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Materials and Methods

Purchased Chemicals:

C-N Coupling: 9,9-Dimethyl-9,10-dihydroacridine was purchased from Ark Pharm. Bromobenzene, 2-bromonaphthalene, 1-bromonaphthalene, 4-bromobenzonitrile, and 4-bromoanisole were purchased from VWR. Bis(dibenzylideneacetone) palladium(0) and 1M tri-*tert*-butylphosphine in toluene were purchased from Sigma Aldrich. Dicyclohexylphosphino-2,6-diisopropoxybiphenyl (RuPhos) and chloro-(2-dicyclohexylphosphino-2,6-diisopropoxy-1,1-biphenyl_[2-(2-aminoethyl)phenyl]palladium(II)-methyl-t-butyl ether adduct (RuPhos precatalyst) were purchased from Sigma Aldrich. Sodium tert-butoxide was purchased from Sigma Aldrich. Dioxane was purified using an mBraun MB-SPS-800 solvent purification system and kept under nitrogen atmosphere. Anhydrous 99.8% toluene was purchased from Sigma Aldrich and kept under nitrogen atmosphere.
Bromination: *N*-bromosuccinimide was purchased from VWR. HPLC grade THF was purchased from VWR.
Suzuki Coupling: Tetrakis(triphenylphosphine) palladium(0) was purchased from Sigma Aldrich. Potassium carbonate was purchased from VWR. 4-biphenylboronic acid was purchased from TCI America. 4-cyanobenzeneboronic acid and 4-methoxyphenylboronic acid were purchased from Sigma Aldrich.
Polymerizations: All monomers and initiators were purchased from Sigma Aldrich. Anhydrous *N,N*-dimethylacetamide (DMAc), dimethylsulfoxide (DMSO), and anhydrous benzene were purchased from Sigma Aldrich. Tetrahydrofuran (THF) and *N,N*-dimethylformamide (DMF) were purified using an mBraun MB-SPS-800 solvent purification system and kept under nitrogen atmosphere.

Chemical Preparation and Storage:

All reagents for catalyst synthesis were used as received. All monomers and initiators for polymerizations were dried with calcium hydride overnight, distilled under vacuum, and freeze-pump-thawed 3 times. All monomers and initiators were stored under inert atmosphere at -10 ºC and in the dark.

Instrumentation for Photocatalyst and Precursors Characterization:

Structural analysis was performed by a Varian 400 MHz NMR Spectrometer. UV-visible spectroscopy was carried out using a Cary 5000 UV-Vis-NIR spectrophotometer from Agilent. Steady state photoluminescence spectroscopy and absolute fluorescence quantum yields measurements were performed using a FS5 Spectrofluorometer from Edinburgh Instruments. Time-resolved spectral emission measurements were performed on an LP980 spectrometer from Edinburgh Instruments equipped with a Nd:Yag laser

operating at 355 nm and an intensified CCD camera for detection. Cyclic Voltammetry experiments were conducted using a Gamry Interface 1010B potentiostat. For full experimental details see each characterization section below.

Instrumentation for Polymer Characterization:

Monomer conversion was determined by a Varian 400 MHz NMR Spectrometer. Molecular weight analysis was performed using gel permeation chromatography (GPC) coupled with multi-angle light scattering (MALS) using an Agilent HPLC system fitted with one guard column and 3 PL-gel mixed C columns running THF as eluent at 1.0 mL/minute. The detectors used for GPC were a Wyatt Technology TrEX differential refractometer (RI) and a Wyatt Technology miniDAWN Treos light scattering detector (MALS). A dn/dc value of 0.065 was used for all poly(butyl acrylate) analyses and 0.080 for poly(methyl methacrylate). dn/dc values for all other polymers was determined through analysis with a known sample concentration.

Batch Reactor Supplies:

Batch polymerizations were performed in a 100 mL beaker wrapped in aluminum foil with a 12-inch strip of 12 V 365 nm LEDs purchased from LED Lighting Hut (365nm UV LED Light Strip, 60 SMD5050 LEDs/M, 5M/reel, DC12V Input from ledlightinghut.com). Polymerizations using 380 nm and 455 nm light sources were performed with 12 V LED strips from Creative Lighting Solutions (CL-FRS5050WPDD-5M-12V-UV and CL-FRS5050WPDD-5M-12V-BL from creativelightings.com).

Flow Reactor Supplies:

Flow polymerizations were performed using a Hepatochem Photoredox Temperature Controlled reactor with a 2 mL flow attachment. The light source used was a 18W 365 nm EvoluChem bulb (part no. HCK1012-01-011 from Hepatochem). The flow tubing was 1/16 in O.D. and 0.003 in I.D. with PFA as the tubing material. The flow rate was controlled using a Pump 11 Elite Syringe Pump from Harvard Apparatus with a 50 mL stainless steel syringe with 1/16 tubing fitting. See detailed reactor set-up and design details in polymerization section.

Computational Details

All calculations were performed using computational chemistry software package Gaussian 09 ver. D01.[1] We acknowledge the use of computational resource provided by XSEDE - Comet supercomputer.

a) Reduction Potentials

Standard reduction potentials (E^0) were calculated following previously reported procedures.[2,3,4,5] A value of -100.5 kcal/mol was assumed for the reduction free energy of the standard hydrogen electrode (SHE). Thus, $E^0 = (-100.5 - \Delta G_{red})/23.06$ (V vs. SHE); for E^0 ($^2PC^{\bullet+}/^3PC^*$), $\Delta G_{red} = G(^3PC^*) - G(^2PC^{\bullet+})$ while for E^0 ($^2PC^{\bullet+}/^1PC$), $\Delta G_{red} = G(^1PC) - G(^2PC^{\bullet+})$.

The Gibbs free energies of $^3PC^*$, $^2PC^{\bullet+}$, 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 unrestricted M06/6-31+G** level of theory in CPCM-H_2O solvent.

To reference to the Saturated Calomel Electrode (SCE), E^0 (vs. SHE) is converted to E^0 (vs. SCE) using E^0 (vs. SCE) = E^0 (vs. SHE) - 0.24 V. Triplet energies (in eV) of PCs were obtained by [$G(^3PC^*) - G(^1PC)$, in kcal/mol]/23.06.

Based on the comparison of our large experimental and computational data set, the choice of CPCM solvation model is justified as the computed reduction potential closely approximates the experimental values. For example, the computed ground state oxidation potentials between the $^2PC^{\bullet+}/^1PC$ redox couple is typically within ~0.2 to 0.3 V from the experimental values.

b) Excited State Calculation

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.[6] rCAM-B3LYP was chosen because it gave better λ_{max} predictions that are closer to experimental values in comparison to rωB97xd level of theory. TD-DFT calculations (with our chosen CAM-B3LYP method) corroborate experimental observations that UV-vis absorption becomes increasingly red-shifted with higher molar absorptivity as the aryl conjugation at the core position is increased.

Summary of PC Properties

Table S1: Summary of experimental photophysical and electrochemical data for PCs 1-7.

PC	$\lambda_{max,abs}$ (nm)[a]	ε ($M^{-1}cm^{-1}$)	$\lambda_{max,em}$ (nm)[b]	$E_{S1,exp}$ (eV)[c]	$E_{T1,77\ K,exp}$ (eV)[c,d]	$E_{1/2}$ ($^2PC^{\bullet+}/^1PC$) (V vs. SCE)[e]	$E^{0*}_{S1,exp.}$ ($^2PC^{\bullet+}/^1PC^*$) (V vs. SCE)[f]	$E^{0*}_{T1,exp.\ 77\ K}$ ($^2PC^{\bullet+}/^3PC^*$) (V vs. SCE)[e,f]
1	361	46,270	487	2.55	2.34	0.76	-1.79	-1.58
2	340	38,560	509	2.44	2.33	0.71	-1.73	-1.62
3	382	44,340	458	2.71	2.39	0.90	-1.81	-1.49
4	360	49,780	453	2.74	2.34	0.77	-1.98	-1.57
5	361	31,500	443	2.80	2.35	0.76	-2.04	-1.59
6	363	43,120	444	2.79	2.34	0.75	-2.04	-1.59
7	355	50,140	535	2.32	2.37	0.82	-1.50	-1.55

[a]Absorption wavelength measured using ultraviolet-visible spectroscopy in DMF. [b]Emission wavelength measured using steady-state fluorescence spectroscopy in DMF. [c]Singlet and triplet energies were calculated using the maximum wavelength of emission. [d]Spectral emission measured at 77 K after 1 ms gate-delay. . [e]All measurements were performed in a 3-compartment electrochemical cell with an $Ag/AgNO_3$ reference electrode in MeCN (0.01 M) and 0.1 M NBu_4PF_6 electrolyte solution. DMF was used to solvate the PCs. Platinum was used at the working and counter electrodes. [f]Excited state redox potentials were calculated using the singlet energies estimated from the maximum wavelength of emission and the experimentally measured $E_{1/2}$.

Table S2: Summary of computationally-predicted photophysical and electrochemical data for PCs 1-7.

PC	$\lambda_{max,abs}$ (nm)	f	$E_{T1,calc}$ (eV)	E^0_{ox} ($^2PC^{\bullet+}/^1PC$) (V vs. SCE)	$E^{0*}_{T1,calc.}$ ($^2PC^{\bullet+}/^3PC^*$) (V vs. SCE)
1	326	1.689	2.41	0.55	-1.86
2	311	1.211	2.36	0.42	-1.94
3	343	1.446	2.43	0.74	-1.69
4	328	1.655	2.30	0.53	-1.77
5	329	1.748	2.29	0.54	-1.75
6	329	1.741	2.28	0.50	-1.78
7	324	1.749	2.39	0.61	-1.78

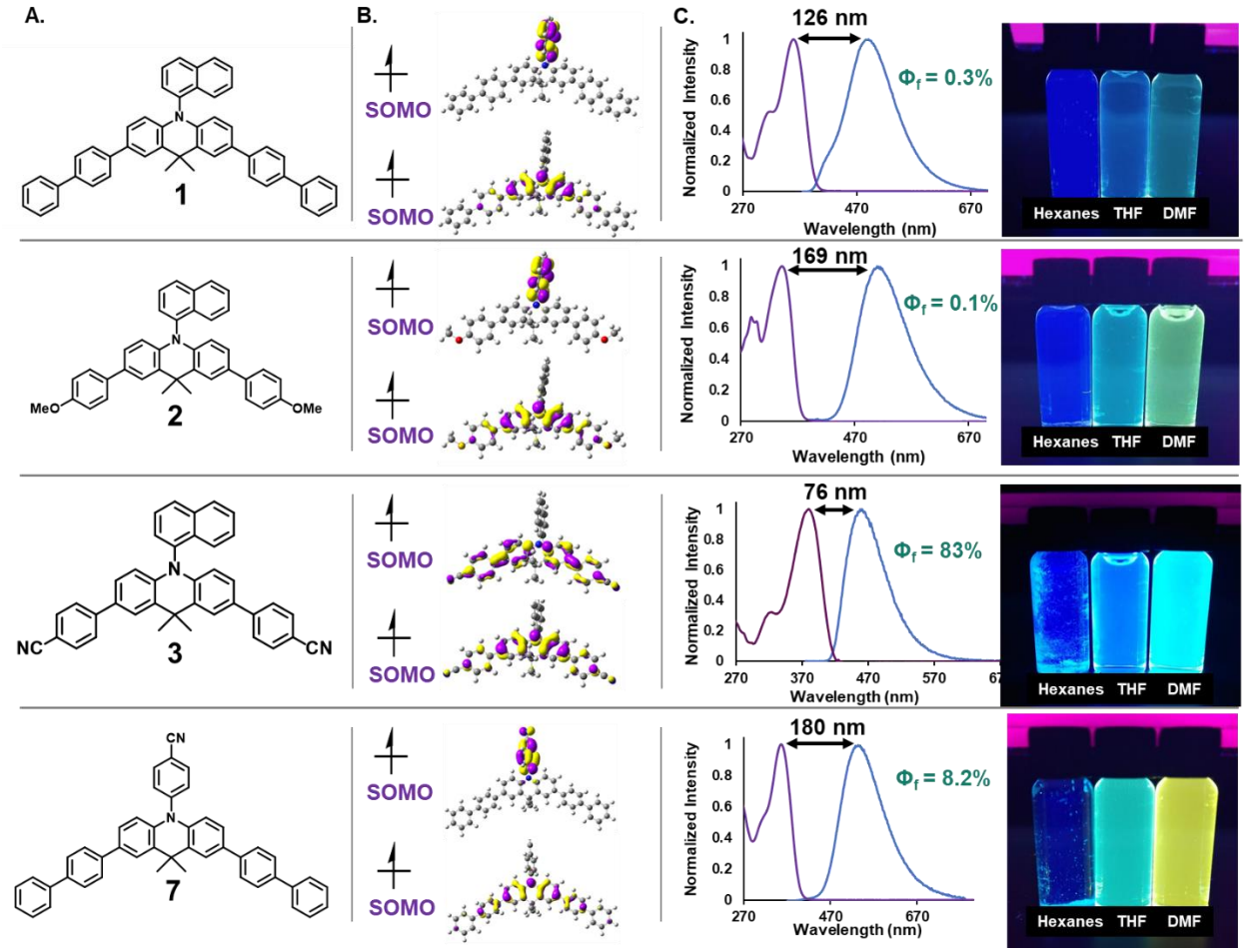
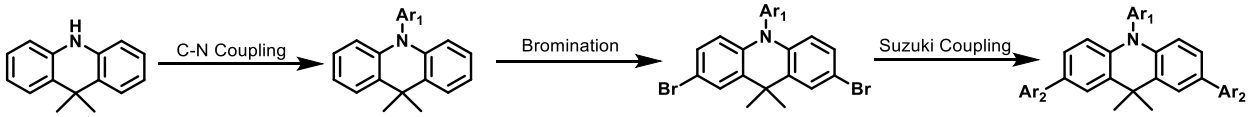


Figure S1. Higher-lying SOMOs (top) and low-lying SOMO (bottom) for PCs 1, 2, 3, and 7 (b). Overlays of the absorption profiles (purple) and emission profiles (blue) with the experimentally determined Stokes Shifts for each PC (c). Photographs of the PCs dissolved in solvents with increasing polarity (d). All CV, absorption, and emission experiments were performed in DMF.

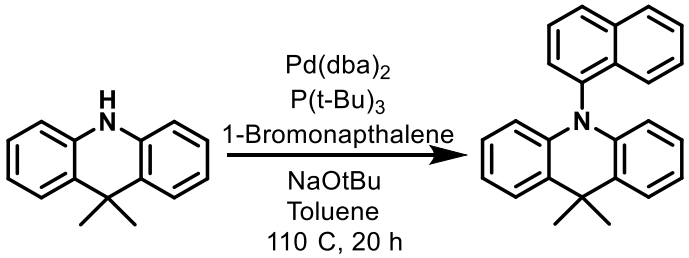
Photocatalyst Synthesis

General Synthetic Scheme:



Scheme 1: The general synthetic scheme for PCs 1-7 follows a previously developed synthetic strategy.[7,8]

Synthesis of 9,9-dimethyl-10-(naphthalen-1-yl)-9,10-dihydroacridine



A storage tube was loaded with 5.0 g (23.9 mmol, 1 eq.) 9,10-Dihydro-9,9-dimethylacridine, 7.42 g 1-bromonaphthalene (36.0 mmol, 1.5 eq.), 137.5 mg of Bis(dibenzylideneacetone)palladium(0) (0.89 µmol, 1 mol%), 717 µL of 1M in toluene Tri-*tert*-butylphosphine (0.717 mmol, 3 mol %), 6.0 g sodium *tert*-butoxide (71.7 mmol), and 100 mL toluene under nitrogen atmosphere. The solution was heated to 110 ºC. After 20 hours, the brown-orange liquid was poured directly through a silica plug and rinsed with toluene. All blue fluorescent portions were collected and concentrated to 50 mL volume via rotary evaporation. The product was precipitated by slow addition of ~75 mL of ethyl acetate. The product, a white solid, was isolated by vacuum filtration and washed with ethyl acetate and methanol. The product was dried overnight under vacuum to yield 5.88 g (73.4% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.06 – 7.95 (m, 2H), 7.68 (ddd, *J* = 8.4, 4.1, 3.0 Hz, 2H), 7.57 – 7.46 (m, 4H), 7.36 (ddd, *J* = 8.3, 6.8, 1.2 Hz, 1H), 6.96 – 6.78 (m, 4H), 6.03 (dd, *J* = 8.1, 1.4 Hz, 2H), 1.85 (s, 3H), 1.75 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.51, 137.71, 135.47, 131.84, 129.71, 129.04, 128.80, 128.67, 127.10, 126.93, 126.68, 126.54, 125.60, 123.78, 120.47, 114.20, 77.34, 77.02, 76.70, 36.03, 33.02, 31.89. HRMS (ESI) calculated for (M+H)+ for $C_{25}H_{21}N$, 336.17468; Found, 336.17468.

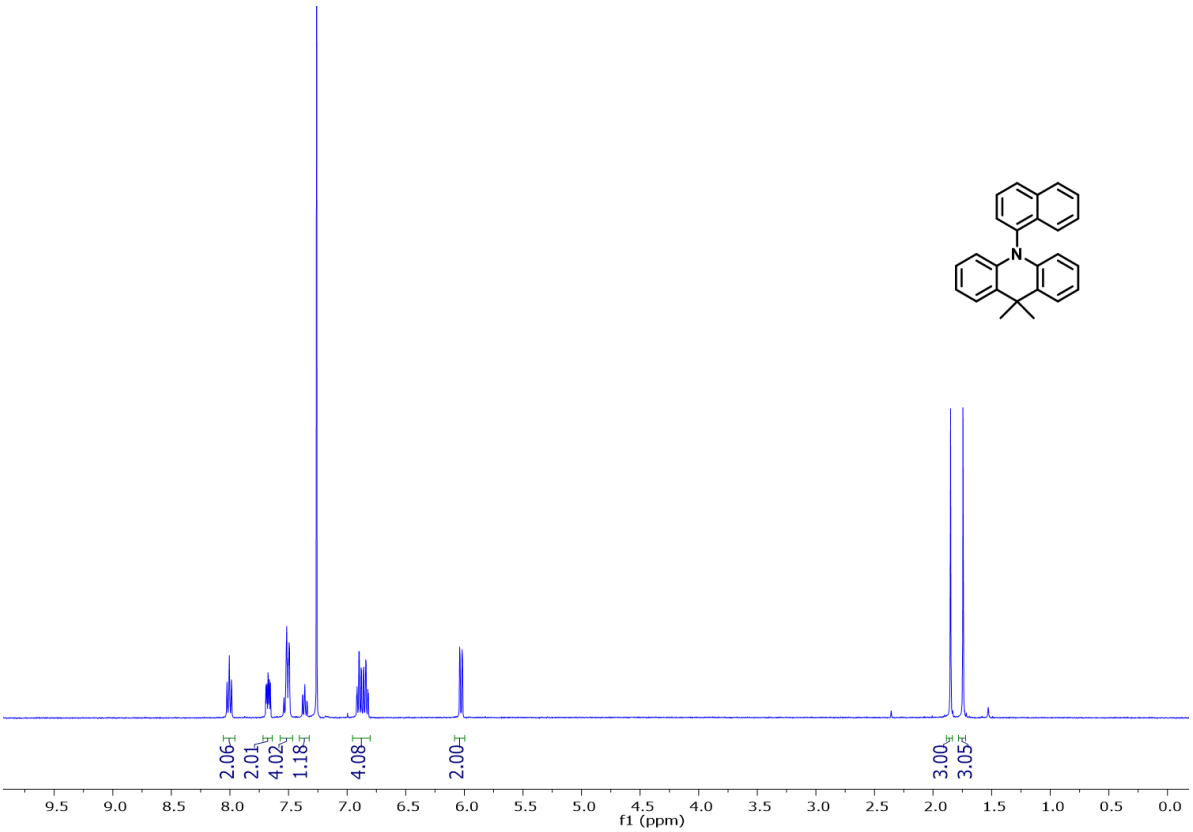


Figure S2: ^{1}H NMR spectrum of 9,9-dimethyl-10-(naphthalen-1-yl)-9,10-dihydroacridine in $CDCl_3$.

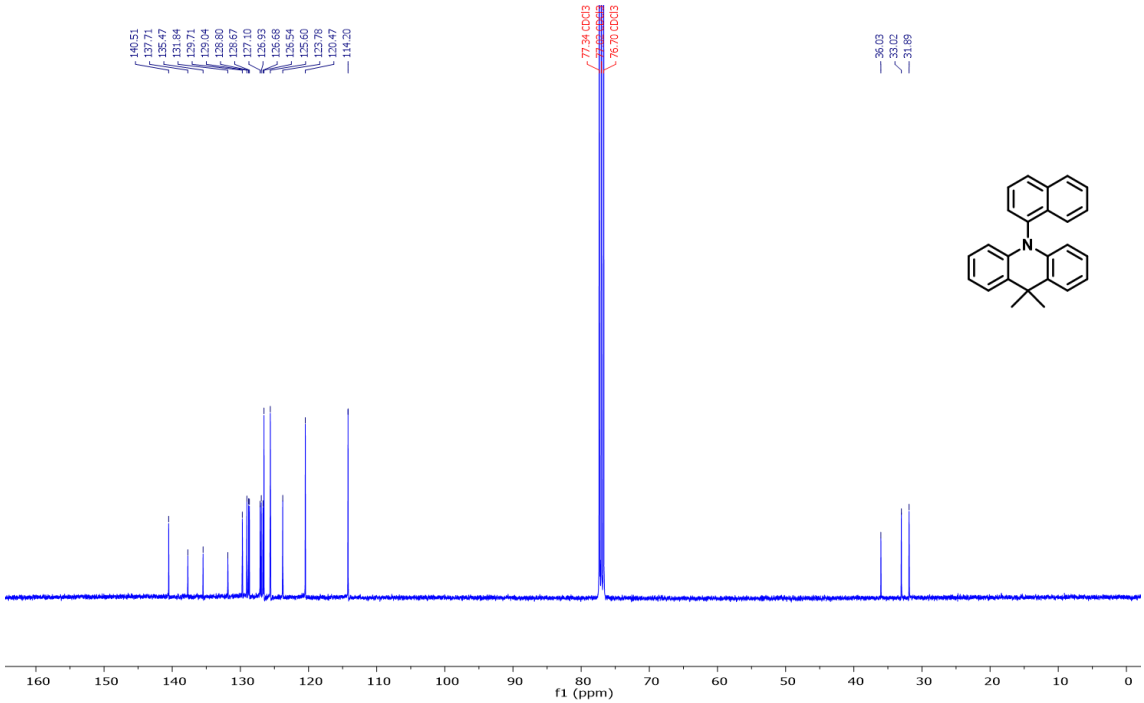
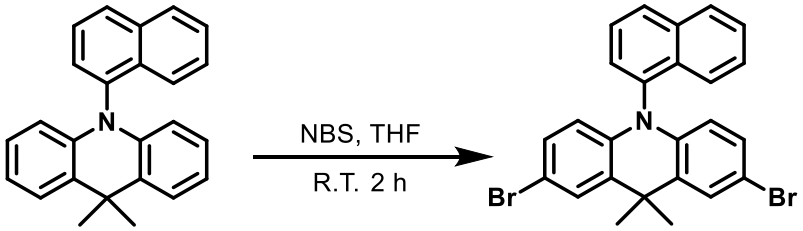


Figure S3: ^{13}C NMR spectrum of 9,9-dimethyl-10-(naphthalen-1-yl)-9,10-dihydroacridine in $CDCl_3$.

Synthesis of 2,7-dibromo-9,9-dimethyl-10-(naphthalen-1-yl)-9,10-dihydroacridine



5.0 g of 9,10-dihydro-9,9-dimethyl-10-(1-napthalenyl)-acridine (14.9 mmol, 1.0 eq.) was dissolved in 200 mL THF under ambient atmosphere. 5.83 g of *N*-Bromosuccinimide (32.8 mmol, 2.2 eq.) was slowly added to make a light brown solution. The reaction then stirred for 2 hours. The solution was then concentrated via rotary evaporation, washed with water 3 times, and dried with magnesium sulfate. The product was recrystallized using DCM layered with methanol at -10 ºC overnight. The product was isolated by filtration and dried under vacuum to give a pale brown solid, which was used without further purification. Yield: 6.4 g, 87%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.08 – 7.97 (m, 2H), 7.67 (dd, *J* = 8.3, 7.2 Hz, 1H), 7.59 – 7.50 (m, 4H), 7.47 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.44 – 7.36 (m, 1H), 6.93 (dd, *J* = 8.8, 2.3 Hz, 2H), 5.90 (d, *J* = 8.8 Hz, 2H), 1.82 (s, 3H), 1.69 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 139.32, 136.71, 135.50, 131.37, 131.18, 129.54, 129.35, 128.88, 128.72, 128.42, 127.44, 126.94, 126.91, 123.24, 116.04, 113.27, 36.35, 32.87, 31.30.

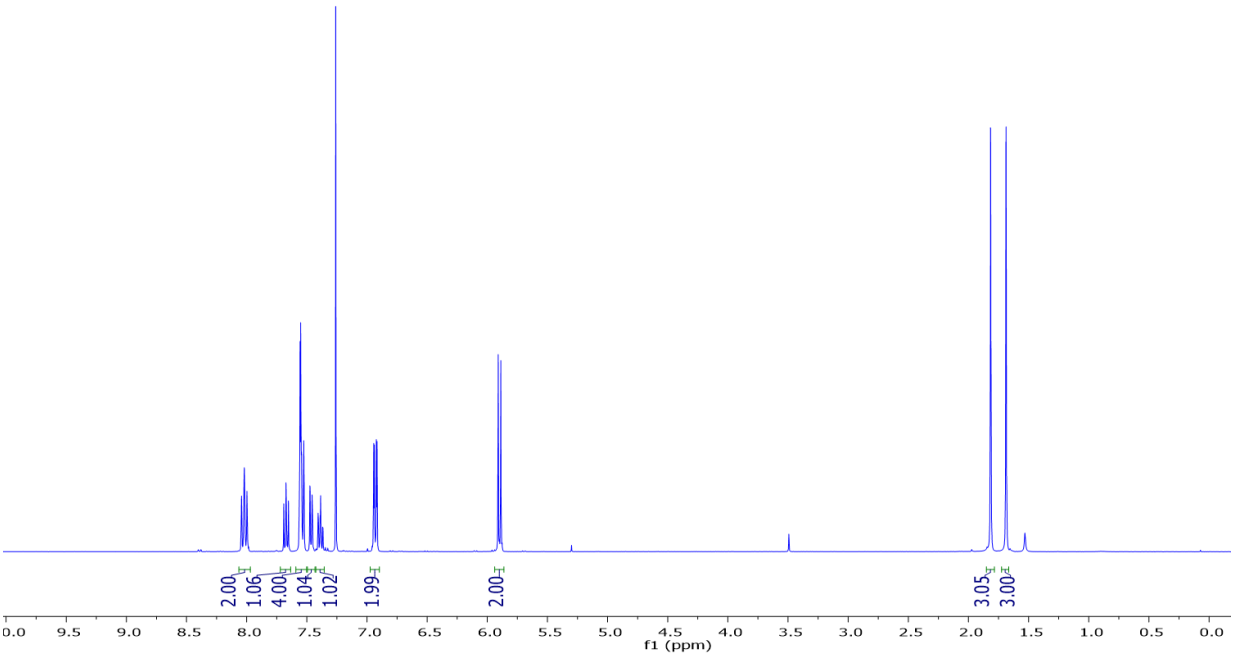


Figure S4: ^{1}H NMR spectrum of 2,7-dibromo-9,9-dimethyl-10-(naphthalen-1-yl)-9,10-dihydroacridine in $CDCl_3$.

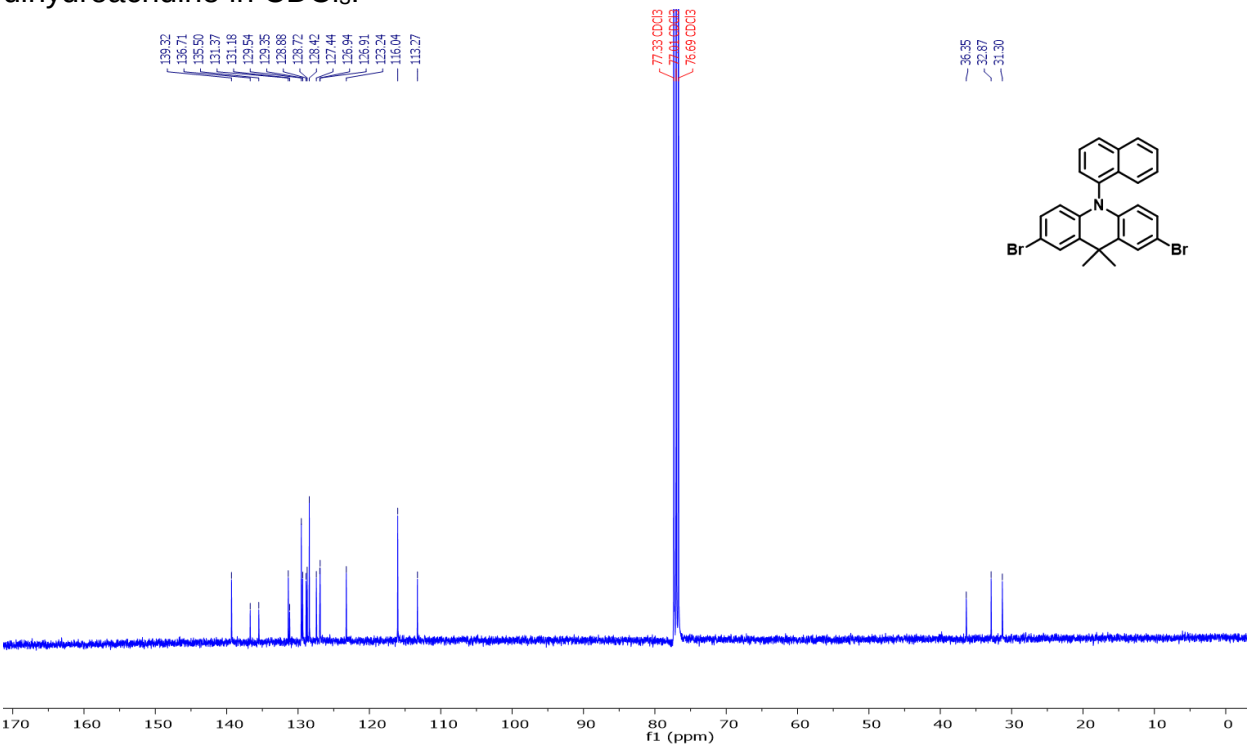
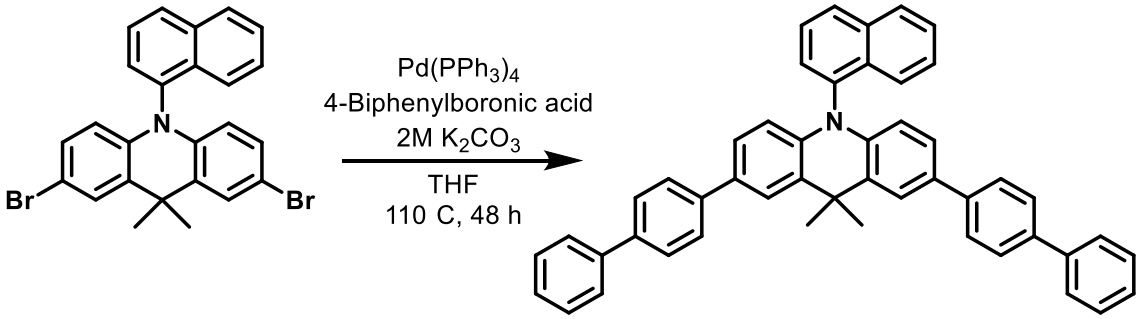


Figure S5: ^{13}C NMR spectrum of 2,7-dibromo-9,9-dimethyl-10-(naphthalen-1-yl)-9,10-dihydroacridine in $CDCl_3$.

Synthesis of 2,7-di([1,1'-biphenyl]-4-yl)-9,9-dimethyl-10-(naphthalen-1-yl)-9,10-dihydroacridine



2.0 g 2,7-dibromo-9,10-dihydro-9,9-dimethyl-10-(1-napthalenyl)-acridine (4.1 mmol, 1 eq.) was loaded into a storage tube. 3.2 g 4-Biphenylboronic acid (16.2 mmol, 4 eq.) was added under ambient conditions. The flask was brought into a nitrogen-filled glovebox. Then, 0.468 g Tetrakis(triphenylphosphine)palladium(0) (0.41 mmol, 10 mol %) was added. 60 mL of THF was added to produce a yellow solution. The flask was taken out of the glovebox, where 45 mL of degassed 2M K_2CO_3 was added using a long needle and syringe. The biphasic solution was then sealed and heated to 110 ºC for 48 hours. At that time, the solution was cooled to room temperature and concentrated on rotovap to produce a reddish-brown oil. The crude mixture was redissolved in DCM then passed through a silica plug. The yellow filtrate was collected and concentrated, then purified by column chromatography with hexanes: ethyl acetate ramping from 100:0 to 70:30. The product, a white solid, was then recrystallized with DCM/MeOH at -25 ºC to give 1.61 g of a fluffy white solid with 62% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.12 – 8.01 (m, 2H), 7.82 (d, *J* = 2.1 Hz, 2H), 7.79 – 7.71 (m, 2H), 7.68 – 7.54 (m, 14H), 7.45 (dd, *J* = 8.4, 7.1 Hz, 5H), 7.38 – 7.30 (m, 2H), 7.16 (dd, *J* = 8.5, 2.1 Hz, 2H), 6.16 (d, *J* = 8.5 Hz, 2H), 2.01 (s, 3H), 1.91 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 140.84, 140.15, 139.85, 139.28, 137.48, 135.52, 132.98, 131.71, 130.09, 129.05, 128.96, 128.79, 127.44, 127.33, 127.18, 126.98, 126.84, 125.31, 124.62, 123.67, 114.80, 36.44, 33.50, 32.48. HRMS (ESI) calculated for (M+H)+ for $C_{49}H_{37}N$, 640,29988; Found, 640.29710.

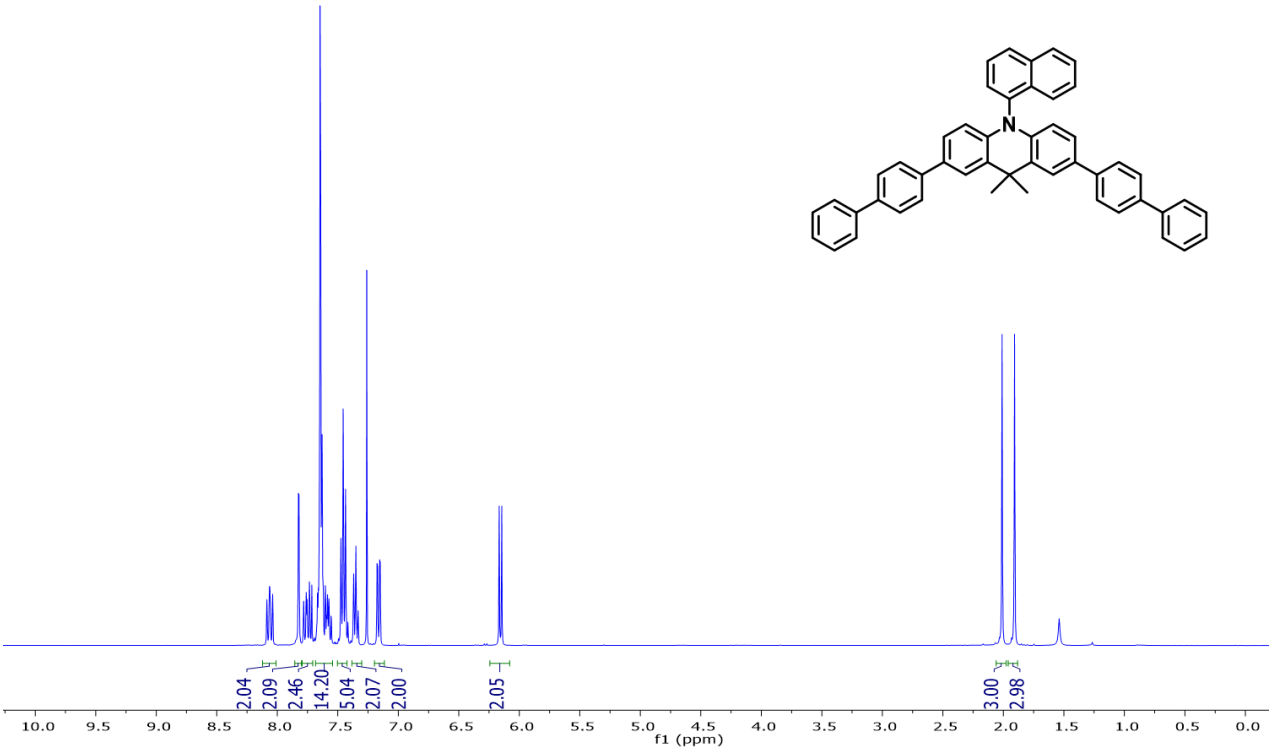


Figure S6: ^{1}H NMR spectrum of 2,7-di([1,1'-biphenyl]-4-yl)-9,9-dimethyl-10-(naphthalen-1-yl)-9,10-dihydroacridine in $CDCl_3$.

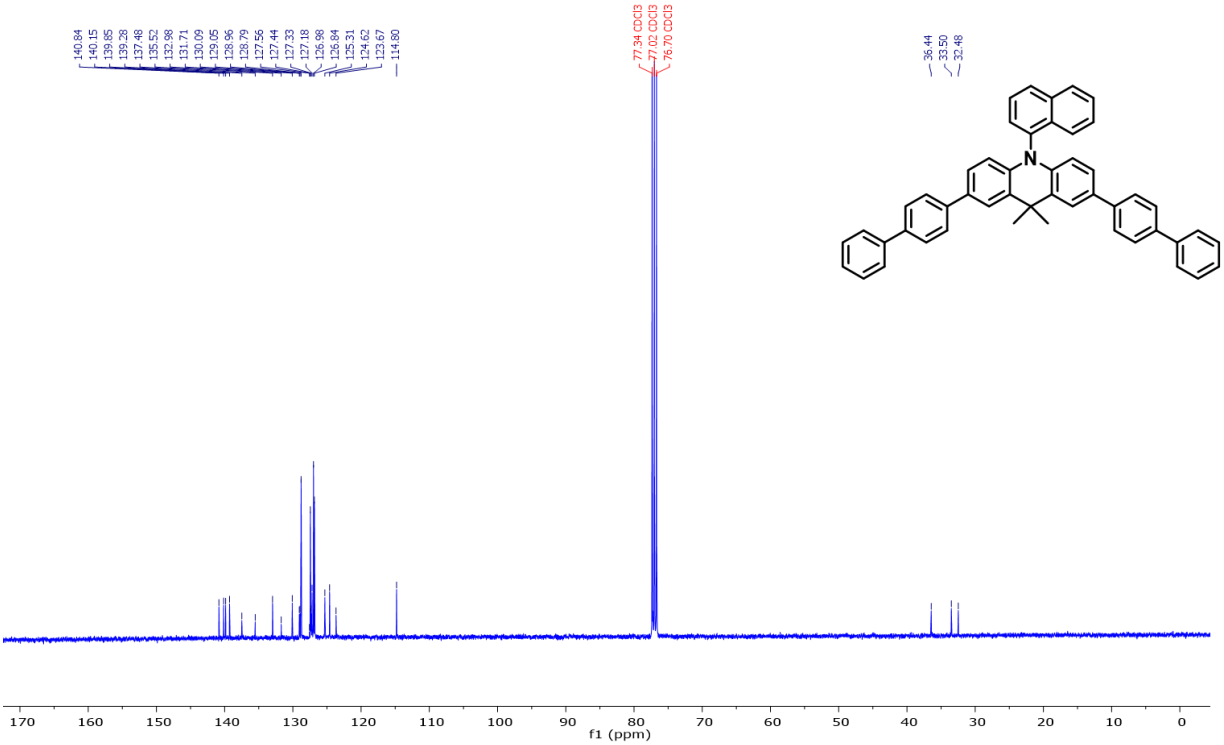
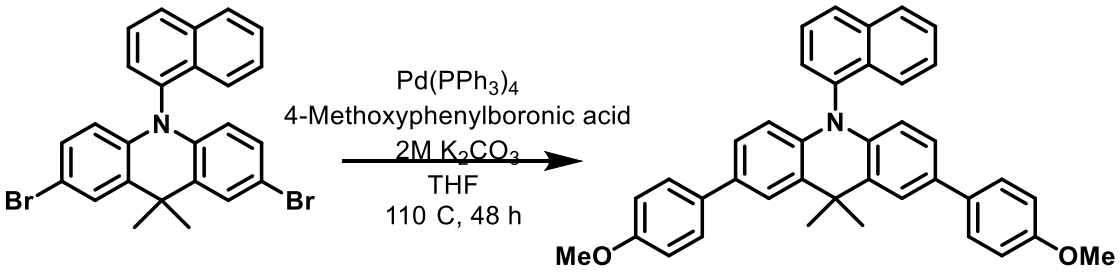


Figure S7: ^{13}C NMR spectrum of 2,7-di([1,1'-biphenyl]-4-yl)-9,9-dimethyl-10-(naphthalen-1-yl)-9,10-dihydroacridine in $CDCl_3$.

Synthesis of 2,7-bis(4-methoxyphenyl)-9,9-dimethyl-10-(naphthalen-1-yl)-9,10-dihydroacridine



2.5 g 2,7-dibromo-9,10-dihydro-9,9-dimethyl-10-(1-napthalenyl)-acridine (5.1 mmol, 1 eq.) was loaded into a storage tube. 3.1 g 4-Methoxyphenylboronic acid (20.2 mmol, 4 eq.) was added under ambient conditions. The flask was brought into a nitrogen-filled glovebox. Then, 0.586 Tetrakis(triphenylphosphine)palladium(0) (0.51 mmol, 10 mol %) was added. 80 mL of THF was added to produce a yellow solution. The flask was taken out of the glovebox, where 56 mL of degassed 2M K_2CO_3 was added using a long needle and syringe. The biphasic solution was then sealed and heated to 110 ºC for 24 hours. At that time, the solution was cooled to room temperature and concentrated on rotovap to produce a reddish oil. The crude mixture was dissolved in 200 mL ethyl acetate and washed 3 times with water. The organic layer was dried with magnesium sulfate, filtered, and concentrated. The product was isolated by column chromatography using 80:20 hexane:ethyl acetate. TLC indicated decomposition of the product when using DCM on silica coated plates. Then, the product was recrystallized 3 times using ethyl acetate layered with methanol to yield a white solid. Yield: 1.76 g, 63.3% yield. ^{1}H NMR (400 MHz, Benzene-d_6) δ 7.97 – 7.90 (m, 1H), 7.86 (d, *J* = 2.1 Hz, 2H), 7.72 (dd, *J* = 8.2, 3.8 Hz, 2H), 7.54 – 7.45 (m, 4H), 7.40 – 7.28 (m, 2H), 7.25 – 7.19 (m, 1H), 7.11 (td, *J* = 7.6, 6.8, 1.3 Hz, 1H), 7.02 (dd, *J* = 8.5, 2.1 Hz, 2H), 6.92 – 6.84 (m, 4H), 6.30 (d, *J* = 8.5 Hz, 2H), 3.36 (s, 6H), 1.91 (s, 3H), 1.81 (s, 3H). HRMS (ESI) calculated for M+ for $C_{39}H_{33}NO_2$, 547.25058; Found, 547.25074.

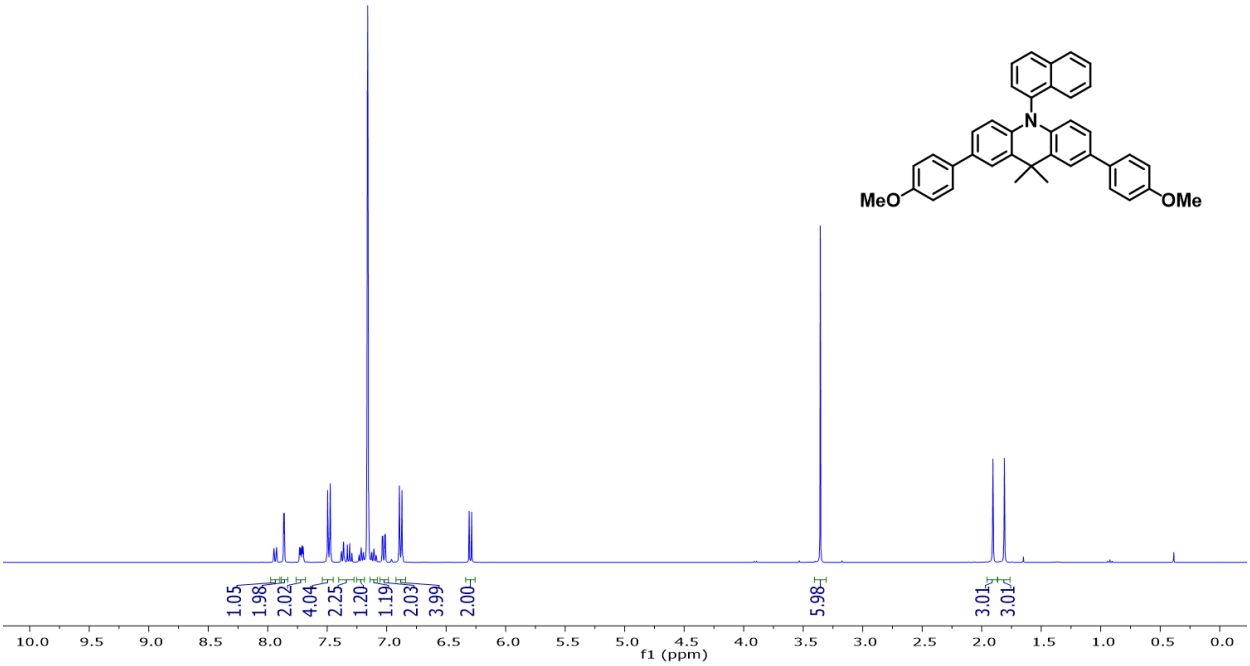


Figure S8: ^{1}H NMR spectrum of 2,7-bis(4-methoxyphenyl)-9,9-dimethyl-10-(naphthalen-1-yl)-9,10-dihydroacridine in C_6D_6.

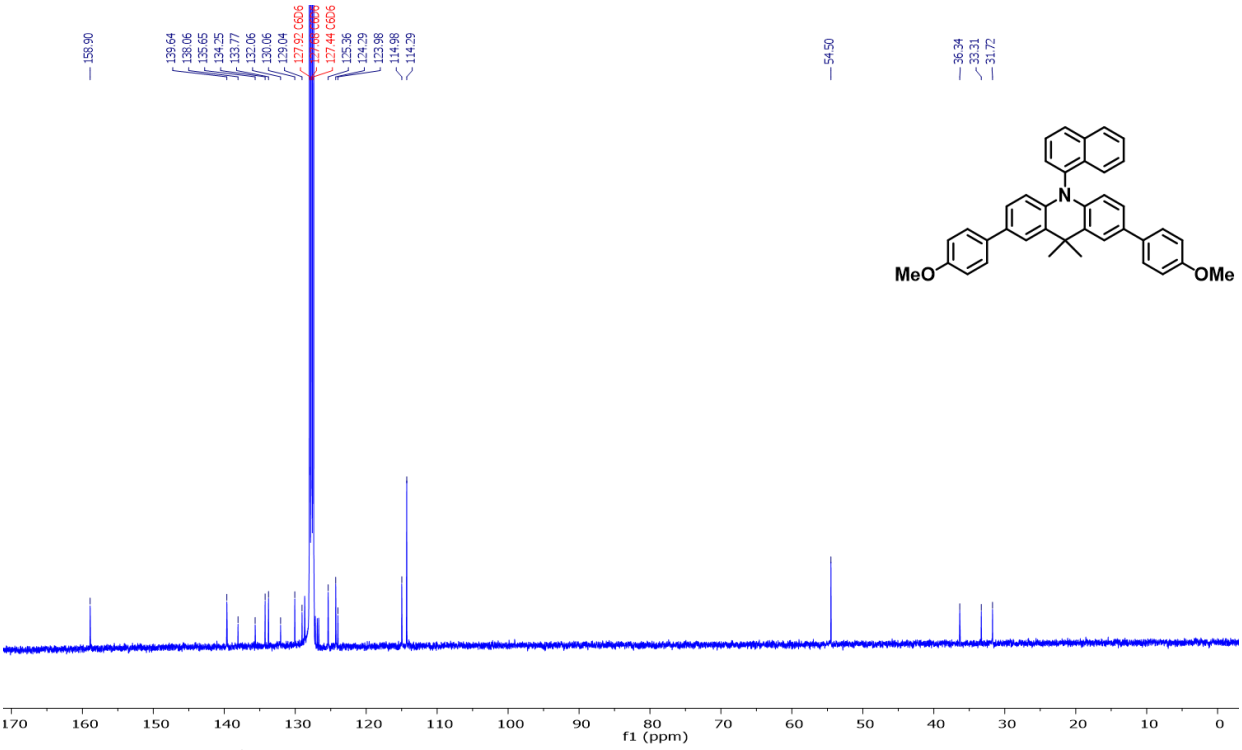
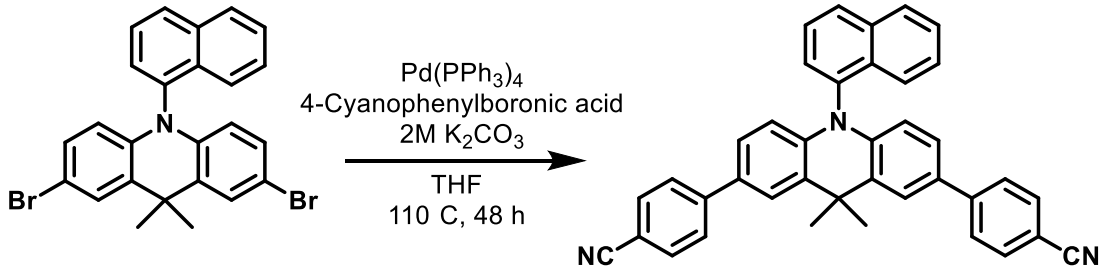


Figure S9: ^{13}C NMR spectrum of 2,7-bis(4-methoxyphenyl)-9,9-dimethyl-10-(naphthalen-1-yl)-9,10-dihydroacridine in C_6D_6.

Synthesis of 4,4'-(9,9-dimethyl-10-(naphthalen-1-yl)-9,10-dihydroacridine-2,7-diyl)dibenzonitrile



0.3 g of 2,7-dibromo-9,10-dihydro-9,9-dimethyl-10-(1-napthalenyl)-acridine (0.61 mmol, 1 eq.) and 0.36 g of 4-Cyanophenylboronic acid (2.4 mmol, 4 eq.) was loaded into a storage tube under ambient atmosphere. The storage tube was taken into a nitrogen-filled glovebox, then loaded with 0.105 g Tetrakis(triphenylphosphine)palladium(0) (0.09 mmol, 15 mol %). The solids were dissolved in 50 mL THF. The storage tube was sealed and brought out of the glovebox, where 8.0 mL of degassed 2M K_2CO_3 was added using a long needle and syringe to produce a biphasic yellow and colorless solution. The solution was heated to 110 ºC for 46 hours, then brought to room temperature. The solution turned reddish-brown upon exposure to air. The solution was concentrated and extracted into DCM, then passed through a silica plug and rinsed with DCM. The yellow filtrate was collected and concentrated to give a pale-yellow solid. Pure product was obtained by recrystallizing with ethyl acetate layered with methanol at -25 ºC to give a yield of 0.287 g, 87%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.15 – 8.05 (m, 2H), 7.82 – 7.55 (m, 14H), 7.45 (ddd, *J* = 8.3, 6.9, 1.2 Hz, 1H), 7.15 (dd, *J* = 8.6, 2.2 Hz, 2H), 6.19 (d, *J* = 8.6 Hz, 2H), 2.00 (s, 3H), 1.88 (s, 3H). ^{13}C NMR (101 MHz, C_6D_6) δ 144.75, 140.56, 137.14, 135.62, 132.27, 132.01, 131.50, 130.19, 129.19, 127.92, 127.68, 127.44, 126.49, 125.87, 124.51, 123.38, 118.70, 115.29, 110.40, 36.22, 33.35, 31.36. HRMS (ESI) calculated for M+ for $C_{39}H_{27}N_3$, 536.21267; Found, 536.16531.

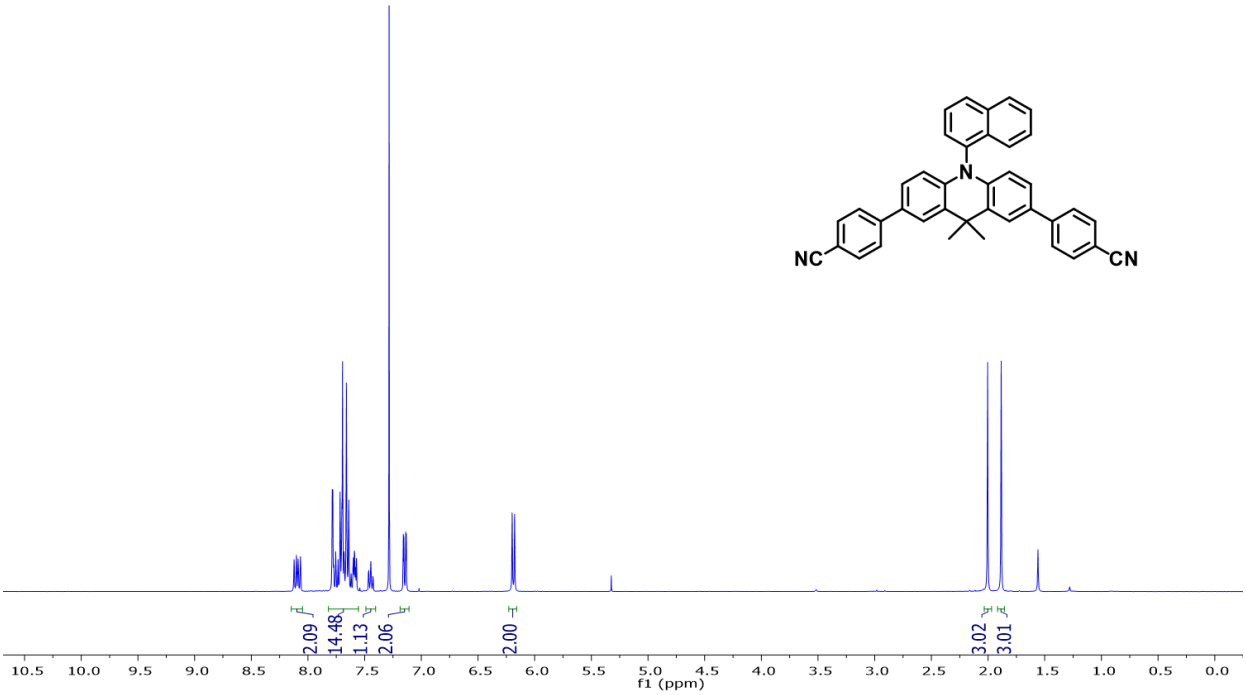


Figure S10: ^{1}H NMR spectrum of 4,4'-(9,9-dimethyl-10-(naphthalen-1-yl)-9,10-dihydroacridine-2,7-diyl)dibenzonitrile in $CDCl_3$.

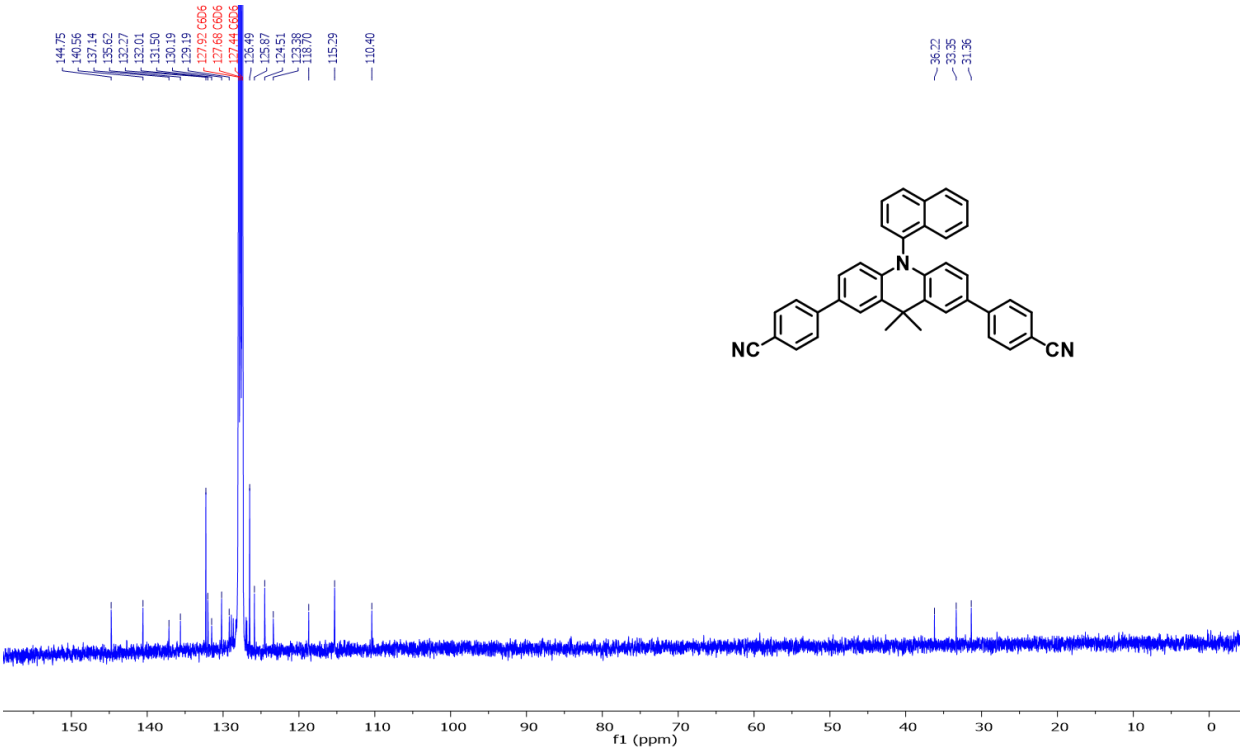
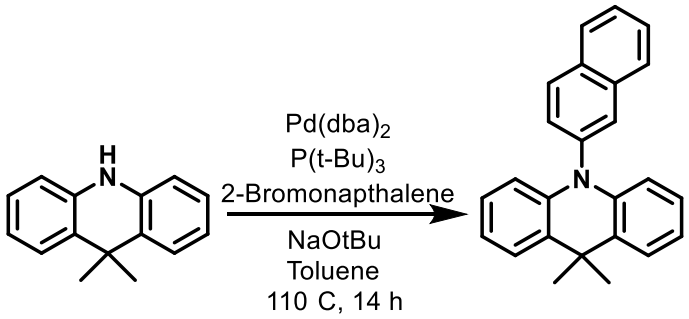


Figure S11: ^{13}C NMR spectrum of 4,4'-(9,9-dimethyl-10-(naphthalen-1-yl)-9,10-dihydroacridine-2,7-diyl)dibenzonitrile in C_6D_6.

Synthesis of 9,9-dimethyl-10-(naphthalen-2-yl)-9,10-dihydroacridine



A storage tube was loaded with 1.0 g (4.8 mmol, 1 eq.) 9,10-Dihydro-9,9-dimethylacridine, 1.48 g 2-bromonaphthalene (7.1 mmol, 1.5 eq.), 27.5 mg of Bis(dibenzylideneacetone)palladium(0) (0.48 µmol, 1 mol%), 134 µL of 1M in toluene Tri-*tert*-butylphosphine (0.134 mmol, 3 mol %), 1.4 g sodium *tert*-butoxide (14.4 mmol, 3 eq.), and 50 mL toluene under nitrogen atmosphere. The solution was heated to 110 ºC. After 14 hours, the reddish-purple liquid with a white precipitate was passed directly through a silica plug and rinsed with toluene. All blue fluorescent portions were collected and concentrated via rotary evaporation. The product was recrystallized 3 times with DCM/methanol at -25 ºC. The product was collected via vacuum filtration, washed with methanol, and dried overnight under vacuum to yield 1.16 g (72.6% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.14 (d, *J* = 8.6 Hz, 1H), 8.04 – 7.98 (m, 1H), 7.91 (dt, *J* = 4.7, 1.8 Hz, 2H), 7.60 (dqd, *J* = 8.3, 6.9, 1.5 Hz, 2H), 7.55 – 7.48 (m, 2H), 7.44 (dd, *J* = 8.6, 2.0 Hz, 1H), 7.03 – 6.90 (m, 4H), 6.39 – 6.27 (m, 2H), 1.77 (s, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 140.97, 138.49, 134.81, 132.85, 130.95, 130.13, 130.00, 128.93, 128.02, 127.89, 126.73, 126.43, 126.32, 125.22, 120.55, 114.16, 36.02, 31.31. HRMS (ESI) calculated for M+ for $C_{25}H_{21}N$, 336.17468; Found, 336.1755.

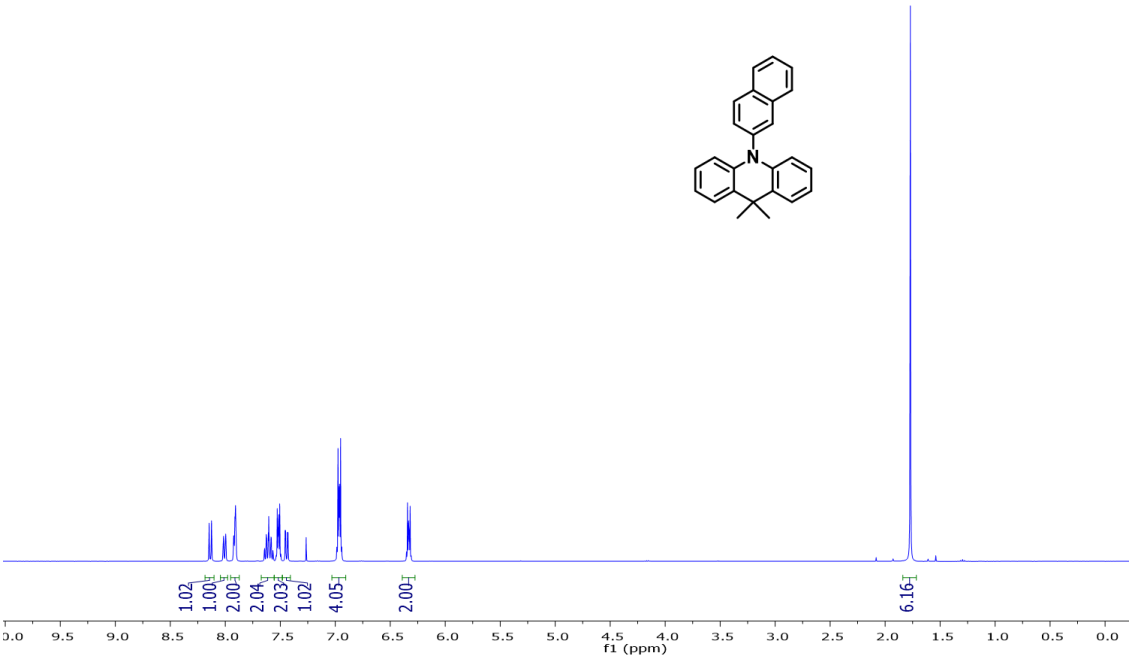


Figure S12: ^{1}H NMR spectrum of 9,9-dimethyl-10-(naphthalen-2-yl)-9,10-dihydroacridine in $CDCl_3$.

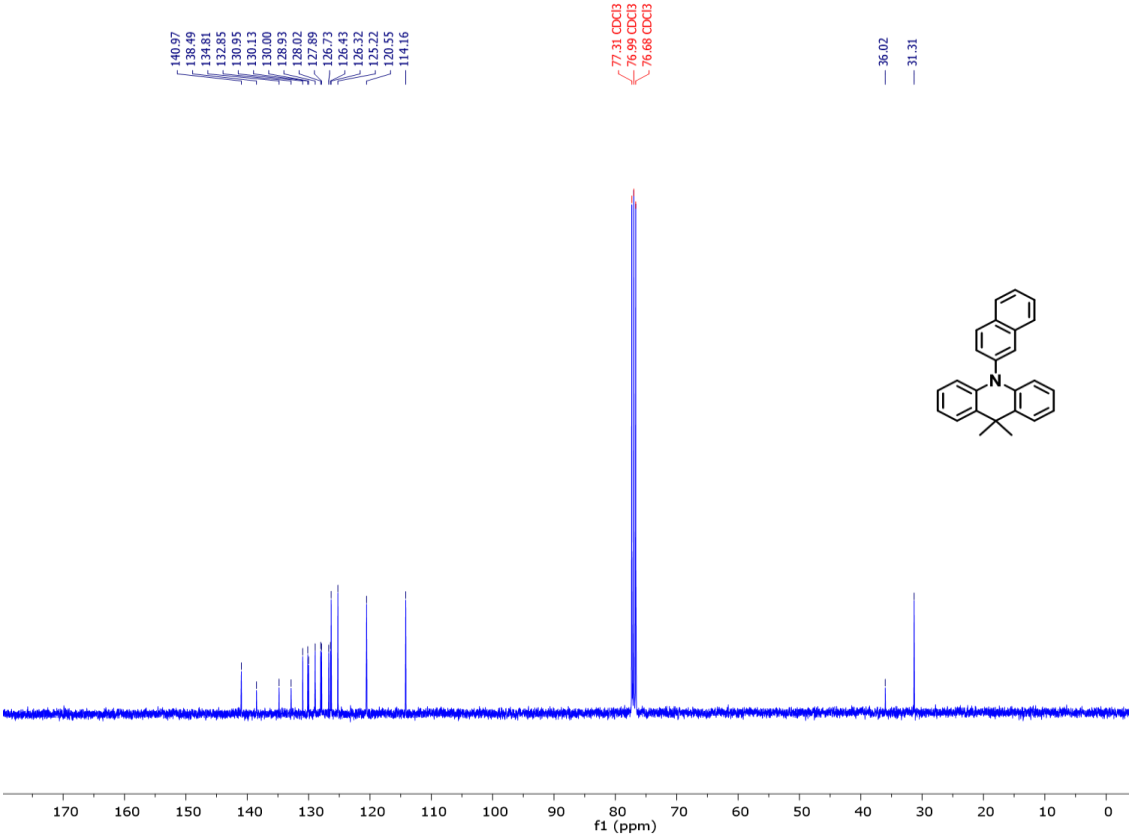
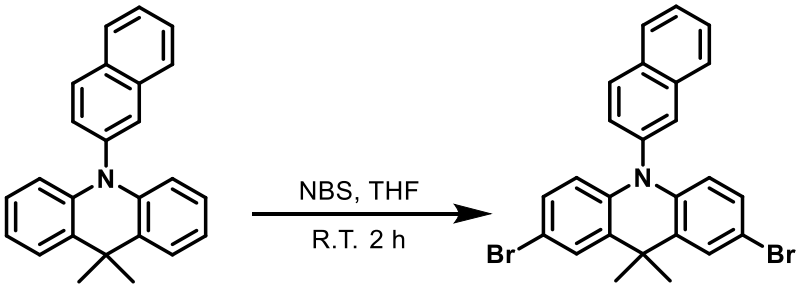


Figure S13: ^{13}C NMR spectrum of 9,9-dimethyl-10-(naphthalen-2-yl)-9,10-dihydroacridine in $CDCl_3$.

Synthesis of 2,7-dibromo-9,9-dimethyl-10-(naphthalen-2-yl)-9,10-dihydroacridine



0.75 g of 9,10-dihydro-9,9-dimethyl-10-(2-napthalenyl)-acridine (2.2 mmol, 1.0 eq.) was dissolved in 20 mL THF under ambient atmosphere. 0.90 g of *N*-Bromosuccinimide (5.0 mmol, 2.25 eq.) was slowly added to make a light brown solution. The reaction then stirred at room temperature for 2 hours. The solution was then concentrated via rotary evaporation, washed with water 3 times, and dried with magnesium sulfate. The product was recrystallized using DCM layered with methanol at -25 ºC overnight. The product was isolated by filtration and dried under vacuum to give a pale brown crystalline solid. ^{1}H NMR revealed a mix of products, which was carried over to the next step without further purification. Yield: 0.95 g, 86%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.01 (d, *J* = 8.6 Hz, 1H), 7.93 – 7.84 (m, 1H), 7.84 – 7.70 (m, 2H), 7.56 – 7.39 (m, 5H), 7.31 – 7.19 (m, 1H), 6.92 (ddd, *J* = 8.8, 4.4, 2.3 Hz, 3H), 6.06 (d, *J* = 8.8 Hz, 2H), 1.58 (s, 7H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.83, 137.96, 137.62, 134.73, 132.99, 131.65, 131.57, 131.39, 129.82, 129.57, 129.31, 128.60, 128.08, 128.05, 127.97, 127.83, 127.12, 126.78, 116.01, 115.31, 113.38, 77.33, 77.01, 76.70, 36.34, 31.00, 30.43.

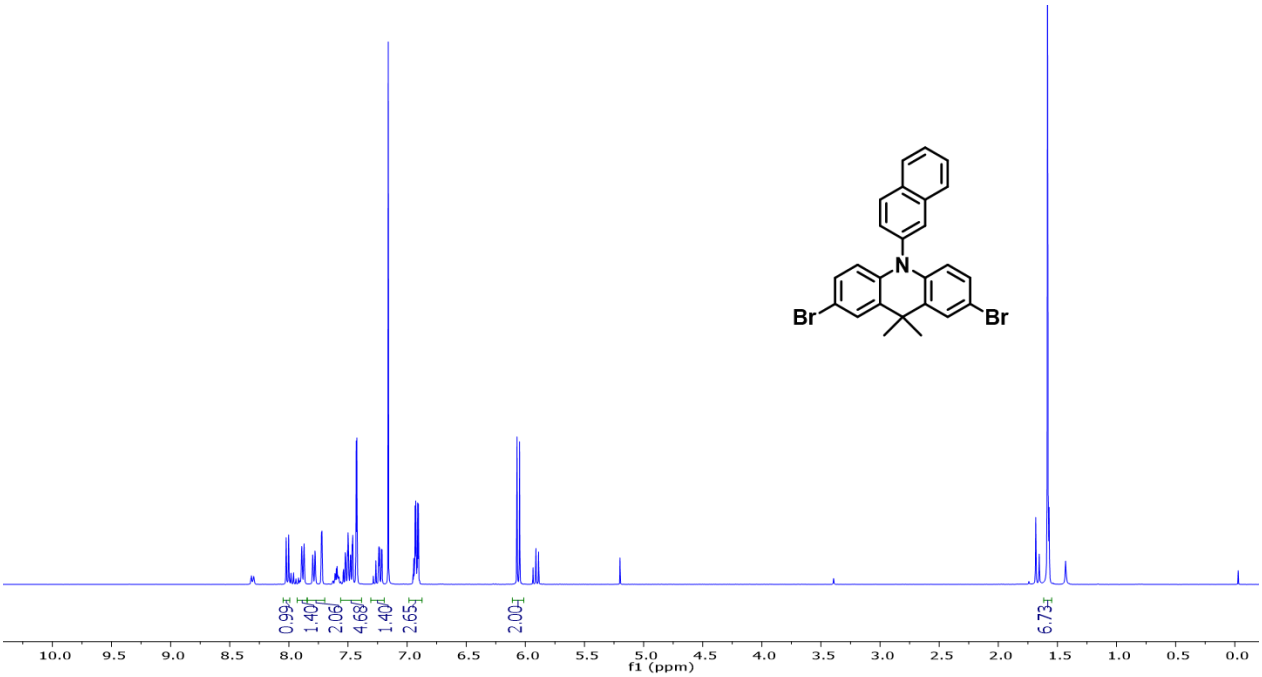


Figure S14: ^{1}H NMR spectrum 2,7-dibromo-9,9-dimethyl-10-(naphthalen-2-yl)-9,10-dihydroacridinein C_6D_6.

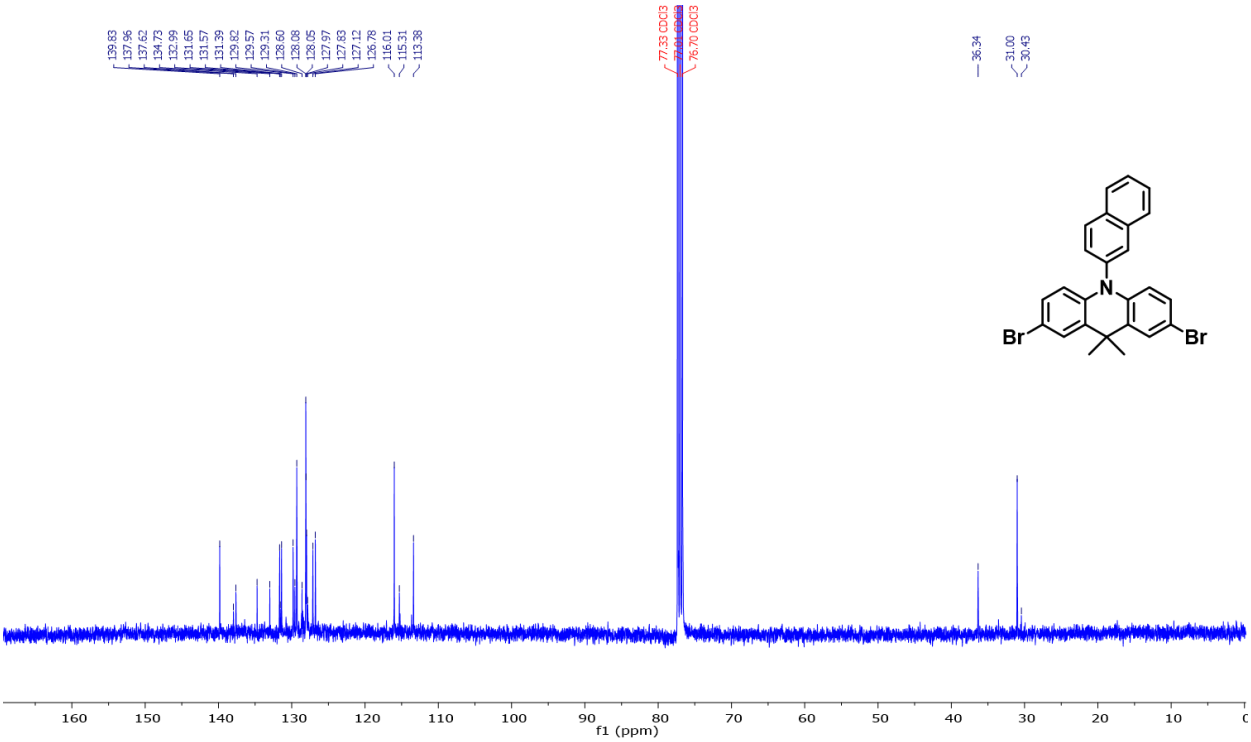
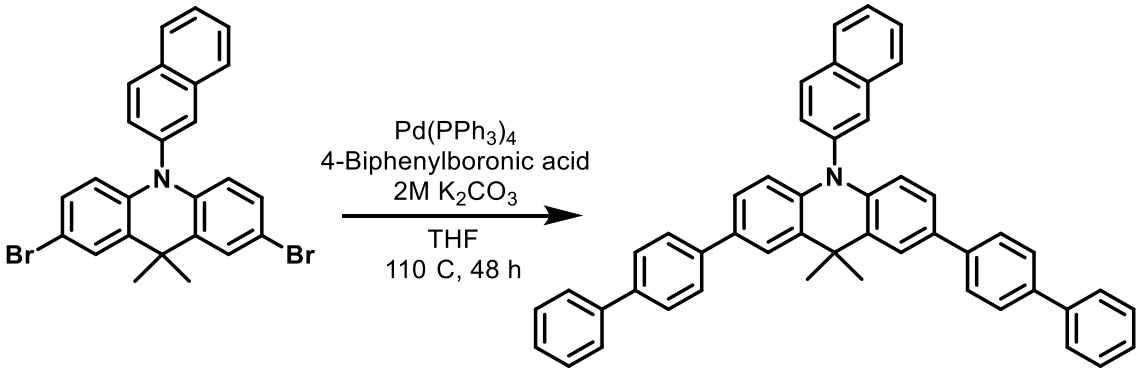


Figure S15: ^{13}C NMR spectrum 2,7-dibromo-9,9-dimethyl-10-(naphthalen-2-yl)-9,10-dihydroacridinein $CDCl_3$.

Synthesis of 2,7-di([1,1'-biphenyl]-4-yl)-9,9-dimethyl-10-(naphthalen-2-yl)-9,10-dihydroacridine



0.8 g of 2,7-dibromo-9,10-dihydro-9,9-dimethyl-10-(2-napthalenyl)-acridine (1.6 mmol, 1 eq.) and 1.28 g of 4-Biphenylboronic acid (6.5 mmol, 4 eq.) was loaded into a storage tube under ambient atmosphere. The storage tube was taken into a nitrogen-filled glovebox, then loaded with 0.281 g Tetrakis(triphenylphosphine)palladium(0) (0.243 mmol, 15 mol %). The solids were dissolved in 50 mL THF. The storage tube was sealed and brought out of the glovebox, where 18 mL of degassed 2M K_2CO_3 (22 eq.) was added using a long needle and syringe to produce a biphasic yellow and colorless solution. The solution was heated to 110 ºC for 48 hours, then brought to room temperature. The solution turned reddish-brown upon exposure to air. The solution was concentrated and extracted into DCM, then dried using magnesium sulfate, filtered, and concentrated. The crude mixture was redissolved in DCM then passed through a silica plug. The yellow filtrate was collected and concentrated, then recrystallized with DCM/MeOH at -25 ºC to give a white crystalline solid with a yield of 59.4%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.17 (d, *J* = 8.6 Hz, 1H), 8.06 – 8.00 (m, 1H), 7.98 – 7.90 (m, 2H), 7.79 (d, *J* = 2.1 Hz, 2H), 7.77 – 7.57 (m, 17H), 7.46 (td, *J* = 8.2, 6.4 Hz, 6H), 7.40 – 7.29 (m, 3H), 7.23 (d, *J* = 2.1 Hz, 1H), 6.41 (d, *J* = 8.5 Hz, 2H), 1.89 (s, 6H). ^{13}C NMR (101 MHz, C_6D_6) δ 141.12, 140.54, 140.52, 139.53, 138.58, 134.97, 133.63, 133.06, 131.12, 130.50, 130.14, 128.79, 127.92, 127.68, 127.44, 125.41, 124.26, 115.15, 36.38, 31.60. HRMS (ESI) calculated for (M+H)+ for $C_{49}H_{37}N$, 640,29988; Found, 640.2991.

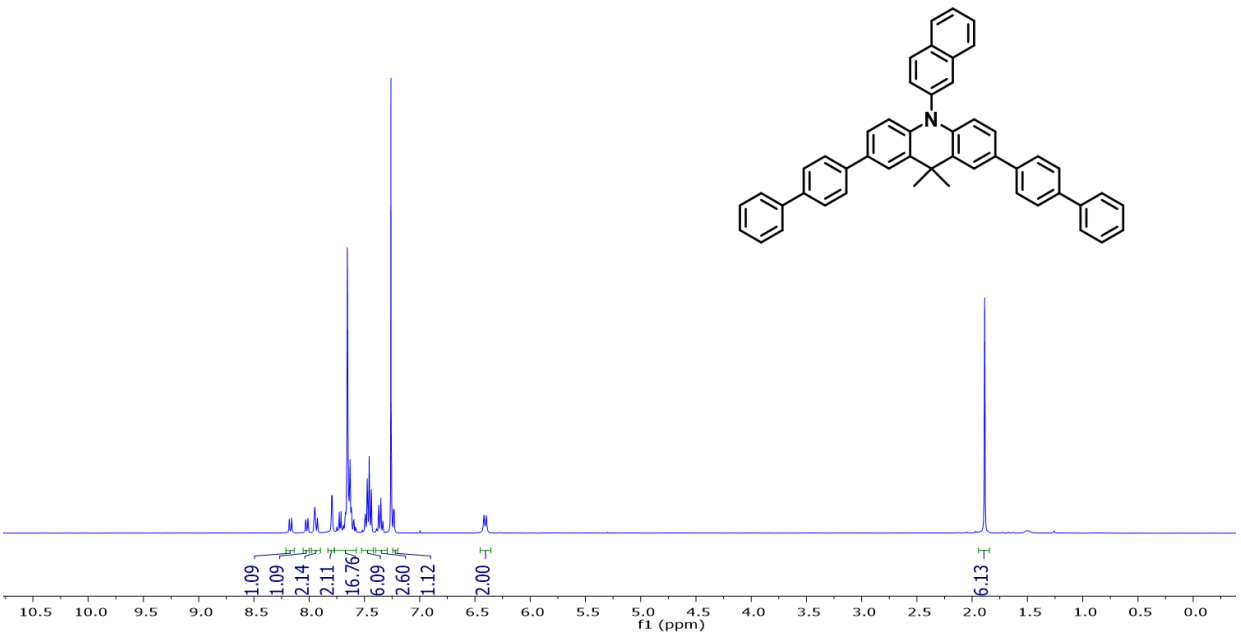


Figure S16: ^{1}H NMR spectrum of 2,7-di([1,1'-biphenyl]-4-yl)-9,9-dimethyl-10-(naphthalen-2-yl)-9,10-dihydroacridine in $CDCl_3$.

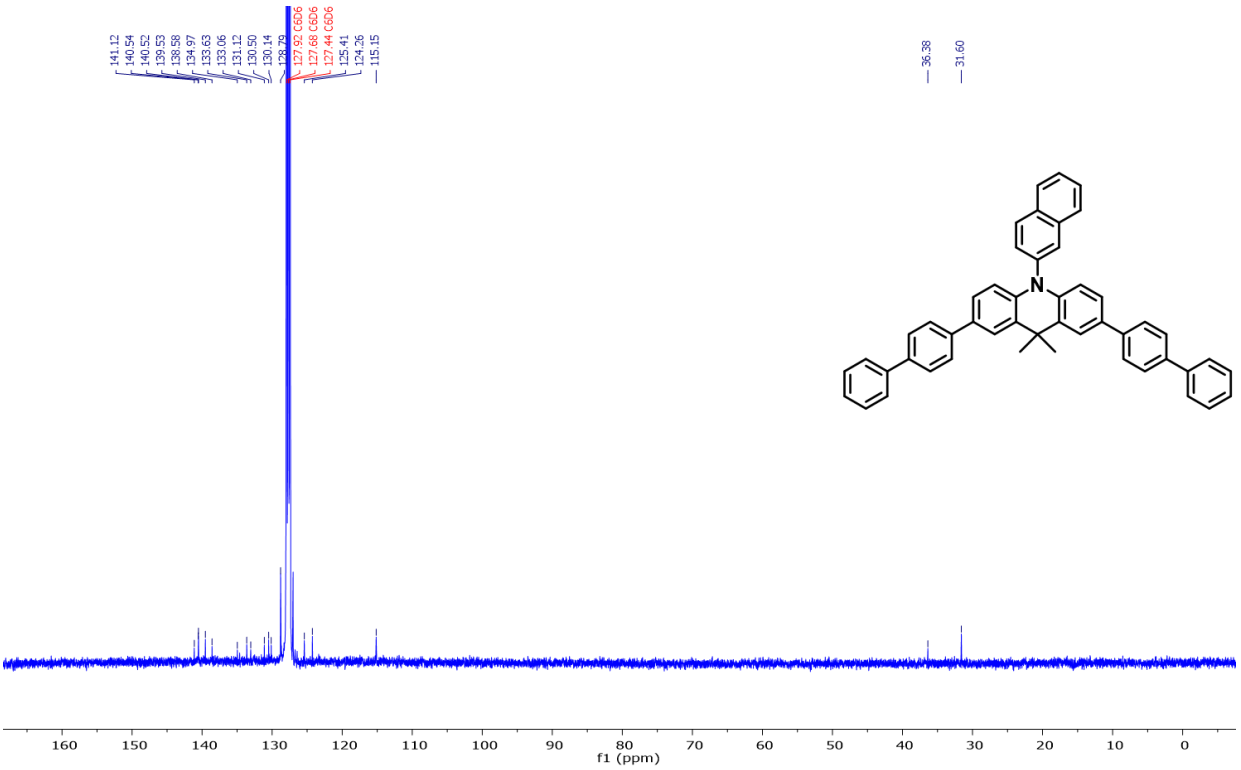
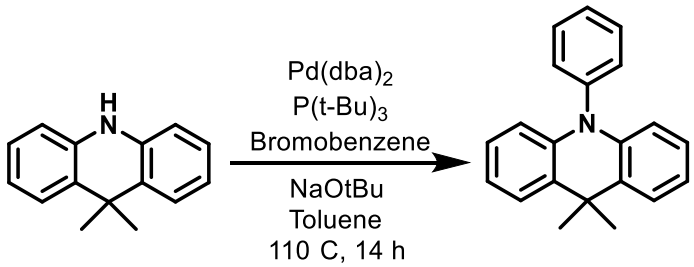


Figure S17: ^{1}H NMR spectrum of 2,7-di([1,1'-biphenyl]-4-yl)-9,9-dimethyl-10-(naphthalen-2-yl)-9,10-dihydroacridine in C_6D_6.

Synthesis of 9,9-dimethyl-10-phenyl-9,10-dihydroacridine



A storage tube was loaded with 1.0 g (4.8 mmol, 1 eq.) 9,10-Dihydro-9,9-dimethylacridine, 1.48 g bromobenzene (7.2 mmol, 1.5 eq.), 27.5 mg of Bis(dibenzylideneacetone)palladium(0) (0.48 µmol, 1 mol%), 143 µL of 1M in toluene Tri-*tert*-butylphosphine (0.134 mmol, 3 mol %), 1.4 g sodium *tert*-butoxide (14.4 mmol, 3 eq.), and 27 mL toluene under nitrogen atmosphere. The solution was heated to 110 ºC. After 14 hours, the reddish liquid with a white precipitate was passed directly through a silica plug and rinsed with toluene. All blue fluorescent portions were collected and concentrated via rotary evaporation. The product was recrystallized with ethyl acetate/methanol at -25 ºC for 4 hours. The product was collected via vacuum filtration, washed with methanol, and dried overnight under vacuum to yield 1.0 g (73.5% yield) of a white crystalline solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.67 – 7.59 (m, 2H), 7.54 – 7.47 (m, 1H), 7.46 (dd, *J* = 7.5, 1.8 Hz, 2H), 7.37 – 7.30 (m, 2H), 7.01 – 6.87 (m, 4H), 6.26 (dd, *J* = 7.9, 1.5 Hz, 2H), 1.70 (s, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 141.20, 140.93, 131.32, 130.83, 129.95, 128.19, 126.32, 125.17, 120.48, 114.01, 35.98, 31.24. HRMS (ESI) calculated for (M+H)+ for $C_{21}H_{19}N$, 285.15175; Found, 285.1514.

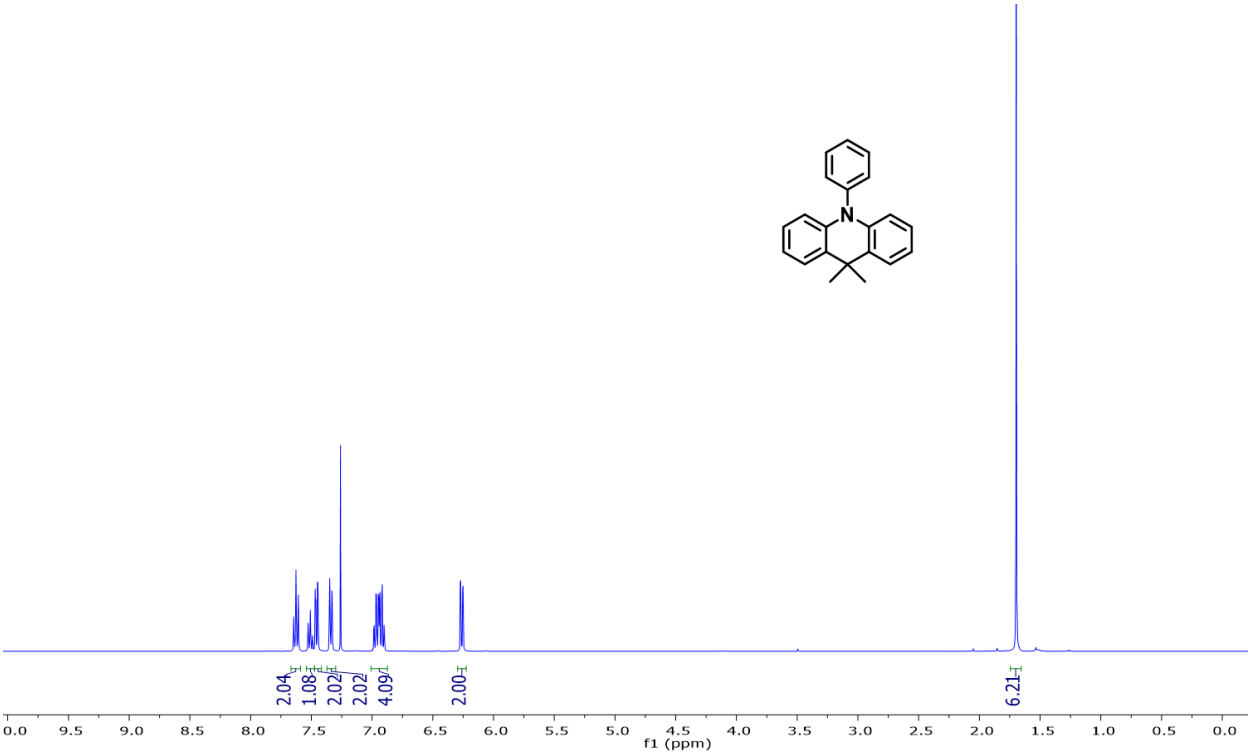


Figure S18: ^{1}H NMR spectrum of 9,9-dimethyl-10-phenyl-9,10-dihydroacridine in $CDCl_3$.

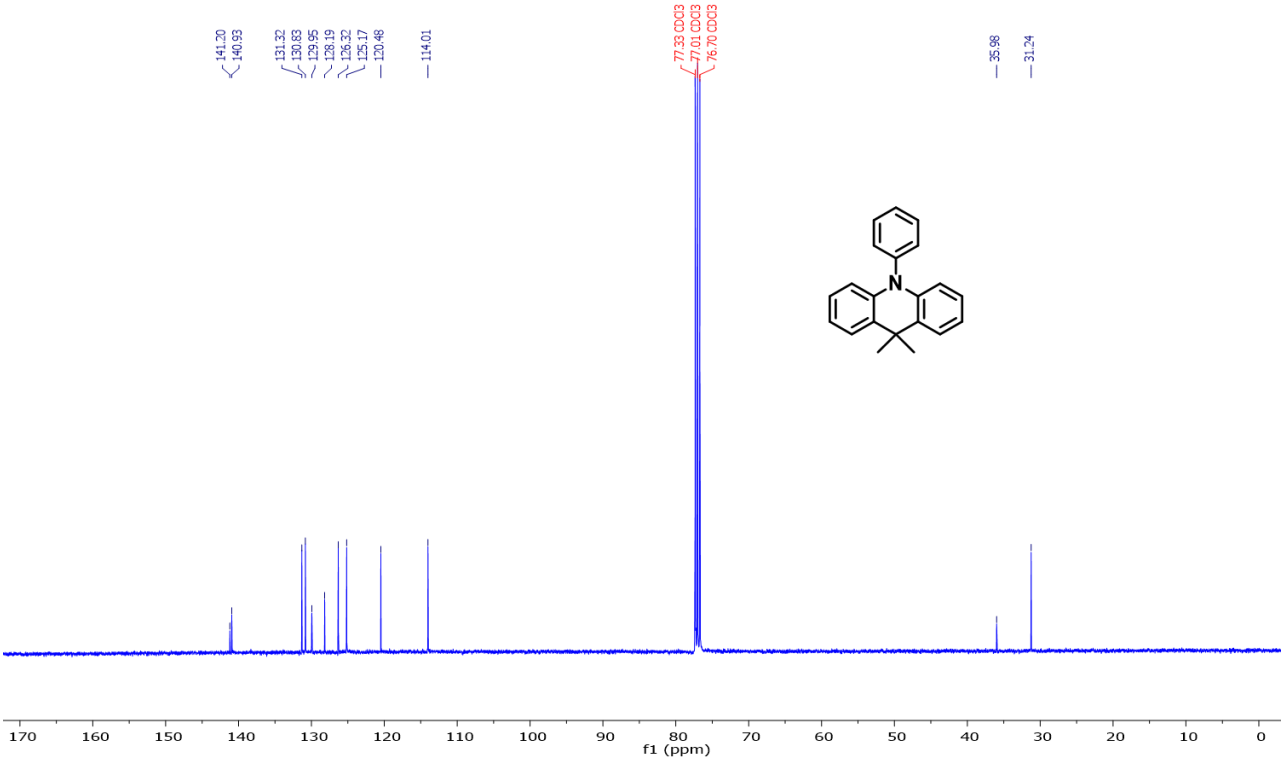
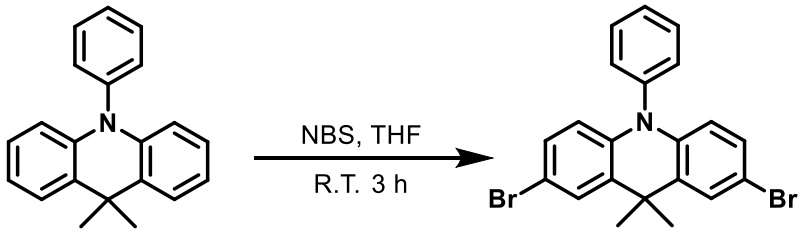


Figure S19: ^{13}C NMR spectrum of 9,9-dimethyl-10-phenyl-9,10-dihydroacridine in $CDCl_3$.

Synthesis of 2,7-dibromo-9,9-dimethyl-10-phenyl-9,10-dihydroacridine



0.75 g of 9,10-dihydro-9,9-dimethyl-10-(phenyl)-acridine (2.2 mmol, 1.0 eq.) was dissolved in 50 mL THF under ambient atmosphere. 1.16 g of *N*-Bromosuccinimide (5.0 mmol, 2.5 eq.) was slowly added to make a light brown solution. The reaction then stirred at room temperature for 3 hours. The solution was then concentrated via rotary evaporation, washed with water 3 times, and dried with magnesium sulfate. The product was recrystallized using DCM layered with methanol at -25 ºC overnight. The product was isolated by filtration and dried under vacuum to give a white solid. ^{1}H NMR analysis revealed a mix of brominated substitutions, which was carried over to the next step without further purification. Yield: 0.78 g, 67%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.71 – 7.63 (m, 1H), 7.59 – 7.48 (m, 1H), 7.48 – 7.37 (m, 2H), 7.22 – 7.17 (m, 1H), 7.12 – 7.04 (m, 1H), 6.96 (ddd, *J* = 8.9, 7.9, 2.3 Hz, 2H), 6.02 (dd, *J* = 8.8, 3.0 Hz, 2H), 1.54 (d, *J* = 4.5 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.39, 139.76, 139.45, 139.42, 134.52, 132.70, 131.73, 131.60, 131.12, 130.81, 129.39, 129.29, 128.72, 128.19, 128.02, 122.71, 115.85, 115.70, 113.64, 113.29, 77.33, 77.01, 76.70, 36.28, 30.93.

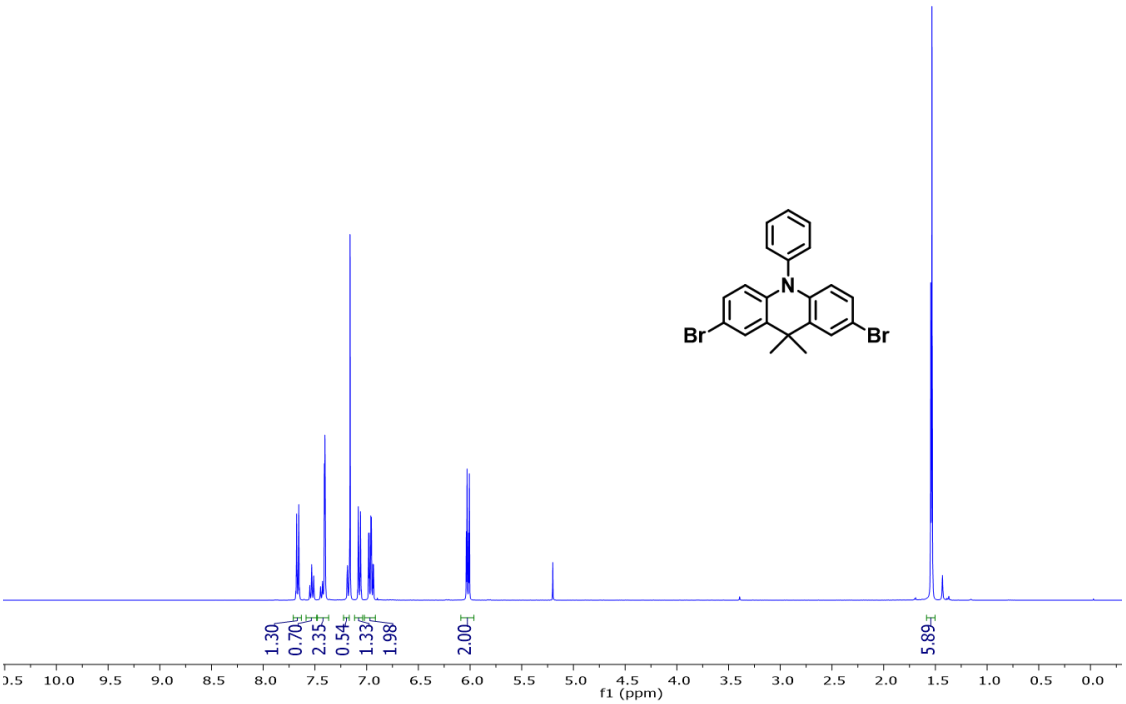


Figure S20: ^{1}H NMR spectrum of 2,7-dibromo-9,9-dimethyl-10-phenyl-9,10-dihydroacridine in $CDCl_3$.

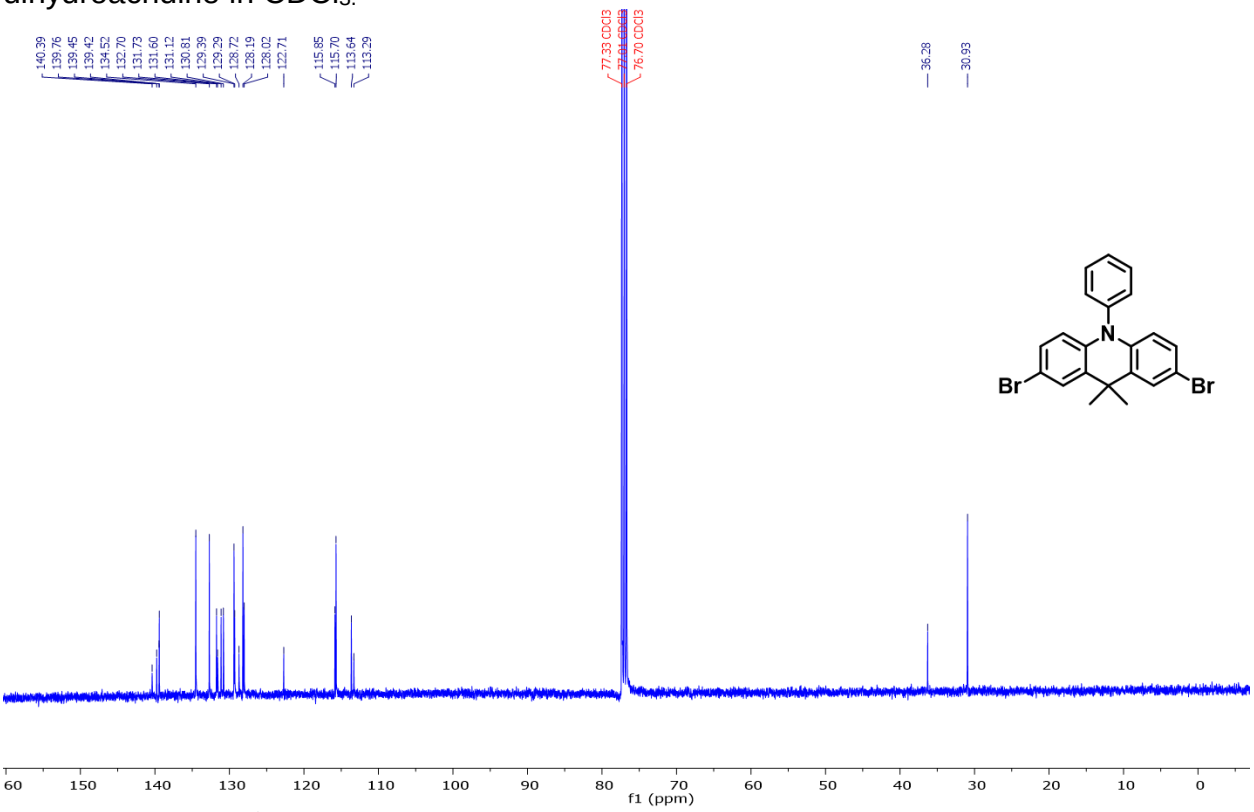
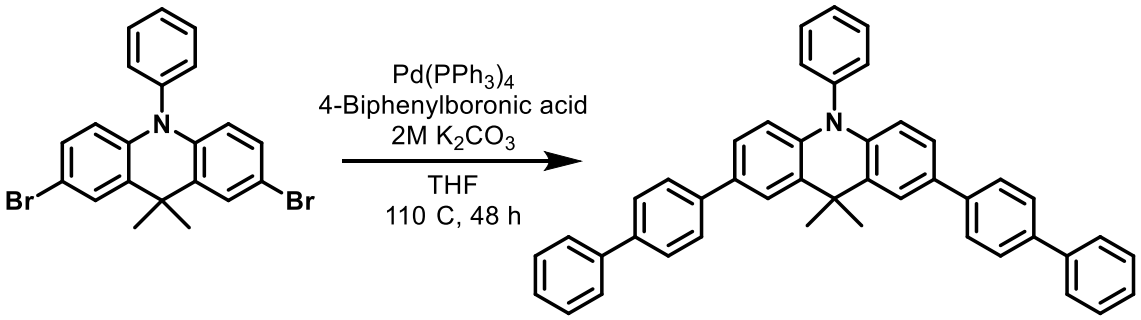


Figure S21: ^{13}C NMR spectrum of 2,7-dibromo-9,9-dimethyl-10-phenyl-9,10-dihydroacridine in $CDCl_3$.

Synthesis of 2,7-di([1,1'-biphenyl]-4-yl)-9,9-dimethyl-10-phenyl-9,10-dihydroacridine



0.5 g of 2,7-dibromo-9,10-dihydro-9,9-dimethyl-10-(phenyl)-acridine (1.1 mmol, 1 eq.) and 0.89 g of 4-Biphenylboronic acid (4.5 mmol, 4 eq.) was loaded into a storage tube under ambient atmosphere. The storage tube was taken into a nitrogen-filled glovebox, then loaded with 0.194 g Tetrakis(triphenylphosphine)palladium(0) (0.168 mmol, 15 mol %). The solids were dissolved in 20 mL THF. The storage tube was sealed and brought out of the glovebox, where 12 mL of degassed 2M K_2CO_3 (22 eq.) was added using a long needle and syringe to produce a biphasic yellow and colorless solution. The solution was heated to 110 ºC for 48 hours, then brought to room temperature. The solution turned reddish-brown upon exposure to air. The solution was concentrated and extracted into DCM, then dried using magnesium sulfate, filtered, and concentrated. The crude mixture was redissolved in DCM then passed through a silica plug. The yellow filtrate was collected and concentrated, then purified by column chromatography with hexanes: ethyl acetate ramping from 100:0 to 70:30. The product, a white solid, was then recrystallized with Ethyl acetate/MeOH at -25 ºC to give 0.665 g of a white crystalline solid with a yield of 62%. ^{1}H NMR (400 MHz, Benzene-d_6) δ 7.94 (d, J = 2.1 Hz, 2H), 7.74 – 7.54 (m, 19H), 7.40 – 7.25 (m, 10H), 6.68 (d, J = 8.5 Hz, 2H), 1.83 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.01, 140.86, 140.21, 139.33, 133.12, 133.03, 131.52, 131.16, 131.00, 130.36, 130.27, 129.52, 128.89, 128.83, 128.80, 128.46, 127.69, 127.59, 127.56, 127.49, 127.47, 127.38, 127.19, 127.08, 127.05, 126.99, 126.90, 126.89, 125.09, 124.23, 114.61, 77.34, 77.02, 76.70, 36.38, 31.85. HRMS (ESI) calculated for (M+H)+ for $C_{45}H_{35}N$, 589.27694; Found, 589.2764.

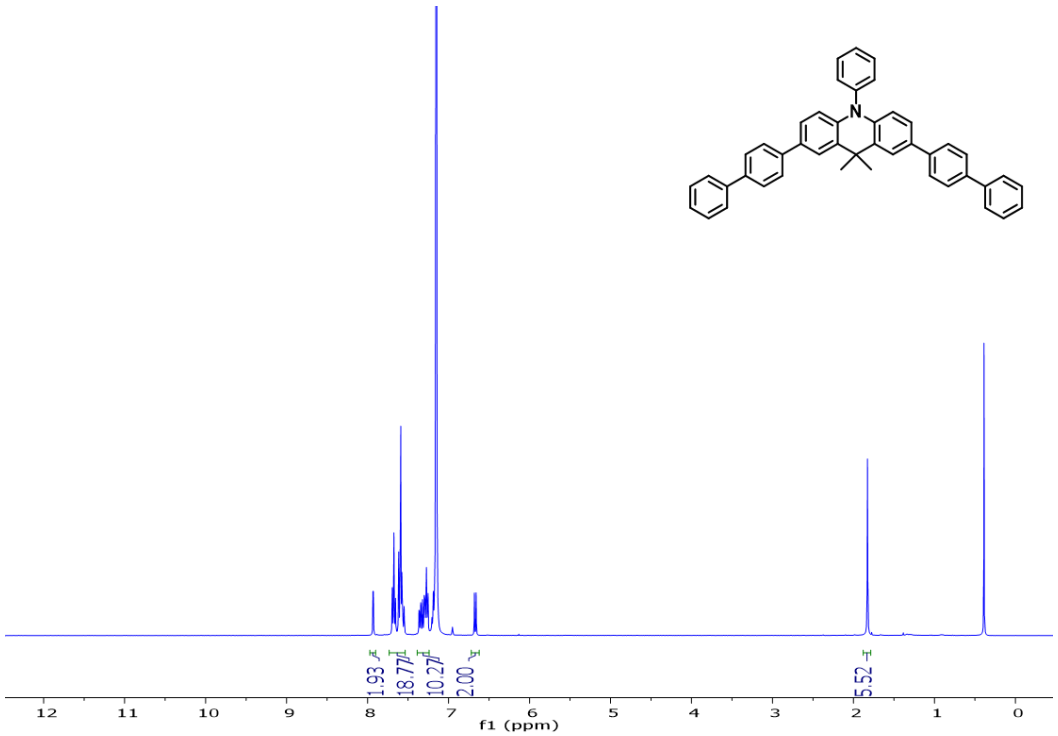


Figure S22: ^{1}H NMR spectrum of 2,7-di([1,1'-biphenyl]-4-yl)-9,9-dimethyl-10-phenyl-9,10-dihydroacridine in C_6D_6.

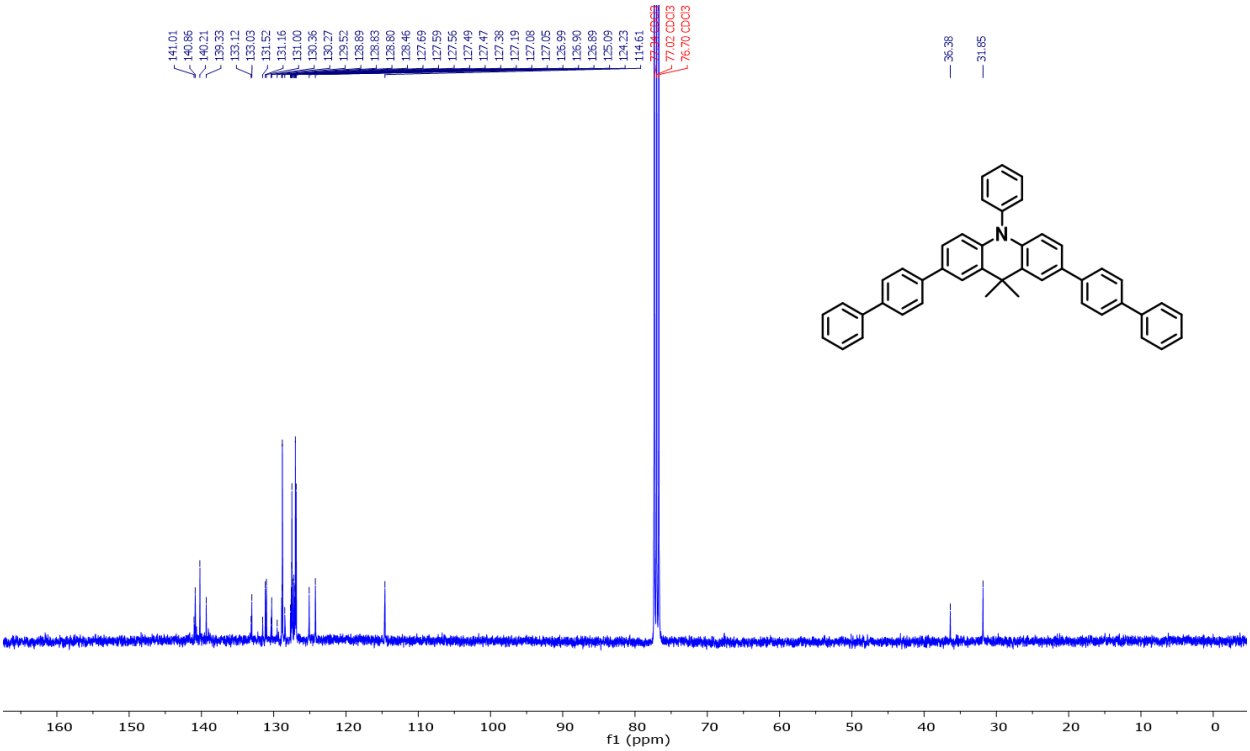
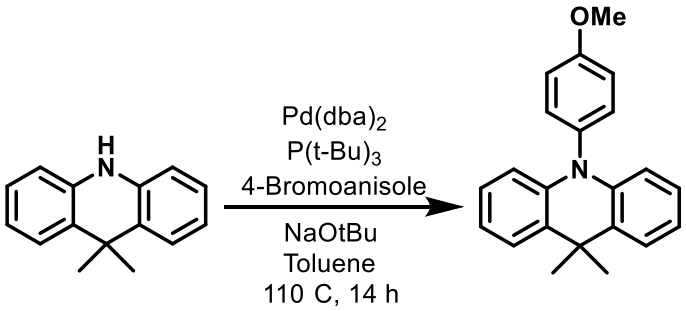


Figure S23: ^{13}C NMR spectrum of 2,7-di([1,1'-biphenyl]-4-yl)-9,9-dimethyl-10-phenyl-9,10-dihydroacridine in $CDCl_3$.

Synthesis of 10-(4-methoxyphenyl)-9,9-dimethyl-9,10-dihydroacridine



A storage tube was loaded with 1.0 g (4.8 mmol, 1 eq.) 9,10-Dihydro-9,9-dimethylacridine, 0.9 mL 4-Bromoanisole (7.2 mmol, 1.5 eq.), 27.5 mg of Bis(dibenzylideneacetone)palladium(0) (0.48 µmol, 1 mol%), 143 µL of 1M in toluene Tri-*tert*-butylphosphine (0.134 mmol, 3 mol %), 1.4 g sodium *tert*-butoxide (14.4 mmol, 3 eq.), and 27 mL toluene under nitrogen atmosphere. The solution was heated to 110 ºC. After 14 hours, the brown liquid with a white precipitate was passed directly through a silica plug and rinsed with toluene. All fluorescent blue portions were collected and concentrated via rotary evaporation. The product was recrystallized with DCM/methanol at -25 ºC for 2 hours. The product was collected via vacuum filtration, washed with methanol, and dried overnight under vacuum to yield 1.25 g (82.8% yield) of white crystalline needles. ^{1}H NMR (400 MHz, Benzene-d_6) δ 7.45 – 7.36 (m, 2H), 7.02 – 6.88 (m, 6H), 6.82 – 6.73 (m, 2H), 6.56 – 6.44 (m, 2H), 3.29 (s, 3H), 1.65 (s, 6H). ^{13}C NMR (101 MHz, C_6D6) δ 159.16, 141.52, 133.83, 132.15, 129.97, 126.43, 125.22, 120.62, 115.89, 114.28, 54.61, 35.89, 31.09. HRMS (ESI) calculated for (M+H)+ for $C_{22}H_{21}NO$, 316.16959; Found, 316.16916.

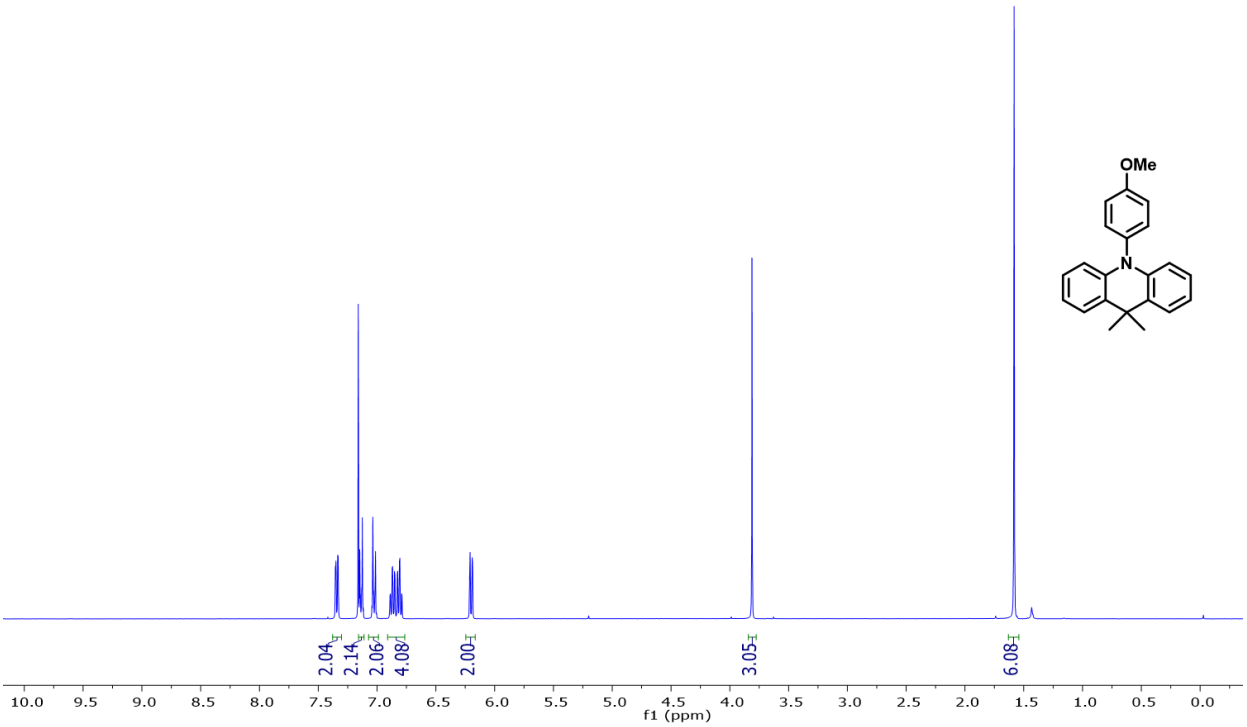


Figure S24: ^{1}H NMR spectrum of 10-(4-methoxyphenyl)-9,9-dimethyl-9,10-dihydroacridine in C_6D_6.

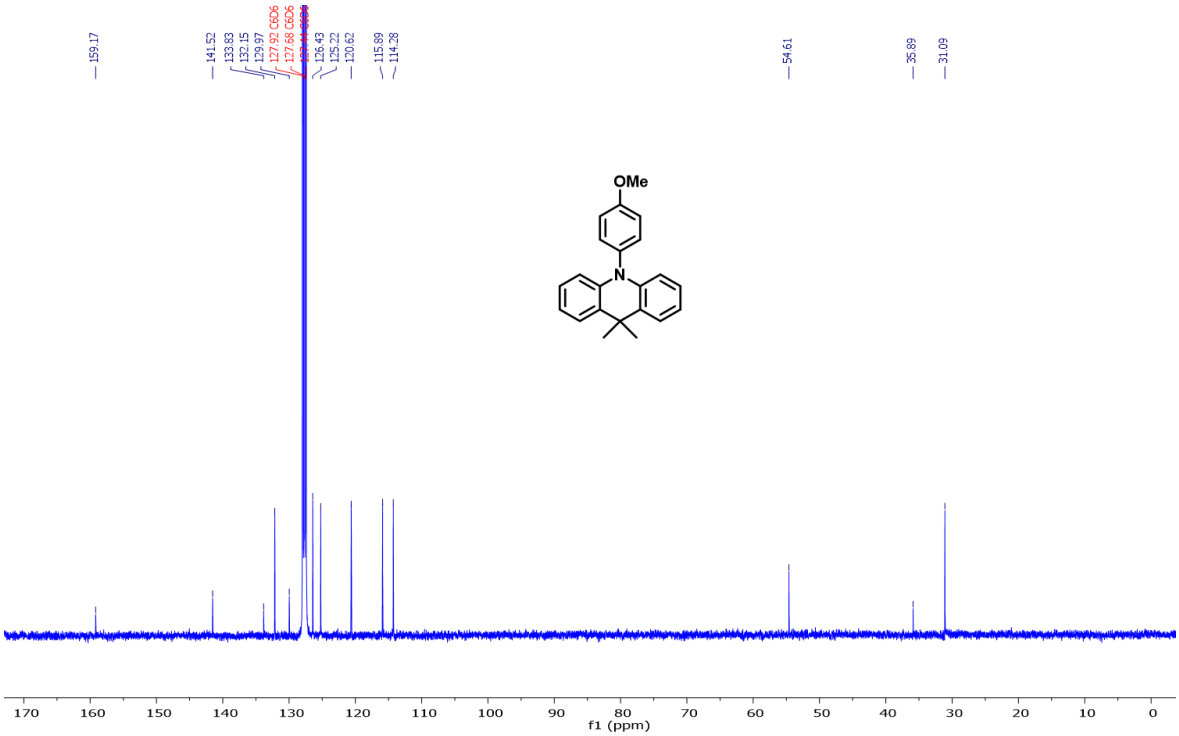
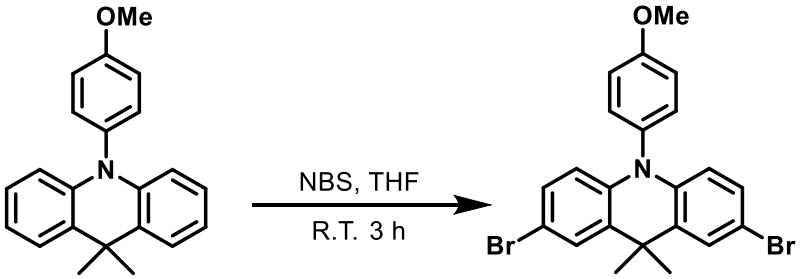


Figure S25: ^{13}C NMR spectrum of 10-(4-methoxyphenyl)-9,9-dimethyl-9,10-dihydroacridine in C_6D_6.

Synthesis of 2,7-dibromo-10-(4-methoxyphenyl)-9,9-dimethyl-9,10-dihydroacridine



1.0 g of 9,10-dihydro-9,9-dimethyl-10-(4-Methoxyphenyl)-acridine (3.2 mmol, 1.0 eq.) was dissolved in 50 mL THF under ambient atmosphere. 1.41 g of *N*-Bromosuccinimide (7.9 mmol, 2.5 eq.) was slowly added to make a light brown solution. The reaction then stirred at room temperature for 3 hours. The solution was then concentrated via rotary evaporation, washed with water 3 times, and dried with magnesium sulfate. The product was recrystallized using DCM layered with methanol at -25 ºC overnight. The product was isolated by filtration and dried under vacuum to give a brownish-white solid, which was used without further purification. Yield: 1.16 g, 77.6%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.49 (d, *J* = 2.3 Hz, 2H), 7.21 – 7.09 (m, 4H), 7.05 (dd, *J* = 8.8, 2.3 Hz, 2H), 6.17 (d, *J* = 8.7 Hz, 2H), 3.91 (s, 3H), 1.63 (s, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.46, 140.08, 132.78, 131.71, 131.60, 129.27, 127.97, 116.22, 115.86, 113.17, 55.56, 36.26, 30.93.

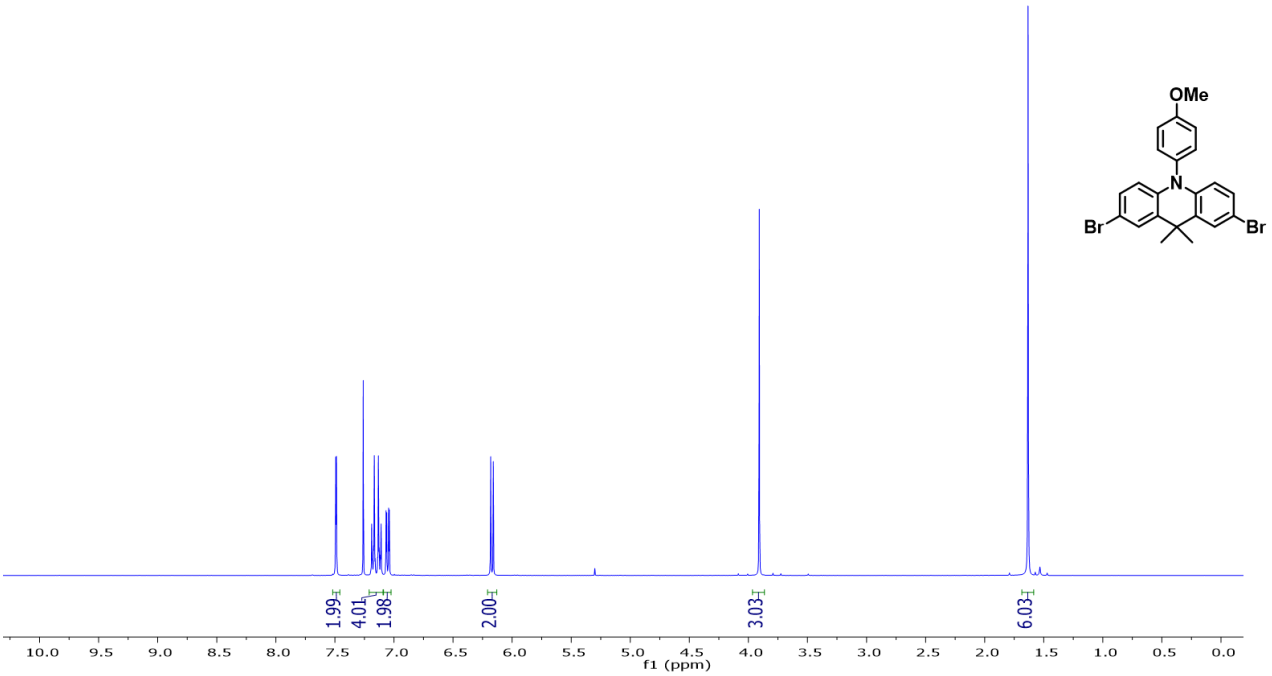


Figure S26: ^{1}H NMR spectrum of 2,7-dibromo-10-(4-methoxyphenyl)-9,9-dimethyl-9,10-dihydroacridine in $CDCl_3$.

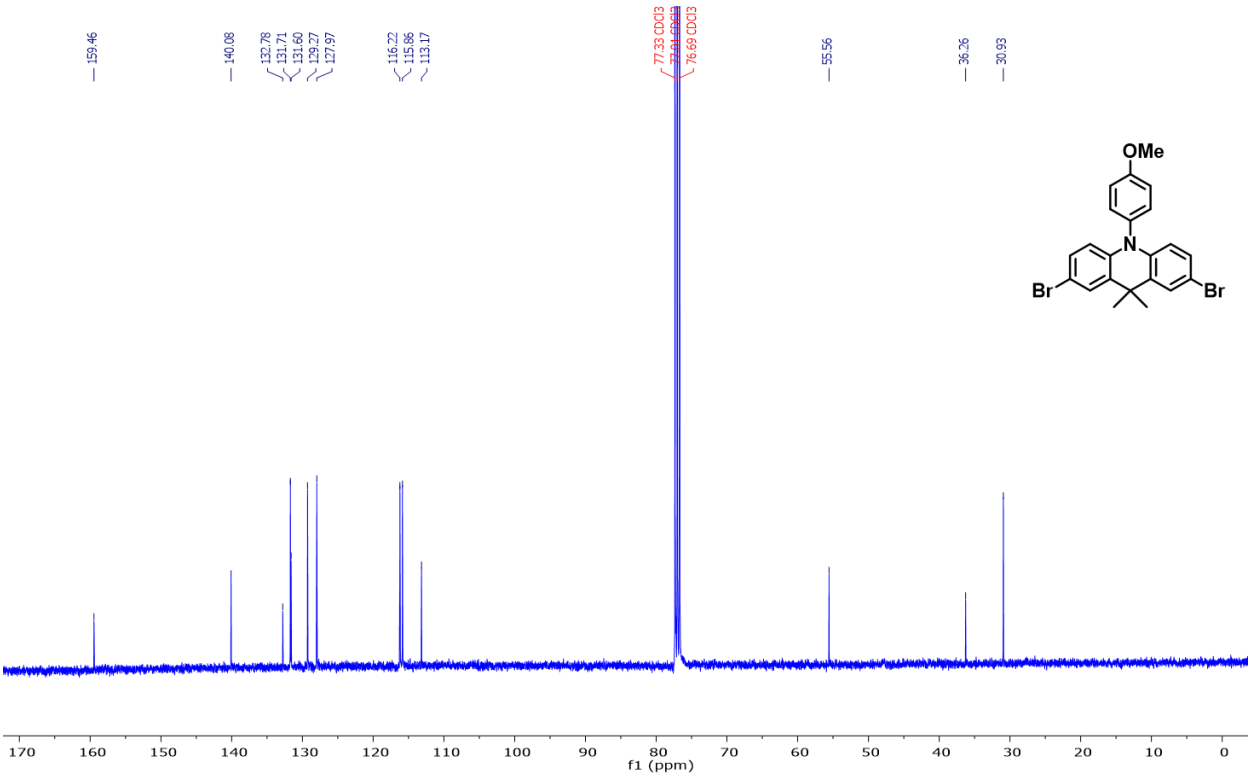
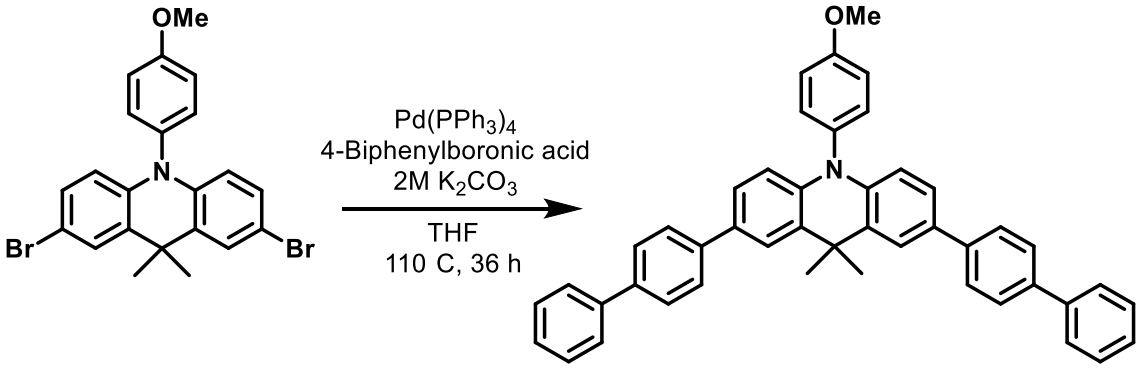


Figure S27: ^{13}C NMR spectrum of 2,7-dibromo-10-(4-methoxyphenyl)-9,9-dimethyl-9,10-dihydroacridine in $CDCl_3$.

Synthesis of 2,7-di([1,1'-biphenyl]-4-yl)-10-(4-methoxyphenyl)-9,9-dimethyl-9,10-dihydroacridine



0.5 g of 2,7-dibromo-9,10-dihydro-9,9-dimethyl-10-(4-Methoxyphenyl)-acridine (1.1 mmol, 1 eq.) and 0.89 g of 4-Biphenylboronic acid (4.5 mmol, 4 eq.) was loaded into a storage tube under ambient atmosphere. The storage tube was taken into a nitrogen-filled glovebox, then loaded with 0.184 g Tetrakis(triphenylphosphine)palladium(0) (0.159 mmol, 15 mol %). The solids were dissolved in 40 mL THF. The storage tube was sealed and brought out of the glovebox, where 12 mL of degassed 2M K_2CO_3 (22 eq.) was added using a long needle and syringe to produce a biphasic yellow and colorless solution. The solution was heated to 110 ºC for 36 hours, then brought to room temperature. The solution turned reddish-brown upon exposure to air. The solution was concentrated and extracted into DCM, then dried using magnesium sulfate, filtered, and concentrated. The crude mixture was redissolved in DCM then passed through a silica plug. The filtrate was concentrated, then dissolved in toluene and passed through an additional silica plug to remove residual palladium. The filtrate was collected and concentrated, then purified by column chromatography with hexanes: ethyl acetate ramping from 100:0 to 80:20. The product, a white solid, was then recrystallized with Ethyl acetate/MeOH at -25 ºC to give 0.385 g of a white solid with a yield of 58.6%. ^{1}H NMR (400 MHz, Benzene-d_6) δ 7.91 (d, J = 2.1 Hz, 2H), 7.73 – 7.65 (m, 4H), 7.64 – 7.50 (m, 11H), 7.40 – 7.33 (m, 3H), 7.27 (td, J = 7.7, 2.4 Hz, 5H), 6.91 – 6.84 (m, 2H), 6.64 (d, J = 8.5 Hz, 2H), 3.34 (s, 3H), 1.81 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.32, 140.86, 140.68, 140.53, 140.24, 139.58, 139.30, 132.93, 132.02, 130.27, 128.83, 128.79, 127.56, 127.46, 127.38, 127.18, 127.05, 126.99, 126.88, 125.08, 124.21, 116.12, 114.61, 77.33, 77.01, 76.70, 55.59, 36.34, 31.86. HRMS (ESI) calculated for (M+H)+ for $C_{46}H_{37}NO$, 619.28751; Found, 619.2877.

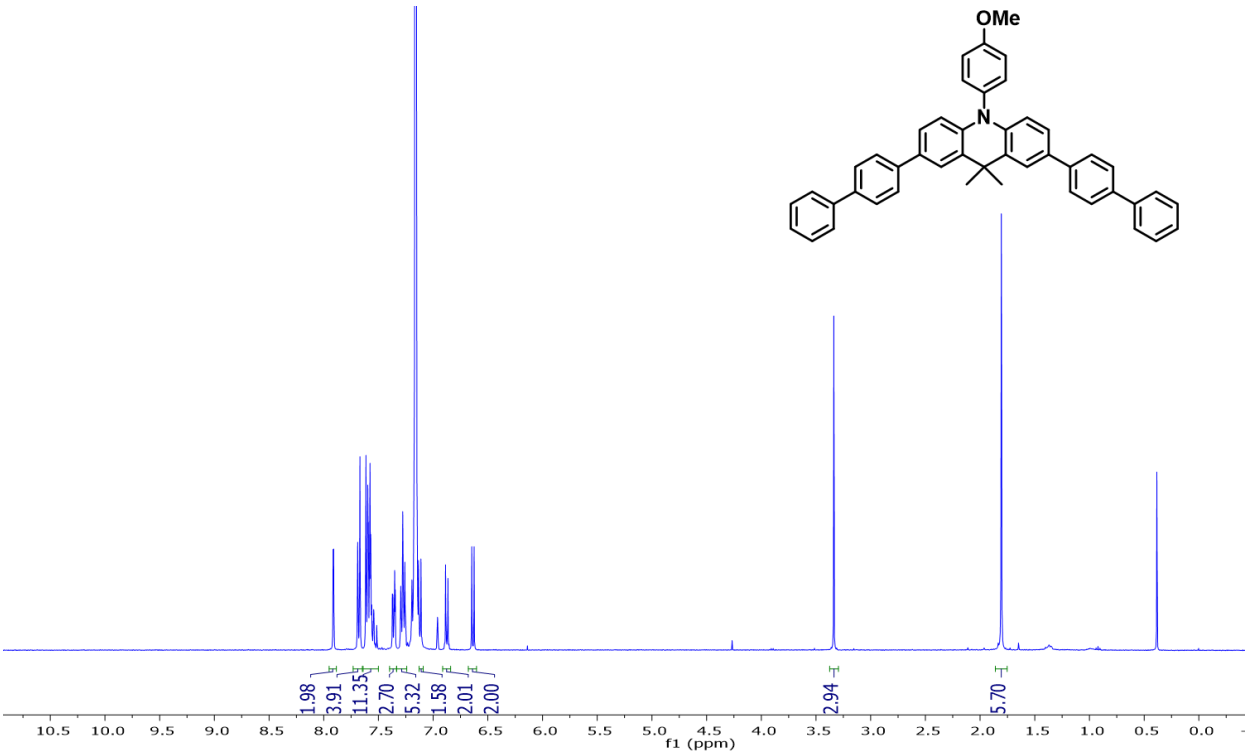


Figure S28: ^{1}H NMR spectrum of 2,7-di([1,1'-biphenyl]-4-yl)-10-(4-methoxyphenyl)-9,9-dimethyl-9,10-dihydroacridine in C_6D_6.

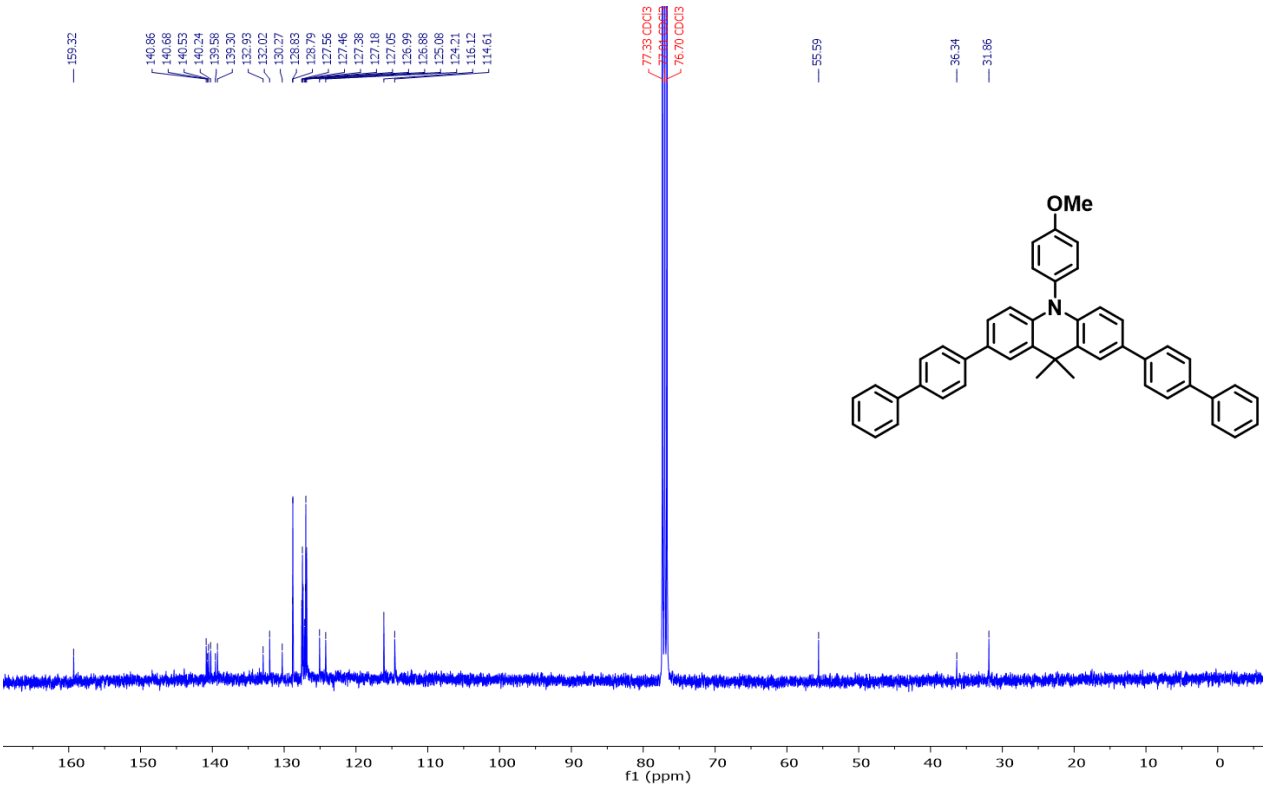
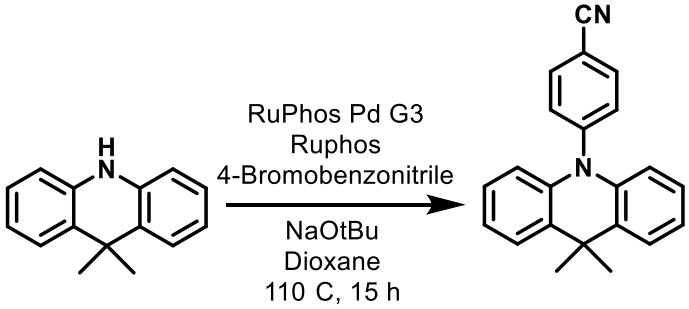


Figure S29: ^{13}C NMR spectrum of 2,7-di([1,1'-biphenyl]-4-yl)-10-(4-methoxyphenyl)-9,9-dimethyl-9,10-dihydroacridine in C_6D_6.

Synthesis of 4-(9,9-dimethylacridin-10(9*H*)-yl)benzonitrile



A storage tube was loaded with 2.0 g (9.6 mmol, 1 eq.) 9,10-Dihydro-9,9-dimethylacridine, 3.5 g 4-Bromobenzonitrile (19.1 mmol, 2.0 eq.), 0.118 g RuPhos ligand (0.28 mmol, 0.03 eq.), and 1.8 g sodium *tert*-butoxide (19.1 mmol, 2 eq.) under ambient atmosphere, then brought into a nitrogen-filled glovebox. Then, 0.244 g RuPhos Pd G3 precatalyst (0.28 mmol, 0.03 eq.) and 15 mL of degassed dioxane was added. The solution was sealed and brought outside of the glovebox, then heated to 110 ºC for 15 hours. The solution was cooled to room temperature, then transferred to a flask and concentrated. The brown solid was dissolved in toluene then passed through a silica plug. The filtrate was concentrated, then recrystallized with DCM/MeOH at -25 ºC overnight. The product was collected via vacuum filtration, washed with methanol, and dried overnight under vacuum to yield 1.7 g (57.3% yield) of pale-yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.21 – 8.12 (m, 2H), 7.79 – 7.70 (m, 4H), 7.32 – 7.19 (m, 4H), 6.59 – 6.51 (m, 2H), 1.93 (s, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 146.12, 140.17, 134.76, 131.53, 131.06, 126.48, 125.45, 121.69, 118.39, 114.81, 111.38, 36.21, 30.85. HRMS (ESI) calculated for (M+H)+ for $C_{22}H_{18}N_2$, 311.15428; Found, 311.15351.

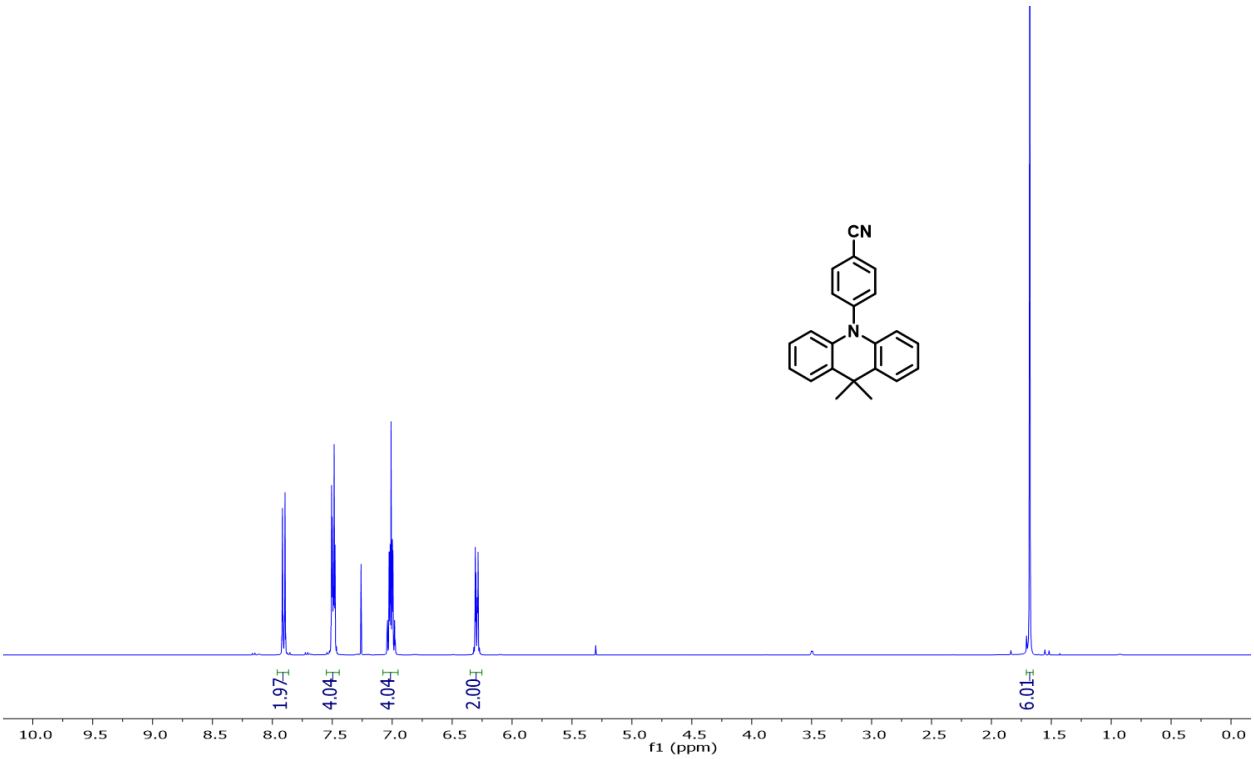


Figure S30: ^{1}H NMR spectrum of 4-(9,9-dimethylacridin-10(9H)-yl)benzonitrile in $CDCl_3$.

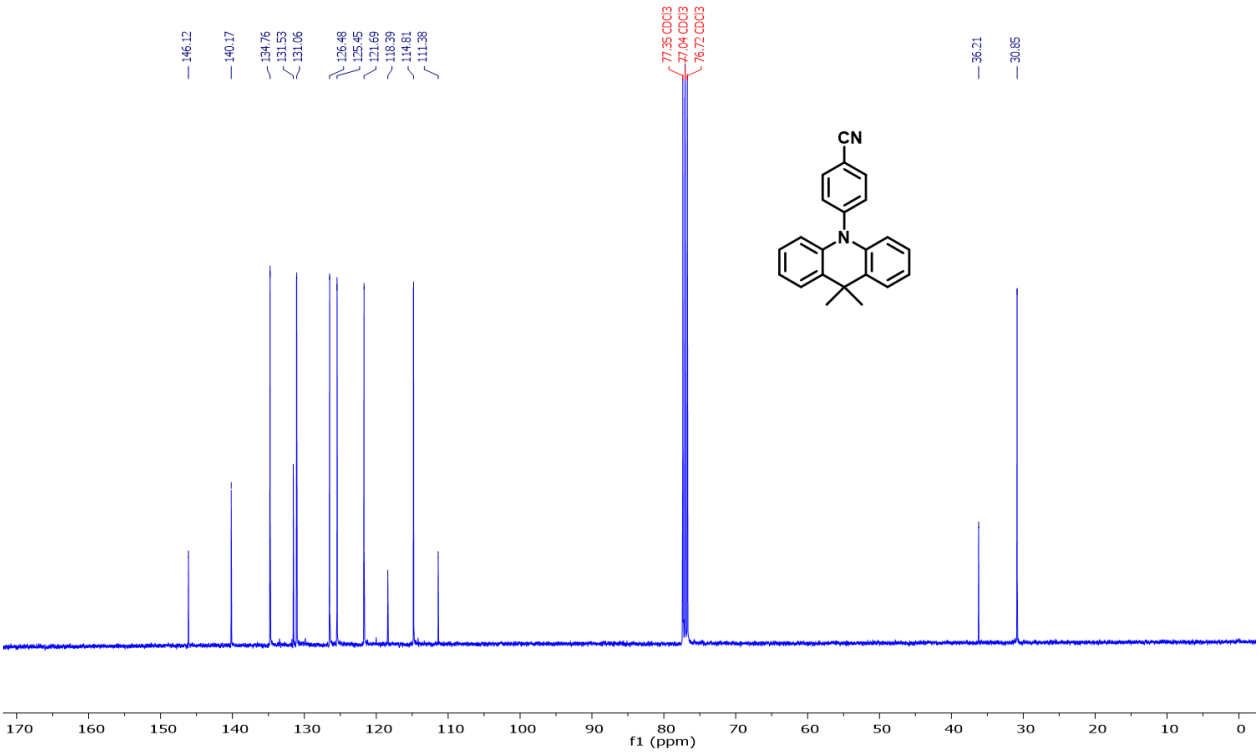
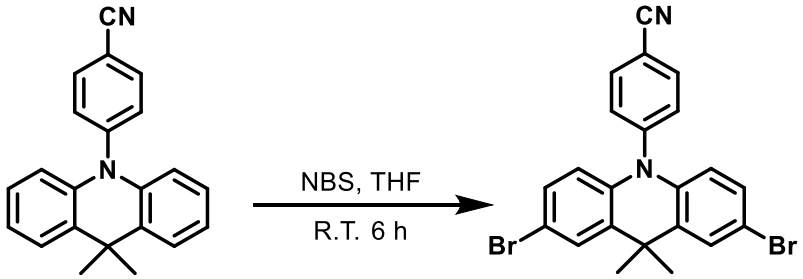


Figure S31: ^{13}C NMR spectrum of 4-(9,9-dimethylacridin-10(9H)-yl)benzonitrile in $CDCl_3$.

Synthesis of 4-(2,7-dibromo-9,9-dimethylacridin-10(9*H*)-yl)benzonitrile



1.0 g of 9,10-dihydro-9,9-dimethyl-10-(4-cyanophenyl)-acridine (3.2 mmol, 1.0 eq.) was dissolved in 20 mL THF under ambient atmosphere. 1.26 g of *N*-Bromosuccinimide (7.1 mmol, 2.2 eq.) was slowly added to make a colorless solution. The reaction then stirred at room temperature for 6 hours. The solution was then concentrated via rotary evaporation, washed with water 3 times, and dried with magnesium sulfate. The product was recrystallized using DCM layered with methanol at -25 ºC overnight. The product was isolated by filtration and dried under vacuum to give a pale yellow crystalline solid, which was used without further purification. Yield: 1.0g, 66%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.91 – 7.82 (m, 2H), 7.46 (d, *J* = 2.3 Hz, 2H), 7.41 – 7.35 (m, 2H), 7.02 (dd, *J* = 8.8, 2.3 Hz, 2H), 6.01 (d, *J* = 8.8 Hz, 2H), 1.57 (s, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 145.00, 138.97, 135.07, 132.42, 131.65, 129.50, 128.41, 117.97, 115.93, 114.34, 112.59, 36.40, 30.78.

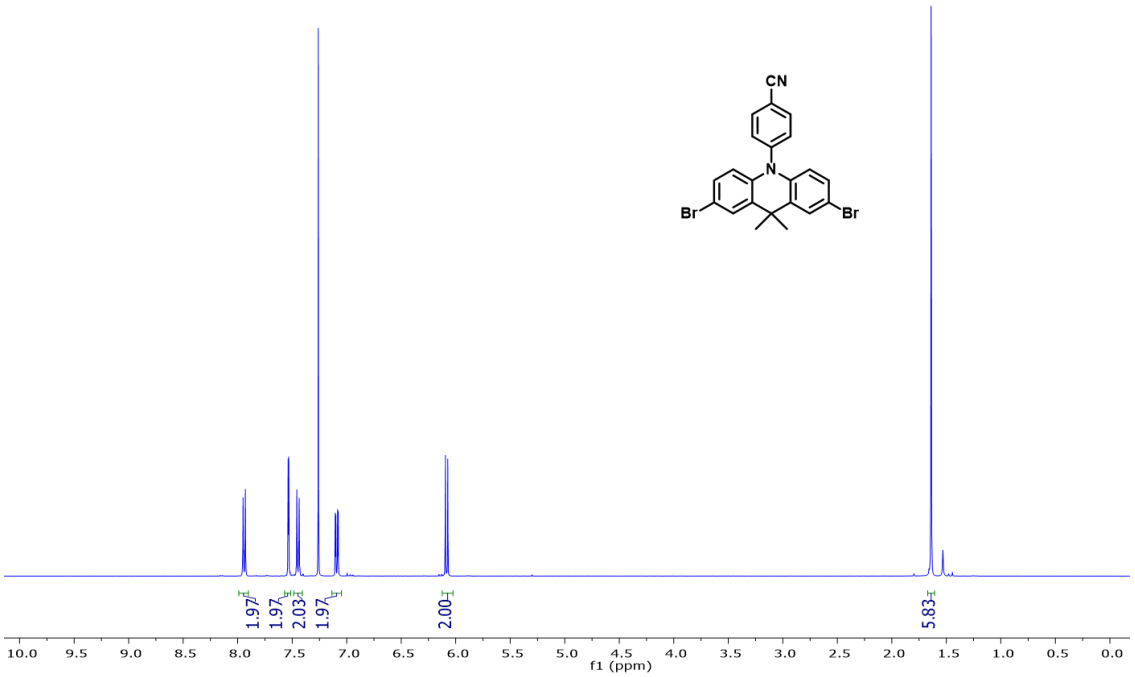


Figure S32: ^{1}H NMR spectrum of 4-(2,7-dibromo-9,9-dimethylacridin-10(9H)-yl)benzonitrile in $CDCl_3$.

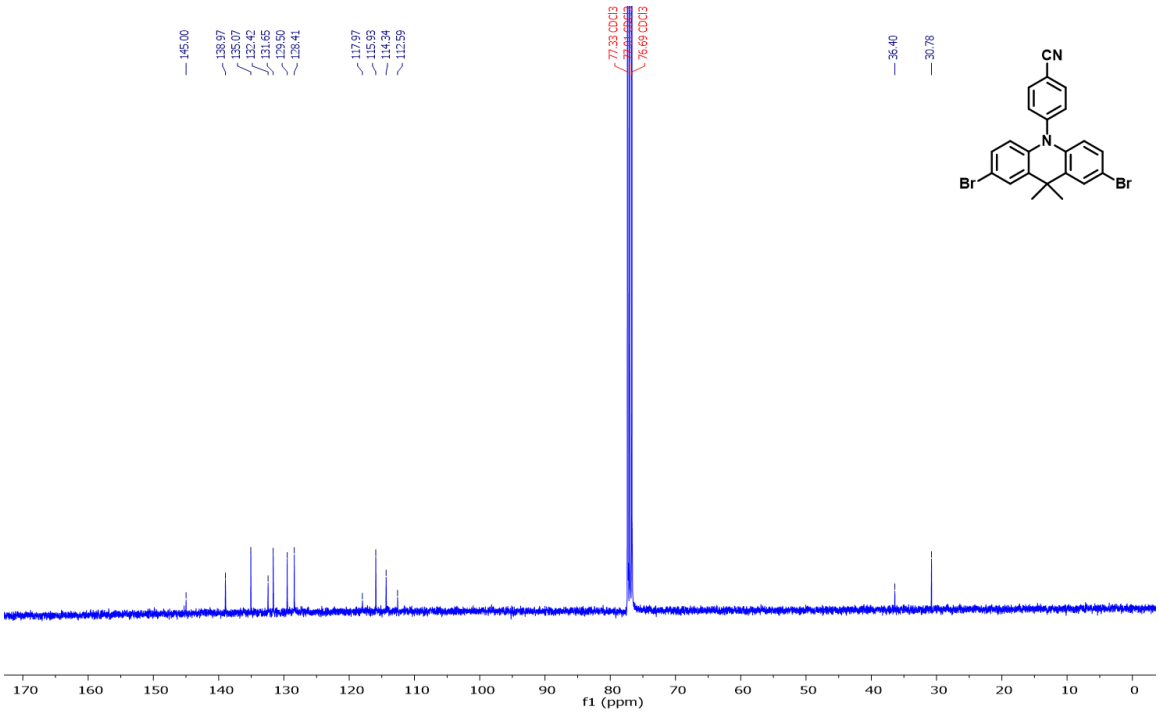
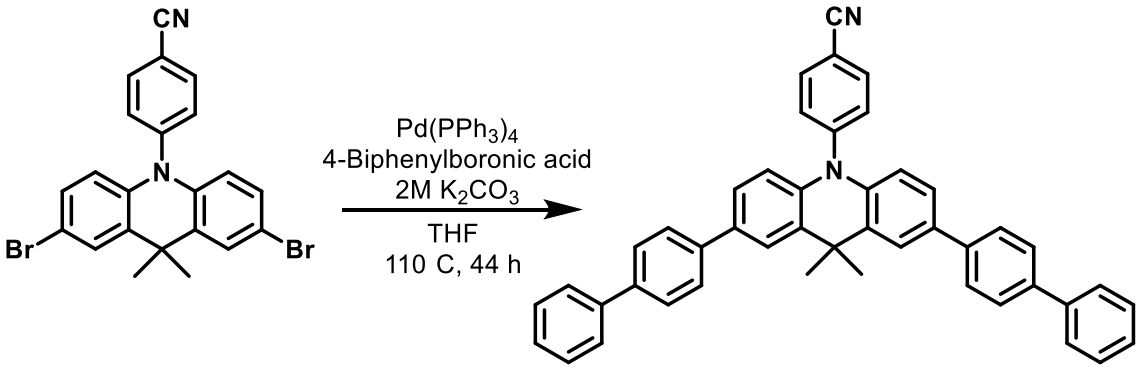


Figure S33: ^{13}C NMR spectrum of 4-(2,7-dibromo-9,9-dimethylacridin-10(9H)-yl)benzonitrile in $CDCl_3$.

Synthesis of 4-(2,7-di([1,1'-biphenyl]-4-yl)-9,9-dimethylacridin-10(9*H*)-yl)benzonitrile



0.8 g of 2,7-dibromo-9,10-dihydro-9,9-dimethyl-10-(4-cyanophenyl)-acridine (1.7 mmol, 1 eq.) and 1.4 g of 4-Biphenylboronic acid (6.8 mmol, 4 eq.) was loaded into a storage tube under ambient atmosphere. The storage tube was taken into a nitrogen-filled glovebox, then loaded with 0.296 g Tetrakis(triphenylphosphine)palladium(0) (0.257 mmol, 15 mol %). The solids were dissolved in 50 mL degassed THF. The storage tube was sealed and brought out of the glovebox, where 19 mL of degassed 2M K_2CO_3 (22 eq.) was added using a long needle and syringe to produce a biphasic yellow and colorless solution. The solution was heated to 110 ºC for 44 hours, then brought to room temperature. The solution turned red upon exposure to air. The solution was concentrated and extracted into DCM. A yellow emulsion formed, which was filtered and washed with methanol to produce the crude product as a pale-yellow powder. The solid was dissolved in DCM and washed with water 3 times, then dried with magnesium sulfate and concentrated. The product was recrystallized with DCM/MeOH at room temperature 2 times to give 0.88 g at 84% yield. ^{1}H NMR (400 MHz, Benzene-d_6) δ 7.87 (d, J = 2.1 Hz, 2H), 7.72 – 7.55 (m, 12H), 7.38 – 7.24 (m, 6H), 7.24 – 7.18 (m, 2H), 7.11 – 7.03 (m, 2H), 6.84 – 6.75 (m, 2H), 6.23 (d, J = 8.5 Hz, 2H), 1.73 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.01, 141.04, 140.22, 139.99, 139.64, 134.51, 134.47, 131.34, 131.25, 128.92, 128.00, 127.76, 127.52, 127.18, 127.10, 125.39, 124.46, 118.01, 115.07, 112.21, 36.42, 31.27. HRMS (ESI) calculated for (M+H)+ for $C_{46}H_{34}N_2$, 614.2722; Found, 614.2736.

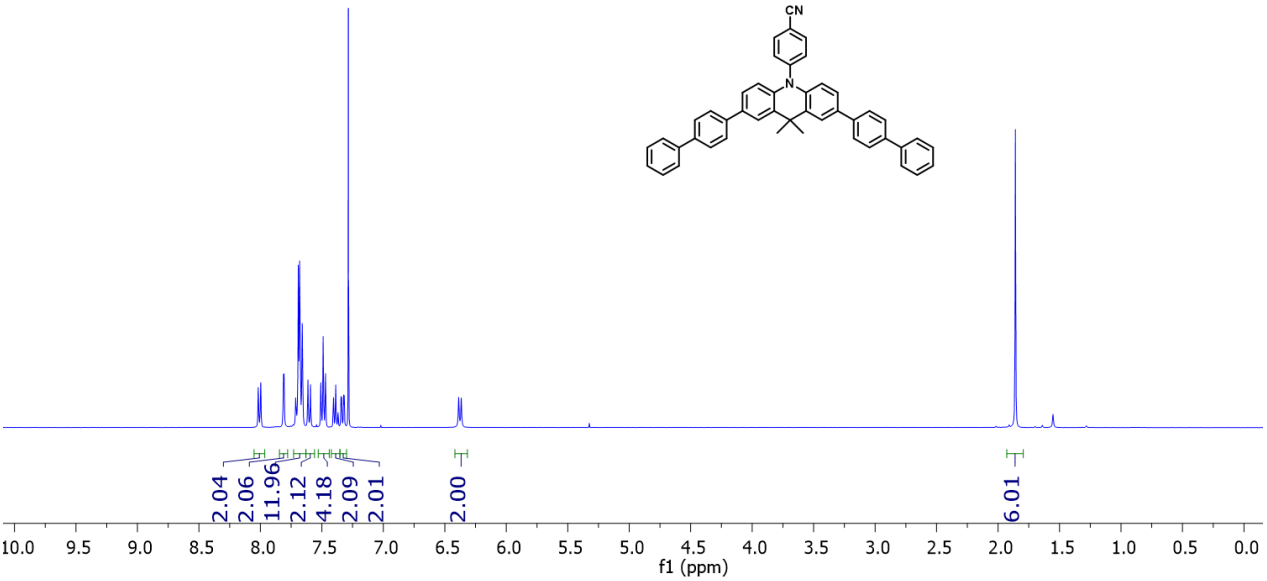


Figure S34: ^{1}H NMR spectrum of 4-(2,7-di([1,1'-biphenyl]-4-yl)-9,9-dimethylacridin-10(9H)-yl)benzonitrile in $CDCl_3$.

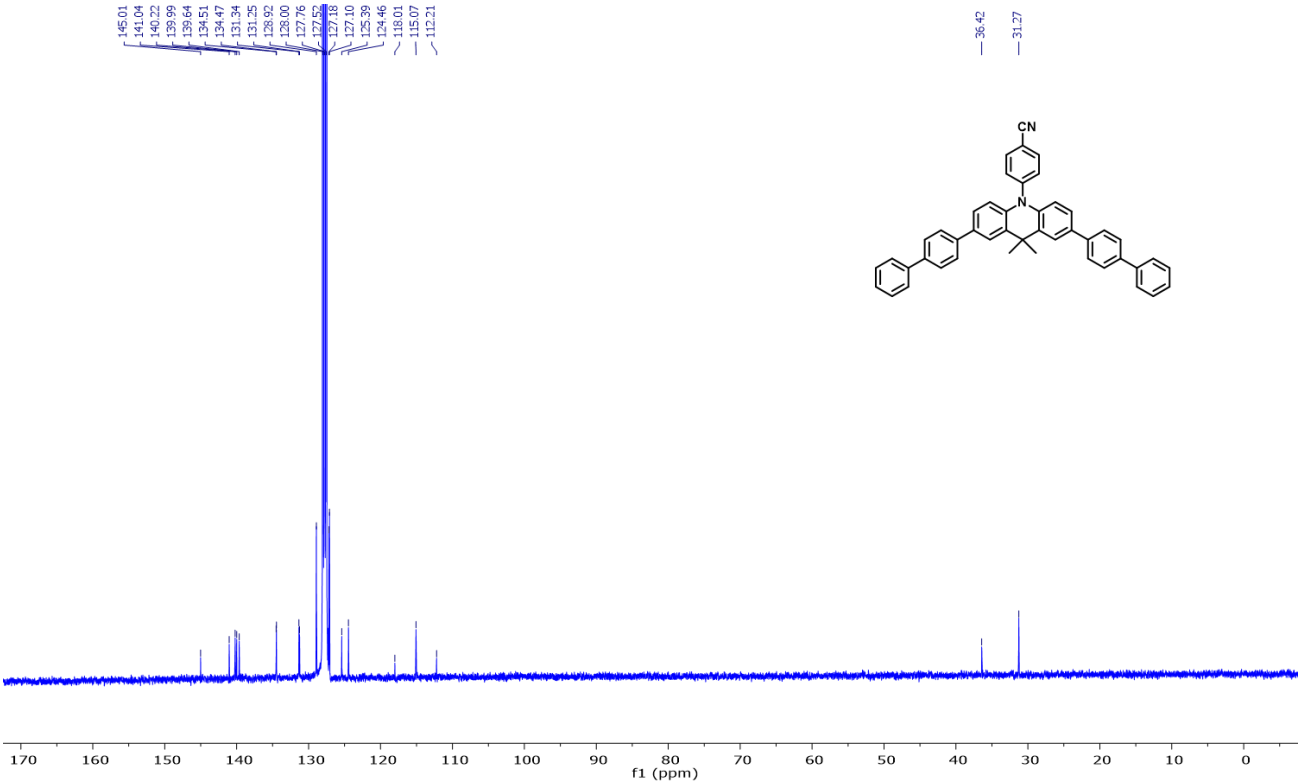


Figure S35: ^{13}C NMR spectrum of 4-(2,7-di([1,1'-biphenyl]-4-yl)-9,9-dimethylacridin-10(9H)-yl)benzonitrile in C_6D_6.

Photocatalyst and Precursors Characterization

UV-visible Spectroscopy:

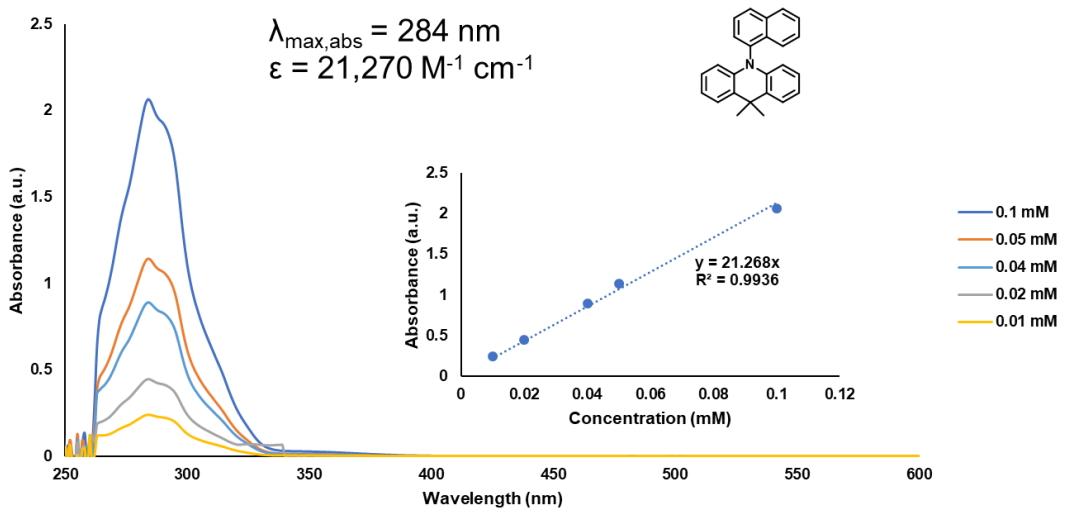


Figure S36: UV-vis spectrum of Acrid-1N (parent compound for **PCs 1, 2,** and **3**) at different concentrations in DMF with a path length of 1 cm. Graph in the lower left demonstrates the Beer-Lambert law relationship at the maximum wavelength of absorbance.

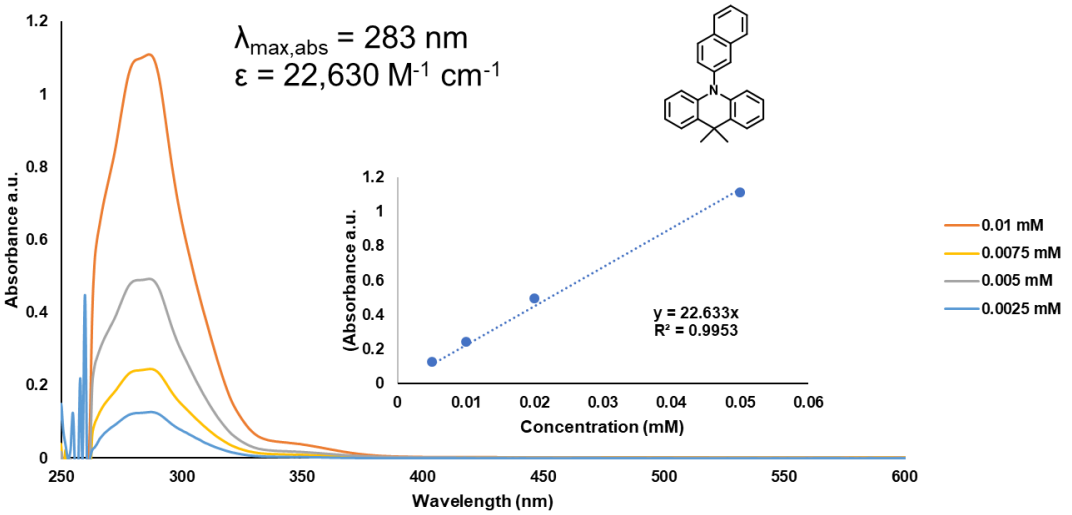


Figure S37: UV-vis spectrum of Acrid-2N (parent compound for **PC 4**) at different concentrations in DMF with a path length of 1 cm. Graph in the lower left demonstrates the Beer-Lambert law relationship at the maximum wavelength of absorbance.

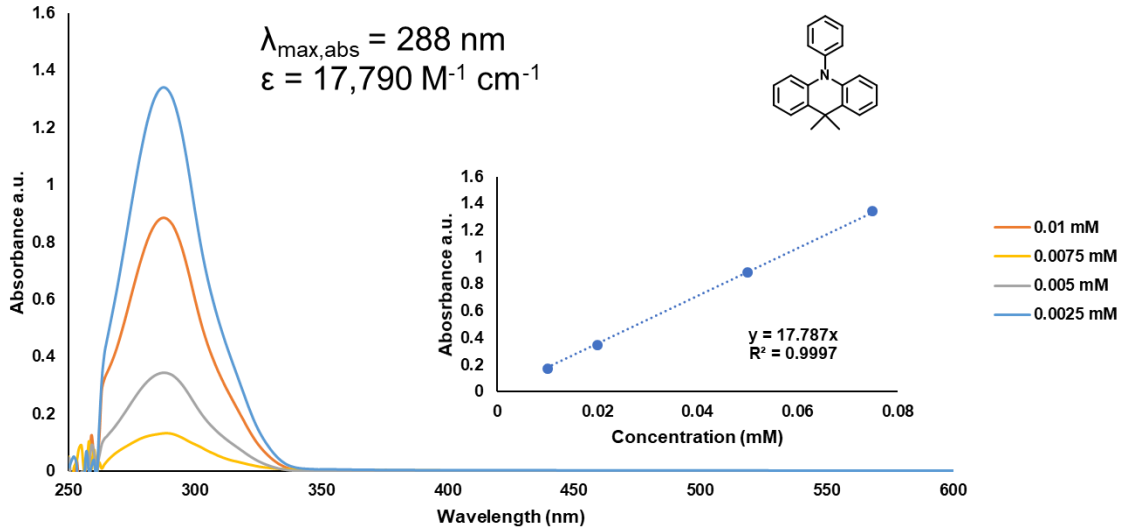


Figure S38: UV-vis spectrum of Acrid-Ph (parent compound for **PC 5**) at different concentrations in DMF with a path length of 1 cm. Graph in the lower left demonstrates the Beer-Lambert law relationship at the maximum wavelength of absorbance.

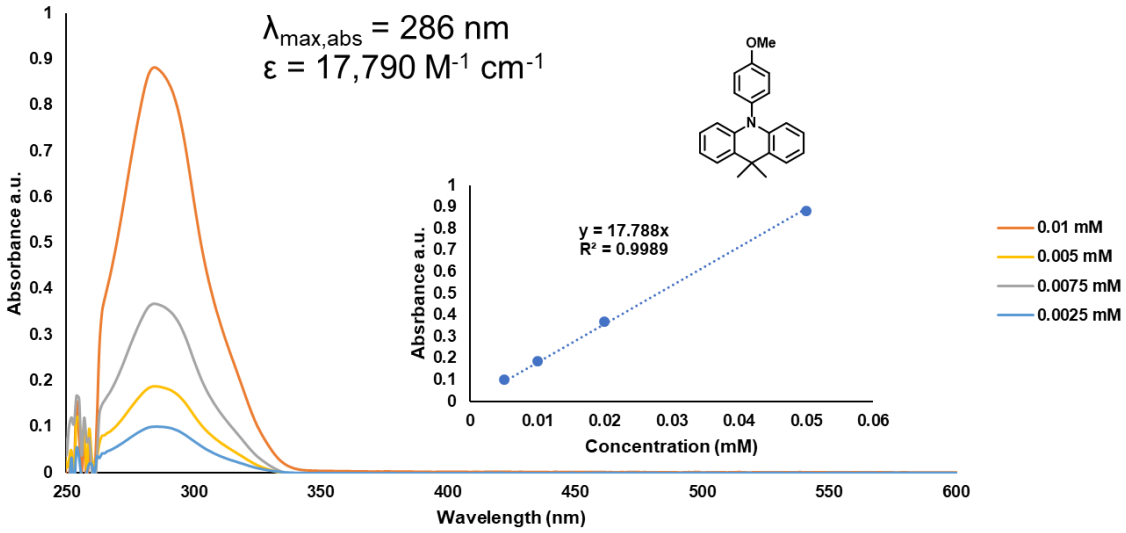


Figure S39: UV-vis spectrum of Acrid-OMe (parent compound for **PC 6**) at different concentrations in DMF with a path length of 1 cm. Graph in the lower left demonstrates the Beer-Lambert law relationship at the maximum wavelength of absorbance.

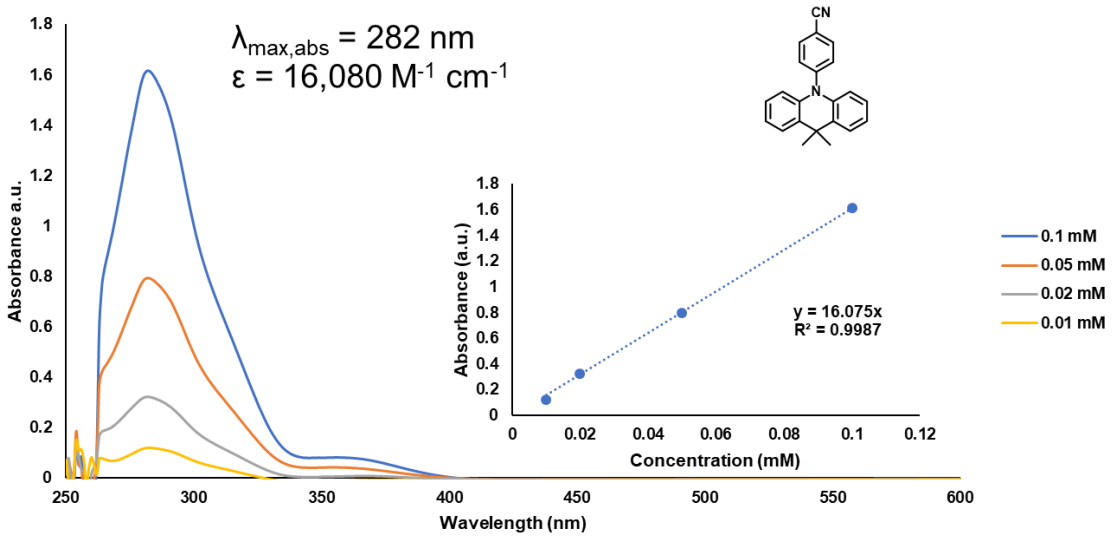


Figure S40: UV-vis spectrum of Acrid-CN (parent compound for **PC 7**) at different concentrations in DMF with a path length of 1 cm. Graph in the lower left demonstrates the Beer-Lambert law relationship at the maximum wavelength of absorbance.

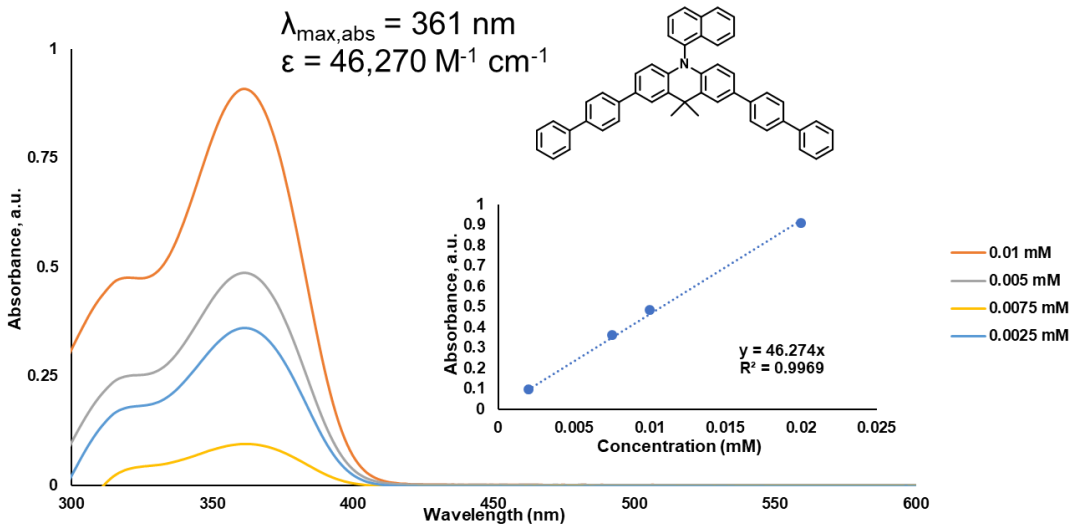


Figure S41: UV-vis spectrum of **PC 1** at different concentrations in DMF with a path length of 1 cm. Graph in the lower left demonstrates the Beer-Lambert law relationship at the maximum wavelength of absorbance.

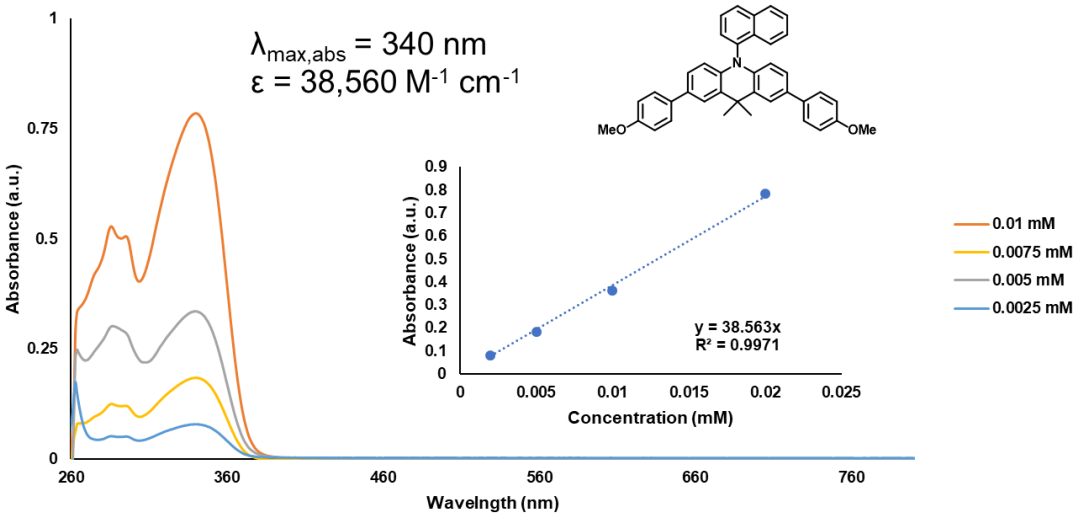


Figure S42: UV-vis spectrum of **PC 2** at different concentrations in DMF with a path length of 1 cm. Graph in the lower left demonstrates the Beer-Lambert law relationship at the maximum wavelength of absorbance.

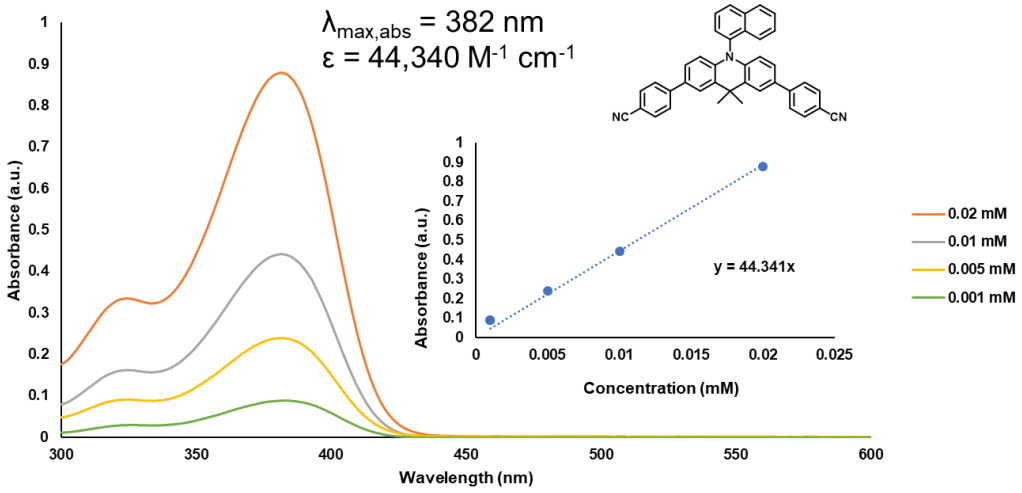


Figure S43: UV-vis spectrum of **PC 3** at different concentrations in DMF with a path length of 1 cm. Graph in the lower left demonstrates the Beer-Lambert law relationship at the maximum wavelength of absorbance.

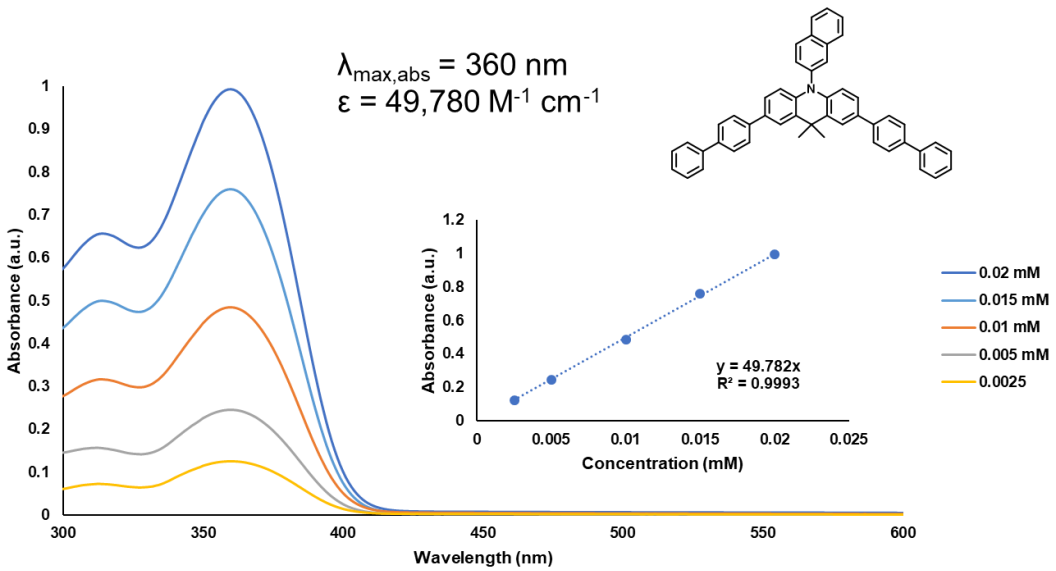


Figure S44: UV-vis spectrum of **PC 4** at different concentrations in DMF with a path length of 1 cm. Graph in the lower left demonstrates the Beer-Lambert law relationship at the maximum wavelength of absorbance.

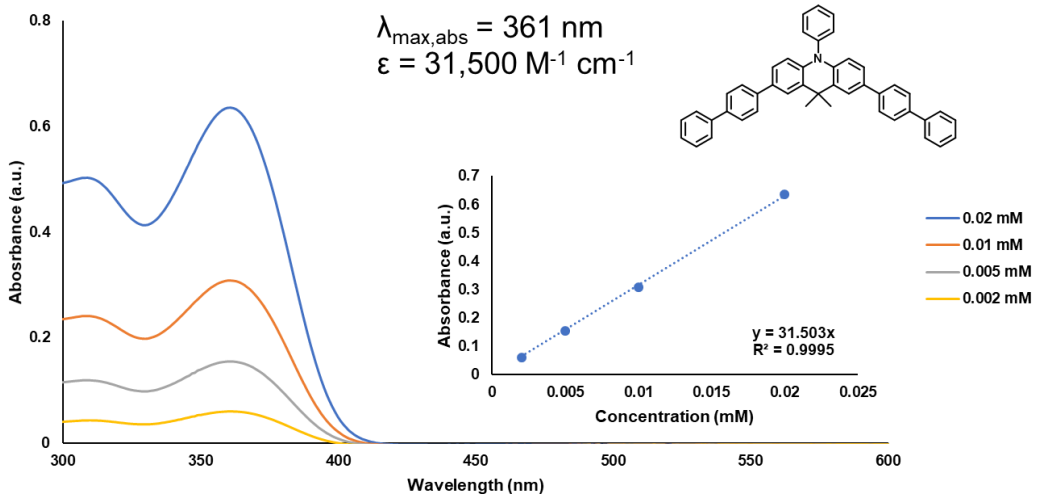


Figure S45: UV-vis spectrum of **PC 5** at different concentrations in DMF with a path length of 1 cm. Graph in the lower left demonstrates the Beer-Lambert law relationship at the maximum wavelength of absorbance.

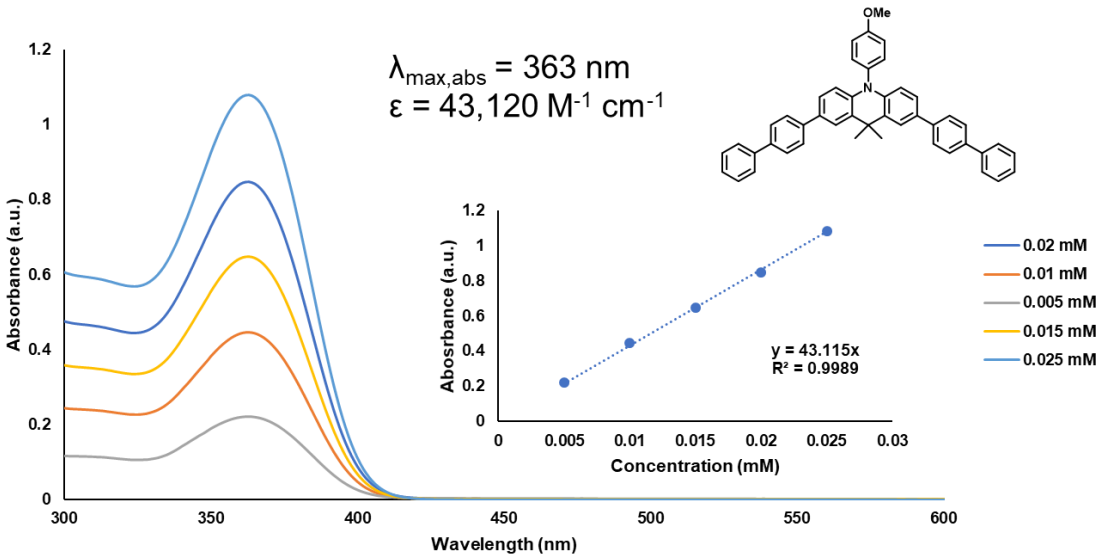


Figure S46: UV-vis spectrum of **PC 6** at different concentrations in DMF with a path length of 1 cm. Graph in the lower left demonstrates the Beer-Lambert law relationship at the maximum wavelength of absorbance.

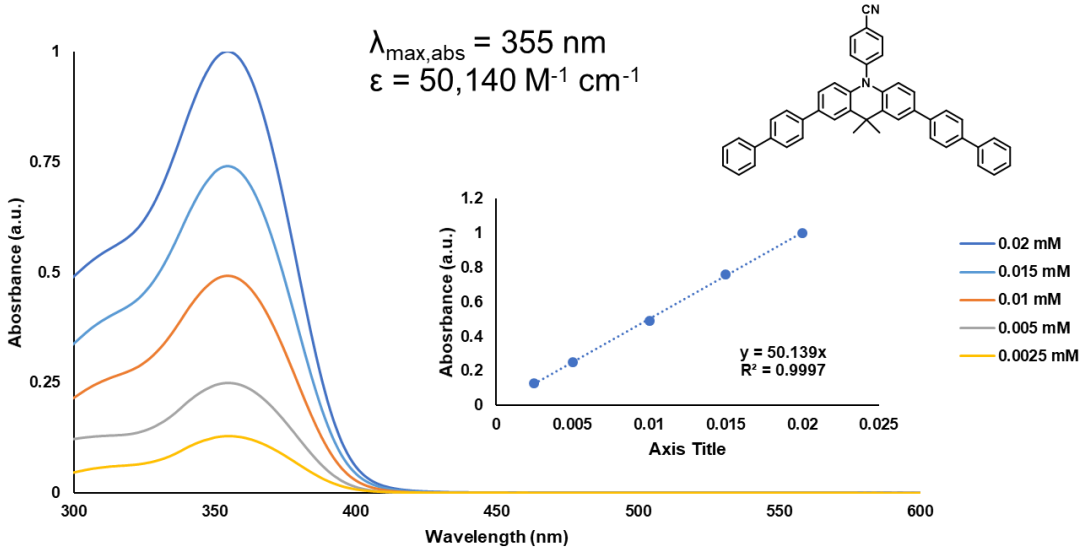


Figure S47: UV-vis spectrum of **PC 7** at different concentrations in DMF with a path length of 1 cm. Graph in the lower left demonstrates the Beer-Lambert law relationship at the maximum wavelength of absorbance.

Fluorescence Spectroscopy

Emission data was measured using an FS5 spectrofluorometer from Edinburg Instruments. All samples were prepared at 0.1 mM concentrations inside a nitrogen-filled glovebox. Measurements were taken in a 1 cm quartz cuvette, sealed with electrical tape. All precursor molecules were excited at 280 nm. All PCs were excited at 365 nm. Each measurement used a step size of 1 nm, a dwell time of 0.1 s, with 3 averaged scans.

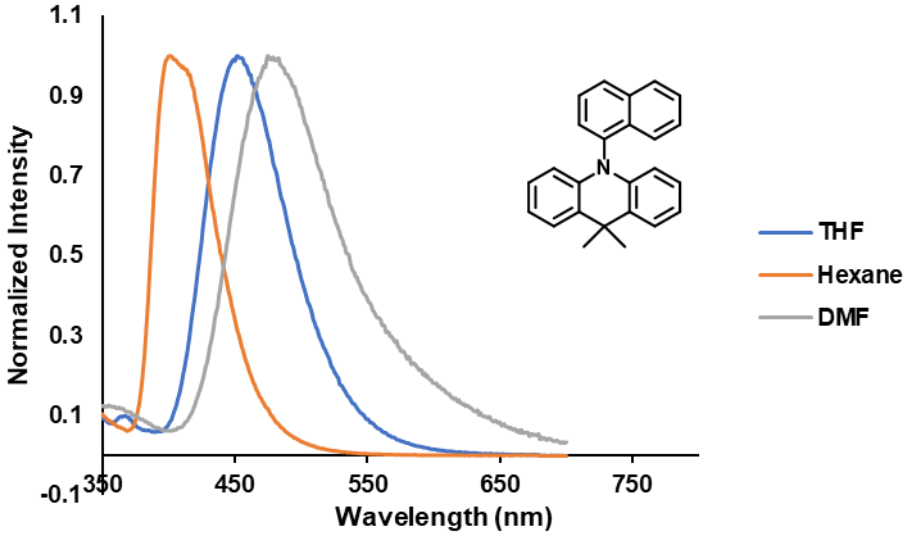


Figure S48: Normalized emission for Acrid-1N (precursor for **PCs 1, 2,** and **3**) measured in Hexane (orange), THF (blue) and DMF (grey).

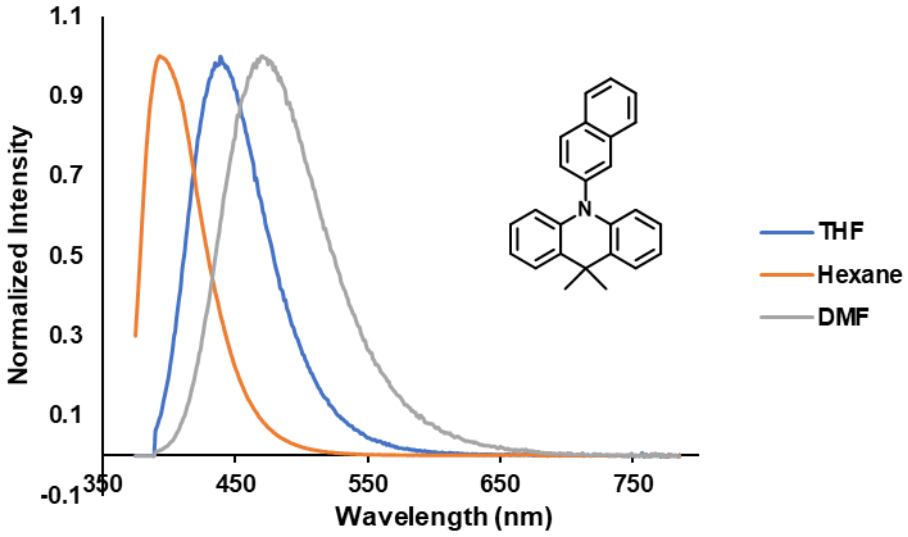


Figure S49: Normalized emission for Acrid-2N (precursor for **PC 4**) measured in Hexane (orange), THF (blue) and DMF (grey).

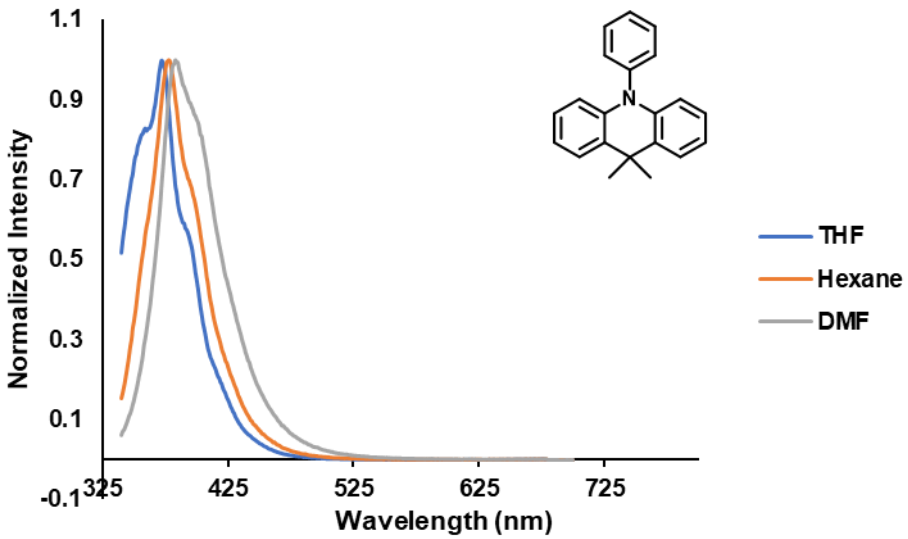


Figure S50: Normalized emission for Acrid-2N (precursor for **PC 5**) measured in Hexane (orange), THF (blue) and DMF (grey).

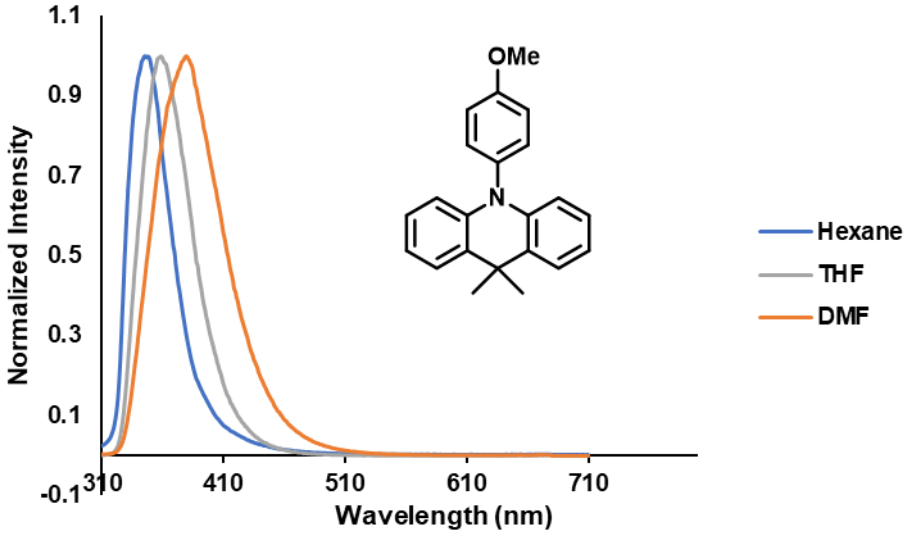


Figure S51: Normalized emission for Acrid-2N (precursor for **PC 6**) measured in Hexane (orange), THF (blue) and DMF (grey).

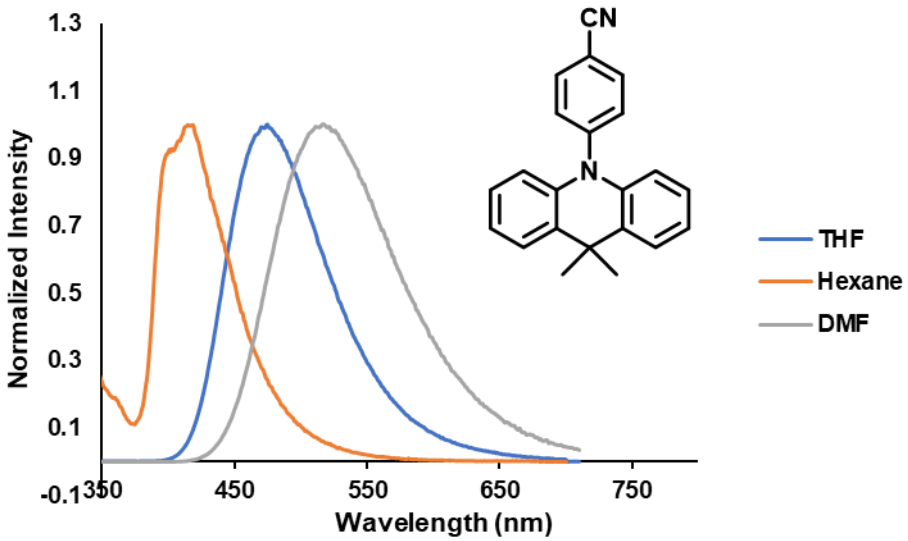


Figure S52: Normalized emission for Acrid-2N (precursor for **PC 7**) measured in Hexane (orange), THF (blue) and DMF (grey).

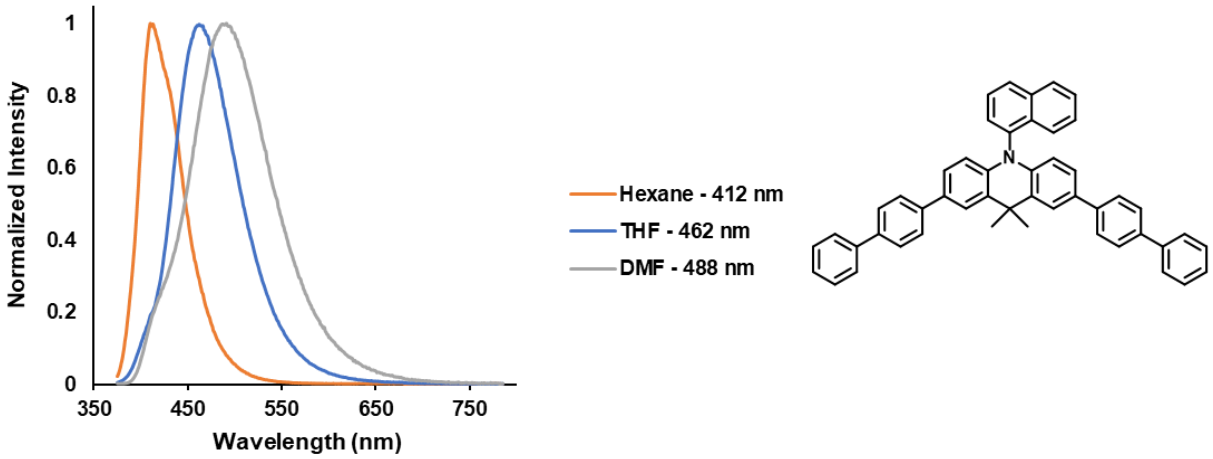


Figure S53: Normalized emission for **PC 1** measured in Hexane (orange), THF (blue) and DMF (grey).

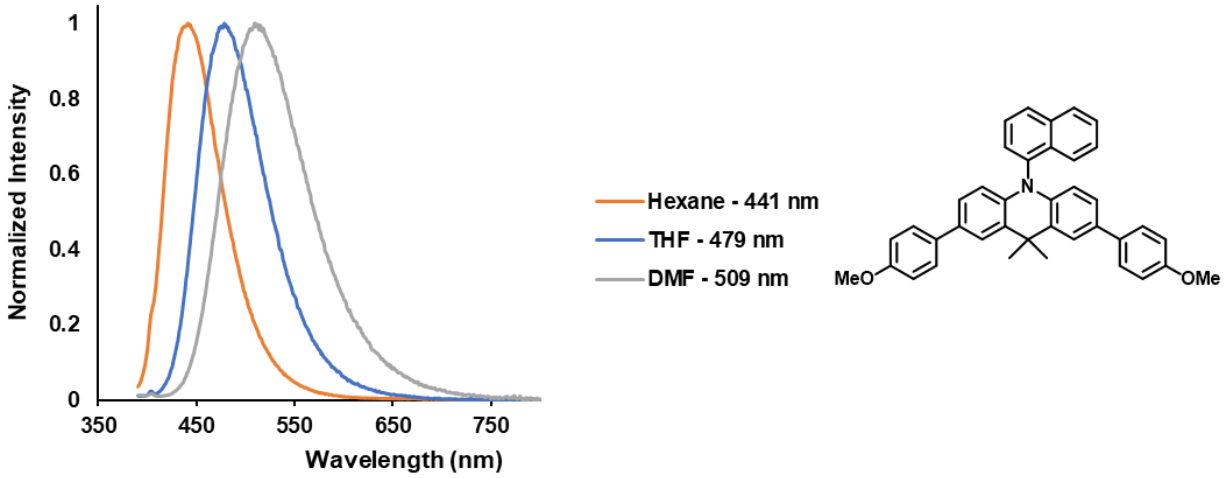


Figure S54: Normalized emission for **PC 2** measured in Hexane (orange), THF (blue) and DMF (grey).

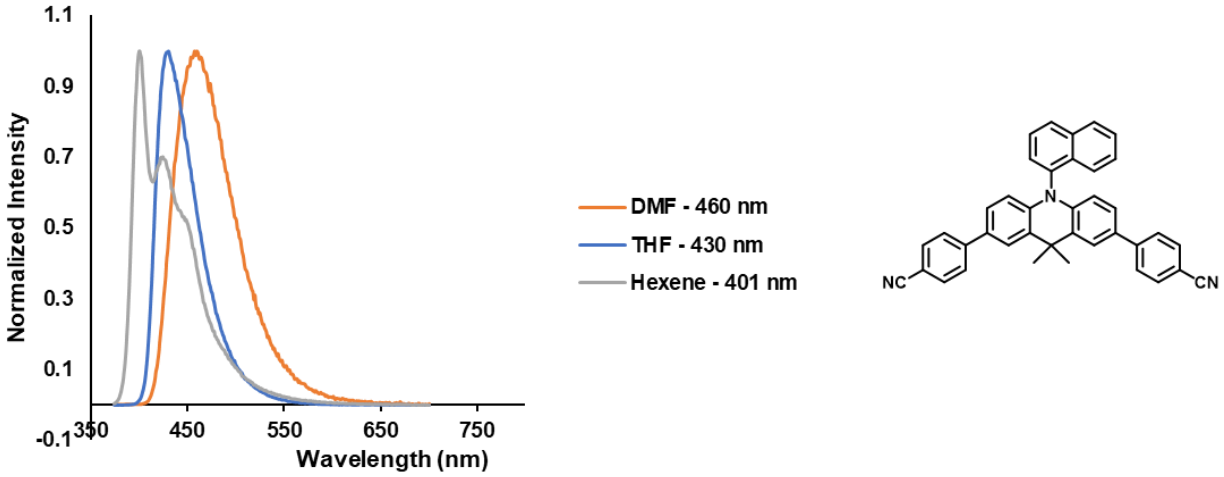


Figure S55: Normalized emission for **PC 3** measured in Hexane (orange), THF (blue) and DMF (grey).

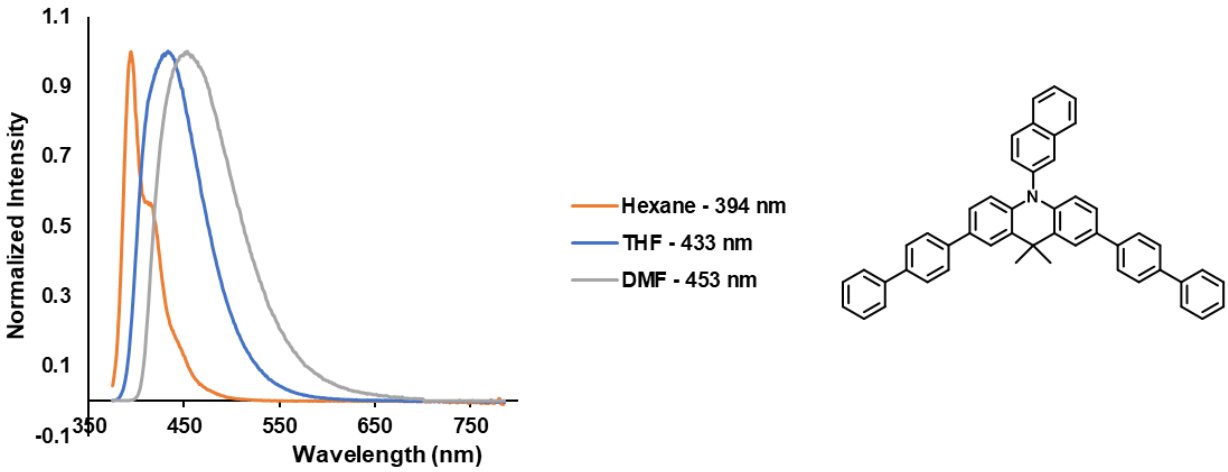


Figure S56: Normalized emission for **PC 4** measured in Hexane (orange), THF (blue) and DMF (grey).

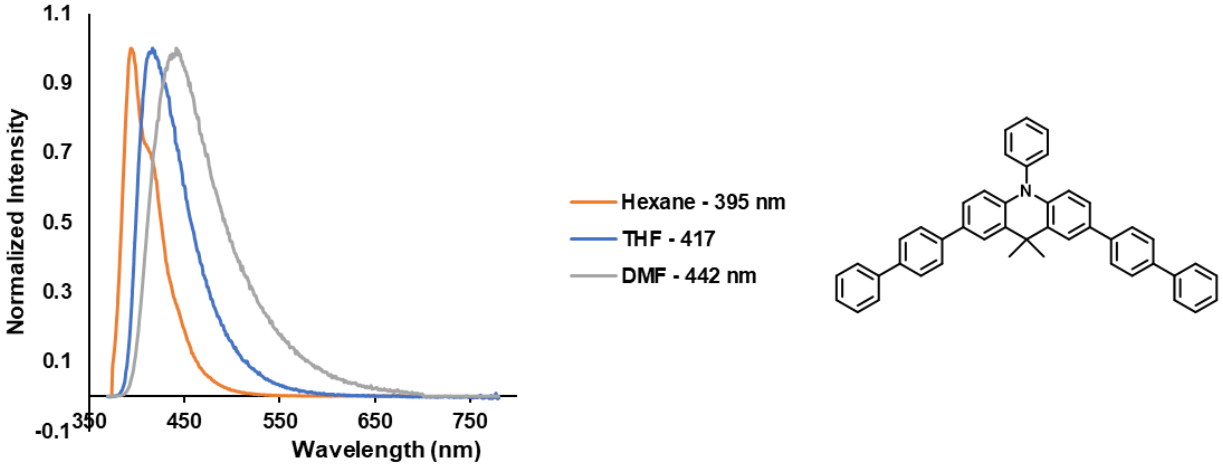


Figure S57: Normalized emission for **PC 5** measured in Hexane (orange), THF (blue) and DMF (grey).

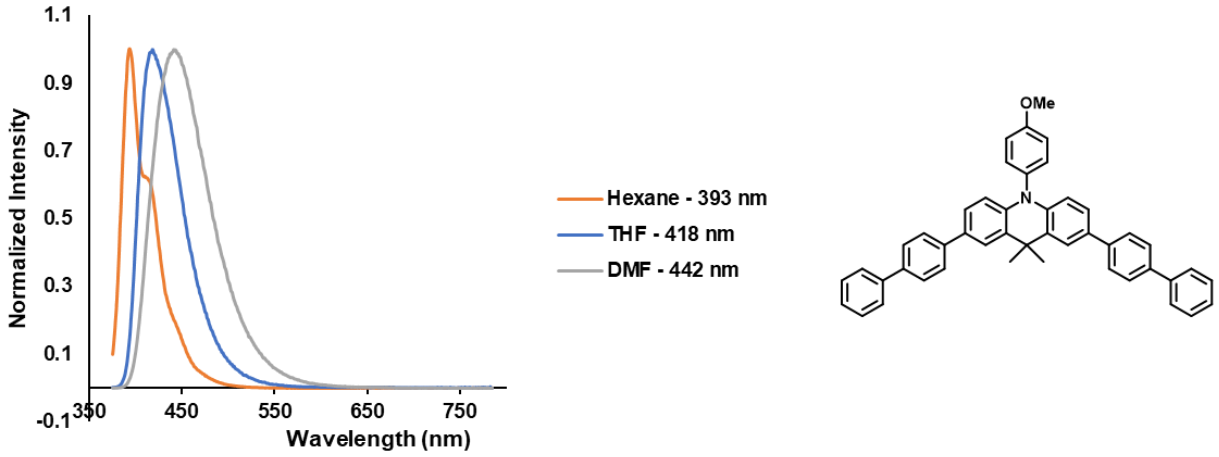


Figure S58: Normalized emission for **PC 6** measured in Hexane (orange), THF (blue) and DMF (grey).

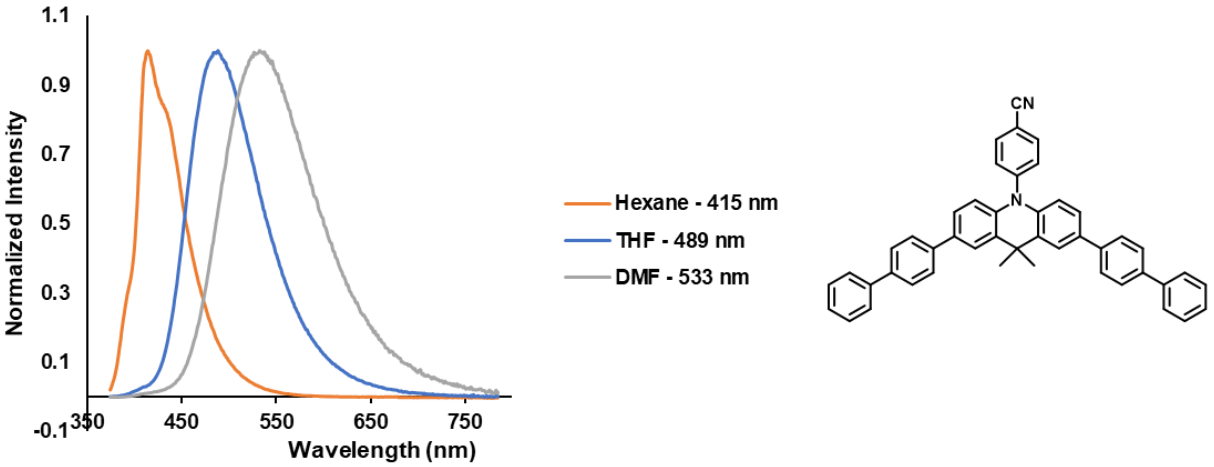


Figure S59: Normalized emission for **PC 7** measured in Hexane (orange), THF (blue) and DMF (grey).

Absolute Fluorescence Quantum Yields

Absolute fluorescence quantum yields (AFQY) of PCs 1-7 were measured using an FS5 Spectrofluorometer from Edinburg Instruments with an SC-30 Integrating Sphere accessory using a direct excitation measurement method. 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 as follows:

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

Scattering and emission spectral regions were measured separately. An O.D. filter for the scattering region with a correction of 9.67 x for R_s and S_s (in the case of excitation at 365 nm) after measurement. The transmission of the O.D. filter was measured at O.D. 0.103 using a Cary 5000 with diffuse reflectance accessory. All samples were prepared inside a nitrogen-filled glovebox at concentrations of 0.1 mM in degassed spectrochemical grade DMAc. Quartz cuvettes with white Teflon caps and a path length of 1 cm were used. The AFQY value was calculated using the Fluoracle software using the equation described above.

To represent reaction conditions, AFQY values were measured at 365 nm. PCs 3,4,5, and 6 showed some emission at 365 nm and so all PCs were also measured at 325 nm, with PC 2 measured with excitation at 305 nm due to strong absorption at 325 nm.

Table S3: Results of measurement of fluorescence quantum yields of PCs 1-7 with excitation at 365 nm and 325 nm.

PC	$\Phi_{f,\ 365\ nm}$	$\Phi_{f,\ 325\ nm}$
1	0.1	0.3
2	0.7	0.1[a]
3	94	83
4	5.7	3.8
5	38	27
6	98	70
7	6.4	8.2

[a]Due to strong PC absorption at 325 nm, 305 nm was used for excitation wavelength.

Time Resolved Emission Measurements

Time-resolved spectral emission measurements were performed on an LP980 spectrometer from Edinburgh Instruments equipped with a Continuum Minilight flashlamp pumped Q-switched Nd:Yag laser operating at 355 nm with a pulse-width of 2 ns and an intensified CCD camera for detection.

General Procedure: 0.5 mL of a 50 uM solution of PC dissolved in DMF was loaded into an NMR tube under inert atmosphere. The tube was frozen under liquid nitrogen, then placed into the sample chamber for analysis before thawing. Time-resolved emission was measured at time = 0 (no gate delay) with a 100 ns integration time and also with a delay of 1 ms with 30 ms integration time. Room temperature measurements were performed with time = 0, or no gate delay. To confirm that the 1 ms delayed emission at 77 K can be attributed to phosphorescence, room temperature measurements were also performed under the same conditions and no emission was detected for any PC. To evaluate influences of solvent polarity on time-resolved measurements, the above procedures were repeated in 2-MeTHF and Toluene for **PC 2**. In the case of measurements at 77 K with no gate delay, some scattering signals at 355 nm and 710 nm from the laser was observed.

Table S4: Summary of results of time-resolved emission for PCs 1-7 at room temperature and 77 K compared to computationally predicted triplet energies.

PC	$\lambda_{max,em,\ RT}$ (nm)[a]	$\lambda_{max,em,\ 77\ K}$ (nm)[b]	$\lambda_{max,em,77\ K,\ 1\ ms}$ (nm)[c]	$E_{S1,\ exp}$ (eV)[d]	$E_{S1,\ exp,\ 77\ K}$ (eV)[d]	$E_{T1,\ exp,\ 77\ K}$ (eV)[d]	$\Delta E_{ST,\ 77\ K}$ (eV)[e]	$E_{T1,\ Calc}$ (eV)[f]	$E^{0*}_{S1,exp.}$ ($^2PC^{\bullet+}/^1PC^*$) (V vs. SCE)[g]	$E^{0*}_{S1,exp,\ 77\ K.}$ ($^2PC^{\bullet+}/^1PC^*$) (V vs. SCE)[g]	$E^{0*}_{T1,exp.,\ 77\ K}$ ($^2PC^{\bullet+}/^3PC^*$) (V vs. SCE)[g]
1	494	428	530	2.55	2.90	2.34	0.56	2.41	-1.79	-2.14	-1.58
2	505	455	531	2.44	2.72	2.33	0.39	2.36	-1.73	-2.01	-1.62
2[h]	482	456	538	2.57	2.72	2.30	0.42	2.36	-1.86	-2.01	-1.59
2[i]	459	435	532	2.70	2.85	2.33	0.52	2.36	-1.99	-2.14	-1.62
3	459	435	518	2.71	2.85	2.39	0.46	2.43	-1.81	-1.95	-1.49
4	471	423	530	2.74	2.93	2.34	0.59	2.30	-1.98	-2.16	-1.57
5	442	421	527	2.80	2.95	2.35	0.60	2.29	-2.04	-2.19	-1.59
6	446	419	530	2.79	2.96	2.34	0.62	2.28	-2.04	-2.21	-1.59
7	529	458	524	2.32	2.71	2.37	0.34	2.39	-1.50	-1.89	-1.55

[a]Room temperature emission measured with no delay. [b]Emission measured at 77 K with no delay. [c]Emission measured at 77 K after 1 ms delay. [d]Energies were calculated from the maximum wavelength of emission. [e]Calculated from $\Delta E_{ST} = E_{S1,\ exp.} - E_{T1,\ exp.}$. [f] DFT calculations performed at uM06/6-311+Gdp/uM06/6-31+Gdp level of theory with CPCM-described solvation in aqueous solvent. [g] Excited-state redox potentials were calculated using the energies estimated from the maximum wavelength of emission and the experimentally measured $E_{1/2}$; $E^{0*}_{S1,\ exp.} = E_{1/2} - E_{S1,exp.}$ [h]Measurements performed in 2-methyl tetrahydrofuran. [i]Measurements performed in toluene. All other measurements were performed in DMF.

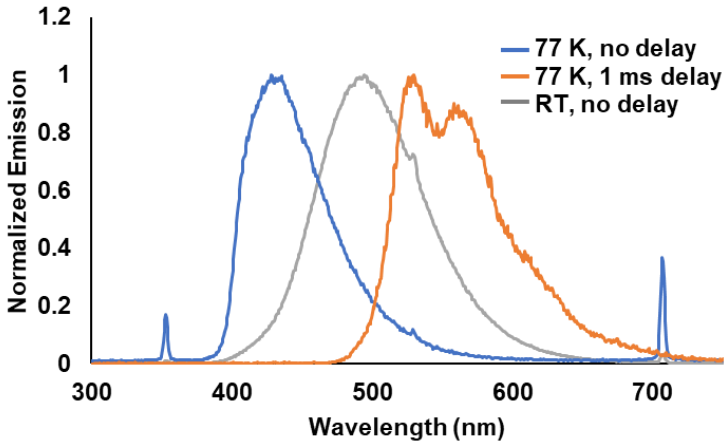


Figure S60: Normalized emission for **PC 1** measured at 77 K with no gate delay (blue), a 1 ms gate delay (orange) and at room temperature with no gate delay (grey) in DMF.

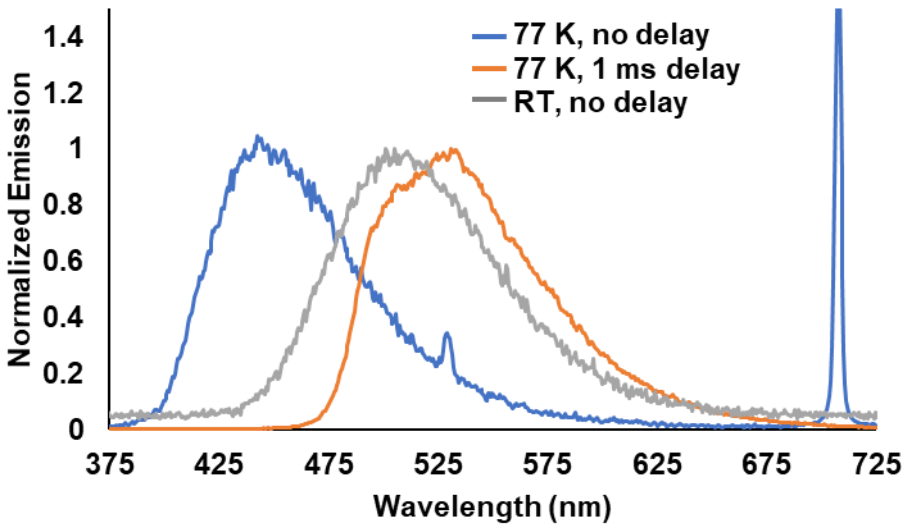


Figure S61: Normalized emission for **PC 2** measured at 77 K with no gate delay (blue), a 1 ms gate delay (orange) and at room temperature with no gate delay (grey) in DMF.

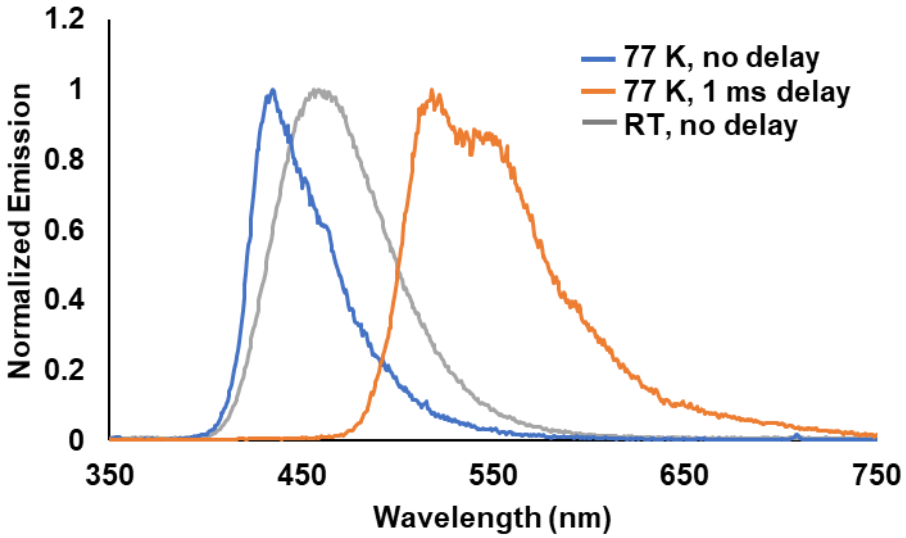


Figure S62: Normalized emission for **PC 3** measured at 77 K with no gate delay (blue), a 1 ms gate delay (orange) and at room temperature with no gate delay (grey) in DMF.

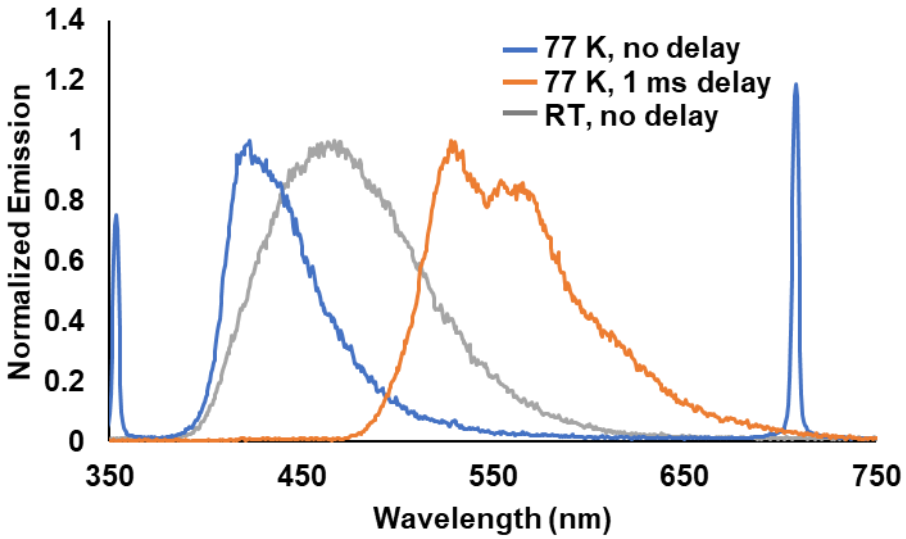


Figure S63: Normalized emission for **PC 4** measured at 77 K with no gate delay (blue), a 1 ms gate delay (orange) and at room temperature with no gate delay (grey) in DMF.

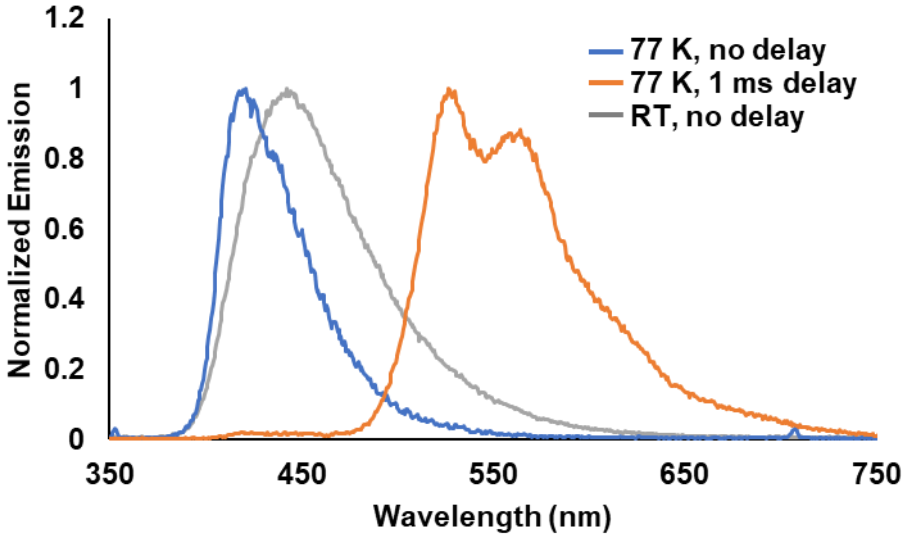


Figure S64: Normalized emission for **PC 5** measured at 77 K with no gate delay (blue), a 1 ms gate delay (orange) and at room temperature with no gate delay (grey) in DMF.

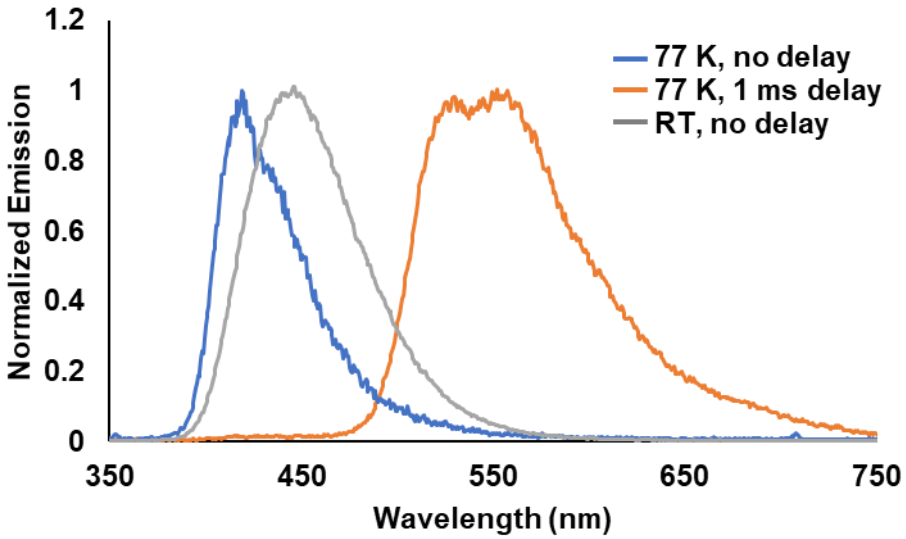


Figure S65: Normalized emission for **PC 6** measured at 77 K with no gate delay (blue), a 1 ms gate delay (orange) and at room temperature with no gate delay (grey) in DMF.

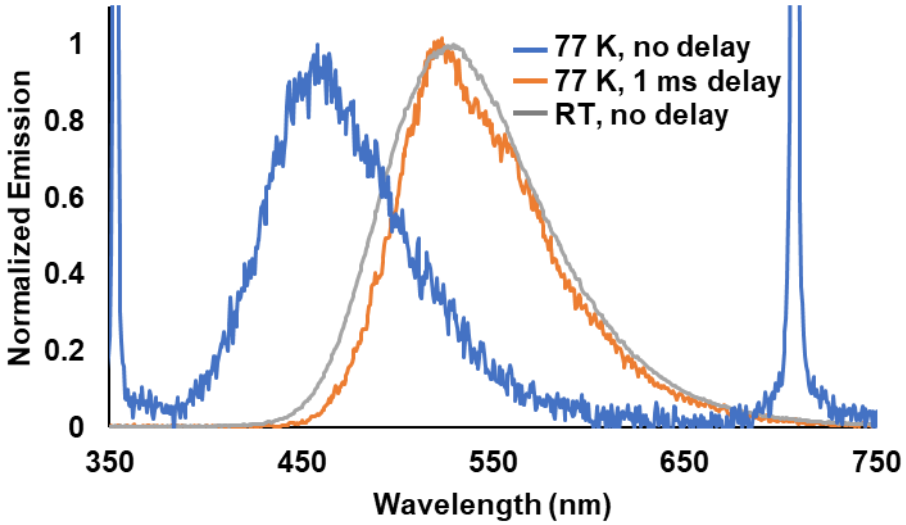


Figure S66: Normalized emission for **PC 7** measured at 77 K with no gate delay (blue), a 1 ms gate delay (orange) and at room temperature with no gate delay (grey) in DMF.

Cyclic Voltammetry

General Procedure for ATRP Initiators: Cyclic voltammetry of ATRP initiators was performed in a 3-compartment electrochemical cell with $Ag/AgNO_3$ (0.01 M) in acetonitrile as the reference electrode, $TBAPF_6$ in DMF (0.1 M) as the electrolyte solution, and platinum for the working and counter electrodes. All solutions were prepared on the benchtop, then sparged with nitrogen for 15 minutes before analysis. 1 mM solutions of analyte were used. Scans were performed at 100 mV/s with 2 cycles each. $E_{p/2}$ values were determined from the average of the onset of reduction and peak potential on the first cycle.

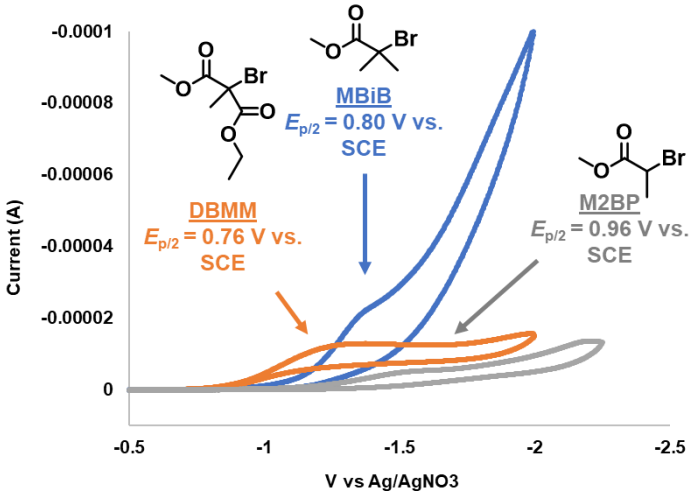


Figure S67: Cyclic voltammograms for Diethyl 2-bromo-2-methyl malonate (orange), methyl α-bromoisobutyate (blue) and methyl 2-bromopropionate (grey).

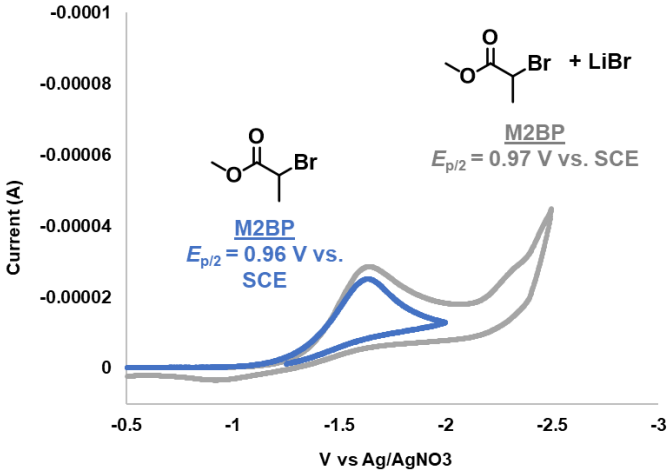


Figure S68: Cyclic voltammograms for methyl 2-bromopropionate (blue) and methyl 2-bromopropionate with 3 mM LiBr additive (grey).

General Procedure for PCs: Cyclic voltammetry of PCs 1-7 and their precursor compounds were performed in a 3-compartment electrochemical cell with $Ag/AgNO_3$ (0.01 M) in acetonitrile as the reference electrode, $TBAPF_6$ in DMF (0.1 M) as the electrolyte solution, and platinum for the working and counter electrodes. All solutions were prepared on the benchtop, then sparged with nitrogen for 15 minutes before analysis. For the non-reversible PC precursors, scans were conducted at 20 mV/s and 100 mV/s. Analysis of PCs 1-7 was conducted at 20 mV/s, 50 mV/s, 80 mV/s, and 100 mV/s with 5 cycles each.

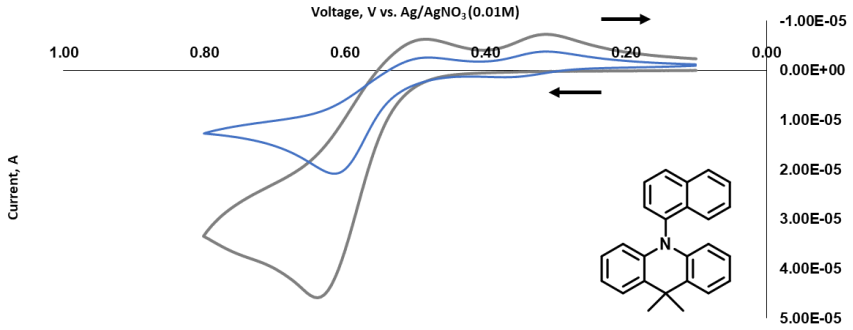


Figure S69: Cyclic voltammogram of Acrid-1N (precursor for **PCs 1, 2, and 3**) at 20 mV/s (blue) and 100 mV/s (grey).

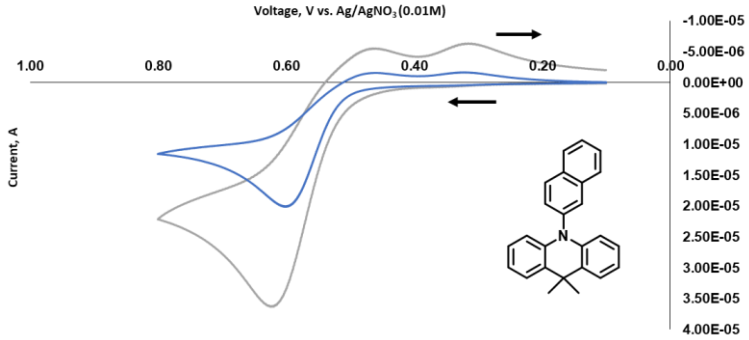


Figure S70: Cyclic voltammogram of Acrid-2N (precursor for **PC 4**) at 20 mV/s (blue) and 100 mV/s (grey).

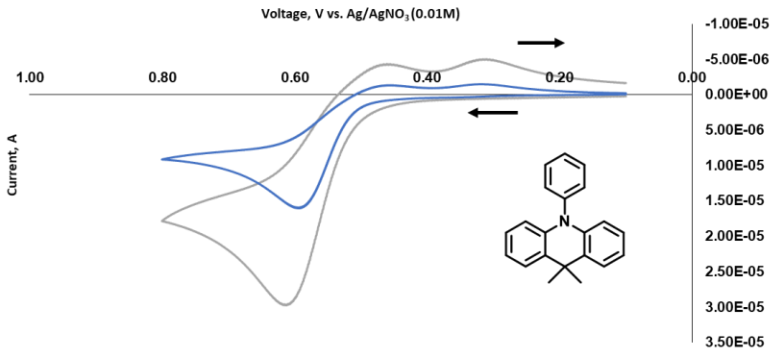


Figure S71: Cyclic voltammogram of Acrid-Ph (precursor for **PC 5**) at 20 mV/s (blue) and 100 mV/s (grey).

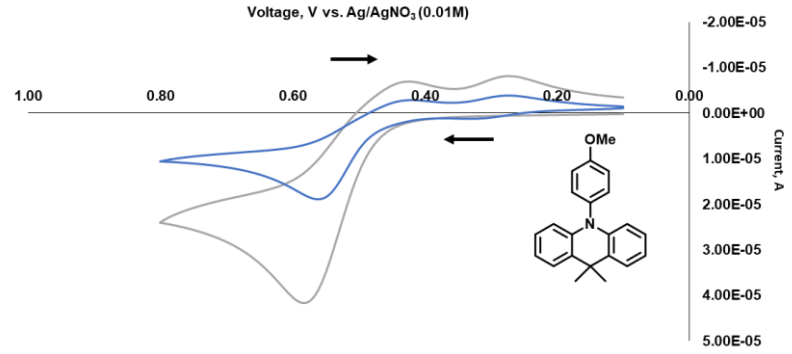


Figure S72: Cyclic voltammogram of Acrid-OMe (precursor for **PC 6**) at 20 mV/s (blue) and 100 mV/s (grey).

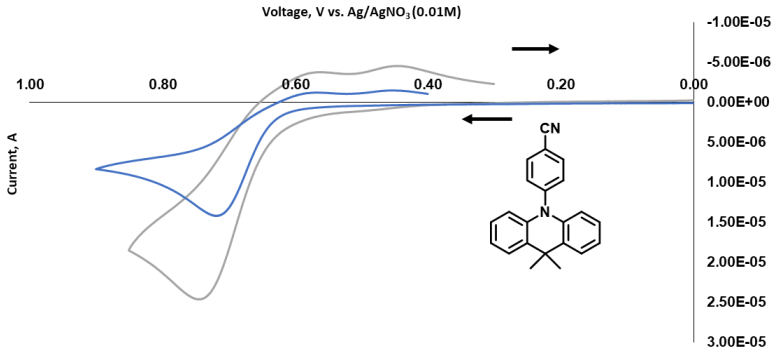


Figure S73: Cyclic voltammogram of Acrid-CN (precursor for **PC 7**) at 20 mV/s (blue) and 100 mV/s (grey).

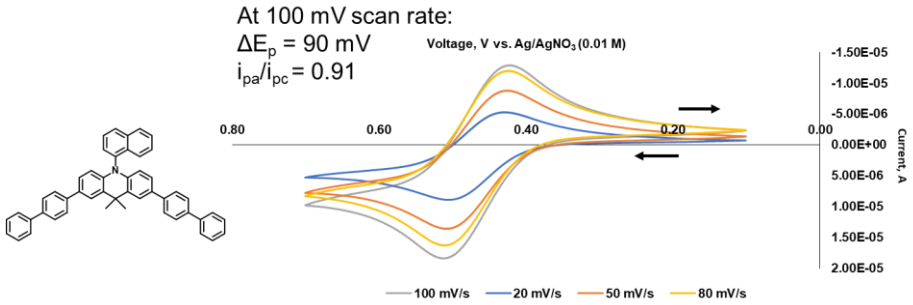


Figure S74: Cyclic voltammogram of **PC 1** at 20 mV/s (blue), 50 mV/s (orange), 80 mV/s (yellow) and 100 mV/s (grey).

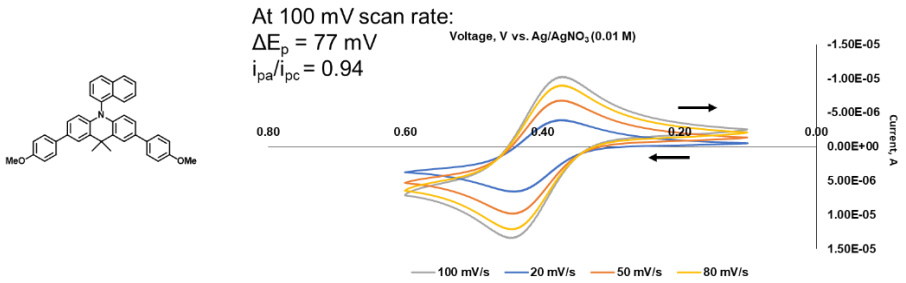


Figure S75: Cyclic voltammogram of **PC 2** at 20 mV/s (blue), 50 mV/s (orange), 80 mV/s (yellow) and 100 mV/s (grey).

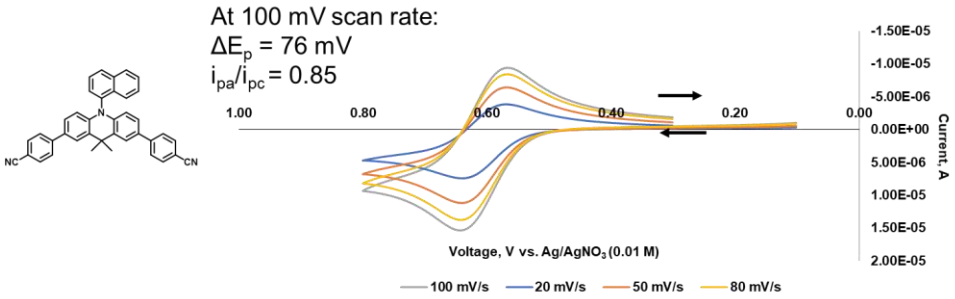


Figure S76: Cyclic voltammogram of **PC 3** at 20 mV/s (blue), 50 mV/s (orange), 80 mV/s (yellow) and 100 mV/s (grey).

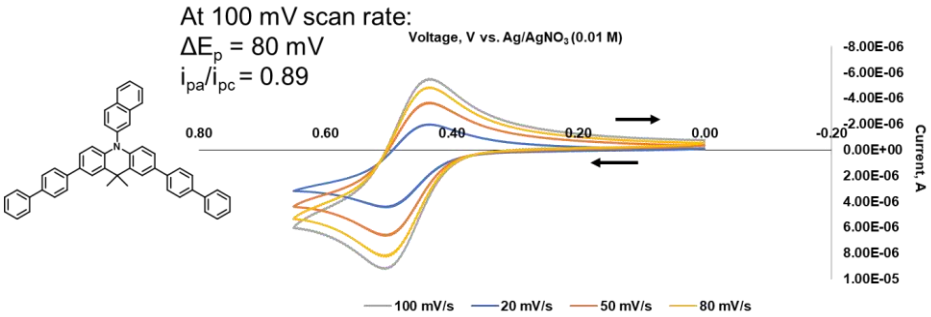


Figure S77: Cyclic voltammogram of **PC 4** at 20 mV/s (blue), 50 mV/s (orange), 80 mV/s (yellow) and 100 mV/s (grey).

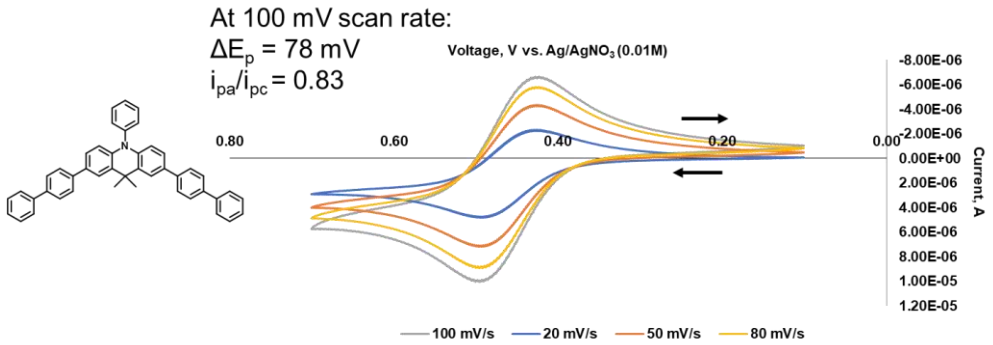


Figure S78: Cyclic voltammogram of **PC 5** at 20 mV/s (blue), 50 mV/s (orange), 80 mV/s (yellow) and 100 mV/s (grey).

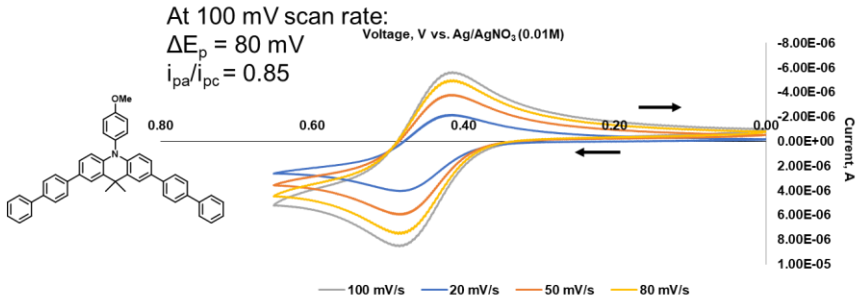


Figure S79: Cyclic voltammogram of **PC 6** at 20 mV/s (blue), 50 mV/s (orange), 80 mV/s (yellow) and 100 mV/s (grey).

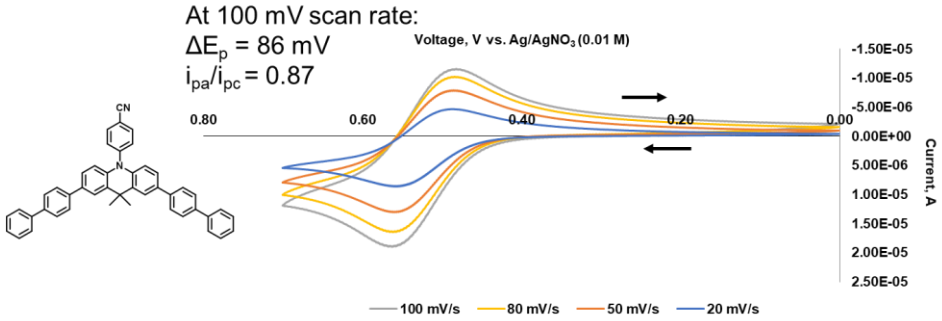


Figure S80: Cyclic voltammogram of **PC 7** at 20 mV/s (blue), 50 mV/s (orange), 80 mV/s (yellow) and 100 mV/s (grey).

Singly Occupied Molecular Orbital Calculations

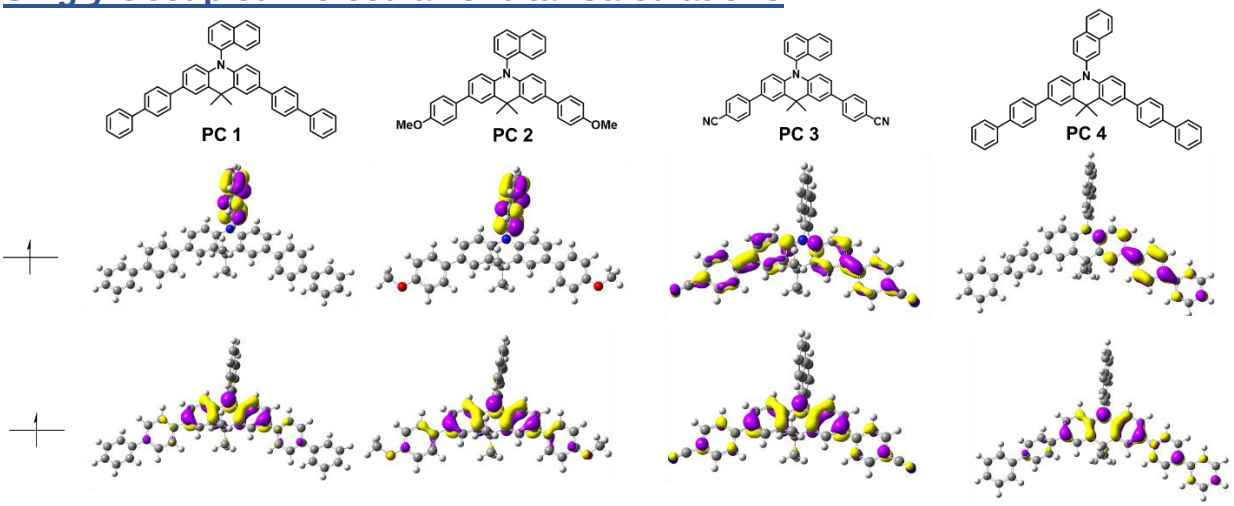


Figure S81: Computed singly occupied molecular orbitals (SOMOs) for PCs 1, 2, 3, and 4 (from left to right); the lower lying SOMO (bottom) and higher lying SOMO (top) for each PC in the triplet excited state are shown.

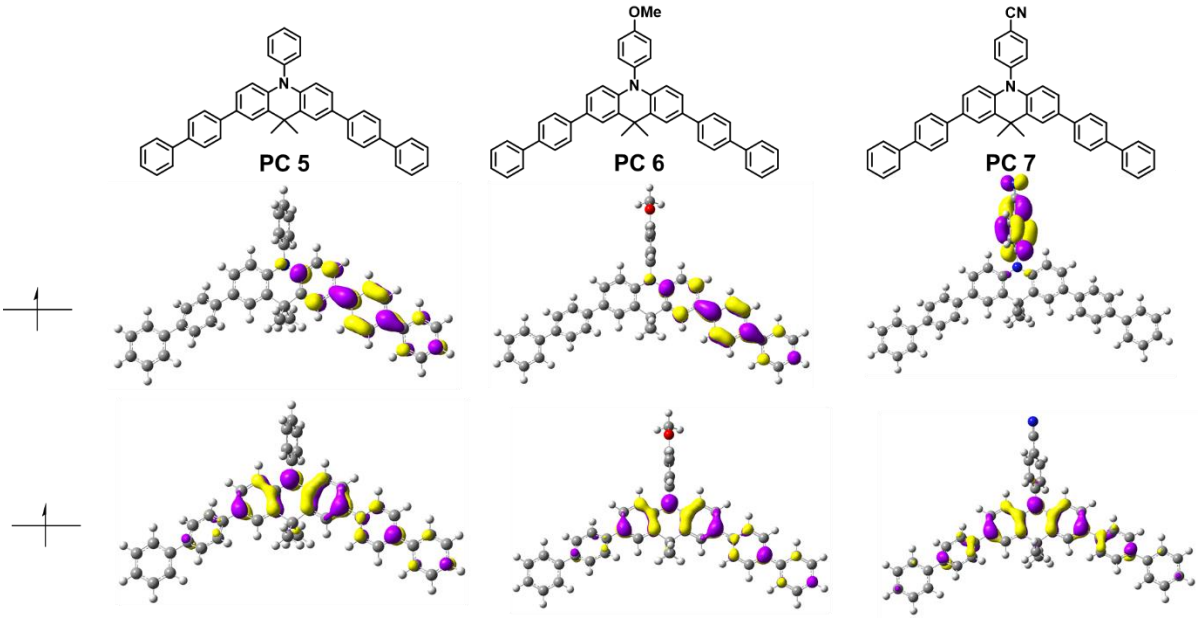


Figure S82: Computed singly occupied molecular orbitals (SOMOs) for PCs 5, 6, and 7 (from left to right); the lower lying SOMO (bottom) and higher lying SOMO (top) for each PC in the triplet excited state are shown.

Characterization of PC 2 in Presence of LiBr

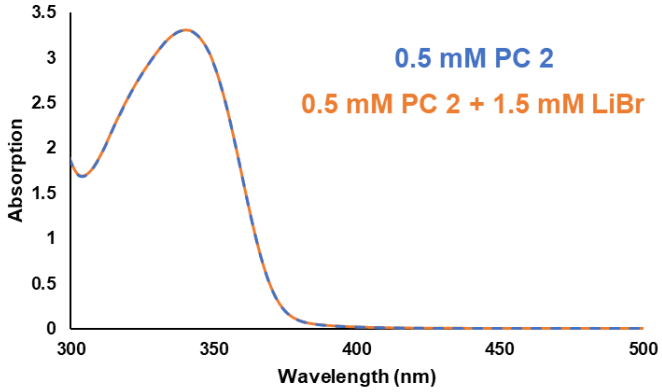


Figure S83: Absorption spectra of a 0.5 mM solution of PC 2 in DMF (blue) compared to absorption of a 0.5 mM solution of PC 2 and 1.5 mM solution of LiBr in DMF.

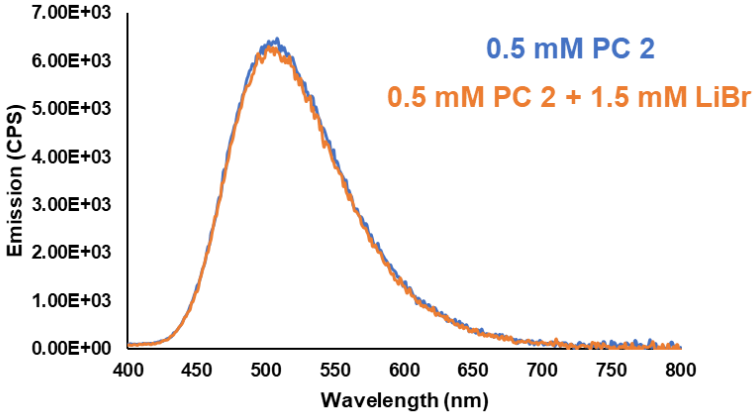


Figure S84: Emission spectra of a 0.5 mM solution of PC 2 in DMF (blue) compared to emission of a 0.5 mM solution of PC 2 and 1.5 mM solution of LiBr in DMF.

Polymerization Results in Batch

Batch Photoreactor Design:

Batch polymerizations were performed in a 100 mL beaker wrapped in aluminum foil with a 12-inch strip of 12 V 365 nm LEDs purchased from LED Lighting Hut. Polymerizations using 380 nm and 455 nm light sources were performed with 12 V LED strips from Creative Lighting Solutions.

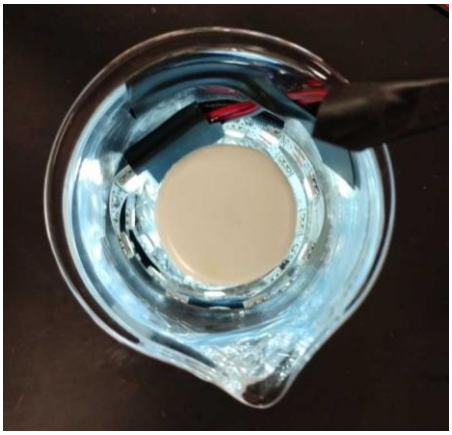


Figure S85: Batch photoreactor used for O-ATRP using dimethyl-dihydroacridines.

General Polymerization Procedure in Batch:

In a typical polymerization procedure, a scintillation vial with a small stir bar was loaded with 3.82 mg of PC 2 (6.97 µmol, 1 eq) and brought into a nitrogen-filled glovebox. Under red-light irradiation, 1 mL of *N,N*-dimethylacetamide (DMAc) was added to dissolve the PC, followed by 1 mL of butyl acrylate (6.97 mmol, 1000 eq.) and 13.3 µL of Diethyl 2-bromo-2-methylmalonate (DBMM) (0.70 µmol, 10 eq). The vial was then closed and placed into the photoreactor. Aliquots were taken by withdrawing 0.1 mL of reaction solution and quenching by injecting into a sealed vial with 0.8 mL of $CDCl_3$ containing 250 ppm BHT with air headspace. The sample was then taken out of the glovebox, where ^1H NMR analysis was performed. The sample was then dried under ambient conditions, dissolved in THF and molecular weight analysis was performed by GPC.

Polymerization Optimization In Batch Conditions

Control polymerizations:

Table S5: Results of control experiments of O-ATRP of butyl acrylate using **PC 2** in batch reactor.[a]

Entry	[BA]:[DBMM]:[PC 2]	Time (min.)	Conv. (%)	$M_{n,\,calc.}$ (kDa)	$Đ$ (M_w/M_n)
1	[1000]:[0]:[1]	150	86	169	2.01

2	[1000]:[0]:[1][b]	120	0	--	--
3	[1000]:[10]:[0]	150	71	218	1.81
4	[1000]:[0]:[0]	60	30	327	1.63
5	[1000]:[0]:[0][c]	60	0	--	--
6	[1000]:[0]:[0][d]	60	0	--	--
7	[1000]:[10]:[1][e]	120	0	--	--

[a]Conditions are 1:1.5 of BA:DMAc by volume, irradiated by 365 nm LEDs, and performed at ambient temperatures. [b]Performed in the presence of air. [c]380 nm LEDs. [d]455 nm LEDs. [e]Conducted in the dark.

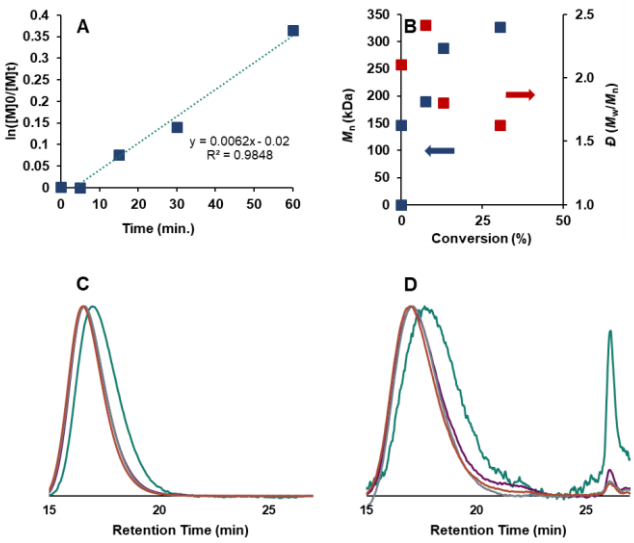


Figure S86: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) for reaction of BA and DMAc under 365 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces.

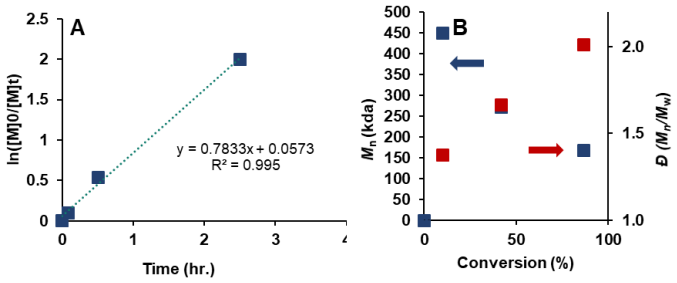


Figure S87: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) for reaction of BA and **PC 2** in DMAc under 355 nm irradiation in a batch reactor.

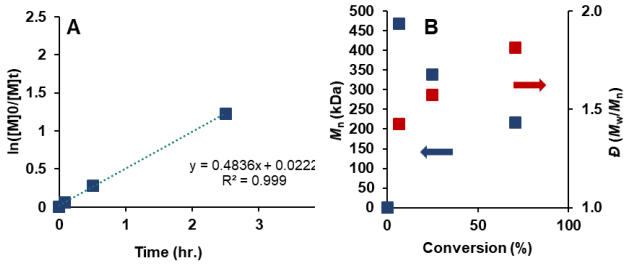


Figure S88: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) for reaction of BA and DBMM in DMAc under 365 nm irradiation in a batch reactor.

Light Source Optimization

Table S6: Results of light source optimizations using **PC 2** conducted in batch reactor.[a]

Entry	Light Source (nm)	Time (min.)	Conv. (%)	$M_{n,\,calc.}$ (kDa)	$Đ$ (M_w/M_n)	I^* (%)
1	365	77	10.6	10.2	1.53	96
2	380	120	73	21.4	9.6	45
3	455	120	86	31.2	3.79	37

[a]Conditions are [1000]:[10]:[1] of [BA]:[DBMM]:[PC 2] with 1 mL of BA to 1 mL of DMAc in 100 mL batch reactor beaker and performed at ambient temperatures.

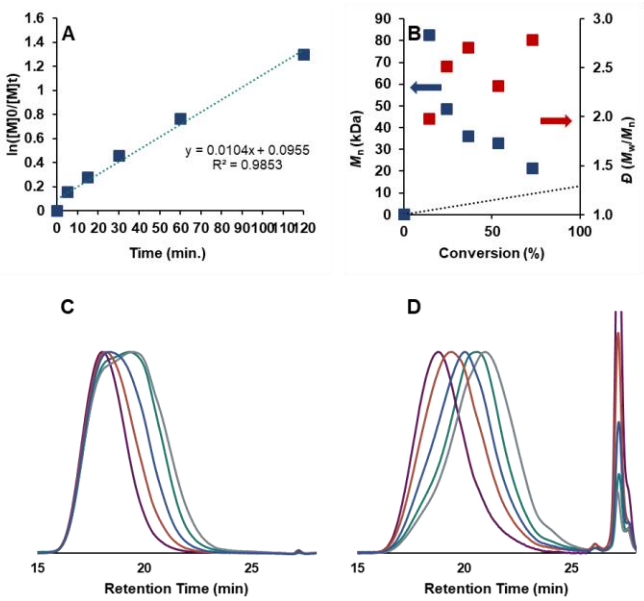


Figure S89: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 380 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces.

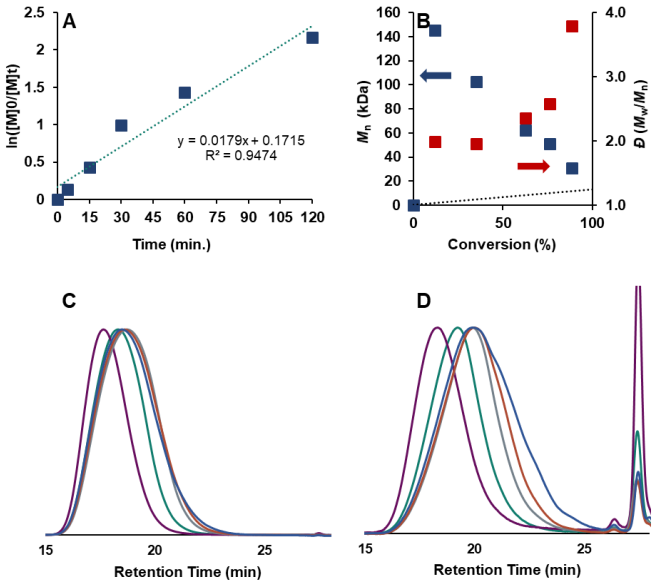


Figure S90: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 455 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces.

Common Organic Photocatalysts Screen

Table S7: Results of O-ATRP of butyl acrylate using well-studied organic PCs.[a]

Entry	PC	Time (min.)	Conv. (%)[b]	$M_{n,\,calc.}$ (kDa)[c]	$M_{n,\,theo.}$ (kDa)[d]	$Đ$ (M_w/M_n [c]	I^* (%)[e]
1	PhenO	240	81	10.3	10.6	2.29	103
2	PhenN	240	82	16.2	10.7	1.47	66
3	4-CzIPN	120	86	63.1	11.3	3.15	18

[a]Conditions are [1000]:[10]:[1] of [BA]:[DBMM]:[PC] with 1 eq of DMAc to BA by volume. Reactions were irradiated by 365 nm LEDs in batch conditions at ambient temperatures. [b]Determined by ^{1}H NMR. [c]Measured using GPC. [d]Calculated by $(Conv \times [Mon]/[Init.] \times Mw_{Mon})/1000$. [e]Initiator efficiency (I^*) calculated by $(Theo.M_n/Calc.M_n) \times 100$.

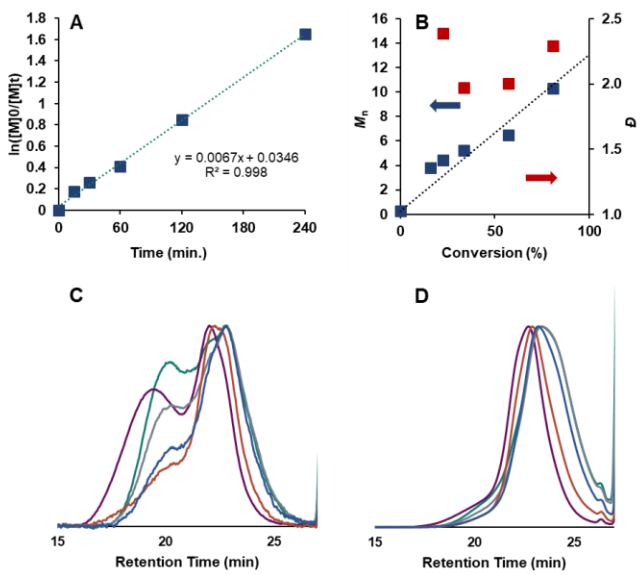


Figure S91: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PhenO** under 365 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1 mL DMAc to 1 mL BA.

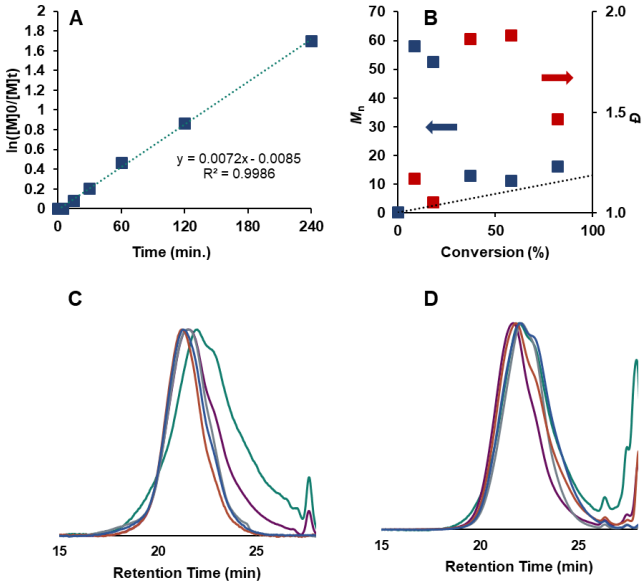


Figure S92: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PhenN** under 365 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1 mL DMAc to 1 mL BA.

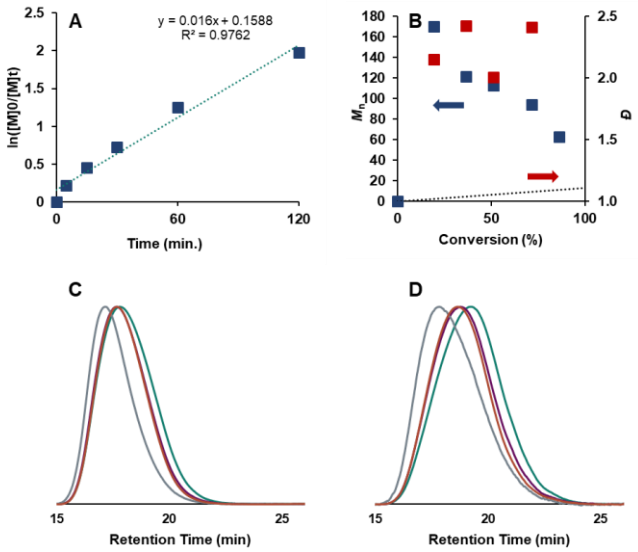


Figure S93: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **4-CzIPN** under 365 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1 mL DMAc to 1 mL BA.

Dimethyl-dihydroacridine Photocatalyst Screen

Table S8: Results of O-ATRP of butyl acrylate using **PCs 1-7** after 60 minutes irradiation.[a]

Entry	PC	Conv. (%)[b]	$M_{n,\,calc.}$ (kDa)[c]	$M_{n,\,theo.}$ (kDa)[d]	$Đ$ (M_w/M_n [c]	I^* (%)[e]
1	1	65	9.3	8.6	1.64	92
2	2	77	10.6	10.2	1.53	96
3	3	42	31.4	11.0	4.93	35
4	4	68	9.6	8.9	1.62	93
5	5	59	8.7	7.8	1.70	90
6	6	72	25.8	9.5	3.52	37
7	7	76	10.9	10.1	1.89	92

[a]Conditions are [1000]:[10]:[1] of [BA]:[DBMM]:[PC] with 1 eq of DMAc to BA by volume. Reactions were irradiated by 365 nm LEDs in batch conditions at ambient temperatures. [b]Determined by ^{1}H NMR. [c]Measured using GPC. [d]Calculated by $(Conv \times [Mon]/[Init.] \times Mw_{Mon})/1000$. [e]Initiator efficiency (I^*) calculated by $(Theo.M_n/Calc.M_n) \times 100$.

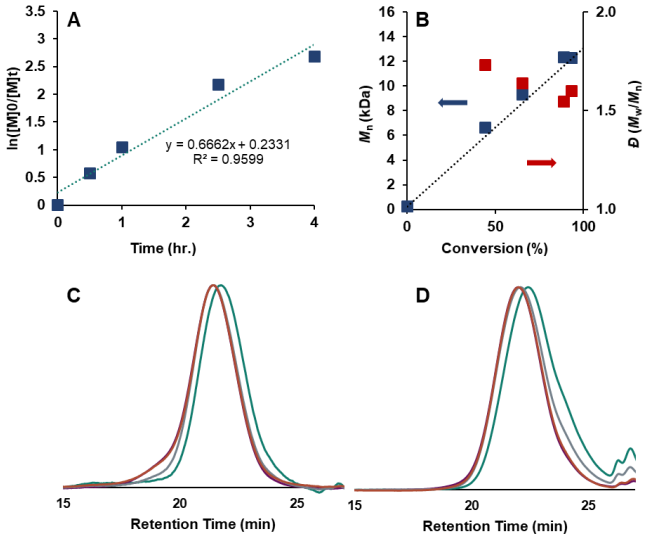


Figure S94: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 1** under 365 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1 mL DMAc to 1 mL BA.

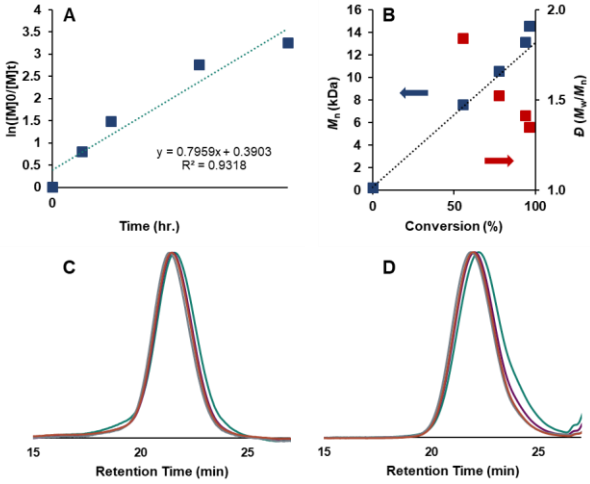


Figure S95: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1 mL DMAc to 1 mL BA.

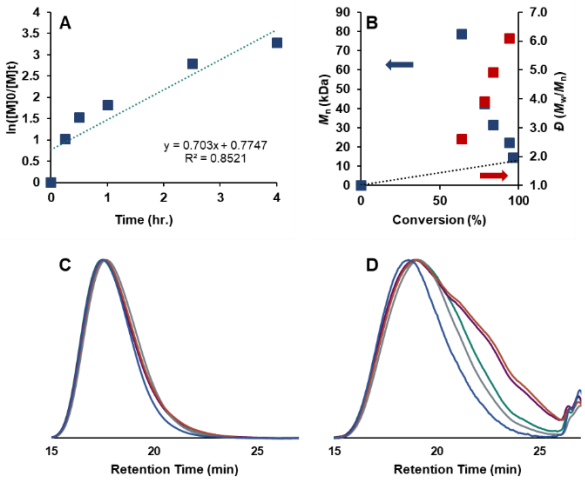


Figure S96: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 3** under 365 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1 mL DMAc to 1 mL BA.

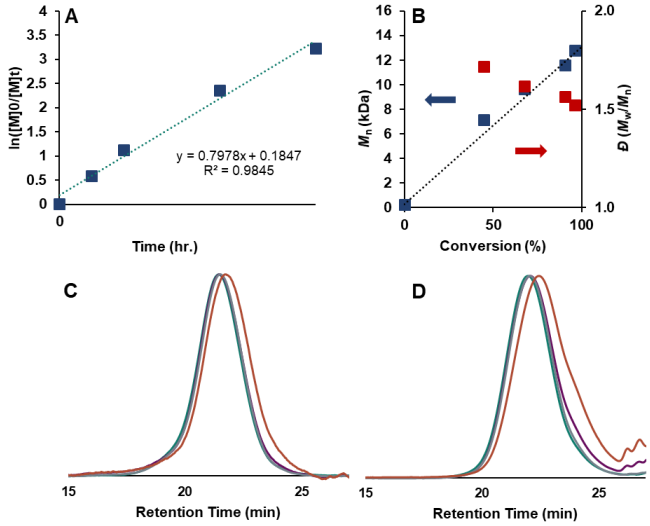


Figure S97: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 4** under 365 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1 mL DMAc to 1 mL BA.

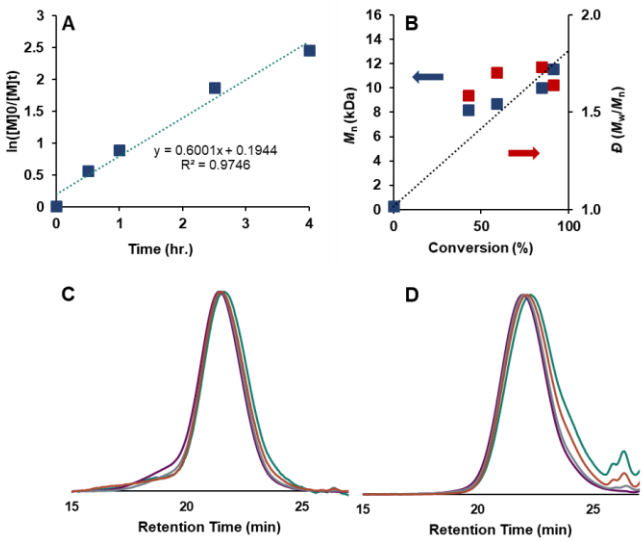


Figure S98: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 5** under 365 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1 mL DMAc to 1 mL BA.

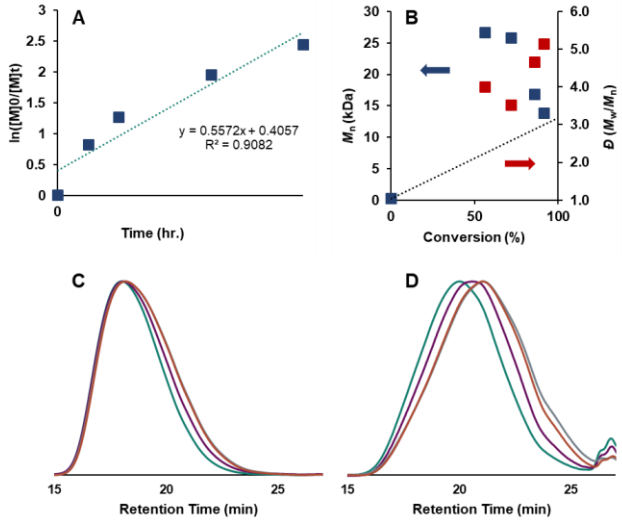


Figure S99: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 6** under 365 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1 mL DMAc to 1 mL BA.

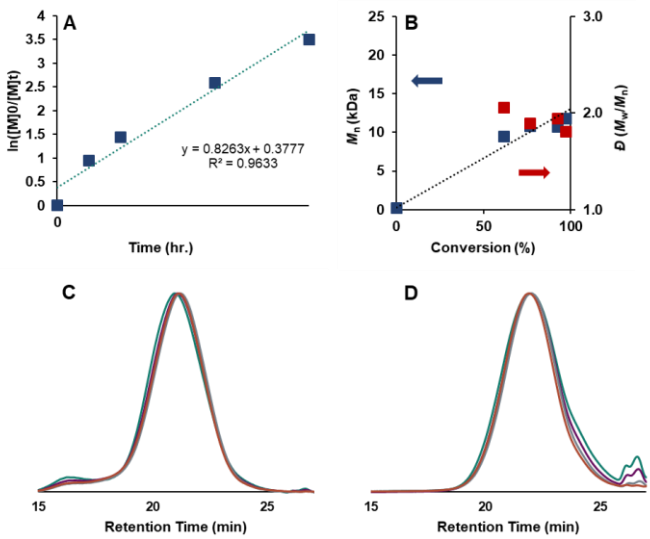


Figure S100: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 7** under 365 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1 mL DMAc to 1 mL BA.

Solvent Screen

Table S9: Results of different solvents on the O-ATRP of butyl acrylate using **PC 2** after 60 minutes.[a]

Entry	Solvent	Conv. (%)[b]	$M_{n,\,calc.}$ (kDa)	$M_{n,\,theo.}$ (kDa)	$Đ$ (M_w/M_n)	I^* (%)
1	DMAc	77	10.6	10.2	1.53	96
2	DMF	67	9.3	8.8	1.58	94
3	DMSO	71	9.7	9.4	2.37	97
4	THF	88	11.2	11.6	2.42	103
5	Benzene	92	24.6	12.1	4.47	49

[a]Conditions are [1000]:[10]:[1] of [BA]:[DBMM]:[PC] with 1 eq of solvent to BA by volume. Reactions were irradiated by 365 nm LEDs in batch conditions at ambient temperatures.

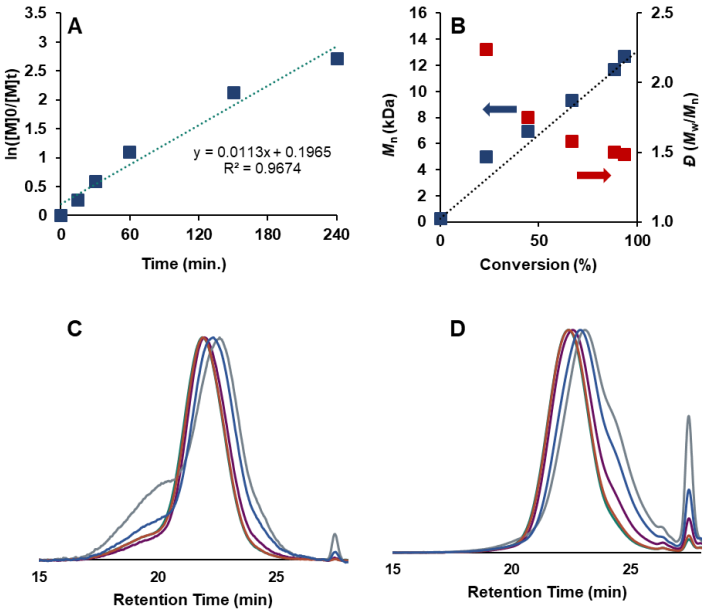


Figure S101: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1 mL DMF to 1 mL BA.

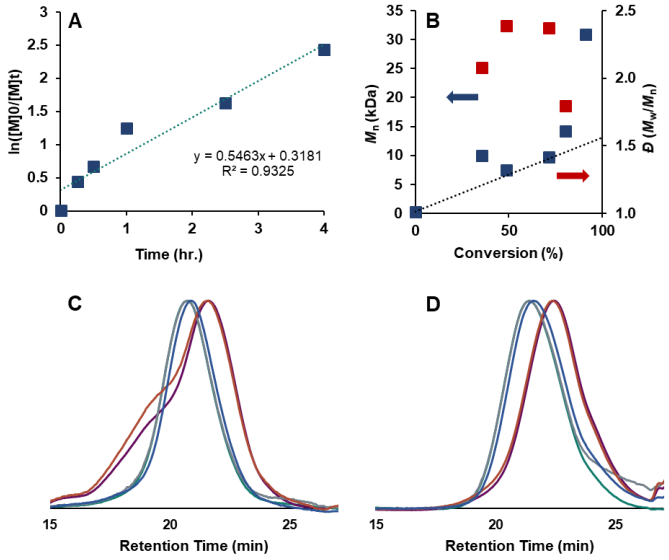


Figure S102: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1 mL DMSO to 1 mL BA.

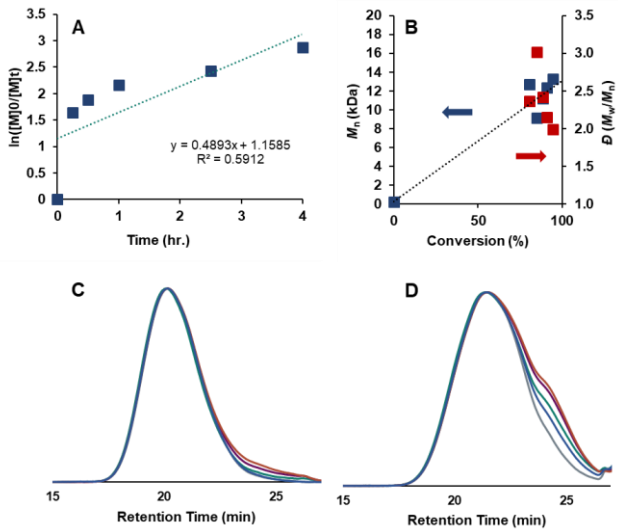


Figure S103: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1 mL THF to 1 mL BA.

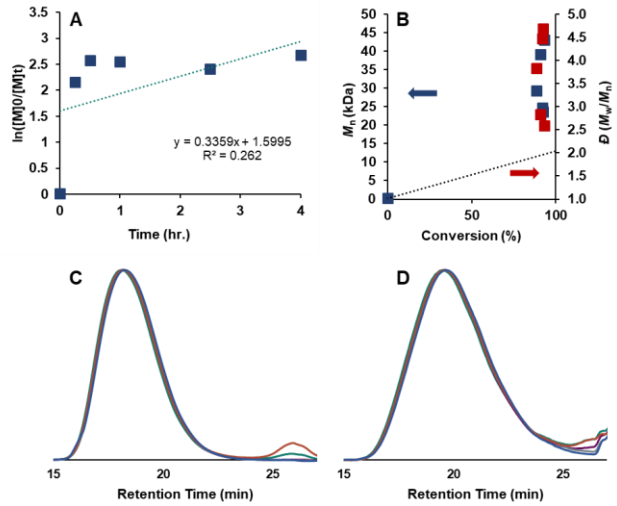


Figure S104: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1 mL Benzene to 1 mL BA.

Initiator Screen

Table S10: Results of differing alkyl halide initiators on the O-ATRP of BA using **PC 2** after 60 minutes.[a]

Entry	Initiator	Conv. (%)[b]	$M_{n,\ calc.}$ (kDa)	$M_{n,\ theo.}$ (kDa)	$Đ$ (M_w/M_n)	I^* (%)
1	DBMM	77	10.6	10.2	1.53	96
2	M2BP	76	17.5	9.9	1.97	57
3	2BrCN	57	8.8	7.5	1.66	85

[a]Conditions are [1000]:[10]:[1] of [BA]:[RX]:[PC 2] with 1 eq DMAc relative to 1 mL BA and were irradiated by 365 nm light in batch reactor conditions with ambient temperature.

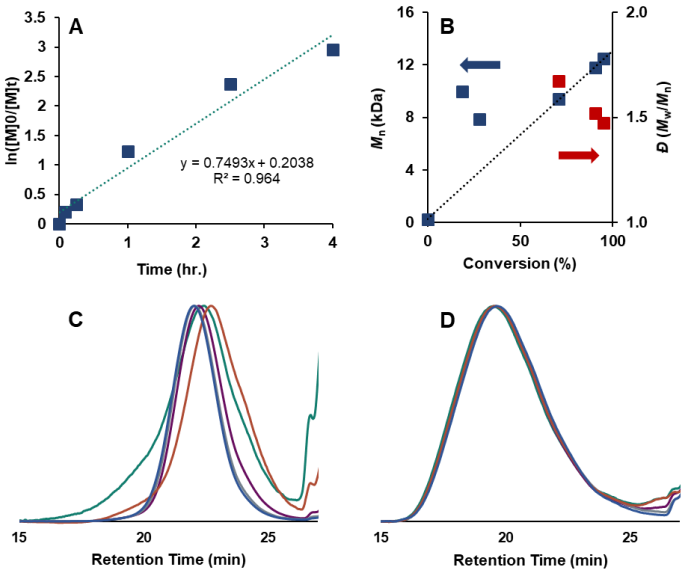


Figure S105: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1 mL DMAc to 1 mL BA.

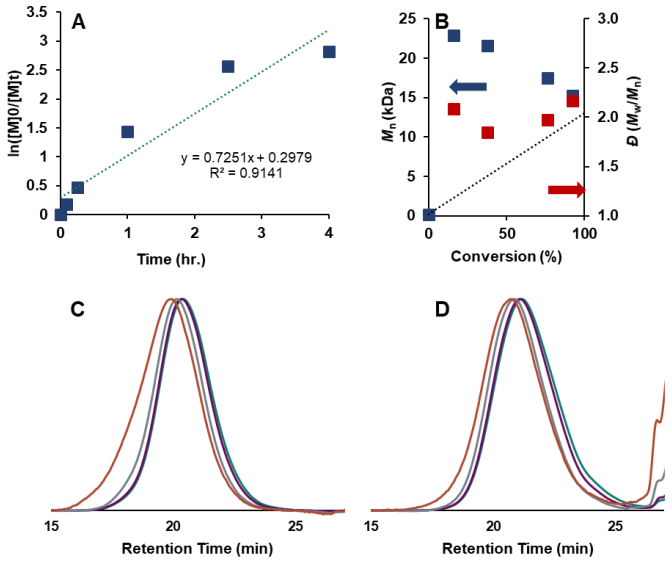


Figure S106: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[M2BP]:[PC] with 1 mL DMAc to 1 mL BA.

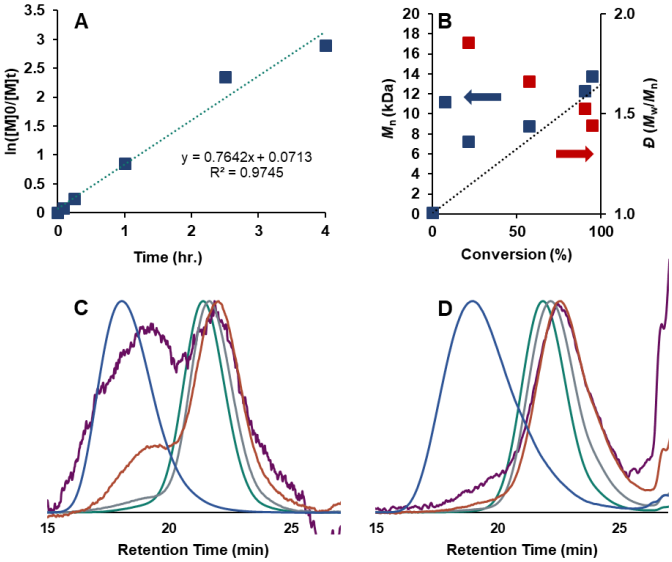


Figure S107: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[2BrCN]:[PC] with 1 mL DMAc to 1 mL BA.

Effect of Reaction Concentration

Table S11: Results of changing reaction concentration on the O-ATRP of BA using **PC** 2 after 2.5 hours.[a]

Entry	DMAc:BA (v/v)	Conv. (%)[b]	$M_{n,\ calc.}$ (kDa)	$M_{n,\ theo.}$ (kDa)	$Đ$ (M_w/M_n)	I^* (%)
1	2:1	90	12/0	11/7	1.43	98
2	1.5:1	89	11.1	11.6	1.52	104
3	1:1	92	10.3	1.52	12.0	117
4	1:2	91	12.7	1.64	12.0	94

[a]Conditions are [1000]:[10]:[1] of [BA]:[DBMM]:[PC 2] and were irradiated by 365 nm light in batch reactor conditions with ambient temperature.

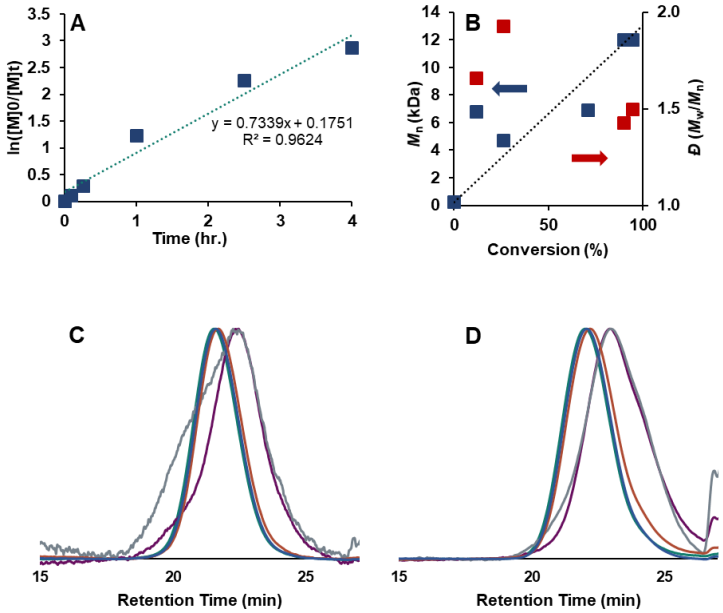


Figure S108: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 2 mL DMAc to 1 mL BA.

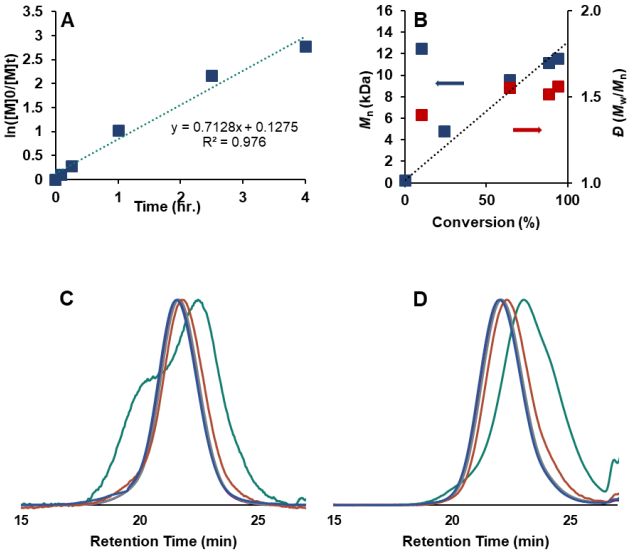


Figure S109: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1.5 mL DMAc to 1 mL BA.

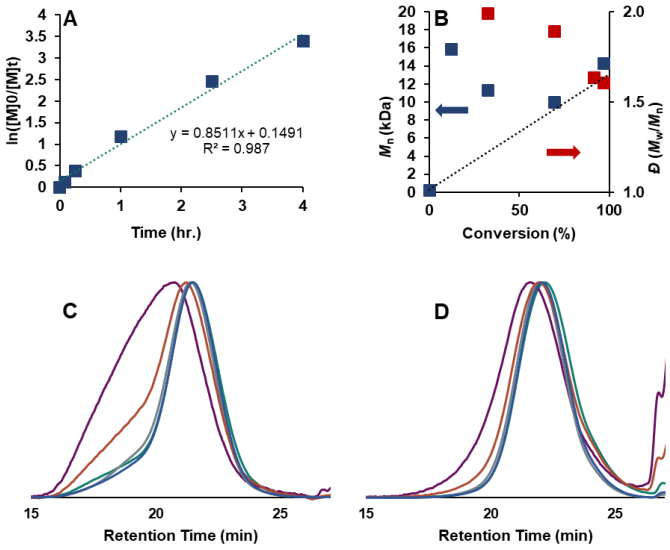


Figure S110: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1 mL DMAc to 1.5 mL BA.

PC loadings:

Table S12: Results of O-ATRP of BA after 1 hour testing the effect of **PC 2** loadings.[a]

Entry	Mol % **PC 2**	Conv. (%)[b]	$M_{n,\ calc.}$ (kDa)	$M_{n,\ theo.}$ (kDa)	$Đ$ (M_w/M_n)	I^* (%)
1	0.1	89	11.1	11.6	1.52	104
2	0.075	77	10.2	10.1	1.57	100
3	0.05	77	10.9	10.1	1.55	92
4	0.025	86	10.7	11.2	1.70	104
5	0.01	88	16.3	11.5	2.13	71

[a]Conditions are [1000]:[10]:[X] of [BA]:[DBMM]:[**PC 2**] with 1.5 equivalents of DMAc to BA by volume. Polymerizations were irradiated by 365 nm light in batch reactor conditions with ambient temperature.

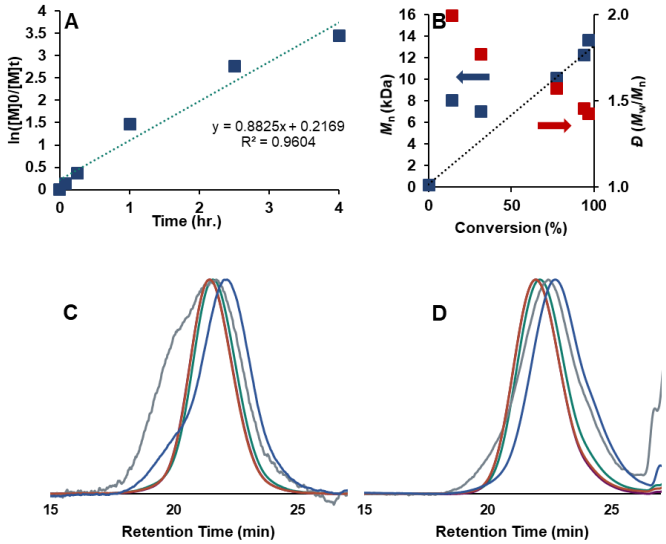


Figure S111: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[0.75] of [BA]:[DBMM]:[PC] with 1.5 mL DMAc to 1 mL BA.

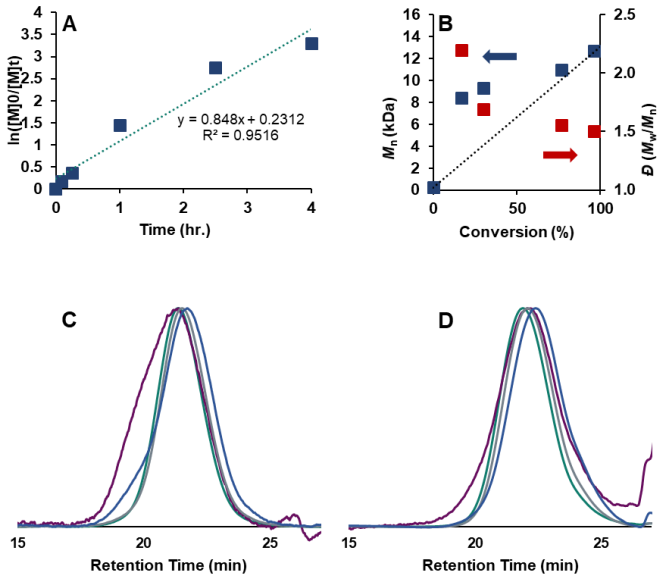


Figure S112: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[0.5] of [BA]:[DBMM]:[PC] with 1.5 mL DMAc to 1 mL BA.

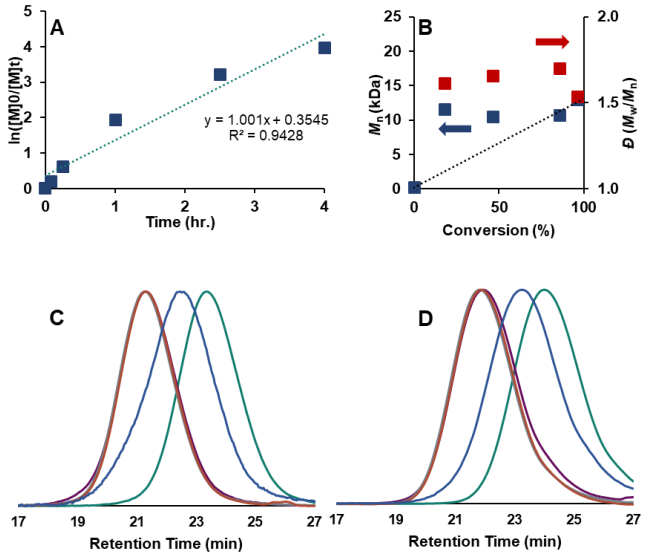


Figure S113: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[0.25] of [BA]:[DBMM]:[PC] with 1.5 mL DMAc to 1 mL BA.

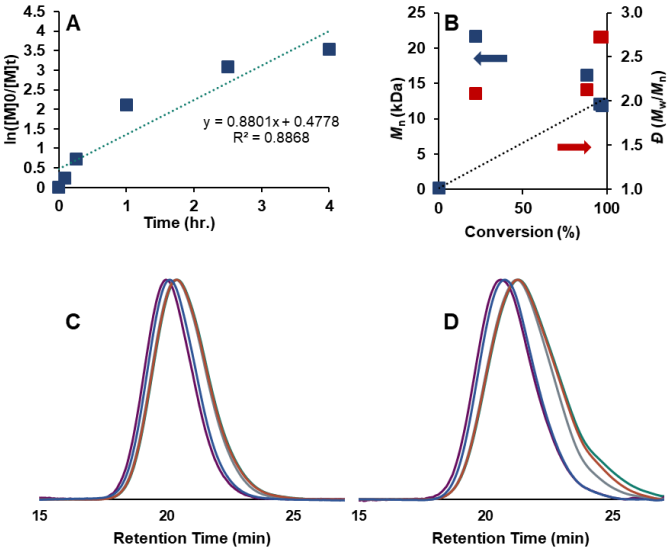


Figure S114: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in batch reactor with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[0.1] of [BA]:[DBMM]:[PC] with 1.5 mL DMAc to 1 mL BA.

Pulsed Irradiation (On/off) Experiment:

A pulsed irradiation experiment was conducted using the same protocols as a typical batch experiment (described above). After 5 minutes of irradiation by 365 nm LED, an aliquot was taken. Then, the reaction was wrapped in foil and stirred at ambient temperatures for 5 minutes. After that time, another aliquot was taken. This procedure was repeated for intervals of 10, 15, 30, 60, and minutes, followed by an extended "off" period of 16 hours.

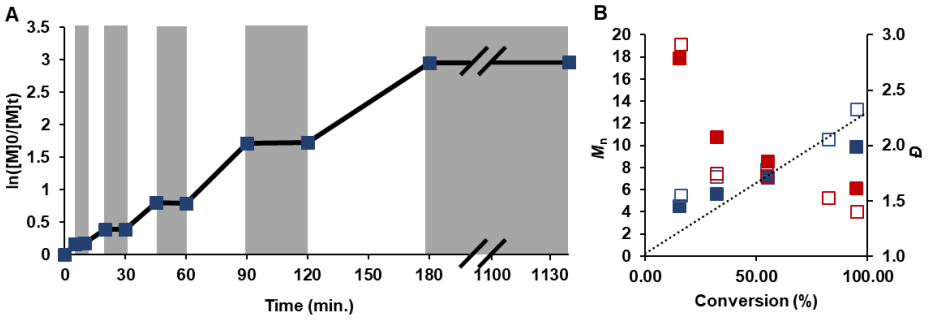


Figure S115: First order kinetic plot for the O-ATRP of BA with period on (white) and off (periods) (A). Plot of M_n (blue) and dispersity (red) versus conversion for on (filled squares) and off (open squares) periods (B). Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[**PC 2**] with 1.5 mL DMAc to 1 mL BA, irradiated by 365 nm LEDs in batch conditions at ambient temperature.

Polymerization Results in Flow

Flow Reactor Design:

Flow polymerizations were performed using a Hepatochem Photoredox Temperature Controlled reactor with a 2 mL flow attachment, also purchased directly from Hepatochem and especially configured for this photoreactor. The light source used was a 18 W 365 nm EvoluChem bulb (part no. HCK1012-01-011 from Hepatochem). The flow tubing was 1/16 in O.D. and 0.003 in I.D. with PFA as the tubing material, with inlet and outlet tubing purchased from IDEX Health and Science. All ferrules and fittings were purchased from IDEX Health and Science. The flow rate was controlled using a Pump 11 Elite Syringe Pump from Harvard Apparatus with a 50 mL stainless steel syringe fitted with chemically resistant Kalrez O-rings.

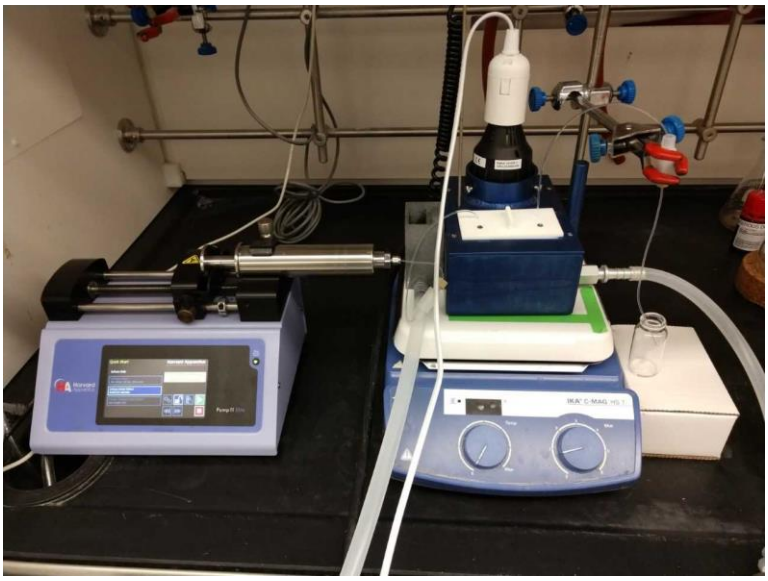


Figure S116: Flow reactor setup consisting of syringe pump and stainless-steel syringe (left) and temperature-controlled flow reactor with 18W 365 LED purchased from Hepatochem (right).

General Polymerization Procedure in Flow:

In a typical polymerization experiment, a vial was loaded with 26.7 mg of Acrid-1N-OMe (0.048 µmol, 1 eq.), then brought into a nitrogen-filled glovebox. Under red light irradiation, 7 mL of DMAc and 7 mL of butyl acrylate (0.048 mol, 1000 eq.) was then added. Once all catalyst was fully dissolved, 93.3 µL of DBMM (0.488 µmol, 10 eq.) was added using a glass syringe. The reaction mixture was then transferred to a 50 mL stainless steel syringe and the first section of tubing attached. The syringe was then removed from the glovebox. Excess gas was pushed out of the syringe, then the first section of tubing was quickly connected to the reactor. The reaction was started with the initial flow rate using a syringe pump. The temperature of the reactor was controlled using a recirculator set to 22 ºC, which recirculated a 1/1 v/v mixture of ethylene glycol and water. The timing for the first equilibration period was set after 1 mL of initial infusion volume. For all timepoints, an equilibration period of 1.25 times the residence time was performed, followed by 0.125 times of collection time (see Table S8). The resulting polymer was collected directly into a vial containing 1 mL of BHT-deuterated chloroform. Conversion analysis was performed using ^{1}H NMR and molecular weight analysis was performed using SEC-MALS GPC.

Table S13: Example of calculations used for O-ATRP experiments performed in 2 mL continuous flow reactor. Residence time is determined by flow rate/reactor volume.

Entry	Res. Time (min.)	Flow Rate (mL/min)	Equilibration Time (min.)	Collection Time (min.)
1	1.5	1.333	1.88	0.1875
2	5	0.400	6.25	0.625
3	15	0.133	18.75	1.875
4	30	0.067	37.50	3.75
5	45	0.044	56.25	5.625
6	60	0.033	75	7.5

Polymerization Optimization in Flow Conditions

Control Polymerizations

Table S14: Results of control experiments of O-ATRP of butyl acrylate using **PC 2** in flow reactor.[a]

Entry	[BA]:[DBMM]:[PC 2]	Res. Time (min.)	Conv. (%)	$M_{n,\ calc.}$ (kDa)	$Đ$ (M_w/M_n)
1	[1000]:[0]:[1]	45	86	53	3.15
3	[1000]:[10]:[0]	45	0	--	--
4	[1000]:[0]:[0]	60	0	--	--
7	[1000]:[10]:[1][b]	45	59	9.3	1.65

[a]Conditions are 1:1.5 of BA:DMAc by volume, irradiated by 365 nm LEDs, and performed at 22 ºC. [b]Catalyzed by Phenoxazine photocatalyst.

PC Screen

Table S15: Results of O-ATRP of BA using **PCs 1-7** in continuous flow.[a]

Entry	PC	Res. Time (min.)	Conv. (%)[b]	$M_{n,\ calc.}$ (kDa)[c]	$M_{n,\ theo.}$ (kDa)[d]	$Đ$ (M_w/M_n)[c]	I* (%)[e]
1	1	45	67	8.9	8.9	1.59	100
2	2	45	81	11.0	10.6	1.35	97
3	3	30	71	13.1	9.5	4.57	72
4	4	45	81	11.1	10.7	1.48	96
5	5	45	79	10.2	10.4	1.48	102
6	6	30	82	11.4	10.7	3.58	94
7	7	45	73	9.6	9.6	1.54	100

[a]Conditions are [1000]:[10]:[1] of [BA]:[DBMM]:[PC] with 1 eq of DMAc to BA by volume. Reactions were performed in continuous flow and irradiated by 18W 365 nm LEDs at 22 ºC.

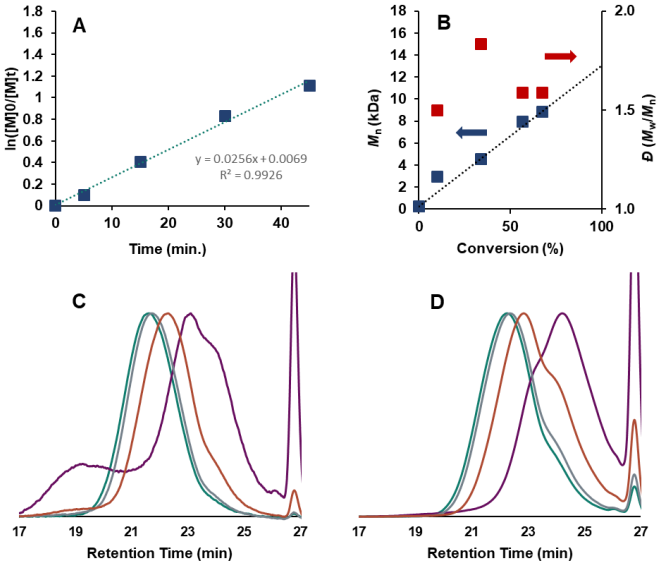


Figure S117: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 1** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1 mL DMAc to 1 mL BA.

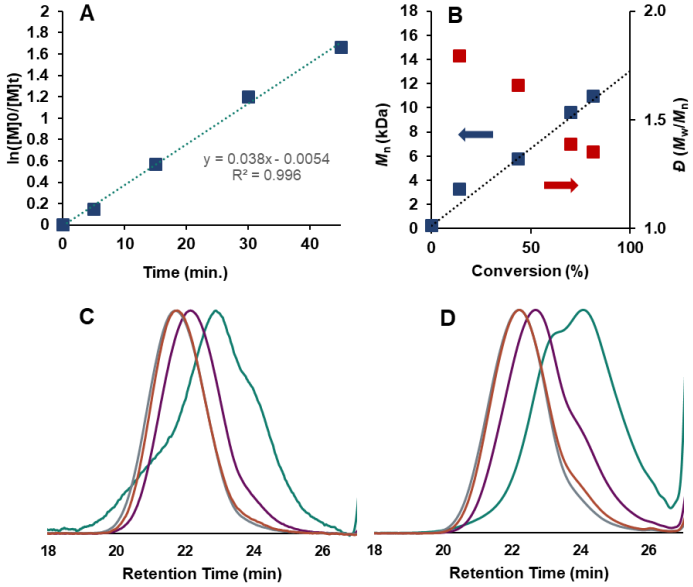


Figure S118: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1 mL DMAc to 1 mL BA.

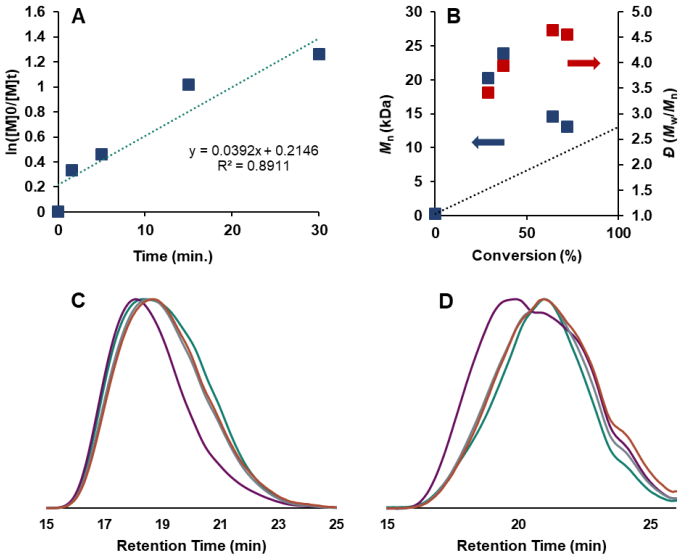


Figure S119: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 3** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1 mL DMAc to 1 mL BA.

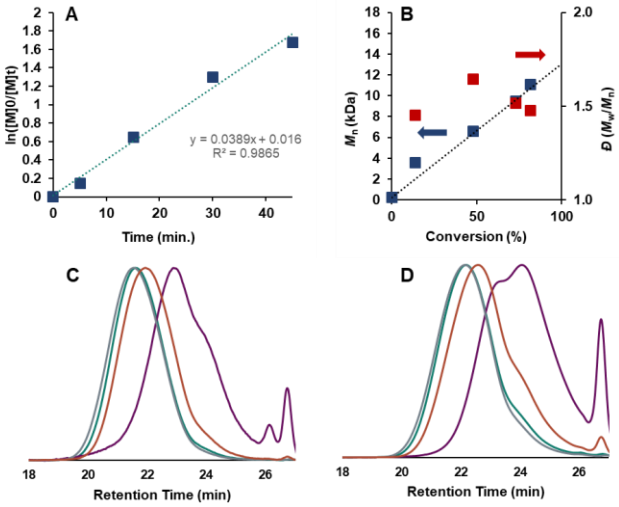


Figure S120: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 4** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1 mL DMAc to 1 mL BA.

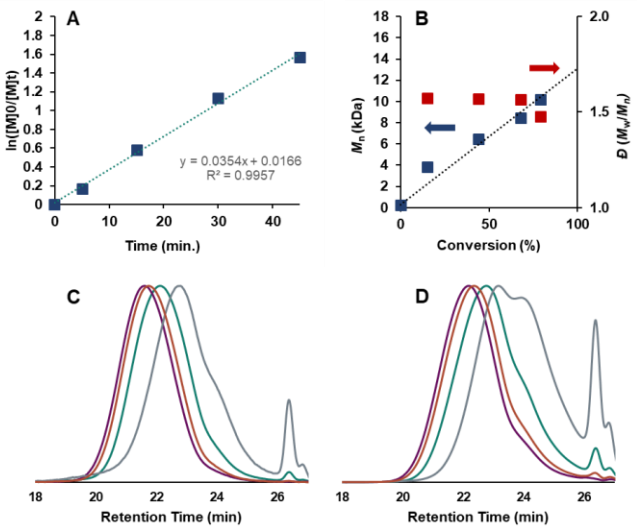


Figure S121: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 5** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1 mL DMAc to 1 mL BA.

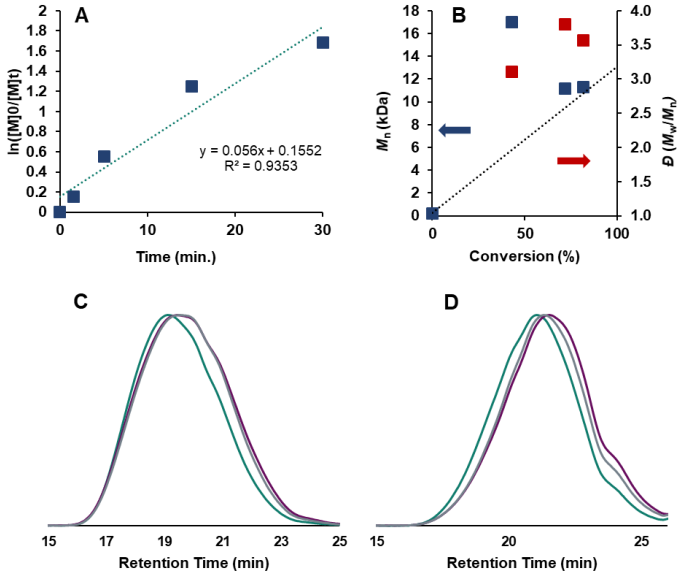


Figure S122: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 6** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1 mL DMAc to 1 mL BA.

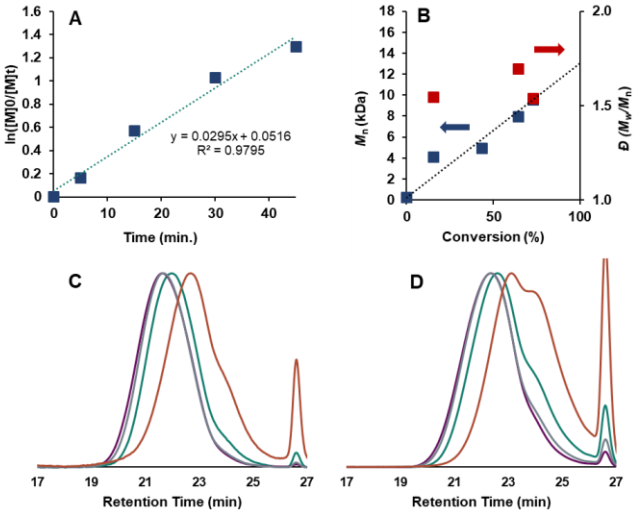


Figure S123: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 7** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1 mL DMAc to 1 mL BA.

Initiator Screen

Table S16: Results of differing alkyl halide initiators on the O-ATRP of BA in continuous flow using **PC 2** after 45 minutes residence time.[a]

Entry	Initiator	Conv. (%)[b]	$M_{n,\,calc.}$ (kDa)	$M_{n,\,theo.}$ (kDa)	$Đ$ (M_w/M_n)	I^* (%)
1	DBMM	81	11.0	10.6	1.35	97
2	MBiB	79	10.8	10.3	1.43	96
3	2BrPN	74	10.8	9.8	1.34	91

[a]Conditions are [1000]:[10]:[1] of [BA]:[RX]:[PC 2] with 1 eq DMAc relative to 1 mL BA and were irradiated by 365 nm light in continuous flow conditions at 22º.

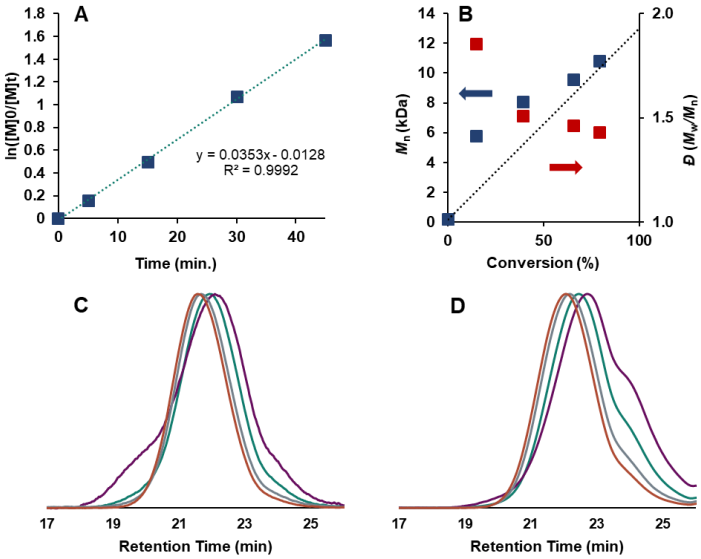


Figure S124: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[MBiB]:[PC] with 1 mL DMAc to 1 mL BA.

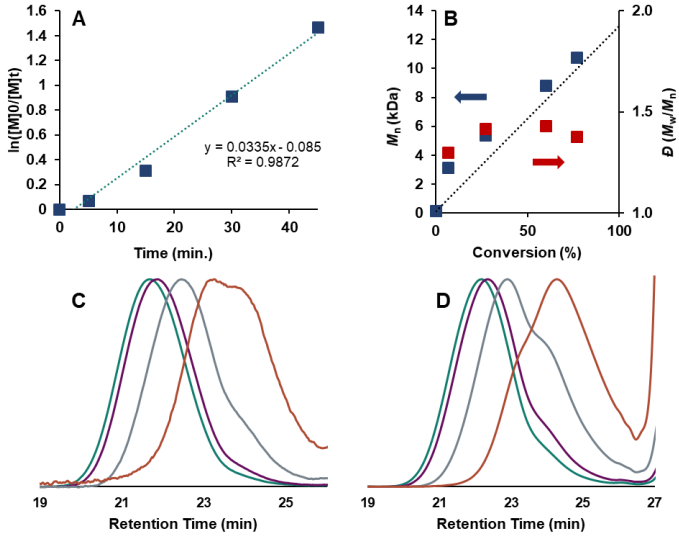


Figure S125: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[2BrPN]:[PC] with 1 mL DMAc to 1 mL BA.

Reaction Concentration

Table S17: Results of changing reaction concentration on the O-ATRP of BA using **PC 2** in continuous flow after 45 minutes residence time.[a]

Entry	DMAc:BA (v/v)	Conv. (%)[b]	$M_{n,\ calc.}$ (kDa)	$M_{n,\ theo.}$ (kDa)	$Đ$ (M_w/M_n)	I^* (%)
1	2:1	87	13.4	11.9	1.31	89
2	1.5:1	80	10.6	10.6	1.37	100
4	1:1	81	11.0	10.6	1.35	97

[a]Conditions are [1000]:[10]:[1] of [BA]:[DBMM]:[PC 2] and were irradiated by 365 nm light in flow conditions at 22 ºC.

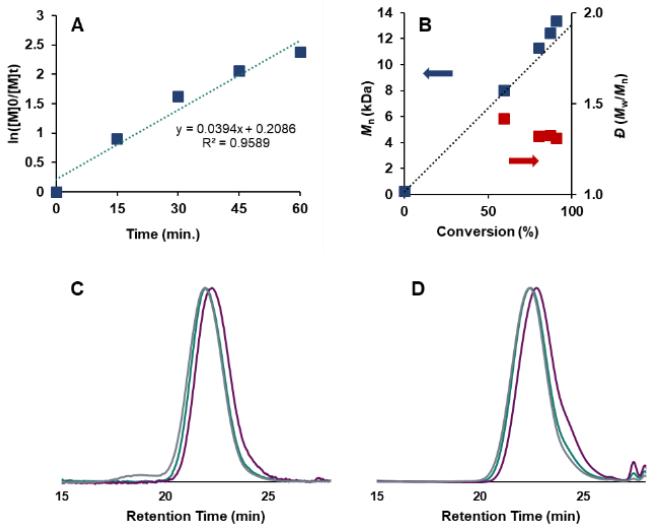


Figure S126: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 2 mL DMAc to 1 mL BA.

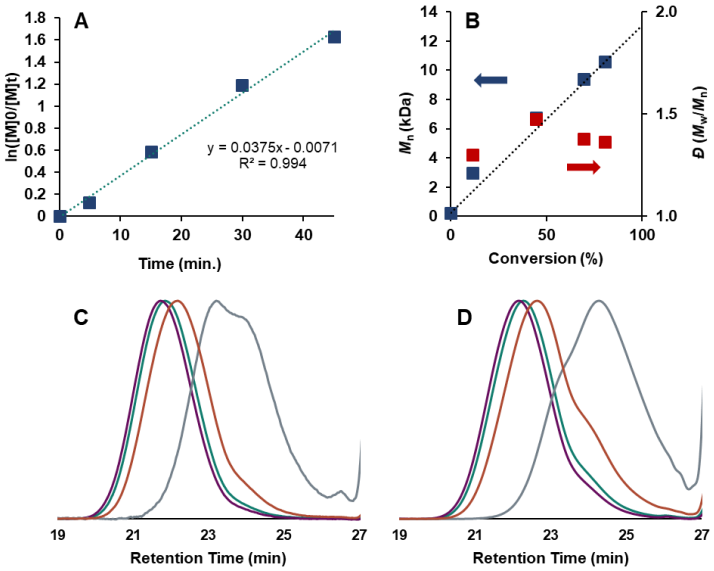


Figure S127: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1.5 mL DMAc to 1 mL BA.

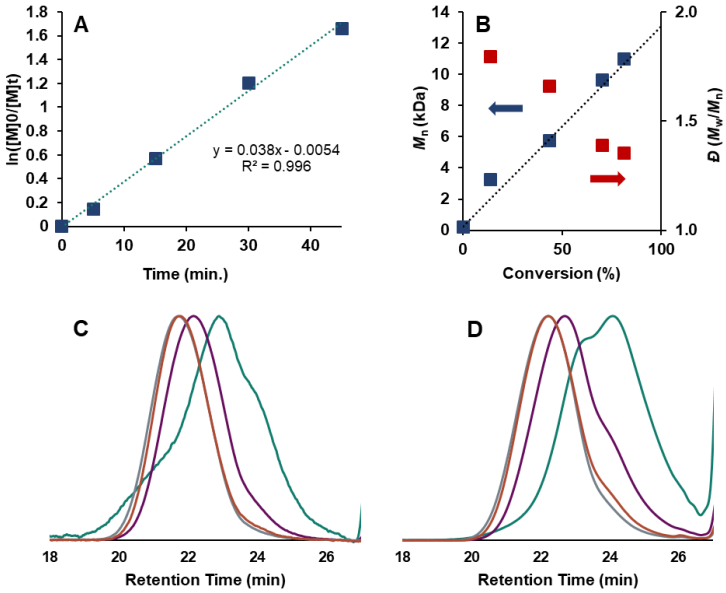


Figure S128: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1 mL DMAc to 1 mL BA.

Catalyst Loading

Table S18: Results of O-ATRP of BA in continuous flow after 45 minutes residence time testing the effect of **PC 2** loadings.[a]

Entry	Mol % **PC 2**	Conv. (%)[b]	$M_{n,\ calc.}$ (kDa)	$M_{n,\ theo.}$ (kDa)	$Đ$ (M_w/M_n)	I^* (%)
1	0.1	80	10.6	10.6	1.37	100
2	0.075	80	10.1	10.6	1.43	105
5	0.05	81	10.2	10.6	1.41	104

[a]Conditions are [1000]:[10]:[X] of [BA]:[DBMM]:[**PC 2**] with 1.5 equivalents of DMAc to BA by volume. Polymerizations were irradiated by 365 nm light in continuous flow reactor conditions at 22 ºC.

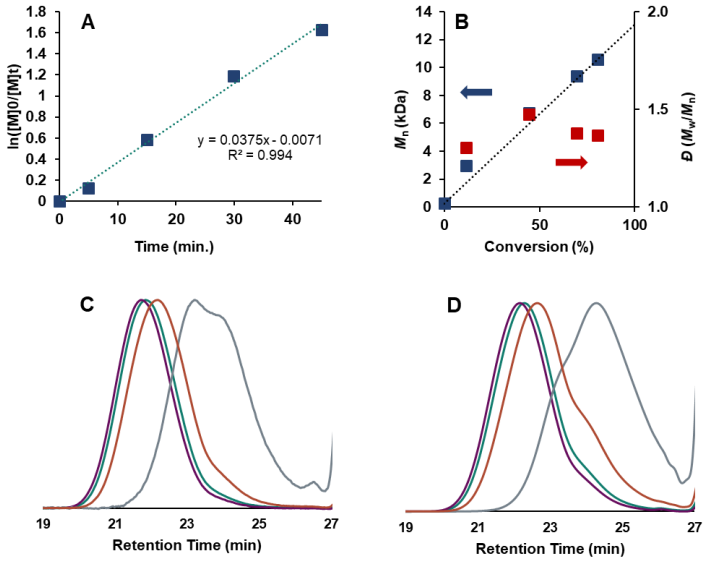


Figure S129: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1] of [BA]:[DBMM]:[PC] with 1.5 mL DMAc to 1 mL BA.

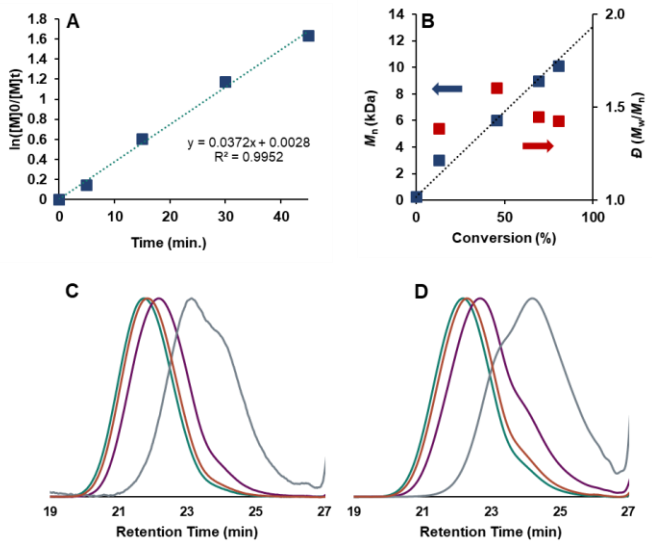


Figure S130: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[0.75] of [BA]:[DBMM]:[PC] with 1.5 mL DMAc to 1 mL BA.

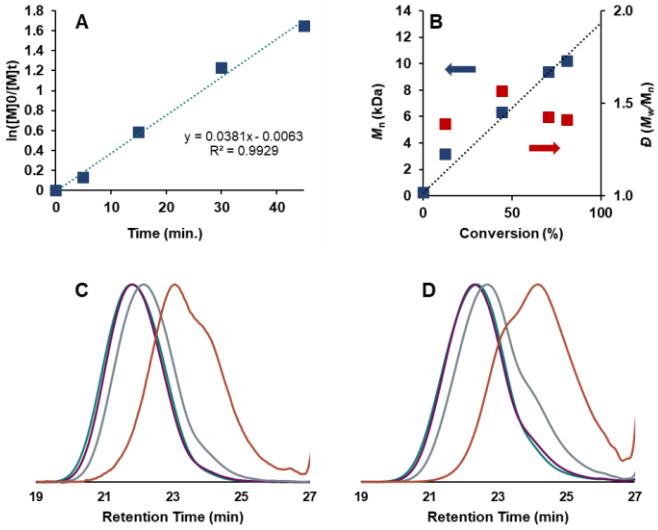


Figure S131: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[0.5] of [BA]:[DBMM]:[PC] with 1.5 mL DMAc to 1 mL BA.

Salt Additives

Table S19: Results of O-ATRP of butyl acrylate using **PC 2** in continuous flow testing the effect of various salt additives on polymerization.[a]

Entry	Salt	Res. Time (min.)	Conv. (%)	k_{app} (s^{-1})	$M_{n,\,calc.}$ (kDa)	$Đ$ (M_w/M_n)	I^* (%)
1	LiBr	90	79	0.0177	10.0	1.23	104
2	LiBr[b]	60	0	--	--	--	--
3	NaBr	90	81	0.0187	9.2	1.36	116
4	KBr	60	80	0.0278	9.4	1.41	112
5	TBABr	90	82	0.0201	15.0	1.20	72
6	LiCl	60	87	0.0354	27.2	1.98	42
7	LiI	60	0	--	--	--	--
9	$LiPF_6$	60	92	0.0424	14.7	1.31	82

[a]Conditions are [1000]:[10]:[1]:[10] of [BA]:[DBMM]:[PC 2]:[Salt] with 1.5 equivalents of DMAc to BA by volume. Polymerizations were irradiated by 18 W 365 nm light in flow reactor conditions at 22 ºC. [b]No DBMM.

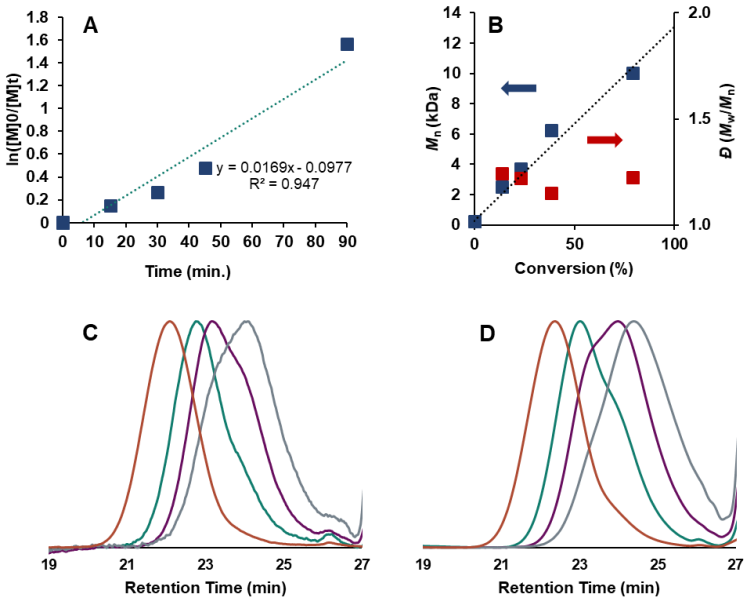


Figure S132: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1]:[10] of [BA]:[DBMM]:[PC]:[LiBr] with 1.5 mL DMAc to 1 mL BA.

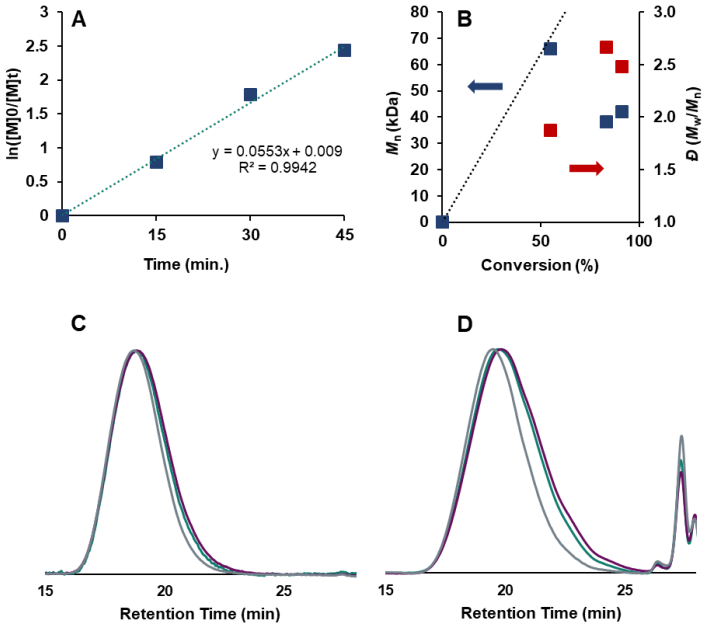


Figure S133: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[0]:[1]:[10] of [BA]:[DBMM]:[PC]:[LiBr] with 1.5 mL DMAc to 1 mL BA.

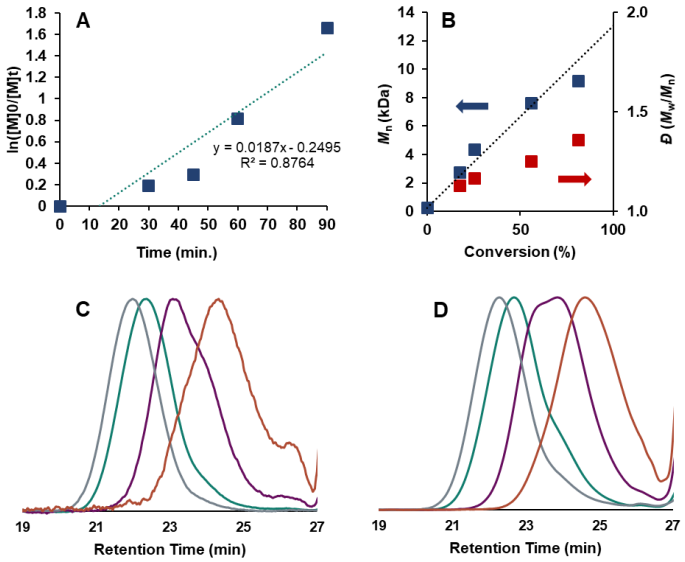


Figure S134: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1]:[10] of [BA]:[DBMM]:[PC]:[NaBr] with 1.5 mL DMAc to 1 mL BA.

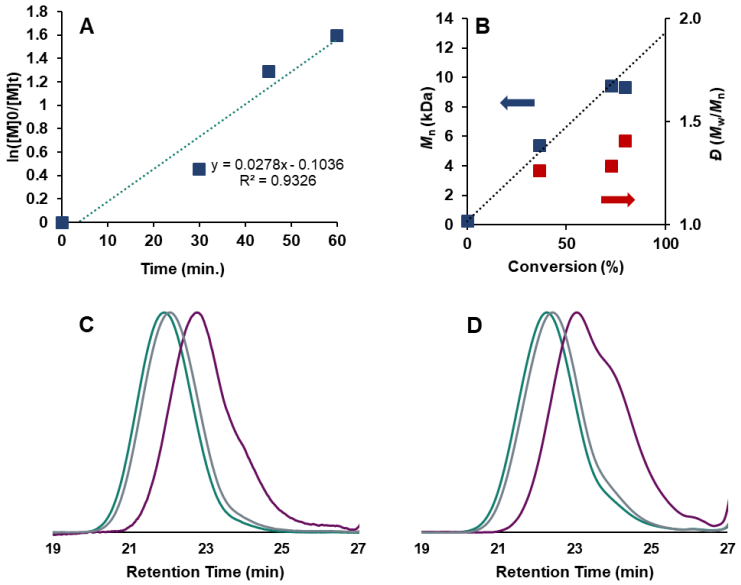


Figure S135: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1]:[10] of [BA]:[DBMM]:[PC]:[KBr] with 1.5 mL DMAc to 1 mL BA.

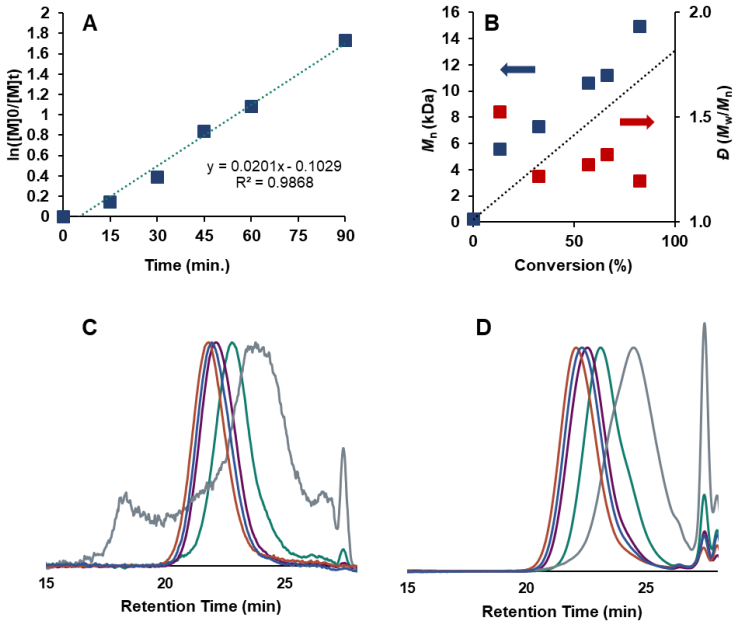


Figure S136: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1]:[10] of [BA]:[DBMM]:[PC]:[TBABr] with 1.5 mL DMAc to 1 mL BA.

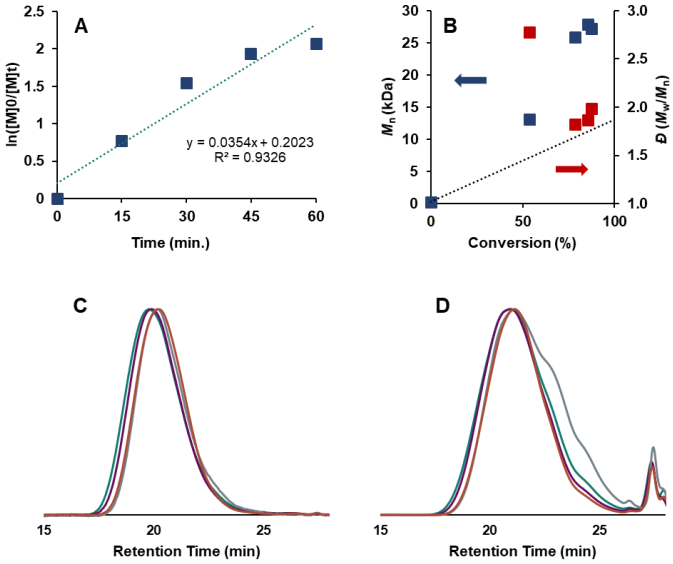


Figure S137: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1]:[10] of [BA]:[DBMM]:[PC]:[LiCl] with 1.5 mL DMAc to 1 mL BA.

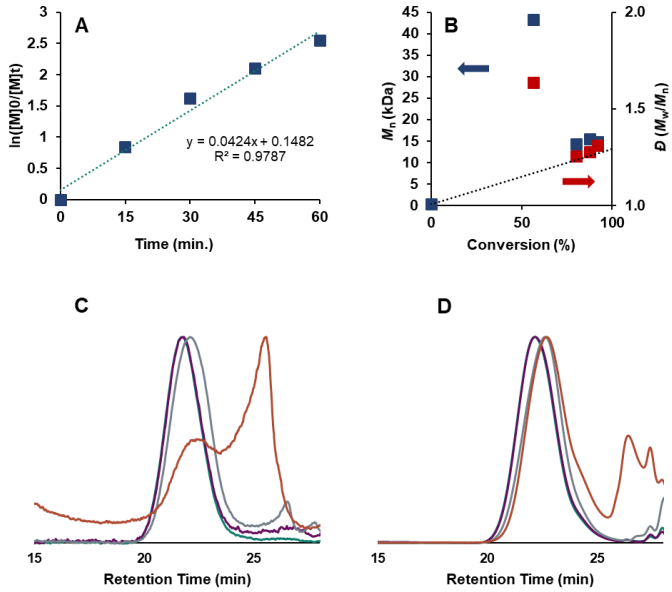


Figure S138: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1]:[10] of [BA]:[DBMM]:[PC]:[$LiPF_6$] with 1.5 mL DMAc to 1 mL BA.

LiBr Loadings

Table S20: Results of O-ATRP of BA using **PC 2** in continuous flow testing the effect of LiBr concentration on polymerization.[a]

Entry	[LiBr]:[PC 2]	Res. Time (min.)	Conv. (%)	k_{app} (s^{-1})	$M_{n,\ calc.}$ (kDa)	$Đ$ (M_w/M_n)	I^* (%)
1	[5]:[1]	60	73	0.0227	9.1	1.30	106
2	[10]:[1]	90	79	0.0177	10.0	1.23	104
3	[20]:[1]	90	60	0.0101	7.7	1.30	104
4	[30]:[1]	120	73	0.0111	9.4	1.20	103
5	[50]:[1]	120	83	10.1	10.9	1.23	108

[a]Conditions are [1000]:[10]:[1]:[X] of [BA]:[DBMM]:[PC 2]:[LiBr] with 1.5 equivalents of DMAc to BA by volume. Polymerizations were irradiated by 18 W 365 nm light in flow reactor conditions at 22 ºC.

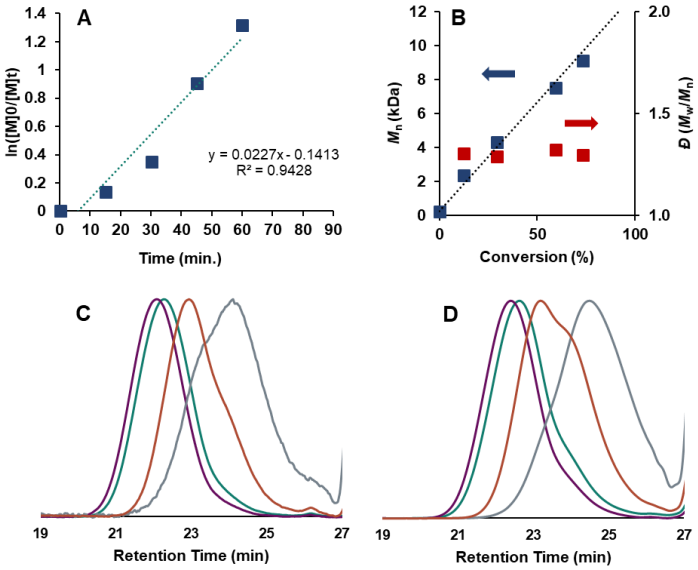


Figure S139: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1]:[5] of [BA]:[DBMM]:[PC]:[LiBr] with 1.5 mL DMAc to 1 mL BA.

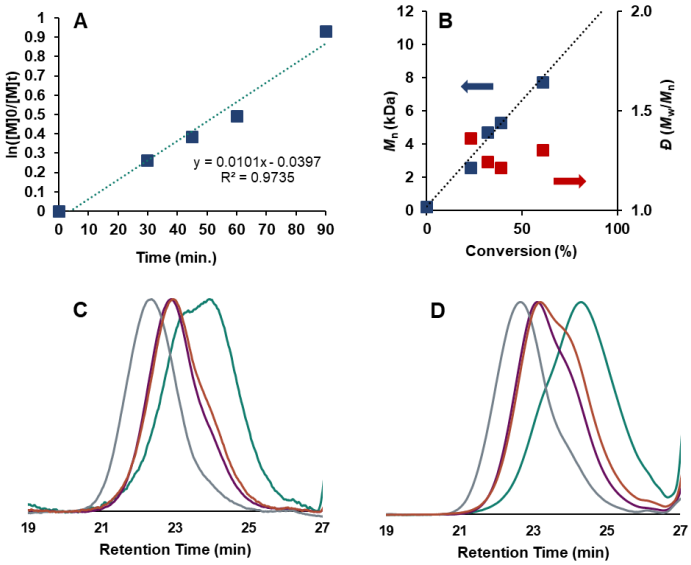


Figure S140: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1]:[20] of [BA]:[DBMM]:[PC]:[LiBr] with 1.5 mL DMAc to 1 mL BA.

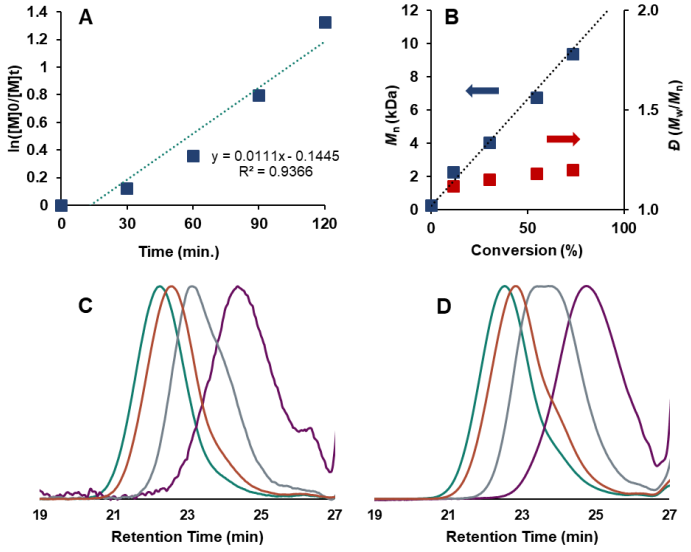


Figure S141: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1]:[30] of [BA]:[DBMM]:[PC]:[LiBr] with 1.5 mL DMAc to 1 mL BA.

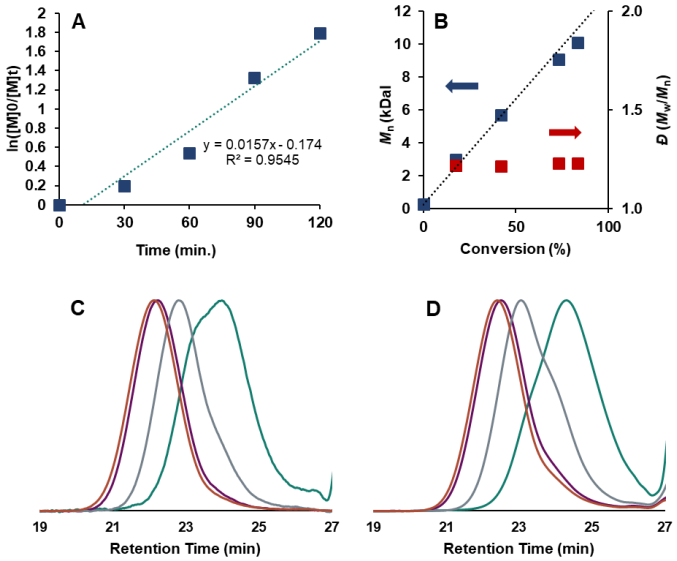


Figure S142: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1]:[50] of [BA]:[DBMM]:[PC]:[LiBr] with 1.5 mL DMAc to 1 mL BA.

Application of other organic PCs to optimized reaction conditions

Table S21: Results of O-ATRP of butyl acrylate using well-studied organic PCs in continuous-flow.[a]

Entry	PC	Res. Time (min.)	Conv. (%)	$M_{n,\ calc.}$ (kDa)	$M_{n,\ theo.}$ (kDa)	$Đ$ (M_w/M_n)	I^* (%)
1	PhenO	90	77	11.5	10.1	1.35	88
2	PhenO[b]	45	59	9.3	7.8	1.65	84
3	PhenN	120	76	9.2	10.0	1.14	109
4	4-CzIPN	90	0	--	--	--	--
5	4-CzIPN[b]	45	77	40	10.2	2.17	20

[a]Conditions are [1000]:[10]:[1]:[30] of [BA]:[DBMM]:[PC]:[LiBr] with 1.5 equivalents of DMAc to BA by volume. Polymerizations were irradiated by 18 W 365 nm light in flow reactor conditions at 22 ºC. [b]Performed in absence of LiBr.

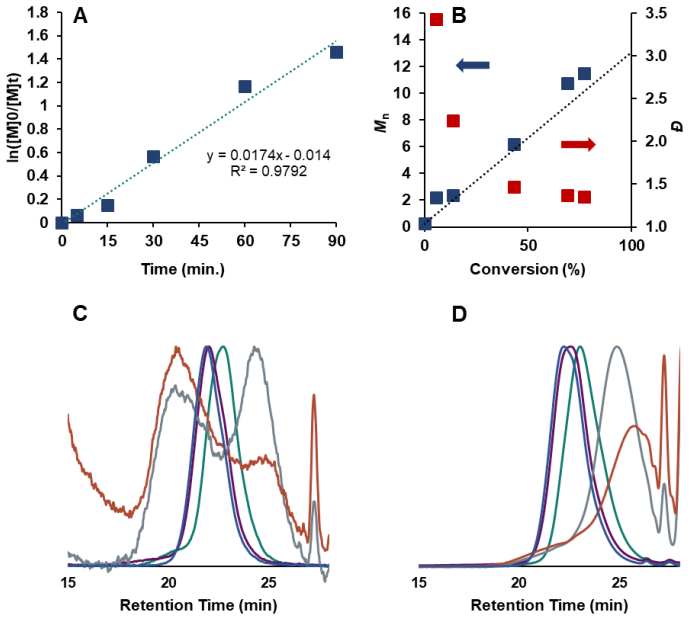


Figure S143: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PhenO** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1]:[30] of [BA]:[DBMM]:[PC]:[LiBr] with 1.5 mL DMAc to 1 mL BA.

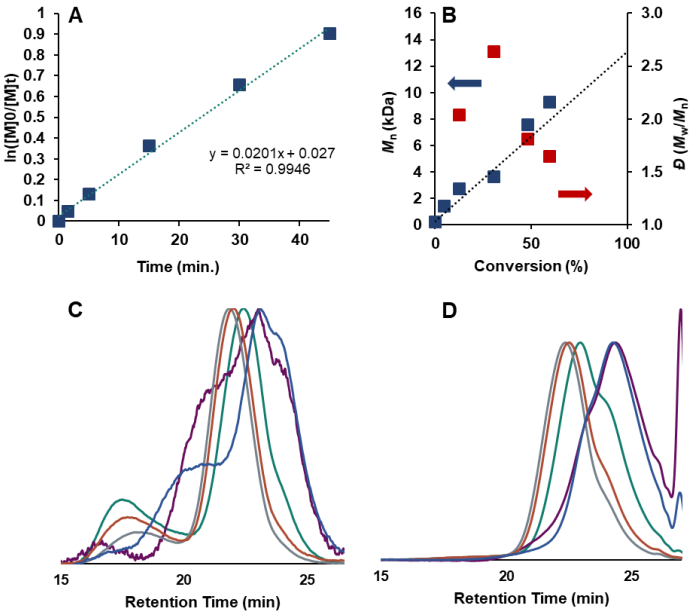


Figure S144: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PhenO** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1]:[0] of [BA]:[DBMM]:[PC]:[LiBr] with 1.5 mL DMAc to 1 mL BA.

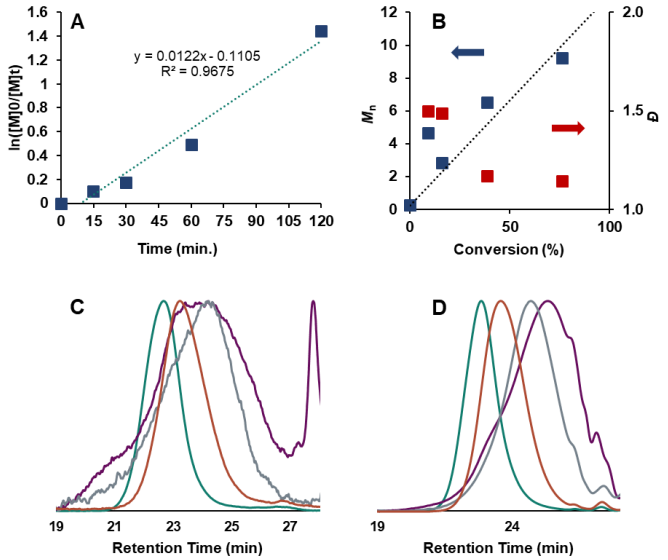


Figure S145: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PhenN** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1]:[30] of [BA]:[DBMM]:[PC]:[LiBr] with 1.5 mL DMAc to 1 mL BA.

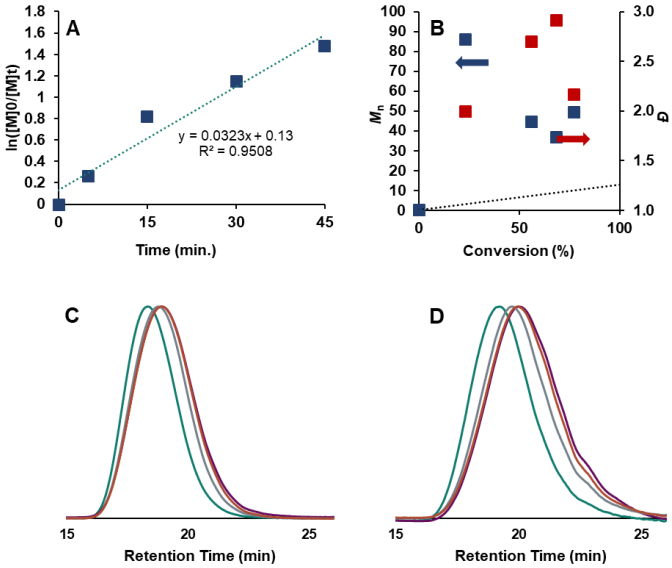


Figure S146: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **4-CzIPN** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1]:[0] of [BA]:[DBMM]:[PC]:[LiBr] with 1.5 mL DMAc to 1 mL BA.

Oxygen Tolerance of PC 2

General Procedure: The oxygen tolerance of the O-ATRP of BA under the optimized reaction conditions was tested by removing the reagents from the nitrogen-filled glovebox, bubbling compressed air through the DMAc, BA, and DBMM inside the fume hood for 30 minutes. The components, including **PC 2** and LiBr were then mixed together and then loaded into the stainless-steel syringe, where the polymerization was then conducted under the standard procedures, including the same equilibration times. Batch reactions conducted under air did not show any monomer conversion.

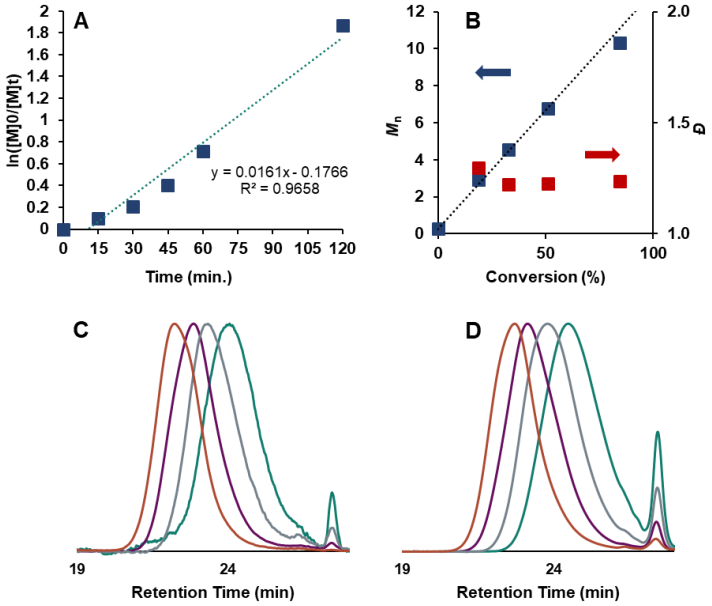


Figure S147: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º using reagents sparged with air. Corresponding SEC-MALS (C) and dRI (D) GPC traces are shown. Conditions are [1000[:[10]:[1]:[30] of [BA]:[DBMM]:[PC]:[LiBr] with 1.5 mL DMAc to 1 mL BA.

MW Control using PC 2

Table S22: Results of O-ATRP of BA using **PC 2** in continuous flow targeting different MW polymers through adjustment of stoichiometry of monomer and initiator.[a]

Entry	[BA]:[DBMM]	Res. Time (min.)	Conv. (%)	$M_{n,\ calc.}$ (kDa)	$M_{n,\ theo.}$ (kDa)	$Đ$ (M_w/M_n)	I^* (%)
1	[1000]:[2.5]	90	89	26.4	45.7	1.35	173
2	[1000]:[5]	120	88	15.2	22.8	1.32	150
3	[1000]:[10]	120	73	9.4	9.7	1.20	103
4	[1000]:[20]	180	80	7.3	5.4	1.19	74
5	[1000]:[40]	180	67	5.4	2.4	1.18	44

[a]Conditions are [1000]:[X]:[1]:[30] of [BA]:[DBMM]:[PC 2]:[LiBr] with 1.5 equivalents of DMAc to BA by volume. Polymerizations were irradiated by 18 W 365 nm light in flow reactor conditions at 22 ºC.

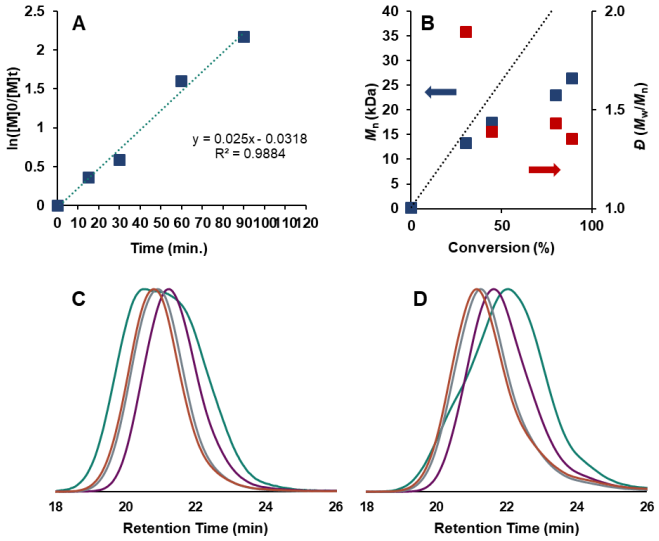


Figure S148: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[2.5]:[1]:[30] of [BA]:[DBMM]:[PC]:[LiBr] with 1.5 mL DMAc to 1 mL BA.

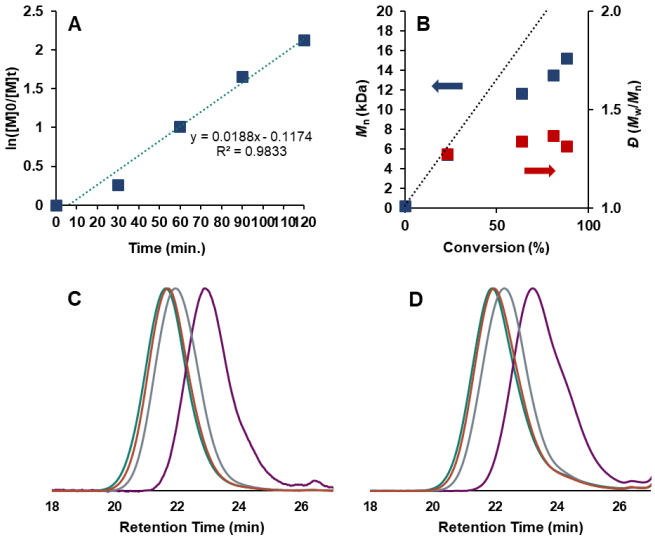


Figure S149: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[5]:[1]:[30] of [BA]:[DBMM]:[PC]:[LiBr] with 1.5 mL DMAc to 1 mL BA.

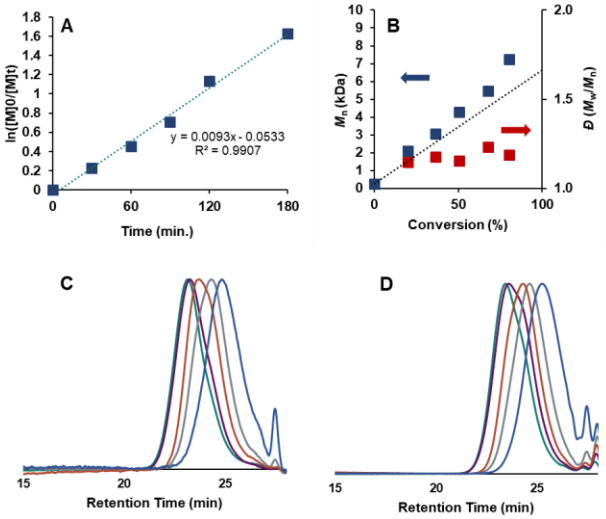


Figure S150: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[20]:[1]:[30] of [BA]:[DBMM]:[PC]:[LiBr] with 1.5 mL DMAc to 1 mL BA.

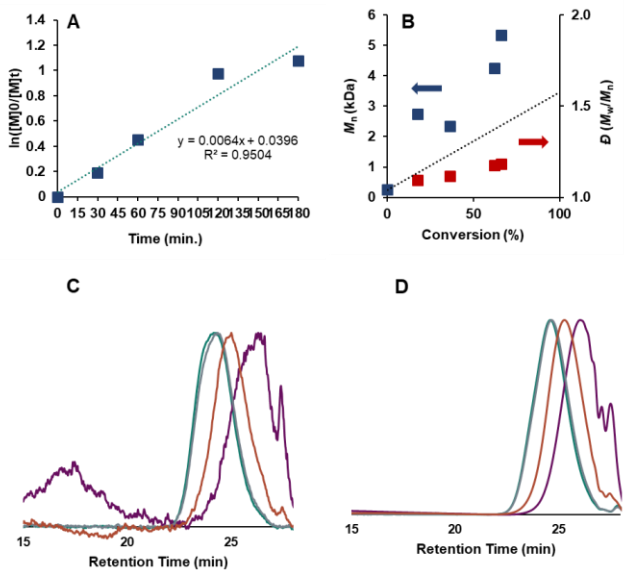


Figure S151: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[40]:[1]:[30] of [BA]:[DBMM]:[PC]:[LiBr] with 1.5 mL DMAc to 1 mL BA.

Monomer Scope

Table S23: Results of O-ATRP of acrylate and methacrylate monomers using **PC 2** in continuous flow.[a]

Entry	Monomer	Res. Time (min.)	Conv. (%)	$M_{n,\,calc.}$ (kDa)	$M_{n,\,theo.}$ (kDa)	$Đ$ (M_w/M_n)	I^* (%)
1	*t*-BA	120	92	13.8	12.1	1.23	88
2	MA	90	92	10	8.1	1.30	81
3	EA	90	76	7.5	7.8	1.19	105
4	2-EHA	90	90	16.3	16.8	1.53	104
5	EGMEA	60	92	10.5	12.3	1.37	117
6	MMA	600	72	8.8	7.4	1.17	85

[a]Conditions are [1000]:[10]:[1]:[30] of [Monomer]:[DBMM]:[PC 2]:[LiBr] with 1.5 equivalents of DMAc to BA by volume. Polymerizations were irradiated by 18 W 365 nm light in flow reactor conditions at 22 ºC.

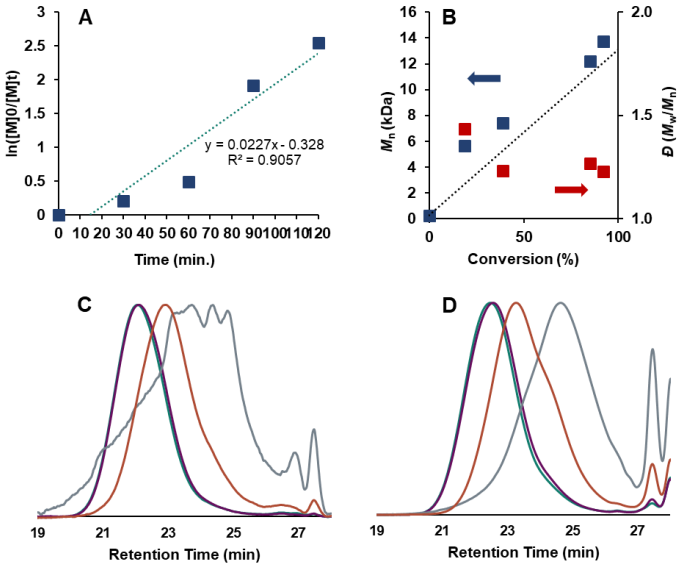


Figure S152: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1]:[30] of [*t*-BA]:[DBMM]:[PC]:[LiBr] with 1.5 mL DMAc to 1 mL BA.

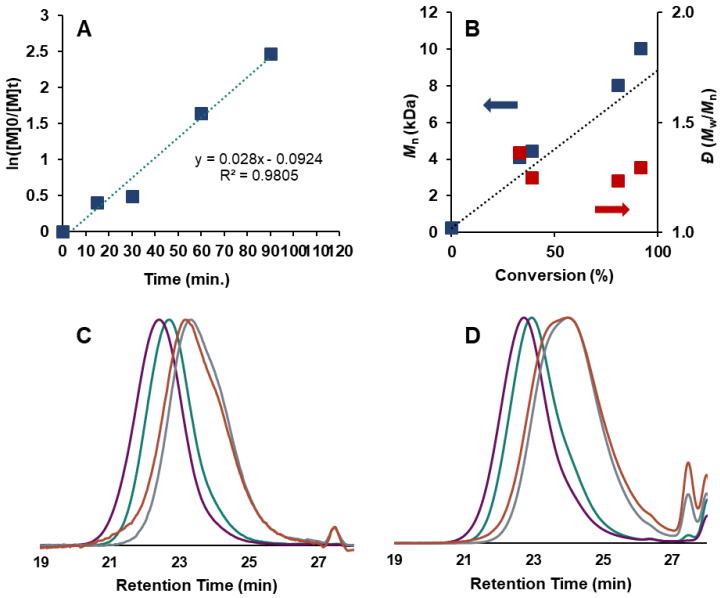


Figure S153: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1]:[30] of [MA]:[DBMM]:[PC]:[LiBr] with 1.5 mL DMAc to 1 mL BA.

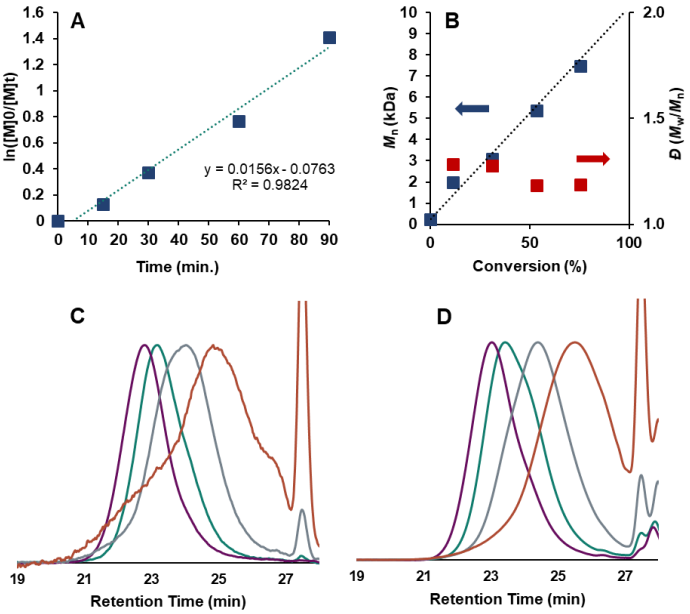


Figure S154: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1]:[30] of [EA]:[DBMM]:[PC]:[LiBr] with 1.5 mL DMAc to 1 mL BA.

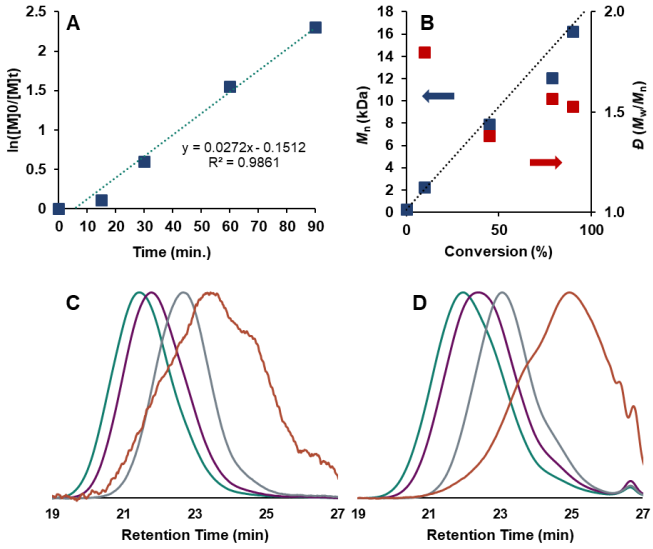


Figure S155: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1]:[30] of [2-EHA]:[DBMM]:[PC]:[LiBr] with 1.5 mL DMAc to 1 mL BA.

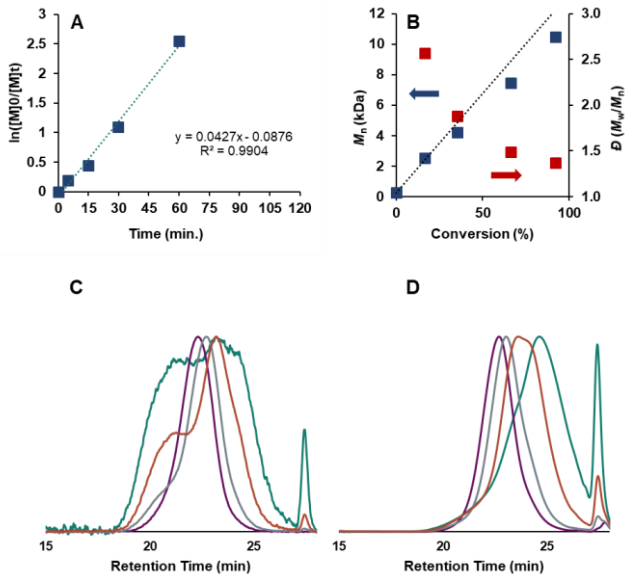


Figure S156: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1]:[30] of [EGMEA]:[DBMM]:[PC]:[LiBr] with 1.5 mL DMAc to 1 mL BA.

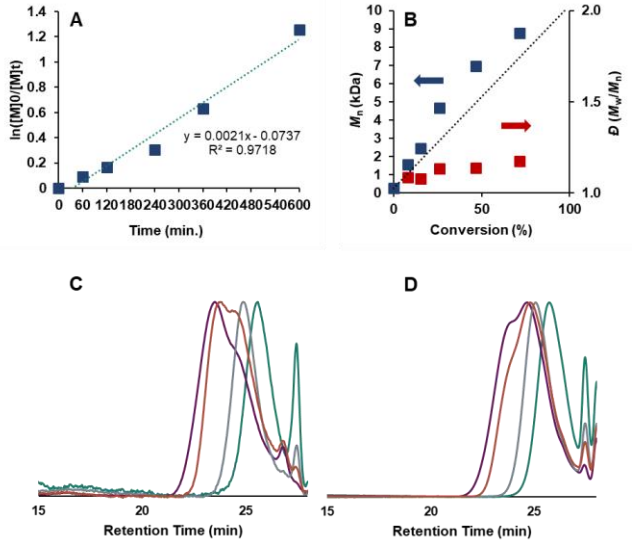
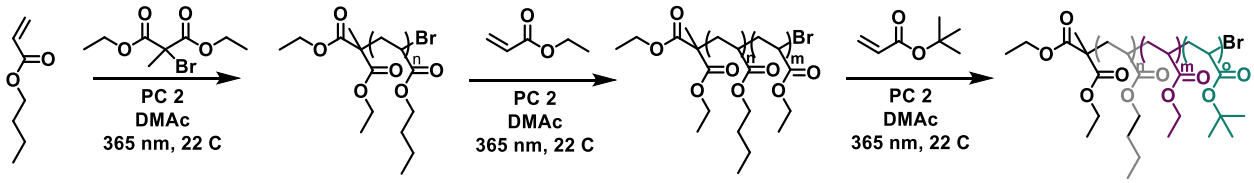


Figure S157: First order kinetic plot (A) and plot of M_n (blue) and dispersity (red) versus conversion (B) plotted against the theoretical M_n for O-ATRP of BA using **PC 2** under 365 nm irradiation in flow conditions at 22 º with corresponding SEC-MALS (C) and dRI (D) GPC traces. Conditions are [1000[:[10]:[1]:[30] of [MMA]:[DBMM]:[PC]:[LiBr] with 1.5 mL DMAc to 1 mL BA.

Chain-extension Experiments



Scheme S2: Synthetic route for the synthesis of triblock copolymers using a chain-extension approach.

Macroinitiator Synthesis: A p(BA) macroinitiator was synthesized using optimized O-ATRP conditions. Inside a nitrogen-filled glovebox, 107.4 mg (1.24 mmol, 30 eq.) of LiBr was dissolved in 9 mL of DMAc. Then, the solution was transferred to a vial with 22.8 mg (0.041 mmol, 1 eq.) of PC 2. 6 mL of BA (41.7 mmol, 1000 eq.) was added, followed by 79.6 µL DBMM (0.41 mmol, 10 eq.). The solution was then transferred to a stainless-steel syringe, which was then fitted with the first section of PFA tubing. The syringe was taken out of the glovebox and quickly connected to the flow reactor, which was set to a 30 minute residence time. After equilibration for 1.25 x residence time, the product was collected for 2 hours. Monomer conversion was measured at 27.5%. After precipitation in cold methanol/water, the polymer was dried to constant weight under vacuum at 50 ºC to give 1.32 g with M_n = 4.57 kDa, $Đ$ = 1.26, and I^* = 83%.

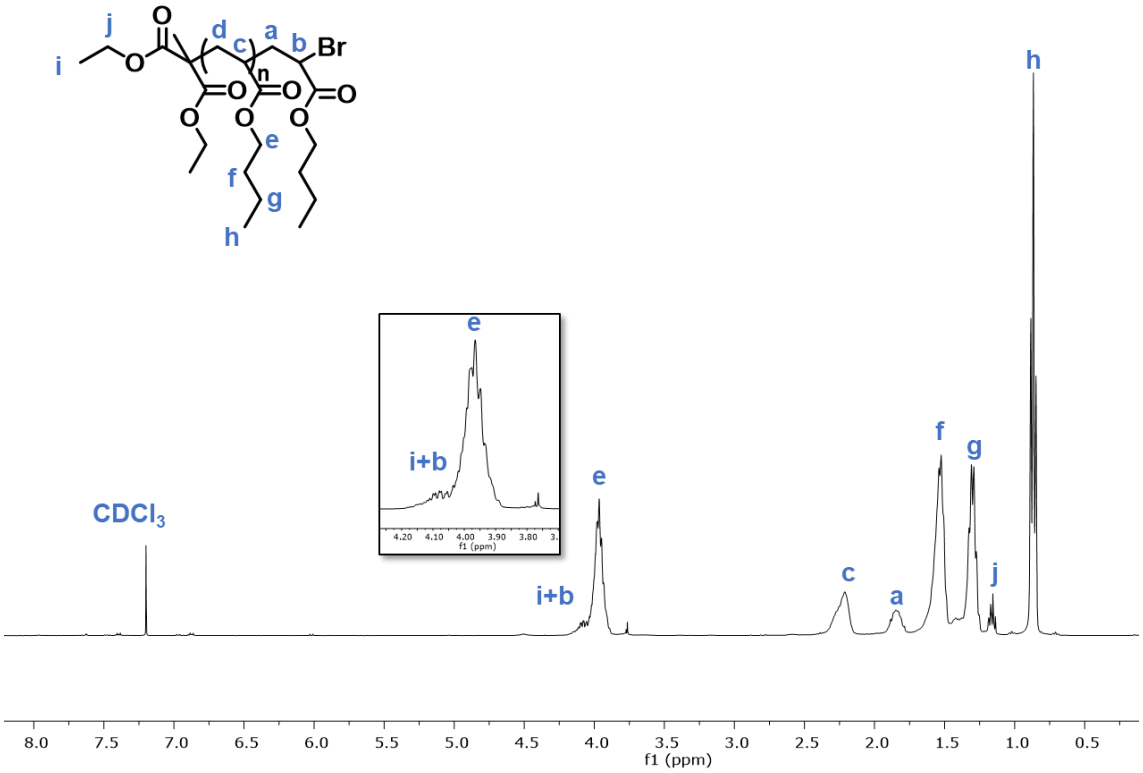


Figure 158: ^{1}H NMR spectrum of p(n-BA) in $CDCl_3$.

Block Copolymer Synthesis: A p(BA)-c-p(EA) block copolymer was synthesized using a [200]:[1]:[0.1]:[3] ratio of [EA]:[pBA]:[PC 2]:[LiBr]. 22.6 mg LiBr (0.262 mmol) was dissolved in 3.72 mL of DMAc. The solution was then transferred to a vial with 4.79 mg PC 2 (0.0087 mmol), which was then transferred to a vial with 400 mg of p(BA) macroinitiator (0.087 mmol). After the polymer was dissolved, 1.86 mL of EA (17.5 mmol) was added. The solution was then transferred to a stainless-steel syringe, which was then fitted with the first section of PFA tubing. The syringe was taken out of the glovebox and quickly connected to the flow reactor, which was set to a 60 minute residence time. After equilibration for 1.25 x residence time, the product was collected for 1 hour. After precipitation in cold methanol/water, the polymer was dried to constant weight under vacuum at 50 ºC to give 0.45 g with M_n = 12.6 kDa, $Đ$ = 1.16.

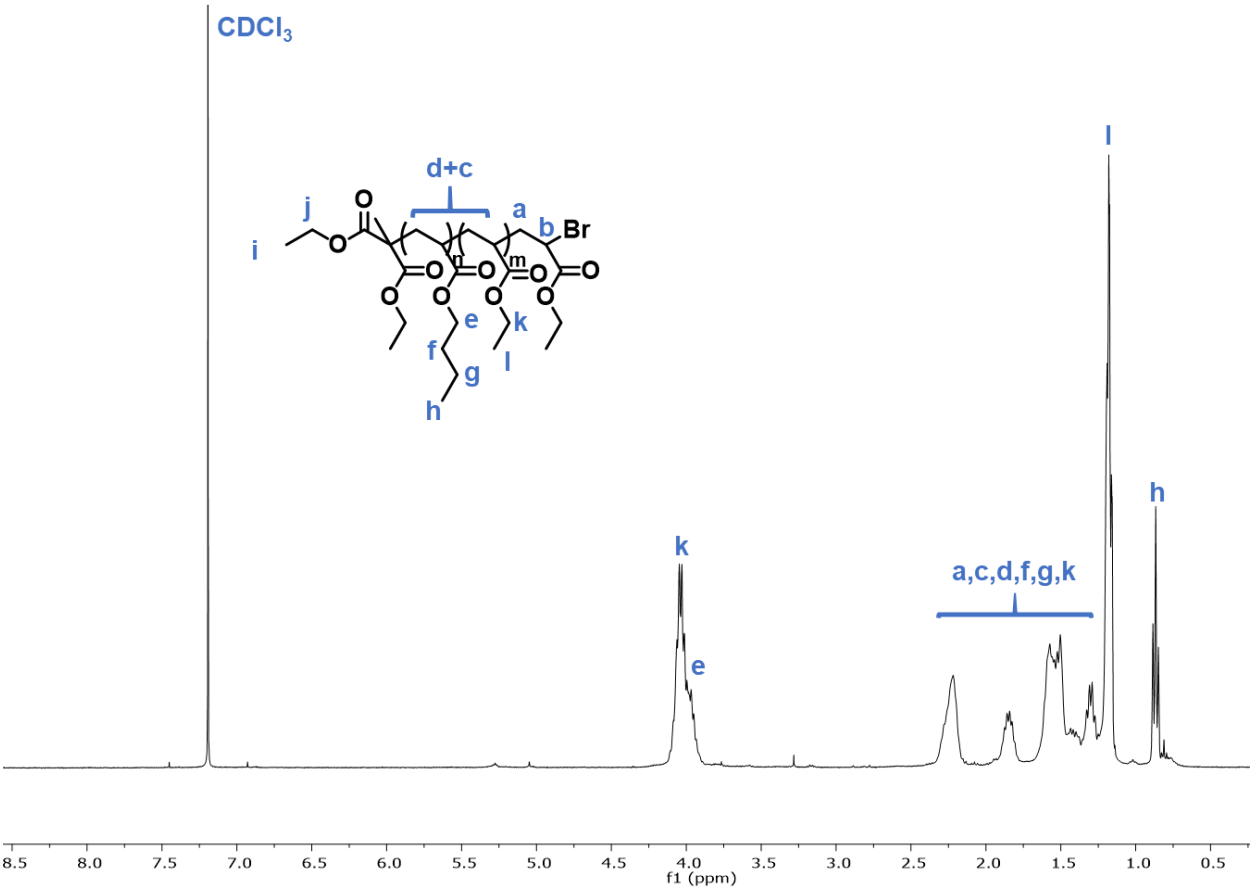


Figure S159: ^{1}H NMR spectrum of p(*n*-BA)-*b*-p(EA) in $CDCl_3$.

Triblock Copolymer Synthesis: A p(BA)-c-p(EA)-c-(*t*-BA) triblock copolymer was synthesized using a [200]:[1]:[0.1]:[3] ratio of [t-BA]:[block copolymer]:[PC 2]:[LiBr]. 8.2 mg LiBr (0.095 mmol) was dissolved in 2.80 mL of DMAc. The solution was then transferred to a vial with 1.7 mg PC 2 (3.18 µmol), which was then transferred to a vial with 400 mg of p(BA)-c-p(EA) macroinitiator (0.032 mmol). After the polymer was dissolved, 0.93 mL of *t*-BA (6.4 mmol) was added. The solution was then transferred to a stainless-steel syringe, which was then fitted with the first section of PFA tubing. The syringe was taken out of the glovebox and quickly connected to the flow reactor, which was set to a 60 minute residence time. After equilibration for 1.25 x residence time, the product was collected for 30 minutes. After precipitation in cold methanol/water, the polymer was dried to constant weight under vacuum at 50 ºC to give 0.2 g with M_n = 20 kDa, $Đ$ = 1.44.

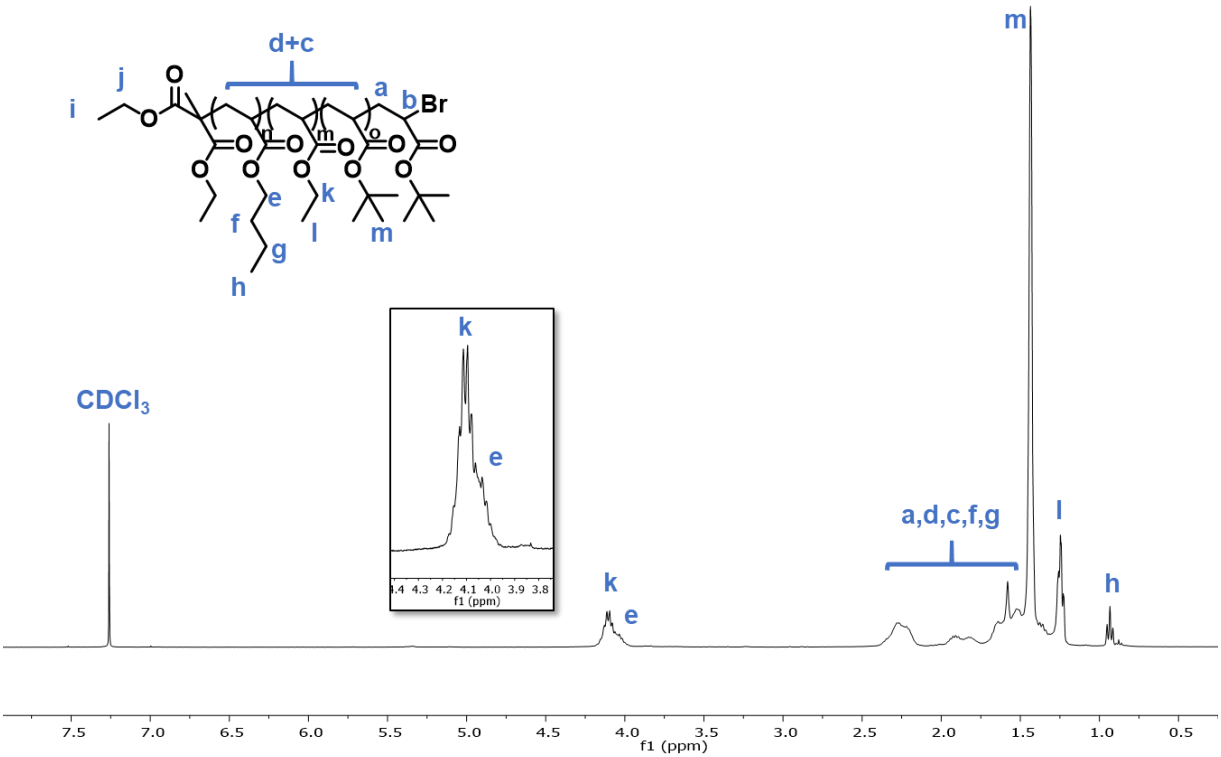


Figure S160: ^{1}H NMR spectrum of p(*n*-BA)-*b*-p(EA)-*b*-p(*t*-BA) in $CDCl_3$.

MALDI-MS Analysis

MALDI-TOF MS analysis was performed on a Bruker Microflex LRF Instrument using NaTFA as ionization agent and trans-2-[3-(4-tert-Butylphenyl)-2-methyl-2-propenylidene]malononitrile as matrix. Two polymers were selected for analysis, both synthesized in continuous-flow. Conditions are [1000]:[10]:[1]:[X] of [BA]:[DBMM]:[PC 2]:[LiBr] with 1.5 eq. DMAc.

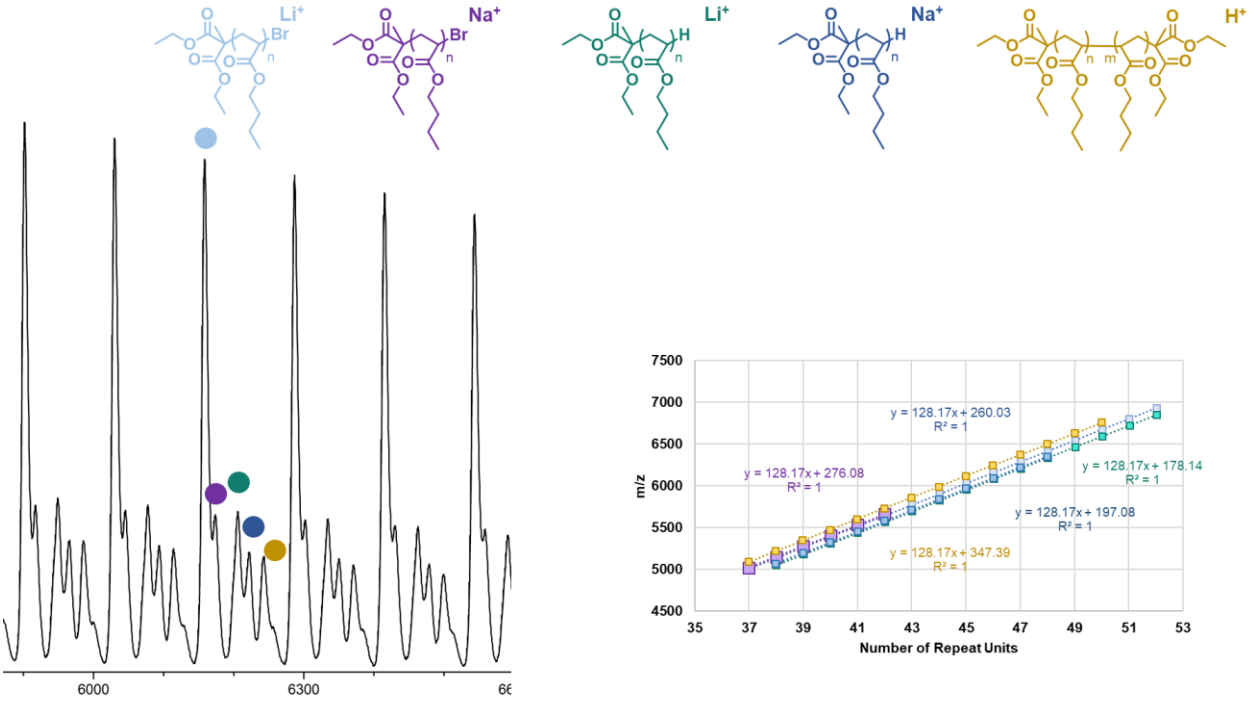


Figure S161: MALDI-TOF analysis of p(BA) synthesized in continuous-flow with 30 eq. of LiBr.

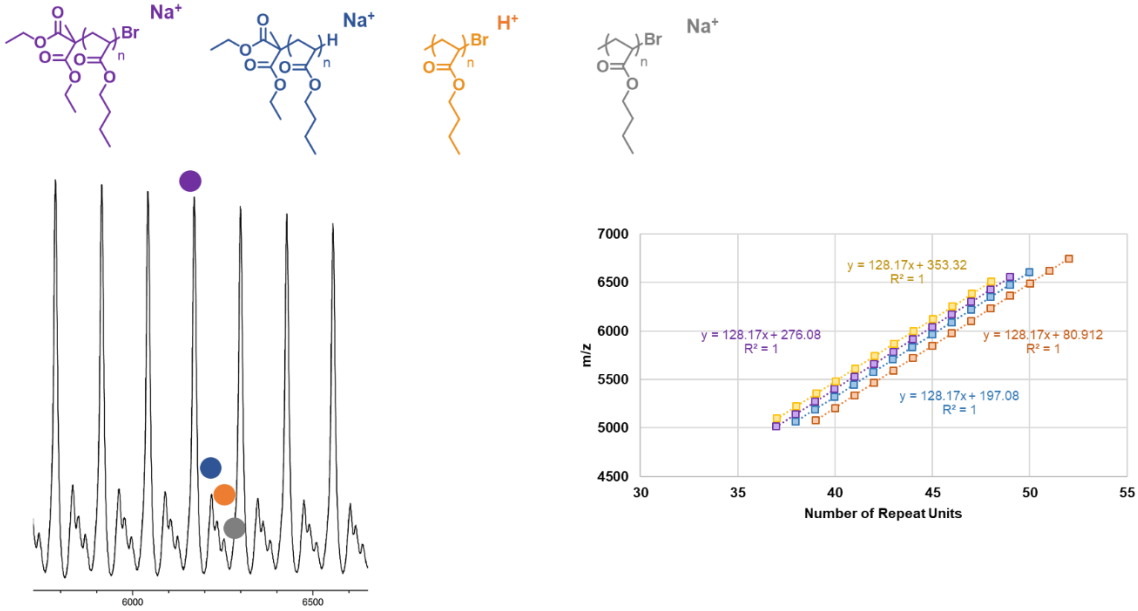
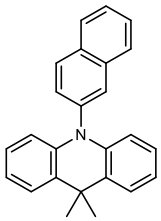


Figure S162: MALDI-TOF analysis of p(BA) synthesized in continuous-flow with no LiBr additives.

Coordinates of Molecular Structures

All coordinates are reported as XYZ Cartesian coordinates. Energies computed at uM06/6-311+G**/CPCM-H_2O level of theory (reported in parentheses) are arranged in the following order: E_{0K} (not ZPE and thermally corrected), H (298 K) and G (298 K). They are stated in Hartrees units. All energies reported were calculated using the GAUSSIAN 09 ver. D.01 computational chemistry package.



Neutral Ground State (-1019.540675, -1019.133186, -1019.203726)

C	-6.67693	-0.80995	0.04879
C	-5.28827	-0.83138	0.10963
C	-4.51158	0.32795	0.03535
C	-5.17666	1.55758	-0.11810
C	-6.58110	1.58520	-0.17705
C	-7.32188	0.41512	-0.09344
C	-3.06175	2.78209	-0.04897
C	-2.33520	1.58903	0.11275
C	-0.94916	1.68147	0.26503
H	-0.37135	0.76612	0.37843
C	-0.27412	2.89680	0.26851
C	-1.00667	4.06973	0.11203
C	-2.38405	4.01432	-0.04531
H	-4.78882	-1.79299	0.21276
H	-7.09647	2.53465	-0.29295
H	-2.94314	4.93741	-0.17122
H	-8.40703	0.46774	-0.14189
H	-0.50930	5.03695	0.10935
N	-4.45181	2.75234	-0.22273
C	-2.99228	0.21480	0.07120
C	-2.52460	-0.51204	-1.20359
H	-2.81606	0.05329	-2.09782
H	-1.43372	-0.62639	-1.21223
H	-2.97004	-1.51208	-1.27103
C	-2.56807	-0.59667	1.30699
H	-1.48097	-0.72405	1.34684
H	-2.88776	-0.09451	2.22822
H	-3.00703	-1.60041	1.29465
C	-5.16383	3.98735	-0.33294
C	-5.43148	4.51664	-1.56989
C	-5.58595	4.65066	0.84430
C	-6.13791	5.73919	-1.69146

H	-5.09929	3.99108	-2.46489
C	-6.27173	5.83575	0.75567
H	-5.35616	4.20261	1.80958
C	-6.56636	6.41132	-0.50772
C	-6.43108	6.31276	-2.95440
H	-6.59948	6.35178	1.65656
C	-7.27339	7.63371	-0.63053
C	-7.11839	7.49939	-3.04113
H	-6.10190	5.79488	-3.85381
C	-7.54353	8.16622	-1.86828
H	-7.59808	8.14326	0.27530
H	-7.33771	7.93165	-4.01440
H	-8.08640	9.10467	-1.95078
H	-7.24311	-1.73575	0.10987
H	0.80585	2.92447	0.38756

Neutral Triplet State (-1019.443813, -1019.040567, -1019.112914)

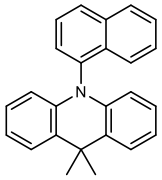
C	-6.66348	-0.85734	0.14692
C	-5.27582	-0.84478	0.12239
C	-4.53154	0.33913	0.09408
C	-5.23122	1.55917	0.10246
C	-6.63617	1.54938	0.09957
C	-7.34330	0.35764	0.12487
C	-3.12714	2.81000	0.10599
C	-2.37367	1.62541	0.04606
C	-0.98135	1.73448	0.05286
H	-0.38195	0.82810	-0.00795
C	-0.32808	2.95948	0.13386
C	-1.08554	4.12237	0.23799
C	-2.47034	4.04868	0.23696
H	-4.74597	-1.79528	0.10964
H	-7.18308	2.48581	0.07193
H	-3.05650	4.95602	0.35574
H	-8.43022	0.38473	0.12433
H	-0.60246	5.09158	0.33548
N	-4.52864	2.78206	0.07479
C	-3.01608	0.24971	-0.02114
C	-2.66479	-0.39572	-1.37486
H	-3.05567	0.20849	-2.20294
H	-1.57853	-0.48187	-1.49705
H	-3.09180	-1.40237	-1.45498
C	-2.46378	-0.62049	1.12180
H	-1.37698	-0.73299	1.04414
H	-2.69271	-0.17120	2.09575
H	-2.89446	-1.62745	1.09958
C	-5.20578	4.01738	-0.07678

C	-5.02542	4.73598	-1.33430
C	-6.04087	4.52155	0.88202
C	-5.73464	5.91971	-1.59524
H	-4.36853	4.31178	-2.09239
C	-6.73791	5.73320	0.65394
H	-6.17244	3.98698	1.82060
C	-6.61287	6.44768	-0.57673
C	-5.61108	6.62247	-2.81248
H	-7.37877	6.14210	1.43275
C	-7.30150	7.62984	-0.82867
C	-6.32485	7.83044	-3.04112
H	-4.95086	6.22572	-3.58213
C	-7.15556	8.32855	-2.07257
H	-7.96457	8.02949	-0.06280
H	-6.20718	8.34766	-3.99017
H	-7.70931	9.24976	-2.23504
H	-7.20395	-1.79998	0.17001
H	0.75788	3.00108	0.13356

Cation Radical State (-1019.345649, -1018.937946, -1019.008939)

C	-6.66433	-0.78982	-0.07694
C	-5.27806	-0.83600	0.01305
C	-4.49965	0.31794	-0.01393
C	-5.17332	1.55739	-0.13755
C	-6.58430	1.60569	-0.23167
C	-7.31828	0.44161	-0.19974
C	-3.06911	2.77870	-0.07994
C	-2.33231	1.57515	0.03510
C	-0.94576	1.67477	0.10990
H	-0.34798	0.77130	0.19574
C	-0.29514	2.90273	0.07881
C	-1.03525	4.08612	-0.02568
C	-2.40832	4.03027	-0.10491
H	-4.79521	-1.80496	0.10825
H	-7.08904	2.56088	-0.33081
H	-2.98378	4.94625	-0.18651
H	-8.40062	0.48534	-0.27105
H	-0.53347	5.04869	-0.04591
N	-4.45044	2.73865	-0.17022
C	-2.99521	0.21818	0.08958
C	-2.46990	-0.64298	-1.07923
H	-2.71658	-0.18363	-2.04285
H	-1.38315	-0.75658	-1.01774
H	-2.90906	-1.64514	-1.05017
C	-2.63592	-0.45061	1.43499
H	-1.55183	-0.56591	1.53213

H	-2.99734	0.15049	2.27682
H	-3.08328	-1.44717	1.50396
C	-5.17316	3.98739	-0.28351
C	-5.40253	4.51696	-1.52554
C	-5.61698	4.61261	0.90108
C	-6.11289	5.73630	-1.64115
H	-5.04323	4.00624	-2.41788
C	-6.30776	5.79423	0.80579
H	-5.40699	4.15083	1.86318
C	-6.57442	6.38455	-0.45605
C	-6.37612	6.32746	-2.90199
H	-6.66015	6.29401	1.70565
C	-7.28729	7.60345	-0.57525
C	-7.06884	7.51057	-2.98378
H	-6.02052	5.82783	-3.80107
C	-7.52875	8.15351	-1.81068
H	-7.63866	8.09477	0.33015
H	-7.26611	7.95894	-3.95417
H	-8.07619	9.08915	-1.89161
H	-7.23725	-1.71238	-0.05227
H	0.78873	2.94004	0.13844



Neutral Ground State (-1019.5428, -1019.135282, -1019.204519)

C	-6.70176	-0.80010	0.07146
C	-5.31250	-0.81669	0.07711
C	-4.54353	0.35067	0.06494
C	-5.21786	1.58418	0.04912
C	-6.62346	1.60629	0.04207
C	-7.35631	0.42861	0.05265
C	-3.10189	2.81102	0.07397
C	-2.36748	1.61310	0.09685
C	-0.97277	1.69870	0.13995
H	-0.39074	0.77868	0.15194
C	-0.29685	2.91282	0.15715
C	-1.03702	4.09152	0.12647
C	-2.42260	4.04230	0.08507
H	-7.26229	-1.73128	0.07888
H	-4.80315	-1.77874	0.08508
H	-7.14671	2.55869	0.03179
H	0.78924	2.93618	0.18896
H	-2.99019	4.96877	0.06388
H	-8.44264	0.47767	0.04668
H	-0.53868	5.05817	0.13515
N	-4.50354	2.79134	0.04050
C	-5.21123	4.01119	-0.18962
C	-5.64729	4.76586	0.87160
C	-5.45884	4.42073	-1.53034
C	-6.35678	5.96720	0.65209
H	-5.43834	4.42222	1.88308
C	-6.18247	5.63130	-1.74584
C	-6.61981	6.38762	-0.62873
H	-6.69378	6.55344	1.50297
H	-7.16899	7.31084	-0.80616
C	-6.44551	6.04500	-3.07678
C	-5.01903	3.67068	-2.65043
C	-5.28970	4.10073	-3.92718
H	-4.94892	3.51757	-4.77923
C	-6.01098	5.29754	-4.14391
H	-6.21892	5.62382	-5.15994
H	-6.99955	6.96879	-3.23557
H	-4.46407	2.74785	-2.48646
C	-3.02493	0.24059	0.03867
C	-2.60406	-0.44842	-1.27277

H	-2.92809	0.14301	-2.13901
H	-1.51485	-0.56282	-1.32685
H	-3.04924	-1.44704	-1.35626
C	-2.55641	-0.60383	1.23633
H	-1.46739	-0.72357	1.23737
H	-2.84928	-0.13017	2.18131
H	-2.99303	-1.60867	1.20817

Neutral Triplet State (-1019.448164, -1019.044641, -1019.117175)

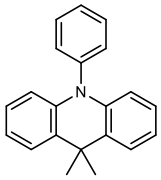
C	-6.69680	-0.76672	0.03885
C	-5.30872	-0.80662	0.09789
C	-4.51949	0.34656	0.05323
C	-5.17402	1.58335	-0.06986
C	-6.57747	1.63207	-0.11400
C	-7.33091	0.46894	-0.06320
C	-3.05078	2.79073	0.04174
C	-2.33580	1.59027	0.19726
C	-0.95220	1.67416	0.37149
H	-0.37885	0.75540	0.47920
C	-0.27245	2.88747	0.39515
C	-0.99220	4.06610	0.22179
C	-2.36694	4.01891	0.04017
H	-7.27335	-1.68740	0.07468
H	-4.82108	-1.77666	0.17464
H	-7.07804	2.59498	-0.19007
H	0.80560	2.90807	0.53169
H	-2.92161	4.94188	-0.11211
H	-8.41573	0.53357	-0.10103
H	-0.48596	5.02853	0.21908
N	-4.43971	2.77742	-0.13664
C	-5.12460	4.00585	-0.31677
C	-5.45106	4.80312	0.84962
C	-5.49216	4.42037	-1.62450
C	-6.17463	5.94313	0.70684
H	-5.11960	4.44579	1.82269
C	-6.25873	5.63529	-1.76054
C	-6.59513	6.37230	-0.60059
H	-6.44412	6.54043	1.57399
H	-7.17280	7.28825	-0.70870
C	-6.63584	6.04787	-3.04578
C	-5.13472	3.70664	-2.77342
C	-5.53708	4.15101	-4.07382
H	-5.25296	3.56793	-4.94587
C	-6.27278	5.29476	-4.20554
H	-6.58814	5.64281	-5.18579
H	-7.21485	6.96337	-3.15517

H	-4.53782	2.80102	-2.67267
C	-3.00117	0.22385	0.08748
C	-2.53876	-0.43027	-1.22835
H	-2.83155	0.18753	-2.08761
H	-1.44809	-0.54669	-1.24584
H	-2.98967	-1.42273	-1.35099
C	-2.58161	-0.65838	1.27431
H	-1.49493	-0.78871	1.31044
H	-2.90527	-0.21268	2.22271
H	-3.01962	-1.65953	1.20008

Cation Radical State (-1019.346591, -1018.938716, -1019.009186)

C	-6.69011	-0.77405	0.08967
C	-5.30187	-0.82312	0.13181
C	-4.52338	0.33032	0.08951
C	-5.19852	1.57131	-0.00291
C	-6.61146	1.62248	-0.05011
C	-7.34591	0.45938	-0.00231
C	-3.09183	2.79014	0.02482
C	-2.35556	1.58551	0.13142
C	-0.96976	1.68422	0.21885
H	-0.37314	0.77927	0.29560
C	-0.31937	2.91259	0.20082
C	-1.05782	4.09622	0.08493
C	-2.43025	4.04089	-0.00443
H	-7.26358	-1.69588	0.12569
H	-4.81635	-1.79316	0.19503
H	-7.11682	2.58005	-0.12134
H	0.76387	2.94967	0.27114
H	-3.00596	4.95641	-0.09259
H	-8.42994	0.50528	-0.03646
H	-0.55503	5.05821	0.06417
N	-4.47415	2.75210	-0.05837
C	-5.19313	3.99333	-0.24749
C	-5.59625	4.70415	0.85342
C	-5.45957	4.41763	-1.57549
C	-6.31183	5.90717	0.67835
H	-5.36306	4.33262	1.84902
C	-6.19099	5.63248	-1.73426
C	-6.60298	6.35550	-0.58663
H	-6.62961	6.47020	1.55092
H	-7.15762	7.28107	-0.72794
C	-6.48691	6.08454	-3.04495
C	-5.04287	3.70119	-2.72542
C	-5.34740	4.17053	-3.98007
H	-5.02539	3.61404	-4.85636

C	-6.07673	5.37002	-4.14319
H	-6.30971	5.72505	-5.14360
H	-7.04615	7.01090	-3.16143
H	-4.47892	2.77604	-2.61646
C	-3.01620	0.22747	0.08912
C	-2.58914	-0.46200	-1.22866
H	-2.90853	0.12768	-2.09651
H	-1.50046	-0.57309	-1.26724
H	-3.03731	-1.45831	-1.30274
C	-2.55536	-0.61549	1.29356
H	-1.46846	-0.73849	1.29070
H	-2.84866	-0.14137	2.23642
H	-2.99404	-1.61732	1.25819



Neutral Ground State (-865.9816177, -865.6235294, -865.6879324)

C	-6.66114	-0.83253	-0.15834
C	-5.27482	-0.84606	-0.05744
C	-4.50715	0.32142	-0.04796
C	-5.17887	1.55353	-0.14175
C	-6.58115	1.57280	-0.24521
C	-7.31264	0.39389	-0.25300
C	-3.06487	2.78130	-0.08341
C	-2.33153	1.58498	0.00917
C	-0.93761	1.67153	0.05463
H	-0.35748	0.75384	0.13401
C	-0.25929	2.88410	0.00958
C	-0.99781	4.06041	-0.08007
C	-2.38353	4.01110	-0.12560
H	-4.76790	-1.80614	0.02394
H	-7.10317	2.52284	-0.31910
H	-2.94719	4.93733	-0.19471
H	-8.39624	0.44077	-0.33258
H	-0.49865	5.02609	-0.11578
N	-4.46440	2.75823	-0.13199
C	-2.99441	0.21656	0.09905
C	-2.43680	-0.69525	-1.00751
H	-2.64160	-0.27115	-1.99814
H	-1.35319	-0.82382	-0.90809
H	-2.88676	-1.69345	-0.96327
C	-2.67572	-0.39531	1.47611
H	-1.59367	-0.49945	1.62066
H	-3.06851	0.24088	2.27912
H	-3.12350	-1.39110	1.57955
C	-5.17972	3.99319	-0.22763
C	-5.44161	4.54738	-1.47871
C	-5.60965	4.63288	0.93221
C	-6.13855	5.74935	-1.56875
H	-5.09507	4.02949	-2.37156
C	-6.30778	5.83449	0.83976
H	-5.39382	4.18034	1.89853
C	-6.57183	6.39287	-0.41006
H	-6.64537	6.33525	1.74377
H	-7.22080	-1.76427	-0.16032
H	0.82662	2.90774	0.04718
H	-6.34286	6.18448	-2.54397

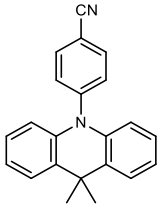
H	-7.11677	7.33096	-0.48152

Neutral Triplet State (-865.8645597, -865.5106975, -865.5778625)

C	-6.66197	-0.84277	-0.48061
C	-5.29011	-0.87712	-0.22796
C	-4.51410	0.27715	-0.18386
C	-5.16335	1.51926	-0.37338
C	-6.54599	1.55798	-0.63345
C	-7.28475	0.38605	-0.68774
C	-3.06828	2.76294	-0.18074
C	-2.36309	1.46815	-0.41724
C	-0.96946	1.56269	-0.70639
H	-0.42189	0.67210	-1.01149
C	-0.29290	2.74283	-0.57473
C	-0.97301	3.96519	-0.12999
C	-2.35120	3.94853	0.01602
H	-4.81438	-1.84165	-0.06733
H	-7.03972	2.51257	-0.79276
H	-2.88351	4.87393	0.22809
H	-8.35096	0.43707	-0.89437
H	-0.40747	4.87887	0.02411
N	-4.44179	2.72027	-0.28012
C	-3.02764	0.23532	0.12969
C	-2.36279	-1.03782	-0.39049
H	-2.45440	-1.12003	-1.48062
H	-1.29909	-1.04675	-0.13057
H	-2.79931	-1.93306	0.06374
C	-2.87947	0.27560	1.67604
H	-1.81605	0.25538	1.94785
H	-3.32470	1.18874	2.09333
H	-3.37810	-0.58917	2.13247
C	-5.16441	3.95797	-0.19789
C	-5.29623	4.75456	-1.33031
C	-5.69698	4.34892	1.02660
C	-5.97898	5.96406	-1.23437
H	-4.86504	4.42020	-2.27195
C	-6.37574	5.56177	1.11657
H	-5.57338	3.70113	1.89311
C	-6.51563	6.36800	-0.01199
H	-6.79225	5.87881	2.06922
H	-7.23140	-1.76761	-0.52184
H	0.76914	2.78512	-0.81008
H	-6.09072	6.59201	-2.11441
H	-7.04573	7.31430	0.06064

Cation Radical State (-865.7868048, -865.4283847, -865.4932297)

C	-6.65960	-0.79816	-0.11104
C	-5.27358	-0.84247	-0.01667
C	-4.49768	0.31323	-0.02766
C	-5.17340	1.55309	-0.13625
C	-6.58427	1.59955	-0.23352
C	-7.31567	0.43341	-0.22060
C	-3.06987	2.77556	-0.07729
C	-2.33167	1.57191	0.02667
C	-0.94460	1.67136	0.09047
H	-0.34684	0.76755	0.17302
C	-0.29423	2.89925	0.05359
C	-1.03519	4.08254	-0.04541
C	-2.40911	4.02696	-0.10952
H	-4.78813	-1.81087	0.07089
H	-7.09141	2.55471	-0.31993
H	-2.98485	4.94332	-0.18533
H	-8.39783	0.47578	-0.29552
H	-0.53354	5.04502	-0.07270
N	-4.45234	2.73556	-0.15074
C	-2.99433	0.21544	0.09090
C	-2.45464	-0.66484	-1.05589
H	-2.68451	-0.21953	-2.03021
H	-1.36963	-0.78279	-0.97602
H	-2.89762	-1.66490	-1.01835
C	-2.65192	-0.43093	1.45226
H	-1.56860	-0.53927	1.56600
H	-3.02789	0.18198	2.27918
H	-3.09741	-1.42789	1.52984
C	-5.17574	3.98560	-0.24944
C	-5.42358	4.52196	-1.50716
C	-5.59754	4.60909	0.91823
C	-6.11929	5.72412	-1.59280
H	-5.07553	4.00237	-2.39729
C	-6.29258	5.81081	0.81801
H	-5.38280	4.15637	1.88372
C	-6.55205	6.36599	-0.43367
H	-6.63036	6.31258	1.72043
H	-7.23074	-1.72209	-0.09913
H	0.79013	2.93661	0.10394
H	-6.32136	6.15915	-2.56753
H	-7.09498	7.30436	-0.50670



Neutral Ground State (-958.1944652, -957.8358095, -957.9047975)

C	-6.66737	-0.82199	-0.15286
C	-5.28112	-0.83597	-0.05233
C	-4.51315	0.33129	-0.04515
C	-5.18630	1.56150	-0.14043
C	-6.58772	1.58252	-0.24471
C	-7.31939	0.40362	-0.25024
C	-3.06742	2.79189	-0.08544
C	-2.33651	1.59505	0.00702
C	-0.94256	1.68157	0.05044
H	-0.36235	0.76401	0.12946
C	-0.26454	2.89415	0.00393
C	-1.00207	4.07083	-0.08452
C	-2.38795	4.02176	-0.12811
H	-4.77454	-1.79600	0.03032
H	-7.11236	2.53099	-0.32127
H	-2.94872	4.94995	-0.19536
H	-8.40280	0.45035	-0.33032
H	-0.50279	5.03626	-0.12060
N	-4.46878	2.76656	-0.13179
C	-3.00016	0.22717	0.09955
C	-2.44487	-0.68574	-1.00723
H	-2.65124	-0.26257	-1.99787
H	-1.36123	-0.81467	-0.90934
H	-2.89510	-1.68365	-0.96098
C	-2.67941	-0.38268	1.47697
H	-1.59720	-0.48684	1.61965
H	-3.07077	0.25456	2.27978
H	-3.12704	-1.37827	1.58225
C	-5.18218	3.99709	-0.23229
C	-5.43186	4.55122	-1.48713
C	-5.62427	4.63258	0.92656
C	-6.12765	5.74699	-1.58913
H	-5.07582	4.03670	-2.37688
C	-6.32289	5.82832	0.83664
H	-5.41761	4.17999	1.89364
C	-6.57370	6.38479	-0.42405
H	-6.67392	6.33299	1.73227
H	-7.22703	-1.75365	-0.15293
H	0.82136	2.91749	0.03989

H	-6.32752	6.18980	-2.56084
C	-7.29288	7.61807	-0.52363
N	-7.87760	8.62083	-0.60529

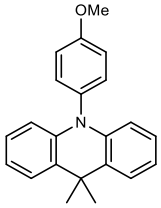
Neutral Triplet State (-958.0959499, -957.7403154, -957.8106704)

C	-6.66286	-0.79211	0.10261
C	-5.27462	-0.82890	0.17451
C	-4.49910	0.32458	0.08025
C	-5.17348	1.55860	-0.07107
C	-6.58224	1.59095	-0.18717
C	-7.31642	0.42726	-0.09310
C	-3.07328	2.77787	-0.08779
C	-2.33224	1.57534	-0.02491
C	-0.94238	1.67010	-0.02599
H	-0.34496	0.76267	0.01779
C	-0.28768	2.89629	-0.06726
C	-1.02987	4.08010	-0.08347
C	-2.40781	4.02608	-0.08587
H	-4.78628	-1.79262	0.29672
H	-7.07879	2.53899	-0.36377
H	-2.99290	4.93959	-0.07525
H	-8.39815	0.46477	-0.18182
H	-0.52915	5.04393	-0.08395
N	-4.46449	2.75559	-0.13292
C	-2.99017	0.21840	0.09031
C	-2.55292	-0.65795	-1.10221
H	-2.87647	-0.21286	-2.05007
H	-1.46383	-0.76688	-1.12629
H	-2.98489	-1.66133	-1.02706
C	-2.53750	-0.43465	1.41259
H	-1.44942	-0.55353	1.43489
H	-2.83538	0.17870	2.27073
H	-2.98131	-1.42870	1.52827
C	-5.17933	3.98756	-0.25204
C	-5.11591	4.73166	-1.46405
C	-5.95784	4.46922	0.83812
C	-5.80917	5.90454	-1.58993
H	-4.52756	4.34716	-2.29613
C	-6.64060	5.64985	0.72844
H	-5.98618	3.90046	1.76658
C	-6.59973	6.41551	-0.49517
H	-7.22140	6.02248	1.56934
H	-7.23193	-1.71458	0.17825
H	0.79822	2.92921	-0.06612
H	-5.77091	6.46200	-2.52320
C	-7.30171	7.61392	-0.61606

N	-7.89642	8.62958	-0.71910

Cation Radical State (-957.9962549, -957.6373759, -957.7067189)

C	-6.66485	-0.79012	-0.10793
C	-5.27881	-0.83369	-0.01394
C	-4.50358	0.32227	-0.02664
C	-5.18120	1.56093	-0.13658
C	-6.59182	1.60730	-0.23378
C	-7.32219	0.44081	-0.21909
C	-3.07539	2.78641	-0.07790
C	-2.33772	1.58249	0.02656
C	-0.95087	1.68283	0.09051
H	-0.35252	0.77949	0.17284
C	-0.30137	2.91114	0.05373
C	-1.04262	4.09448	-0.04532
C	-2.41624	4.03841	-0.10985
H	-4.79295	-1.80171	0.07436
H	-7.10300	2.56014	-0.32157
H	-2.98934	4.95645	-0.18546
H	-8.40429	0.48237	-0.29360
H	-0.54146	5.05710	-0.07212
N	-4.45816	2.74288	-0.15223
C	-3.00020	0.22612	0.09054
C	-2.46110	-0.65325	-1.05751
H	-2.69244	-0.20779	-2.03135
H	-1.37598	-0.77032	-0.97866
H	-2.90322	-1.65362	-1.01958
C	-2.65602	-0.42087	1.45145
H	-1.57256	-0.52881	1.56352
H	-3.03131	0.19125	2.27916
H	-3.10085	-1.41809	1.52854
C	-5.18074	3.99023	-0.25417
C	-5.42549	4.52252	-1.51451
C	-5.60453	4.61409	0.91301
C	-6.11889	5.72037	-1.61108
H	-5.07632	4.00322	-2.40335
C	-6.29887	5.81168	0.81712
H	-5.39226	4.16474	1.87969
C	-6.55382	6.36149	-0.44487
H	-6.64184	6.32053	1.71278
H	-7.23544	-1.71428	-0.09460
H	0.78289	2.94911	0.10418
H	-6.32259	6.15948	-2.58296
C	-7.26927	7.59845	-0.54488
N	-7.84982	8.60263	-0.62682



Neutral Ground State (-980.4768749, -980.0837207, -980.1536317)

C	-6.64277	-0.86018	-0.15293
C	-5.25848	-0.87429	-0.02611
C	-4.48722	0.29094	-0.03822
C	-5.15280	1.52145	-0.18316
C	-6.55317	1.54085	-0.31309
C	-7.28840	0.36450	-0.29750
C	-3.03808	2.74501	-0.12247
C	-2.30930	1.55050	0.02090
C	-0.91625	1.63598	0.08976
H	-0.33981	0.72031	0.20849
C	-0.23413	2.84532	0.02071
C	-0.96796	4.01985	-0.11839
C	-2.35264	3.97147	-0.18857
H	-4.75727	-1.83317	0.09473
H	-7.06905	2.49025	-0.42698
H	-2.91393	4.89537	-0.29710
H	-8.37026	0.41181	-0.39829
H	-0.46590	4.98311	-0.17416
N	-4.43626	2.72488	-0.20028
C	-2.97783	0.18727	0.14300
C	-2.40069	-0.76397	-0.91915
H	-2.58470	-0.37473	-1.92799
H	-1.31963	-0.89127	-0.79374
H	-2.85401	-1.75917	-0.84862
C	-2.68944	-0.37694	1.54702
H	-1.61089	-0.47989	1.71685
H	-3.09514	0.28940	2.31857
H	-3.14373	-1.36672	1.67672
C	-5.14907	3.95836	-0.31557
C	-5.40441	4.50841	-1.56550
C	-5.59748	4.61416	0.83249
C	-6.10430	5.70791	-1.68660
H	-5.05118	3.99097	-2.45603
C	-6.29580	5.80599	0.72759
H	-5.39495	4.17670	1.80862
C	-6.55268	6.35863	-0.53380
H	-6.65378	6.32992	1.61046
H	-7.20521	-1.79012	-0.13632
H	0.85099	2.86782	0.07777

H	-6.29191	6.11938	-2.67367
O	-7.24298	7.52453	-0.53704
C	-7.51964	8.13289	-1.78735
H	-8.06726	9.04976	-1.56651
H	-6.59371	8.38227	-2.32062
H	-8.14025	7.48271	-2.41682

Neutral Triplet State (-980.3598742, -979.9706979, -980.0435839)

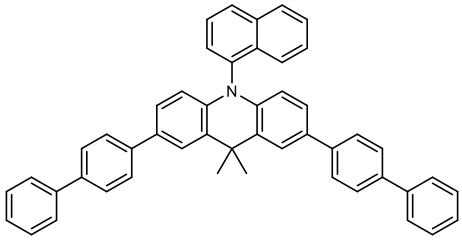
C	-6.60724	-0.93954	-0.38032
C	-5.24229	-0.93637	-0.09250
C	-4.47918	0.22699	-0.12407
C	-5.13640	1.44294	-0.42367
C	-6.51154	1.44274	-0.72247
C	-7.23629	0.26078	-0.70342
C	-3.06287	2.72406	-0.27142
C	-2.34020	1.42512	-0.40960
C	-0.93693	1.51806	-0.66946
H	-0.37488	0.61835	-0.91545
C	-0.27640	2.70959	-0.58203
C	-0.97878	3.94637	-0.22618
C	-2.36283	3.92505	-0.12321
H	-4.76017	-1.87873	0.15657
H	-7.01096	2.37527	-0.96998
H	-2.90910	4.85608	0.01497
H	-8.29667	0.28165	-0.94287
H	-0.42642	4.87401	-0.11267
N	-4.43295	2.65915	-0.39766
C	-2.99752	0.22438	0.21268
C	-2.31187	-1.07175	-0.21752
H	-2.38701	-1.22144	-1.30174
H	-1.25197	-1.05263	0.05745
H	-2.74619	-1.94216	0.28444
C	-2.86627	0.36593	1.75421
H	-1.80540	0.37716	2.03637
H	-3.32767	1.29738	2.10834
H	-3.35780	-0.47441	2.26127
C	-5.17535	3.88693	-0.39824
C	-5.28785	4.63220	-1.56270
C	-5.76087	4.33379	0.78599
C	-5.99254	5.83448	-1.56110
H	-4.82217	4.27074	-2.47756
C	-6.46197	5.52870	0.79893
H	-5.66130	3.73674	1.69116
C	-6.57985	6.28448	-0.37493
H	-6.92454	5.90032	1.70976
H	-7.16607	-1.87154	-0.36083

H	0.79176	2.75059	-0.78899
H	-6.07400	6.40530	-2.48064
O	-7.28153	7.43744	-0.26527
C	-7.41874	8.24881	-1.42019
H	-8.01009	9.11370	-1.11763
H	-6.44107	8.58767	-1.78511
H	-7.94339	7.71380	-2.22155

Cation Radical State (-980.2828065, -979.8893145, -979.9600725)

C	-6.64320	-0.82311	-0.09306
C	-5.25852	-0.86753	0.02071
C	-4.47989	0.28610	-0.01035
C	-5.15098	1.52408	-0.15952
C	-6.56028	1.57007	-0.27917
C	-7.29470	0.40617	-0.24514
C	-3.04678	2.74349	-0.10597
C	-2.31174	1.54137	0.03530
C	-0.92524	1.64034	0.11120
H	-0.32973	0.73819	0.22195
C	-0.27211	2.86602	0.05217
C	-1.00986	4.04791	-0.08068
C	-2.38321	3.99267	-0.15748
H	-4.77687	-1.83454	0.13943
H	-7.06245	2.52405	-0.40032
H	-2.95784	4.90728	-0.25791
H	-8.37557	0.44860	-0.33706
H	-0.50644	5.00892	-0.12337
N	-4.42865	2.70600	-0.19426
C	-2.97805	0.18836	0.12878
C	-2.42734	-0.72497	-0.98631
H	-2.63924	-0.30345	-1.97524
H	-1.34455	-0.84881	-0.88694
H	-2.87836	-1.72054	-0.92971
C	-2.65346	-0.42043	1.51168
H	-1.57169	-0.52583	1.64225
H	-3.03972	0.21532	2.31638
H	-3.10051	-1.41482	1.61109
C	-5.14964	3.95281	-0.32052
C	-5.36986	4.49187	-1.57878
C	-5.61490	4.58603	0.83036
C	-6.07052	5.68822	-1.70283
H	-4.99638	3.97874	-2.46248
C	-6.31073	5.77550	0.71111
H	-5.43046	4.14386	1.80701
C	-6.54290	6.33260	-0.55458
H	-6.68656	6.29475	1.58844

H	-7.21633	-1.74546	-0.06460
H	0.81177	2.90255	0.11282
H	-6.23970	6.10278	-2.69127
O	-7.23138	7.49205	-0.56573
C	-7.49016	8.11016	-1.81806
H	-8.04124	9.02430	-1.59657
H	-6.55574	8.36361	-2.33311
H	-8.10162	7.46295	-2.45849



Neutral Ground State (-1943.264512, -1942.515656, -1942.629532)

C	-6.69778	-0.81461	0.08751
C	-5.30078	-0.80754	0.09124
C	-4.53614	0.35876	0.07897
C	-5.20991	1.59223	0.06602
C	-6.61479	1.60573	0.06351
C	-7.34182	0.42808	0.07166
C	-3.10020	2.81945	0.08427
C	-2.36316	1.62340	0.10321
C	-0.97211	1.70859	0.14218
H	-0.39852	0.78291	0.12346
C	-0.27235	2.91830	0.16517
C	-1.03249	4.09331	0.13715
C	-2.41541	4.04658	0.09666
H	-4.78140	-1.76473	0.06992
H	-7.14571	2.55378	0.06763
H	-2.97747	4.97648	0.08899
H	-8.42857	0.48212	0.09122
H	-0.54296	5.06458	0.17482
N	-4.49962	2.79951	0.05350
C	-5.21240	4.01780	-0.17443
C	-5.64053	4.77399	0.88877
C	-5.47799	4.41808	-1.51428
C	-6.36189	5.96868	0.67166
H	-5.41782	4.43647	1.89935
C	-6.21571	5.62071	-1.72665
C	-6.64537	6.37909	-0.60801
H	-6.69317	6.55659	1.52356
H	-7.20579	7.29586	-0.78349
C	-6.50112	6.02393	-3.05613
C	-5.04567	3.66617	-2.63595
C	-5.33804	4.08615	-3.91124
H	-5.00300	3.50140	-4.76444
C	-6.07444	5.27421	-4.12484
H	-6.30029	5.59188	-5.13975
H	-7.06654	6.94116	-3.21257
H	-4.47903	2.75008	-2.47510
C	-3.01759	0.24950	0.03487
C	-2.61004	-0.42323	-1.28920

H	-2.94602	0.17583	-2.14540
H	-1.52124	-0.53336	-1.35700
H	-3.05262	-1.42247	-1.37795
C	-2.53569	-0.60690	1.21860
H	-1.44682	-0.72695	1.20622
H	-2.81761	-0.14248	2.17138
H	-2.97271	-1.61132	1.18542
C	1.20174	2.94713	0.21329
C	1.93221	3.96556	-0.41506
C	1.92560	1.95462	0.88930
C	3.32023	3.98861	-0.37150
H	1.40870	4.73712	-0.97652
C	3.31329	1.97538	0.92901
H	1.39457	1.16767	1.42170
C	4.04234	2.99231	0.29865
H	3.85321	4.77789	-0.89860
H	3.83835	1.20337	1.48849
C	-7.45818	-2.07853	0.09073
C	-8.67596	-2.19323	-0.59441
C	-6.98998	-3.20885	0.77554
C	-9.39123	-3.38352	-0.59763
H	-9.05427	-1.34591	-1.16348
C	-7.70418	-4.39973	0.77018
H	-6.06627	-3.14729	1.34838
C	-8.92025	-4.51405	0.08345
H	-10.31660	-3.44523	-1.16766
H	-7.32553	-5.24746	1.33843
C	-9.67871	-5.78191	0.07684
C	-9.01467	-7.01671	0.06148
C	-11.08047	-5.78318	0.08531
C	-9.72776	-8.21142	0.05569
H	-7.92696	-7.04218	0.03020
C	-11.79459	-6.97746	0.07759
H	-11.61813	-4.83724	0.12172
C	-11.12117	-8.19768	0.06324
H	-9.19165	-9.15756	0.03581
H	-12.88176	-6.95419	0.09199
H	-11.67882	-9.13112	0.05791
C	5.51898	3.01135	0.33803
C	6.25442	1.81823	0.30557
C	6.22345	4.22162	0.40717
C	7.64513	1.83360	0.34308
H	5.73239	0.86638	0.22543
C	7.61430	4.23826	0.44197
H	5.67493	5.16057	0.45755
C	8.33227	3.04422	0.41086

H	8.19460	0.89557	0.30927
H	8.13903	5.18898	0.50362

Neutral Triplet State (-1943.170318, -1942.425272, -1942.541009)

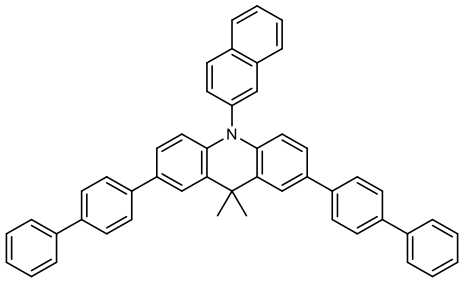
C	3.67645	0.06456	-0.19904
C	2.47837	-0.55825	0.17142
C	1.24850	0.09579	0.17858
C	1.21629	1.44370	-0.22450
C	2.40688	2.09017	-0.58571
C	3.61507	1.41144	-0.56997
C	-1.21636	1.44371	-0.22452
C	-1.24858	0.09581	0.17857
C	-2.47846	-0.55822	0.17141
H	-2.52319	-1.58953	0.51330
C	-3.67654	0.06460	-0.19904
C	-3.61514	1.41149	-0.56995
C	-2.40695	2.09021	-0.58568
H	2.52310	-1.58955	0.51331
H	2.38406	3.13284	-0.89457
H	-2.38411	3.13290	-0.89448
H	4.51740	1.93639	-0.87775
H	-4.51748	1.93645	-0.87770
N	-0.00004	2.14006	-0.26137
C	-0.00003	3.49336	-0.69800
C	-0.00015	3.76925	-2.12294
C	0.00019	4.53865	0.25871
C	0.00021	5.05381	-2.56133
H	-0.00048	2.92418	-2.80901
C	0.00055	5.89948	-0.22307
C	0.00060	6.13873	-1.61682
H	0.00017	5.27593	-3.62525
H	0.00089	7.16661	-1.97399
C	0.00083	6.94074	0.71457
C	0.00007	4.30474	1.63908
C	0.00035	5.39004	2.57453
H	0.00026	5.17261	3.63922
C	0.00072	6.67800	2.12218
H	0.00096	7.51240	2.81852
H	0.00114	7.96934	0.35782
H	-0.00024	3.27856	2.00073
C	-0.00005	-0.56056	0.75727
C	-0.00006	-0.30247	2.27876
H	0.00001	0.77244	2.49893
H	-0.89203	-0.74560	2.74037
H	0.89185	-0.74572	2.74038
C	-0.00008	-2.07248	0.52201

H	-0.87228	-2.54582	0.98323
H	0.00001	-2.31299	-0.54814
H	0.87198	-2.54589	0.98340
C	-4.95476	-0.67191	-0.17249
C	-6.15128	-0.03523	0.18611
C	-5.01756	-2.03381	-0.49902
C	-7.35383	-0.72911	0.21943
H	-6.13721	1.01301	0.47884
C	-6.21960	-2.72830	-0.46257
H	-4.11539	-2.55393	-0.81608
C	-7.41456	-2.09164	-0.10170
H	-8.25694	-0.20903	0.53404
H	-6.23392	-3.77753	-0.75190
C	4.95464	-0.67199	-0.17250
C	6.15120	-0.03537	0.18612
C	5.01739	-2.03389	-0.49904
C	7.35371	-0.72932	0.21945
H	6.13718	1.01286	0.47888
C	6.21939	-2.72844	-0.46258
H	4.11519	-2.55397	-0.81610
C	7.41438	-2.09185	-0.10171
H	8.25684	-0.20929	0.53409
H	6.23365	-3.77768	-0.75189
C	8.69236	-2.83207	-0.05997
C	8.73591	-4.17044	0.35504
C	9.89419	-2.21493	-0.43417
C	9.93893	-4.86869	0.39354
H	7.81930	-4.66413	0.67326
C	11.09794	-2.91166	-0.39408
H	9.88367	-1.18398	-0.78321
C	11.12619	-4.24226	0.01930
H	9.94940	-5.90419	0.72590
H	12.01705	-2.41467	-0.69617
H	12.06669	-4.78711	0.04945
C	-8.69259	-2.83178	-0.05998
C	-8.73624	-4.17015	0.35506
C	-9.89438	-2.21456	-0.43416
C	-9.93931	-4.86830	0.39358
H	-7.81967	-4.66390	0.67328
C	-11.09819	-2.91119	-0.39404
H	-9.88379	-1.18361	-0.78321
C	-11.12653	-4.24179	0.01935
H	-9.94985	-5.90380	0.72596
H	-12.01726	-2.41414	-0.69612
H	-12.06707	-4.78655	0.04953

Cation Radical State (-1943.07344, -1942.324576, -1942.440306)

C	-6.67612	-0.85743	-0.03437
C	-5.27360	-0.86738	-0.00706
C	-4.50662	0.28614	-0.04432
C	-5.18363	1.52660	-0.11188
C	-6.59544	1.55867	-0.15613
C	-7.32098	0.39302	-0.11971
C	-3.08758	2.75164	-0.06906
C	-2.34216	1.55159	-0.00085
C	-0.96261	1.65051	0.07685
H	-0.37764	0.73433	0.09279
C	-0.28044	2.87691	0.08963
C	-1.05027	4.05501	0.00605
C	-2.42047	3.99815	-0.07003
H	-4.76622	-1.82872	0.00979
H	-7.11532	2.51022	-0.20271
H	-2.99375	4.91871	-0.11549
H	-8.40584	0.44967	-0.12345
H	-0.56665	5.02757	0.03360
N	-4.46879	2.71217	-0.13951
C	-5.19404	3.95567	-0.26369
C	-5.60290	4.60284	0.87394
C	-5.45835	4.45707	-1.56486
C	-6.31803	5.81439	0.76744
H	-5.37298	4.17415	1.84709
C	-6.18292	5.68274	-1.65618
C	-6.60017	6.33820	-0.47050
H	-6.64129	6.32492	1.66987
H	-7.15234	7.27171	-0.56052
C	-6.46643	6.21378	-2.93955
C	-5.04116	3.80531	-2.75227
C	-5.33322	4.35018	-3.97934
H	-5.00911	3.84415	-4.88503
C	-6.05196	5.56369	-4.07566
H	-6.27364	5.98032	-5.05471
H	-7.02030	7.14843	-3.00450
H	-4.48496	2.87089	-2.69096
C	-2.99546	0.18724	-0.08099
C	-2.59586	-0.44975	-1.43071
H	-2.94180	0.16739	-2.26920
H	-1.50727	-0.54940	-1.50158
H	-3.03738	-1.44721	-1.53094
C	-2.50479	-0.69351	1.08182
H	-1.41812	-0.81632	1.04951
H	-2.77457	-0.25030	2.04681
H	-2.94252	-1.69500	1.02704

C	1.18108	2.92485	0.18314
C	1.91111	3.98479	-0.37930
C	1.89874	1.90924	0.83624
C	3.29446	4.01883	-0.30346
H	1.39482	4.77325	-0.92194
C	3.28071	1.95137	0.92002
H	1.36833	1.09420	1.32338
C	4.01100	3.00342	0.34714
H	3.83019	4.83229	-0.78767
H	3.80097	1.16807	1.46664
C	-7.44261	-2.10516	0.02481
C	-8.70193	-2.21244	-0.58751
C	-6.94361	-3.23142	0.69986
C	-9.42359	-3.39441	-0.53602
H	-9.10573	-1.37283	-1.14884
C	-7.67245	-4.40801	0.75966
H	-5.99192	-3.17584	1.22355
C	-8.92629	-4.51860	0.14025
H	-10.37661	-3.45590	-1.05684
H	-7.27512	-5.24800	1.32516
C	-9.69440	-5.77712	0.19722
C	-9.03888	-7.01681	0.18472
C	-11.09479	-5.76462	0.26412
C	-9.76029	-8.20465	0.23571
H	-7.95398	-7.05340	0.10784
C	-11.81627	-6.95270	0.31721
H	-11.62430	-4.81430	0.30030
C	-11.15197	-8.17799	0.30269
H	-9.23308	-9.15552	0.21508
H	-12.90141	-6.92069	0.37799
H	-11.71604	-9.10659	0.34299
C	5.48378	3.03860	0.42577
C	6.23205	1.85338	0.39017
C	6.17045	4.25634	0.53573
C	7.62063	1.88398	0.46242
H	5.72481	0.89713	0.27726
C	7.55905	4.28694	0.60941
H	5.61069	5.18816	0.58964
C	8.29038	3.10119	0.57290
H	8.18218	0.95360	0.42383
H	8.07111	5.24157	0.70456
H	9.37574	3.12585	0.62984



Neutral Ground State (-1943.262417, -1942.513497, -1942.628359)

C	-6.68692	-0.82044	-0.07011
C	-5.28923	-0.81689	-0.05986
C	-4.52141	0.34535	-0.11324
C	-5.19219	1.57899	-0.19032
C	-6.59689	1.59625	-0.20625
C	-7.32709	0.42151	-0.14683
C	-3.08258	2.80349	-0.13391
C	-2.34727	1.60772	-0.06102
C	-0.95960	1.69415	0.03881
H	-0.38524	0.76900	0.05185
C	-0.26198	2.90504	0.08196
C	-1.02078	4.07900	0.01801
C	-2.40046	4.03146	-0.08846
H	-4.77440	-1.77630	-0.04080
H	-7.12537	2.54416	-0.25671
H	-2.95942	4.96215	-0.12958
H	-8.41378	0.47912	-0.13525
H	-0.53375	5.05056	0.07588
N	-4.47574	2.77867	-0.25827
C	-3.00194	0.23461	-0.15085
C	-2.59052	-0.41916	-1.48332
H	-2.92332	0.19132	-2.33222
H	-1.50090	-0.52740	-1.54671
H	-3.03543	-1.41656	-1.58424
C	-2.52246	-0.64088	1.01929
H	-1.43443	-0.76485	1.00472
H	-2.80300	-0.19134	1.97952
H	-2.95904	-1.64447	0.97105
C	1.20915	2.93724	0.18629
C	1.96028	3.94881	-0.42876
C	1.90926	1.95602	0.90272
C	3.34561	3.97598	-0.33440
H	1.45564	4.71073	-1.02003
C	3.29461	1.98104	0.99356
H	1.36027	1.17510	1.42569
C	4.04433	2.99076	0.37593

H	3.89611	4.75871	-0.85313
H	3.80046	1.21822	1.58267
C	-7.45092	-2.08056	-0.00404
C	-8.67031	-2.22691	-0.68036
C	-6.98722	-3.17467	0.74036
C	-9.39161	-3.41201	-0.61757
H	-9.04611	-1.40986	-1.29369
C	-7.70689	-4.36069	0.80028
H	-6.06320	-3.08715	1.30917
C	-8.92478	-4.50633	0.12288
H	-10.31851	-3.49969	-1.18170
H	-7.33113	-5.17856	1.41260
C	-9.68702	-5.77044	0.18442
C	-9.02537	-7.00585	0.22771
C	-11.08869	-5.76829	0.19911
C	-9.74048	-8.19799	0.28380
H	-7.93786	-7.03479	0.19283
C	-11.80489	-6.96017	0.25329
H	-11.62440	-4.82059	0.19024
C	-11.13383	-8.18104	0.29625
H	-9.20617	-9.14504	0.30881
H	-12.89195	-6.93408	0.27107
H	-11.69313	-9.11254	0.33896
C	5.51877	3.01394	0.46579
C	6.25762	1.82262	0.47047
C	6.21765	4.22696	0.54335
C	7.64656	1.84237	0.55087
H	5.74059	0.86851	0.38479
C	7.60672	4.24795	0.62142
H	5.66503	5.16465	0.56481
C	8.32825	3.05565	0.62589
H	8.19930	0.90568	0.54461
H	8.12690	5.20083	0.68839
H	9.41363	3.07207	0.68700
C	-5.19051	4.01510	-0.33898
C	-5.45326	4.57290	-1.56451
C	-5.61444	4.65055	0.85232
C	-6.15530	5.80005	-1.65954
H	-5.11737	4.06917	-2.47062
C	-6.29853	5.83857	0.78858
H	-5.38773	4.18027	1.80763
C	-6.58682	6.44459	-0.46186
C	-6.43896	6.40543	-2.90968
H	-6.62871	6.33360	1.70024
C	-7.28930	7.67212	-0.55847
C	-7.12074	7.59680	-2.97090

H	-6.10622	5.90871	-3.81962
C	-7.55024	8.23593	-1.78428
H	-7.61760	8.16022	0.35780
H	-7.33244	8.05403	-3.93439
H	-8.08951	9.17799	-1.84659

Neutral Triplet State (-1943.172055, -1942.426199, -1942.543911)

C	-6.69142	-0.80753	-0.05008
C	-5.29415	-0.81308	-0.00764
C	-4.51920	0.34332	-0.06025
C	-5.18528	1.57757	-0.17084
C	-6.59003	1.60579	-0.21921
C	-7.32599	0.43720	-0.15919
C	-3.07978	2.79924	-0.11848
C	-2.33304	1.59352	-0.00265
C	-0.96574	1.67370	0.10797
H	-0.41381	0.74177	0.17715
C	-0.22463	2.90522	0.11506
C	-1.02340	4.09625	-0.00497
C	-2.38392	4.03846	-0.11558
H	-4.78683	-1.77498	0.03882
H	-7.11100	2.55584	-0.29449
H	-2.94443	4.96518	-0.20276
H	-8.41200	0.49915	-0.17211
H	-0.55212	5.07445	-0.00726
N	-4.45885	2.77203	-0.23487
C	-3.00181	0.22571	-0.05534
C	-2.56573	-0.47660	-1.35668
H	-2.86484	0.11271	-2.23244
H	-1.47749	-0.60384	-1.38533
H	-3.02492	-1.46867	-1.43874
C	-2.56040	-0.61216	1.15703
H	-1.47469	-0.75133	1.17010
H	-2.85515	-0.12373	2.09344
H	-3.01215	-1.60970	1.13397
C	1.17832	2.93910	0.22046
C	1.93391	4.17502	0.18514
C	1.97940	1.74040	0.36236
C	3.29309	4.20162	0.25746
H	1.41142	5.12278	0.08626
C	3.33762	1.77493	0.43213
H	1.49388	0.77038	0.42845
C	4.08523	3.00456	0.37514
H	3.78488	5.16986	0.20734
H	3.86187	0.83073	0.55287
C	-7.46168	-2.06275	0.01437

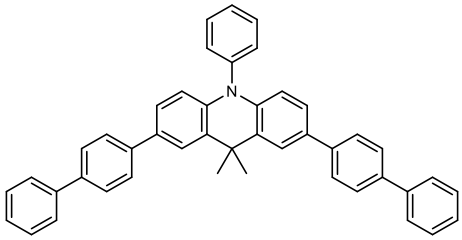
C	-8.66930	-2.20953	-0.68291
C	-7.01378	-3.15244	0.77497
C	-9.39315	-3.39312	-0.62683
H	-9.03215	-1.39618	-1.30865
C	-7.73736	-4.33588	0.82964
H	-6.10064	-3.06372	1.36070
C	-8.94198	-4.48350	0.12908
H	-10.30926	-3.48300	-1.20782
H	-7.37538	-5.15037	1.45448
C	-9.70635	-5.74646	0.18264
C	-9.04616	-6.98179	0.24548
C	-11.10797	-5.74313	0.16957
C	-9.76301	-8.17318	0.29345
H	-7.95822	-7.01136	0.23218
C	-11.82578	-6.93431	0.21617
H	-11.64273	-4.79522	0.14529
C	-11.15633	-8.15522	0.27842
H	-9.23006	-9.12044	0.33385
H	-12.91293	-6.90764	0.21264
H	-11.71698	-9.08615	0.31496
C	5.52315	3.03157	0.43340
C	6.29452	1.83760	0.42639
C	6.25099	4.25096	0.49797
C	7.67825	1.86466	0.48063
H	5.80098	0.87145	0.36332
C	7.63504	4.26935	0.55266
H	5.72246	5.20013	0.51761
C	8.36895	3.07907	0.54481
H	8.22954	0.92661	0.46847
H	8.15182	5.22549	0.60622
H	9.45492	3.09763	0.58724
C	-5.17569	4.01035	-0.34861
C	-5.43837	4.53246	-1.58870
C	-5.60275	4.66458	0.82954
C	-6.15262	5.74981	-1.71135
H	-5.09896	4.00858	-2.48176
C	-6.29728	5.84440	0.73618
H	-5.37331	4.21710	1.79473
C	-6.59126	6.41703	-0.52834
C	-6.44399	6.32174	-2.97530
H	-6.63220	6.35762	1.63573
C	-7.30822	7.63340	-0.65301
C	-7.14062	7.50258	-3.06327
H	-6.10625	5.80769	-3.87354
C	-7.57707	8.16418	-1.89153
H	-7.64140	8.13918	0.25168

H	-7.35900	7.93438	-4.03686
H	-8.12777	9.09782	-1.97565

Cation Radical State (-1943.072237, -1942.323601, -1942.439961)

C	-6.67593	-0.81368	-0.06512
C	-5.27642	-0.82682	0.02827
C	-4.50327	0.32289	-0.00260
C	-5.17083	1.56318	-0.13337
C	-6.58000	1.59905	-0.23406
C	-7.31140	0.43675	-0.20174
C	-3.07109	2.78011	-0.07577
C	-2.33242	1.57936	0.04228
C	-0.95220	1.67361	0.11398
H	-0.37264	0.75558	0.17128
C	-0.26259	2.89543	0.08082
C	-1.02722	4.07487	-0.02874
C	-2.39752	4.02312	-0.10362
H	-4.77420	-1.78847	0.10017
H	-7.09331	2.55049	-0.32792
H	-2.96498	4.94534	-0.17461
H	-8.39497	0.49659	-0.25270
H	-0.53853	5.04525	-0.02653
N	-4.45024	2.74443	-0.16708
C	-2.99464	0.21731	0.09248
C	-2.47858	-0.63559	-1.08393
H	-2.73174	-0.16944	-2.04286
H	-1.39120	-0.75121	-1.03282
H	-2.91816	-1.63808	-1.06017
C	-2.62987	-0.45669	1.43143
H	-1.54530	-0.57341	1.52543
H	-2.98707	0.14177	2.27725
H	-3.07727	-1.45358	1.50119
C	1.20014	2.93937	0.15888
C	1.92663	3.98784	-0.42907
C	1.92327	1.93239	0.81933
C	3.31083	4.01966	-0.36989
H	1.40634	4.76933	-0.97779
C	3.30632	1.97149	0.88518
H	1.39732	1.12606	1.32521
C	4.03250	3.01230	0.28728
H	3.84286	4.82435	-0.87253
H	3.83122	1.19479	1.43677
C	-7.44819	-2.05901	-0.02288
C	-8.67643	-2.17245	-0.69424
C	-6.98405	-3.17741	0.68884
C	-9.40089	-3.35368	-0.66482

H	-9.05111	-1.33904	-1.28430
C	-7.71530	-4.35358	0.72512
H	-6.05853	-3.11651	1.25702
C	-8.93710	-4.47061	0.04592
H	-10.32831	-3.42095	-1.22956
H	-7.34661	-5.18818	1.31746
C	-9.70615	-5.72944	0.07680
C	-9.04935	-6.96819	0.10224
C	-11.10797	-5.71816	0.08012
C	-9.77110	-8.15667	0.12864
H	-7.96204	-7.00316	0.07458
C	-11.82993	-6.90685	0.10888
H	-11.63917	-4.76813	0.08569
C	-11.16438	-8.13132	0.13266
H	-9.24252	-9.10696	0.13826
H	-12.91673	-6.87595	0.12064
H	-11.72887	-9.06029	0.15399
C	5.50622	3.04384	0.34662
C	6.25022	1.85585	0.31492
C	6.19795	4.26057	0.43344
C	7.63969	1.88278	0.36842
H	5.73821	0.90020	0.21981
C	7.58747	4.28752	0.48853
H	5.64168	5.19469	0.48392
C	8.31458	3.09904	0.45602
H	8.19786	0.95024	0.33300
H	8.10381	5.24144	0.56591
H	9.40067	3.12082	0.49832
C	-5.17194	3.99161	-0.28282
C	-5.39733	4.52430	-1.52450
C	-5.62491	4.61606	0.89908
C	-6.11068	5.74179	-1.64290
H	-5.03207	4.01596	-2.41592
C	-6.31952	5.79541	0.80273
H	-5.41905	4.15339	1.86179
C	-6.58169	6.38662	-0.45967
C	-6.36898	6.33411	-2.90428
H	-6.67900	6.29252	1.70136
C	-7.29927	7.60257	-0.58143
C	-7.06629	7.51441	-2.98867
H	-6.00589	5.83734	-3.80202
C	-7.53612	8.15354	-1.81739
H	-7.65821	8.09095	0.32266
H	-7.25967	7.96335	-3.95962
H	-8.08740	9.08680	-1.90005



Neutral Ground State (-1789.70333, -1789.003797, -1789.112474)

C	-6.69989	-0.81898	-0.02825
C	-5.30238	-0.81197	-0.01853
C	-4.53743	0.35291	-0.04825
C	-5.21063	1.58693	-0.09291
C	-6.61559	1.60058	-0.11006
C	-7.34293	0.42293	-0.07913
C	-3.10149	2.81303	-0.04073
C	-2.36387	1.61707	-0.00101
C	-0.97441	1.70270	0.06973
H	-0.40018	0.77725	0.06348
C	-0.27575	2.91299	0.11070
C	-1.03596	4.08725	0.07358
C	-2.41767	4.04056	-0.00081
H	-4.78389	-1.76975	-0.01681
H	-7.14669	2.54800	-0.13643
H	-2.97708	4.97166	-0.01791
H	-8.42979	0.47762	-0.06783
H	-0.54800	5.05849	0.12946
N	-4.49744	2.78971	-0.12214
C	-3.01797	0.24326	-0.08123
C	-2.60078	-0.42499	-1.40459
H	-2.92897	0.17713	-2.26110
H	-1.51137	-0.53604	-1.46300
H	-3.04479	-1.42327	-1.49867
C	-2.54363	-0.61867	1.10152
H	-1.45478	-0.73819	1.09579
H	-2.83226	-0.15942	2.05478
H	-2.97833	-1.62369	1.06075
C	1.19694	2.94440	0.18874
C	1.93736	3.96344	-0.42695
C	1.90944	1.95526	0.88154
C	3.32406	3.99075	-0.35478
H	1.42289	4.73202	-1.00080
C	3.29603	1.98049	0.95021
H	1.36966	1.16781	1.40434
C	4.03501	2.99827	0.33282
H	3.86540	4.78011	-0.87312
H	3.81163	1.21134	1.52230

C	-7.46038	-2.08219	0.01355
C	-8.67949	-2.21922	-0.66514
C	-6.99296	-3.18890	0.73671
C	-9.39722	-3.40749	-0.62467
H	-9.05782	-1.39145	-1.26236
C	-7.70923	-4.37786	0.77461
H	-6.06873	-3.10925	1.30640
C	-8.92708	-4.51411	0.09519
H	-10.32412	-3.48731	-1.18998
H	-7.33107	-5.20593	1.37152
C	-9.68682	-5.78060	0.13535
C	-9.02318	-7.01548	0.16020
C	-11.08850	-5.78098	0.14913
C	-9.73645	-8.20946	0.19802
H	-7.93560	-7.04226	0.12573
C	-11.80285	-6.97466	0.18496
H	-11.62575	-4.83412	0.15455
C	-11.12983	-8.19494	0.21006
H	-9.20058	-9.15589	0.20907
H	-12.88996	-6.95059	0.20256
H	-11.68767	-9.12784	0.23868
C	5.51053	3.02259	0.40175
C	6.25087	1.83224	0.38646
C	6.20908	4.23574	0.48091
C	7.64064	1.85296	0.44982
H	5.73412	0.87815	0.29893
C	7.59899	4.25773	0.54162
H	5.65601	5.17265	0.51798
C	8.32188	3.06636	0.52697
H	8.19424	0.91700	0.42874
H	8.11884	5.21066	0.61042
H	9.40790	3.08360	0.57503
C	-5.21346	4.02684	-0.19195
C	-5.48858	4.59209	-1.43448
C	-5.62452	4.65757	0.97987
C	-6.18072	5.79861	-1.50480
H	-5.15594	4.08037	-2.33591
C	-6.31731	5.86325	0.90663
H	-5.39682	4.19655	1.93953
C	-6.59465	6.43391	-0.33509
H	-6.64008	6.35809	1.81923
H	-6.39560	6.24324	-2.47337
H	-7.13541	7.37545	-0.39088

Neutral Triplet State (-1789.613053, -1788.916577, -1789.028301)

C	-6.70454	-0.81677	-0.02960

C	-5.30717	-0.81828	0.00443
C	-4.53627	0.34119	-0.03495
C	-5.20665	1.57554	-0.11723
C	-6.61178	1.59949	-0.15998
C	-7.34361	0.42744	-0.11721
C	-3.10303	2.80086	-0.07160
C	-2.35223	1.59519	0.01374
C	-0.98334	1.67584	0.10161
H	-0.42946	0.74370	0.15120
C	-0.24364	2.90810	0.11169
C	-1.04575	4.09905	0.01591
C	-2.40801	4.04086	-0.06952
H	-4.79589	-1.77881	0.03477
H	-7.13669	2.54876	-0.21503
H	-2.97062	4.96799	-0.13575
H	-8.42989	0.48576	-0.12518
H	-0.57560	5.07780	0.01462
N	-4.48431	2.77328	-0.15646
C	-3.01887	0.22649	-0.03665
C	-2.58560	-0.47761	-1.33783
H	-2.88806	0.10976	-2.21367
H	-1.49749	-0.60406	-1.37010
H	-3.04274	-1.47071	-1.41756
C	-2.57250	-0.60808	1.17663
H	-1.48614	-0.74318	1.18773
H	-2.86686	-0.11845	2.11258
H	-3.02222	-1.60674	1.15630
C	1.16041	2.94320	0.20101
C	1.91394	4.18035	0.16895
C	1.96423	1.74465	0.32608
C	3.27350	4.20857	0.23447
H	1.38947	5.12788	0.07833
C	3.32274	1.78087	0.39004
H	1.48068	0.77315	0.38479
C	4.06807	3.01220	0.34161
H	3.76340	5.17795	0.18810
H	3.84887	0.83633	0.49882
C	-7.46995	-2.07542	0.02393
C	-8.68030	-2.21928	-0.66911
C	-7.01431	-3.17137	0.77090
C	-9.39965	-3.40603	-0.62176
H	-9.04896	-1.40052	-1.28434
C	-7.73364	-4.35771	0.81724
H	-6.09859	-3.08526	1.35301
C	-8.94127	-4.50234	0.12125
H	-10.31819	-3.49326	-1.19930

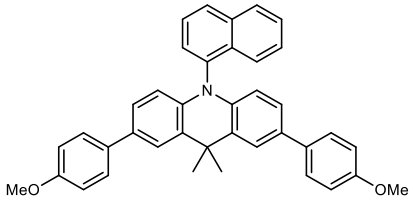
H	-7.36604	-5.17704	1.43236
C	-9.70186	-5.76790	0.16764
C	-9.03826	-7.00195	0.21895
C	-11.10353	-5.76814	0.16035
C	-9.75187	-8.19550	0.26165
H	-7.95032	-7.02873	0.20105
C	-11.81810	-6.96147	0.20164
H	-11.64090	-4.82151	0.14510
C	-11.14528	-8.18103	0.25271
H	-9.21626	-9.14159	0.29323
H	-12.90532	-6.93762	0.20288
H	-11.70337	-9.11364	0.28534
C	5.50608	3.04155	0.39859
C	6.27960	1.84899	0.38944
C	6.23193	4.26205	0.46517
C	7.66329	1.87833	0.44378
H	5.78789	0.88196	0.32566
C	7.61596	4.28273	0.51975
H	5.70198	5.21039	0.48612
C	8.35197	3.09377	0.50997
H	8.21614	0.94121	0.43046
H	8.13103	5.23972	0.57478
H	9.43790	3.11417	0.55260
C	-5.20346	4.01271	-0.24971
C	-5.47669	4.55206	-1.50278
C	-5.61614	4.65472	0.91391
C	-6.17462	5.75381	-1.59080
H	-5.14101	4.02698	-2.39508
C	-6.31426	5.85558	0.81991
H	-5.38772	4.20856	1.88007
C	-6.59280	6.40449	-0.43109
H	-6.63994	6.36325	1.72412
H	-6.39036	6.18254	-2.56603
H	-7.13793	7.34223	-0.50236

Cation Radical State (-1789.513356, -1788.813909, -1788.923804)

C	-6.69679	-0.80216	-0.04078
C	-5.29701	-0.81322	0.04716
C	-4.52706	0.33876	0.03456
C	-5.19813	1.57999	-0.06768
C	-6.60785	1.61390	-0.16205
C	-7.33598	0.44903	-0.15159
C	-3.09912	2.79847	-0.01277
C	-2.35774	1.59722	0.07937
C	-0.97665	1.69148	0.13293
H	-0.39627	0.77314	0.17572

C	-0.28835	2.91398	0.10076
C	-1.05510	4.09365	0.01199
C	-2.42645	4.04199	-0.04072
H	-4.79121	-1.77422	0.10072
H	-7.12463	2.56545	-0.23313
H	-2.99483	4.96485	-0.09405
H	-8.41988	0.50695	-0.19803
H	-0.56660	5.06414	0.01398
N	-4.47994	2.76284	-0.07939
C	-3.01865	0.23485	0.13137
C	-2.49820	-0.62513	-1.03728
H	-2.74541	-0.16403	-2.00015
H	-1.41155	-0.74382	-0.98021
H	-2.93953	-1.62667	-1.01018
C	-2.65831	-0.43111	1.47610
H	-1.57364	-0.54352	1.57510
H	-3.02106	0.17103	2.31700
H	-3.10431	-1.42859	1.54862
C	1.17528	2.95910	0.15931
C	1.89226	4.01247	-0.43148
C	1.90849	1.94919	0.80382
C	3.27705	4.04672	-0.38953
H	1.36359	4.79627	-0.96883
C	3.29215	1.99082	0.85275
H	1.39027	1.13848	1.31070
C	4.00879	3.03705	0.25274
H	3.80126	4.85555	-0.89378
H	3.82535	1.21186	1.39306
C	-7.46499	-2.05039	-0.01694
C	-8.69406	-2.15796	-0.68765
C	-6.99529	-3.17784	0.67666
C	-9.41429	-3.34209	-0.67442
H	-9.07282	-1.31721	-1.26458
C	-7.72251	-4.35684	0.69716
H	-6.06863	-3.12202	1.24354
C	-8.94552	-4.46779	0.01912
H	-10.34258	-3.40426	-1.23831
H	-7.34975	-5.19857	1.27668
C	-9.71162	-5.72871	0.03507
C	-9.05255	-6.96649	0.04449
C	-11.11347	-5.72005	0.04118
C	-9.77218	-8.15648	0.05845
H	-7.96523	-6.99933	0.01446
C	-11.83330	-6.91026	0.05745
H	-11.64635	-4.77113	0.05920
C	-11.16550	-8.13371	0.06567

H	-9.24189	-9.10586	0.05587
H	-12.92011	-6.88146	0.07176
H	-11.72828	-9.06389	0.07752
C	5.48300	3.07142	0.29601
C	6.22880	1.88495	0.25148
C	6.17344	4.28897	0.38172
C	7.61862	1.91401	0.29201
H	5.71756	0.92884	0.15691
C	7.56339	4.31807	0.42360
H	5.61622	5.22192	0.44216
C	8.29221	3.13105	0.37893
H	8.17798	0.98259	0.24717
H	8.07880	5.27253	0.50054
H	9.37860	3.15458	0.41134
C	-5.20232	4.01213	-0.17097
C	-5.45039	4.55799	-1.42481
C	-5.62618	4.63061	0.99899
C	-6.14597	5.76088	-1.50477
H	-5.10143	4.04399	-2.31796
C	-6.32141	5.83293	0.90619
H	-5.41226	4.17194	1.96199
C	-6.57998	6.39592	-0.34236
H	-6.66033	6.32921	1.81131
H	-6.34710	6.20173	-2.47725
H	-7.12316	7.33472	-0.40995



Neutral Ground State (-1710.393301, -1709.744942, -1709.848553)

C	-6.72230	-0.77498	0.08538
C	-5.32545	-0.76469	0.09801
C	-4.56208	0.40350	0.09003
C	-5.23730	1.63574	0.06805
C	-6.64188	1.64647	0.05638
C	-7.36705	0.46731	0.06520
C	-3.12943	2.86678	0.10234
C	-2.39073	1.67232	0.13290
C	-0.99952	1.75989	0.18814
H	-0.42442	0.83481	0.17816
C	-0.30119	2.97017	0.21975
C	-1.06378	4.14324	0.18105
C	-2.44629	4.09449	0.12007
H	-4.80441	-1.72127	0.08206
H	-7.17453	2.59369	0.05469
H	-3.00943	5.02375	0.10306
H	-8.45411	0.51932	0.07943
H	-0.57603	5.11529	0.22519
N	-4.52900	2.84483	0.05672
C	-5.24106	4.06052	-0.18299
C	-5.67777	4.82209	0.87301
C	-5.49720	4.45474	-1.52661
C	-6.39772	6.01560	0.64491
H	-5.46242	4.48959	1.88687
C	-6.23353	5.65617	-1.75039
C	-6.67160	6.41999	-0.63879
H	-6.73562	6.60745	1.49149
H	-7.23090	7.33577	-0.82296
C	-6.50931	6.05266	-3.08393
C	-5.05666	3.69742	-2.64135
C	-5.33974	4.11089	-3.92092
H	-4.99842	3.52193	-4.76874
C	-6.07479	5.29778	-4.14582
H	-6.29344	5.61027	-5.16392
H	-7.07391	6.96888	-3.24913
H	-4.49133	2.78222	-2.47099
C	-3.04264	0.29712	0.05935
C	-2.62149	-0.37579	-1.26039
H	-2.95061	0.22218	-2.12007

H	-1.53181	-0.48359	-1.31793
H	-3.06145	-1.37589	-1.35265
C	-2.57005	-0.55847	1.24748
H	-1.48089	-0.67647	1.24547
H	-2.86186	-0.09458	2.19759
H	-3.00498	-1.56369	1.21025
C	1.17297	3.00337	0.29036
C	1.91146	4.01215	-0.33534
C	1.89051	2.02059	0.99291
C	3.30352	4.05546	-0.27284
H	1.39541	4.78003	-0.90903
C	3.27361	2.04473	1.06119
H	1.35385	1.23188	1.51721
C	3.99204	3.06428	0.42794
H	3.83261	4.85553	-0.78188
H	3.82096	1.28418	1.61340
C	-7.48313	-2.03979	0.08300
C	-8.68664	-2.15929	-0.61808
C	-7.02750	-3.17035	0.78170
C	-9.41785	-3.34579	-0.63389
H	-9.05997	-1.31224	-1.19114
C	-7.73970	-4.35853	0.77483
H	-6.10705	-3.11125	1.36027
C	-8.94218	-4.45559	0.06620
H	-10.34199	-3.38982	-1.20199
H	-7.38700	-5.22727	1.32618
O	5.34377	3.00705	0.55043
O	-9.57079	-5.65878	0.11913
C	6.11097	4.02085	-0.07376
H	7.15540	3.79226	0.14269
H	5.95928	4.02306	-1.16070
H	5.86743	5.01189	0.33026
C	-10.80124	-5.79613	-0.56885
H	-10.67391	-5.63934	-1.64768
H	-11.14010	-6.81763	-0.39141
H	-11.55188	-5.09335	-0.18494

Neutral Triplet State (-1710.298892, -1709.654666, -1709.761732)

C	-6.66205	-0.76215	-0.03037
C	-5.26530	-0.76625	-0.02159
C	-4.49196	0.39500	-0.06686
C	-5.15916	1.62738	-0.14791
C	-6.56273	1.65555	-0.13006
C	-7.29815	0.48570	-0.07794
C	-3.04990	2.85198	-0.06996
C	-2.32084	1.65663	0.06110

C	-0.93744	1.74688	0.20198
H	-0.36209	0.82437	0.26254
C	-0.24029	2.96019	0.21936
C	-0.99003	4.13048	0.05419
C	-2.36458	4.07874	-0.10122
H	-4.75591	-1.72849	-0.00367
H	-7.08029	2.61213	-0.14071
H	-2.91963	5.00190	-0.24669
H	-8.38400	0.54704	-0.04110
H	-0.49764	5.10084	0.05719
N	-4.44165	2.83286	-0.21111
C	-5.13784	4.05616	-0.35660
C	-5.32554	4.89390	0.81170
C	-5.65662	4.42739	-1.62930
C	-6.09030	6.01423	0.72095
H	-4.88437	4.57143	1.75270
C	-6.45060	5.62852	-1.71081
C	-6.66912	6.39351	-0.53645
H	-6.27374	6.62976	1.59785
H	-7.27370	7.29607	-0.60318
C	-6.96281	6.00951	-2.95785
C	-5.40462	3.69695	-2.79499
C	-5.94176	4.10805	-4.05174
H	-5.73715	3.51265	-4.93784
C	-6.70806	5.24055	-4.13043
H	-7.12446	5.56354	-5.08130
H	-7.56098	6.91694	-3.02434
H	-4.78284	2.80405	-2.73993
C	-2.97309	0.28585	-0.06605
C	-2.52894	-0.33373	-1.40510
H	-2.84371	0.29950	-2.24501
H	-1.43796	-0.43895	-1.44509
H	-2.97231	-1.32768	-1.54061
C	-2.52248	-0.61614	1.09457
H	-1.43384	-0.73219	1.10962
H	-2.83591	-0.19452	2.05722
H	-2.94870	-1.62105	1.00641
C	1.22602	2.99618	0.37935
C	2.00745	3.95424	-0.27385
C	1.89115	2.06703	1.19741
C	3.39303	3.99816	-0.12993
H	1.53267	4.67655	-0.93571
C	3.26698	2.09517	1.35097
H	1.31673	1.32112	1.74365
C	4.02974	3.06171	0.68653
H	3.95831	4.75534	-0.66477

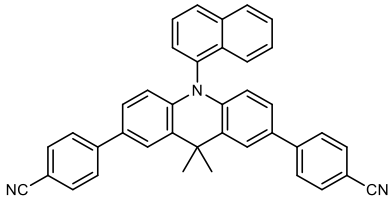
H	3.77443	1.37954	1.99370
C	-7.43614	-2.01711	0.02408
C	-8.65395	-2.14694	-0.65023
C	-6.98337	-3.12502	0.76027
C	-9.40222	-3.32186	-0.60471
H	-9.02620	-1.31773	-1.24944
C	-7.71263	-4.30098	0.81472
H	-6.05332	-3.05650	1.32196
C	-8.92963	-4.40888	0.13253
H	-10.33765	-3.37492	-1.15326
H	-7.36317	-5.15151	1.39559
O	5.37018	3.01054	0.89568
O	-9.57306	-5.59888	0.24804
C	6.18236	3.96676	0.23767
H	7.21163	3.74154	0.51985
H	6.08117	3.89087	-0.85248
H	5.93494	4.98756	0.55608
C	-10.82061	-5.74730	-0.40639
H	-10.71625	-5.63476	-1.49306
H	-11.16696	-6.75669	-0.18093
H	-11.55383	-5.02071	-0.03331

Cation Radical State (-1710.206299, -1709.557807, -1709.664188)

C	-6.69941	-0.80099	-0.00086
C	-5.29534	-0.80560	0.03467
C	-4.52896	0.34798	0.00021
C	-5.20442	1.58792	-0.08094
C	-6.61579	1.61704	-0.12999
C	-7.34131	0.45188	-0.08955
C	-3.10987	2.81457	-0.03169
C	-2.36469	1.61656	0.06266
C	-0.98703	1.71713	0.16247
H	-0.40422	0.80019	0.19735
C	-0.30161	2.94340	0.17427
C	-1.07306	4.11878	0.06072
C	-2.44171	4.05977	-0.04029
H	-4.78404	-1.76457	0.05756
H	-7.13678	2.56781	-0.18200
H	-3.01397	4.97972	-0.10846
H	-8.42582	0.51275	-0.09455
H	-0.59285	5.09313	0.08483
N	-4.49044	2.77403	-0.11914
C	-5.21593	4.01089	-0.28788
C	-5.63449	4.69727	0.82305
C	-5.48197	4.46270	-1.60726
C	-6.36284	5.89592	0.66973

H	-5.40386	4.30712	1.81221
C	-6.22536	5.67254	-1.74674
C	-6.65247	6.36751	-0.58715
H	-6.69263	6.43702	1.55184
H	-7.21759	7.28909	-0.71276
C	-6.51838	6.14764	-3.04999
C	-5.05204	3.77342	-2.76904
C	-5.35310	4.26450	-4.01632
H	-5.01999	3.72910	-4.90166
C	-6.09372	5.45987	-4.15989
H	-6.32408	5.83290	-5.15443
H	-7.08747	7.06985	-3.15148
H	-4.47980	2.85205	-2.67153
C	-3.01601	0.24962	-0.01784
C	-2.59700	-0.39584	-1.35667
H	-2.93096	0.21539	-2.20445
H	-1.50734	-0.49518	-1.41206
H	-3.03647	-1.39426	-1.45765
C	-2.54112	-0.62310	1.15713
H	-1.45370	-0.74327	1.14353
H	-2.82756	-0.17529	2.11529
H	-2.97511	-1.62633	1.10166
C	1.15508	2.99309	0.29721
C	1.89416	4.06738	-0.22100
C	1.86912	1.96159	0.93963
C	3.27811	4.12141	-0.12064
H	1.38572	4.87168	-0.74740
C	3.24339	2.00477	1.05542
H	1.33640	1.12582	1.38710
C	3.96245	3.08464	0.52246
H	3.81049	4.96367	-0.55120
H	3.78927	1.21518	1.56542
C	-7.46506	-2.04606	0.05498
C	-8.75377	-2.13265	-0.49331
C	-6.93936	-3.20286	0.66529
C	-9.49441	-3.30623	-0.44865
H	-9.18665	-1.27207	-0.99794
C	-7.66614	-4.37402	0.72601
H	-5.95712	-3.17590	1.13095
C	-8.95151	-4.43858	0.16800
H	-10.48101	-3.32822	-0.90020
H	-7.26516	-5.25960	1.21235
O	5.30037	3.03686	0.67926
O	-9.58089	-5.62532	0.27711
C	6.07992	4.10644	0.16376
H	7.11751	3.86492	0.39545

H	5.96015	4.19350	-0.92276
H	5.81197	5.05596	0.64246
C	-10.88792	-5.75153	-0.26433
H	-10.88313	-5.58510	-1.34818
H	-11.20469	-6.77367	-0.05619
H	-11.58228	-5.05021	0.21363



Neutral Ground State (-1665.834996, -1665.255578, -1665.356775)

C	-6.69400	-0.81796	0.07243
C	-5.29666	-0.81681	0.08389
C	-4.53052	0.34705	0.06763
C	-5.20277	1.58182	0.04681
C	-6.60784	1.59983	0.03838
C	-7.33741	0.42507	0.04661
C	-3.09323	2.80582	0.07076
C	-2.35704	1.60878	0.09653
C	-0.96743	1.69346	0.14355
H	-0.39488	0.76741	0.12894
C	-0.26983	2.90490	0.16436
C	-1.02798	4.08125	0.12913
C	-2.40959	4.03392	0.08408
H	-4.77883	-1.77462	0.06775
H	-7.13604	2.54912	0.03711
H	-2.97200	4.96327	0.07271
H	-8.42371	0.48285	0.06252
H	-0.54005	5.05289	0.16821
N	-4.49083	2.78631	0.03104
C	-5.20261	4.00716	-0.19402
C	-5.63211	4.75897	0.87150
C	-5.46397	4.41104	-1.53327
C	-6.35173	5.95500	0.65670
H	-5.41214	4.41746	1.88130
C	-6.20001	5.61523	-1.74276
C	-6.63145	6.36992	-0.62234
H	-6.68445	6.54029	1.50976
H	-7.19040	7.28791	-0.79594
C	-6.48203	6.02359	-3.07134
C	-5.02988	3.66265	-2.65661
C	-5.31909	4.08774	-3.93088
H	-4.98282	3.50569	-4.78541
C	-6.05372	5.27730	-4.14177
H	-6.27691	5.59890	-5.15599
H	-7.04612	6.94195	-3.22564
H	-4.46452	2.74524	-2.49890
C	-3.01225	0.23564	0.02543
C	-2.60508	-0.43381	-1.30028
H	-2.94000	0.16744	-2.15528

H	-1.51639	-0.54496	-1.36758
H	-3.04869	-1.43237	-1.39110
C	-2.53254	-0.62314	1.20805
H	-1.44404	-0.74548	1.19585
H	-2.81424	-0.16024	2.16147
H	-2.97022	-1.62707	1.17262
C	1.20165	2.93524	0.21850
C	1.92575	3.96822	-0.39837
C	1.91890	1.93136	0.88939
C	3.30976	4.00273	-0.34984
H	1.39878	4.74529	-0.94653
C	3.30292	1.94952	0.94067
H	1.38432	1.13518	1.40176
C	4.00783	2.98910	0.31986
H	3.85638	4.80474	-0.83876
H	3.84323	1.16821	1.46856
C	-7.45742	-2.07733	0.07940
C	-8.67789	-2.18035	-0.60725
C	-6.98603	-3.20506	0.77073
C	-9.40373	-3.36011	-0.60805
H	-9.05188	-1.32973	-1.17198
C	-7.69945	-4.39255	0.77530
H	-6.05796	-3.14438	1.33432
C	-8.91576	-4.47635	0.08464
H	-10.34246	-3.42744	-1.15142
H	-7.32665	-5.25549	1.32061
C	5.43487	3.01557	0.36943
C	-9.65694	-5.69723	0.08696
N	6.59872	3.03664	0.40916
N	-10.26056	-6.69330	0.08890

Neutral Triplet State (-1665.740922, -1665.161865, -1665.267554)

C	-6.69542	-0.84416	0.05508
C	-5.27664	-0.84128	0.08233
C	-4.50912	0.30012	0.00494
C	-5.18069	1.55447	-0.10669
C	-6.60061	1.58070	-0.15424
C	-7.32952	0.42714	-0.07836
C	-3.08486	2.77170	-0.08017
C	-2.33330	1.56483	0.04051
C	-0.96440	1.66249	0.15667
H	-0.39308	0.74002	0.20551
C	-0.25655	2.89227	0.15831
C	-1.03987	4.07521	0.00728
C	-2.40115	4.01746	-0.10536
H	-4.76313	-1.79750	0.12392

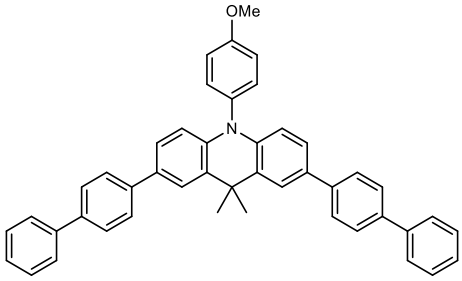
H	-7.11984	2.53106	-0.23599
H	-2.96676	4.93998	-0.19910
H	-8.41241	0.50457	-0.08760
H	-0.56682	5.05256	0.01147
N	-4.45817	2.72609	-0.16625
C	-5.18049	3.96494	-0.33734
C	-5.58997	4.65660	0.77328
C	-5.45399	4.41415	-1.65549
C	-6.31502	5.85761	0.62119
H	-5.35451	4.26821	1.76205
C	-6.19408	5.62608	-1.79477
C	-6.61133	6.32681	-0.63508
H	-6.63716	6.40266	1.50383
H	-7.17399	7.25004	-0.76009
C	-6.49416	6.09706	-3.09820
C	-5.03434	3.71909	-2.81766
C	-5.34221	4.20573	-4.06491
H	-5.01719	3.66552	-4.95041
C	-6.07977	5.40334	-4.20822
H	-6.31593	5.77315	-5.20268
H	-7.06070	7.02094	-3.19961
H	-4.46480	2.79664	-2.71775
C	-2.99528	0.20193	-0.05847
C	-2.62442	-0.39576	-1.43675
H	-2.98863	0.24341	-2.25113
H	-1.53694	-0.48876	-1.53359
H	-3.06978	-1.38975	-1.55614
C	-2.47831	-0.72105	1.05745
H	-1.39436	-0.85325	0.99158
H	-2.71735	-0.31011	2.04495
H	-2.92167	-1.71852	0.98212
C	1.18194	2.93819	0.29459
C	1.91869	4.11062	-0.02058
C	1.92352	1.81583	0.75001
C	3.29059	4.15866	0.09853
H	1.40653	4.99281	-0.39431
C	3.29440	1.85540	0.87781
H	1.40999	0.90255	1.03772
C	4.00525	3.02978	0.55100
H	3.82929	5.06584	-0.16363
H	3.83363	0.98371	1.24005
C	-7.45538	-2.06960	0.15040
C	-8.82921	-2.11663	-0.20672
C	-6.86898	-3.27981	0.60749
C	-9.56196	-3.28020	-0.12289
H	-9.32385	-1.22736	-0.58696

C	-7.59443	-4.44694	0.70098
H	-5.83050	-3.29754	0.92615
C	-8.95723	-4.46981	0.33477
H	-10.60853	-3.28727	-0.41692
H	-7.12172	-5.35473	1.06760
C	5.41738	3.07602	0.67940
C	-9.70768	-5.66989	0.42774
N	6.58044	3.11393	0.78517
N	-10.32513	-6.65910	0.50416

Cation Radical State (-1665.636921, -1665.057501, -1665.160744)

C	-6.66904	-0.83808	0.02270
C	-5.26910	-0.85968	0.04938
C	-4.49807	0.29251	0.00332
C	-5.17362	1.53369	-0.07333
C	-6.58575	1.57356	-0.11005
C	-7.31449	0.41076	-0.06455
C	-3.07572	2.75492	-0.04895
C	-2.33334	1.55334	0.03729
C	-0.95292	1.65210	0.12054
H	-0.36655	0.73722	0.15343
C	-0.27725	2.87953	0.11970
C	-1.04052	4.05893	0.01522
C	-2.41014	4.00237	-0.06676
H	-4.76713	-1.82378	0.07263
H	-7.10131	2.52704	-0.15922
H	-2.98328	4.92175	-0.12857
H	-8.39928	0.46810	-0.06307
H	-0.55414	5.03020	0.03225
N	-4.45612	2.71648	-0.11935
C	-5.18104	3.95968	-0.26769
C	-5.57330	4.63745	0.85790
C	-5.46447	4.42113	-1.57952
C	-6.29403	5.84296	0.72666
H	-5.32735	4.23784	1.83943
C	-6.19869	5.63914	-1.69422
C	-6.59965	6.32732	-0.52160
H	-6.60411	6.37925	1.61861
H	-7.15829	7.25491	-0.63019
C	-6.50917	6.12924	-2.98758
C	-5.06088	3.73839	-2.75416
C	-5.37932	4.24411	-3.99131
H	-5.06676	3.71367	-4.88696
C	-6.11053	5.44780	-4.11092
H	-6.35449	5.83216	-5.09779
H	-7.07106	7.05759	-3.07043

H	-4.49502	2.81108	-2.67713
C	-2.98871	0.19109	-0.02939
C	-2.58704	-0.45969	-1.37334
H	-2.92868	0.14956	-2.21903
H	-1.49864	-0.56260	-1.43868
H	-3.03044	-1.45697	-1.46382
C	-2.50172	-0.68031	1.14280
H	-1.41558	-0.80637	1.11208
H	-2.77157	-0.22812	2.10332
H	-2.94155	-1.68106	1.09535
C	1.18757	2.93186	0.22772
C	1.91724	3.94495	-0.41355
C	1.88167	1.97064	0.97949
C	3.29781	3.99680	-0.31418
H	1.40446	4.68519	-1.02200
C	3.26120	2.01608	1.09133
H	1.33573	1.19496	1.50995
C	3.97450	3.03091	0.44147
H	3.85622	4.77727	-0.82301
H	3.78964	1.27516	1.68431
C	-7.44670	-2.08372	0.08652
C	-8.66494	-2.19760	-0.60115
C	-6.99046	-3.17558	0.84131
C	-9.40679	-3.36564	-0.54381
H	-9.02316	-1.37339	-1.21255
C	-7.72784	-4.34586	0.91252
H	-6.06500	-3.10007	1.40641
C	-8.94006	-4.44434	0.21803
H	-10.34288	-3.44977	-1.08834
H	-7.37603	-5.18218	1.50979
C	5.39946	3.08219	0.55046
C	-9.70520	-5.65043	0.28915
N	6.55914	3.12344	0.63903
N	-10.32738	-6.63217	0.34807



Neutral Ground State (-1904.198697, -1903.46407, -1903.578044)

C	-6.67987	-0.82389	-0.09715
C	-5.28233	-0.82001	-0.07810
C	-4.51411	0.34217	-0.12798
C	-5.18350	1.57669	-0.20740
C	-6.58838	1.59268	-0.23700
C	-7.31906	0.41807	-0.18281
C	-3.07429	2.79914	-0.14915
C	-2.33925	1.60300	-0.07452
C	-0.95120	1.68800	0.02146
H	-0.37834	0.76194	0.04078
C	-0.25159	2.89791	0.05658
C	-1.00901	4.07246	-0.01480
C	-2.38906	4.02616	-0.11595
H	-4.76708	-1.77906	-0.05141
H	-7.11563	2.54102	-0.29141
H	-2.94784	4.95678	-0.16034
H	-8.40584	0.47584	-0.18023
H	-0.52026	5.04366	0.03474
N	-4.46837	2.77779	-0.25991
C	-2.99452	0.22927	-0.14860
C	-2.56919	-0.44875	-1.46436
H	-2.88988	0.14824	-2.32735
H	-1.47942	-0.56187	-1.51361
H	-3.01535	-1.44656	-1.55422
C	-2.52940	-0.62547	1.04285
H	-1.44085	-0.74686	1.04555
H	-2.82391	-0.15987	1.99121
H	-2.96411	-1.63054	1.00596
C	1.21924	2.92894	0.16473
C	1.97409	3.93522	-0.45446
C	1.91523	1.95278	0.89214
C	3.35893	3.96273	-0.35269
H	1.47275	4.69285	-1.05405
C	3.30006	1.97805	0.99034
H	1.36307	1.17630	1.41838
C	4.05340	2.98304	0.36945
H	3.91262	4.74132	-0.87424

H	3.80249	1.21978	1.58823
C	-7.44468	-2.08322	-0.02631
C	-8.66173	-2.23406	-0.70592
C	-6.98526	-3.17153	0.72923
C	-9.38515	-3.41746	-0.63483
H	-9.03442	-1.42198	-1.32769
C	-7.70693	-4.35585	0.79735
H	-6.06336	-3.08026	1.30090
C	-8.92287	-4.50566	0.11740
H	-10.31032	-3.50872	-1.20124
H	-7.33455	-5.16854	1.41857
C	-9.68759	-5.76775	0.18890
C	-9.02812	-7.00377	0.24603
C	-11.08929	-5.76326	0.20005
C	-9.74527	-8.19417	0.31209
H	-7.94059	-7.03481	0.21422
C	-11.80754	-6.95343	0.26408
H	-11.62346	-4.81486	0.18059
C	-11.13862	-8.17491	0.32078
H	-9.21259	-9.14179	0.34803
H	-12.89460	-6.92539	0.27890
H	-11.69951	-9.10504	0.37135
C	5.52721	3.00712	0.46863
C	6.26614	1.81598	0.48621
C	6.22539	4.22076	0.54289
C	7.65451	1.83646	0.57581
H	5.74968	0.86130	0.40351
C	7.61392	4.24246	0.63024
H	5.67241	5.15842	0.55437
C	8.33554	3.05033	0.64744
H	8.20738	0.89984	0.57951
H	8.13356	5.19583	0.69449
H	9.42048	3.06734	0.71582
C	-5.18248	4.01411	-0.34248
C	-5.45096	4.58125	-1.58129
C	-5.61117	4.65613	0.82113
C	-6.14608	5.78613	-1.67695
H	-5.11159	4.07428	-2.48292
C	-6.30435	5.85253	0.74101
H	-5.39617	4.20590	1.78885
C	-6.57535	6.42318	-0.50985
H	-6.64741	6.36669	1.63541
H	-6.34410	6.21215	-2.65566
O	-7.25977	7.59206	-0.48777
C	-7.55375	8.21735	-1.72582
H	-8.10126	9.12923	-1.48496

H	-6.63525	8.47711	-2.26694
H	-8.18040	7.57421	-2.35650

Neutral Triplet State (-1904.10853, -1903.377049, -1903.494435)

C	-6.68667	-0.81733	-0.08136
C	-5.28967	-0.82194	-0.03105
C	-4.51490	0.33450	-0.08517
C	-5.18042	1.56877	-0.20191
C	-6.58499	1.59510	-0.26336
C	-7.32081	0.42646	-0.20395
C	-3.07631	2.78980	-0.14975
C	-2.32881	1.58452	-0.03096
C	-0.96125	1.66464	0.07645
H	-0.40989	0.73282	0.15236
C	-0.21951	2.89583	0.07662
C	-1.01806	4.08627	-0.05201
C	-2.37876	4.02846	-0.15798
H	-4.78216	-1.78321	0.02603
H	-7.10487	2.54505	-0.34657
H	-2.93991	4.95430	-0.24999
H	-8.40675	0.48774	-0.22599
H	-0.54615	5.06414	-0.06348
N	-4.45597	2.76476	-0.25655
C	-2.99775	0.21635	-0.06594
C	-2.55030	-0.51069	-1.34959
H	-2.84077	0.06266	-2.23869
H	-1.46212	-0.63990	-1.36639
H	-3.00913	-1.50387	-1.41807
C	-2.56810	-0.59806	1.16688
H	-1.48254	-0.73737	1.19263
H	-2.87073	-0.09034	2.09049
H	-3.02153	-1.59520	1.15980
C	1.18319	2.93034	0.18688
C	1.93871	4.16585	0.14862
C	1.98341	1.73295	0.34115
C	3.29742	4.19349	0.23327
H	1.41708	5.11278	0.03778
C	3.34120	1.76848	0.42318
H	1.49777	0.76297	0.40751
C	4.08864	2.99792	0.36728
H	3.78932	5.16154	0.18016
H	3.86465	0.82506	0.55337
C	-7.45696	-2.07198	-0.00732
C	-8.66187	-2.22712	-0.70748
C	-7.01253	-3.15240	0.76847
C	-9.38662	-3.40955	-0.63899

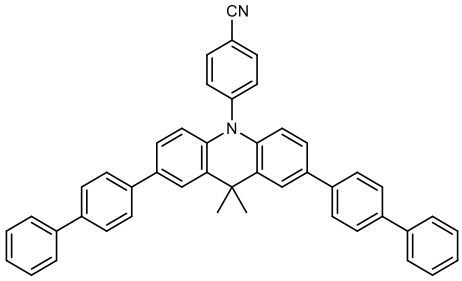
H	-9.02224	-1.42166	-1.34474
C	-7.73693	-4.33467	0.83548
H	-6.10180	-3.05670	1.35684
C	-8.93916	-4.49045	0.13259
H	-10.30065	-3.50623	-1.22216
H	-7.37767	-5.14114	1.47216
C	-9.70475	-5.75200	0.20016
C	-9.04576	-6.98694	0.28040
C	-11.10635	-5.74779	0.18364
C	-9.76365	-8.17708	0.34178
H	-7.95782	-7.01751	0.27018
C	-11.82520	-6.93775	0.24358
H	-11.64030	-4.79986	0.14599
C	-11.15692	-8.15827	0.32300
H	-9.23162	-9.12419	0.39581
H	-12.91232	-6.91027	0.23707
H	-11.71835	-9.08826	0.37007
C	5.52614	3.02619	0.44160
C	6.29836	1.83290	0.44787
C	6.25233	4.24623	0.50998
C	7.68147	1.86115	0.51770
H	5.80620	0.86617	0.38271
C	7.63575	4.26589	0.58037
H	5.72295	5.19509	0.52038
C	8.37062	3.07623	0.58520
H	8.23347	0.92343	0.51528
H	8.15112	5.22267	0.63640
H	9.45604	3.09577	0.63990
C	-5.17248	4.00304	-0.36794
C	-5.43214	4.54436	-1.61899
C	-5.61041	4.65588	0.78476
C	-6.13254	5.74362	-1.73643
H	-5.08438	4.02419	-2.50960
C	-6.30842	5.84695	0.68000
H	-5.40064	4.22028	1.75996
C	-6.57315	6.39651	-0.58178
H	-6.65982	6.37330	1.56379
H	-6.32581	6.15350	-2.72278
O	-7.26215	7.56107	-0.58271
C	-7.54687	8.16933	-1.83209
H	-8.09491	9.08488	-1.60740
H	-6.62402	8.42047	-2.36955
H	-8.16983	7.51784	-2.45761

Cation Radical State (-1904.009308, -1903.274911, -1903.3907)

C	-6.66879	-0.82254	-0.09147

C	-5.26959	-0.83516	0.00582
C	-4.49656	0.31463	-0.02567
C	-5.16353	1.55507	-0.15980
C	-6.57237	1.58965	-0.26801
C	-7.30368	0.42718	-0.23631
C	-3.06426	2.77052	-0.10550
C	-2.32571	1.57003	0.01734
C	-0.94534	1.66386	0.08876
H	-0.36637	0.74599	0.15399
C	-0.25501	2.88493	0.04864
C	-1.01861	4.06382	-0.07185
C	-2.38914	4.01244	-0.14437
H	-4.76726	-1.79633	0.08347
H	-7.08452	2.54121	-0.36659
H	-2.95678	4.93409	-0.22099
H	-8.38703	0.48650	-0.29287
H	-0.52910	5.03380	-0.07810
N	-4.44431	2.73740	-0.18878
C	-2.98882	0.20922	0.08110
C	-2.46401	-0.66246	-1.07718
H	-2.70480	-0.20922	-2.04548
H	-1.37785	-0.78279	-1.01281
H	-2.90830	-1.66255	-1.04358
C	-2.63583	-0.44451	1.43357
H	-1.55188	-0.55687	1.53985
H	-3.00296	0.16542	2.26689
H	-3.08212	-1.44127	1.51317
C	1.20748	2.92903	0.13466
C	1.93849	3.97170	-0.45771
C	1.92524	1.92897	0.81114
C	3.32219	4.00498	-0.38652
H	1.42237	4.74758	-1.01827
C	3.30771	1.96944	0.88876
H	1.39511	1.12770	1.32070
C	4.03849	3.00488	0.28735
H	3.85832	4.80514	-0.89205
H	3.82815	1.19863	1.45272
C	-7.44142	-2.06754	-0.04210
C	-8.66821	-2.18624	-0.71509
C	-6.97979	-3.17968	0.68088
C	-9.39396	-3.36649	-0.67594
H	-9.04098	-1.35784	-1.31341
C	-7.71222	-4.35480	0.72673
H	-6.05550	-3.11428	1.25057
C	-8.93283	-4.47702	0.04641
H	-10.32041	-3.43813	-1.24177

H	-7.34555	-5.18418	1.32763
C	-9.70310	-5.73486	0.08819
C	-9.04722	-6.97375	0.12630
C	-11.10489	-5.72263	0.08972
C	-9.76974	-8.16147	0.16325
H	-7.95989	-7.00966	0.10028
C	-11.82767	-6.91056	0.12887
H	-11.63549	-4.77227	0.08551
C	-11.16301	-8.13520	0.16525
H	-9.24180	-9.11198	0.18285
H	-12.91446	-6.87883	0.13898
H	-11.72813	-9.06357	0.19479
C	5.51163	3.03869	0.36042
C	6.25732	1.85150	0.34470
C	6.20094	4.25695	0.44475
C	7.64622	1.88064	0.41118
H	5.74731	0.89454	0.25199
C	7.58988	4.28612	0.51289
H	5.64282	5.19057	0.48274
C	8.31874	3.09841	0.49611
H	8.20592	0.94863	0.38804
H	8.10430	5.24127	0.58811
H	9.40435	3.12195	0.54856
C	-5.16446	3.98445	-0.30042
C	-5.39675	4.53288	-1.55262
C	-5.61815	4.61376	0.85737
C	-6.09578	5.73181	-1.66396
H	-5.03253	4.02425	-2.44287
C	-6.31351	5.80523	0.75225
H	-5.42505	4.16576	1.82980
C	-6.55638	6.37009	-0.50782
H	-6.68053	6.31991	1.63606
H	-6.27292	6.15312	-2.64820
O	-7.24367	7.53127	-0.50579
C	-7.51386	8.15603	-1.75201
H	-8.06570	9.06741	-1.52091
H	-6.58432	8.41517	-2.27319
H	-8.12860	7.51119	-2.39181



Neutral Ground State (-1881.916031, -1881.215888, -1881.329213)

C	-6.70258	-0.81554	-0.04454
C	-5.30514	-0.80874	-0.03429
C	-4.54009	0.35601	-0.06831
C	-5.21489	1.58796	-0.11893
C	-6.61898	1.60304	-0.13842
C	-7.34629	0.42538	-0.10222
C	-3.10135	2.81724	-0.06612
C	-2.36602	1.62104	-0.02130
C	-0.97680	1.70721	0.05411
H	-0.40230	0.78201	0.05167
C	-0.27891	2.91781	0.09576
C	-1.03828	4.09210	0.05428
C	-2.41986	4.04507	-0.02525
H	-4.78690	-1.76651	-0.02822
H	-7.15294	2.54874	-0.17102
H	-2.97654	4.97782	-0.04512
H	-8.43304	0.47993	-0.09236
H	-0.55058	5.06329	0.11079
N	-4.49877	2.79108	-0.15333
C	-3.02049	0.24734	-0.10084
C	-2.60332	-0.42090	-1.42415
H	-2.93181	0.18077	-2.28081
H	-1.51388	-0.53143	-1.48230
H	-3.04699	-1.41934	-1.51752
C	-2.54609	-0.61373	1.08241
H	-1.45734	-0.73328	1.07649
H	-2.83468	-0.15416	2.03546
H	-2.98031	-1.61887	1.04202
C	1.19362	2.94958	0.18000
C	1.93634	3.96535	-0.43799
C	1.90239	1.96445	0.88201
C	3.32268	3.99323	-0.35932
H	1.42426	4.73050	-1.01853
C	3.28861	1.99048	0.95747
H	1.36004	1.18000	1.40662
C	4.03021	3.00486	0.33769
H	3.86655	4.77962	-0.87947

H	3.80169	1.22490	1.53656
C	-7.46309	-2.07871	0.00412
C	-8.68065	-2.22017	-0.67617
C	-6.99720	-3.17969	0.73666
C	-9.39874	-3.40795	-0.62820
H	-9.05752	-1.39682	-1.28037
C	-7.71399	-4.36806	0.78226
H	-6.07416	-3.09587	1.30765
C	-8.93042	-4.50898	0.10130
H	-10.32447	-3.49186	-1.19477
H	-7.33742	-5.19168	1.38626
C	-9.69057	-5.77496	0.14948
C	-9.02711	-7.00968	0.18347
C	-11.09223	-5.77488	0.16177
C	-9.74063	-8.20326	0.22849
H	-7.93950	-7.03681	0.15039
C	-11.80682	-6.96817	0.20492
H	-11.62928	-4.82790	0.16013
C	-11.13402	-8.18835	0.23891
H	-9.20499	-9.14970	0.24654
H	-12.89393	-6.94381	0.22122
H	-11.69205	-9.12095	0.27318
C	5.50541	3.02990	0.41348
C	6.24598	1.83967	0.40643
C	6.20312	4.24362	0.49074
C	7.63546	1.86106	0.47574
H	5.72975	0.88514	0.32060
C	7.59274	4.26624	0.55762
H	5.64948	5.18044	0.52128
C	8.31596	3.07499	0.55096
H	8.18944	0.92522	0.46087
H	8.11207	5.21956	0.62483
H	9.40175	3.09275	0.60369
C	-5.21281	4.02412	-0.22552
C	-5.47664	4.59140	-1.47070
C	-5.63448	4.64920	0.94683
C	-6.16682	5.79272	-1.55046
H	-5.13583	4.08407	-2.37026
C	-6.32667	5.84978	0.87874
H	-5.41539	4.18650	1.90649
C	-6.59159	6.42087	-0.37287
H	-6.66143	6.34766	1.78431
H	-6.37753	6.24677	-2.51460
C	-7.30370	7.66007	-0.44856
N	-7.88247	8.66765	-0.50996

Neutral Triplet State (-1881.820979, -1881.124393, -1881.241494)

C	-6.68978	-0.81419	-0.01918
C	-5.29196	-0.82622	0.09172
C	-4.51925	0.32529	0.06933
C	-5.18445	1.56703	-0.06096
C	-6.59082	1.59725	-0.19933
C	-7.32276	0.43366	-0.17630
C	-3.09252	2.77918	0.00647
C	-2.34957	1.57801	0.08417
C	-0.96682	1.67044	0.13232
H	-0.38606	0.75143	0.16298
C	-0.27882	2.89276	0.11813
C	-1.04542	4.07351	0.06849
C	-2.41798	4.02213	0.01883
H	-4.78941	-1.78813	0.16302
H	-7.09073	2.55243	-0.32225
H	-2.99877	4.93880	0.00484
H	-8.40497	0.49081	-0.25774
H	-0.55661	5.04357	0.10468
N	-4.47595	2.75953	-0.07417
C	-3.01034	0.21643	0.14843
C	-2.51006	-0.64688	-1.02663
H	-2.77741	-0.18959	-1.98612
H	-1.42189	-0.76150	-0.99074
H	-2.94822	-1.64962	-0.98813
C	-2.62969	-0.44806	1.48758
H	-1.54405	-0.56651	1.56867
H	-2.97423	0.15837	2.33321
H	-3.07983	-1.44292	1.57135
C	1.18724	2.93672	0.16703
C	1.89994	3.98857	-0.42999
C	1.92460	1.92853	0.80788
C	3.28566	4.02394	-0.39618
H	1.36653	4.77117	-0.96487
C	3.30931	1.97033	0.84770
H	1.40876	1.11806	1.31803
C	4.02175	3.01591	0.24264
H	3.80655	4.83284	-0.90407
H	3.84636	1.19165	1.38490
C	-7.46028	-2.06341	0.01029
C	-8.66688	-2.18713	-0.69609
C	-7.01229	-3.17483	0.74154
C	-9.38695	-3.37209	-0.68021
H	-9.02789	-1.35861	-1.30162
C	-7.73805	-4.35570	0.76264
H	-6.10274	-3.10522	1.33433

C	-8.93865	-4.48256	0.04932
H	-10.29803	-3.44702	-1.27030
H	-7.38172	-5.18611	1.36860
C	-9.70262	-5.74545	0.06436
C	-9.04161	-6.98123	0.10807
C	-11.10398	-5.74039	0.03386
C	-9.75879	-8.17294	0.11982
H	-7.95373	-7.01089	0.10721
C	-11.82162	-6.93214	0.04714
H	-11.63886	-4.79244	0.02450
C	-11.15186	-8.15375	0.08968
H	-9.22652	-9.12095	0.14453
H	-12.90854	-6.90579	0.03227
H	-11.71274	-9.08513	0.09933
C	5.49681	3.05121	0.27746
C	6.24338	1.86574	0.22411
C	6.18716	4.26859	0.36435
C	7.63352	1.89542	0.25792
H	5.73203	0.90972	0.12871
C	7.57746	4.29859	0.39847
H	5.62951	5.20090	0.43136
C	8.30703	3.11240	0.34573
H	8.19307	0.96437	0.20686
H	8.09254	5.25325	0.47605
H	9.39358	3.13654	0.37257
C	-5.18951	4.00016	-0.19011
C	-5.19798	4.69850	-1.42583
C	-5.89456	4.51943	0.92700
C	-5.88811	5.87642	-1.54729
H	-4.65816	4.28495	-2.27721
C	-6.58112	5.70082	0.81960
H	-5.87615	3.97575	1.87104
C	-6.60825	6.42916	-0.42581
H	-7.11300	6.10025	1.68074
H	-5.89760	6.40520	-2.49820
C	-7.30738	7.62940	-0.54188
N	-7.90007	8.64770	-0.64073

Cation Radical State (-1881.723271, -1881.023358, -1881.137948)

C	-6.68859	-0.81795	-0.04896
C	-5.28878	-0.82776	0.04327
C	-4.51919	0.32410	0.02760
C	-5.19124	1.56371	-0.08280
C	-6.60015	1.59740	-0.18271
C	-7.32786	0.43246	-0.16875
C	-3.08952	2.78503	-0.02553

C	-2.34948	1.58384	0.07412
C	-0.96891	1.67874	0.13172
H	-0.38880	0.76062	0.17988
C	-0.28017	2.90126	0.09668
C	-1.04678	4.08063	0.00060
C	-2.41781	4.02853	-0.05607
H	-4.78262	-1.78809	0.10308
H	-7.12043	2.54646	-0.26105
H	-2.98274	4.95322	-0.11439
H	-8.41147	0.49018	-0.21940
H	-0.55891	5.05132	0.00019
N	-4.47082	2.74634	-0.09679
C	-3.01079	0.22153	0.12927
C	-2.48691	-0.64232	-1.03502
H	-2.73069	-0.18421	-2.00015
H	-1.40055	-0.76141	-0.97375
H	-2.92876	-1.64355	-1.00601
C	-2.65427	-0.43937	1.47749
H	-1.56985	-0.55017	1.58052
H	-3.02072	0.16498	2.31513
H	-3.09903	-1.43724	1.55166
C	1.18255	2.94674	0.15977
C	1.90119	4.00185	-0.42664
C	1.91427	1.93559	0.80468
C	3.28555	4.03634	-0.38042
H	1.37423	4.78651	-0.96428
C	3.29747	1.97774	0.85816
H	1.39510	1.12387	1.30883
C	4.01570	3.02551	0.26228
H	3.81099	4.84613	-0.88172
H	3.82916	1.19816	1.39899
C	-7.45650	-2.06550	-0.02014
C	-8.68859	-2.17383	-0.68575
C	-6.98459	-3.19202	0.67402
C	-9.40924	-3.35733	-0.66728
H	-9.06939	-1.33425	-1.26294
C	-7.71237	-4.37027	0.69991
H	-6.05599	-3.13587	1.23754
C	-8.93829	-4.48196	0.02689
H	-10.33959	-3.42011	-1.22759
H	-7.33796	-5.21085	1.27997
C	-9.70479	-5.74228	0.04843
C	-9.04605	-6.98029	0.05979
C	-11.10667	-5.73300	0.05805
C	-9.76607	-8.16990	0.07873
H	-7.95884	-7.01373	0.02703

C	-11.82681	-6.92286	0.07960
H	-11.63926	-4.78390	0.07480
C	-11.15937	-8.14651	0.08947
H	-9.23618	-9.11949	0.07739
H	-12.91357	-6.89368	0.09671
H	-11.72244	-9.07644	0.10530
C	5.48950	3.06041	0.31012
C	6.23586	1.87411	0.26841
C	6.17915	4.27839	0.39725
C	7.62549	1.90383	0.31282
H	5.72541	0.91773	0.17270
C	7.56888	4.30803	0.44337
H	5.62144	5.21116	0.45566
C	8.29826	3.12124	0.40124
H	8.18542	0.97268	0.26991
H	8.08371	5.26270	0.52150
H	9.38453	3.14523	0.43678
C	-5.19197	3.99230	-0.19508
C	-5.43275	4.53397	-1.45265
C	-5.62277	4.61124	0.97264
C	-6.12669	5.73181	-1.54631
H	-5.07881	4.02025	-2.34296
C	-6.31810	5.80865	0.88137
H	-5.41465	4.15626	1.93770
C	-6.56802	6.36583	-0.37850
H	-6.66614	6.31189	1.77833
H	-6.32635	6.17667	-2.51653
C	-7.28464	7.60225	-0.47443
N	-7.86633	8.60617	-0.55285

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