Electronic Supplementary Material (ESI) for Materials Advances.

Exploring Color Space: An Investigation of Heteroaryl-Substituted Benzobis[1,2-*d*:4,5-*d*']oxazoles and Their Application in Organic Light-Emitting Diodes

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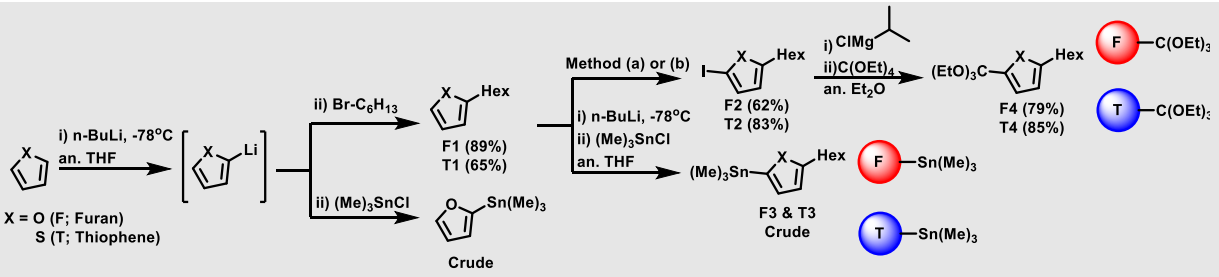
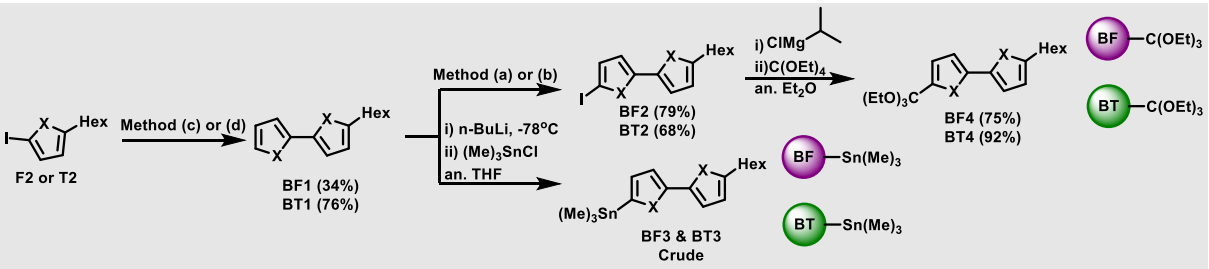
Precursors



Scheme S1. Synthesis of precursors **F3**, **T3**, **F4**, and **T4**. Method a) *n*-Butyllithium (-78°C), I_2, an. THF. Method b) NIS in DCM/AcOH.



Scheme S2. Synthesis of precursors **BF3**, **BT3**, **BF4**, and **BT4**. Method a) *n*-Butyllithium (-78°C), I_2, an. THF. Method b) NIS in DCM/AcOH. Method c) 2-trimethylstannyl-furan, $Pd(PPh_3)_4$, toluene. Method d) thiophen-2-ylmagnesium bromide, $Ni(dppp)Cl_2$, an. THF.

*2-hexylfuran (**F1**)*

This compound was prepared according to previous literature.[4] (89%, 60 mmol scale) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 (d, J = 1.9 Hz, 1H), 6.29 (dd, J = 1.9, 3.1 Hz, 1H), 5.99 (d, J = 3.1 Hz, 1H), 2.64 (t, J = 7.6 Hz, 2H), 1.66 (p, J = 7.5 Hz, 2H), 1.41 – 1.28 (m, 6H), 0.92 (t, J = 6.7 Hz, 3H).

*5-iodo-2-hexylfuran (**F2**)*

This compound was prepared according to previous literature.[4] (62%, 40 mmol scale) ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.41 (d, *J* = 3.2 Hz, 1H), 5.92 (d, *J* = 3.2 Hz, 1H), 2.65 (t, *J* = 7.7 Hz, 2H), 1.62 (p, *J* = 7.4 Hz, 3H), 1.39 – 1.25 (m, 11H), 0.90 (t, *J* = 6.8 Hz, 6H).

*2-hexyl-5-(trimethylstannyl)furan (**F3**)*

This compound was prepared according to previous literature and used without further purification or identification.[4]

*2-hexyl-5-(triethoxymethyl)furan (**F4**)*

To an oven-dried, N_2 filled round bottom flask equipped with stir bar was added 1.22 g (50 mmol) of magnesium turnings. The solid was purged with N_2 twice before the addition of a small iodine crystal. These solids were stirred at 50 °C for 1 hour. After cooling to room temperature, 50 mL of anhydrous diethyl ether was added via cannula along with 4.6 mL (50 mmol) of 2-chloropropane. This suspension was fitted with a condenser and stirred at 35 °C for 1 hour, or until minimum magnesium was noticed. Upon cooling to room temperature, 5.56 g (20 mmol) of 5-iodo-2-hexylfuran was added through the top of the condenser and the solution was refluxed for 20 hours to produce a cloudy yellow-grey suspension. After cooling to room temperature, 6.3 mL (30 mmol) of tetraethylorthocarbonate was added through the top of the condenser and solution was returned to reflux for an addition 20 hours. Suspension becomes a milky-orange color after the reflux period ends. This solution is poured into ice-cold, conc. aqueous NH_4Cl and extracted with diethyl ether. The organic layer is separated and washed with distilled water once, dried over sodium sulfate, and concentrated. Distillation via Kugelrohr at 85 °C remove excess tetraethylorthocarbonate and other volatiles to produce an orange oil as the final product. This oil was used without further purification. (4.72 g, 79%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.39 (d, 1H), 5.89 (d, 1H), 3.41 (q, 6H), 2.58 (t, 2H), 1.59 (p, 2H), 1.32 – 1.22 (m, 6H), 1.14 (t, 9H), 0.84 (t, 3H)

*5-hexyl-2,2'-bifuran (**BF1**)*

This compound was prepared according to previous literature.[4] Purification was performed via Kugelrohr distillation at 135 °C for over 12 hours. The collected fraction was then subjected to second distillation at 105 °C to remove volatiles. The orange oil was subjected to a second column (silica, hexanes) to remove color. Resulting product was noted as a clear oil. (34%, 57 mmol scale) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 (d, *J* = 1.8 Hz, 1H), 6.50 (d, *J* = 3.1 Hz, 1H), 6.47 (dd, *J* = 3.4, 1.5 Hz, 1H), 6.45 (dd, *J* = 3.6, 1.8 Hz, 1H), 6.06 (d, *J* = 2.7 Hz, 1H), 2.68 (t, *J* = 7.6 Hz, 2H), 1.69 (p, *J* = 7.3 Hz, 2H), 1.44 – 1.26 (m, 6H), 0.93 (t, *J* = 3.0 Hz, 3H).

*5-hexyl-5'-iodo-2,2'-bifuran (**BF2**)*

To an oven-dried, N_2 filled round bottom flask equipped with stirbar was added 5-hexyl-2,2'-bifuran (4.10 g, 18.8 mmol) and 50 mL of anhydrous THF. The solution was brought to -78 °C before the dropwise addition of n-BuLi (2.5 M, 8.0 mL, 20 mmol). This solution was brought to room temperature for 1 hour of stirring. Solution was returned to -78 °C before the addition of a separate solution of iodine (5.08 g, 20 mmol, in 50 mL of an. THF) via cannula. Solution turned a dark purple color and was brought to room temperature for overnight stirring. Next, a conc. sodium thiosulfate solution was added to quench the reaction followed by addition of hexanes. The aqueous layer was removed and organic layer was washed twice with distilled water, dried over sodium sulfate, and concentrated to a dark oil. Column chromatography (silica, hexanes) was used to produce a clear oil. (5.09 g, 79%) **Note** – this oil gradually darkens in the presence of light and air and was used immediately upon purification. Due to impurities, certain coupling constants were unable to be obtained. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.57 (d, J = 3.4 Hz, 1H), 6.47 (d, J = 3.3 Hz, 1H), 6.37 (d, J = 3.3 Hz, 1H), 6.03 (d, J = 3.3 Hz, 1H), 2.65 (t, J = 7.7 Hz, 2H), 1.66 (p, 2H), 1.41-1.24 (m, 6H), 0.90 (t, 3H)

*5-hexyl-5'-(trimethylstannyl)-2,2'-bifuran (**BF3**)*

This compound was prepared according to previous literature without purification or identificaiton.[4]

*5-hexyl-5'-(triethoxymethyl)-2,2'-bifuran (**BF4**)*

This product was formed identically to 2-hexyl-5-(triethoxymethyl)furan using 5-hexyl-5'-iodo-2,2'-bifuran. (75%, 14.8 mmol scale) ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.57 (d, *J* = 3.3 Hz, 1H), 6.52 (d, *J* = 3.2 Hz, 1H), 6.42 (d, *J* = 3.3 Hz, 1H), 6.02 (d, *J* = 3.2 Hz, 1H), 3.46 (q, *J* = 7.1 Hz, 6H), 2.63 (t, *J* = 7.6 Hz, 2H), 1.64 (p, *J* = 7.5 Hz, 2H), 1.39 – 1.27 (m, 6H), 1.18 (t, *J* = 7.1 Hz, 9H), 0.87 (t, *J* = 6.8 Hz, 3H).

*2-hexylthiophene (**T1**)*

This compound was prepared analogously to compound **1**. After purification with a hexanes column, the oil was subjected to distillation (Kugelrohr; 103 °C) to give a colorless oil. (65%, 75 mmol scale) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.13 (dd, J = 6.4, 1.6 Hz, 1H), 6.95 (dd, J = 5.1, 3.3 Hz, 1H), 6.81 (dd, J = 2.6, 1.2 Hz, 1H), 2.86 (t, J = 7.7 Hz, 2H), 1.72 (p, J = 7.5 Hz, 2H), 1.46 – 1.30 (m, 6H), 0.94 (t, J = 5.9 Hz, 3H).

*5-iodo-2-hexylthiophene (**T2**)*

This compound was prepared according to previous literature.[5] (83%, 50 mmol scale) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.05 (d, *J* = 3.5 Hz, 1H), 6.49 (d, *J* = 3.5 Hz, 1H), 2.81 (t, *J* = 7.6 Hz, 2H), 1.65 (p, *J* = 7.5 Hz, 2H), 1.42 – 1.25 (m, 6H), 0.91 (t, *J* = 6.9 Hz, 3H).

*2-hexyl-5-(trimethylstannyl)thiophene (**T3**)*

This compound was prepared according to previous literature and used without further purification or identification.

*2-hexyl-5-(triethoxymethyl)thiophene (**T4**)*

This product was prepared analogously to compound **4** using compound **10** as aryl halide. (85%, 20 mmol scale) ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.95 (d, *J* = 3.5 Hz, 1H), 6.61 (d, *J* = 3.6 Hz, 1H), 3.43 (q, *J* = 7.1 Hz, 6H), 2.74 (t, *J* = 7.1 Hz, 2H), 1.64 (p, *J* = 7.4 Hz, 2H), 1.36-1.25 (m, 6H), 1.17 (t, *J* = 7.1 Hz, 9H), 0.86 (t, *J* = 6.9 Hz 3H).

*5-hexyl-2,2'-bithiophene (**BT1**)*

This compound was prepared according to previous literature with minor modifications.[6] To an oven-dried round bottom flask with stir-bar was added ## mmol of magnesium turnings. This flask with equipped with condenser and backfilled with nitrogen three times. Through the condenser was added ~50 mL of anhydrous diethyl ether (an. Et_2O). This mixture was cooled to 0 °C and ## mmol of 2-bromothiophene was added dropwise. The solution stirred at RT for 2 hours. The Grignard reagent was added to an addition funnel via cannula that was equipped to a second nitrogen purged, oven-dried flask with ## mmol of **10**, ## mmol of $Pd(dppf)Cl_2 \cdot DCM$, and 50 mL of an. Et_2O. The Grignard was added dropwise at 0 °C until complete addition, at which the solution was brought to room temperature for overnight stirring. This solution was poured into cold concentrated ammonium chloride and stirred for 30 minutes. Et_2O was added and the organic layer was separated, washed with distilled water twice, dried over Na_2SO_4, and concentrated. Column chromatography with a hexanes eluent was used to isolate a light green oil. (76%, 42 mmol scale) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.19 (d, *J* = 5.1 Hz, 1H), 7.15 (d, *J* = 3.5 Hz, 1H), 7.05 – 7.02 (m, 2H), 6.73 (d, *J* = 3.5 Hz, 1H), 2.84 (t, *J* = 7.6 Hz, 2H), 1.74 (p, *J* = 7.6 Hz, 2H), 1.48 – 1.34 (m, 6H), 0.97 (t, *J* = 6.1 Hz, 3H).

*5-hexyl-5'-iodo-2,2'-bithiophene (**BT2**)*

This product was prepared analogously to compound **10** using compound **13**.[5] (68%, 15 mmol scale) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.12 (d, *J* = 3.8 Hz, 1H), 6.92 (d, *J* = 3.6 Hz, 1H), 6.76 (d, *J* = 3.8 Hz, 1H), 6.67 (d, *J* = 3.6 Hz, 1H), 2.78 (t, *J* = 7.9 Hz, 2H), 1.68 (p, *J* = 7.5 Hz, 2H), 1.35 (m, 6H), 0.91 (t, *J* = 6.8 Hz, 3H).

*5-hexyl-5'-(trimethylstannyl)-2,2'-bithiophene (**BT3**)*

This compound was prepared according to previous literature without purification and matched reference 400 MHz (^{1}H) spectra.[4] (90% crude)

*5-hexyl-5'-(triethoxymethyl)-2,2'- bithiophene (**BT4**)*

This product was prepared analogously to compound **4** using compound **14** as aryl halide. (92%, 20 mmol scale)^{1}H NMR (500 MHz, $CDCl_3$) δ 7.05 (d, *J* = 3.7 Hz, 1H), 6.96 (d, *J* = 3.9 Hz, 2H), 6.65 (d, *J* = 3.6 Hz, 1H), 3.49 (q, *J* = 7.1 Hz, 7H), 2.77 (t, *J* = 7.0 Hz, 2H), 1.66 (p, *J* = 7.5 Hz, 2H), 1.40 – 1.28 (m, 6H), 1.21 (t, *J* = 7.2 Hz, 9H), 0.89 (t, *J* = 6.8 Hz, 3H).

General procedure for formation of intermediates 26F48Br, 2BF48Br, 26T48Br and 26BT48Br.

To an oven-dried, N_2 filled round bottom flask equipped with stir bar was added corresponding orthoeseter (3 mol eq), an. THF, and an. DMAc. The solution was degassed with N_2 for appx. 25 minutes. Afterwards, $Yb(OTf)_3$ (5 mol%) was added to the flask and the solution was then brought to 40 °C. Br-DAHQ (1 mol eq) is added portion-wise to the solution over a period of 5 minutes. Solution is heated to 60 °C for 24 hours. After cooling to room temperature, the solution is poured into MeOH, which precipitates the product out of solution. Filtering the solid gives the following pure products in the following yields:

*4,8-dibromo-2,6-bis(5-hexylfuran-2-yl)benzo[1,2-d:4,5-d']bis(oxazole) – **26F48Br***

(77%) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 (d, J = 3.4, 2H), 6.26 (d, J = 3.5 Hz, 2H), 2.79 (t, J = 7.6, 4H), 1.75 (p, J = 7.5 Hz, 4H), 1.44-1.28 (m, 12H), 0.94-0.88 (m, 6H). ^{13}C (125 MHz, $CDCl_3$) δ 162.42, 156.65, 146.32, 139.78, 139.31, 117.65, 108.28, 91.37, 31.47, 28.85, 28.39, 27.72, 22.53, 14.03.

*4,8-dibromo-2,6-bis(5'-hexyl-[2,2'-bifuran]-5-yl)benzo[1,2-d:4,5-d']bis(oxazole) – **26BF48Br***

(33%).^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49 (d, *J* = 3.7 Hz, 2H), 6.85 (d, *J* = 3.3 Hz, 2H), 6.70 (d, *J* = 3.7 Hz, 2H), 6.14 (d, *J* = 3.3 Hz, 2H), 2.70 (t, *J* = 7.6 Hz, 4H), 1.70 (p, *J* = 7.5 Hz, 4H), 1.44 – 1.30 (m, 12H), 0.90 (d, *J* = 7.0 Hz, 6H). Unable to obtain ^{13}C NMR.

*4,8-dibromo-2,6-bis(5-hexylthiophen-2-yl)benzo[1,2-d:4,5-d']bis(oxazole) – **26T48Br***

(56%) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (d, *J* = 3.7 Hz, 2H), 6.88 (d, *J* = 3.8 Hz, 2H), 2.90 (t, *J* = 7.6 Hz, 4H), 1.74 (p, *J* = 7.6 Hz, 4H), 1.46 – 1.28 (m, 12H), 0.90 (t, *J* = 7.2 Hz, 6H). ^{13}C (125 MHz, $CDCl_3$) δ 160.39, 153.71, 146.49, 139.41, 131.55, 125.84, 125.49, 90.95, 31.49, 31.35, 30.44, 28.69, 22.53, 14.04.

*4,8-dibromo-2,6-bis(5'-hexyl-[2,2'-bithiophen]-5-yl)benzo[1,2-d:4,5-d']bis(oxazole) – **26BT48Br***

(34%) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (d, *J* = 3.9 Hz, 2H), 7.10 (d, *J* = 3.7 Hz, 4H), 6.70 (d, *J* = 3.6 Hz, 2H), 2.78 (t, *J* = 7.6 Hz, 4H), 1.68 (p, *J* = 7.6 Hz, 4H), 1.35 (m, 12H), 0.90 (t, *J* = 6.7 Hz, 8H). ^{13}C NMR unable to be obtained.

General procedure for 26F, 26BF, 26T and 26BT.

To an oven-dried, N_2 filled round bottom flask equipped with stir bar was added corresponding orthoeseter (3 mol eq), $Y(OTf)_3$ (5 mol%), and an. THF. To a separate oven-dried, N_2 filled round bottom flask equipped with stir bar was added an. DMSO, an. Pyridine, and DAHQ · 2HCl (1 mol eq). Both solutions were degassed with N_2 for appx. 25 minutes. The DAHQ · 2HCl solution is added dropwise to the second flask and the collective solution is heated to 60 °C for 24 hours. After cooling to room temperature, the solution is diluted with MeOH, which precipitates the product out of solution. Filtering the solid gives the following products in the following yields:

2,6-bis(5-hexylfuran-2-yl)benzo[1,2-d:4,5-d']bis(oxazole) ***– 26F***

(30%) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 (s, 2H), 7.19 (d, J = 3.3 Hz, 2H), 6.23 (d, J = 3.3 Hz, 2H), 2.76 (t, J = 7.6 Hz, 4H), 1.74 (p, J = 7.5 Hz, 4H), 1.43-1.26 (m, 12H), 0.89 (t, J = 6.7, 6H). ^{13}C (125 MHz, $CDCl_3$) δ 161.39, 156.60, 147.94, 140.57, 139.95, 115.81, 107.97, 100.67, 31.48, 28.85, 28.34, 27.81, 22.52, 14.04. HRMS (ESI) *m/z:* $[M + H]^+$ calcd for $C_{28}H_{33}N_2O_4$: 461.2440; found: 461.2439.

2,6-bis(5'-hexyl-[2,2'-bifuran]-5-yl)benzo[1,2-d:4,5-d']bis(oxazole) ***– 26BF***

(11%) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (s, 2H), 7.33 (d, J = 3.6 Hz, 2H), 6.80 (d, J = 3.3 Hz, 2H), 6.68 (d, J = 3.6 Hz, 2H), 6.12 (d, J = 3.3 Hz, 2H), 2.69 (t, J = 7.5 Hz, 4H), 1.69 (p, J = 7.4 Hz, 4H), 1.43-1.20 (m, 12H), 0.90 (t, J = 6.9 Hz, 6H). ^{13}C (125 MHz, $CDCl_3$) δ 158.03, 156.31, 150.22, 148.12, 143.55, 140.56, 140.17, 116.82, 109.02, 107.21, 106.39, 100.74, 31.53, 28.85, 28.14, 27.92, 22.56, 14.06. HRMS (ESI) *m/z:* $[M + H]^+$ calcd for $C_{36}H_{37}N_2O_6$: 593.2652; found: 593.2654.

2,6-bis(5-hexylthiophen-2-yl)benzo[1,2-d:4,5-d']bis(oxazole) – ***26T***

(16%) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 (s, 2H), 7.74 (d, *J* = 3.7 Hz, 2H), 6.87 (d, *J* = 3.7 Hz, 2H), 2.89 (t, *J* = 7.6 Hz, 4H), 1.74 (p, *J* = 7.6 Hz, 4H), 1.40 (m, 4H), 1.32 (m, 8H), 0.92 – 0.87 (m, 6H). Unable to obtain ^{13}C NMR. HRMS (ESI) *m/z:* $[M + H]^+$ calcd for $C_{28}H_{33}N_2O_2S_2$: 493.1983; found: 493.1963.

2,6-bis(5'-hexyl-[2,2'-bithiophen]-5-yl)benzo[1,2-d:4,5-d']bis(oxazole) – ***26BT***

(13%) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 (m, 4H), 7.16 (d, *J* = 3.3 Hz, 2H), 7.13 (d, *J* = 3.6 Hz, 2H), 6.74 (d, *J* = 3.7 Hz, 2H), 2.82 (t, *J* = 7.6 Hz, 4H), 1.70 (p, *J* = 7.6 Hz, 4H), 1.40 (m, 4H), 1.33 (m, 8H), 0.89 (m, 6H). HRMS (ESI) *m/z:* $[M + H]^+$ calcd for $C_{36}H_{37}N_2O_2S_4$: 657.1738; found: 657.1764.

General procedure for final molecules via Stille cross-coupling

The general procedure is as follows: 1 mol eq. of 4,8-dibromo-2,6-diethylbenzobisoxazole, 26F48Br, 26BF48Br, 26T48Br, or 26BT48Br was added to an oven-dried round bottom flask equipped with stirbar and anhydrous toluene. To the flask was added 2.5 mol % equivalent of $Pd_2(dba)_3$, 10 mol % tri(o-tolyl)phosphine, and 4 mol eq. of corresponding stannane. These contents were degassed for 20-30 minutes and afterwards heated to 120 ^oC for 24 hours. After cooling to room temperature, the crude solution was worked-up using either *method A* or *method B* (descriptions below; specified for each compound before yield) and purified using column chromatography (hexanes:$CHCl_3$ gradient). Concentrated fractions were sonicated in minimal hexanes and filtered to produce pure materials in the following yields: (NOTE – ^{13}C NMR peaks which are believed to be *completely* overlapping are italicized.)

Method A. Reaction mixture was diluted with DCM, washed with 1M potassium fluoride solution three times, distilled water once, dried over sodium sulfate, and concentrated onto silica gel.

Method B. Reaction mixture was diluted with $CHCl_3$ and poured into a 1:1 mixture of K_2CO_3:silica gel and stirred for 15-30 minutes. The solid was filtered and washed with excess $CHCl_3$. Filtrate was concentrated onto silica gel.

2,6-diethyl-4,8-bis(5-hexylfuran-2-yl)benzo[1,2-d:4,5-d']bis(oxazole) ***– 48F***

Work-up: Method A. (63%) ^1H NMR (500 MHz, $CDCl_3$) δ 7.42 (d, J = 3.2 Hz, 2H), 6.24 (d, J = 3.1 Hz, 2H), 3.10 (q, J = 7.6 Hz, 4H), 2.83 (t, J = 7.6 Hz, 4H), 1.80 (p, J = 7.5 Hz, 4H), 1.55 (t, J = 7.5 H, 6H), 1.51 – 1.43 (m, 4H), 1.40 – 1.32 (m, 8H), 0.91 (t, J = 6.7 Hz, 6H). ^{13}C (125 MHz, $CDCl_3$) δ 168.78, 157.50, 145.75, 143.52, 134.56, 112.95, 107.28, 104.11, 31.63, 28.91, 28.35, 27.86, 22.62, 22.56, 14.08, 10.96. HRMS (ESI) *m/z:* $[M + H]^+$ calcd for $C_{32}H_{41}N_2O_4$: 517.3066; found: 517.3063.

2,6-diethyl-4,8-bis(5'-hexyl-[2,2'-bifuran]-5-yl)benzo[1,2-d:4,5-d']bis(oxazole) ***– 48BF***

Work-up: Method A. (67%) ^1H NMR (500 MHz, $CDCl_3$) δ 7.62 (d, J = 3.6 Hz, 2H), 6.73 (d, J = 3.5 Hz, 2H), 6.67 (d, J = 3.2 Hz, 2H), 6.12 (d, J = 3.2 Hz, 2H), 3.14 (q, J = 7.6 Hz, 4H), 2.71 (t, J = 7.6 Hz, 4H), 1.72 (p, J = 7.4 Hz, 4H), 1.60 (t, J = 7.6, 6H), 1.45-1.30 (m, 12H), 0.91 (t, J = 7.0 Hz, 6H). ^{13}C (125 MHz, $CDCl_3$) δ 168.93, 156.80, 147.07, 146.39, 144.84, 143.52, 134.77, 114.07, 106.81, 106.67, 106.50, 103.85, 31.57, 28.88, 28.18, 28.01, 22.64, 22.58, 14.07, 10.93. HRMS (ESI) *m/z:* $[M + H]^+$ calcd for $C_{40}H_{45}N_2O_6$: 649.3278; found: 649.3291.

2,6-diethyl-4,8-bis(5-hexylthiophen-2-yl)benzo[1,2-d:4,5-d']bis(oxazole) ***– 48T***

Work-up: Method B. (83%) ^1H NMR (500 MHz, $CDCl_3$) δ 8.12 (d, J = 3.7 Hz, 2H), 6.91 (d, J = 3.7 Hz, 2H), 3.12 (q, J = 7.6 Hz, 4H), 2.91 (t, J = 7.9 Hz, 4H), 1.77 (p, J = 7.5 Hz, 4H), 1.56 (t, J = 7.6 Hz, 6H), 1.46 – 1.39 (m, 4H), 1.36 – 1.30 (m, 8H), 0.90 (t, J = 6.9, 6H). ^{13}C (125 MHz, $CDCl_3$) δ 168.15, 147.97, 144.29, 135.20, 131.70, 128.60, 124.59, 107.59, 31.70, 31.61, 30.20, 28.85, 22.65, 22.60, 14.09, 11.18. HRMS (ESI) *m/z:* $[M + H]^+$ calcd for $C_{32}H_{41}N_2O_2S_2$: 549.2609; found: 549.2595.

2,6-diethyl-4,8-bis(5'-hexyl-[2,2'-bithiophen]-5-yl)benzo[1,2-d:4,5-d']bis(oxazole) ***– 48BT***

Work-up: Method B. (73%) ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.20 (d, J = 3.9 Hz, 2H), 7.21 (d, J = 3.9 Hz, 2H), 7.14 (d, J = 3.6 Hz, 2H), 6.73 (d, J = 3.5 Hz, 2H), 3.13 (q, J = 7.5 Hz, 4H), 2.83 (t, J = 7.7 Hz, 4H), 1.72 (p, J = 7.4 Hz, 4H), 1.58 (t, J = 7.6 Hz, 6H), 1.48-1.30 (m, 12H), 0.91 (t, J = 7.1 Hz, 6H). ^{13}C (125 MHz, $CDCl_3$) δ 168.22, 145.73, 144.24, 139.48, 135.23, 134.89, 132.61, 129.54, 124.88, 123.60, 123.35, 107.40, 31.58, 30.25, 28.79, 22.61, 22.58, 14.08, 11.12. HRMS (ESI) *m/z:* $[M + H]^+$ calcd for $C_{40}H_{45}N_2O_2S_4$: 713.2364; found: 713.2396.

2,4,6,8-tetrakis(5-hexylfuran-2-yl)benzo[1,2-d:4,5-d']bis(oxazole) ***– 26F48F***

Work-up: Method A. (72%) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 (d, *J* = 3.3 Hz, 2H), 7.27 (d, *J* = 3.4 Hz, 2H), 6.28 (d, *J* = 3.3 Hz, 2H), 6.25 (d, *J* = 3.4 Hz, 2H), 2.87 (t, *J* = 7.6 Hz, 4H), 2.81 (t, *J* = 7.6 Hz, 4H), 1.86 (p, *J* = 7.6 Hz, 4H), 1.78 (p, *J* = 7.6 Hz, 4H), 1.54 – 1.31 (m, 10H), 0.94 – 0.88 (m, 12H). ^{13}C (125 MHz, $CDCl_3$) δ 161.05, 157.55, 156.39, 145.49, 143.19, 141.01, 135.53, 115.69, 113.37, 107.82, 107.42, 104.32, 31.68, 31.53, 29.00, 28.89, 28.44, 28.38, 27.88, 27.74, 22.59, 22.57, 14.09, 14.06. HRMS (ESI) *m/z:* $[M + H]^+$ calcd for $C_{48}H_{61}N_2O_6$: 761.4530; found: 761.4544.

4,8-bis(5'-hexyl-[2,2'-bifuran]-5-yl)-2,6-bis(5-hexylfuran-2-yl)benzo[1,2-d:4,5-d']bis(oxazole) ***– 26F48BF***

Work-up: Method A. (48%) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75 (d, *J* = 3.5 Hz, 2H), 7.32 (d, *J* = 3.3 Hz, 2H), 6.77 (d, *J* = 1.0 Hz, 2H), 6.76 (d, *J* = 1.2 Hz, 2H), 6.28 (d, *J* = 3.3 Hz, 2H), 6.14 (d, *J* = 3.3 Hz, 2H), 2.84 (t, *J* = 7.7 Hz, 4H), 2.73 (t, *J* = 7.6 Hz, 4H), 1.81 (p, *J* = 7.6 Hz, 4H), 1.73 (p, *J* = 7.6 Hz, 4H), 1.49 – 1.31 (m, 24H), 0.95 – 0.89 (m, 12H). ^{13}C (125 MHz, $CDCl_3$) δ 161.12, 156.79, 156.50, 147.08, 146.17, 145.02, 143.15, 141.02, 135.75, 115.84, 114.45, 107.97, 106.81, 106.67, 106.59, 103.97, 31.58, 31.54, 28.94, 28.91, 28.44, 28.22, 28.03, 27.81, *22.59*, *14.08*. HRMS (ESI) *m/z:* $[M + H]^+$ calcd for $C_{56}H_{65}N_2O_8$: 893.4741; found: 893.4734.

2,6-bis(5'-hexyl-[2,2'-bifuran]-5-yl)-4,8-bis(5-hexylfuran-2-yl)benzo[1,2-d:4,5-d']bis(oxazole) ***– 26BF48F***

Work-up: Method A. (53%) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57 (d, *J* = 3.3 Hz, 2H), 7.41 (d, *J* = 3.6 Hz, 2H), 6.80 (d, *J* = 3.3 Hz, 2H), 6.71 (d, *J* = 3.6 Hz, 2H), 6.30 (d, *J* = 3.3 Hz, 2H), 6.14 (d, *J* = 3.3 Hz, 2H), 2.89 (t, *J* = 7.6 Hz, 4H), 2.71 (t, *J* = 7.6 Hz, 4H), 1.88 (p, *J* = 7.6 Hz, 4H), 1.71 (p, *J* = 7.6 Hz, 4H), 1.55 – 1.31 (m, 24H), 0.96 – 0.89 (m, 12H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.84, 157.64, 156.04, 149.92, 145.44, 143.84, 143.34, 141.05, 135.73, 116.59, 113.48, 108.73, 107.52, 107.13, 106.35, 104.32, 31.67, 31.54, 29.02, 28.87, 28.47, 28.16, *27.94*, 22.61, 22.57, 14.09, 14.07. HRMS (ESI) *m/z:* $[M + H]^+$ calcd for $C_{56}H_{65}N_2O_8$: 893.4741; found: 893.4766.

2,4,6,8-tetrakis(5'-hexyl-[2,2'-bifuran]-5-yl)benzo[1,2-d:4,5-d']bis(oxazole) ***– 26BF48BF***

Work-up: Method A. (26%) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (d, *J* = 3.5 Hz, 2H), 7.42 (d, *J* = 3.6 Hz, 2H), 6.82 (d, *J* = 3.3 Hz, 2H), 6.80 (d, *J* = 3.2 Hz, 2H), 6.75 (d, *J* = 3.5 Hz, 2H), 6.71 (d, *J* = 3.5 Hz, 2H), 6.15 (dd, *J* = 5.1, 3.1 Hz, 4H), 2.73 (t, *J* = 7.2 Hz, 4H), 2.72 (t, *J* = 7.2 Hz, 4H), 1.74 (p, *J* = 7.7 Hz, 4H), 1.73 (p, *J* = 7.7 Hz, 4H), 1.46 – 1.31 (m, 24H), 0.95 – 0.90 (m, 12H).^{13}C (125 MHz, $CDCl_3$) δ 157.86, 156.80, 156.08, 149.93, 147.08, 146.10, 145.07, 143.86, 143.26, 141.07, 135.88, 116.65, 114.48, 108.74, 107.11, 106.78, 106.57, 106.46, 103.89, 31.60, 31.56, 28.95, 28.91, 28.24, 28.19, 28.04, 27.93, 22.62, 22.58, 14.09, 14.08. HRMS (ESI) *m/z:* $[M + H]^+$ calcd for $C_{64}H_{69}N_2O_{10}$: 1025.4952; found: 1025.4916.

2,6-bis(5-hexylfuran-2-yl)-4,8-bis(5-hexylthiophen-2-yl)benzo[1,2-d:4,5-d']bis(oxazole) **– *26F48T***

Work-up: Method B. (71%) ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.23 (d, *J* = 3.7 Hz, 2H), 7.31 (d, *J* = 4.0 Hz, 2H), 6.94 (d, *J* = 3.7 Hz, 2H), 6.25 (d, *J* = 3.4 Hz, 2H), 2.94 (t, *J* = 7.7 Hz, 4H), 2.82 (t, *J* = 7.7 Hz, 4H), 1.80 (p, *J* = 8.0 Hz, 4H), 1.78 (p, *J* = 8.0 Hz, 4H), 1.49 – 1.30 (m, 24H), 0.95 – 0.89 (m, 12H). ^{13}C (125 MHz, $CDCl_3$) δ 161.30, 155.73, 148.10, 143.93, 140.80, 136.25, 131.44, 128.91, 124.69, 116.03, 107.87, 107.84, 31.68, 31.63, 31.53, 30.24, 28.89, 28.38, 27.71, 22.62, 22.57, 14.10, 14.07. HRMS (ESI) *m/z:* $[M + H]^+$ calcd for $C_{48}H_{61}N_2O_4S_2$: 793.4073; found: 793.4091.

4,8-bis(5'-hexyl-[2,2'-bithiophen]-5-yl)-2,6-bis(5-hexylfuran-2-yl)benzo[1,2-d:4,5-d']bis(oxazole) – ***26F48BT***

Work-up: Method B. (56%) ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.26 (d, *J* = 3.9 Hz, 2H), 7.28 (d, *J* = 3.4 Hz, 2H), 7.20 (d, *J* = 3.9 Hz, 2H), 7.14 (d, *J* = 3.5 Hz, 2H), 6.73 (d, *J* = 3.5 Hz, 2H), 6.23 (d, *J* = 3.4 Hz, 2H), 2.83 (t, *J* = 7.1 Hz, 4H), 2.82 (t, *J* = 7.1 Hz, 4H), 1.78 (p, *J* = 7.6 Hz, 4H), 1.73 (p, *J* = 7.6 Hz, 4H), 1.50 – 1.31 (m, 24H), 0.96 – 0.90 (m, 12H). ^{13}C (125 MHz, $CDCl_3$) δ 161.35, 155.63, 145.61, 143.85, 140.65, 139.49, 136.22, 135.03, 132.33, 129.81, 124.85, 123.58, 123.46, 116.19, 107.88, 107.54, *31.61*, 31.56, 30.27, 28.95, 28.83, 28.40, 27.68, *22.60*, *14.10*. HRMS (ESI) *m/z:* $[M + H]^+$ calcd for $C_{56}H_{65}N_2O_4S_4$: 957.3827; found: 957.3847.

2,6-bis(5'-hexyl-[2,2'-bifuran]-5-yl)-4,8-bis(5-hexylthiophen-2-yl)benzo[1,2-d:4,5-d']bis(oxazole) – ***26BF48T***

Work-up: Method B. (59%) ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.24 (d, *J* = 3.7 Hz, 2H), 7.43 (d, *J* = 3.6 Hz, 2H), 6.95 (d, *J* = 3.7 Hz, 2H), 6.82 (d, *J* = 3.3 Hz, 2H), 6.70 (d, *J* = 3.7 Hz, 2H), 6.14 (d, *J* = 3.2 Hz, 2H), 2.95 (t, *J* = 7.6 Hz, 4H), 2.71 (t, *J* = 7.6 Hz, 4H), 1.81 (p, *J* = 7.6 Hz, 4H), 1.72 (p, *J* = 7.6 Hz, 4H), 1.50 – 1.31 (m, 24H), 0.95 – 0.89 (m, 12H). ^{13}C (125 MHz, $CDCl_3$) δ 157.86, 155.32, 150.02, 148.16, 144.06, 143.82, 140.88, 136.43, 131.36, 129.00, 124.71, 116.86, 108.90, 107.84, 107.16, 106.41, 31.67, 31.65, 31.56, 30.25, 28.91, 28.88, 28.18, 27.92, 22.64, 22.57, 14.12, 14.07. HRMS (ESI) *m/z:* $[M + H]^+$ calcd for $C_{56}H_{65}N_2O_6S_2$: 925.4284; found: 925.4260.

2,6-bis(5'-hexyl-[2,2'-bifuran]-5-yl)-4,8-bis(5'-hexyl-[2,2'-bithiophen]-5-yl)benzo[1,2-d:4,5-d']bis(oxazole) – ***26BF48BT***

Work-up: Method B. (31%) ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.22 (d, *J* = 3.8 Hz, 2H), 7.33 (d, *J* = 3.6 Hz, 2H), 7.16 (d, *J* = 3.9 Hz, 2H), 7.11 (d, *J* = 3.5 Hz, 2H), 6.80 (d, *J* = 3.2 Hz, 2H), 6.71 (d, *J* = 3.5 Hz, 2H), 6.64 (d, *J* = 3.6 Hz, 2H), 6.14 (d, *J* = 3.2 Hz, 2H), 2.83 (t, *J* = 7.7 Hz, 4H), 2.72 (t, *J* = 7.7 Hz, 4H), 1.73 (m, 8H), 1.50-1.32 (m, 29H), 0.96 – 0.91 (m, 12H). ^{13}C (125 MHz, $CDCl_3$) δ 157.76, 155.08, 149.92, 145.47, 143.87, 143.84, 140.69, 139.42, 136.29, 135.09, 132.22, 129.82, 124.81, 123.45, 123.35, 116.90, 108.88, 107.39, 107.15, 106.39, 31.63, 31.61, 31.59, 30.28, 28.95, 28.89, 28.20, 27.93, 22.63, 22.61, 14.11, 14.09. HRMS (ESI) *m/z:* $[M + H]^+$ calcd for $C_{64}H_{69}N_2O_6S_4$: 1089.4039; found: 1089. 4006.

4,8-bis(5-hexylfuran-2-yl)-2,6-bis(5-hexylthiophen-2-yl)benzo[1,2-d:4,5-d']bis(oxazole) – ***26T48F***

Work-up: Method B. (75%) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 (d, *J* = 3.6 Hz, 2H), 7.52 (d, *J* = 3.3 Hz, 2H), 6.88 (d, *J* = 3.7 Hz, 2H), 6.27 (d, *J* = 3.2 Hz, 2H), 2.91 (t, *J* = 7.6 Hz, 4H), 2.86 (t, *J* = 7.6 Hz, 4H), 1.88 (p, *J* = 7.6 Hz, 4H), 1.76 (p, *J* = 7.6 Hz, 4H), 1.55-1.30 (m, 24H), 0.97-0.90 (m, 12H). ^{13}C (125 MHz, $CDCl_3$) δ 159.90, 157.37, 151.93, 145.73, 143.35, 135.70, 129.96, 127.11, 125.48, 113.13, 107.40, 103.96, 31.73, 31.53, 31.48, 30.43, 29.03, 28.72, 28.48, 27.94, 22.59, 22.56, 14.12, 14.05. HRMS (ESI) *m/z:* $[M + H]^+$ calcd for $C_{48}H_{61}N_2O_4S_2$: 793.4073; found: 793.4060.

4,8-bis(5'-hexyl-[2,2'-bifuran]-5-yl)-2,6-bis(5-hexylthiophen-2-yl)benzo[1,2-d:4,5-d']bis(oxazole) – ***26T48BF***

Work-up: Method B. (24%) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.80 (d, *J* = 3.6 Hz, 2H), 7.66 (d, *J* = 3.5 Hz, 2H), 6.87 (d, *J* = 3.7 Hz, 2H), 6.71 (d, *J* = 3.2 Hz, 2H), 6.70 (d, *J* = 3.4 Hz, 2H), 6.14 (d, *J* = 3.2 Hz, 2H), 2.90 (t, *J* = 7.6 Hz, 4H), 2.74 (t, *J* = 7.6 Hz, 4H), 1.82 – 1.71 (m, 8H), 1.47 – 1.32 (m, 24H), 0.95 – 0.89 (m, 12H). ^{13}C (125 MHz, $CDCl_3$) δ159.88, 156.60, 151.91, 146.90, 146.37, 145.08, 143.21, 135.83, 129.95, 127.02, 125.45, 114.19, 106.85, 106.55, 106.50, 103.53, 31.61, 31.57, 31.40, 30.43, 28.97, 28.79, 28.24, 28.03, 22.62, 22.58, 14.09, 14.08. HRMS (ESI) *m/z:* $[M + H]^+$ calcd for $C_{56}H_{65}N_2O_6S_2$: 925.4284; found: 925.4278.

2,6-bis(5'-hexyl-[2,2'-bithiophen]-5-yl)-4,8-bis(5-hexylfuran-2-yl)benzo[1,2-d:4,5-d']bis(oxazole) – ***26BT48F***

Work-up: Method B. (39%) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77 (d, *J* = 3.8 Hz, 2H), 7.48 (d, *J* = 3.2 Hz, 2H), 7.11 (m, 4H), 6.71 (d, *J* = 3.5 Hz, 2H), 6.25 (d, *J* = 3.2 Hz, 2H), 2.86 (t, *J* = 7.7 Hz, 4H), 2.81 (t, *J* = 7.7 Hz, 4H), 1.89 (p, *J* = 7.6 Hz, 4H), 1.70 (p, *J* = 7.6 Hz, 4H), 1.56 – 1.47 (m, 4H), 1.47 – 1.31 (m, 24H), 0.96-0.89 (m, 12H). ^{13}C (125 MHz, $CDCl_3$) δ 159.40, 157.39, 147.06, 145.62, 143.40, 142.80, 135.82, 133.92, 130.56, 127.16, 125.12, 124.66, 123.59, 113.24, 107.42, 103.91, 31.76, 31.56, 31.53, 30.24, 29.11, 28.77, 28.50, 27.96, 22.65, 22.57, 14.13, 14.07. HRMS (ESI) *m/z:* $[M + H]^+$ calcd for $C_{56}H_{65}N_2O_4S_4$: 957.3827; found: 957.3815.

4,8-bis(5'-hexyl-[2,2'-bifuran]-5-yl)-2,6-bis(5'-hexyl-[2,2'-bithiophen]-5-yl)benzo[1,2-d:4,5-d']bis(oxazole) – ***26BT48BF***

Work-up: Method B. (27%) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 (d, *J* = 3.8 Hz, 2H), 7.50 (d, *J* = 3.4 Hz, 2H), 7.03 (d, *J* = 3.4 Hz, 2H), 7.00 (d, *J* = 3.8 Hz, 2H), 6.69 (d, *J* = 3.5 Hz, 2H), 6.62 (d, *J* = 3.2 Hz, 2H), 6.59 (d, *J* = 3.4 Hz, 2H), 6.09 (d, *J* = 3.1 Hz, 2H), 2.81 (t, *J* = 7.7 Hz, 4H), 2.71 (t, *J* = 7.7 Hz, 4H), 1.80 – 1.66 (m, 8H), 1.49 – 1.31 (m, 24H), 0.98 – 0.91 (m, 12H). ^{13}C (125 MHz, $CDCl_3$) δ 159.12, 156.39, 146.69, *146.21*, 145.13, 143.02, 142.47, 135.78, 134.11, 130.31, 127.06, 124.99, 124.39, 123.42, 114.17, 106.74, 106.46, 106.42, 103.23, 31.68, 31.61, 31.50, 30.25, 29.09, 28.87, 28.26, 28.00, 22.68, 22.62, 14.13, 14.10. HRMS (ESI) *m/z:* $[M + H]^+$ calcd for $C_{64}H_{69}N_2O_6S_4$: 1089.4039; found: 1089.4016.

2,4,6,8-tetrakis(5-hexylthiophen-2-yl)benzo[1,2-d:4,5-d']bis(oxazole) – ***26T48T***

Work-up: Method B. (81%) ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.23 (d, *J* = 3.7 Hz, 2H), 7.83 (d, *J* = 3.6 Hz, 2H), 6.93 (d, *J* = 3.7 Hz, 2H), 6.88 (d, *J* = 3.7 Hz, 2H), 2.94 (t, *J* = 7.6 Hz, 4H), 2.91 (t, *J* = 7.6 Hz, 4H), 1.80 (p, *J* = 7.6 Hz, 4H), 1.77 (p, *J* = 7.6 Hz, 4H), 1.50 – 1.31 (m, 24H), 0.96 – 0.89 (m, 12H). ^{13}C (125 MHz, $CDCl_3$) δ 159.15, 152.06, 147.91, 144.04, 136.34, 131.74, 130.15, 128.79, 126.87, 125.51, 124.62, 107.43, 31.71, 31.66, 31.55, 31.50, 30.46, 30.22, 28.92, 28.78, 22.66, 22.58, 14.13, 14.07. HRMS (ESI) *m/z:* $[M + H]^+$ calcd for $C_{48}H_{61}N_2O_2S_4$: 825.3616; found: 825.3610.

4,8-bis(5'-hexyl-[2,2'-bithiophen]-5-yl)-2,6-bis(5-hexylthiophen-2-yl)benzo[1,2-d:4,5-d']bis(oxazole) – ***26T48BT***

Work-up: Method B. (39%) ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.16 (d, *J* = 3.9 Hz, 2H), 7.70 (d, *J* = 3.7 Hz, 2H), 7.11 (d, *J* = 3.9 Hz, 2H), 7.10 (d, *J* = 3.5 Hz, 2H), 6.81 (d, *J* = 3.6 Hz, 2H), 6.72 (d, *J* = 3.5 Hz, 2H), 2.87 (t, *J* = 7.7 Hz, 4H), 2.84 (t, *J* = 7.7 Hz, 4H), 1.77 (p, *J* = 7.3 Hz, 4H), 1.75 (p, *J* = 7.3 Hz, 4H), 1.48 – 1.33 (m, 24H), 0.97 – 0.92 (m, 12H). ^{13}C (125 MHz, $CDCl_3$) δ 159.03, 152.11, 145.44, 143.86, 139.24, 136.25, 135.17,

132.64, 130.23, 129.61, 126.67, 125.45, 124.80, 123.47, 123.41, 107.06, 31.64, 31.62, 31.58, 31.45, 30.47, 30.29, *28.87*, *22.62*, 14.11, 14.10. HRMS (ESI) *m/z:* $[M + Li]^+$ calcd for $C_{56}H_{65}N_2O_2S_6$: 989.3370; found: 989.3542.

2,6-bis(5'-hexyl-[2,2'-bithiophen]-5-yl)-4,8-bis(5-hexylthiophen-2-yl)benzo[1,2-d:4,5-d']bis(oxazole) – ***26BT48T***

Work-up: Method B. (73%) ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (dd, *J* = 3.6, 1.6 Hz, 2H), 7.76 (dd, *J* = 3.9, 2.1 Hz, 2H), 7.11 (d, *J* = 3.5 Hz, 2H), 7.08 (dd, *J* = 3.9, 1.5 Hz, 2H), 6.89 (d, *J* = 3.6 Hz, 2H), 6.71 (d, *J* = 3.6 Hz, 2H), 2.93 (t, *J* = 7.7 Hz, 4H), 2.81 (t, *J* = 7.7 Hz, 4H), 1.80 (p, *J* = 7.6 Hz, 4H), 1.70 (p, *J* = 7.6 Hz, 4H), 1.52 – 1.30 (m, 24H), 0.99 – 0.89 (m, 12H). ^{13}C (125 MHz, $CDCl_3$) δ 158.45, 147.76, 146.90, 143.98, 142.74, 136.37, 133.94, 131.64, 130.61, 128.78, 126.88, 125.04, 124.61, 124.50, 123.47, 107.28, 31.71, 31.64, 31.59, 31.50, 30.25, 30.23, 29.02, 28.83, 22.71, 22.60, 14.17, 14.09. HRMS (ESI) *m/z:* $[M + H]^+$ calcd for $C_{56}H_{65}N_2O_2S_6$: 989.3370; found: 989.3510.

2,4,6,8-tetrakis(5'-hexyl-[2,2'-bithiophen]-5-yl)benzo[1,2-d:4,5-d']bis(oxazole) – ***26BT48BT***

Work-up: Method B. (25%) ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.01 (d, *J* = 3.8 Hz, 2H), 7.57 (d, *J* = 3.8 Hz, 2H), 7.06 (d, *J* = 3.4 Hz, 2H), 7.04 (d, *J* = 3.3 Hz, 2H), 7.03 (d, *J* = 3.8 Hz, 2H), 6.97 (d, *J* = 3.8 Hz, 2H), 6.70 (d, *J* = 3.5 Hz, 2H), 6.67 (d, *J* = 3.4 Hz, 2H), 2.82 (t, *J* = 6.7 Hz, 4H), 2.81 (t, *J* = 6.7 Hz, 4H), 1.78 – 1.69 (m, 10H), 1.49 – 1.32 (m, 32H), 0.98 – 0.91 (m, 15H). ^{13}C (125 MHz, $CDCl_3$) δ158.28, 146.67, 145.16, 143.69, 142.72, 139.10, 136.15, 135.28, 134.13, 132.42, 130.69, 129.55, 126.67, 124.99, 124.71, 124.59, 123.47, 123.35, 123.30, 106.78, 31.67, 31.62, 31.59, 31.54, 30.30, 30.29, 28.98, 28.90, 22.67, 22.63, 14.14, 14.11. HRMS (ESI) *m/z:* $[M + H]^+$ calcd for $C_{64}H_{69}N_2O_2S_8$: 1153.3125; found: 1153.3071.

Characterization

NMR Spectra

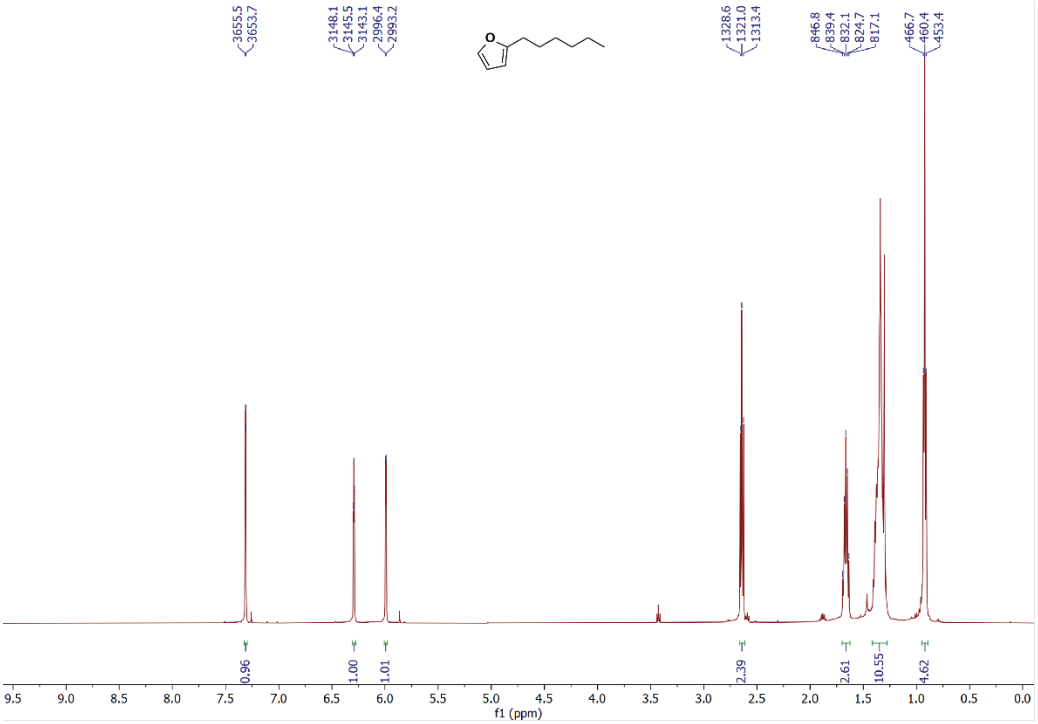


Figure S1. ^{1}H NMR of F1

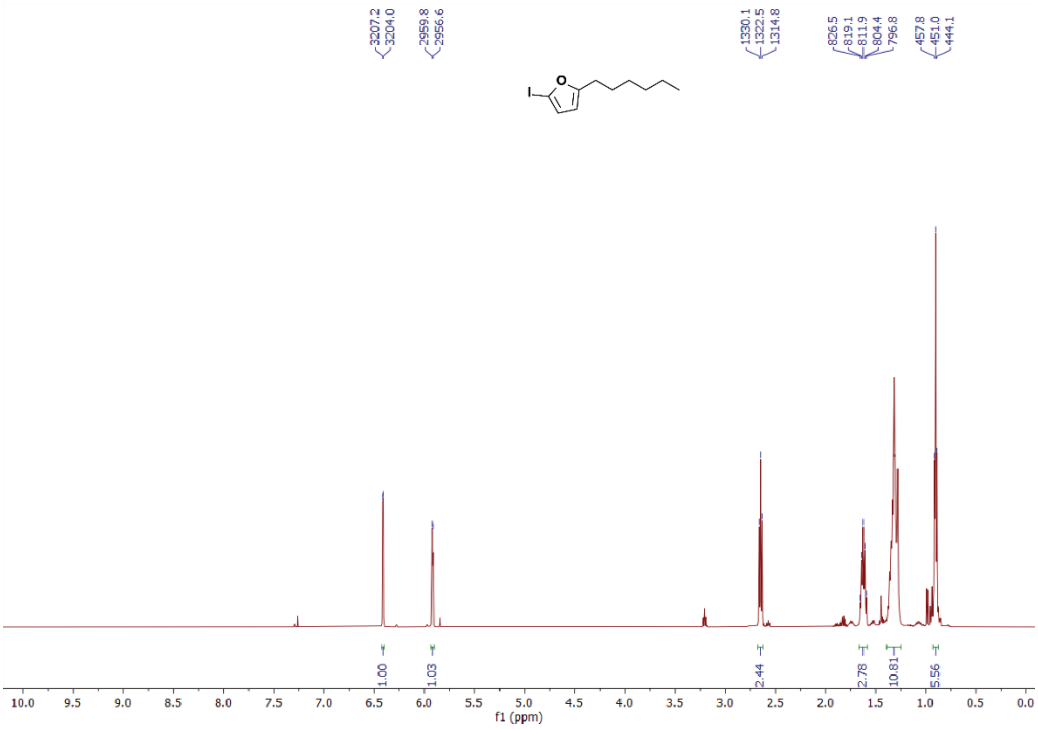


Figure S2. ^{1}H NMR of F2

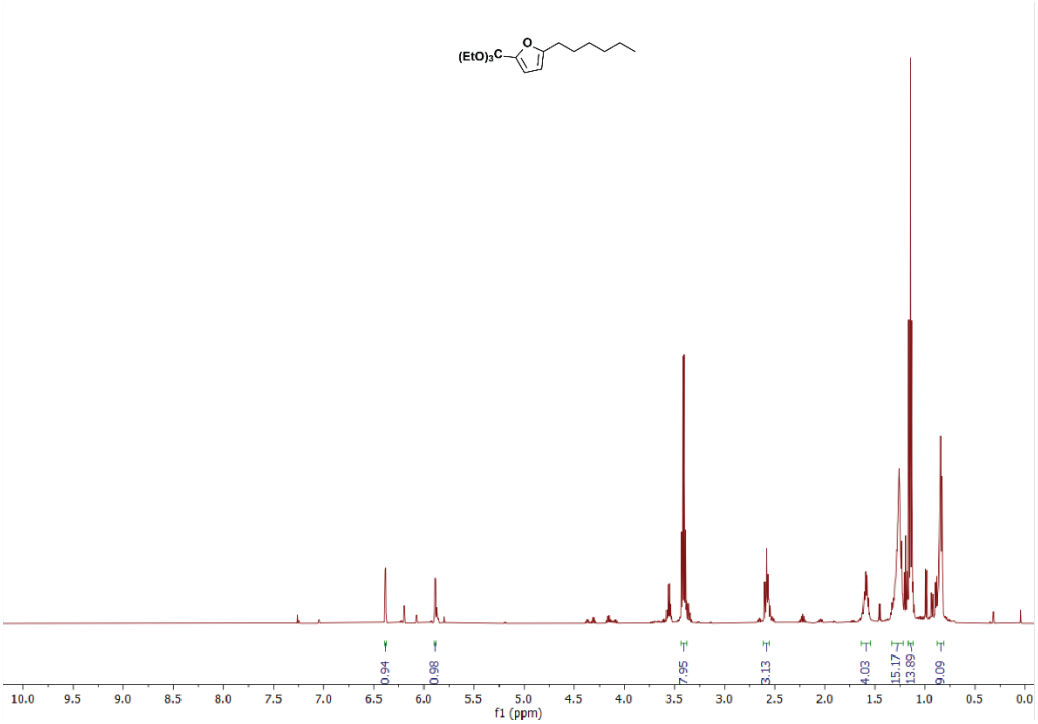


Figure S3. ^{1}H NMR of F4

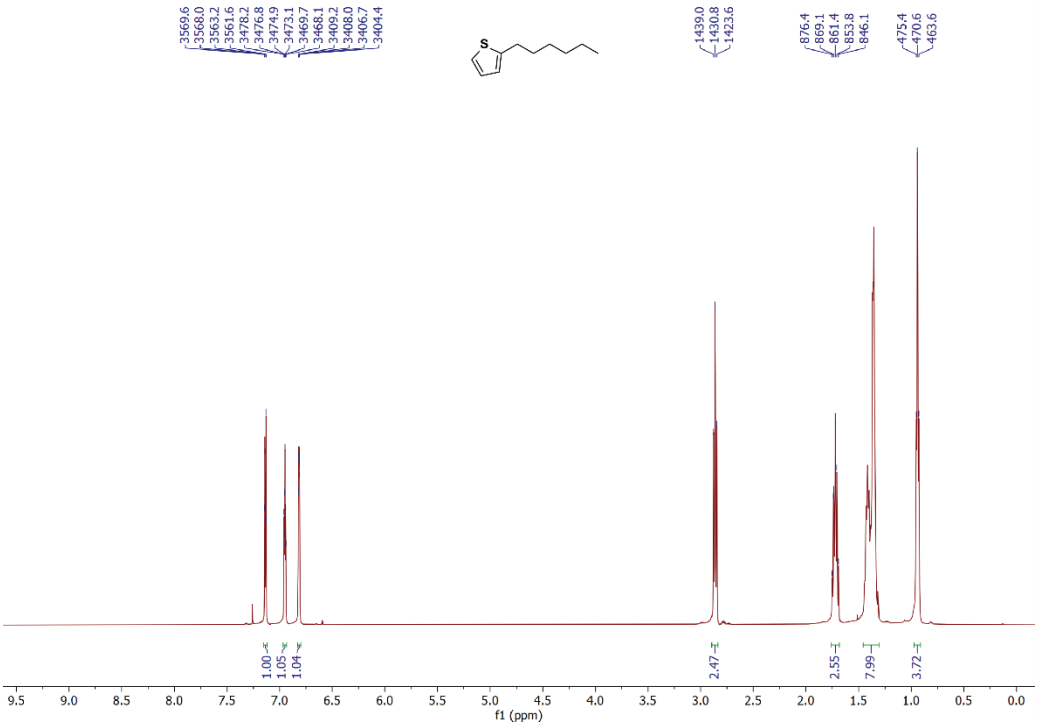


Figure S4. ^{1}H NMR of T1

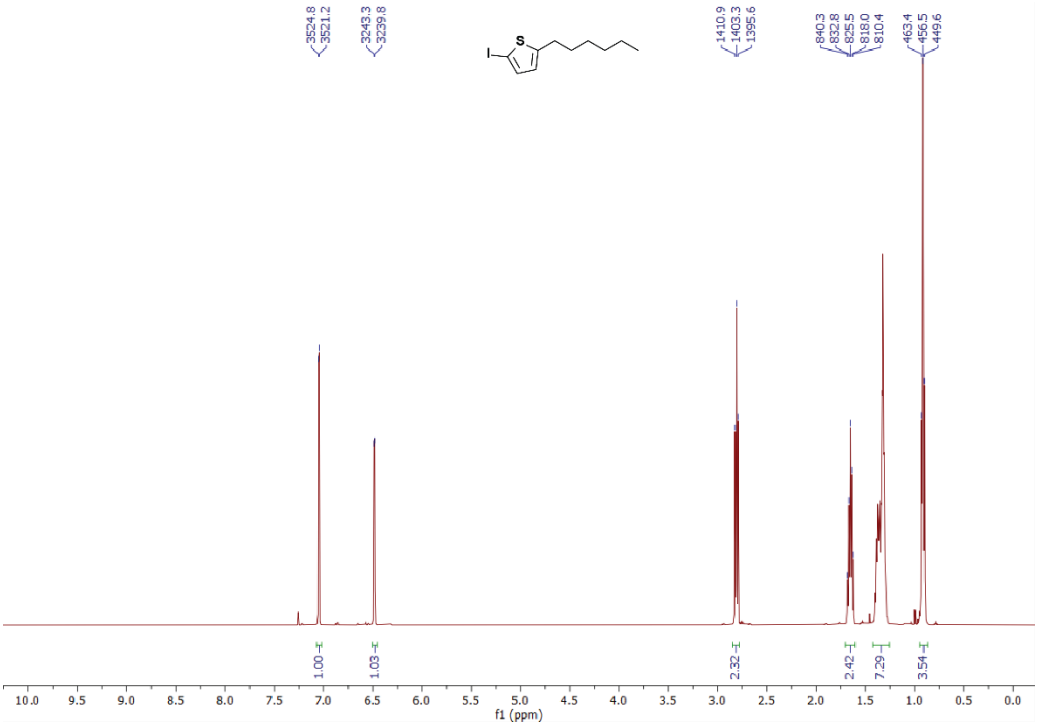


Figure S5. ^{1}H NMR of T2

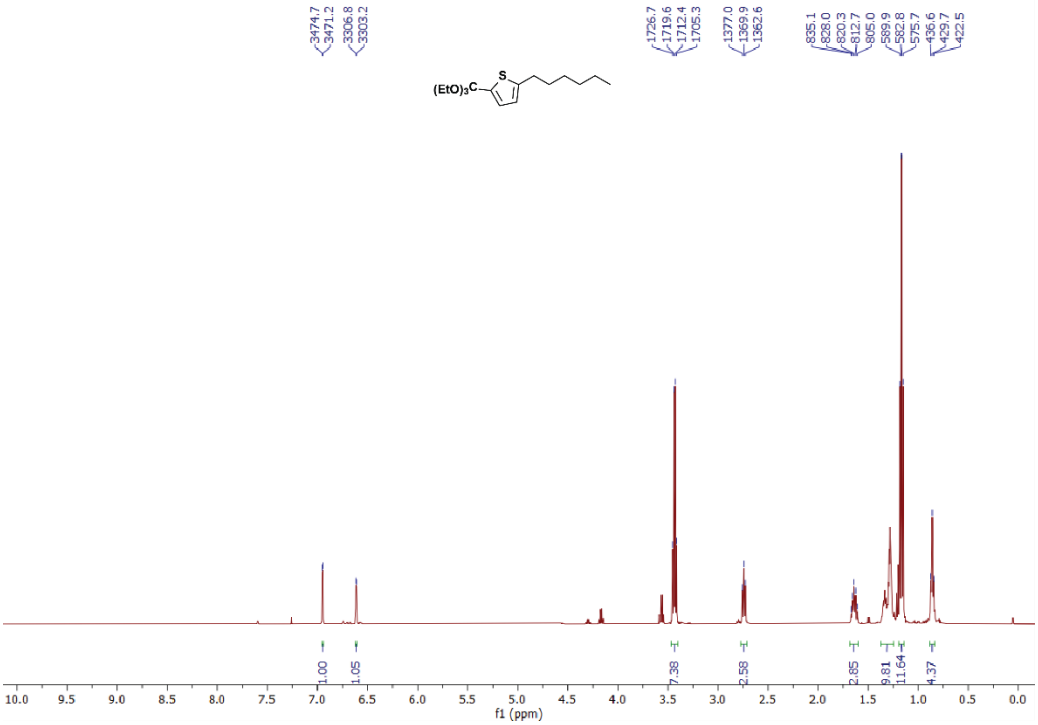


Figure S6. ^{1}H NMR of T4

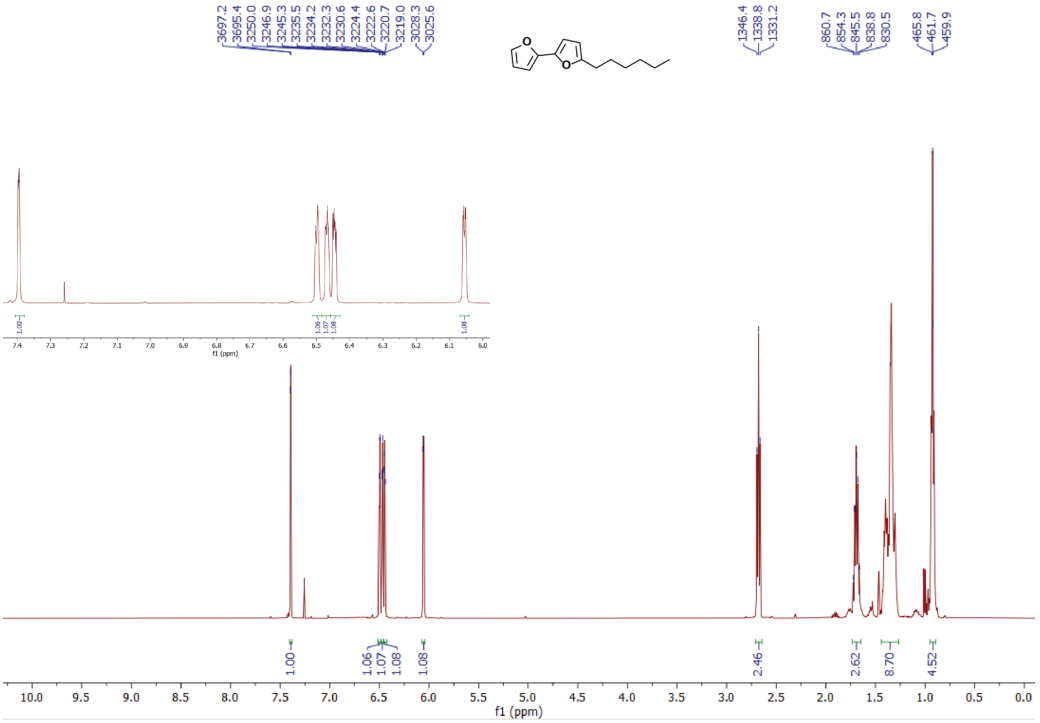


Figure S7. ^{1}H NMR of BF1

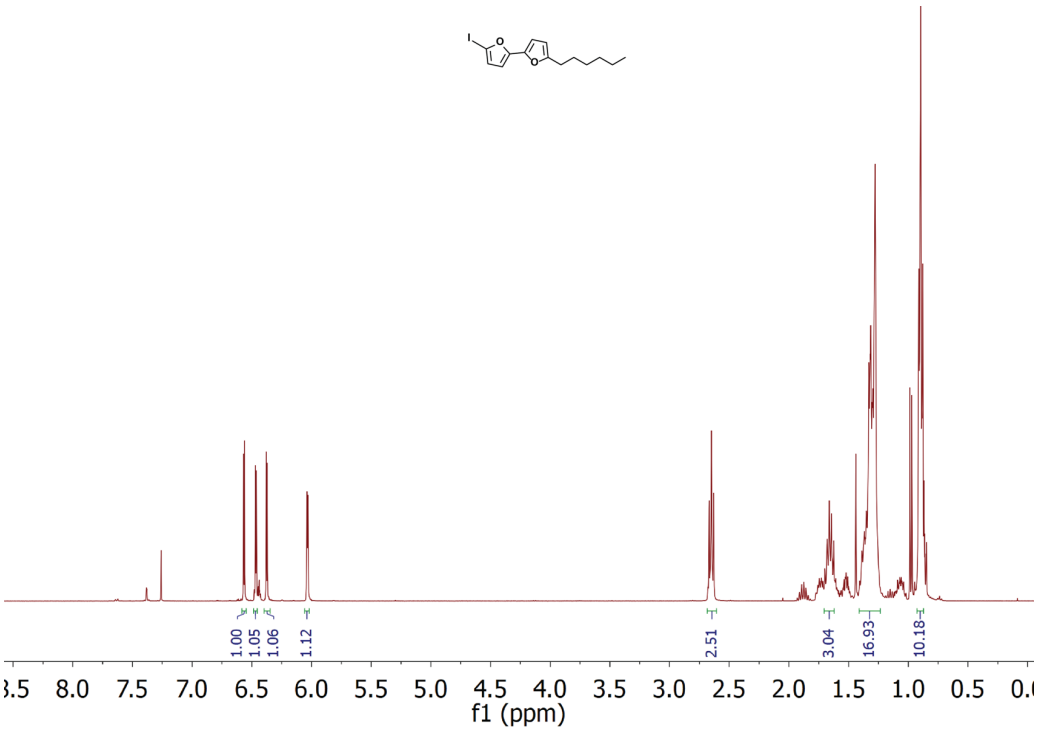


Figure S8. ^{1}H NMR of BF2

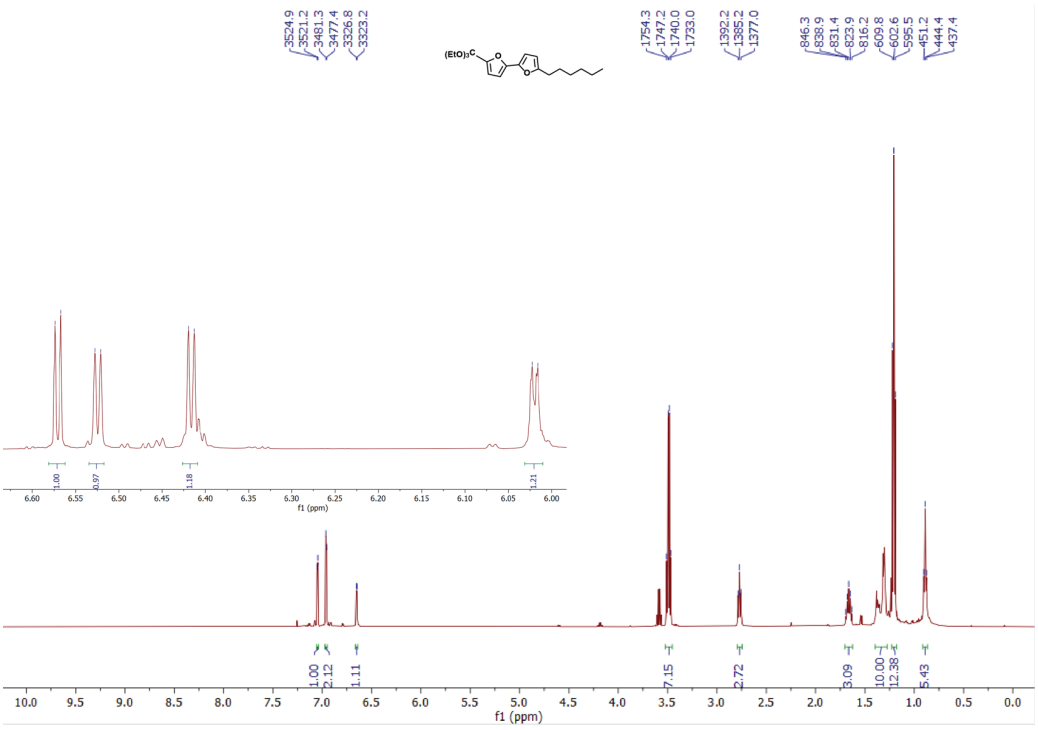


Figure S9. ^{1}H NMR of BF4

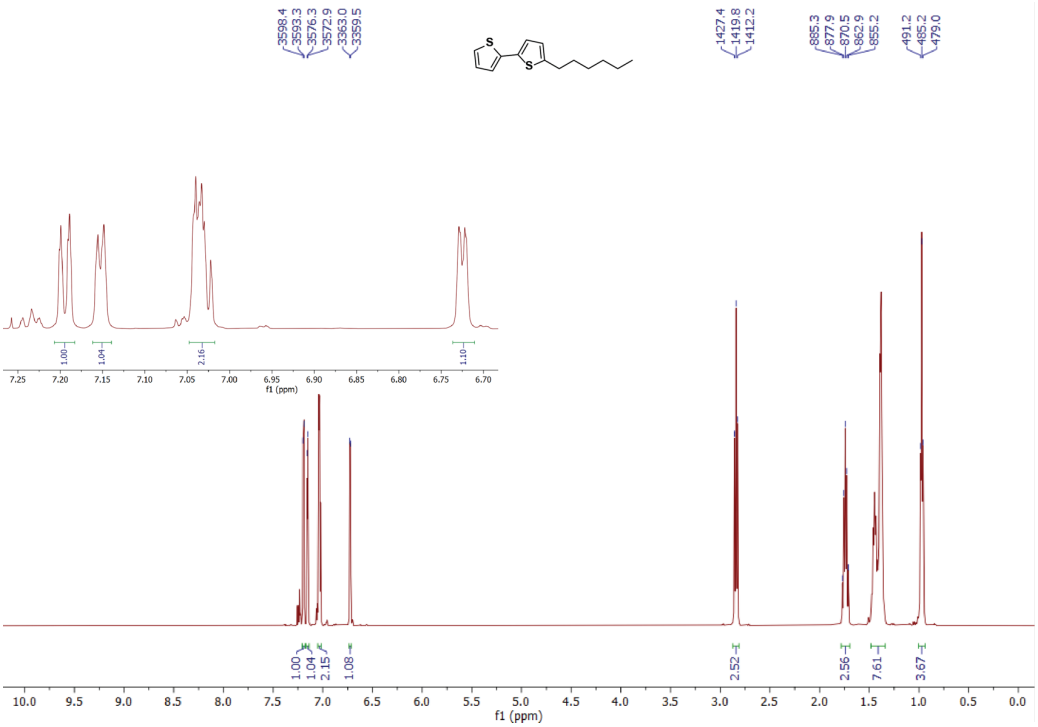


Figure S10. ^{1}H NMR of BT1

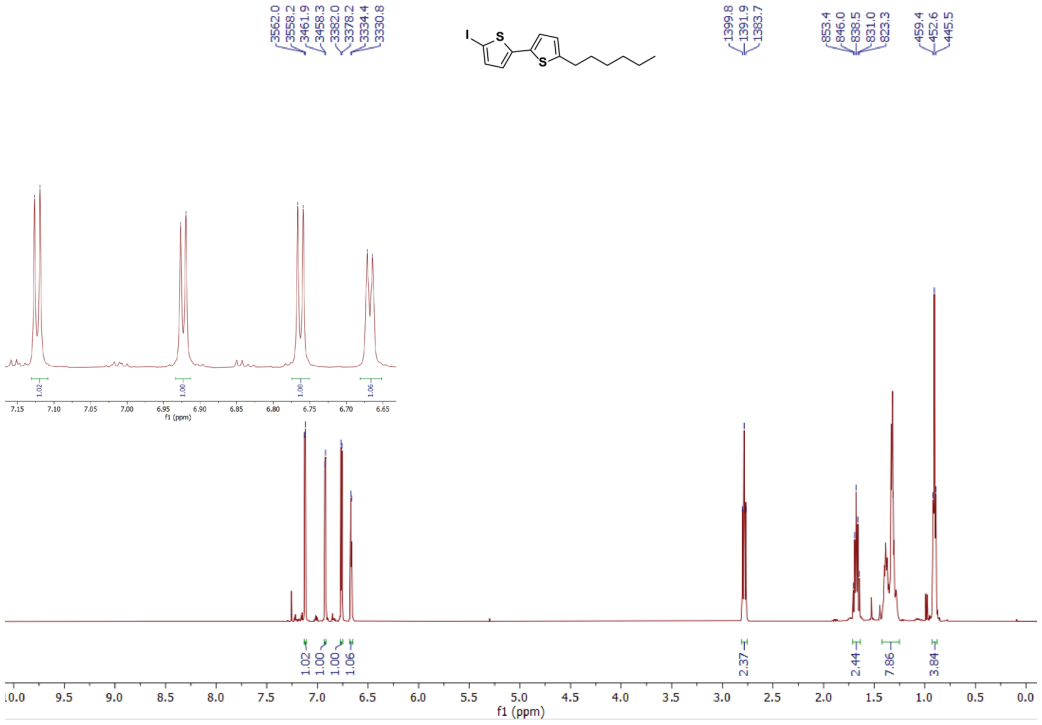


Figure S12. ^{1}H NMR of BT2

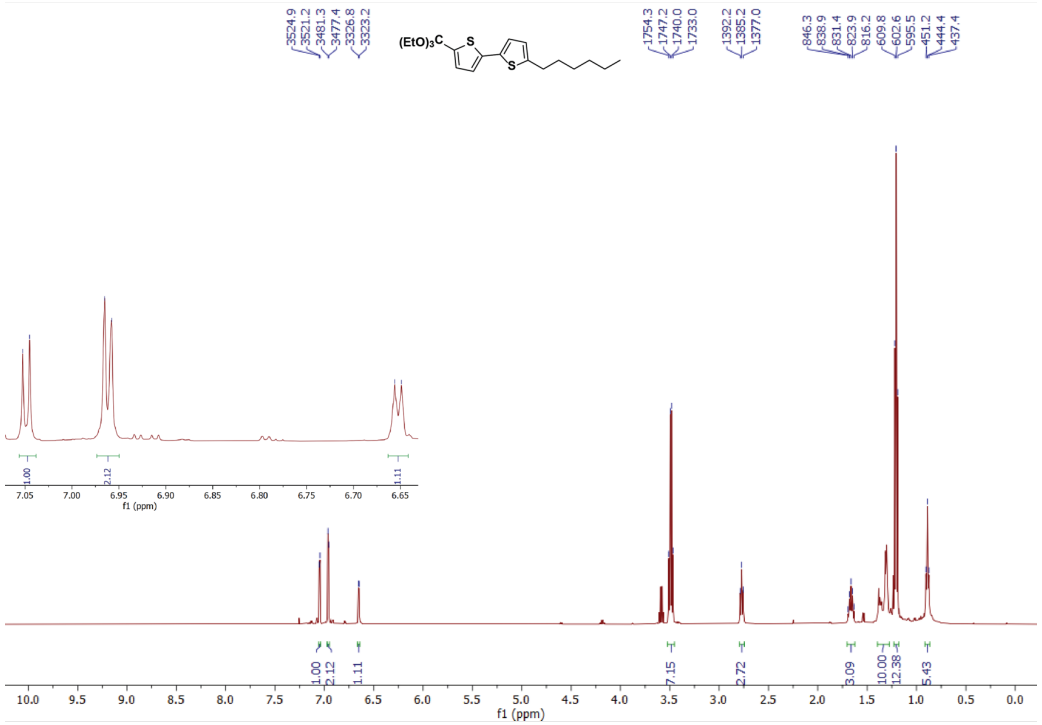


Figure S13. ^{1}H NMR of BT4

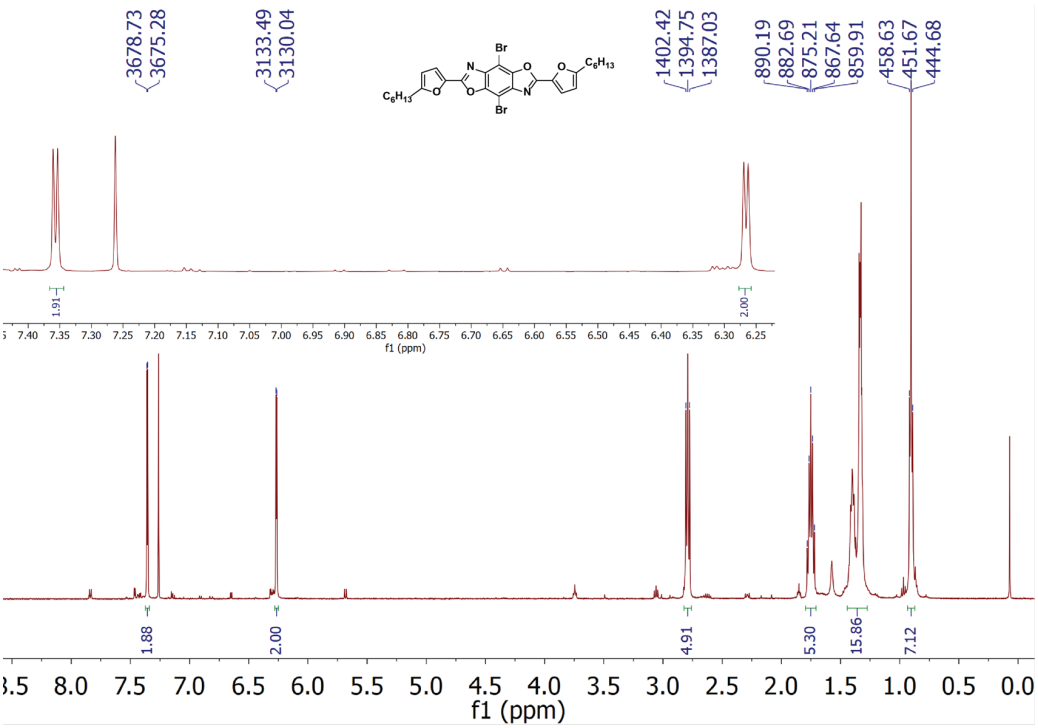


Figure S14. ^{1}H NMR of 26F48Br

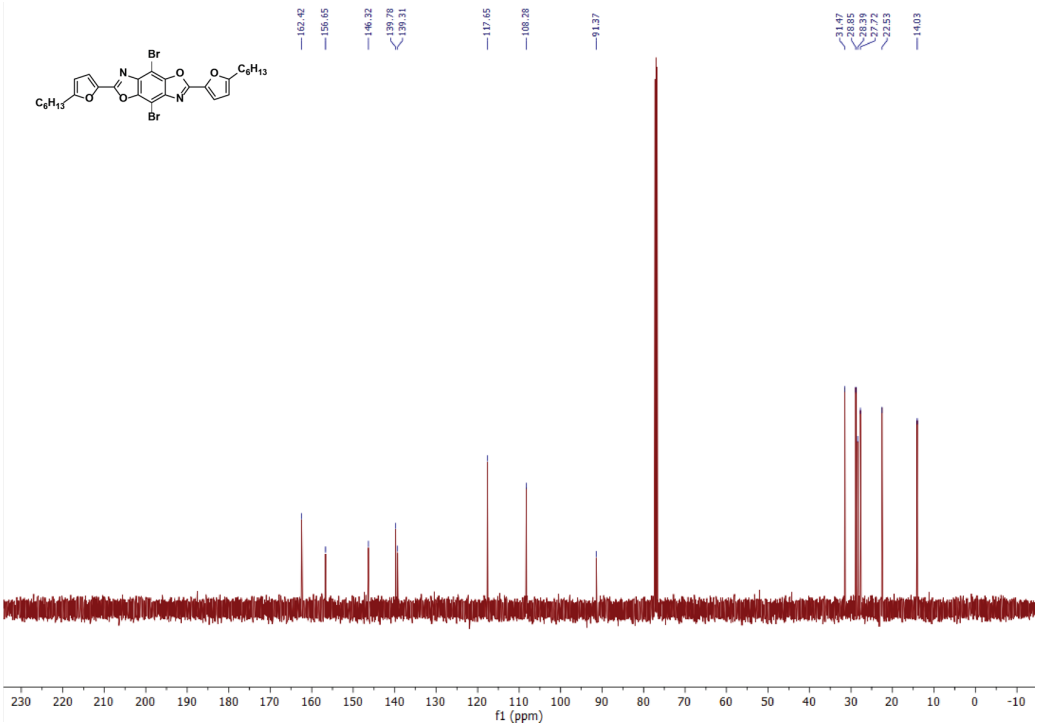


Figure S15. ^{13}C NMR of 26F48Br

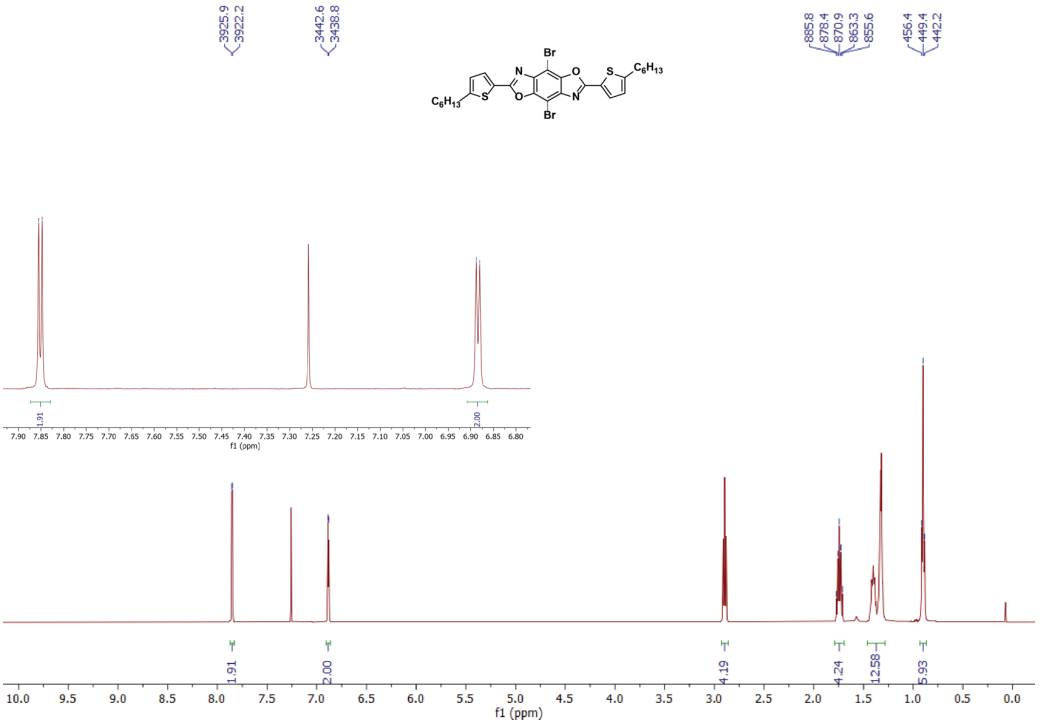


Figure S16. ^{1}H NMR of 26T48Br

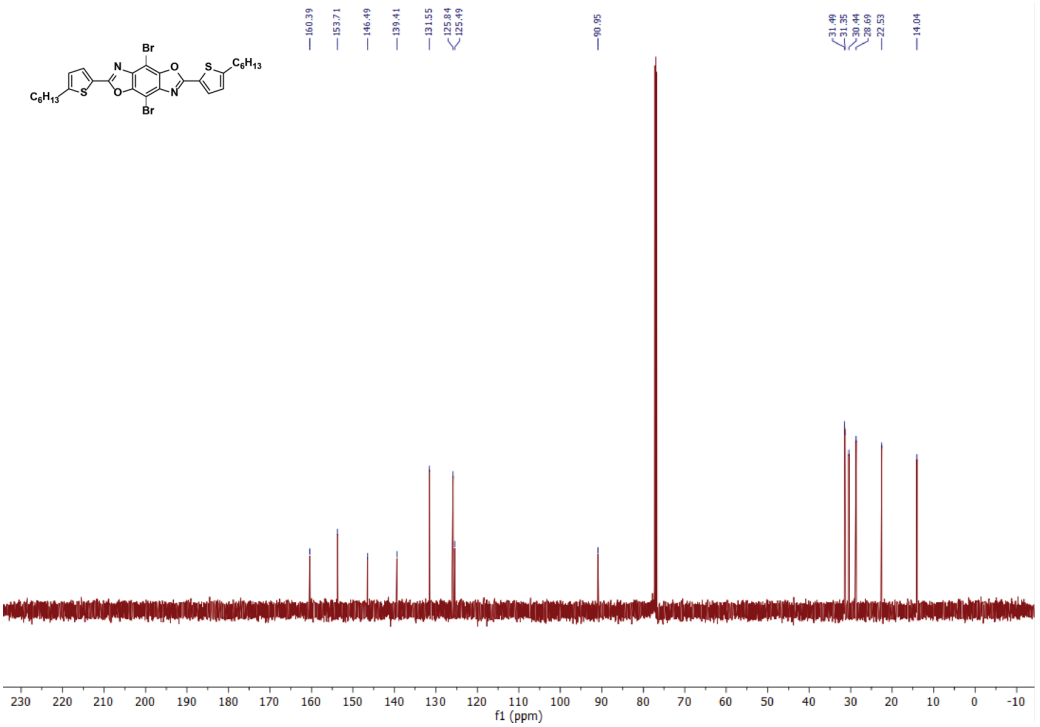


Figure S17. ^{13}C NMR of 26T48Br

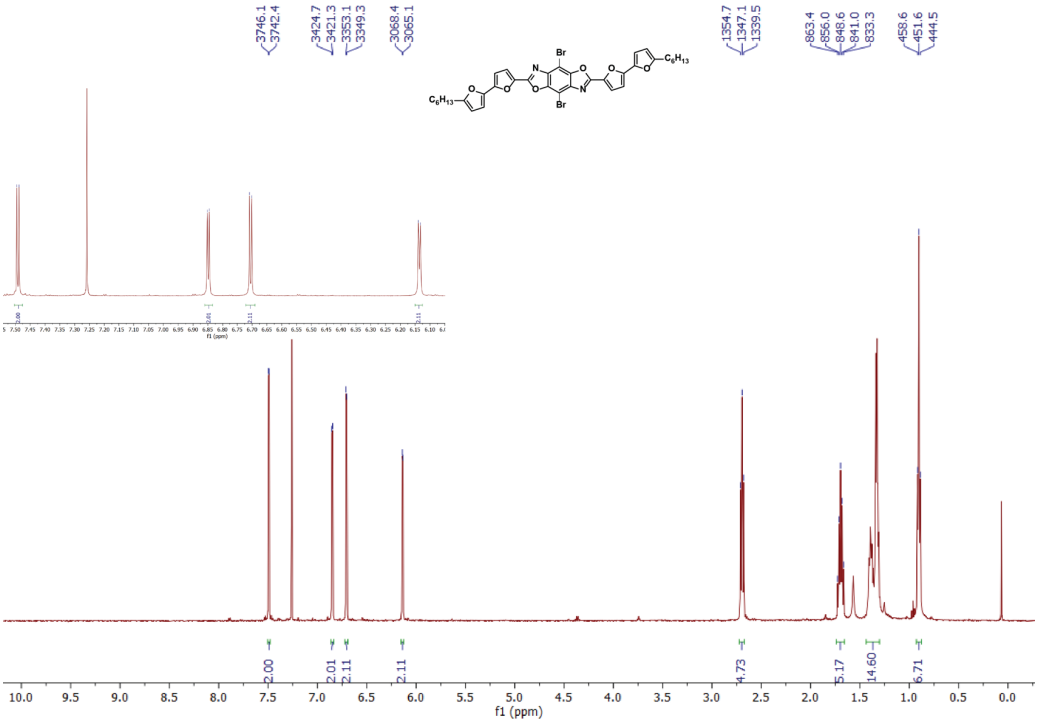


Figure S18. ^{1}H NMR of 26BF48Br

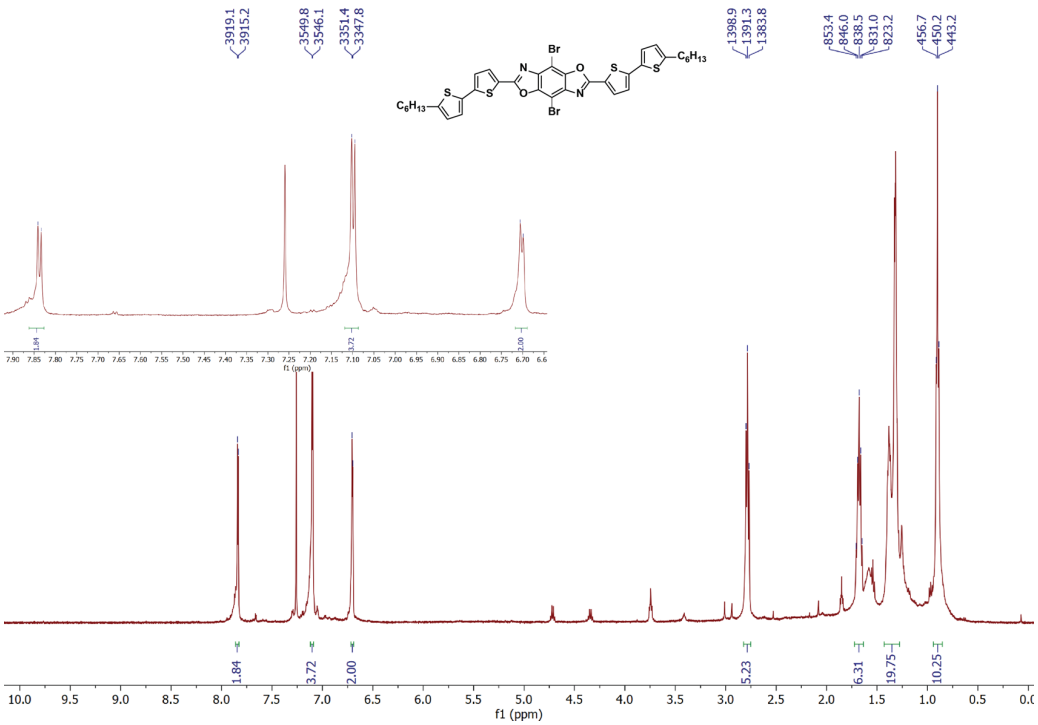


Figure S19. ^{1}H NMR of 26BT48Br

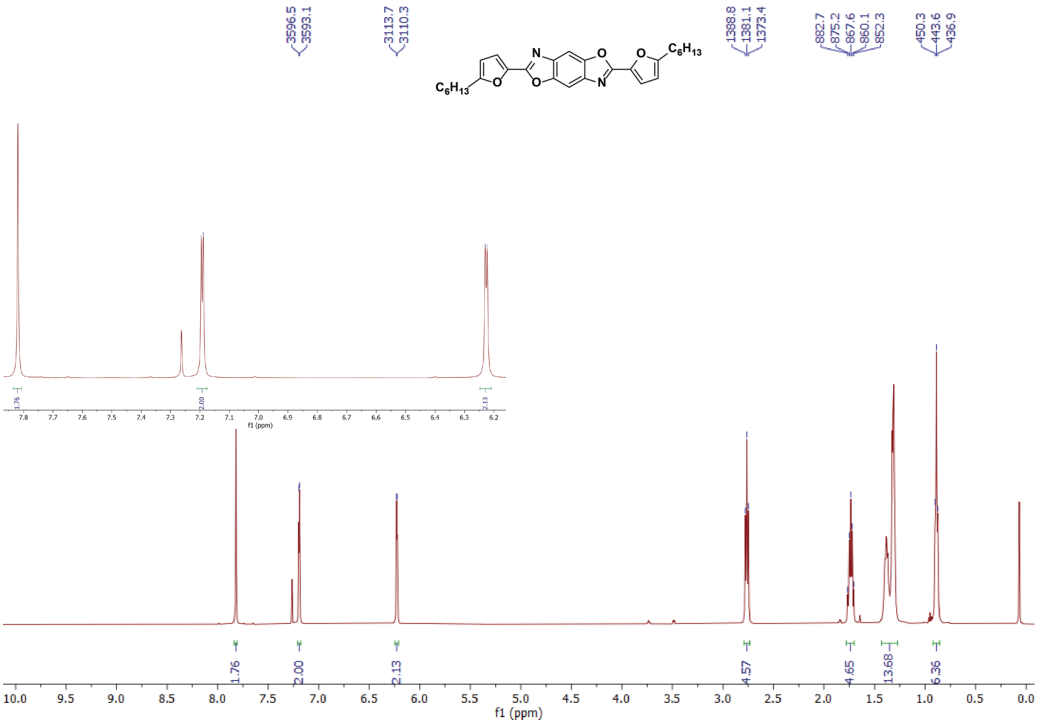


Figure S20. ^{1}H NMR of 26F

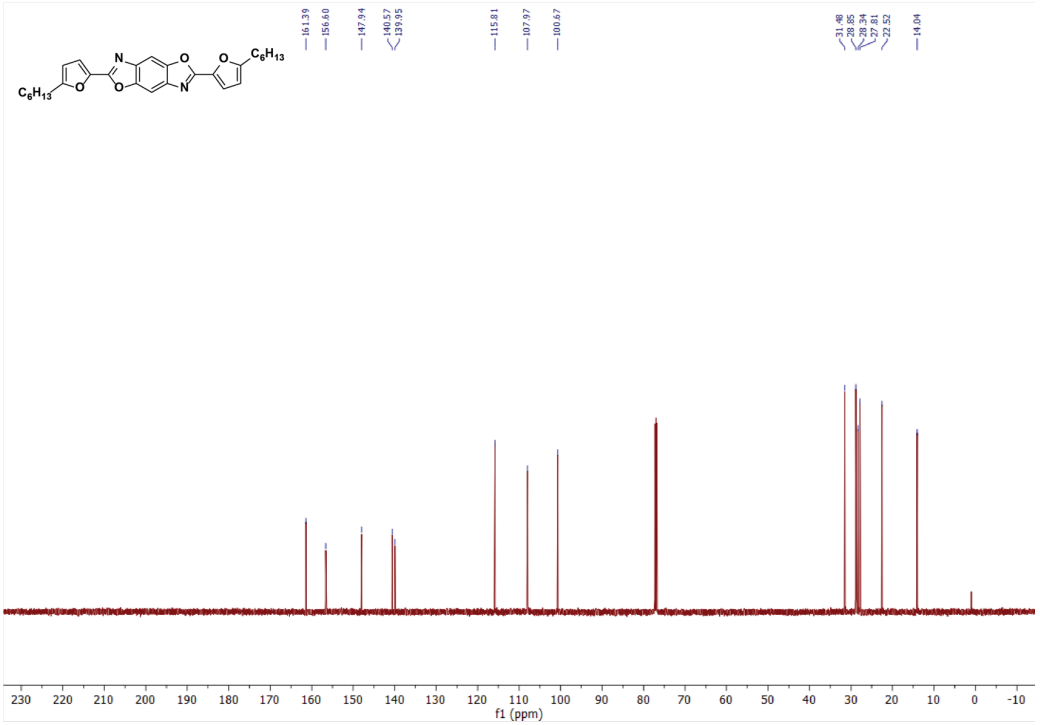


Figure S21. ^{13}C NMR of 26F

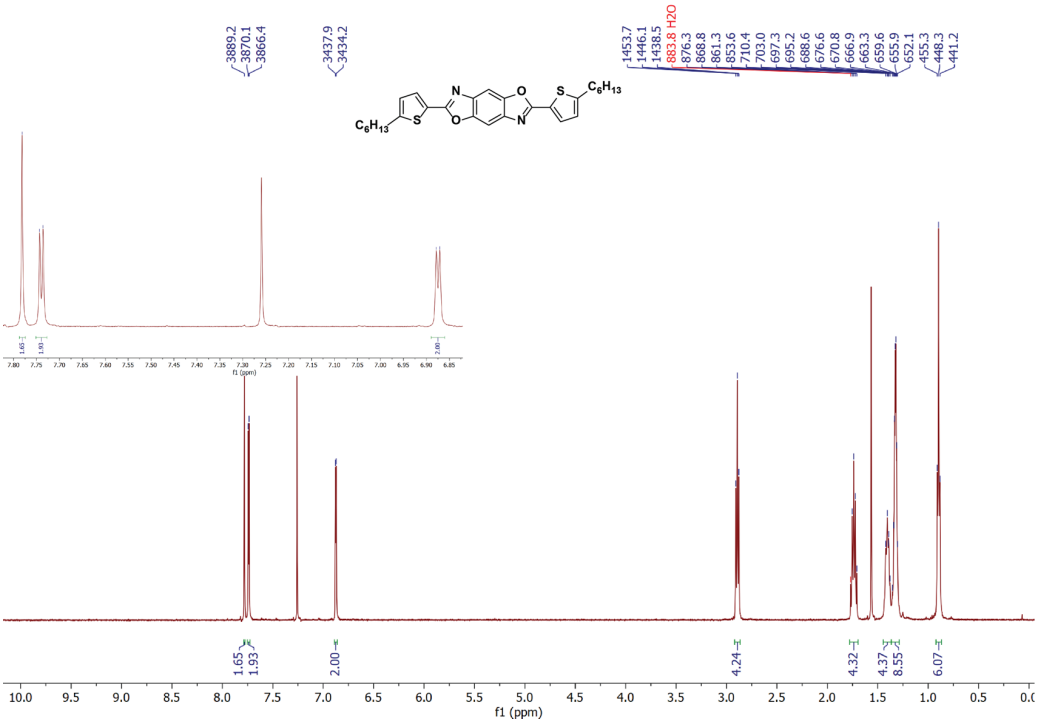


Figure S22. ^{1}H NMR of 26T

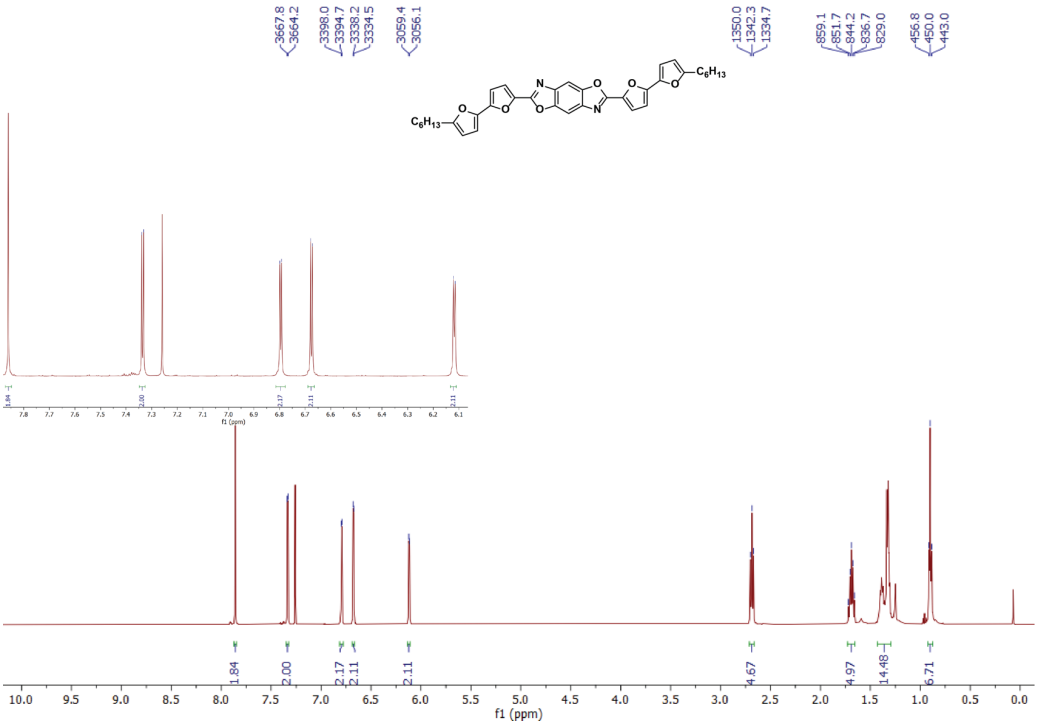


Figure S23. ^{1}H NMR of 26BF

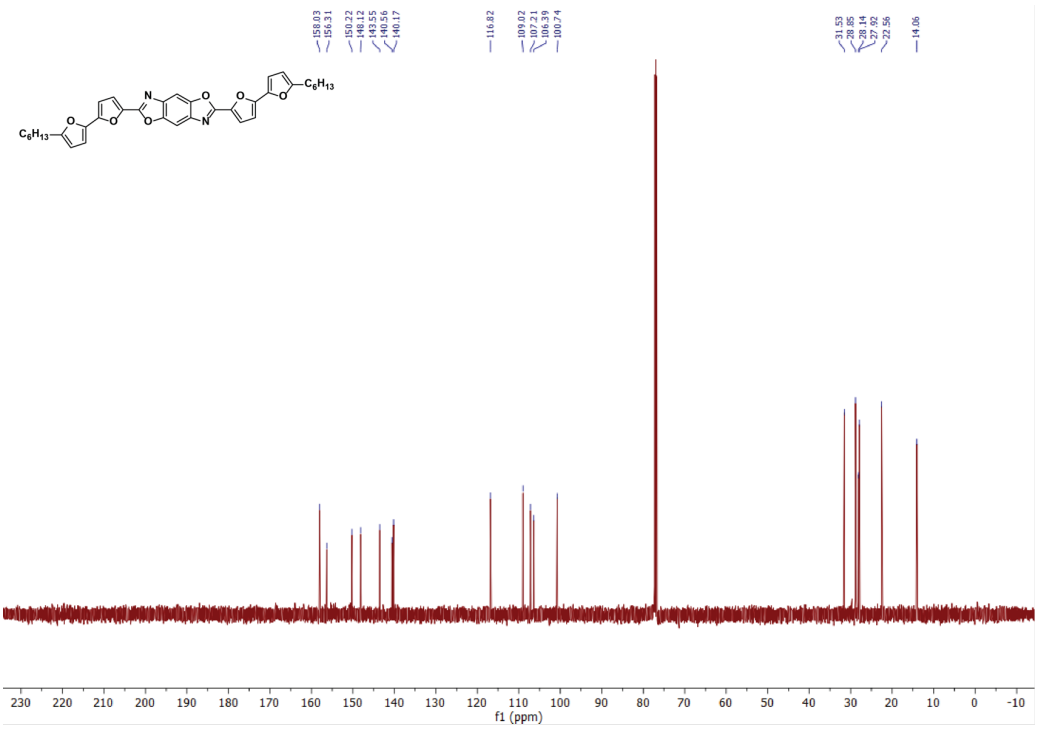


Figure S24. ^{13}C NMR of 26BF

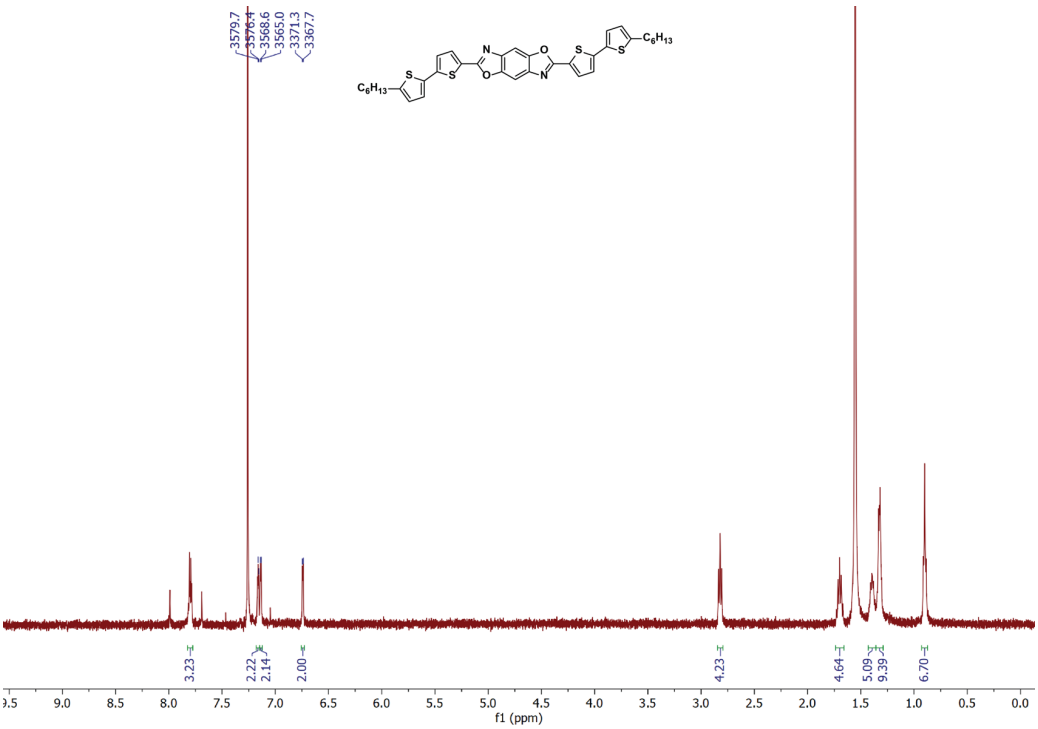


Figure S25. ^{1}H NMR of 26BT

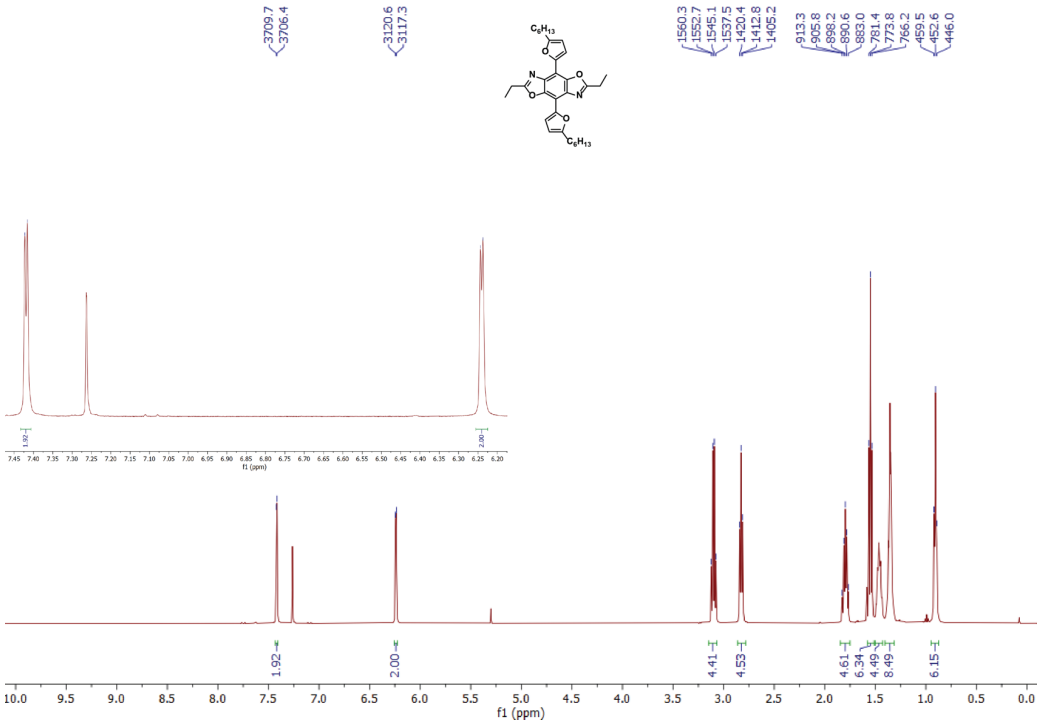


Figure S26. ^{1}H NMR of 48F

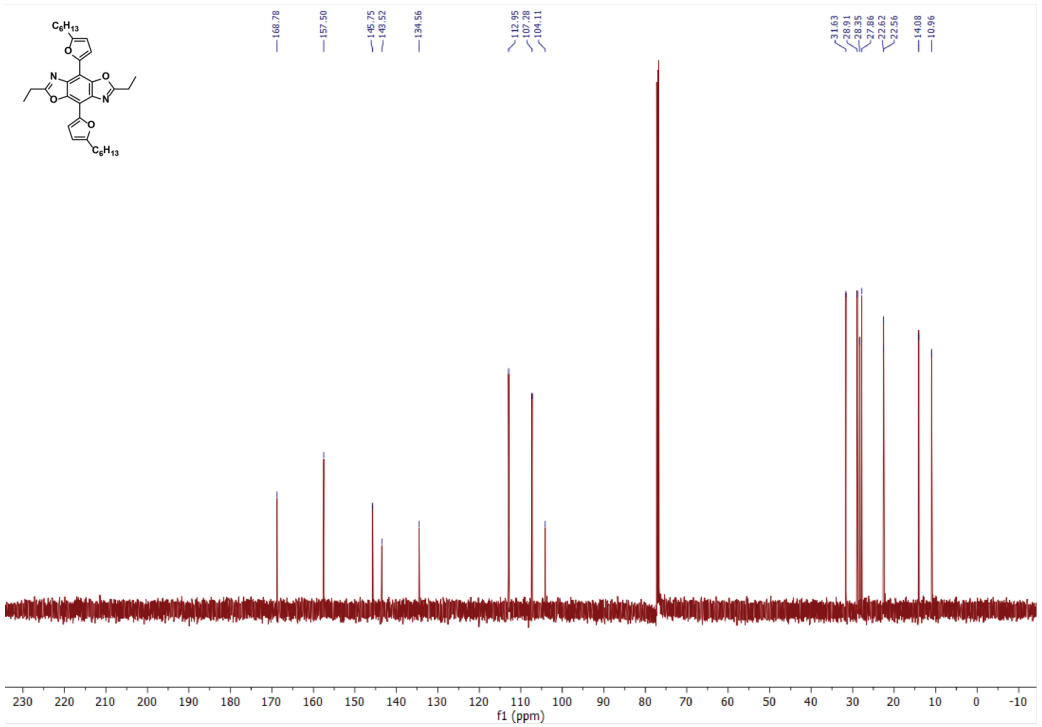


Figure S27. ^{13}C NMR of 48F

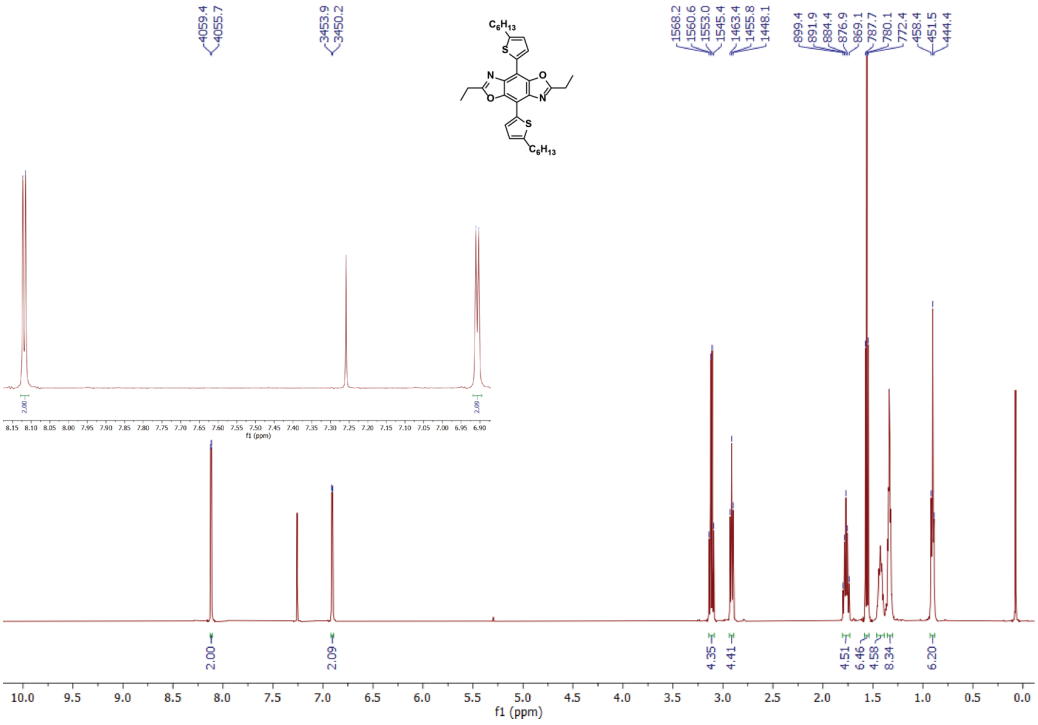


Figure S28. ^{1}H NMR of 48T

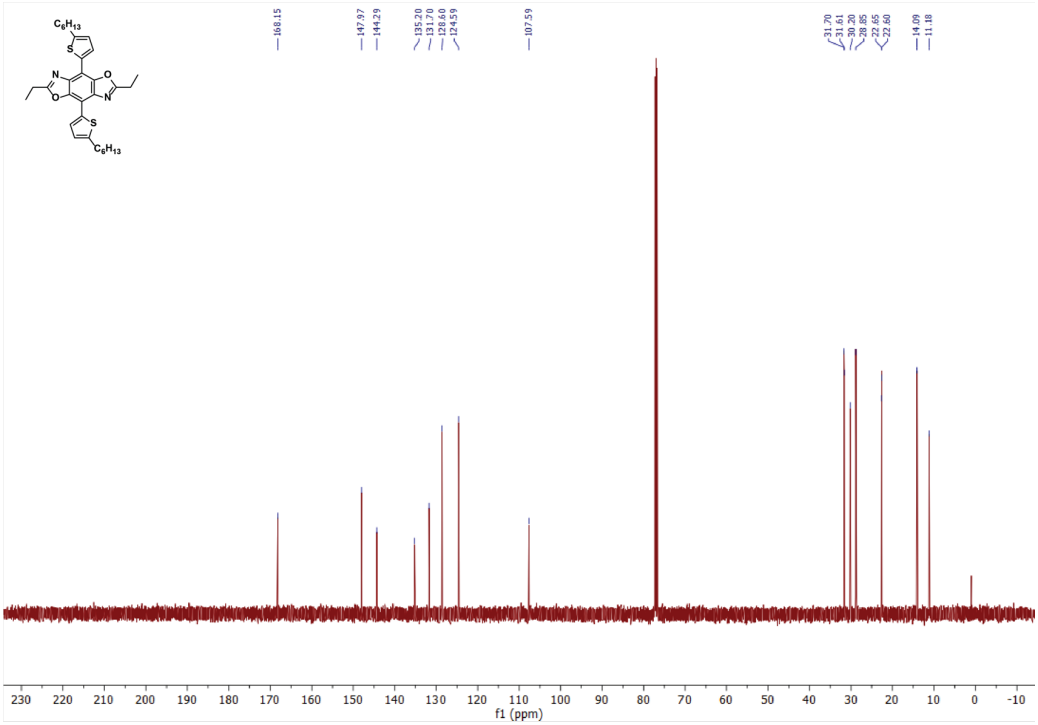


Figure S29. ^{13}C NMR of 48T

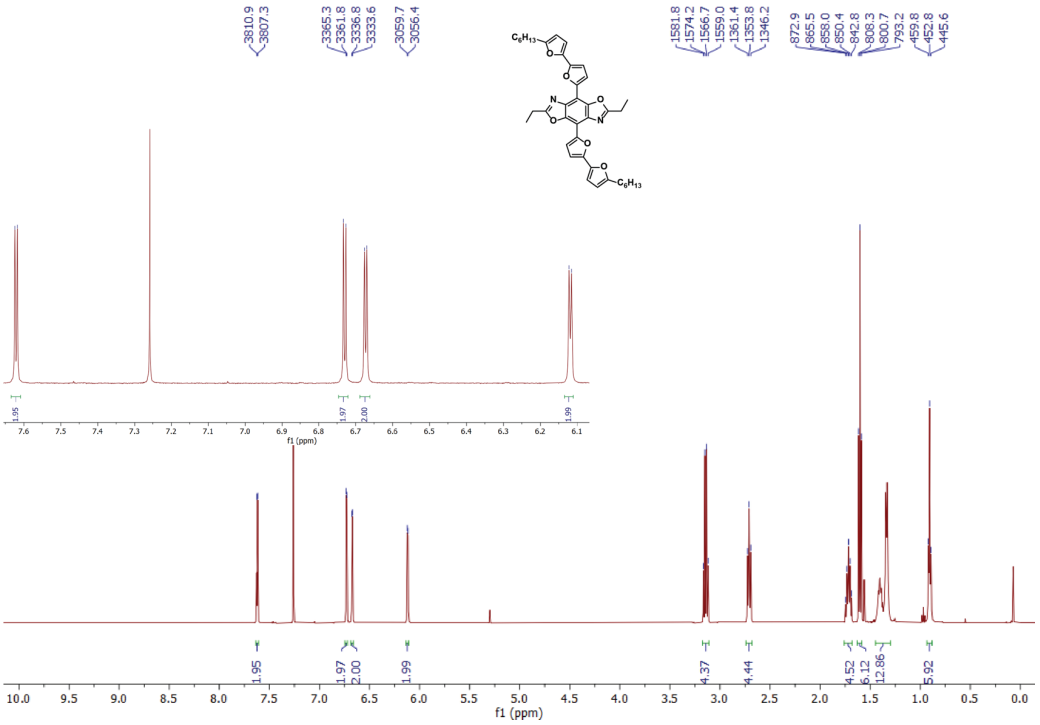


Figure S30. ^{1}H NMR of 48BF

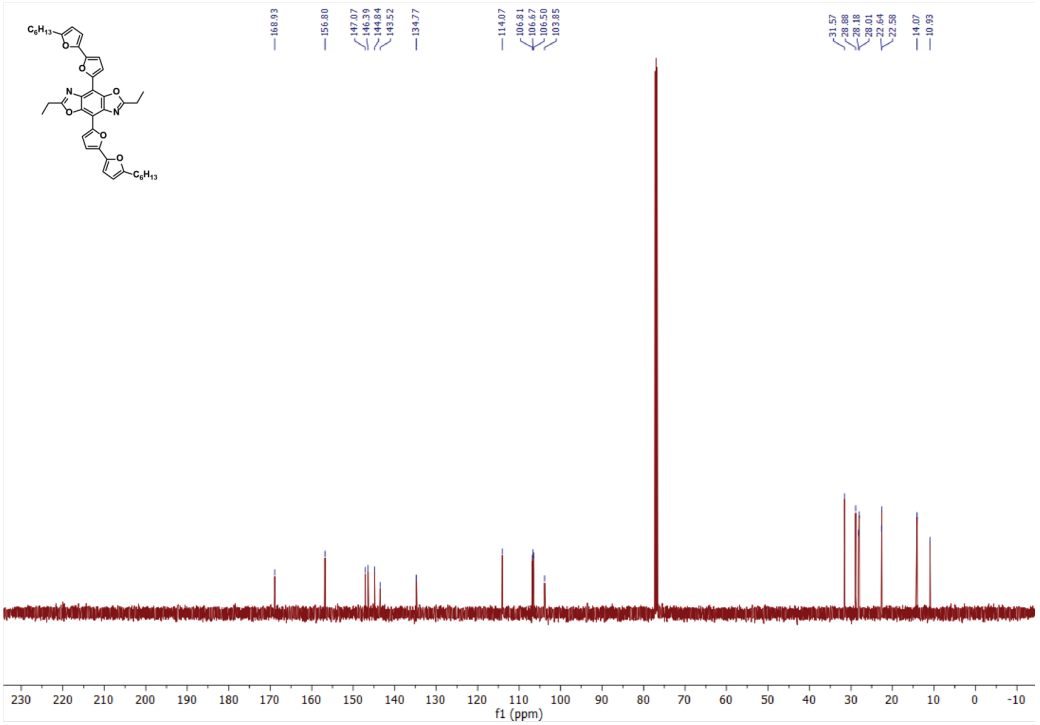


Figure S31. ^{13}C NMR of 48BF

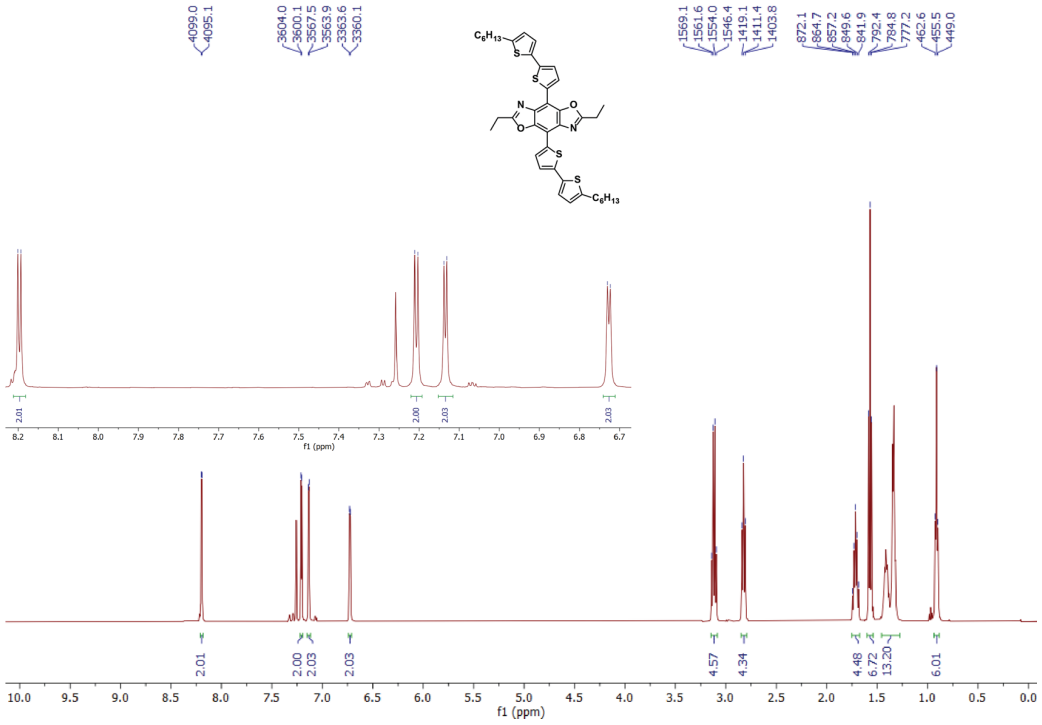


Figure S32. ^{1}H NMR of 48BT

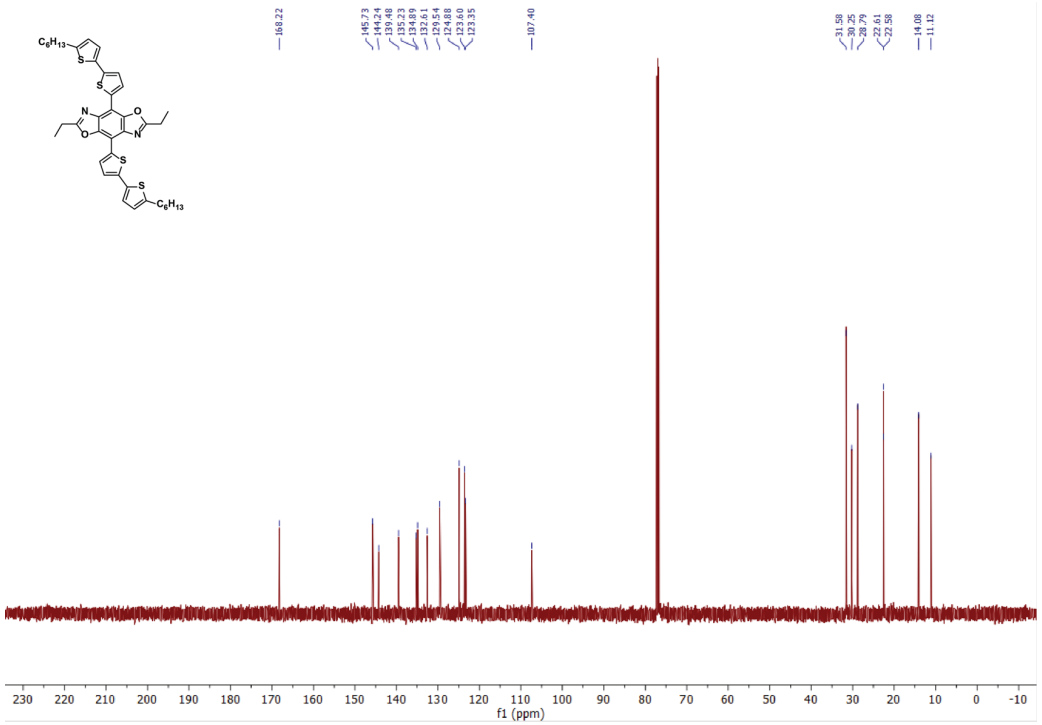


Figure S33. ^{13}C NMR of 48BT

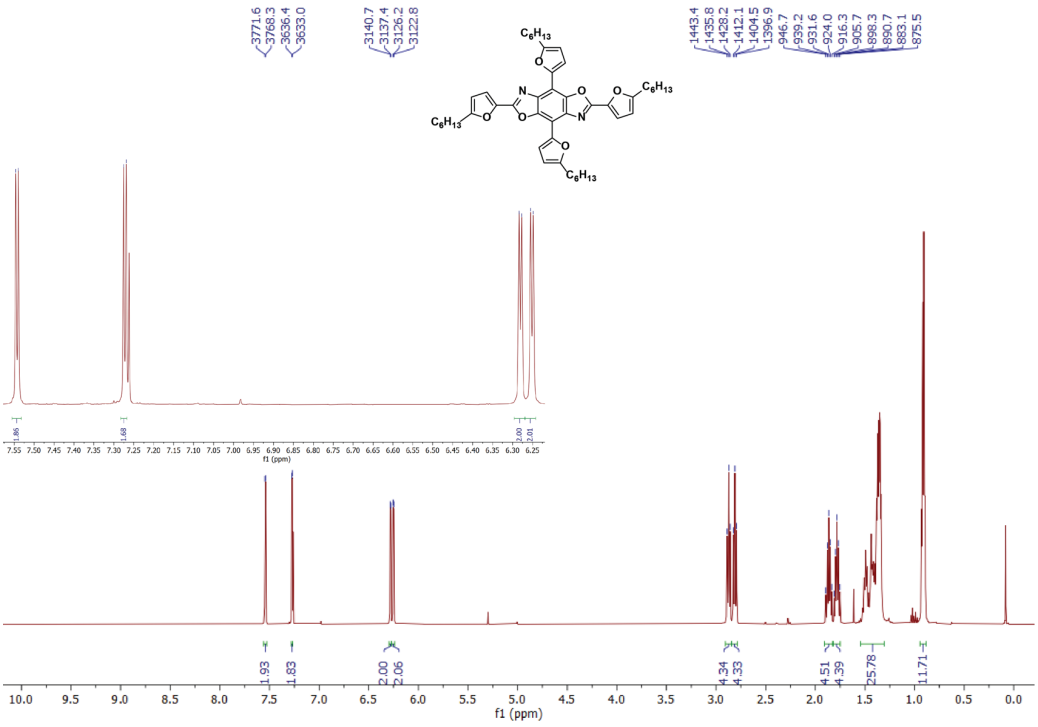


Figure S34. ^{1}H NMR of 26F48F

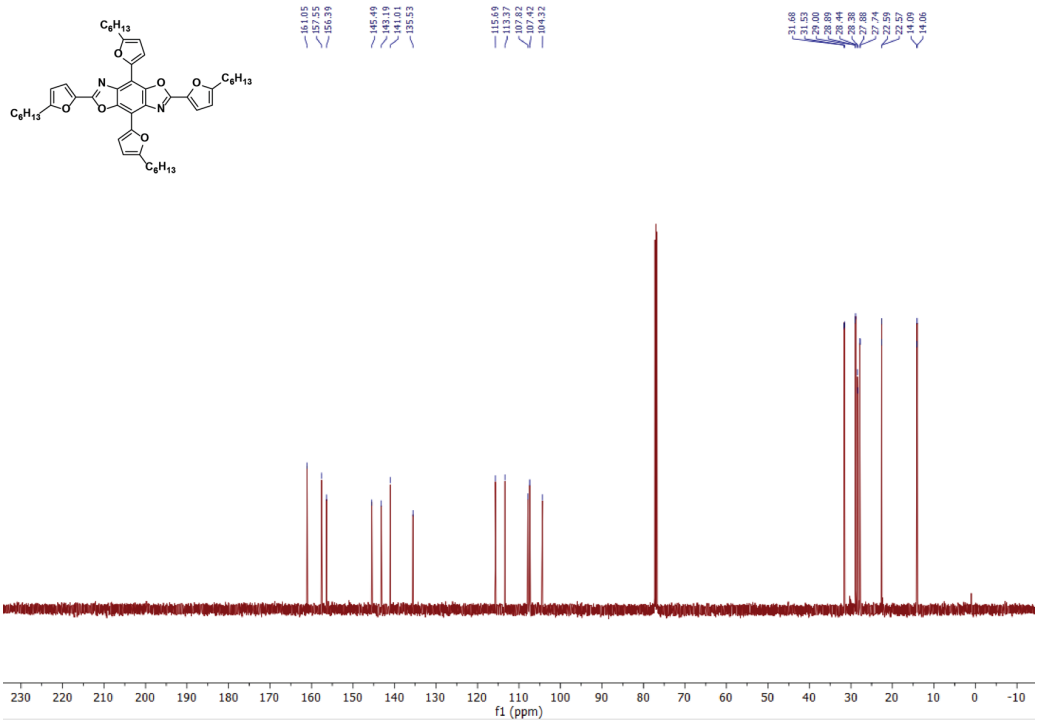


Figure S35. ^{13}C NMR of 26F48F

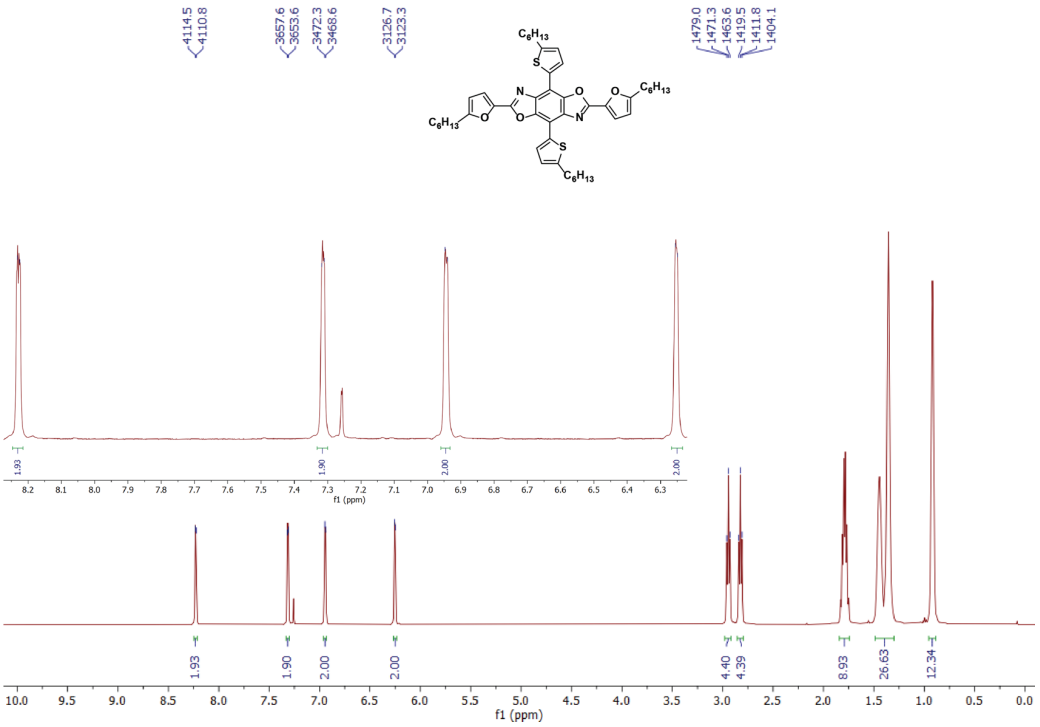


Figure S36. ^{1}H NMR of 26F48T

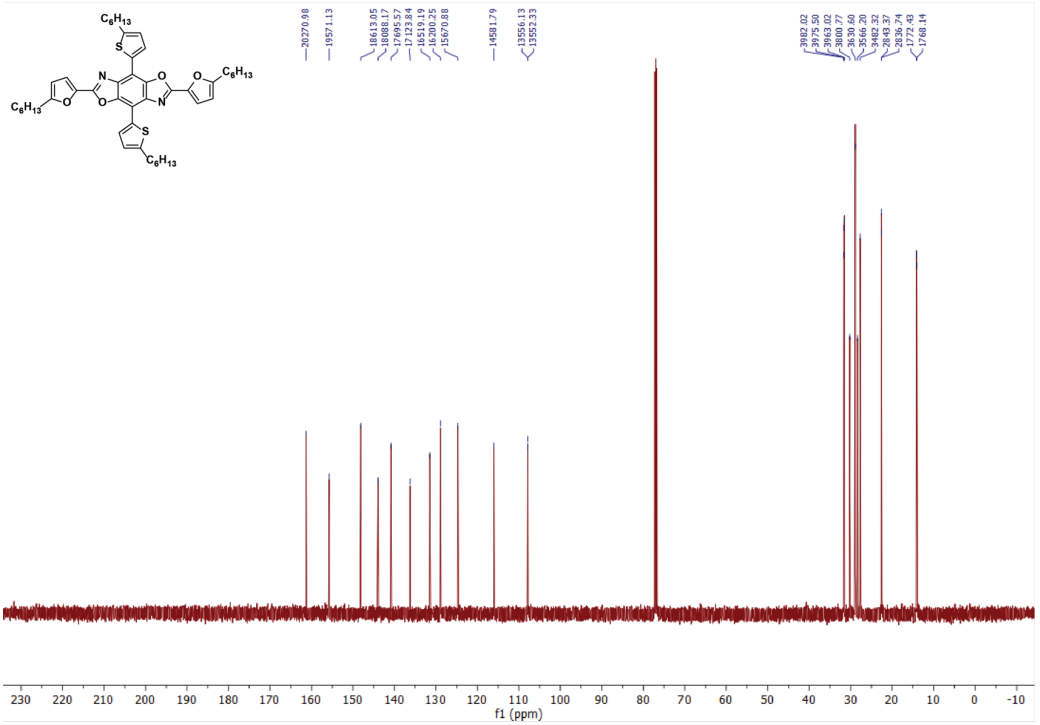


Figure S37. ^{13}C NMR of 26F48T

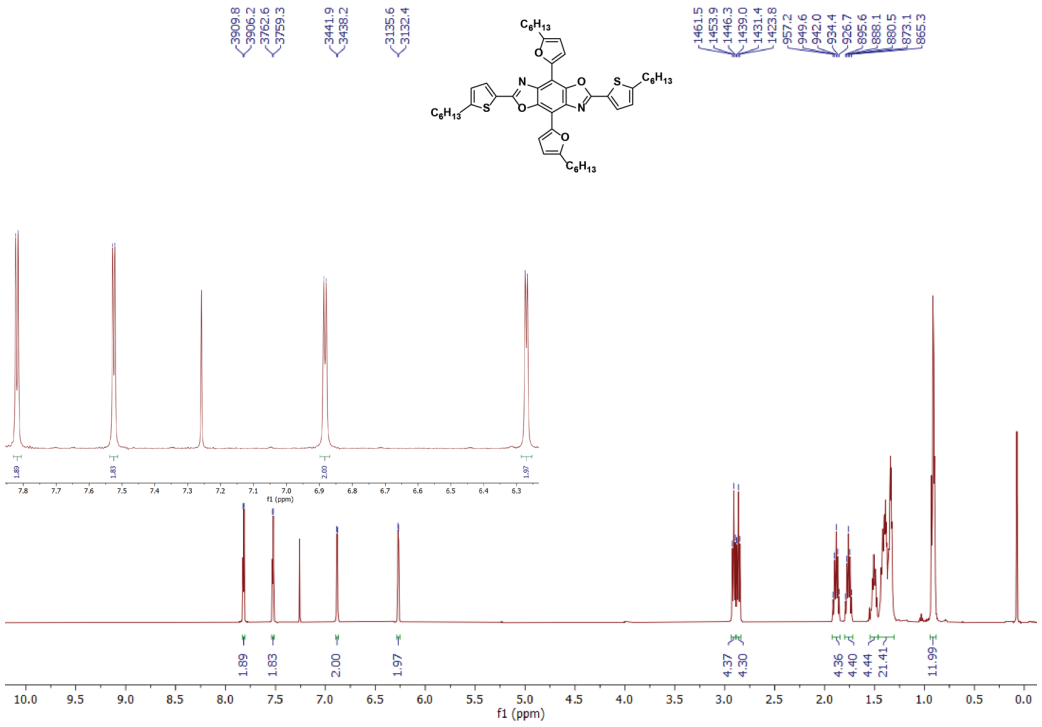


Figure S38. ^{1}H NMR of 26T48F

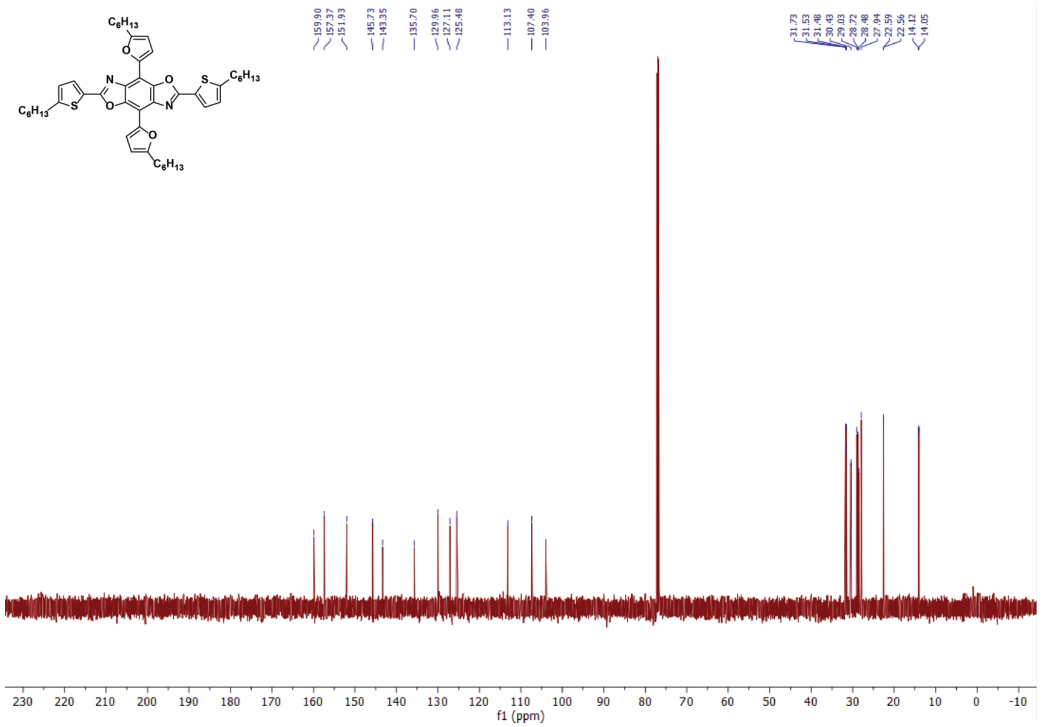


Figure S39. ^{13}C NMR of 26T48F

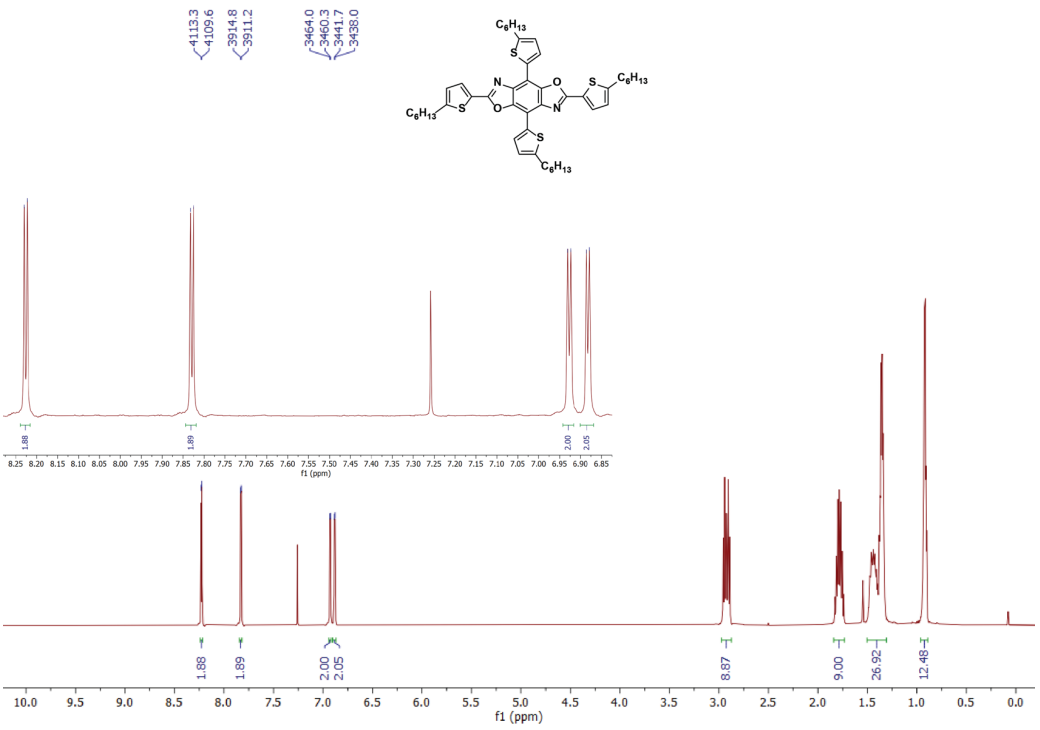


Figure S40. ^{1}H NMR of 26T48T

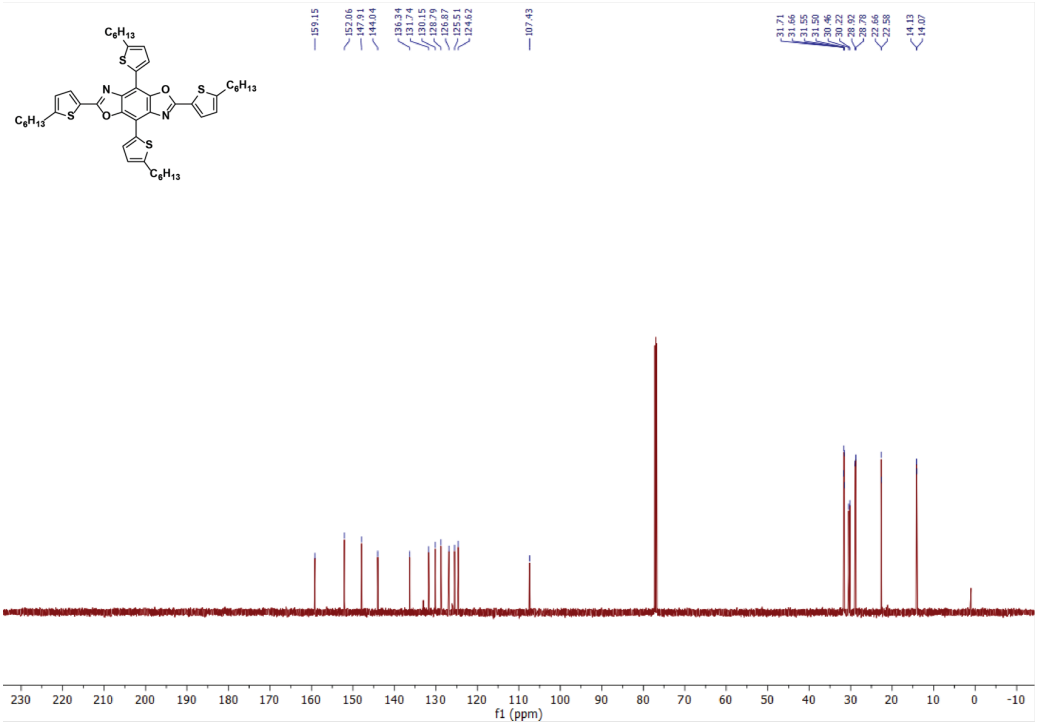


Figure S41. ^{13}C NMR of 26T48T

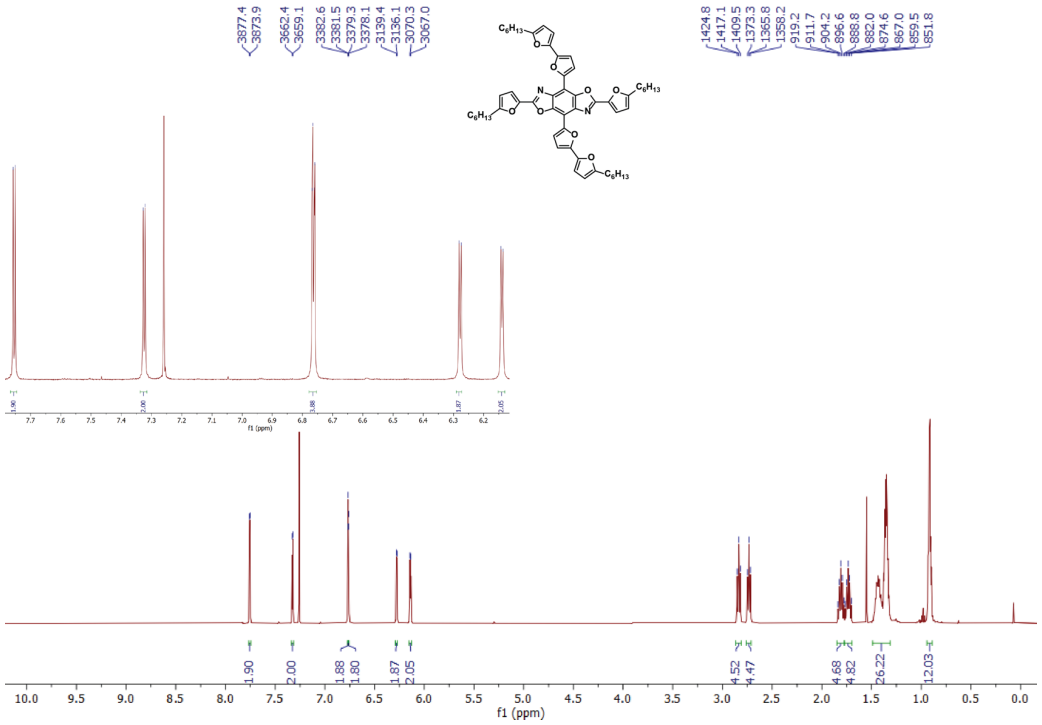


Figure S42. ^{1}H NMR of 26F48BF

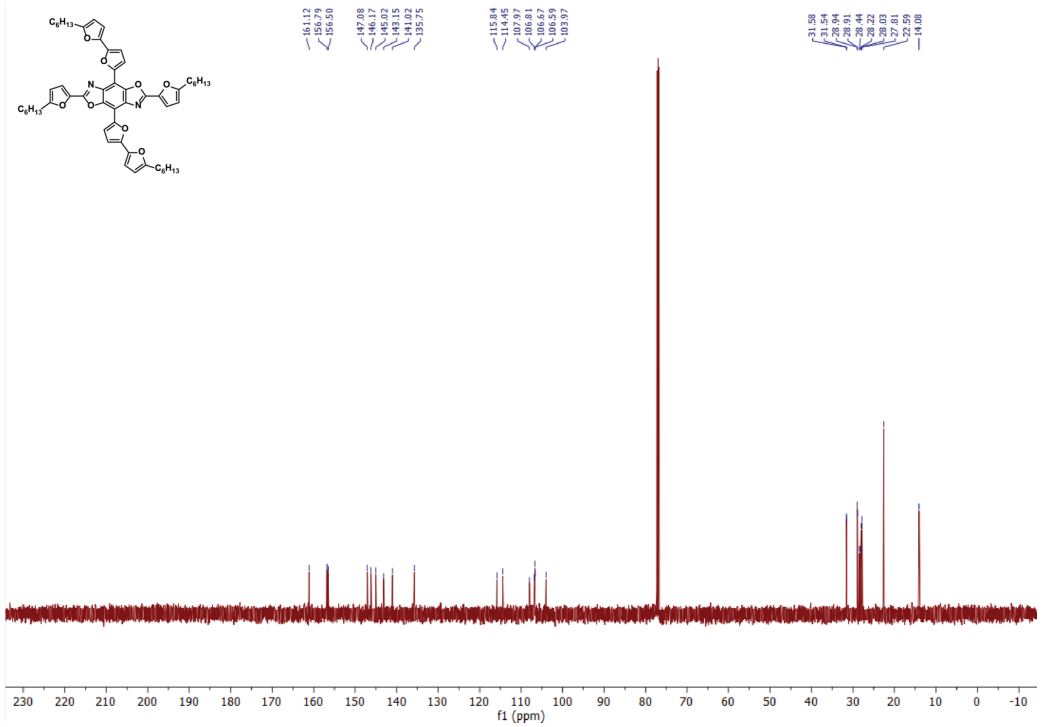


Figure S43. ^{13}C NMR of 26F48BF

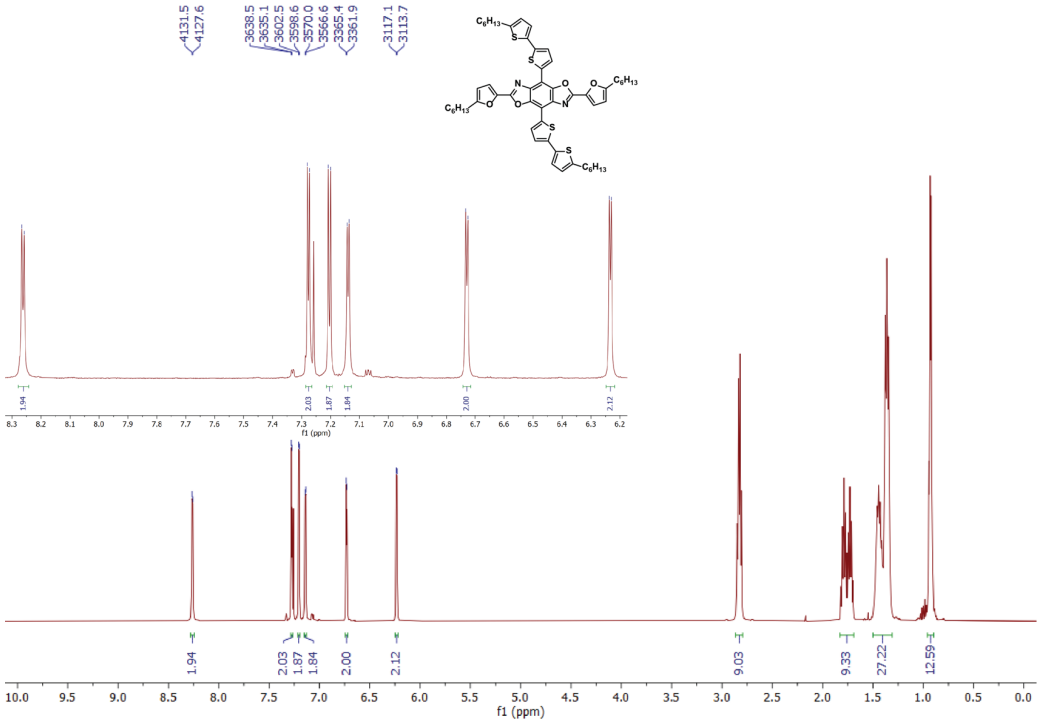


Figure S44. ^{1}H NMR of 26F48BT

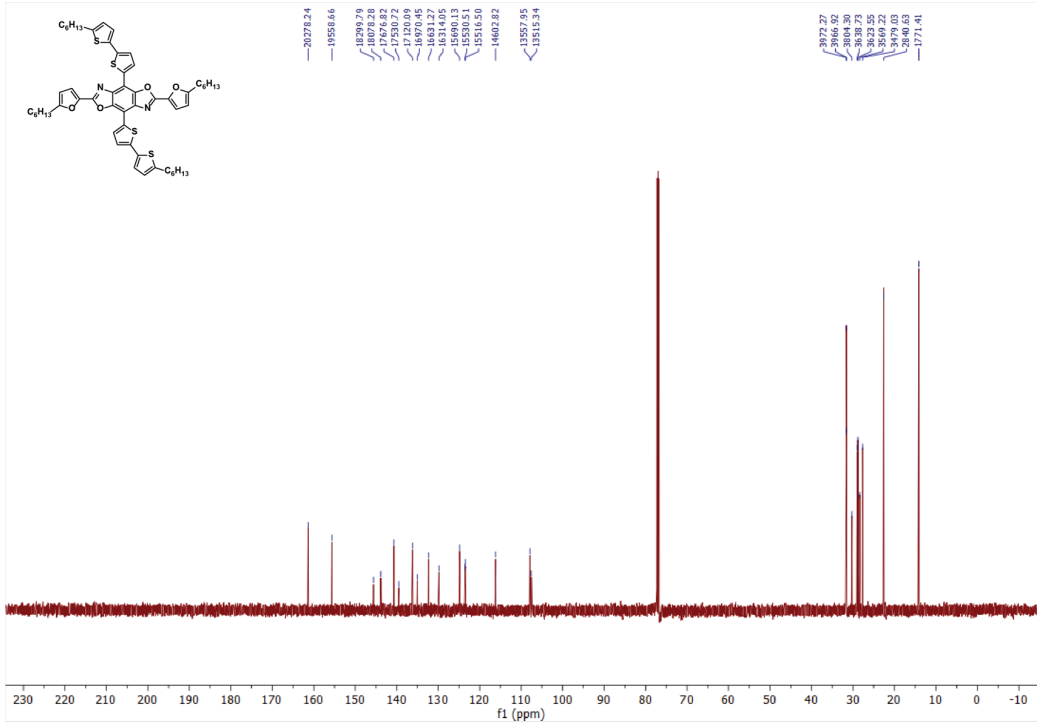


Figure S45. ^{13}C NMR of 26F48BT

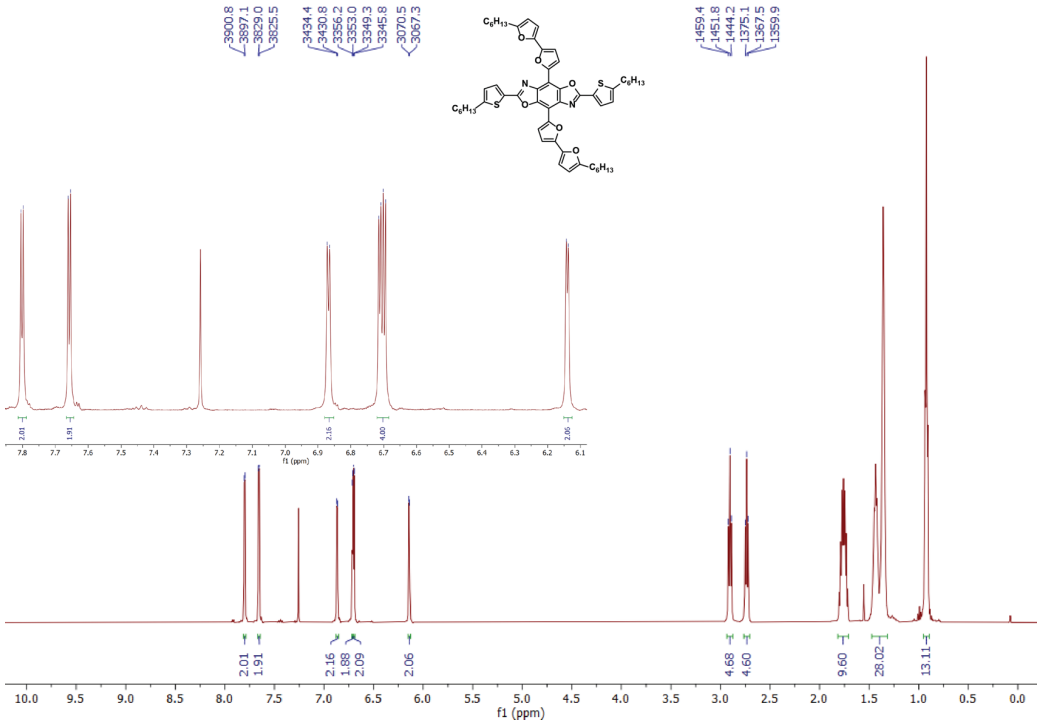


Figure S46. ^{1}H NMR of 26T48BF

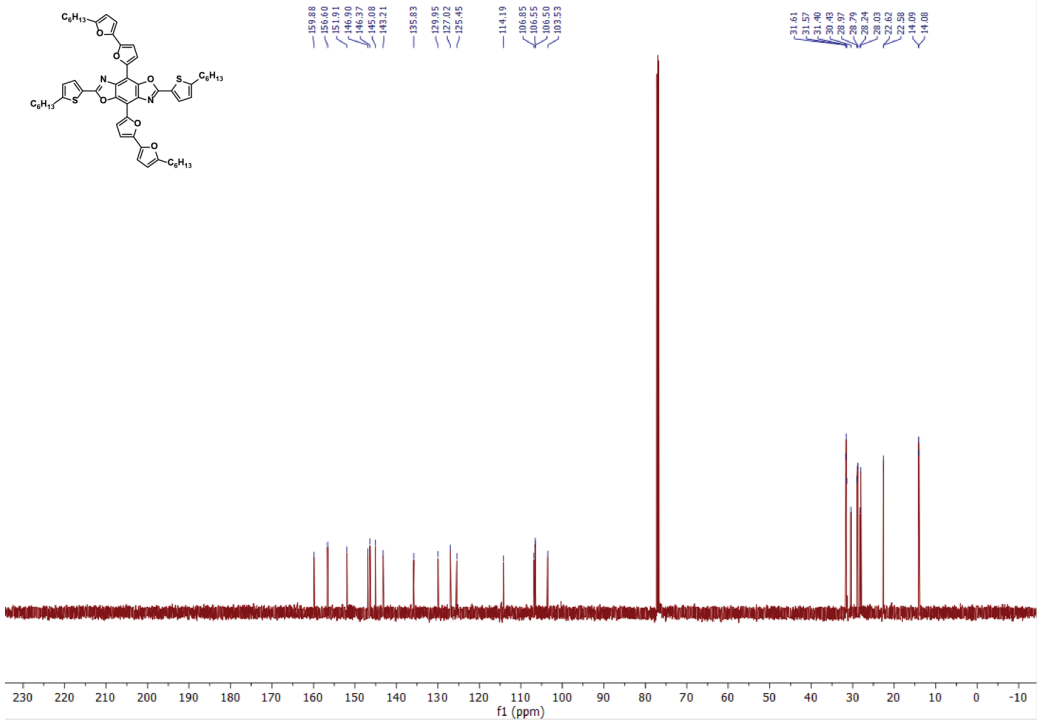


Figure S47. ^{13}C NMR of 26T48BF

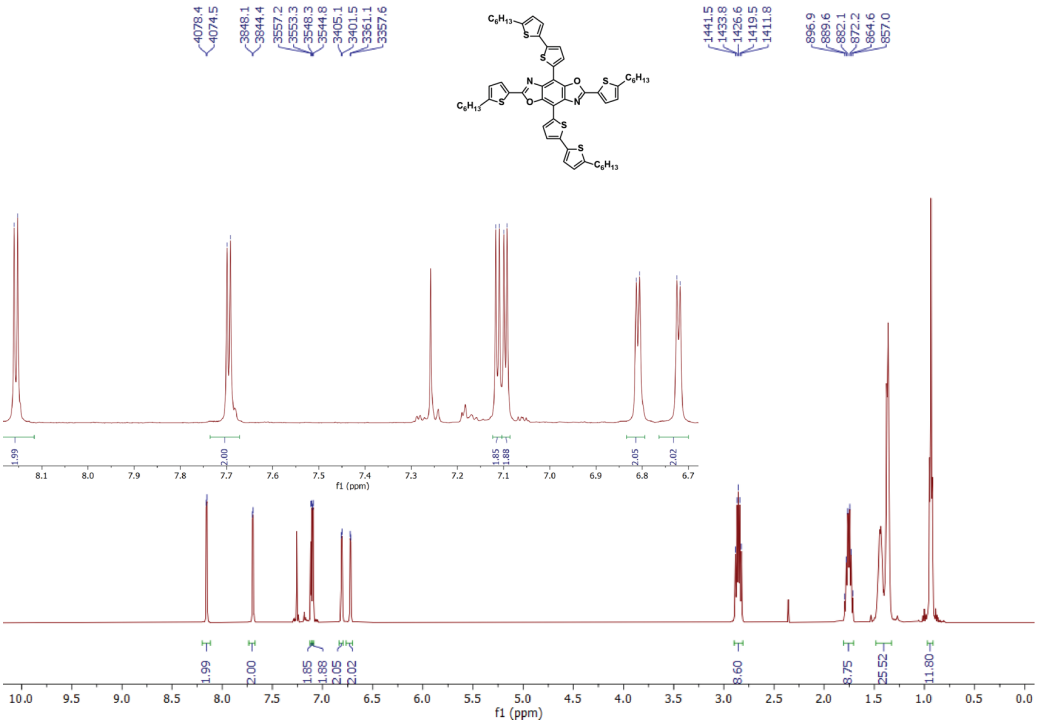


Figure S48. ^{1}H NMR of 26T48BT

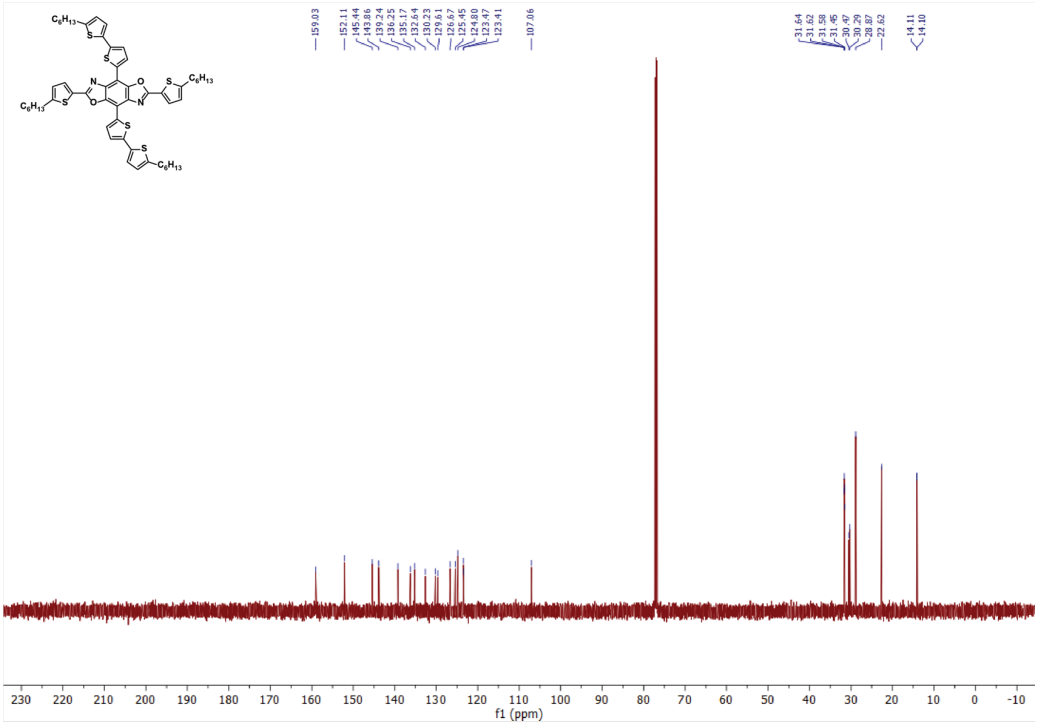


Figure S49. ^{13}C NMR of 26T48BT

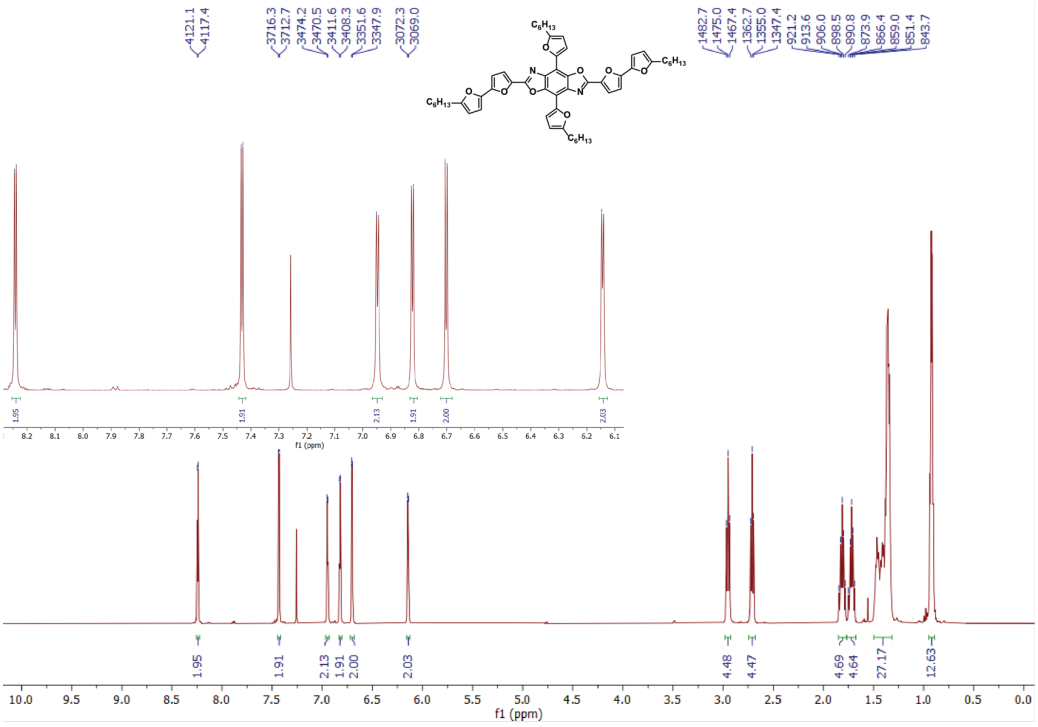


Figure S50. ^{1}H NMR of 26BF48F

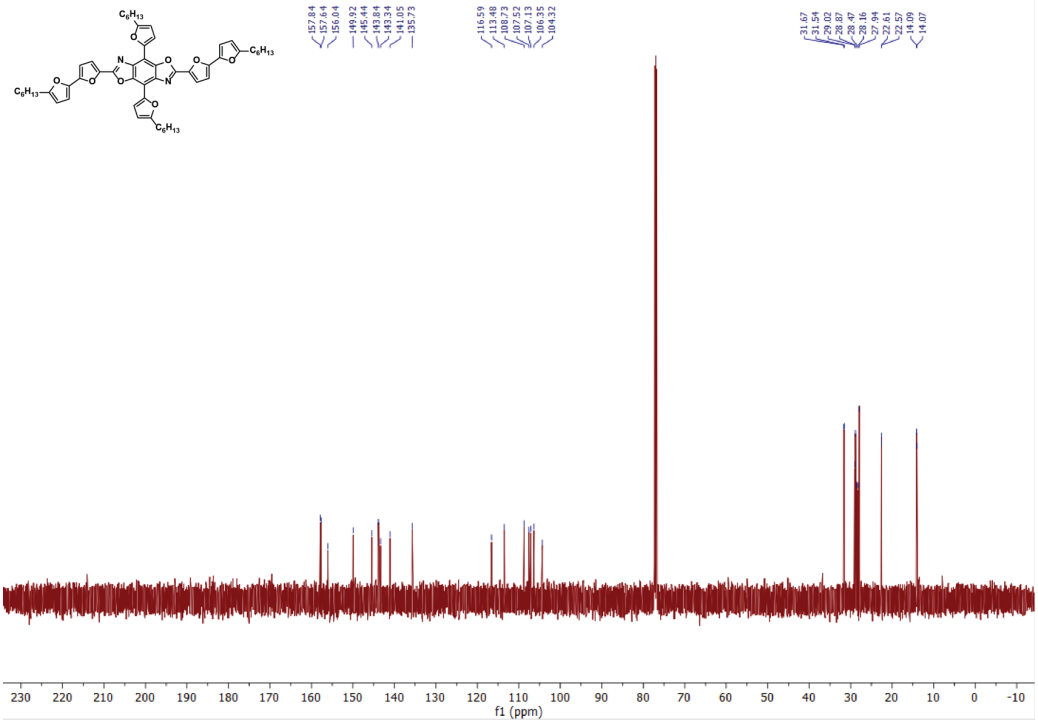


Figure S51. ^{13}C NMR of 26BF48F

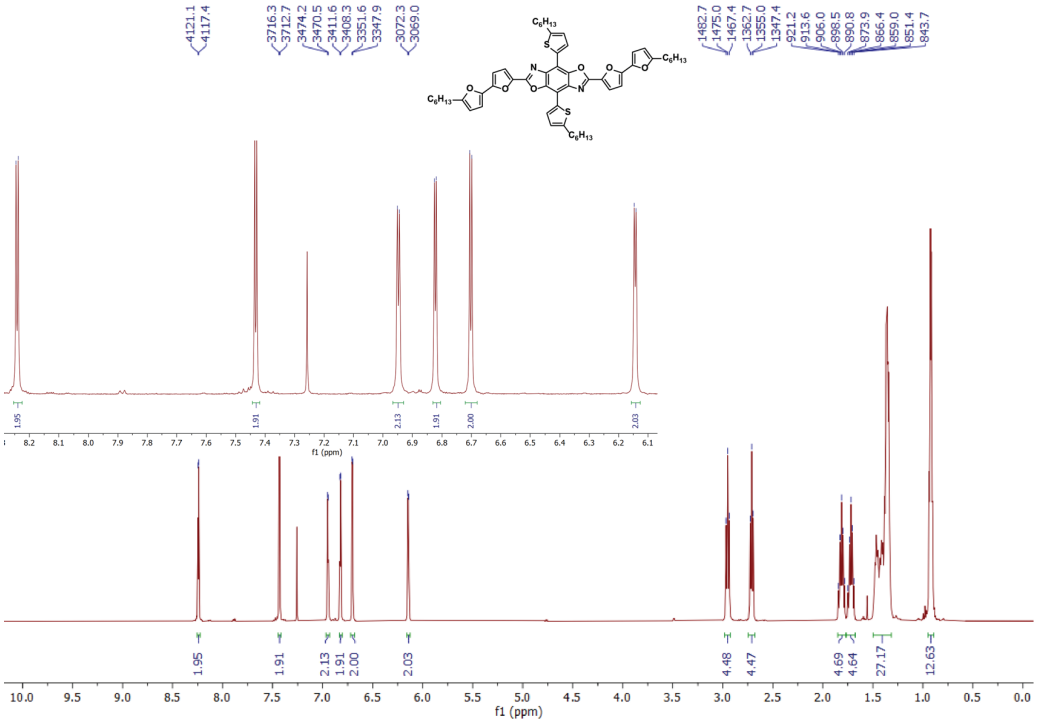


Figure S52. ^{1}H NMR of 26BF48T

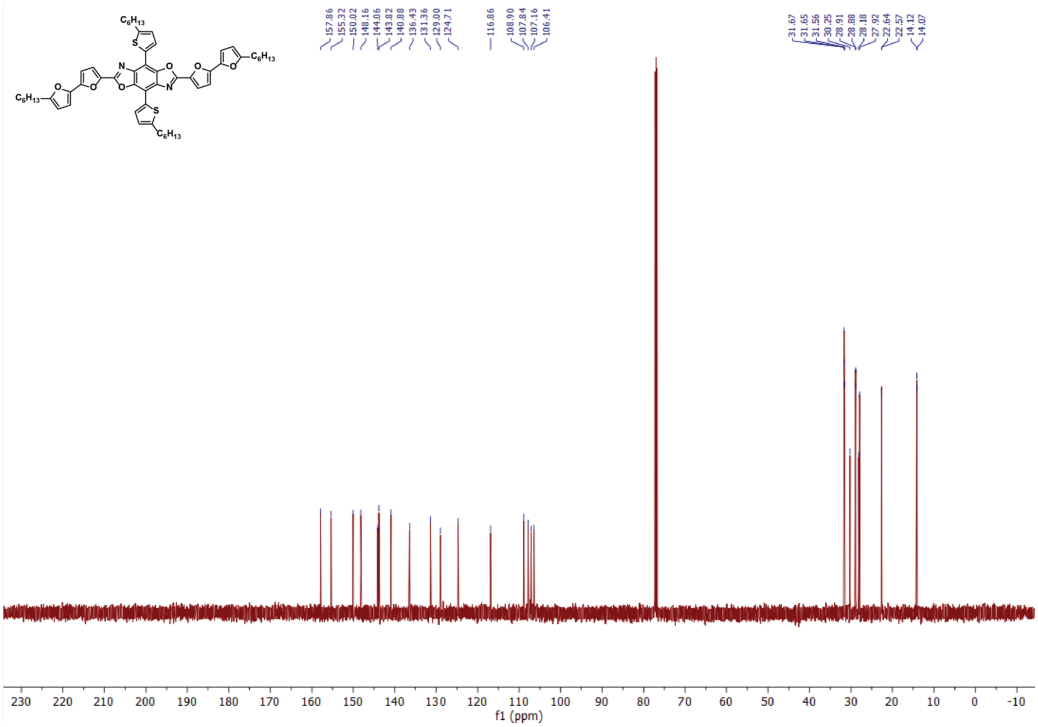


Figure S53. ^{13}C NMR of 26BF48T

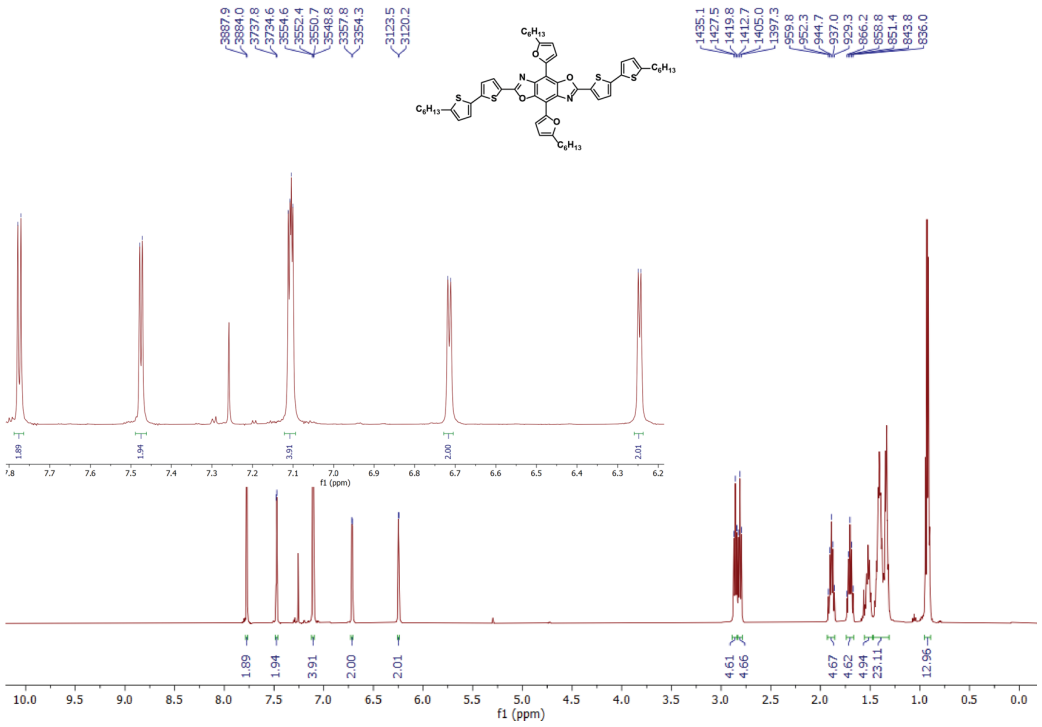


Figure S54. ^{1}H NMR of 26BT48F

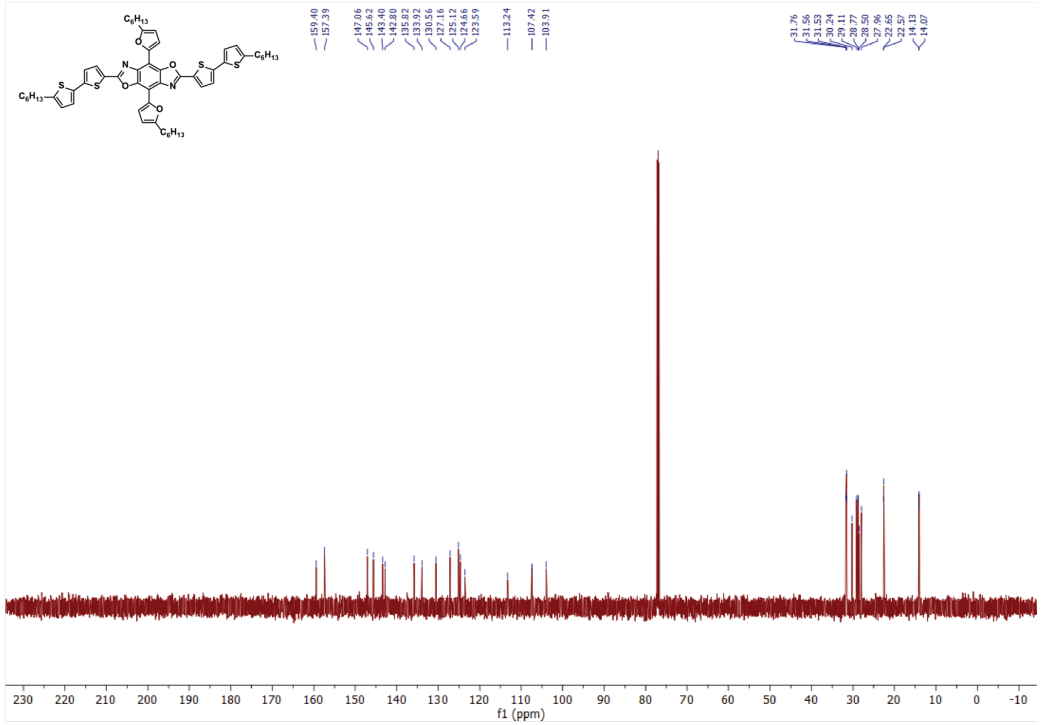


Figure S55. ^{13}C NMR of 26BT48F

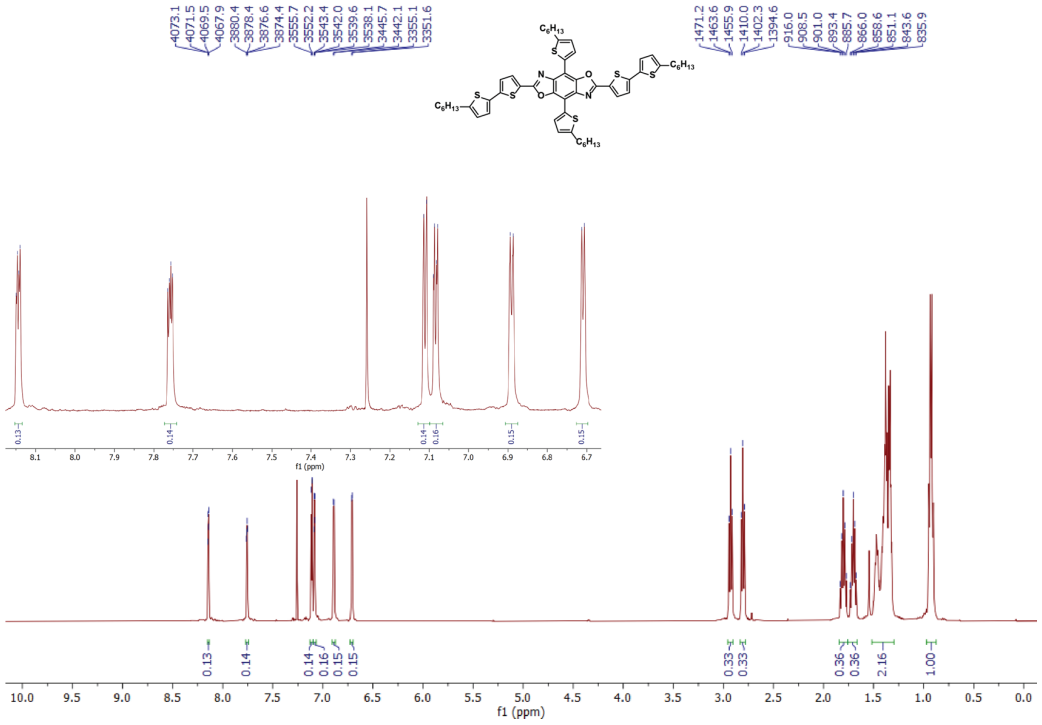


Figure S56. ^{1}H NMR of 26BT48T

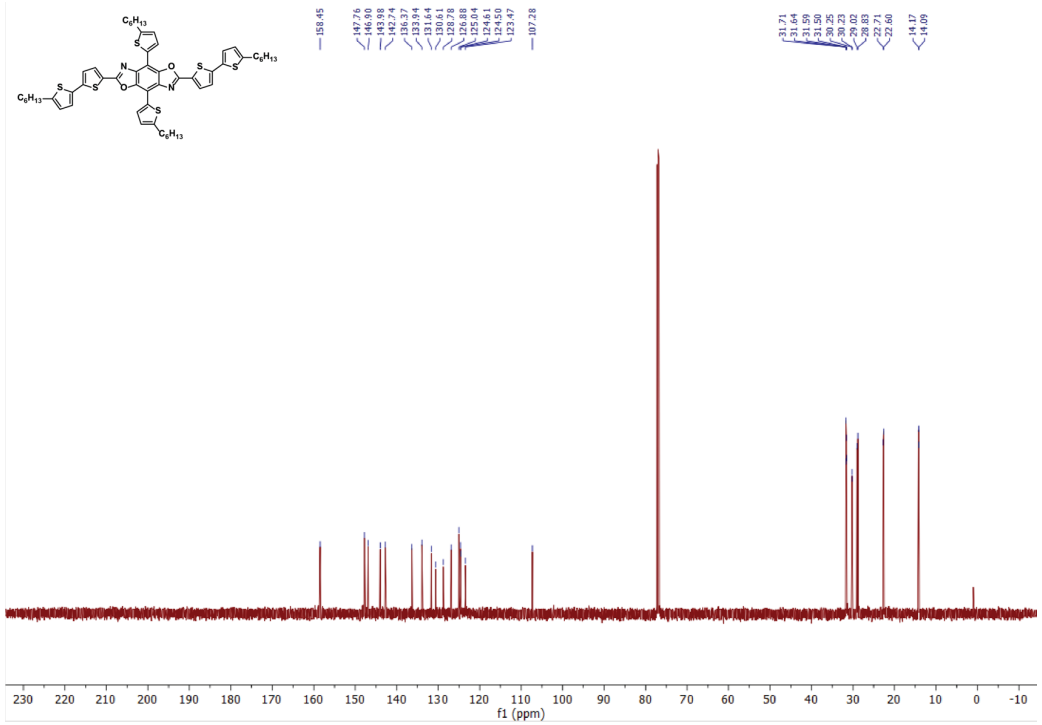


Figure S57. ^{13}C NMR of 26BT48T

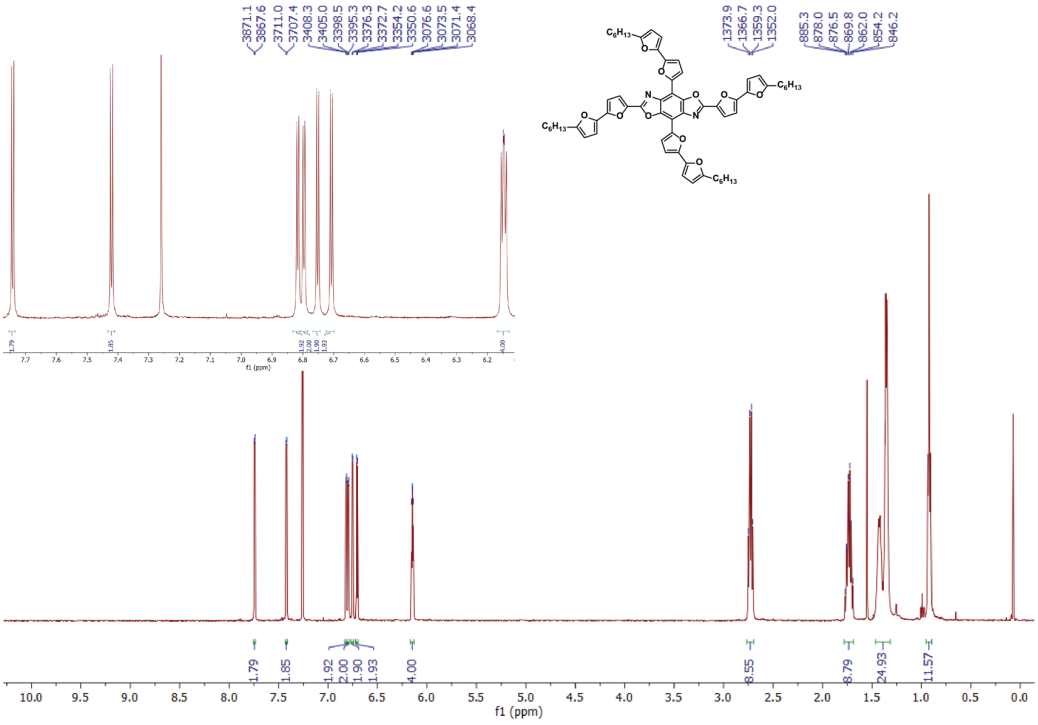


Figure S58. ^{1}H NMR of 26BF48BF

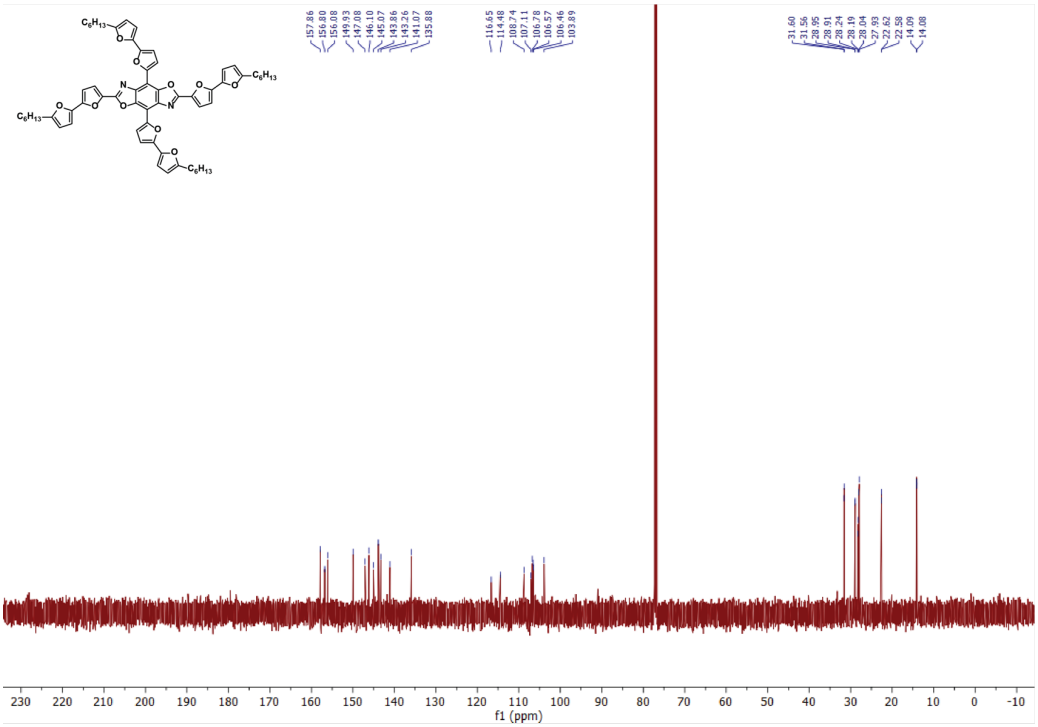


Figure S59. ^{13}C NMR of 26BF48BF

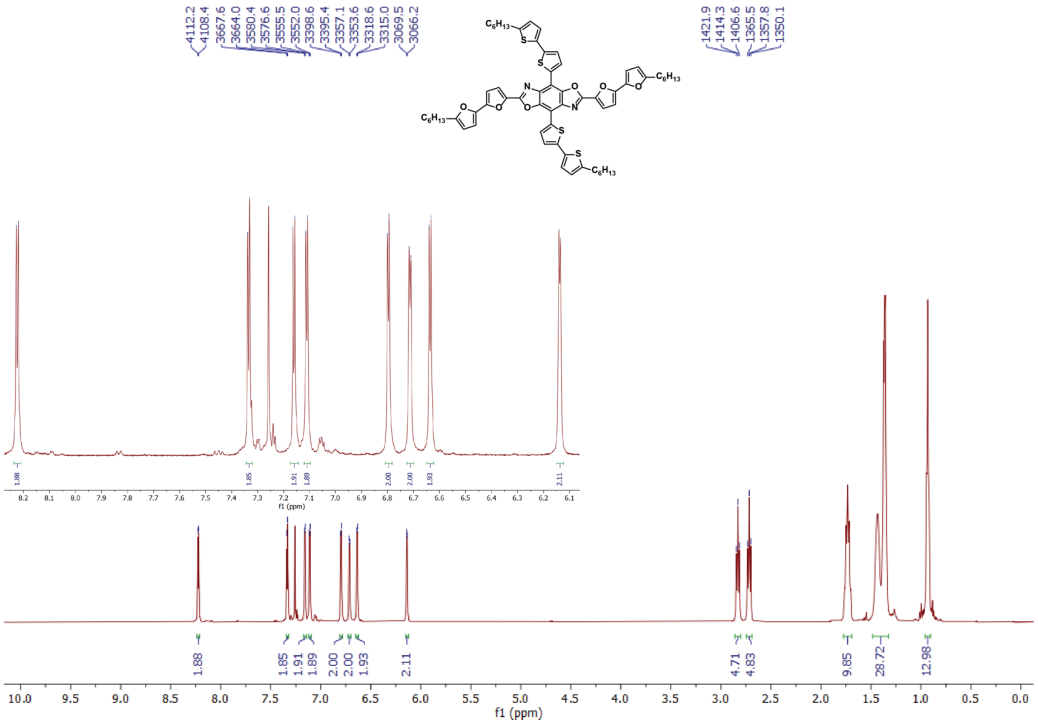


Figure S60. ^{1}H NMR of 26BF48BT

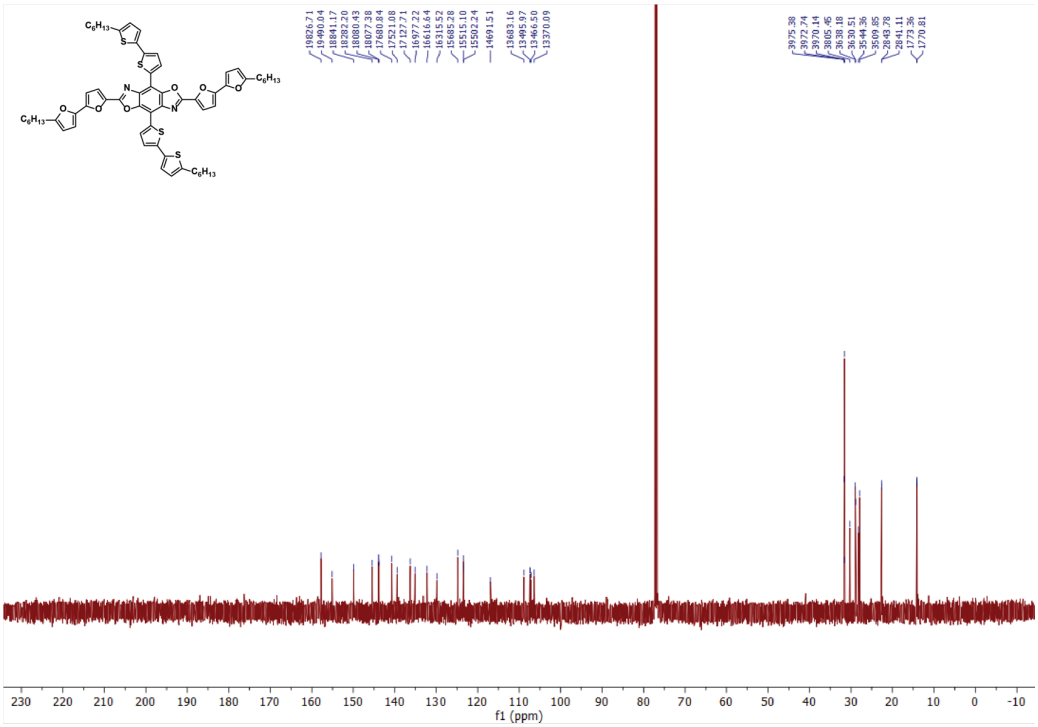


Figure S61. ^{13}C NMR of 26BF48BT

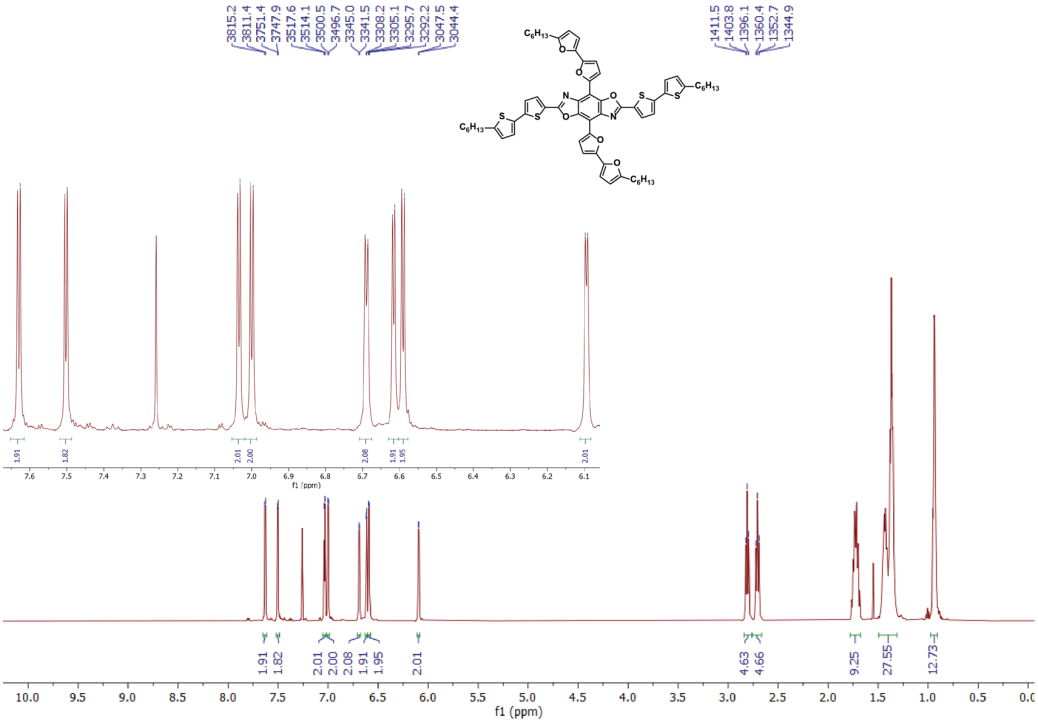


Figure S62. ^{1}H NMR of 26BT48BF

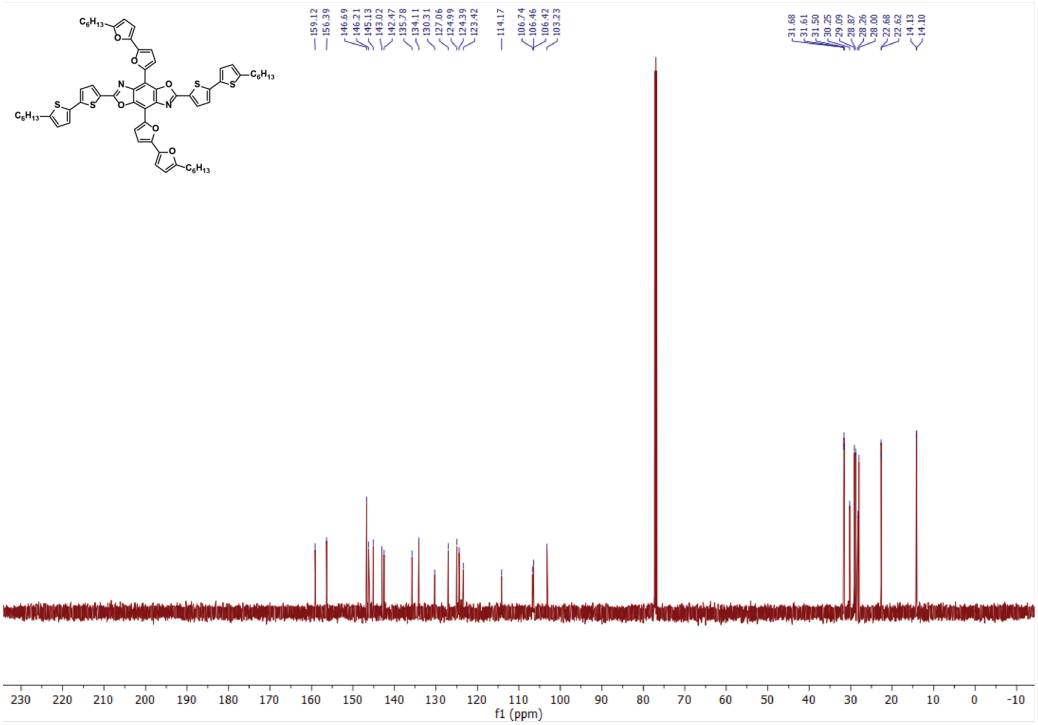


Figure S63. ^{13}C NMR of 26BT48BF

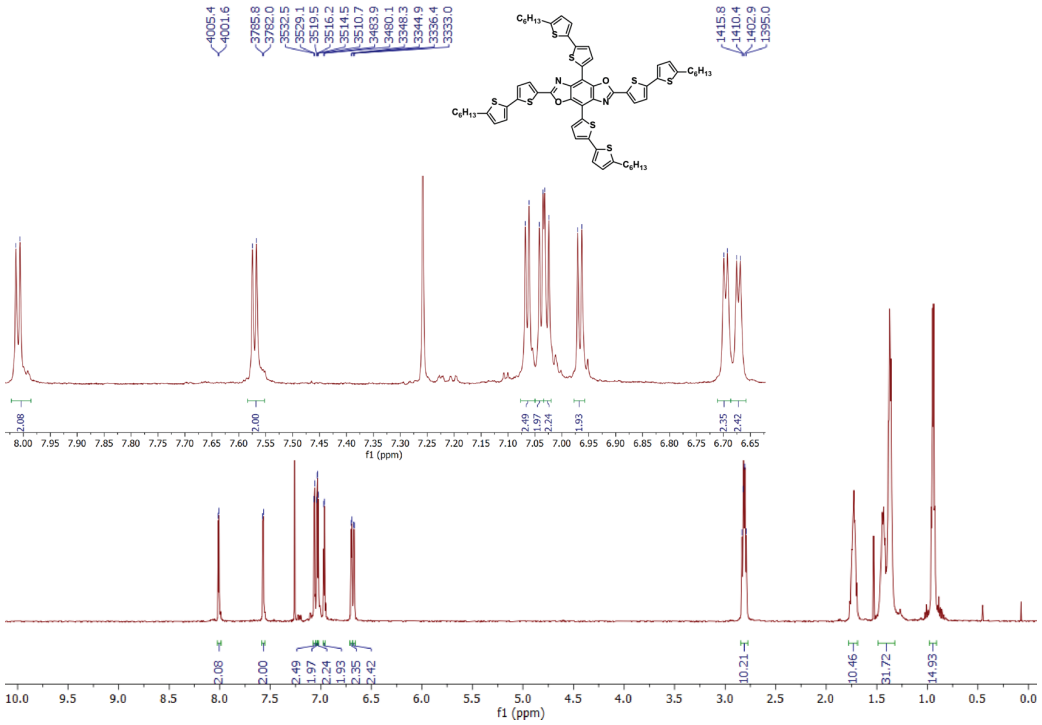


Figure S64. ^{1}H NMR of 26BT48BT

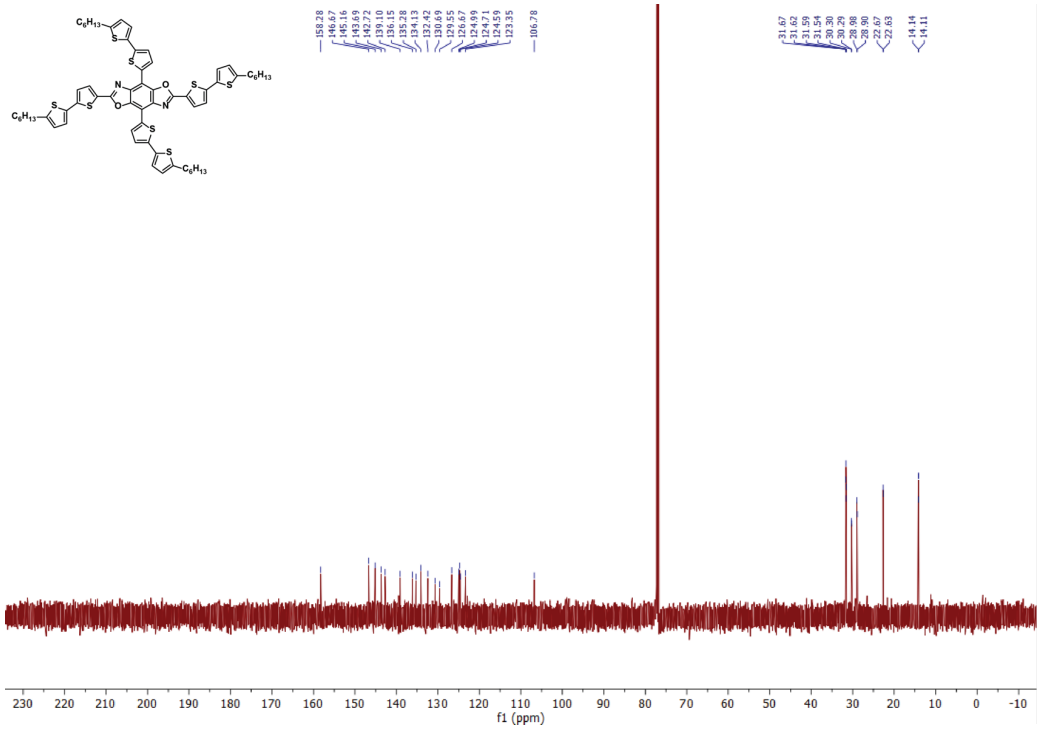


Figure S65. ^{13}C NMR of 26BT48BT

Cyclic Voltammograms

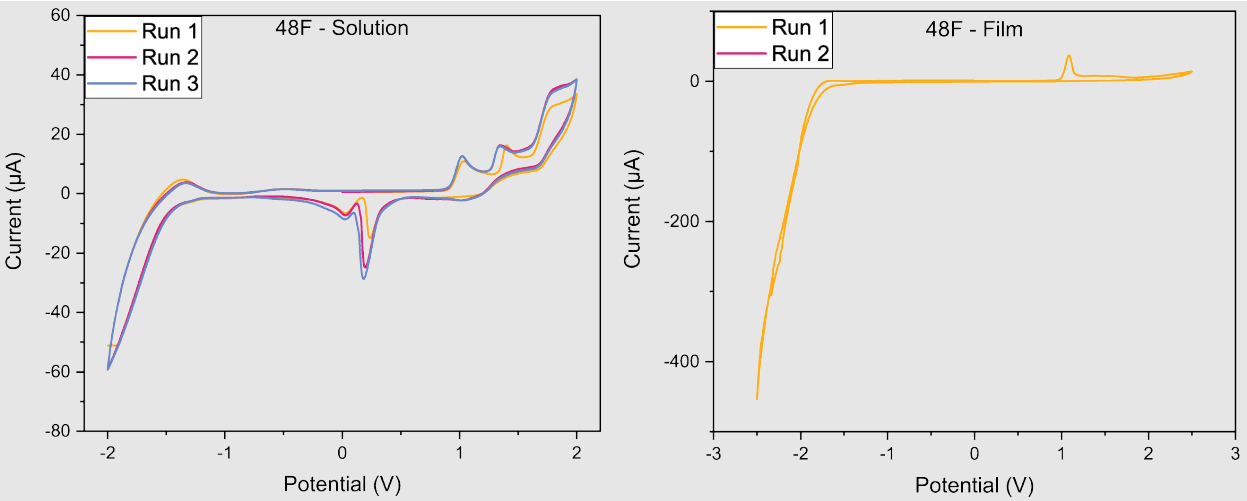


Figure S66. Cyclic voltammograms of 48F in solution (left) and film (right).

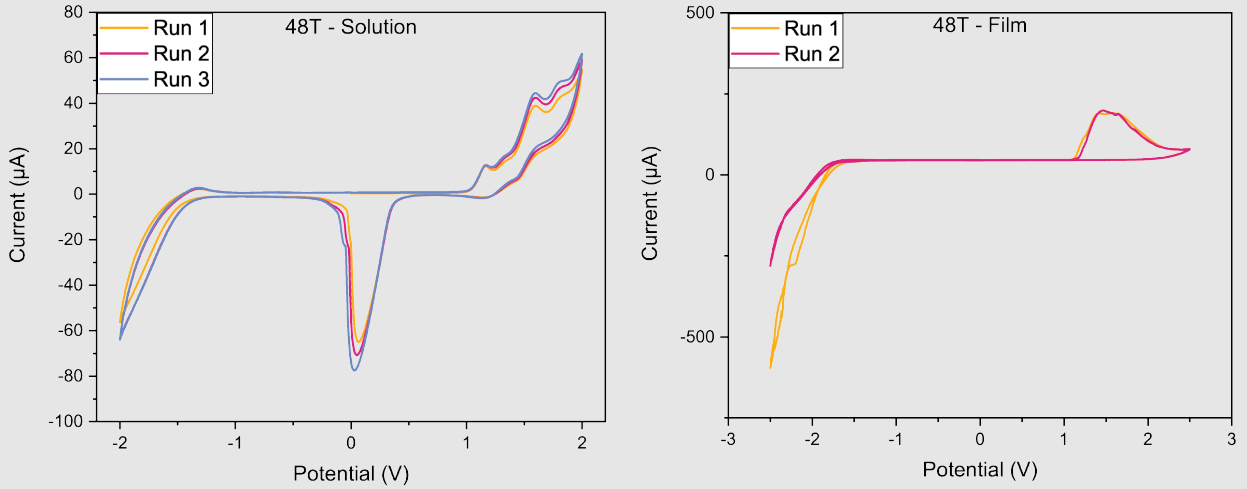


Figure S67. Cyclic voltammograms of 48T in solution (left) and film (right).

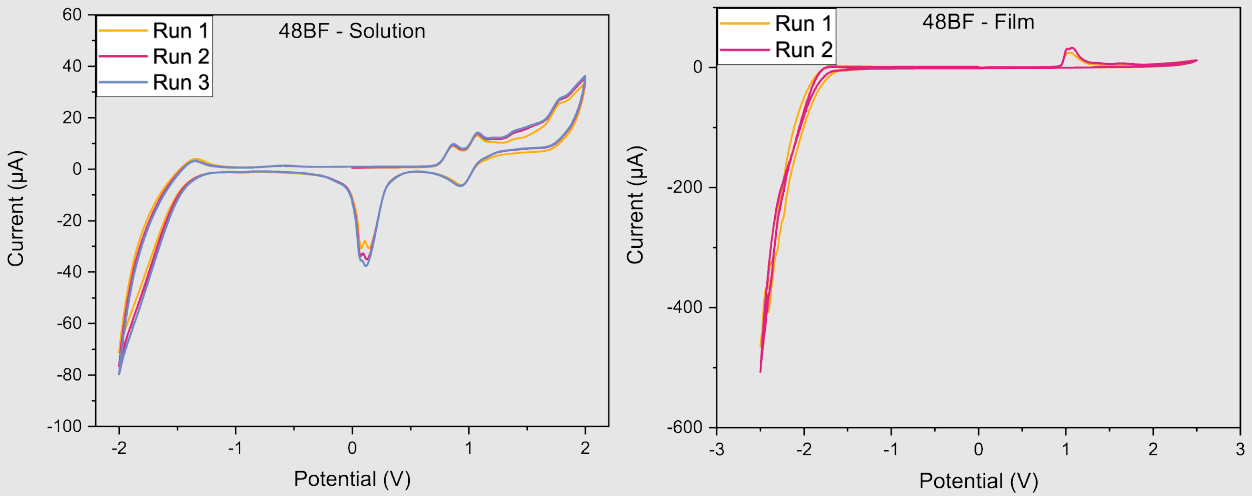


Figure S68. Cyclic voltammograms of 48BF in solution (left) and film (right).

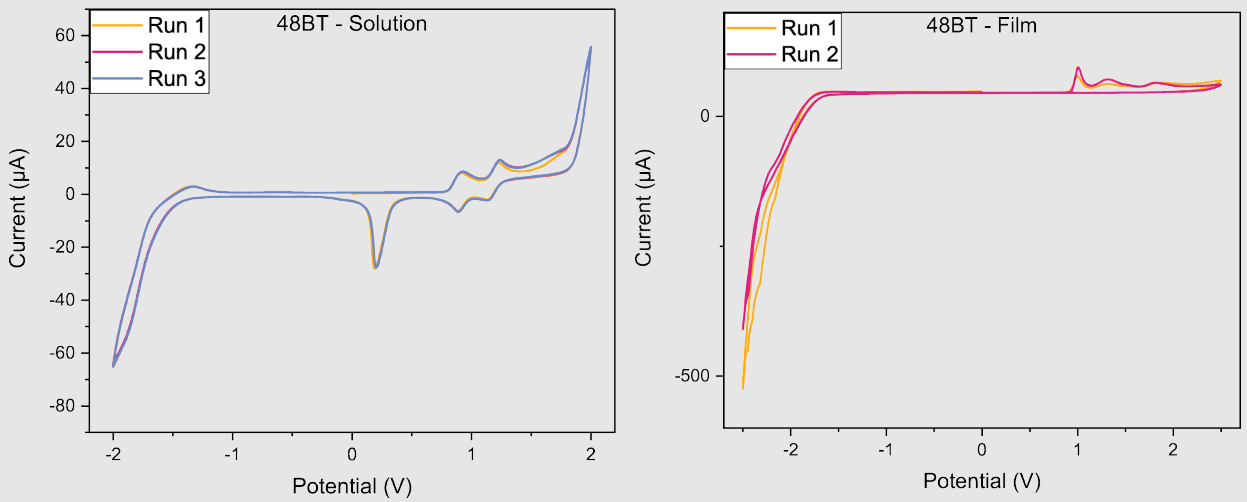


Figure S69. Cyclic voltammograms of 48BT in solution (left) and film (right).

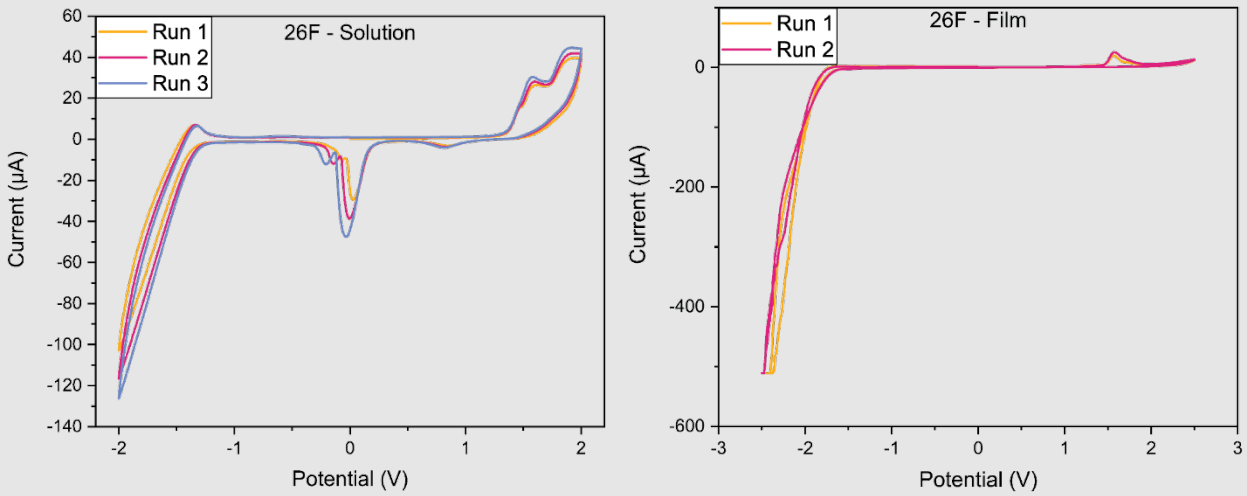


Figure S70. Cyclic voltammograms of 26F in solution (left) and film (right).

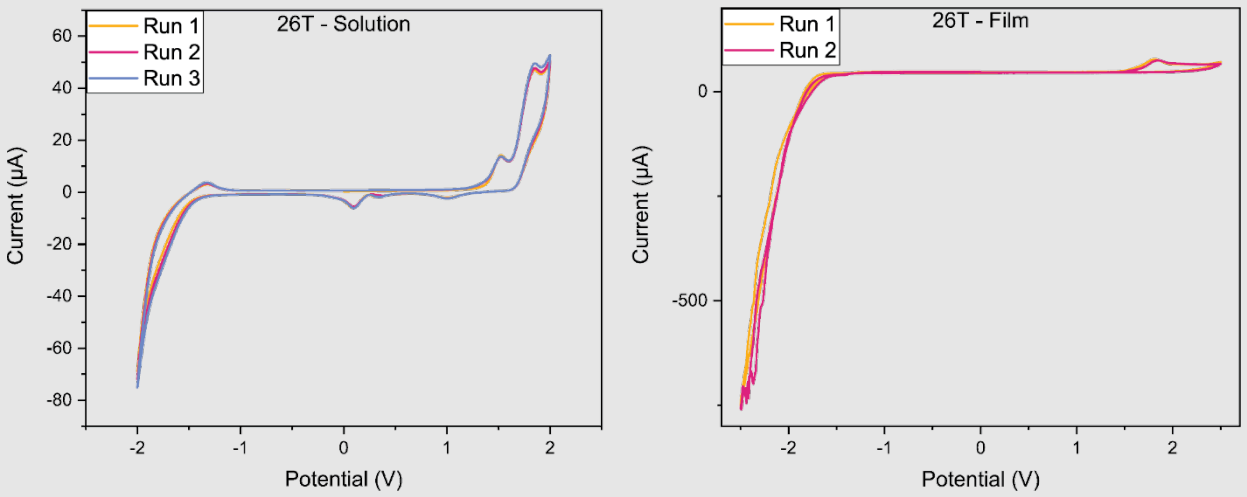


Figure S71. Cyclic voltammograms of 26T in solution (left) and film (right).

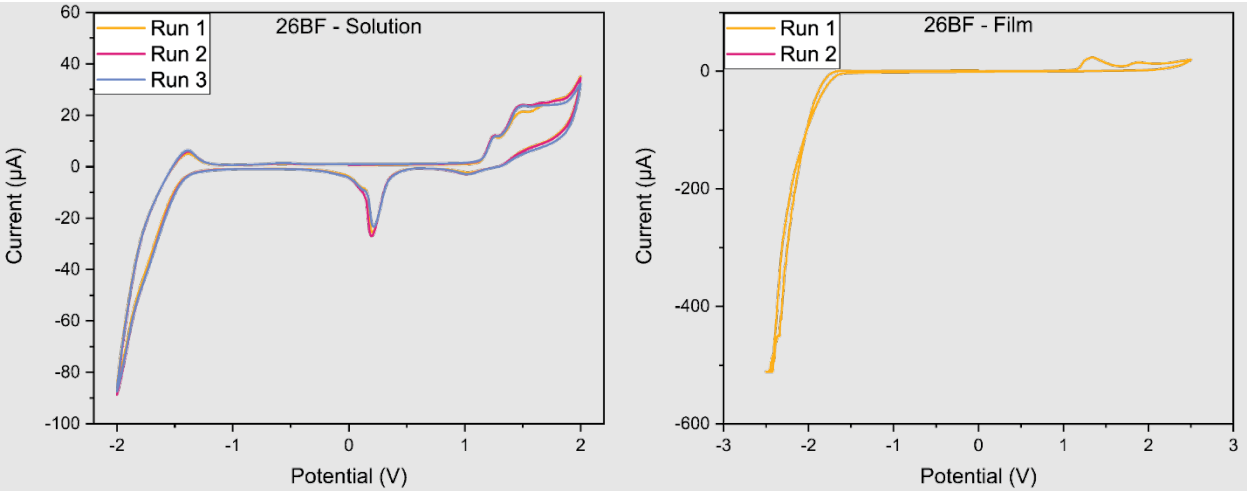


Figure S72. Cyclic voltammograms of 26BF in solution (left) and film (right).

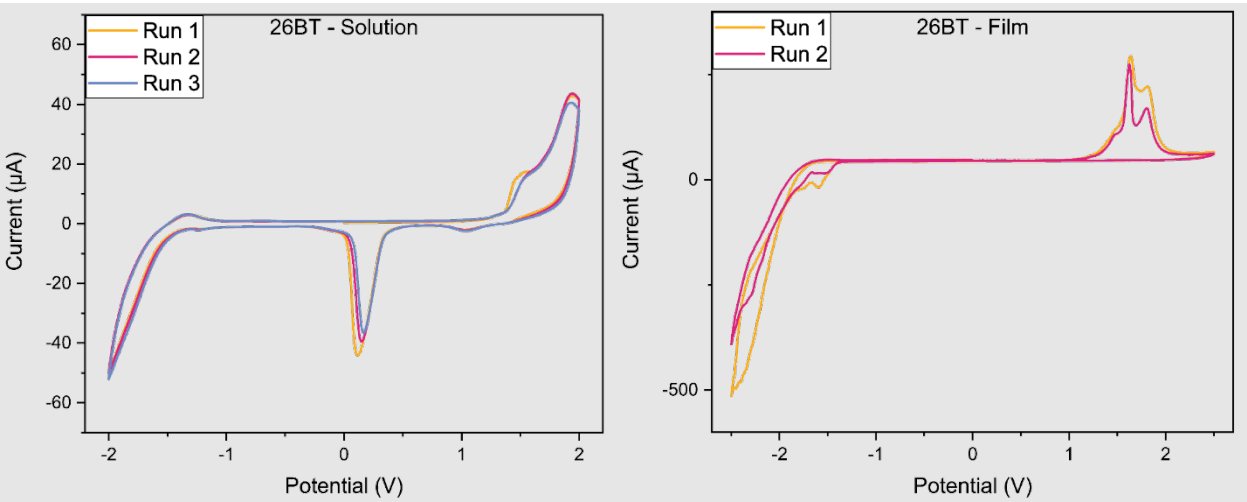


Figure S73. Cyclic voltammograms of 26BT in solution (left) and film (right).

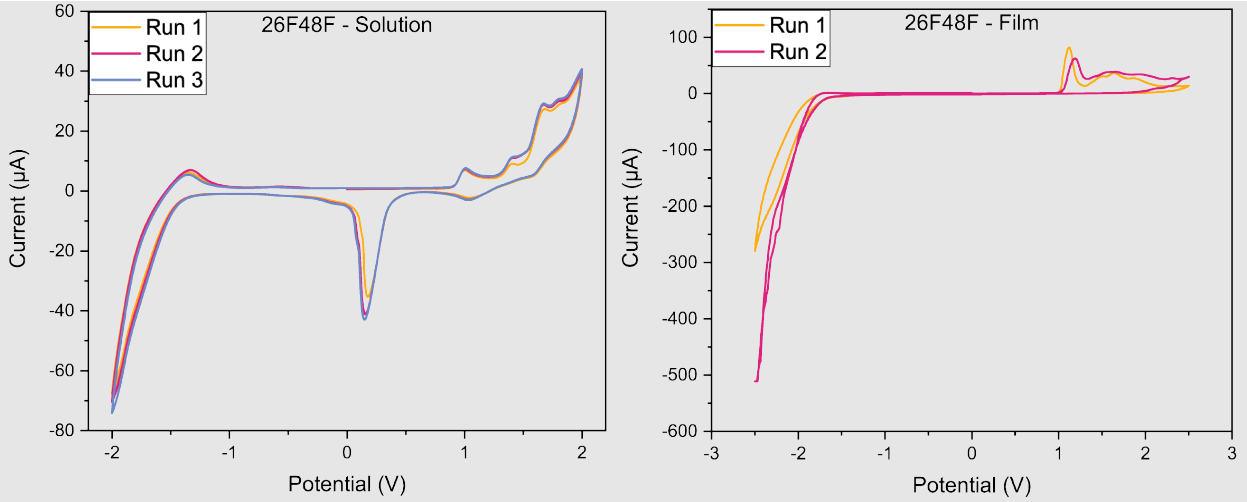


Figure S74. Cyclic voltammograms of 26F48F in solution (left) and film (right).

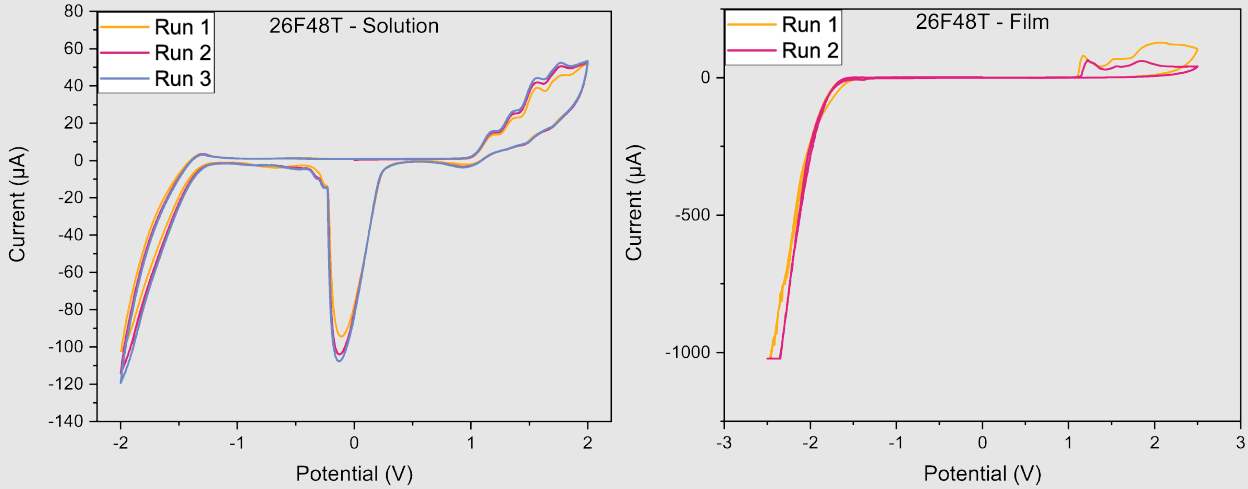


Figure S75. Cyclic voltammograms of 26F48T in solution (left) and film (right).

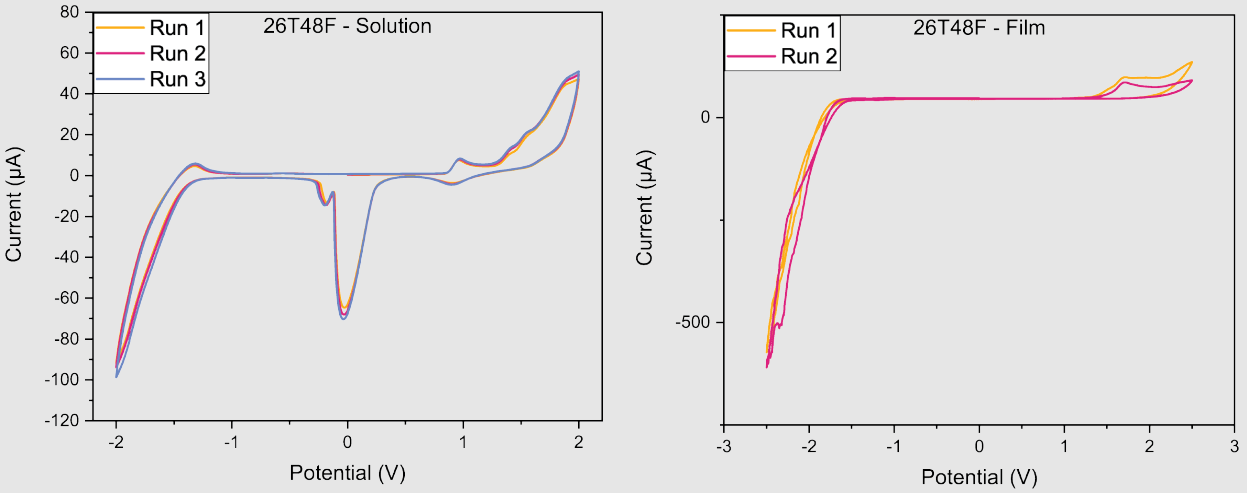


Figure S76. Cyclic voltammograms of 26T48F in solution (left) and film (right).

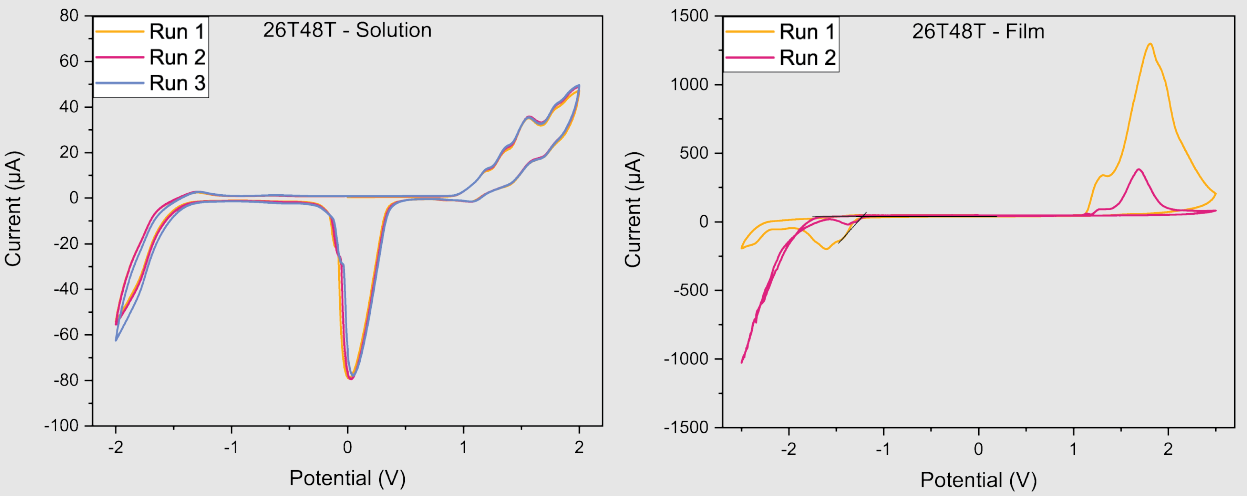


Figure S77. Cyclic voltammograms of 26T48T in solution (left) and film (right).

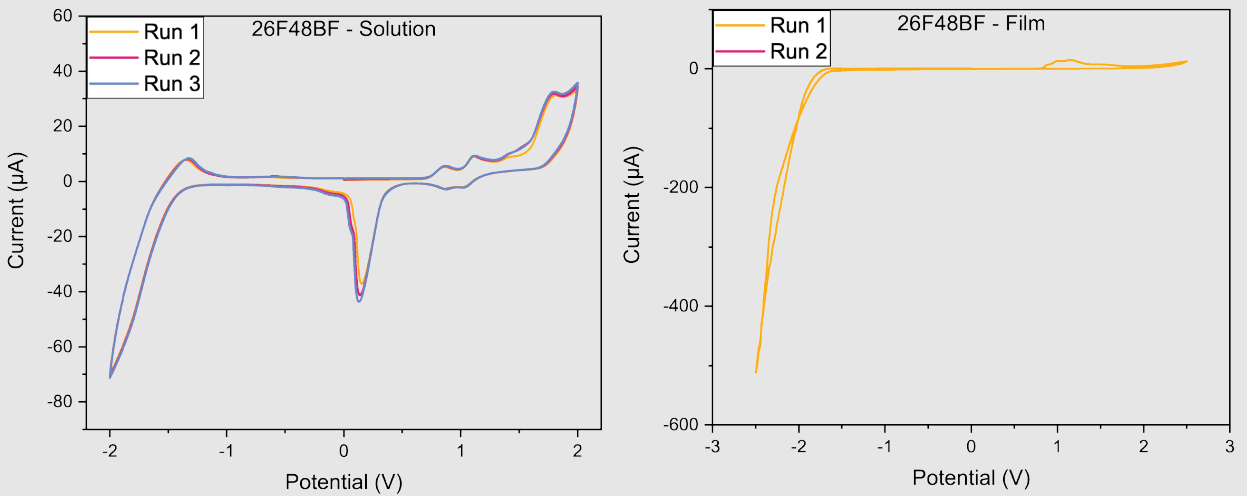


Figure S78. Cyclic voltammograms of 26F48BF in solution (left) and film (right).

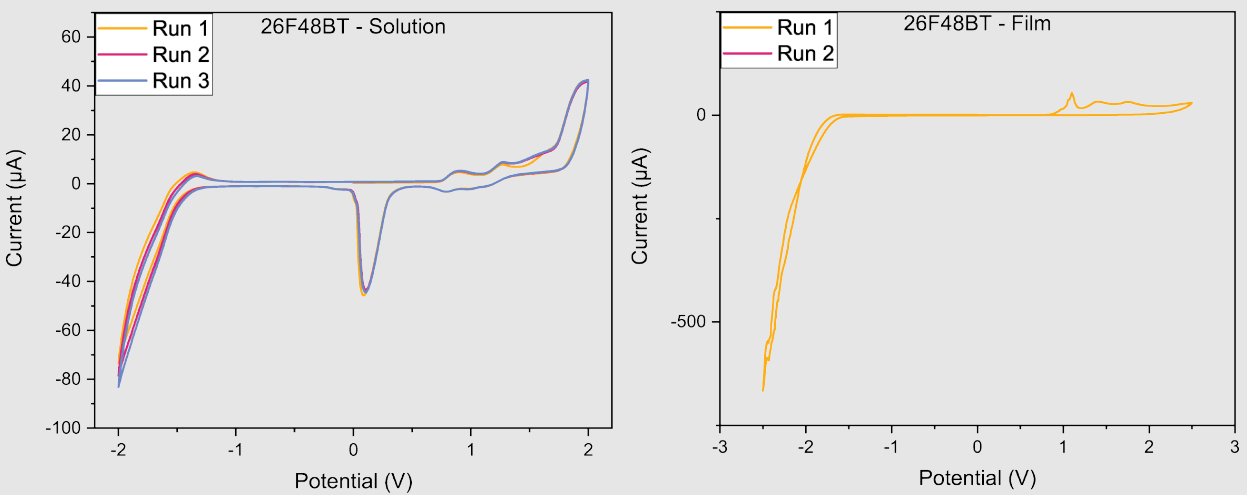


Figure S79. Cyclic voltammograms of 26F48BT in solution (left) and film (right).

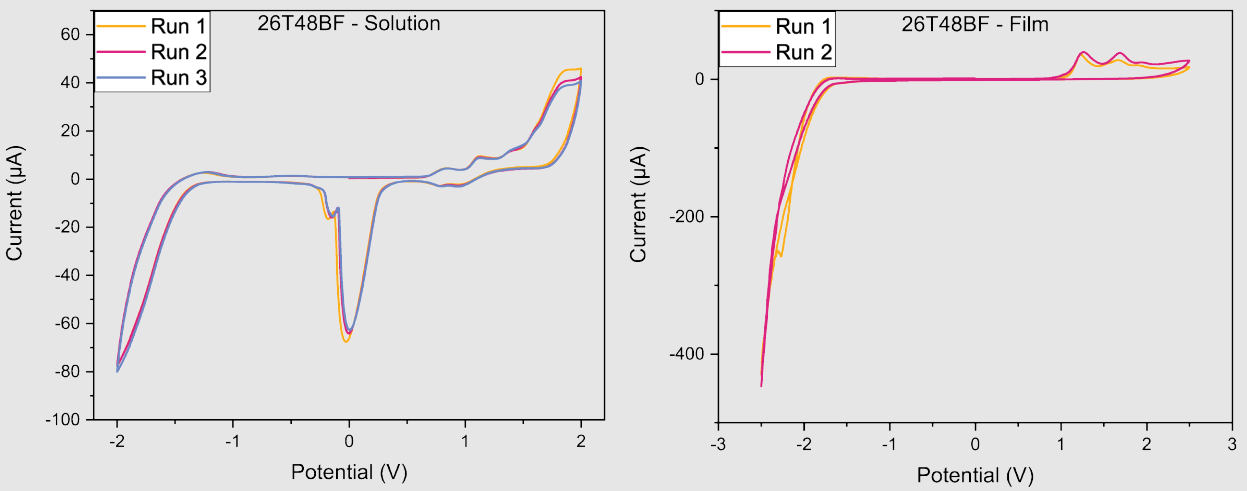


Figure S80. Cyclic voltammograms of 26T48BF in solution (left) and film (right).

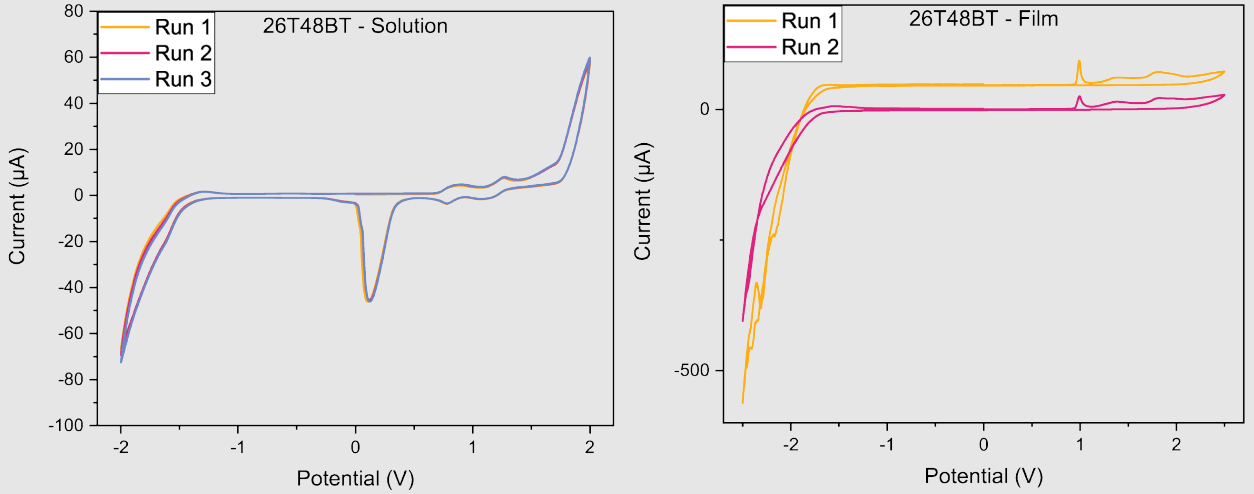


Figure S81. Cyclic voltammograms of 26T48BT in solution (left) and film (right).

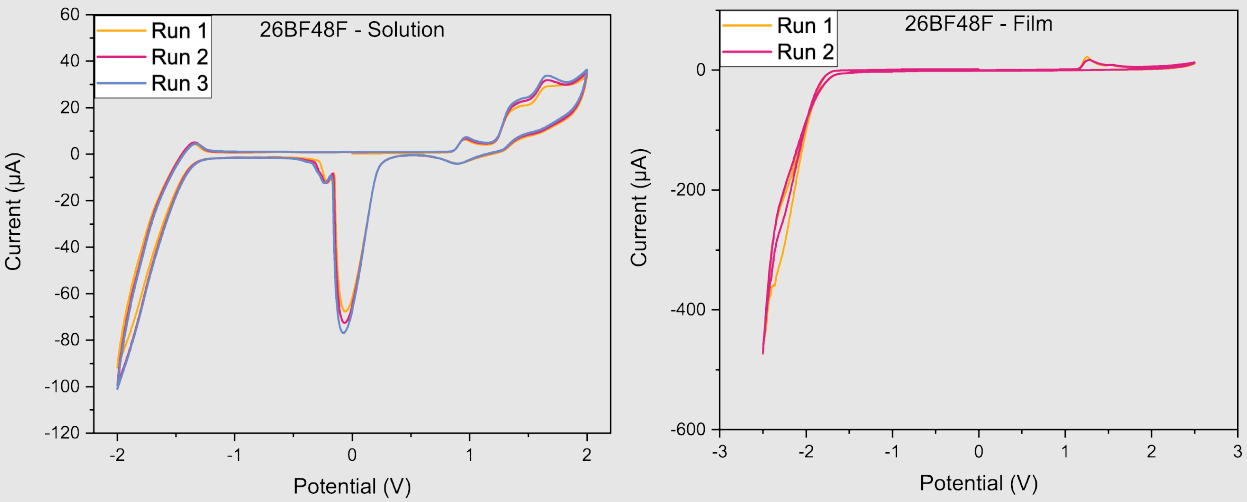


Figure S82. Cyclic voltammograms of 26BF48F in solution (left) and film (right).

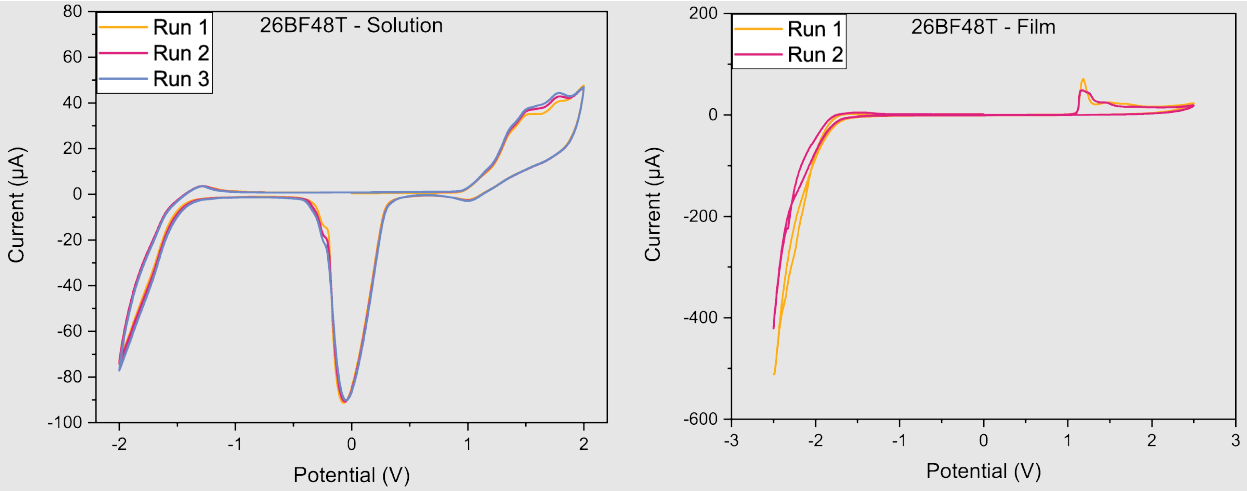


Figure S83. Cyclic voltammograms of 26BF48T in solution (left) and film (right).

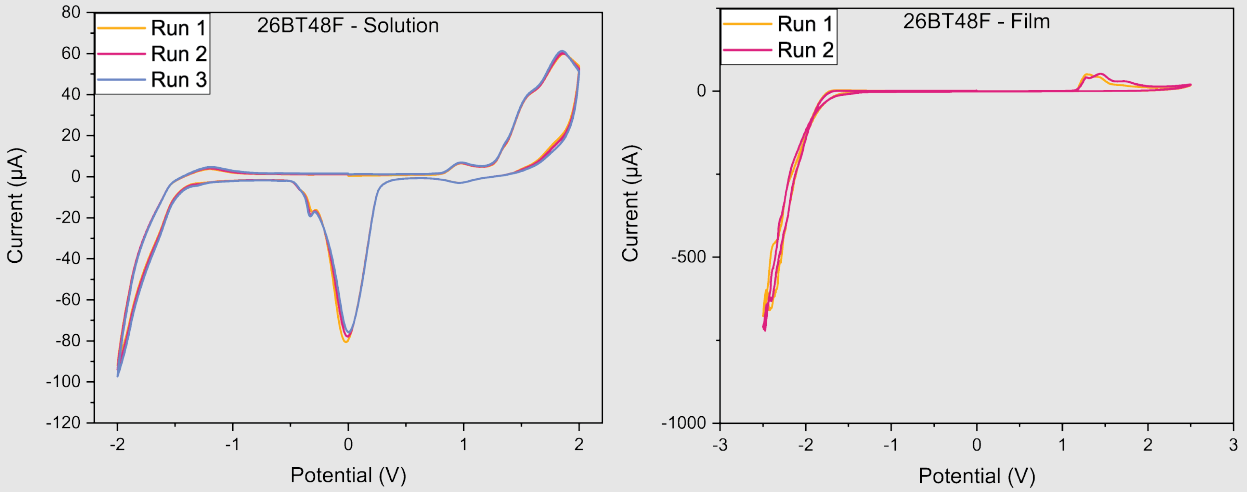


Figure S84. Cyclic voltammograms of 26BT48F in solution (left) and film (right).

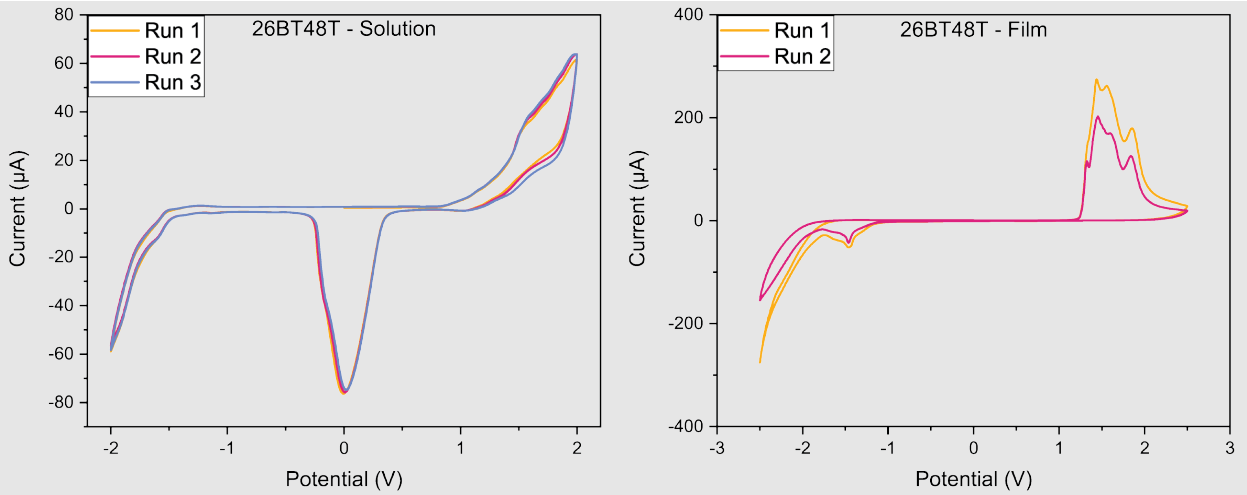


Figure S85. Cyclic voltammograms of 26BT48T in solution (left) and film (right).

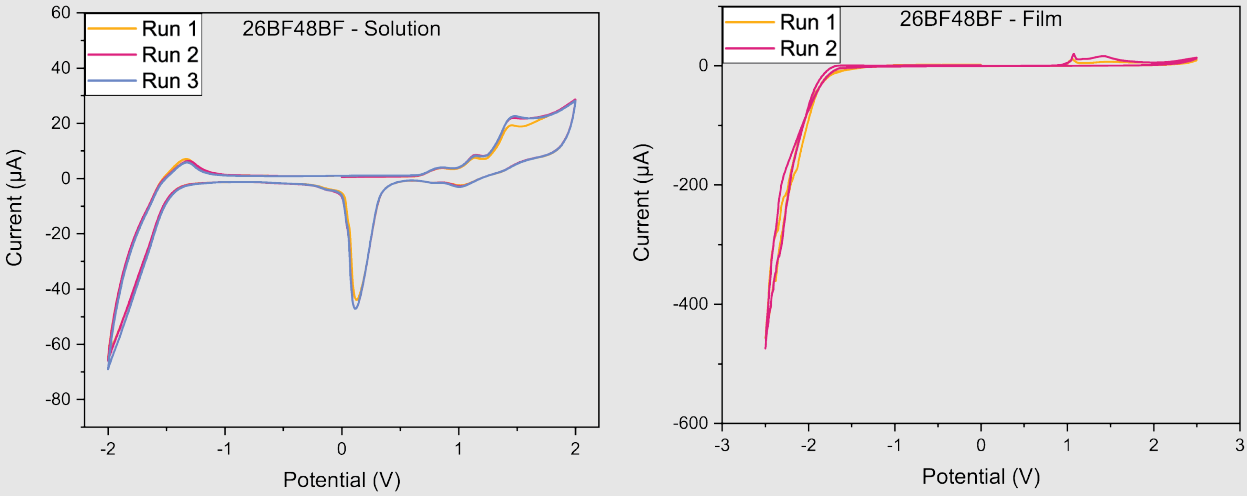


Figure S86. Cyclic voltammograms of 26BF48BF in solution (left) and film (right).

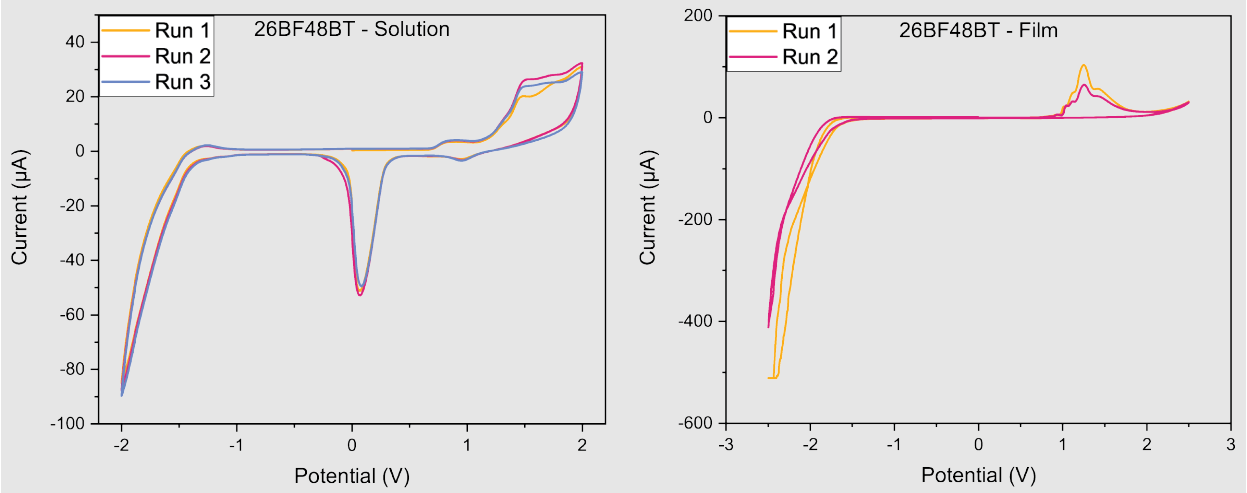


Figure S87. Cyclic voltammograms of 26BF48BT in solution (left) and film (right).

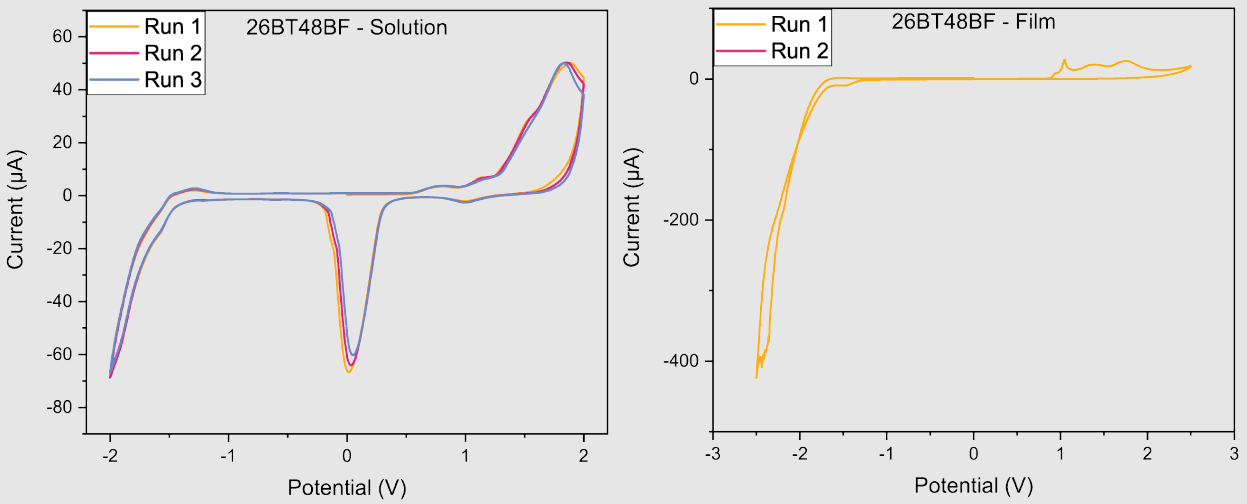


Figure S88. Cyclic voltammograms of 26BF48BT in solution (left) and film (right).

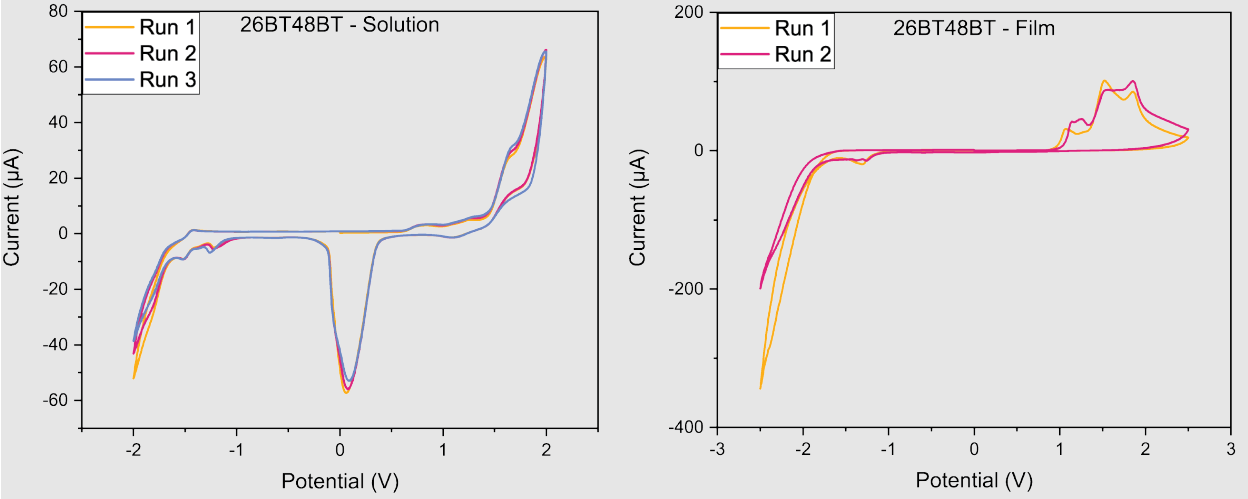


Figure S89. Cyclic voltammograms of 26BT48BT in solution (left) and film (right).

Experimental Absorbance and Emission Spectra

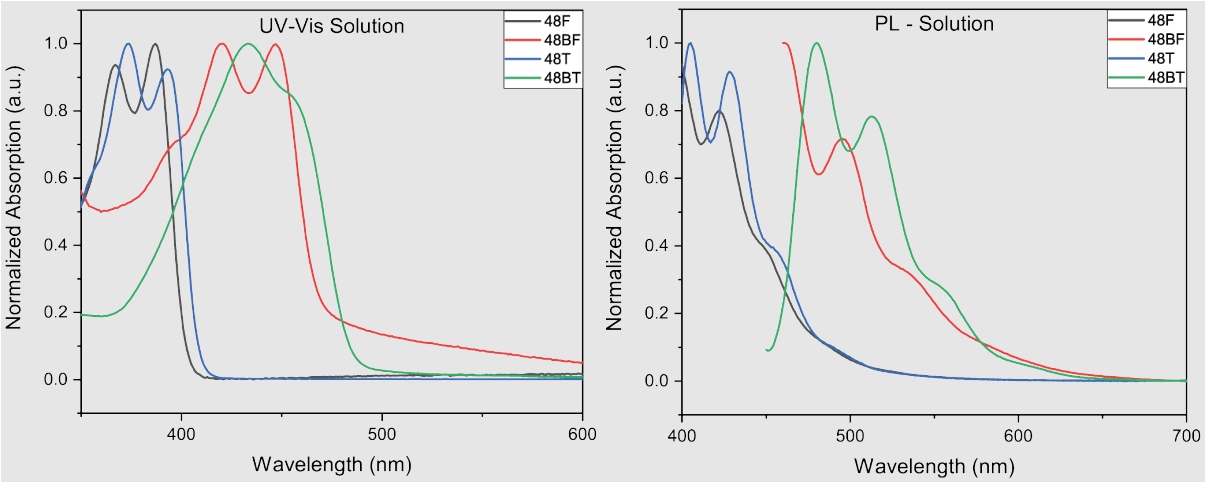


Figure S90. Absorbance (left) and photoluminescence (right) spectra of the 4,8-parents in chloroform.

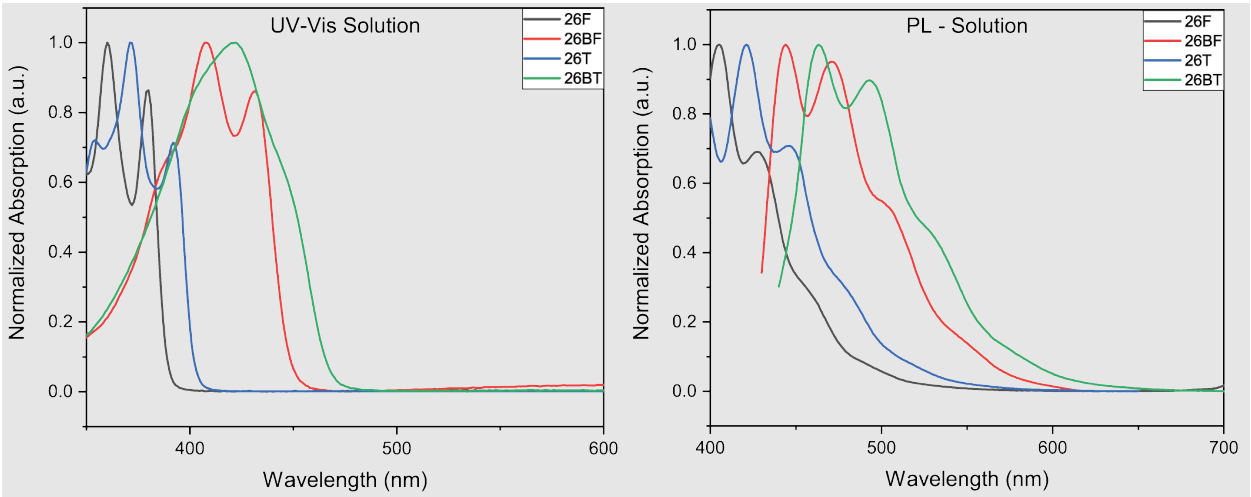


Figure S91. Absorbance (left) and photoluminescence (right) spectra of the 2,6-parents in chloroform.

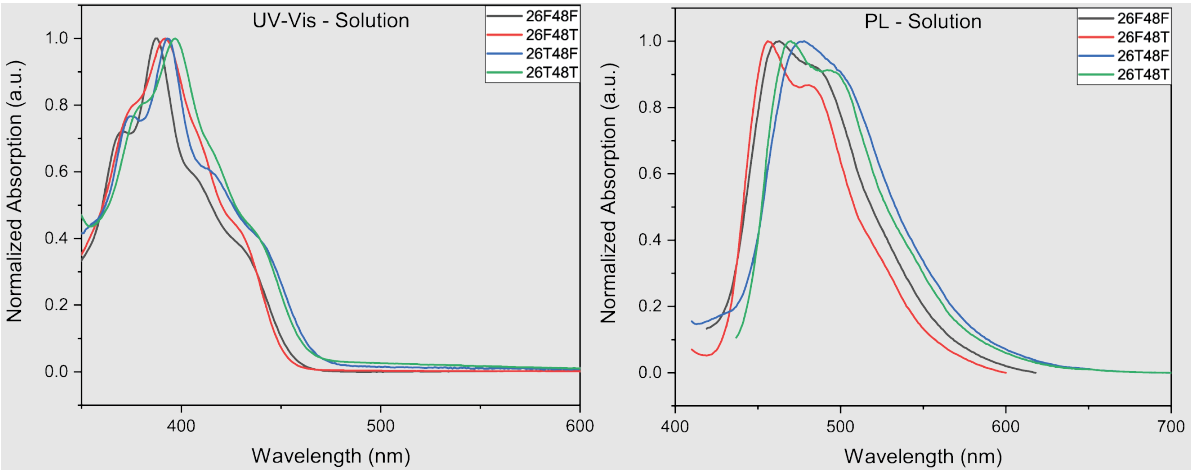


Figure S92. Absorbance (left) and photoluminescence (right) spectra of the 26X48X series in chloroform.

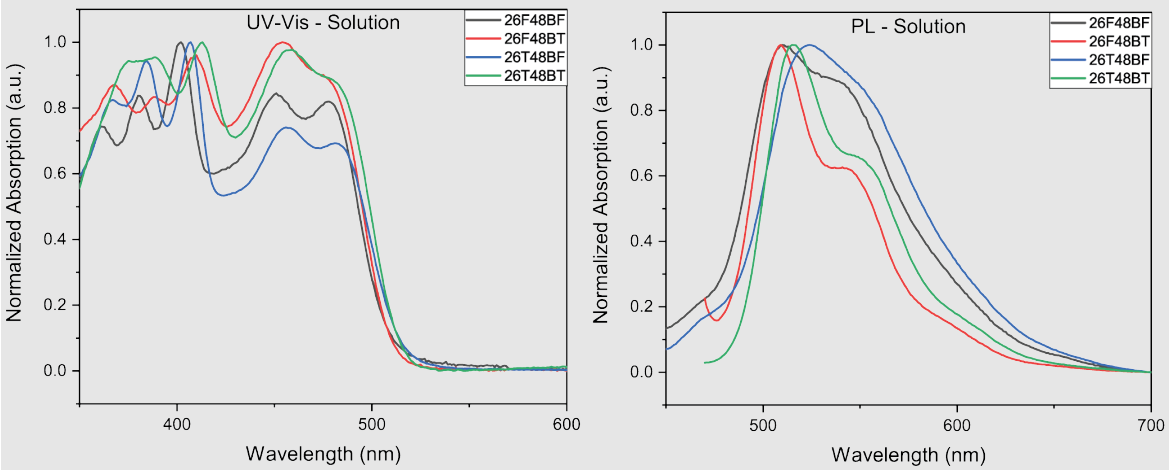


Figure S93. Absorbance (left) and photoluminescence (right) spectra of the 26X48BX series in chloroform.

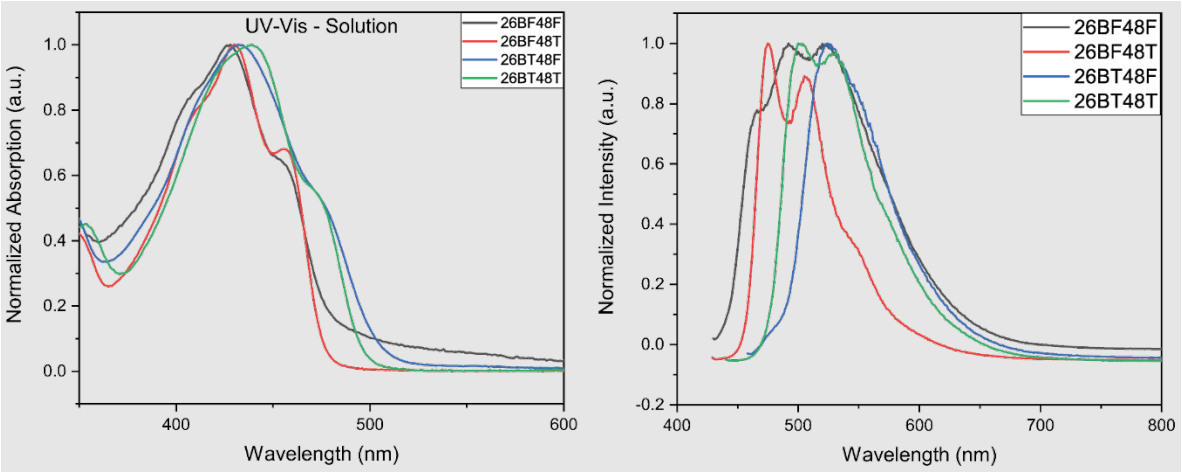


Figure S94. Absorbance (left) and photoluminescence (right) spectra of the 26BX48X series in chloroform.

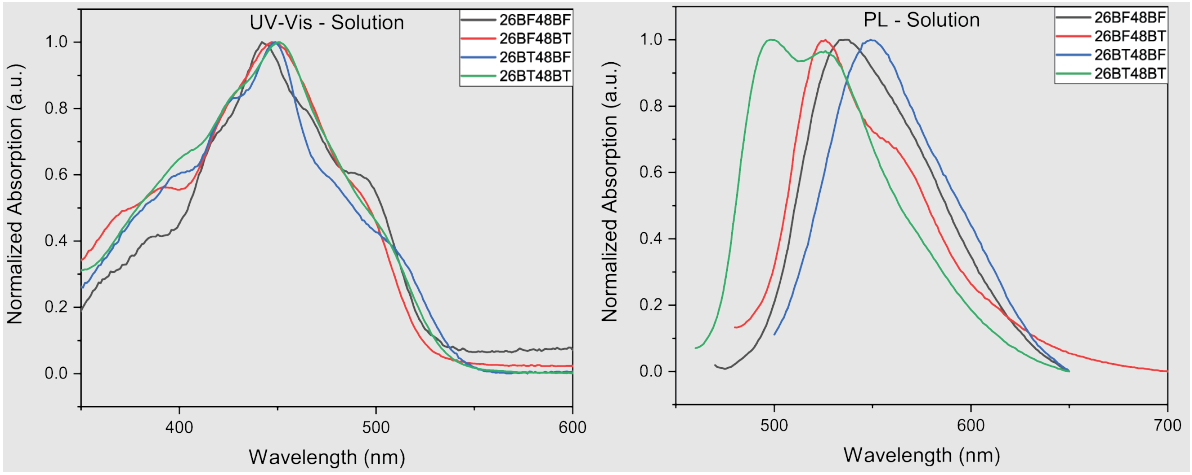


Figure S95. Absorbance (left) and photoluminescence (right) spectra of the 26BX48BX series in chloroform.

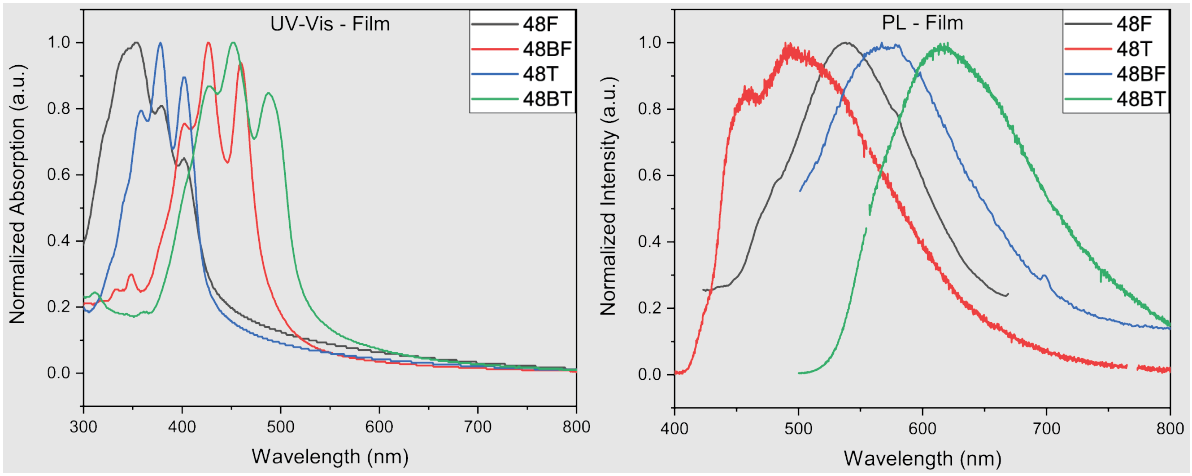


Figure S96. Absorbance (left) and photoluminescence (right) spectra of the 4,8-parents in film-state.

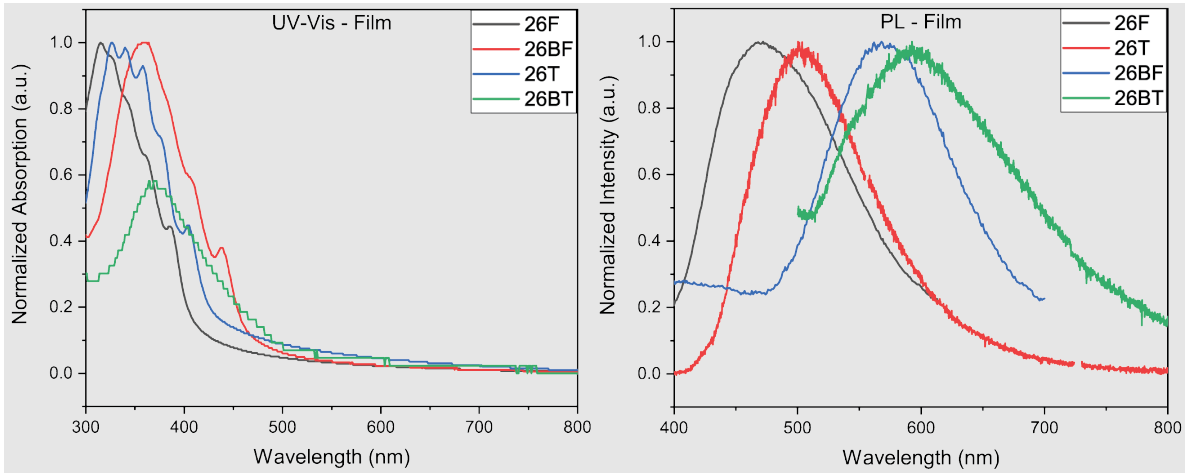


Figure S97. Absorbance (left) and photoluminescence (right) spectra of the 2,6-parents in film-state.

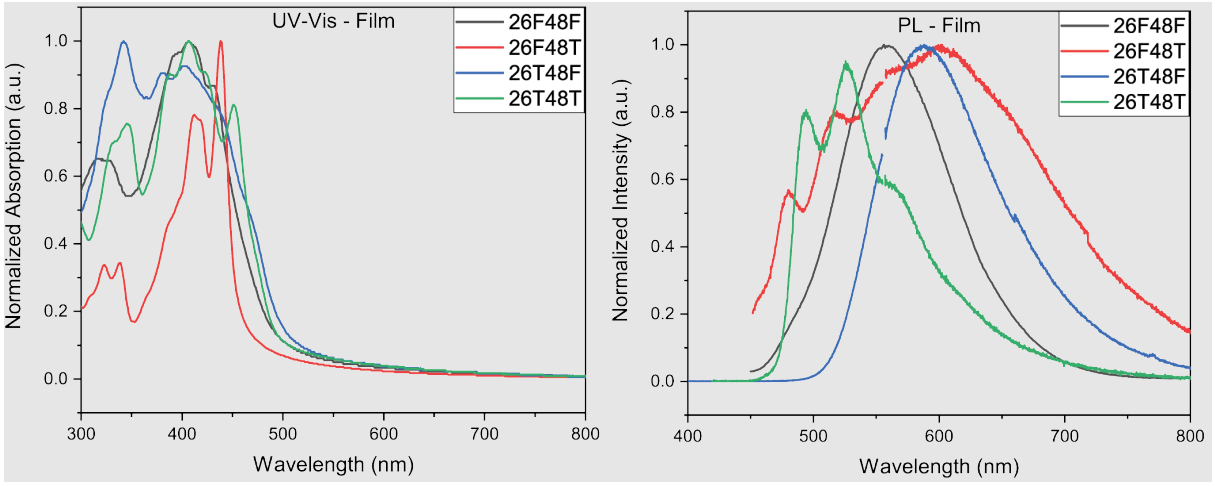


Figure S98. Absorbance (left) and photoluminescence (right) spectra of the 26X48X series in film-state.

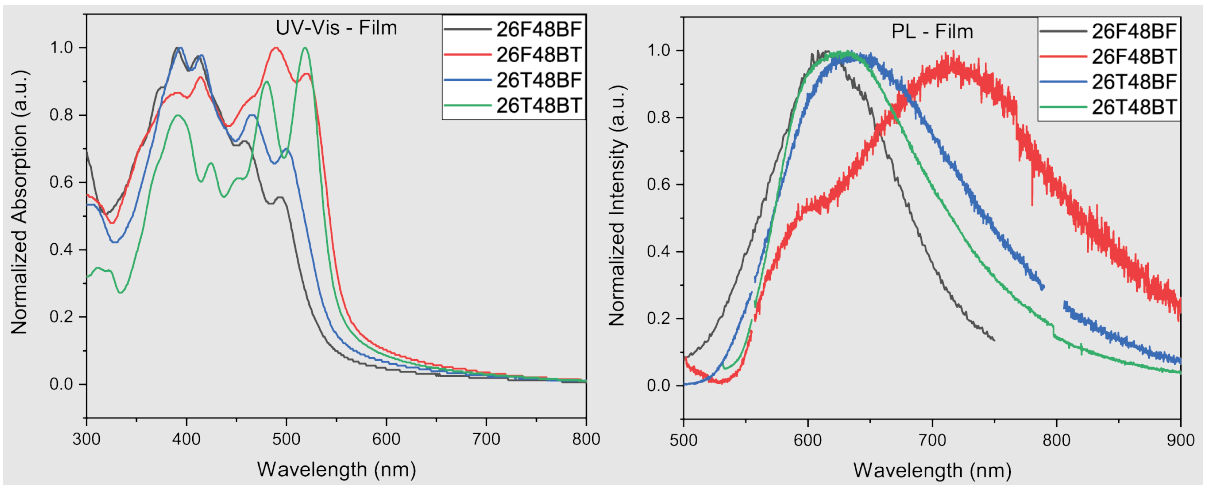


Figure S99. Absorbance (left) and photoluminescence (right) spectra of the 26X48BX series in film-state.

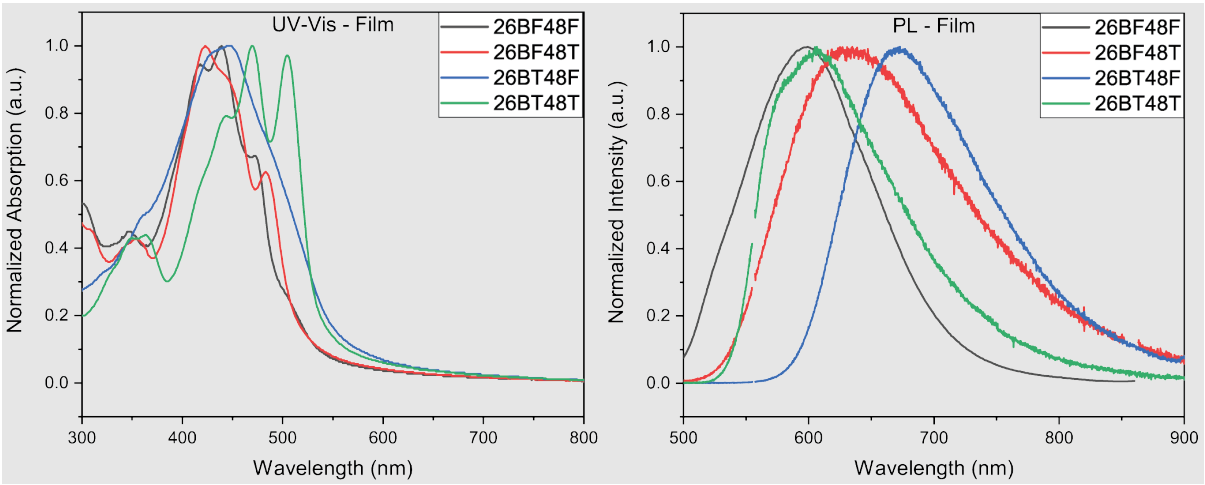


Figure S100. Absorbance (left) and photoluminescence (right) spectra of the 26BX48X series in film-state.

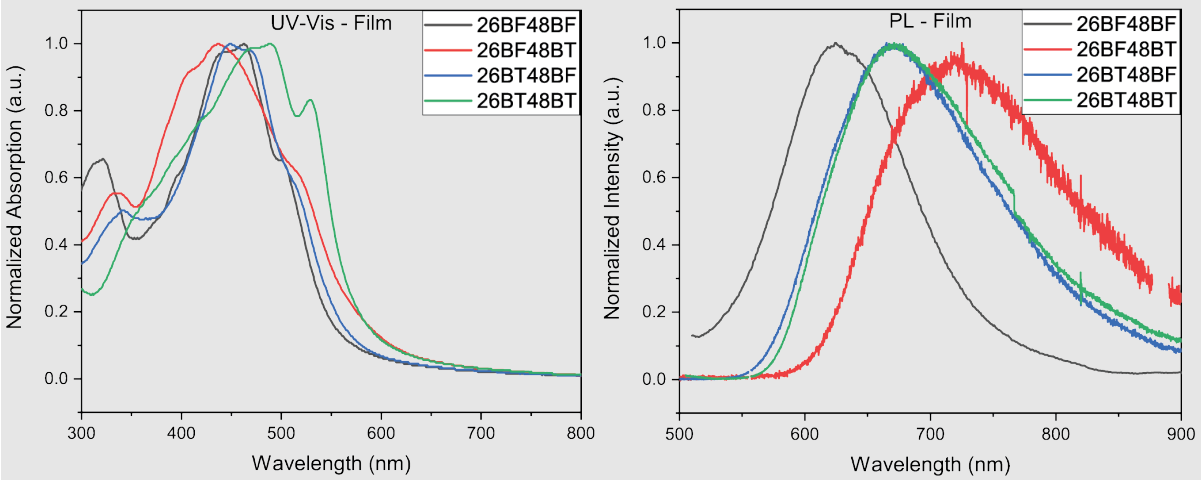


Figure S101. Absorbance (left) and photoluminescence (right) spectra of the 26BX48BX series in film-state.

Electroluminescent Emission

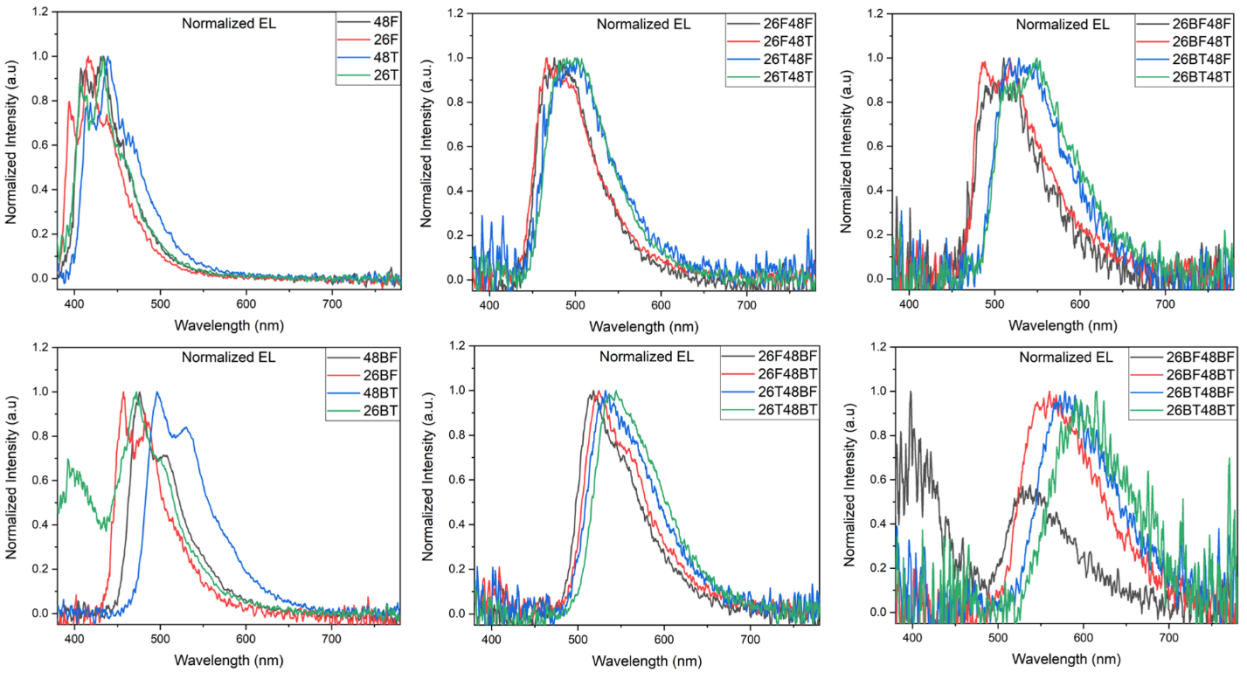


Figure S102. Electroluminescence of the 24 molecules investigated.

Thermal Analysis

Thermogravimetric Analysis

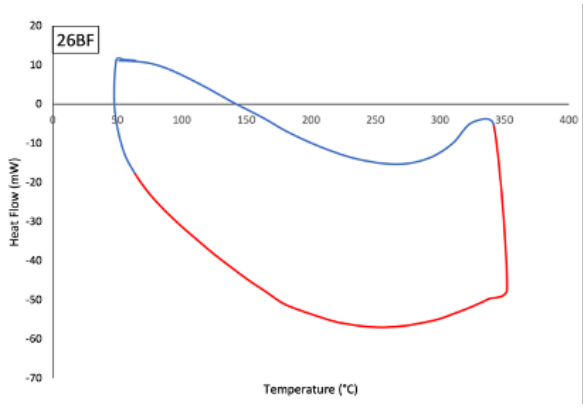
All thermal gravimetric analysis (TGA) measurements were performed on a Mettler-Toledo TGA/DSC instrument using standard 40 μl aluminum pans. Each sample was heated at a rate of 10 °C/min up to 600 °C. The 5% decomposition temperatures are summarized in Table S1 below.

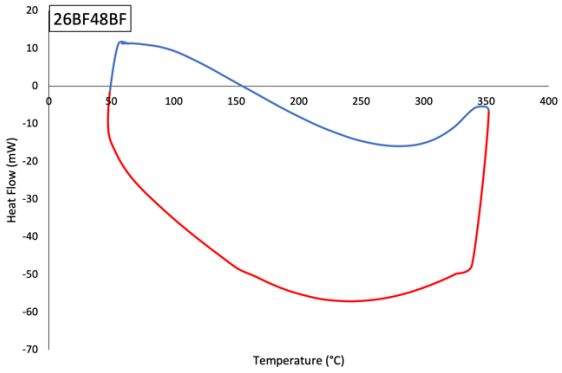
Table S1. Summary of 5% decomposition temperature for BBO cruciforms.

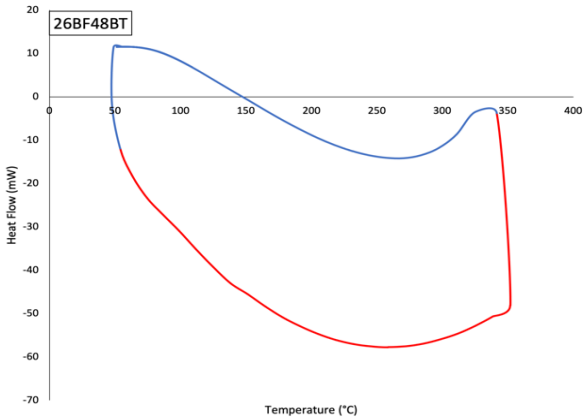
Compound	T_g (°C)
26BF	368.25
26BF48BT	406.26
26BF48BT	394.96
26BF48F	409.27
26BF48T	393.74
26BT	381.55
26BT48BF	388.37
26BT48BT	398.41
26BT48F	388.06
26BT48T	421.17
26F	395.73
26F48BF	395.91
26F48BT	396.45
26F48F	416.15
26F48T	400.03
26T	432.67
26T48BF	392.22
26T48BT	408.17
26T48F	441.84
26T48T	451.84
48BF	366.70
48BT	411.10
48F	414.98
48T	441.98

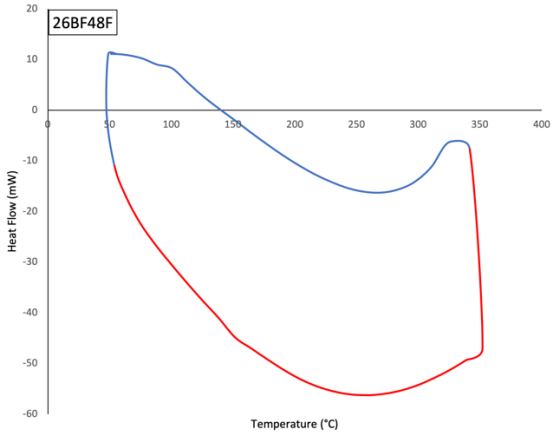
Differential Scanning Calorimetry

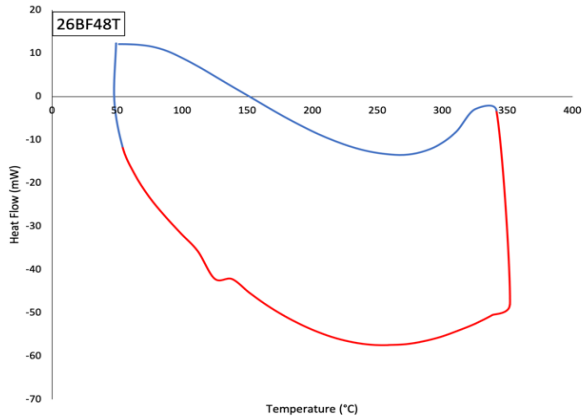
All differential scanning calorimetry (DSC) measurements were performed in the Mettler-Toledo TGA/DSC instrument under nitrogen atmosphere. The data shows the heating cycle in red and cooling cycle in blue.

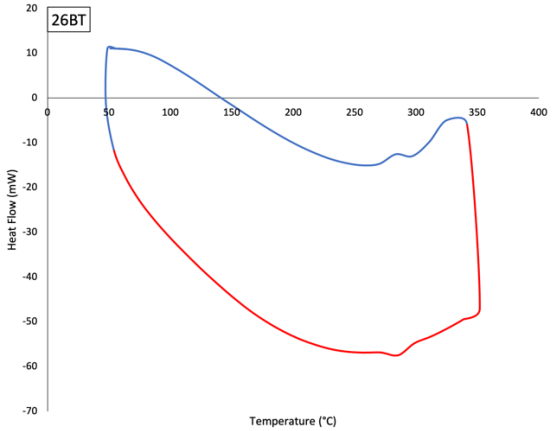

26BF
Heat Flow (mW)
Temperature (°C)

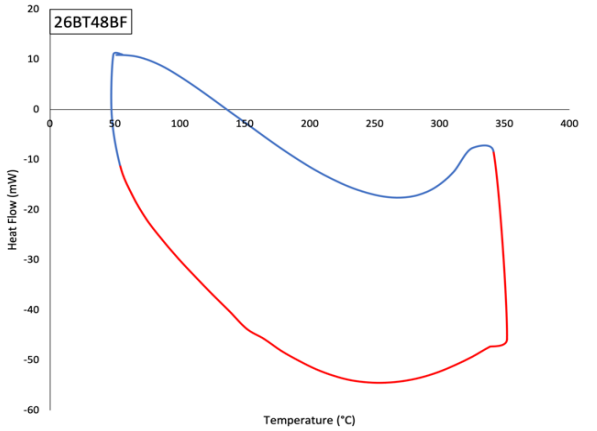

26BF48BF
Heat Flow (mW)
Temperature (°C)

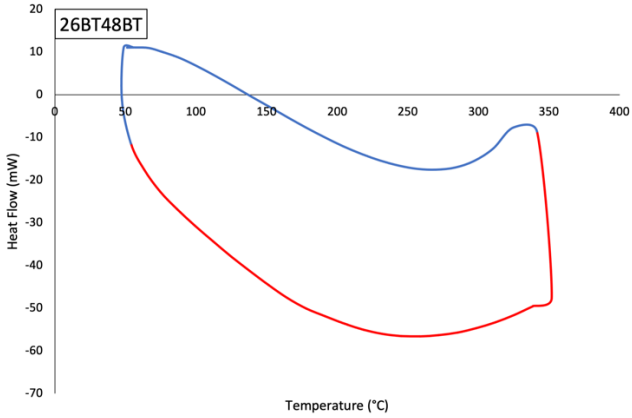

26BF48BT
Heat Flow (mW)
Temperature (°C)

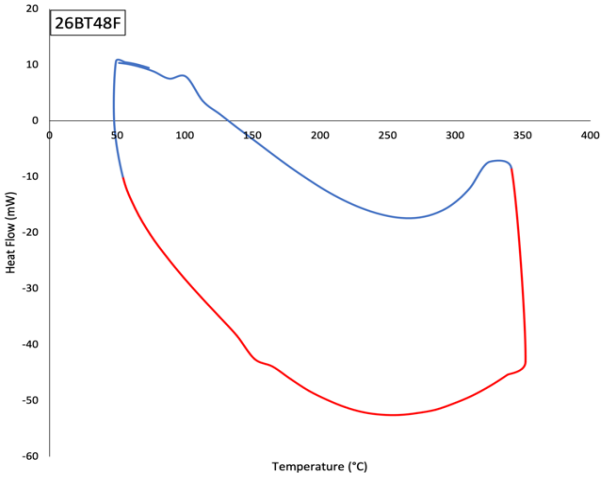

26BF48F
Heat Flow (mW)
Temperature (°C)

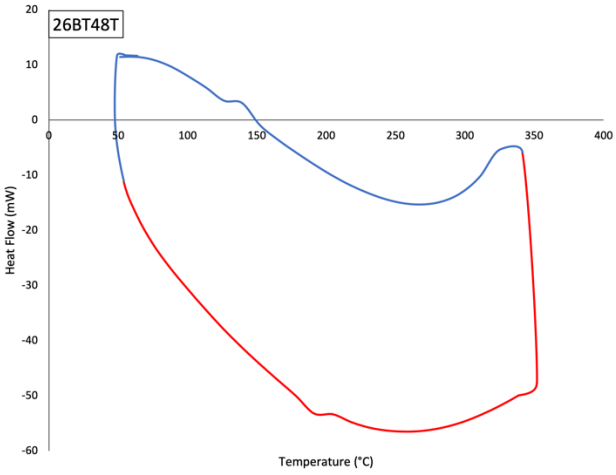

26BF48T
Heat Flow (mW)
Temperature (°C)

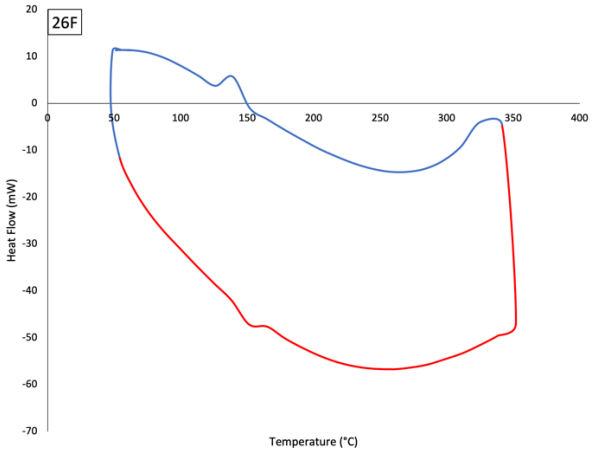

26BT
Heat Flow (mW)
Temperature (°C)

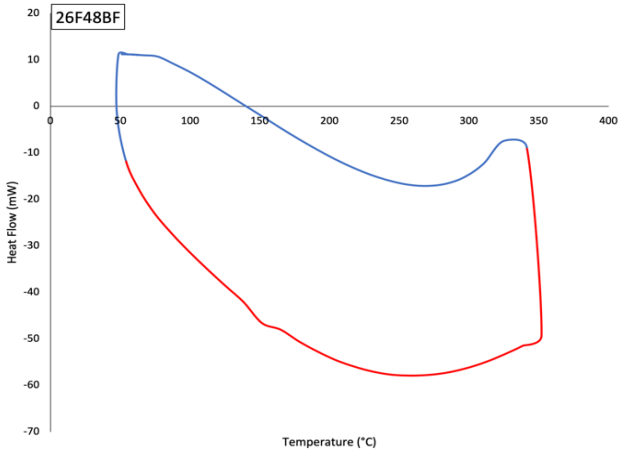

26BT48BF
Heat Flow (mW)
Temperature (°C)

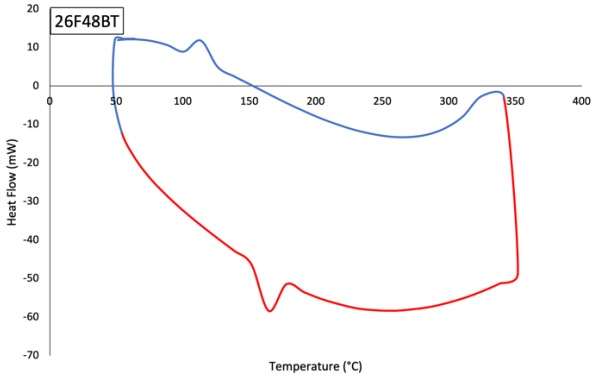

26BT48BT
Heat Flow (mW)
Temperature (°C)

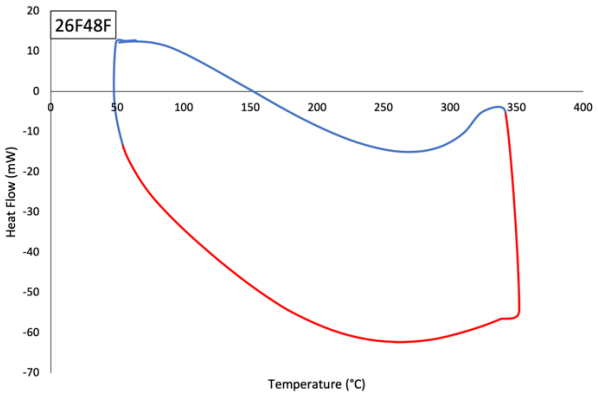

26BT48F
Heat Flow (mW)
Temperature (°C)

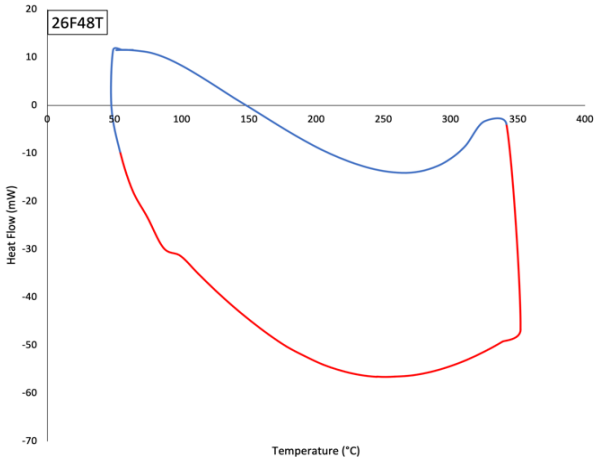

26BT48T
Heat Flow (mW)
Temperature (°C)

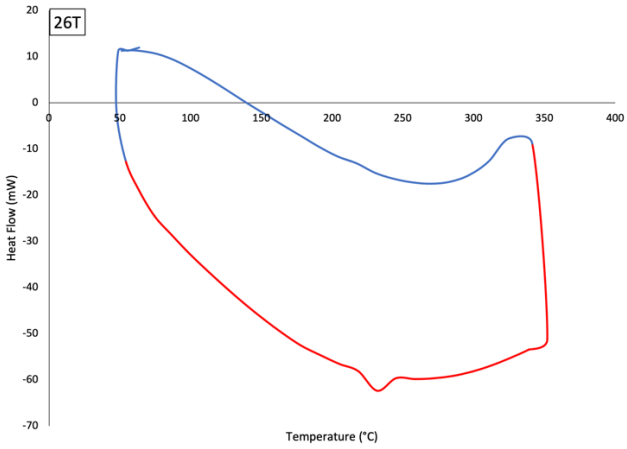

26F
Heat Flow (mW)
Temperature (°C)

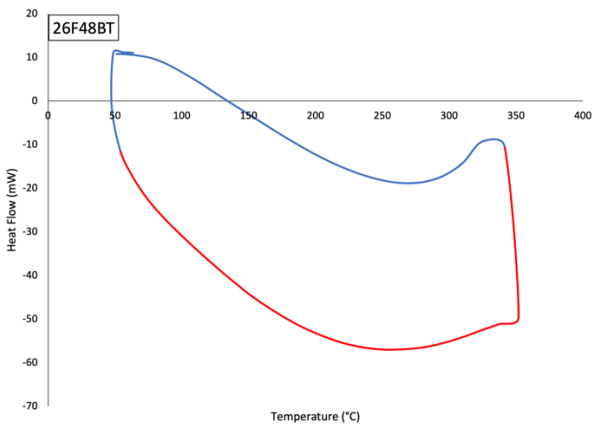

26F48BF
Heat Flow (mW)
Temperature (°C)

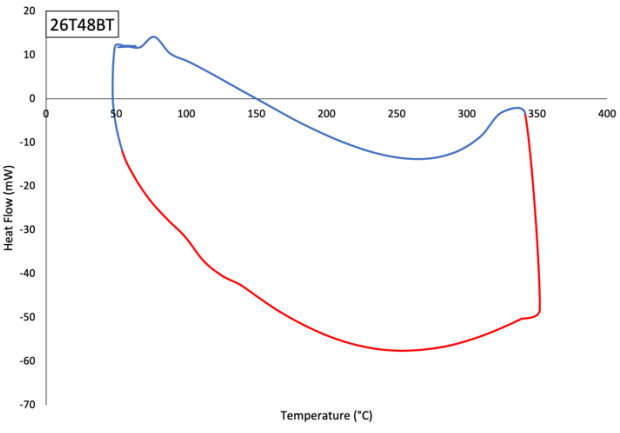

26F48BT
Heat Flow (mW)
Temperature (°C)


26F48F
Heat Flow (mW)
Temperature (°C)


26F48T
Heat Flow (mW)
Temperature (°C)


26T
Heat Flow (mW)
Temperature (°C)


26F48BT
Heat Flow (mW)
Temperature (°C)


26T48BT
Heat Flow (mW)
Temperature (°C)

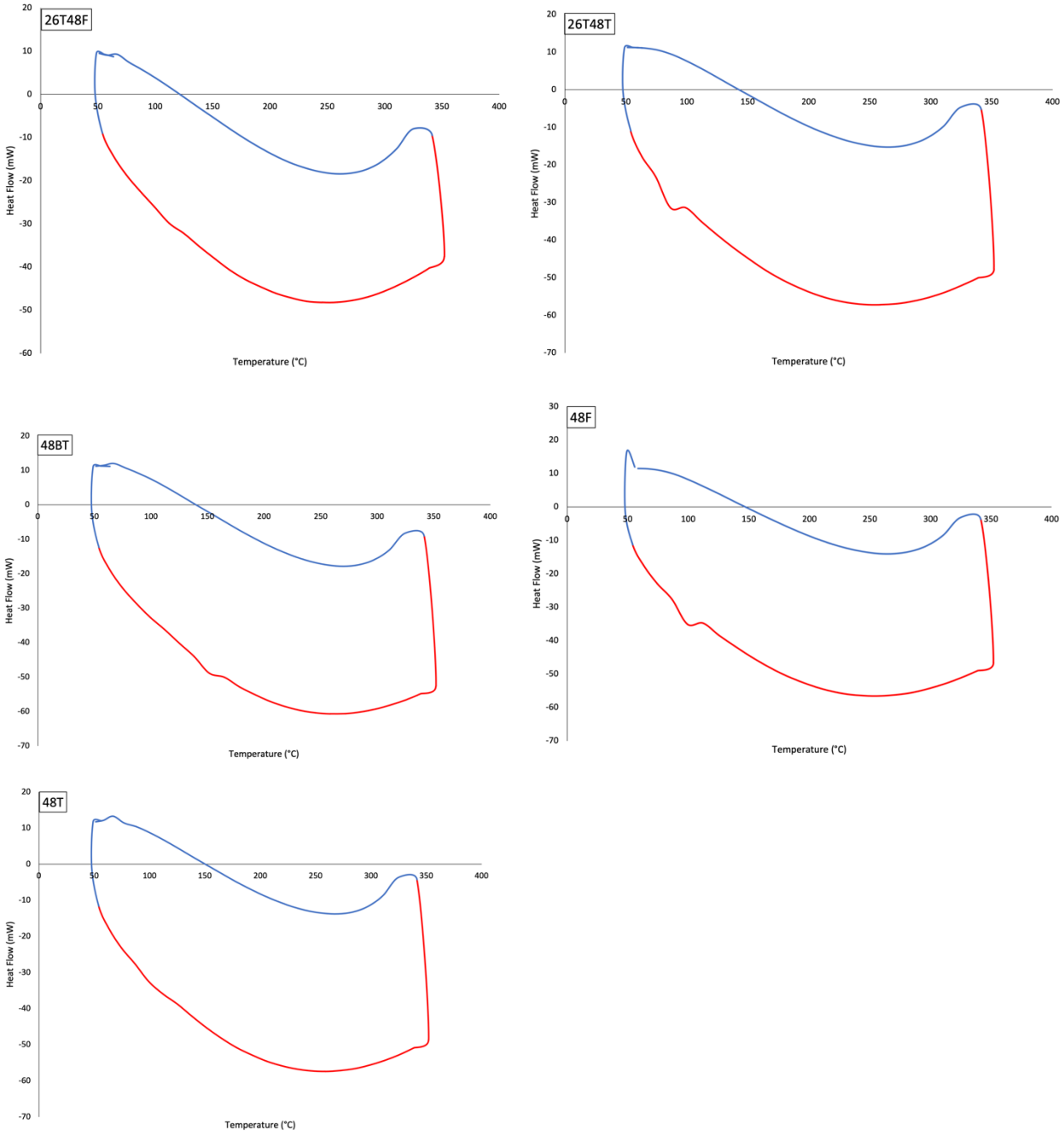


Fig. S102; DSC curves for all compounds with the DSCname in top left corner of each graph (note: 48BF sample was unavailable for DSC).

Theoretical Calculations

Gaussian Setups

All calculations were carried out with the Gaussian 09 series of programs[7] using density function theory (DFT). Becke's three parameter exchange functional combined with the Lee–Yang–Parr correlation functional (B3LYP) and with the 6-31G(d) basis set was used for all calculations.[8-11]

FMOs

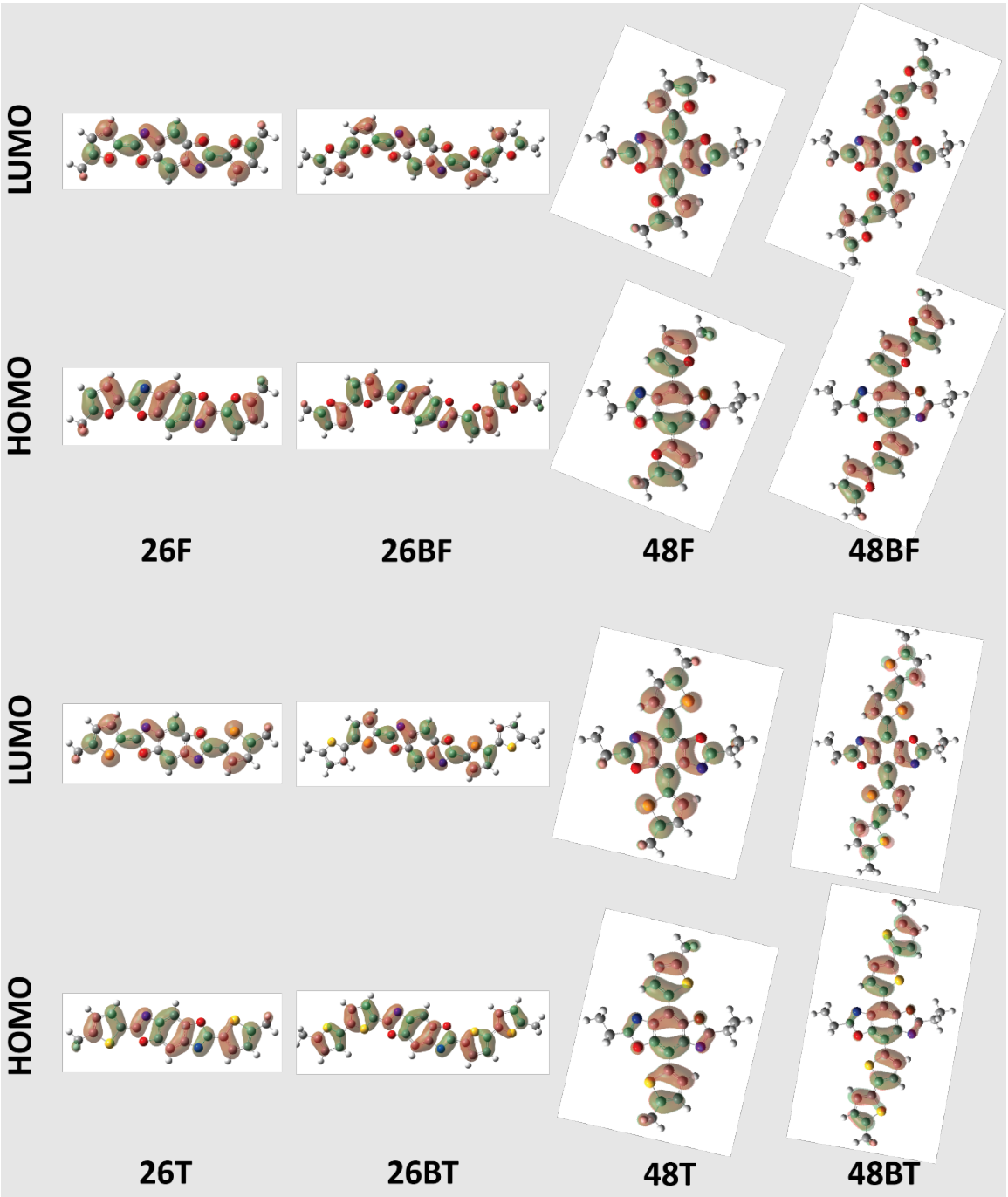


Figure S103. Parent molecules HOMO and LUMO mappings.

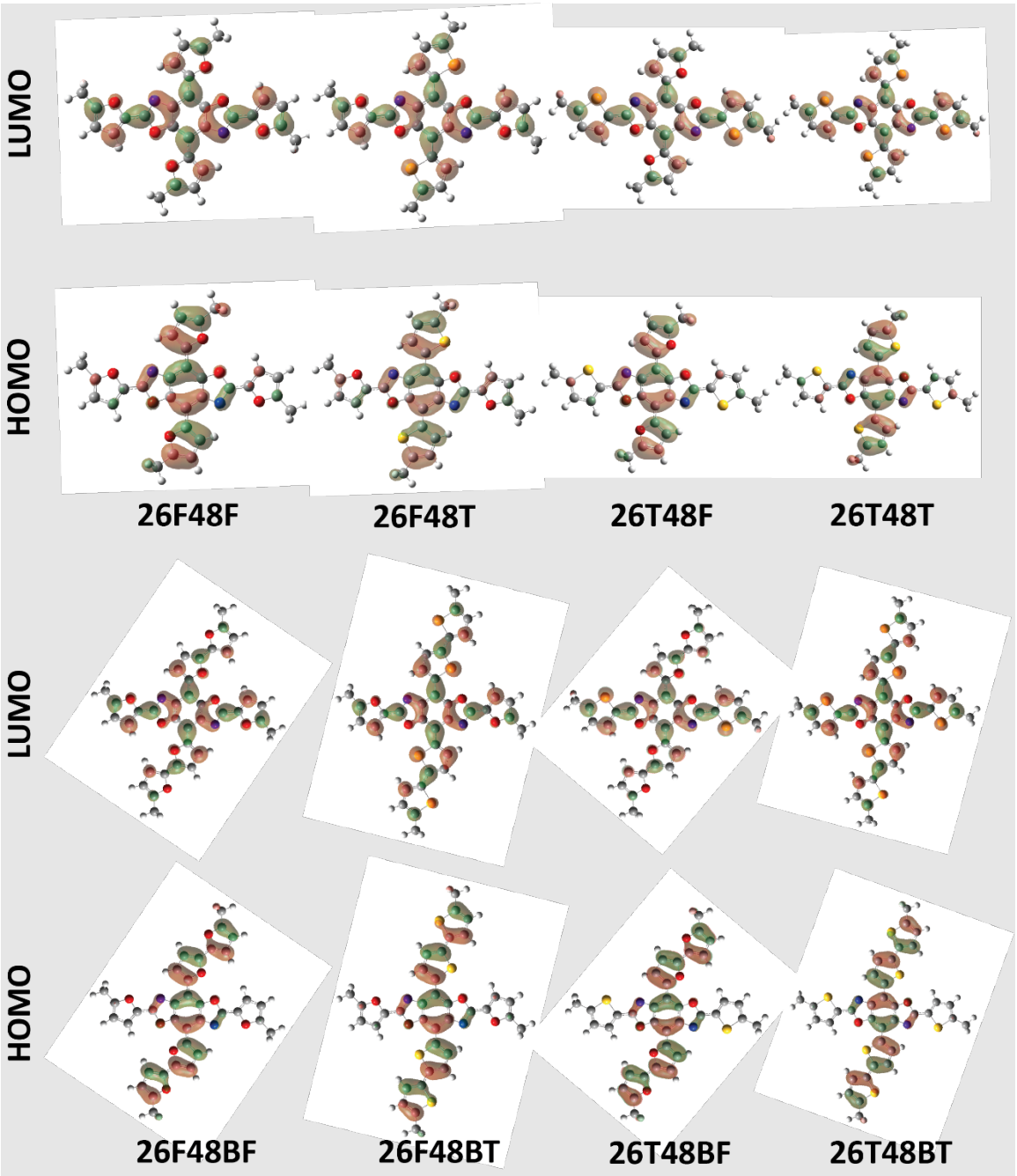


Figure S104. 1X1 and 1X2 series HOMO and LUMO mappings.

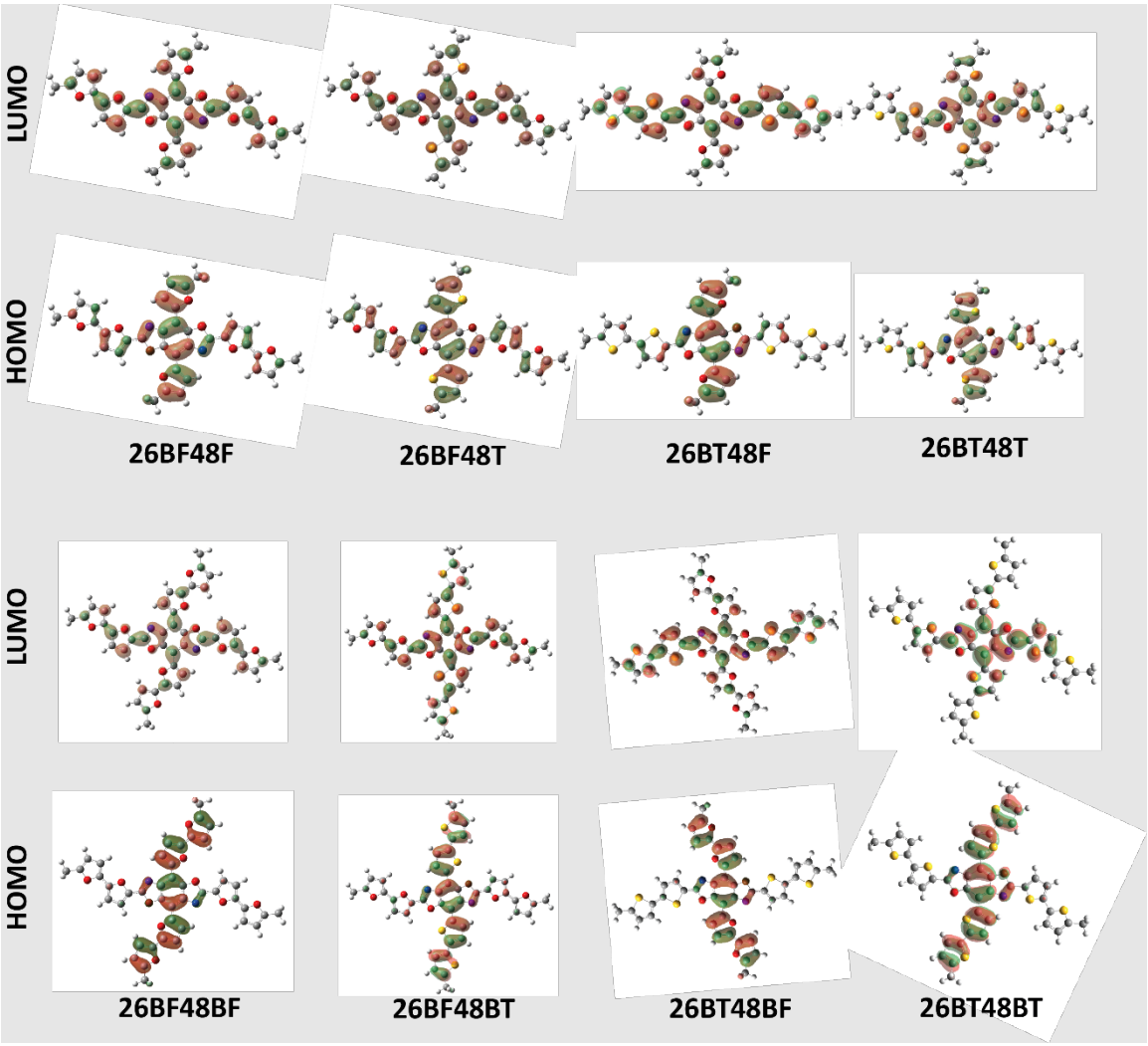


Figure S105. 2X1 and 2X2 series HOMO and LUMO mappings.

Calculated Absolute Energy (Hartree)

Molecule	Energy (Hartree)
48F	-1260.797095
26F	-1103.523541
48T	-1906.745549
26T	-1749.470941
48BF	-1718.478805
26BF	-1561.204012
48BT	-3010.37657

26BT	-2852.079057
26F48F	-1639.843126
26F48T	-2285.791352
26T48F	-2285.799061
26T48T	-2931.747081
26F48BF	-2097.524138
26F48BT	-3389.42235
26T48BF	-2743.479904
26T48BT	-4035.377896
26BF48F	-2097.523507
26BF48T	-2743.47168
26BT48F	-3389.429079
26BT48T	-4033.831109
26BF48BF	-2555.204498
26BF48BT	-3847.102682
26BT48BF	-3847.103852
26BT48BT	-5137.497186

Excitation energies and oscillator strengths

48F

```
Excited State   1: Singlet-A 3.2098 eV 386.27 nm f=0.8634 <S**2>=0.000
      99 ->100         0.70083
```

26F

```
Excited State   1: Singlet-A 3.3998 eV 364.69 nm f=1.5708 <S**2>=0.000
      83 -> 84         0.7054
```

48T

```
Excited State   1: Singlet-A 3.7012 eV 334.99 nm f=0.6302 <S**2>=0.000
107 ->108         0.69046
```

26T

```
Excited State   1: Singlet-A 3.8895 eV 318.76 nm f=1.3593 <S**2>=0.000
91 -> 92         0.69739
```

48BF

```
Excited State   1: Singlet-A 2.6516 eV 467.58 nm f=1.5020 <S**2>=0.000
133 ->134         0.70588
```

26BF

Excited State 1: Singlet-A 2.8259 eV 438.74 nm f=2.0607 <S**2>=0.000
117 ->118 0.70494

48BT

Excited State 1: Singlet-A 3.4099 eV 363.60 nm f=0.9292 <S**2>=0.000
149 ->150 0.69847

26BT

Excited State 1: Singlet-A 3.6203 eV 342.47 nm f=1.7341 <S**2>=0.000
133 ->134 0.69900

26F48F

Excited State 1: Singlet-A 2.7064 eV 458.12 nm f=0.4163 <S**2>=0.000
125 ->126 0.68899 125 ->128 0.13100

26F48T

Excited State 1: Singlet-A 2.7375 eV 452.92 nm f=0.5171 <S**2>=0.000
132 ->134 -0.10247 133 ->134 0.68939 133 ->136
0.12066

26T48F

Excited State 1: Singlet-A 2.5556 eV 485.15 nm f=0.3233 <S**2>=0.000
133 ->134 0.69229 133 ->136 0.12307

26T48T

Excited State 1: Singlet-A 3.3670 eV 368.23 nm f=0.4886 <S**2>=0.000
141 ->142 0.69189

26F48BF

Excited State 1: Singlet-A 2.3441 eV 528.92 nm f=0.8153 <S**2>=0.000
159 ->160 0.69736

26F48BT

Excited State 1: Singlet-A 2.3634 eV 524.59 nm f=1.1988 <S**2>=0.000
175 ->176 0.70046

26T48BF

Excited State 1: Singlet-A 2.2260 eV 556.99 nm f=0.6074 <S**2>=0.000
167 ->168 0.69729

26T48BT

Excited State 1: Singlet-A 3.1341 eV 395.60 nm f=0.6365 <S**2>=0.000
183 ->184 0.69715

26BF48F

Excited State 1: Singlet-A 2.5052 eV 494.90 nm f=0.5147 <S**2>=0.000
159 ->160 0.69512 159 ->162 -0.10292

26BF48T

Excited State 1: Singlet-A 2.5409 eV 487.95 nm f=0.7590 <S**2>=0.000
167 ->168 0.69919

26BT48F

```
Excited State   1: Singlet-A 2.2851 eV 542.57 nm f=0.3866 <S**2>=0.000
175 ->176         0.69815
```

26BT48T

```
Excited State   1: Singlet-A 3.3063 eV 375.00 nm f=0.6313 <S**2>=0.000
183 ->184         0.69698
```

26BF48BF

```
Excited State   1: Singlet-A 2.2022 eV 563.00 nm f=0.6116 <S**2>=0.000
193 ->194         0.69700
```

26BF48BT

```
Excited State   1: Singlet-A 2.2573 eV 549.25 nm f=0.9261 <S**2>=0.000
209 ->210         0.69879
```

26BT48BF

```
Excited State   1: Singlet-A 2.0096 eV 616.95 nm f=0.3723 <S**2>=0.000
209 ->210         0.70030
```

26BT48BT

```
Excited State   1: Singlet-A 3.0973 eV 400.30 nm f=0.4248 <S**2>=0.000
225 ->226         0.70075
```

Cartesian Coordinates

48F

C	-0.9032	1.13327	0.17047
C	-1.34121	-0.073	0.52536
C	-0.40105	-1.29318	0.5408
C	0.89355	-1.03308	0.23975
C	1.38598	0.32193	-0.15541
C	0.57369	1.40587	-0.17393
N	-2.02329	2.0538	0.15457
C	-3.06686	1.31355	0.42318
O	-2.73196	-0.03269	0.86923
N	2.0446	-1.90714	0.24195
C	3.08476	-1.13387	-0.02837
O	2.77241	0.23167	-0.48518
C	-4.51534	1.81531	0.27538
H	-4.8649	1.60936	-0.7147
H	-5.14028	1.31516	0.98551
C	4.53383	-1.63004	0.13096
H	5.16239	-1.12813	-0.57463
H	4.57105	-2.68478	-0.04526
C	5.0247	-1.33062	1.55958
H	6.03153	-1.67555	1.6704

H	4.98762	-0.27586	1.73571
H	4.39602	-1.83244	2.26526
C	-4.56138	3.33331	0.53069
H	-3.93655	3.83364	-0.17941
H	-5.56773	3.68181	0.42806
H	-4.21187	3.53921	1.52085
C	1.0886	2.813	-0.52933
C	0.31707	3.91516	-0.56423
O	2.47117	3.11862	-0.86706
C	1.24925	5.08359	-0.75765
H	-0.74734	3.95526	-0.46232
C	2.49314	4.57335	-0.82047
H	0.97677	6.11644	-0.82022
C	-0.89649	-2.70925	0.88854
C	-0.10967	-3.80081	0.9191
O	-2.27515	-3.03608	1.22225
C	-1.02595	-4.9832	1.10352
H	0.95543	-3.82556	0.81959
C	-2.27686	-4.49062	1.16643
H	-0.73935	-6.01254	1.16063
C	3.77817	5.42192	-0.83785
H	3.57739	6.36369	-1.30444
H	4.11153	5.5849	0.16571
H	4.53843	4.90672	-1.38697
C	-3.54995	-5.35709	1.17505
H	-4.31865	-4.85608	1.72547
H	-3.87857	-5.51826	0.16955
H	-3.33719	-6.29894	1.63607

26F

C	-0.96964	1.04831	0.28333
C	-1.3363	-0.2111	0.51237
C	-0.32128	-1.36717	0.43301
C	0.95876	-1.00059	0.18508
C	1.3709	0.41378	-0.0686
C	0.49255	1.44288	-0.00016
N	-2.14529	1.8956	0.32944
C	-3.14427	1.0702	0.50282
O	-2.73227	-0.28932	0.82741
N	2.16227	-1.79885	0.12771
C	3.15568	-0.94116	-0.04679
O	2.76492	0.44062	-0.37692
C	-4.61885	1.49375	0.36933
C	4.63069	-1.36119	0.09291

C	-5.02429	2.74082	0.06626
C	-6.5131	2.6643	-0.15542
C	-6.86189	1.37847	0.03533
O	-5.74922	0.59506	0.55209
C	5.03794	-2.60823	0.39368
C	6.53655	-2.61883	0.23361
C	6.88849	-1.37717	-0.14826
O	5.75972	-0.46017	-0.08669
H	-0.6062	-2.3888	0.57441
H	0.79215	2.46002	-0.14362
H	-4.40905	3.61258	-0.01379
H	-7.16273	3.47105	-0.42381
H	4.41862	-3.43304	0.67831
H	7.19042	-3.45265	0.38225
C	8.30646	-0.97759	-0.59692
H	9.02535	-1.59203	-0.09637
H	8.39707	-1.11208	-1.65456
H	8.48217	0.04897	-0.35157
C	-8.26138	0.80721	-0.25907
H	-8.99583	1.57252	-0.11843
H	-8.29882	0.45836	-1.26991
H	-8.46187	-0.00618	0.4066

48T

C	0.18224	1.31167	-0.0017
C	-1.12793	0.79711	-0.00596
C	-1.48335	-0.55711	-0.05767
C	-0.33723	-1.38426	-0.10743
C	0.97278	-0.86937	-0.1033
C	1.32829	0.48504	-0.05148
N	0.1106	2.70407	0.05743
C	-1.15601	2.97101	0.08533
O	-1.98029	1.87649	0.05051
N	-0.26595	-2.77634	-0.16597
C	1.00131	-3.04374	-0.19628
O	1.82505	-1.94814	-0.16116
C	-1.82616	4.30376	0.14976
H	-2.49878	4.39268	-0.71437
H	-2.47914	4.31797	1.03317
C	1.66246	-4.37929	-0.25253
H	2.27654	-4.43156	-1.1614
H	0.86901	-5.12543	-0.34945
C	2.54175	-4.6699	0.97679
H	3.0121	-5.654	0.88106

H	3.33197	-3.91993	1.07851
H	1.94522	-4.66429	1.89507
C	-0.83795	5.47126	0.18845
H	-0.2026	5.47732	-0.70199
H	-1.37957	6.42137	0.23495
H	-0.1829	5.40224	1.06181
C	2.67627	1.00439	-0.04692
C	3.1889	2.27829	-0.00297
C	4.60845	2.14393	-0.02525
H	2.60156	3.18246	0.03972
C	4.88083	0.80533	-0.08107
H	5.33972	2.94051	-0.00277
C	-2.83101	-1.07708	-0.0612
C	-3.34288	-2.35123	-0.10827
C	-4.7624	-2.21766	-0.08314
H	-2.75489	-3.25483	-0.15488
C	-5.03539	-0.8793	-0.0226
H	-5.49329	-3.01453	-0.10703
C	6.13959	0.01307	-0.12739
H	7.0025	0.68452	-0.11337
H	6.21958	-0.6664	0.73062
H	6.19612	-0.59984	-1.03583
C	-6.29442	-0.08776	0.0282
H	-6.35017	0.5215	0.93915
H	-6.37518	0.59525	-0.82686
H	-7.15709	-0.75948	0.01234
S	3.71215	0.09927	-0.09473
S	-3.86717	-0.17273	-0.00863

26T

C	-1.06336	0.88458	-0.00006
C	-1.23658	-0.5214	-0.00009
C	-0.21568	-1.45549	-0.0001
C	1.06336	-0.88457	-0.00013
C	1.23658	0.5214	-0.00008
C	0.21568	1.4555	-0.00004
N	-2.3131	1.48871	-0.00008
C	-3.15351	0.49302	-0.00008
O	-2.58981	-0.76271	-0.00012
N	2.3131	-1.48871	-0.00019
C	3.15351	-0.49302	-0.00014
O	2.58982	0.76271	-0.00007
C	-4.58759	0.58094	-0.00008
C	4.58759	-0.58094	-0.00008

C	-5.43347	1.65992	-0.00028
C	-6.75408	1.12629	-0.00018
C	-6.63163	-0.23787	0.00013
C	5.43347	-1.65992	-0.00022
C	6.75408	-1.1263	-0.00006
C	6.63163	0.23787	0.00015
H	-0.38028	-2.52624	-0.00013
H	0.38028	2.52624	0.
H	-5.13058	2.69684	-0.0005
H	-7.68235	1.68063	-0.0003
H	5.13057	-2.69684	-0.0004
H	7.68234	-1.68064	-0.00008
C	7.61265	1.35617	0.0004
H	8.63077	0.95818	0.00035
H	7.4913	1.99422	-0.88349
H	7.49126	1.99386	0.88455
C	-7.61265	-1.35618	0.00039
H	-8.63077	-0.95818	0.00024
H	-7.49125	-1.99427	-0.88346
H	-7.49131	-1.99381	0.88457
S	-5.31117	-0.58253	0.00022
S	5.31117	0.58253	0.00011

48BF

C	-0.93966	1.08256	0.13841
C	-1.32404	-0.12469	0.54768
C	-0.33184	-1.30126	0.60773
C	0.94809	-0.99777	0.2857
C	1.38034	0.35851	-0.17086
C	0.5217	1.40432	-0.22831
N	-2.09718	1.9538	0.09084
C	-3.10681	1.18442	0.40238
O	-2.71325	-0.12754	0.90051
N	2.13443	-1.82213	0.31512
C	3.13928	-1.02016	0.00056
O	2.76754	0.31216	-0.50855
C	-4.57535	1.61994	0.25175
H	-4.92756	1.35617	-0.72344
H	-5.17023	1.12631	0.99177
C	4.60729	-1.45518	0.16418
H	5.2104	-0.96184	-0.56928
H	4.68132	-2.51429	0.03296
C	5.09966	-1.07658	1.57282
H	6.11916	-1.37979	1.68819

H	5.02562	-0.01732	1.70354
H	4.49567	-1.56957	2.30549
C	-4.68097	3.14536	0.44045
H	-4.08606	3.63877	-0.29954
H	-5.70223	3.44764	0.33674
H	-4.32829	3.40921	1.41568
C	0.96527	2.81892	-0.64473
C	0.13601	3.87554	-0.71804
O	2.32789	3.18434	-1.00471
C	1.00174	5.08358	-0.96063
H	-0.92852	3.86177	-0.6123
C	2.26998	4.63943	-1.01125
H	0.67327	6.09731	-1.05949
C	-0.75812	-2.72348	1.01812
C	0.0839	-3.77024	1.08983
O	-2.11823	-3.10764	1.37177
C	-0.76891	-4.99003	1.32157
H	1.14898	-3.74352	0.98956
C	-2.04367	-4.56284	1.36977
H	-0.42802	-5.99973	1.41667
C	3.5015	5.56009	-1.06509
C	4.77393	5.12596	-1.11875
O	3.43293	7.01311	-1.05905
C	5.64727	6.34344	-0.95076
H	5.1006	4.11499	-1.24316
C	4.8154	7.39252	-0.81215
H	6.71715	6.36782	-0.93352
C	-3.26542	-5.50146	1.41352
C	-4.54438	-5.08364	1.47022
O	-3.18048	-6.95495	1.39402
C	-5.40241	-6.30963	1.28909
H	-4.88471	-4.07835	1.60491
C	-4.55969	-7.34819	1.14258
H	-6.47174	-6.34558	1.26791
C	5.26671	8.81585	-0.43589
H	6.25701	8.98436	-0.80326
H	4.59842	9.52873	-0.87204
H	5.25848	8.92391	0.62862
C	-5.00109	-8.77177	0.75345
H	-4.32628	-9.4848	1.17928
H	-5.99006	-8.9515	1.12321
H	-4.99523	-8.86752	-0.31283

26BF

C	-0.81567	1.18077	0.24469
C	-1.32355	-0.01192	0.56327
C	-0.49178	-1.30151	0.46123
C	0.80206	-1.11232	0.1419
C	1.39134	0.24022	-0.13651
C	0.67251	1.37813	-0.07954
N	-1.91022	2.1307	0.25076
C	-2.9798	1.4418	0.50918
O	-2.68101	0.10539	0.98464
N	1.90306	-2.04766	0.02204
C	2.98442	-1.32039	-0.14773
O	2.75956	0.09735	-0.4567
C	-4.43453	1.87039	0.33403
C	4.42162	-1.78284	-0.02891
C	-4.93747	2.96963	-0.27232
C	-6.42094	2.69699	-0.44681
C	-6.62376	1.48227	0.10375
O	-5.47035	1.02494	0.82565
C	4.95797	-3.02062	0.01356
C	6.46873	-2.80686	-0.01612
C	6.63524	-1.46491	-0.0474
O	5.40454	-0.76954	0.08127
C	-7.84247	0.56193	0.05924
C	7.86191	-0.58286	-0.18478
C	-7.71934	-0.62392	0.65552
C	-9.04334	-1.28144	0.60087
C	-9.87526	-0.44151	-0.02003
O	-9.1776	0.75085	-0.54628
C	7.62763	0.72573	-0.17339
C	8.9329	1.39889	-0.08766
C	9.85391	0.43465	-0.04995
O	9.291	-0.89781	-0.30645
C	-11.34971	-0.84998	-0.09582
C	11.27787	0.85714	0.24876
H	-0.90276	-2.26873	0.64837
H	1.10763	2.33834	-0.26023
H	-4.40389	3.83588	-0.5903
H	-7.14634	3.3248	-0.91911
H	4.43479	-3.95364	0.04733
H	7.23243	-3.556	-0.01496
H	-6.8276	-1.02034	1.0999
H	-9.29631	-2.24425	0.99483

H	6.67132	1.19845	-0.20524
H	9.11043	2.45473	-0.0503
H	-11.86531	-0.48679	0.76855
H	-11.7909	-0.43161	-0.97629
H	11.46566	0.76153	1.2978
H	11.95648	0.23233	-0.29346
H	-11.42281	-1.91684	-0.13268
H	11.41714	1.87595	-0.04711

48BT

C	0.19927	1.32244	0.0155
C	-1.10812	0.80411	-0.00155
C	-1.45813	-0.55282	-0.05437
C	-0.3082	-1.37742	-0.0898
C	0.9991	-0.8588	-0.07278
C	1.3492	0.49837	-0.02078
N	0.12338	2.71421	0.07087
C	-1.14423	2.97818	0.0848
O	-1.96453	1.88046	0.04341
N	-0.23281	-2.76886	-0.14325
C	1.03551	-3.03345	-0.15816
O	1.85536	-1.93467	-0.11739
C	-1.81889	4.30894	0.1393
H	-2.48202	4.39417	-0.73254
H	-2.48103	4.32306	1.0159
C	1.70069	-4.36737	-0.19821
H	2.34602	-4.41409	-1.0853
H	0.91254	-5.11449	-0.32566
C	2.53585	-4.66299	1.06073
H	3.01175	-5.6454	0.97639
H	3.3202	-3.91204	1.19693
H	1.9063	-4.66406	1.95662
C	-0.83456	5.4795	0.18621
H	-0.18975	5.48575	-0.69738
H	-1.37972	6.42787	0.22475
H	-0.1891	5.41449	1.06696
C	2.69184	1.02108	-0.00382
C	3.20242	2.29979	0.05261
C	4.61618	2.17921	0.03977
H	2.60926	3.20013	0.09696
C	4.89283	0.83326	-0.02418
H	5.34657	2.97455	0.0724
C	-2.80061	-1.07561	-0.07121
C	-3.31148	-2.3545	-0.12136

C	-4.72522	-2.23321	-0.11205
H	-2.71842	-3.25524	-0.15977
C	-5.00137	-0.88668	-0.0568
H	-5.45587	-3.02842	-0.14201
C	6.11116	0.07923	-0.0672
C	6.38403	-1.26217	-0.14074
C	7.8079	-1.37897	-0.1504
H	5.65088	-2.05443	-0.18379
C	8.31353	-0.11165	-0.08304
H	8.38719	-2.29079	-0.20147
C	-6.21864	-0.13058	-0.02247
C	-6.48824	1.21235	0.03231
C	-7.91182	1.33236	0.04172
H	-5.75272	2.00301	0.06158
C	-8.42036	0.06533	-0.00742
H	-8.4891	2.24607	0.08023
C	9.69141	0.44836	-0.05621
H	10.42269	-0.36322	-0.10207
H	9.87038	1.11953	-0.90569
H	9.87496	1.02389	0.85988
C	-9.79955	-0.49185	-0.02527
H	-9.97935	-1.15068	0.83366
H	-10.52894	0.32197	0.00982
H	-9.9852	-1.07972	-0.93307
S	7.28337	0.79128	-0.03155
S	3.72962	0.11937	-0.05079
S	-3.83798	-0.17331	-0.03155
S	-7.39233	-0.84061	-0.04708

26BT

C	-0.93538	1.01939	-0.00021
C	-1.2954	-0.35136	-0.00022
C	-0.4091	-1.4136	-0.00021
C	0.93537	-1.01936	-0.00021
C	1.2954	0.35138	-0.00021
C	0.40909	1.41364	-0.00021
N	-2.09154	1.78541	-0.00025
C	-3.05907	0.91086	-0.00023
O	-2.66861	-0.40945	-0.00023
N	2.09153	-1.78539	-0.00025
C	3.05906	-0.91085	-0.00021
O	2.66862	0.40946	-0.00022
C	-4.46518	1.19142	-0.00025
C	4.46518	-1.19142	-0.00019

C	-5.15976	2.37755	-0.00021
C	-6.5363	2.03858	-0.00014
C	-6.59823	0.662	-0.00007
C	5.15975	-2.37755	-0.00026
C	6.53629	-2.03859	-0.00009
C	6.59822	-0.662	-0.00003
C	-7.68817	-0.26858	0.0001
C	7.68817	0.26857	0.00013
C	-7.75804	-1.63757	0.00019
C	-9.14784	-1.96404	0.00035
C	-9.83626	-0.78323	0.00037
C	7.75805	1.63756	0.00023
C	9.14786	1.96402	0.00038
C	9.83627	0.7832	0.00037
C	-11.28221	-0.43428	0.00051
C	11.28222	0.43424	0.00044
H	-0.71556	-2.45265	-0.00018
H	0.71557	2.45268	-0.00019
H	-4.71639	3.36266	-0.00031
H	-7.38221	2.71008	-0.00018
H	4.71638	-3.36266	-0.00039
H	7.3822	-2.71008	-0.00005
H	-6.91726	-2.31603	0.00014
H	-9.58456	-2.95321	0.00049
H	6.91729	2.31603	0.00022
H	9.58459	2.95318	0.00052
H	-11.55314	0.15605	0.88473
H	-11.55332	0.15598	-0.88369
H	11.5532	-0.1561	0.88462
H	11.55328	-0.15599	-0.8838
H	-11.88416	-1.34688	0.00063
H	11.88418	1.34684	0.00053
S	8.95273	-0.26338	0.0002
S	5.33954	-0.13583	-0.00011
S	-5.33954	0.13584	-0.0001
S	-8.95274	0.26337	0.00022

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C	-0.93966	1.08256	0.13841
C	-1.32404	-0.12469	0.54768
C	-0.33184	-1.30126	0.60773
C	0.94809	-0.99777	0.2857
C	1.38034	0.35851	-0.17086
C	0.5217	1.40432	-0.22831

N	-2.09718	1.9538	0.09084
C	-3.10681	1.18442	0.40238
O	-2.71325	-0.12754	0.90051
N	2.13443	-1.82213	0.31512
C	3.13928	-1.02016	0.00056
O	2.76754	0.31216	-0.50855
C	0.96527	2.81892	-0.64473
C	0.13601	3.87554	-0.71804
O	2.32789	3.18434	-1.00471
C	1.00174	5.08358	-0.96063
H	-0.92852	3.86177	-0.6123
C	2.26998	4.63943	-1.01125
H	0.67327	6.09731	-1.05949
C	-0.75812	-2.72348	1.01812
C	0.0839	-3.77024	1.08983
O	-2.11823	-3.10764	1.37177
C	-0.76891	-4.99003	1.32157
H	1.14898	-3.74352	0.98956
C	-2.04367	-4.56284	1.36977
H	-0.42802	-5.99973	1.41667
C	-4.57616	1.62018	0.25166
C	-5.80391	1.03905	0.49284
O	-4.74722	2.91206	-0.24767
C	-6.80553	2.01804	0.12526
H	-6.0038	0.04502	0.8813
C	-6.1232	3.13296	-0.31625
H	-7.8803	1.87957	0.1926
C	4.60746	-1.45523	0.1642
C	5.83701	-0.87337	-0.06577
O	4.77472	-2.74706	0.66496
C	6.83581	-1.85199	0.31037
H	6.03984	0.12084	-0.45223
C	6.15015	-2.96737	0.7455
H	7.91107	-1.71293	0.2527
C	-3.2644	-5.50067	1.41348
H	-3.93879	-5.17294	2.17682
H	-3.76191	-5.4829	0.46635
H	-2.94065	-6.49777	1.62765
C	3.50266	5.56096	-1.06514
H	4.0021	5.54425	-0.119
H	4.17097	5.21846	-1.82734
H	3.19136	6.56045	-1.28652
C	6.5426	-4.35617	1.28292
H	6.16337	-4.47436	2.27646

H	6.12832	-5.11343	0.6506
H	7.60878	-4.44566	1.29511
C	-6.51972	4.52181	-0.85056
H	-6.10009	5.27902	-0.22172
H	-6.14863	4.63982	-1.84718
H	-7.58594	4.61155	-0.85401

26F48T

C	1.14585	0.7616	0.00004
C	1.17433	-0.64897	0.00003
C	0.0629	-1.49937	0.00005
C	-1.14586	-0.7616	0.0001
C	-1.17433	0.64897	0.0001
C	-0.0629	1.49937	0.00008
N	2.44988	1.2369	0.00008
C	3.18778	0.16448	0.00003
O	2.49812	-1.02191	0.
N	-2.44988	-1.2369	0.00012
C	-3.18778	-0.16447	0.00014
O	-2.49812	1.02191	0.00008
C	-0.10168	2.94293	0.00002
C	0.8795	3.90474	-0.00002
C	0.21016	5.16391	-0.00005
H	1.94076	3.7088	0.00003
C	-1.13171	4.9022	-0.00009
H	0.66588	6.14478	-0.00004
C	0.10167	-2.94293	0.00002
C	-0.8795	-3.90475	0.0001
C	-0.21015	-5.16392	0.00002
H	-1.94076	-3.70881	0.00019
C	1.13172	-4.90219	-0.00009
H	-0.66587	-6.14478	0.00003
C	4.61984	0.05586	0.
C	5.4598	-1.02827	-0.00005
O	5.34868	1.21395	0.00005
C	6.78398	-0.50171	-0.00005
H	5.1544	-2.0646	-0.00009
C	6.66701	0.8626	0.00001
H	7.70961	-1.06043	-0.00009
C	-4.61984	-0.05586	0.00005
C	-5.45981	1.02827	-0.00001
O	-5.34868	-1.21395	0.00004
C	-6.78399	0.5017	-0.00007
H	-5.15442	2.0646	0.

C	-6.66701	-0.8626	-0.00003
H	-7.70962	1.06042	-0.00012
C	2.34685	-5.76107	-0.00019
H	2.97015	-5.57688	-0.88448
H	2.97028	-5.57692	0.88401
H	2.0571	-6.81545	-0.0002
C	-2.34684	5.76107	-0.00015
H	-2.97016	5.5769	-0.88443
H	-2.97025	5.5769	0.88407
H	-2.05709	6.81545	-0.00014
C	-7.65284	-1.97666	-0.00006
H	-7.53336	-2.61492	-0.884
H	-7.53338	-2.61495	0.88387
H	-8.66946	-1.5748	-0.00006
C	7.65285	1.97665	0.00005
H	7.53334	2.61499	-0.88383
H	7.53342	2.61485	0.88404
H	8.66947	1.57478	-0.00003
S	-1.33633	3.55198	-0.00008
S	1.33633	-3.55198	-0.00008

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C	1.14585	0.7616	0.00004
C	1.17433	-0.64897	0.00003
C	0.0629	-1.49937	0.00005
C	-1.14586	-0.7616	0.0001
C	-1.17433	0.64897	0.0001
C	-0.0629	1.49937	0.00008
N	2.44988	1.2369	0.00008
C	3.18778	0.16448	0.00003
O	2.49812	-1.02191	0.
N	-2.44988	-1.2369	0.00012
C	-3.18778	-0.16447	0.00014
O	-2.49812	1.02191	0.00008
C	-0.10168	2.94293	0.00002
C	0.8795	3.90474	-0.00002
O	-1.33633	3.55198	-0.00008
C	0.21016	5.16391	-0.00005
H	1.94076	3.7088	0.00003
C	-1.13171	4.9022	-0.00009
H	0.66588	6.14478	-0.00004
C	0.10167	-2.94293	0.00002
C	-0.8795	-3.90475	0.0001
O	1.33633	-3.55198	-0.00008

C	-0.21015	-5.16392	0.00002
H	-1.94076	-3.70881	0.00019
C	1.13172	-4.90219	-0.00009
H	-0.66587	-6.14478	0.00003
C	4.61984	0.05586	0.
C	5.4598	-1.02827	-0.00005
C	6.78398	-0.50171	-0.00005
H	5.1544	-2.0646	-0.00009
C	6.66701	0.8626	0.00001
H	7.70961	-1.06043	-0.00009
C	-4.61984	-0.05586	0.00005
C	-5.45981	1.02827	-0.00001
C	-6.78399	0.5017	-0.00007
H	-5.15442	2.0646	0.
C	-6.66701	-0.8626	-0.00003
H	-7.70962	1.06042	-0.00012
C	2.34685	-5.76107	-0.00019
H	2.97015	-5.57688	-0.88448
H	2.97028	-5.57692	0.88401
H	2.0571	-6.81545	-0.0002
C	-2.34684	5.76107	-0.00015
H	-2.97016	5.5769	-0.88443
H	-2.97025	5.5769	0.88407
H	-2.05709	6.81545	-0.00014
C	-7.65284	-1.97666	-0.00006
H	-7.53336	-2.61492	-0.884
H	-7.53338	-2.61495	0.88387
H	-8.66946	-1.5748	-0.00006
C	7.65285	1.97665	0.00005
H	7.53334	2.61499	-0.88383
H	7.53342	2.61485	0.88404
H	8.66947	1.57478	-0.00003
S	-5.34868	-1.21395	0.00004
S	5.34868	1.21395	0.00005

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C	-0.22241	0.40362	0.
C	-0.23254	-1.0072	0.00001
C	0.88985	-1.84307	0.
C	2.08891	-1.08965	-0.00005
C	2.09905	0.32117	-0.00005
C	0.97666	1.15704	-0.00003
N	-1.5325	0.86194	-0.00003
C	-2.2564	-0.21999	0.00002

O	-1.55137	-1.39731	0.00005
N	3.399	-1.54796	-0.00007
C	4.1229	-0.46603	-0.00009
O	3.41787	0.71128	-0.00004
C	0.99667	2.60099	0.00002
C	0.00306	3.54997	0.00006
C	0.65599	4.81773	0.00009
H	-1.05556	3.34025	0.00001
C	2.00114	4.57348	0.00013
H	0.18755	5.79259	0.00009
C	0.86984	-3.28702	0.00002
C	1.86343	-4.236	-0.00006
C	1.2105	-5.50376	0.00003
H	2.92206	-4.02629	-0.00015
C	-0.13465	-5.2595	0.00013
H	1.67894	-6.47862	0.00002
C	-3.68693	-0.34721	0.00004
C	-4.51272	-1.44217	0.0001
C	-5.84364	-0.93287	0.00009
H	-4.19388	-2.47444	0.00013
C	-5.74441	0.43285	0.00004
H	-6.76193	-1.50357	0.00013
C	5.55343	-0.33882	-0.00001
C	6.37923	0.75614	0.00005
C	7.71015	0.24683	0.00011
H	6.0604	1.78842	0.00005
C	7.61091	-1.11888	0.00007
H	8.62844	0.81753	0.00016
C	-1.33851	-6.1341	0.00024
H	-1.96416	-5.95803	0.88453
H	-1.96429	-5.95807	-0.88397
H	-1.03508	-7.18463	0.00024
C	3.20501	5.44808	0.00019
H	3.83067	5.27203	0.88447
H	3.83076	5.27203	-0.88403
H	2.90157	6.4986	0.00018
C	8.61114	-2.22003	0.0001
H	8.49996	-2.85979	0.88404
H	8.49998	-2.85981	-0.88383
H	9.62245	-1.80499	0.0001
C	-6.74465	1.53399	-0.00001
H	-6.63344	2.17383	0.88387
H	-6.63353	2.17369	-0.884
H	-7.75596	1.11894	0.00007

S	6.29726	-1.48734	0.
S	-4.43076	0.80131	0.
S	2.22329	3.22604	0.00012
S	-0.35679	-3.91206	0.00013

26F48BF

C	-0.93966	1.08256	0.13841
C	-1.32404	-0.12469	0.54768
C	-0.33184	-1.30126	0.60773
C	0.94809	-0.99777	0.2857
C	1.38034	0.35851	-0.17086
C	0.5217	1.40432	-0.22831
N	-2.09718	1.9538	0.09084
C	-3.10681	1.18442	0.40238
O	-2.71325	-0.12754	0.90051
N	2.13443	-1.82213	0.31512
C	3.13928	-1.02016	0.00056
O	2.76754	0.31216	-0.50855
C	0.96527	2.81892	-0.64473
C	0.13601	3.87554	-0.71804
O	2.32789	3.18434	-1.00471
C	1.00174	5.08358	-0.96063
H	-0.92852	3.86177	-0.6123
C	2.26998	4.63943	-1.01125
H	0.67327	6.09731	-1.05949
C	-0.75812	-2.72348	1.01812
C	0.0839	-3.77024	1.08983
O	-2.11823	-3.10764	1.37177
C	-0.76891	-4.99003	1.32157
H	1.14898	-3.74352	0.98956
C	-2.04367	-4.56284	1.36977
H	-0.42802	-5.99973	1.41667
C	3.5015	5.56009	-1.06509
C	4.77393	5.12596	-1.11875
O	3.43293	7.01311	-1.05905
C	5.64727	6.34344	-0.95076
H	5.1006	4.11499	-1.24316
C	4.8154	7.39252	-0.81215
H	6.71715	6.36782	-0.93352
C	-3.26542	-5.50146	1.41352
C	-4.54438	-5.08364	1.47022
O	-3.18048	-6.95495	1.39402
C	-5.40241	-6.30963	1.28909
H	-4.88471	-4.07835	1.60491

C	-4.55969	-7.34819	1.14258
H	-6.47174	-6.34558	1.26791
C	5.26671	8.81585	-0.43589
H	6.25701	8.98436	-0.80326
H	4.59842	9.52873	-0.87204
H	5.25848	8.92391	0.62862
C	-5.00109	-8.77177	0.75345
H	-4.32628	-9.4848	1.17928
H	-5.99006	-8.9515	1.12321
H	-4.99523	-8.86752	-0.31283
C	-4.57616	1.62018	0.25166
C	-5.80391	1.03905	0.49284
O	-4.74722	2.91206	-0.24767
C	-6.80553	2.01804	0.12526
H	-6.0038	0.04502	0.8813
C	-6.1232	3.13296	-0.31625
H	-7.8803	1.87957	0.1926
C	4.60746	-1.45523	0.1642
C	5.83701	-0.87337	-0.06577
O	4.77472	-2.74706	0.66496
C	6.83581	-1.85199	0.31037
H	6.03984	0.12084	-0.45223
C	6.15015	-2.96737	0.7455
H	7.91107	-1.71293	0.2527
C	-6.51972	4.52181	-0.85056
H	-6.10709	5.27887	-0.21692
H	-6.14142	4.64308	-1.84408
H	-7.58614	4.60846	-0.86191
C	6.5426	-4.35617	1.28292
H	6.15418	-4.47853	2.27239
H	6.13736	-5.11322	0.64452
H	7.60894	-4.44169	1.30525

26F48BT

C	-0.40104	1.31944	0.00029
C	0.95378	0.92794	0.00021
C	1.46285	-0.37661	0.00012
C	0.40104	-1.31944	0.00012
C	-0.95378	-0.92794	0.0002
C	-1.46285	0.37661	0.00031
N	-0.46268	2.70605	0.00038
C	0.77813	3.09639	0.00032
O	1.70416	2.08058	0.00023
N	0.46268	-2.70605	-0.00003

C	-0.77813	-3.09639	0.00001
O	-1.70416	-2.08058	0.00014
C	-2.86761	0.73782	0.00039
C	-3.41584	2.00895	0.00021
C	-4.82782	2.02006	0.00056
H	-2.79746	2.89683	0.
C	-5.39978	0.76236	0.00102
H	-5.41361	2.93349	0.00082
C	2.86761	-0.73782	0.00001
C	3.41585	-2.00895	-0.00012
C	4.82782	-2.02006	-0.00022
H	2.79746	-2.89683	-0.00015
C	5.39978	-0.76235	-0.00016
H	5.41361	-2.93348	-0.00032
C	-6.79953	0.40153	0.00155
C	-7.37962	-0.84843	0.00716
C	-8.80213	-0.81876	0.00581
H	-6.80087	-1.76618	0.0125
C	-9.332	0.44452	-0.00076
H	-9.41982	-1.71152	0.00977
C	6.79953	-0.40152	-0.00023
C	7.37962	0.84845	-0.00003
C	8.80213	0.81878	-0.00018
H	6.80086	1.76621	0.00022
C	9.332	-0.44453	-0.00048
H	9.41982	1.71155	-0.00006
C	-10.77358	0.85456	-0.00383
H	-11.41003	-0.03598	0.00003
H	-11.03217	1.45551	0.87696
H	-11.03086	1.44692	-0.89079
C	10.77358	-0.85456	-0.00073
H	11.03146	-1.45088	-0.88487
H	11.41003	0.03599	-0.00043
H	11.03157	-1.45157	0.8829
C	1.30461	4.43132	0.00036
C	2.58724	4.91794	0.00031
O	0.40998	5.46685	0.00048
C	2.47035	6.3376	0.00041
H	3.4907	4.32532	0.00022
C	1.13112	6.62455	0.0005
H	3.27529	7.05931	0.00041
C	-1.30462	-4.43132	-0.00012
C	-2.58724	-4.91794	-0.00027
O	-0.40998	-5.46685	-0.00013

C	-2.47035	-6.3376	-0.00042
H	-3.4907	-4.32532	-0.00032
C	-1.13112	-6.62455	-0.00031
H	-3.27529	-7.05931	-0.00058
C	0.35414	7.89297	0.00062
H	-0.29109	7.96487	-0.88333
H	-0.291	7.96476	0.88465
H	1.03563	8.74762	0.00064
C	-0.35414	-7.89297	-0.00034
H	0.29119	-7.9647	-0.88423
H	0.2909	-7.96493	0.88374
H	-1.03563	-8.74762	-0.00056
S	-8.05189	1.63895	-0.00572
S	-4.15325	-0.47001	0.00074
S	4.15325	0.47001	0.00001
S	8.05189	-1.63897	-0.0006

26T48BF

C	0.02878	1.37542	-0.00234
C	1.20404	0.59665	-0.00135
C	1.268	-0.80266	-0.00062
C	-0.02877	-1.37542	-0.00135
C	-1.20404	-0.59665	-0.00236
C	-1.268	0.80265	-0.00266
N	0.37934	2.71734	-0.00277
C	1.68126	2.71527	-0.00205
O	2.2644	1.47263	-0.00113
N	-0.37934	-2.71734	-0.00183
C	-1.68126	-2.71527	-0.00319
O	-2.2644	-1.47262	-0.00345
C	-2.47011	1.59667	-0.00311
C	-2.69335	2.95676	-0.00738
O	-3.67761	0.93692	0.00152
C	-4.09966	3.14189	-0.00524
H	-1.91986	3.7093	-0.01121
C	-4.65978	1.88561	0.00034
H	-4.64199	4.07621	-0.0072
C	2.47012	-1.59667	0.00046
C	2.69335	-2.95676	0.00087
O	3.67763	-0.93691	0.00143
C	4.09966	-3.1419	0.00205
H	1.91986	-3.70931	0.00028
C	4.65979	-1.88561	0.00236
H	4.64199	-4.07622	0.00261

C	-6.01404	1.41595	0.00558
C	-6.57874	0.16695	0.01498
O	-6.99959	2.37064	0.00116
C	-7.99315	0.36791	0.01639
H	-6.04012	-0.76933	0.02091
C	-8.20468	1.71743	0.00785
H	-8.76045	-0.39418	0.02306
C	6.01406	-1.41594	0.00346
C	6.5788	-0.16693	0.00388
O	6.99959	-2.37067	0.00431
C	7.9932	-0.36791	0.00508
H	6.0402	0.76938	0.00338
C	8.2047	-1.71746	0.00534
H	8.76052	0.39419	0.00569
C	-9.42385	2.56977	0.00451
H	-10.31726	1.93941	0.01039
H	-9.46043	3.22452	0.88435
H	-9.46377	3.21278	-0.88379
C	9.42385	-2.56984	0.00636
H	9.46303	-3.21847	-0.87788
H	10.31728	-1.93947	0.00749
H	9.46113	-3.21899	0.8903
C	2.57929	3.83577	-0.00218
C	3.94796	3.92342	-0.00147
C	4.25546	5.31458	-0.00209
H	4.6362	3.0907	-0.00063
C	3.06052	5.98332	-0.00312
H	5.23746	5.76685	-0.00181
C	-2.5793	-3.83576	-0.005
C	-3.94796	-3.9234	-0.00999
C	-4.25548	-5.31455	-0.00983
H	-4.63618	-3.09067	-0.01388
C	-3.06055	-5.9833	-0.0048
H	-5.23747	-5.76681	-0.01309
C	2.69165	7.42442	-0.00413
H	2.09679	7.68297	-0.88857
H	2.0958	7.68395	0.87936
H	3.59472	8.04038	-0.00396
C	-2.6917	-7.4244	-0.00202
H	-2.09297	-7.68428	-0.88345
H	-2.09975	-7.68261	0.88447
H	-3.59478	-8.04036	-0.00489
S	-2.03023	-5.08931	-0.00182
S	2.0302	5.08932	-0.00319

26T48BT

C	-0.0234	1.37552	-0.00238
C	1.18056	0.64188	-0.00143
C	1.29753	-0.754	-0.00074
C	0.02341	-1.37552	-0.00146
C	-1.18055	-0.64187	-0.00243
C	-1.29752	0.754	-0.00269
N	0.27603	2.72977	-0.00277
C	1.57709	2.77707	-0.00208
O	2.20694	1.55743	-0.0012
N	-0.27603	-2.72977	-0.00198
C	-1.5771	-2.77706	-0.0033
O	-2.20694	-1.55742	-0.00353
C	-2.52887	1.50186	-0.0031
C	-2.80352	2.85251	-0.00733
C	-4.21584	2.98419	-0.00515
H	-2.05912	3.63384	-0.01115
C	-4.72793	1.70757	0.0004
H	-4.79321	3.89727	-0.00708
C	2.52888	-1.50186	0.0003
C	2.80352	-2.85252	0.00066
C	4.21584	-2.98419	0.00182
H	2.05912	-3.63385	0.00007
C	4.72794	-1.70756	0.00215
H	4.79321	-3.89728	0.00233
C	-6.06341	1.1869	0.00566
C	-6.58034	-0.08262	0.01503
C	-8.00135	0.06457	0.01647
H	-6.00661	-0.9978	0.02092
C	-8.2639	1.4051	0.00798
H	-8.73921	-0.72607	0.02313
C	6.06343	-1.18689	0.00323
C	6.58039	0.08264	0.00369
C	8.0014	-0.06457	0.00485
H	6.00668	0.99786	0.00321
C	8.26392	-1.40513	0.00507
H	8.73928	0.72608	0.00547
C	-9.51451	2.2106	0.00468
H	-10.38338	1.54681	0.01056
H	-9.57587	2.86347	0.88453
H	-9.5788	2.85166	-0.88361
C	9.51451	-2.21067	0.00605
H	9.57824	-2.85732	-0.87822

H	10.3834	-1.54688	0.00718
H	9.57639	-2.85797	0.88996
C	2.43199	3.93081	-0.0022
C	3.79636	4.0703	-0.00151
C	4.05089	5.47211	-0.00209
H	4.51567	3.26427	-0.0007
C	2.83145	6.09506	-0.00308
H	5.01503	5.96129	-0.00182
C	-2.432	-3.9308	-0.00513
C	-3.79636	-4.07027	-0.0101
C	-4.05091	-5.47208	-0.00997
H	-4.51566	-3.26424	-0.01395
C	-2.83148	-6.09505	-0.00498
H	-5.01505	-5.96125	-0.01323
C	2.4082	7.52114	-0.00404
H	1.80395	7.75697	-0.88847
H	1.80296	7.75787	0.87946
H	3.28727	8.1709	-0.00388
C	-2.40826	-7.52112	-0.00225
H	-1.80012	-7.75809	-0.88369
H	-1.80692	-7.75673	0.88423
H	-3.28733	-8.17088	-0.00512
S	-1.8358	-5.16263	-0.002
S	1.83577	5.16264	-0.00316
S	-3.71049	0.7968	0.00153
S	-7.08444	2.10353	0.00127
S	3.71051	-0.79679	0.00126
S	7.08444	-2.10356	0.00405

26BF48F

C	-0.93966	1.08256	0.13841
C	-1.32404	-0.12469	0.54768
C	-0.33184	-1.30126	0.60773
C	0.94809	-0.99777	0.2857
C	1.38034	0.35851	-0.17086
C	0.5217	1.40432	-0.22831
N	-2.09718	1.9538	0.09084
C	-3.10681	1.18442	0.40238
O	-2.71325	-0.12754	0.90051
N	2.13443	-1.82213	0.31512
C	3.13928	-1.02016	0.00056
O	2.76754	0.31216	-0.50855
C	0.96527	2.81892	-0.64473
C	0.13601	3.87554	-0.71804

O	2.32789	3.18434	-1.00471
C	1.00174	5.08358	-0.96063
H	-0.92852	3.86177	-0.6123
C	2.26998	4.63943	-1.01125
H	0.67327	6.09731	-1.05949
C	-0.75812	-2.72348	1.01812
C	0.0839	-3.77024	1.08983
O	-2.11823	-3.10764	1.37177
C	-0.76891	-4.99003	1.32157
H	1.14898	-3.74352	0.98956
C	-2.04367	-4.56284	1.36977
H	-0.42802	-5.99973	1.41667
C	-4.57616	1.62018	0.25166
C	-5.80391	1.03905	0.49284
O	-4.74722	2.91206	-0.24767
C	-6.80553	2.01804	0.12526
H	-6.0038	0.04502	0.8813
C	-6.1232	3.13296	-0.31625
H	-7.8803	1.87957	0.1926
C	4.60746	-1.45523	0.1642
C	5.83701	-0.87337	-0.06577
O	4.77472	-2.74706	0.66496
C	6.83581	-1.85199	0.31037
H	6.03984	0.12084	-0.45223
C	6.15015	-2.96737	0.7455
H	7.91107	-1.71293	0.2527
C	6.5426	-4.35617	1.28292
C	5.85758	-5.47178	1.71813
O	7.91824	-4.57679	1.36343
C	6.8559	-6.45083	2.09445
H	4.78227	-5.61071	1.77593
C	8.08524	-5.86842	1.86408
H	6.653	-7.445	2.48085
C	-6.51972	4.52181	-0.85056
C	-5.83804	5.63696	-1.29215
O	-7.89592	4.74292	-0.91936
C	-6.83917	6.61639	-1.6599
H	-4.76321	5.77542	-1.35931
C	-8.06671	6.03458	-1.41864
H	-6.63921	7.61034	-2.04838
C	-9.53606	6.4703	-1.56945
H	-10.01949	6.43075	-0.61571
H	-9.57446	7.47052	-1.94758
H	-10.03514	5.81237	-2.24985

C	9.55341	-6.30352	2.02763
H	9.58895	-7.30379	2.40589
H	10.04514	-6.26356	1.07815
H	10.04624	-5.6455	2.71249
C	-3.2644	-5.50067	1.41348
H	-3.93879	-5.17294	2.17682
H	-3.76191	-5.4829	0.46635
H	-2.94065	-6.49777	1.62765
C	3.50266	5.56096	-1.06514
H	4.0021	5.54425	-0.119
H	4.17097	5.21846	-1.82734
H	3.19136	6.56045	-1.28652

26BF48T

C	1.28577	0.49093	0.00003
C	1.00254	-0.89186	0.
C	-0.26857	-1.47672	0.
C	-1.28576	-0.49091	0.00002
C	-1.00252	0.89187	0.00003
C	0.26858	1.47673	0.00006
N	2.66133	0.66767	0.00006
C	3.14571	-0.54184	-0.00002
O	2.21121	-1.54744	-0.00004
N	-2.66133	-0.66766	0.00001
C	-3.1457	0.54185	-0.00006
O	-2.2112	1.54745	0.00002
C	0.54796	2.89344	0.00004
C	1.71638	3.61636	0.00011
C	1.33992	4.99177	0.00004
H	2.70862	3.19205	0.00025
C	-0.02668	5.03112	-0.0001
H	1.99983	5.84867	0.0001
C	-0.54797	-2.89342	0.
C	-1.7164	-3.61632	0.00015
C	-1.33996	-4.99174	0.00006
H	-2.70863	-3.192	0.00027
C	0.02664	-5.03111	-0.00012
H	-1.99989	-5.84863	0.00011
C	4.516	-0.96249	-0.00005
C	5.09856	-2.20787	-0.00011
O	5.48222	0.00716	0.00001
C	6.50117	-1.99679	-0.0001
H	4.56946	-3.14987	-0.00015
C	6.68727	-0.63187	-0.00003

H	7.28231	-2.74262	-0.00014
C	-4.516	0.9625	-0.00005
C	-5.09856	2.20788	-0.0001
O	-5.48221	-0.00715	0.00003
C	-6.50117	1.99678	-0.00007
H	-4.56947	3.14988	-0.00017
C	-6.68726	0.63186	0.00002
H	-7.28232	2.74262	-0.0001
C	-7.85712	-0.1962	0.00009
C	-8.04955	-1.55327	0.00023
O	-9.06881	0.44739	-0.00001
C	-9.46311	-1.75355	0.00022
H	-7.27254	-2.30388	0.00034
C	-10.04269	-0.5157	0.00007
H	-9.987	-2.69947	0.0003
C	7.85713	0.19619	0.00003
C	8.04958	1.55325	0.00009
O	9.06882	-0.44742	0.00004
C	9.46314	1.75352	0.00014
H	7.27258	2.30387	0.00009
C	10.04271	0.51567	0.0001
H	9.98704	2.69943	0.00019
C	11.45154	0.03837	0.00012
H	11.6687	-0.5738	-0.88412
H	12.13294	0.89331	0.00017
H	11.66865	-0.57388	0.88431
C	-11.45153	-0.03842	-0.00002
H	-12.13292	-0.89336	0.00005
H	-11.66869	0.57388	0.88412
H	-11.66864	0.57369	-0.88431
C	1.02353	-6.13582	-0.00026
H	1.67197	-6.09297	-0.88461
H	1.6722	-6.093	0.88392
H	0.50939	-7.10087	-0.00021
C	-1.02359	6.13582	-0.00025
H	-1.67205	6.09294	-0.88458
H	-1.67224	6.09299	0.88395
H	-0.50947	7.10087	-0.00022
S	-0.52274	3.75878	-0.00013
S	0.52272	-3.75877	-0.00014

26BT48F

C	-1.22627	0.62551	0.
C	-1.09151	-0.77988	-0.01

C	0.10982	-1.49724	-0.01
C	1.22627	-0.62551	0.
C	1.09151	0.77988	0.01
C	-0.10982	1.49724	0.00999
N	-2.57574	0.94247	-0.00001
C	-3.18874	-0.20874	-0.01
O	-2.36239	-1.30403	-0.02
N	2.57574	-0.94247	-0.00001
C	3.18874	0.20874	0.01
O	2.36239	1.30403	0.01999
C	-0.23336	2.93596	0.01999
C	-1.31524	3.78288	0.01999
O	0.92558	3.67895	0.01998
C	-0.7906	5.10871	0.02999
H	-2.34841	3.47182	0.01999
C	0.57208	4.99797	0.02998
H	-1.35287	6.03258	0.03
C	0.23336	-2.93596	-0.02
C	1.31524	-3.78288	-0.01999
O	-0.92558	-3.67895	-0.02
C	0.7906	-5.10871	-0.03
H	2.34841	-3.47182	-0.01999
C	-0.57208	-4.99797	-0.03
H	1.35287	-6.03258	-0.03
C	-4.60223	-0.45816	-0.02
C	-5.25081	-1.67585	-0.04999
C	-6.65816	-1.55179	-0.05999
H	-4.71724	-2.61905	-0.06999
C	-7.10012	-0.2401	-0.04
H	-7.33298	-2.40103	-0.09999
C	4.60223	0.45816	0.02
C	5.25081	1.67585	0.05
C	6.65816	1.55179	0.06
H	4.71724	2.61905	0.07
C	7.10012	0.2401	0.04
H	7.33298	2.40103	0.09999
C	8.45801	-0.25574	0.05999
C	8.90888	-1.55788	0.21988
C	10.32646	-1.67027	0.17991
H	8.24167	-2.41365	0.37977
C	10.97906	-0.46494	-0.01996
H	10.85234	-2.61971	0.29983
C	-8.45801	0.25574	-0.06
C	-8.90888	1.55788	-0.21995

C	-10.32646	1.67027	-0.17996
H	-8.24167	2.41365	-0.3799
C	-10.97906	0.46494	0.01998
H	-10.85234	2.61971	-0.29993
C	-12.45458	0.20189	0.10995
H	-12.74031	-0.24594	1.08387
H	-12.99816	1.15178	-0.00002
H	-12.80029	-0.48587	-0.68402
C	12.45458	-0.20189	-0.1099
H	12.99816	-1.15178	0.00003
H	12.74033	0.24599	-1.08378
H	12.80028	0.48583	0.68411
C	-1.68411	-5.98665	-0.03999
H	-2.32391	-5.87279	0.84432
H	-2.32391	-5.87279	-0.92431
H	-1.27895	-7.00224	-0.03999
C	1.68411	5.98665	0.03997
H	2.32392	5.87279	0.92427
H	2.3239	5.87278	-0.84435
H	1.27895	7.00224	0.03997
S	9.82672	0.8507	-0.15986
S	5.73962	-0.86871	0.00001
S	-5.73962	0.86871	0.
S	-9.82672	-0.8507	0.15994

26BT48T

C	-1.28095	0.50339	-0.00004
C	-1.01115	-0.88208	0.
C	0.25422	-1.47926	0.
C	1.28094	-0.50337	-0.00002
C	1.01114	0.88209	-0.00003
C	-0.25422	1.47927	-0.00006
N	-2.65473	0.69348	-0.00007
C	-3.15083	-0.51127	0.00002
O	-2.22613	-1.52589	0.00003
N	2.65472	-0.69347	-0.00001
C	3.15081	0.51129	0.00005
O	2.22612	1.52591	-0.00002
C	-0.51984	2.89862	-0.00005
C	-1.68119	3.63285	-0.00011
C	-1.29139	5.00454	-0.00005
H	-2.6775	3.2182	-0.00025
C	0.07553	5.03063	0.0001
H	-1.94295	5.86781	-0.00011

C	0.51985	-2.8986	0.
C	1.68121	-3.63281	-0.00015
C	1.29143	-5.00451	-0.00006
H	2.67751	-3.21815	-0.00028
C	-0.07548	-5.03061	0.00012
H	1.94301	-5.86777	-0.00011
C	-4.52514	-0.9186	0.00005
C	-5.11975	-2.15827	0.00011
C	-6.52026	-1.93357	0.0001
H	-4.59982	-3.10536	0.00015
C	-6.69309	-0.56691	0.00002
H	-7.3086	-2.67179	0.00013
C	4.52513	0.91861	0.00005
C	5.11975	2.15827	0.0001
C	6.52025	1.93357	0.00006
H	4.59983	3.10537	0.00017
C	6.69308	0.5669	-0.00003
H	7.3086	2.67178	0.0001
C	7.85484	-0.27248	-0.00009
C	8.03409	-1.63135	-0.00024
C	9.44563	-1.84535	-0.00022
H	7.24983	-2.37438	-0.00034
C	10.03721	-0.61318	-0.00007
H	9.96032	-2.79631	-0.00031
C	-7.85486	0.27247	-0.00004
C	-8.03412	1.63134	-0.00009
C	-9.44567	1.84532	-0.00014
H	-7.24986	2.37437	-0.0001
C	-10.03723	0.61315	-0.0001
H	-9.96036	2.79627	-0.00019
C	-11.45063	0.14955	-0.00012
H	-11.67372	-0.46048	0.88411
H	-12.1237	1.01107	-0.00018
H	-11.67367	-0.46055	-0.88432
C	11.45062	-0.1496	0.00002
H	12.12367	-1.01112	-0.00006
H	11.67371	0.46056	-0.88413
H	11.67366	0.46037	0.8843
C	-1.08306	-6.12559	0.00026
H	-1.73105	-6.07645	0.88461
H	-1.73128	-6.07647	-0.88392
H	-0.57831	-7.09559	0.00021
C	1.08312	6.12559	0.00024
H	1.73113	6.07641	0.88458

H	1.73132	6.07647	-0.88395
H	0.57839	7.09559	0.00022
S	-9.07274	-0.35934	-0.00004
S	-5.48189	0.06039	-0.00002
S	-0.55919	-3.75352	0.00013
S	0.55921	3.75352	0.00013
S	5.48188	-0.06038	-0.00003
S	9.07272	0.35932	0.00001

26BF48BF

C	-0.93966	1.08256	0.13841
C	-1.32404	-0.12469	0.54768
C	-0.33184	-1.30126	0.60773
C	0.94809	-0.99777	0.2857
C	1.38034	0.35851	-0.17086
C	0.5217	1.40432	-0.22831
N	-2.09718	1.9538	0.09084
C	-3.10681	1.18442	0.40238
O	-2.71325	-0.12754	0.90051
N	2.13443	-1.82213	0.31512
C	3.13928	-1.02016	0.00056
O	2.76754	0.31216	-0.50855
C	0.96527	2.81892	-0.64473
C	0.13601	3.87554	-0.71804
O	2.32789	3.18434	-1.00471
C	1.00174	5.08358	-0.96063
H	-0.92852	3.86177	-0.6123
C	2.26998	4.63943	-1.01125
H	0.67327	6.09731	-1.05949
C	-0.75812	-2.72348	1.01812
C	0.0839	-3.77024	1.08983
O	-2.11823	-3.10764	1.37177
C	-0.76891	-4.99003	1.32157
H	1.14898	-3.74352	0.98956
C	-2.04367	-4.56284	1.36977
H	-0.42802	-5.99973	1.41667
C	3.5015	5.56009	-1.06509
C	4.77393	5.12596	-1.11875
O	3.43293	7.01311	-1.05905
C	5.64727	6.34344	-0.95076
H	5.1006	4.11499	-1.24316
C	4.8154	7.39252	-0.81215
H	6.71715	6.36782	-0.93352
C	-3.26542	-5.50146	1.41352

C	-4.54438	-5.08364	1.47022
O	-3.18048	-6.95495	1.39402
C	-5.40241	-6.30963	1.28909
H	-4.88471	-4.07835	1.60491
C	-4.55969	-7.34819	1.14258
H	-6.47174	-6.34558	1.26791
C	5.26671	8.81585	-0.43589
H	6.25701	8.98436	-0.80326
H	4.59842	9.52873	-0.87204
H	5.25848	8.92391	0.62862
C	-5.00109	-8.77177	0.75345
H	-4.32628	-9.4848	1.17928
H	-5.99006	-8.9515	1.12321
H	-4.99523	-8.86752	-0.31283
C	-4.57616	1.62018	0.25166
C	-5.80391	1.03905	0.49284
O	-4.74722	2.91206	-0.24767
C	-6.80553	2.01804	0.12526
H	-6.0038	0.04502	0.8813
C	-6.1232	3.13296	-0.31625
H	-7.8803	1.87957	0.1926
C	4.60746	-1.45523	0.1642
C	5.83701	-0.87337	-0.06577
O	4.77472	-2.74706	0.66496
C	6.83581	-1.85199	0.31037
H	6.03984	0.12084	-0.45223
C	6.15015	-2.96737	0.7455
H	7.91107	-1.71293	0.2527
C	6.5426	-4.35617	1.28292
C	5.85758	-5.47178	1.71813
O	7.91824	-4.57679	1.36343
C	6.8559	-6.45083	2.09445
H	4.78227	-5.61071	1.77593
C	8.08524	-5.86842	1.86408
H	6.653	-7.445	2.48085
C	-6.51972	4.52181	-0.85056
C	-5.83804	5.63696	-1.29215
O	-7.89592	4.74292	-0.91936
C	-6.83917	6.61639	-1.6599
H	-4.76321	5.77542	-1.35931
C	-8.06671	6.03458	-1.41864
H	-6.63921	7.61034	-2.04838
C	-9.53606	6.4703	-1.56945
H	-10.01949	6.43075	-0.61571

H	-9.57446	7.47052	-1.94758
H	-10.03514	5.81237	-2.24985
C	9.55341	-6.30352	2.02763
H	9.58895	-7.30379	2.40589
H	10.04514	-6.26356	1.07815
H	10.04624	-5.6455	2.71249

26BF48BT

C	1.12967	0.79184	0.00011
C	1.17858	-0.61818	0.00006
C	0.09725	-1.50758	0.00004
C	-1.12967	-0.79184	0.00006
C	-1.17858	0.61818	0.00011
C	-0.09725	1.50758	0.00015
N	2.42716	1.28165	0.00015
C	3.18506	0.22298	0.00009
O	2.507	-0.97338	0.00005
N	-2.42717	-1.28165	-0.00001
C	-3.18506	-0.22297	0.00001
O	-2.50701	0.97338	0.00009
C	-0.1911	2.95489	0.00022
C	0.84636	3.87142	-0.00007
C	0.4177	5.21677	0.00031
H	1.88248	3.55973	-0.00038
C	-0.95552	5.36918	0.0009
H	1.10344	6.05776	0.00046
C	0.1911	-2.95489	-0.00002
C	-0.84636	-3.87142	-0.00007
C	-0.4177	-5.21677	-0.00014
H	-1.88248	-3.55973	-0.00008
C	0.95552	-5.36918	-0.00014
H	-1.10344	-6.05776	-0.00022
C	-1.73374	6.58727	0.00149
C	-3.10211	6.74993	0.00679
C	-3.51627	8.11114	0.00564
H	-3.79444	5.91453	0.01174
C	-2.48042	9.0076	-0.00047
H	-4.55686	8.42056	0.00938
C	1.73374	-6.58727	-0.00021
C	3.10212	-6.74993	-0.00058
C	3.51628	-8.11114	-0.00052
H	3.79446	-5.91452	-0.00091
C	2.48041	-9.0076	-0.00011
H	4.55687	-8.42055	-0.00078

C	-2.53903	10.5052	-0.00322
H	-3.58334	10.83313	0.00039
H	-2.04858	10.93767	0.87782
H	-2.0558	10.93415	-0.88996
C	2.53902	-10.50521	0.00002
H	2.05215	-10.93599	-0.88384
H	3.58334	-10.83313	0.00002
H	2.05219	-10.93584	0.88396
C	4.61461	0.13768	0.00009
C	5.47873	-0.9323	0.00003
O	5.32085	1.31067	0.00016
C	6.78936	-0.39162	0.00007
H	5.19322	-1.9744	-0.00002
C	6.64335	0.97861	0.00015
H	7.72613	-0.92899	0.00005
C	-4.61461	-0.13768	-0.00007
C	-5.47873	0.9323	-0.00023
O	-5.32085	-1.31067	-0.00002
C	-6.78936	0.39162	-0.00031
H	-5.19322	1.9744	-0.00033
C	-6.64335	-0.97861	-0.00017
H	-7.72614	0.929	-0.00045
C	-7.5815	-2.0617	-0.00015
C	-7.44465	-3.42563	-0.00002
O	-8.91166	-1.72563	-0.00029
C	-8.76932	-3.95714	-0.00011
H	-6.51117	-3.96953	0.0001
C	-9.62749	-2.89301	-0.00026
H	-9.05244	-5.00068	-0.00006
C	7.58149	2.0617	0.00022
C	7.44464	3.42563	0.00031
O	8.91166	1.72563	0.0002
C	8.76932	3.95714	0.00036
H	6.51117	3.96953	0.00035
C	9.62749	2.89301	0.00028
H	9.05244	5.00069	0.00043
C	11.10948	2.76578	0.00028
H	11.46611	2.22308	-0.88401
H	11.56718	3.75858	0.00036
H	11.4661	2.22292	0.88447
C	-11.10948	-2.76578	-0.0004
H	-11.56718	-3.75858	-0.00038
H	-11.46618	-2.22294	0.88378
H	-11.46603	-2.22305	-0.88471

S	-0.9471	8.16238	-0.0052
S	-1.73891	3.8011	0.00073
S	1.73891	-3.8011	-0.00003
S	0.94709	-8.16238	0.00024

26BT48BF

C	1.09264	0.8558	0.00027
C	1.21335	-0.55059	0.00019
C	0.17661	-1.49159	0.00013
C	-1.09268	-0.85589	0.00018
C	-1.21341	0.5505	0.00026
C	-0.17665	1.4915	0.0003
N	2.36276	1.4117	-0.00965
C	3.17477	0.39431	-0.00969
O	2.55724	-0.83818	-0.0098
N	-2.36281	-1.41179	-0.00986
C	-3.17483	-0.39443	-0.0098
O	-2.55729	0.83808	-0.00972
C	-0.4071	2.91492	0.00038
C	-1.55532	3.68108	-0.009
O	0.68566	3.74429	-0.00026
C	-1.14646	5.03899	-0.00927
H	-2.56646	3.3047	-0.00841
C	0.2292	5.02876	-0.00003
H	-1.77494	5.91758	-0.00894
C	0.40708	-2.915	0.00005
C	1.55531	-3.68114	-0.00985
O	-0.68567	-3.7444	-0.00018
C	1.14647	-5.03906	-0.00002
H	2.56644	-3.30474	-0.00966
C	-0.22919	-5.02885	-0.00022
H	1.77496	-5.91764	-0.01
C	1.22322	6.06105	0.00939
C	2.59357	6.04007	0.00872
O	0.77585	7.35815	-0.00048
C	3.01167	7.40589	0.01839
H	3.20798	5.1515	0.01847
C	1.87953	8.17098	0.00892
H	4.02738	7.77732	0.01784
C	-1.2232	-6.06116	0.00953
C	-2.59354	-6.0402	0.0093
O	-0.77581	-7.35825	-0.0005
C	-3.01163	-7.40603	0.00912
H	-3.20797	-5.15163	0.01927

C	-1.87948	-8.1711	0.00925
H	-4.02733	-7.77746	0.01891
C	1.62658	9.6369	0.00896
H	2.57708	10.17736	0.00845
H	1.06516	9.94749	-0.88489
H	1.04605	9.9476	0.88335
C	-1.62651	-9.63702	0.00918
H	-1.05572	-9.94773	0.8834
H	-2.577	-10.17749	0.00894
H	-1.05534	-9.94758	-0.88484
C	4.61143	0.41524	-0.01962
C	5.42321	1.53066	-0.03929
C	6.79928	1.21504	-0.05932
H	5.01965	2.53607	-0.05903
C	7.06025	-0.1445	-0.03966
H	7.58387	1.96403	-0.08908
C	-4.61151	-0.4153	-0.0198
C	-5.42333	-1.53069	-0.03984
C	-6.79939	-1.21501	-0.04981
H	-5.01985	-2.53613	-0.05987
C	-7.06029	0.14454	-0.03976
H	-7.584	-1.96397	-0.08982
C	-8.33663	0.82257	-0.04972
C	-8.60491	2.17428	-0.21944
C	-9.99371	2.47967	-0.16949
H	-7.82703	2.93089	-0.37919
C	-10.80517	1.37502	0.03019
H	-10.38464	3.49217	-0.2893
C	8.33664	-0.82244	-0.04978
C	8.60501	-2.17414	-0.22008
C	9.99384	-2.47943	-0.18011
H	7.82719	-2.93081	-0.39027
C	10.80522	-1.37473	0.03017
H	10.38483	-3.49191	-0.30032
C	12.30283	-1.31583	0.12023
H	12.64311	-0.91673	1.09432
H	12.71144	-2.33111	0.01001
H	12.74316	-0.67631	-0.67359
C	-12.30278	1.31623	0.12005
H	-12.71132	2.33154	0.01025
H	-12.74305	0.68715	-0.67406
H	-12.6432	0.90675	1.09386
S	5.56036	-1.05479	0.00003
S	9.84375	0.0863	0.18048

S	-5.56029	1.05474	0.00024
S	-9.84381	-0.08607	0.16994

26BT48BT

C	-0.25493	0.13158	0.
C	-0.73812	-1.09704	-0.17236
C	-2.23629	-1.40017	0.01736
C	-3.01422	-0.32764	0.29762
C	-2.47214	1.05246	0.4881
C	-1.15822	1.33689	0.3239
N	1.18684	0.09476	-0.14532
C	1.47241	-1.1688	-0.31915
O	0.30311	-2.00939	-0.54366
N	-4.44782	-0.23418	0.45211
C	-4.70955	1.05202	0.62244
O	-3.54359	1.9234	0.85414
C	-0.59523	2.76333	0.46383
C	0.70431	3.07655	0.31361
C	0.78746	4.58003	0.33137
H	1.51748	2.3919	0.19277
C	-0.46985	5.02924	0.4915
H	1.67134	5.17375	0.22392
C	-2.81663	-2.82093	-0.11485
C	-4.12002	-3.1184	0.03524
C	-4.21894	-4.62143	0.03067
H	-4.92654	-2.4242	0.14819
C	-2.96644	-5.08743	-0.12391
H	-5.10964	-5.20381	0.14123
C	-0.87314	6.51034	0.38721
C	-2.12728	6.97031	0.54845
C	-2.10001	8.42738	0.16192
H	-2.97784	6.40937	0.87423
C	-0.83168	8.70301	-0.19466
H	-2.92764	9.10602	0.16019
C	-2.5803	-6.57491	-0.00602
C	-1.33131	-7.05196	-0.16718
C	-1.37396	-8.50425	0.23419
H	-0.47484	-6.50532	-0.50219
C	-2.64338	-8.76391	0.59666
H	-0.55322	-9.19094	0.24205
C	-0.37687	10.02819	-0.83353
H	-1.00282	10.82363	-0.48781
H	0.63771	10.22718	-0.55776
H	-0.44931	9.9551	-1.89858

C	-3.10437	-10.08133	1.24838
H	-4.12277	-10.27493	0.98287
H	-2.48657	-10.88495	0.90254
H	-3.0224	-9.99995	2.31272
C	2.90983	-1.72034	-0.28399
C	3.48996	-2.96351	-0.42971
C	4.91779	-2.77507	-0.27942
H	2.99359	-3.91028	-0.61993
C	5.1156	-1.42873	-0.05183
H	5.66885	-3.55691	-0.33841
C	-6.14737	1.60152	0.57444
C	-6.72999	2.84478	0.70906
C	-8.15654	2.65367	0.55026
H	-6.23609	3.79323	0.89734
C	-8.35116	1.30582	0.32896
H	-8.90894	3.43488	0.59966
C	-9.57134	0.3996	0.08092
C	-9.76662	-0.94804	-0.14041
C	-11.19307	-1.13981	-0.29931
H	-9.01412	-1.72921	-0.18996
C	-11.77513	0.1038	-0.1644
H	-11.68688	-2.08826	-0.48754
C	6.33859	-0.52544	0.19306
C	6.53707	0.82068	0.42068
C	7.9648	1.00979	0.57105
H	5.78593	1.60252	0.47949
C	8.54434	-0.23379	0.42539
H	8.46107	1.95655	0.76131
C	9.98175	-0.78534	0.46066
H	10.20822	-1.25084	-0.47578
H	10.66755	0.01724	0.63509
H	10.06818	-1.50565	1.24716
C	-13.21297	0.65329	-0.21231
H	-13.89658	-0.15113	-0.38691
H	-13.44629	1.12363	0.72002
H	-13.29504	1.36916	-1.00332
S	-3.5227	-7.6422	0.29894
S	-2.02878	-4.0099	-0.41184
S	-10.79567	1.06929	0.07077
S	-7.12719	0.63603	0.3392
S	-1.39552	3.94027	0.77074
S	0.05794	7.58931	0.09585
S	3.89246	-0.75735	-0.05022
S	7.56206	-1.19676	0.19163

Device Properties

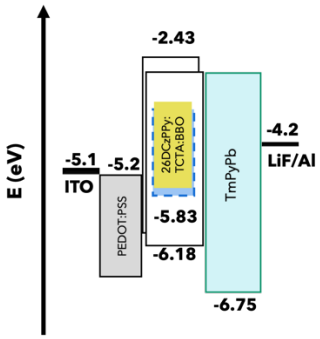

Fig S106. Band Diagram of the WOLED Device architecture.

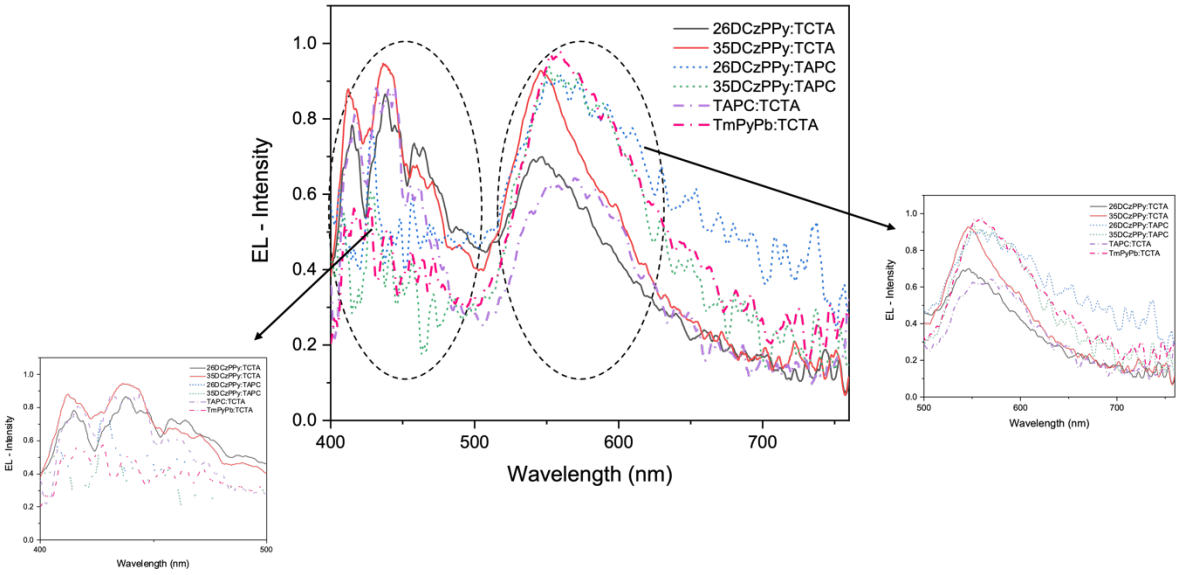

Figure S107. EL spectra of the mixed host combinations at 9V.

References

(1) Tlach, B. C.; Tomlinson, A. L.; Bhuwalka, A.; Jeffries-EL, M. Tuning the Optical and Electronic Properties of 4,8-Disubstituted Benzobisoxazoles via Alkyne Substitution. *J. Org. Chem.* **2011**, *76* (21), 8670–8681. https://doi.org/10.1021/jo201078w.

(2) Tlach, B. C.; Tomlinson, A. L.; Ryno, A. G.; Knoble, D. D.; Drochner, D. L.; Krager, K. J.; Jeffries-El, M. Influence of Conjugation Axis on the Optical and Electronic Properties of Aryl-Substituted Benzobisoxazoles. *J. Org. Chem.* **2013**, *78* (13), 6570–6581. https://doi.org/10.1021/jo4007927.

(3) Mike, J. F.; Makowski, A. J.; Jeffries-EL, M. An Efficient Synthesis of 2,6-Disubstituted Benzobisoxazoles: New Building Blocks for Organic Semiconductors. *Org. Lett.* **2008**, *10* (21), 4915–4918. https://doi.org/10.1021/ol802011y.

(4) Gidron, O.; Dadvand, A.; Sheynin, Y.; Bendikov, M.; Perepichka, D. F. Towards "Green" Electronic Materials. α-Oligofurans as Semiconductors. *Chem. Commun.* **2011**, *47* (7), 1976–1978. https://doi.org/10.1039/C0CC04699J.

(5) Liu, Y.; Wu, P.; Jiang, J.; Wu, J.; Chen, Y.; Tan, Y.; Tan, C.; Jiang, Y. Conjugated Polyelectrolyte Nanoparticles for Apoptotic Cell Imaging. *ACS Appl. Mater. Interfaces* **2016**, *8* (34), 21984–21989. https://doi.org/10.1021/acsami.6b09347.

(6) Shcherbina, M. A.; Borshchev, O. V; Pleshkova, A. P.; Ponomarenko, S. A.; Chvalun, S. N. When Dendrimers Are Not Better – Rational Design of Nanolayers for High-Performance Organic Electronic Devices. *Nanoscale* **2019**, *11* (10), 4463–4470. https://doi.org/10.1039/C8NR09241A.

(7) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, Williams, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, D. J. Fox, Wallingford, CT, 2016.

(8) J.-L. Calais, 'Density-functional theory of atoms and molecules. R.G. Parr and W. Yang, Oxford University Press, New York, Oxford, 1989., 1993, 47, 101-101.

(9) C. Lee, W. Yang, R. G. Parr, 'Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density', Phys. Rev. B 1988, 37, 785-789.

(10) A. D. Becke, 'Density-functional thermochemistry. III. The role of exact exchange', J. Chem. Phys. 1993, 98, 5648-5652.

(11) W. Koch, M. C. Holthausen, A chemist's guide to density functional theory, Wiley-VCH, 2000.