiator and the isolated pMMA-*b*-nBA block copolymer.

^{1}H-NMR SPECTRA OF CATALYSTS & RELEVANT INTERMEDIATES

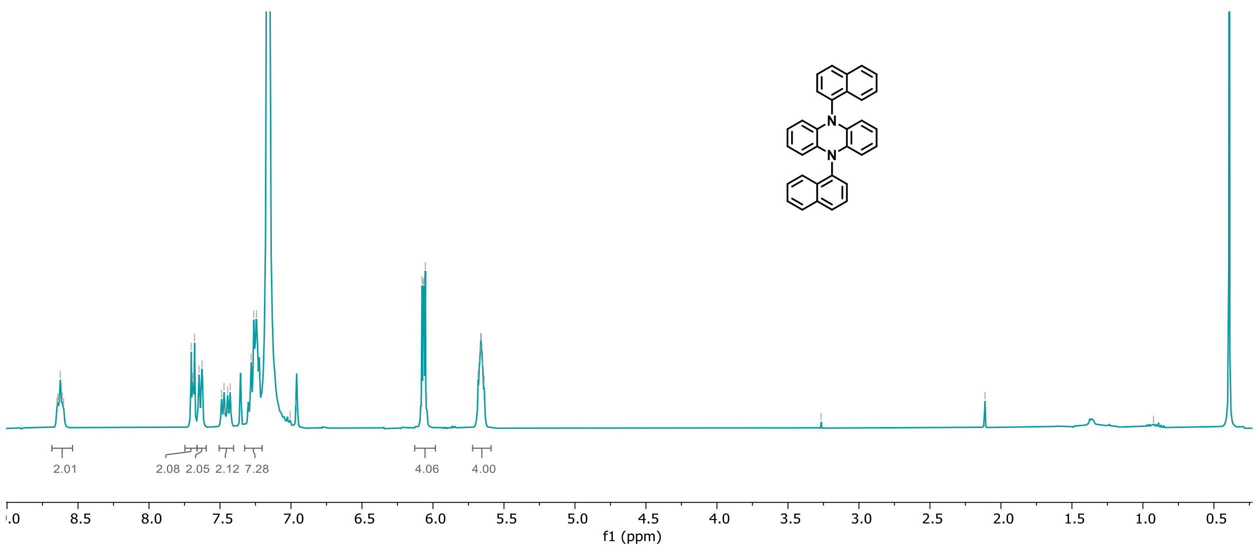


Figure S109. ^{1}H-NMR spectrum of **PC 3** in C_6D_6 after recrystallization.

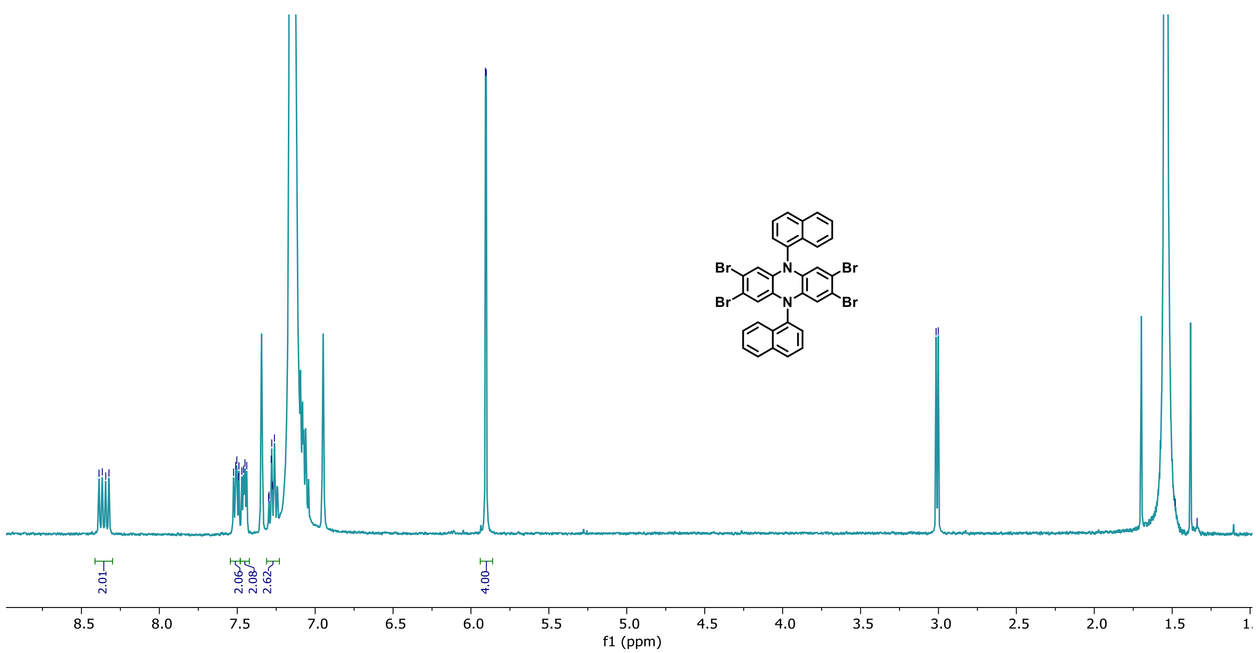


Figure S110. ^{1}H-NMR spectrum of unpurified **PC 3-4Br** in C_6D_6.

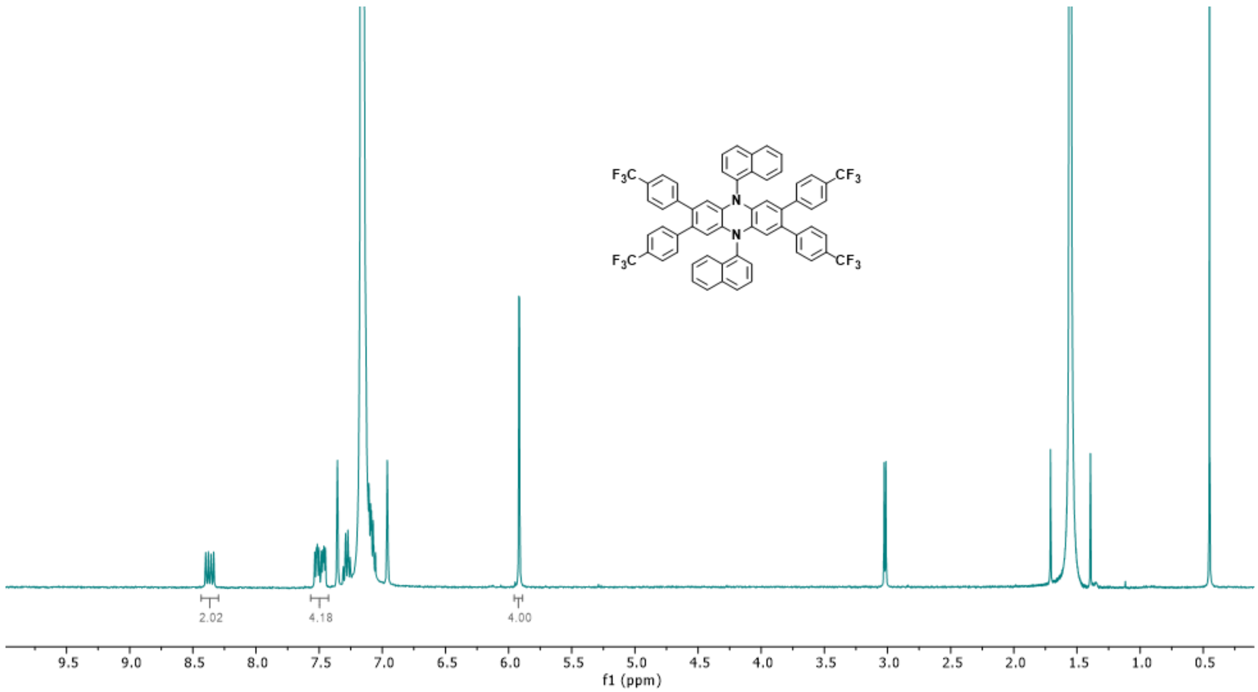


Figure S111. ^{1}H-NMR spectrum of **PC 3a** in C_6D_6 after recrystallization.

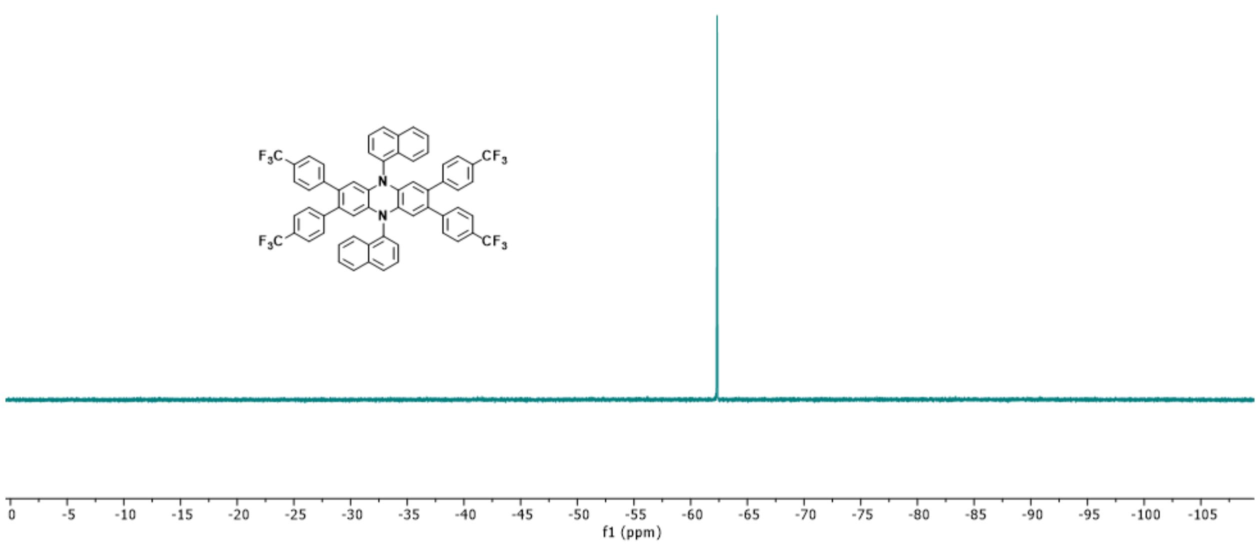


Figure S112. ^{19}F-NMR spectrum of **PC 3a** in C_6D_6.

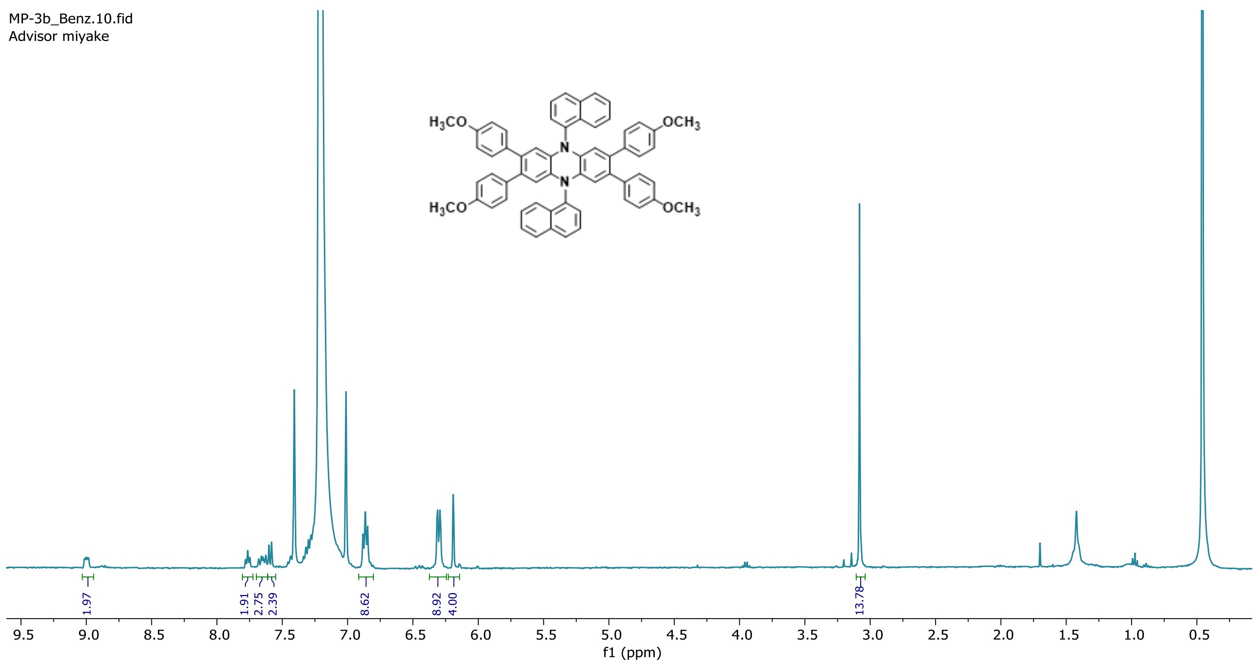


Figure S113. ^{1}H-NMR spectrum of **PC 3b** in C_6D_6.

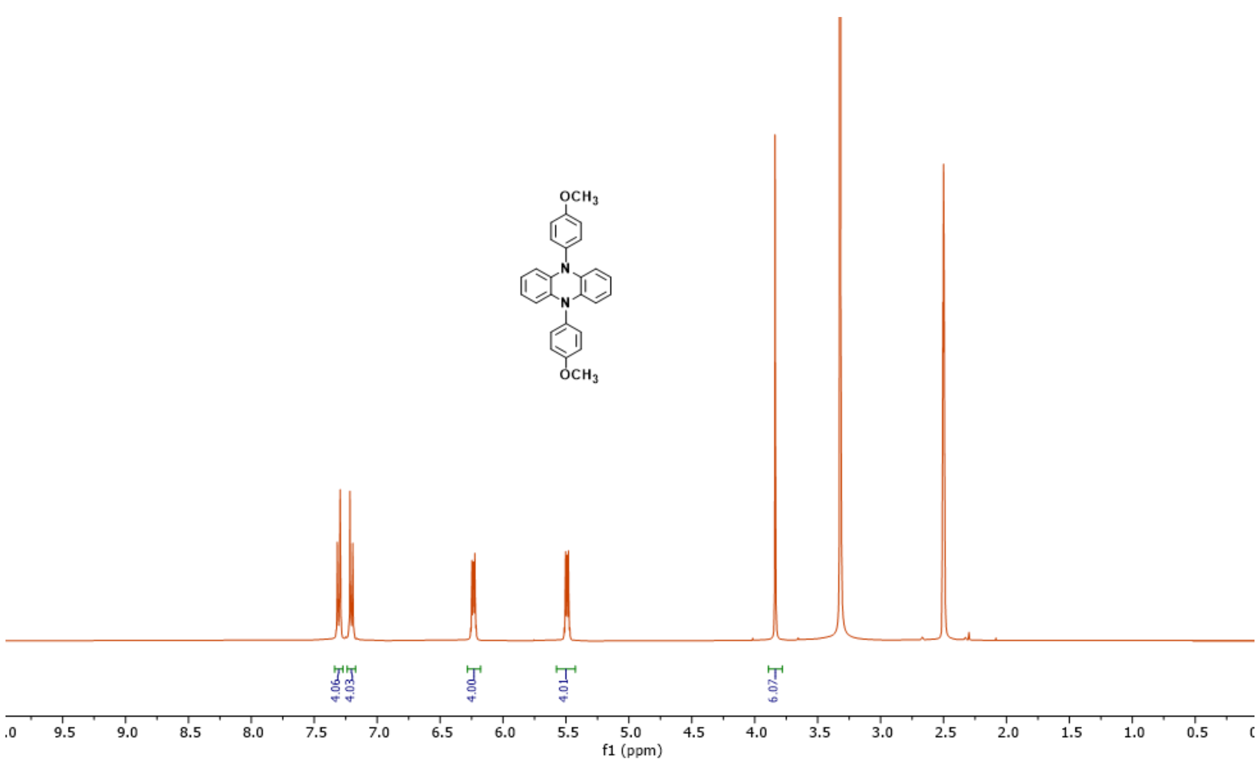


Figure S114. ^{1}H-NMR spectrum of PC **4** recrystallization from toluene-hexanes DMSO-d_6.

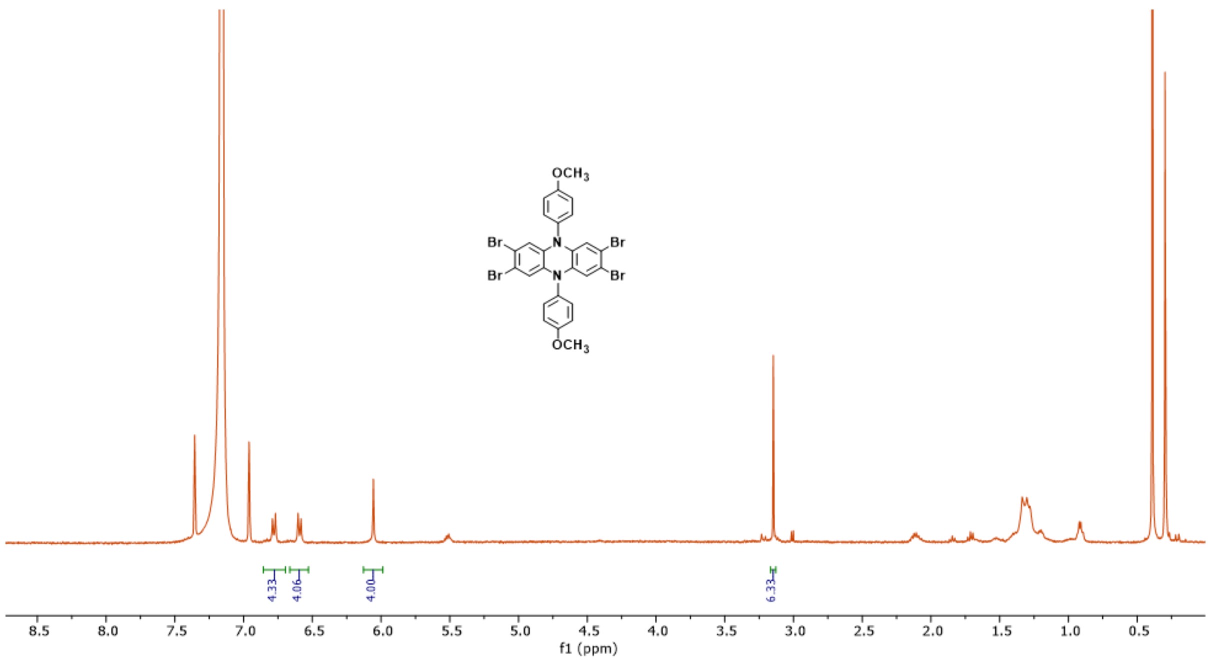


Figure S115. ^{1}H-NMR spectrum of unpurified **4-4Br** in C_6D_6.

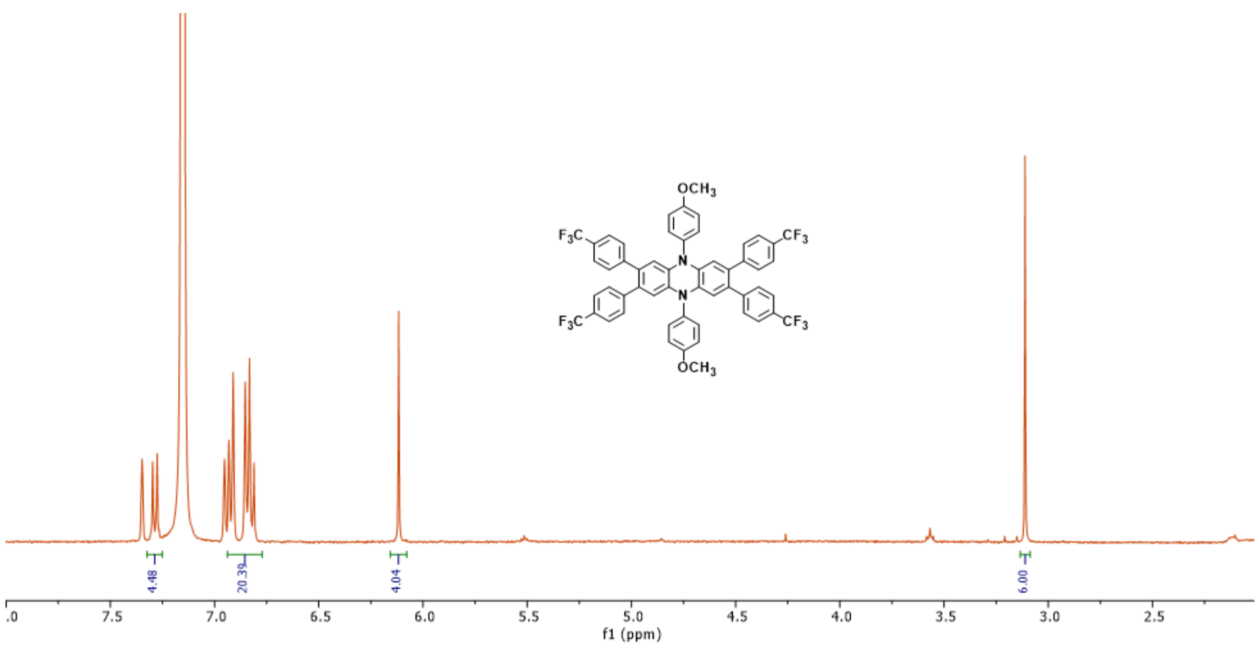


Figure S116. ^{1}H-NMR spectrum of **4a** in C_6D_6 after recrystallization.

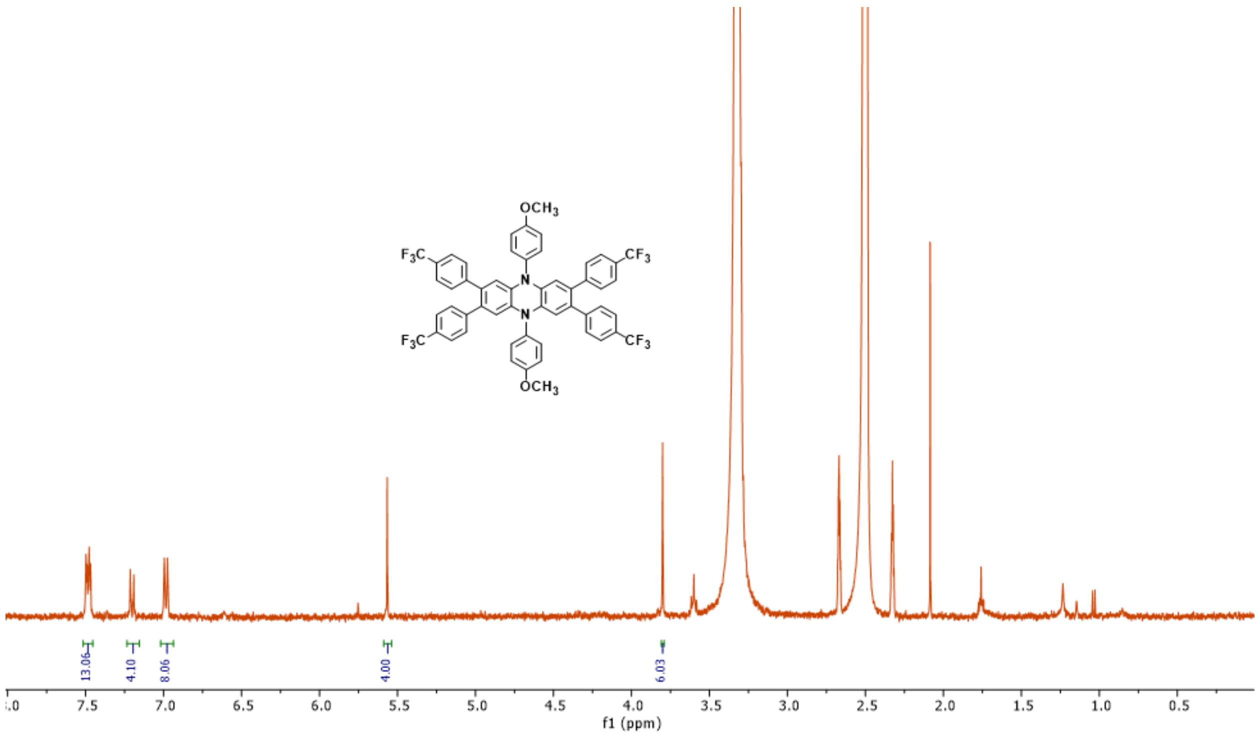


Figure S117. ^{1}H-NMR spectrum of **4a** in DMSO-d_6 after recrystallization.

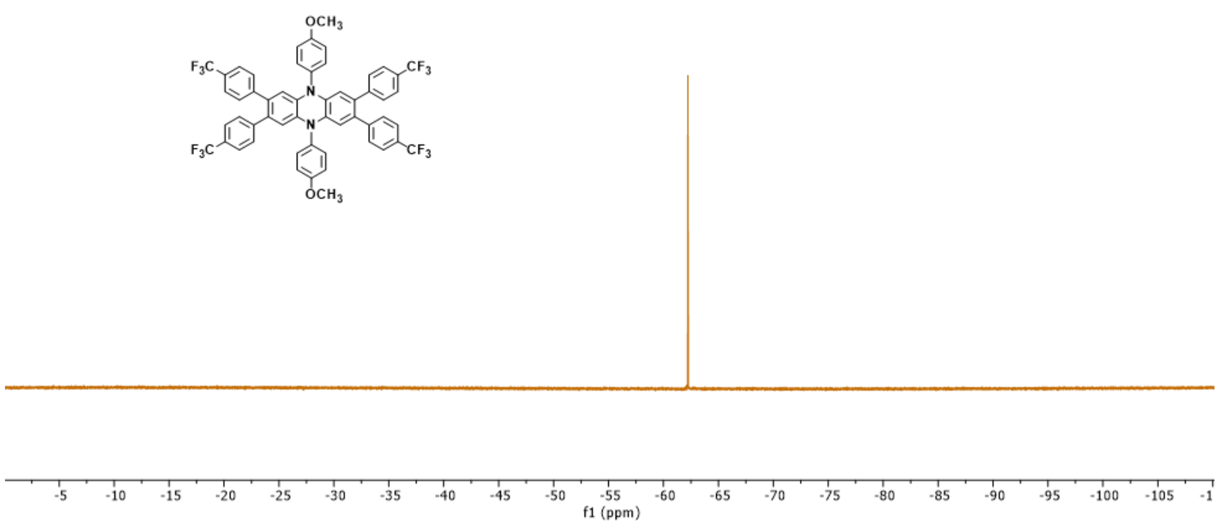


Figure S118. ^{19}F-NMR spectrum of **PC 4a** in C_6D_6 after recrystallization.

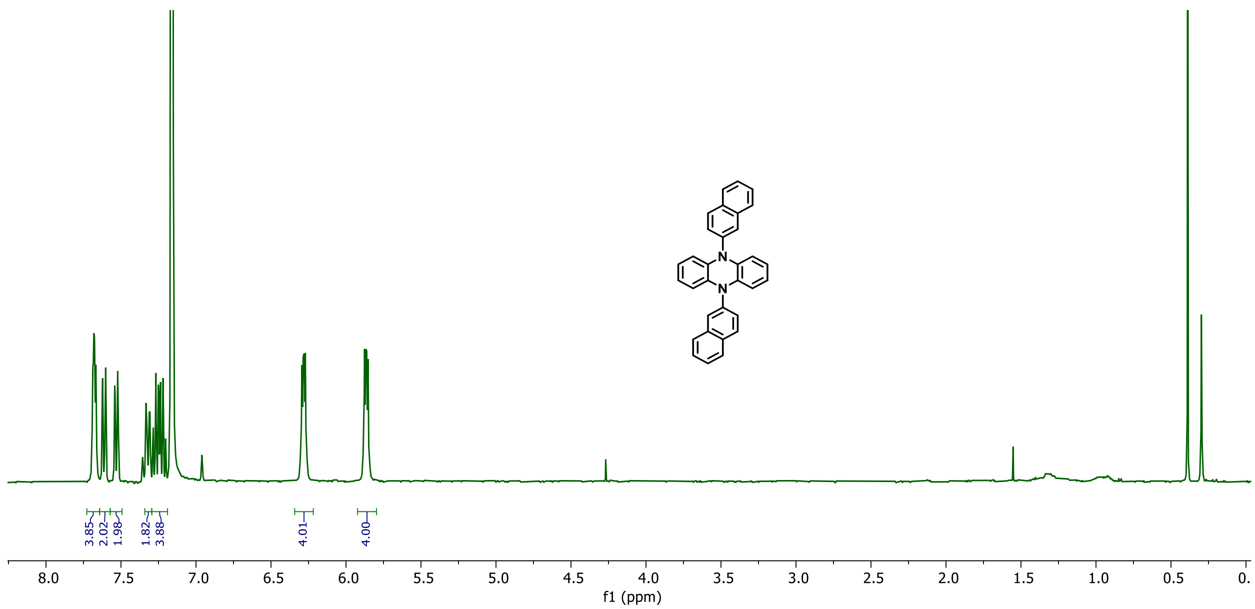


Figure S119. ^{1}H-NMR spectrum of PC **5** in C_6D_6 after recrystallization.

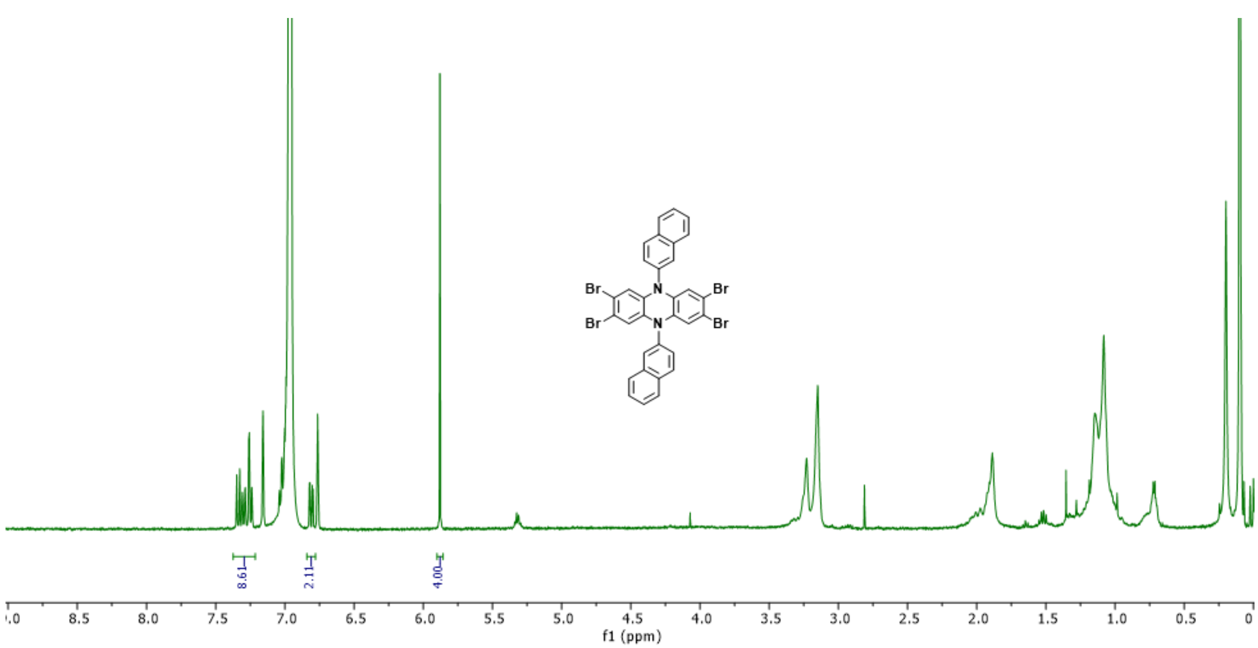


Figure S120. ^{1}H-NMR spectrum of unpurified **5-4Br** in C_6D_6.

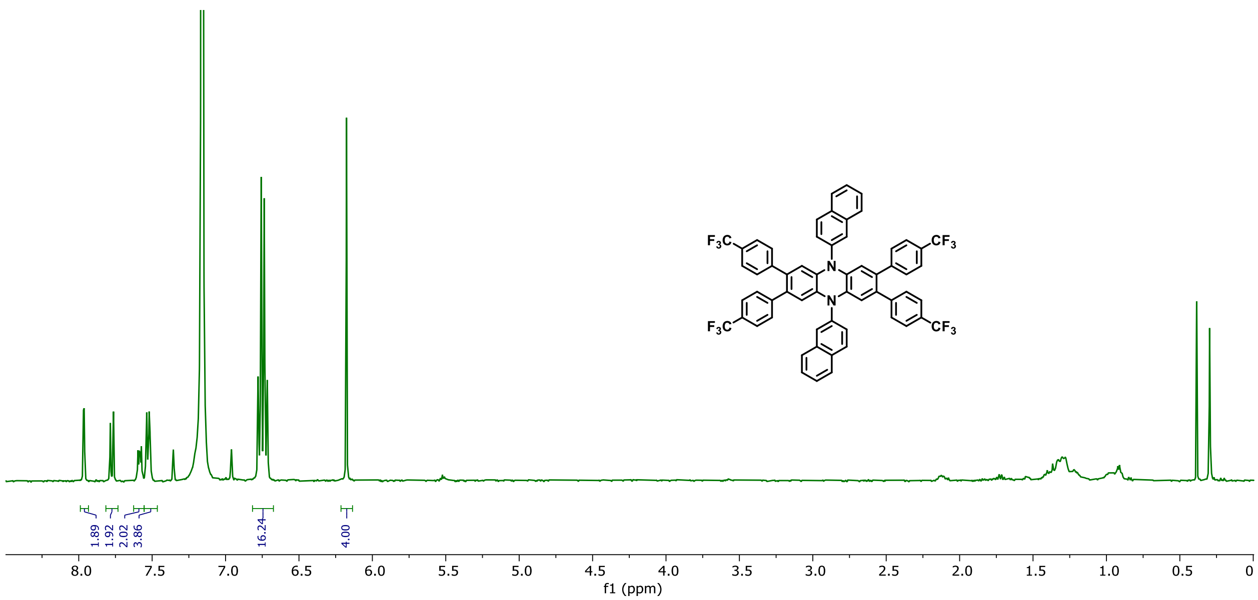


Figure S121. ^{1}H-NMR spectrum of PC **5a** in C_6D_6 after recrystallization.

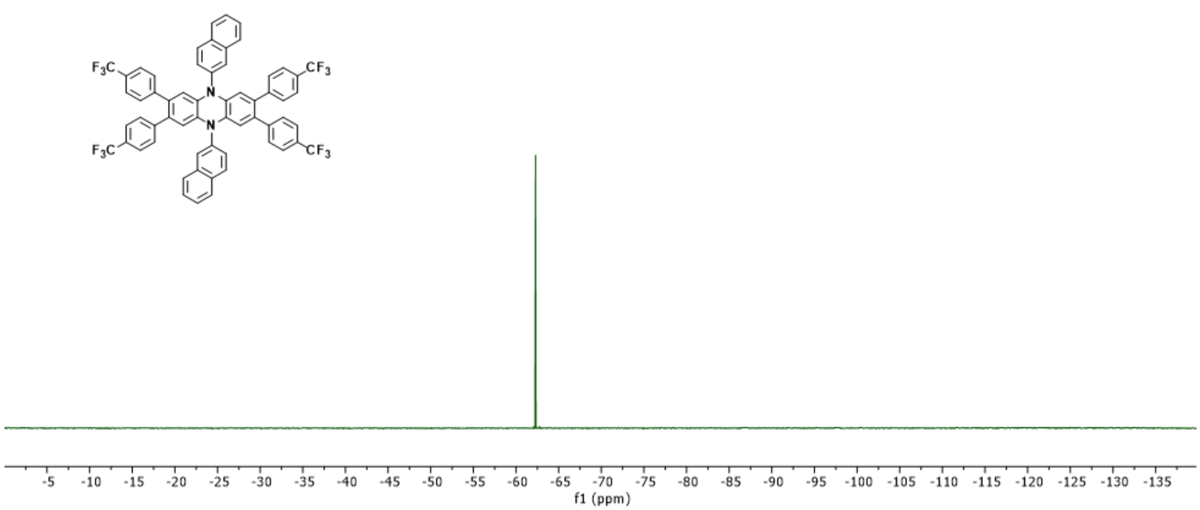


Figure S122. ^{19}F-NMR spectrum of **PC 5a** in C_6D_6 after recrystallization.

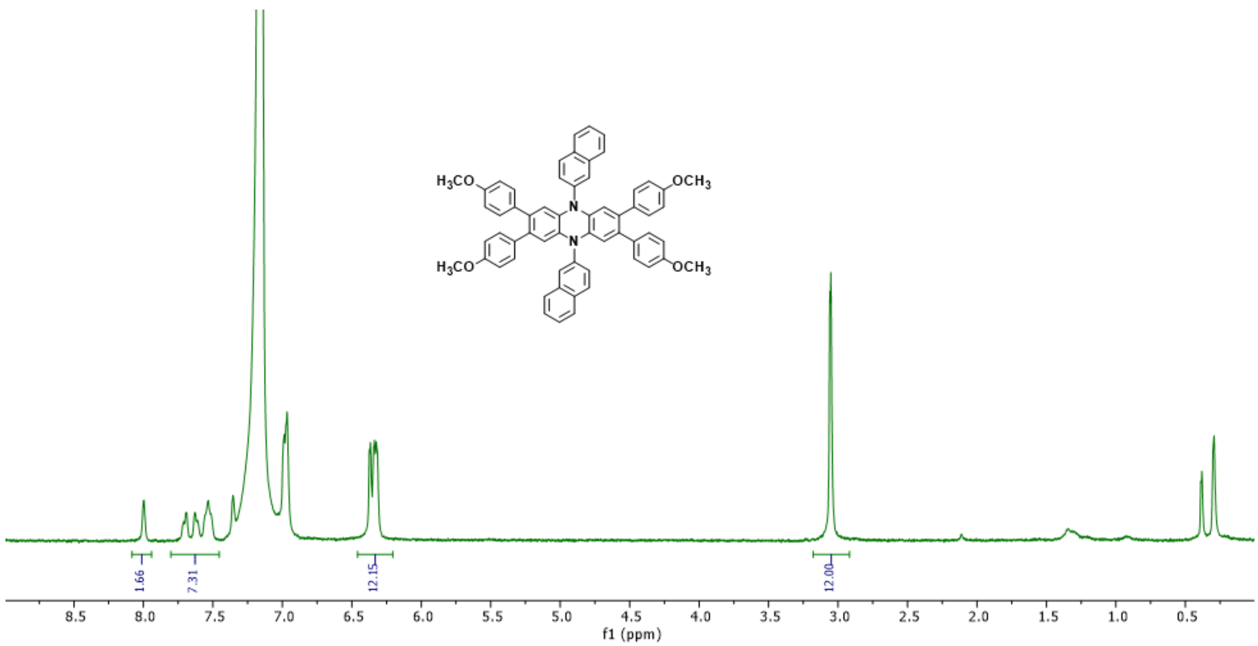


Figure S123. ^{1}H-NMR spectrum of PC **5b** in C_6D_6 after recrystallization.

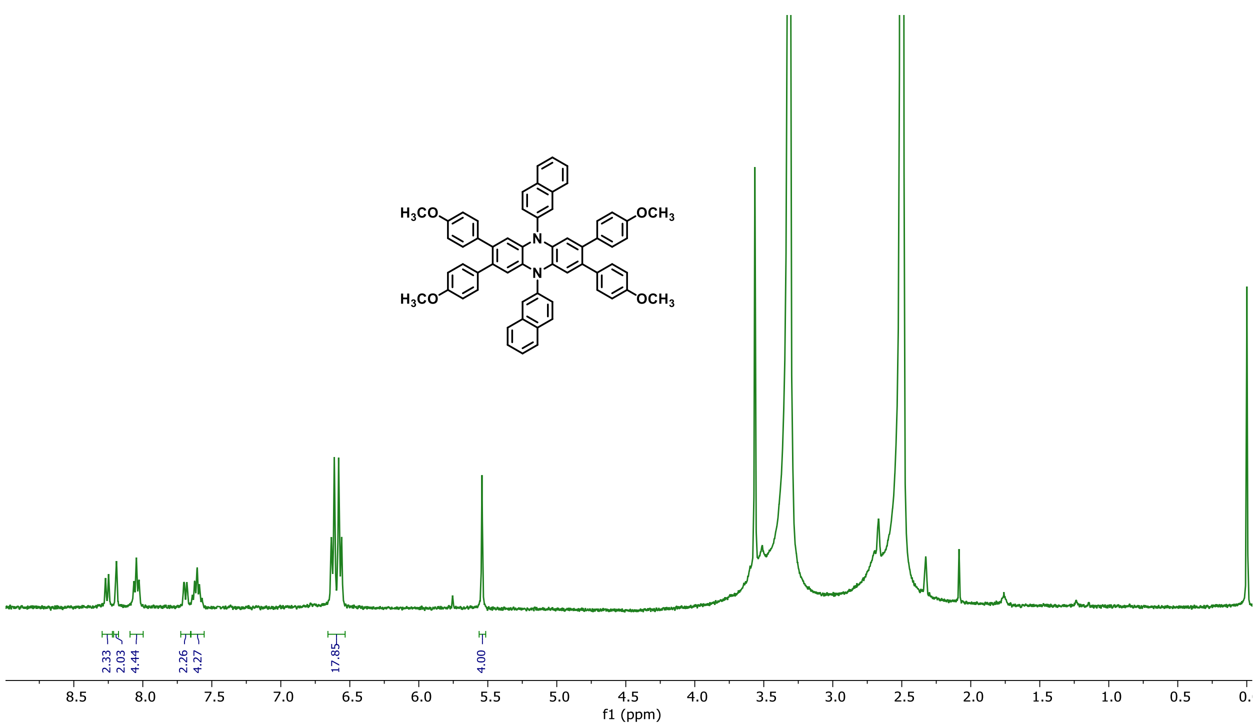


Figure S124. ^{1}H-NMR spectrum of PC **5b** in DMSO-d6 after recrystallization.

COMPUTATIONAL DETAILS

All calculations were performed using computational chemistry software package Gaussian 16. This work used the Extreme Science and Engineering Discovery Environment (XSEDE).

Reduction Potentials

Standard reduction potentials (E^0) of **3**, **4, 5, 3a, 3b, 4a, 4b** and **5a, 5b** were calculated following previously reported procedures.[5,6,7,8] A value of -100.5 kcal/mol was assumed for the reduction free energy of the standard hydrogen electrode (SHE). Thus, $E^{0*}_{T1,comp}$ ($^2PC^{•+}/^3PC^*$) was calculated as $E^{0*}_{T1,comp}$ = (-100.5 - ΔG_{red})/23.06 (V vs. SHE) where ΔG_{red} = G($^3PC^*$) – G($^2PC^{•+}$). $E^0_{ox,comp}$ ($^2PC^{•+}/^1PC$) was calculated as ΔG_{red} = G(^1PC) – G($^2PC^{•+}$).

For **3**, **4, 5, 3a, 3b, 4a, 4b** and **5a, 5b** Gibbs free energies of $^3PC^*$, $^2PC^{•+}$, and ^1PC were calculated at the unrestricted M06/6-311+G** level of theory in CPCM-H_2O solvent (single point energy) using geometries optimized at the unrestricted M06/6-31G** level of theory in CPCM-H_2O solvent. Values were converted from V vs. SHE to V vs. SCE by E^0 (V vs. SCE) = E^0 (V vs. SHE) – 0.24 V. The triplet energies ($E_{T1,comp}$) of DHPs and CE-DHPs were obtained by $E_{T1,comp}$(kcal/mol) = [G($^3PC^*$) – G(^1PC)] then converted from kcal/mol to eV by dividing $E_{T1,comp}$(kcal/mol) by 23.06. A CPCM-H_2O solvation model was chosen based on the results of previous work where the computed reduction potential approximates the experimental values within ~0.2 V to ~0.4 V.

Excited State Calculations (TD-DFT)

Using optimized ground state geometries, single point time dependent density functional theory (TD-DFT) calculations were performed using the rCAM-B3LYP/6- 31+G(d,p)/CPCM-DMA level of theory.[9] rCAM-B3LYP was chosen because it gave better λ_{max} predictions that are closer to experimental values in comparison to rωB97xd level of theory.[10]

Electrostatic Potential (ESP) Calculations

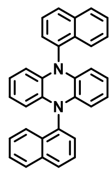
For geometries optimized using uM06/6-31G** (ground state singlets and excited state triplets), single point energy calculations with CHELPG[11] ESP population analyses were performed at uM06/6-31G** level of theory using a CPCM-DMAc solvation model. Total electron density of ^1PC and $^3PC^*$ were first plotted and then were mapped with ESP derived charges to show distribution of charges on the dihydrophenazine derivatives. Molecular orbitals of ^1PC (highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO)) and molecular orbitals of $^3PC^*$ (high lying singly occupied molecular orbitals (SOMOs)) were mapped then visualized.

Molecular Coordinates

All coordinates are reported as XYZ Cartesian coordinates. Energies (E_{0K} (not ZPE and thermally corrected)) are computed at uM06/6-311+G**/CPCM-H2O level of theory and are reported in parentheses. Energies are reported in Hartrees units.

PC 3 – (ground state)

(-1341.480383)



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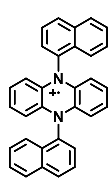
C	0.10437400	-6.85423600	-0.46515200
C	0.82601300	-6.85128900	0.72477600
C	0.80991900	-8.00140600	1.54129300
C	0.08422200	-9.11518900	1.12996800
C	-0.63151100	-9.10764700	-0.06859700
C	2.26948800	-6.87543500	3.15480600
C	2.28550900	-5.72529300	2.33831900
C	3.01109400	-4.61145600	2.74971300
H	3.02034300	-3.72623400	2.11958000
C	3.72686600	-4.61901300	3.94825100
C	3.71954300	-5.75049200	4.74412400
C	2.99120100	00	4.34468700
H	0.11702900	-5.96660800	-1.09176600
H	0.07489800	- DC6014600	
H	2.97867700	-7.76018800	4.97123800
N	1.57040300	-5.72795600	1.12746900
N	1.52509800	-7.99878000	2.75210100
H	-1.18992200	-9.99239500	-0.36275200
H	-1.17685000	-7.94909400	-1.79982100
H	4.28518800	-3.73422600	4.24246100
H	4.27242000	-5.77764700	5.67935400
C	1.50356600	-4.53359700	0.35095400
C	0.47380500	-3.58694800	0.61468100
C	2.42550400	-4.31319300	-0.64293200
C	-0.49338500	-3.77674800	1.63097000
C	0.42156300	-2.40543000	-0.18155600
C	2.36880600	-3.14091200	-1.42619500
H	3.19809200	-5.05938900	-0.81621400
C	-1.46942300	-2.83605400	1.84763900
H	-0.45042900	-4.67937900	2.23718500
C	-0.59962400	-1.45633700	0.06847500
C	1.38731400	-2.20982200	-1.19935400

H	3.10607300	-2.98318600	-2.20871900
C	-1.52480500	-1.66508400	1.05983200
H	-2.20722300	-2.99132800	2.63087700
H	-0.63440400	-0.55670600	-0.54370200
H	1.33458600	-1.30306500	-1.79945500
H	-2.30418100	-0.92975300	1.24294600
C	1.59195100	-9.19315300	3.52859900
C	0.67013700	-9.41347900	4.52261900
C	2.62159300	-10.13988500	3.26471900
C	0.72686100	-10.58575400	5.30589000
H	-0.10236400	-8.66721800	4.69600700
C	2.67385900	-11.32139900	4.06096200
C	3.58864700	-9.95017200	2.24828600
C	1.70825100	-11.51691900	5.07891400
H	-0.01030800	-10.74341800	6.08851800
C	3.69493100	-12.27057700	3.81078700
C	4.56457700	-10.89094900	2.03148000
H	3.54568200	-9.04753900	1.64207600
H	1.76101100	-12.42367200	5.67901700
C	4.61998000	-12.06191500	2.81928800
H	3.72973400	-13.17020300	4.42297100
H	5.30227200	-10.73574200	1.24813000
H	5.39927100	-12.79731100	2.63606800

PC 3 – (radical cation)

(-1341.309566)



C	-0.63362100	-7.94070200	-0.82768400
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C	0.84544500	-8.00671800	1.53988800
C	0.14076400	-9.14289800	1.11547500
C	-0.58833300	-9.10851200	-0.05389200
C	2.28701200	-6.89823400	3.12783900
C	2.25002500	-5.72006700	2.33953500
C	2.95469200	-4.58388100	2.76395600
H	2.92186200	-3.68218300	2.16154800
C	3.68378300	-4.61826500	3.93332700
C	3.72907500	-5.78607600	4.70711700

C	3.03983800	-6.91238200	4.31153000
H	0.02495000	-5.91124800	-1.03241200
H	0.17358700	-10.04459400	1.71788700
H	3.07051000	-7.81553200	4.91184100
N	1.51472300	-5.71269700	1.16681300
N	1.58074600	-8.01408700	2.71261200
H	-1.13011500	-9.99378800	-0.37198900
H	-1.21223000	-7.91835900	-1.74587400
H	4.22555500	-3.73298500	4.25143000
H	4.30767800	-5.80841700	5.62531000
C	1.46551000	-4.51150600	0.37009300
C	0.44011200	-3.56455400	0.62798700
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C	0.41406800	-2.39198900	-0.18319200
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H	3.16981100	-5.08498300	-0.76895100
C	-1.50369800	-2.77577200	1.82881800
H	-0.52492600	-4.62551600	2.25778000
C	-0.59658700	-1.42707400	0.04514300
C	1.39258900	-2.22035700	-1.19250300
H	3.11259300	-3.02098200	-2.18109300
C	-1.53469300	-1.61326700	1.02827500
H	-2.25186500	-2.91306100	2.60496500
H	-0.61202200	-0.53447400	-0.57721700
H	1.35634900	-1.31934800	-1.80163800
H	-2.30609600	-0.86632700	1.19502200
C	1.62992800	-9.21526300	3.50935500
C	0.69019600	-9.39897700	4.49110200
C	2.65531100	-10.16224200	3.25150100
C	0.72845400	-10.56411900	5.28400600
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C	2.68131900	-11.33478700	4.06271100
C	3.63469000	-9.99381000	2.24375000
C	1.70277800	-11.50637500	5.07201000
H	-0.01722500	-10.70569000	6.06055300
C	3.69195900	-12.29972800	3.83441900
C	4.59912800	-10.95109400	2.05072500
H	3.62040100	-9.10134200	1.62169700
H	1.73899100	-12.40736900	5.68116900
C	4.63008700	-12.11357800	2.85130000
H	3.70736600	-13.19231100	4.45680400
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PC 3 – (neutral triplet)

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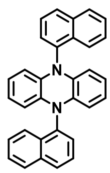

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C	0.86474100	-8.01124600	1.53108500
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C	-0.56128100	-9.11693000	-0.07005900
C	2.29685000	-6.90536300	3.11743500
C	2.23044400	-5.71553500	2.34860600
C	2.91534200	-4.57209200	2.78823900
H	2.85093000	-3.66541900	2.19497900
C	3.65656200	-4.60979100	3.94961300
C	3.73982100	-5.79329400	4.69910000
C	3.06649400	-6.92452800	4.29120400
H	-0.02047800	-5.88406000	-0.98830400
H	0.24427900	-10.06142400	1.68451300
H	3.11590000	-7.84261700	4.86803100
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N	1.59219700	-8.02466500	2.70868100
H	-1.08334500	-10.00948800	-0.40174000
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H	4.17865400	-3.71722200	4.28122000
H	4.33476800	-5.82197200	5.60707100
C	1.46459300	-4.50599900	0.36835100
C	0.43974100	-3.55687700	0.62637000
C	2.41823700	-4.33067500	-0.62864900
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C	0.41603100	-2.38042900	-0.19394300
C	2.37856000	-3.17894100	-1.41615000
H	3.17844900	-5.09433800	-0.77984600
C	-1.51265500	-2.75090400	1.83192900
H	-0.52135500	-4.61105000	2.25613400
C	-0.59442400	-1.41843700	0.03969000
C	1.39655600	-2.22055400	-1.20460200
H	3.12146500	-3.03681300	-2.19707600
C	-1.54096200	-1.60102400	1.03450600
H	-2.25814200	-2.88971800	2.61161000
H	-0.61222200	-0.52561700	-0.58406000
H	1.36404700	-1.32212700	-1.81903900
H	-2.30908500	-0.84797200	1.19652100

C	1.63083800	-9.22085500	3.51119700
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C	4.60795700	-10.97554600	2.04744300
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C	4.63638300	-12.12556300	2.84479800
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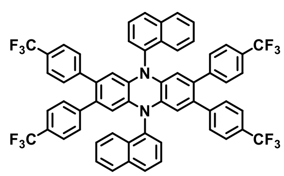
PC 3a – (ground state)

(-3613.344380)



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C	3.10597100	-4.66890200	2.69574500
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C	4.40955500	-5.83279700	6.06916500
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H	-3.23277500	-8.45987700	-1.39042700
C	-1.29851400	-7.35671100	-4.55275200
H	0.43444200	-7.28431300	-3.29018600
C	-2.66265900	-7.63182200	-4.62556400
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C	6.43993900	-6.25001000	9.82476900
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F	6.29997800	1.21036800	4.22787500
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F	-4.64164300	-7.79676900	-5.89844500
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PC 3a – radical cation

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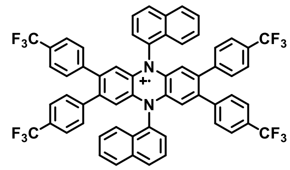

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C	2.16053100	-6.91404500	3.18500000
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C	2.98296000	-4.67724400	2.74046700
H	2.99646200	-3.79269200	2.11018300
C	3.66701600	-4.65992900	3.94604400
C	3.63065200	-5.81175900	4.77942800
C	2.87051300	-6.90336200	4.38911200
H	0.10683600	-6.01393600	-1.08650800
H	-0.03459300	-10.01100100	1.82004200
H	2.85446400	-7.78950300	5.01704200
N	1.55759200	-5.79692700	1.12826900
N	1.40390700	-8.00659300	2.80216400
C	1.64849600	-4.65569100	0.25085500
C	0.69458100	-3.61295800	0.38153600
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C	2.75659500	-3.52043300	-1.55588700
H	3.35703300	-5.44868100	-0.74060400
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H	-0.44183200	-4.46563400	2.02349300
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C	4.17663700	-2.82443600	5.57450600
C	5.86497200	-1.60711400	3.72691600
H	5.39169800	-3.24988000	2.42975700
C	4.81313600	-1.63518800	5.90138100
H	3.50842000	-3.29198200	6.29383800
C	5.65960500	-1.03080000	4.97840800
H	6.53174200	-1.13062700	3.01206100
H	4.64855300	-1.17672600	6.87163800
C	4.40586300	-5.91946900	6.03505400
C	5.76972200	-5.61290200	6.06768800
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C	6.49852600	-5.75972200	7.23960500
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H	2.72093800	-6.60962300	7.18943800
C	5.86488900	-6.20943300	8.39280800
H	7.55912700	-5.52841300	7.25509500
H	4.01756700	-6.86729700	9.28282200
C	-1.41238000	-10.38757500	-0.39304600
C	-1.21470000	-10.97888600	-1.64464300
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H	0.24009900	-7.19328300	-3.25906300
C	-2.90392600	-7.59419100	-4.46202600
H	-4.59780300	-8.27586500	-3.32415900
H	-1.05692800	-6.93567200	-5.35222200
C	6.61152200	-6.38072000	9.67728300
C	6.36528600	0.25062300	5.28913400
C	-3.40241500	-14.05465800	-1.35973300
C	-3.65079500	-7.42292700	-5.74636600
F	5.99617200	1.22896800	4.44804000
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F	-3.16340300	-14.48629300	-2.60108700
F	-3.03400100	-15.03286000	-0.51817300
F	-4.93545300	-7.77504000	-5.64654400
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PC 3a – neutral triplet

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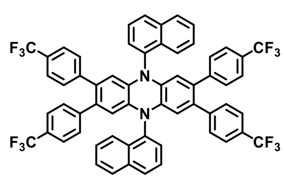

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C	3.09474900	-4.62990800	2.71119900
H	3.08645500	-3.74957100	2.07426000
C	3.73830600	-4.56098100	3.95063200
C	3.75246700	-5.78126900	4.78675000

C	2.92125200	-6.83954400	4.40794900
H	0.30668100	-6.03272100	-1.16468300
H	-0.09161500	-9.89331100	1.88535100
H	2.90571900	-7.73860100	5.01822000
N	1.68884200	-5.76961300	1.09241300
N	1.42279400	-7.92341900	2.83312800
C	1.79723900	-4.64853200	0.19953200
C	0.83893900	-3.60457600	0.29128200
C	2.81977700	-4.61653800	-0.71386900
C	-0.22045300	-3.60891800	1.23027700
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C	2.93645700	-3.52617400	-1.60074200
H	3.53080800	-5.43902500	-0.74420700
C	-1.11671300	-2.57022700	1.26775400
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C	0.02196300	-1.45571800	-0.54523300
C	2.02824200	-2.49910600	-1.54922000
H	3.74783400	-3.50893000	-2.32264000
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H	-1.92661600	-2.58134500	1.99255300
H	0.12366800	-0.62259900	-1.23823800
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H	-1.71620000	-0.67072100	0.41531700
C	1.30221400	-9.04931000	3.71836900
C	0.31189100	-9.05120600	4.66713400
C	2.22231900	-10.12348000	3.59070800
C	0.18504600	-10.14437100	5.54911500
H	-0.36676500	-8.20347900	4.72815700
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C	4.23287000	-3.27441700	4.40717000
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C	5.11413200	-0.73163700	5.27213100
H	5.54580400	-0.35613600	3.19167900
H	4.58511200	-1.40087300	7.24867400
C	4.68064600	-5.98292400	5.88521600
C	5.96439800	-5.39071700	5.89131000
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H	6.26592200	-4.76256600	5.05743300
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H	3.36046000	-7.25863600	7.04036700
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H	4.96025500	-7.67242700	8.84840900
C	-1.41843900	-10.30740800	-0.34487700
C	-1.22307400	-10.95825900	-1.56820500
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C	-2.78559100	-12.67204500	-0.93699600
H	-1.73466700	-12.63386700	-2.81363400
H	-3.68668200	-12.46278400	1.00768400
C	-1.27736600	-7.87382200	-2.16897600
C	-2.64837600	-8.14061200	-2.25643800
C	-0.59645300	-7.47100200	-3.32534900
C	-3.32172600	-8.01466500	-3.46339300
H	-3.19581400	-8.43904800	-1.36524500
C	-1.26363900	-7.34584900	-4.53342200
H	0.47194100	-7.27261900	-3.27469400
C	-2.62822400	-7.61905300	-4.60251900
H	-4.38731900	-8.21656700	-3.51751500
H	-0.72529800	-7.04038900	-5.42793800
C	7.43920800	-6.69443100	9.12206100
C	5.60827400	0.60715300	5.68817700
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F	4.99449600	1.59996100	5.01775300
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F	6.99327700	-6.13448900	10.26365100
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F	-3.30373600	-14.41242300	-2.44123200
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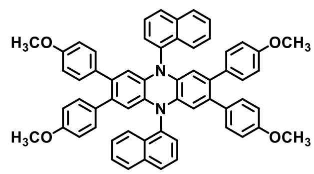
PC 3b – ground state



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C	-0.62983900	-9.17060500	-0.09412600
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C	2.94471100	-4.65951000	2.81767200
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C	3.69068100	-4.65556100	4.00675600
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C	3.02663200	-6.95289300	4.31866100
H	-0.02691500	-5.95320700	-0.98296100
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H	3.08770000	-7.87293400	4.89563200
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C	-0.39546300	-3.60347800	1.40390100
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C	2.69823200	-3.43725100	-1.48625800
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H	3.49409800	-3.40010300	-2.22515600

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H	0.03310900	-6.93140200	-3.23142100
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H	-4.70436100	-8.34529700	-3.21626900
H	-1.34180300	-6.58925800	-5.23296900
O	5.96201000	0.25903700	5.62393400
O	7.03240100	-6.50920800	9.31336500
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PC 3b – radical cation

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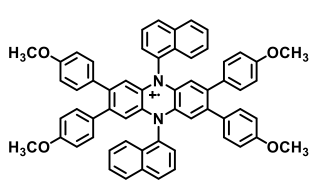

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H	0.01597600	-5.95023200	-1.00334200
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H	3.04473900	-7.87591400	4.91597500
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C	1.61524200	-4.61884300	0.30521700
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C	2.61286500	-4.55630700	-0.63419800
C	-0.38466300	-3.62652500	1.42000600
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C	2.70267300	-3.43829000	-1.48777400
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H	3.00892000	-6.91527500	7.13395700
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C	-3.63132600	-8.06371100	-3.18643600
H	-3.27422400	-8.70499400	-1.18018700
C	-1.76719300	-7.04879900	-4.34245900

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C	-3.09852600	-7.46660600	-4.33602900
H	-4.67402700	-8.37063300	-3.19780700
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O	7.00834600	-6.48664000	9.29242600
O	-2.89789000	-14.04895400	-1.70532300
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H	7.58476500	0.50936300	4.34685500
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H	7.00138000	1.91423600	5.27727600
C	6.51981900	-7.09276300	10.47354100
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H	7.35038600	-7.10473800	11.18058100
C	-3.63191800	-14.85639900	-0.80509700
H	-3.01620100	-15.16731700	0.04872500
H	-4.52401700	-14.33554200	-0.43422800
H	-3.94061400	-15.74040300	-1.36465500
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H	-2.62774800	-7.30587800	-6.99206600
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PC 3b – neutral triplet

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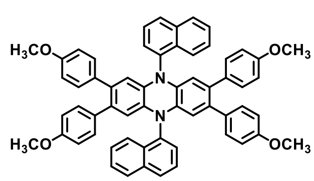

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C	3.77321100	-5.86405200	4.79666500
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C	4.50085900	-1.75726600	6.34523500

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C	5.99166700	-5.42615400	5.88698200
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H	6.25765700	-4.75858700	5.07101300
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PC 4 – ground state

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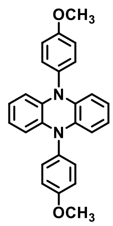

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C	1.82028100	-9.13278100	3.61145500
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H	3.48256200	-10.08699700	2.63913300
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H	0.06238900	-10.40732300	6.22371500

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C	0.80569000	-3.48091300	0.74945500
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H	0.11499200	-3.63619100	1.57552700
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C	0.68868000	-0.03541900	-1.63650200
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PC 4 – radical cation

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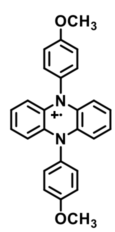

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H	-1.10410200	-9.82343000	-0.18201800
H	-1.13961200	-7.75161400	-1.56324200
H	4.88129100	-3.88241800	4.08095900
H	4.89867400	-5.94552700	5.47546600
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H	-0.09229400	-12.69336200	6.62897500
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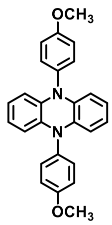
PC 4 – neutral triplet

(-1263.259559) 

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C	2.65229000	-6.91507900	3.13472200
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C	3.46309400	-6.93720800	4.28821200
H	0.17582200	-5.81580100	-0.91757400
H	0.31735900	-9.97089200	1.82750300
H	3.46540900	-7.82800700	4.91087900
N	1.83205400	-5.68543000	1.19605400
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C	2.80301000	-10.15651600	3.38971900
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H	0.16315900	-8.48571100	4.71560700
C	1.82622900	-11.40924900	5.20738500
H	0.11947200	-10.48688900	6.17321300
C	1.79384300	-4.49035000	0.40375700
C	0.90532200	-3.47841700	0.73410000
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C	2.58966800	-3.20901500	-1.46424100
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C	1.69454100	-2.18306600	-1.13632500
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H	-1.10336100	-9.86817000	-0.17477500
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PC 4a – ground state

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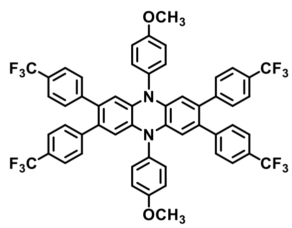

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F	-2.55162300	-2.86845700	9.94008400
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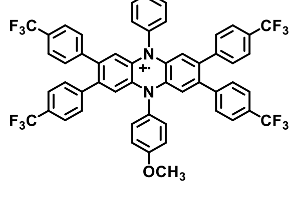
PC 4a – radical cation



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PC 4a – neutral triplet

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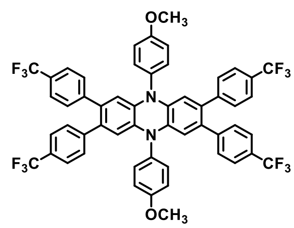

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PC 4b – ground state

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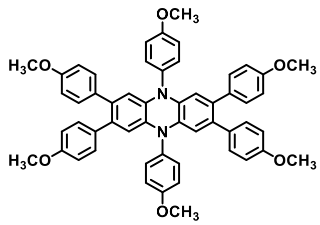

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C	0.60707800	5.24471300	5.06547500
H	-1.49020300	5.01090800	5.54975300
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C	-5.44384500	-1.74563700	-4.54209400
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C	-7.77672600	-1.15598100	-4.72279800
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C	-2.58018700	-4.40942100	-3.96775500
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C	-3.99439200	-6.25850600	-4.57808200
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H	-5.94729000	-6.26672300	-3.69565300
O	5.23150900	-0.11449000	6.20748800
O	0.87549600	6.35916300	5.79068300
O	-8.84438500	-1.05839600	-5.55392600
O	-4.29488600	-7.41525700	-5.22030400
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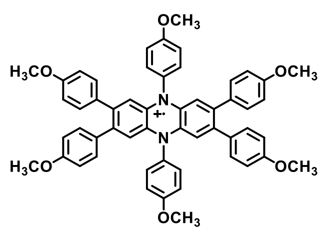
PC 4b – radical cation

(-2644.878597)



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C	0.93033800	0.62137100	2.59116600

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H	-0.62435200	-3.72724200	1.42912300
C	2.13293800	-4.55841700	-0.37710500
H	3.00938000	-3.36007600	-1.92504200
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N	-0.71001600	-1.47655000	0.01141200
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C	3.05197000	0.53143600	5.71788600
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O	-8.74159400	-0.98944200	-5.63374700
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H	0.32323300	7.87296200	6.88887800
H	-0.93835400	7.29888000	5.76599200
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H	7.19041600	-0.52949900	6.52214000

H	6.47370000	-1.47996100	5.19351800
C	-3.23039100	-7.91034500	-6.11591900
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H	-2.91693500	-7.22582100	-6.91469400
C	-9.97388300	-0.52758100	-5.11494500
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PC 4b – neutral triplet

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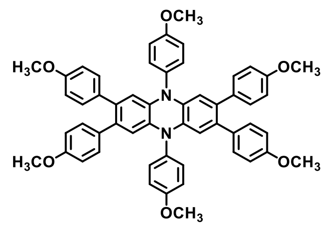

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C	-3.95861700	-0.48002900	-1.40029600
C	-4.21338800	-1.50085400	-2.30693800
C	-1.41872000	0.63587300	1.06333600
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H	-1.43919900	-3.37181000	-1.67455600
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C	1.29052100	-2.36079100	-1.06576600
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C	2.23742100	-3.35958100	-1.20649400
H	1.33260900	-1.46230600	-1.67762000
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C	0.35405000	7.57604000	5.55938900
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PC 5 – ground state

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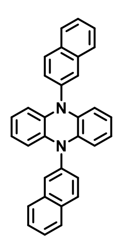

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PC 5 – radical cation

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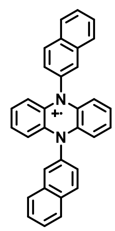

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C	-0.39782600	-5.45430700	2.52472000
C	-1.62007500	-4.86287400	2.17270400
H	-1.62305700	-3.88543500	1.70219500
C	-2.80535400	-5.52084400	2.42381400
C	-2.80107900	-6.78262300	3.03341600
C	-1.61151900	-7.38170000	3.38960900
H	3.23028700	-3.79176300	1.86182700
H	3.24521700	-8.26624900	4.01813700
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N	0.80582900	-4.81564200	2.28525500
N	0.81436500	-7.30969700	3.48924300
C	0.80179100	-3.51623000	1.66003700
C	0.84971100	-3.44590700	0.25144700
C	0.75270000	-2.39426300	2.44474300
H	0.88799300	-4.36566200	-0.32719100
C	0.74939100	-1.11612600	1.83803600
H	0.71637200	-2.48402800	3.52918600
H	5.36946500	-7.12334100	3.52262900

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C	0.84719400	-2.21554700	-0.35295900
C	0.79749000	-1.02598300	0.41533700
C	0.79420600	0.25415100	-0.18947600
C	0.74567000	1.38941400	0.57949100
H	0.74365900	2.36758900	0.10562000
C	0.69815100	1.29813400	1.98871900
H	0.66015700	2.20657900	2.58412300
C	0.69987600	0.07268800	2.60534200
H	0.83091000	0.31854000	-1.27523600
H	0.66348400	-0.00553300	3.69015500
H	0.88372200	-2.13785900	-1.43750600
C	0.81783600	-8.60241600	4.12816200
C	0.77841400	-8.67266800	5.49588500
C	0.86102100	-9.75714300	3.31806300
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H	0.89153200	-9.64893100	2.23655800
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H	0.70821200	-9.15660100	8.14627100
C	0.82411600	-12.37791800	5.96780400
C	0.78523500	-12.46816900	7.33639700
H	0.71272700	-11.38773500	9.21293000
H	0.85640700	-13.27465500	5.35192400
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PC 5 – neutral triplet

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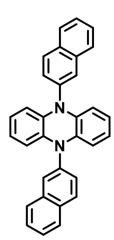

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C	2.00679900	-6.57406400	3.46953700
C	3.23604800	-7.16905500	3.80136200

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C	-0.40678300	-6.62537500	3.38530100
C	-0.40746900	-5.33696300	2.78699400
C	-1.63109800	-4.72301600	2.47369900
H	-1.61361800	-3.73421600	2.02699900
C	-2.81966500	-5.36805200	2.73871400
C	-2.81753600	-6.65086700	3.31309700
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H	3.18253600	-3.63599100	2.18681700
H	3.24616300	-8.15814500	4.24760900
H	-1.62927800	-8.26204000	4.07632200
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C	0.79378400	-3.49817300	1.73038000
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C	0.75803900	-2.26944800	2.40860700
H	0.85798100	-4.56350200	-0.13008300
C	0.76168800	-1.05954400	1.66365600
H	0.72905600	-2.24582100	3.49737400
H	5.35901600	-6.96820500	3.82623100
H	5.33756800	-4.69235200	2.80744100
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C	0.80111900	-1.12991700	0.22338300
C	0.80537300	0.07284300	-0.50866000
C	0.77284100	1.31926100	0.12786600
H	0.77739800	2.23162200	-0.46620100
C	0.73466500	1.38640100	1.51578600
H	0.70915300	2.35277600	2.01711400
C	0.72906500	0.21218700	2.27510600
H	0.83550000	0.01440100	-1.59737700
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H	0.86442100	-2.45523000	-1.49451300
C	0.81432600	-8.56592700	4.20783400
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H	0.73329300	-7.94201000	6.24950700
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H	0.91748400	-11.75319700	3.04637200

C	0.75333000	-11.68010800	7.89828700
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H	0.72169100	-11.88370200	8.96547800
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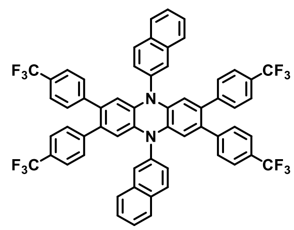
PC 5a – ground state

(-3613.340800)



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N	1.58697000	0.95838300	-0.57831900
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C	2.68728500	1.40790600	0.16641800
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C	2.98848100	7.21819400	-0.82855000
H	3.12495000	5.38238700	-1.93788700
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C	2.56214900	7.84595000	0.36797200
H	3.47357400	7.82265600	-1.59269800
C	1.69335200	9.03048200	2.76284300

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C	2.32642200	9.80992500	1.76766900
H	1.36197800	9.50260000	3.68427900
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C	1.33255800	-0.44519300	-0.66555900
C	1.88637400	-1.18095400	-1.68165300
C	0.51449000	-1.05933300	0.31316600
C	1.65094900	-2.57484900	-1.76721900
H	2.51528000	-0.69063200	-2.42341600
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H	2.40008600	-5.31530500	-3.65101100
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C	7.12080100	4.57774400	3.71156900
H	5.01390300	4.37569800	3.35484800
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F	7.14093600	-3.60823200	5.18874300
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PC 5a – radical cation

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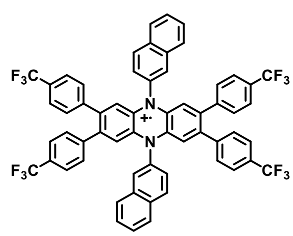

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C	-0.22843200	4.08467600	-1.23352900
C	-1.34771300	3.61424000	-1.90318200
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H	-0.11403200	5.15415600	-1.08272200
N	1.46000600	0.95475400	-0.27007500
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C	3.48508200	0.56003600	1.00519200
C	2.76631200	2.82593400	0.52513600
C	4.60217200	1.02742700	1.67963100
H	3.29643000	-0.50891900	0.97041100
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C	2.69762800	5.78965100	-0.95816200
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H	1.08438900	5.21730700	2.00261500
C	2.89149500	7.14303700	-0.85999600
H	3.03682000	5.22553900	-1.82355700
C	1.33237800	7.88521900	2.46205600
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H	3.39654500	7.68313500	-1.65796000
C	1.53173300	9.23965100	2.54745100
H	0.82816500	7.34469400	3.26069400
C	2.63250200	9.26165300	0.39510800
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H	1.18566500	9.78657900	3.42057300
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C	1.82256600	-1.17641200	-1.37881600
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C	1.60600100	-2.57190200	-1.47024100
H	2.44882100	-0.67087900	-2.11215600
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H	2.81503400	-2.85688800	-3.23925000
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C	6.05553600	3.01346500	2.34242400
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H	4.97203000	4.43095900	3.54848300
C	8.46413100	3.12931400	2.51207700
H	7.42182000	1.74027200	1.25776200
C	8.34670100	4.17773200	3.42425000
H	7.00571400	5.46306000	4.50811800
H	9.44944100	2.77539000	2.21805500
C	5.47517900	0.03399800	2.34272600
C	5.85012300	0.18896300	3.68426700
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H	5.51978600	1.06340800	4.24014900
C	6.67773800	-2.06653300	2.27266200
H	5.62295300	-1.22469500	0.60220400
C	7.03584800	-1.90176500	3.60439800
H	6.89849100	-0.65481300	5.35718400
H	7.00779000	-2.94352500	1.72439800
C	-2.62096400	1.61807700	-2.85687000
C	-2.94090900	2.08748700	-4.13803500
C	-3.33877300	0.54088200	-2.33105900
C	-3.95628400	1.49378900	-4.86811000
H	-2.38021000	2.91403700	-4.56797900
C	-4.36267500	-0.05325000	-3.05845900
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C	-1.94296400	5.73630500	-3.06895300
C	-3.70670900	4.44333900	-2.05168500
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C	-4.63202500	5.39252800	-2.44910400
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H	-5.68365400	5.26746000	-2.20139800
C	-5.24709700	7.50626500	-3.59277800
C	-5.76122500	-0.18653300	-5.14505500
C	7.86371900	-2.92164900	4.31926300
C	9.60036600	4.75008800	4.00452900
F	-4.72627500	8.53780900	-4.26278800
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F	-6.17000200	6.93963800	-4.38489900
F	-5.28742200	-0.68588800	-6.29682600
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F	8.17067800	-3.96833800	3.54797600
F	7.22621500	-3.39406800	5.40129800
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PC 5a – neutral triplet

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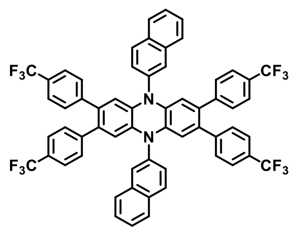

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C	0.70704600	3.23492800	-0.59453400
C	-0.27667400	4.11784700	-1.05227800
C	-1.39250000	3.68946100	-1.75789300
H	-0.65947000	0.36508400	-1.81327200
H	-0.18616700	5.17227800	-0.80595400
N	1.48227400	0.95497200	-0.35370700
N	1.81661000	3.67517300	0.10365900
C	2.61007500	1.37850400	0.32761500
C	3.54521800	0.49506200	0.84549200
C	2.78453300	2.80105500	0.56704900
C	4.66923900	0.91124500	1.56316600
H	3.33777200	-0.56871900	0.76919500
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H	4.11404200	4.30414200	1.26663600

C	1.98951300	5.08379900	0.32944600
C	1.56304400	5.63591800	1.50882000
C	2.60956900	5.86118300	-0.67317600
C	1.74145500	7.01980600	1.74475200
H	1.08947900	5.01057800	2.26411300
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H	2.93263000	5.37883900	-1.59290500
C	1.31679200	7.63300300	2.94837400
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C	1.24295200	-0.45477000	-0.49677700
C	1.81788500	-1.14640000	-1.53017000
C	0.41130000	-1.08968300	0.45187200
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C	0.16477200	-2.43275700	0.33635700
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H	-0.47458000	-2.93877000	1.05683100
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C	6.22450000	2.91915100	2.02269500
C	6.32200100	4.18569500	2.64117500
C	7.43736400	2.24257900	1.74933700
C	7.54583700	4.74730600	2.95885700
H	5.41406700	4.72376900	2.90563400
C	8.65911900	2.80777600	2.05501800
H	7.40914400	1.27396300	1.25725100
C	8.72668900	4.06346400	2.66792000
H	7.58664900	5.71717500	3.44698000
H	9.57702900	2.27575300	1.81119000

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H	5.92249100	1.19891300	3.97008700
C	6.28566000	-2.36449700	2.50347000
H	5.17942800	-1.65623600	0.82366600
C	6.85575800	-2.05358100	3.73881100
H	7.15011600	-0.51799100	5.22187600
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C	-2.41294800	4.69852400	-2.11154400
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H	-5.77161800	5.25804000	-1.96474100
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PC 5b – ground state

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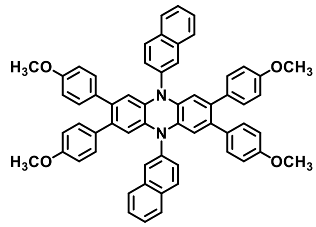

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N	1.10438900	0.85275800	-0.35561700
N	1.02288500	3.41302200	-1.46460100
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C	4.20525000	0.80590200	-2.44217400
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C	4.18765900	2.10640500	-2.96620200
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C	1.01575800	4.74305300	-1.98134800
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H	-0.01191600	4.19611300	-3.76931000
C	1.62634200	7.06124200	-1.71008900
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C	-0.12866400	6.62537700	-4.98471300
C	1.04913700	7.36741600	-2.96811100
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C	2.23346200	-3.64337800	3.64932200
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C	1.07188500	-4.41580800	1.67573800
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H	5.04316700	0.06464800	-4.92749300
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H	8.64844200	2.98158400	-4.06542600
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C	-6.61144000	8.08807600	1.08317900
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H	-7.28392400	8.75891800	1.62022000
H	-5.92766800	8.68508900	0.46532700
C	-5.84118900	-0.82021100	5.50200500
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C	8.74099800	-3.82084800	-2.89883500
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PC 5a – cation radical

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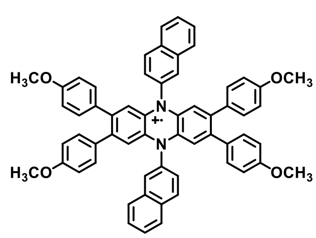

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N	1.09808100	0.85713500	-0.36798300
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C	4.17830200	0.79854800	-2.42824200
H	3.15800400	-0.61195100	-1.18905900
C	3.11757800	2.96856900	-2.61043300
C	4.17104500	2.12729500	-2.94439600
H	3.12258500	3.98909800	-2.98167300
C	1.00973100	4.74290400	-1.99396200
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H	-0.03766300	4.14373300	-3.75738600
C	1.60943100	7.05390900	-1.76202300
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C	5.19743500	-0.20219700	-2.80269400
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H	3.89098600	3.56179200	-5.20753900
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O	8.30576700	4.32265600	-6.08217600
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PC 5b – neutral triplet

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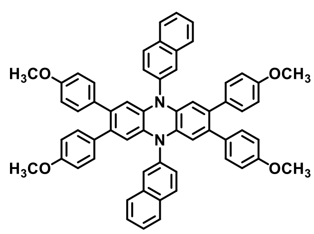

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C	1.06417200	3.52336300	-0.98316000
C	0.38930800	3.64283900	-2.19071700
H	-0.22675000	0.33355600	-2.70264200
H	1.40341200	4.42796300	-0.48525900
N	1.00551000	-0.11579100	-0.38181300
N	1.93489800	2.18988400	0.86131900
C	1.66477800	-0.23674900	0.82886000
C	1.94185300	-1.46555800	1.41622100
C	2.13717200	0.97263300	1.48806700
C	2.61532500	-1.59781500	2.62948500
H	1.69904700	-2.36445900	0.85475300
C	2.73664800	0.86034000	2.73619400

C	2.94131600	-0.36072800	3.37916000
H	2.97186700	1.77797300	3.26989100
C	2.50512100	3.36483500	1.45430200
C	1.73187400	4.17534400	2.24475200
C	3.86647900	3.64982600	1.21273100
C	2.29361500	5.33491400	2.83274200
H	0.68497200	3.92954900	2.41698200
C	4.43208400	4.76548500	1.77458400
H	4.44177900	2.97547200	0.58253200
C	1.53131100	6.20266200	3.65094600
C	3.66800500	5.63406500	2.59426200
H	5.47946400	5.00101200	1.59605700
C	2.10387600	7.31865800	4.20905200
H	0.48336000	5.96732700	3.82799000
C	4.22804400	6.79271300	3.18413800
C	3.46407700	7.61630700	3.97333100
H	1.51034400	7.97918900	4.83602000
H	5.27704000	7.01718300	2.99874000
H	3.90483400	8.50350800	4.42100700
C	0.50459600	-1.30439200	-1.00938400
C	1.24626300	-1.91650300	-1.98656200
C	-0.74103800	-1.82266400	-0.59453000
C	0.76296500	-3.09110500	-2.61139000
H	2.20552800	-1.49601600	-2.28505000
C	-1.22682800	-2.96221100	-1.18377300
H	-1.29300200	-1.30626500	0.18746400
C	1.49403500	-3.75117400	-3.62790900
C	-0.49508400	-3.62418900	-2.20152000
H	-2.18657300	-3.37368500	-0.87731400
C	1.00149300	-4.89030900	-4.21435200
H	2.45308300	-3.33736800	-3.93433300
C	-0.97512000	-4.80047900	-2.82635900
C	-0.24424500	-5.41939200	-3.80993900
H	1.56973500	-5.39062400	-4.99436900
H	-1.93578800	-5.20371600	-2.51074800
H	-0.62292100	-6.32207900	-4.28271900
C	0.15455000	5.00121600	-2.72486100
C	1.18811400	5.93906600	-2.77002200
C	-1.11631400	5.41330400	-3.15800800
C	0.98510000	7.23828000	-3.22954700
H	2.18720300	5.64375400	-2.45321100
C	-1.33590400	6.69931900	-3.61431900
H	-1.94646400	4.71048900	-3.12447400
C	-0.28512000	7.62318900	-3.65650500

H	1.82097400	7.93077300	-3.25582100
H	-2.32210600	7.02116400	-3.94033500
C	-0.74278200	2.46200900	-4.15436500
C	-1.90376700	1.72027100	-4.38146900
C	-0.19652000	3.16335700	-5.24172900
C	-2.51399500	1.67093700	-5.63279200
H	-2.35707000	1.17687900	-3.55381800
C	-0.78742800	3.12321100	-6.49043000
H	0.71498300	3.74109200	-5.10176800
C	-1.95425400	2.37778700	-6.69626400
H	-3.42128800	1.08837200	-5.76088600
H	-0.35865000	3.65828300	-7.33438800
C	3.07355600	-2.92243900	3.03379300
C	4.30980800	-3.12137600	3.68932300
C	2.32120900	-4.07680500	2.75042100
C	4.76086800	-4.38530200	4.01789300
H	4.93630200	-2.26219800	3.91664800
C	2.76139800	-5.35272700	3.08034300
H	1.34505000	-3.97330300	2.27914400
C	3.99197900	-5.51584000	3.72040400
H	5.72241300	-4.52734700	4.50650200
H	2.13221000	-6.20703100	2.84786400
C	3.33610700	-0.35602700	4.78249400
C	2.86862600	-1.31690300	5.69946400
C	4.18297200	0.64882500	5.30256100
C	3.20423200	-1.27965800	7.04830300
H	2.19942300	-2.10083000	5.35340100
C	4.52721800	0.69365100	6.63865800
H	4.60201400	1.39508000	4.62956000
C	4.04030000	-0.27164700	7.52936000
H	2.80173800	-2.03781300	7.71411400
H	5.19149300	1.46517000	7.02164800
O	-0.60028400	8.85626300	-4.12424100
O	-2.45988700	2.40561800	-7.95409200
O	4.44021700	-0.14504800	8.82245700
O	4.51857200	-6.71222600	4.09384900
C	0.43065700	9.82049900	-4.18055900
H	1.24338500	9.50375000	-4.84754900
H	-0.01892500	10.73311700	-4.57493700
H	0.84577000	10.02589900	-3.18492000
C	-3.63443300	1.66213100	-8.20587800
H	-4.47465100	2.01556200	-7.59356500
H	-3.87484700	1.80881900	-9.26001100
H	-3.48186400	0.59106000	-8.01792400

C	3.77152800	-7.87367300	3.80348900
H	3.60701700	-7.98971700	2.72360400
H	4.35636800	-8.72014500	4.16753400
H	2.79770400	-7.86664800	4.31169400
C	3.97332700	-1.10377700	9.74657500
H	4.29988600	-2.11759300	9.47775100
H	4.39983500	-0.83737200	10.71518600
H	2.87752400	-1.09285400	9.82264500

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