Supporting Information for

Donor Modification of Thermally Activated Delayed Fluorescence Photosensitizers for Organocatalyzed Atom Transfer Radical Polymerization

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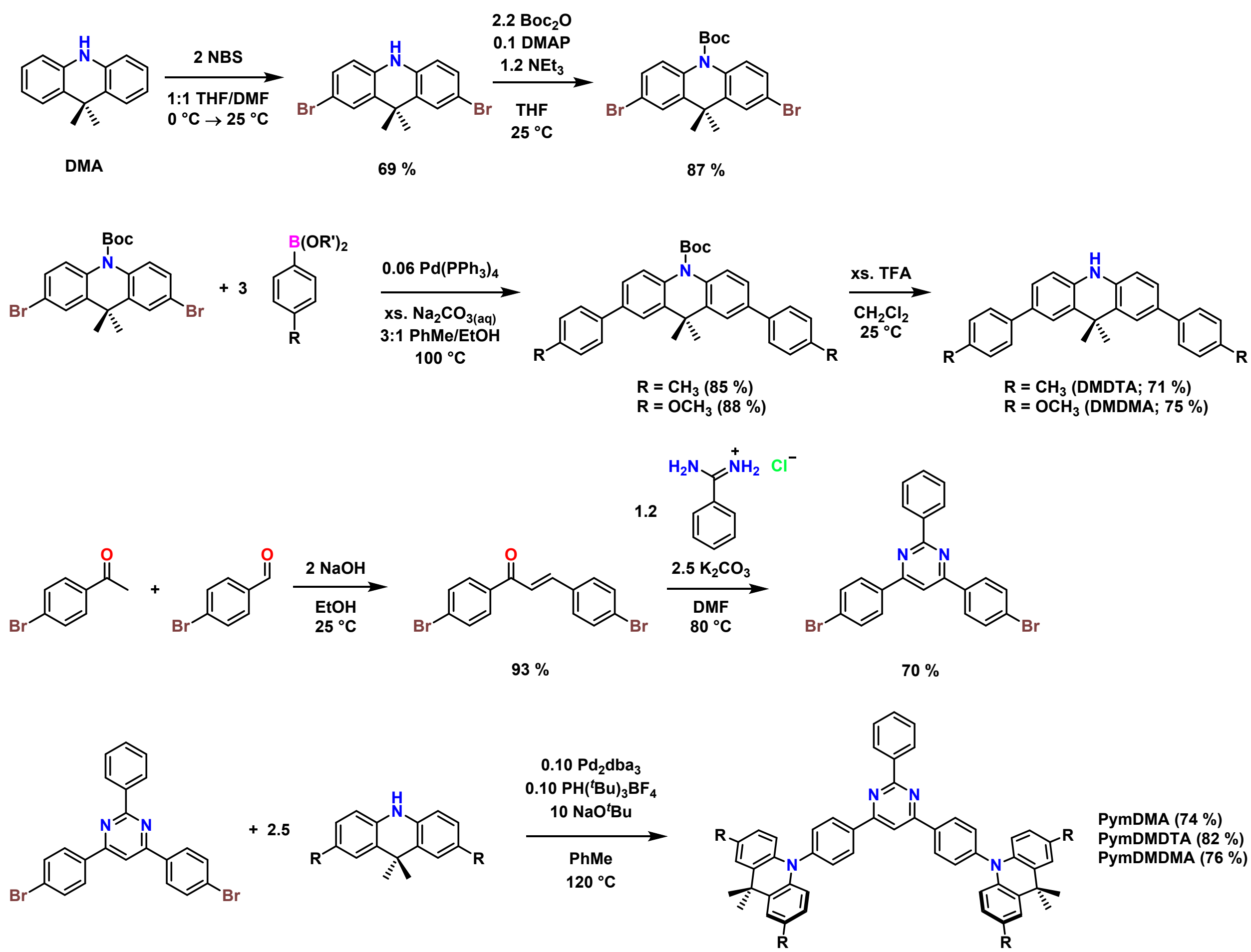
S1 – Synthetic Methods

S1.1 – General Considerations

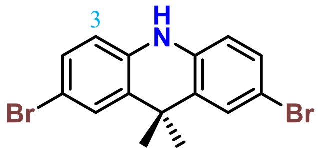
All reactions were performed in air unless otherwise stated. Solvents were of reagent grade or higher and obtained from commercial sources. CH_2Cl_2 was freshly distilled from P_4O_{10} prior to use. Tetrahydrofuran and toluene were dried using an Innovative Technologies Inc. solvent purification system. 9,9-dimethyl-9,10-dihydroacridine[1] and benzamidinium hydrochloride[2] were prepared according to literature methods. Phenox O-PC A0202 was purchased from Sigma. Other chemicals were purchased from commercial sources and used as received without further purification.

S1.2 – Photocatalyst Synthetic Scheme



S2 – Small Molecule Synthesis and Characterization Data

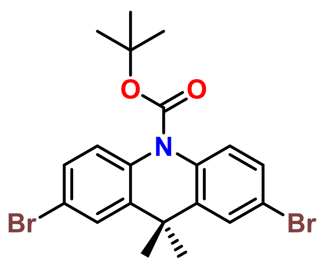
2,7-dibromo-9,9-dimethyl-9,10-dihydroacridine



A round bottom flask was charged with 9,9-dimethyl-9,10-dihydroacridine (7.00 g, 33.4 mmol, 1.00 eq.), a magnetic stir bar, and 50 mL of tetrahydrofuran. The flask was cooled in an ice bath. In a separate flask, *N*-bromosuccinimide (11.9 g, 66.9 mmol, 2.00 eq.) was dissolved in 50 mL *N,N*-dimethylformamide. The solution of *N*-bromosuccinimide was added dropwise with stirring. The mixture was allowed to warm and stirred at ambient temperature for 16 hours. Tetrahydrofuran was removed by rotary evaporation and the remaining solution was poured into 250 mL water and extracted with dichloromethane. The organic phase was washed 5× with water, once with brine, then dried over $MgSO_4$. The crude residue was purified on silica using 10% ethyl acetate/hexanes (v/v). Product fractions were recrystallized from dichloromethane/hexanes to afford the title compound as light green crystals that darken in the presence of oxygen. Yield = 8.40 g (69%). The spectral data are consistent with the literature.[3]

^{1}H NMR (400 MHz, C_6D_6): δ 7.36 (d, *J* = 2.2 Hz, 2H, CH^1), 7.09 (dd, *J* = 8.4, 2.2 Hz, 2H, CH^2), 5.93 – 5.75 (m, 2H, CH^3), 5.09 (s, 1H, N*H*), 1.08 (s, 6H, CH_3).

***tert*-butyl 2,7-dibromo-9,9-dimethylacridine-10(9H)-carboxylate**

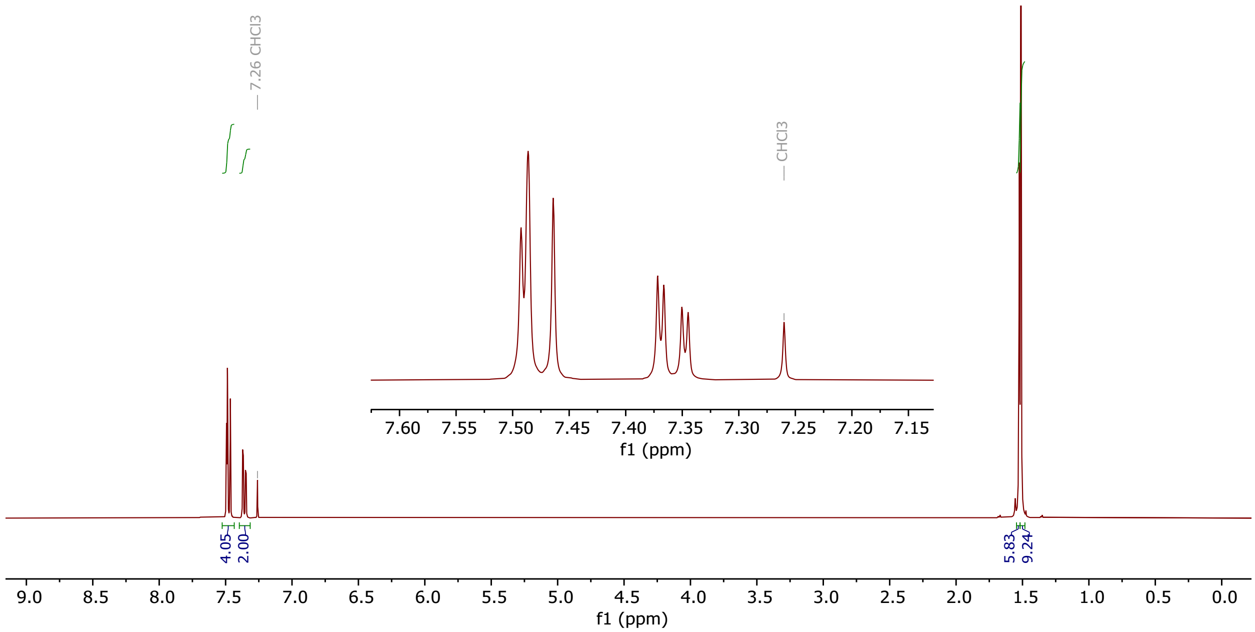


A side-arm flask was charged with 2,7-dibromo-9,9-dimethyl-9,10-dihydroacridine (7.60 g, 23.2 mmol, 1.00 eq.), *N,N*-dimethylaminopyridine (283 mg, 2.32 mmol, 0.10 eq.), and a magnetic stir bar. The flask was capped with a rubber septum and subjected to three vacuum and N_2-backfill cycles. Dry tetrahydrofuran (30 mL) and triethylamine (3.90 mL, 27.8 mmol, 1.20 eq.) were added *via* syringe through the septum cap. The mixture was heated to 50 °C under a positive pressure of N_2. In a separate side-arm flask, di-*tert*-butyl dicarbonate (11.2 g, 51.1 mmol, 2.20 eq.) was dissolved in 20 mL dry tetrahydrofuran after 3× vacuum-backfill cycles. This solution was transferred to the other flask *via* syringe and added dropwise through the septum cap. The mixture was stirred at 50 °C for 16 hours. Tetrahydrofuran was removed by rotary evaporation and the crude residue was dissolved in 50 mL dichloromethane. This was washed 3× with water, once with brine, then dried over $MgSO_4$. The crude residue was purified on silica using 2:1 dichloromethane/hexanes (v/v) to afford a white solid. Yield = 9.20 g (87%).

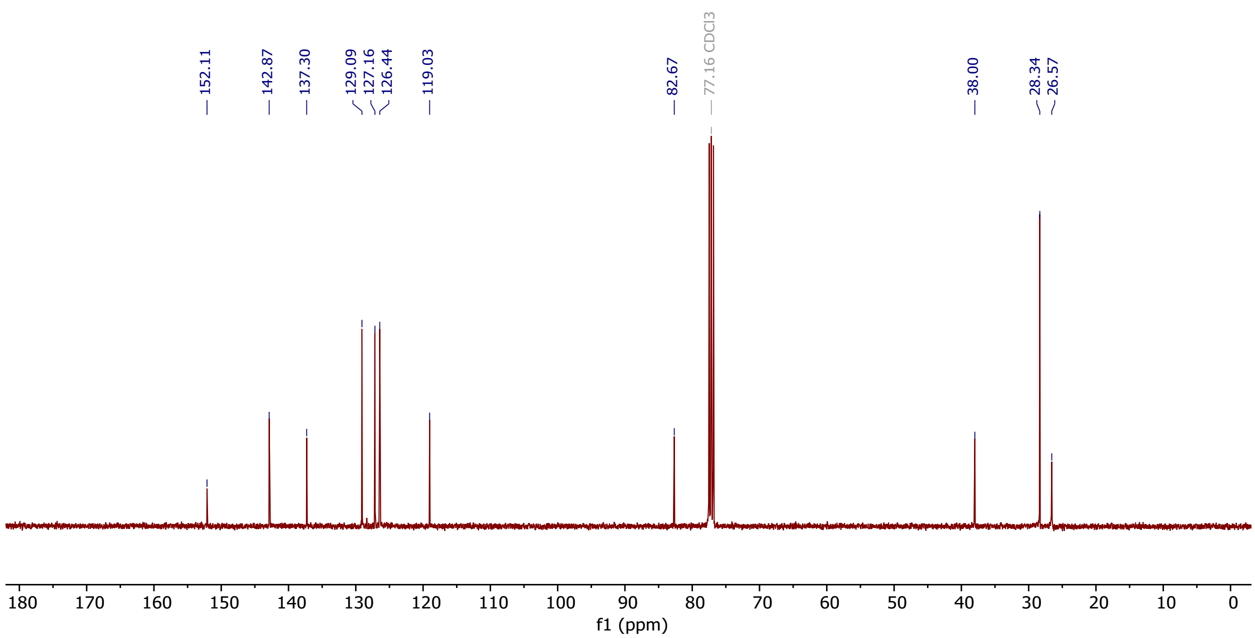
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.53 – 7.42 (m, 4H, CH^1 and CH^3), 7.36 (dd, *J* = 8.6, 2.2 Hz, 2H, CH^2), 1.52 (s, 6H, $C(CH_3)_2$), 1.51 (s, 9H, $C(CH_3)_3$).

^{13}C NMR (101 MHz, $CDCl_3$): δ 152.1, 142.9, 137.3, 129.1, 127.2, 126.4, 119.0, 82.7, 38.0, 28.3, 26.6.

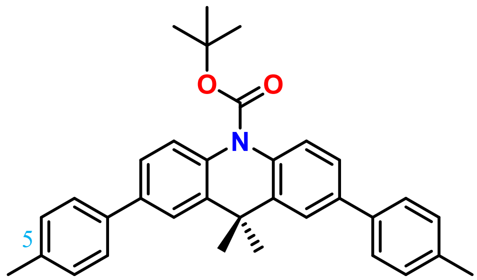
HRMS (FD) *m/z*: $[M+H]^+$ calc'd for $[C_{20}H_{22}Br_2NO_2]^+$ 466.0017; found 466.0019; difference 0.39 ppm.



[1]H NMR spectrum (25 °C, $CDCl_3$) of *tert*-butyl 2,7-dibromo-9,9-dimethylacridine-10(9H)-carboxylate.



[13]C{[1]H} NMR spectrum (25 °C, $CDCl_3$) of *tert*-butyl 2,7-dibromo-9,9-dimethylacridine-10(9H)-carboxylate.



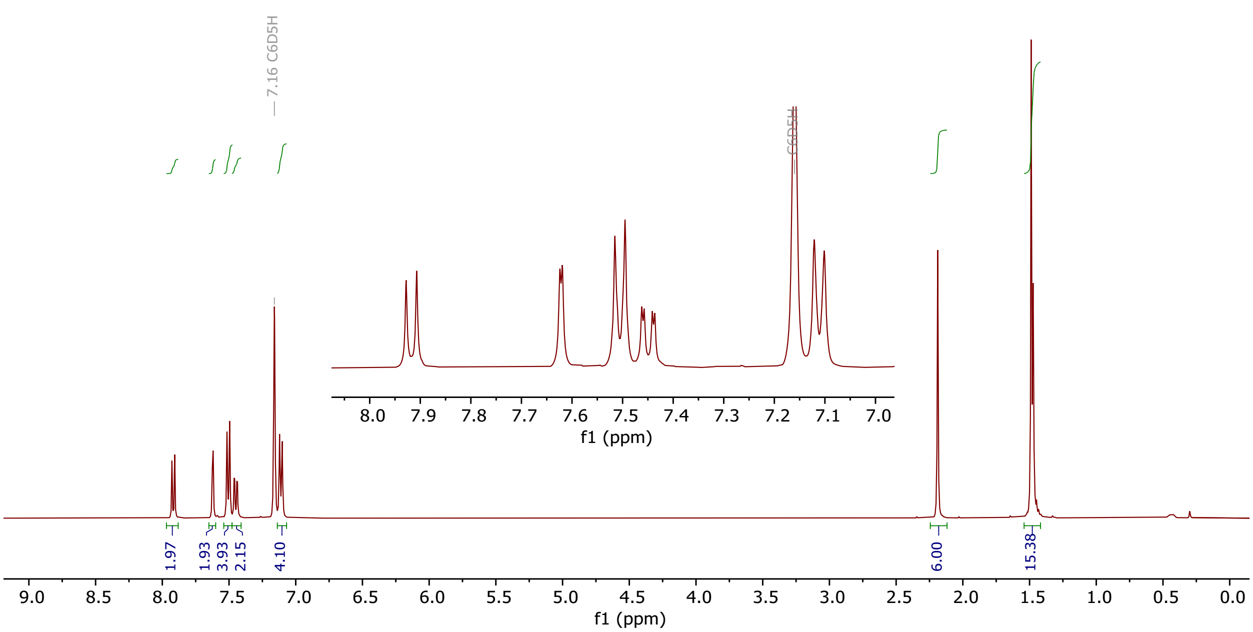
tert-butyl 9,9-dimethyl-2,7-di-p-tolylacridine-10(9H)-carboxylate

A side-arm flask was charged with *tert*-butyl 2,7-dibromo-9,9-dimethylacridine-10(9H)-carboxylate (974 mg, 2.08 mmol, 1.00 eq.), 4,4,5,5-tetramethyl-2-(p-tolyl)-1,3,2-dioxaborolane (1.37 g, 6.26 mmol, 3.00 eq.), and a magnetic stir bar. The flask was transferred into an inert atmosphere glovebox and $Pd(PPh_3)_4$ (145 mg, 0.125 mmol, 0.06 eq.) was added. The flask was sealed with a rubber septum and transferred to a Schlenk line. Under a positive pressure of N_2, a reflux condenser was fitted to the mouth of the flask. 60 mL of pre-sparged 3:1 toluene/ethanol was added through the side arm via syringe. 10 mL of pre-sparged of a saturated aqueous solution of Na_2CO_3 was then added by cannula transfer. The mixture was heated to 90 °C for 16 hours then cooled to room temperature and extracted from water with dichloromethane. Palladium was removed using a 3-inch plug of silica, eluting with 3:1 dichloromethane/hexanes (v/v). The solvent was removed to afford a colourless oil which solidifies upon application of high vacuum. This was washed with methanol and collected by vacuum filtration to provide the title compound as an analytically pure white solid. Yield = 976 mg (85 %).

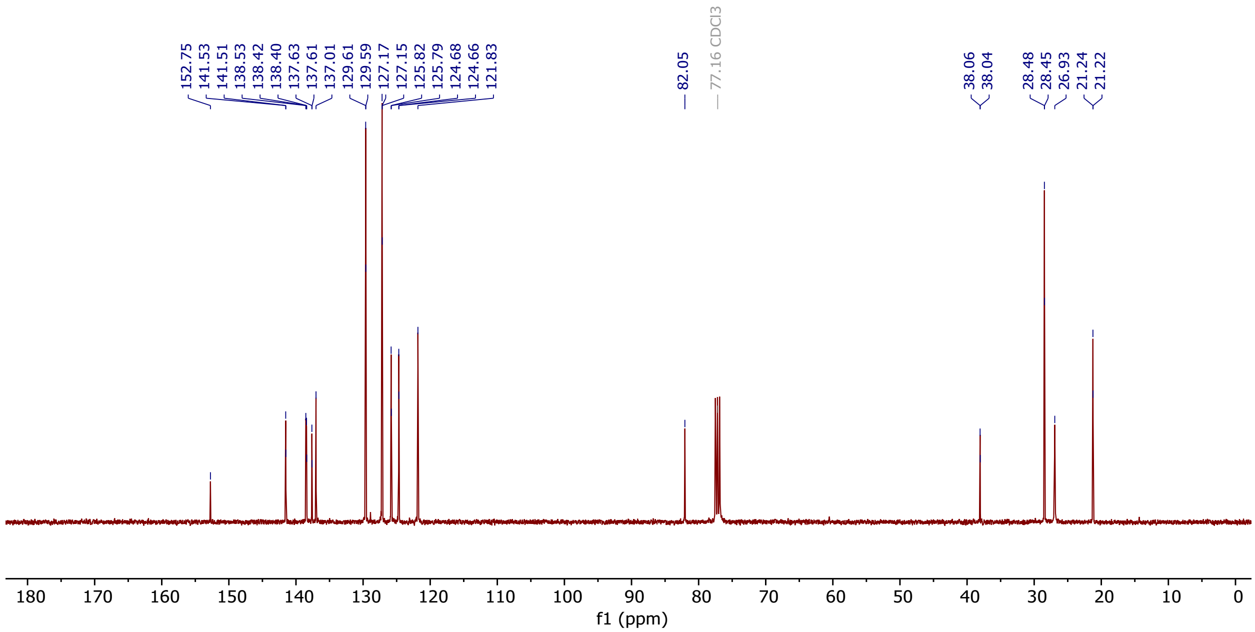
^{1}H NMR (400 MHz, C_6D_6): δ 7.92 (d, *J* = 8.3 Hz, 2H, CH^3), 7.62 (d, *J* = 2.1 Hz, 2H, CH^1), 7.51 (d, *J* = 8.1 Hz, 4H, $CH^{4/5}$), 7.45 (dd, *J* = 8.3, 2.1 Hz, 2H, CH^2), 7.11 (d, *J* = 7.8 Hz, 4H, $CH^{4/5}$), 2.19 (s, 6H, CH_3), 1.49 (s, 9H, $C(CH_3)_3$), 1.47 (s, 6H, $C(CH_3)_2$).

^{13}C NMR (101 MHz, $CDCl_3$): δ 152.7, 141.5, 141.5, 138.5, 138.4, 138.4, 137.6, 137.6, 137.0, 129.6, 129.6, 127.2, 127.1, 125.8, 125.8, 124.7, 124.7, 121.8, 82.0, 38.1, 38.0, 28.5, 28.5, 26.9, 21.2, 21.2.

HRMS (ESI) *m/z*: $[M]^+$ calc'd for $[C_{34}H_{35}NO_2]^+$ 489.2668; found 489.2673; difference 0.97 ppm.

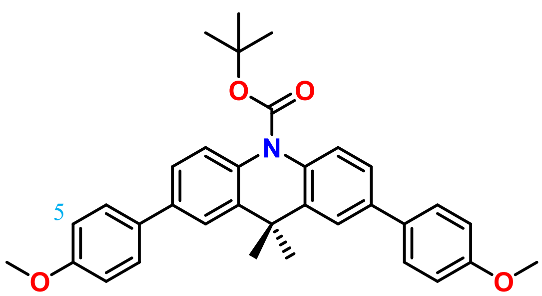


^{1}H NMR spectrum (25 °C, C_6D_6) of *tert*-butyl 9,9-dimethyl-2,7-di-p-tolylacridine-10(9H)-carboxylate.



$^{13}C\{^1H\}$ NMR spectrum (25 °C, $CDCl_3$) of *tert*-butyl 9,9-dimethyl-2,7-di-p-tolylacridine-10(9H)-carboxylate.

tert-butyl 2,7-bis(4-methoxyphenyl)-9,9-dimethylacridine-10(9H)-carboxylate

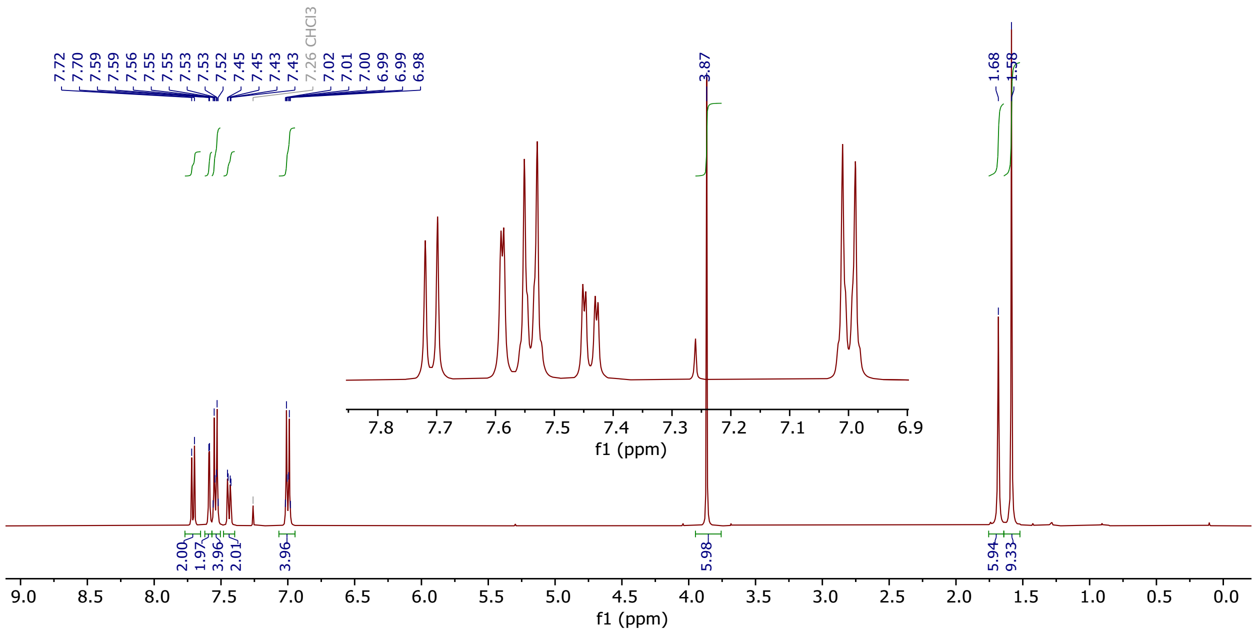


A side-arm flask was charged with *tert*-butyl 2,7-dibromo-9,9-dimethylacridine-10(9H)-carboxylate (1.00 g, 2.14 mmol, 1.00 eq.), 4-methoxyphenyl boronic acid (976 mg, 6.42 mmol, 3.00 eq.), and a magnetic stir bar. The flask was transferred into an inert atmosphere glovebox and $Pd(PPh_3)_4$ (148 mg, 0.128 mmol, 0.06 eq.) was added. The flask was sealed with a rubber septum and transferred to a Schlenk line. Under a positive pressure of N_2, a reflux condenser was fitted to the mouth of the flask. 60 mL of pre-sparged 3:1 toluene/ethanol was added through the side arm via syringe. 10 mL of pre-sparged of a saturated aqueous solution of Na_2CO_3 was then added by cannula transfer. The mixture was heated to 90 °C for 16 hours then cooled to room temperature and extracted from water with dichloromethane. Palladium was removed using a 3-inch plug of silica, eluting with 3:1 dichloromethane/hexanes (v/v). The solvent was removed to afford a colourless oil which solidifies upon application of high vacuum. This was washed with methanol and collected by vacuum filtration to provide the title compound as an analytically pure white solid. Yield = 976 mg (88 %).

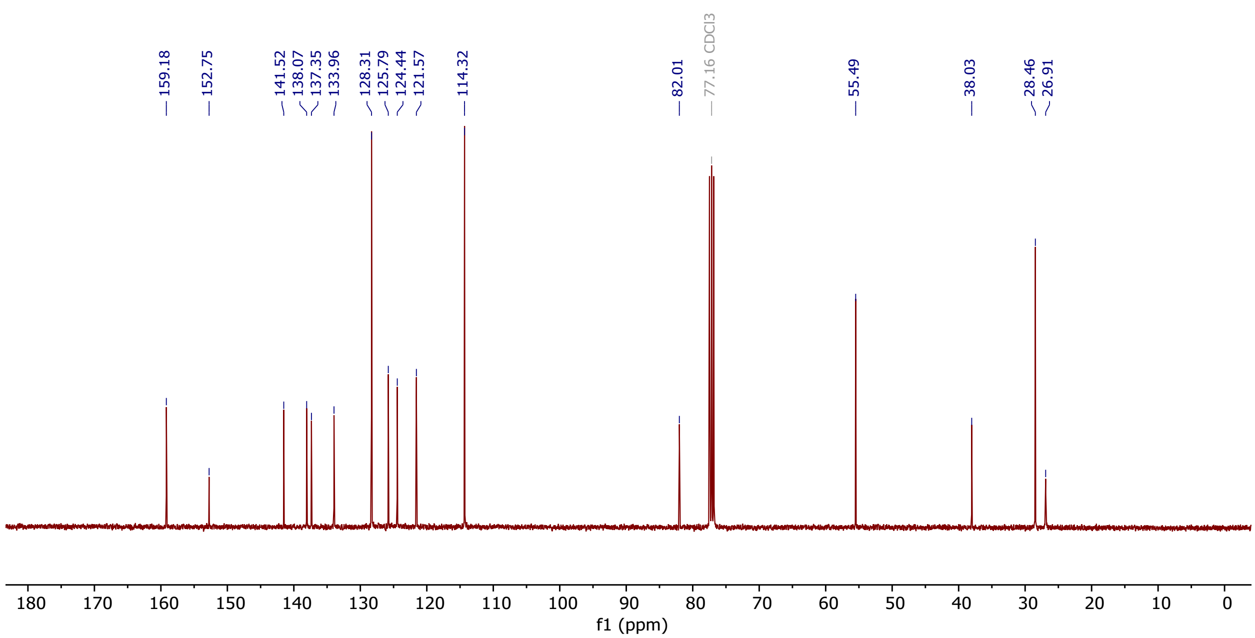
^1H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, *J* = 8.3 Hz, 2H, CH^3), 7.59 (d, *J* = 2.1 Hz, 2H, CH^1), 7.54 (d, *J* = 8.7 Hz, 4H, $CH^{4/5}$), 7.44 (dd, *J* = 8.3, 2.1 Hz, 2H, CH^2), 7.00 (d, *J* = 8.7 Hz, 4H, $CH^{4/5}$), 3.87 (s, 6H, OCH_3), 1.68 (s, 6H, $C(CH_3)_2$), 1.58 (s, 9H, $C(CH_3)_3$).

^{13}C NMR (101 MHz, $CDCl_3$): δ 159.2, 152.7, 141.5, 138.1, 137.4, 134.0, 128.3, 125.8, 124.4, 121.6, 114.3, 82.0, 55.5, 38.0, 28.5, 26.9.

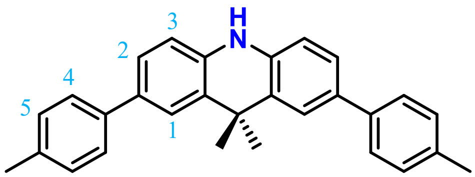
HRMS (ESI) *m/z*: $[M]^+$ calc'd for $[C_{34}H_{35}NO_4]^+$ 521.2566; found 521.2569; difference 0.62 ppm.



^{1}H NMR spectrum (25 °C, $CDCl_3$) of *tert*-butyl 2,7-bis(4-methoxyphenyl)-9,9-dimethylacridine-10(9H)-carboxylate.



$^{13}C\{^1H\}$ NMR spectrum (25 °C, $CDCl_3$) of *tert*-butyl 2,7-bis(4-methoxyphenyl)-9,9-dimethylacridine-10(9H)-carboxylate.



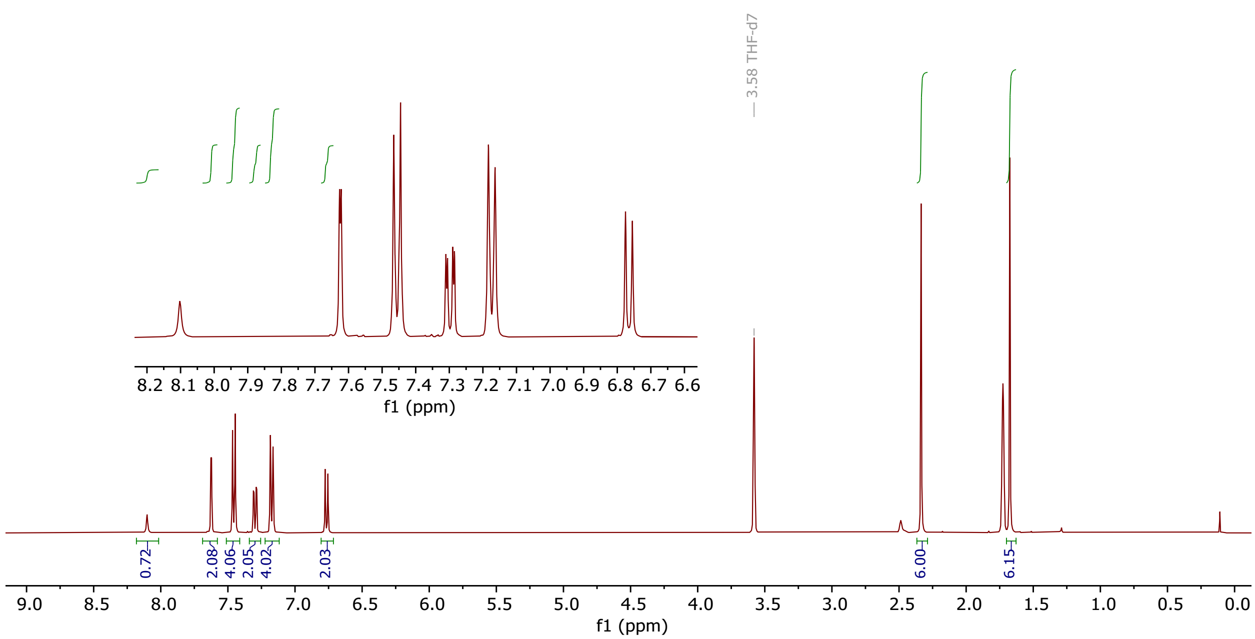
9,9-dimethyl-2,7-di-*p*-tolyl-9,10-dihydroacridine (DMDTA)

A side-arm flask was charged with *tert*-butyl 9,9-dimethyl-2,7-di-*p*-tolylacridine-10(9H)-carboxylate (512 mg, 1.00 mmol) and a stir bar. The flask was capped with a rubber septum and subjected to three vacuum-N_2 backfill cycles. 10 mL of freshly distilled dichloromethane were added *via* syringe through the septum cap. 4.0 mL of trifluoracetic acid were added dropwise to the solution with stirring. After 1 hour, the mixture was neutralized with aqueous sodium bicarbonate and extracted with dichloromethane. The solvent was removed, and the crude product was recrystallized from dichloromethane/hexanes at room temperature. Light green crystals were collected by vacuum filtration. Yield = 274 mg (71%).

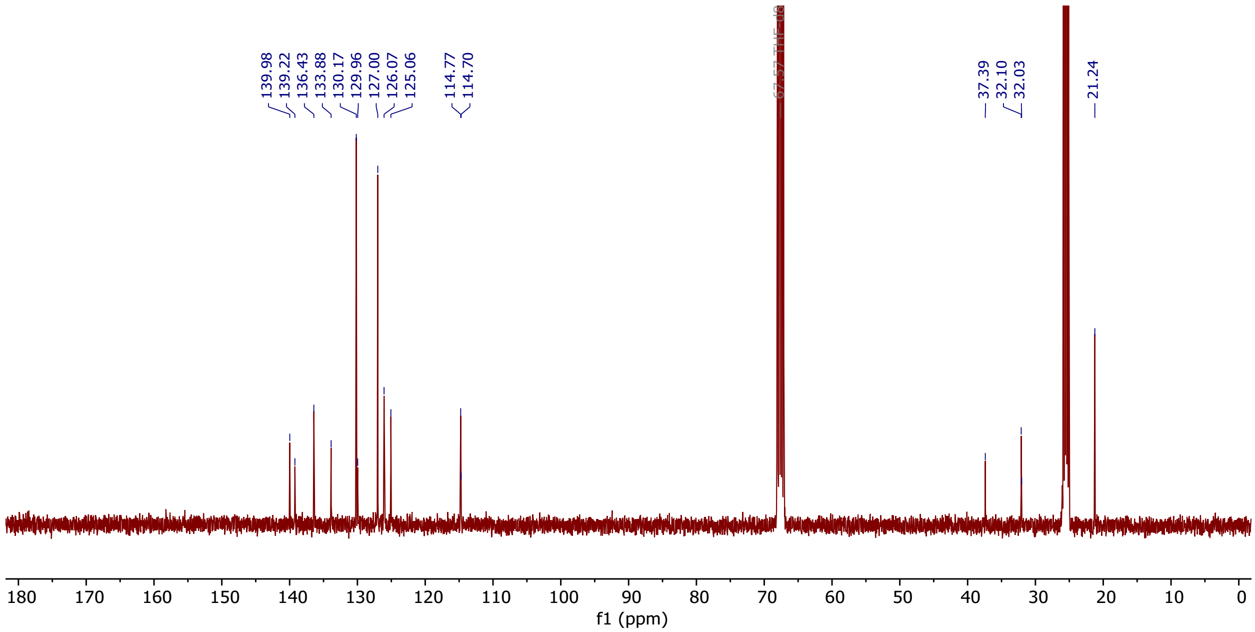
^{1}H NMR (400 MHz, THF-*d_8*): δ 8.10 (s, 1H, NH), 7.62 (d, *J* = 2.0 Hz, 2H, CH^1), 7.52 – 7.41 (d, *J* = 7.9Hz, 4H, $CH^{4/5}$), 7.30 (dd, *J* = 8.2, 2.0 Hz, 2H, CH^2), 7.17 (d, *J* = 7.9 Hz, 4H, $CH^{4/5}$), 6.77 (d, *J* = 8.2 Hz, 2H, CH^3), 2.34 (s, 6H, CH_3), 1.67 (s, 6H, $C(CH_3)_2$).

^{13}C NMR (101 MHz, THF-*d_8*): δ 140.0, 139.2, 136.4, 133.9, 130.2, 130.0, 127.0, 126.1, 125.1, 114.8, 114.7, 37.4, 32.1, 32.0, 21.2.

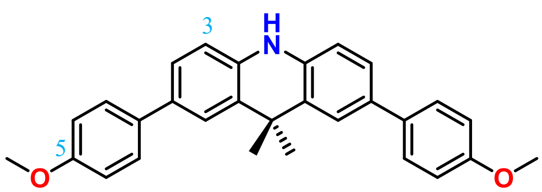
HRMS (ESI) *m/z:* $[M]^+$ calc'd for $[C_{29}H_{27}N]^+$ 389.2143; found 389.2149; difference 1.41 ppm.



^{1}H NMR spectrum (25 °C, THF-*d_8*) of 9,9-dimethyl-2,7-di-*p*-tolyl-9,10-dihydroacridine.



$^{13}C\{^1H\}$ NMR spectrum (25 °C, THF-d_8) of 9,9-dimethyl-2,7-di-*p*-tolyl-9,10-dihydroacridine.



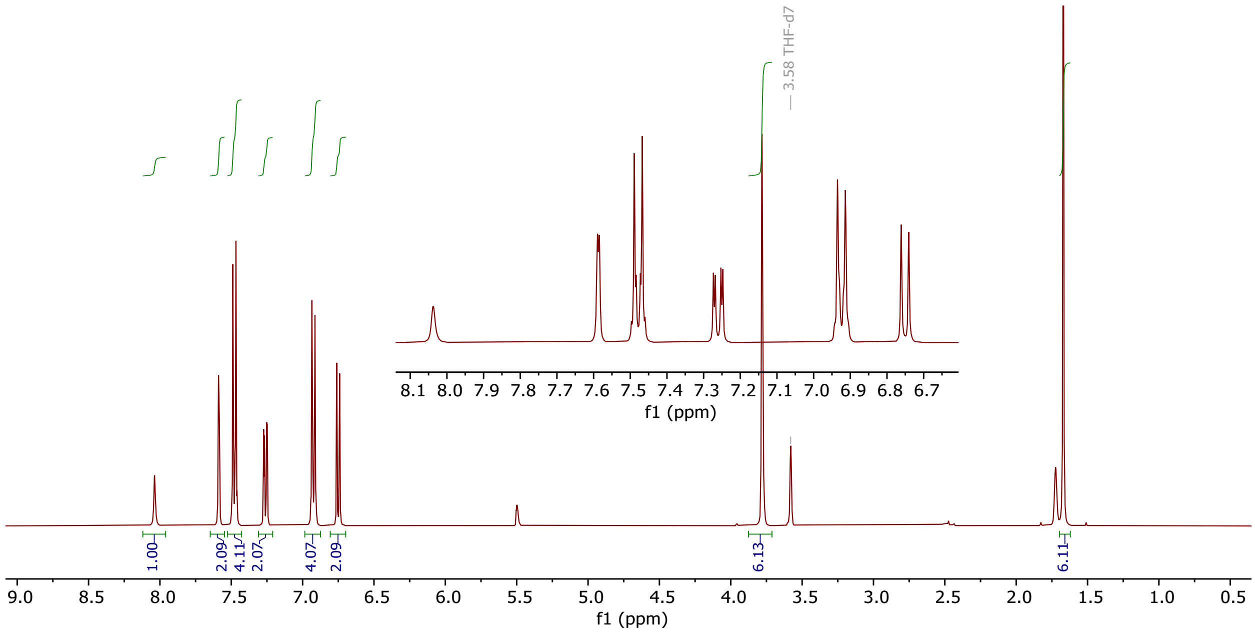
9,9-dimethyl-2,7-bis(4-methoxyphenyl)-9,10-dihydroacridine (DMDMA)

A side-arm flask was charged with *tert*-butyl 2,7-bis(4-methoxyphenyl)-9,9-dimethylacridine-10(9H)-carboxylate (522 mg, 1.00 mmol) and a stir bar. The flask was capped with a rubber septum and subjected to three vacuum-N_2 backfill cycles. 10 mL of freshly distilled dichloromethane were added *via* syringe through the septum cap. 4.0 mL of trifluoracetic acid were added dropwise to the solution with stirring. After 1 hour, the mixture was neutralized with aqueous sodium bicarbonate and extracted with dichloromethane. The solvent was removed, and the crude product was recrystallized from dichloromethane/hexanes at room temperature. Light green crystals were collected by vacuum filtration. Yield = 316 mg (75%).

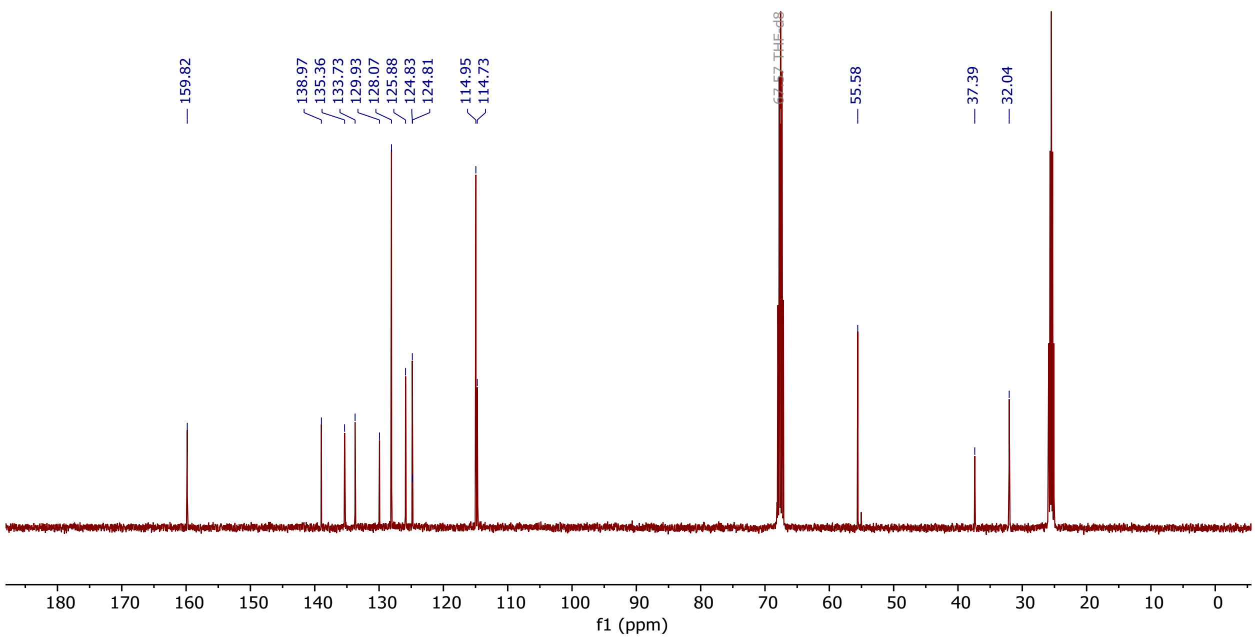
^{1}H NMR (400 MHz, THF-d_8): δ 8.04 (s, 1H, NH), 7.59 (d, J = 2.0 Hz, 2H, CH^1), 7.48 (d, J = 8.7 Hz, 4H, $CH^{4/5}$), 7.26 (dd, J = 8.2, 2.0 Hz, 2H, CH^2), 6.92 (d, J = 8.7 Hz, 4H, $CH^{4/5}$), 6.75 (d, J = 8.2 Hz, 2H, CH^3), 3.87 – 3.71 (s, 6H, OCH_3), 1.67 (s, 6H, $C(CH_3)_2$).

^{13}C NMR (101 MHz, THF-d_8) δ 159.8, 139.0, 135.4, 133.7, 129.9, 128.1, 125.9, 124.8, 124.8, 115.0, 114.7, 55.6, 37.4, 32.0.

HRMS (ESI) *m/z*: $[M]^+$ calc'd for $[C_{29}H_{27}NO_2]^+$ 421.2042; found 421.2039; difference -0.71 ppm

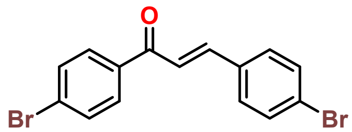


[1]H NMR spectrum (25 °C, THF-d_8) of 2,7-bis(4-methoxyphenyl)-9,9-dimethyl-9,10-dihydroacridine.



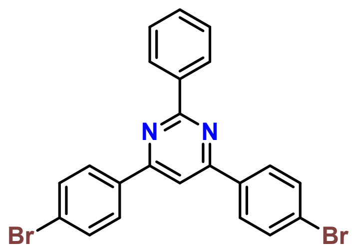
[13]C{[1]H} NMR spectrum (25 °C, THF-d_8) of 2,7-bis(4-methoxyphenyl)-9,9-dimethyl-9,10-dihydroacridine.

(E)-1,3-bis(4-bromophenyl)prop-2-en-1-one



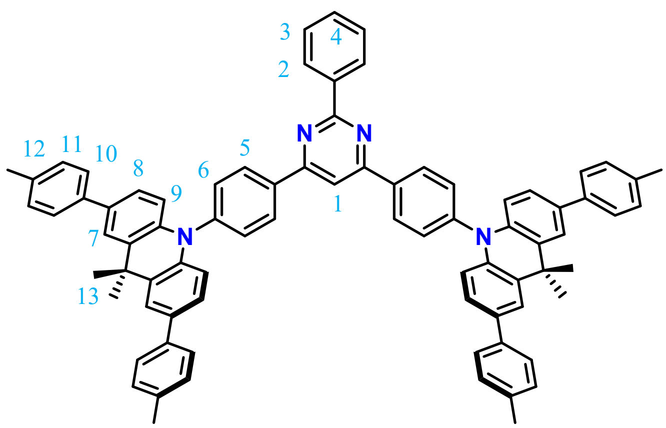
4-bromoacetophenone (5.37 g, 27.0 mmol, 1.00 eq.), 4-bromobenzaldehyde (5.00 g, 27.0 mmol, 1.00 eq.), and powdered sodium hydroxide (2.16 g, 54.0 mmol, 2.00 eq.) were added to a round-bottom flask equipped with a magnetic stir bar. 100 mL ethanol was added and the mixture stirred at room temperature for 24 hours. The flask was then cooled to -25 °C for 1 hour to fully precipitate the product. A white solid was collected by vacuum filtration and washed with water. Yield = 9.19 g (93 %). The spectral data are consistent with literature reports.[4]

4,6-bis(4-bromophenyl)-2-phenylpyrimidine (Pym-Br$_2$)



(E)-1,3-bis(4-bromophenyl)prop-2-en-1-one (1.95 g, 5.32 mmol, 1.00 eq.), benzamidinium hydrochloride (1.00 g, 6.39 mmol, 1.20 eq.), and potassium carbonate (1.84 g, 13.3 mmol, 2.50 eq.) were added to a round bottom flask equipped with a magnetic stir bar. 100 mL of *N,N*-dimethylformamide was added and the mixture was heated to 80 °C for 20 hours with stirring. The mixture was cooled to room temperature and 150 mL of water was added to precipitate the product. A white solid was collected by Buchner filtration and washed with water and ethanol. Yield = 1.73 g (70 %). The spectral data are consistent with literature reports.[5]

PymDMDTA

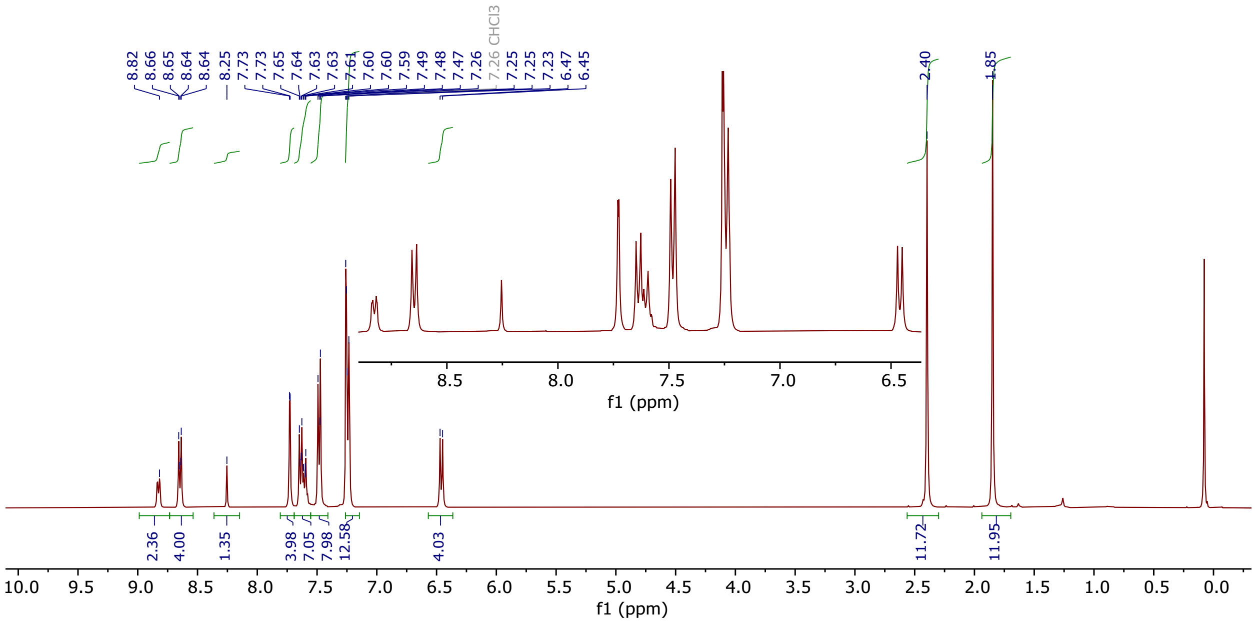


A side-arm flask was charged with DMDTA (200 mg, 0.513 mmol, 2.50 eq.), Pym-Br$_2$ (96 mg, 0.21 mmol, 1.0 eq.), and a magnetic stir bar. The flask was transferred into a nitrogen-filled glovebox and charged with sodium *tert*-butoxide (197 mg, 2.05 mmol, 10.0 eq.), Pd$_2$dba$_3$ (19 mg, 0.021 mmol, 0.10 eq.) and PH^{t}Bu$_3$BF$_4$ (6 mg, 0.02 mmol, 0.1 eq.). The flask was sealed with a rubber septum and transferred to a Schlenk line. Under a positive pressure of N$_2$, a reflux condenser was fitted to the mouth of the flask. 10 mL of dry, degassed toluene was added through the side arm via syringe. The mixture was heated to 120 °C for 16 hours then cooled to room temperature and extracted from water with dichloromethane. Palladium was removed with using a 3-inch plug of silica, eluting with dichloromethane. The solvent was removed, and the crude solid was recrystallized from dichloromethane/ethanol. The resulting yellow solid was collected by vacuum filtration. Yield = 183 mg (82 %)

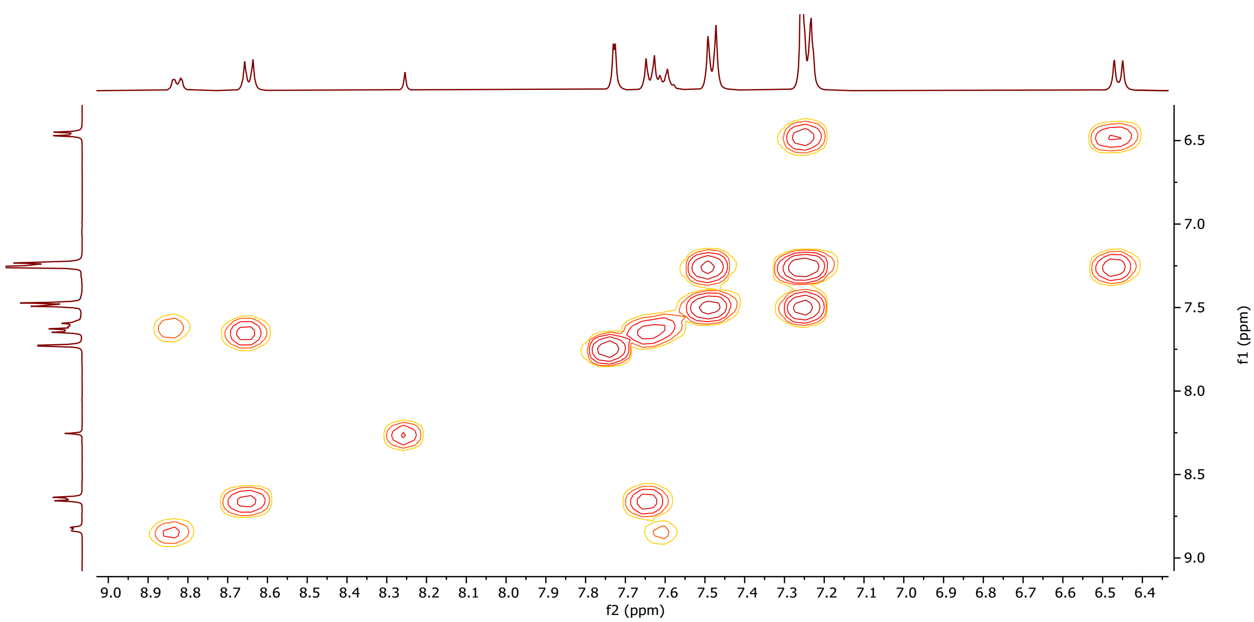
^{1}H NMR (400 MHz, CDCl$_3$) δ 8.83 (dd, 2H, J = 8.1, 2.1 Hz, CH^2), 8.65 (d, J = 8.4 Hz, 4H, CH$^{5/6}$), 8.25 (s, 1H, CH^1), 7.73 (d, J = 2.2 Hz, 4H, CH^7), 7.69 – 7.56 (m, 7H, CH^3, CH^4, and CH$^{5/6}$), 7.48 (d, J = 8.0 Hz, 8H, CH$^{10/11}$), 7.24 (m, 12H, CH^8 and CH$^{10/11}$), 6.46 (d, J = 8.5 Hz, 4H, CH^9), 2.40 (s, 12H, CH^{12}), 1.85 (s, 12H, CH^{13}).

^{13}C NMR (101 MHz, CDCl$_3$) δ 165.1, 164.4, 144.0, 139.8, 138.5, 137.6, 136.4, 134.0, 132.0, 131.2, 130.5, 130.2, 129.6, 129.6, 128.8, 128.7, 126.6, 125.2, 124.5, 114.7, 110.9, 36.5, 32.1, 21.2.

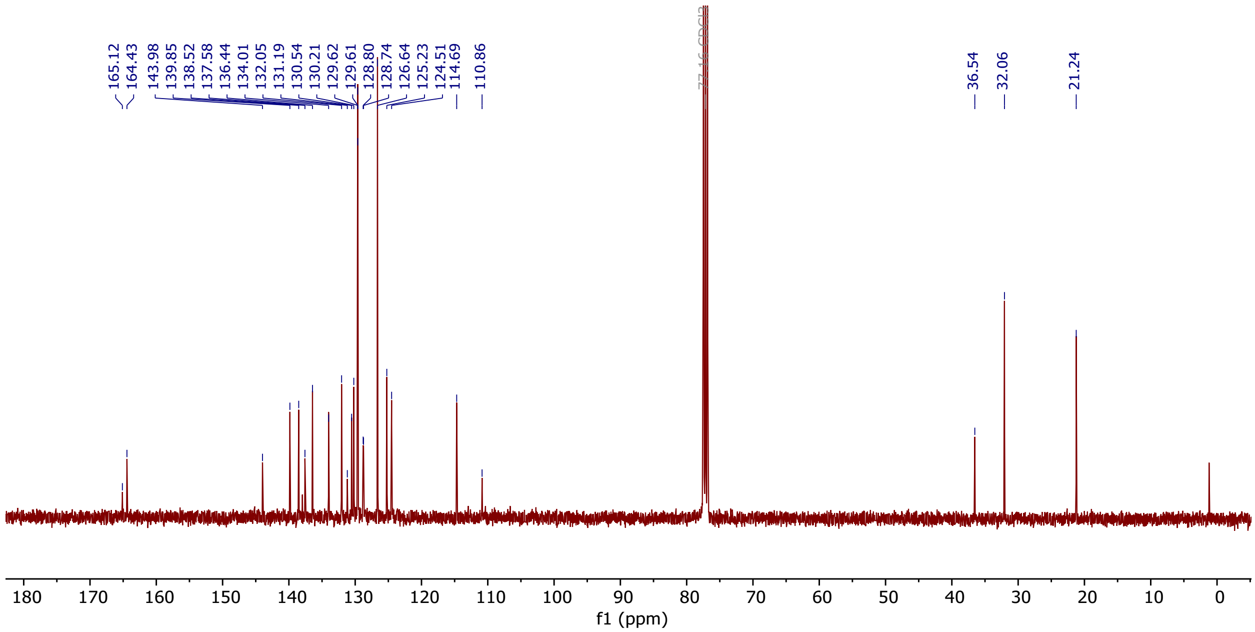
HRMS (ESI) *m/z*: [M]$^+$ calc'd for [C$_{80}$H$_{66}$N$_4$]$^+$ 1082.5287; found 1082.5293; difference 0.50 ppm



[1]H NMR spectrum (25 °C, $CDCl_3$) of **PymDMDTA**.

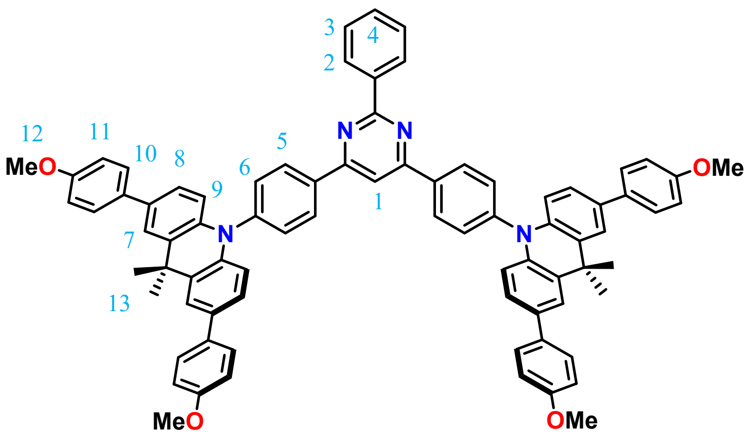


COSY (25 °C, $CDCl_3$) of **PymDMDTA**.



$^{13}C\{^{1}H\}$ NMR spectrum (25 °C, $CDCl_3$) of **PymDMDTA**.

PymDMDMA

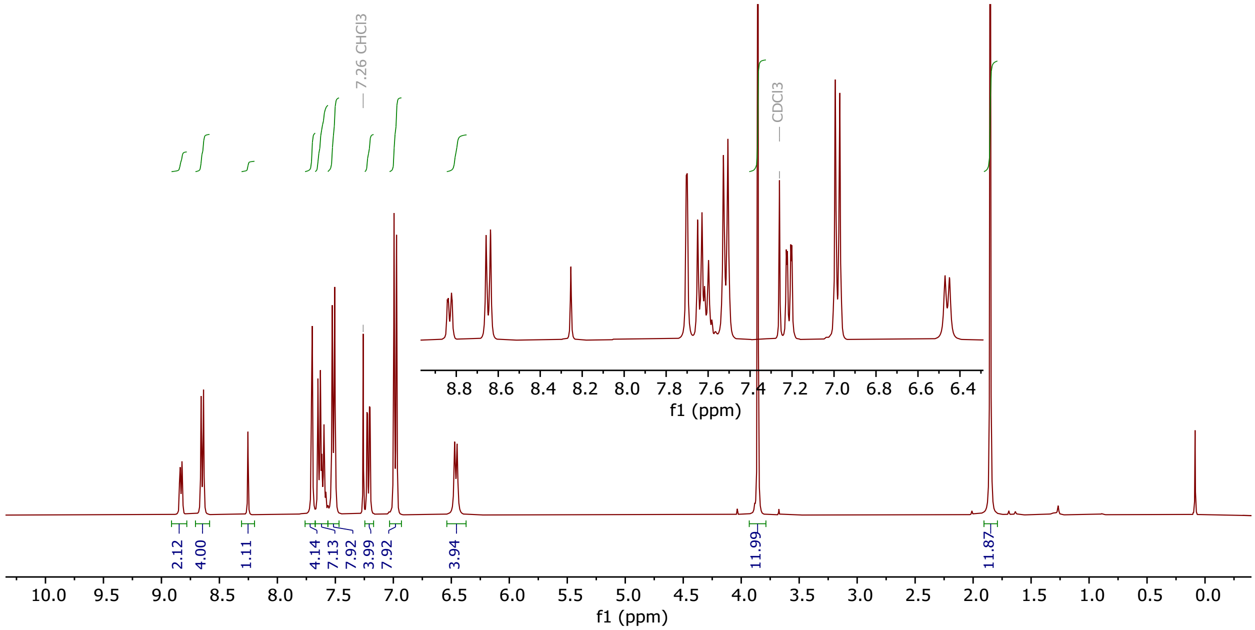


A side-arm flask was charged with DMDMA (250 mg, 0.590 mmol, 2.50 eq.), Pym-Br_2 (111 mg, 0.240 mmol, 1.00 eq.), and a magnetic stir bar. The flask was transferred into a nitrogen-filled glovebox and charged with sodium *tert*-butoxide (231 mg, 2.40 mmol, 10.0 eq.), Pd_2dba_3 (22 mg, 0.024 mmol, 0.10 eq.) and $PH^{t}Bu_3BF_4$ (7 mg, 0.02 mmol, 0.1 eq.). The flask was sealed with a rubber septum and transferred to a Schlenk line. Under a positive pressure of N_2, a reflux condenser was fitted to the mouth of the flask. 10 mL of dry, degassed toluene was added through the side arm via syringe. The mixture was heated to 120 °C for 16 hours then cooled to room temperature and extracted from water with dichloromethane. Palladium was removed with using a 3-inch plug of silica, eluting with dichloromethane. The solvent was removed, and the crude solid was recrystallized from dichloromethane/ethanol. The resulting yellow solid was collected by vacuum filtration. Yield = 207 mg (76 %).

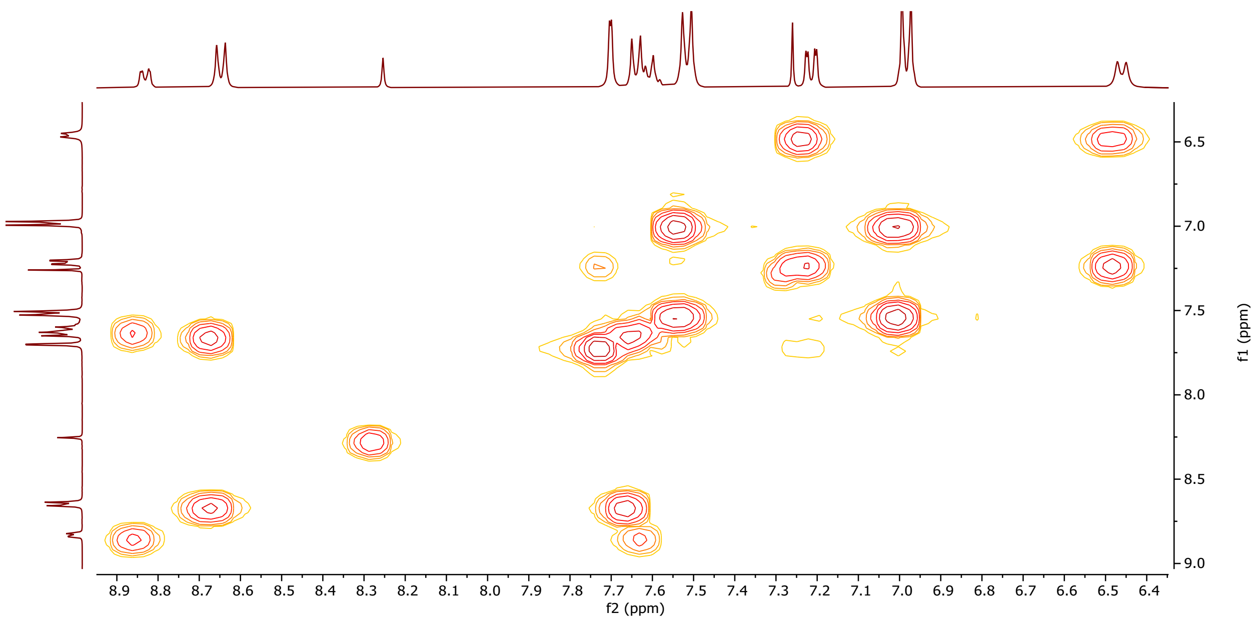
^{1}H NMR (400 MHz, CDCl$_3$) δ 8.85 (dd, 2H, J = 8.1, 2.1 Hz, CH^{2}), 8.65 (d, J = 8.3 Hz, 4H, $CH^{5/6}$), 8.25 (s, 1H, CH^{1}), 7.70 (d, J = 2.2 Hz, 4H, CH^{7}), 7.67 – 7.56 (m, 7H, CH^{3}, CH^{4}, and $CH^{5/6}$), 7.52 (d, J = 8.8 Hz, 8H, $CH^{10/11}$), 7.21 (dd, J = 8.6, 2.1 Hz, 4H, CH^{8}), 6.98 (d, J = 8.8 Hz, 8H, $CH^{10/11}$), 6.46 (d, J = 8.5 Hz, 4H, CH^{9}), 3.86 (s, 12H, CH^{12}), 1.85 (s, 12H, CH^{13}).

^{13}C NMR (101 MHz, CDCl$_3$) δ 165.1, 164.4, 158.8, 144.0, 139.6, 137.9, 137.5, 134.0, 133.7, 132.0, 131.2, 130.5, 130.2, 128.8, 128.7, 127.8, 125.0, 124.2, 114.7, 114.4, 110.8, 55.5, 36.5, 32.0.

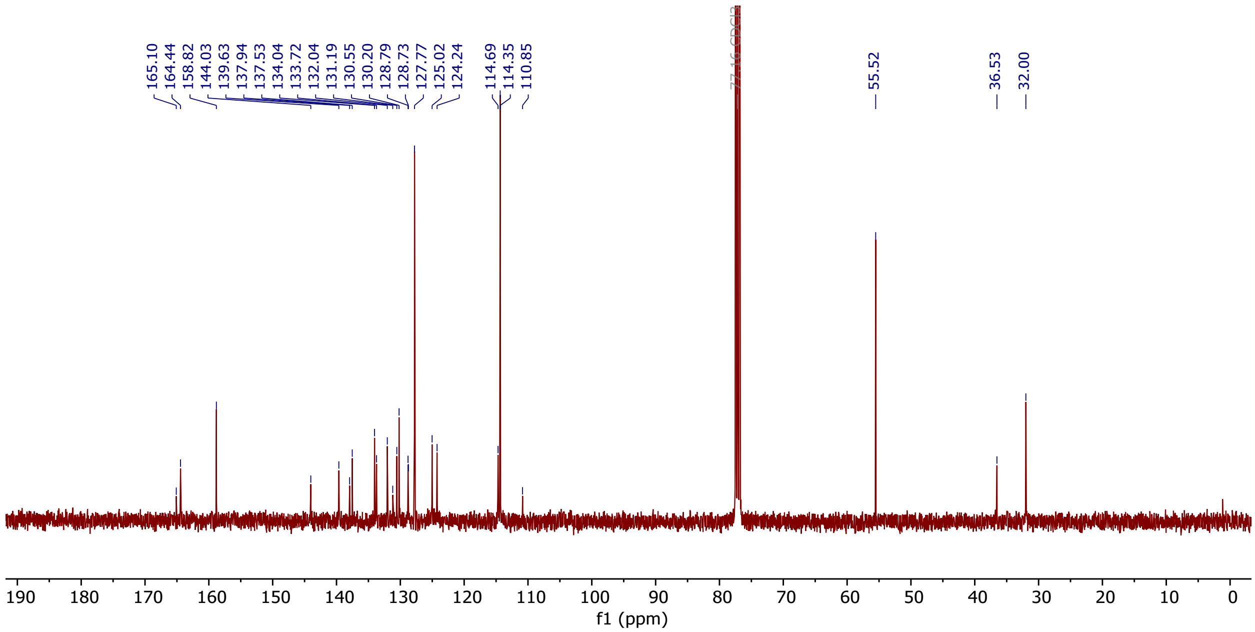
HRMS (ESI) *m/z*: $[M]^{+}$ calc'd for $[C_{80}H_{66}N_4O_4]^{+}$ 1146.5084; found 1146.5103; difference 1.68 ppm



^{1}H NMR spectrum (25 °C, $CDCl_3$) of **PymDMDMA**.

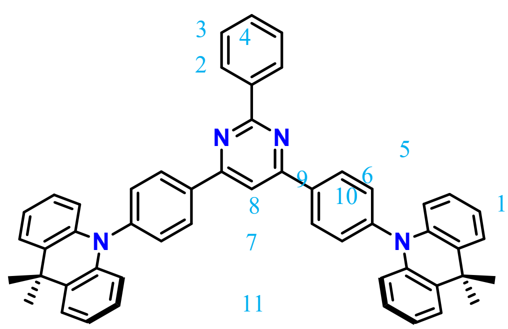


COSY (25 °C, $CDCl_3$) of **PymDMDMA**.



$^{13}C\{^1H\}$ NMR spectrum (25 °C, $CDCl_3$) of **PymDMDMA**.

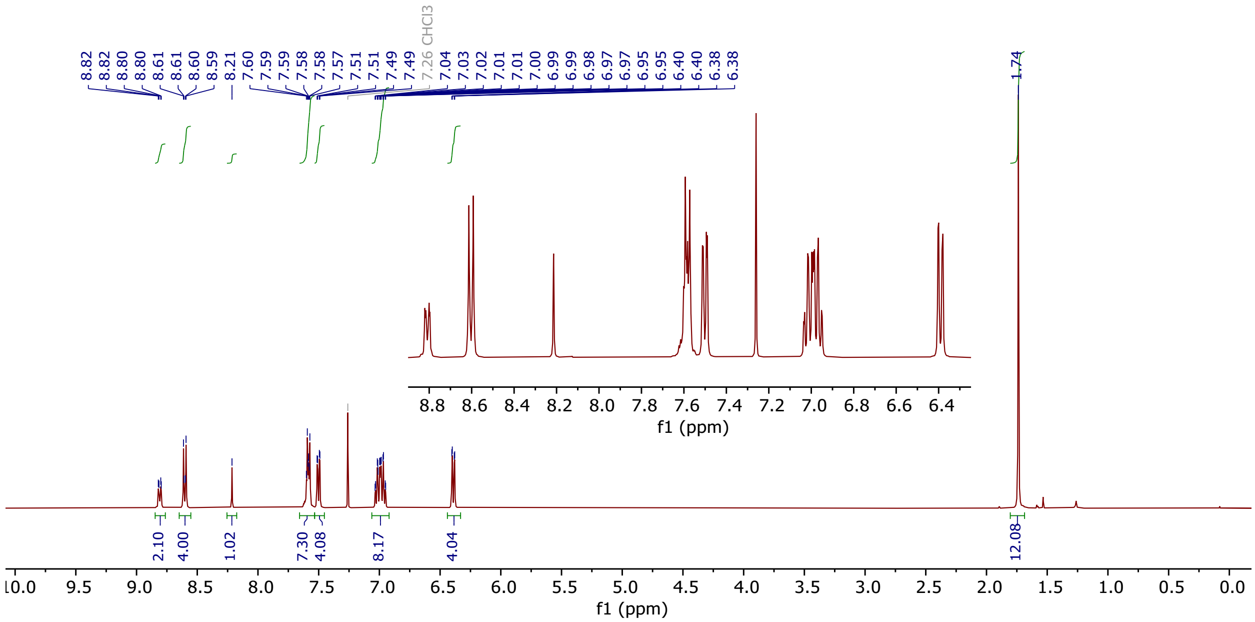
PymDMA



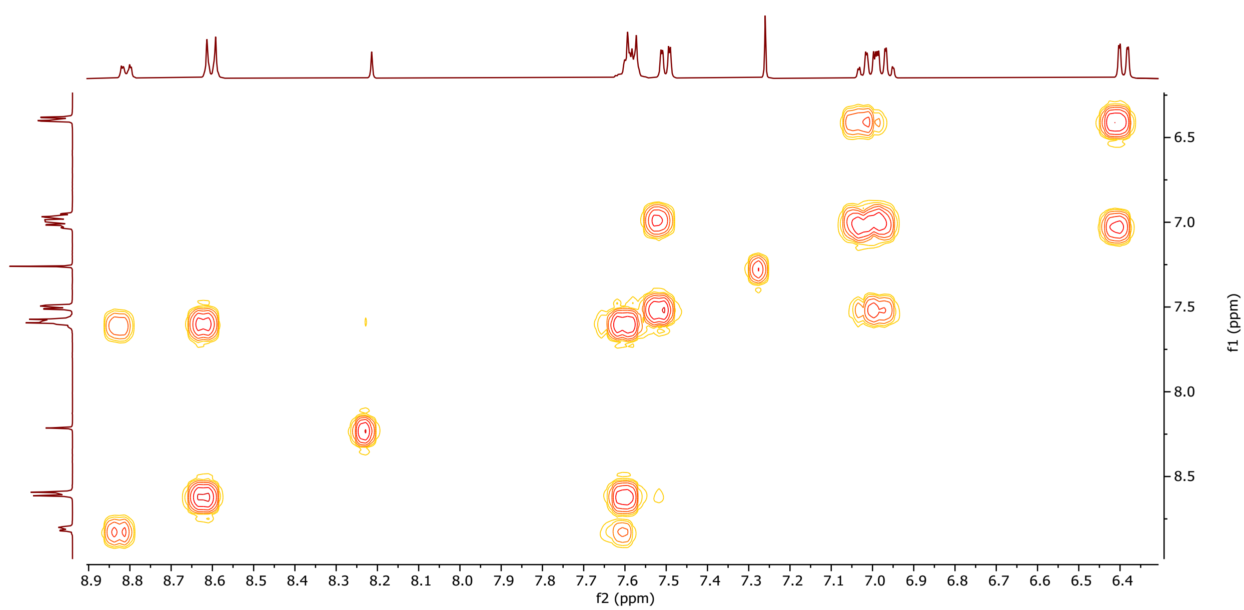
A side-arm flask was charged with 9,9-dimethyl-9,10-dihydroacridine (404 mg, 1.93 mmol, 3.00 eq.), Pym-Br_2 (300 mg, 0.644 mmol, 1.00 eq.), and a magnetic stir bar. The flask was transferred into a nitrogen-filled glovebox and charged with sodium *tert*-butoxide (619 mg, 6.44 mmol, 10.0 eq.), Pd_2dba_3 (59 mg, 0.064 mmol, 0.10 eq.) and $PH^tBu_3BF_4$ (19 mg, 0.064 mmol, 0.10 eq.). The flask was sealed with a rubber septum and transferred to a Schlenk line. Under a positive pressure of N_2, a reflux condenser was fitted to the mouth of the flask. 10 mL of dry, degassed toluene was added through the side arm via syringe. The mixture was heated to 120 °C for 48 hours then cooled to room temperature and extracted from water with dichloromethane. Palladium was removed with using a 3-inch plug of silica, eluting with dichloromethane. The solvent was removed, and the crude solid was recrystallized from dichloromethane/ethanol. The resulting pale yellow solid was collected by vacuum filtration. Yield = 345 mg (74%). The characterization data match earlier reports.[6]

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.81 (dd, J = 7.8, 1.9 Hz, 2H, CH^{2}), 8.60 (d, J = 8.4 Hz, 4H, CH$^{5/6}$), 8.21 (s, 1H, CH^{1}), 7.65 – 7.54 (m, 7H, CH^{3}, CH^{4}, and CH$^{5/6}$), 7.50 (dd, J = 7.5, 1.8 Hz, 4H, CH^{7}), 7.06 – 6.92 (m, 8H, CH$^{8/9}$), 6.39 (dd, J = 8.0, 1.5 Hz, 4H, CH^{10}), 1.74 (s, 12H, CH^{11}).

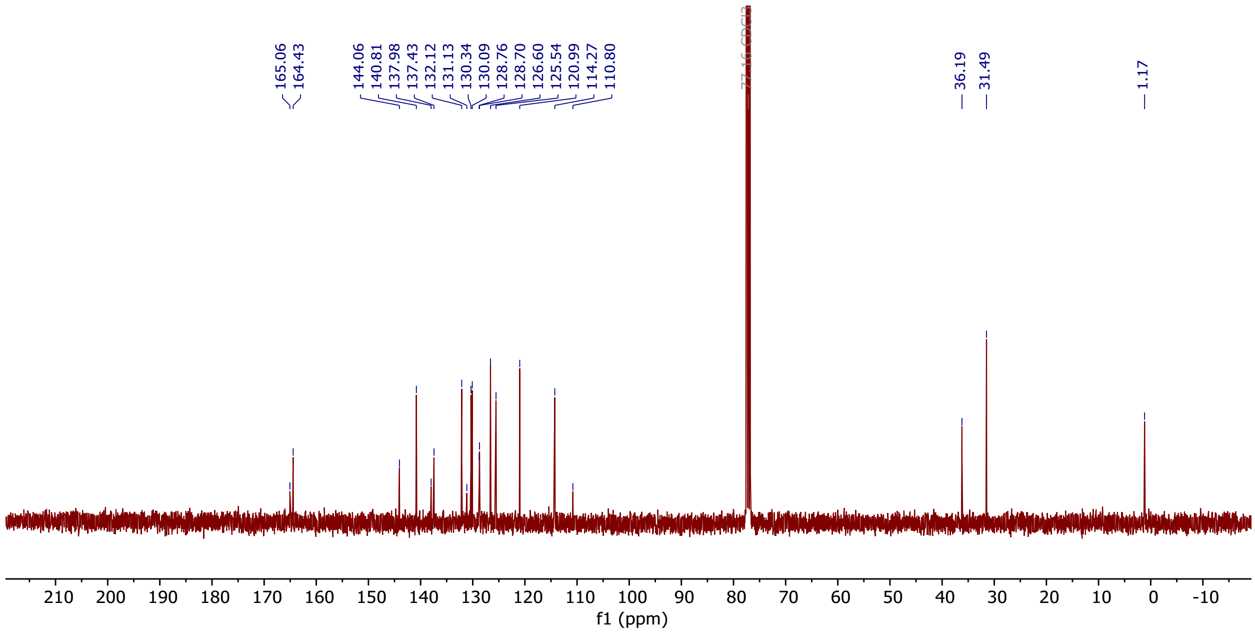
^{13}C NMR (101 MHz, $CDCl_3$) δ 165.1, 164.4, 144.1, 140.8, 138.0, 137.4, 132.1, 131.1, 130.3, 130.1, 128.8, 128.7, 126.6, 125.5, 121.0, 114.3, 110.8, 36.2, 31.5, 1.2.



^{1}H NMR spectrum (25 °C, $CDCl_3$) of **PymDMA**.



COSY (25 °C, $CDCl_3$) of **PymDMA**.



$^{13}C\{^{1}H\}$ NMR spectrum (25 °C, $CDCl_3$) of **PymDMA**.

S3 – Ph

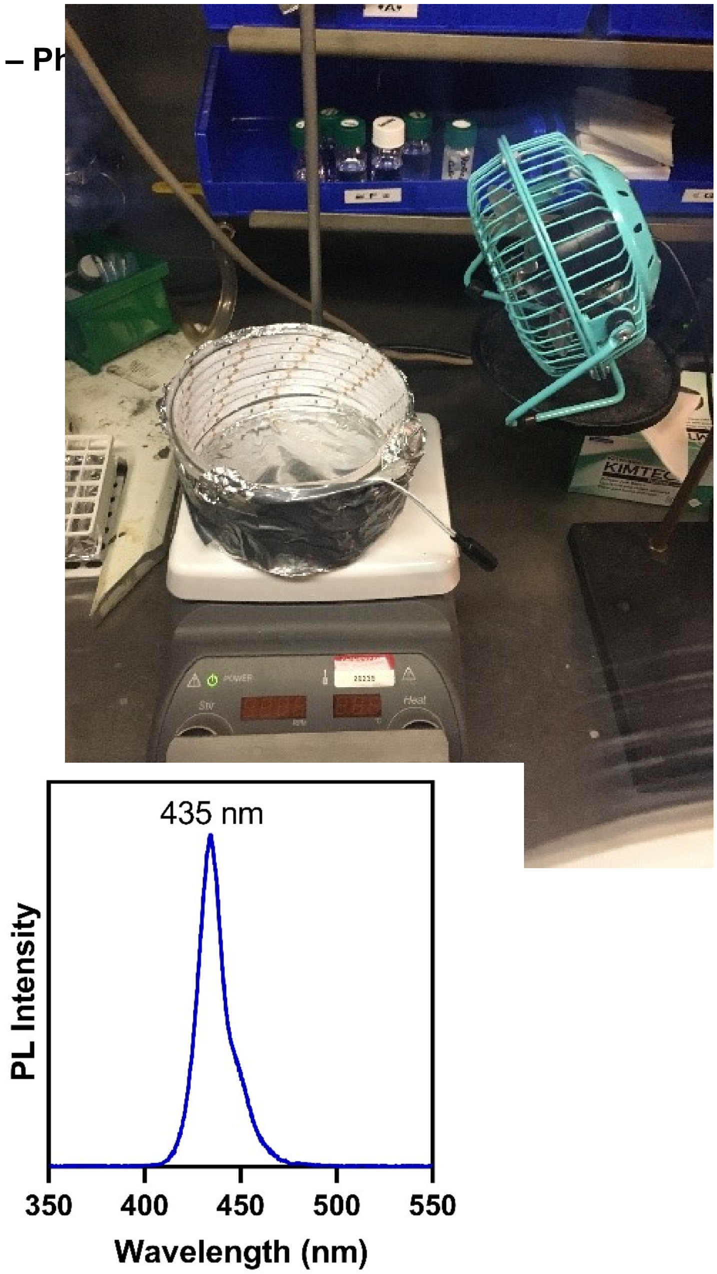


Fig. S1 Photograph of the photopolymerization setup used and emission spectrum of the LED.

S4 – Additional Data

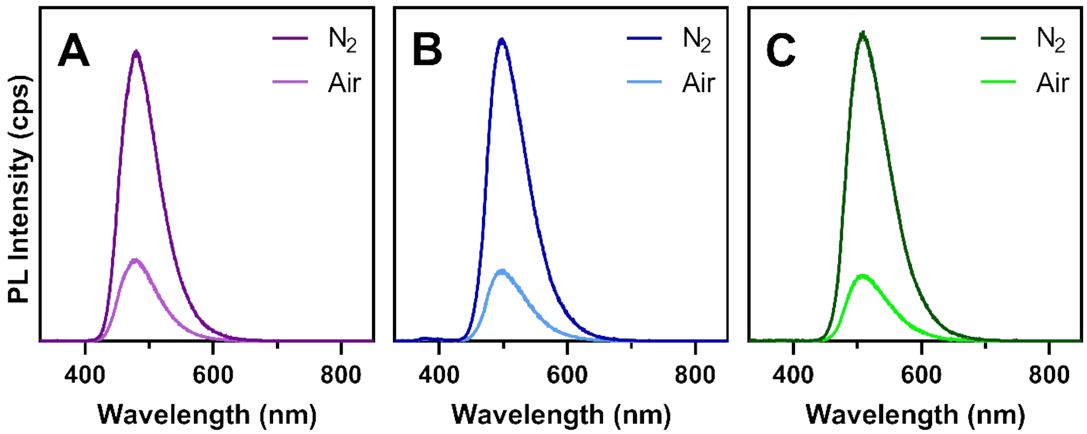


Fig. S2 Photoluminscence spectra of (A) **PymDMA** (B) **PymDMDTA** and (C) **PymDMDMA** in toluene (2 µg mL^{-1}) under N_2- or air-sparged conditions.

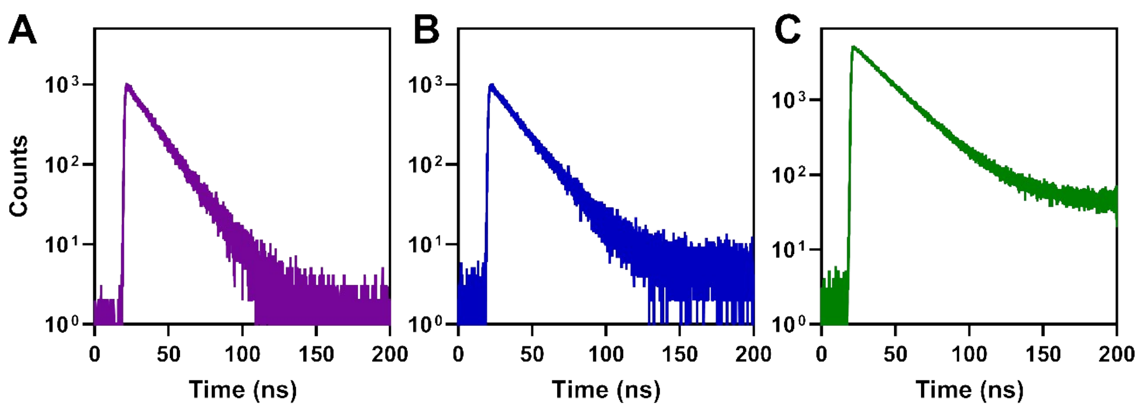


Fig. S3 Prompt fluorescence decays of (A) **PymDMA** (B) **PymDMDTA**, and (C) **PymDMDMA** in degassed toluene at 2 µg mL^{-1}. Excited at 313 nm and emission collected at the emission maxima (A – 485 nm, B – 505 nm, C – 515 nm).

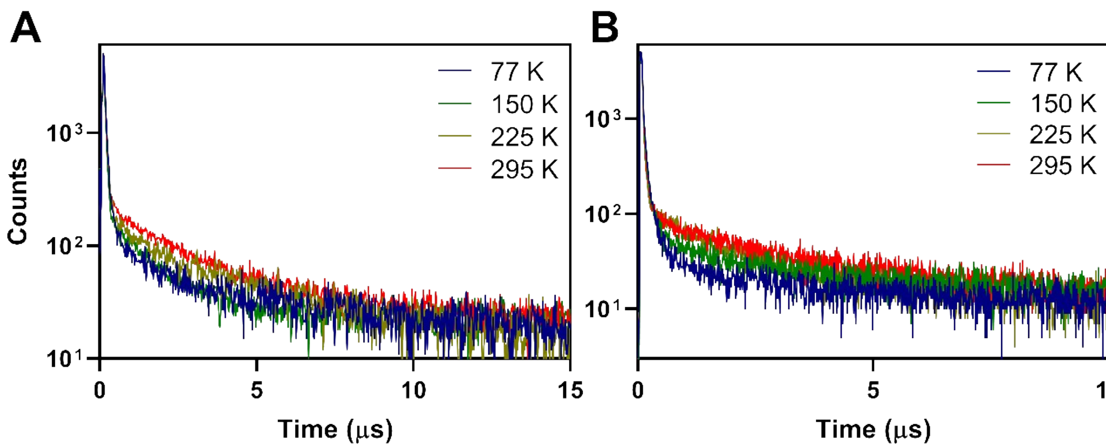


Fig. S4 Temperature dependence of the transient photoluminescence decays of (A) **PymDMDTA** and (B) **PymDMDMA** at 10 wt% in PMMA. Samples were excited at 380 nm and their decays recorded at 530 nm

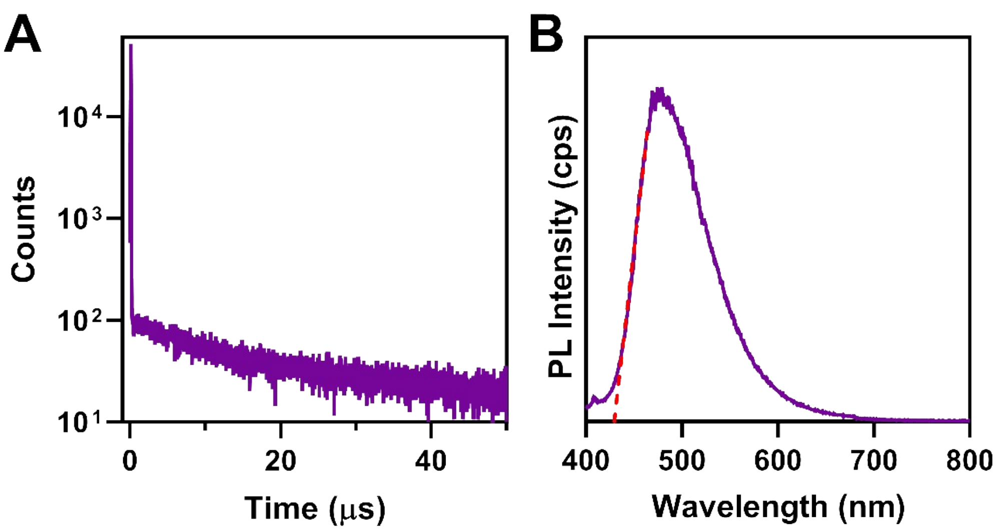


Fig. S5 (A) Delayed fluorescence decay of **PymDMA** in toluene in degassed toluene at 2 μg mL^{-1}. Excited at 313 nm and emission collected at 485 nm. (B) Photoluminescence spectrum of **PymDMA** in 2-MeTHF at 77 K excited at 365 nm.

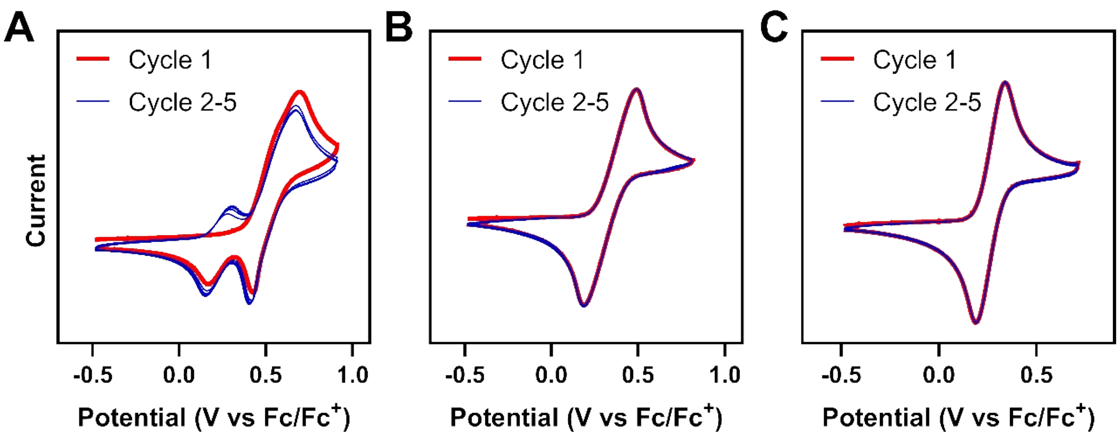


Fig. S6 First five cycles of CV for (A) **PymDMA** (B) **PymDMDTA** and (C) **PymDMDMA** at 4 mM in $CHCl_3$. 200 mM ($^{n}Bu_4N)PF_6$ was used as supporting electrolyte. Scan rate 20 mV/s.

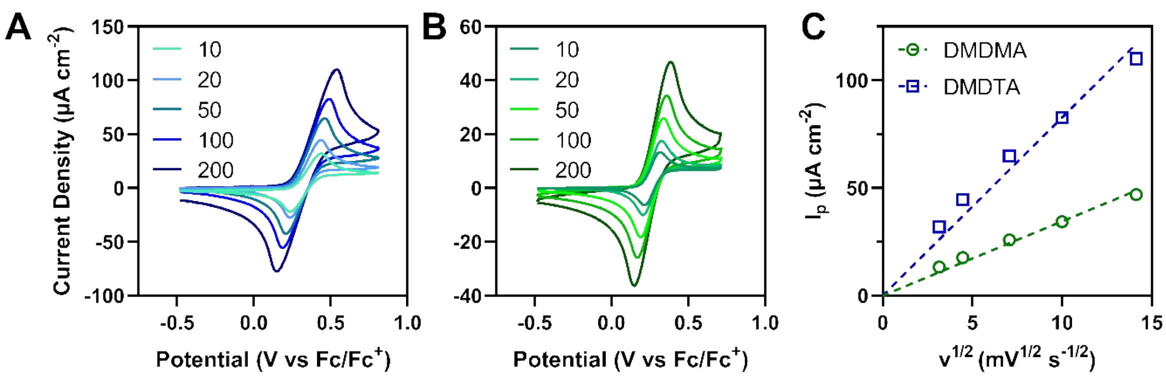


Fig. S7 Cyclic voltammograms of (A) **PymDMDTA** and (B) **PymDMDMA** at scan rates of 10, 20, 50, 100, and 200 mV s^{-1} recorded at 4 mM in $CHCl_3$. 200 mM ($^{n}Bu_4N)PF_6$ was used as supporting electrolyte. (C) Randles–Ševčík plot of peak anodic current against the square root of the potential scan rate.

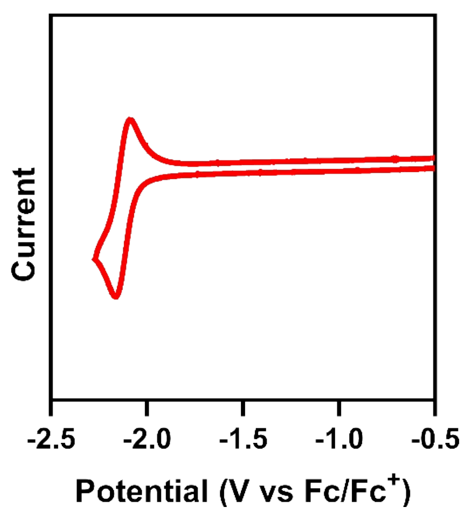


Fig. S8 CV of 2,4,6-triphenylpyrimidine (4 mM) in DMF. 200 mM ($^{n}Bu_4N)PF_6$ was used as supporting electrolyte. Scan rate 20 mV/s.

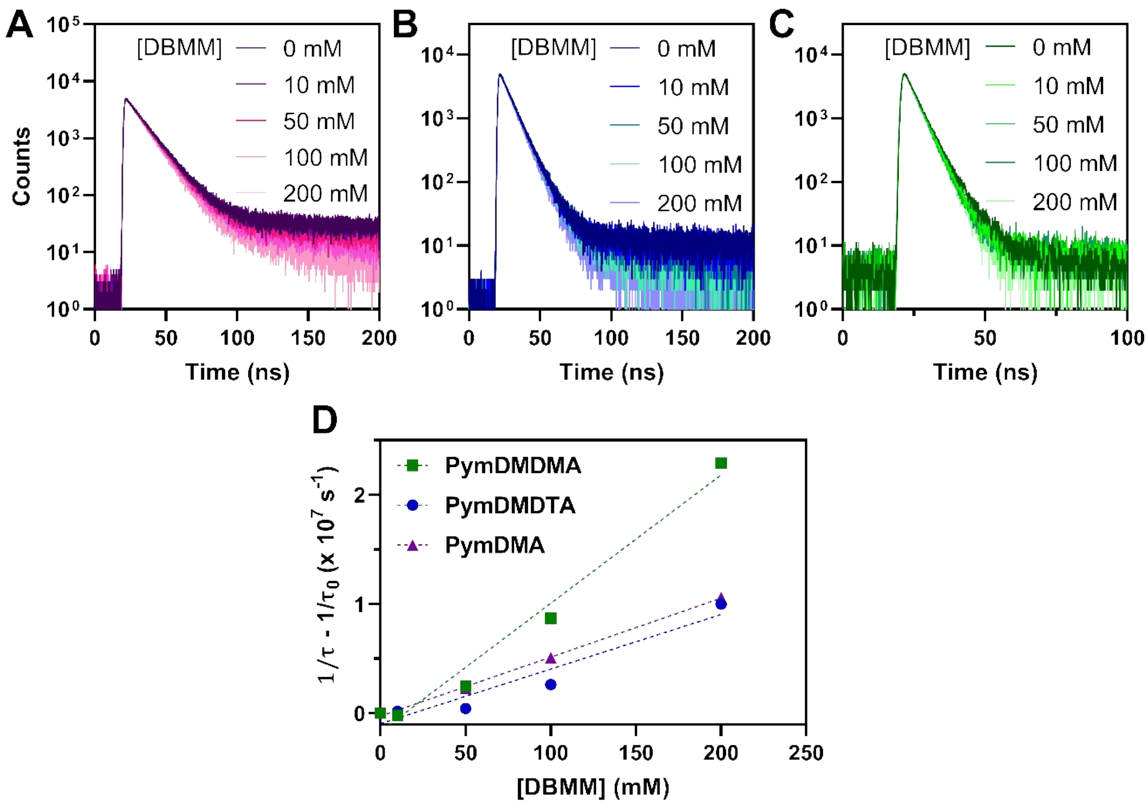


Fig. S9 Prompt fluorescence decays of (A) **PymDMA**, (B) **PymDMDTA**, and (C) **PymDMDMA** dissolved in DMAC (100 µM; degassed by three freeze-pump-thaw cycles) with the presence of varying amounts of DBMM initiator. Excited at 380 nm and emission collected at 600 nm. (D) Stern-Volmer plot of the change in prompt fluorescence lifetime as a function of DBMM concentration.

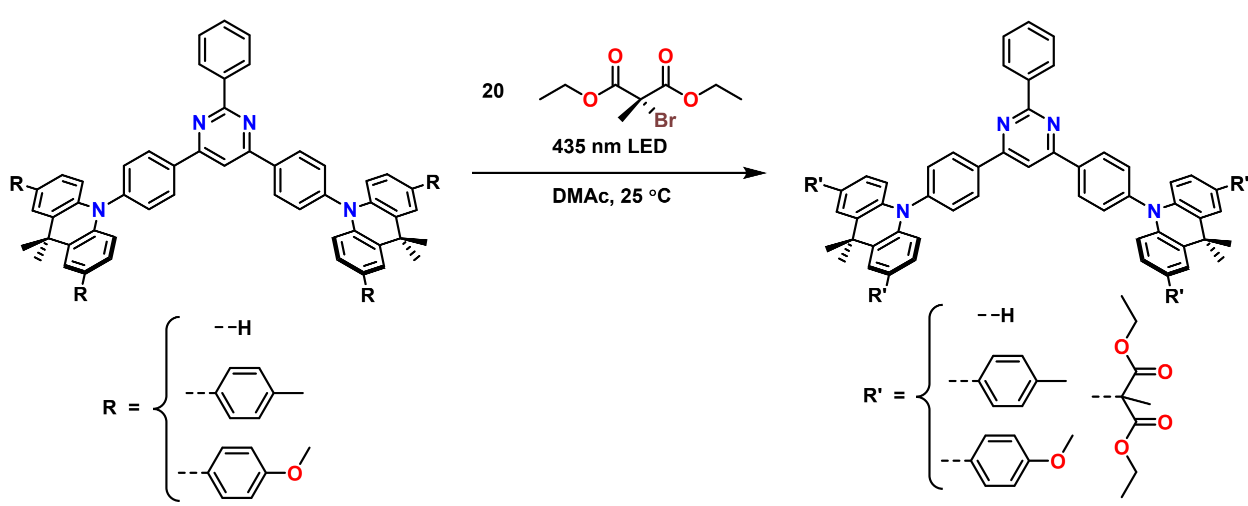


Fig. S10 Photosubstitution experiments of **PymDMA**, **PymDMDTA**, and **PymDMDMA** in DMAc with DBMM as a radical alkylation agent. Conditions: 10 mg PC, 2 mL DMAc, 900 rpm stir speed. 500 µL aliquots were removed every 2 hours and extracted from CH_2Cl_2/H_2O prior to NMR analysis.

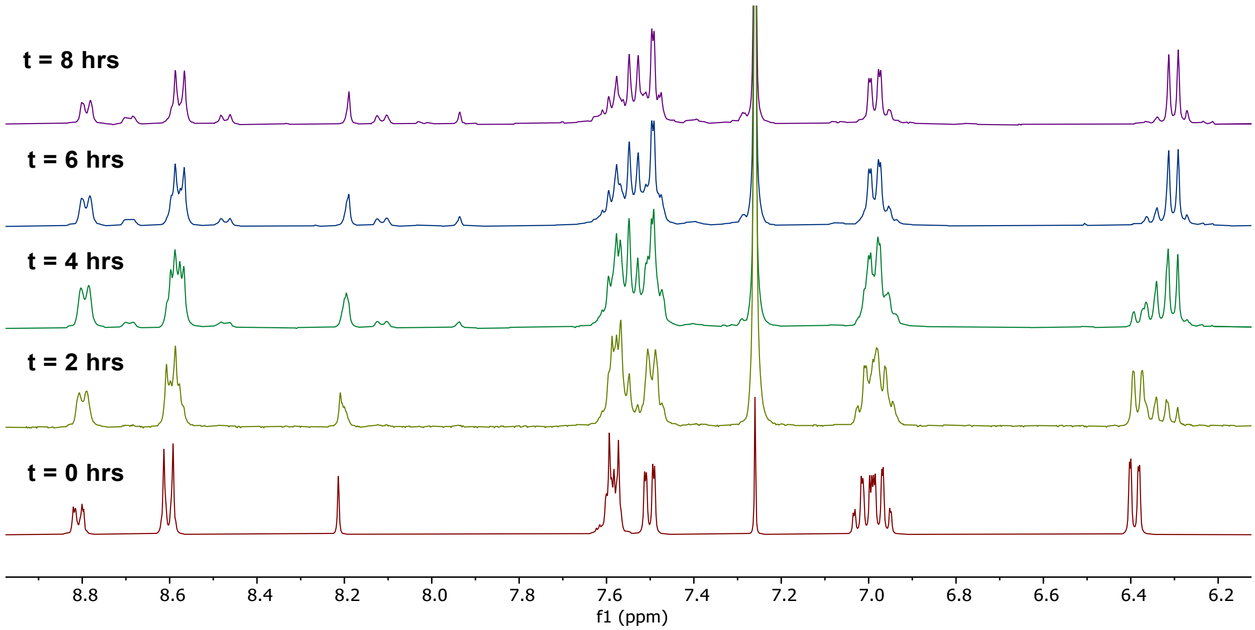


Fig. S11 Evolution of the aromatic portion of the ^{1}H NMR spectrum of **PymDMA** ($CDCl_3$, 25 °C) upon irradiation with 435 nm light in the presence of DBMM.

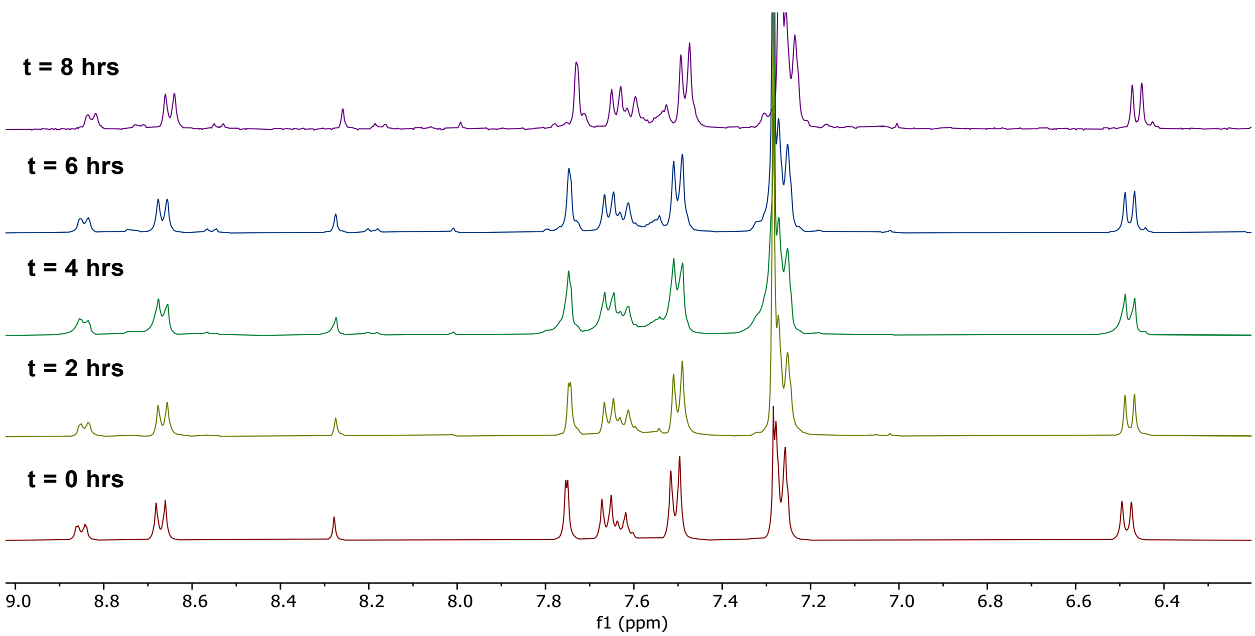


Fig. S12 Evolution of the aromatic portion of the ^{1}H NMR spectrum of **PymDMDTA** ($CDCl_3$, 25 °C) upon irradiation with 435 nm light in the presence of DBMM.

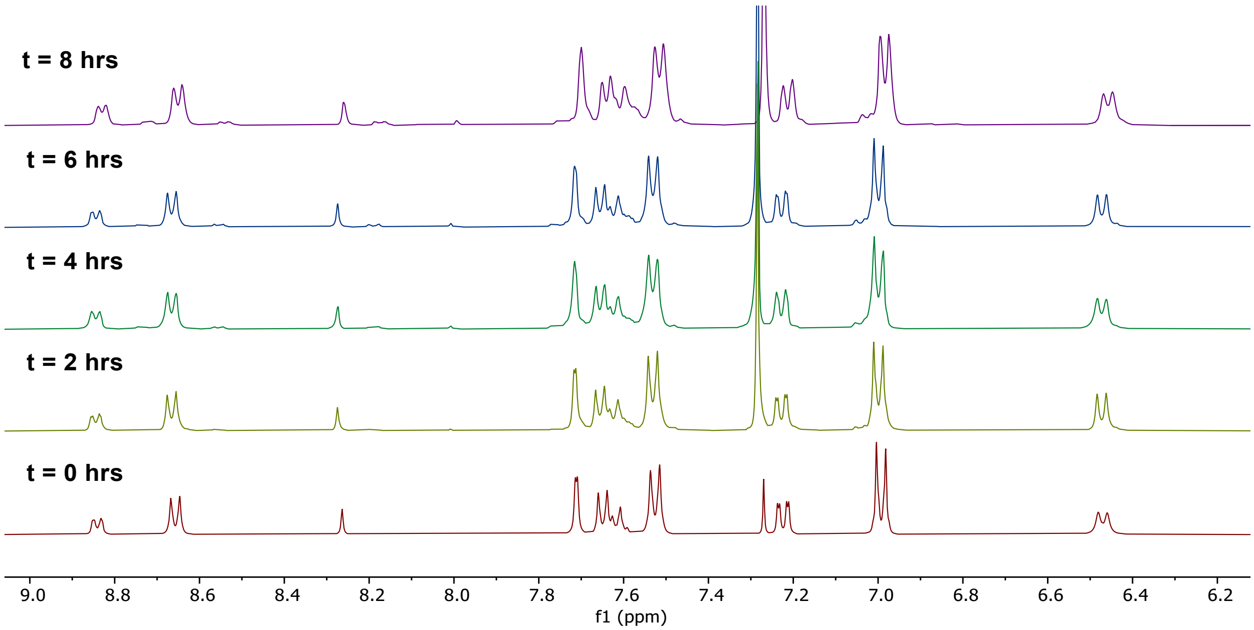


Fig. S13 Evolution of the aromatic portion of the [1]H NMR spectrum of **PymDMDMA** ($CDCl_3$, 25 °C) upon irradiation with 435 nm light in the presence of DBMM.

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S5 – Polymer Characterization

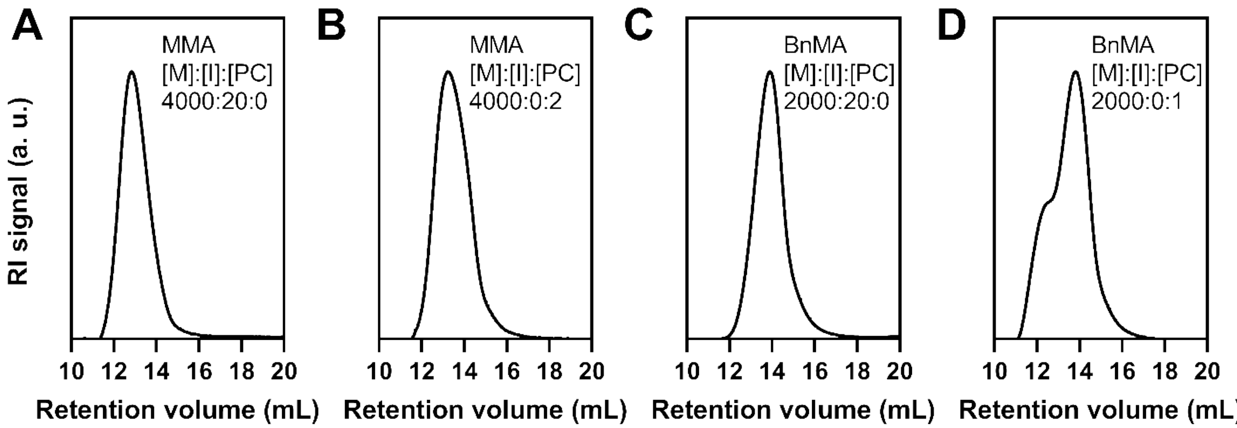

Fig. S14 RI chromatograms of control polymerization experiments with MMA and BnMA, corresponding to the first four entries of Tab. 4 in the main text.

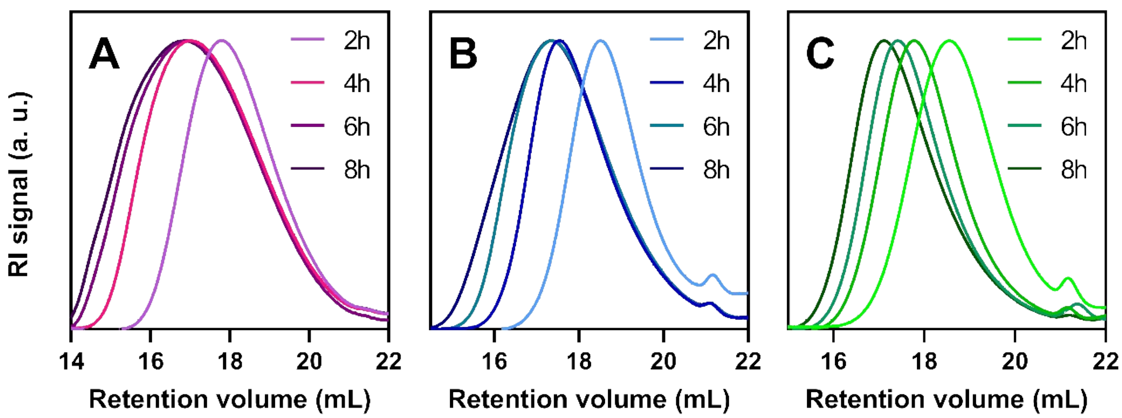

Fig. S15 RI Chromatograms of PMMA prepared using 500 ppm of photocatalysts (A) **PymDMA**, (B) **PymDMDTA**, and (C) **PymDMDMA** taken from the reaction mixture 2, 4, 6, and 8 hours after initiation.

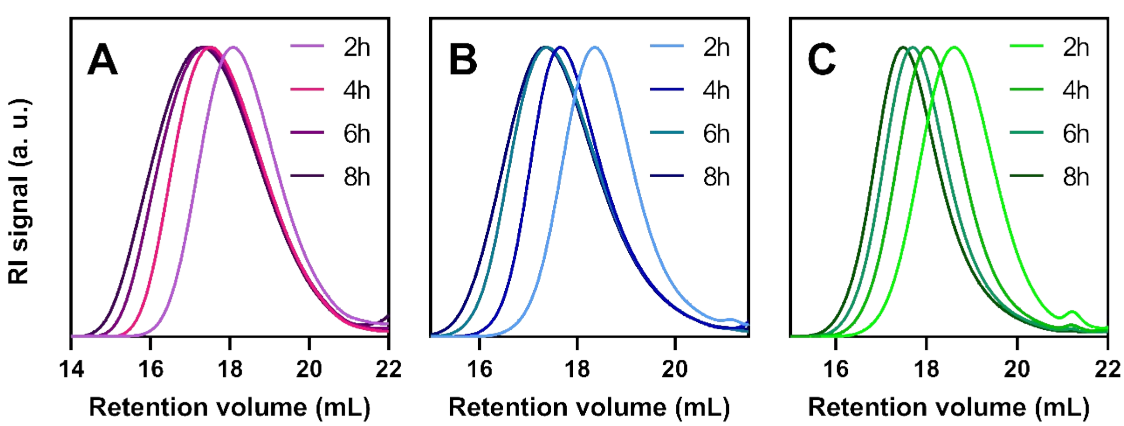

Fig. S16 RI Chromatograms of p(BnMA) prepared using 500 ppm of photocatalysts (A**) PymDMA**, (B) **PymDMDTA**, and (C) **PymDMDMA** taken from the reaction mixture 2, 4, 6, and 6 hours after initiation.

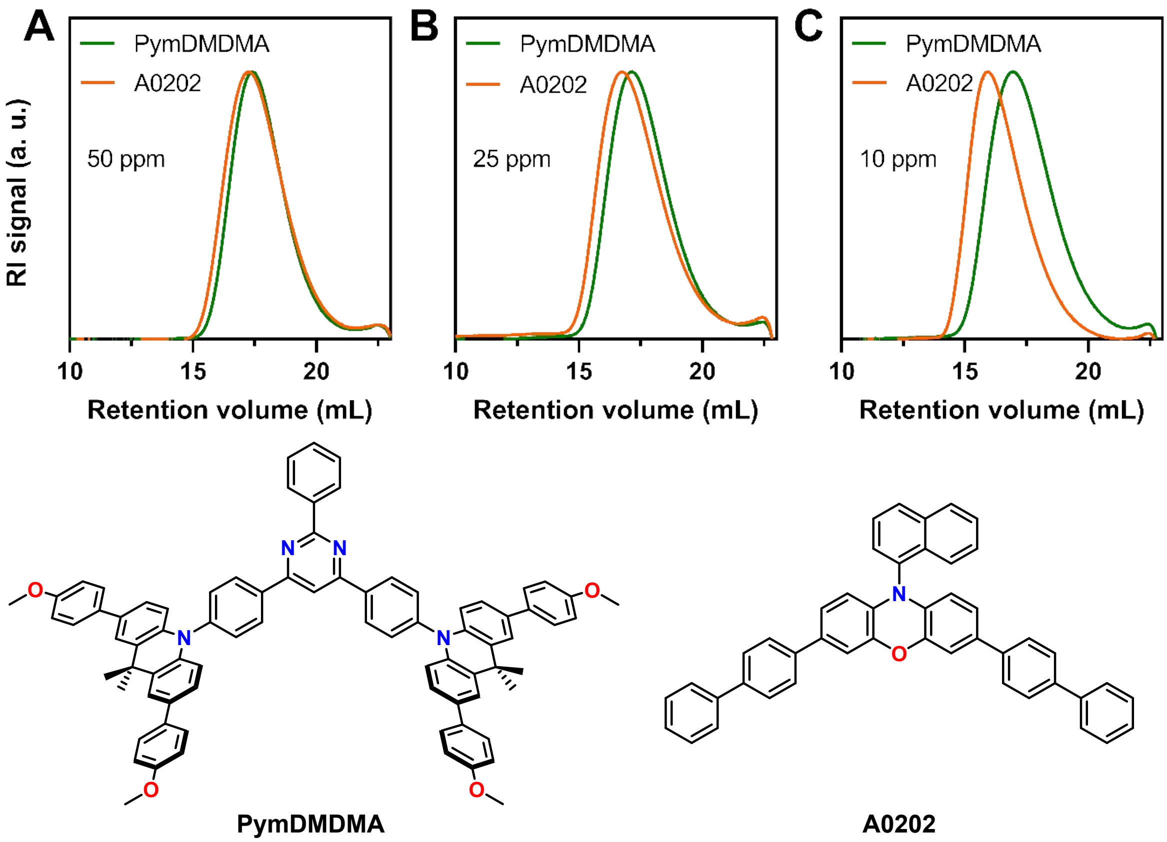

Fig. S17 RI chromatograms of PMMA prepared using (A) 50 ppm, (B) 25 ppm, and (C) 10 ppm (relative to monomer) of the photocatalysts **PymDMDMA** and **Phenox O-PC A0202** (structures below).

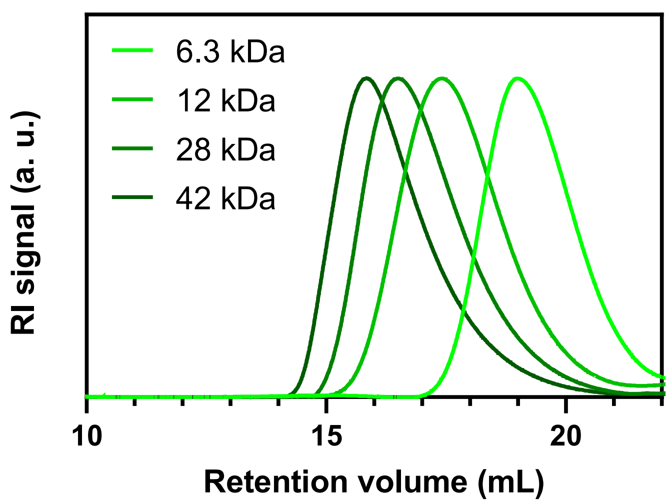

Fig. S18 RI chromatograms of PMMA at molecular weights between 6 and 42 kDa prepared with 50 ppm **PymDMDMA**.

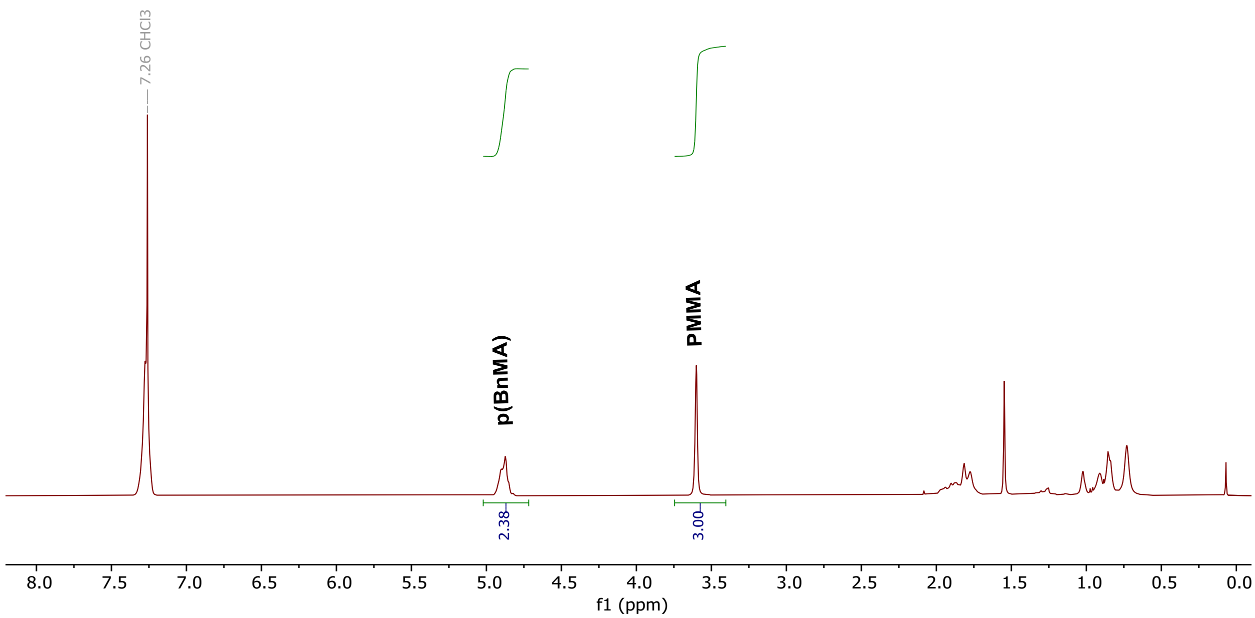

Fig. S19 ^{1}H NMR spectrum (25 °C, $CDCl_3$) of PMMA-*b*-p(BnMA).

S6 – Density Functional Theory Optimized Structures

Cartesian coordinates (Å) for the optimized structures of **PymDMA**.

PymDMA (S_0)				PymDMA (T_1)				PymDMA$^{\bullet+}$			
H	-6.80E-05	-0.20735	-0.03122	H	-0.03925	-0.23448	-0.05539	H	-1.80E-05	-0.26723	-0.03116
C	-3.50E-05	0.867236	0.097964	C	-0.0134	0.833342	0.118859	C	-1.00E-05	0.807211	0.10124
C	1.198591	1.580521	0.21697	C	1.226694	1.525235	0.262026	C	1.195803	1.524764	0.223754
N	1.191505	2.899989	0.463576	N	1.205878	2.87577	0.524685	N	1.190281	2.841591	0.470113
C	-1.60E-05	3.50688	0.582772	C	0.027115	3.469179	0.63915	C	-7.00E-06	3.455172	0.588492
N	-1.19155	2.900012	0.463603	N	-1.18844	2.878479	0.514766	N	-1.1903	2.841592	0.470133
C	-1.19864	1.580543	0.216986	C	-1.19447	1.551364	0.242377	C	-1.19582	1.524765	0.223769
C	-2.00E-06	4.967486	0.858692	C	0.018481	4.93124	0.931363	C	-4.00E-06	4.912607	0.86082
C	1.209631	5.66768	0.989856	C	1.218678	5.624335	1.153985	C	1.210461	5.612958	0.990499
H	2.14235	5.126266	0.8808	H	2.151823	5.07428	1.109882	H	2.144483	5.073745	0.882645
C	1.207939	7.035883	1.250927	C	1.208294	6.98981	1.427519	C	1.20852	6.981162	1.24881
H	2.151236	7.566415	1.349984	H	2.146035	7.512377	1.599741	H	2.150981	7.512628	1.346912
C	1.40E-05	7.724762	1.383427	C	-0.0014	7.687711	1.481457	C	-2.00E-06	7.669514	1.379892
H	2.00E-05	8.792459	1.586724	H	-0.00864	8.753752	1.694576	H	-1.00E-06	8.737236	1.581089
C	-1.20792	7.035889	1.250966	C	-1.20007	7.007128	1.259446	C	-1.20853	6.98116	1.24883
H	-2.15121	7.566427	1.350055	H	-2.14541	7.542638	1.297549	H	-2.15099	7.512626	1.346949
C	-1.20963	5.667688	0.989895	C	-1.1917	5.639932	0.987375	C	-1.21047	5.612956	0.990519
H	-2.14235	5.126276	0.880869	H	-2.11648	5.103031	0.810789	H	-2.14449	5.073741	0.882681
C	-2.52704	0.923325	0.104302	C	-2.52757	0.906313	0.114853	C	-2.53011	0.873807	0.113304
C	-2.69131	-0.29926	-0.56638	C	-2.7085	-0.30444	-0.57481	C	-2.70596	-0.34626	-0.55793
H	-1.84351	-0.77651	-1.04824	H	-1.86592	-0.78133	-1.06644	H	-1.86385	-0.83324	-1.03916
C	-3.9442	-0.90116	-0.65553	C	-3.96652	-0.89382	-0.67113	C	-3.96478	-0.93643	-0.65021
H	-4.06869	-1.84202	-1.18291	H	-4.09958	-1.82579	-1.21273	H	-4.09773	-1.87522	-1.17901
C	-5.05983	-0.29235	-0.07245	C	-5.07721	-0.2824	-0.08082	C	-5.06683	-0.30796	-0.06688
C	-4.90791	0.92903	0.592842	C	-4.91247	0.92853	0.599246	C	-4.91177	0.90923	0.601618
H	-5.77767	1.397717	1.043443	H	-5.77771	1.401936	1.054397	H	-5.77551	1.389565	1.051201
C	-3.65632	1.532019	0.67536	C	-3.65422	1.51732	0.690691	C	-3.65215	1.495053	0.68519
H	-3.53393	2.479891	1.186998	H	-3.52096	2.458187	1.212376	H	-3.51966	2.441869	1.195672
C	2.526988	0.9233	0.104259	C	2.494499	0.892146	0.14879	C	2.53009	0.873809	0.113277
C	2.691215	-0.29944	-0.56617	C	2.657505	-0.52486	-0.12676	C	2.705924	-0.34632	-0.55785
H	1.843368	-0.77683	-1.0478	H	1.784024	-1.14589	-0.29004	H	1.863803	-0.83336	-1.03899
C	3.944099	-0.90133	-0.65534	C	3.891871	-1.1031	-0.20824	C	3.964749	-0.93649	-0.65014
H	4.06854	-1.84231	-1.18252	H	3.985328	-2.16088	-0.43734	H	4.097679	-1.87532	-1.17886
C	5.059801	-0.29235	-0.07255	C	5.082612	-0.31914	-0.06245	C	5.066822	-0.30795	-0.06692
C	4.907936	0.929172	0.592479	C	4.94837	1.087956	0.190482	C	4.911775	0.909297	0.601479
H	5.77773	1.397986	1.042865	H	5.845933	1.681679	0.339363	H	5.775535	1.38968	1.050984
C	3.656339	1.532143	0.675034	C	3.716684	1.660825	0.308835	C	3.652151	1.495114	0.685058
H	3.533984	2.480126	1.186473	H	3.615232	2.713414	0.541041	H	3.519675	2.441972	1.195464
N	-6.34949	-0.91377	-0.16095	N	-6.37476	-0.89061	-0.17995	N	-6.37354	-0.91567	-0.16191

PymDMA (S_0)				PymDMA (T_1)				PymDMA$^{\bullet+}$			
C	-6.74152	-1.82592	0.837937	C	-6.77867	-1.8104	0.805106	C	-6.78089	-1.80629	0.8403
C	-7.19092	-0.59802	-1.24561	C	-7.20899	-0.55791	-1.26359	C	-7.1935	-0.59115	-1.25128
C	-8.46334	-1.19437	-1.3667	C	-8.4855	-1.14343	-1.39868	C	-8.47999	-1.16904	-1.37667
C	-9.0062	-2.20612	-0.34965	C	-9.04077	-2.16235	-0.39563	C	-9.04317	-2.15856	-0.35735
C	-7.9995	-2.46111	0.779152	C	-8.04094	-2.43697	0.734594	C	-8.05446	-2.42167	0.777738
C	-6.75978	0.321857	-2.22239	C	-6.76728	0.370493	-2.22804	C	-6.72767	0.319486	-2.2278
C	-7.56947	0.651335	-3.30266	C	-7.56932	0.717725	-3.30819	C	-7.51975	0.655437	-3.31325
C	-8.8293	0.07039	-3.43492	C	-8.83268	0.147165	-3.45403	C	-8.79151	0.091882	-3.44985
C	-9.25197	-0.83842	-2.46873	C	-9.26637	-0.7696	-2.50034	C	-9.24869	-0.80487	-2.4868
H	-10.2342	-1.29013	-2.5746	H	-10.2513	-1.21323	-2.6159	H	-10.2381	-1.23457	-2.60503
H	-5.78343	0.781732	-2.13267	H	-5.78843	0.822199	-2.12639	H	-5.74467	0.76047	-2.12725
H	-7.20866	1.364633	-4.03894	H	-7.19987	1.437394	-4.03405	H	-7.14533	1.357319	-4.05206
H	-9.47338	0.317986	-4.27357	H	-9.47087	0.409093	-4.29298	H	-9.42122	0.3478	-4.29617
C	-5.871	-2.10859	1.909662	C	-5.91525	-2.11184	1.878065	C	-5.91054	-2.08789	1.918704
C	-6.23178	-3.00516	2.908218	C	-6.287	-3.01682	2.864645	C	-6.29055	-2.96494	2.921136
C	-7.47066	-3.64169	2.86196	C	-7.53009	-3.64463	2.806299	C	-7.54425	-3.58074	2.871031
C	-8.329	-3.35912	1.802911	C	-8.38152	-3.3441	1.746602	C	-8.40047	-3.30166	1.808226
H	-4.90563	-1.62036	1.959584	H	-4.94741	-1.62978	1.936436	H	-4.93928	-1.61301	1.963837
H	-9.29447	-3.85589	1.769906	H	-9.35048	-3.83354	1.7036	H	-9.37127	-3.7859	1.782255
H	-5.53851	-3.20169	3.721787	H	-5.59873	-3.22676	3.679288	H	-5.60932	-3.16737	3.741944
H	-7.76665	-4.34493	3.634818	H	-7.83454	-4.35421	3.570199	H	-7.8531	-4.26974	3.650897
C	-9.30136	-3.54623	-1.07713	C	-9.34277	-3.49212	-1.13918	C	-9.35576	-3.50214	-1.07687
H	-9.70769	-4.29062	-0.38441	H	-9.75754	-4.24131	-0.45654	H	-9.78162	-4.22895	-0.37881
H	-8.38671	-3.95635	-1.51758	H	-8.42897	-3.90381	-1.58001	H	-8.44763	-3.93479	-1.50834
H	-10.0319	-3.40681	-1.88081	H	-10.0686	-3.33844	-1.94472	H	-10.0794	-3.35358	-1.88375
C	-10.3225	-1.65301	0.261693	C	-10.3559	-1.60659	0.21576	C	-10.3556	-1.57537	0.241235
H	-10.1393	-0.70681	0.781214	H	-10.1679	-0.66758	0.746433	H	-10.1635	-0.62789	0.754361
H	-10.7506	-2.35816	0.981809	H	-10.7925	-2.31641	0.926337	H	-10.7986	-2.26967	0.96129
H	-11.0739	-1.47402	-0.51444	H	-11.1025	-1.41327	-0.56179	H	-11.0959	-1.39436	-0.54357
N	6.349461	-0.91376	-0.16107	N	6.360238	-0.92063	-0.16455	N	6.373529	-0.91566	-0.16195
C	7.190683	-0.5984	-1.24601	C	7.263447	-0.48125	-1.15687	C	7.193414	-0.59131	-1.25143
C	8.463137	-1.19467	-1.36706	C	8.562534	-1.02948	-1.25446	C	8.479909	-1.16918	-1.3768
C	9.00626	-2.20594	-0.34966	C	9.036096	-2.19483	-0.38726	C	9.043181	-2.1585	-0.35735
C	7.999787	-2.46054	0.779416	C	7.962157	-2.61726	0.613767	C	8.054567	-2.42144	0.777854
C	6.741746	-1.82547	0.838121	C	6.719467	-1.95357	0.727864	C	6.780973	-1.80609	0.840389
C	8.329554	-3.35806	1.803514	C	8.228986	-3.66263	1.50546	C	8.400672	-3.30124	1.808479
C	5.871399	-2.1078	1.910081	C	5.841962	-2.29191	1.783191	C	5.91069	-2.08756	1.918886
C	7.471397	-3.64028	2.862808	C	7.333246	-4.04199	2.501962	C	7.544519	-3.58017	2.87138
C	6.232442	-3.00389	2.908967	C	6.139483	-3.33408	2.648189	C	6.290791	-2.96441	2.921446
H	4.905968	-1.61968	1.959917	H	4.934644	-1.72126	1.927308	H	4.93941	-1.61272	1.963986
H	9.295077	-3.85473	1.770573	H	9.175067	-4.18935	1.428484	H	9.371482	-3.78544	1.782535
H	7.767597	-4.34314	3.635937	H	7.579122	-4.86014	3.172295	H	7.853445	-4.26901	3.651352

PymDMA (S_0)				PymDMA (T_1)				PymDMA$^{\bullet+}$			
H	5.539303	-3.20017	3.722713	H	5.445065	-3.57931	3.446303	H	5.609617	-3.16674	3.742321
C	6.759278	0.321013	-2.22311	C	6.840485	0.483942	-2.09884	C	6.727502	0.319155	-2.22808
C	7.56875	0.650104	-3.30366	C	7.71549	0.971916	-3.05755	C	7.519506	0.654938	-3.31363
C	8.828621	0.06923	-3.43589	C	9.021876	0.485215	-3.12128	C	8.791274	0.091388	-3.45022
C	9.251548	-0.83912	-2.46938	C	9.416866	-0.51504	-2.23668	C	9.248526	-0.80518	-2.48705
H	10.23379	-1.29077	-2.57522	H	10.42051	-0.9195	-2.3232	H	10.23796	-1.23488	-2.60526
H	5.782896	0.780828	-2.13343	H	5.818779	0.837936	-2.08015	H	5.744499	0.760137	-2.12754
H	7.207743	1.363044	-4.0402	H	7.368647	1.720149	-3.76405	H	7.145028	1.356685	-4.05254
H	9.472532	0.316532	-4.27476	H	9.717237	0.857797	-3.86749	H	9.420922	0.347172	-4.29662
C	9.301391	-3.54635	-1.07661	C	9.377576	-3.3974	-1.31148	C	9.355745	-3.50219	-1.07668
H	8.386681	-3.95675	-1.51669	H	8.497183	-3.71215	-1.88072	H	8.447583	-3.93497	-1.50795
H	9.707908	-4.29041	-0.38363	H	9.728683	-4.25299	-0.72615	H	9.781743	-4.22885	-0.37855
H	10.03179	-3.40724	-1.88049	H	10.16661	-3.13461	-2.02269	H	10.07932	-3.35373	-1.88368
C	10.32261	-1.65248	0.261212	C	10.30809	-1.76685	0.397561	C	10.35561	-1.57518	0.241006
H	10.13952	-0.70603	0.780287	H	10.08968	-0.92442	1.061453	H	10.16361	-0.62762	0.754007
H	11.0739	-1.47386	-0.51512	H	11.10637	-1.46326	-0.28682	H	11.09586	-1.39425	-0.54391
H	10.75084	-2.35725	0.981617	H	10.6893	-2.59129	1.007783	H	10.7988	-2.26935	0.961119

Cartesian coordinates (Å) for the optimized structures of **PymDMDTA**.

PymDMDTA (S_0)				PymDMDTA (T_1)				PymDMDTA$^{\bullet+}$			
C	4.91E+00	-0.55698	1.832072	C	4.953467	0.014544	1.920713	C	4.91E+00	-0.49926	1.824501
C	5.057036	-0.30012	0.465176	C	5.073461	0.27217	0.516815	C	5.06409	-0.26425	0.45545
C	3.94041	-0.36323	-0.37397	C	3.881352	0.346123	-0.26857	C	3.957392	-0.32461	-0.3942
C	3.66E+00	-0.87052	2.35308	C	3.725463	-0.1406	2.498378	C	3.65E+00	-0.7931	2.340247
C	2.524541	-0.92477	1.522031	C	2.50274	-0.08938	1.723486	C	2.527209	-0.84888	1.502466
C	2.687545	-0.67168	0.150573	C	2.653286	0.157675	0.303912	C	2.699251	-0.61496	0.129124
C	1.20E+00	-1.2498	2.104333	C	1.239881	-0.27306	2.357006	C	1.19E+00	-1.16183	2.084431
H	3.533683	-1.07336	3.411026	H	3.632686	-0.29402	3.566235	H	3.523372	-0.98244	3.399517
H	5.777857	-0.50705	2.47886	H	5.852675	-0.00673	2.530422	H	5.778393	-0.4505	2.476684
N	6.347405	0.020907	-0.07364	N	6.348326	0.448496	-0.08222	N	6.368499	0.033981	-0.08422
H	1.838812	-0.74063	-0.52285	H	1.777604	0.183484	-0.33507	H	1.854461	-0.68472	-0.54866
H	4.06E+00	-0.1769	-1.43647	H	3.965081	0.506669	-1.33989	H	4.09E+00	-0.15399	-1.45846
C	-2.65E-03	-0.8935	1.475151	C	-0.00285	-0.23866	1.658703	C	-2.41E-03	-0.8139	1.445381
N	1.189132	-1.88795	3.285157	N	1.230325	-0.50002	3.71378	N	1.186847	-1.78167	3.272625
C	-0.00226	-2.17704	3.832326	C	0.058522	-0.68308	4.30593	C	-0.00403	-2.06568	3.827208
N	-1.19383	-1.88845	3.28528	N	-1.15919	-0.65253	3.712278	N	-1.19418	-1.78137	3.271199
C	-1.20107	-1.25035	2.104445	C	-1.17591	-0.41864	2.376084	C	-1.19917	-1.16167	2.082952
H	-0.00288	-0.31796	0.558576	H	-0.03408	-0.10759	0.584718	H	-0.00193	-0.25369	0.519162
C	-2.52977	-0.92583	1.522279	C	-2.51167	-0.39698	1.724943	C	-2.53198	-0.84836	1.499276
C	-0.0021	-2.88027	5.141789	C	0.066404	-0.94177	5.775132	C	-0.00499	-2.74978	5.143403
C	-2.69327	-0.67434	0.150597	C	-2.72882	0.221171	0.481522	C	-2.70276	-0.61828	0.125146
C	-3.94628	-0.36629	-0.3738	C	-3.98849	0.218134	-0.11182	C	-3.9601	-0.32738	-0.3998
C	-3.66002	-0.8704	2.353757	C	-3.60711	-1.0031	2.363704	C	-3.65794	-0.78822	2.336268
C	-4.91201	-0.55699	1.832916	C	-4.86758	-1.00954	1.772578	C	-4.91589	-0.49327	1.818965
C	-5.06249	-0.30175	0.465715	C	-5.06621	-0.40074	0.529545	C	-5.06707	-0.26211	0.449077
H	-1.84476	-0.74425	-0.52302	H	-1.91401	0.734238	-0.02018	H	-1.85758	-0.6916	-0.55181
H	-4.07004	-0.18106	-1.43644	H	-4.14867	0.704468	-1.06971	H	-4.08924	-0.15961	-1.46462
H	-3.53819	-1.07214	3.411876	H	-3.44675	-1.46951	3.328934	H	-3.5295	-0.97484	3.396152
H	-5.78256	-0.50614	2.480009	H	-5.70748	-1.4871	2.26915	H	-5.78291	-0.44095	2.470499
C	1.207611	-3.21678	5.769544	C	1.277051	-1.07367	6.473005	C	1.204819	-3.07783	5.776572
C	1.206028	-3.87309	6.9981	C	1.28222	-1.31688	7.844404	C	1.201975	-3.71727	7.013537
C	-0.00186	-4.20404	7.616711	C	0.077626	-1.43074	8.543775	C	-0.00692	-4.03945	7.635025
C	-1.20986	-3.87579	6.996896	C	-1.13164	-1.2992	7.858374	C	-1.21484	-3.71988	7.010327
C	-1.21168	-3.21943	5.768363	C	-1.13846	-1.0575	6.485428	C	-1.21578	-3.08038	5.773388
H	-2.14449	-2.96529	5.278213	H	-2.07161	-0.95057	5.94456	H	-2.1492	-2.8339	5.280672
H	-2.1531	-4.13311	7.471403	H	-2.07352	-1.38421	8.394751	H	-2.15781	-3.97098	7.488033
H	2.140332	-2.96054	5.280314	H	2.205978	-0.98372	5.921363	H	2.139014	-2.82931	5.286342
H	2.149355	-4.12823	7.473607	H	2.2284	-1.41838	8.370452	H	2.144201	-3.96624	7.49382
H	-0.00177	-4.71654	8.575164	H	0.082386	-1.62003	9.614378	H	-0.00766	-4.5387	8.600099
N	-6.35268	0.019357	-0.0735	N	-6.36712	-0.40231	-0.08211	N	-6.37046	0.037716	-0.09221

PymDMDTA (S_0)				PymDMDTA (T_1)				PymDMDTA$^{\bullet+}$			
C	-6.74994	1.366659	-0.14733	C	-7.25287	0.655858	0.182697	C	-6.78157	1.373338	-0.17151
C	-7.18876	-1.01995	-0.52057	C	-6.72198	-1.45722	-0.9391	C	-7.18582	-1.01631	-0.52087
C	-8.46227	-0.74258	-1.05852	C	-7.98659	-1.49195	-1.56344	C	-8.47065	-0.763	-1.05604
C	-8.00425	1.722404	-0.6845	C	-8.53083	0.699425	-0.41302	C	-8.04621	1.708522	-0.70976
C	-9.00884	0.684256	-1.2025	C	-9.03918	-0.39333	-1.36298	C	-9.03425	0.652255	-1.21296
C	-5.8918	2.382083	0.317877	C	-6.8692	1.695172	1.053322	C	-5.92869	2.401397	0.287806
C	-6.25822	3.718126	0.253338	C	-7.72202	2.752955	1.329419	C	-6.31179	3.727569	0.217146
C	-7.49715	4.104319	-0.27831	C	-8.99754	2.826129	0.750273	C	-7.56067	4.096186	-0.3178
C	-8.33766	3.079496	-0.73344	C	-9.36192	1.782585	-0.11114	C	-8.39328	3.05767	-0.76787
C	-6.75875	-2.35842	-0.43412	C	-5.81014	-2.50304	-1.18493	C	-6.72699	-2.3485	-0.41886
C	-7.56458	-3.40118	-0.86623	C	-6.13503	-3.55746	-2.02459	C	-7.51518	-3.40531	-0.83369
C	-8.83678	-3.15828	-1.40415	C	-7.38468	-3.62086	-2.65873	C	-8.79974	-3.18888	-1.36784
C	-9.2457	-1.82026	-1.48303	C	-8.2778	-2.57175	-2.40259	C	-9.23555	-1.85622	-1.46065
C	-10.3273	0.804234	-0.39048	C	-10.3247	-1.02819	-0.76589	C	-10.3529	0.76264	-0.39719
H	-10.7587	1.806338	-0.48209	H	-11.1075	-0.2762	-0.62209	H	-10.7966	1.757386	-0.50075
H	-11.0749	0.087314	-0.74555	H	-10.7256	-1.80285	-1.42803	H	-11.0902	0.033133	-0.7459
H	-10.1466	0.608444	0.67149	H	-10.1133	-1.48764	0.205161	H	-10.17	0.580504	0.666544
C	-9.3005	0.967739	-2.70135	C	-9.37349	0.247297	-2.73772	C	-9.33109	0.915647	-2.71589
H	-8.38426	0.888527	-3.29551	H	-8.48078	0.70227	-3.17921	H	-8.41634	0.84378	-3.31284
H	-10.0285	0.25617	-3.10427	H	-9.75597	-0.50034	-3.44038	H	-10.0503	0.189696	-3.10692
H	-9.70868	1.974409	-2.83929	H	-10.1358	1.026599	-2.63411	H	-9.7551	1.913988	-2.86098
H	-4.9227	2.12173	0.725373	H	-5.88742	1.675897	1.509768	H	-4.95623	2.152695	0.692881
H	-5.55685	4.472768	0.597898	H	-7.37753	3.547536	1.985339	H	-5.62039	4.493198	0.554412
H	-9.3124	3.356915	-1.12287	H	-10.3561	1.806773	-0.5471	H	-9.3715	3.32252	-1.15452
H	-5.78708	-2.58478	-0.01266	H	-4.84154	-2.49266	-0.70086	H	-5.75057	-2.55094	0.002085
H	-7.2075	-4.42134	-0.75719	H	-5.4142	-4.35804	-2.16541	H	-7.14274	-4.41755	-0.71307
H	-10.2162	-1.61035	-1.92199	H	-9.24001	-2.58856	-2.90537	H	-10.2105	-1.66994	-1.89804
C	-9.70908	-4.2634	-1.86889	C	-7.74533	-4.74315	-3.55749	C	-9.65148	-4.31083	-1.81059
C	-9.1717	-5.39923	-2.49821	C	-6.78931	-5.34009	-4.39723	C	-9.08877	-5.47545	-2.3651
C	-9.99084	-6.43738	-2.93549	C	-7.12766	-6.3947	-5.24187	C	-9.89172	-6.52991	-2.78726
C	-11.3806	-6.3887	-2.76621	C	-8.43336	-6.89983	-5.28875	C	-11.2879	-6.47478	-2.66895
C	-11.1033	-4.21653	-1.7009	C	-9.05456	-5.25163	-3.60707	C	-11.053	-4.25522	-1.69677
C	-11.919	-5.25518	-2.144	C	-9.38952	-6.3031	-4.45713	C	-11.8502	-5.31477	-2.11697
C	-12.2638	-7.52931	-3.21493	C	-8.79098	-8.06322	-6.1839	C	-12.1539	-7.63407	-3.09659
H	-13.2665	-7.17934	-3.48313	H	-9.83842	-8.01847	-6.50168	H	-13.1406	-7.29675	-3.4304
H	-11.8421	-8.04497	-4.08459	H	-8.16593	-8.08416	-7.08339	H	-11.6928	-8.19988	-3.91259
H	-12.3837	-8.27897	-2.42084	H	-8.6495	-9.02345	-5.66908	H	-12.314	-8.33408	-2.26553
H	-8.1008	-5.45581	-2.67403	H	-5.77408	-4.95274	-4.40946	H	-8.013	-5.54115	-2.50119
H	-9.54259	-7.29734	-3.42904	H	-6.36452	-6.82625	-5.88659	H	-9.4276	-7.40982	-3.22642
H	-11.5527	-3.36543	-1.19629	H	-9.81543	-4.83234	-2.95426	H	-11.5229	-3.3856	-1.2461
H	-12.9948	-5.18801	-1.99464	H	-10.4125	-6.67422	-4.46719	H	-12.9298	-5.24489	-2.00754
C	-7.90224	5.528469	-0.3549	C	-9.91955	3.951368	1.035407	C	-7.98006	5.509732	-0.40083

PymDMDTA (S_0)				PymDMDTA (T_1)				PymDMDTA$^{\bullet+}$			
C	-7.54727	6.441772	0.652348	C	-9.97232	4.545849	2.30794	C	-7.57834	6.445424	0.570334
C	-7.92297	7.78093	0.577375	C	-10.8346	5.60665	2.574336	C	-7.97469	7.776542	0.492051
C	-8.67433	8.266905	-0.50036	C	-11.6876	6.117157	1.587254	C	-8.78567	8.234483	-0.55612
C	-9.02708	7.358957	-1.50702	C	-11.6352	5.528426	0.317469	C	-9.18066	7.304801	-1.52882
C	-8.64972	6.019846	-1.43866	C	-10.7707	4.470608	0.044984	C	-8.79112	5.971558	-1.454
H	-9.59622	7.708397	-2.3661	H	-12.2729	5.912698	-0.47618	H	-9.79483	7.633954	-2.36367
H	-8.91221	5.350916	-2.25388	H	-10.7325	4.060261	-0.96055	H	-9.08931	5.287705	-2.24372
H	-6.98782	6.093408	1.516407	H	-9.34407	4.157349	3.104935	H	-6.97358	6.121229	1.412538
H	-7.63425	8.46033	1.376819	H	-10.8519	6.040812	3.572061	H	-7.65532	8.473365	1.263416
C	-9.10985	9.712193	-0.56225	C	-12.6468	7.244829	1.888952	C	-9.23838	9.672462	-0.62196
H	-8.39349	10.36953	-0.05757	H	-12.2423	7.924319	2.647249	H	-8.51146	10.34441	-0.15423
H	-9.21287	10.05609	-1.59718	H	-12.8685	7.833435	0.992074	H	-9.38854	9.999012	-1.65618
H	-10.0832	9.858165	-0.07407	H	-13.6039	6.865289	2.272303	H	-10.193	9.809686	-0.09639
C	7.18231	-1.01831	-0.5231	C	7.294459	-0.59046	-0.02126	C	7.180011	-1.02065	-0.51871
C	8.461391	-0.74211	-1.04836	C	8.596465	-0.43165	-0.54954	C	8.465142	-0.76899	-1.054
C	9.027531	0.68097	-1.14697	C	9.033289	0.826538	-1.30001	C	9.048121	0.642385	-1.16983
C	6.747247	1.367731	-0.14202	C	6.657387	1.660179	-0.72747	C	6.784658	1.368462	-0.15569
C	8.012261	1.72138	-0.65493	C	7.901414	1.852118	-1.37257	C	8.056847	1.700832	-0.67765
C	5.881879	2.384577	0.306402	C	5.730936	2.72713	-0.69069	C	5.930578	2.397966	0.298165
C	6.252295	3.71988	0.250357	C	5.983614	3.913525	-1.35454	C	6.320488	3.722706	0.239358
C	8.350014	3.077717	-0.69457	C	8.119789	3.063377	-2.02977	C	8.411615	3.04852	-0.72202
C	7.50272	4.103896	-0.25537	C	7.182059	4.107935	-2.06339	C	7.578144	4.088392	-0.27678
H	4.904275	2.125901	0.694182	H	4.810131	2.616148	-0.13457	H	4.952048	2.151526	0.689793
H	5.545721	4.475803	0.581256	H	5.232445	4.696869	-1.33336	H	5.628295	4.489812	0.571653
H	9.334127	3.353097	-1.06112	H	9.080746	3.228296	-2.50552	H	9.396756	3.310629	-1.09259
C	9.385236	0.982678	-2.62766	C	9.457584	0.426821	-2.74066	C	9.39353	0.926436	-2.65823
H	8.494411	0.921106	-3.26126	H	8.6232	-0.03542	-3.27766	H	8.497046	0.873234	-3.28416
H	10.12333	0.269625	-3.00897	H	10.28743	-0.28608	-2.72201	H	10.1179	0.19956	-3.03787
H	9.809805	1.986108	-2.73491	H	9.786002	1.302414	-3.30905	H	9.832573	1.921792	-2.7754
C	10.31144	0.776173	-0.27807	C	10.24112	1.469794	-0.56208	C	10.34244	0.72549	-0.31239
H	10.08383	0.567196	0.772296	H	9.962254	1.766346	0.453996	H	10.12483	0.529123	0.742232
H	10.75395	1.776083	-0.33662	H	10.59518	2.359829	-1.09119	H	10.79814	1.717571	-0.38666
H	11.06683	0.056667	-0.61087	H	11.07678	0.766239	-0.49409	H	11.0824	-0.007	-0.64902
C	6.745221	-2.35538	-0.45252	C	6.925471	-1.83683	0.535248	C	6.716572	-2.35169	-0.4234
C	7.549036	-3.39793	-0.8889	C	7.84363	-2.86317	0.655058	C	7.500045	-3.40898	-0.84591
C	8.825844	-3.15611	-1.41621	C	9.165729	-2.71152	0.199032	C	8.782079	-3.19378	-1.38648
C	9.242702	-1.81956	-1.47729	C	9.494284	-1.49104	-0.41163	C	9.22327	-1.86229	-1.47091
H	10.23973	-1.61496	-1.85518	H	10.50587	-1.3626	-0.78207	H	10.22149	-1.68151	-1.85485
H	5.760693	-2.5792	-0.0606	H	5.904397	-1.99751	0.853625	H	5.730697	-2.5513	-0.02369
H	7.164521	-4.41286	-0.84241	H	7.519128	-3.81282	1.068694	H	7.100873	-4.41627	-0.78373
C	7.911557	5.527486	-0.32137	C	7.460596	5.367878	-2.78671	C	8.004128	5.500713	-0.34602
C	8.686437	6.01865	-1.38569	C	8.205754	5.374019	-3.97873	C	8.834647	5.964911	-1.38276

PymDMDTA (S_0)				PymDMDTA (T_1)				PymDMDTA$^{\bullet+}$			
C	7.540118	6.438686	0.68197	C	6.991439	6.60327	-2.30594	C	7.595771	6.431196	0.627476
C	7.924228	7.776103	0.620361	C	7.257534	7.787048	-2.9876	C	8.002903	7.759921	0.565997
C	9.072145	7.356027	-1.44062	C	8.466784	6.56123	-4.65736	C	9.234965	7.295811	-1.44084
C	8.696056	8.263594	-0.44218	C	7.996623	7.791209	-4.17856	C	8.827028	8.221894	-0.47014
C	9.086535	9.720849	-0.52162	C	8.254357	9.073938	-4.93223	C	9.240346	9.670899	-0.55186
H	10.03582	9.853991	-1.05177	H	9.174114	9.014486	-5.52349	H	10.21607	9.78362	-1.0356
H	9.191395	10.16287	0.475179	H	8.342325	9.927911	-4.25215	H	9.297322	10.12845	0.441156
H	8.330064	10.30921	-1.05877	H	7.434076	9.296973	-5.6278	H	8.517873	10.25483	-1.13787
H	8.971972	5.349106	-2.19263	H	8.561362	4.435248	-4.39447	H	9.146901	5.283301	-2.16897
H	9.669383	7.703702	-2.28115	H	9.039856	6.531415	-5.58141	H	9.870692	7.625397	-2.25924
H	6.968415	6.087841	1.536943	H	6.44113	6.642027	-1.3701	H	6.983867	6.102524	1.46276
H	7.628755	8.452168	1.420156	H	6.892425	8.72793	-2.582	H	7.684257	8.450825	1.342947
C	9.696863	-4.26023	-1.88567	C	10.1577	-3.80039	0.331366	C	9.627496	-4.31526	-1.84243
C	9.714374	-5.50308	-1.22999	C	10.14148	-4.66147	1.443186	C	9.574665	-5.57023	-1.20762
C	10.5286	-6.54204	-1.67437	C	11.07266	-5.68771	1.570919	C	10.3717	-6.62605	-1.63707
C	10.53192	-4.10853	-3.00556	C	11.14463	-4.01827	-0.64594	C	10.51086	-4.17136	-2.9283
C	11.34805	-5.14902	-3.44352	C	12.07219	-5.04781	-0.51361	C	11.30239	-5.23249	-3.35556
C	11.36583	-6.38601	-2.78666	C	12.05894	-5.9008	0.598045	C	11.25396	-6.48007	-2.71732
C	12.27335	-7.50325	-3.2455	C	13.08537	-6.99692	0.755062	C	12.13812	-7.61931	-3.16148
H	13.24541	-7.46446	-2.73507	H	13.95027	-6.65024	1.336673	H	13.08873	-7.61802	-2.61136
H	12.4706	-7.44346	-4.32131	H	13.46183	-7.3359	-0.21569	H	12.37993	-7.54798	-4.22684
H	11.83778	-8.48634	-3.03603	H	12.66983	-7.86387	1.279716	H	11.6628	-8.58956	-2.98375
H	10.52015	-7.4904	-1.14088	H	11.03719	-6.3324	2.446252	H	10.31438	-7.58095	-1.11992
H	9.097685	-5.65016	-0.3474	H	9.406604	-4.5095	2.228738	H	8.923965	-5.71256	-0.34948
H	10.5188	-3.17355	-3.55925	H	11.1645	-3.39828	-1.53792	H	10.55119	-3.22977	-3.46864
H	11.97434	-5.00113	-4.32097	H	12.81406	-5.19957	-1.29444	H	11.96353	-5.09422	-4.20776

Cartesian coordinates (Å) for the optimized structures of **PymDMDMA**.

PymDMDMA (S_0)				PymDMDMA (T_1)				PymDMDMA$^{\bullet+}$			
C	4.857338	-0.55467	2.021993	C	4.835858	0.847046	1.945808	C	4.859587	-0.49858	1.994065
C	5.018175	-0.3553	0.646727	C	5.018594	0.49625	0.604658	C	5.022419	-0.31705	0.617932
C	3.91E+00	-0.44897	-0.19696	C	3.913378	0.457989	-0.25157	C	3.92E+00	-0.41012	-0.23565
C	3.600572	-0.84174	2.546552	C	3.564433	1.150515	2.42472	C	3.597223	-0.7717	2.512557
C	2.475607	-0.92612	1.710368	C	2.441735	1.102391	1.580018	C	2.477228	-0.85913	1.670002
C	2.65E+00	-0.73062	0.330807	C	2.642876	0.759949	0.231521	C	2.66E+00	-0.67881	0.289783
C	1.141679	-1.22212	2.295687	C	1.096654	1.417186	2.127083	C	1.13935	-1.14813	2.254056
H	3.470867	-1.00018	3.611093	H	3.415429	1.426985	3.462165	H	3.460532	-0.91964	3.577524
H	5.723815	-0.4812	2.672357	H	5.696785	0.878442	2.607614	H	5.722049	-0.42476	2.649561
N	6.31331	-0.06201	0.104208	N	6.331152	0.184593	0.106982	N	6.329958	-0.04086	0.076594
H	1.80E+00	-0.82427	-0.34522	H	1.804538	0.753228	-0.45834	H	1.82E+00	-0.7745	-0.3903
H	4.04E+00	-0.3074	-1.26536	H	4.059803	0.201268	-1.29681	H	4.06E+00	-0.28136	-1.30484
C	-0.05089	-0.88687	1.643839	C	-0.06891	0.995952	1.506758	C	-0.05149	-0.819	1.595745
N	1.123544	-1.81231	3.501138	N	1.067154	2.118634	3.289773	N	1.122789	-1.72671	3.462975
C	-0.07307	-2.07478	4.050308	C	-0.15796	2.395017	3.79538	C	-0.07271	-1.98807	4.018459
N	-1.25944	-1.80412	3.483212	N	-1.32647	2.049689	3.27213	N	-1.25837	-1.72003	3.44535
C	-1.25545	-1.21386	2.27767	C	-1.32123	1.329131	2.099947	C	-1.25369	-1.1412	2.23644
H	-0.04203	-0.34852	0.704981	H	-0.02295	0.401767	0.603023	H	-0.04286	-0.29077	0.650965
C	-2.5783	-0.90849	1.672455	C	-2.58026	0.95371	1.544555	C	-2.58128	-0.8441	1.633068
C	-0.0854	-2.72524	5.38678	C	-0.18256	3.16982	5.070742	C	-0.08439	-2.62702	5.357404
C	-2.73007	-0.71254	0.290378	C	-2.71594	0.199438	0.318043	C	-2.74132	-0.65931	0.25079
C	-3.97775	-0.42187	-0.25611	C	-3.94146	-0.1575	-0.17811	C	-3.99393	-0.38256	-0.29268
C	-3.71486	-0.81523	2.491866	C	-3.81165	1.325639	2.206338	C	-3.71328	-0.75303	2.459054
C	-4.96149	-0.51892	1.948596	C	-5.03614	0.995344	1.694803	C	-4.96639	-0.4719	1.922624
C	-5.1005	-0.31922	0.570919	C	-5.14108	0.234788	0.488689	C	-5.10751	-0.28586	0.544699
H	-1.87652	-0.81282	-0.37298	H	-1.83169	-0.08442	-0.24192	H	-1.89132	-0.75739	-0.41696
H	-4.09253	-0.27974	-1.32636	H	-4.01285	-0.70647	-1.11318	H	-4.11485	-0.24985	-1.3634
H	-3.60215	-0.97409	3.558285	H	-3.73205	1.871363	3.138212	H	-3.5932	-0.90459	3.525506
H	-5.83698	-0.43868	2.585978	H	-5.94376	1.269521	2.22597	H	-5.83817	-0.39554	2.565397
C	1.118284	-3.04093	6.036542	C	1.008915	3.646018	5.639099	C	1.120237	-2.93692	6.009242
C	1.105016	-3.64815	7.290026	C	0.986734	4.370485	6.83001	C	1.107434	-3.53419	7.267082
C	-0.10871	-3.95011	7.912035	C	-0.22486	4.629593	7.473755	C	-0.1064	-3.83176	7.891188
C	-1.31078	-3.64226	7.270586	C	-1.41624	4.159159	6.914893	C	-1.30923	-3.52996	7.248116
C	-1.30091	-3.03498	6.017098	C	-1.39572	3.43704	5.723936	C	-1.30018	-2.93261	5.990276
H	-2.22901	-2.79707	5.510152	H	-2.31422	3.067785	5.281979	H	-2.22954	-2.70012	5.483263
H	-2.25852	-3.87722	7.747712	H	-2.36424	4.355758	7.409954	H	-2.25608	-3.76198	7.727824
H	2.055581	-2.80759	5.544604	H	1.943633	3.441596	5.129867	H	2.058242	-2.70771	5.516863
H	2.043795	-3.88766	7.78238	H	1.918453	4.734252	7.256369	H	2.045818	-3.76946	7.761624
H	-0.11774	-4.42435	8.889952	H	-0.24156	5.193585	8.40316	H	-0.11492	-4.29814	8.87256
N	-6.38482	-0.01629	0.008623	N	-6.41255	-0.12312	-0.03867	N	-6.40517	-0.00088	-0.016
C	-6.77608	1.32843	-0.12543	C	-7.31714	0.882811	-0.41954	C	-6.81194	1.332663	-0.14398

PymDMDMA (S_0)				PymDMDMA (T_1)				PymDMDMA$^{\bullet+}$			
C	-7.22087	-1.0704	-0.40337	C	-6.75284	-1.4796	-0.17395	C	-7.22081	-1.06631	-0.41576
C	-8.4877	-0.81109	-0.96525	C	-7.9862	-1.8764	-0.74154	C	-8.49991	-0.82798	-0.97025
C	-8.02351	1.665908	-0.68936	C	-8.60425	0.566242	-0.91332	C	-8.06984	1.653347	-0.70532
C	-9.0271	0.610558	-1.17364	C	-9.06347	-0.87244	-1.15328	C	-9.0573	0.583296	-1.18175
C	-5.91874	2.359655	0.304885	C	-6.92003	2.238611	-0.35676	C	-5.96168	2.374061	0.288355
C	-6.27874	3.693219	0.179195	C	-7.79792	3.254036	-0.68482	C	-6.33976	3.698242	0.168435
C	-7.51162	4.06174	-0.37873	C	-9.10676	2.972885	-1.11974	C	-7.58239	4.053326	-0.39042
C	-8.35173	3.021052	-0.79749	C	-9.46085	1.618813	-1.237	C	-8.41271	3.000425	-0.81252
C	-6.79804	-2.40578	-0.25654	C	-5.86879	-2.47202	0.309521	C	-6.7692	-2.39595	-0.26446
C	-7.60487	-3.46266	-0.65133	C	-6.15157	-3.81554	0.15341	C	-7.55846	-3.46391	-0.64774
C	-8.8699	-3.23814	-1.21381	C	-7.34105	-4.24194	-0.46687	C	-8.83793	-3.26314	-1.20071
C	-9.27114	-1.90261	-1.35342	C	-8.23608	-3.24177	-0.88105	C	-9.26565	-1.93148	-1.34349
C	-10.3529	0.768681	-0.38032	C	-10.3455	-1.14894	-0.31896	C	-10.3832	0.726003	-0.38343
H	-10.7795	1.767682	-0.51721	H	-11.1467	-0.45401	-0.58891	H	-10.8226	1.718032	-0.52493
H	-11.0999	0.040393	-0.71289	H	-10.7138	-2.16477	-0.49214	H	-11.12	-0.01255	-0.71375
H	-10.1832	0.616092	0.690522	H	-10.1441	-1.0374	0.751138	H	-10.211	0.579774	0.687635
C	-9.30322	0.832797	-2.68573	C	-9.37924	-1.04804	-2.66509	C	-9.33831	0.79555	-2.69548
H	-8.38158	0.725484	-3.26702	H	-8.49071	-0.85054	-3.27312	H	-8.41777	0.700079	-3.28017
H	-10.0304	0.108023	-3.06606	H	-9.71881	-2.06619	-2.87904	H	-10.0562	0.058942	-3.06889
H	-9.70566	1.834483	-2.86924	H	-10.1688	-0.36	-2.98247	H	-9.75709	1.789722	-2.87963
H	-4.95438	2.113488	0.732133	H	-5.90724	2.484325	-0.06761	H	-4.99344	2.13735	0.710624
H	-5.57675	4.459236	0.496648	H	-7.44908	4.281231	-0.64647	H	-5.64717	4.471922	0.484561
H	-9.32228	3.284579	-1.2067	H	-10.4609	1.381401	-1.58414	H	-9.38744	3.252279	-1.21634
H	-5.83186	-2.61838	0.184383	H	-4.96899	-2.17458	0.830777	H	-5.7974	-2.58789	0.172035
H	-7.25419	-4.47875	-0.49351	H	-5.46066	-4.54753	0.559832	H	-7.19052	-4.47197	-0.48503
H	-10.2358	-1.70687	-1.81171	H	-9.16519	-3.55045	-1.34846	H	-10.235	-1.75461	-1.79685
C	-9.74234	-4.35715	-1.64249	C	-7.64645	-5.67528	-0.64812	C	-9.69074	-4.3936	-1.61077
C	-9.20913	-5.51915	-2.2175	C	-6.62571	-6.60938	-0.88562	C	-9.13423	-5.59113	-2.09204
C	-10.0187	-6.58202	-2.62371	C	-6.89421	-7.96604	-1.06235	C	-9.92726	-6.66592	-2.48686
C	-11.4059	-6.49751	-2.46271	C	-8.216	-8.42538	-1.00062	C	-11.3235	-6.56642	-2.40295
C	-11.1415	-4.2988	-1.48847	C	-8.9687	-6.16305	-0.59012	C	-11.0988	-4.31856	-1.53655
C	-11.9611	-5.34367	-1.89084	C	-9.25222	-7.50848	-0.7612	C	-11.9012	-5.37888	-1.92094
O	-12.295	-7.47017	-2.82403	O	-8.59706	-9.72231	-1.15599	O	-12.194	-7.54452	-2.75546
C	-11.7857	-8.66237	-3.39764	C	-7.5918	-10.6998	-1.38514	C	-11.6768	-8.77767	-3.24212
H	-8.13677	-5.59113	-2.37755	H	-5.59707	-6.26952	-0.96489	H	-8.05643	-5.67906	-2.1938
H	-9.55984	-7.45638	-3.07148	H	-6.07411	-8.64781	-1.25581	H	-9.4539	-7.56438	-2.86536
H	-11.5913	-3.42746	-1.02047	H	-9.78483	-5.47945	-0.37466	H	-11.5695	-3.42481	-1.13774
H	-13.038	-5.29608	-1.76067	H	-10.27	-7.88115	-0.70192	H	-12.9825	-5.32242	-1.84811
C	-7.91056	5.482478	-0.51821	C	-10.0547	4.051833	-1.46321	C	-7.99694	5.461899	-0.52579
C	-7.56842	6.434958	0.451808	C	-10.0351	5.278288	-0.78034	C	-7.58895	6.435115	0.402257
C	-7.93489	7.777121	0.332182	C	-10.9239	6.307569	-1.08792	C	-7.97752	7.768166	0.290943
C	-8.66975	8.198278	-0.78141	C	-11.867	6.128131	-2.10785	C	-8.79573	8.166167	-0.77591

PymDMDMA (S_0)				PymDMDMA (T_1)				PymDMDMA$^{\bullet+}$			
C	-9.02421	7.26204	-1.7635	C	-11.902	4.910142	-2.80573	C	-9.21211	7.209574	-1.71801
C	-8.64782	5.933064	-1.63097	C	-11.0135	3.89621	-2.48599	C	-8.82065	5.887947	-1.59033
H	-9.58436	7.604452	-2.62825	H	-12.629	4.790849	-3.60291	H	-9.83376	7.535535	-2.54574
H	-8.90784	5.231472	-2.41883	H	-11.0404	2.975603	-3.06181	H	-9.13112	5.175032	-2.34857
H	-7.02336	6.12142	1.338034	H	-9.33007	5.427228	0.032402	H	-6.98086	6.142964	1.253544
H	-7.65444	8.474535	1.113522	H	-10.8791	7.232429	-0.5245	H	-7.6512	8.480672	1.039573
O	-9.08494	9.480968	-1.00384	O	-12.7806	7.059081	-2.4954	O	-9.2348	9.431925	-0.98747
C	-8.74492	10.46955	-0.04622	C	-12.7852	8.317533	-1.83597	C	-8.84798	10.4513	-0.07318
C	7.146751	-1.1223	-0.29681	C	6.777086	-1.14689	0.13171	C	7.14703	-1.11212	-0.3049
C	8.429377	-0.87322	-0.82669	C	8.063721	-1.49141	-0.33379	C	8.438067	-0.88286	-0.83485
C	9.001345	0.542524	-0.98188	C	9.056042	-0.45007	-0.86831	C	9.023222	0.523386	-1.00143
C	6.717842	1.279519	-0.02116	C	7.139634	1.218026	-0.39504	C	6.746246	1.290077	-0.04891
C	7.98644	1.606692	-0.54249	C	8.439293	0.955019	-0.87679	C	8.023604	1.601445	-0.56995
C	5.85421	2.317907	0.378153	C	6.65572	2.541142	-0.42353	C	5.887726	2.338043	0.349209
C	6.228852	3.648499	0.264228	C	7.432222	3.579945	-0.91361	C	6.276891	3.659731	0.236042
C	8.329392	2.959043	-0.6388	C	9.193073	2.028976	-1.36007	C	8.378578	2.946147	-0.66865
C	7.48314	4.006764	-0.25109	C	8.72893	3.350896	-1.39813	C	7.54004	4.005541	-0.28067
H	4.874014	2.079723	0.77259	H	5.655643	2.752615	-0.06618	H	4.904706	2.108632	0.740194
H	5.522368	4.420021	0.557425	H	7.010794	4.580894	-0.94334	H	5.57812	4.438306	0.525307
H	9.317142	3.214828	-1.01009	H	10.20585	1.835743	-1.70072	H	9.369506	3.190813	-1.03605
C	9.371078	0.779286	-2.4714	C	9.463693	-0.83402	-2.3168	C	9.391843	0.744168	-2.49458
H	8.484627	0.693454	-3.10834	H	8.588238	-0.84571	-2.97431	H	8.505012	0.663576	-3.13132
H	10.10938	0.048092	-2.81629	H	9.925306	-1.82644	-2.34772	H	10.12212	0.002471	-2.83221
H	9.799906	1.775876	-2.61836	H	10.18657	-0.12079	-2.72616	H	9.832377	1.734088	-2.64766
C	10.27928	0.670789	-0.10837	C	10.31906	-0.44335	0.035905	C	10.30353	0.643918	-0.12816
H	10.04303	0.507974	0.94822	H	10.056	-0.17457	1.064113	H	10.06876	0.492455	0.930201
H	10.72575	1.665873	-0.20638	H	11.05835	0.279638	-0.32484	H	10.76045	1.632405	-0.23675
H	11.03446	-0.065	-0.40405	H	10.79608	-1.42901	0.05465	H	11.04906	-0.10184	-0.42084
C	6.705133	-2.45377	-0.17176	C	5.936906	-2.16295	0.629326	C	6.684066	-2.43841	-0.16091
C	7.50702	-3.51656	-0.56069	C	6.351058	-3.48563	0.664028	C	7.472614	-3.51203	-0.53012
C	8.787734	-3.30226	-1.09083	C	7.623514	-3.86011	0.206641	C	8.761686	-3.32016	-1.06308
C	9.209709	-1.97064	-1.20429	C	8.446493	-2.83513	-0.27975	C	9.202197	-1.99175	-1.19572
H	10.21032	-1.78539	-1.58298	H	9.447815	-3.09912	-0.60647	H	10.20603	-1.82437	-1.57132
H	5.718088	-2.6578	0.224733	H	4.945106	-1.91052	0.98314	H	5.693259	-2.62278	0.234148
H	7.117881	-4.52715	-0.47379	H	5.661754	-4.24175	1.029616	H	7.070399	-4.51533	-0.43197
C	7.896543	5.424471	-0.37839	C	9.569545	4.452417	-1.92358	C	7.964974	5.412162	-0.40658
C	8.671211	5.868881	-1.45886	C	10.43767	4.261268	-3.00774	C	8.823373	5.831351	-1.43704
C	7.523479	6.383598	0.583855	C	9.527281	5.740211	-1.35311	C	7.522035	6.394191	0.505917
C	7.904336	7.712984	0.47042	C	10.30942	6.777456	-1.84064	C	7.918677	7.715913	0.395517
C	9.067304	7.201971	-1.5863	C	11.23562	5.292546	-3.50792	C	9.229167	7.15792	-1.56458
C	8.682463	8.134934	-0.61737	C	11.17354	6.562176	-2.92384	C	8.778013	8.113645	-0.64326
O	9.007615	9.461949	-0.63798	O	11.90341	7.645192	-3.32867	O	9.106741	9.429618	-0.6657

PymDMDMA (S_0)				PymDMDMA (T_1)				PymDMDMA$^{\bullet+}$			
C	9.801146	9.939569	-1.7113	C	12.79969	7.478601	-4.41368	C	9.984948	9.897101	-1.68295
H	8.95385	5.165721	-2.23764	H	10.47683	3.290644	-3.49467	H	9.159462	5.114452	-2.18066
H	9.658867	7.499086	-2.44497	H	11.88489	5.097215	-4.35407	H	9.88114	7.437281	-2.38402
H	6.944755	6.073682	1.44964	H	8.886191	5.922456	-0.49511	H	6.882387	6.107275	1.335399
H	7.621374	8.445139	1.220547	H	10.27842	7.764821	-1.39004	H	7.588153	8.464569	1.108354
C	9.655354	-4.42862	-1.50987	C	8.078452	-5.27012	0.238082	C	9.610369	-4.45833	-1.46124
C	9.667666	-5.645	-0.79903	C	7.709053	-6.13448	1.287884	C	9.533733	-5.69771	-0.78914
C	10.47508	-6.70483	-1.18632	C	8.128975	-7.45654	1.323302	C	10.32849	-6.77001	-1.15603
C	10.49505	-4.33174	-2.62815	C	8.891167	-5.80264	-0.77266	C	10.52485	-4.35739	-2.52348
C	11.3176	-5.38664	-3.02924	C	9.327299	-7.12921	-0.75011	C	11.32907	-5.4278	-2.90799
C	11.31016	-6.58458	-2.30659	C	8.94481	-7.96655	0.303194	C	11.23649	-6.64726	-2.22208
O	12.06786	-7.68182	-2.60512	O	9.307134	-9.27903	0.429553	O	11.9675	-7.75426	-2.50449
C	12.93699	-7.61067	-3.72284	C	10.14356	-9.83977	-0.56758	C	12.91422	-7.69607	-3.56519
H	10.48667	-7.63621	-0.62848	H	7.848324	-8.11397	2.140581	H	10.27712	-7.71618	-0.62694
H	9.049944	-5.75058	0.088549	H	7.101561	-5.75286	2.103797	H	8.862144	-5.80953	0.056969
H	10.49185	-3.4207	-3.22044	H	9.173159	-5.17686	-1.61504	H	10.59017	-3.43267	-3.08959
H	11.94326	-5.26658	-3.90653	H	9.94807	-7.49654	-1.55967	H	12.00966	-5.30769	-3.74282
H	10.78027	9.442924	-1.7431	H	13.56998	6.727713	-4.19139	H	10.96139	9.399792	-1.62758
H	9.94432	11.00607	-1.52732	H	13.27609	8.449738	-4.56176	H	10.11092	10.96469	-1.49819
H	9.298474	9.803679	-2.67837	H	12.27344	7.190115	-5.33372	H	9.555392	9.748557	-2.68165
H	13.68596	-6.81621	-3.6034	H	11.10816	-9.3178	-0.6279	H	13.68265	-6.93668	-3.37374
H	12.38322	-7.44403	-4.65663	H	9.664505	-9.82198	-1.55595	H	12.42628	-7.48826	-4.52573
H	13.44223	-8.57714	-3.77218	H	10.31343	-10.8762	-0.26937	H	13.37973	-8.68182	-3.6013
H	-7.65662	10.5751	0.057716	H	-11.8287	8.840927	-1.96228	H	-7.75789	10.57391	-0.049
H	-9.17925	10.24668	0.937664	H	-13.0007	8.209619	-0.76508	H	-9.21457	10.24038	0.93922
H	-9.1633	11.40601	-0.42008	H	-13.5799	8.897926	-2.30739	H	-9.308	11.36936	-0.44097
H	-11.2552	-8.46455	-4.33885	H	-7.04506	-10.5038	-2.31657	H	-11.1014	-8.63324	-4.16507
H	-12.6536	-9.29283	-3.59986	H	-8.11657	-11.6529	-1.4684	H	-12.5466	-9.40168	-3.45146
H	-11.11	-9.18664	-2.7085	H	-6.8805	-10.748	-0.55059	H	-11.0464	-9.27051	-2.49146

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