Supporting Information for

Blue to Yellow Thermally Activated Delayed Fluorescence with Quantum Yields Near Unity in Acrylic Polymers Based on D-π-A Pyrimidines

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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. *N*,*N* dimethylacetamide (DMAc), tris[2-(dimethylamino)ethyl]amine (Me_6TREN), ethyl α-bromoisobutyrate (EBiB), and triethylamine were degassed by three freeze-pump-thaw cycles and stored in an inert atmosphere glovebox. Tetrahydrofuran (THF) was dried using an Innovative Technologies Inc. solvent purification system. N^3,N^3,N^6,N^6-tetra-*p*-tolyl-9*H*-carbazole-3,6-diamine (TTAC)[1] and 9,9-dimethyl-9,10-dihydroacridine (DMA)[2] were synthesized by literature procedures. Other chemicals were purchased from commercial sources and used as received without further purification.

S1.2 General Nucleophilic Aromatic Substitution (A):

Modified from a previously reported procedure.[3] A round-bottom flask was charged with diarylamine (1.0 eq.), potassium phosphate tribasic (5.0 eq.) and dimethylformamide. The flask was sealed with a rubber septum and sparged with N_2 for 15 minutes. The mixture was heated to 135 °C and stirred for 30 minutes. Aryl fluoride (2.0 eq.) was then added under a positive pressure of nitrogen, the flask was resealed, and the temperature was increased to 150 °C. This mixture was stirred under N_2 flow until judged complete by TLC. After cooling to room temperature, it was filtered to remove inorganic salts. The solvent was removed in vacuo at 90 °C. The resulting crude residue was purified by column chromatography on silica.

S1.3 General Synthesis of Donor-Functionalized Acetophenones (B):

Modified from a previously reported procedure.[4] A Schlenk flask was charged with donor-functionalized benzonitrile (1.0 eq.) and a magnetic stir bar, then sealed with a rubber septum. The headspace was cleared by three cycles of vacuum and N_2 backfill. Dry, degassed tetrahydrofuran was added by syringe through the septum cap and the mixture was cooled to -78 °C in a dry ice/acetone bath. A 1.6 M solution of MeLi in diethyl ether (1.5 eq.) was added dropwise to the cold solution through the septum by syringe. The mixture was stirred at this temperature for 3 hours then the reaction was quenched with 1 M HCl in water. The mixture was then poured into water in a separatory funnel and extracted with dichloromethane. The combined organic phases were dried over $MgSO_4$, gravity filtered, and the solvent was removed by rotary evaporation. The solid residue contains only minor contaminants and was purified by column chromatography on a short silica column.

S1.4 General Aldol Condensation (C):

A round-bottom flask was charged with aldehyde (1.0 eq.) and ketone (1.0 eq.) in air. Ethanol was added to the solids and the mixture was heated between 40 °C and 50 °C with stirring. A solution of NaOH (2 eq.) in ethanol was added to this mixture portionwise. The mixture was maintained at this temperature and stirred until the reaction is judged complete by TLC, when the aldehyde is completely consumed. The solvent is removed by rotary evaporation and the solid residue is suspended in water and collected by Buchner filtration. This crude solid is mainly a mixture of the ketone starting material and chalcone product which is purified on silica, eluting with a mixture of toluene/chloroform/ethyl acetate (94.5:5:0.5 v/v).

S1.5 General [3+3] Annulation-oxidation (D):

In air, a round bottom flask was charged with chalcone (1.0 eq.), *p*-bromobenzamidine hydrochloride (1.5 eq.), and potassium carbonate (3.5 eq.). Dimethylformamide was added and the mixture heated to 90°C and stirred until the chalcone is completely consumed, as judged by TLC. Dimethylformamide was removed by rotary evaporation at 90°C and the solid residue suspended in water and collected by Buchner filtration.

This was then washed with a 1:1 mixture (v/v) of methanol and water to removed unreacted p-bromobenzamidine hydrochloride and other salts. The products obtained are of sufficient purity to use in the next step without further purification. For purposes of characterization, a small amount of material can be held back and purified by column chromatography in toluene. The product comes out with the solvent front and elutes with impurities which may be removed by washing with hexanes. This procedure is low-yielding due to the insolubility of the product in the eluent and is not recommended for purifying bulk quantities of the product.

S1.6 General Suzuki-Miyaura Cross-Coupling (E):

Modified from a previously reported procedure.[3] A Schlenk flask was charged with pyrimidine derivative (1.0 eq.) prepared in reaction D, *p*-formylphenylboronic acid (2.0 eq.), and potassium phosphate tribasic (1.8 eq.). A stir bar was added and the flask was transferred into an inert atmosphere glovebox wherein tris(dibenzylideneacetone)dipalladium(0) (0.03 eq.) and SPhos (0.12 eq.) were added. The flask was sealed with a rubber septum and transferred to a Schlenk line and the headspace was cycled three times between vacuum and nitrogen. Degassed toluene was added through the rubber septum cap via syringe, followed by 1/30th that volume of degassed water. The mixture was heated to 100°C and then the flask was sealed. Stirring was continued until the pyrimidine starting material is entirely consumed, as judged by TLC. The mixture was then exposed to air and allowed to cool to ambient temperature. The reaction was diluted in dichloromethane and poured into water in a separatory funnel. The organics were extracted three times with CH_2Cl_2 and the combined organic fractions were dried over $MgSO_4$, gravity filtered and the volatiles were removed by rotary evaporation. This crude solid residue was purified by column chromatography on silica.

S1.7 General Sodium Borohydride Reduction (F):

A previously reported procedure was used without modification.[3] In air, a round bottom flask was charged with pyrimidine derivative (1.0 eq.) which was dissolved in a 3:1 mixture of dichloromethane and ethanol. Solid $NaBH_4$ (1.2 eq.) was added and the mixture was stirred at ambient temperature until the aldehyde is completely consumed, as judged by TLC. The reaction was quenched by the slow addition of aqueous ammonium chloride until gas evolution ceases then poured into a separatory funnel containing water. The organic phase was extracted three times with dichloromethane and the combined organic extracts were dried over $MgSO_4$. The salt was removed by gravity filtration and volatile were removed by rotary evaporation. The crude residue was purified by column chromatography on silica.

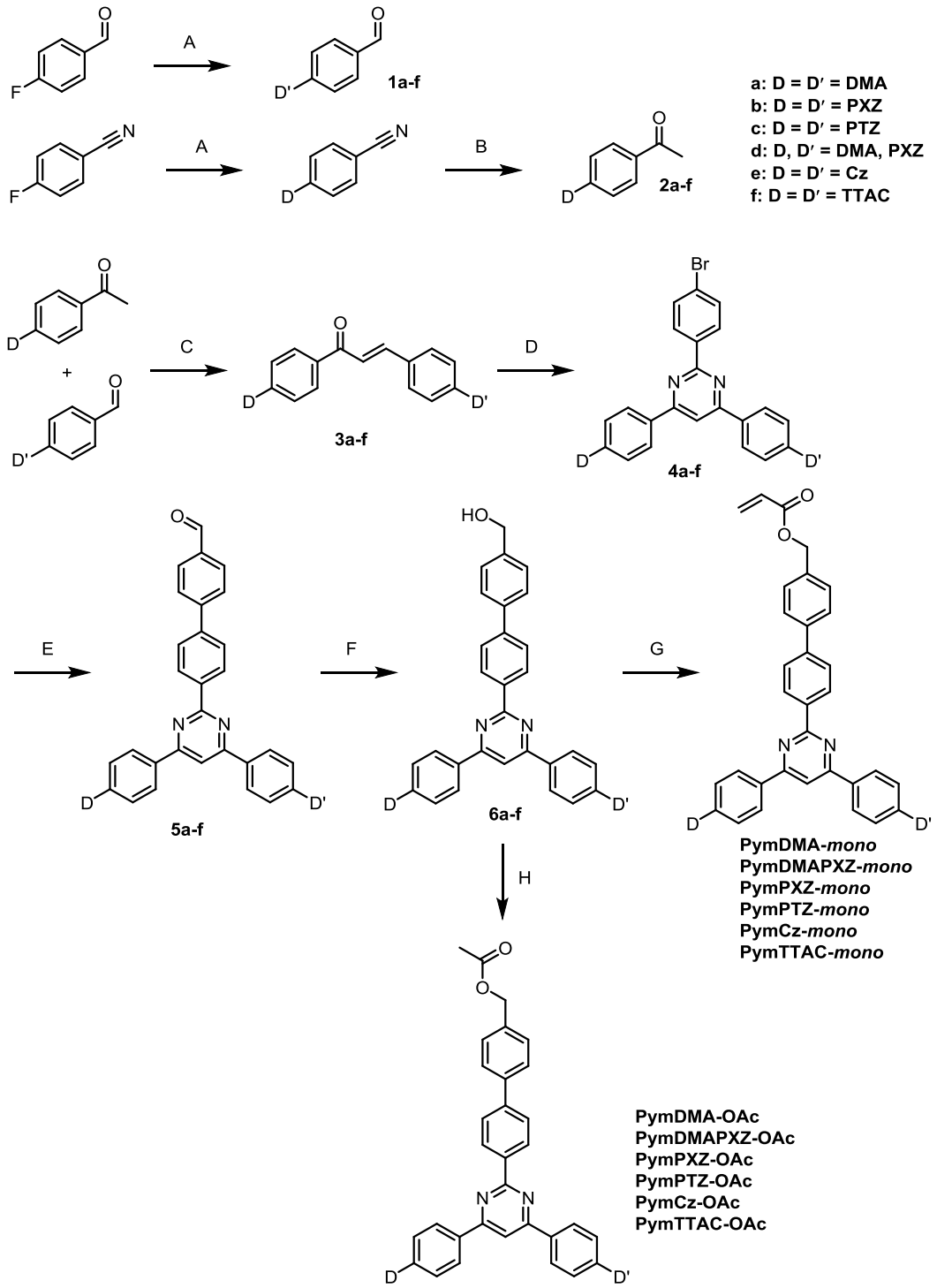
S1.8 General Acrylation (G):

Modified from a previously reported procedure.[3] A flame dried Schlenk flask was charged with pyrimidine derivative (1.0 eq.) and a magnetic stir bar and stoppered with a rubber septum. The headspace was cleared by three vacuum and N_2-backfill cycles. Freshly distilled dichloromethane was added to the solids through the septum cap. A solution of triethylamine in dichloromethane (1.3 eq.) was added through the septum, the mixture was cooled in an ice bath and stirred at this temperature for 30 minutes. Acryloyl chloride (1.2 eq.) diluted in dichloromethane was added dropwise to the mixture through the septum. The reaction was monitored by TLC and immediately quenched with aqueous ammonium chloride once the alcohol is completely consumed. The mixture is poured into a separatory funnel containing water and the organics are extracted three times with dichloromethane. The combined organic extracts are dried over $MgSO_4$, gravity filtered, and the solvent is removed by rotary evaporation at 30 °C, to avoid product losses by thermal decomposition. The crude residue is purified on silica using a short column, again to avoid losses due to decomposition on silica.

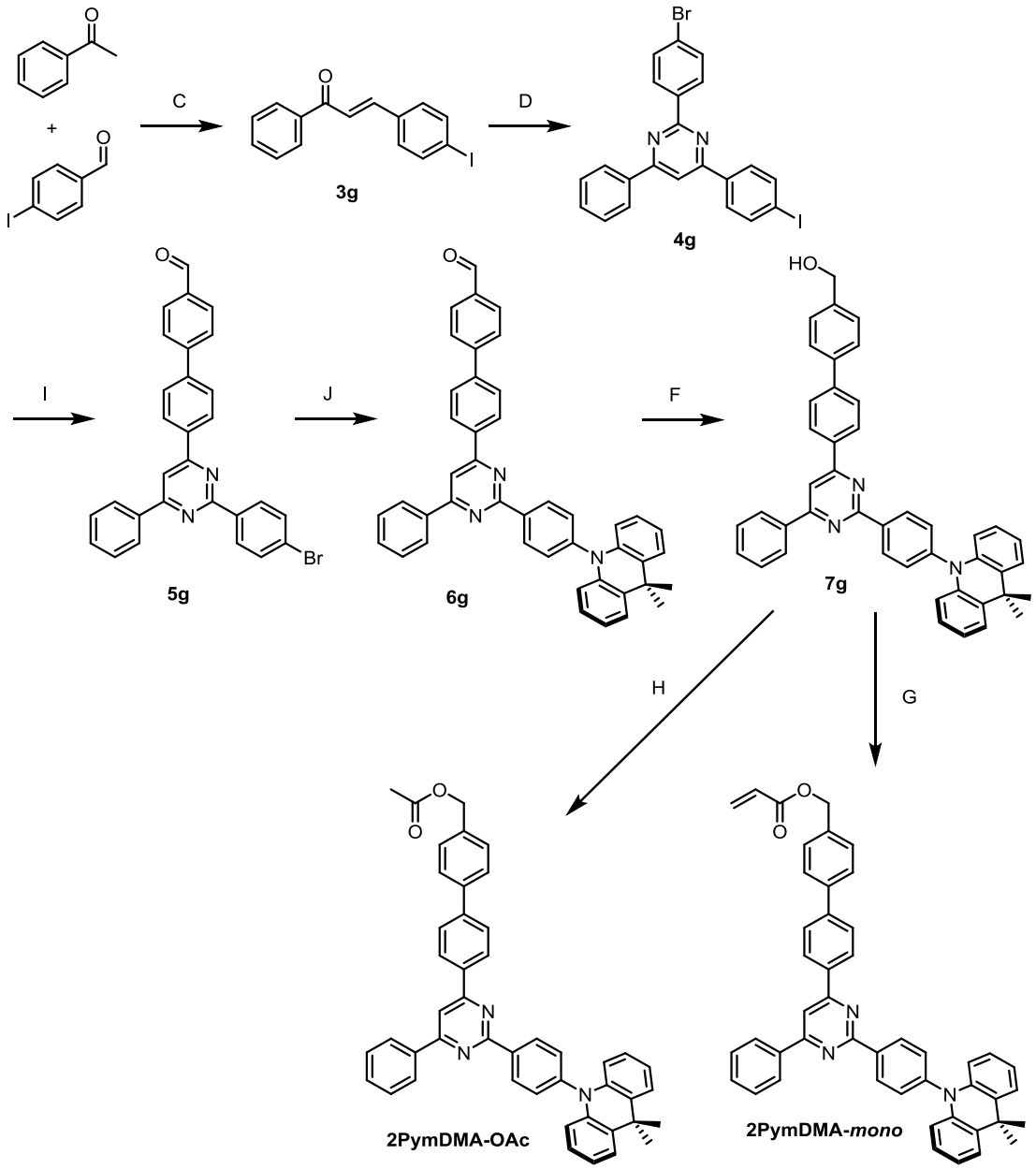
S1.9 General Acetylation (H):

A flame dried Schlenk flask was charged with pyrimidine derivative (1.0 eq.) and a magnetic stir bar and stoppered with a rubber septum. The headspace was cleared by three vacuum and N_2-backfill cycles. Freshly distilled dichloromethane was added to the solids through the septum cap. Triethylamine (15 eq.) and acetyl chloride (15 eq.) were added through the septum, the mixture was stirred at ambient temperature for 30 minutes then quenched with aqueous ammonium chloride. The mixture is poured into a separatory funnel containing water and the organic are extracted three times with dichloromethane. The combined organic extracts are dried over $MgSO_4$, gravity filtered, and the solvent is removed by rotary evaporation. The crude residue is purified on silica using a short column.

S1.10 Synthetic Schemes



Scheme S1. Synthetic scheme towards the monomers and acetate derivatives. See sections S2.2 – S2.9 for details regarding reactions A – H. Characterization for all compounds is given in section S2.11.



Scheme S2. Synthetic scheme towards the monomer **2PymDMA-*mono*** and acetate derivative. See section S1.11 for details regarding reactions I and J. Characterization for all compounds is given in section S1.11.

S1.11 Characterization Data

p-bromobenzamidinium hydrochloride. In air, a vial was charged with *p*-bromobenzonitrile (1.00 g, 5.49 mmol, 1.0 eq.), sodium methoxide (594 mg, 11.0 mmol, 2.0 eq.) and a magnetic stir bar were added. The vial was charged with 20 mL MeOH, sealed, and stirred at 35 °C for 48 h. The cap was removed and ammonium chloride (588 mg, 11.0 mmol, 2.0 eq.) was added. The vial was resealed and stirred for 24 h. The reaction mixture was filtered, and the filtrate concentrated to dryness. The crude solid residue was purified on silica (gradient 1:9 MeOH/CH_2Cl_2 to 1:1 MeOH/CH_2Cl_2 v/v). White solid. Yield 853 mg (66%). **^{1}H NMR:** (400 MHz, DMSO-d_6) δ 9.78 – 9.23 (br, 4H, NH_2), 7.92 – 7.73 (m, 4H, CH_{Ph}). These data are consistent with literature values.[5]

4-(9,9-dimethylacridin-10(9H)-yl)benzaldehyde (**1a**). Prepared according to general reaction A, using 9,9-dimethyl-9,10-dihydroacridine (1.00 g, 4.78 mmol, 1.0 eq.), *p*-fluorobenzaldehyde (1.03 mL, 9.56 mmol, 2.0 eq.) in 100 mL DMF for 48 h. Purified on silica (1:11 EtOAc/Hexanes v/v). Pale yellow solid. Yield 1.02 g (68%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 10.13 (s, 1H, CHO), 8.13 (d, J = 8.4 Hz, 2H, CH_{Ph}), 7.54 (d, J = 8.4 Hz, 2H, CH_{Ph}), 7.51 – 7.40 (dd, ^3J = 7.5 HZ, ^4J = 1.8 Hz, 2H, CH_{DMA}), 7.14 – 6.85 (m, 4H, CH_{DMA}), 6.33 (dd, ^3J = 7.9 Hz, ^4J = 2.2 Hz, 2H, CH_{DMA}), 1.69 (s, 6H, CH_3). These data are consistent with literature values.[6]

4-(10H-phenoxazin-10-yl)benzaldehyde (**1b**). Prepared according to general reaction A, using phenoxazine (920 mg, 5.02 mmol, 1.0 eq.), *p*-fluorobenzaldehyde (1.25 g, 10.0 mmol, 2.0 eq.) in 90 mL DMF for 28 h. Purified on silica (1:19 EtOAc/Hexanes v/v). Orange solid. Yield 1.07 g (74%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 10.11 (s, 1H, CHO), 8.12 (d, J = 8.4 Hz, 2H, CH_{Ph}), 7.56 (d, J = 8.4 Hz, 2H, CH_{Ph}), 6.77 – 6.66 (m, 4H, CH_{PXZ}), 6.62 (ddd, ^3J = 9.0, 7.2, ^4J = 1.9 Hz, 2H, CH_{PXZ}), 5.96 (dd, ^3J = 7.9, ^4J = 1.9 Hz, 2H, CH_{PXZ}). These data are consistent with literature values.[7]

4-(10H-phenothiazin-10-yl)benzaldehyde (**1c**). Prepared according to general reaction A, using phenothiazine (5.00 g, 25.1 mmol, 1.0 eq.), *p*-fluorobenzaldehyde (5.38 mL, 50.2 mmol, 2.0 eq.) in 500 mL DMF for 48 h. Purified on silica (1:11 EtOAc/Hexanes v/v). Off-white solid. Yield 3.87 g (51%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 9.86 (s, 1H, CHO), 7.76 (d, J = 8.1 Hz, 2H, CH_{Ph}), 7.42 (d, J = 8.1 Hz, 2H, CH_{Ph}), 7.34 – 7.24 (m, 4H, CH_{PTZ}), 7.22 – 7.11 (m, 4H, CH_{PTZ}). These data are consistent with literature values.[7]

(4-(9H-carbazol-9-yl)benzaldehyde (**1e**). Prepared according to general reaction A, using carbazole (6.00 g, 35.9 mmol, 1.0 eq.), *p*-fluorobenzaldehyde (7.70 mL, 71.8 mmol, 2.0 eq.) in 500 mL DMF for 48 h. Purified on silica (1:11 EtOAc/Hexanes v/v). Off-white solid. Yield 4.28 g (44%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 10.12 (s, 1H, CHO), 8.18 – 8.10 (m, 4H, CH_{Ph} and CH_{Cz}), 7.80 (d, J = 8.4 Hz, 2H, CH_{Ph}), 7.51 (d, J = 8.2 Hz, 2H, CH_{Cz}), 7.45 (dd, J = 8.2, 8.2 Hz, 2H, CH_{Cz}), 7.34 (dd, J = 8.2, 8.2 Hz, 2H, CH_{Cz}). These data are consistent with literature values.[8]

4-(3,6-bis(di-p-tolylamino)-9H-carbazol-9-yl)benzaldehyde (**1f**) Prepared according to general reaction A, using N^3,N^3,N^6,N^6-tetra-*p*-tolyl-9*H*-carbazole-3,6-diamine (900 mg, 1.61 mmol, 1.0 eq.), *p*-fluorobenzaldehyde (350 µL, 3.23 mmol, 2.0 eq.) in 150 mL DMF for 40 h. Purified on silica (1:11 EtOAc/Hexanes v/v). Orange solid. Yield = 812 mg (76%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 10.10 (s, 1H, CHO), 8.11 (d, J = 8.5 Hz, 2H, CH_{Ph}), 7.79 (d, J = 8.5 Hz, 2H, CH_{Ph}), 7.70 (d, ^4J = 2.1 Hz, 2H, CH_{Cz}), 7.39 (d, J = 8.8 Hz, 2H, CH_{Cz}), 7.18 (dd, ^3J = 8.8, ^4J = 2.1 Hz, 2H, CH_{Cz}), 7.02 (d, J = 8.4 Hz, 8H, CH_{tol}), 6.96 (d, J = 8.4 Hz, 8H, CH_{tol}), 2.29 (s, 12H, CH_3). **^{13}C{^{1}H} NMR:** (101 MHz, Chloroform-*d*) δ 191.0, 146.3, 143.6, 142.1, 137.9, 134.5, 131.6, 131.4, 129.1, 126.5, 125.4, 124.9, 123.2, 117.8, 111.7, 21.5. **HRMS (APCI) *m/z*:** $[M]^+$ calc'd for $[C_{47}H_{39}N_3O]^+$ 661.3093; found 661.3091; difference -0.3 ppm.

4-(9,9-dimethylacridin-10(9H)-yl)benzonitrile. Prepared according to general reaction A, using 9,9-dimethyl-9,10-dihydroacridine (2.09 g, 10.0 mmol, 1.0 eq.), *p*-fluorobenzonitrile (2.42 g, 20.0 mmol, 2.0 eq.) in 170 mL DMF for 48 h. Purified on silica (1:11 EtOAc/Hexanes v/v). Pale yellow solid. Yield 2.65 g (85%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 7.91 (d, *J* = 8.5 Hz, 2H, CH_{Ph}), 7.53 – 7.46 (m, 4H, CH_{Ph} and CH_{DMA}), 7.10 – 6.83 (m, 4H, CH_{DMA}), 6.45 – 6.13 (dd, ^3J = 7.9 Hz, ^4J = 2.2 HZ, 2H, CH_{DMA}), 1.69 (s, 6H, CH_3). These data are consistent with literature values.[9]

4-(10H-phenoxazin-10-yl)benzonitrile. Prepared according to general reaction A, using phenoxazine (1.20 g, 6.55 mmol, 1.0 eq.), *p*-fluorobenzonitrile (1.59 g, 13.1 mmol, 2.0 eq.) in 100 mL DMF for 20 h. Purified on silica (1:9 EtOAc/Hexanes v/v). Yellow solid. Yield 1.35 g (72%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 7.90 (d, *J* = 8.5 Hz, 2H, CH_{Ph}), 7.51 (d, *J* = 8.5 Hz, 2H, CH_{Ph}), 6.88 – 6.68 (m, 4H, CH_{PXZ}), 6.63 (ddd, ^3J = 7.9, 6.9 Hz, ^4J = 2.1 Hz, 2H, CH_{PXZ}), 5.93 (dd, ^4J = 6.9, ^3J = 1.4 Hz, 2H, CH_{PXZ}). These data are consistent with literature values.[10]

4-(10H-phenothiazin-10-yl)benzonitrile. Prepared according to general reaction A, using phenothiazine (5.00 g, 25.1 mmol, 1.0 eq.), *p*-fluorobenzonitrile (6.08 g, 50.2 mmol, 2.0 eq.) in 500 mL DMF for 18 h. Purified on silica (1:9 EtOAc/Hexanes v/v). Yellow solid. Yield 4.88 g (65%). **^{1}H NMR:** ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.48 (d, *J* = 9.0 Hz, 2H, CH_{Ph}), 7.44 (dd, ^3J = 7.7 Hz, ^4J = 1.7 Hz, 2H, CH_{PTZ}), 7.36 – 7.24 (m, 4H, CH_{PTZ}), 7.20 (ddd, ^3J = 7.7, 6.8 Hz, ^4J = 1.7 Hz, 2H, CH_{PTZ}), 7.07 (d, *J* = 9.0 Hz, 2H, CH_{Ph}).These data are consistent with literature values.[11]

4-(3,6-bis(di-p-tolylamino)-9H-carbazol-9-yl)benzonitrile. Prepared according to general reaction A, using N^3,N^3,N^6,N^6-tetra-*p*-tolyl-9*H*-carbazole-3,6-diamine (900 mg, 1.61 mmol, 1.0 eq.), *p*-fluorobenzonitrile (391 mg, 3.23 mmol, 2.0 eq.) in 150 mL DMF for 16 h. Purified on silica (1:11 EtOAc/Hexanes v/v). Recrystallized from CH_2Cl_2/MeOH. Yellow solid. Yield = 894 mg (84%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 7.89 (d, *J* = 8.5 Hz, 2H, CH_{Ph}), 7.73 (d, *J* = 8.5 Hz, 2H, CH_{Ph}), 7.69 (d, ^4J = 2.1 Hz, 2H, CH_{Cz}), 7.34 (d, *J* = 8.8 Hz, 2H, CH_{Cz}), 7.18 (dd, ^3J = 8.8, ^4J = 2.1 Hz, 2H, CH_{Cz}), 7.02 (d, *J* = 8.4 Hz, 8H, CH_{tol}), 6.95 (d, *J* = 8.4 Hz, 8H, CH_{tol}), 2.29 (s, 12H, CH_3). **^{13}C{^{1}H} NMR:** (101 MHz, Chloroform-*d*) δ 146.3, 142.3, 142.3, 136.9, 134.1, 131.5, 129.9, 126.8, 125.4, 124.9, 123.2, 118.5, 117.7, 110.5, 110.2, 20.9. **HRMS (APCI) *m/z*:** $[M]^+$ calc'd for $[C_{47}H_{38}N_4]^+$ 658.3096; found 658.3094; difference -0.3 ppm.

1-(4-(9,9-dimethylacridin-10(9H)-yl)phenyl)ethan-1-one (**2a**). Prepared according to general reaction B, using (9,9-dimethylacridin-10(9*H*)-yl)benzonitrile (1.33 g, 4.29 mmol, 1.0 eq.) and 4.00 mL (1.5 eq.) 1.6 M MeLi in diethyl ether, in 25 mL THF for 3 h. Purified on silica (1:11 EtOAc/Hexanes v/v). Pale yellow solid. Yield 1.31 g (93%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 8.22 (d, *J* = 8.5 Hz, 2H, CH_{Ph}), 7.57 – 7.39 (m, 4H, CH_{Ph} and CH_{DMA}), 7.11 – 6.86 (m, 4H, CH_{DMA}), 6.28 (dd, ^3J = 7.6, ^4J = 1.9 Hz, 2H, CH_{DMA}), 2.71 (s, 3H, $C(O)CH_3$), 1.70 (s, 6H, CH_3). **^{13}C{^{1}H} NMR:** (101 MHz, Chloroform-*d*) δ 197.4, 146.2, 140.6, 136.7, 131.3, 131.1, 130.8, 126.6, 125.5, 121.2, 114.4, 36.2, 31.2, 26.9. **HRMS (APCI) *m/z*:** $[M+H]^+$ calc'd for $[C_{23}H_{22}NO]^+$ 328.1701; found 328.1703; difference +0.6 ppm.

1-(4-(10H-phenoxazin-10-yl)phenyl)ethan-1-one (**2b**). Prepared according to general reaction B, using 4-(10*H*-phenoxazin-10-yl)benzonitrile (875 mg, 3.08 mmol, 1.0 eq.) and 2.90 mL (1.5 eq.) 1.6 M MeLi in diethyl ether, in 30 mL THF for 3 h. Purified on silica (1:9 EtOAc/Hexanes v/v). Orange solid. Yield 828 mg (89%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 8.18 (d, *J* = 8.5 Hz, 2H, CH_{Ph}), 7.47 (d, *J* = 8.5 Hz, 2H, CH_{Ph}), 6.70 (m, 4H, CH_{PXZ}), 6.60 (ddd, ^3J = 7.9, 7.2 Hz, ^4J = 1.6 Hz, 2H, CH_{PXZ}), 5.94 (dd, ^3J = 7.2, ^4J = 1.6 Hz, 2H, CH_{PXZ}), 2.68 (s, 3H, $C(O)CH_3$). These data are consistent with literature values.[12]

1-(4-(10H-phenothiazin-10-yl)phenyl)ethan-1-one (**2c**). Prepared according to general reaction B, using 4-(10*H*-phenothiazin-10-yl)benzonitrile (2.00 g, 6.66 mmol, 1.0 eq.) and 6.24 mL (1.5 eq.) 1.6 M MeLi in diethyl ether, in 25 mL THF for 3 h. Purified on silica (1:7 EtOAc/Hexanes v/v gradient to 1:1

EtOAc/Hexanes). Orange solid. Yield 1.82 g (87%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 7.95 (d, *J* = 8.8 Hz, 2H, CH_{Ph}), 7.31 (dd, ^3J = 7.7, ^4J = 1.6 Hz, 2H, CH_{PTZ}), 7.24 – 7.13 (m, 4H, CH_{Ph} and CH_{PTZ}), 7.08 (ddd, ^3J = 7.6, 7.6 Hz, ^4J = 1.6 Hz, 2H, CH_{PTZ}), 6.98 (dd, *J* = 7.6 Hz, ^4J = 1.6 Hz, 2H, CH_{PTZ}), 2.57 (s, 3H, $C(O)CH_3$). These data are consistent with literature values.[12]

1-(4-(9H-carbazol-9-yl)phenyl)ethan-1-one (**2e**). Prepared according to general reaction A, using carbazole (2.00 g, 12.0 mmol, 1.0 eq.), *p*-fluoroacetophenone (2.90 mL, 23.9 mmol, 2.0 eq.) in 170 mL DMF for 72 h. Purified on silica (1:9 EtOAc/Hexanes v/v). Off-white solid. Yield 1.30 g (38%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 8.21 (d, *J* = 8.3 Hz, 2H, CH_{Ph}), 8.16 (d, *J* = 7.6 Hz, 2H, CH_{Cz}), 7.71 (d, *J* = 8.3 Hz, 2H, CH_{Ph}), 7.49 (d, *J* = 8.2 Hz, 2H, CH_{Cz}), 7.44 (dd, *J* = 8.2, 8.2 Hz, 2H, CH_{Cz}), 7.37 – 7.29 (dd, *J* = 8.2, 8.2 Hz, 2H, CH_{Cz}), 2.71 (s, 3H, $C(O)CH_3$). These data are consistent with literature values.[13]

1-(4-(3,6-bis(di-p-tolylamino)-9H-carbazol-9-yl)phenyl)ethan-1-one (**2f**). Prepared according to general reaction B, using 4-(3,6-bis(di-*p*-tolylamino)-9*H*-carbazol-9-yl)benzonitrile (800 mg, 1.21 mmol, 1.0 eq.) and 1.10 mL (1.82 mmol, 1.5 eq.) 1.6 M MeLi in diethyl ether, in 30 mL THF for 3 h. Purified on silica (1:9 EtOAc/Hexanes v/v). Yellow solid. Yield 802 mg (98%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 8.19 (d, *J* = 8.2 Hz, 2H, CH_{Ph}), 7.71 (m, 4H, CH_{Ph} and CH_{Cz}), 7.37 (d, *J* = 8.8 Hz, 2H, CH_{Cz}), 7.18 (dd, *J* = 8.8, 2.2 Hz, 2H, CH_{Cz}), 7.02 (d, *J* = 8.2 Hz, 8H, CH_{tol}), 6.96 (d, *J* = 8.2 Hz, 8H, CH_{tol}), 2.69 (s, 3H, $C(O)CH_3$), 2.29 (s, 12H, CH_3). **^{13}C{^{1}H} NMR:** (101 MHz, Chloroform-*d*) δ 196.3, 148.0, 143.2, 141.9, 137.3, 135.4, 131.4, 130.3, 129.9, 126.7, 125.4, 124.7, 123.1, 119.0, 111.3, 26.8, 20.9. **HRMS (APCI) *m/z*:** $[M]^+$ calc'd for $[C_{48}H_{41}N_3O]^+$ 675.3250; found 675.3253; difference +0.4 ppm.

(E)-1,3-bis(4-(9,9-dimethylacridin-10(9H)-yl)phenyl)prop-2-en-1-one (**3a**). Prepared according to general reaction C using **2a** (500 mg, 1.53 mmol, 1.0 eq.) and **1a** (479 mg, 1.53 mmol, 1.0 eq.) in 80 mL ethanol, with 122 mg sodium hydroxide (3.05 mmol, 2.0 eq.) in 20 mL ethanol at 40 °C for 24 hours. Yellow solid. Yield 698 mg (73 %). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 8.32 (d, *J* = 8.4 Hz, 2H, CH_{Ph}), 8.01 (d, J_{trans} = 15.7 Hz, 1H, CH_{vinyl}), 7.95 (d, *J* = 8.4 Hz, 2H, CH_{Ph}), 7.71 (d, J_{trans} = 15.7 Hz, 1H, CH_{vinyl}), 7.53 (d, *J* = 8.4 Hz, 2H, CH_{Ph}), 7.51 – 7.46 (m, 4H, CH_{DMA}), 7.44 (d, *J* = 8.4 Hz, 2H, CH_{Ph}), 7.04 – 6.92 (m, 8H, CH_{DMA}), 6.37 – 6.29 (m, 4H, CH_{DMA}), 1.71 (s, 12H, CH_3). **^{13}C{^{1}H} NMR:** (101 MHz, Chloroform-*d*) δ 189.5, 146.0, 144.2, 143.7, 140.7, 140.6, 137.7, 134.8, 132.1, 131.3, 131.2, 131.1, 130.9, 130.4, 126.6, 125.5, 125.5, 122.7, 121.3, 121.0, 114.5, 114.2, 36.2, 36.2, 31.4, 31.3. **HRMS (APCI) *m/z*:** $[M+H]^+$ calc'd for $[C_{45}H_{39}N_2O]^+$ 623.3062; found 623.3063; difference +0.2 ppm.

(E)-1,3-bis(4-(10H-phenoxazin-10-yl)phenyl)prop-2-en-1-one (**3b**). Prepared according to general reaction C using **2b** (500 mg, 1.66 mmol, 1.0 eq.) and **1b** (477 mg, 1.66 mmol, 1.0 eq.) in 80 mL ethanol, with 133 mg sodium hydroxide (3.32 mmol, 2.0 eq.) in 20 mL ethanol at 40 °C for 22 hours. Recrystallized from minimal CH_2Cl_2 and methanol. Red solid. Yield 347 mg (37 %). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 8.28 (d, *J* = 8.4 Hz, 2H, CH_{Ph}), 7.95 (d, J_{trans} = 15.7 Hz, 1H, CH_{vinyl}), 7.90 (d, *J* = 8.4 Hz, 2H, CH_{Ph}), 7.64 (d, J_{trans} = 15.7 Hz, 1H, CH_{vinyl}), 7.54 (d, *J* = 8.4 Hz, 2H, CH_{Ph}), 7.45 (d, *J* = 8.4 Hz, 2H, CH_{Ph}), 6.82 – 6.55 (m, 12H, CH_{PXZ}), 5.99 (d, *J* = 7.9, 4H, CH_{PXZ}). **^{13}C{^{1}H} NMR:** (101 MHz, Chloroform-*d*) δ 189.9, 144.2, 144.1, 143.7, 141.4, 138.0, 135.0, 134.0, 133.8, 131.7, 131.4, 131.3, 131.2, 123.5, 122.8, 122.0, 121.8, 115.9, 115.8, 113.5, 113.4. **HRMS (APCI) *m/z*:** $[M]^+$ calc'd for $[C_{39}H_{26}N_2O_3]^+$ 570.1943; found 570.1948; difference +0.9 ppm.

(E)-1,3-bis(4-(10H-phenothiazin-10-yl)phenyl)prop-2-en-1-one (**3c**). Prepared according to general reaction C using **2c** (1.70 g, 5.60 mmol, 1.0 eq.) and **1c** (1.78 g, 5.60 mmol, 1.0 eq.) in 100 mL ethanol, with 448 mg sodium hydroxide (11.2 mmol, 2.0 eq.) in 20 mL ethanol at 40 °C for 18 hours. Orange solid. Yield 2.89 g (86 %). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 8.06 (d, *J* = 8.7 Hz, 2H, CH_{Ph}), 7.86 (d, J_{trans} = 15.6 Hz, 1H, CH_{vinyl}), 7.75 (d, *J* = 8.5 Hz, 2H, CH_{Ph}), 7.54 (d, J_{trans} = 15.6 Hz, 1H, CH_{vinyl}), 7.37 – 7.30 (m,

4H, CH_{Ph} and CH_{PTZ}), 7.27 (d, J = 8.7 Hz, 2H, CH_{Ph}), 7.22 – 7.14 (m, 4H, CH_{PTZ}), 7.10 (ddd, ^3J = 7.5, 7.5 Hz, ^4J = 1.4 Hz, 2H, CH_{PTZ}), 7.05 – 6.98 (m, 4H, CH_{PTZ}), 6.95 (ddd, ^3J = 7.5, 7.5 Hz, ^4J = 1.4 Hz, 2H), 6.60 (dd, J = 7.5, 1.4 Hz, 2H). **$^{13}C\{^1H\}$ NMR:** (101 MHz, Chloroform-*d*) δ 188.6, 148.2, 144.5, 143.4, 143.3, 142.2, 133.5, 132.9, 130.8, 130.6, 129.5, 128.4, 127.6, 127.3, 127.2, 126.7, 125.2, 124.7, 123.9, 123.2, 121.7, 120.7, 119.5. **HRMS (APCI) *m/z*:** $[M]^+$ calc'd for $[C_{39}H_{26}N_2OS_2]^+$ 602.1487; found 602.1493; difference +1.0 ppm.

(E)-1-(4-(10H-phenoxazin-10-yl)phenyl)-3-(4-(9,9-dimethylacridin-10(9H)-yl)phenyl)prop-2-en-1-one (**3d**). Prepared according to general reaction C using **2b** (600 mg, 1.99 mmol, 1.0 eq.) and **1a** (623 mg, 1.99 mmol, 1.0 eq.) in 120 mL ethanol, with 159 mg sodium hydroxide (3.98 mmol, 2.0 eq.) in 20 mL ethanol at 40 °C for 18 hours. Orange solid. Yield 962 mg (81 %). **^1H NMR:** (400 MHz, Chloroform-*d*) δ 8.32 (d, J = 8.4 Hz, 2H, CH_{Ph}), 8.02 (d, J_{trans} = 15.7 Hz, 1H, CH_{vinyl}), 7.97 (d, J = 8.3 Hz, 2H, CH_{Ph}), 7.69 (d, J_{trans} = 15.7 Hz, 1H, CH_{vinyl}), 7.57 (d, J = 8.4 Hz, 2H, CH_{Ph}), 7.51 (dd, J = 7.4, 1.9 Hz, 2H, CH_{DMA}), 7.46 (d, J = 8.3 Hz, 2H, CH_{Ph}), 7.11 – 6.90 (m, 4H, CH_{DMA}), 6.80 – 6.69 (m, 4H, CH_{PXZ}), 6.66 (ddd, ^3J = 7.6, 7.6 Hz, ^4J = 1.9 Hz, 2H, CH_{PXZ}), 6.35 (dd, J = 7.9, 1.6 Hz, 2H, CH_{DMA}), 6.03 (dd, ^3J = 7.6 Hz, ^4J = 1.9 Hz, 2H, CH_{PXZ}), 1.73 (s, 6H). **$^{13}C\{^1H\}$ NMR:** (101 MHz, Chloroform-*d*) δ 189.2, 144.3, 144.1, 143.6, 143.5, 140.6, 137.9, 134.6, 133.7, 131.9, 131.3, 131.2, 131.0, 130.4, 126.4, 125.4, 123.3, 122.5, 121.9, 120.9, 115.8, 114.1, 113.4, 36.0, 31.2. **HRMS (APCI) *m/z*:** $[M]^+$ calc'd for $[C_{42}H_{32}N_2O_2]^+$ 596.2464; found 596.2463; difference -0.2 ppm.

(E)-1,3-bis(4(9H-carbazol-9-yl)phenyl)prop-2-en-1-one (**3e**). Prepared according to general reaction C using **2e** (1.35 g, 4.73 mmol, 1.0 eq.) and **1e** (1.28 g, 4.73 mmol, 1.0 eq.) in 150 mL ethanol, with 378 mg sodium hydroxide (9.46 mmol, 2.0 eq.) in 50 mL ethanol at 40 °C for 18 hours. Yellow solid. Yield 1.73 g (68 %). **^1H NMR:** (400 MHz, Chloroform-*d*) δ 8.34 (d, J = 8.5 Hz, 2H, CH_{Ph}), 8.17 (d, J = 7.8 Hz, 4H, CH_{Cz}), 8.02 (d, J_{trans} = 15.7 Hz, 1H, CH_{vinyl}), 7.94 (d, J = 8.4 Hz, 2H, CH_{Ph}), 7.80 (d, J = 8.4 Hz, 2H, CH_{Ph}), 7.72 (d, J_{trans} = 15.7 Hz, 1H, CH_{vinyl}), 7.70 (d, J = 8.4 Hz, 2H, CH_{Ph}), 7.58 – 7.41 (m, 8H, CH_{Cz}), 7.39 – 7.29 (m, 4H, CH_{Cz}). **$^{13}C\{^1H\}$ NMR:** (101 MHz, Chloroform-*d*) δ 188.3, 144.2, 142.2, 140.6, 140.4, 140.0, 136.7, 134.6, 130.5, 130.2, 127.9, 126.8, 126.4, 126.3, 124.0, 123.9, 122.8, 120.8, 120.6, 120.6, 109.9. **HRMS (APCI) *m/z*:** $[M]^+$ calc'd for $[C_{39}H_{26}N_2O]^+$ 538.2045; found 538.2050; difference +0.9 ppm.

(E)-1,3-bis(4-(3,6-bis(di-p-tolylamino)-9H-carbazol-9-yl)phenyl)prop-2-en-1-one (**3f**). Prepared according to general reaction C using **2f** (715 mg, 1.06 mmol, 1.0 eq.) and **1f** (700 mg, 1.06 mmol, 1.0 eq.) in 180 mL ethanol, with 85 mg sodium hydroxide (2.12 mmol, 2.0 eq.) in 20 mL ethanol at 50 °C for 36 hours. Orange solid. Yield 797 mg (57 %). **^1H NMR:** (400 MHz, Chloroform-*d*) δ 8.30 (d, J = 8.3 Hz, 2H, CH_{Ph}), 7.99 (d, J_{trans} = 15.6 Hz, 1H, CH_{vinyl}), 7.91 (d, J = 8.2 Hz, 2H, CH_{Ph}), 7.77 (d, J = 8.3 Hz, 2H, CH_{Ph}), 7.74 – 7.64 (m, 7H, CH_{Cz} (4H), CH_{Ph} (2H) and CH_{vinyl} (1H)), 7.41 (d, J = 8.8 Hz, 2H, CH_{Cz}), 7.38 (d, J = 8.8 Hz, 2H, CH_{Cz}), 7.20 (d, J = 8.8, 4H, CH_{Cz}), 7.03 (d, J = 8.1 Hz, 16H, CH_{tol}), 6.97 (d, J = 8.1 Hz, 16H, CH_{tol}), 2.30 (s, 32H, CH_3). **$^{13}C\{^1H\}$ NMR:** (101 MHz, Chloroform-*d*) δ 189.0, 146.3, 144.1, 141.9, 141.7, 137.6, 137.3, 136.4, 133.5, 131.4, 131.3, 130.5, 130.2, 129.9, 129.2, 128.4, 126.9, 126.3, 123.1, 123.1, 122.1, 118.3, 110.8, 20.9. **HRMS (FD) *m/z*:** $[M]^+$ calc'd for $[C_{95}H_{78}N_6O]^+$ 1318.6237; found 1318.6248; difference +0.8 ppm.

(E)-3-(4-iodophenyl)-1-phenylprop-2-en-1-one (**3g**). Prepared according to general reaction C using acetophenone (0.50 mL, 4.28 mmol, 1.0 eq.) and 4-iodobenzaldehyde (995 mg, 4.28 mmol, 1.0 eq.) with 341 mg sodium hydroxide (8.56 mmol, 2.0 eq.) in 50 mL ethanol at 25 °C for 20 hours**. ^1H NMR:** (400 MHz, Chloroform-*d*) δ 8.08 – 7.94 (d, J = 7.8 Hz, 2H), 7.76 (d, J = 8.2 Hz, 2H, CH_{PhI}), 7.72 (d, J_{trans} = 15.8 Hz, 1H, CH_{vinyl}), 7.63 – 7.56 (t, 1H, J = 7.2 Hz, CH_{Ph}), 7.56 – 7.45 (m, 3H, CH_{Ph} and CH_{vinyl}), 7.37 (d, J = 8.2 Hz, 2H, CH_{PhI}). These data are consistent with literature values.[14]

10,10'-((2-(4-bromophenyl)pyrimidine-4,6-diyl)bis(4,1-phenylene))bis(9,9-dimethyl-9,10-dihydroacridine) (**4a**). Prepared according to general reaction D using 500 mg **3a** (0.801 mmol, 1.0 eq.), 284 mg *p*-bromobenzamidine hydrochloride (1.20 mmol, 1.5 eq.) and 388 mg K_2CO_3 (2.81 mmol, 3.5 eq.) in 120 mL dimethylformamide for 18 hours at 90 °C. Yellow solid. Yield 531 mg (83 %; purity ~75 – 80%). After column chromatography, the purity can be improved to ~90 – 95%, with loss of yield. **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 8.67 (d, *J* = 8.6 Hz, 2H, CH_{PhBr}), 8.57 (d, *J* = 8.4 Hz, 4H, CH_{Ph}), 8.22 (s, 1H, CH_{Pym}), 7.71 (d, *J* = 8.6 Hz, 2H, CH_{PhBr}), 7.58 (d, *J* = 8.4 Hz, 4H, CH_{Ph}), 7.50 (dd, *J* = 7.5, 1.8 Hz, 4H, CH_{DMA}), 7.05 – 6.93 (m, 8H, CH_{DMA}), 6.38 (dd, *J* = 7.9, 1.6 Hz, 4H, CH_{DMA}), 1.73 (s, 12H, CH_3). **^{13}C{^{1}H} NMR:** (101 MHz, Chloroform-*d*) δ 164.5, 164.1, 144.2, 140.8, 137.2, 136.9, 132.2, 132.0, 130.4, 130.3, 130.1, 129.0, 126.6, 125.5, 121.0, 114.3, 111.6, 36.6, 31.5. **HRMS (FD) *m/z*:** $[M]^+$ calc'd for $[C_{52}H_{41}BrN_4]^+$ 802.2494; found 802.2482; difference -1.5 ppm.

10,10'-((2-(4-bromophenyl)pyrimidine-4,6-diyl)bis(4,1-phenylene))bis(10H-phenoxazine) (**4b**). Prepared according to general reaction D using 350 mg **3b** (0.613 mmol, 1.0 eq.), 217 mg *p*-bromobenzamidine hydrochloride (0.920 mmol, 1.5 eq.) and 297 mg K_2CO_3 (2.15 mmol, 3.5 eq.) in 50 mL dimethylformamide for 18 hours at 90 °C. Yellow solid. Yield 342 mg (74 %). The solubility of this compound is insufficient for characterization by NMR spectroscopy. **HRMS (FD) *m/z*:** $[M]^+$ calc'd for $[C_{46}H_{29}BrN_4O_2]^+$ 748.1474; found 748.1446; difference -3.7 ppm.

10,10'-((2-(4-bromophenyl)pyrimidine-4,6-diyl)bis(4,1-phenylene))bis(10H-phenothiazine) (**4c**). Prepared according to general reaction D using 2.13 g **3c** (3.54 mmol, 1.0 eq.), 1.25 g *p*-bromobenzamidine hydrochloride (5.31 mmol, 1.5 eq.) and 1.71 g K_2CO_3 (12.4 mmol, 3.5 eq.) in 250 mL dimethylformamide for 18 hours at 80 °C. The starting materials were removed by column chromatography on silica using toluene as eluent. Yellow solid. Yield 528 mg (19 %). **^{1}H NMR**: (400 MHz, Chloroform-*d*) δ 8.62 (d, *J* = 8.5 Hz, 2H, CH_{PhBr}), 8.43 (d, *J* = 8.6 Hz, 4H, CH_{Ph}), 8.07 (s, 1H, CH_{Pym}), 7.68 (d, *J* = 8.6 Hz, 2H, CH_{PhBr}), 7.51 (d, *J* = 8.5 Hz, 4H, CH_{Ph}), 7.17 (dd, ^3J = 7.5 Hz, ^4J = 1.7 Hz, 4H, CH_{PTZ}), 6.98 (ddd, ^3J = 8.0, 7.5, ^4J = 1.5 Hz, 8H, CH_{PTZ}), 6.61 (dd, *J* = 8.0, 1.4 Hz, 4H, CH_{PTZ}). **^{13}C NMR**: (101 MHz, Chloroform-*d*) δ 164.3, 164.0, 145.0, 143.5, 137.0, 135.4, 131.9, 130.6, 130.2, 129.6, 129.2, 128.4, 127.6, 127.6, 127.2, 125.8, 124.1, 123.8, 119.0, 110.3. **HRMS (FD) *m/z*:** $[M]^+$ calc'd for $[C_{46}H_{29}BrN_4S_2]^+$ 780.1017; found 780.0987; difference -3.8 ppm.

10-(4-(2-(4-bromophenyl)-6-(4-(9,9-dimethylacridin-10(9H)-yl)phenyl)pyrimidin-4-yl)phenyl)-10H-phenoxazine (**4d**). Prepared according to general reaction D using 380 mg **3d** (0.637 mmol, 1.0 eq.), 225 mg *p*-bromobenzamidine hydrochloride (0.955 mmol, 1.5 eq.) and 308 mg K_2CO_3 (2.23 mmol, 3.5 eq.) in 100 mL dimethylformamide for 24 hours at 90 °C. Yellow solid. Yield 483 mg (98 %; Purity ~70 – 75%). After column chromatography, the purity can be improved to ~90 – 95%, with loss of yield. **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 8.66 (d, *J* = 8.2 Hz, 2H, CH_{PhBr}), 8.60 – 8.49 (m, 4H, CH_{Ph}), 8.18 (s, 1H, CH_{Pym}), 7.71 (d, *J* = 8.2 Hz, 2H, CH_{PhBr}), 7.63 – 7.54 (m, 4H, CH_{Ph}), 7.50 (d, *J* = 7.5 Hz, 2H, CH_{DMA}), 7.05 – 6.91 (m, 4H, CH_{DMA}), 6.81 – 6.58 (m, 6H, CH_{PXZ}), 6.37 (d, *J* = 7.9 Hz, 2H, CH_{DMA}), 6.05 (d, *J* = 7.8 Hz, 2H, CH_{PXZ}), 1.73 (s, 6H, CH_3). **^{13}C{^{1}H} NMR:** (101 MHz, Chloroform-*d*) δ 164.6, 164.3, 164.2, 144.2, 144.1, 141.8, 140.8, 137.5, 137.1, 136.9, 134.2, 132.1, 132.0, 131.7, 130.4, 130.3, 130.2, 130.1, 126.6, 126.0, 125.6, 123.5, 121.8, 121.0, 115.8, 114.2, 113.5, 111.0, 36.2, 31.5. **HRMS (FD) *m/z*:** $[M]^+$ calc'd for $[C_{49}H_{35}BrN_4O]^+$ 774.1994; found 774.2024; difference +3.9 ppm.

9,9'-((2-(4-bromophenyl)pyrimidine-4,6-diyl)bis(4,1-phenylene))bis(9H-carbazole) (**4e**). Prepared according to general reaction D using 1.00 g **3e** (1.86 mmol, 1.0 eq.), 656 mg *p*-bromobenzamidine hydrochloride (2.79 mmol, 1.5 eq.) and 898 mg K_2CO_3 (6.50 mmol, 3.5 eq.) in 100 mL dimethylformamide for 18 hours at 90 °C. White solid. Yield 1.16 g (87 %). The solubility of this compound is insufficient for

characterization by NMR spectroscopy. **HRMS (FD) *m/z*:** $[M]^+$ calc'd for $[C_{46}H_{29}BrN_4]^+$ 716.1576; found 716.1556; difference -2.8 ppm.

9,9'-((2-(4-bromophenyl)pyrimidine-4,6-diyl)bis(4,1-phenylene))bis(N3,N3,N6,N6-tetra-p-tolyl-9H-carbazole-3,6-diamine) (**4f**). Prepared according to general reaction D using 745 mg **3f** (0.565 mmol, 1.0 eq.), 199 mg *p*-bromobenzamidine hydrochloride (0.847 mmol, 1.5 eq.) and 273 mg K_2CO_3 (1.98 mmol, 3.5 eq.) in 250 mL dimethylformamide for 40 hours at 90 °C. Yellow solid. Yield 790 mg (91 %; Purity ~70 – 75%). After column chromatography, the purity can be increased to >95%, with loss of yield. **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 8.66 (d, *J* = 8.5 Hz, 2H, CH_{PhBr}), 8.54 (d, *J* = 8.5 Hz, 4H, CH_{Ph}), 8.18 (s, 1H, CH_{Pym}), 7.82 (d, *J* = 8.5 Hz, 4H, CH_{Ph}), 7.76 – 7.67 (m, 6H, CH_{Cz} (4H) and CH_{PhBr} (2H)), 7.42 (d, *J* = 8.7 Hz, 4H, CH_{Cz}), 7.21 (dd, *J* = 8.7, 2.1 Hz, 4H, CH_{Cz}), 7.03 (d, *J* = 8.4 Hz, 16H, CH_{tol}), 6.97 (d, *J* = 8.4 Hz, 16H, CH_{tol}), 2.30 (s, 24H, CH_3). **^{13}C{^{1}H} NMR:** (101 MHz, Chloroform-*d*) δ 164.3, 164.1, 146.4, 141.7, 140.6, 137.7, 137.0, 135.8, 131.9, 131.3, 130.3, 129.9, 129.8, 129.1, 127.0, 125.5, 124.6, 123.1, 118.0, 110.8, 110.5, 20.9. **HRMS (FD) *m/z*:** $[M]^+$ calc'd for $[C_{102}H_{81}BrN_8]^+$ 1496.5768; found 1496.5745; difference -1.5 ppm.

2-(4-bromophenyl)-4-(4-iodophenyl)-6-phenylpyrimidine (**4g**). Prepared according to general reaction D using 2.01 g **3g** (6.02 mmol, 1.0 eq.), 2.12 g *p*-bromobenzamidine hydrochloride (9.02 mmol, 1.5 eq.) and 2.91 g K_2CO_3 (21.05 mmol, 3.5 eq.) in 250 mL dimethylformamide for 18 hours at 80 °C. White solid. Yield 2.60 g (84 %). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 8.57 (d, *J* = 8.6 Hz, 2H, CH_{PhBr}), 8.34 – 8.18 (dd, ^3J = 7.6 Hz, ^4J = 2.3 Hz, 2H, CH_{Ph}), 8.03 – 7.95 (m, 3H, CH_{PhI} (2H) and CH_{Pym} (1H)), 7.90 (d, *J* = 8.5 Hz, 2H, CH_{PhI}), 7.66 (d, *J* = 8.6 Hz, 2H, CH_{PhBr}), 7.59 – 7.52 (m, 3H, CH_{Ph}). **^{13}C NMR**: (101 MHz, Chloroform-*d*) δ 165.3, 164.0, 163.9, 138.3, 137.3, 137.0, 137.0, 131.8, 131.2, 130.2, 129.1, 129.0, 127.4, 125.7, 110.3, 97.9. **HRMS (APCI) *m/z*:** $[M]^+$ calc'd for $[C_{22}H_{14}BrIN_2]^+$ 511.9384; found 511.9387; difference +0.6 ppm.

4'-(4,6-bis(4-(9,9-dimethylacridin-10(9H)-yl)phenyl)pyrimidin-2-yl)-[1,1'-biphenyl]-4-carbaldehyde (**5a**). Prepared according to general reaction E using 420 mg **4a** (0.524 mmol, 1.0 eq.), 157 mg *p*-formylphenylboronic acid (1.05 mmol, 2.0 eq.), 200 mg potassium phosphate tribasic (0.943 mmol, 1.8 eq.), 14 mg tris(dibenzylideneacetone)-dipalladium(0) (0.0157 mmol, 0.03 eq.) and 26 mg SPhos (0.0629 mmol, 0.12 eq.) in 15 mL toluene and 0.5 mL H_2O for 24 hours at 100 °C. Purified on silica using dichloromethane as eluent. Yellow solid. Yield 295 mg (68%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 10.10 (s, 1H, CHO), 8.92 (d, *J* = 8.5 Hz, 2H, CH_{biphen}), 8.62 (d, *J* = 8.5 Hz, 4H, CH_{Ph}), 8.24 (s, 1H, CH_{Pym}), 8.02 (d, *J* = 8.3 Hz, 2H, CH_{biphen}), 7.90 (d, *J* = 8.5 Hz, 2H, CH_{biphen}), 7.87 (d, *J* = 8.3 Hz, 2H, CH_{biphen}), 7.60 (d, *J* = 8.5 Hz, 4H, CH_{Ph}), 7.51 (dd, ^3J = 7.5 Hz, ^4J = 1.8 Hz, 4H, CH_{DMA}), 7.10 – 6.89 (m, 8H, CH_{DMA}), 6.40 (dd, ^3J = 8.0 Hz, ^4J = 1.5 Hz, 4H, CH_{DMA}), 1.74 (s, 12H, CH_3). **^{13}C{^{1}H} NMR:** (101 MHz, Chloroform-*d*) δ 192.0, 164.5, 146.7, 144.9, 142.1, 140.8, 138.1, 137.3, 135.7, 132.1, 130.5, 130.4, 130.1, 129.4, 127.9, 127.7, 126.6, 125.6, 121.0, 114.3, 111.0, 36.2, 31.5. **HRMS (APCI) *m/z*:** $[M+H]^+$ calc'd for $[C_{59}H_{47}N_4O]^+$ 827.3750; found 827.3751; difference +0.1 ppm.

4'-(4,6-bis(4-(10H-phenoxazin-10-yl)phenyl)pyrimidin-2-yl)-[1,1'-biphenyl]-4-carbaldehyde (**5b**). Prepared according to general reaction E using 340 mg **4b** (0.453 mmol, 1.0 eq.), 136 mg *p*-formylphenylboronic acid (0.907 mmol, 2.0 eq.), 173 mg potassium phosphate tribasic (0.816 mmol, 1.8 eq.), 13 mg tris(dibenzylideneacetone)dipalladium(0) (0.0136 mmol, 0.03 eq.) and 23 mg SPhos (0.0544 mmol, 0.12 eq.) in 15 mL toluene and 0.5 mL H_2O for 18 hours at 100 °C. Purified on silica using dichloromethane as eluent. Yellow solid. Yield 150 mg (43%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 10.10 (s, 1H, CHO), 8.88 (d, *J* = 8.5 Hz, 2H, CH_{biphen}), 8.56 (d, *J* = 8.4 Hz, 4H, CH_{Ph}), 8.16 (s, 1H, CH_{Pym}), 8.02 (d, *J* = 8.1 Hz, 2H, CH_{biphen}), 7.89 (d, *J* = 8.5 Hz, 2H, CH_{biphen}), 7.86 (d, *J* = 8.1 Hz, 2H, CH_{biphen}), 7.60 (d, *J* = 8.4 Hz, 4H, CH_{Ph}), 6.78 – 6.59 (m, 12H, CH_{PXZ}), 6.06 (dd, ^3J = 7.9 Hz, ^4J = 1.6 Hz, 4H). **^{13}C{^{1}H}**

NMR: (101 MHz, Chloroform-*d*) δ 192.0, 164.5, 164.3, 146.7, 144.1, 142.2, 141.9, 138.0, 137.5, 135.7, 134.1, 131.7, 130.5, 130.2, 129.3, 127.9, 127.7, 123.5, 121.8, 115.8, 113.5, 110.9. **HRMS (APCI) *m/z*:** $[M]^+$ calc'd for $[C_{53}H_{34}N_4O_3]^+$ 774.2631; found 774.2634; difference +0.4 ppm.

4'-(4,6-bis(4-(10H-phenothiazin-10-yl)phenyl)pyrimidin-2-yl)-[1,1'-biphenyl]-4-carbaldehyde (**5c**). Prepared according to general reaction E using 500 mg **4c** (0.640 mmol, 1.0 eq.), 192 mg *p*-formylphenylboronic acid (1.28 mmol, 2.0 eq.), 244 mg potassium phosphate tribasic (1.15 mmol, 1.8 eq.), 18 mg tris(dibenzylideneacetone)dipalladium(0) (0.0192 mmol, 0.03 eq.) and 32 mg SPhos (0.0767 mmol, 0.12 eq.) in 30 mL toluene and 1.0 mL H_2O for 14 hours at reflux. Orange solid. Yield 416 mg (81 %). **^{1}H NMR:** (400 MHz, THF-d_8) δ 10.05 (s, 1H, CHO), 8.92 (d, *J* = 8.5 Hz, 2H, CH_{biphen}), 8.67 (d, *J* = 8.6 Hz, 4H, CH_{Ph}), 8.48 (s, 1H, CH_{Pym}), 8.13 – 7.84 (m, 6H, CH_{biphen}), 7.58 (d, *J* = 8.6 Hz, 4H, CH_{Ph}), 7.12 (dd, *J* = 7.5, 1.7 Hz, 4H, CH_{PTZ}), 7.05 – 6.91 (m, 8H, CH_{PTZ}), 6.57 (dd, *J* = 8.2, 1.3 Hz, 4H, CH_{PTZ}). **^{13}C NMR** (101 MHz, THF-d_8) δ 191.8, 165.3, 165.0, 147.1, 145.8, 144.8, 143.0, 139.3, 137.3, 137.0, 131.0, 130.7, 130.1, 129.8, 129.4, 129.3, 128.8, 128.6, 128.3, 128.1, 128.0, 124.3, 124.3, 119.3, 111.3. **HRMS (FD) *m/z*:** $[M]^+$ calc'd for $[C_{53}H_{34}N_4OS_2]^+$ 806.2174; found 806.2172; difference -0.2 ppm.

4'-(4-(4-(10H-phenoxazin-10-yl)phenyl)-6-(4-(9,9-dimethylacridin-10(9H)-yl)phenyl)pyrimidin-2-yl)-[1,1'-biphenyl]-4-carbaldehyde (**5d**). Prepared according to general reaction E using 450 mg **4d** (0.580 mmol, 1.0 eq.), 174 mg *p*-formylphenylboronic acid (1.16 mmol, 2.0 eq.), 222 mg potassium phosphate tribasic (1.04 mmol, 1.8 eq.), 16 mg tris(dibenzylideneacetone)-dipalladium(0) (0.0174 mmol, 0.03 eq.) and 29 mg SPhos (0.0696 mmol, 0.12 eq.) in 30 mL toluene and 1 mL H_2O for 45 hours at 100 °C. Purified on silica using toluene as eluent. Orange solid. Yield 297 mg (64%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 10.10 (s, 1H, CHO), 8.91 (d, *J* = 8.4 Hz, 2H, CH_{biphen}), 8.61 (d, *J* = 8.4 Hz, 2H, CH_{Ph}), 8.58 (d, *J* = 8.4 Hz, 2H, CH_{Ph}), 8.20 (s, 1H, CH_{Pym}), 8.02 (d, *J* = 8.4 Hz, 2H, CH_{biphen}), 7.89 (d, *J* = 8.4 Hz, 2H, CH_{biphen}), 7.87 (d, *J* = 8.4 Hz, 2H, CH_{biphen}), 7.66 – 7.57 (m, 4H, CH_{Ph}), 7.51 (dd, ^3J = 7.5 Hz, ^4J = 1.9 Hz, 2H, CH_{DMA}), 7.13 – 6.91 (m, 4H, CH_{DMA}), 6.85 – 6.57 (m, 6H, CH_{PXZ}), 6.40 (dd, ^3J = 7.9, ^4J = 1.9 Hz, 2H, CH_{DMA}), 6.07 (d, *J* = 7.8 Hz, 2H, CH_{PXZ}), 1.74 (s, 6H, CH_3). **^{13}C{^{1}H} NMR:** (101 MHz, Chloroform-*d*) δ 192.0, 164.5, 164.5, 164.3, 146.7, 144.2, 144.1, 142.2, 141.8, 140.8, 138.0, 137.5, 137.2, 135.6, 134.1, 132.1, 131.7, 130.5, 130.4, 130.3, 130.1, 129.4, 127.9, 127.7, 126.6, 125.6, 123.5, 121.8, 121.0, 115.8, 114.3, 113.5, 111.0, 36.2, 31.5. **HRMS (FD) *m/z*:** $[M]^+$ calc'd for $[C_{56}H_{40}N_4O_2]^+$ 800.3151; found 800.3140; difference -1.4 ppm.

4'-(4,6-bis(4-(9H-carbazol-9-yl)phenyl)pyrimidin-2-yl)-[1,1'-biphenyl]-4-carbaldehyde (**5e**). Prepared according to general reaction E using 1.15 g **4e** (1.60 mmol, 1.0 eq.), 481 mg *p*-formylphenylboronic acid (3.21 mmol, 2.0 eq.), 612 mg potassium phosphate tribasic (2.88 mmol, 1.8 eq.), 44 mg tris(dibenzylideneacetone)dipalladium(0) (0.0480 mmol, 0.03 eq.) and 80 mg SPhos (0.192 mmol, 0.12 eq.) in 45 mL toluene and 1.5 mL H_2O for 16 hours at 100 °C. Purified on silica using toluene to remove starting material (bromide), and then 10% ethyl acetate/toluene (v/v) to remove the product. Off-white solid. Yield 756 mg (64%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 10.09 (s, 1H, CHO), 8.92 (d, *J* = 8.0 Hz, 2H, CH_{biphen}), 8.60 (d, *J* = 8.1 Hz, 4H, CH_{Ph}), 8.20 (s, 1H, CH_{Pym}), 8.19 (d, *J* = 8.4 Hz, 4H, CH_{Cz}), 8.01 (d, *J* = 8.0 Hz, 2H, CH_{biphen}), 7.95 – 7.75 (m, 8H, CH_{biphen} (4H), CH_{Ph} (4H)), 7.57 (d, *J* = 8.2 Hz, 4H, CH_{Cz}), 7.48 (dd, *J* = 8.2, 7.4 Hz, 4H, CH_{Cz}), 7.35 (dd, *J*=8.4 Hz, *J* = 7.4 Hz, 4H, CH_{Cz}). **^{13}C{^{1}H} NMR:** (101 MHz, Chloroform-*d*) δ 192.0, 164.4, 164.3, 146.7, 142.1, 140.6, 140.5, 138.2, 136.2, 135.6, 131.2, 129.3, 129.1, 127.9, 127.7, 127.4, 126.3, 123.9, 120.6, 120.6, 110.5, 110.0. **HRMS (FD) *m/z*:** $[M]^+$ calc'd for $[C_{53}H_{34}N_4O]^+$ 742.2733; found 742.2755; difference +3.0 ppm.

4'-(4,6-bis(4-(3,6-bis(di-p-tolylamino)-9H-carbazol-9-yl)phenyl)pyrimidin-2-yl)-[1,1'-biphenyl]-4-carbaldehyde (**5f**). Prepared according to general reaction E using 715 mg **4f** (0.468 mmol, 1.0 eq.), 140 mg *p*-formylphenylboronic acid (0.935 mmol, 2.0 eq.), 179 mg potassium phosphate tribasic (0.842 mmol,

1.8 eq.), 13 mg tris(dibenzylideneacetone)dipalladium(0) (0.0140 mmol, 0.03 eq.) and 23 mg SPhos (0.0560 mmol, 0.12 eq.) in 30 mL toluene and 1 mL H_2O for 45 hours at 100 °C. Purified on silica using toluene as eluent. All pure fractions were combined and recrystallized from CH_2Cl_2/MeOH. Orange solid. Yield 458 mg (64%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 10.10 (s, 1H, CHO), 8.90 (d, *J* = 8.4 Hz, 2H, CH_{biphen}), 8.58 (d, *J* = 8.6 Hz, 4H, CH_{Ph}), 8.20 (s, 1H, CH_{Pym}), 8.02 (d, *J* = 8.3 Hz, 2H, CH_{biphen}), 7.89 (d, *J* = 8.3 Hz, 2H, CH_{biphen}), 7.87 (d, *J* = 8.4 Hz, 2H, CH_{biphen}), 7.84 (d, *J* = 8.6 Hz, 4H, CH_{Ph}), 7.75 (d, ^4J = 2.1 Hz, 4H, CH_{Cz}), 7.44 (d, *J* = 8.8 Hz, 4H, CH_{Cz}), 7.24 (dd, *J* = 8.8 Hz, *J* = 2.1 Hz, 4H, CH_{Cz}), 7.03 (d, *J* = 8.5 Hz, 16H, CH_{tol}), 6.98 (d, *J* = 8.5 Hz, 16H, CH_{tol}), 2.30 (s, 24H, CH_3). **^{13}C{^{1}H} NMR:** (101 MHz, Chloroform-*d*) δ 192.0, 164.4, 164.3, 146.7, 146.4, 142.1, 141.7, 140.6, 138.2, 137.7, 135.9, 135.6, 131.3, 130.5, 129.9, 129.3, 129.1, 127.9, 127.7, 127.0, 125.5, 124.6, 123.1, 118.0, 110.8, 110.4, 20.9. **HRMS (FD) *m/z*:** $[M]^+$ calc'd for $[C_{109}H_{86}N_8O]^+$ 1522.6925; found 1522.6951; difference +1.7 ppm.

4'-(2-(4-bromophenyl)-6-phenylpyrimidin-4-yl)-[1,1'-biphenyl]-4-carbaldehyde (**5g**). Modified from a reported procedure.[15] A Schlenk flask was charged with **4g** (463 mg, 0.902 mmol, 1.0 eq.), *p*-formylphenylboronic acid (156 mg, 1.04 mmol, 1.15 eq.), $Pd(OAc)_2$ (10 mg, 0.045 mmol, 0.05 eq.), and XPhos (43 mg, 0.090 mmol, 0.010 eq.). The flask was evacuated and backfilled with dry N_2. To this flask was added 20 mL of diglyme and 10 mL of a saturated aqueous solution of K_2CO_3 (both sparged with N_2). The reaction mixture was refluxed for 48 hours. After cooling to room temperature, the mixture was washed with water and extracted with 3x 50 mL EtOAc. The combined organics were dried over $MgSO_4$ and filtered. The organic residue was purified by column chromatography on silica (2:1 CH_2Cl_2/Hexanes v/v). White solid. Yield 131 mg (30% yield). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 10.09 (s, 1H, CHO), 8.60 (d, *J* = 8.6 Hz, 2H, CH_{PhBr}), 8.37 (d, *J* = 8.4 Hz, 2H, CH_{biphen}), 8.29 (dd, ^4J = 7.6 Hz, ^3J = 2.0 Hz,2H, CH_{Ph}), 8.05 (s, 1H, CH_{Pym}), 8.00 (d, *J* = 8.3 Hz, 2H, CH_{biphen}), 7.84 (d, *J* = 8.4 Hz, 2H, CH_{biphen}), 7.82 (d, *J* = 8.3 Hz, 2H, CH_{biphen}), 7.67 (d, *J* = 8.6 Hz, 2H, CH_{PhBr}), 7.61 – 7.54 (m, 3H, CH_{Ph}). **^{13}C NMR:** (101 MHz, Chloroform-*d*) δ 191.9, 165.2, 164.2, 163.9, 146.3, 142.2, 137.4, 137.4, 137.1, 135.8, 131.8, 131.2, 130.5, 130.2, 129.1, 128.1, 128.0, 127.9, 127.4, 125.7, 110.6. **HRMS (APCI) *m/z*:** $[M]^+$ calc'd for $[C_{29}H_{19}BrN_2O]^+$ 490.0681; found 490.0683; difference +0.4 ppm.

4'-(2-(4-(9,9-dimethylacridin-10(9H)-yl)phenyl)-6-phenylpyrimidin-4-yl)-[1,1'-biphenyl]-4-carbaldehyde (**6g**) Modified from a reported procedure.[16] A Schlenk flask was charged with **5g** (225 mg, 0.458 mmol, 1.0 eq.), 9,9-dimethyl-9,10-dihydroacridine (192 mg, 0.916 mmol, 2.0 eq.), $Pd(OAc)_2$ (5 mg, 0.0228 mmol, 0.05 eq.), *rac*-BINAP (14 mg, 0.0228 mmol, 0.05 eq.), and Cs_2CO_3 (448 mg, 1.374 mmol, 3.0 eq.). The flask was evacuated and backfilled with dry N_2. 30 mL of dry, degassed toluene was added through a septum cap. The mixture was heated to reflux for 24 hours. After cooling, the mixture was washed with water and extracted with 3x 50 mL ethyl acetate. The combined organic phases were dried over $MgSO_4$ and flitered. The crude organic residue was purified by column chromatography on silica (1:1 dichloromethane/hexanes v/v gradient up to pure dichloromethane). Light yellow solid. Yield 224 mg (79%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 10.10 (s, 1H, CHO), 8.99 (d, *J* = 8.1 Hz, 2H, CH_{Ph}), 8.46 (d, *J* = 8.0 Hz, 2H, CH_{biphen}), 8.36 (dd, ^3J = 7.6 Hz, ^4J = 2.5 Hz, 2H, CH_{Ph}), 8.14 (s, 1H, CH_{Pym}), 8.02 (d, *J* = 8.0 Hz, 2H, CH_{biphen}), 7.87 (d, *J* = 8.0 Hz, 4H, CH_{biphen}), 7.65 – 7.57 (m, 3H, CH_{Ph}), 7.54 (d, *J* = 8.1 Hz, 2H, CH_{Ph}), 7.50 (d, *J* = 7.2 Hz, 2H, CH_{DMA}), 7.07 – 6.89 (m, 4H, CH_{DMA}), 6.41 (d, *J* = 8.1 Hz, 2H, CH_{DMA}), 1.74 (s, 6H, CH_3). **^{13}C NMR:** (101 MHz, Chloroform-*d*) δ 192.0, 165.3, 164.3, 164.2, 146.3, 143.7, 142.3, 140.9, 138.1, 137.5, 137.4, 135.8, 131.6, 131.2, 131.2, 130.5, 130.2, 129.2, 128.1, 128.1, 127.9, 127.5, 126.6, 125.4, 120.8, 114.3, 110.6, 36.2, 31.5. **HRMS (APCI) *m/z*:** $[M]^+$ calc'd for $[C_{44}H_{33}N_3O]^+$ 619.2624; found 619.2629; difference +0.8 ppm.

(4'-(4,6-bis(4-(9,9-dimethylacridin-10(9H)-yl)phenyl)pyrimidin-2-yl)-[1,1'-biphenyl]-4-yl)methanol (**6a**). Prepared according to general reaction F using 341 mg **5a** (0.412 mmol, 1.0 eq.) and 19 mg $NaBH_4$ (0.495

mmol, 1.2 eq.) in 15 mL CH_2Cl_2 and 5 mL ethanol for 3 hours at ambient temperature. Purified on silica using dichloromethane as eluent. Pale yellow solid. Yield 306 mg (90%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 8.87 (d, *J* = 8.5 Hz, 2H, CH_{biphen}), 8.61 (d, *J* = 8.4 Hz, 4H, CH_{Ph}), 8.22 (s, 1H, CH_{Pym}), 7.83 (d, *J* = 8.5 Hz, 2H, CH_{biphen}), 7.74 (d, *J* = 8.2 Hz, 2H, CH_{biphen}), 7.59 (d, *J* = 8.4 Hz, 4H, CH_{Ph}), 7.53 – 7.47 (m, 6H, CH_{DMA} (4H) and CH_{biphen} (2H)), 7.07 – 6.91 (m, 8H, CH_{DMA}), 6.40 (dd, ^3J = 8.0 Hz, ^4J = 1.5 Hz, 4H, CH_{DMA}), 4.79 (s, 2H, C*H*$_2$OH – coupling to -OH is not observed), 1.74 (s, 12H, CH_3). **^{13}C{^{1}H} NMR:** (101 MHz, Chloroform-*d*) δ 164.8, 164.4, 144.1, 143.4, 140.8, 140.6, 137.4, 136.7, 132.1, 130.3, 130.1, 129.2, 127.7, 127.6, 127.4, 126.6, 125.5, 121.0, 114.3, 110.8, 65.3, 36.2, 31.5. **HRMS (FD) *m/z*:** $[M]^+$ calc'd for $[C_{59}H_{48}N_4O]^+$ 828.3828; found 828.3847; difference +2.3 ppm.

(4'-(4,6-bis(4-(10H-phenoxazin-10-yl)phenyl)pyrimidin-2-yl)-[1,1'-biphenyl]-4-yl)methanol (**6b**). Prepared according to general reaction F using 150 mg **5b** (0.194 mmol, 1.0 eq.) and 9 mg $NaBH_4$ (0.232 mmol, 1.2 eq.) in 15 mL CH_2Cl_2 and 5 mL ethanol for 2 hours at ambient temperature. Purified on silica using 2% ethyl acetate/dichloromethane to remove the starting materials then gradient to 10% ethyl acetate/dichloromethane to collect the product. Yellow solid. Yield 140 mg (93%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 8.84 (d, *J* = 8.4 Hz, 2H, CH_{biphen}), 8.56 (d, *J* = 8.5 Hz, 4H, CH_{Ph}), 8.14 (s, 1H, CH_{Pym}), 7.81 (d, *J* = 8.4 Hz, 2H, CH_{biphen}), 7.73 (d, *J* = 8.5 Hz, 2H, CH_{biphen}), 7.59 (d, *J* = 8.5 Hz, 4H, CH_{Ph}), 7.51 (d, *J* = 8.5 Hz, 2H, CH_{biphen}), 6.77 – 6.60 (m, 12H, CH_{PXZ}), 6.06 (dd, ^3J = 7.8, ^4J = 1.6 Hz, 4H, CH_{PXZ}), 4.79 (d, *J* = 5.9 Hz, 2H, C*H*$_2$OH), 1.70 (t, *J* = 5.9, 1H, CH_2O*H*). **^{13}C{^{1}H} NMR:** (101 MHz, Chloroform-*d*) δ 164.8, 164.3, 144.1, 143.4, 141.7, 140.6, 140.1, 137.6, 136.9, 134.2, 131.6, 130.2, 129.2, 127.7, 127.5, 127.4, 123.5, 121.8, 115.8, 113.5, 110.7, 65.3. **HRMS (APCI) *m/z*:** $[M]^+$ calc'd for $[C_{53}H_{36}N_4O_3]^+$ 776.2787; found 776.2790; difference +0.4 ppm.

(4'-(4,6-bis(4-(10H-phenothiazin-10-yl)phenyl)pyrimidin-2-yl)-[1,1'-biphenyl]-4-yl)methanol (**6c**). Prepared according to general reaction F using 280 mg **5c** (0.347 mmol, 1.0 eq.) and 16 mg $NaBH_4$ (0.416 mmol, 1.2 eq.) in 15 mL CH_2Cl_2 and 5 mL ethanol for 2 hours at ambient temperature. Purified on silica using 5% ethyl acetate/dichloromethane. Yellow solid. Yield 224 mg (80%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 8.84 (d, *J* = 8.5 Hz, 2H, CH_{biphen}), 8.50 (d, *J* = 8.6 Hz, 4H, CH_{Ph}), 8.10 (s, 1H, CH_{Pym}), 7.82 (d, *J* = 8.5 Hz, 2H, CH_{biphen}), 7.75 (d, *J* = 8.2 Hz, 2H, CH_{biphen}), 7.56 (d, *J* = 8.6 Hz, 4H, CH_{Ph}), 7.52 (d, *J* = 8.2 Hz, 2H, CH_{biphen}), 7.18 (dd, *J* = 7.5, 1.7 Hz, 4H, CH_{PTZ}), 7.09 – 6.89 (m, 8H, CH_{PTZ}), 6.61 (dd, *J* = 8.0, 1.4 Hz, 4H, CH_{PTZ}), 4.81 (d, *J* = 5.8 Hz, 2H, C*H*$_2$OH), 1.72 (t, *J* = 5.8 Hz, 1H, CH_2O*H*). **^{13}C NMR:** (101 MHz, Chloroform-*d*) δ 164.6, 164.2, 144.7, 143.6, 143.2, 140.5, 140.2, 137.1, 135.8, 129.6, 129.1, 128.1, 127.7, 127.6, 127.5, 127.3, 127.1, 123.6, 118.7, 110.1, 65.3. **HRMS (APCI) *m/z*:** $[M]^+$ calc'd for $[C_{53}H_{36}N_4OS_2]^+$ 808.2331; found 808.2334; difference +0.4 ppm.

(4'-(4-(4-(10H-phenoxazin-10-yl)phenyl)-6-(4-(9,9-dimethylacridin-10(9H)-yl)phenyl)pyrimidin-2-yl)-[1,1'-biphenyl]-4-yl)methanol (**6d**). Prepared according to general reaction F using 265 mg **5d** (0.331 mmol, 1.0 eq.) and 15 mg $NaBH_4$ (0.397 mmol, 1.2 eq.) in 30 mL CH_2Cl_2 and 10 mL ethanol for 3 hours at ambient temperature. Purified on silica using dichloromethane as eluent. Recrystallized from CH_2Cl_2/MeOH. Yellow solid. Yield 239 mg (90%). **^{1}H NMR:** (400 MHz, Benzene-d_6) δ 9.19 (d, *J* = 8.2 Hz, 2H, CH_{biphen}), 8.28 (d, *J* = 8.0 Hz, 2H, CH_{Ph}), 8.21 (d, *J* = 8.1 Hz, 2H, CH_{Ph}), 7.84 (d, *J* = 8.2 Hz, 2H, CH_{biphen}), 7.63 (s, 1H, CH_{Pym}), 7.58 (d, *J* = 7.9 Hz, 2H, CH_{biphen}), 7.44 (d, *J* = 7.6 Hz, 2H, CH_{DMA}), 7.32 (d, *J* = 8.0 Hz, 2H, CH_{Ph}), 7.26 (d, *J* = 7.9 Hz, 2H, CH_{biphen}), 7.16 (d, *J* = 8.1 Hz, 2H, CH_{Ph}) 7.07 – 6.93 (m, 4H, CH_{DMA}), 6.89 – 6.82 (m, 2H, CH_{PXZ}), 6.66 – 6.48 (m, 6H, CH_{PXZ} (4H) and CH_{DMA} (2H)), 6.11 (dd, *J* = 7.0, 2.5 Hz, 2H, CH_{PXZ}), 4.37 (d, *J* = 5.7 Hz, 2H, C*H*$_2$OH), 1.70 (s, 6H, CH_3), 0.92 (t, *J* = 5.9 Hz, 1H, CH_2O*H*). **^{13}C{^{1}H} NMR:** (101 MHz, Chloroform-*d*) δ 164.8, 164.5, 164.2, 144.1, 143.4, 140.8, 140.6, 140.2, 137.7, 137.3, 137.0, 132.1, 130.4, 130.3, 130.1, 129.2, 127.7, 127.6, 127.4, 126.6, 125.5, 123.1, 121.0, 114.3, 113.5, 110.7, 65.3, 36.2, 31.5. **HRMS (FD) *m/z*:** $[M]^+$ calc'd for $[C_{56}H_{42}N_4O_2]^+$ 802.3308; found 802.3327; difference +2.4 ppm.

(4'-(4,6-bis(4-(9H-carbazol-9-yl)phenyl)pyrimidin-2-yl)-[1,1'-biphenyl]-4-yl)methanol (**6e**). Prepared according to general reaction F using 500 mg **5e** (0.673 mmol, 1.0 eq.) and 31 mg $NaBH_4$ (0.808 mmol, 1.2 eq.) in 45 mL CH_2Cl_2 and 15 mL ethanol for 4 hours at ambient temperature. Purified on silica using dichloromethane to remove residual starting material then gradient up to 20% ethyl acetate in dichloromethane (v/v) to remove the product. Pale yellow solid. Yield 404 mg (81%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 8.88 (d, *J* = 8.6 Hz, 2H, CH_{biphen}), 8.61 (d, *J* = 8.6 Hz, 4H, CH_{Ph}), 8.21 (s, 1H, CH_{Pym}), 8.19 (d, *J* = 7.8 Hz, 4H, CH_{Cz}), 7.84 (d, *J* = Hz, 4H, CH_{Ph}), 7.83 (d, *J* = Hz, 2H, CH_{biphen}), 7.74 (d, *J* = 8.6 Hz, 2H, CH_{biphen}), 7.56 (d, *J* = 8.2 Hz, 4H, CH_{Cz}), 7.54 – 7.42 (m, 6H, CH_{Cz} (4H) and CH_{biphen} (2H)), 7.34 (ddd, *J* = 8.2, 7.1, 1.0 Hz, 4H, CH_{Cz}), 4.79 (d, *J* = 5.3 Hz, 2H, C*H*$_2$OH), 1.71 (t, *J* = 5.3 Hz, 1H, CH_2O*H*). **^{13}C{^{1}H} NMR:** (101 MHz, Chloroform-*d*) δ 164.8, 164.3, 142.7, 140.7, 140.6, 140.4, 140.2, 137.1, 136.37, 129.2, 129.1, 128.2, 127.6, 127.4, 126.3, 123.9, 120.6, 120.5, 110.3, 110.0, 66.0. **HRMS (APCI) *m/z*:** $[M+H]^+$ calc'd for $[C_{53}H_{37}N_4O]^+$ 745.2967; found 745.2966; difference -0.1 ppm.

(4'-(4,6-bis(4-(3,6-bis(di-p-tolylamino)-9H-carbazol-9-yl)phenyl)pyrimidin-2-yl)-[1,1'-biphenyl]-4-yl)methanol (**6f**). Prepared by modification of general reaction F using 458 mg **5f** (0.301 mmol, 1.0 eq.) and 14 mg $NaBH_4$ (0.361 mmol, 1.2 eq.) in 40 mL THF and 10 mL ethanol for 2 hours at ambient temperature. Purified by dissolving the solid residue in THF and fusing to 500 mg silica gel by removing the solvent, then transferring this to the top of a silica column and eluting with dichloromethane to remove starting materials, then gradient up to 1:1 ethyl acetate/dichloromethane to remove product. Pure fractions were combined and recrystallized from CH_2Cl_2/MeOH. Yellow solid. Yield 351 mg (76%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 8.86 (d, *J* = 8.1 Hz, 2H, CH_{biphen}), 8.58 (d, *J* = 8.2 Hz, 4H, CH_{Ph}), 8.18 (s, 1H, CH_{Pym}), 7.88 – 7.79 (m, 6H, CH_{Ph} (4H) and CH_{biphen} (2H)), 7.78 – 7.69 (m, 6H, CH_{Cz} (4H) and CH_{biphen} (2H)), 7.51 (d, *J* = 8.1 Hz, 2H, CH_{biphen}), 7.44 (d, *J* = 8.8 Hz, 4H, CH_{Cz}), 7.22 (dd, *J* = 8.8, 2.1 Hz, 4H, CH_{Cz}), 7.03 (d, *J* = 8.3 Hz, 16H, CH_{tol}), 6.98 (d, *J* = 8.3 Hz, 16H, CH_{tol}), 4.79 (d, *J* = 5.9 Hz, 2H, C*H*$_2$OH), 2.30 (s, 24H, CH_3), 1.69 (t, *J* = 5.9 Hz, 1H, CH_2O*H*). **^{13}C{^{1}H} NMR:** (101 MHz, Chloroform-*d*) δ 164.7, 164.2, 146.4, 143.3, 141.7, 140.5, 140.2, 137.7, 137.1, 136.1, 131.3, 129.9, 129.2, 129.1, 127.7, 127.6, 127.4, 127.0, 125.5, 124.6, 123.1, 118.0, 110.9, 110.3, 65.3, 20.9. **HRMS (FD) *m/z*:** $[M]^+$ calc'd for $[C_{109}H_{88}N_8O]^+$ 1524.7081; found 1524.7110; difference +2.0 ppm.

(4'-(2-(4-(9,9-dimethylacridin-10(9H)-yl)phenyl)-6-phenylpyrimidin-4-yl)-[1,1'-biphenyl]-4-yl)methanol (**7g**). Prepared according to general reaction F using 200 mg **6g** (0.323 mmol, 1.0 eq.) and 15 mg $NaBH_4$ (0.387 mmol, 1.2 eq.) in 15 mL CH_2Cl_2 and 5 mL ethanol for 30 minutes at ambient temperature. Purified on silica using dichloromethane as eluent. White solid. Yield 173 mg (86%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 8.99 (d, *J* = 8.1 Hz, 2H, CH_{Ph}), 8.42 (d, *J* = 8.1 Hz, 2H, CH_{biphen}), 8.36 (dd, ^3J = 7.9, ^4J = 2.12, 2H, CH_{Ph}), 8.12 (s, 1H, CH_{Pym}), 7.82 (d, *J* = 8.1 Hz, 2H, CH_{Ph}), 7.71 (d, *J* = 7.9 Hz, 2H, CH_{biphen}), 7.64 – 7.57 (m, 3H, CH_{Ph}), 7.57 – 7.42 (m, 6H, CH_{biphen} (4H) and CH_{DMA} (2H)), 7.06 – 6.89 (m, 4H, CH_{DMA}), 6.42 (dd, *J* = 8.0, 1.5 Hz, 2H, CH_{DMA}), 4.78 (d, *J* = 5.8 Hz, 2H, C*H*$_2$OH), 1.81 – 1.67 (m, 7H, CH_3 and CH_2O*H*). **^{13}C NMR:** (101 MHz, Chloroform-*d*) δ 165.1, 164.6, 164.1, 143.6, 143.5, 140.9, 140.8, 139.8, 138.3, 137.5, 136.4, 131.5, 131.2, 131.1, 130.2, 129.2, 127.9, 127.7, 127.7, 127.5, 127.4, 126.6, 125.4, 120.8, 114.3, 110.5, 65.2, 36.2, 31.5. **HRMS (APCI) *m/z*:** $[M]^+$ calc'd for $[C_{44}H_{35}N_3O]^+$ 621.2780; found 621.2784; difference +0.6 ppm.

(4'-(4,6-bis(4-(9,9-dimethylacridin-10(9H)-yl)phenyl)pyrimidin-2-yl)-[1,1'-biphenyl]-4-yl)methyl acrylate (**PymDMA**). Prepared according to general reaction G using 200 mg **6a** (0.241 mmol, 1.0 eq.), 43 µL NEt_3 (0.314 mmol, 1.3 eq.), and 24 µL acryloyl chloride (0.289 mmol, 1.2 eq.) in 10 mL CH_2Cl_2 for 15 minutes at 0 °C. Purified on silica using dichloromethane as eluent. White solid. Yield 77 mg (36%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 8.87 (d, *J* = 8.5 Hz, 2H, CH_{biphen}), 8.61 (d, *J* = 8.4 Hz, 4H, CH_{Ph}), 8.22 (s, 1H,

CH_{Pym}), 7.82 (d, J = 8.5 Hz, 2H, CH_{biphen}), 7.74 (d, J = 8.2 Hz, 2H, CH_{biphen}), 7.59 (d, J = 8.4 Hz, 4H, CH_{Ph}), 7.55 – 7.44 (m, 6H, CH_{DMA} (4H) and CH_{biphen} (2H)), 7.11 – 6.89 (m, 8H, CH_{DMA}), 6.49 (dd, J_{trans} = 17.3 Hz, J_{gem} = 1.4 Hz, 1H, CH_{vinyl}), 6.39 (dd, ^3J = 8.0 Hz, ^4J = 1.5 Hz, 4H, CH_{DMA}), 6.21 (dd, J_{trans} = 17.3 Hz, J_{cis} = 10.4 Hz, 1H, CH_{vinyl}), 5.88 (dd, J_{cis} = 10.4, J_{gem} = 1.4 Hz, 1H, CH_{vinyl}), 5.28 (s, 2H, CH_2), 1.74 (s, 12H, CH3). **$^{13}C\{^1H\}$ NMR:** (101 MHz, Chloroform-*d*) δ 166.2, 164.8, 164.5, 144.1, 143.2, 140.8, 140.8, 137.4, 135.5, 132.1, 131.4, 130.4, 130.1, 129.2, 129.0, 128.5, 127.6, 127.5, 126.6, 125.5, 121.0, 114.3, 110.8, 66.2, 36.2, 31.5. **HRMS (APCI) *m/z*:** $[M+H]^+$ calc'd for $[C_{62}H_{51}N_4O_2]^+$ 883.4012; found 883.4015; difference +0.3 ppm.

(4'-(4,6-bis(4-(10H-phenoxazin-10-yl)phenyl)pyrimidin-2-yl)-[1,1'-biphenyl]-4-yl)methyl acrylate (**PymPXZ**). Prepared according to general reaction G using 130 mg **6b** (0.167 mmol, 1.0 eq), 30 µL NEt_3 (0.218 mmol, 1.3 eq.), and 16 µL acryloyl chloride (0.201 mmol, 1.2 eq.) in 4 mL CH_2Cl_2 for 1 hour at 0 °C. Purified on silica using dichloromethane as eluent. Yellow solid. Yield 62 mg (45%). **^1H NMR:** (400 MHz, Chloroform-*d*) δ 8.84 (d, J = 8.1 Hz, 2H, CH_{biphen}), 8.56 (d, J = 8.1 Hz, 4H, CH_{Ph}), 8.14 (s, 1H, CH_{Pym}), 7.81 (d, J = 8.1 Hz, 2H, CH_{biphen}), 7.73 (d, J = 7.9 Hz, 2H, CH_{biphen}), 7.60 (d, J = 8.1 Hz, 4H, CH_{Ph}), 7.52 (d, J = 7.9 Hz, 2H, CH_{biphen}), 6.85 – 6.58 (m, 12H, CH_{PXZ}), 6.51 (d, J_{trans} = 17.3 Hz, 1H, CH_{vinyl}), 6.21 (dd, J_{trans} = 17.3 Hz, J_{cis} = 10.4 Hz, 1H, CH_{vinyl}), 6.13 – 6.00 (d, J = 7.7 Hz, 4H, CH_{PXZ}), 5.91 (d, J_{cis} = 10.4 Hz, 1H, CH_{vinyl}), 5.28 (s, 2H, CH_2). **$^{13}C\{^1H\}$ NMR:** (101 MHz, Chloroform-*d*) δ 166.2, 164.8, 164.3, 144.1, 143.2, 141.8, 140.8, 137.6, 137.0, 135.6, 134.2, 131.7, 131.4, 130.2, 129.2, 129.0, 128.4, 127.6, 127.4, 123.5, 121.8, 115.8, 113.5, 110.7, 66.2. **HRMS (APCI) *m/z*:** $[M+H]^+$ calc'd for $[C_{56}H_{39}N_4O_4]^+$ 831.2971; found 831.2968; difference -0.4 ppm.

(4'-(4,6-bis(4-(10H-phenothiazin-10-yl)phenyl)pyrimidin-2-yl)-[1,1'-biphenyl]-4-yl)methyl acrylate (**PymPTZ**). Prepared according to general reaction G using 200 mg **6c** (0.247 mmol, 1.0 eq), 44.5 µL NEt_3 (0.321 mmol, 1.3 eq.), and 24.1 µL acryloyl chloride (0.297 mmol, 1.2 eq.) in 10 mL CH_2Cl_2 for 90 minutes at 0 °C. Purified on silica using 3:1 dichloromethane/hexanes (v/v) as eluent. Yellow solid. Yield 72 mg (34%). **^1H NMR:** (400 MHz, Chloroform-*d*) δ 8.82 (d, J = 8.3 Hz, 2H, CH_{biphen}), 8.47 (d, J = 8.5 Hz, 4H, CH_{Ph}), 8.08 (s, 1H, CH_{Pym}), 7.79 (d, J = 8.3 Hz, 2H, CH_{biphen}), 7.72 (d, J = 8.2 Hz, 2H, CH_{biphen}), 7.57 – 7.47 (m, 6H, CH_{Ph} (4H) and CH_{biphen} (2H)), 7.16 (dd, J = 7.4, 1.7 Hz, 4H, CH_{PTZ}), 7.05 – 6.89 (m, 8H, CH_{PTZ}), 6.59 (dd, ^3J = 8.0 Hz, ^4J = 1.4 Hz, 4H, CH_{PTZ}), 6.49 (dd, J_{trans} = 17.3 Hz, J_{gem} = 1.5 Hz, 1H, CH_{vinyl}), 6.21 (dd, J_{trans} = 17.3 Hz, J_{cis} = 10.5 Hz, 1H, CH_{vinyl}), 5.88 (dd, J_{cis} = 10.5 Hz, J_{gem} = 1.5 Hz, 1H, CH_{vinyl}), 5.28 (s, 2H, CH_2). **^{13}C NMR:** (101 MHz, Chloroform-*d*) δ 166.2, 164.6, 164.2, 144.8, 143.6, 143.1, 140.8, 137.3, 135.7, 135.5, 131.4, 129.6, 129.1, 129.0, 128.4, 128.0, 127.6, 127.5, 127.4, 127.1, 123.7, 123.7, 118.7, 110.1, 66.2. **HRMS (APCI) *m/z*:** $[M]^+$ calc'd for $[C_{56}H_{38}N_4O_2S_2]^+$ 862.2436; found 862.2445; difference +1.0 ppm.

(4'-(4-(4-(10H-phenoxazin-10-yl)phenyl)-6-(4-(9,9-dimethylacridin-10(9H)-yl)phenyl)pyrimidin-2-yl)-[1,1'-biphenyl]-4-yl)methyl acrylate (**PymDMAPXZ**). Prepared according to general reaction G using 225 mg **6d** (0.280 mmol, 1.0 eq), 50 µL NEt_3 (0.364 mmol, 1.3 eq.), and 7 µL acryloyl chloride (0.336 mmol, 1.2 eq.) in 15 mL CH_2Cl_2 for 1 hour at 0 °C. Purified on silica using dichloromethane as eluent. Yellow solid. Yield 86 mg (36%). **^1H NMR:** (400 MHz, Benzene-d_6) δ 9.16 (d, J = 8.1 Hz, 2H, CH_{biphen}), 8.28 (d, J = 8.1 Hz, 2H, CH_{Ph}), 8.21 (d, J = 8.1 Hz, 2H, CH_{Ph}), 7.77 (d, J = 8.1 Hz, 2H, CH_{biphen}), 7.63 (s, 1H, CH_{Pym}), 7.50 (d, J = 7.9 Hz, 2H, CH_{biphen}), 7.44 (d, J = 7.5 Hz, 2H, CH_{DMA}), 7.32 (d, J = 8.1 Hz, 2H, CH_{Ph}), 7.26 (d, J = 7.9 Hz, 2H, CH_{biphen}), 7.16 (d, J = 7.9 Hz, CH_{biphen}), 7.08 – 6.94 (m, 4H, CH_{DMA}), 6.88 – 6.81 (m, 2H, CH_{PXZ}), 6.63 – 6.50 (m, 6H, CH_{PXZ} (4H) and CH_{DMA} (2H)), 6.34 (dd, J_{trans} = 17.3 Hz, 1H, CH_{vinyl}), 6.11 (dd, J = 6.9, 2.4 Hz, 2H, CH_{PXZ}), 6.02 (dd, J_{trans} = 17.3 Hz, J_{cis} = 10.4 Hz, 1H, CH_{vinyl}), 5.26 (d, J_{cis} = 10.4 Hz, 1H, CH_{vinyl}), 5.10 (s, 2H, CH_2), 1.70 (s, 6H, CH_3). **$^{13}C\{^1H\}$ NMR:** (101 MHz, Chloroform-*d*) δ 166.2, 164.7, 164.5, 164.2, 144.1, 143.2, 140.8,

137.3, 137.1, 135.5, 132.1, 131.4, 130.4, 130.3, 130.1, 129.2, 129.0, 129.0, 128.4, 127.6, 127.4, 126.6, 125.5, 121.0, 114.3, 110.8, 66.2, 36.2, 31.5. **HRMS (FD) *m/z*:** $[M]^+$ calc'd for $[C_{59}H_{44}N_4O_3]^+$ 856.3413; found 856.3411; difference -0.2 ppm.

(4'-(4,6-bis(4-(9H-carbazol-9-yl)phenyl)pyrimidin-2-yl)-[1,1'-biphenyl]-4-yl)methyl acrylate (**PymCz**). Prepared according to general reaction G using 350 mg **6e** (0.470 mmol, 1.0 eq), 85 µL NEt_3 (0.611 mmol, 1.3 eq.), and 46 µL acryloyl chloride (0.564 mmol, 1.2 eq.) in 8 mL CH_2Cl_2 for 1 hour at 0 °C. Purified on silica using dichloromethane as eluent. White solid. Yield 114 mg (30%). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 8.89 (d, *J* = 8.4 Hz, 2H, CH_{biphen}), 8.61 (d, *J* = 8.5 Hz, 4H, CH_{Ph}), 8.21 (s, 1H, CH_{Pym}), 8.19 (d, *J* = 7.7 Hz, 4H, CH_{Cz}), 7.88 – 7.79 (m, 6H, CH_{Ph} (4H) and CH_{biphen} (2H)), 7.74 (d, *J* = 8.4 Hz, 2H, CH_{biphen}), 7.61 – 7.43 (m, 10H, CH_{Cz} (8H) and CH_{biphen} (2H)), 7.35 (ddd, ^3J = 7.9, 7.9 Hz ^4J = 1.0 Hz, 4H, CH_{Cz}), 6.49 (dd, J_{trans} = 17.3 Hz, J_{gem} = 1.5 Hz, 1H, CH_{vinyl}), 6.21 (dd, J_{trans} = 17.3 Hz, J_{cis} = 10.4 Hz, 1H, CH_{vinyl}), 5.89 (dd, J_{cis} = 10.4 Hz, J_{gem} = 1.5 Hz, 1H, CH_{vinyl}), 5.29 (s, 2H, CH_2). **^{13}C{^{1}H} NMR:** (101 MHz, Chloroform-*d*) δ 166.2, 164.7, 164.3, 143.2, 140.8, 140.7, 140.4, 137.2, 136.3, 135.5, 131.4, 129.2, 129.1, 129.0, 128.5, 127.6, 127.4, 127.4, 126.3, 123.9, 120.6, 120.5, 110.3, 110.0, 66.2. **HRMS (APCI) *m/z*:** $[M+H]^+$ calc'd for $[C_{56}H_{39}N_4O_2]^+$ 799.3073; found 799.3076; difference +0.4 ppm.

(4'-(4,6-bis(4-(3,6-bis(di-p-tolylamino)-9H-carbazol-9-yl)phenyl)pyrimidin-2-yl)-[1,1'-biphenyl]-4-yl)methyl acrylate (**PymTTAC**). Prepared according to general reaction G using 110 mg **6f** (0.0720 mmol, 1.0 eq), 13 µL NEt_3 (0.0937 mmol, 1.3 eq.), and 7 µL acryloyl chloride (0.0865 mmol, 1.2 eq.) in 15 mL THF for 1 h at 0 °C. Purified on silica using dichloromethane as eluent. Yellow solid. Yield 32 mg (28% yield). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 8.87 (d, *J* = 8.1 Hz, 2H, CH_{biphen}), 8.58 (d, *J* = 8.1 Hz, 4H, CH_{Ph}), 8.19 (s, 1H, CH_{Pym}), 7.87 – 7.79 (m, 6H, CH_{Ph} (4H) and CH_{biphen} (2H)), 7.78 – 7.69 (m, 6H, CH_{Cz} (4H) and CH_{biphen} (2H)), 7.52 (d, *J* = 8.1 Hz, 2H, CH_{biphen}), 7.44 (d, *J* = 8.8 Hz, 4H, CH_{Cz}), 7.22 (dd, *J* = 8.8, 2.2 Hz, 4H, CH_{Cz}), 7.04 (d, *J* = 8.2 Hz, 16H, CH_{tol}), 6.98 (d, *J* = 8.2 Hz, 16H, CH_{tol}), 6.50 (d, J_{trans} = 17.3 Hz, 1H, CH_{vinyl}), 6.22 (dd, J_{trans} = 17.3 Hz, J_{cis} = 10.4 Hz, 1H, CH_{vinyl}), 5.89 (d, J_{cis} = 10.4 Hz, 1H, CH_{vinyl}), 5.29 (s, 2H, CH_2), 2.30 (s, 24H, CH_3). **^{13}C{^{1}H} NMR:** (101 MHz, Chloroform-*d*) δ 166.2, 164.7, 164.2, 146.4, 143.1, 141.7, 140.9, 140.5, 137.7, 137.2, 136.1, 135.5, 131.4, 131.3, 129.9, 129.2, 129.1, 129.0, 128.5, 127.6, 127.4, 127.0, 125.5, 124.5, 123.1, 118.0, 110.9, 110.2, 66.2, 20.9. **HRMS (FD) *m/z*:** $[M]^+$ calc'd for $[C_{112}H_{90}N_8O_2]^+$ 1578.7187; found 1578.7160; difference -1.7 ppm.

(4'-(2-(4-(9,9-dimethylacridin-10(9H)-yl)phenyl)-6-phenylpyrimidin-4-yl)-[1,1'-biphenyl]-4-yl)methyl acrylate (**2PymDMA**). Prepared according to general reaction G using 140 mg **7g** (0.225 mmol, 1.0 eq), 40.6 µL NEt_3 (0.293 mmol, 1.3 eq.), and 22.0 µL acryloyl chloride (0.270 mmol, 1.2 eq.) in 10 mL CH_2Cl_2 for 90 minutes at 0 °C. Purified on silica using 2:1 dichloromethane/hexanes as eluent. White solid. Yield 46 mg (30% yield). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 8.99 (d, *J* = 8.2 Hz, 2H, CH_{Ph}), 8.43 (d, *J* = 8.1 Hz, 2H, CH_{biphen}), 8.37 – 8.30 (dd, ^3J = 8.4 Hz, ^4J = 2.6 Hz, 2H, CH_{Ph}), 8.13 (s, 1H, CH_{Pym}), 7.82 (d, *J* = 8.2 Hz, 2H, CH_{Ph}), 7.71 (d, *J* = 7.8 Hz, 2H, CH_{biphen}), 7.65 – 7.57 (m, 3H, CH_{Ph}), 7.57 – 7.45 (m, 6H, CH_{biphen} (4H) and CH_{DMA} (2H)), 7.05 – 6.90 (m, 4H, CH_{DMA}), 6.50 (d, J_{trans} = 17.4 Hz, 1H, CH_{vinyl}), 6.42 (d, *J* = 7.9 Hz, 2H, CH_{DMA}), 6.21 (dd, J_{trans} = 17.3 Hz, J_{cis} = 10.4 Hz, 1H, CH_{vinyl}), 5.89 (d, J_{cis} = 10.5 Hz, 1H, CH_{vinyl}), 5.29 (s, 2H, CH_2), 1.74 (s, 6H, CH_3). **^{13}C NMR:** (101 MHz, Chloroform-*d*) δ 166.2, 165.2, 164.6, 164.2, 143.7, 143.3, 140.9, 140.4, 138.3, 137.5, 136.5, 135.7, 131.5, 131.4, 131.2, 131.1, 130.2, 129.2, 129.0, 128.4, 128.0, 127.8, 127.5, 127.5, 126.6, 125.4, 120.8, 114.3, 110.5, 66.2, 36.2, 31.5. **HRMS (APCI) *m/z*:** $[M]^+$ calc'd for $[C_{47}H_{37}N_3O_2]^+$ 675.2886; found 675.2893; difference +1.0 ppm.

(4'-(4,6-bis(4-(9,9-dimethylacridin-10(9H)-yl)phenyl)pyrimidin-2-yl)-[1,1'-biphenyl]-4-yl)methyl acetate (**PymDMA-OAc**). Prepared according to general reaction H using 30 mg **6a** (0.0362 mmol, 1.0 eq.), 75 µL NEt_3 (0.543 mmol, 15 eq.), and 39 µL acetyl chloride (0.543 mmol, 15 eq.) in 10 mL THF. Purified on

silica using 3:1 dichloromethane/hexanes as eluent. White solid. Yield 27 mg (86 %). **^{1}H NMR:** (400 MHz, Benzene-d_6) δ 9.18 (d, *J* = 8.3 Hz, 2H), 8.29 (d, *J* = 8.4 Hz, 4H), 7.78 (d, *J* = 8.2 Hz, 2H), 7.67 (s, 1H), 7.53 (d, *J* = 8.0 Hz, 2H), 7.44 (dd, *J* = 7.6, 1.7 Hz, 4H), 7.32 (d, *J* = 8.3 Hz, 4H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.00 (dtd, *J* = 20.4, 7.3, 1.5 Hz, 8H), 6.58 (dd, *J* = 8.0, 1.4 Hz, 4H), 5.03 (s, 2H), 1.70 (s, 15H). **^{13}C{^{1}H} NMR:** (101 MHz, Benzene-d_6) δ 170.0, 165.1, 164.6, 144.4, 143.8, 141.3, 140.9, 137.7, 137.6, 136.3, 132.2, 130.6, 130.4, 129.7, 129.3, 127.0, 125.9, 121.5, 114.7, 111.1, 65.9, 36.3, 31.6, 20.5.

(4'-(4,6-bis(4-(10H-phenoxazin-10-yl)phenyl)pyrimidin-2-yl)-[1,1'-biphenyl]-4-yl)methyl acetate (**PymPXZ-OAc**). Prepared according to general reaction H using 25 mg **6b** (0.0322 mmol, 1.0 eq.), 67 µL NEt_3 (0.483 mmol, 15 eq.), and 34 µL acetyl chloride (0.483 mmol, 15 eq.) in 10 mL THF. Purified on silica using 3:1 dichloromethane/hexanes (v/v) as eluent. Yellow solid. Yield 25 mg (95 %). **^{1}H NMR:** (400 MHz, Benzene-d_6) δ 9.15 (d, *J* = 8.5 Hz, 2H), 8.21 (d, *J* = 8.4 Hz, 4H), 7.78 (d, *J* = 8.5 Hz, 2H), 7.61 (s, 1H), 7.52 (d, *J* = 8.2 Hz, 2H), 7.28 (d, *J* = 8.1 Hz, 2H), 6.92 – 6.78 (m, 4H), 6.56 (tt, *J* = 7.5, 5.5 Hz, 8H), 6.19 – 6.04 (m, 4H), 5.03 (s, 2H), 1.70 (s, 3H). **^{13}C{^{1}H} NMR:** (101 MHz, Benzene-d_6) δ 165.2, 164.5, 144.7, 143.9, 142.0, 140.8, 137.7, 137.6, 136.4, 134.7, 131.6, 130.4, 129.7, 129.3, 123.8, 122.3, 116.2, 113.8, 65.9, 20.5.

(4'-(4,6-bis(4-(10H-phenothiazin-10-yl)phenyl)pyrimidin-2-yl)-[1,1'-biphenyl]-4-yl)methyl acetate (**PymPTZ-OAc**). Prepared according to general reaction H using 20 mg **6c** (0.0247 mmol, 1.0 eq.), 51 µL NEt_3 (0.371 mmol, 15 eq.), and 26 µL acetyl chloride (0.371 mmol, 15 eq.) in 5 mL THF. Purified on silica using 3:1 dichloromethane/hexanes (v/v) as eluent. Yellow solid. Yield 17 mg (81 %). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 8.82 (d, *J* = 8.3 Hz, 2H), 8.47 (d, *J* = 8.5 Hz, 4H), 8.08 (s, 1H), 7.78 (d, *J* = 8.4 Hz, 2H), 7.72 (d, *J* = 8.0 Hz, 2H), 7.53 (d, *J* = 8.5 Hz, 4H), 7.49 (d, *J* = 8.1 Hz, 2H), 7.16 (dd, *J* = 7.5, 1.7 Hz, 4H), 6.97 (dtd, *J* = 24.2, 7.5, 1.5 Hz, 8H), 6.59 (dd, *J* = 8.0, 1.4 Hz, 4H), 5.18 (s, 2H), 2.14 (s, 3H). **^{13}C NMR:** (101 MHz, Chloroform-*d*) δ 171.1, 164.6, 164.2, 144.8, 143.6, 143.1, 140.8, 137.3, 135.7, 135.6, 129.6, 129.1, 129.0, 128.0, 127.6, 127.5, 127.4, 127.1, 123.7, 123.7, 118.8, 110.1, 66.2, 21.2.

(4'-(4-(4-(10H-phenoxazin-10-yl)phenyl)-6-(4-(9,9-dimethylacridin-10(9H)-yl)phenyl)pyrimidin-2-yl)-[1,1'-biphenyl]-4-yl)methyl acetate (**PymDMAPXZ-OAc**). Prepared according to general reaction H using 20 mg **6d** (0.0250 mmol, 1.0 eq.), 50 µL NEt_3 (0.373 mmol, 15 eq.), and 27 µL acetyl chloride (0.373 mmol, 15 eq.) in 10 mL THF. Purified on silica using 3:1 dichloromethane/hexanes (v/v) as eluent. Yellow solid. Yield 18 mg (85 %). **^{1}H NMR:** (400 MHz, Benzene-d_6) δ 9.16 (d, *J* = 8.1 Hz, 2H), 8.28 (d, *J* = 7.9 Hz, 2H), 8.22 (d, *J* = 8.1 Hz, 2H), 7.78 (d, *J* = 8.0 Hz, 2H), 7.64 (s, 1H), 7.52 (d, *J* = 7.8 Hz, 2H), 7.44 (d, *J* = 7.5 Hz, 2H), 7.30 (dd, *J* = 17.3, 7.9 Hz, 4H), 7.00 (dt, *J* = 19.5, 7.2 Hz, 4H), 6.90 – 6.79 (m, 2H), 6.57 (d, *J* = 7.3 Hz, 6H), 6.22 – 6.03 (m, 2H), 5.03 (s, 2H), 1.70 (s, 9H). **^{13}C{^{1}H} NMR:** (101 MHz, Benzene-d_6) δ 170.0, 165.1, 164.7, 164.5, 144.7, 144.5, 143.8, 141.9, 141.3, 140.8, 137.8, 137.7, 137.5, 136.3, 134.7, 132.2, 131.6, 130.6, 130.5, 130.4, 129.7, 129.3, 126.9, 125.9, 123.8, 122.3, 121.5, 116.2, 114.7, 113.8, 111.0, 65.9, 36.4, 31.6, 20.5.

(4'-(4,6-bis(4-(9H-carbazol-9-yl)phenyl)pyrimidin-2-yl)-[1,1'-biphenyl]-4-yl)methyl acetate (**PymCz-OAc**). Prepared according to general reaction H using 20 mg **6e** (0.0268 mmol, 1.0 eq.), 56 µL NEt_3 (0.403 mmol, 15 eq.), and 29 µL acetyl chloride (0.403 mmol, 15 eq.) in 10 mL THF. Purified on silica using 3:1 dichloromethane/hexanes (v/v) as eluent. White solid. Yield 15 mg (71 %). **^{1}H NMR:** (400 MHz, Benzene-d_6) δ 9.21 (d, *J* = 8.3 Hz, 2H), 8.27 (d, *J* = 8.5 Hz, 4H), 8.11 (d, *J* = 7.7 Hz, 4H), 7.82 (d, *J* = 8.3 Hz, 2H), 7.71 (s, 1H), 7.54 (d, *J* = 7.4 Hz, 2H), 7.52 (d, *J* = 7.7 Hz, 4H), 7.46 – 7.36 (m, 8H), 7.35 – 7.24 (m, 6H), 5.03 (s, 2H), 1.71 (s, 3H). **^{13}C{^{1}H} NMR:** (101 MHz, Benzene-d_6) δ 170.0, 165.1, 164.5, 143.8, 141.1, 140.8, 140.5, 137.8, 136.5, 136.3, 129.7, 129.3, 129.3, 127.4, 126.6, 124.4, 121.0, 120.9, 110.2, 65.9, 20.5.

(4'-(4,6-bis(4-(3,6-bis(di-p-tolylamino)-9H-carbazol-9-yl)phenyl)pyrimidin-2-yl)-[1,1'-biphenyl]-4-yl)methyl acetate (**PymTTAC-OAc**). Prepared according to general reaction H using 20 mg **6f** (0.0131 mmol, 1.0 eq.), 27 µL NEt_3 (0.197 mmol, 15 eq.), and 14 µL acetyl chloride (0.197 mmol, 15 eq.) in 10 mL THF. Purified on silica using 3:1 dichloromethane/hexanes (v/v) as eluent. Yellow solid. Yield 17 mg (83 %). **^{1}H NMR:** (400 MHz, Benzene-d_6) δ 9.22 (d, *J* = 8.4 Hz, 2H), 8.28 (d, *J* = 8.6 Hz, 4H), 7.93 (s, 4H), 7.81 (d, *J* = 8.4 Hz, 2H), 7.70 (s, 1H), 7.53 (d, 2H), 7.49 (d, 4H), 7.29 (d, 2H), 7.22 (d, *J* = 8.4 Hz, 16H), 6.95 (d, *J* = 8.4 Hz, 16H), 5.03 (s, 2H), 2.12 (s, 24H), 1.70 (s, 3H). **^{13}C{^{1}H} NMR:** (101 MHz, Benzene-d_6) δ 164.4, 147.1, 142.2, 140.8, 138.4, 136.4, 131.2, 130.2, 129.7, 129.3, 127.0, 126.5, 125.4, 123.3, 119.1, 111.2, 65.9, 20.8, 20.5.

(4'-(2-(4-(9,9-dimethylacridin-10(9H)-yl)phenyl)-6-phenylpyrimidin-4-yl)-[1,1'-biphenyl]-4-yl)methyl acetate (**2PymDMA-OAc**). Prepared according to general reaction H using 20 mg **7g** (0.0322 mmol, 1.0 eq.), 49 µL NEt_3 (0.482 mmol, 15 eq.), and 34 µL acetyl chloride (0.482 mmol, 15 eq.) in 5 mL THF. Purified on silica using 3:1 dichloromethane/hexanes (v/v) as eluent. Yellow solid. Yield 12 mg (56 %). **^{1}H NMR:** (400 MHz, Chloroform-*d*) δ 8.99 (d, *J* = 8.5 Hz, 2H), 8.42 (d, *J* = 8.2 Hz, 2H), 8.38 – 8.30 (dd, ^3J = 7.8 Hz, ^4J = 2.2 Hz, 2H), 8.13 (s, 1H), 7.81 (d, *J* = 8.5 Hz, 2H), 7.71 (d, *J* = 8.0 Hz, 2H), 7.64 – 7.56 (m, 3H), 7.57 – 7.41 (m, 6H), 7.07 – 6.87 (m, 4H), 6.41 (dd, *J* = 7.9, 1.6 Hz, 2H), 5.19 (s, 2H), 2.15 (s, 3H), 1.73 (s, 6H). **^{13}C NMR:** (101 MHz, Chloroform-*d*) δ 171.1, 165.2, 164.6, 164.2, 143.7, 143.3, 140.9, 140.4, 138.3, 137.5, 136.5, 135.8, 131.6, 131.2, 131.1, 130.2, 129.2, 129.1, 128.0, 127.8, 127.5, 127.5, 126.6, 125.4, 120.8, 114.3, 110.5, 66.1, 36.2, 31.5, 21.2.

S2 NMR Spectra of New Compounds

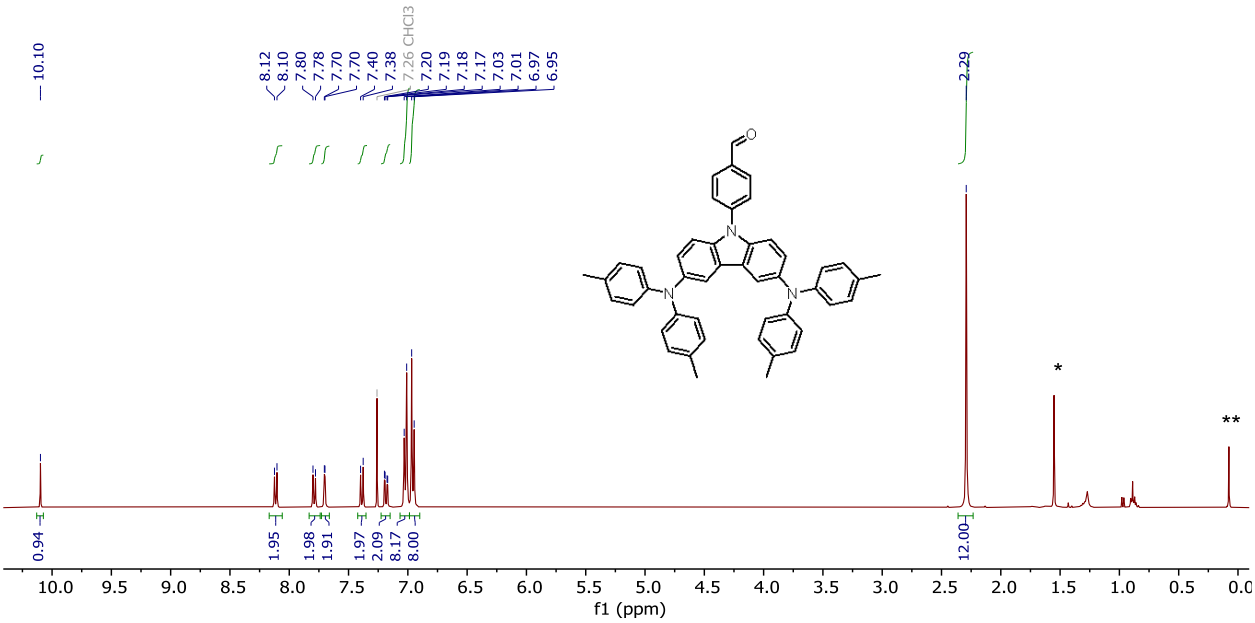


Figure S1a ^{1}H NMR spectrum of **1f** in $CDCl_3$. * = H_2O, ** = PDMS grease.

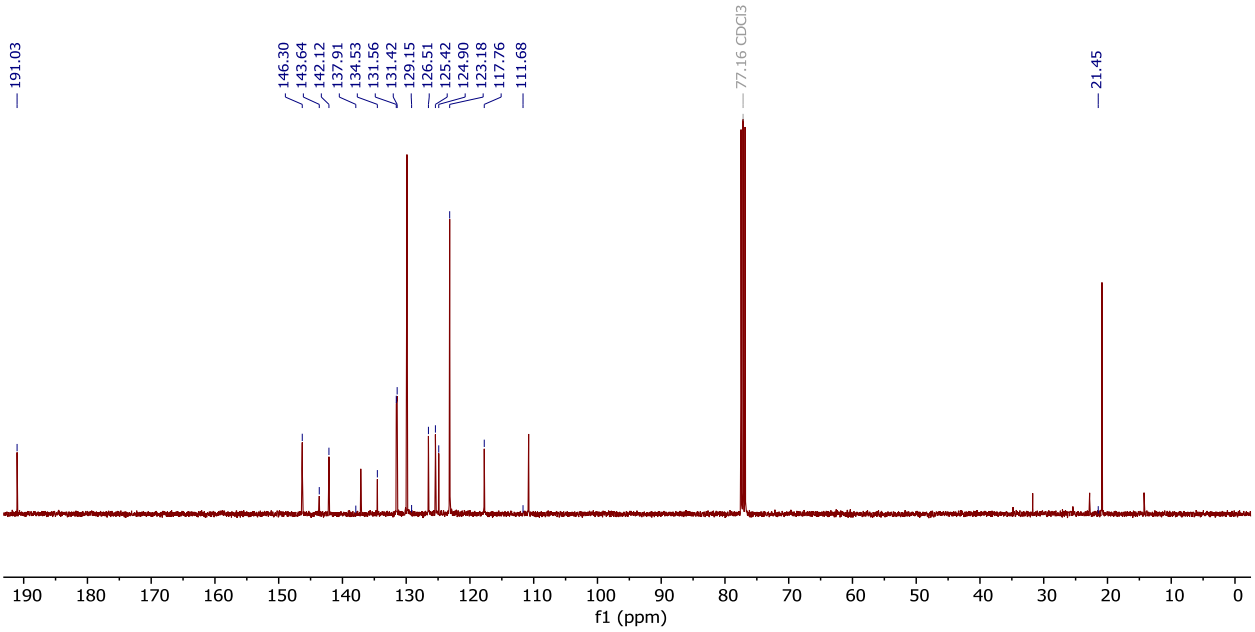


Figure S1b ^{13}C{^{1}H} NMR spectrum of **1f** in $CDCl_3$.

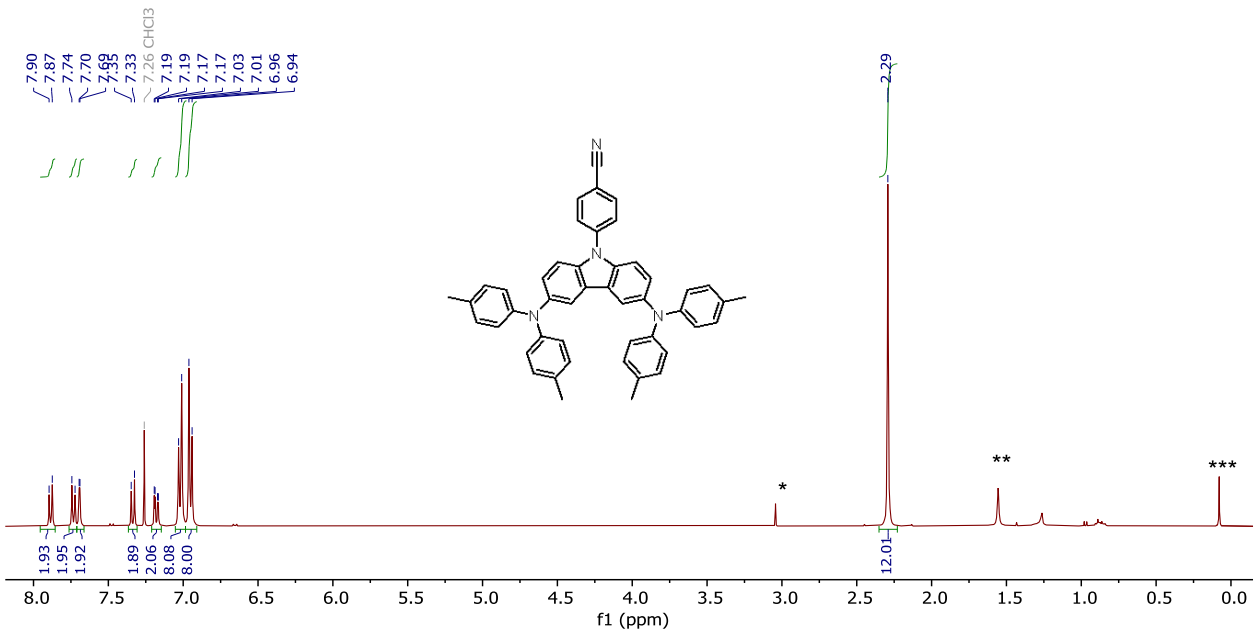


Figure S2a ^{1}H NMR spectrum of 4-(3,6-bis(di-*p*-tolylamino)-9*H*-carbazol-9-yl)benzonitrile in $CDCl_3$. * = methanol, ** = H_2O, *** = PDMS grease.

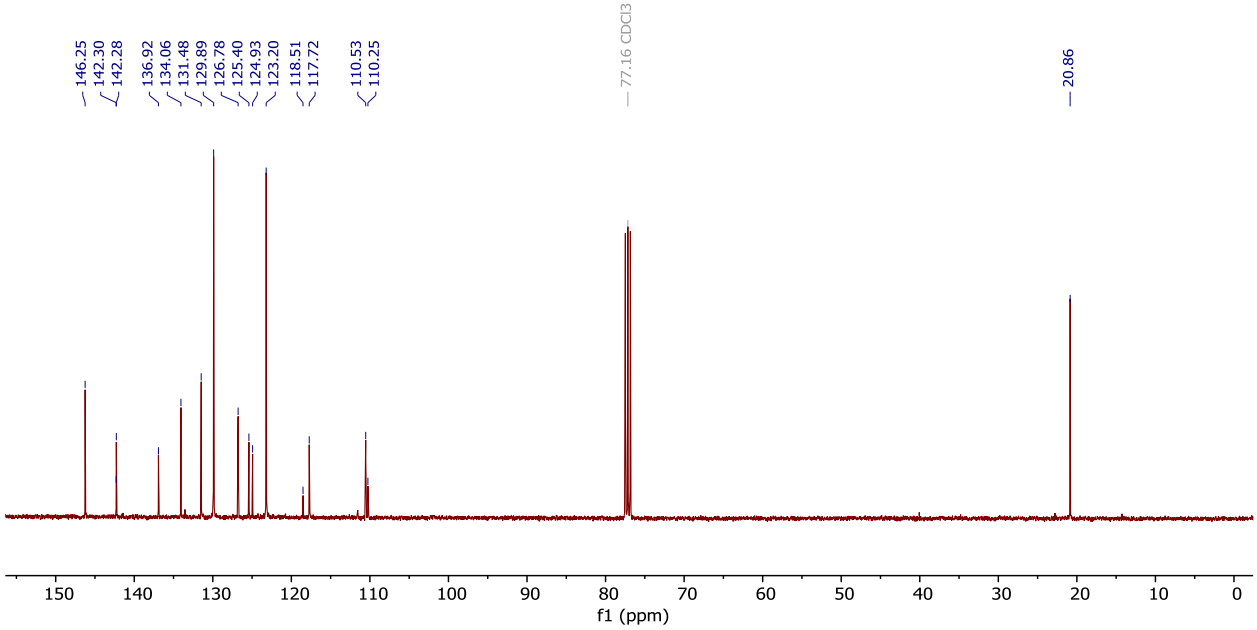


Figure S2b ^{13}C{^{1}H} NMR spectrum of 4-(3,6-bis(di-*p*-tolylamino)-9*H*-carbazol-9-yl)benzonitrile in $CDCl_3$.

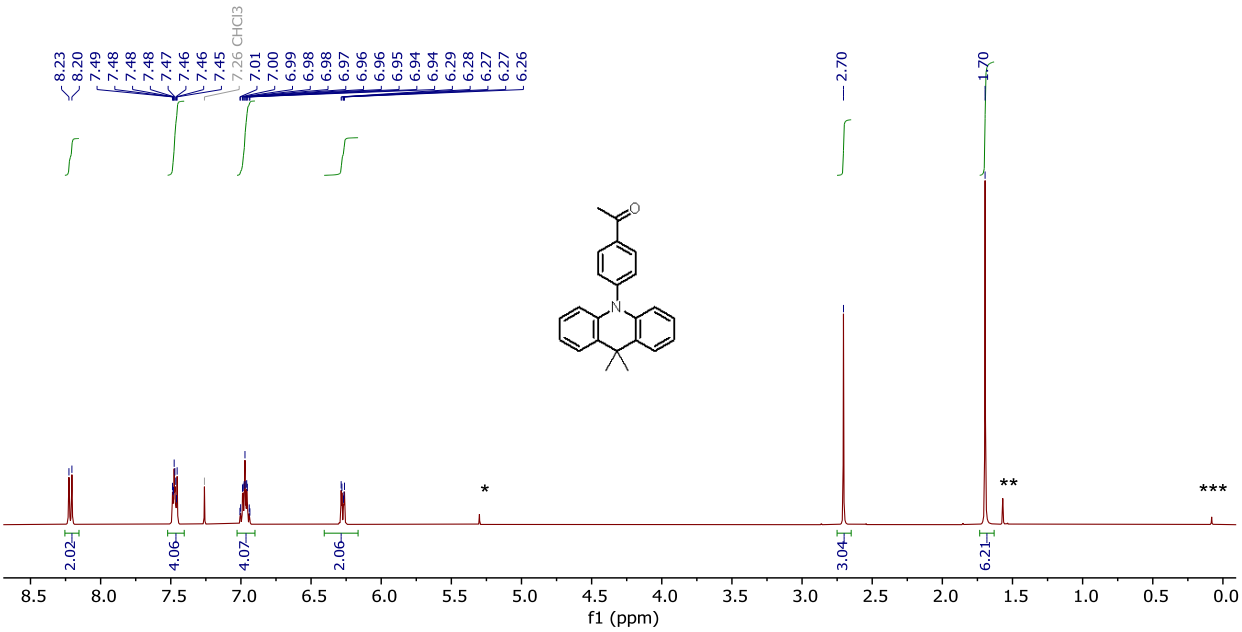


Figure S3a ^{1}H NMR spectrum of **2a** in $CDCl_3$. * = CH_2Cl_2, ** = H_2O, *** = PDMS grease.

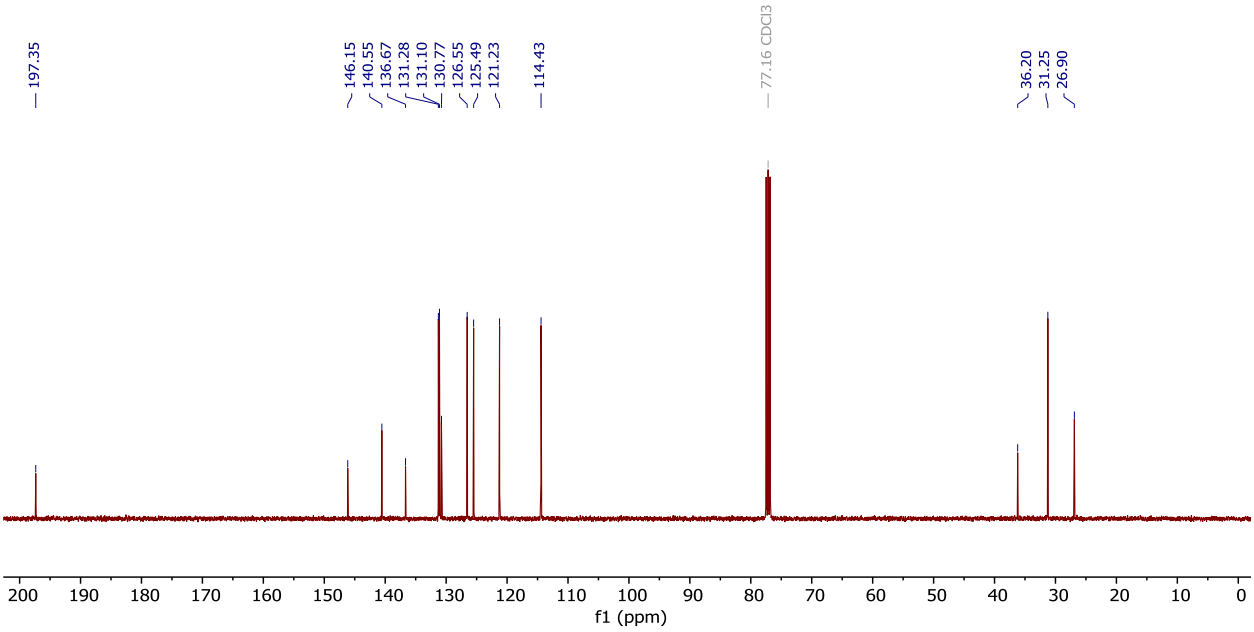


Figure S3b $^{13}C\{^{1}H\}$ NMR spectrum of **2a** in $CDCl_3$.

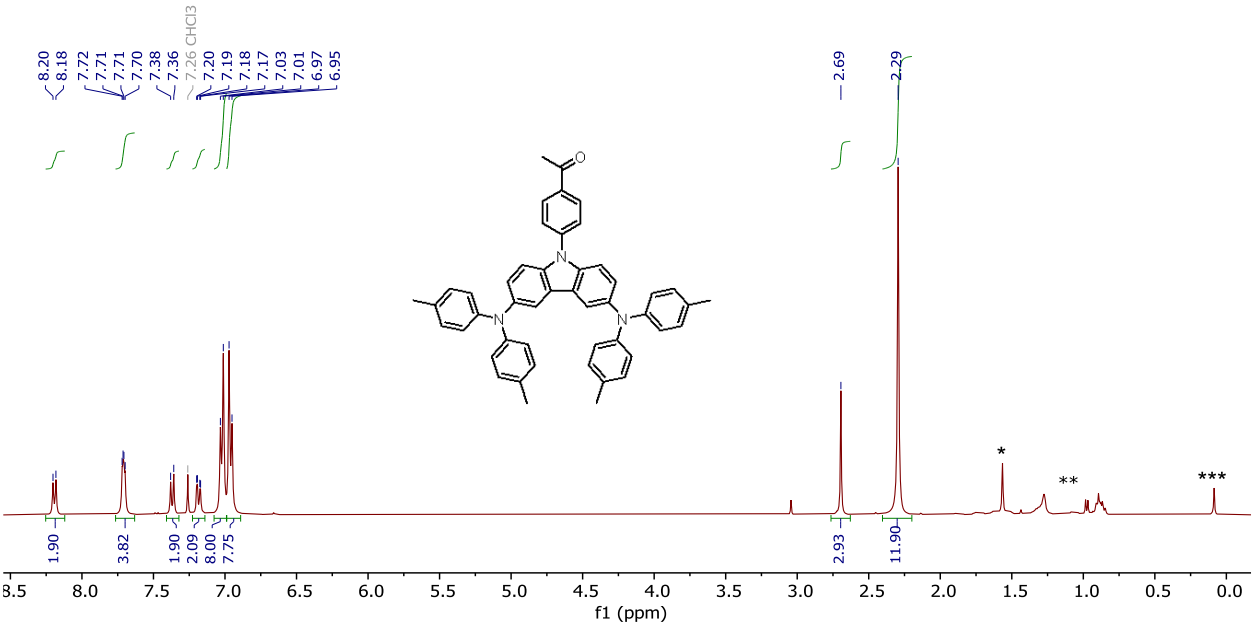


Figure S4a ^{1}H NMR spectrum of **2f** in $CDCl_3$. * = H_2O, ** = hexanes, *** = PDMS grease.

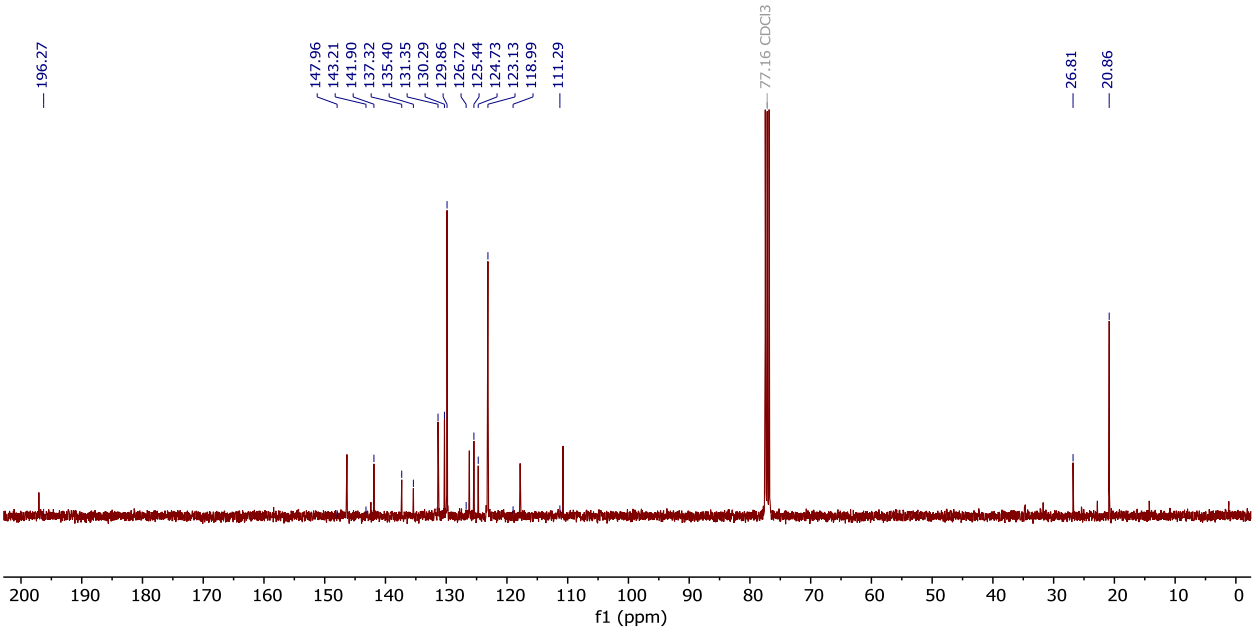


Figure S4b ^{13}C{^{1}H} NMR spectrum of **2f** in $CDCl_3$.

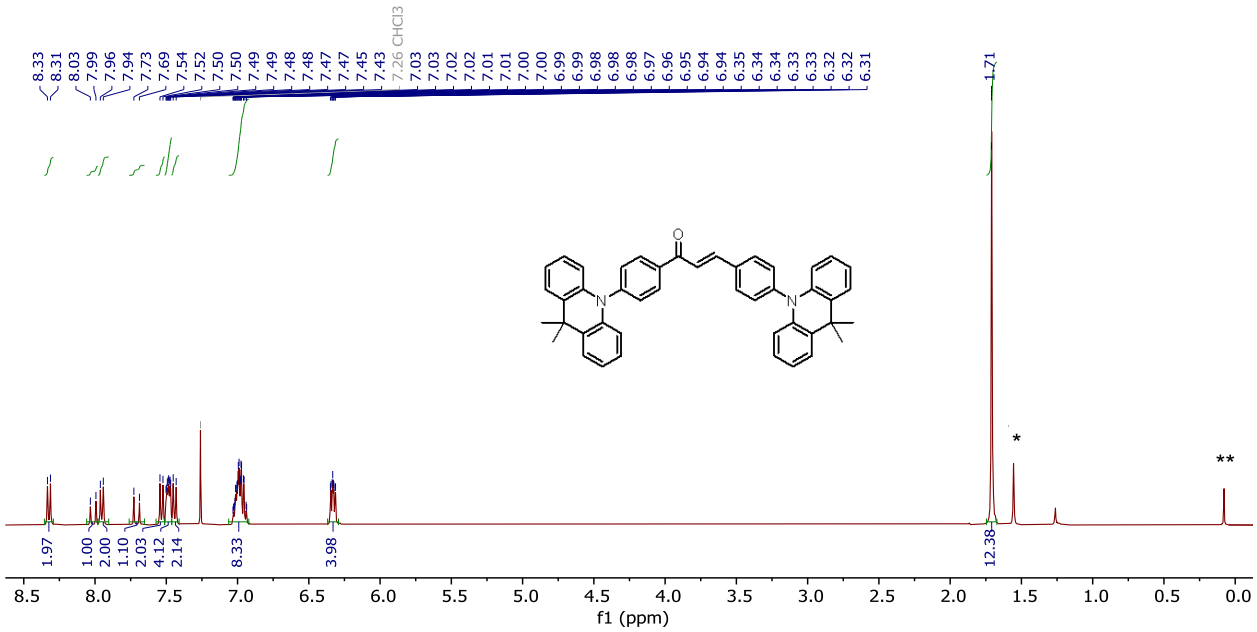


Figure S5a ^{1}H NMR spectrum of **3a** in $CDCl_3$. * = H_2O, ** = PDMS grease.

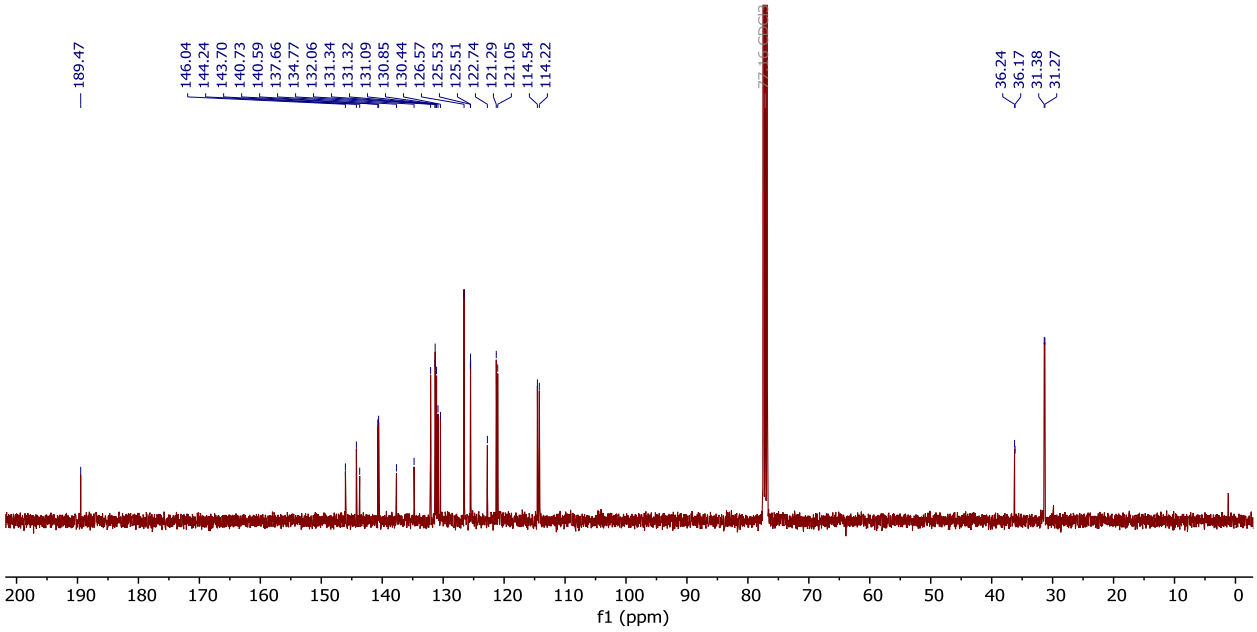


Figure S5b ^{13} {^{1}H} NMR spectrum of **3a** in $CDCl_3$.

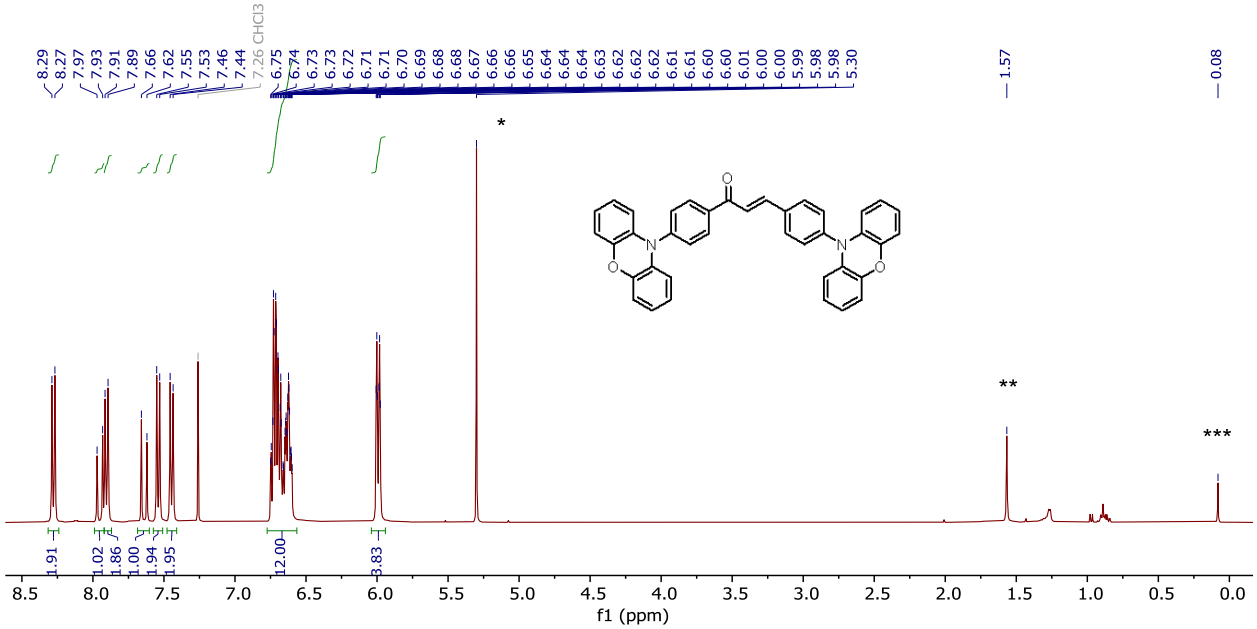


Figure S6a ^{1}H NMR spectrum of **3b** in $CDCl_3$. * = CH_2Cl_2, ** = H_2O, *** = PDMS grease.

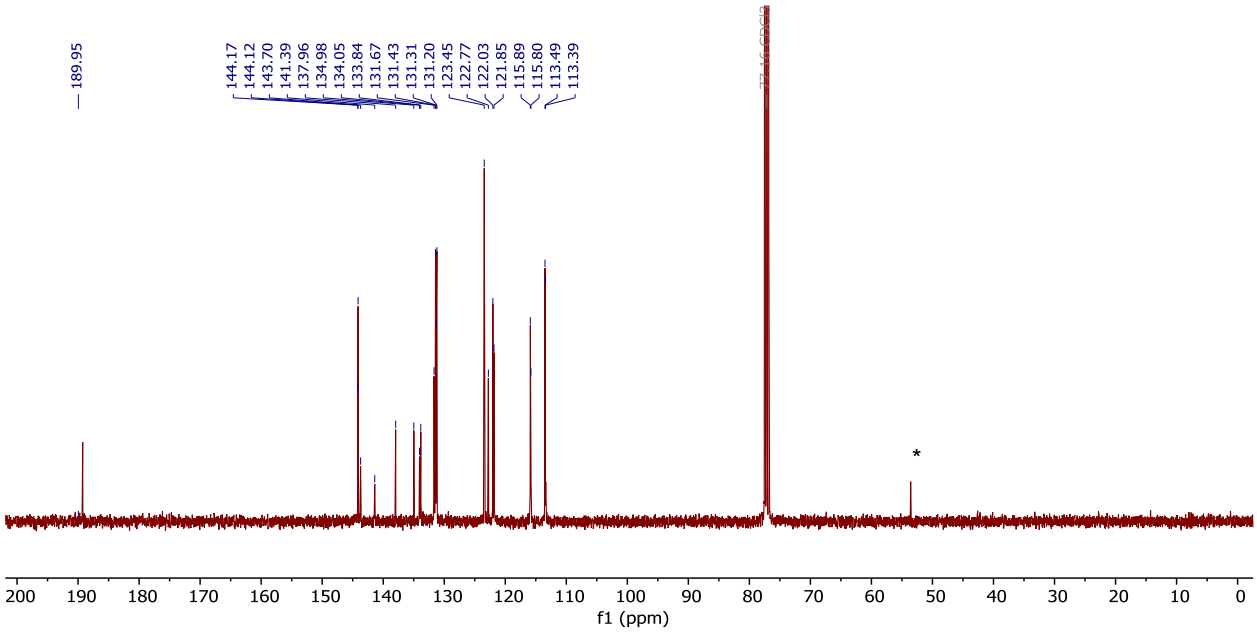


Figure S6b ^{13}C{^{1}H} NMR spectrum of **3b** in $CDCl_3$. * = CH_2Cl_2.

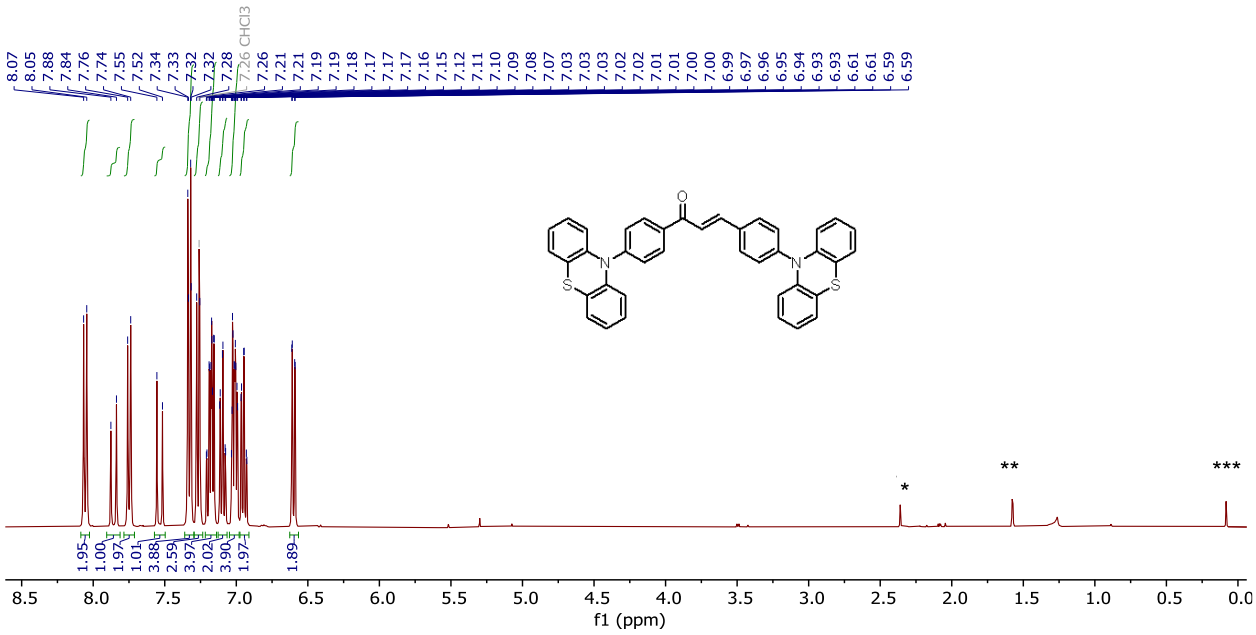


Figure S7a ^{1}H NMR spectrum of **3c** in $CDCl_3$. * = toluene, ** = H_2O, *** = PDMS grease

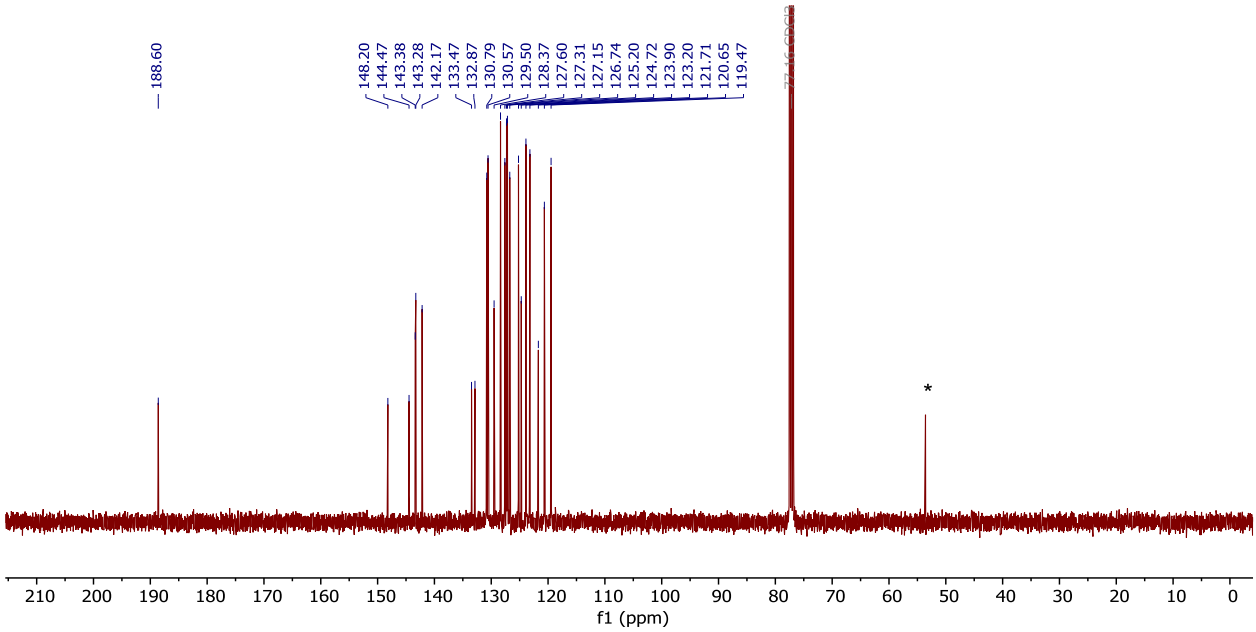


Figure S7b $^{13}C\{^{1}H\}$ NMR spectrum of **3c** in $CDCl_3$. * = CH_2Cl_2

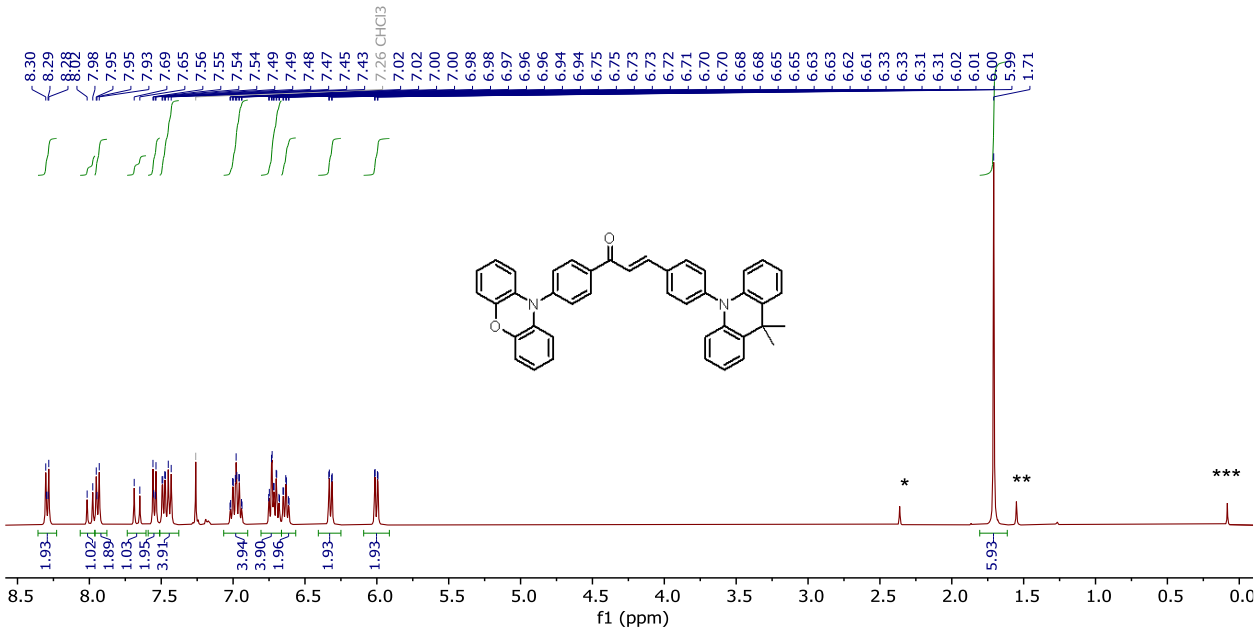


Figure S8a ^{1}H NMR spectrum of **3d** in $CDCl_3$. * = toluene, ** = H_2O, *** = PDMS grease.

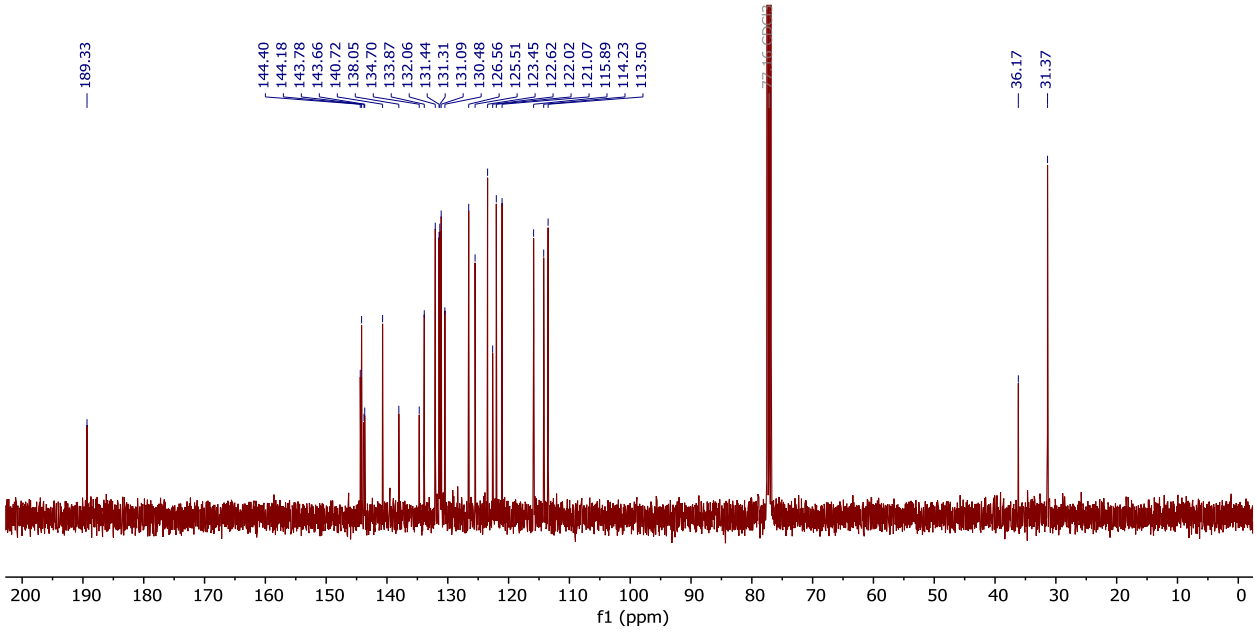


Figure S8b ^{13}C{^{1}H} NMR spectrum of **3d** in $CDCl_3$.

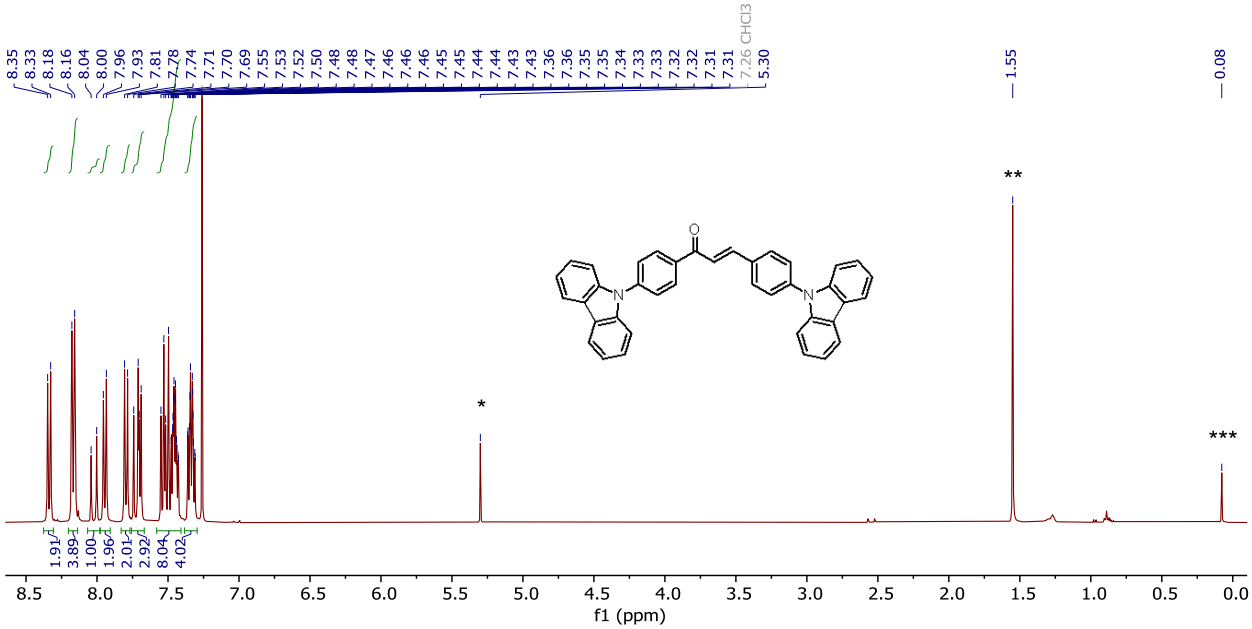


Figure S9a ^{1}H NMR spectrum of **3e** in $CDCl_3$. * = CH_2Cl_2, ** = H_2O, *** = PDMS grease.

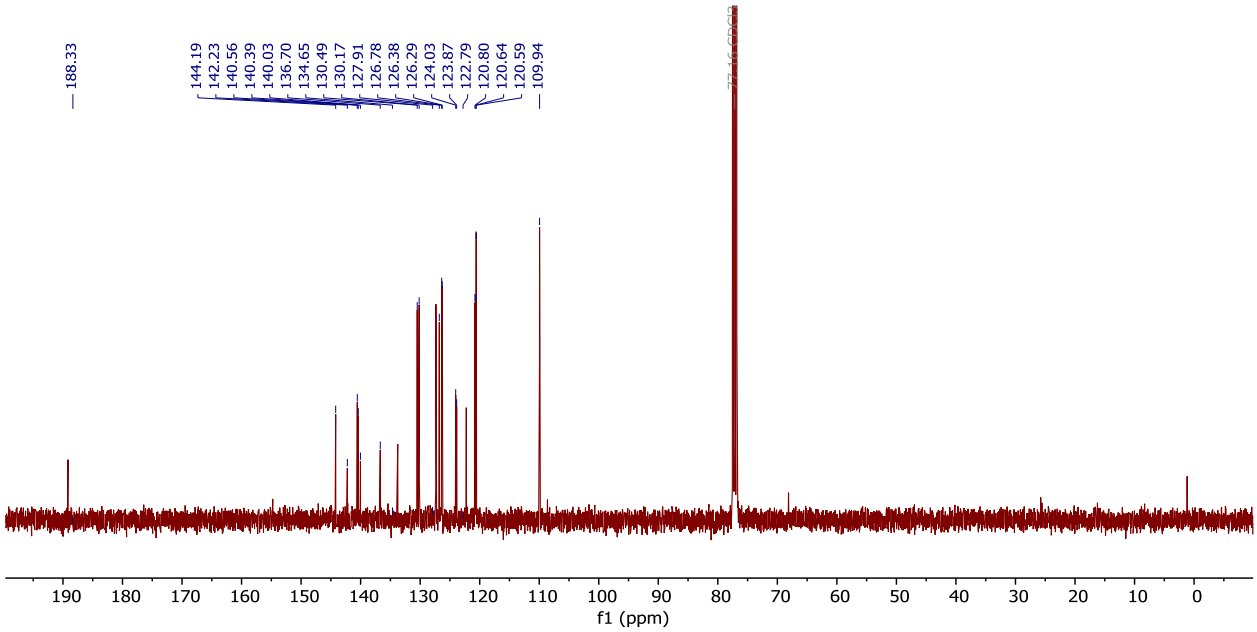


Figure S9b ^{13}C{^{1}H} NMR spectrum of **3e** in $CDCl_3$.

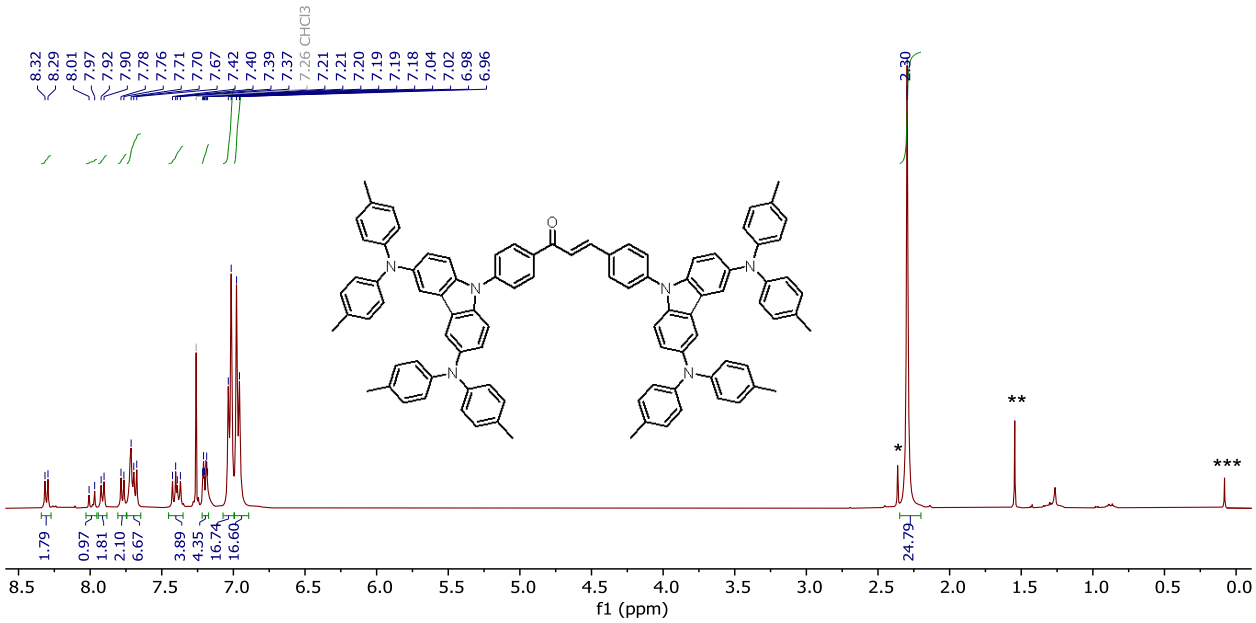


Figure S10a ^{1}H NMR spectrum of **3f** in $CDCl_3$. * = toluene, ** = H_2O, *** = PDMS grease.

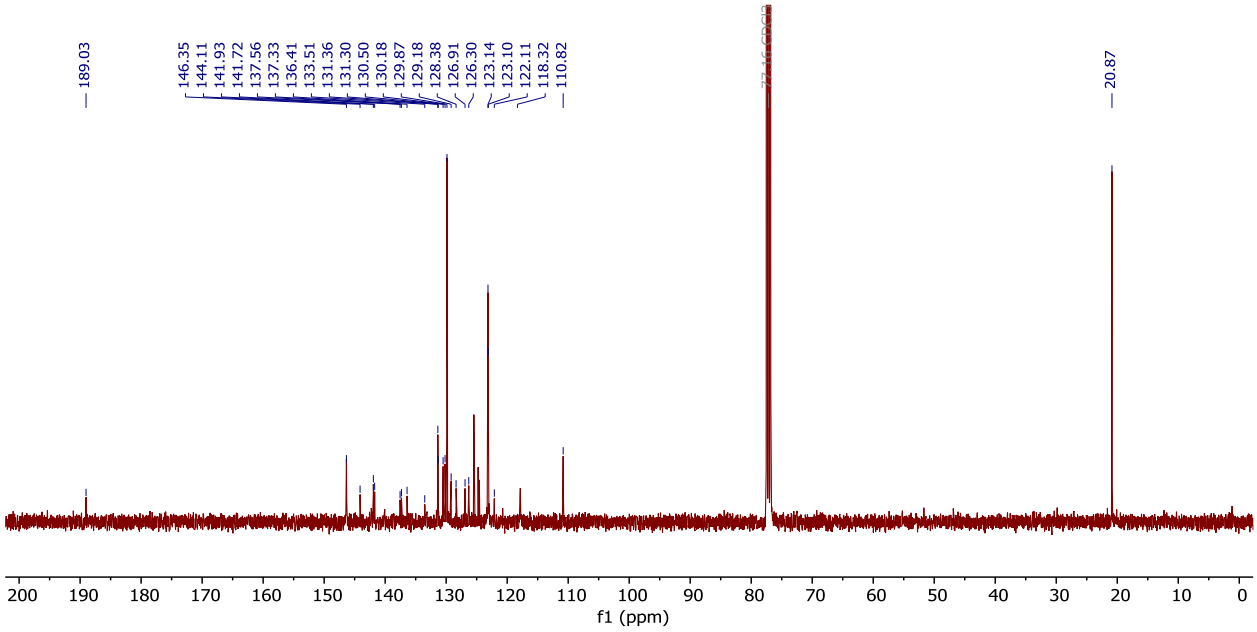


Figure S10b ^{13}C{^{1}H} NMR spectrum of **3f** in $CDCl_3$.

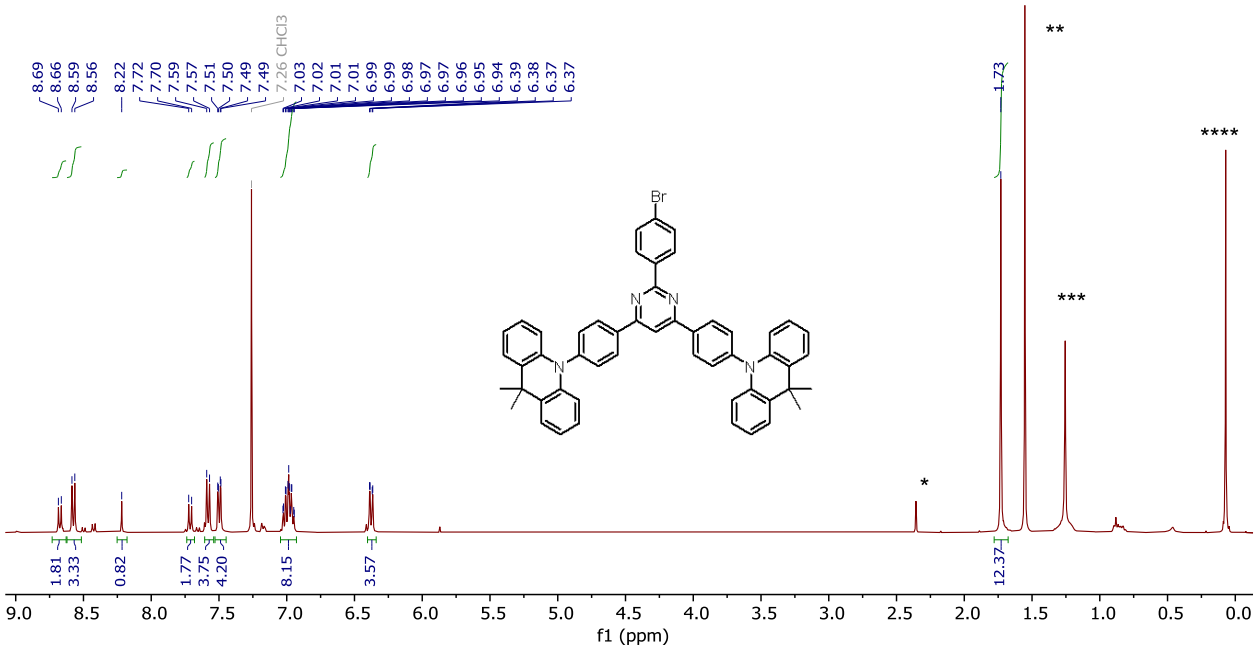


Figure S11a ^{1}H NMR spectrum of **4a** in $CDCl_3$. * = toluene, ** = H_2O, *** = hexanes, **** = PDMS grease.

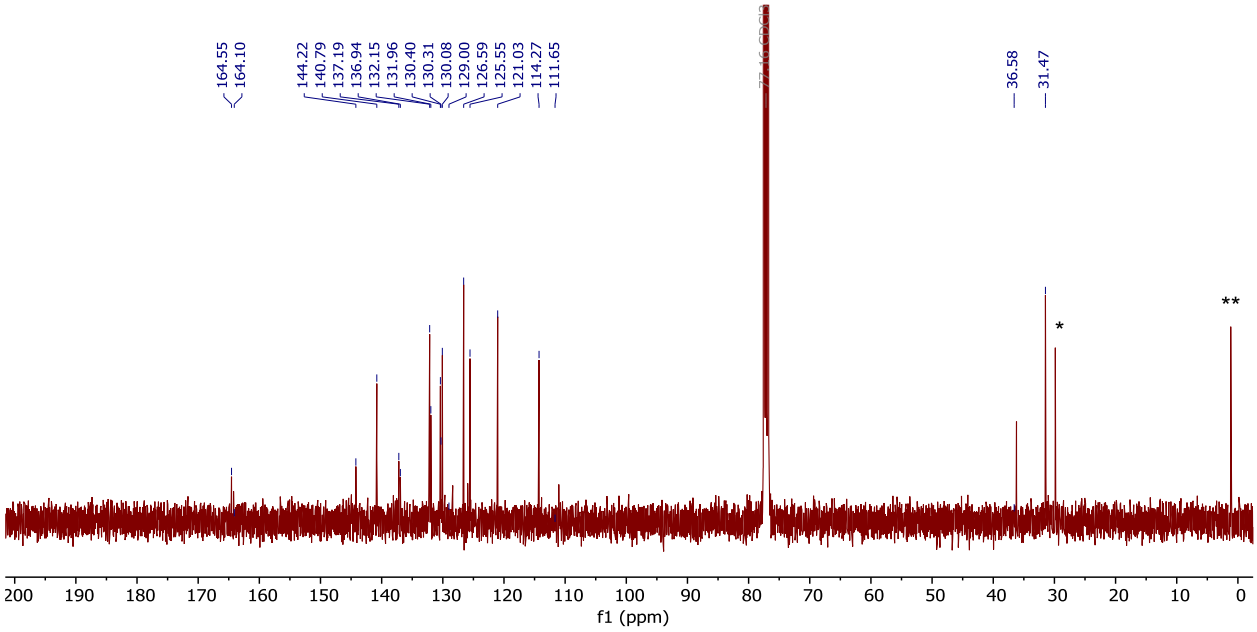


Figure S11b ^{13}C{^{1}H} NMR spectrum of **4a** in $CDCl_3$. * = toluene, ** = PDMS grease.

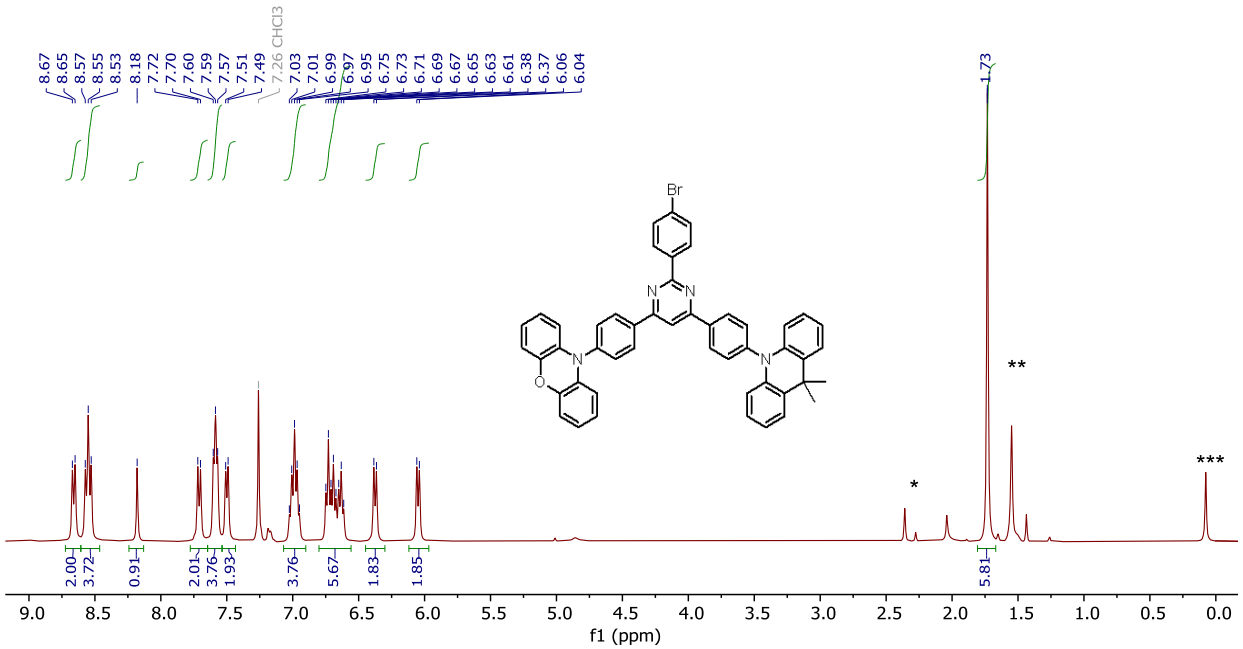


Figure S12a ^{1}H NMR spectrum of **4d** in $CDCl_3$. * = toluene, ** = H_2O, *** = PDMS grease.

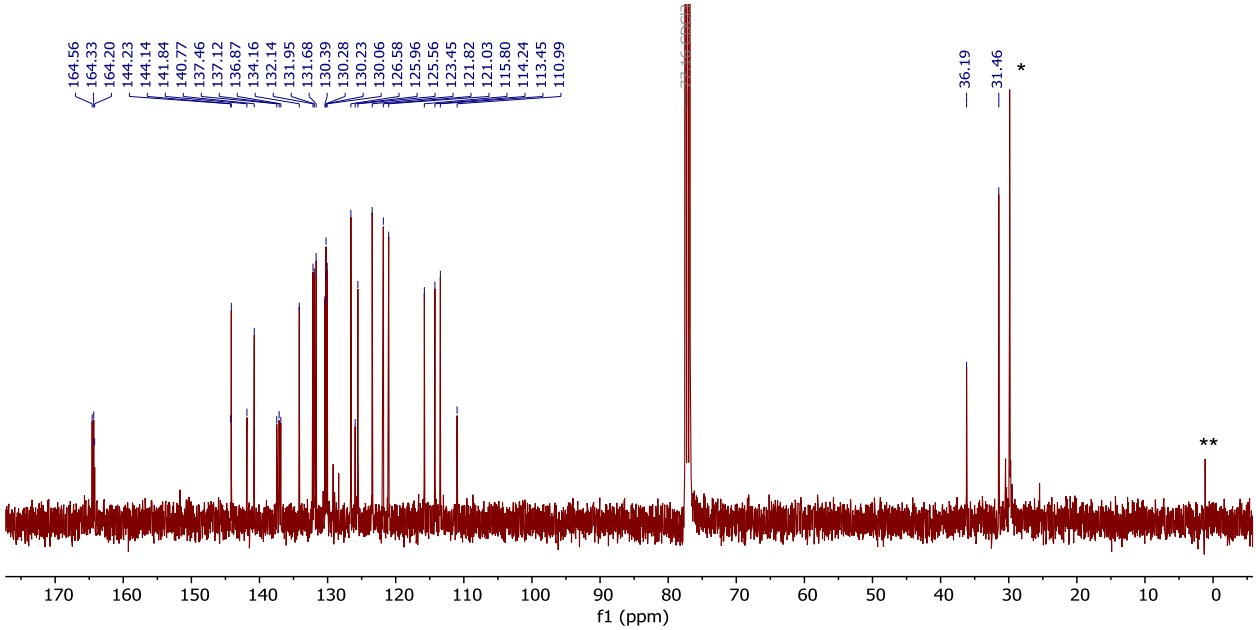


Figure S12b ^{13}C{^{1}H} NMR spectrum of **4d** in $CDCl_3$. * = toluene, ** = PDMS grease.

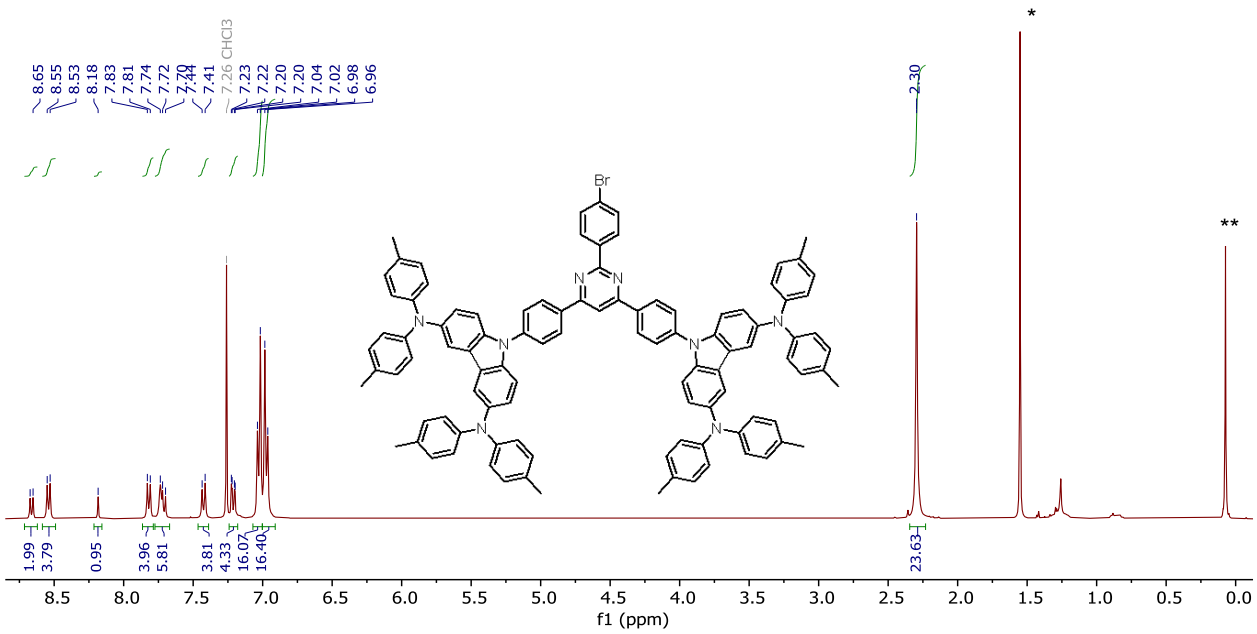


Figure S13a ^{1}H NMR spectrum of **4f** in $CDCl_3$. * = H_2O, ** = PDMS grease.

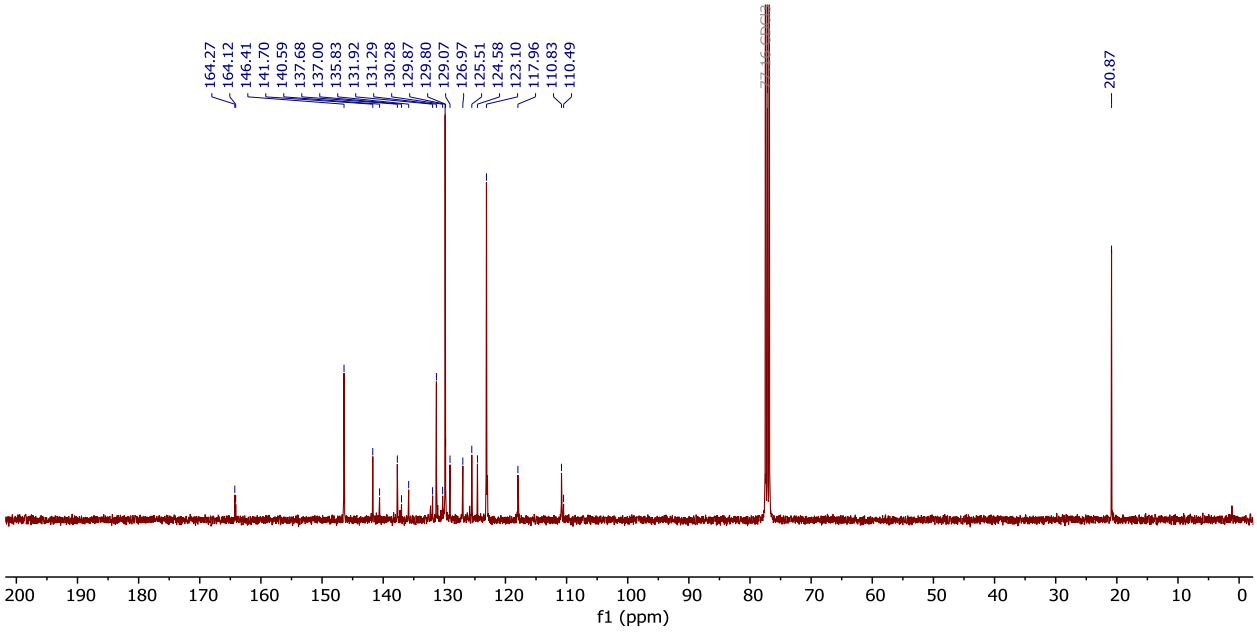


Figure S13b ^{13}C{^{1}H} NMR spectrum of **4f** in $CDCl_3$.

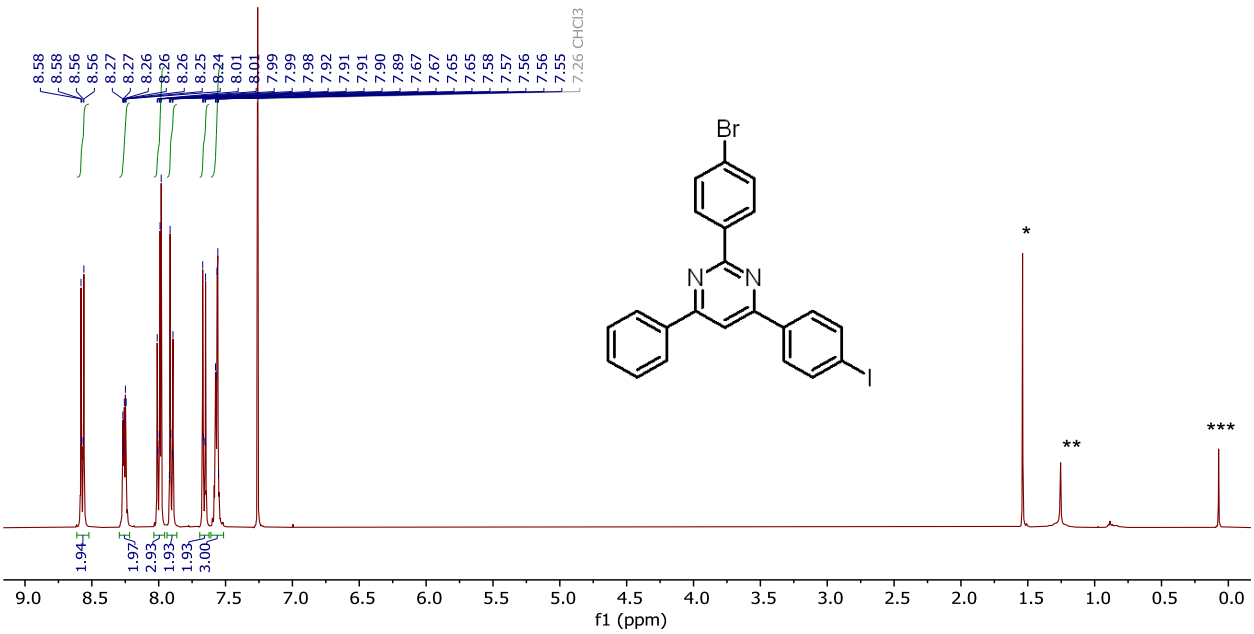


Figure S14a ^{1}H NMR spectrum of **4g** in $CDCl_3$. * = H_2O, ** = hexanes, *** = PDMS grease.

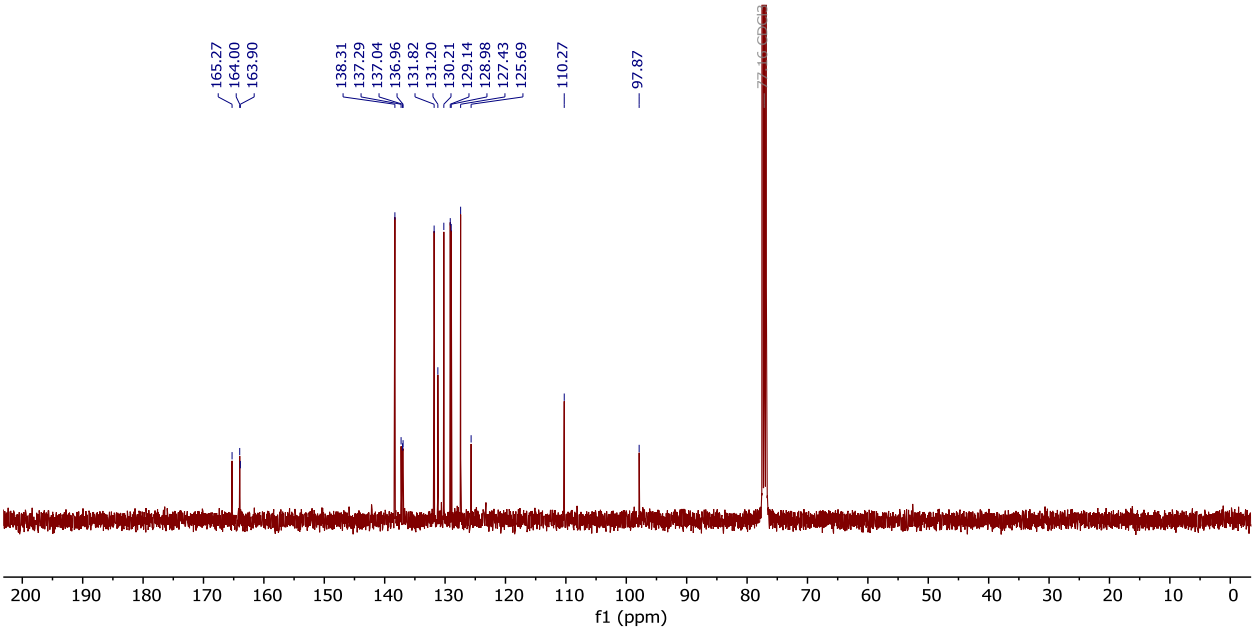


Figure S14b $^{13}C\{^{1}H\}$ NMR spectrum of **4g** in $CDCl_3$.

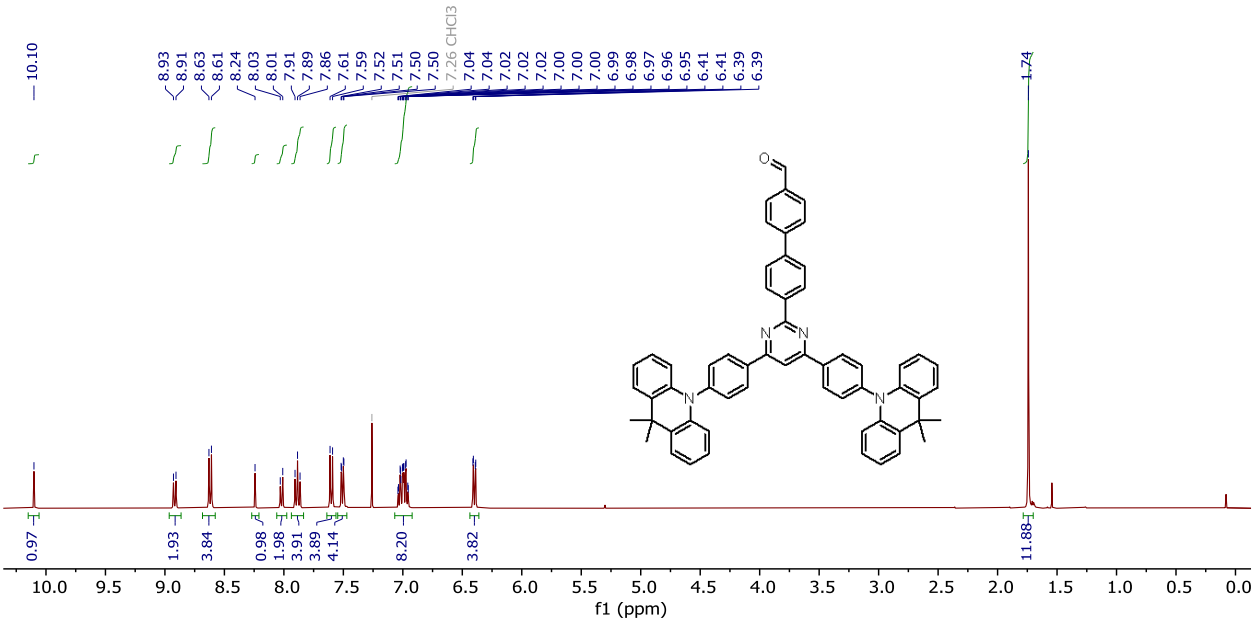


Figure S15a ^{1}H NMR spectrum of **5a** in $CDCl_3$.

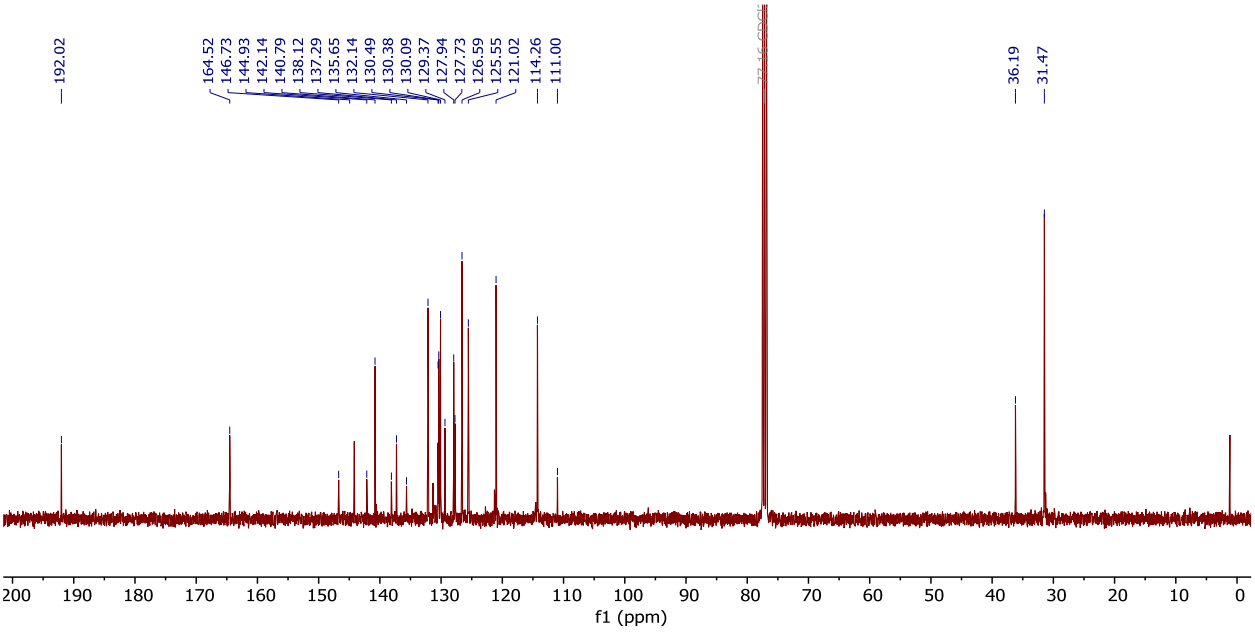


Figure S15b ^{13}C{^{1}H} NMR spectrum of **5a** in $CDCl_3$.

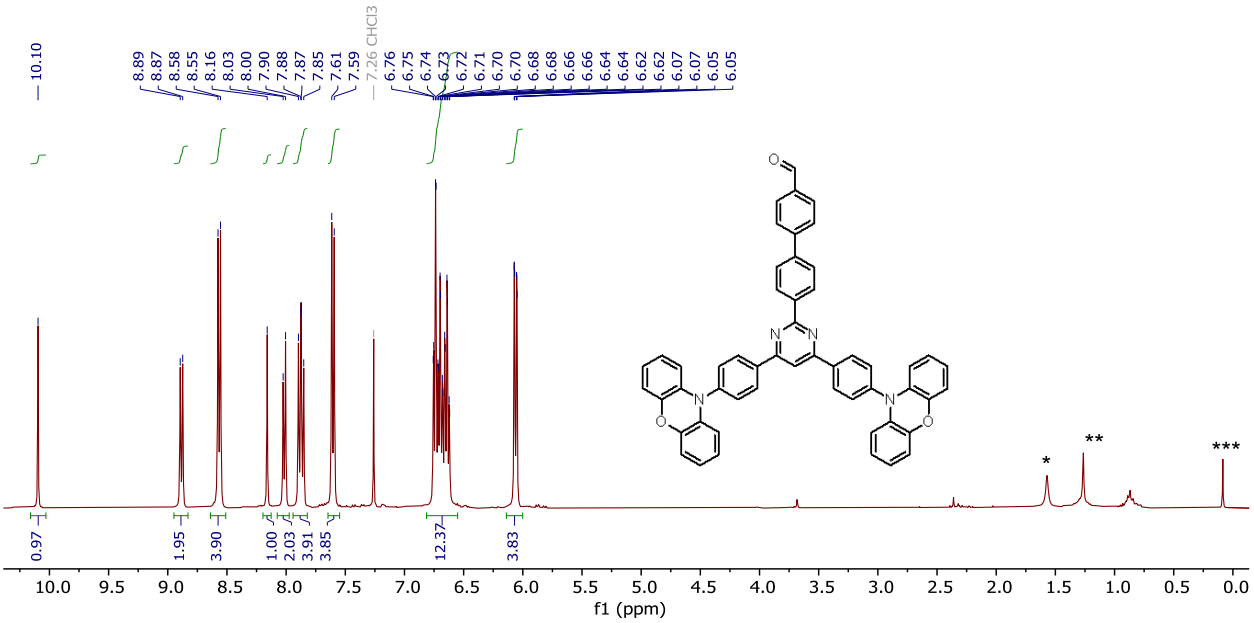


Figure S16a ^{1}H NMR spectrum of **5b** in $CDCl_3$. * = H_2O, ** = hexanes, *** = PDMS grease.

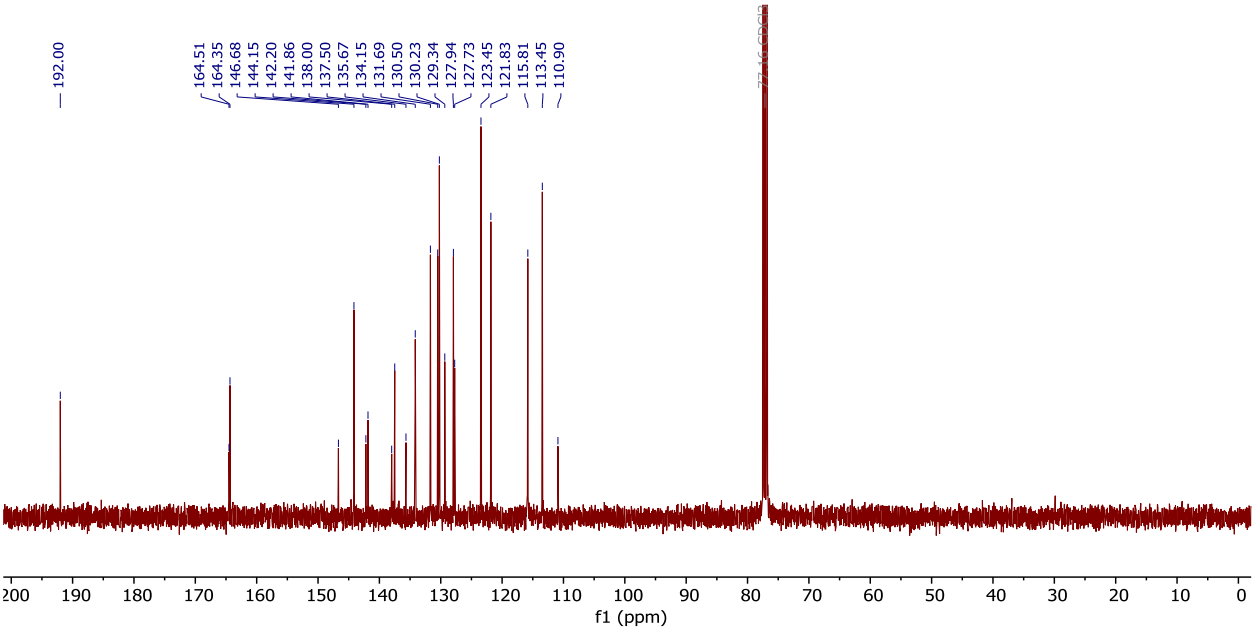


Figure S16b ^{13}C{^{1}H} NMR spectrum of **5b** in $CDCl_3$.

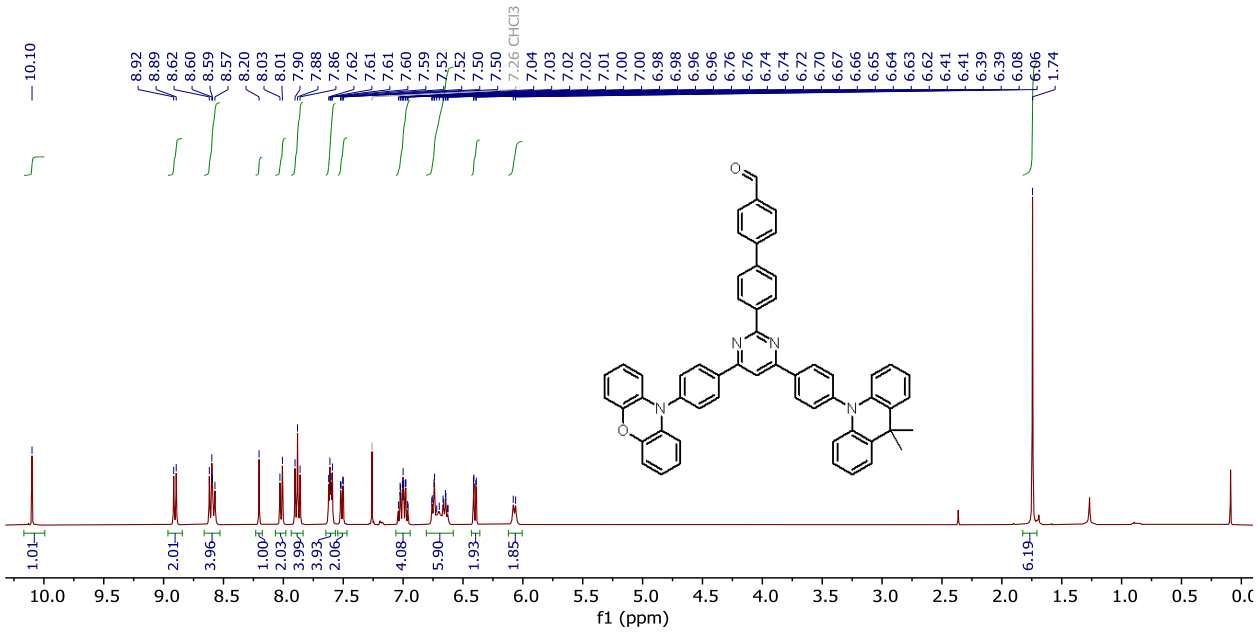


Figure S17a ^{1}H NMR spectrum of **5d** in $CDCl_3$.

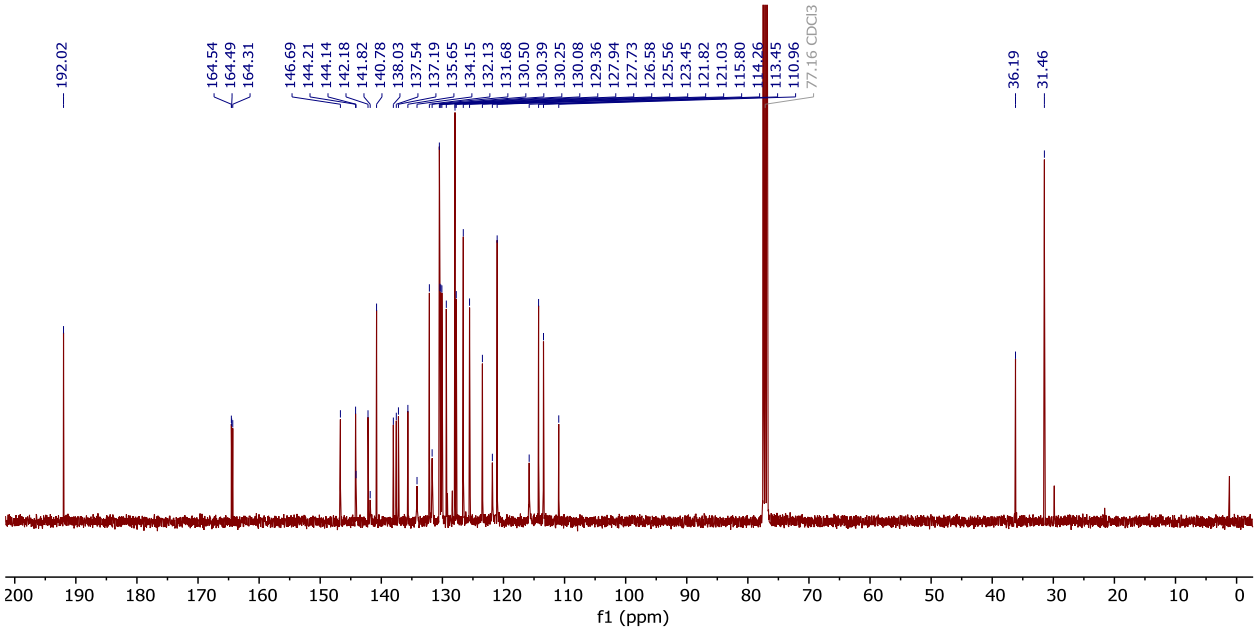


Figure S17b ^{13}C{^{1}H} NMR spectrum of **5d** in $CDCl_3$.

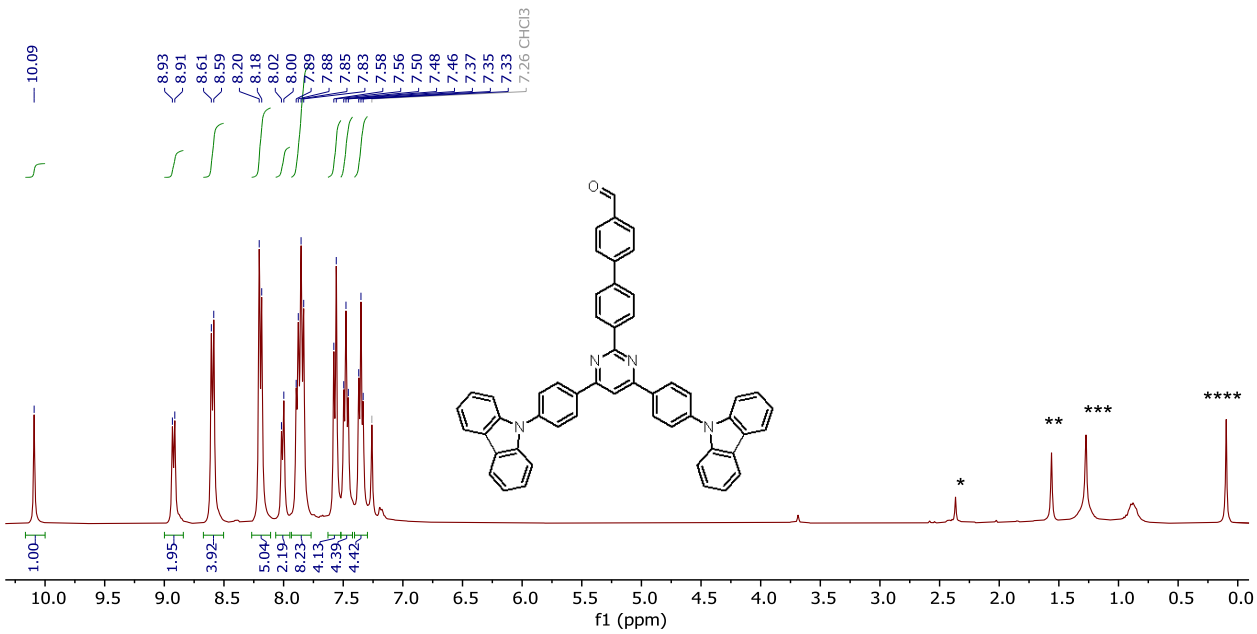


Figure S18a ^{1}H NMR spectrum of **5e** in $CDCl_3$. * = toluene, ** = H_2O, *** = hexanes, **** = PDMS grease.

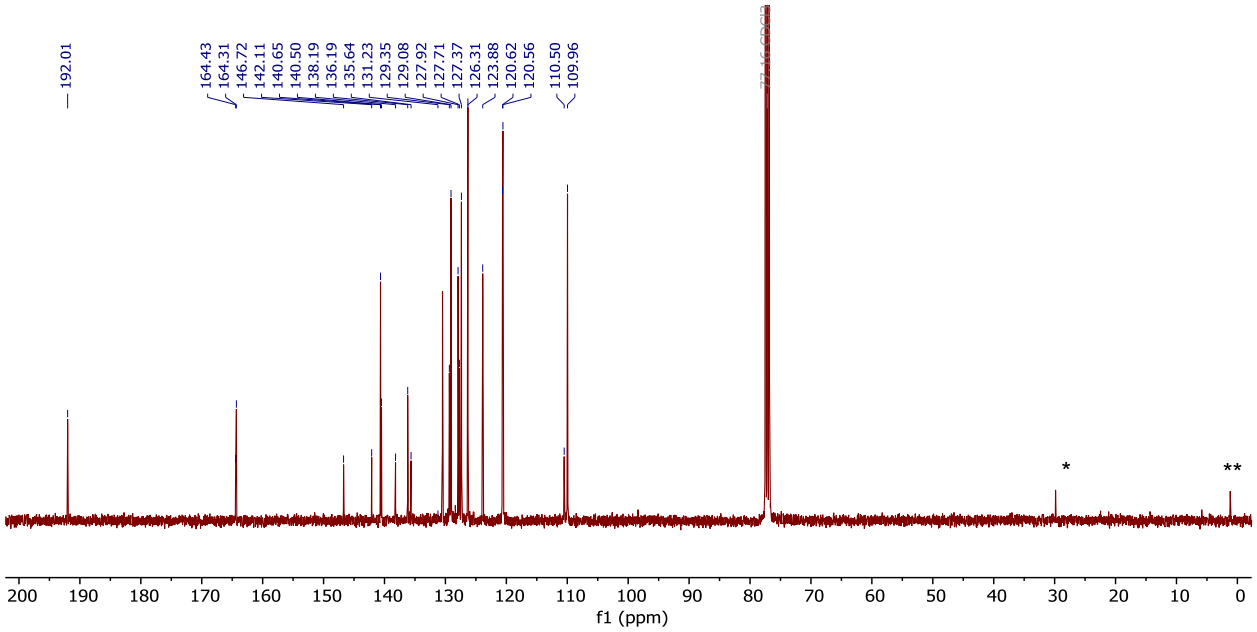


Figure S18b $^{13}C\{^{1}H\}$ NMR spectrum of **5e** in $CDCl_3$. * = hexanes, ** = PDMS grease.

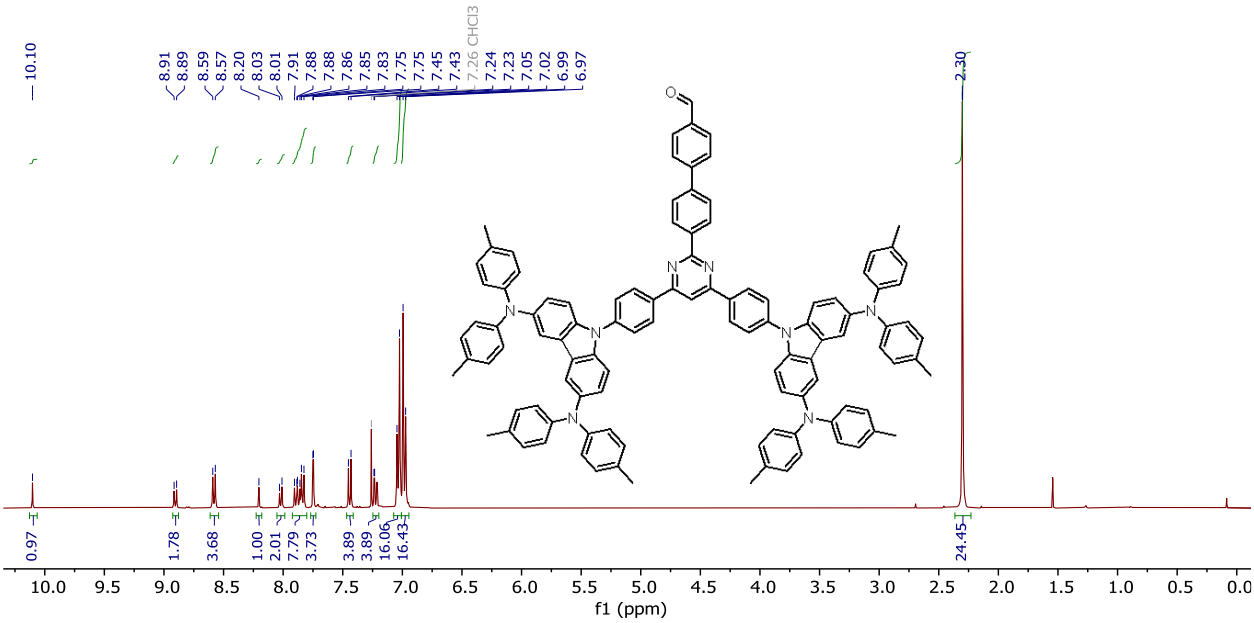


Figure S19a ^{1}H NMR spectrum of **5f** in $CDCl_3$.

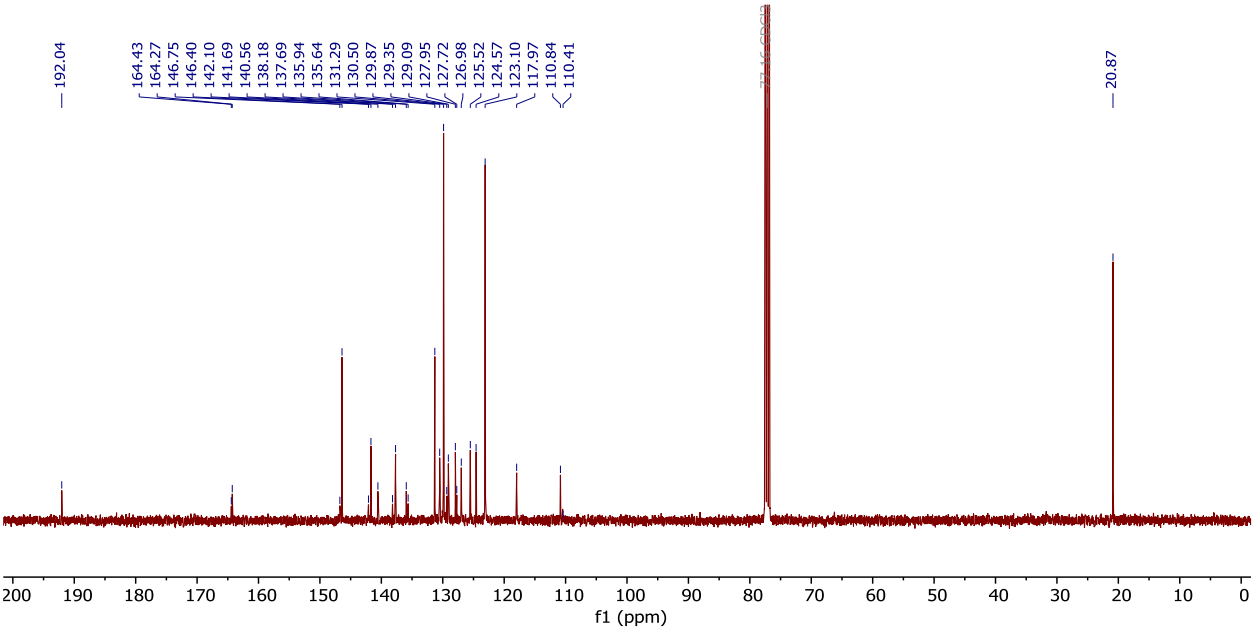


Figure S19b ^{13}C{^{1}H} NMR spectrum of **5f** in $CDCl_3$.

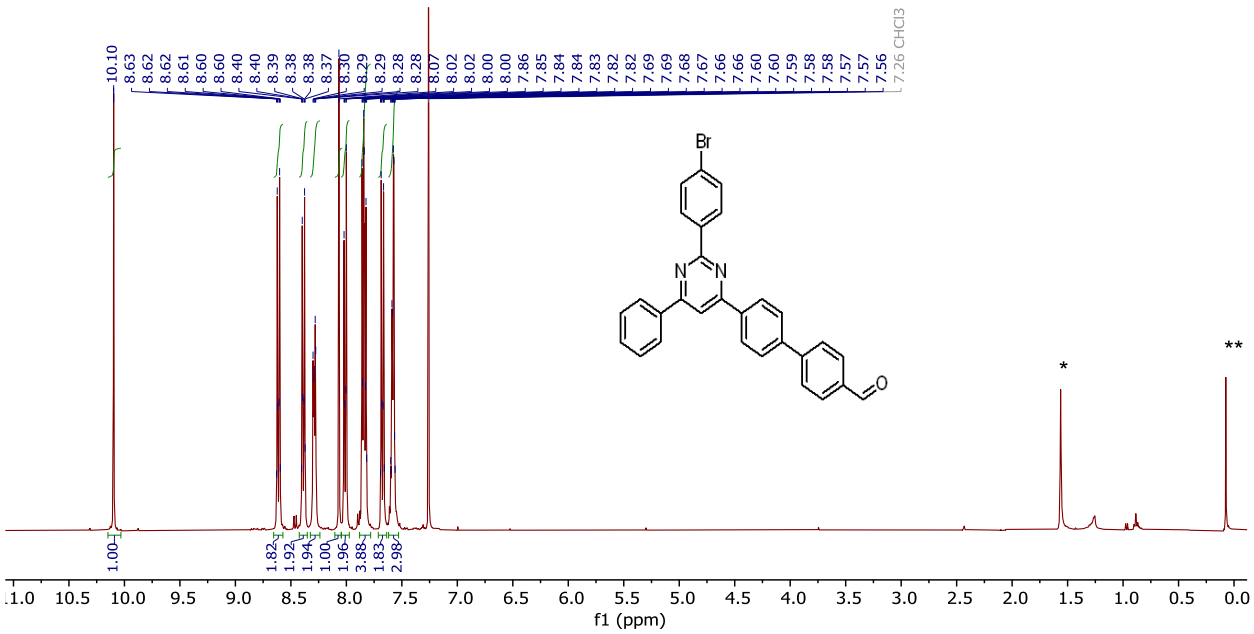


Figure S20a ^{1}H NMR spectrum of **5g** in $CDCl_3$. * = H_2O, ** = PDMS grease.

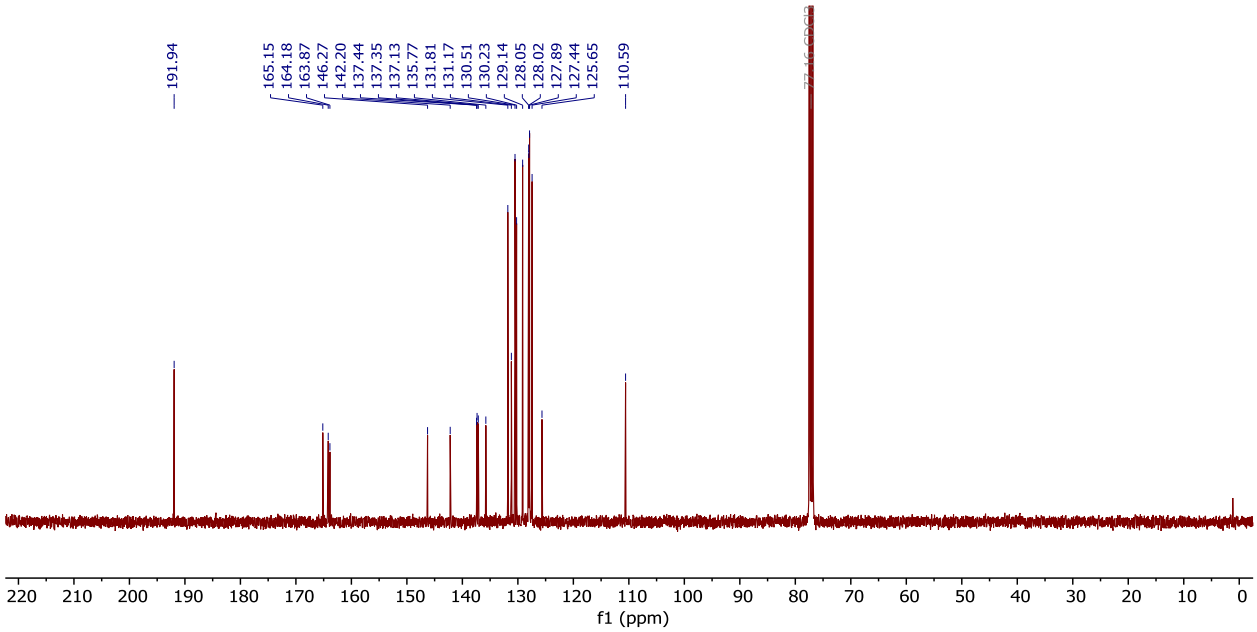


Figure S20b ^{13}C{^{1}H} NMR spectrum of **5g** in $CDCl_3$.

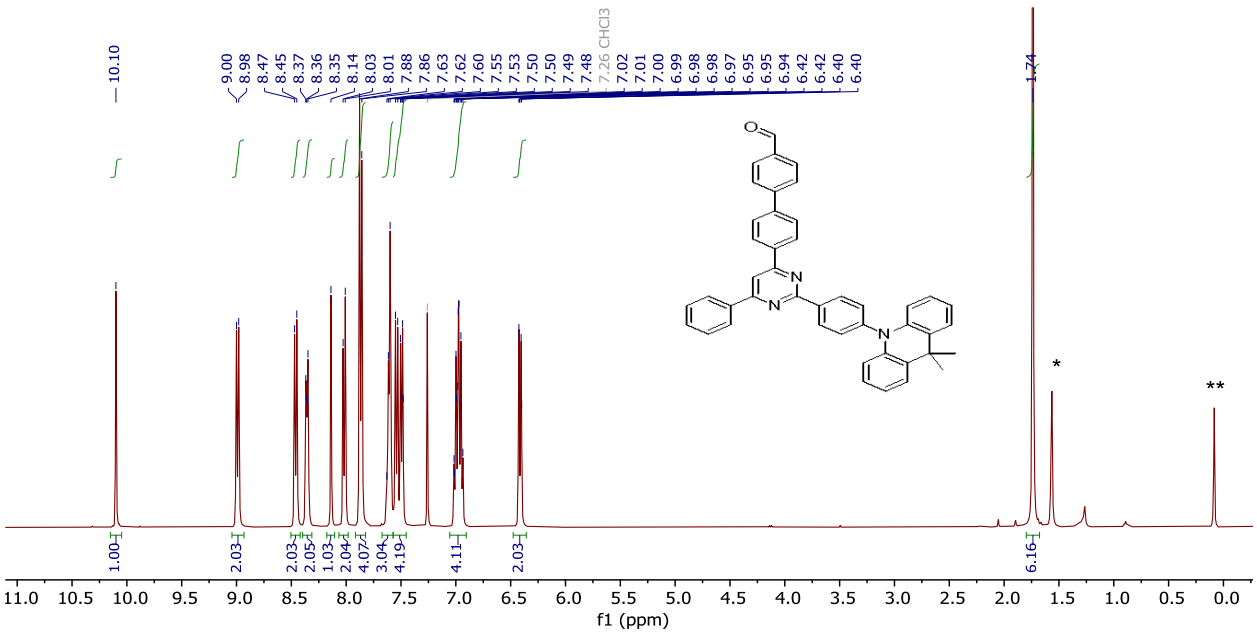


Figure S21a ^{1}H NMR spectrum of **6g** in $CDCl_3$. * = H_2O, ** = PDMS grease.

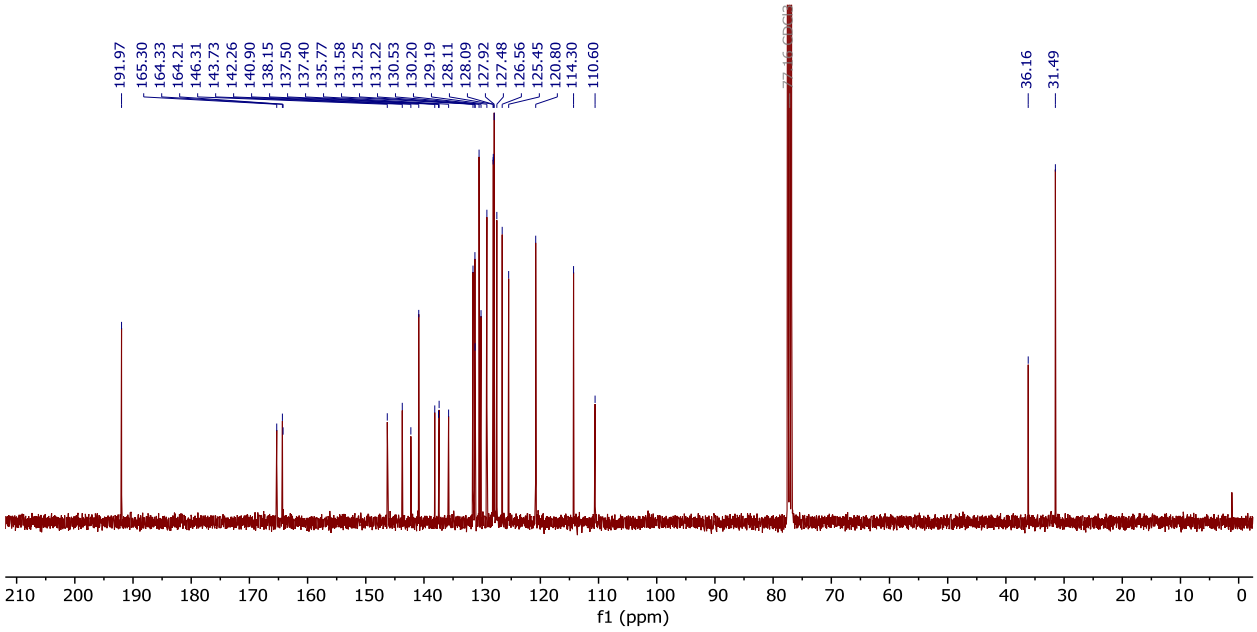


Figure S21b ^{13}C{^{1}H} NMR spectrum of **6g** in $CDCl_3$.

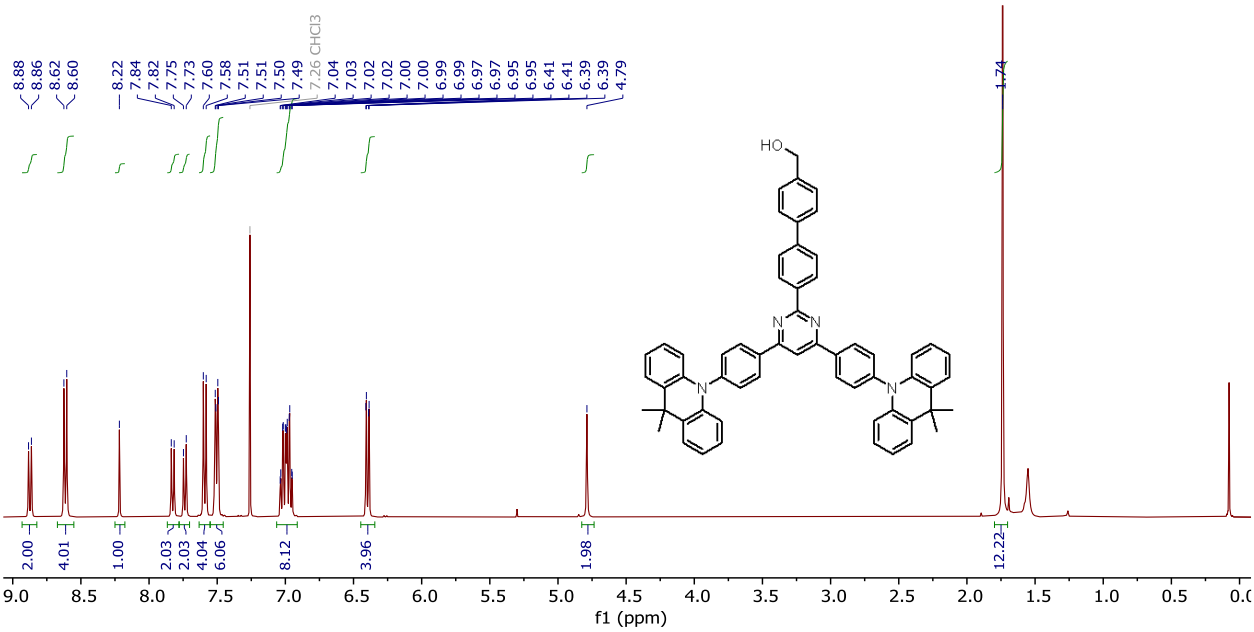


Figure S22a ^{1}H NMR spectrum of **6a** in $CDCl_3$.

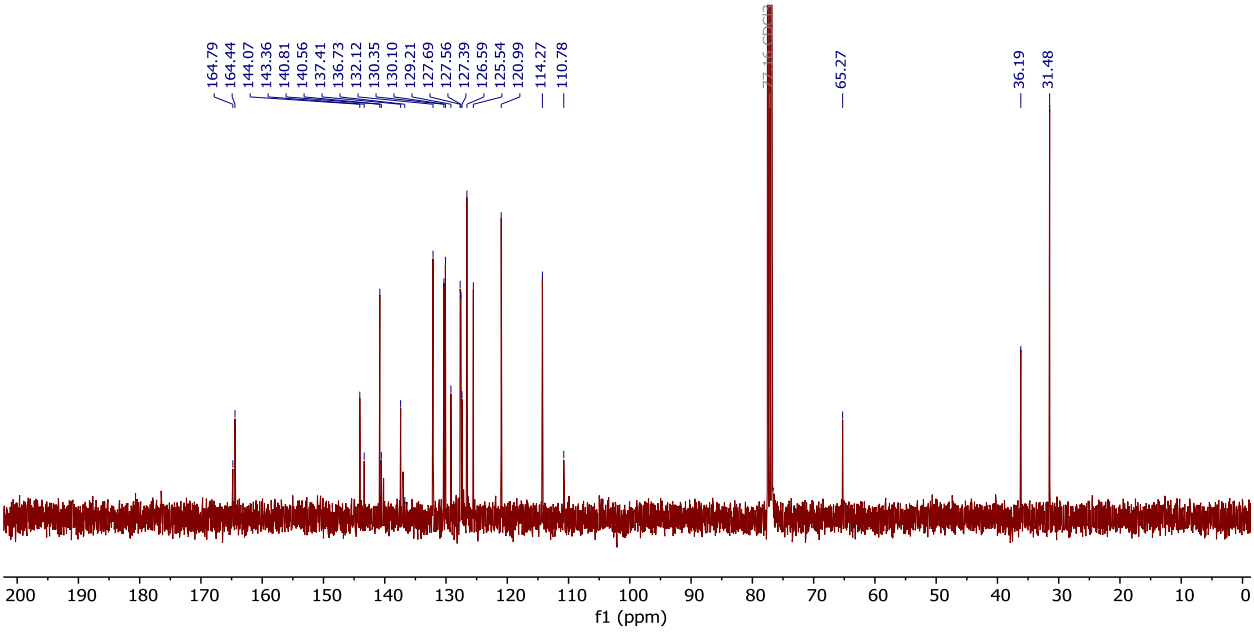


Figure S22b ^{13}C{^{1}H} NMR spectrum of **6a** in $CDCl_3$.

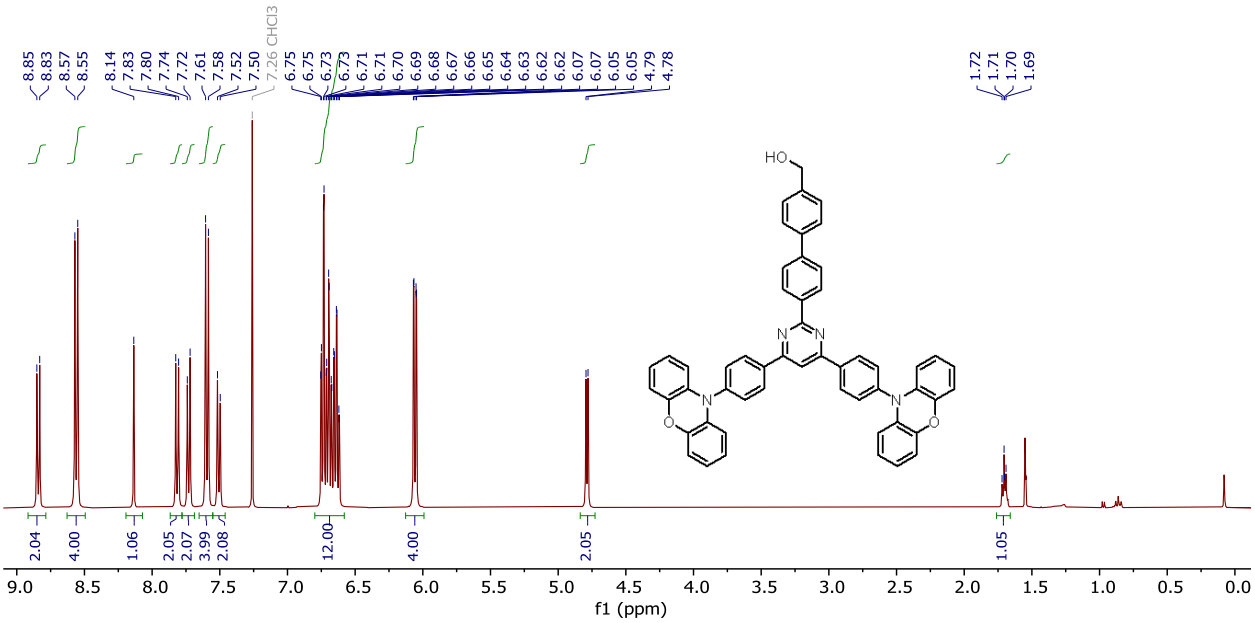


Figure S23a ^{1}H NMR spectrum of **6b** in $CDCl_3$.

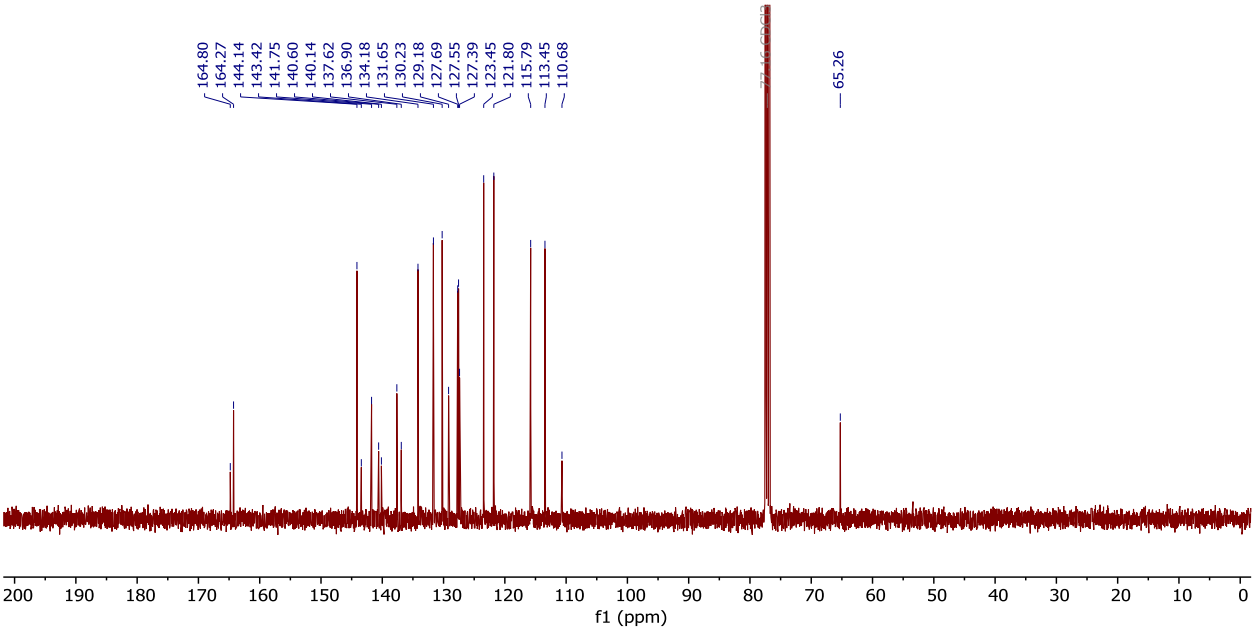


Figure S23b ^{13}C{^{1}H} NMR spectrum of **6b** in $CDCl_3$.

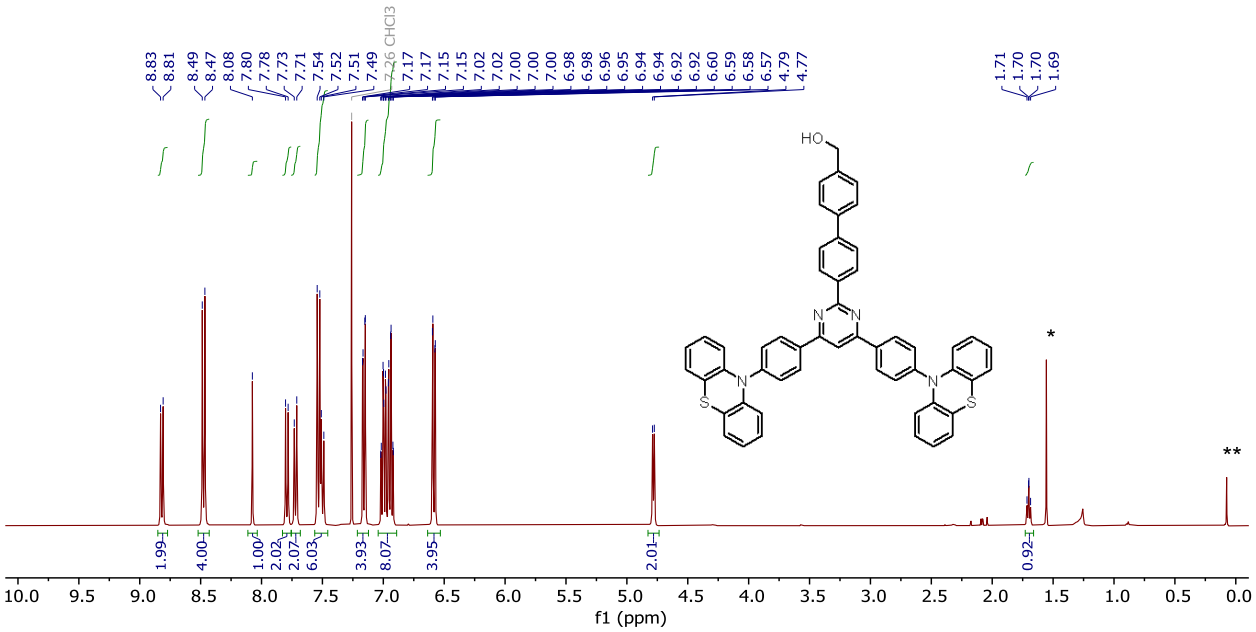


Figure S24a ^{1}H NMR spectrum of **6c** in $CDCl_3$. * = H_2O, ** = PDMS grease.

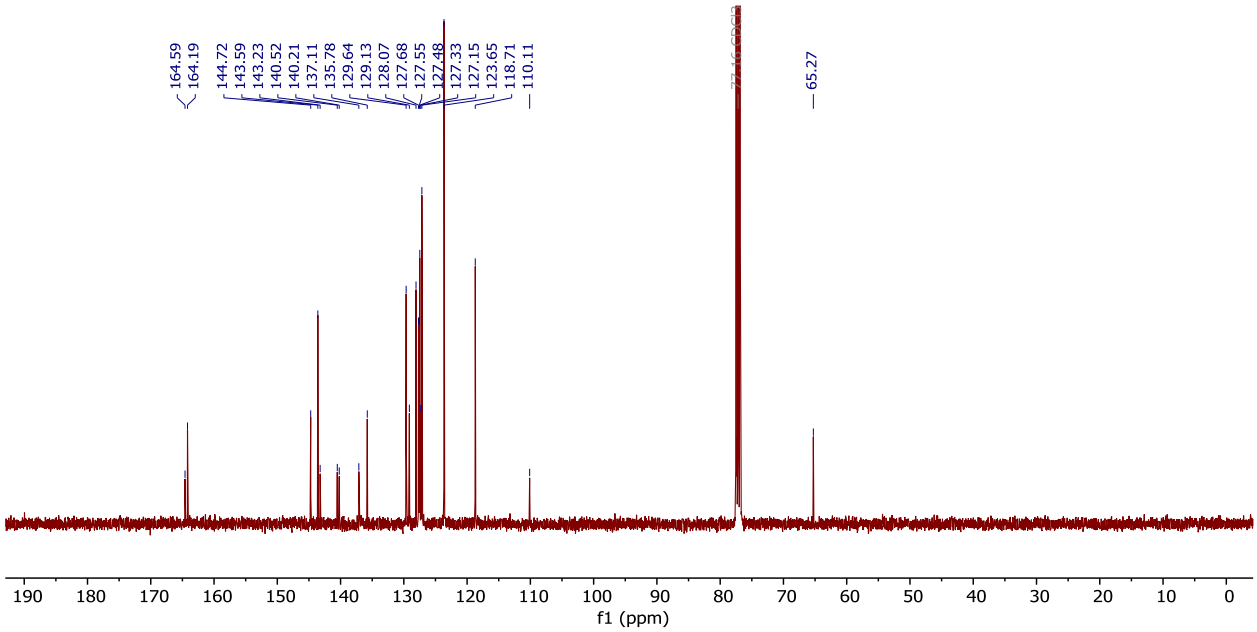


Figure S24b ^{13}C{^{1}H} NMR spectrum of **6c** in $CDCl_3$.

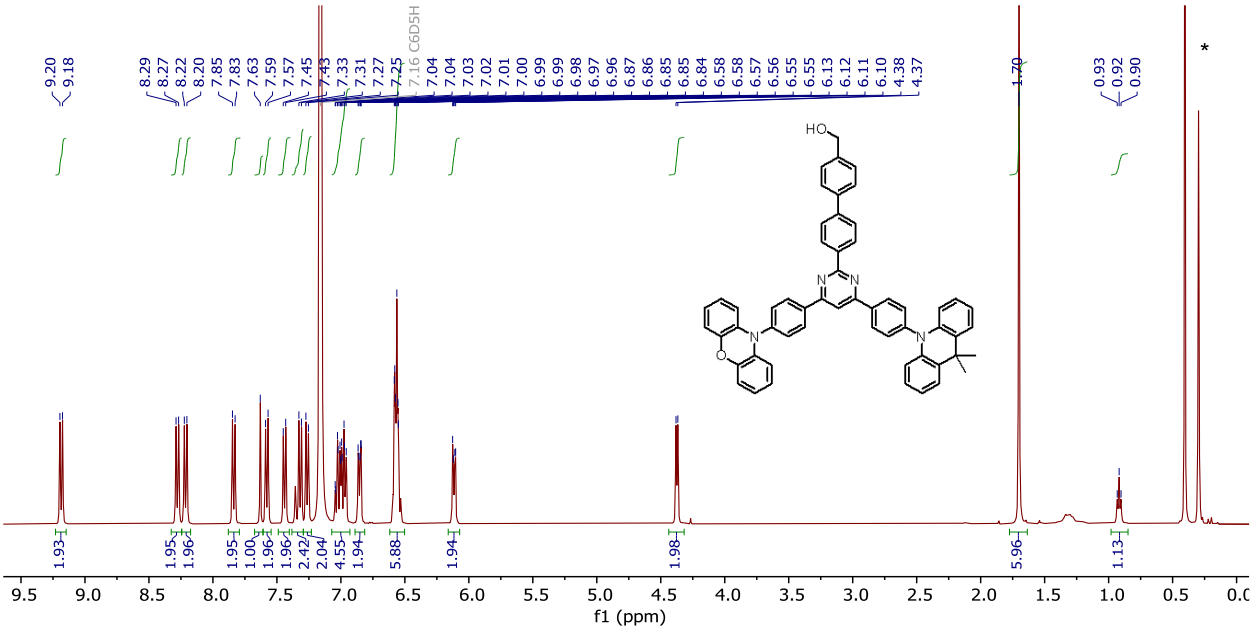


Figure S25a ^{1}H NMR spectrum of **6d** in C_6D_6. * = H_2O.

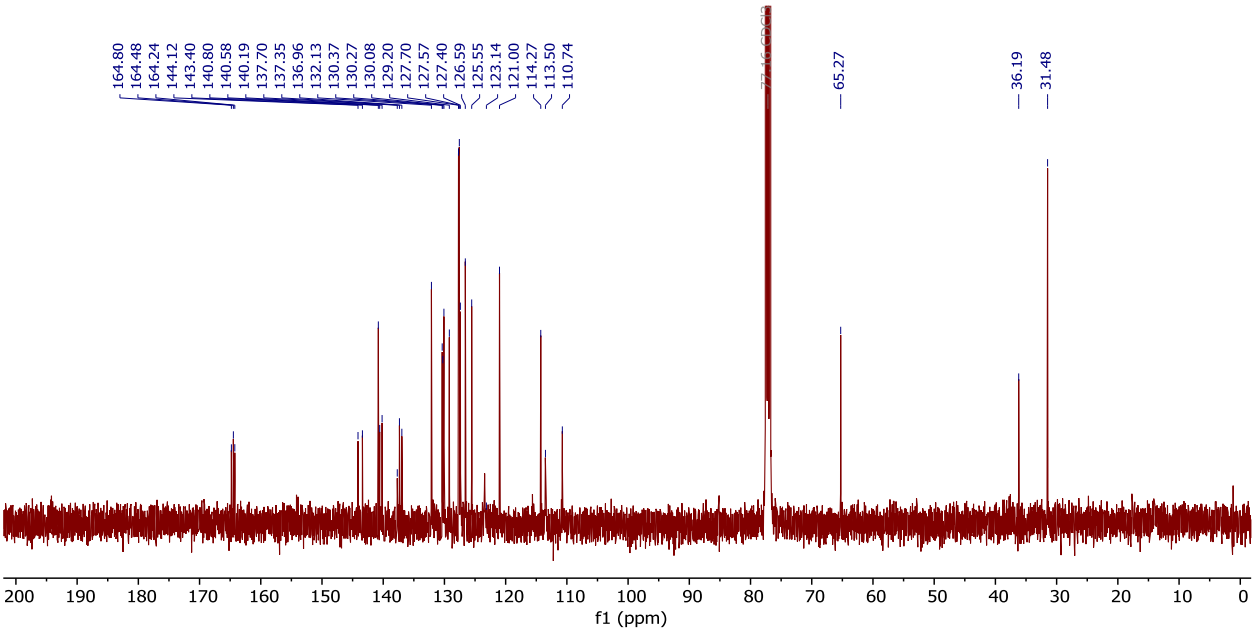


Figure S25b $^{13}C\{^{1}H\}$ NMR spectrum of **6d** in $CDCl_3$.

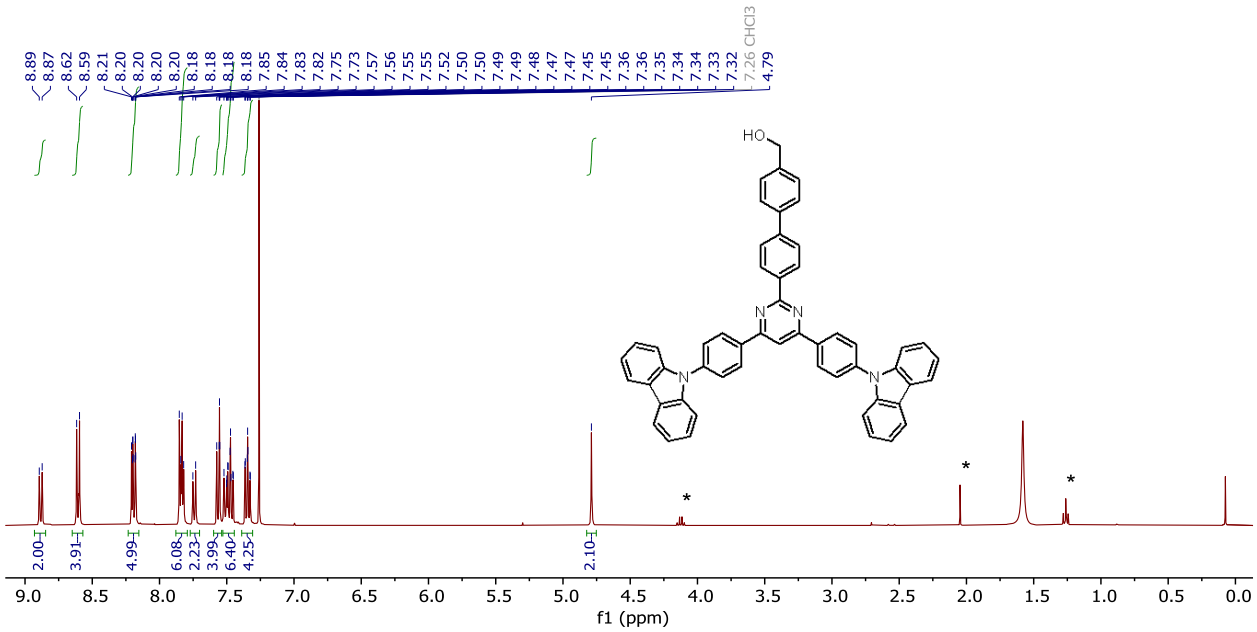


Figure S26a ^{1}H NMR spectrum of **6e** in $CDCl_3$. * = ethyl acetate

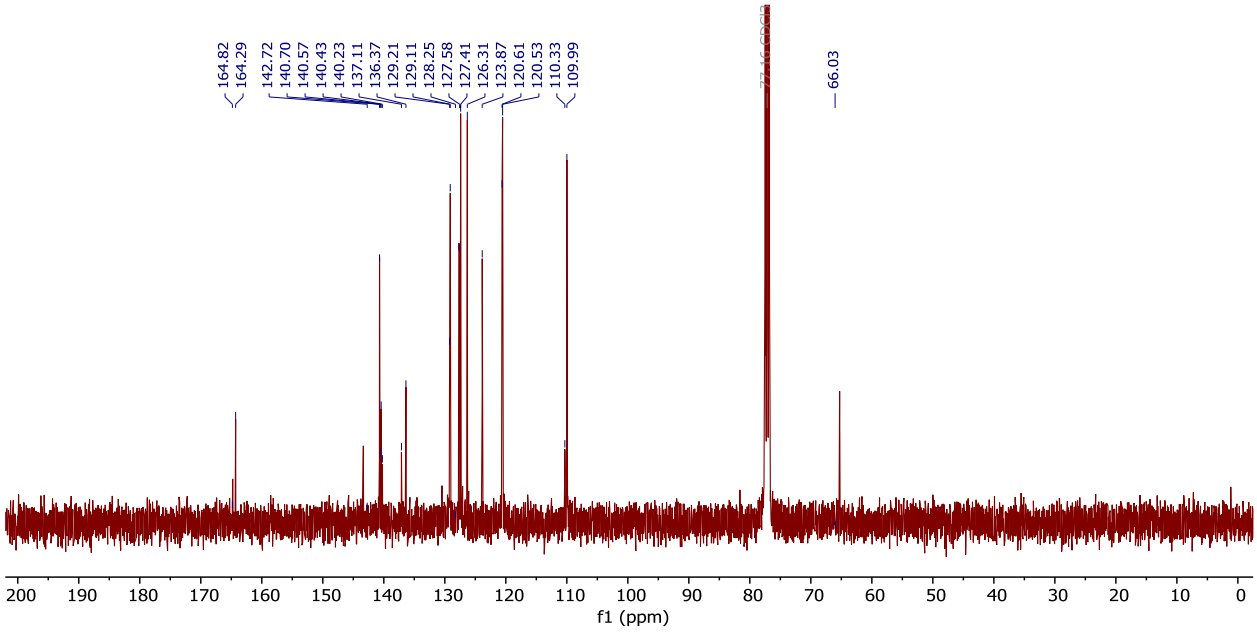


Figure S26b ^{13}C{^{1}H} NMR spectrum of **6e** in $CDCl_3$.

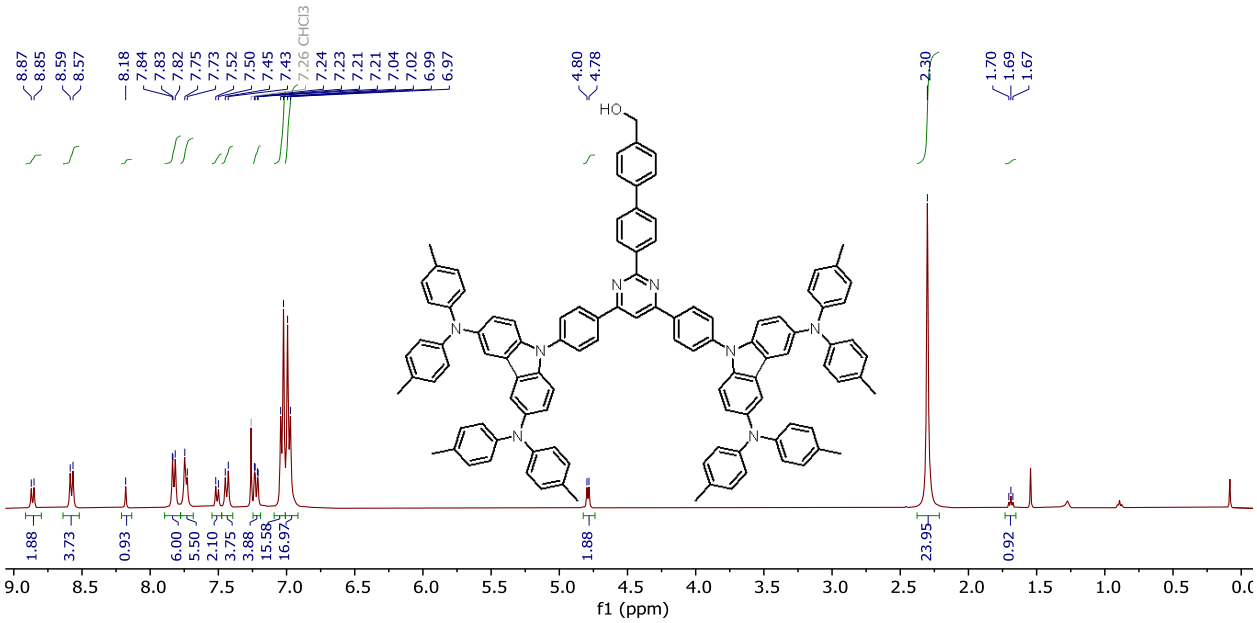


Figure S27a ^{1}H NMR spectrum of **6f** in $CDCl_3$.

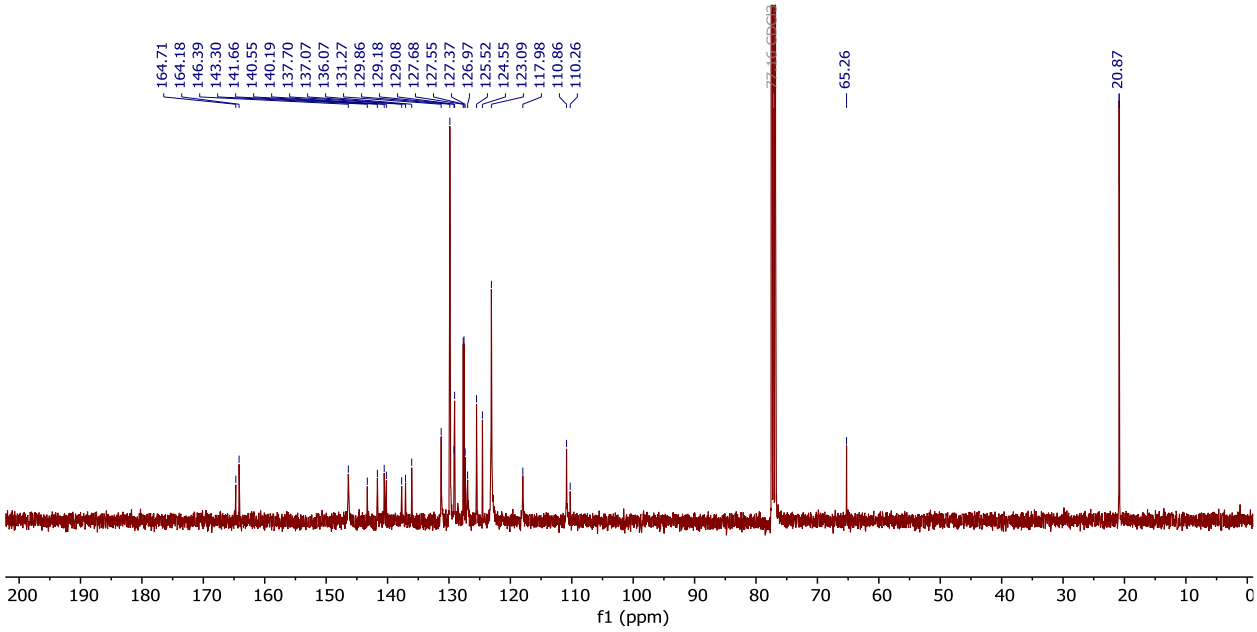


Figure S27b ^{13}C{^{1}H} NMR spectrum of **6f** in $CDCl_3$.

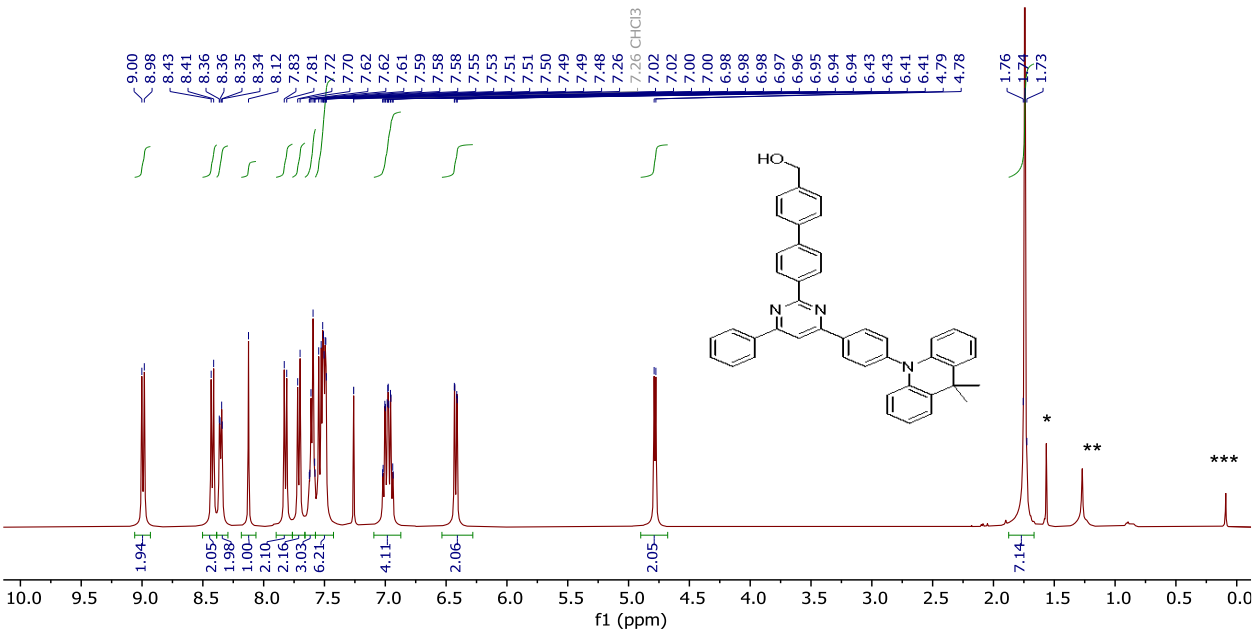


Figure S28a ^{1}H NMR spectrum of **7g** in $CDCl_3$. * = H_2O, ** = hexanes, *** = PDMS grease.

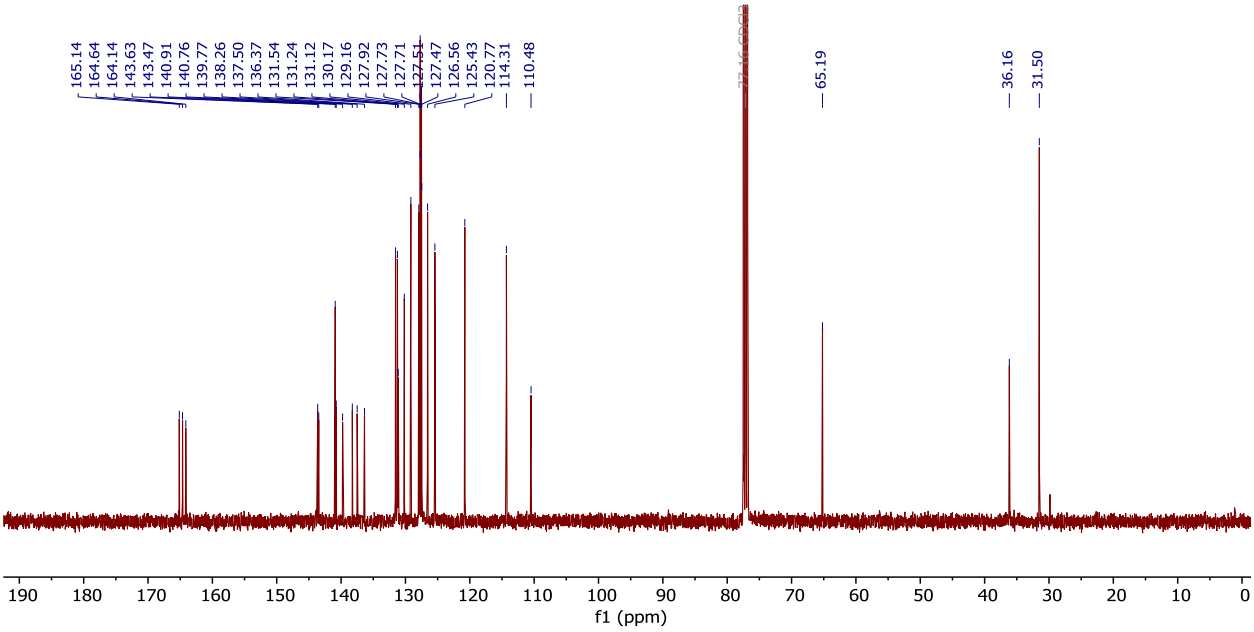


Figure S28b $^{13}C\{^{1}H\}$ NMR spectrum of **7g** in $CDCl_3$.

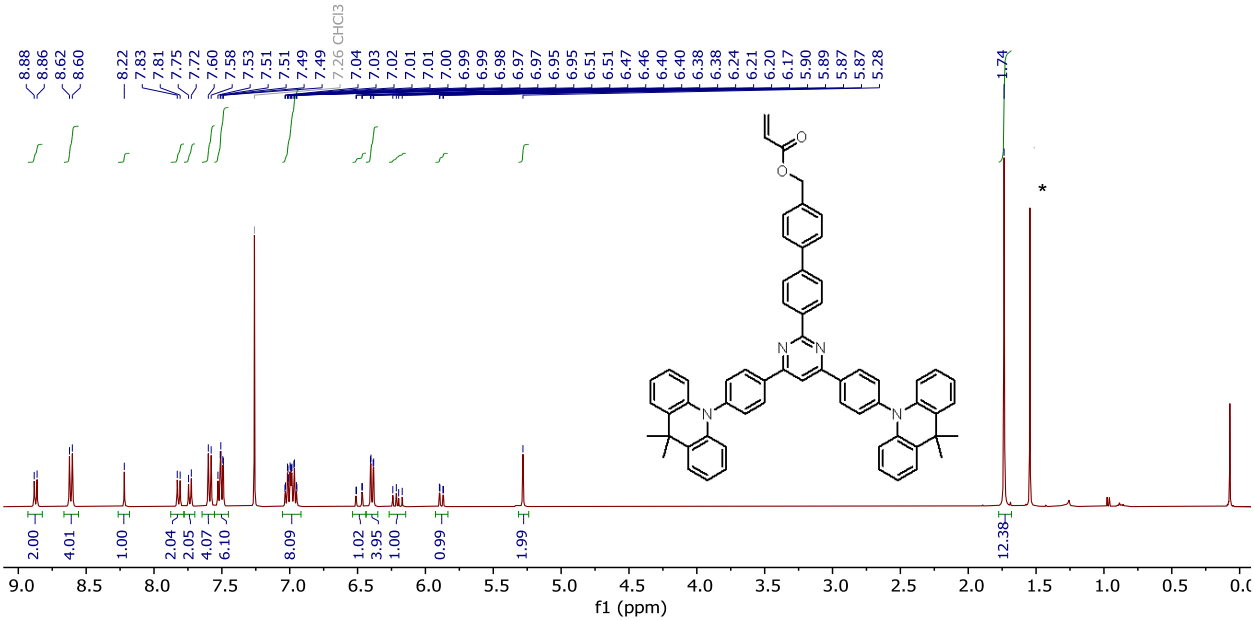


Figure S29a ^{1}H NMR spectrum of **PymDMA** in $CDCl_3$. * = H_2O.

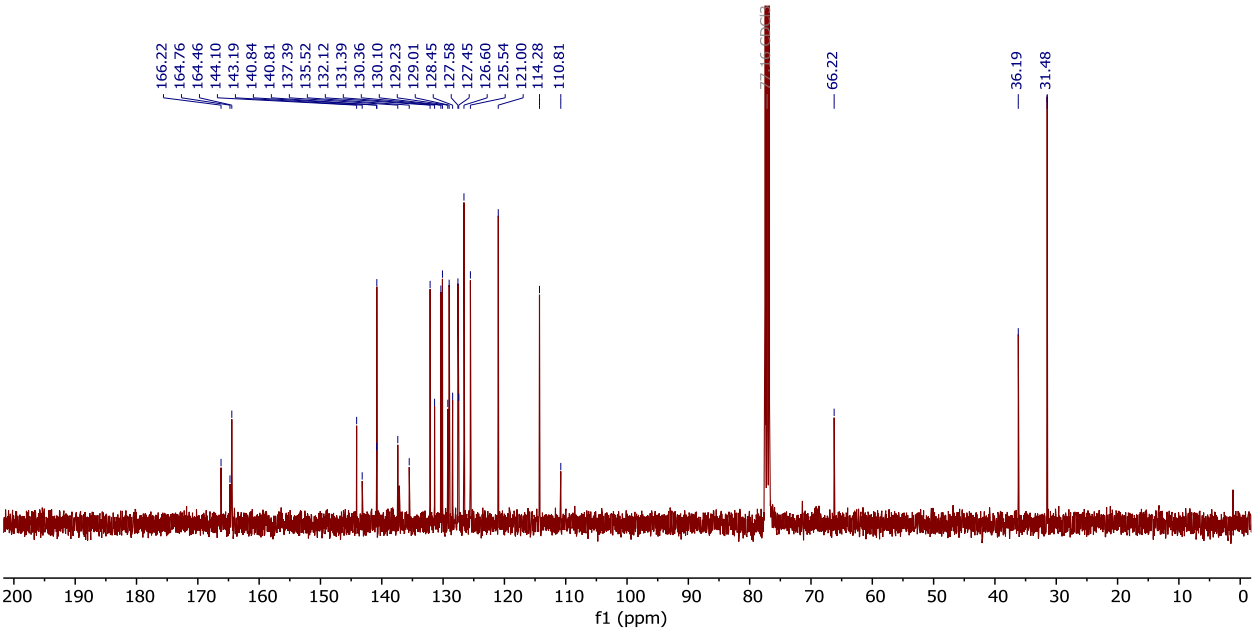


Figure S29b ^{13}C{^{1}H} NMR spectrum of **PymDMA** in $CDCl_3$.

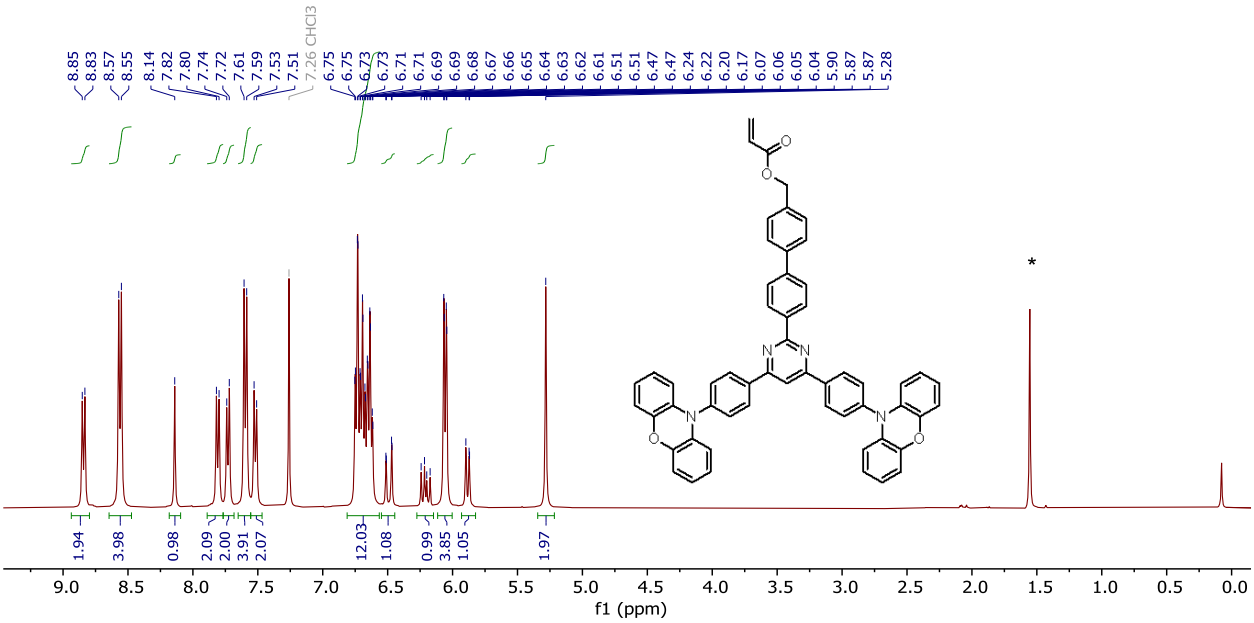


Figure S30a ^{1}H NMR spectrum of **PymPXZ** in $CDCl_3$. * = H_2O.

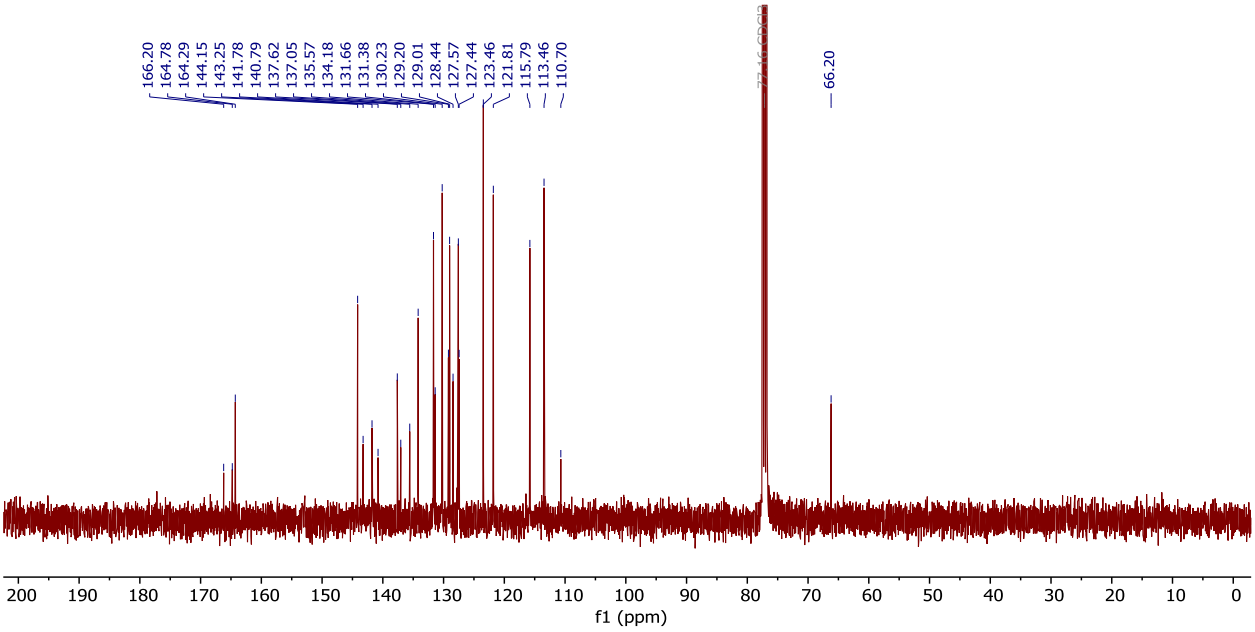


Figure S30b ^{13}C{^{1}H} NMR spectrum of **PymPXZ** in $CDCl_3$.

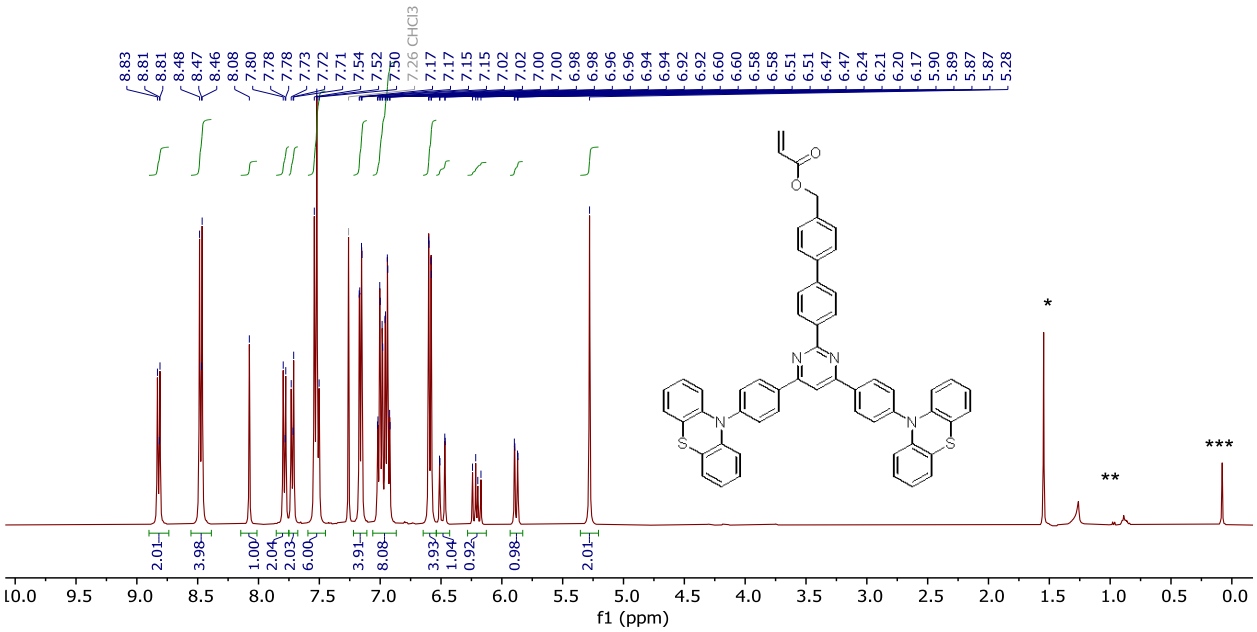


Figure S31a ^{1}H NMR spectrum of **PymPTZ** in $CDCl_3$. * = H_2O, ** = hexanes, *** = PDMS grease.

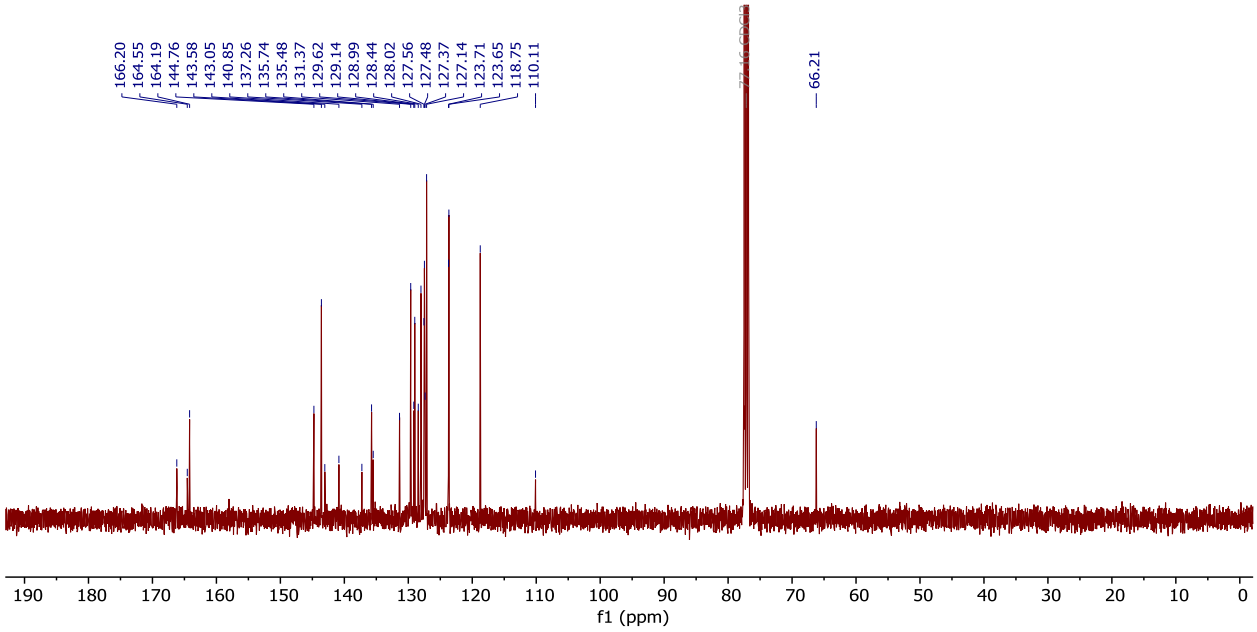


Figure S31b ^{13}C{^{1}H} NMR spectrum of **PymPTZ** in $CDCl_3$.

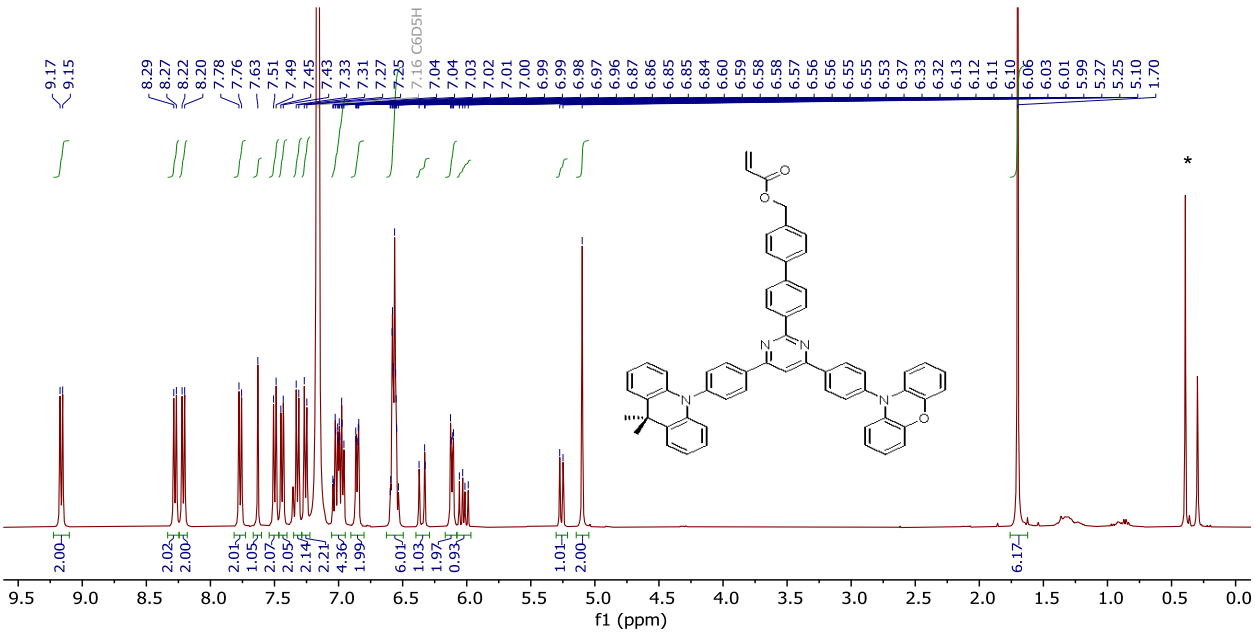


Figure S4a ^{1}H NMR spectrum of **PymDMAPXZ** in C_6D_6. * = H_2O.

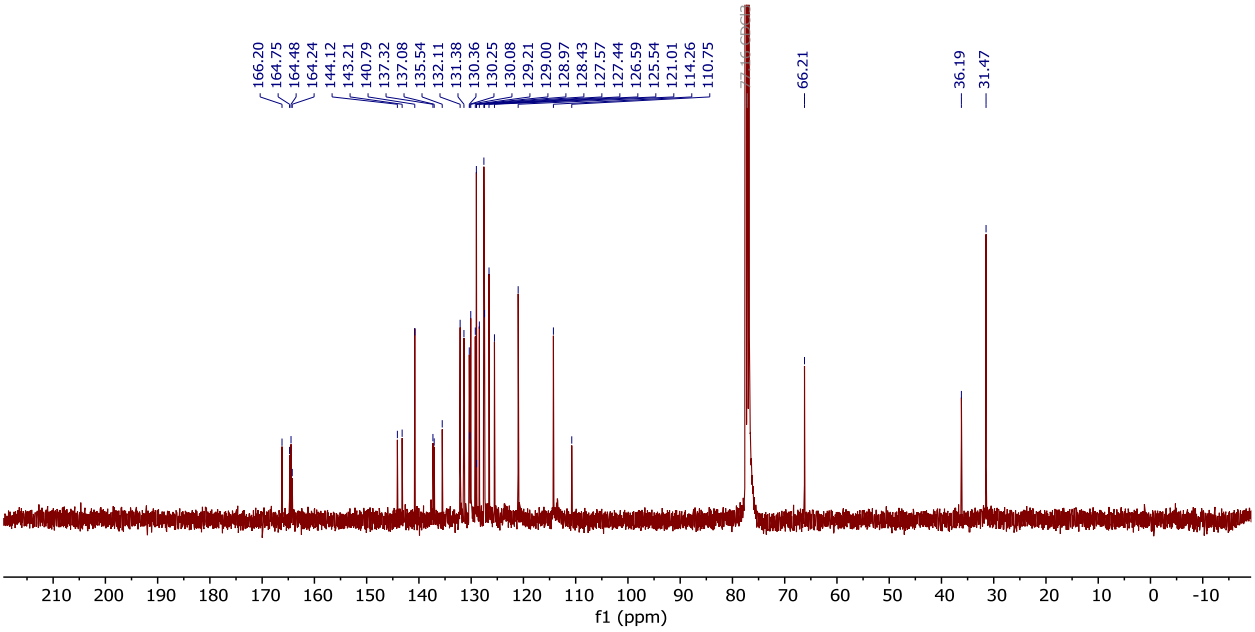


Figure S32b ^{13}C{^{1}H} NMR spectrum of **PymDMAPXZ** in $CDCl_3$.

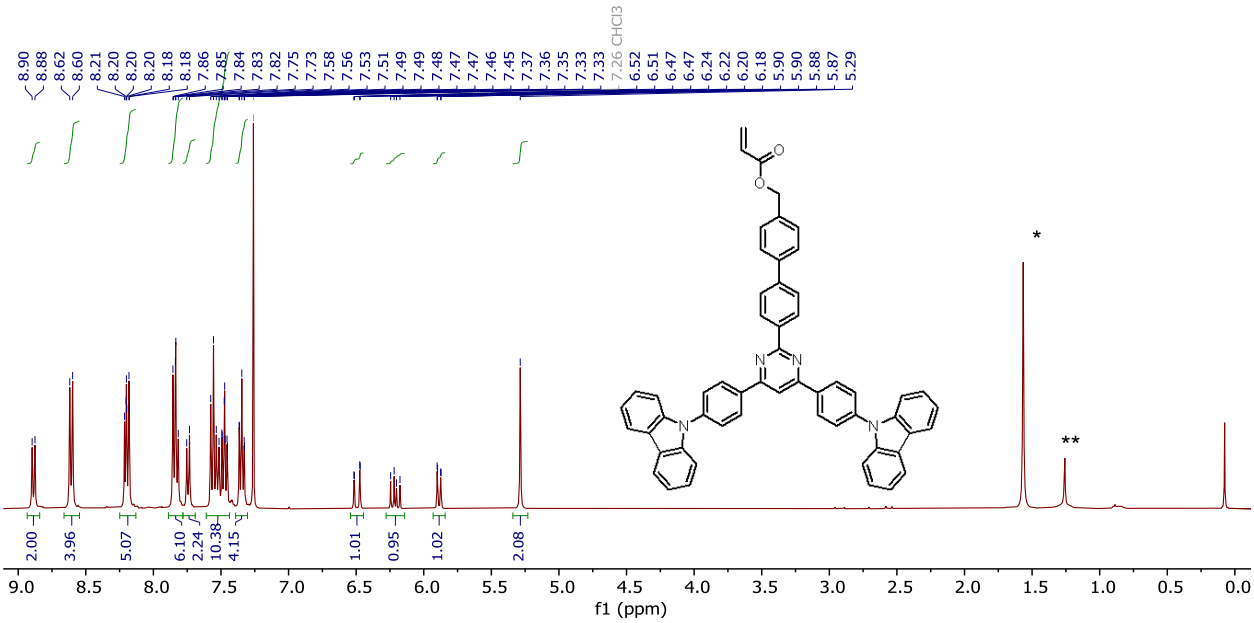


Figure S33a ^{1}H NMR spectrum of **PymCz** in $CDCl_3$. * = H_2O, ** = hexanes.

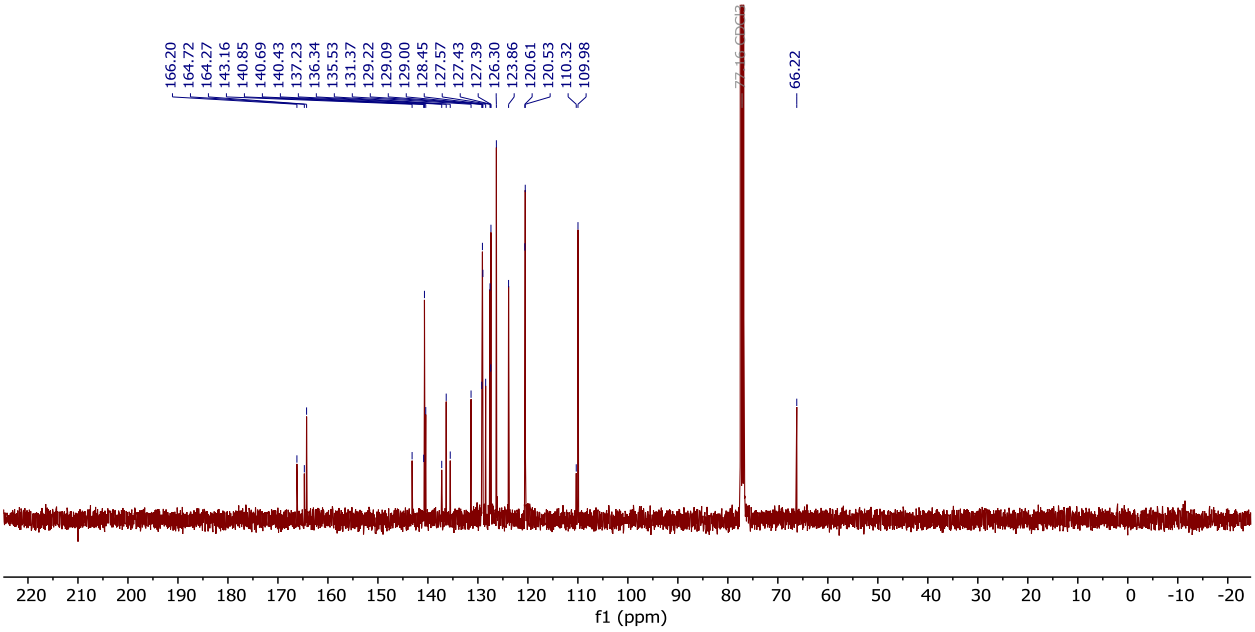


Figure S33b ^{13}C{^{1}H} NMR spectrum of **PymCz** in $CDCl_3$.

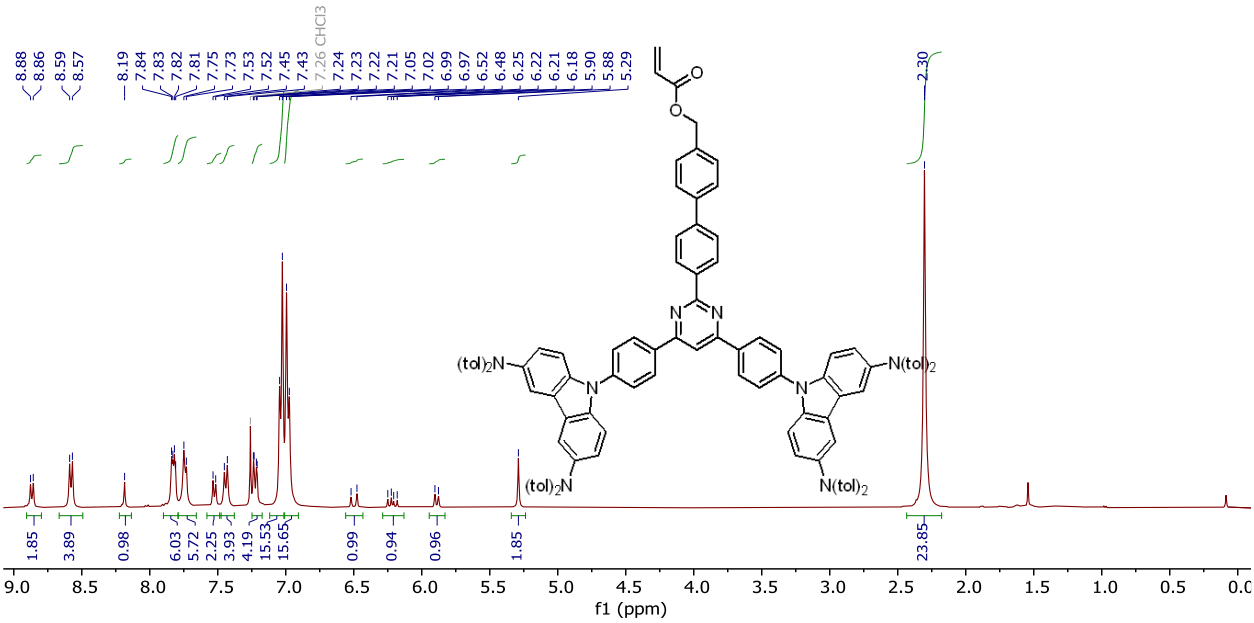


Figure S34a ^{1}H NMR spectrum of **PymTTAC** in $CDCl_3$.

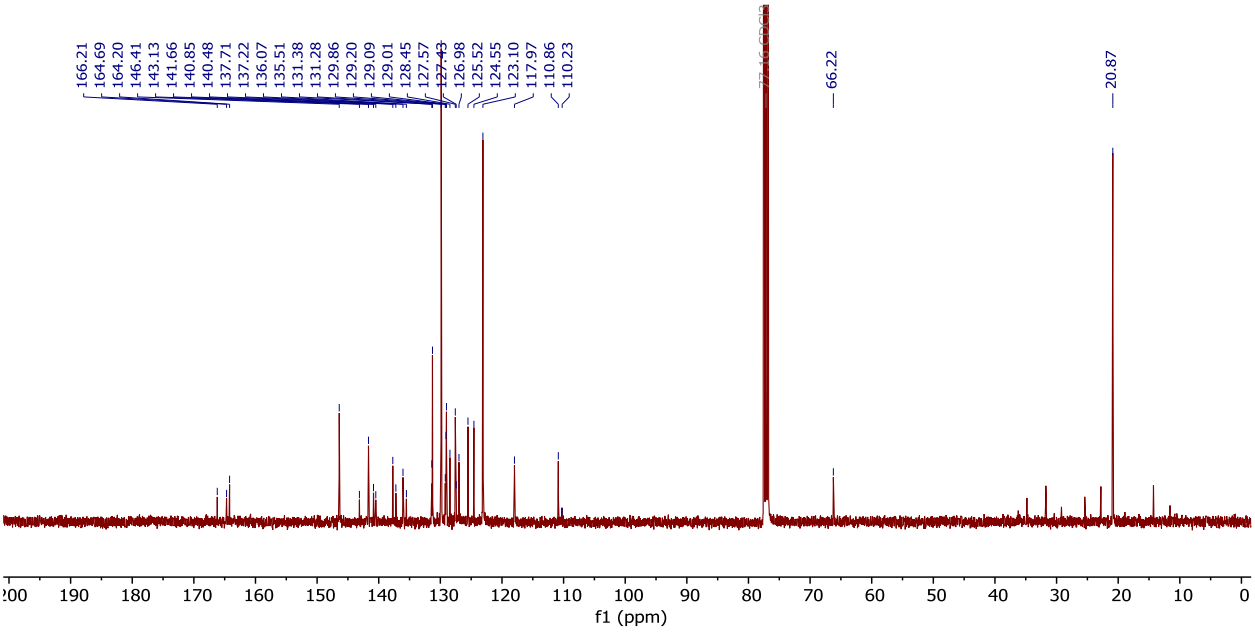


Figure S34b ^{13}C{^{1}H} NMR spectrum of **PymTTAC** in $CDCl_3$.

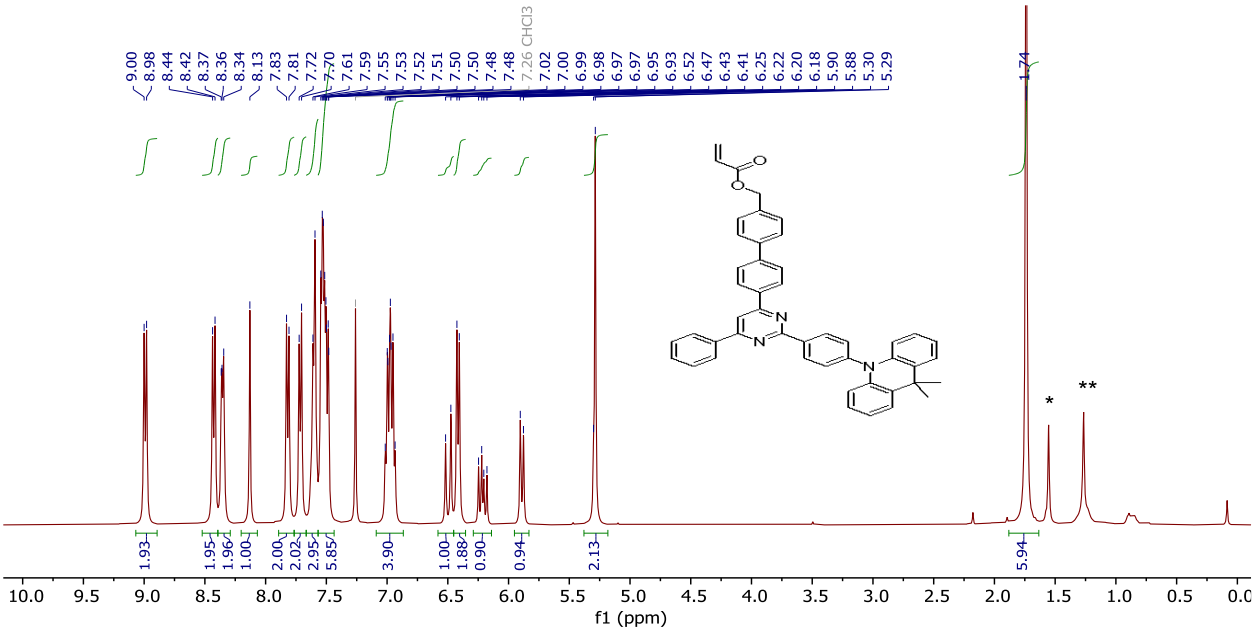


Figure S35a ^{1}H NMR spectrum of **2PymDMA** in $CDCl_3$. * = H_2O, ** = hexanes.

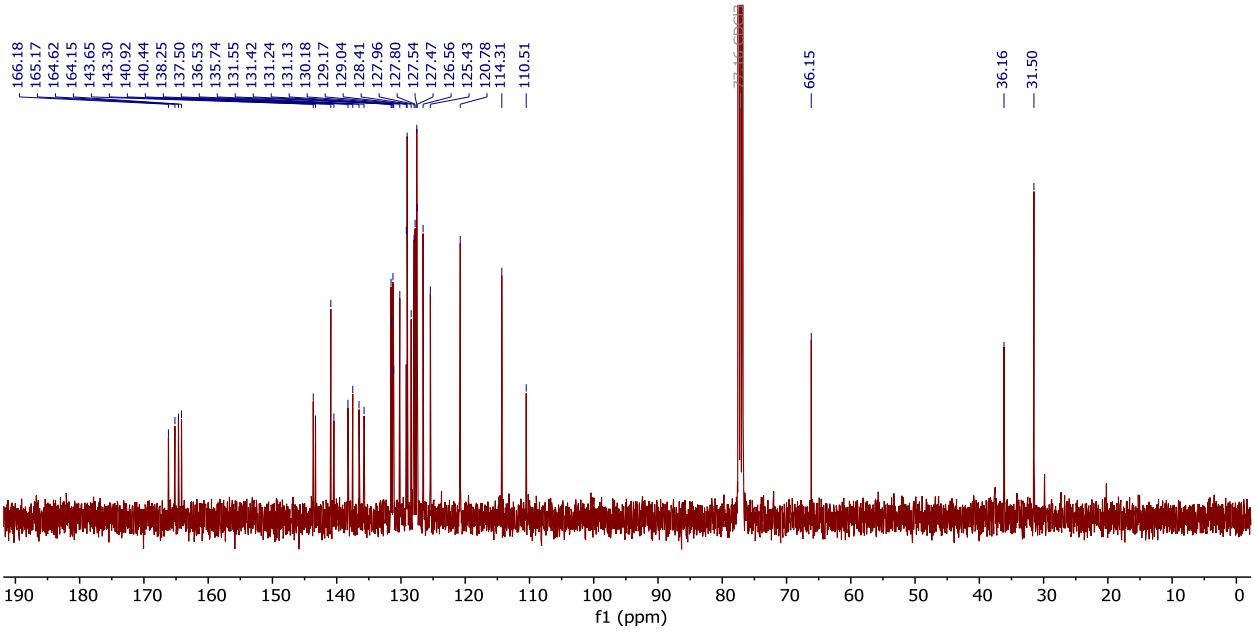


Figure S35b ^{13}C{^{1}H} NMR spectrum of **2PymDMA** in $CDCl_3$.

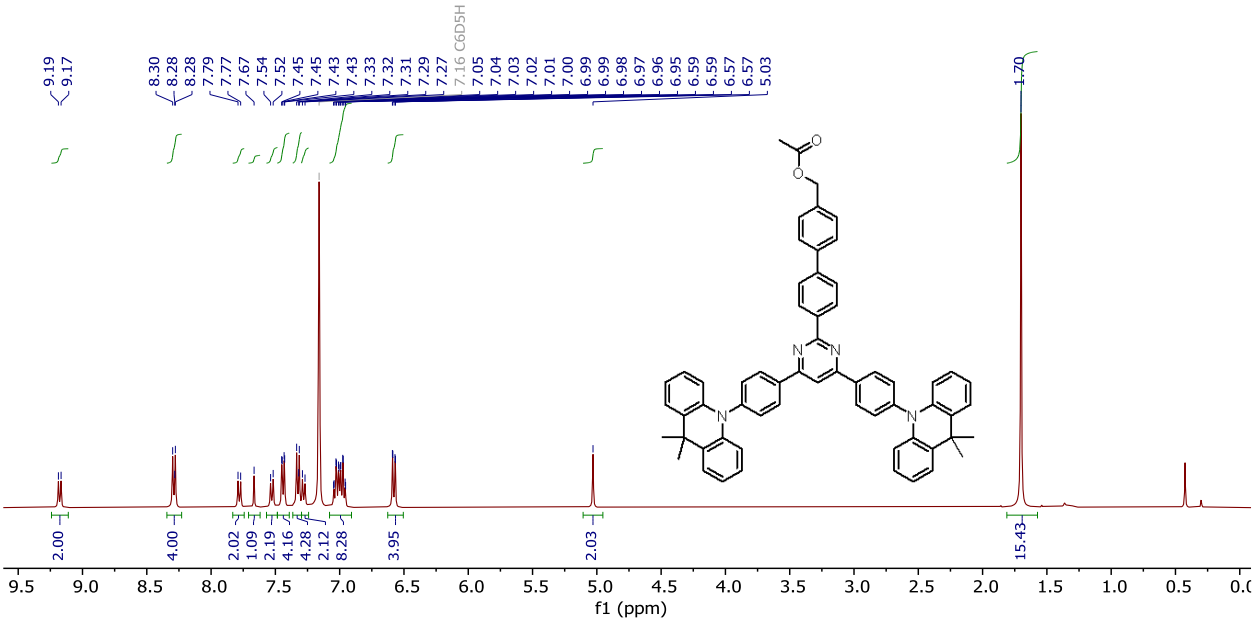


Figure 36a ^{1}H NMR spectrum of **PymDMA-OAc** in C_6D_6.

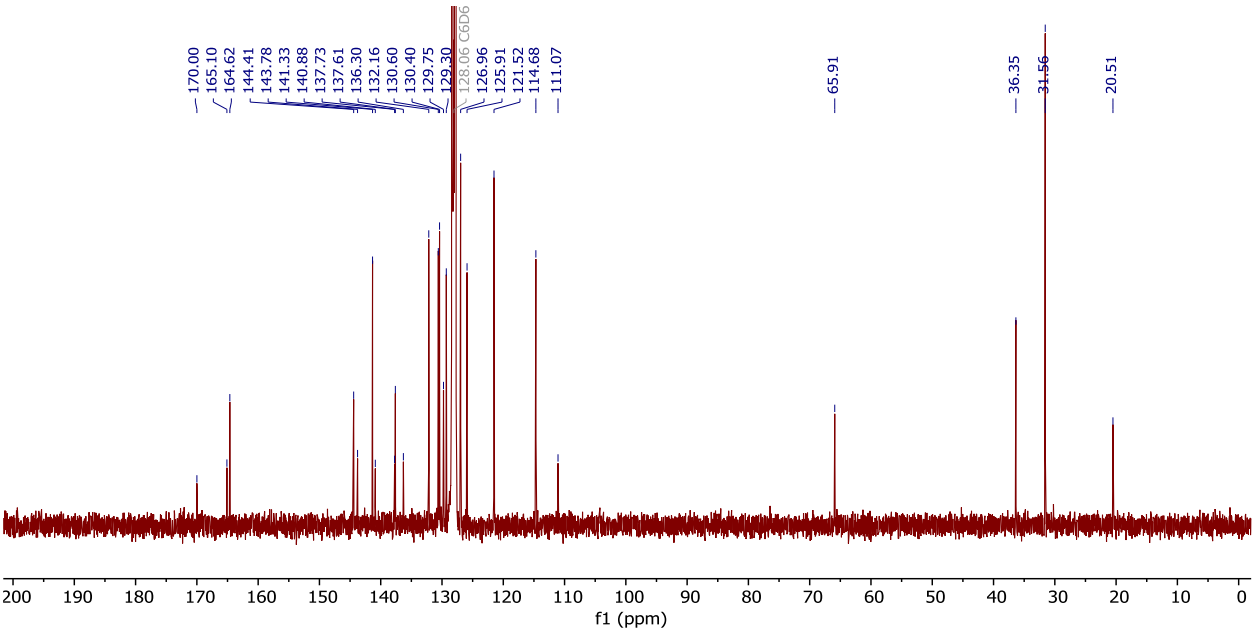


Figure 36b ^{13}C{^{1}H} NMR spectrum of **PymDMA-OAc** in C_6D_6.

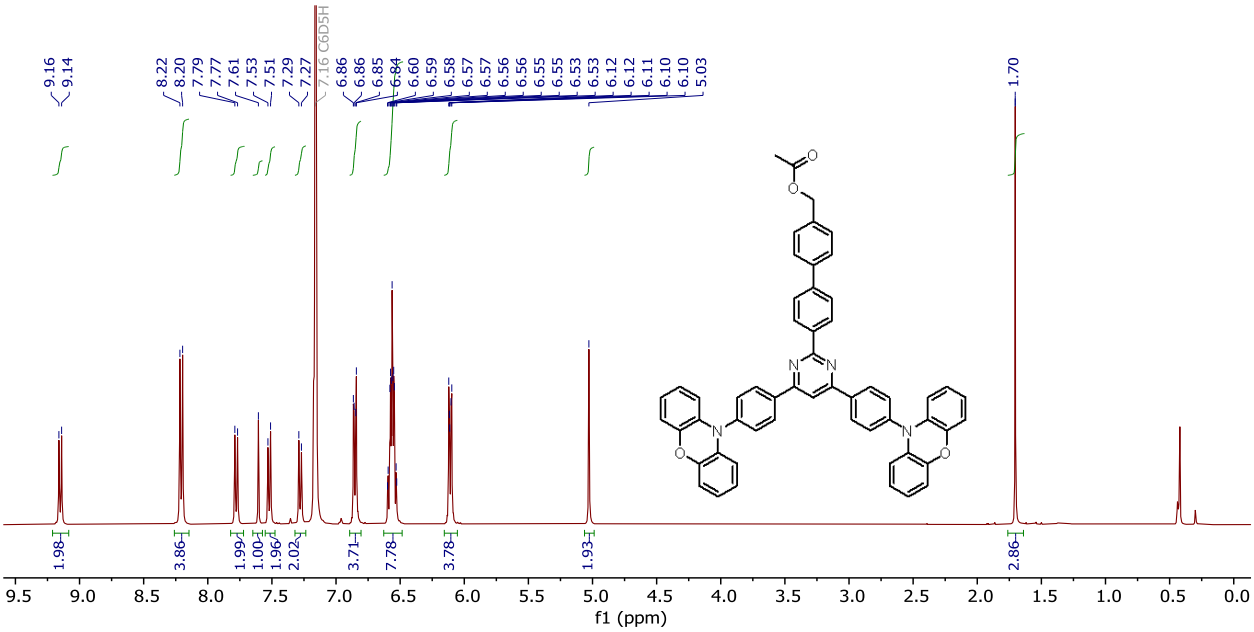


Figure 37a ^{1}H NMR spectrum of **PymPXZ-OAc** in C_6D_6.

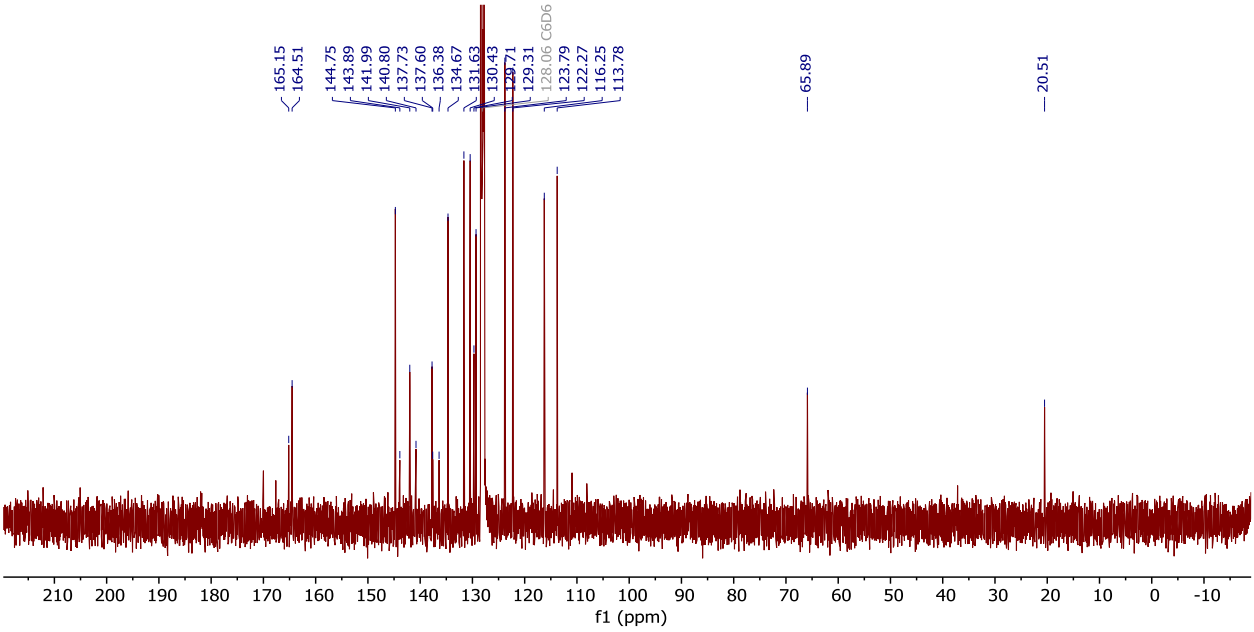


Figure 37b ^{13}C{^{1}H} NMR spectrum of **PymPXZ-OAc** in C_6D_6.

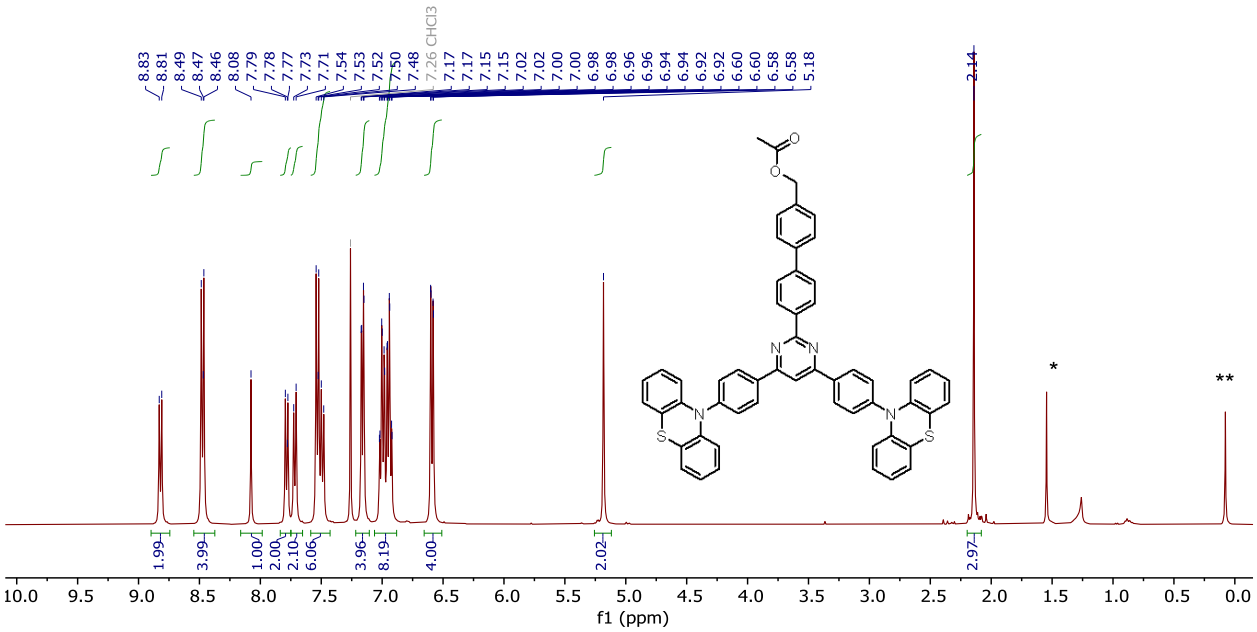


Figure 38a ^{1}H NMR spectrum of **PymPTZ-OAc** in $CDCl_3$. * = H_2O, ** = PDMS grease.

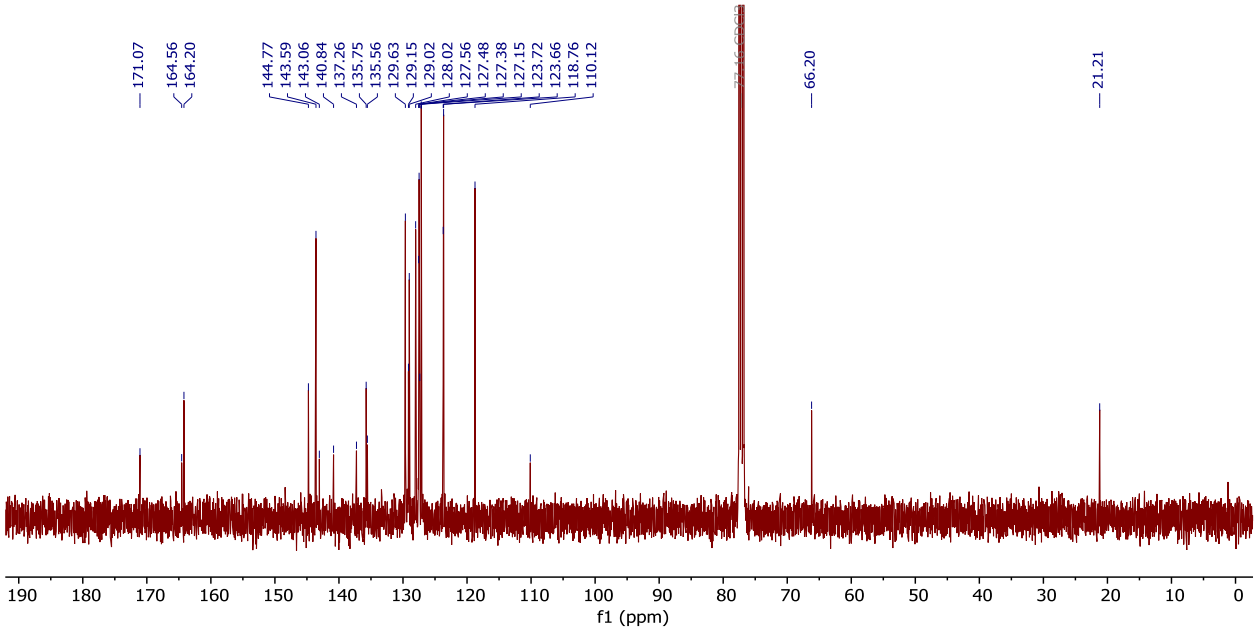


Figure 38b ^{13}C{^{1}H} NMR spectrum of **PymPTZ-OAc** in $CDCl_3$.

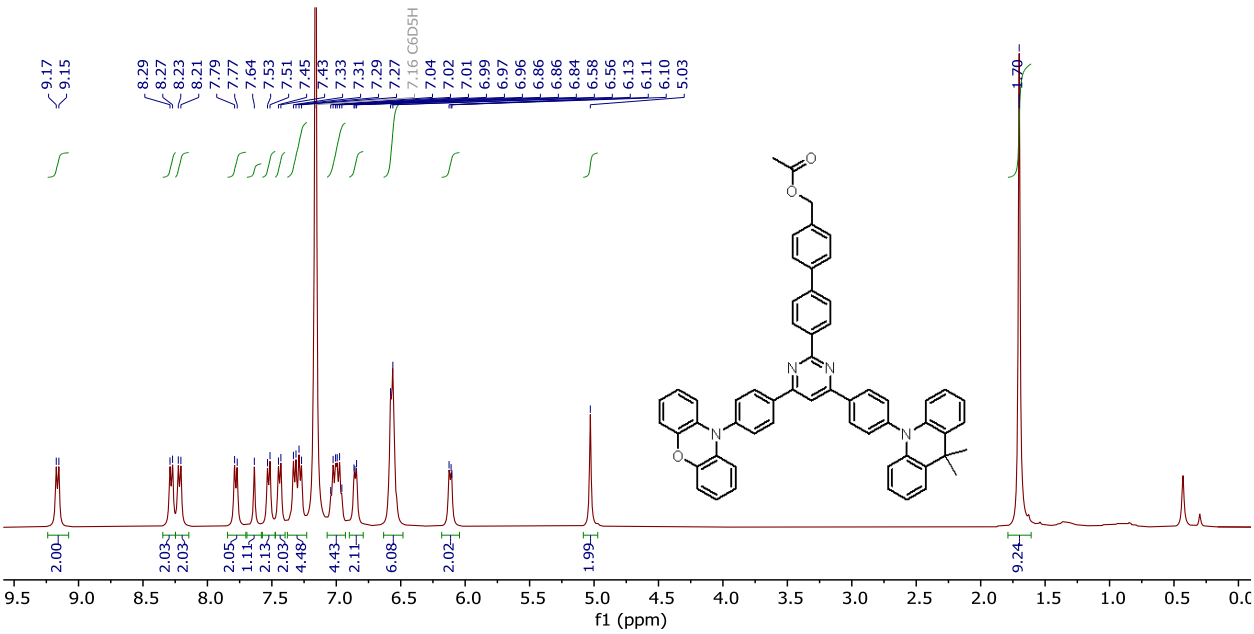


Figure 39a ^{1}H NMR spectrum of **PymDMAPXZ-OAc** in C_6D_6.

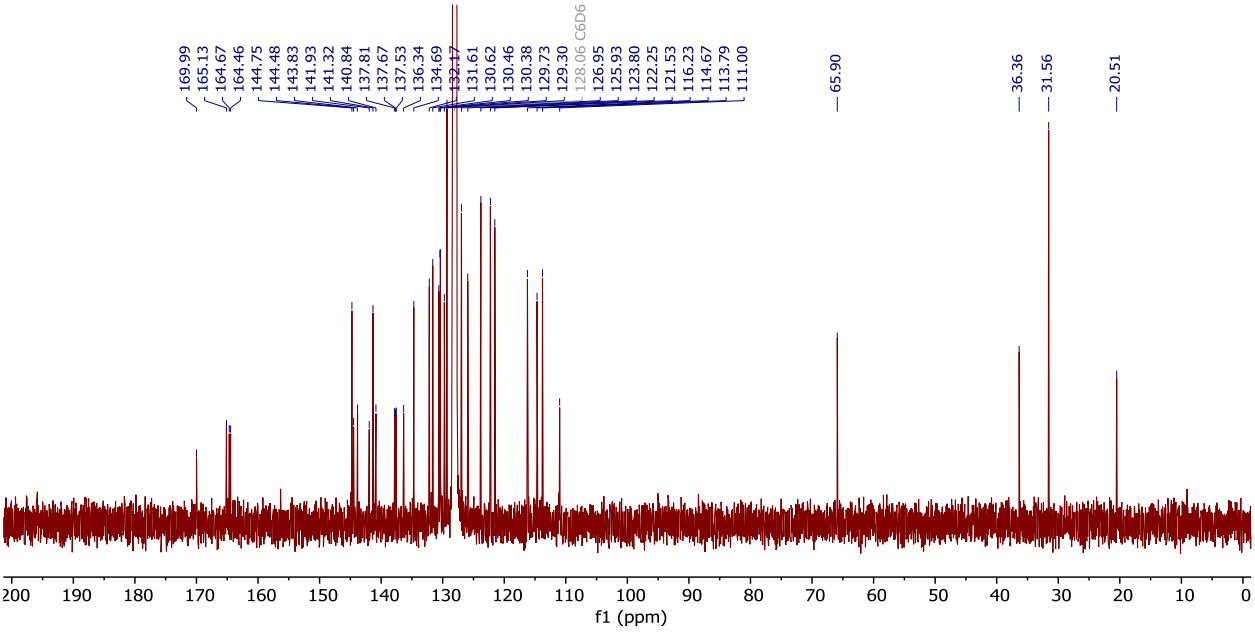


Figure 39b ^{13}C{^{1}H} NMR spectrum of **PymDMAPXZ-OAc** in C_6D_6.

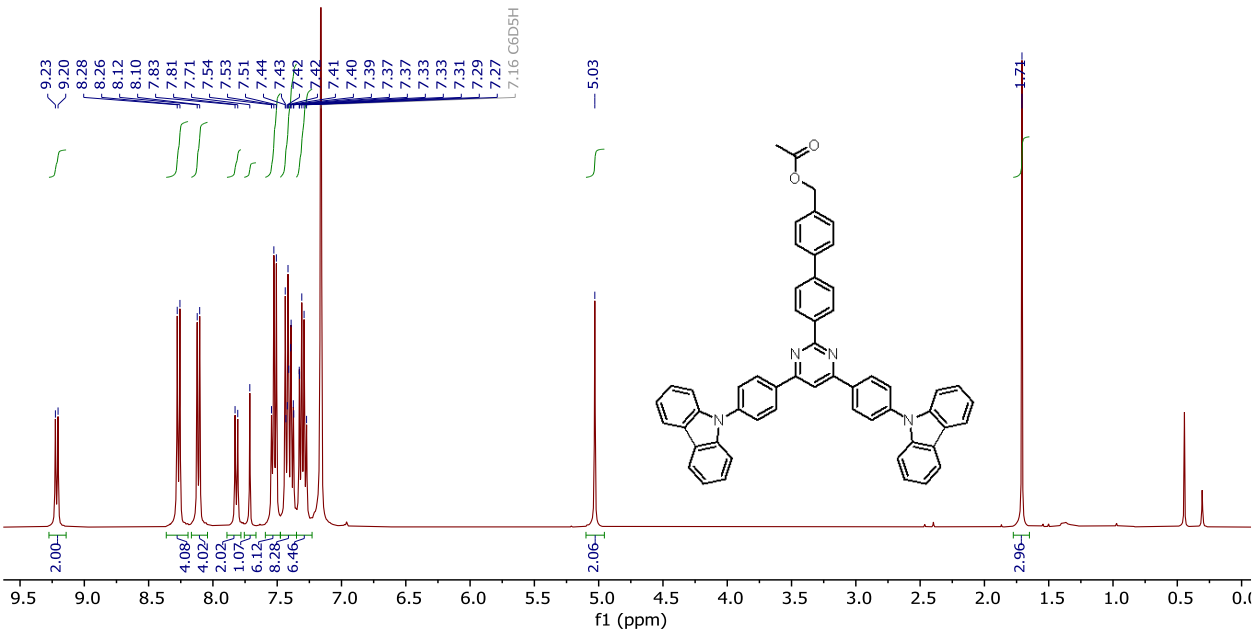


Figure 40a ^{1}H NMR spectrum of **PymCz-OAc** in C_6D_6.

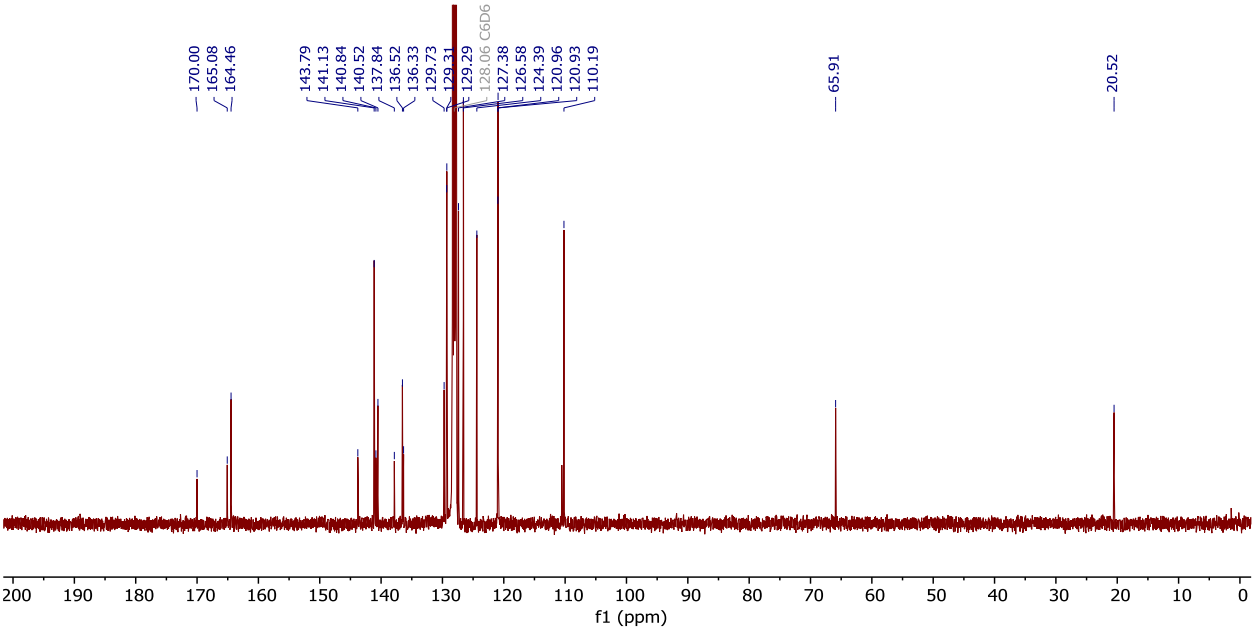


Figure 40b ^{13}C{^{1}H} NMR spectrum of **PymCz-OAc** in C_6D_6.

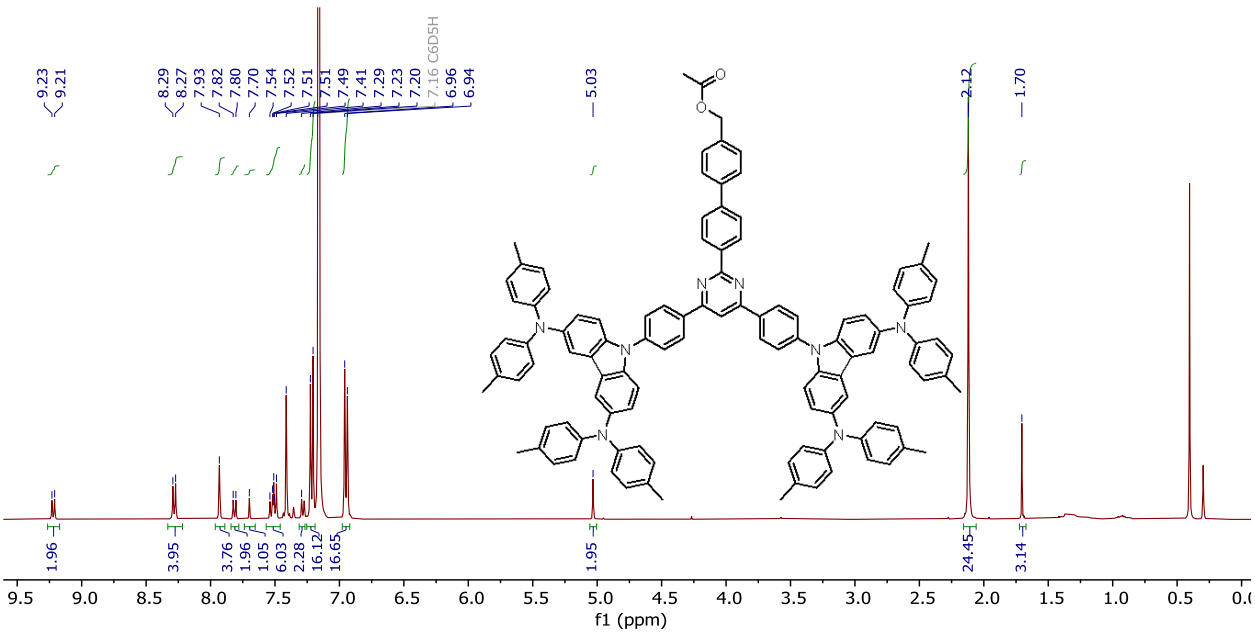


Figure 41a ^{1}H NMR spectrum of **PymTTAC-OAc** in C_6D_6.

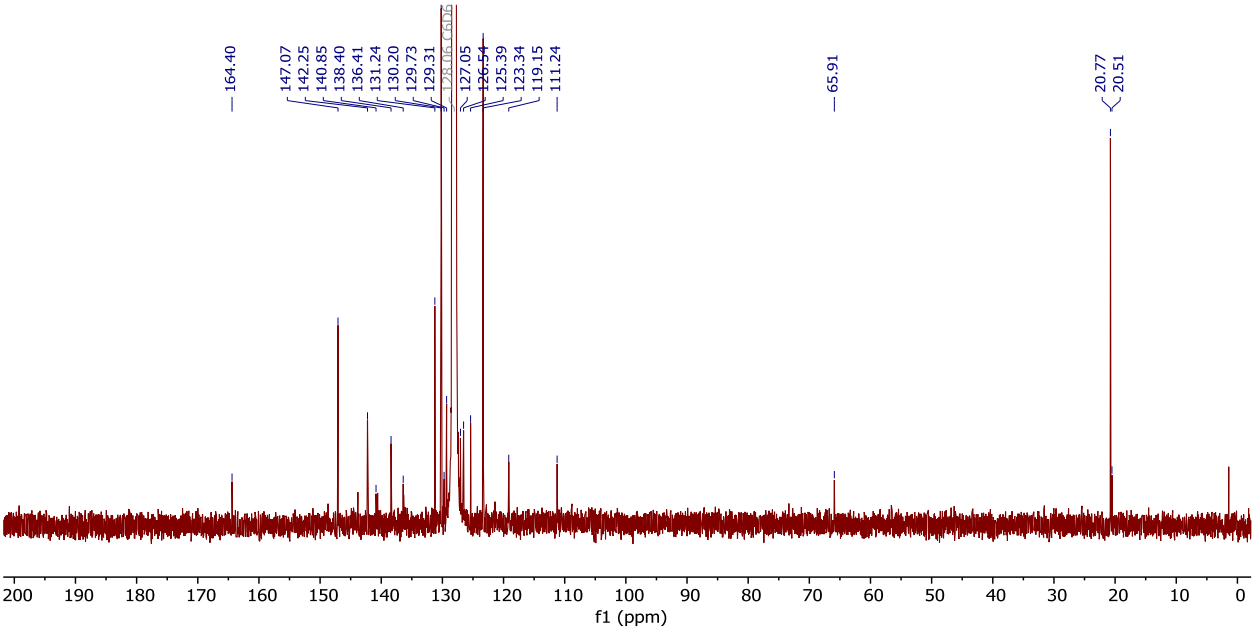


Figure 41b ^{13}C{^{1}H} NMR spectrum of **PymTTAC-OAc** in C_6D_6.

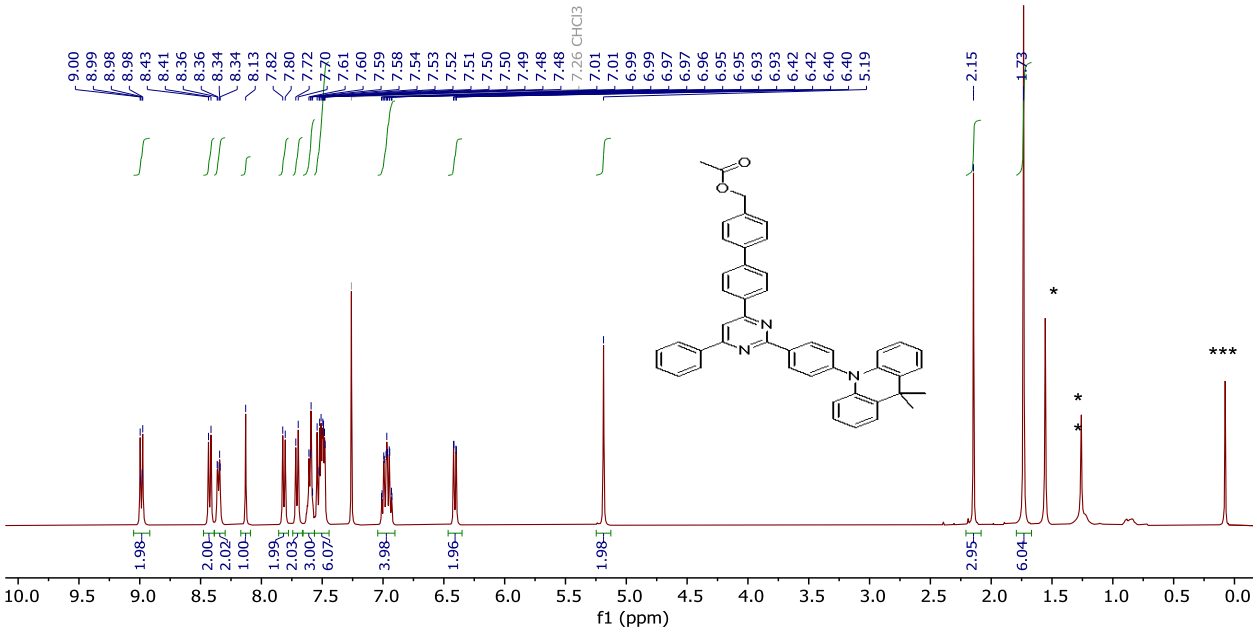


Figure 42a ^{1}H NMR spectrum of **2PymDMA-OAc** in $CDCl_3$. * = H_2O, ** = hexanes, *** = PDMS grease.

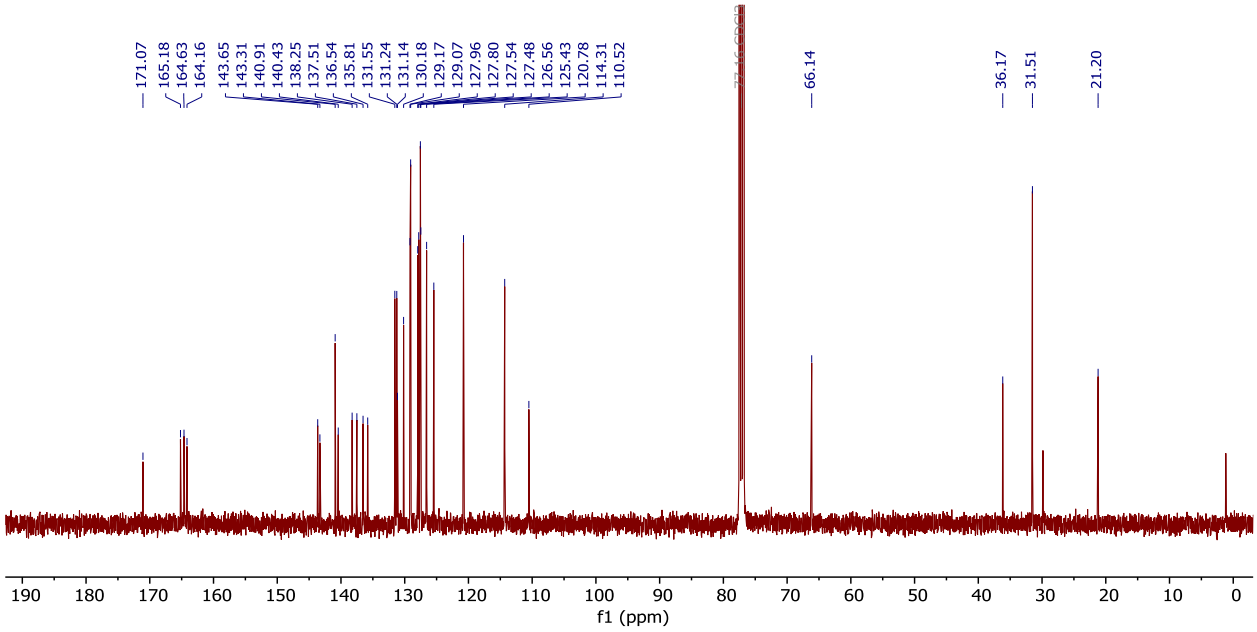


Figure 42b $^{13}C\{^{1}H\}$ NMR spectrum of **2PymDMA-OAc** in $CDCl_3$.

S3 ^{1}H NMR Spectra and Size Exclusion Chromatography of Polymers

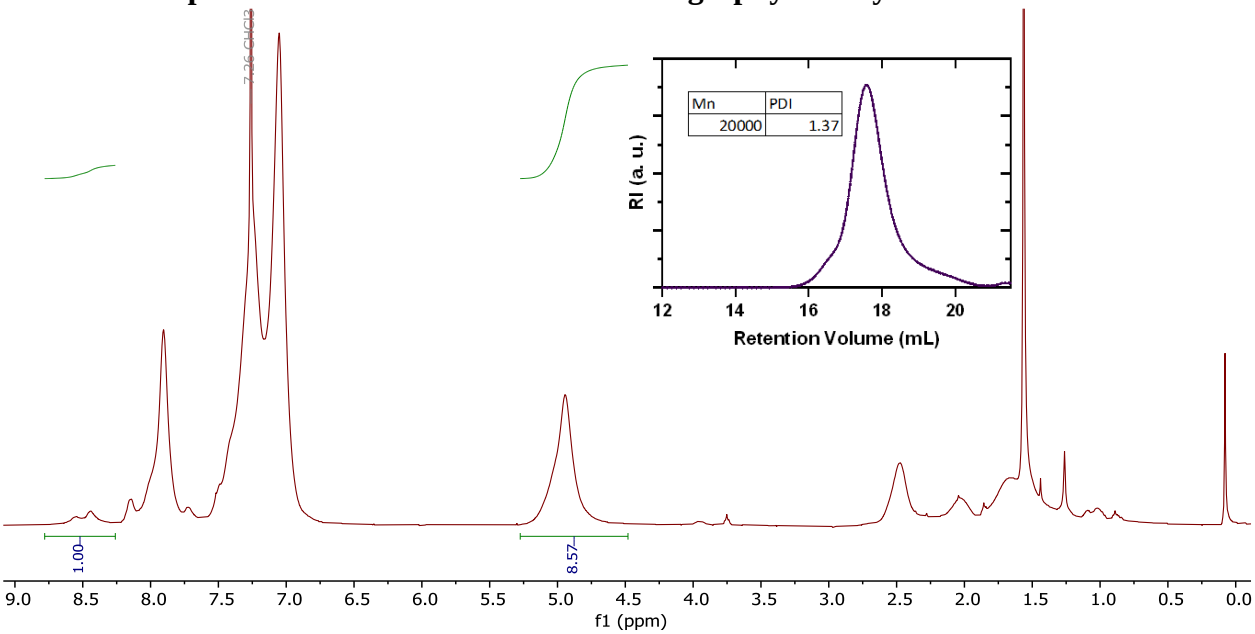


Figure S43 ^{1}H NMR spectrum of **P1** in $CDCl_3$ after SEC and reprecipitation from CH_2Cl_2/MeOH. Inset is the refractive index trace for the same, from gel permeation chromatography.

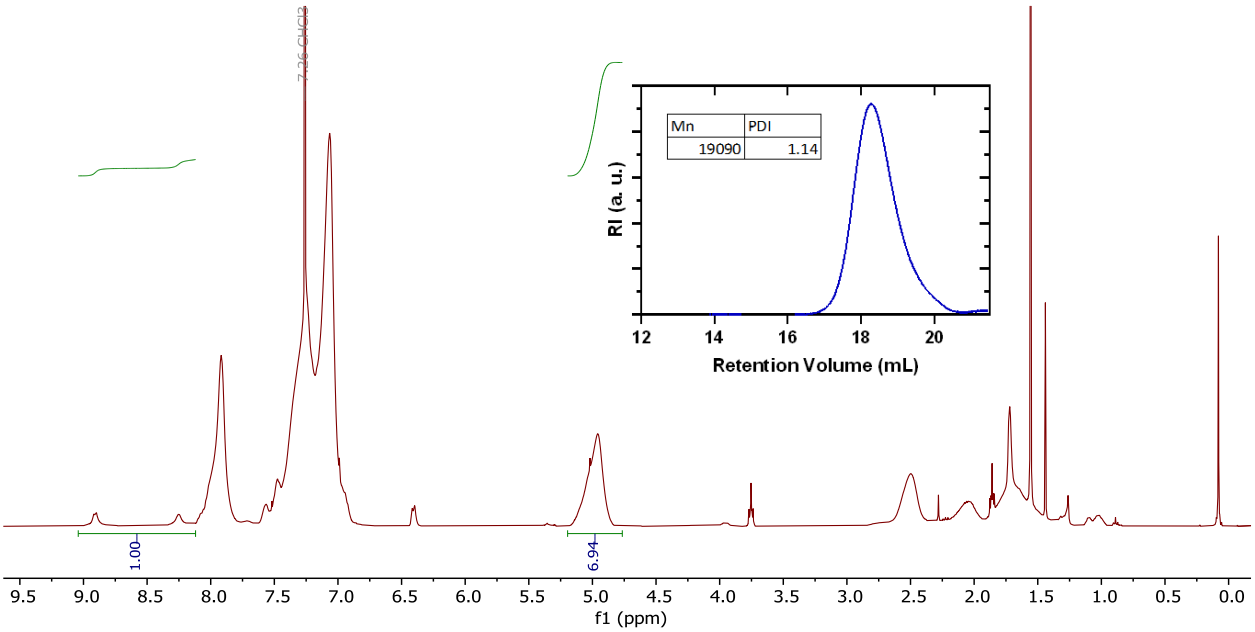


Figure S44 ^{1}H NMR spectrum of **P2** in $CDCl_3$ after SEC and reprecipitation from CH_2Cl_2/MeOH. Inset is the refractive index trace for the same, from gel permeation chromatography.

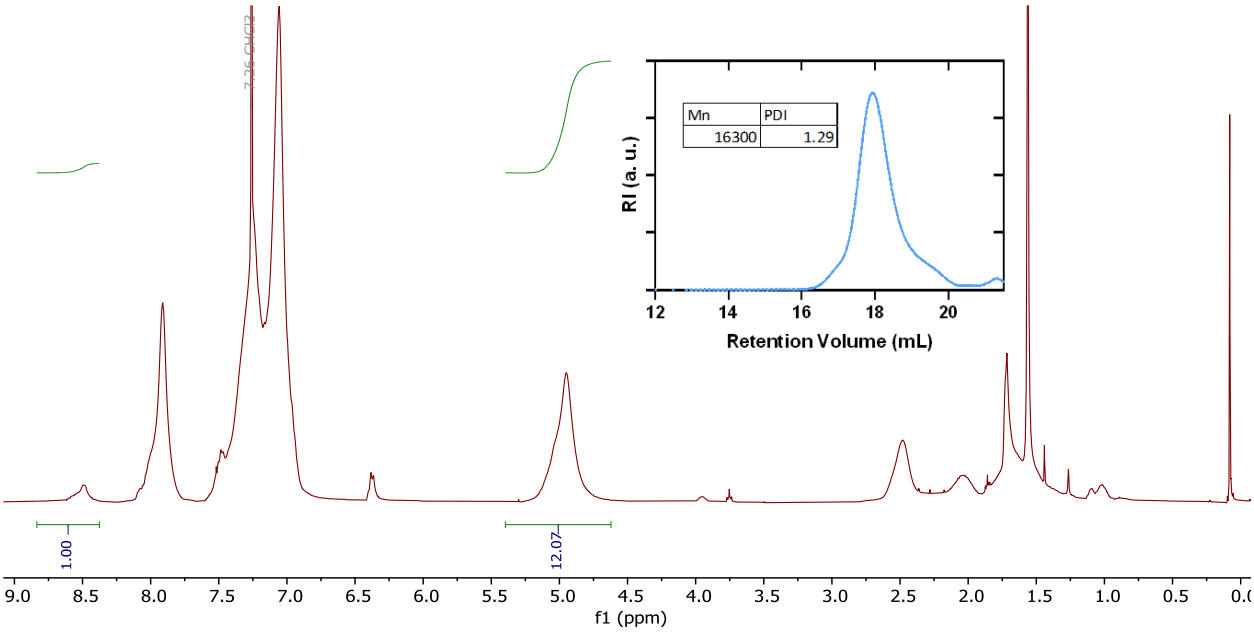


Figure S45 ^{1}H NMR spectrum of **P3** in $CDCl_3$ after SEC and reprecipitation from CH_2Cl_2/MeOH. Inset is the refractive index trace for the same, from gel permeation chromatography.

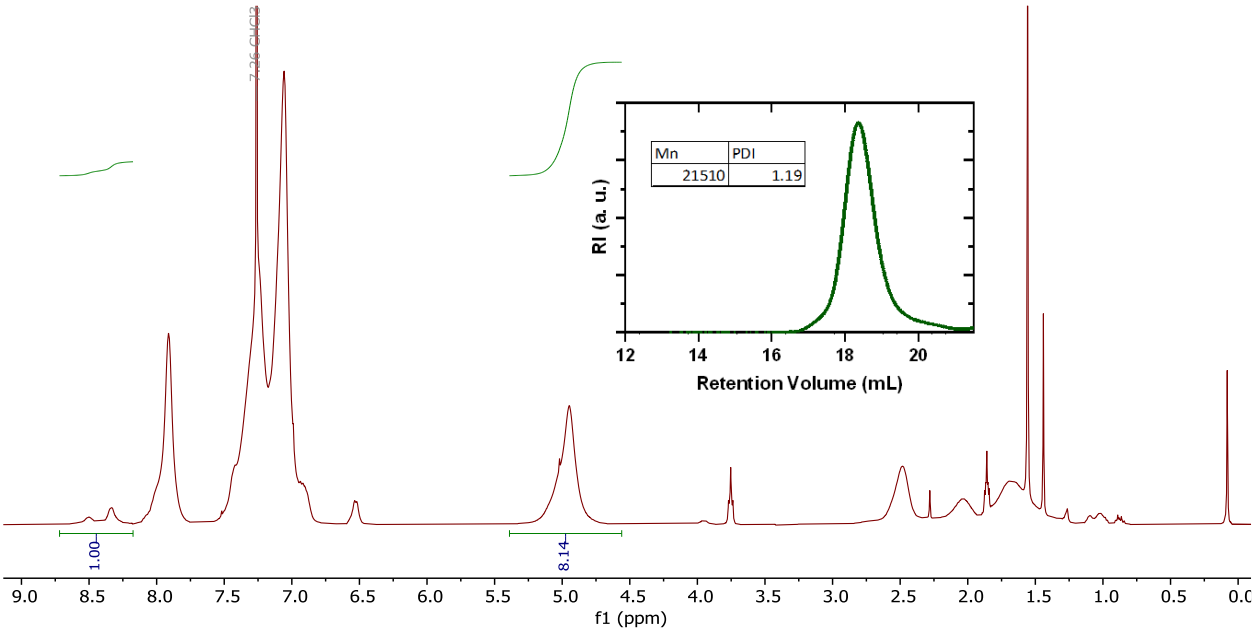


Figure S46 ^{1}H NMR spectrum of **P4** in $CDCl_3$ after SEC and reprecipitation from CH_2Cl_2/MeOH. Inset is the refractive index trace for the same, from gel permeation chromatography.

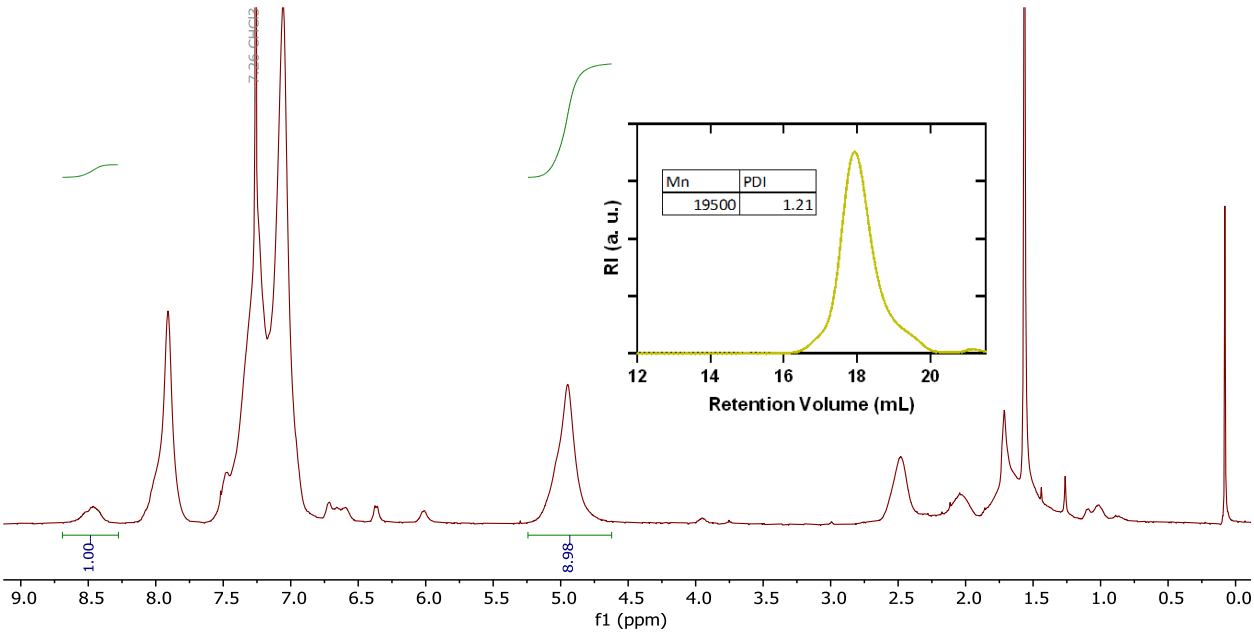


Figure S47 ^{1}H NMR spectrum of **P5** in $CDCl_3$ after SEC and reprecipitation from CH_2Cl_2/MeOH. Inset is the refractive index trace for the same, from gel permeation chromatography.

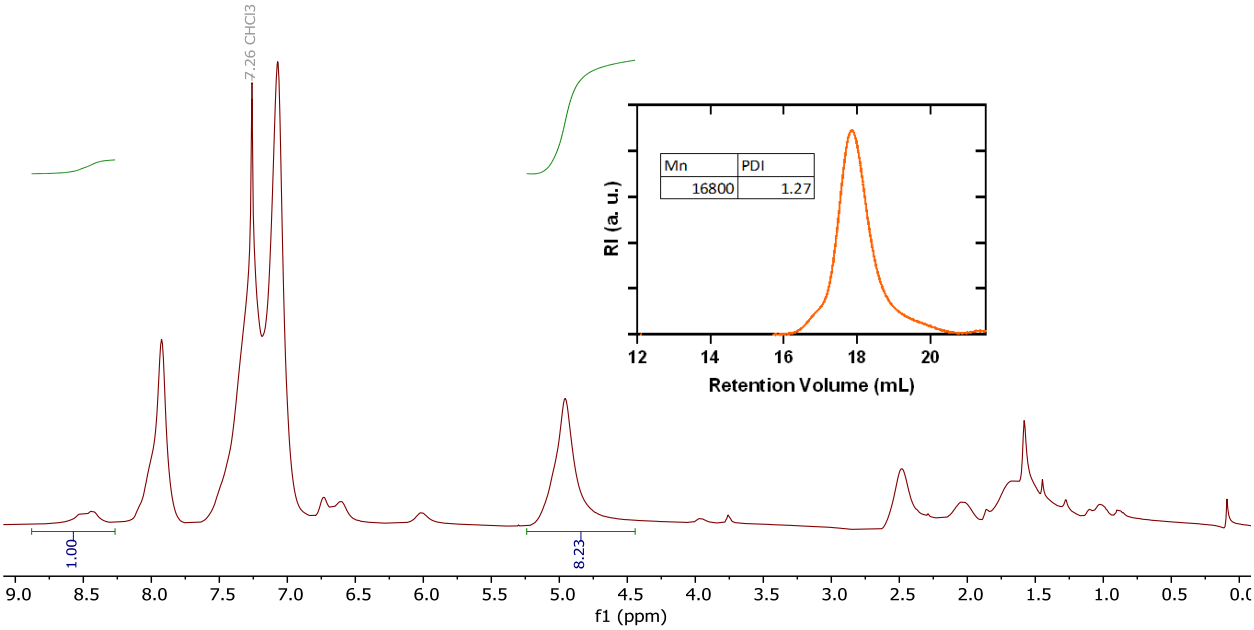


Figure S48 ^{1}H NMR spectrum of **P6** in $CDCl_3$ after SEC and reprecipitation from CH_2Cl_2/MeOH. Inset is the refractive index trace for the same, from gel permeation chromatography.

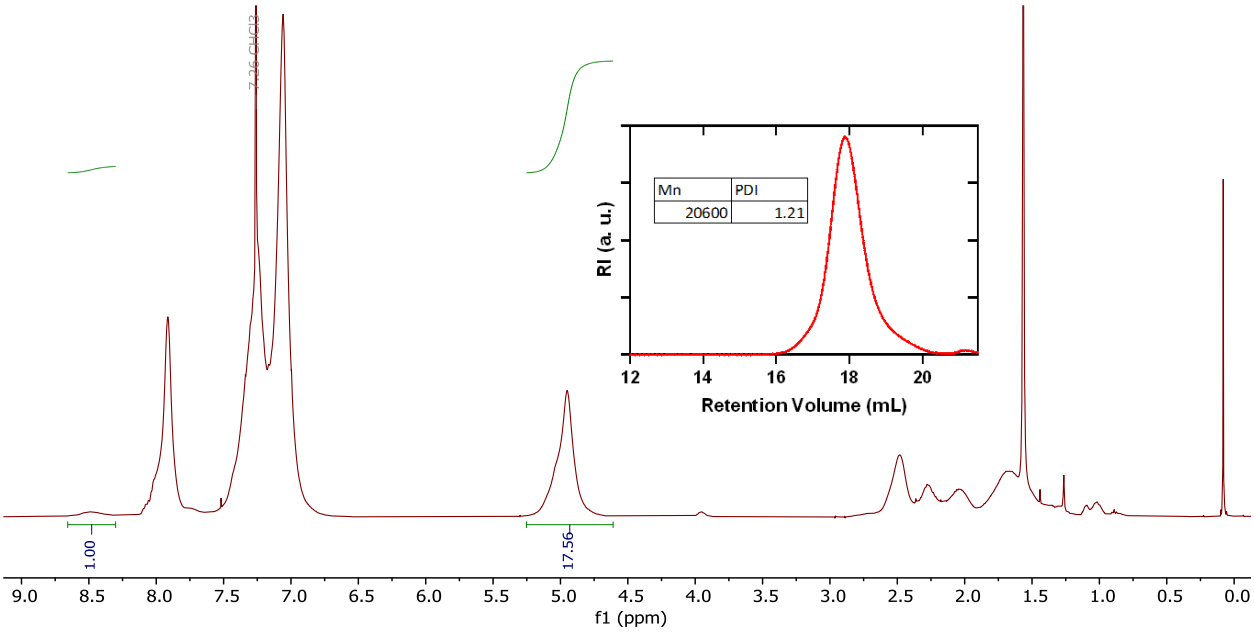


Figure S49 ^{1}H NMR spectrum of **P7** in $CDCl_3$ after SEC and reprecipitation from CH_2Cl_2/MeOH. Inset is the refractive index trace for the same, from gel permeation chromatography.

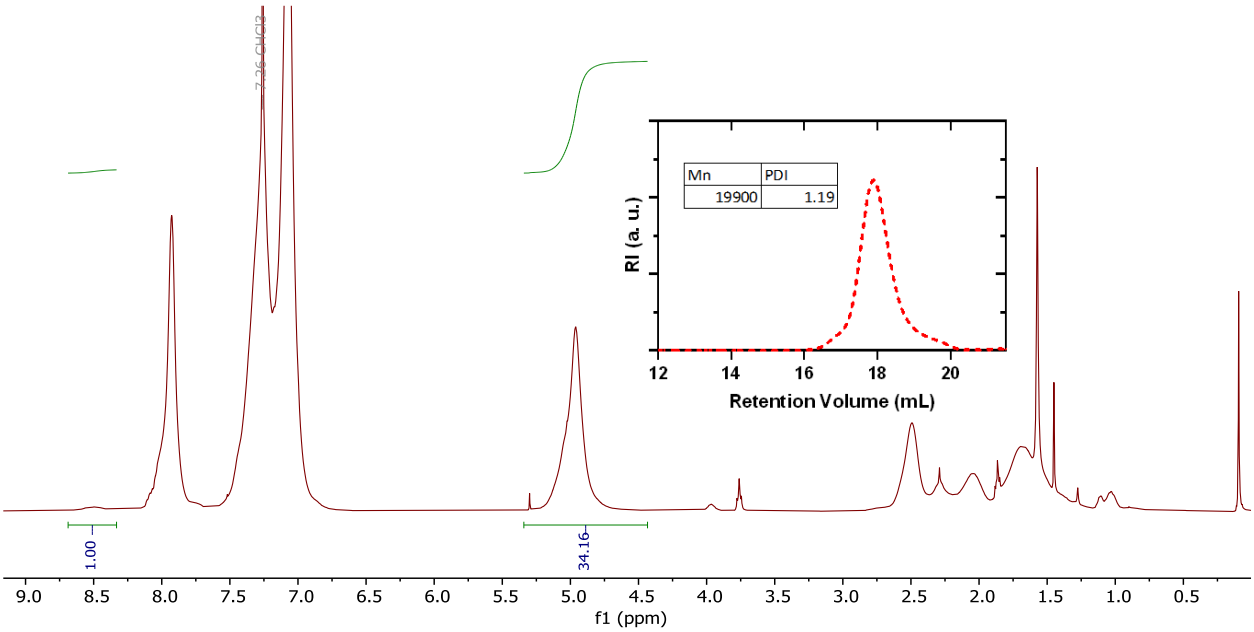


Figure S50 ^{1}H NMR spectrum of **P7a** in $CDCl_3$ after SEC and reprecipitation from CH_2Cl_2/MeOH. Inset is the refractive index trace for the same, from gel permeation chromatography.

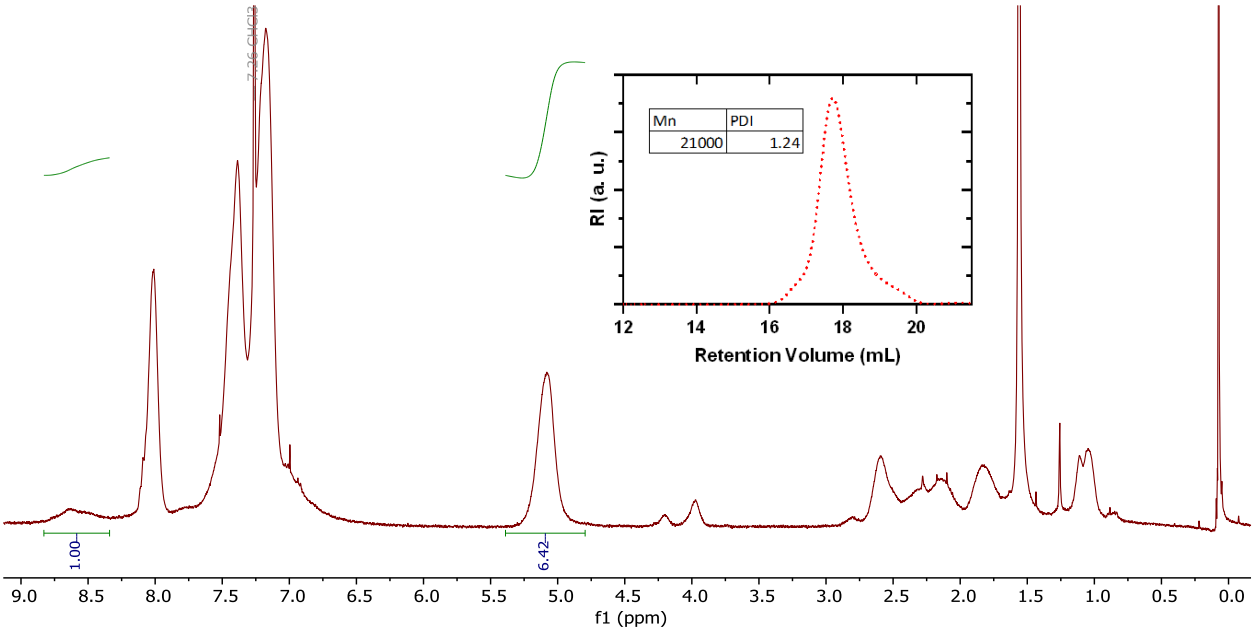


Figure S51 ^{1}H NMR spectrum of **P7b** in $CDCl_3$ after SEC and reprecipitation from CH_2Cl_2/MeOH. Inset is the refractive index trace for the same, from gel permeation chromatography.

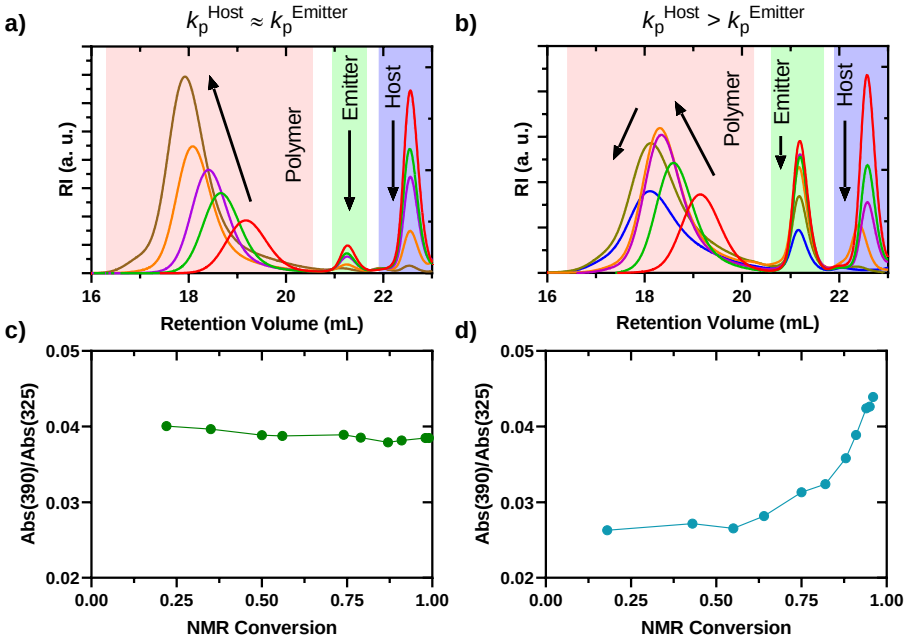


Figure S52 (Top) refractive index trace from gel permeation chromatography for the polymerization of (a) **P6** and (b) **P3** as a function of monomer conversion. The arrows indicate the direction of increasing monomer conversion. (Bottom) Relative absorption of the TADF emitter (absorbance at 390 nm) to the host (absorbance at 325 nm) as a function of monomer conversion for the polymerization of (c) **P6** and (d) **P3**. The absorption was determined by a photodiode array, using absorption traces at the same retention volume as the peak in the RI trace to ensure only polymer is measured.

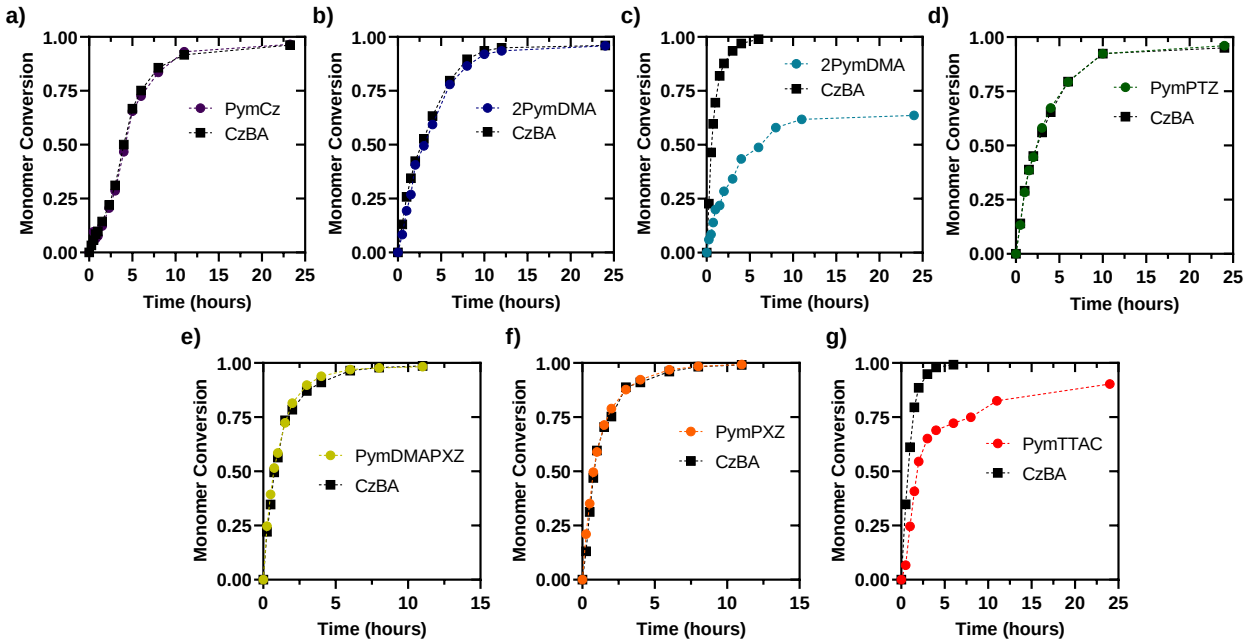


Figure S53 Monomer conversion as a function of time for the polymerization of (a) **P1**, (b) **P2**, (c) **P3**, (d) **P4**, (e) **P5**, (f) **P6**, (g) **P7** by Cu(0)-RDRP. Conversion was determined by ^{1}H NMR spectroscopy, using the integral value for the olefinic signals of the acrylate monomers relative to an internal standard 1,3,5-trimethoxybenzene. Host monomer (CzBA) is plotted as black squares and pyrimidine monomers are plotted as coloured circles.

Here, the method for determining actual doping percentage from ^{1}H NMR data of the polymers is outlined:

Let $I_{8.5}$ be the integral value for the signal occurring at ca. 8.5 ppm in the polymer NMR spectrum, corresponding to 6 protons (2 of the biphenyl moiety, 4 of the bridging phenyl groups). This will be set to the value of 1.00. Let $I_{5.0}$ be the integral value for the signal occurring at 5.0 ppm in the polymer NMR spectrum, corresponding to the sum of the two benzylic protons from the host and dopant monomers. Let n_H be the *relative* number of moles of the host monomer and n_D the same for the dopant in the polymer. Then

$$n_D = \frac{I_{8.5}}{6} = \frac{1}{6} \tag{1}$$

$$n_H = \frac{I_{5.0} - 2 \times n_D}{2} = \frac{I_{5.0}}{2} - \frac{1}{6} \tag{2}$$

$$Mass\ Ratio = \frac{n_D}{n_H} \times \frac{MW_D}{MW_H} \tag{3}$$

$$Mass\ Percentage = \frac{Mass\ Ratio}{1 - Mass\ Ratio} \tag{4}$$

Where MW_D and MW_H are the molecular masses of the dopant and host monomers, respectively. In this scheme, Mass Percentage is analogous to the % mass of monomer fed into the polymerization at the start.

The average number of host and dopant monomer residues per polymer chain (DP_H and DP_D, respectively) and the overall degree of polymerization (DP_n) were calculated from the molar ratio determined from NMR spectroscopy (n_D/n_H) and the number average molecular weight M_n from GPC, using equations (5) – (7).

$$DP_H = \frac{M_n}{MW_H + (n_D/n_H)MW_D} \tag{5}$$

$$DP_D = \frac{M_n}{(n_H/n_D)MW_H + MW_D} \tag{6}$$

$$DP_n = DP_H + DP_D \tag{7}$$

Polymer	$I_{5.0}$	n_H	Molar Ratio	Mass Ratio	TADF Mass Percentage	DP_H	DP_D	DP_n
P1	8.57	4.12	0.0405	0.0988	0.0899	55.6	2.3	57.9
P2	6.94	3.30	0.0505	0.104	0.0944	52.8	2.7	55.5
P3	12.07	5.87	0.0284	0.0767	0.0712	46.2	1.3	47.5
P4	8.14	3.90	0.0427	0.113	0.101	59.0	2.5	61.5
P5	8.98	4.32	0.0386	0.101	0.0917	54.1	2.1	56.2
P6	8.23	3.95	0.0422	0.107	0.0968	46.4	2.0	48.4
P7	17.56	8.61	0.0194	0.935	0.0855	57.5	1.1	58.6
P7a	34.16	16.9	0.00985	0.0476	0.0454	58.0	0.6	58.6
P7b	6.42	3.04	0.0548	0.176	0.149	50.7	2.8	53.5

Table S1. Determination of the actual doping percentage of TADF monomer in the polymers using ^{1}H NMR and Equations 1 – 7. Molar Ratio = n_D/n_H.

S4 Solution-State UV-Visible Absorption and Emission Spectroscopy of Monomers

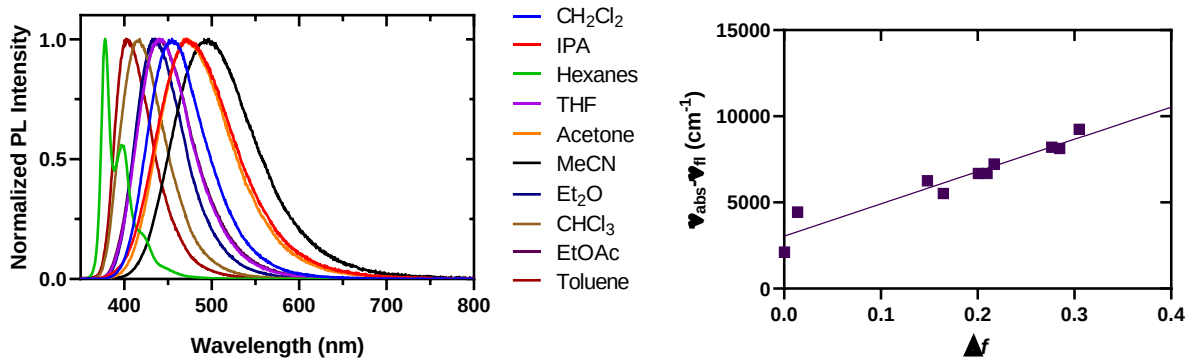


Figure S54 (Left) Normalized steady-state fluorescence spectra of **PymCz** in organic solvents of different polarity. (Right) Stokes shift plotted against the orientation polarizability (Δf) of different organic solvents (Lippert-Mataga plot; violet squares) and linear fit to the data (y = 18737x + 3042, R^2 = 0.9172).

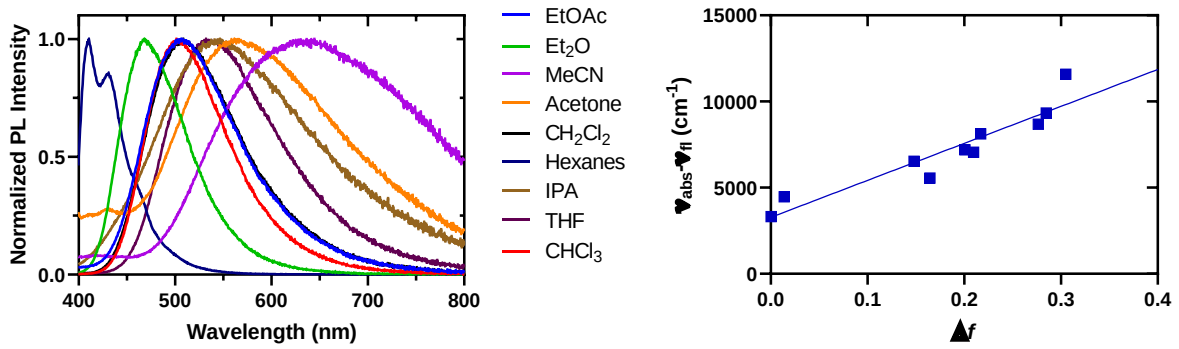


Figure S55 (Left) Normalized steady-state fluorescence spectra of 2**PymDMA** in organic solvents of different polarity. (Right) Stokes shift plotted against the orientation polarizability (Δf) of different organic solvents (Lippert-Mataga plot; blue squares) and linear fit to the data (y = 21457x + 3277, R^2 = 0.8768).

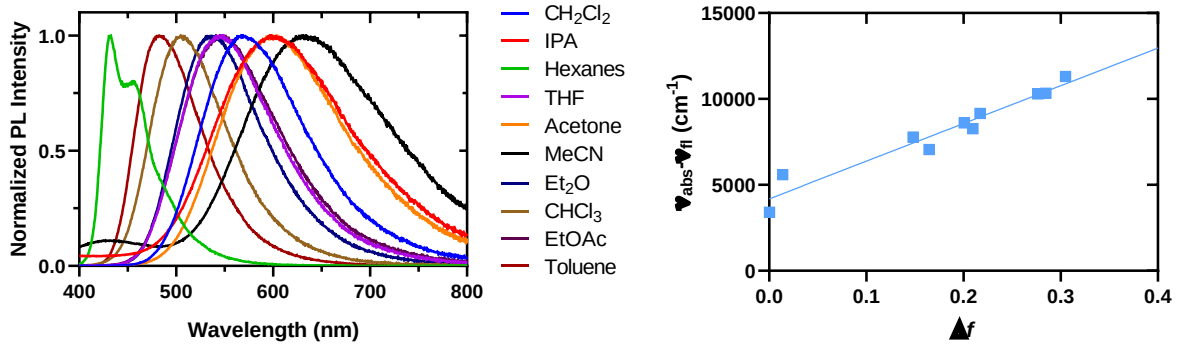


Figure S56 (Left) Normalized steady-state fluorescence spectra of **PymDMA** in organic solvents of different polarity. (Right) Stokes shift plotted against the orientation polarizability (Δf) of different organic solvents (Lippert-Mataga plot; light blue squares) and linear fit to the data (y = 21944x + 4185, R^2 = 0.9411).

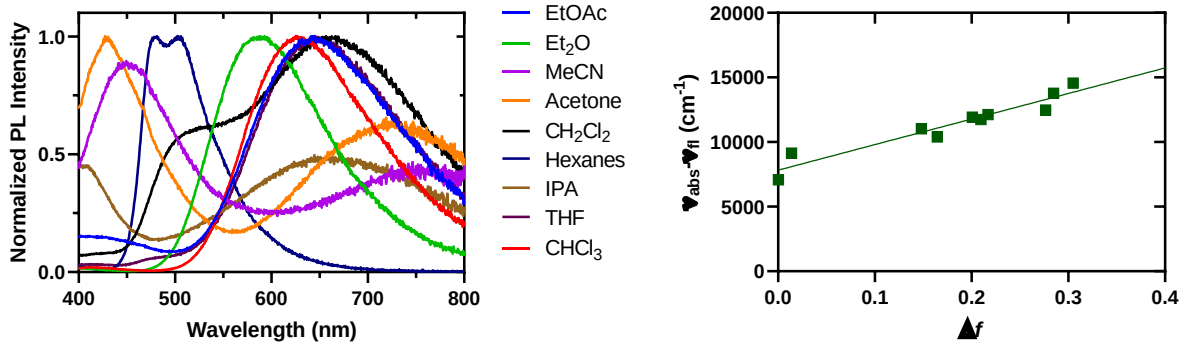


Figure S57 (Left) Normalized steady-state fluorescence spectra of **PymPTZ** in organic solvents of different polarity. (Right) Stokes shift plotted against the orientation polarizability (Δ*f*) of different organic solvents (Lippert-Mataga plot; green squares) and linear fit to the data (y = 19781x + 4185, R^2 = 0.9164).

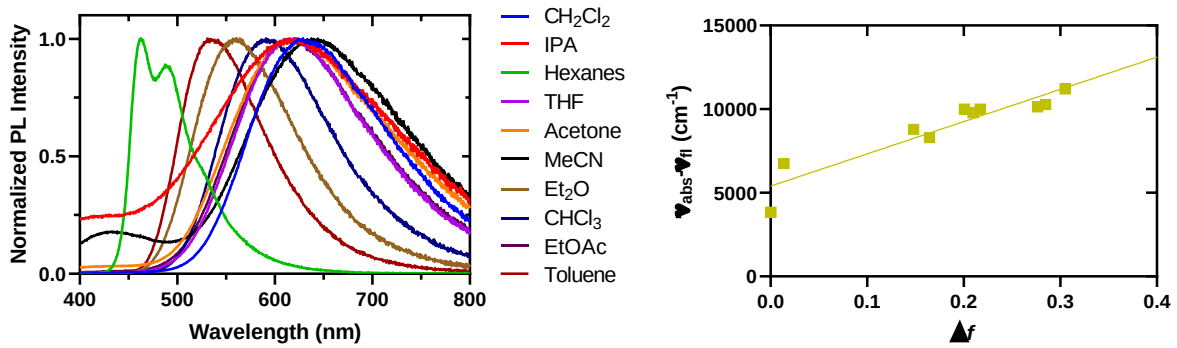


Figure S58 (Left) Normalized steady-state fluorescence spectra of **PymDMAPXZ** in organic solvents of different polarity. (Right) Stokes shift plotted against the orientation polarizability (Δ*f*) of different organic solvents (Lippert-Mataga plot; green squares) and linear fit to the data (y = 19269x + 5400, R^2 = 0.8703).

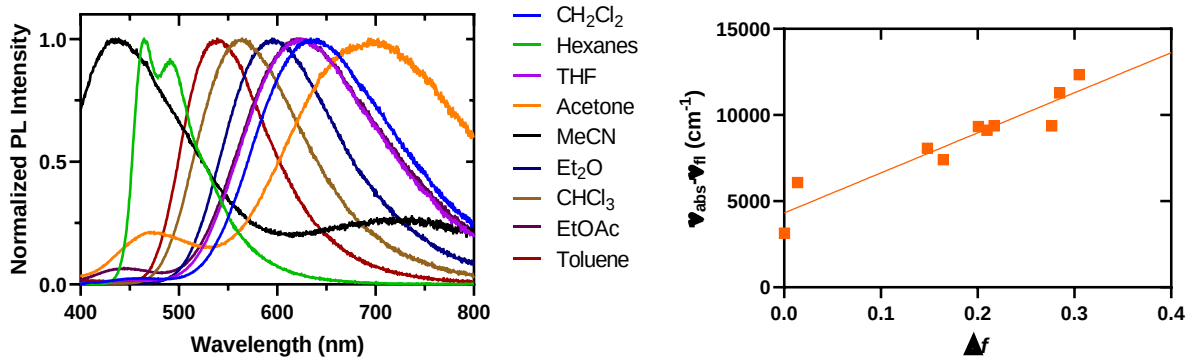


Figure S59 (Left) Normalized steady-state fluorescence spectra of **PymPXZ** in organic solvents of different polarity. (Right) Stokes shift plotted against the orientation polarizability (Δ*f*) of different organic solvents (Lippert-Mataga plot; yellow squares) and linear fit to the data (y = 23250x + 4317, R^2 = 0.8835).

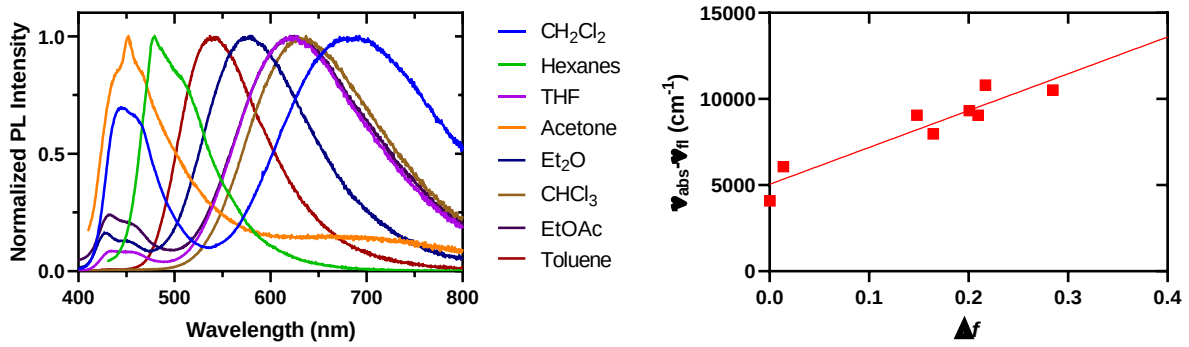


Figure S60 (Left) Normalized steady-state fluorescence spectra of **PymTTAC** in organic solvents of different polarity. (Right) Stokes shift plotted against the orientation polarizability (Δf) of different organic solvents (Lippert-Mataga plot; orange squares) and linear fit to the data (y = 21372x + 5049, R^2 = 0.8788).

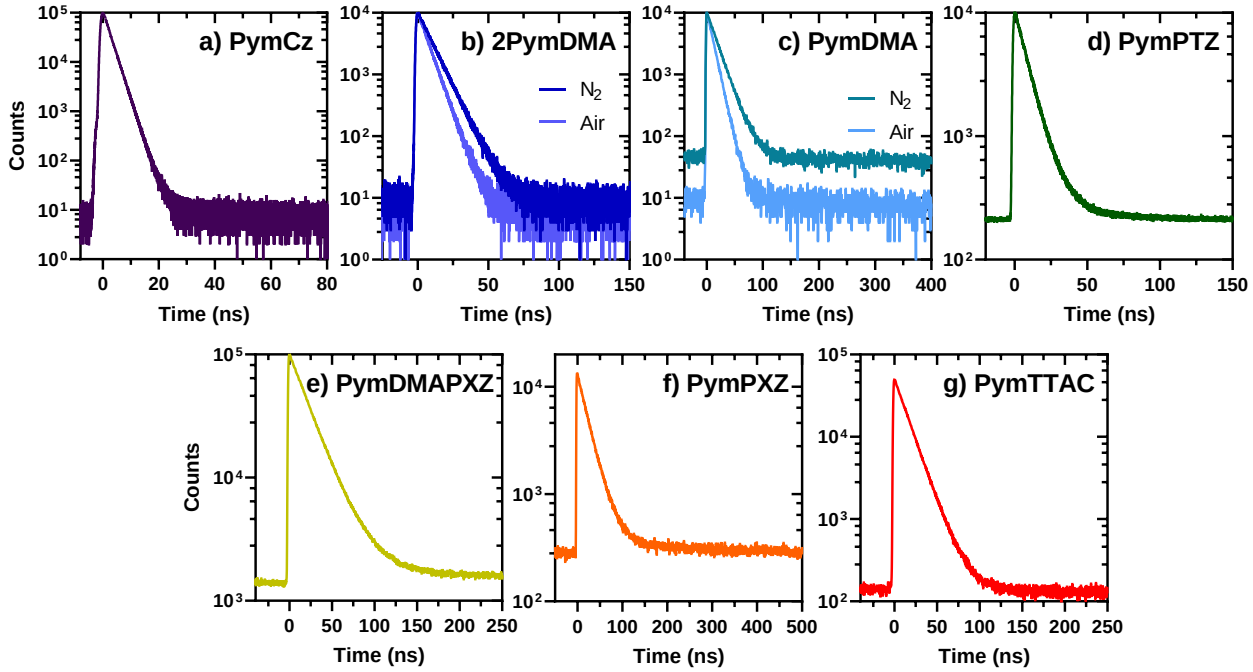


Figure S61 Photoluminescence decays of acrylic monomers (a) **PymCz**, (b) 2**PymDMA**, (c) **PymDMA**, (d) **PymPTZ**, (e) **PymDMAPXZ**, (f) **PymPXZ**, and (g) **2PymTTAC** in N_2-sparged toluene (~10^{-6} M). Note that the different y-axis offsets arise from residual delayed fluorescence build up. All compounds were excited at 313 nm and detected at the wavelength of maximum emission.

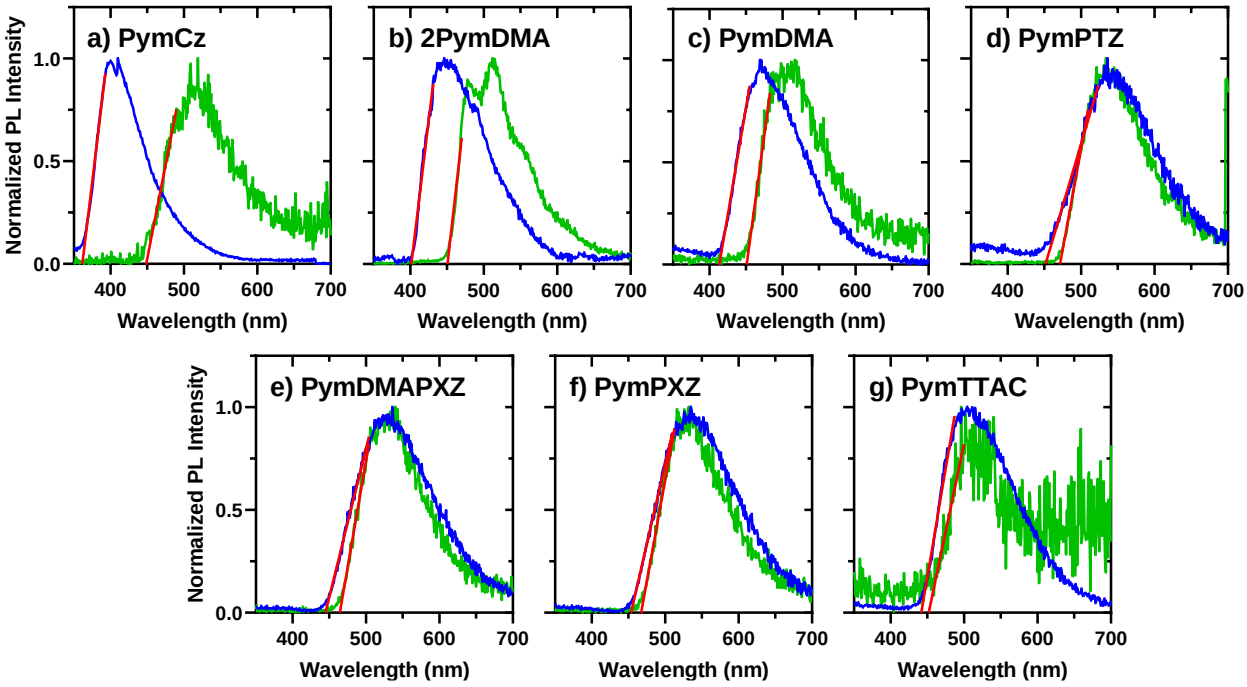


Figure S62 Prompt fluorescence (blue) and phosphorescence (green) spectra of (a) **PymCz**, (b) 2**PymDMA**, (c) **PymDMA**, (d) **PymPTZ**, (e) **PymDMAPXZ**, (f) **PymPXZ**, and (g) **2PymTTAC** in frozen 2-methyltetrahydrofuran matrix at 77 K. The singlet and triplet energies were determined from the onset of emission (red lines). Prompt spectra were acquired within the first microsecond and delayed spectra were acquired between 100 μs and 5 ms, exciting at 313 nm.

S5 Solution-State UV-Visible Absorption and Emission Spectroscopy of Polymers

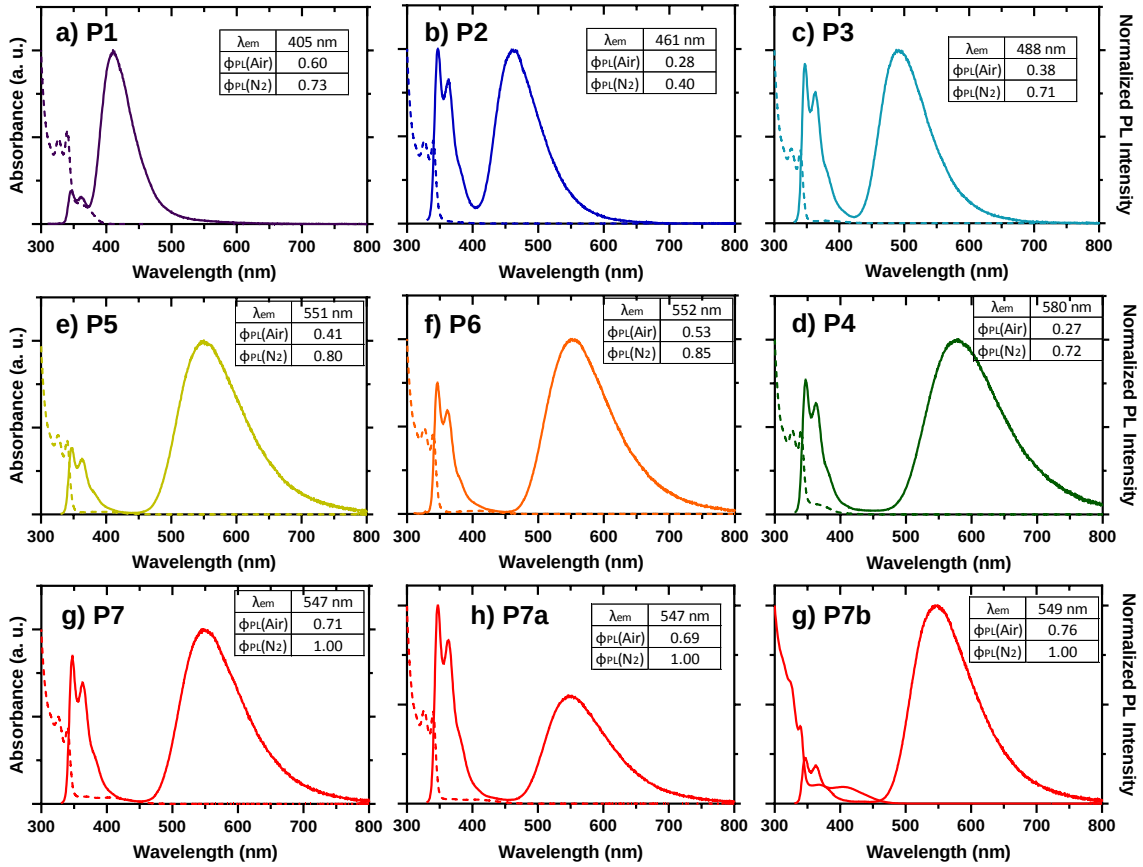


Figure S63 (a) Steady-state UV-Vis absorption (dashed) and normalized photoluminescence (solid) spectra for polymers **P1** – **P7**. Inset are the wavelength of maximum emission (λ_{em}) and quantum yield of emission in the presence or absence of atmospheric oxygen. Absorption spectra were recorded at 0.01 mg mL^{-1} in toluene, and fluorescence spectra were at 0.05 mg mL^{-1} in toluene, λ_{ex} = 310 nm.

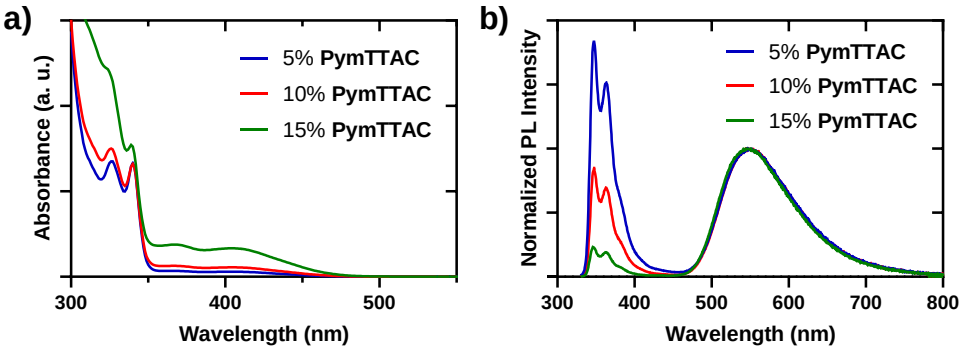


Figure S64 (a) Steady-state UV-Vis absorption spectra and (b) fluorescence spectra for **P7** (red), **P7a** (blue), and **P7b** (green) in toluene. Absorption spectra were recorded at 0.01 mg mL^{-1} in toluene, and fluorescence spectra were at 0.05 mg mL^{-1} in toluene, λ_{ex} = 310 nm.

S6 Emission Spectroscopy of Polymer Films

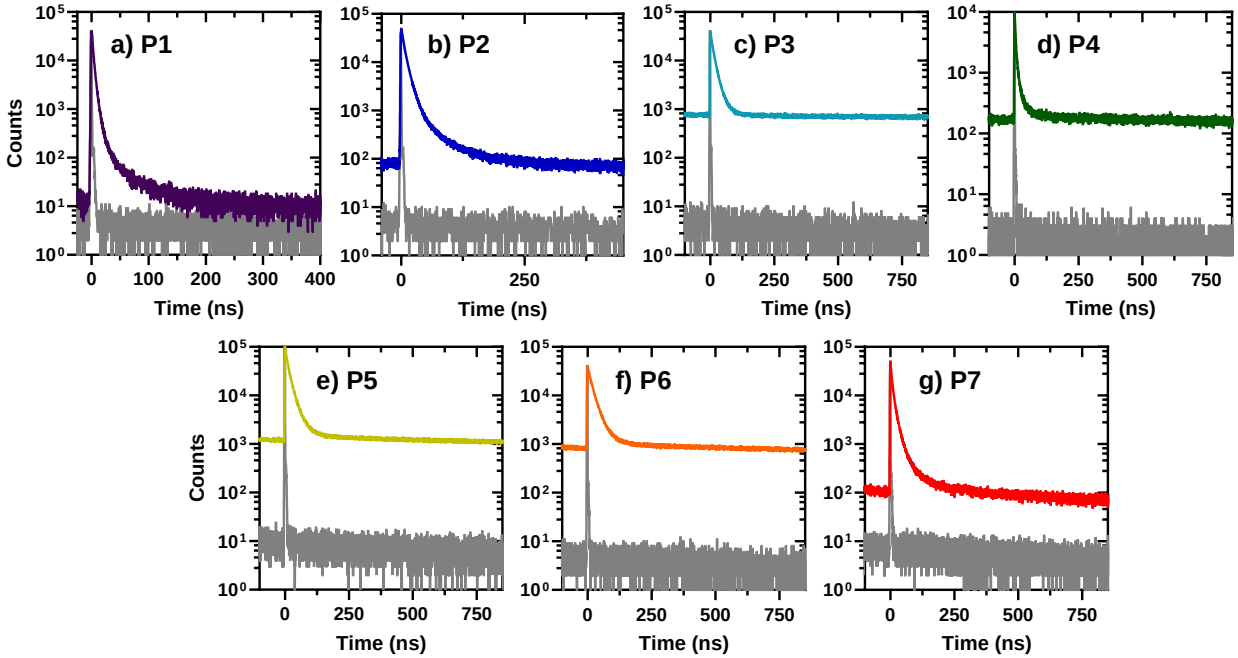


Figure S65 Photoluminescence decays of the polymer films (a) **P1**, (b) **P2**, (c) **P3**, (d) **P4**, (e) **P6**, and (f) **P7** under vacuum on a nanosecond timescale. The instrument response function is plotted as a gray curve. Different y-axis offsets arise from residual delayed fluorescence buildup.

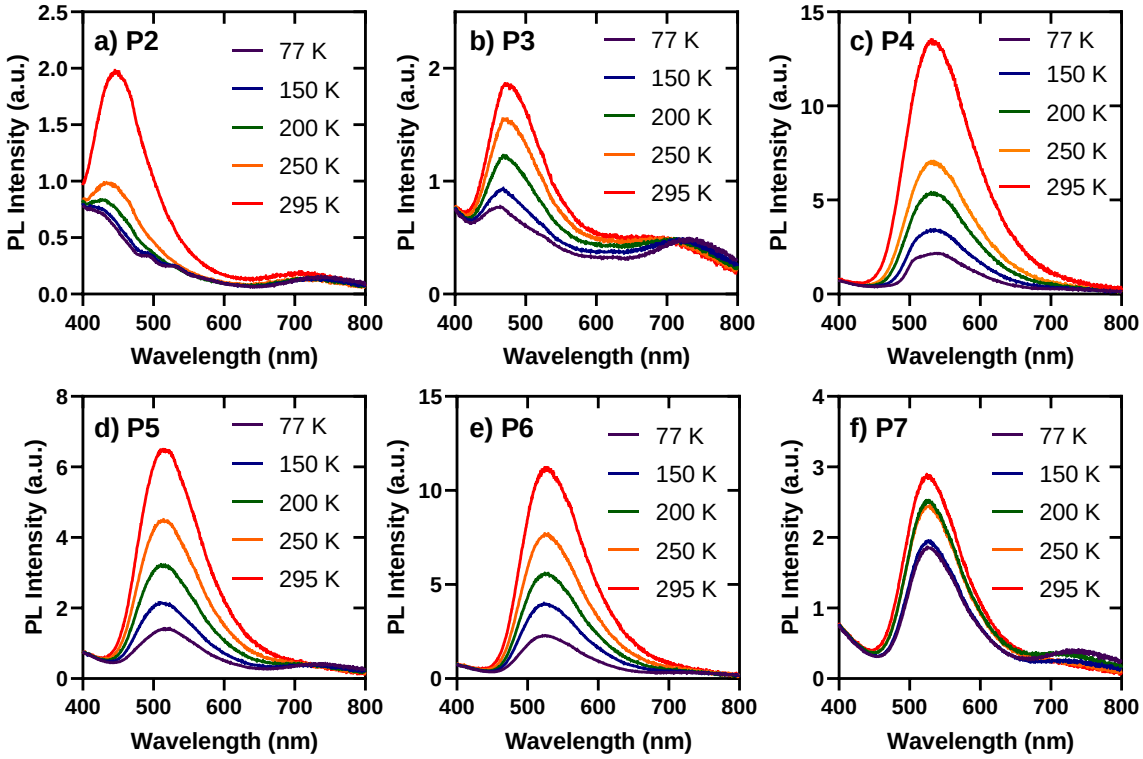


Figure S66 Temperature-dependence of the photoluminescence spectra of (a) **P2**, (b) **P3**, (c) **P4**, (d) **P5**, (e) **P6**, and (f) **P7**. All polymer films were spin-cast on glass slides and excited at 313 nm.

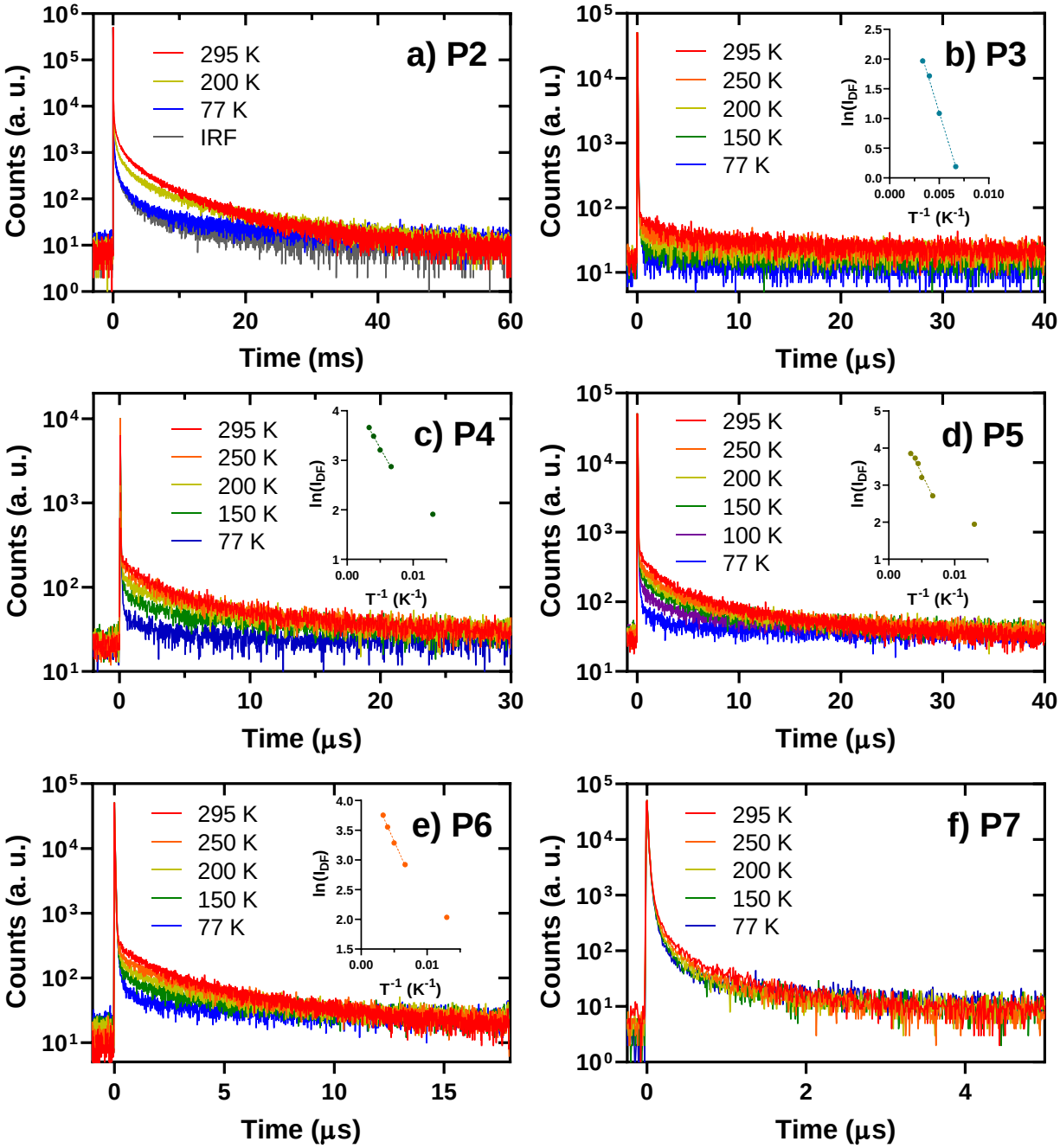


Figure S67 Temperature-dependence of the photoluminescence decays of (a) **P2**, (b) **P3**, (c) **P4**, (d) **P5**, (e) **P6**, and (f) **P7**. All polymer films were spin-cast on glass slides, excited at 313 nm and observed at the emission maximum. Inset are plots of the dependence of the delayed fluorescence emission integral (I_{DF}) as a function of inverse temperature. The activation energy of RISC was estimated from the linear portion of the curves (dashed lines)

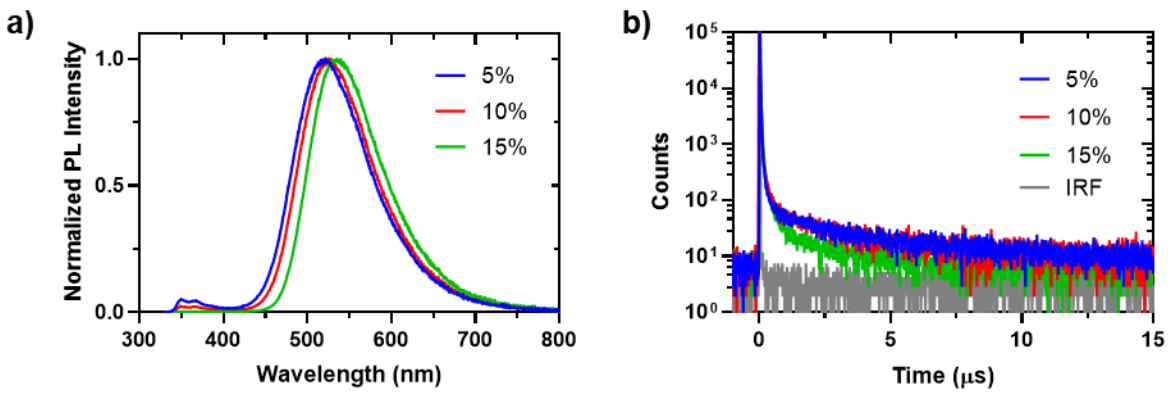


Figure S68 (a) Normalized photoluminescence spectra and (b) photoluminescence decay (λ_{ex} = 313 nm at 1 MHz pulse rate) of **P5** (blue), **P5a** (red), **and P5b** (green) film under vacuum. The instrument response function is plotted as a gray curve.

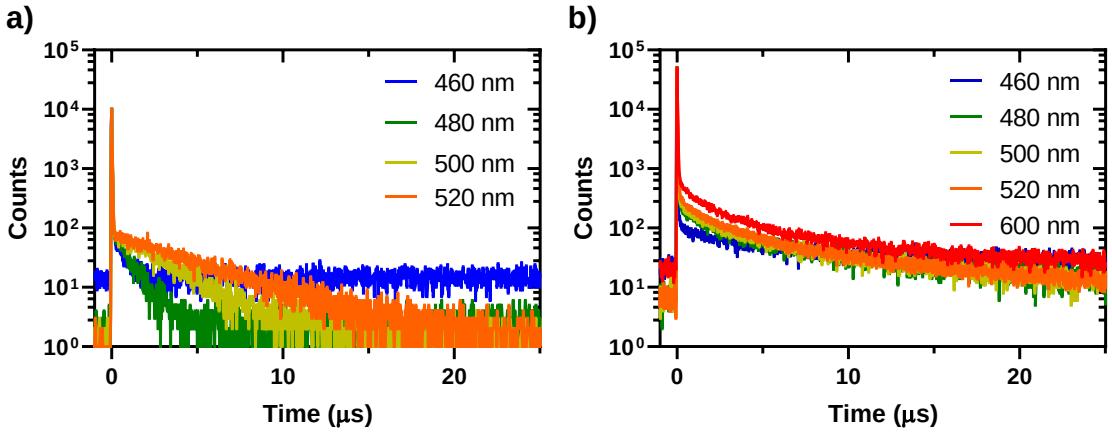


Figure S69 Photoluminescence decays of (a) **PymDMAPXZ** in toluene and (b) a thin film of **P5** at differing emission wavelengths. Excitation was at 313 nm.

S7 Cyclic Voltammetry

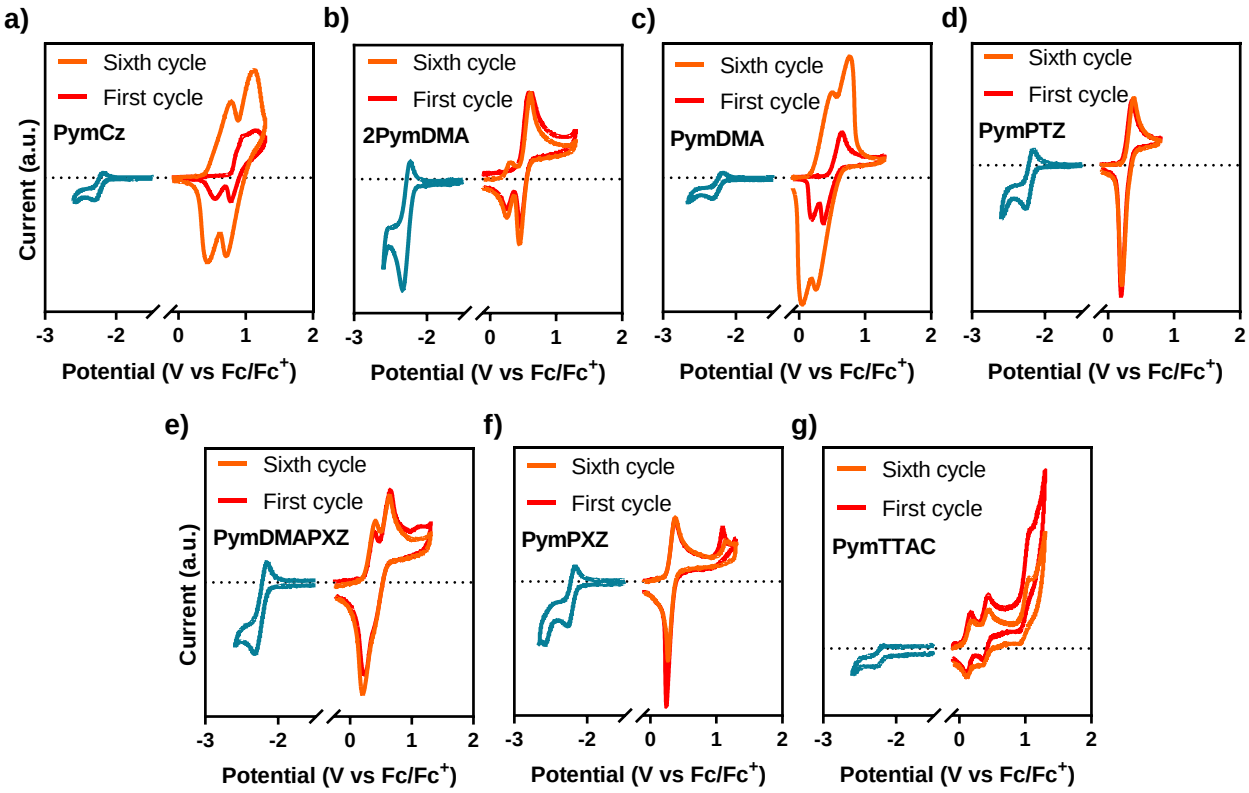


Figure S70 First (red) and final (orange) scans for the cyclic voltammograms of the acetate derivatives of the monomers (a) **PymCz-OAc**, (b) 2**PymDMA-OAc**, (c) **PymDMA-OAc**, (d) **PymPTZ-OAc**, (e) **PymDMAPXZ-OAc**, (f) **PymPXZ-OAc**, and (g) **PymTTAC-OAc** in 1,2-difluorobenzene (1 mM) with a 0.2M [^{n}Bu$_4$N][PF$_6$] supporting electrolyte, recorded at scan rates of 50 mV s^{-1}. The reductive wave does not change significantly between the first and final scans.

S8 Thermal Analyses

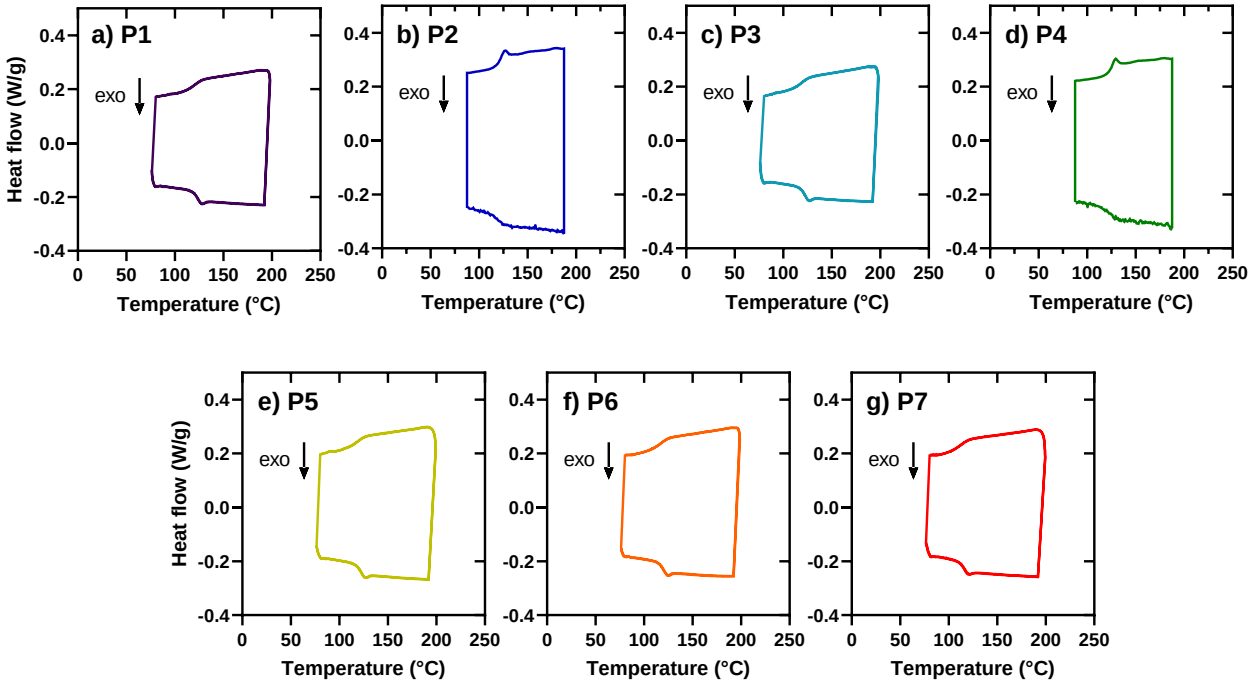


Figure S71 DSC traces of **P1** – **P7**

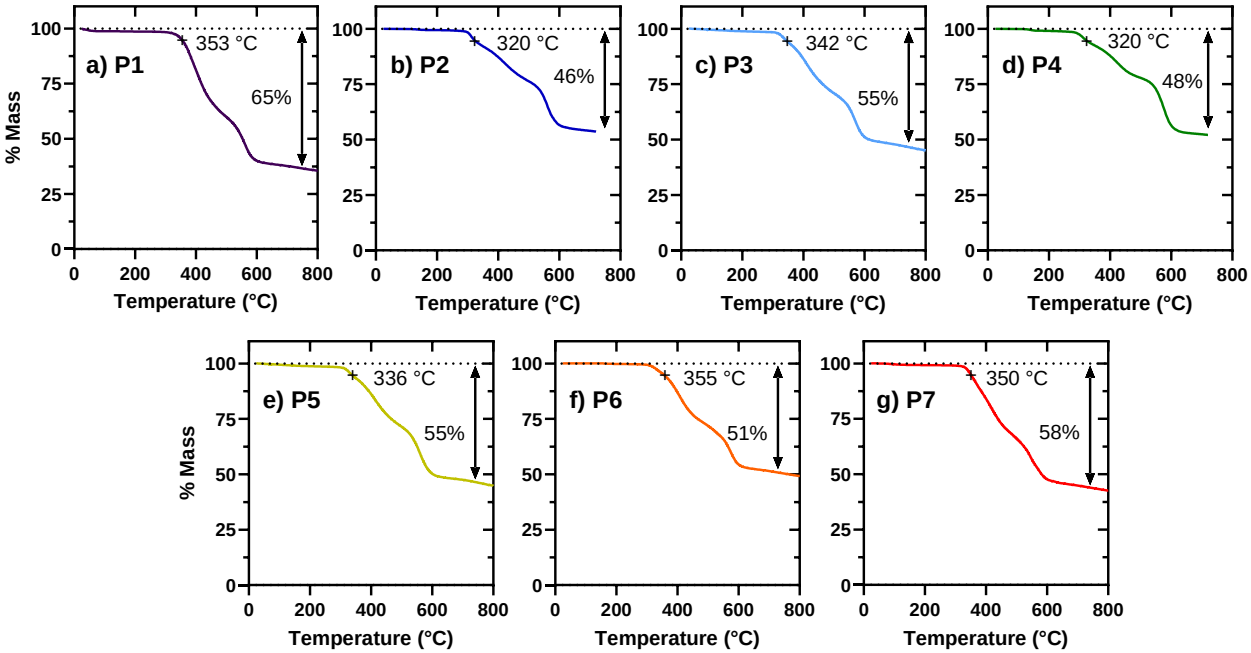


Figure S72 TGA traces of **P1** – **P7**.

S9 X-Ray Crystallography of PymPXZ

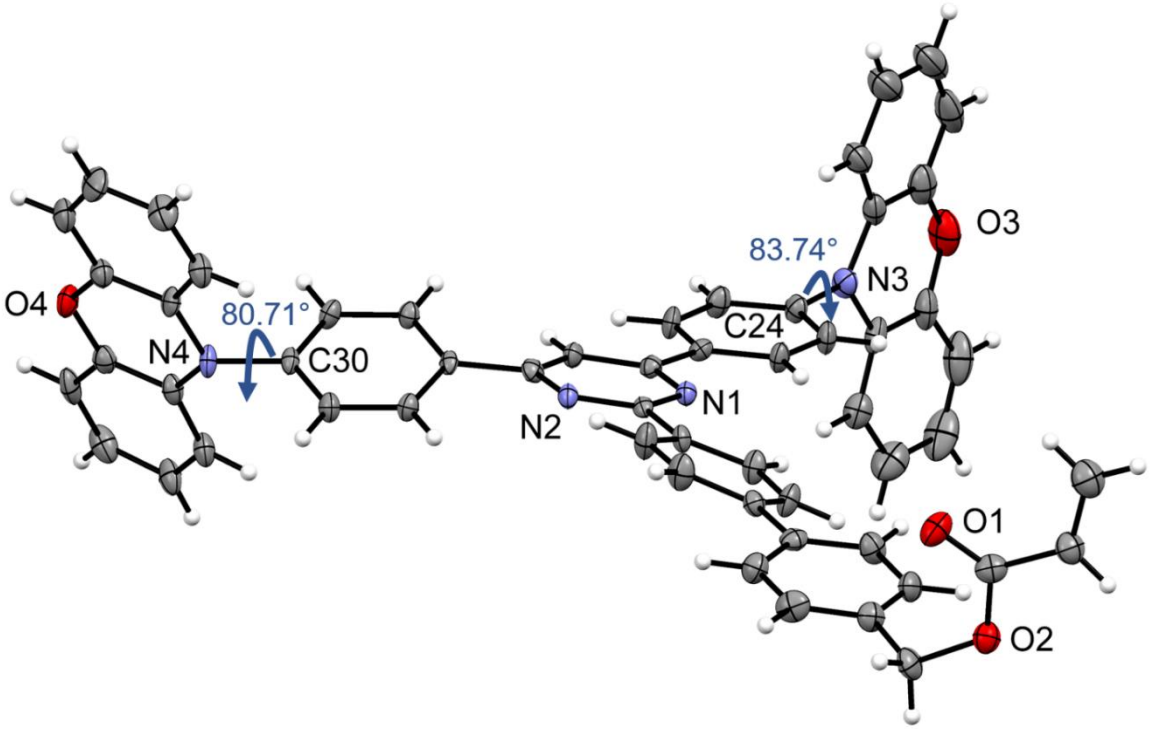


Figure S73 Molecular structure of **PymPXZ** in the crystal. Thermal ellipsoids are plotted at 50% probability. A co-crystallizing water molecule has been removed for clarity.

Compound	**PymPXZ** · 0.29 H_2O
Formula	$C_{56}H_{38}N_4O_4$ · 0.29 H_2O
$D_{calc.}$/ g cm^{-3}	1.372
μ/mm^{-1}	0.088
Formula Weight	836.22
Colour	yellow
Shape	blade
Size/mm^3	0.30×0.09×0.03
T/K	100(2)
Crystal System	triclinic
Space Group	P-1
a/Å	9.1593(6)
b/Å	14.5263(9)
c/Å	15.5079(10)
α/°	95.081(2)
β/°	97.193(2)
γ/°	96.204(2)
V/Å^3	2024.2(2)
Z	2
Z'	1
Wavelength/Å	0.71073
Radiation type	MoK$_\alpha$
Θ_{min}/°	1.418
Θ_{max}/°	22.499
Measured Refl.	22223
Independent Refl.	5287
Reflections with I > 2(I)	3399
R_{int}	0.0640
Largest Peak	0.366
Deepest Hole	-0.223
GooF	1.005
wR_2 (all data)	0.1303
wR_2	0.1109
R_1 (all data)	0.0956
R_1	0.0496

Table S2 Crystallographic data for **PymPXZ**.

S10 Computational Results

Entry	HOMO (eV)	LUMO (eV)	E_g (eV)	$E_{S0\rightarrow S1}$ (eV)	$f_{S0\rightarrow S1}$	$E_{S0\rightarrow T1}$ (eV)	ΔE_{ST} (eV)
PymCz-*s*Bu	-5.72909	-2.26344	3.46564	3.0357	0.4313	2.8369	0.1988
2PymDMA-*s*Bu	-5.09180	-2.22644	2.86536	2.5458	0.0000	2.5436	0.0022
PymDMA-*s*Bu	-5.23112	-2.28603	2.94509	2.4741	0.0000	2.4689	0.0052
PymPTZ-*s*Bu	-5.32092	-2.37882	2.94210	2.5007	0.0001	2.4935	0.0072
PymDMAPXZ-*s*Bu	-5.04826	-2.33474	2.71352	2.2509	0.0001	2.2455	0.0054
PymPXZ-*s*Bu	-5.06377	-2.38726	2.67651	2.2209	0.0000	2.2157	0.0052
PymTTAC-*s*Bu	-4.78975	-2.23351	2.55623	2.2519	0.2451	2.2041	0.0478

Table S3 Computed electronic parameters calculated at B3LYP/6-31G+d on optimized structures of *sec*-butyl analogues of the monomers. TD-DFT was performed for the $S_0 \rightarrow S_1$ and $S_0 \rightarrow T_1$ excitations at the same level of theory on the optimized ground state structure.

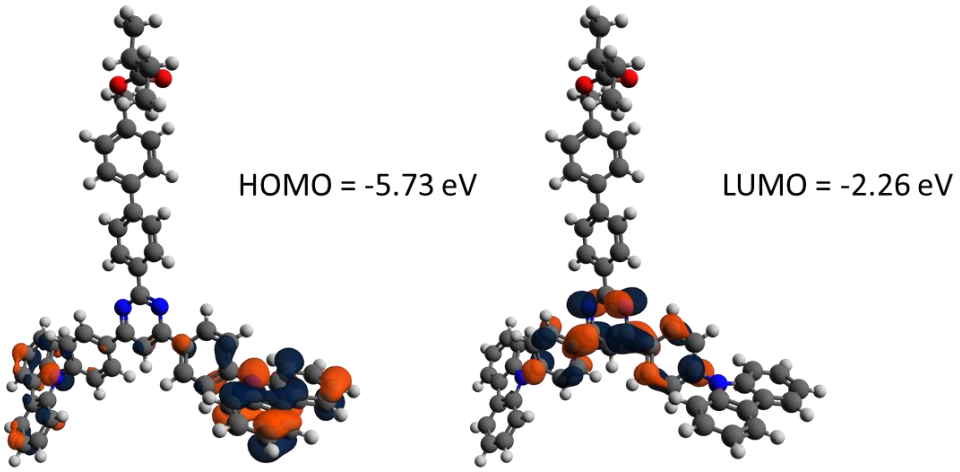


Fig S74 Calculated HOMO and LUMO diagrams for the *sec*-butyl analogues of **PymCz**.

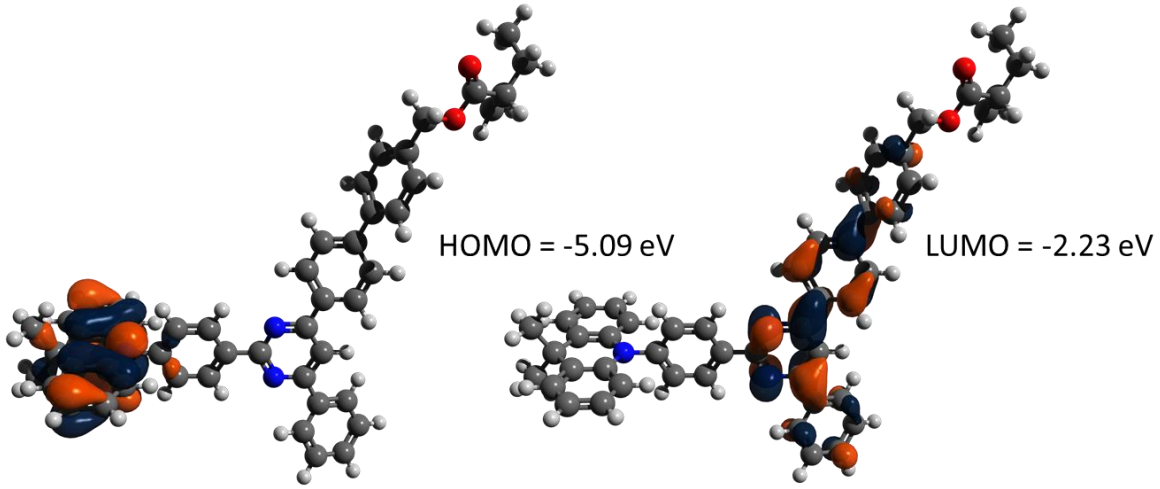


Fig S75 Calculated HOMO and LUMO diagrams for the *sec*-butyl analogues of **2PymDMA**.

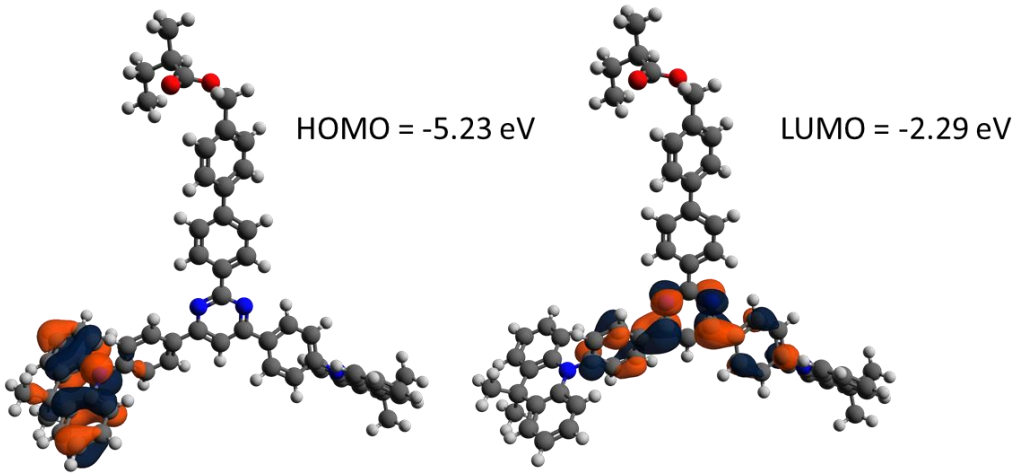


Fig S76 Calculated HOMO and LUMO diagrams for the *sec*-butyl analogues of **PymDMA**.

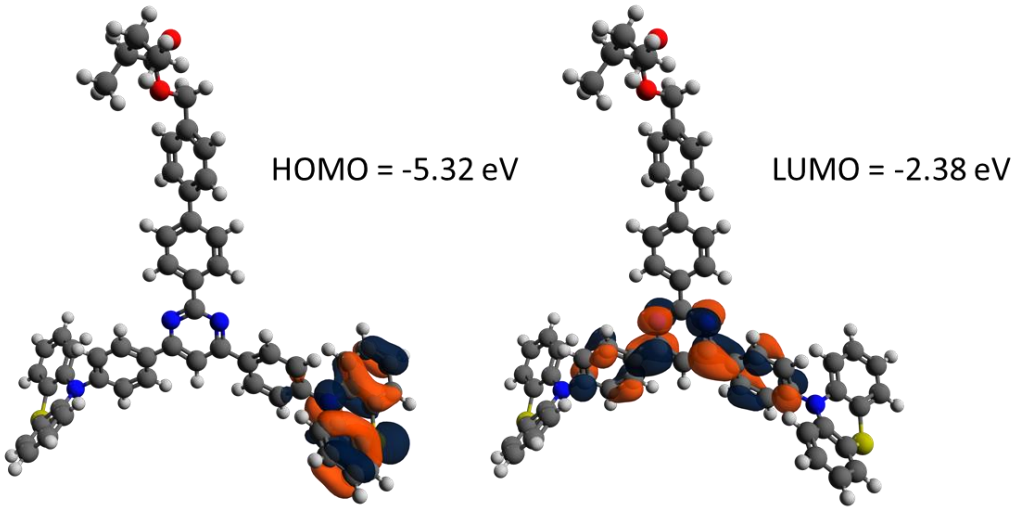


Fig S77 Calculated HOMO and LUMO diagrams for the *sec*-butyl analogues of **PymPTZ**

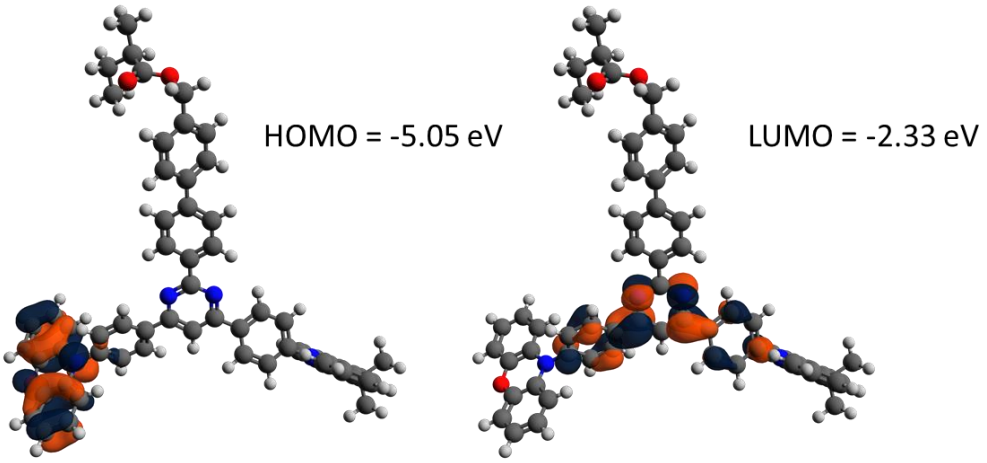


Fig S78 Calculated HOMO and LUMO diagrams for the *sec*-butyl analogues of **PymDMAPXZ**.

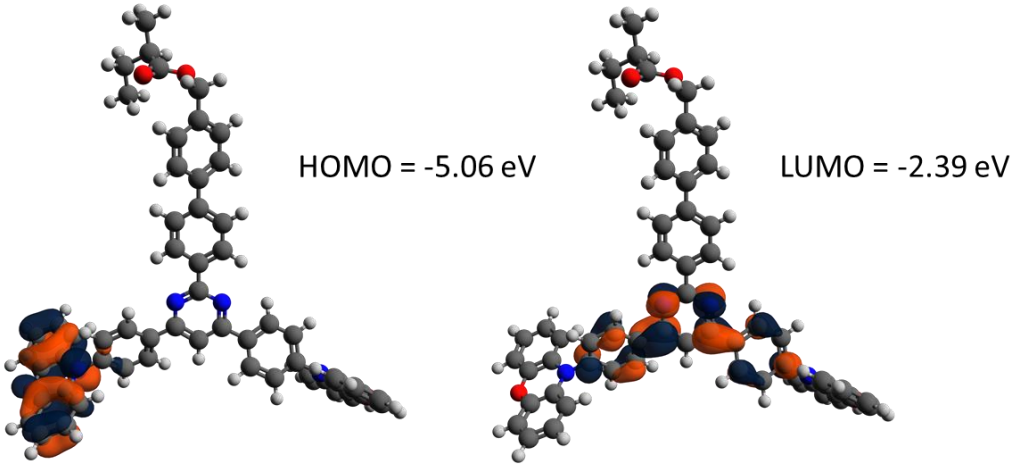


Fig S79 Calculated HOMO and LUMO diagrams for the *sec*-butyl analogues of **PymPXZ**.

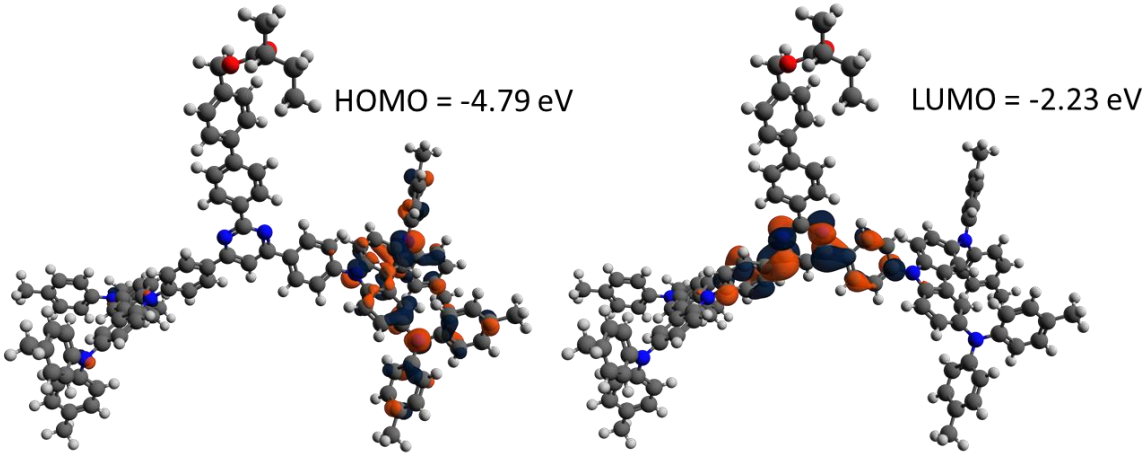


Fig S80 Calculated HOMO and LUMO diagrams for the *sec*-butyl analogues of **PymTTAC**.

Table S4 xyz coordinates of the DFT-optimized structure for the *sec*-butyl analogue of **PymCz**. Units are Angstroms.

C	0.14092	0.40489	-0.25575
N	-0.02515	-0.92750	-0.24633
C	-1.27845	-1.40173	-0.15221
C	-2.37119	-0.52706	-0.09561
C	-2.11141	0.84906	-0.12656
N	-0.85070	1.30818	-0.19277
H	-3.38459	-0.90187	-0.02905
C	1.53182	0.92071	-0.34351
C	2.62905	0.04634	-0.27777
C	1.78099	2.29471	-0.49421
C	3.93129	0.53179	-0.35863
H	2.44948	-1.01538	-0.14867
C	3.08453	2.77612	-0.57788

H	0.94138	2.97813	-0.55895
C	4.18867	1.90661	-0.51122
H	4.76279	-0.16296	-0.27504
H	3.24852	3.84037	-0.72486
C	-3.19662	1.86262	-0.07447
C	-2.91799	3.16412	0.37656
C	-4.51148	1.56273	-0.46918
C	-3.92119	4.12614	0.45419
H	-1.90605	3.40515	0.68401
C	-5.51505	2.52773	-0.41713
H	-4.75484	0.57991	-0.86232
C	-5.22891	3.81646	0.05370
H	-3.69976	5.11800	0.83690
H	-6.51844	2.29280	-0.75927
C	-1.44056	-2.87912	-0.12518
C	-2.58701	-3.49033	0.40986
C	-0.42662	-3.70424	-0.64100
C	-2.72578	-4.87675	0.41667
H	-3.38058	-2.88665	0.84028
C	-0.55576	-5.09042	-0.63139
H	0.46947	-3.24259	-1.04146
C	-1.70983	-5.68839	-0.10564
H	-3.62318	-5.33478	0.82153
H	0.24140	-5.71701	-1.02031
C	5.57839	2.42176	-0.59803
C	5.94264	3.63315	0.01693
C	6.57132	1.71617	-1.30133
C	7.24756	4.11584	-0.06884
H	5.20326	4.19048	0.58585
C	7.87651	2.19966	-1.38591
H	6.31273	0.79183	-1.81096
C	8.23364	3.40673	-0.76840
H	7.50546	5.05218	0.42200
H	8.62809	1.63785	-1.93379
C	9.64434	3.93332	-0.84628
H	10.15001	3.59349	-1.75234
O	10.43999	3.52652	0.30771
H	9.66044	5.02448	-0.80049
C	11.15299	2.37993	0.20157
O	11.15531	1.67874	-0.79224
C	11.97614	2.11246	1.45412
H	11.59273	2.76423	2.24820
C	11.84835	0.64140	1.89393
C	13.44394	2.49328	1.16723
H	12.18040	-0.00139	1.06922
H	12.54792	0.47999	2.72531
C	10.43417	0.24075	2.33057
H	13.85437	1.87331	0.36239
H	13.53657	3.54518	0.87337
H	14.05233	2.33854	2.06568
H	9.71612	0.33794	1.50776

H	10.41167	-0.80295	2.66554
H	10.08056	0.86520	3.16105
C	-1.77106	-7.93650	-1.22097
C	-2.09243	-7.89572	1.02856
C	-1.57862	-7.60342	-2.56590
C	-1.97041	-9.27946	-0.80892
C	-2.20940	-7.52181	2.37148
C	-2.17406	-9.25362	0.62535
C	-1.56810	-8.64244	-3.49700
H	-1.44688	-6.57323	-2.88139
C	-1.95550	-10.30442	-1.76392
C	-2.43213	-8.53044	3.30942
H	-2.12278	-6.48492	2.68063
C	-2.39823	-10.24743	1.58705
C	-1.74998	-9.98141	-3.10400
H	-1.41851	-8.40872	-4.54791
H	-2.10673	-11.33840	-1.46379
C	-2.53093	-9.88057	2.92506
H	-2.52709	-8.26445	4.35902
H	-2.46297	-11.29234	1.29374
H	-1.73475	-10.76767	-3.85378
H	-2.70606	-10.64218	3.67998
C	-7.46980	4.66864	0.79821
C	-6.21499	6.06115	-0.48718
C	-7.94486	3.60891	1.57805
C	-8.22119	5.85991	0.62675
C	-5.22787	6.62963	-1.29913
C	-7.42181	6.74699	-0.19383
C	-9.20000	3.75015	2.17085
H	-7.35844	2.70769	1.72668
C	-9.47888	5.97670	1.23274
C	-5.45771	7.91157	-1.79955
H	-4.31514	6.09430	-1.54087
C	-7.62816	8.03346	-0.70879
C	-9.96492	4.91870	1.99883
H	-9.59082	2.93966	2.78062
H	-10.06639	6.88332	1.11065
C	-6.64240	8.61211	-1.50614
H	-4.70467	8.37474	-2.43185
H	-8.54783	8.57164	-0.49291
H	-10.93955	4.99696	2.47273
H	-6.79019	9.60981	-1.91031
N	-6.25104	4.79785	0.11880
N	-1.84704	-7.10063	-0.09880

Table S5 xyz coordinates of the DFT-optimized structure for the *sec*-butyl analogue of **2PymDMA**. Units are Angstrom.

N	-0.715950	1.396515	-0.077369
C	-1.915535	1.986411	0.031280

N	-2.125687	3.307169	0.136355
C	-1.048891	4.111591	0.146111
C	0.240284	3.578363	0.021769
C	0.370369	2.188562	-0.096443
C	1.690824	1.522163	-0.233328
C	1.834162	0.168437	0.114606
C	3.065469	-0.471111	0.006351
C	4.202165	0.209845	-0.466391
C	4.051808	1.560711	-0.826358
C	2.822544	2.205123	-0.709389
C	-3.114036	1.101857	0.036600
C	-2.988065	-0.274235	-0.216133
C	-4.110134	-1.101423	-0.212124
C	-5.377054	-0.568241	0.048332
C	-5.511414	0.800881	0.302411
C	-4.390186	1.629287	0.294822
C	-1.294542	5.572013	0.279618
C	-0.311311	6.440591	0.783740
C	-0.560587	7.809066	0.897529
C	-1.795053	8.333112	0.503776
C	-2.781669	7.477081	0.004347
C	-2.536663	6.108222	-0.100894
C	5.514691	-0.474029	-0.584581
C	6.367175	-0.224735	-1.675223
C	7.597490	-0.870681	-1.785669
C	8.021034	-1.783916	-0.811074
C	7.174064	-2.037464	0.275500
C	5.941808	-1.394953	0.388452
N	-6.532659	-1.421733	0.054925
C	-7.245285	-1.621658	-1.142497
C	-6.922574	-2.039616	1.258173
C	-8.049515	-2.888805	1.301145
C	-8.908505	-3.190853	0.066303
C	-8.382627	-2.457363	-1.174415
C	-9.047496	-2.614182	-2.399266
C	-8.631066	-1.983054	-3.570323
C	-7.505022	-1.160040	-3.524146
C	-6.820773	-0.981308	-2.326242
C	-6.181098	-1.809702	2.436700
C	-6.542507	-2.406557	3.640136
C	-7.653823	-3.248685	3.697187
C	-8.384074	-3.473412	2.531269
C	9.356024	-2.466810	-0.923879
O	10.353801	-1.616466	-0.290778
C	11.626694	-2.081037	-0.304816
C	12.596185	-1.087092	0.332210
O	11.930652	-3.145768	-0.806590
C	14.018785	-1.673460	0.445784
C	14.199434	-2.779599	1.493936
C	12.058755	-0.511302	1.657335
C	-8.889768	-4.721652	-0.203103

C	-10.370352	-2.739770	0.341643
H	0.964637	-0.375350	0.468148
H	3.141356	-1.523080	0.268253
H	4.911887	2.120358	-1.183929
H	2.748536	3.245976	-1.011182
H	-2.005123	-0.684643	-0.419313
H	-4.012198	-2.165048	-0.411707
H	-6.497532	1.209079	0.506544
H	-4.491090	2.690589	0.493260
H	0.645292	6.048554	1.117452
H	0.207317	8.464222	1.300697
H	-1.988149	9.399326	0.589903
H	-3.744558	7.876718	-0.303467
H	-3.299794	5.438531	-0.483049
H	6.050566	0.457625	-2.459488
H	8.233273	-0.669638	-2.645284
H	7.485080	-2.739465	1.046236
H	5.314074	-1.592822	1.253114
H	-9.924385	-3.254329	-2.440657
H	-9.176317	-2.133060	-4.498003
H	-7.152455	-0.652846	-4.418761
H	-5.948229	-0.339467	-2.306550
H	-5.315969	-1.158208	2.408537
H	-5.950807	-2.209024	4.530509
H	-7.949045	-3.722506	4.629245
H	-9.248374	-4.129873	2.580988
H	9.362222	-3.438318	-0.421230
H	9.649266	-2.622966	-1.966381
H	12.642882	-0.252998	-0.386001
H	14.316314	-2.058062	-0.536350
H	14.697433	-0.840965	0.677596
H	15.231374	-3.149945	1.477569
H	13.998674	-2.419461	2.509854
H	13.539530	-3.629782	1.291963
H	12.791308	0.185935	2.080982
H	11.119673	0.026188	1.503432
H	11.878310	-1.298794	2.397126
H	-7.869192	-5.067108	-0.400670
H	-9.276418	-5.278504	0.657251
H	-9.508759	-4.977331	-1.069854
H	-10.786100	-3.258166	1.212357
H	-10.412751	-1.662461	0.535416
H	-11.018283	-2.956766	-0.514419
H	1.110126	4.222651	0.016797

Table S6 xyz coordinates of the DFT-optimized structure for the *sec*-butyl analogue of **PymDMA**. Units are Angstrom.

C	0.46566	0.69743	-0.26635
N	0.64133	-0.63396	-0.25169

C	-0.44998	-1.40811	-0.14033
C	-1.72773	-0.83859	-0.07077
C	-1.82378	0.55831	-0.10577
N	-0.72168	1.32053	-0.18992
H	-2.61225	-1.45776	0.00792
C	1.67942	1.54712	-0.37634
C	2.96251	0.97719	-0.33402
C	1.57148	2.93953	-0.52606
C	4.09868	1.77489	-0.43706
H	3.05867	-0.09544	-0.20602
C	2.71001	3.73365	-0.63134
H	0.58585	3.38960	-0.57302
C	3.99852	3.17011	-0.58876
H	5.07977	1.31204	-0.37199
H	2.59802	4.80483	-0.77668
C	-3.13086	1.26562	-0.03836
C	-3.18370	2.59250	0.42155
C	-4.32852	0.64226	-0.42801
C	-4.39882	3.26988	0.50383
H	-2.26140	3.08148	0.71634
C	-5.54391	1.32204	-0.35371
H	-4.31765	-0.37087	-0.81933
C	-5.58585	2.63819	0.11710
H	-4.43632	4.29257	0.86893
H	-6.46557	0.83948	-0.66670
C	-0.23387	-2.87971	-0.10931
C	-1.17399	-3.75232	0.46481
C	0.93788	-3.42481	-0.66147
C	-0.95323	-5.12920	0.48054
H	-2.07417	-3.36059	0.92945
C	1.15572	-4.80123	-0.65321
H	1.67080	-2.75562	-1.09922
C	0.21109	-5.66122	-0.08251
H	-1.67795	-5.79861	0.93548
H	2.05886	-5.21912	-1.08942
C	5.21202	4.01830	-0.69935
C	5.27299	5.28115	-0.08317
C	6.33534	3.58599	-1.42711
C	6.41309	6.07606	-0.19079
H	4.42920	5.63389	0.50382
C	7.47525	4.38193	-1.53397
H	6.30646	2.62731	-1.93811
C	7.53082	5.63866	-0.91462
H	6.43794	7.04607	0.30177
H	8.33222	4.02805	-2.10054
C	8.76288	6.50205	-1.01550
H	9.31669	6.30492	-1.93559
O	9.66117	6.30040	0.11715
H	8.50675	7.56222	-0.95752
C	10.63280	5.36630	-0.01541
O	10.78582	4.69210	-1.01612

C	11.52416	5.30356	1.21726
H	11.01308	5.84250	2.02391
C	11.76368	3.84413	1.64948
C	12.85052	6.02651	0.90162
H	12.22399	3.30205	0.81410
H	12.49836	3.85453	2.46605
C	10.49689	3.11351	2.11049
H	13.37927	5.52507	0.08337
H	12.68109	7.07048	0.61378
H	13.49863	6.02055	1.78549
H	9.76010	3.03628	1.30224
H	10.73339	2.09455	2.43882
H	10.01999	3.63274	2.95169
N	0.43631	-7.07862	-0.06906
C	-0.02848	-7.85751	-1.14641
C	1.10980	-7.65639	1.02494
C	-0.69639	-7.23717	-2.22349
C	0.16731	-9.25529	-1.16224
C	1.33967	-9.04804	1.07592
C	1.56062	-6.83821	2.08239
C	-1.16608	-7.98111	-3.30119
H	-0.84735	-6.16433	-2.21674
C	-0.31963	-9.97303	-2.26435
C	0.88432	-10.00609	-0.03257
C	2.01500	-9.56044	2.19320
H	1.38833	-5.76917	2.04712
C	2.22784	-7.38124	3.17573
C	-0.98028	-9.36373	-3.32991
H	-1.67599	-7.47361	-4.11620
H	-0.17735	-11.04973	-2.29215
C	-0.08554	-11.05913	0.57287
C	2.12757	-10.73399	-0.61633
C	2.46128	-8.75544	3.24004
H	2.19992	-10.62959	2.24810
H	2.56321	-6.72421	3.97420
H	-1.34081	-9.95894	-4.16417
H	-0.41797	-11.77304	-0.18835
H	0.39976	-11.62873	1.37265
H	-0.97256	-10.57231	0.99259
H	2.65607	-11.29688	0.16050
H	1.83838	-11.44185	-1.40050
H	2.82921	-10.01363	-1.05072
H	2.98078	-9.19507	4.08686
N	-6.83761	3.33580	0.19714
C	-7.59580	3.25110	1.38091
C	-7.28045	4.08115	-0.91307
C	-7.11128	2.49851	2.47173
C	-8.83791	3.91266	1.48994
C	-8.51294	4.76789	-0.87430
C	-6.48613	4.14375	-2.07755
C	-7.83857	2.39685	3.65333

H	-6.15746	1.99066	2.39352
C	-9.54365	3.78768	2.69543
C	-9.43486	4.75093	0.35201
C	-8.89671	5.49073	-2.01324
H	-5.53852	3.61966	-2.11171
C	-6.89853	4.87129	-3.18934
C	-9.06848	3.04460	3.77485
H	-7.43779	1.81007	4.47605
H	-10.50172	4.29005	2.79557
C	-10.80927	4.14929	-0.05443
C	-9.64353	6.20833	0.85057
C	-8.11499	5.55446	-3.16558
H	-9.84285	6.02451	-2.00022
H	-6.26380	4.90031	-4.07139
H	-9.64873	2.97511	4.69068
H	-11.50137	4.13758	0.79444
H	-11.27496	4.73451	-0.85463
H	-10.69120	3.12019	-0.41078
H	-10.08695	6.83347	0.06816
H	-10.31280	6.23706	1.71709
H	-8.68845	6.65749	1.14382
H	-8.45143	6.12683	-4.02551

Table S7 xyz coordinates of the DFT-optimized structure for the *sec*-butyl analogue of **PymPTZ**. Units are Angstrom.

N	-0.458421	-1.271696	-0.326190
C	-1.772338	-1.011350	-0.233089
C	-2.238984	0.308193	-0.175975
C	-1.293099	1.339134	-0.243901
N	0.017676	1.063573	-0.337484
C	0.385184	-0.227715	-0.371134
C	1.83773	-0.524360	-0.473690
C	2.299835	-1.849915	-0.521004
C	3.660987	-2.125962	-0.615224
C	4.612678	-1.091129	-0.668296
C	4.142345	0.234117	-0.624473
C	2.782032	0.513920	-0.529468
C	-2.690095	-2.180211	-0.170094
C	-4.041201	-2.078385	-0.539731
C	-4.886610	-3.185901	-0.470601
C	-4.398596	-4.417891	-0.026461
C	-3.050973	-4.531511	0.340784
C	-2.206343	-3.426274	0.264574
C	-1.679931	2.774477	-0.192598
C	-0.746790	3.735141	0.234018
C	-1.091116	5.083458	0.298951
C	-2.375598	5.503601	-0.071806
C	-3.307284	4.557433	-0.507603
C	-2.963124	3.206744	-0.565450

C	6.064073	-1.386918	-0.768564
C	6.909783	-0.604207	-1.575270
C	8.271643	-0.885692	-1.671257
C	8.837403	-1.954387	-0.963380
C	7.998739	-2.738408	-0.160666
C	6.635745	-2.461307	-0.063931
N	-2.763535	6.887521	-0.021713
C	-3.163241	7.429893	1.230422
C	-3.851316	8.659210	1.282873
S	-4.370460	9.452163	-0.224063
C	-3.002548	8.989894	-1.265467
C	-2.386552	7.732500	-1.101596
C	-2.618833	9.841835	-2.303911
C	-1.657733	9.441685	-3.234886
C	-1.067608	8.185202	-3.101333
C	-1.415981	7.345058	-2.040904
C	-2.907685	6.763972	2.441106
C	-3.318450	7.308152	3.660478
C	-3.968286	8.541288	3.704445
C	-4.221606	9.217202	2.508816
N	-5.297673	-5.538558	0.035895
C	-5.285471	-6.473255	-1.035763
C	-5.875038	-5.869492	1.292431
C	-6.991058	-6.728530	1.355081
S	-7.783752	-7.266299	-0.145467
C	-6.346546	-7.388649	-1.189014
C	-6.330873	-8.332307	-2.218905
C	-5.291860	-8.350645	-3.152003
C	-4.255071	-7.426072	-3.029186
C	-4.242826	-6.506984	-1.977109
C	-5.374686	-5.347820	2.497423
C	-5.963172	-5.676192	3.721179
C	-7.045759	-6.553653	3.775394
C	-7.547798	-7.085442	2.585553
C	10.309527	-2.245764	-1.055022
O	10.991759	-1.458976	-0.035955
C	12.335155	-1.599536	0.019934
C	12.991146	-0.756511	1.110578
O	12.953457	-2.337447	-0.724448
C	13.681853	-1.694536	2.136925
C	12.735419	-2.592812	2.943167
C	12.071101	0.285836	1.760232
H	-3.290553	0.523324	-0.033788
H	1.579483	-2.660096	-0.495908
H	3.989488	-3.160049	-0.676981
H	4.853247	1.055986	-0.639961
H	2.437925	1.541590	-0.492210
H	-4.438900	-1.138419	-0.910866
H	-5.928604	-3.106882	-0.766703
H	-2.669454	-5.488437	0.686669
H	-1.162049	-3.513768	0.544498

H	0.248409	3.409068	0.516545
H	-0.365247	5.817392	0.638583
H	-4.297060	4.890231	-0.806364
H	-3.697200	2.494431	-0.930419
H	6.491522	0.213566	-2.155890
H	8.902097	-0.272294	-2.311505
H	8.417718	-3.570409	0.401389
H	6.011799	-3.071093	0.583893
H	-3.096345	10.814412	-2.390096
H	-1.380039	10.103138	-4.050533
H	-0.321474	7.849868	-3.816817
H	-0.935996	6.377643	-1.954140
H	-2.395581	5.809222	2.434770
H	-3.114984	6.761516	4.577488
H	-4.277457	8.974026	4.651578
H	-4.730841	10.177390	2.517310
H	-7.152433	-9.039638	-2.296824
H	-5.298244	-9.075463	-3.961019
H	-3.438772	-7.417566	-3.746581
H	-3.420973	-5.805398	-1.898584
H	-4.528144	-4.671798	2.483042
H	-5.558544	-5.246113	4.633556
H	-7.497759	-6.821804	4.726029
H	-8.393700	-7.767740	2.602067
H	10.530470	-3.302358	-0.878067
H	10.722417	-1.972537	-2.030536
H	13.800684	-0.227755	0.588399
H	14.403391	-2.317843	1.596398
H	14.260538	-1.061792	2.823313
H	13.306973	-3.222596	3.635005
H	12.022096	-2.012019	3.538772
H	12.161350	-3.262059	2.290309
H	12.638248	0.866302	2.498149
H	11.671411	0.983053	1.016621
H	11.218643	-0.173893	2.267959

Table S8 xyz coordinates of the DFT-optimized structure for the *sec*-butyl analogue of **PymDMAPXZ**. Units are Angstrom.

C	-0.46954	-0.32432	-0.25251
N	-0.63560	1.00839	-0.22904
C	0.46123	1.77288	-0.10819
C	1.73470	1.19454	-0.03915
C	1.82095	-0.20293	-0.08550
N	0.71341	-0.95604	-0.17805
H	2.62307	1.80730	0.04672
C	-1.68888	-1.16456	-0.37031
C	-2.96806	-0.58597	-0.32599
C	-1.59036	-2.55671	-0.52889
C	-4.10956	-1.37513	-0.43523
H	-3.05707	0.48646	-0.19124

C	-2.73422	-3.34219	-0.64048
H	-0.60786	-3.01335	-0.57760
C	-4.01888	-2.77007	-0.59548
H	-5.08750	-0.90595	-0.36823
H	-2.62947	-4.41316	-0.79251
C	3.12265	-0.92017	-0.02204
C	3.16499	-2.25181	0.42504
C	4.32548	-0.30169	-0.40353
C	4.37498	-2.93882	0.50252
H	2.23868	-2.73695	0.71357
C	5.53572	-0.99103	-0.33398
H	4.32273	0.71526	-0.78495
C	5.56724	-2.31211	0.12372
H	4.40443	-3.96529	0.85754
H	6.46139	-0.51221	-0.64080
C	0.25580	3.24605	-0.06653
C	1.19177	4.10441	0.53391
C	-0.90151	3.80506	-0.63558
C	0.98155	5.48336	0.55985
H	2.07940	3.70000	1.01161
C	-1.10859	5.18274	-0.61901
H	-1.63088	3.14549	-1.09348
C	-0.16733	6.02920	-0.02040
H	1.70130	6.14370	1.03527
H	-1.99989	5.61111	-1.06936
C	-5.23807	-3.60923	-0.71191
C	-5.30752	-4.87578	-0.10429
C	-6.35851	-3.16428	-1.43649
C	-6.45304	-5.66213	-0.21708
H	-4.46613	-5.23828	0.48019
C	-7.50384	-3.95168	-1.54848
H	-6.32321	-2.20240	-1.94100
C	-7.56787	-5.21214	-0.93763
H	-6.48443	-6.63527	0.26887
H	-8.35853	-3.58808	-2.11234
C	-8.80579	-6.06649	-1.04419
H	-9.35954	-5.85764	-1.96172
O	-9.70098	-5.86893	0.09151
H	-8.55654	-7.12879	-0.99592
C	-10.66592	-4.92647	-0.03105
O	-10.81480	-4.24161	-1.02510
C	-11.55572	-4.86931	1.20299
H	-11.04705	-5.41832	2.00435
C	-11.78640	-3.41241	1.64827
C	-12.88653	-5.58184	0.88229
H	-12.24409	-2.86023	0.81809
H	-12.52054	-3.42573	2.46528
C	-10.51502	-2.69334	2.11480
H	-13.41321	-5.07017	0.06906
H	-12.72336	-6.62417	0.58508
H	-13.53373	-5.57998	1.76684

H	-9.77835	-2.61330	1.30671
H	-10.74531	-1.67596	2.45230
H	-10.04063	-3.22279	2.95105
N	-0.37334	7.44660	0.00569
C	0.02715	8.23809	-1.09208
C	-1.18105	8.02533	1.00832
C	0.67647	7.71038	-2.21539
C	-0.22070	9.62349	-1.06025
C	-1.40027	9.41571	0.98865
C	-1.76635	7.28028	2.03992
C	1.07059	8.54094	-3.27139
H	0.87918	6.64600	-2.26316
C	0.16186	10.44795	-2.10949
C	-2.17848	10.03604	1.95640
H	-1.60934	6.20787	2.07915
C	-2.54491	7.90460	3.02189
C	0.81541	9.90968	-3.22458
H	1.57615	8.10391	-4.12804
H	-0.05365	11.50977	-2.03456
C	-2.75568	9.28119	2.98463
H	-2.31660	11.11149	1.89423
H	-2.98302	7.30138	3.81218
H	1.11726	10.55955	-4.04068
H	-3.35951	9.77170	3.74242
N	6.81355	-3.01981	0.19836
C	7.57031	-2.95356	1.38427
C	7.25290	-3.75612	-0.91932
C	7.08966	-2.20897	2.48224
C	8.80711	-3.62578	1.48824
C	8.48010	-4.45251	-0.88588
C	6.46034	-3.79977	-2.08584
C	7.81563	-2.12556	3.66609
H	6.13992	-1.69294	2.40792
C	9.51166	-3.51915	2.69618
C	9.39955	-4.45648	0.34241
C	8.86063	-5.16542	-2.03214
H	5.51667	-3.26837	-2.11587
C	6.86943	-4.51791	-3.20496
C	9.04030	-2.78403	3.78270
H	7.41796	-1.54454	4.49439
H	10.46563	-4.02997	2.79253
C	10.77976	-3.86187	-0.05466
C	9.59510	-5.92090	0.82547
C	8.08071	-5.21035	-3.18657
H	9.80268	-5.70646	-2.02336
H	6.23622	-4.53238	-4.08846
H	9.61945	-2.72884	4.70019
H	11.47020	-3.86527	0.79561
H	11.24225	-4.44212	-0.86030
H	10.67102	-2.82797	-0.39990
H	10.03497	-6.54114	0.03717

H	10.26232	-5.96457	1.69294
H	8.63575	-6.36531	1.11191
H	8.41455	-5.77556	-4.05223
O	-0.82784	10.22716	0.02581

Table S9 xyz coordinates of the DFT-optimized structure for the *sec*-butyl analogue of **PymPXZ**. Units are Angstrom.

C	0.22205	0.48558	-0.23070
N	0.14737	-0.85554	-0.21574
C	-1.06704	-1.41321	-0.08947
C	-2.21655	-0.61726	-0.00600
C	-2.05184	0.77310	-0.04459
N	-0.82882	1.31756	-0.14299
H	-3.19939	-1.06210	0.08464
C	1.57074	1.09556	-0.35324
C	2.72655	0.29804	-0.31924
C	1.72106	2.48386	-0.50503
C	3.98983	0.87189	-0.43110
H	2.62378	-0.77384	-0.19008
C	2.98597	3.05359	-0.61962
H	0.83550	3.10862	-0.54596
C	4.14841	2.26158	-0.58417
H	4.86880	0.23564	-0.37163
H	3.07295	4.12688	-0.76623
C	-3.20384	1.71172	0.03380
C	-3.00270	3.02548	0.48909
C	-4.50063	1.32156	-0.34256
C	-4.06891	3.91897	0.57960
H	-2.00237	3.33374	0.77345
C	-5.56679	2.21637	-0.26057
H	-4.68250	0.32335	-0.73005
C	-5.35606	3.51904	0.20541
H	-3.91242	4.93174	0.94041
H	-6.56503	1.91315	-0.56390
C	-1.12716	-2.89960	-0.05794
C	-2.19739	-3.58191	0.54409
C	-0.09110	-3.65159	-0.63828
C	-2.23579	-4.97640	0.56044
H	-2.99620	-3.02957	1.03033
C	-0.13202	-5.04420	-0.63049
H	0.74137	-3.12916	-1.09735
C	-1.20550	-5.71387	-0.03053
H	-3.05892	-5.50141	1.03682
H	0.66658	-5.62119	-1.08878
C	5.49700	2.87096	-0.70263
C	5.79263	4.10224	-0.09047
C	6.51803	2.23702	-1.43340
C	7.05937	4.67281	-0.20484
H	5.03116	4.60603	0.49887
C	7.78479	2.80863	-1.54691

H	6.31064	1.29903	-1.94148
C	8.07401	4.03486	-0.93151
H	7.26493	5.62268	0.28466
H	8.55937	2.30129	-2.11541
C	9.44383	4.65586	-1.03971
H	9.94813	4.35687	-1.96082
O	10.29380	4.29596	0.09077
H	9.38770	5.74527	-0.98530
C	11.07569	3.19789	-0.04106
O	11.09592	2.50266	-1.03883
C	11.94767	2.97838	1.18752
H	11.54538	3.60139	1.99523
C	11.92530	1.50047	1.62235
C	13.38012	3.45267	0.86360
H	12.27538	0.88329	0.78564
H	12.65564	1.38069	2.43406
C	10.55160	1.00897	2.09403
H	13.80706	2.86306	0.04467
H	13.39803	4.50944	0.57325
H	14.02111	3.33334	1.74461
H	9.80708	1.06329	1.29102
H	10.60446	-0.03528	2.42381
H	10.18135	1.60654	2.93695
N	-1.25371	-7.14539	-0.01312
C	-1.78115	-7.84772	-1.11784
C	-0.57178	-7.86318	0.99303
C	-2.32373	-7.20733	-2.23919
C	-1.77923	-9.25530	-1.09520
C	-0.59918	-9.27030	0.96432
C	0.12379	-7.23849	2.03598
C	-2.85159	-7.94925	-3.30278
H	-2.33787	-6.12360	-2.27958
C	-2.29497	-9.99323	-2.15183
C	0.04676	-10.02316	1.93538
H	0.15751	-6.15541	2.08145
C	0.76953	-7.99544	3.02099
C	-2.83912	-9.34178	-3.26527
H	-3.26929	-7.42498	-4.15782
H	-2.26849	-11.07684	-2.08399
C	0.73554	-9.38739	2.97537
H	-0.00491	-11.10577	1.86608
H	1.29802	-7.48314	3.82012
H	-3.24574	-9.92357	-4.08724
H	1.23516	-9.98075	3.73547
N	-6.44681	4.44330	0.29394
C	-7.28072	4.44543	1.43233
C	-6.82742	5.19675	-0.83732
C	-7.05650	3.62004	2.54160
C	-8.38072	5.32317	1.47159
C	-7.93811	6.05646	-0.74306
C	-6.13954	5.13984	-2.05614

C	-7.90322	3.67010	3.65552
H	-6.21257	2.93880	2.53722
C	-9.22573	5.36975	2.57199
C	-8.34753	6.82509	-1.82410
H	-5.27836	4.48768	-2.15281
C	-6.54625	5.91921	-3.14581
C	-8.98982	4.54162	3.67595
H	-7.70171	3.02090	4.50307
H	-10.06033	6.06438	2.55060
C	-7.64966	6.76252	-3.03621
H	-9.21121	7.47139	-1.69812
H	-5.99052	5.85721	-4.07730
H	-9.65123	4.58537	4.53622
H	-7.97126	7.36928	-3.87756
O	-1.29161	-9.96336	-0.01199
O	-8.65422	6.19322	0.43218

Table S10 xyz coordinates of the DFT-optimized structure for the *sec*-butyl analogue of **PymTTAC**. Units are Angstrom.

C	0.02494	3.38971	-0.47902
N	1.18159	2.71486	-0.38216
C	1.11722	1.38176	-0.22764
C	-0.11958	0.72456	-0.19932
C	-1.27855	1.50171	-0.32194
N	-1.19826	2.83701	-0.44736
H	-0.17779	-0.35045	-0.08658
C	0.10492	4.86572	-0.63357
C	1.33638	5.53379	-0.53437
C	-1.04922	5.62646	-0.88222
C	1.40902	6.91669	-0.67712
H	2.23268	4.95835	-0.33017
C	-0.97223	7.00881	-1.02788
H	-2.00393	5.12019	-0.97393
C	0.25741	7.68523	-0.92766
H	2.36997	7.41189	-0.56565
H	-1.87608	7.56985	-1.25020
C	-2.64014	0.90627	-0.30679
C	-3.74850	1.70107	0.03252
C	-2.86500	-0.44290	-0.62856
C	-5.03376	1.16732	0.05811
H	-3.58818	2.74801	0.26647
C	-4.14767	-0.98584	-0.59830
H	-2.03731	-1.08296	-0.91967
C	-5.24469	-0.18396	-0.25349
H	-5.88232	1.79773	0.30662
H	-4.30276	-2.03403	-0.83525
C	2.40695	0.65362	-0.10540
C	2.49027	-0.61523	0.49248
C	3.58932	1.23643	-0.59287
C	3.70672	-1.28765	0.58715

H	1.60280	-1.08763	0.90326
C	4.80939	0.57349	-0.49570
H	3.53906	2.22288	-1.04110
C	4.87843	-0.69826	0.09203
H	3.75177	-2.27413	1.03850
H	5.71710	1.04313	-0.86274
C	0.33755	9.15992	-1.07983
C	-0.66347	9.99847	-0.55718
C	1.41457	9.76257	-1.75456
C	-0.58697	11.38260	-0.70381
H	-1.49729	9.56438	-0.01197
C	1.49047	11.14732	-1.89996
H	2.18821	9.13868	-2.19412
C	0.49052	11.97773	-1.37423
H	-1.37088	12.00968	-0.28376
H	2.33225	11.59187	-2.42387
C	0.56869	13.47663	-1.51753
H	1.13203	13.76583	-2.40697
O	1.18936	14.10146	-0.35350
H	-0.42816	13.92186	-1.54972
C	2.52863	14.29891	-0.39073
O	3.23012	13.97865	-1.33132
C	3.02718	15.00674	0.86168
H	2.23054	14.95157	1.61312
C	4.29576	14.32631	1.41082
C	3.28212	16.48969	0.51881
H	5.06532	14.33611	0.62899
H	4.67360	14.94293	2.23767
C	4.07133	12.89187	1.90388
H	4.06105	16.58161	-0.24630
H	2.37429	16.97839	0.14675
H	3.61327	17.02841	1.41404
H	3.74415	12.23316	1.09079
H	4.99726	12.47260	2.31483
H	3.30964	12.85541	2.69328
N	-6.55143	-0.73184	-0.22420
C	-7.17842	-1.42204	-1.27106
C	-7.43963	-0.68210	0.85935
C	-6.72278	-1.69593	-2.56500
C	-8.47538	-1.81548	-0.85607
C	-8.64098	-1.34579	0.50514
C	-7.26652	-0.13998	2.13723
C	-7.57402	-2.37827	-3.43004
H	-5.74479	-1.36981	-2.90464
C	-9.30698	-2.52308	-1.73135
C	-9.69125	-1.43319	1.42580
H	-6.33943	0.34289	2.42955
C	-8.31286	-0.25915	3.04799
C	-8.85909	-2.80672	-3.02548
H	-7.24726	-2.59070	-4.44352
H	-10.29747	-2.84178	-1.41981

C	-9.53034	-0.89034	2.70456
H	-10.62167	-1.92701	1.16096
H	-8.19722	0.14333	4.04984
N	-9.69181	-3.51012	-3.94486
N	-10.57699	-0.97995	3.66902
C	-11.05576	-3.13708	-4.08629
C	-9.16422	-4.61018	-4.67133
C	-11.25092	-2.21581	3.86308
C	-10.97133	0.17939	4.38794
C	-11.42697	-1.78130	-4.12286
C	-12.06523	-4.10616	-4.18884
C	-8.27296	-5.51168	-4.06954
C	-9.51155	-4.81632	-6.01883
C	-10.53372	-3.42486	3.89526
C	-12.64401	-2.26438	4.02370
C	-11.02341	1.43399	3.76151
C	-11.30611	0.10154	5.75201
C	-12.76548	-1.41680	-4.25052
H	-10.66036	-1.01548	-4.04880
C	-13.40099	-3.72560	-4.33410
H	-11.80259	-5.15948	-4.15778
C	-7.74340	-6.57895	-4.79841
H	-7.99336	-5.37455	-3.02913
C	-8.98870	-5.89529	-6.72765
H	-10.19403	-4.12632	-6.50629
C	-11.19659	-4.63696	4.07515
H	-9.45417	-3.40862	3.77709
C	-13.29266	-3.48519	4.22081
H	-13.21922	-1.34360	3.99746
C	-11.39255	2.57197	4.48224
H	-10.77169	1.51782	2.70840
C	-11.68924	1.24242	6.45316
H	-11.26448	-0.85828	6.25849
C	-13.78286	-2.37815	-4.36281
H	-13.02257	-0.35918	-4.27658
H	-14.16222	-4.49944	-4.41267
C	-8.09042	-6.79931	-6.13725
H	-7.05408	-7.26153	-4.30495
H	-9.27544	-6.02854	-7.76950
C	-12.58913	-4.69634	4.24543
H	-10.61458	-5.55682	4.09679
H	-14.37396	-3.49172	4.34422
C	-11.73853	2.50393	5.83765
H	-11.42281	3.53161	3.96967
H	-11.94172	1.15112	7.50831
C	-15.23133	-1.96730	-4.50044
C	-7.52484	-7.96088	-6.92256
C	-13.29542	-6.01957	4.43518
C	-12.15240	3.73386	6.61345
H	-15.37685	-1.28129	-5.34478
H	-15.87797	-2.83634	-4.66269

H	-15.59035	-1.45085	-3.60028
H	-8.31806	-8.63196	-7.27720
H	-6.97358	-7.61812	-7.80803
H	-6.83593	-8.55545	-6.31291
H	-12.84331	-6.60480	5.24602
H	-14.35351	-5.87497	4.67864
H	-13.24632	-6.63546	3.52715
H	-12.08657	4.63536	5.99482
H	-13.18656	3.65383	6.97371
H	-11.51578	3.88766	7.49444
N	6.11804	-1.37852	0.18749
C	6.98907	-1.65277	-0.87636
C	6.68165	-1.90280	1.35912
C	6.85653	-1.37053	-2.23999
C	8.11550	-2.35804	-0.38354
C	7.92070	-2.51498	1.04419
C	6.21919	-1.85086	2.67835
C	7.86891	-1.79056	-3.09856
H	5.98383	-0.85848	-2.63283
C	9.13521	-2.74962	-1.25831
C	8.68292	-3.11439	2.05319
H	5.28870	-1.35482	2.93585
C	7.00360	-2.42999	3.67223
C	9.01482	-2.46833	-2.62296
H	7.78251	-1.59319	-4.16279
H	10.00989	-3.27779	-0.88998
C	8.22694	-3.07300	3.37462
H	9.62713	-3.59875	1.82179
H	6.67162	-2.39064	4.70532
N	10.02988	-2.86995	-3.54044
N	8.99132	-3.65974	4.42587
C	10.56358	-4.18482	-3.47000
C	10.53359	-1.93495	-4.48341
C	10.39014	-3.41918	4.49720
C	8.35765	-4.52268	5.35852
C	9.72120	-5.28905	-3.24958
C	11.93985	-4.41689	-3.61466
C	10.73872	-0.59277	-4.12936
C	10.82638	-2.32861	-5.80169
C	10.90842	-2.13410	4.25810
C	11.28866	-4.45271	4.80236
C	7.36253	-5.42302	4.94819
C	8.70226	-4.48707	6.72195
C	10.24729	-6.57663	-3.17091
H	8.65227	-5.13167	-3.13889
C	12.45046	-5.71508	-3.55103
H	12.61042	-3.57891	-3.78053
C	11.21470	0.32399	-5.06943
H	10.52268	-0.26699	-3.11612
C	11.31682	-1.40661	-6.72336
H	10.66789	-3.36121	-6.09864

C	12.28076	-1.90177	4.31723
H	10.22935	-1.31945	4.02389
C	12.66030	-4.20088	4.87544
H	10.91154	-5.45454	4.98552
C	6.73060	-6.25345	5.87652
H	7.08252	-5.47077	3.90000
C	8.07538	-5.33375	7.63306
H	9.46457	-3.79249	7.06245
C	11.62163	-6.82115	-3.32311
H	9.57025	-7.41203	-3.00031
H	13.52209	-5.86444	-3.66844
C	11.51899	-0.05935	-6.38168
H	11.36322	1.35860	-4.76601
H	11.53369	-1.74048	-7.73673
C	13.18815	-2.92667	4.63038
H	12.65279	-0.89621	4.12806
H	13.33320	-5.02185	5.11564
C	7.07328	-6.23348	7.23430
H	5.96209	-6.94117	5.52861
H	8.36284	-5.28275	8.68196
C	12.17823	-8.22400	-3.23365
C	12.04346	0.93149	-7.39608
C	14.67505	-2.65956	4.68995
C	6.39631	-7.14038	8.23686
H	11.66725	-8.90498	-3.92631
H	13.24658	-8.24453	-3.47437
H	12.05826	-8.64094	-2.22479
H	13.03433	0.64053	-7.76865
H	11.38033	1.00422	-8.26808
H	12.13325	1.93380	-6.96360
H	14.90865	-1.83286	5.37307
H	15.22456	-3.54189	5.03530
H	15.07438	-2.38561	3.70435
H	5.63373	-7.76390	7.75783
H	7.11605	-7.81147	8.72366
H	5.90386	-6.56534	9.031

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