Electronic Supplementary Material (ESI) for Polymer Chemistry.

Direct Heteroarylation Polymerization of a π-Conjugated Polymer with Degradable 1,2,4-Oxadiazole Linkers

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General Instrumentation and Characterization

NMR Spectroscopy

NMR spectra were measured with a Bruker Avance III (400 MHz) and an Agilent DD2 (500 MHz). Chemical shifts are reported in parts per million (ppm) and are referenced to the solvent.

Gel Permeation Chromatography (GPC)

Tetrahydrofuran GPC traces were measured at 35 °C using a Viscotek liquid chromatograph (TDA302) equipped with a Viscotek VE 3580 RI detector and a 2500 UV-Vis detector. Reagent grade tetrahydrofuran with 7.75 mM tetrabutylammonium bromide was used as the eluent at a flow rate of 0.6 mL/min. The column was calibrated to linear polymethylmethacrylate standards.

1,2,4-trichlorobenzene GPC traces were measured at 140 °C using a Viscotek HT-SEC module 350A. 1,2,4-trichlorobenzene stabilized with butylated hydroxytoluene was used as eluent. The column was calibrated with narrow weight distribution polystyrene standards using absorption at 486 nm.

Mass Spectrometry

MALDI-TOF mass spectra were measured using a Bruker Autoflex Speed Matrix-assisted laser desorption ionization time-of-flight mass spectrometer (MALDI-TOF/MS) equipped with a 2 kHz frequency tripled Nd:YAG laser (λ = 355 nm). Spectra were collected in linear positive mode.

Thermogravimetric Analysis (TGA)

The TGA-DSC trace of **T-ODA-T** was measured using a Netzsch STA 449 F5 Jupiter with a heating rate of 20 K/min.

Absorption and Photoluminescence Spectroscopy

UV-Visible absorption spectra were measured using a Perkin-Elmer Lambda 365 UV/Vis Spectrophotometer. Fluorescence spectra were measured using a Photon Technology International (PTI) QuantaMaster 40-FNA spectrofluorometer with a photomultiplier detector and xenon arc lamp. All cuvettes used were quartz. Quantum yields are referenced to quinine sulfate hemihydrate in 0.5 M sulfuric acid. Spectroscopic grade solvents were used for all absorption and photoluminescence measurements.

Thin films for absorption and photoluminescence measurements were prepared on glass substrate by spin coating (500 RPM for 1.5 s followed by 1000 RPM for 30 s) from a filtered (0.1 µm PTFE syringe filter) chloroform solution of the polymer sample with a concentration of 15 mg/mL. Before spin coating, the glass slide substrates were cleaned and sonicated with water, methanol, and isopropanol. The slides were dried under a stream of N_2 and treated with O_2 plasma.

Cyclic Voltammetry

Cyclic voltammetry was performed under N_2 using a BASi Epsilon EC potentiostat with polymer films drop cast onto a glassy carbon button electrode from a 15 mg/mL solution in chloroform. The electrolyte solution was prepared with anhydrous, degassed acetonitrile.

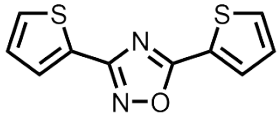
Materials and Synthesis

General

2-bromo-3-dodecylthiophene and 2-bromo-3-(2-ethylhexyl)thiophene purchased from TCI. Thionyl chloride purchased from Fluka. All other reagents purchased from Sigma Aldrich. All reagents were used as received. Dry solvents were obtained from a solvent purification system. $Pd_2(dba)_3$ and $P(o\text{-}MeOPh)_3$ were stored and weighed out in a glove box.

Small Molecule Model Synthesis and Degradation Studies

Synthesis of 3,5-di(thiophen-2-yl)-1,2,4-oxadiazole (T-ODA-T)



The synthesis of T-ODA-T was adapted from Agneeswari et al.[1] Hydroxylamine (50% wt/wt aqueous solution; 0.5 mL) was added to a stirring solution of thiophene-2-carbonitrile (3.5 mL; 3.8 mmol) in ethanol (7 mL). The solution was heated to a reflux for 2 hours. After cooling, the reaction mixture was concentrated under vacuum and redissolved in ethyl acetate (15 mL). The solution was washed with DI water (3x 15 mL), dried over Na_2SO_4, and concentrated under vacuum to afford thiophene-2-amidoxime as a white solid (435 mg, 81%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (dd, J = 5.1, 1.1 Hz, 1H), 7.28 (dd, J = 3.7, 1.1 Hz, 1H), 7.05 (dd, J = 5.1, 3.7 Hz, 1H), 4.86 (s, 2H).

Thiophene-2-carbonyl chloride (0.32 mL; 3.0 mmol) was added to a stirring solution of thiophene-2-amidoxime (414 mg; 2.91 mmol) and pyridine (0.5 mL; 6 mmol) in toluene (10 mL) cooled in an ice bath. The mixture was left stirring in an ice bath for 2 hours. Following this period, the solution was heated to reflux for 19 hours. The reaction mixture was filtered while hot and the filtrate was concentrated under vacuum. The crude product was purified by recrystallization from hexanes/ethyl acetate (1:90) to afford the product as off-white crystals (281 mg; 40%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (dd, J = 3.8, 1.2 Hz, 1H), 7.86 (dd, J = 3.7, 1.2 Hz, 1H), 7.67 (dd, J = 5.0, 1.2 Hz, 1H), 7.53 (dd, J = 5.0, 1.2 Hz, 1H), 7.22 (dd, J = 5.0, 3.8 Hz, 1H), 7.18 (dd, J = 5.0, 3.7 Hz, 1H). HRMS (DART-TOF): [M+H$^+$] Calculated for $C_{10}H_7N_2OS$ = 235.00, found = 235.00.

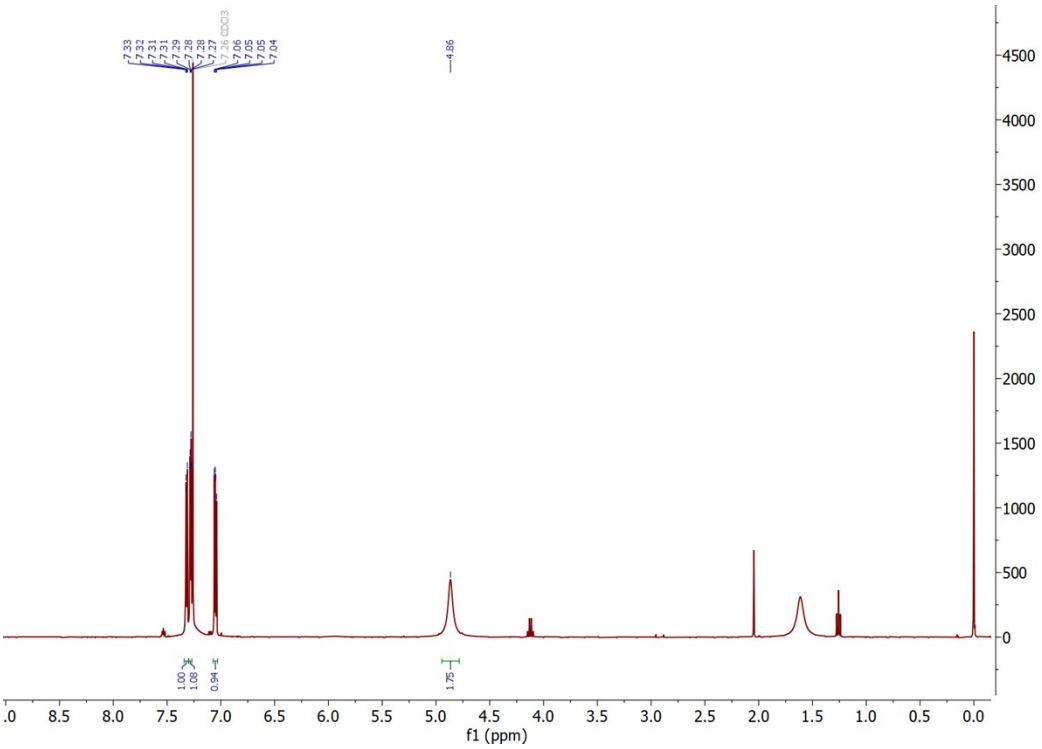


Figure S1. ^{1}H NMR spectrum (400 MHz) of thiophene-2-amidoxime in $CDCl_3$.

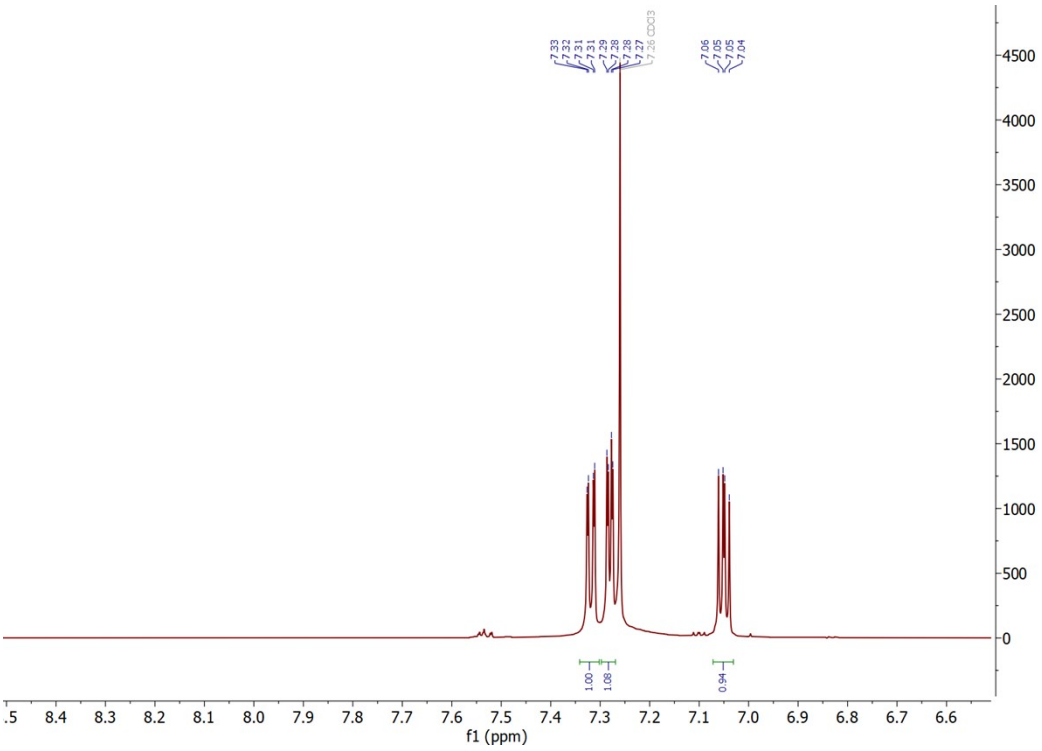


Figure S2. Aromatic region of ^{1}H NMR spectrum (400 MHz) of thiophene-2-amidoxime in $CDCl_3$.

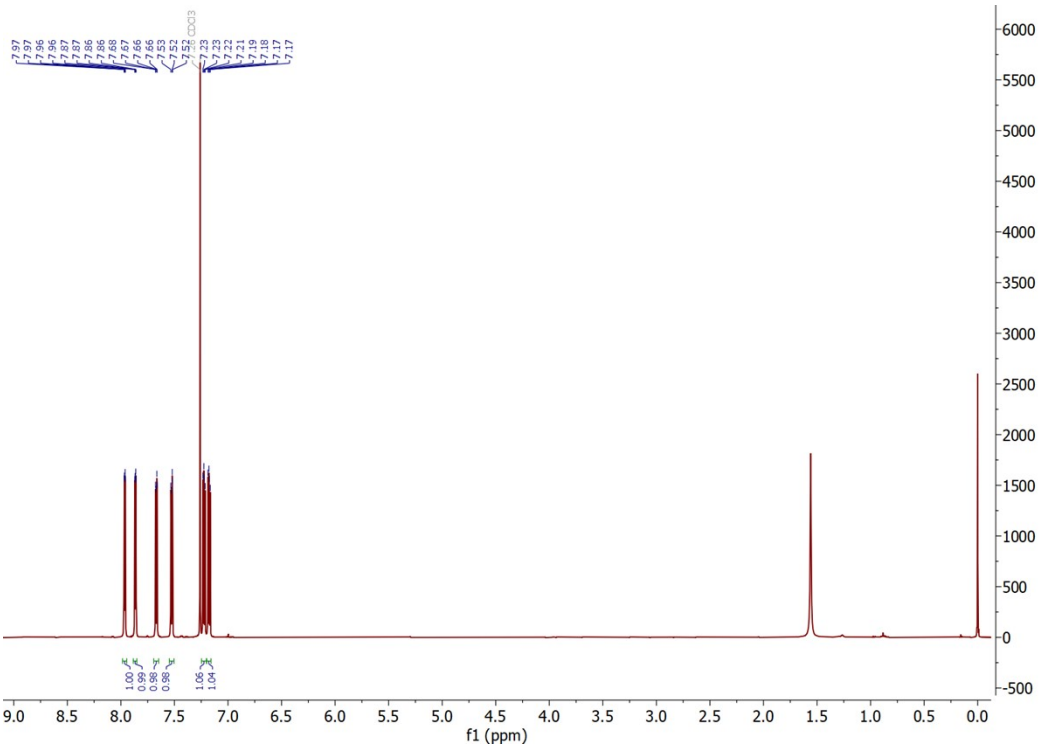


Figure S3. ^{1}H NMR spectrum (400 MHz) of 3,5-di(thiophen-2-yl)-1,2,4-oxadiazole in $CDCl_3$.

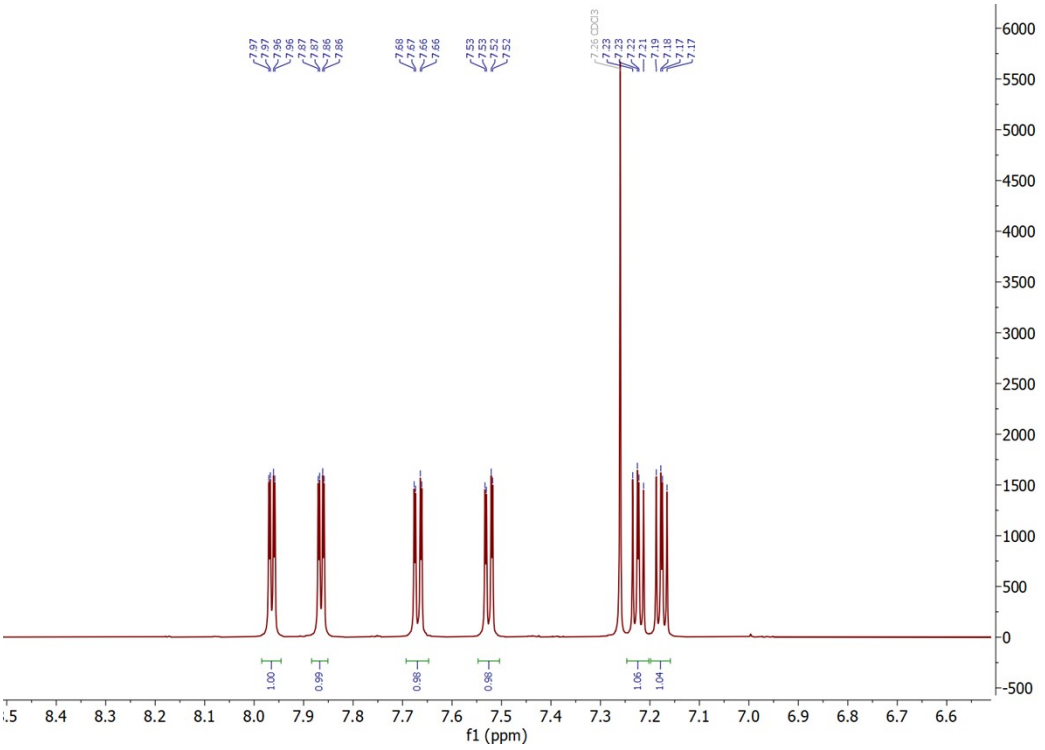


Figure S4. Aromatic region of ^{1}H NMR spectrum (400 MHz) of 3,5-di(thiophen-2-yl)-1,2,4-oxadiazole in $CDCl_3$.

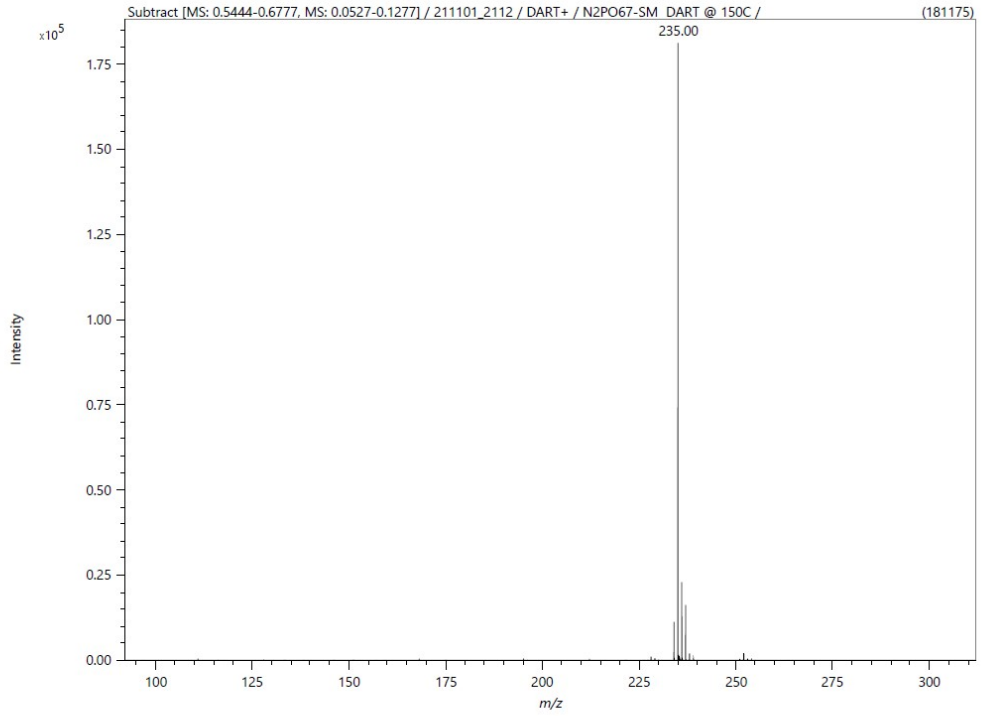


Figure S 5. Mass spectrum (DART, positive mode) of 3,5-di(thiophen-2-yl)-1,2,4-oxadiazole in $CDCl_3$.

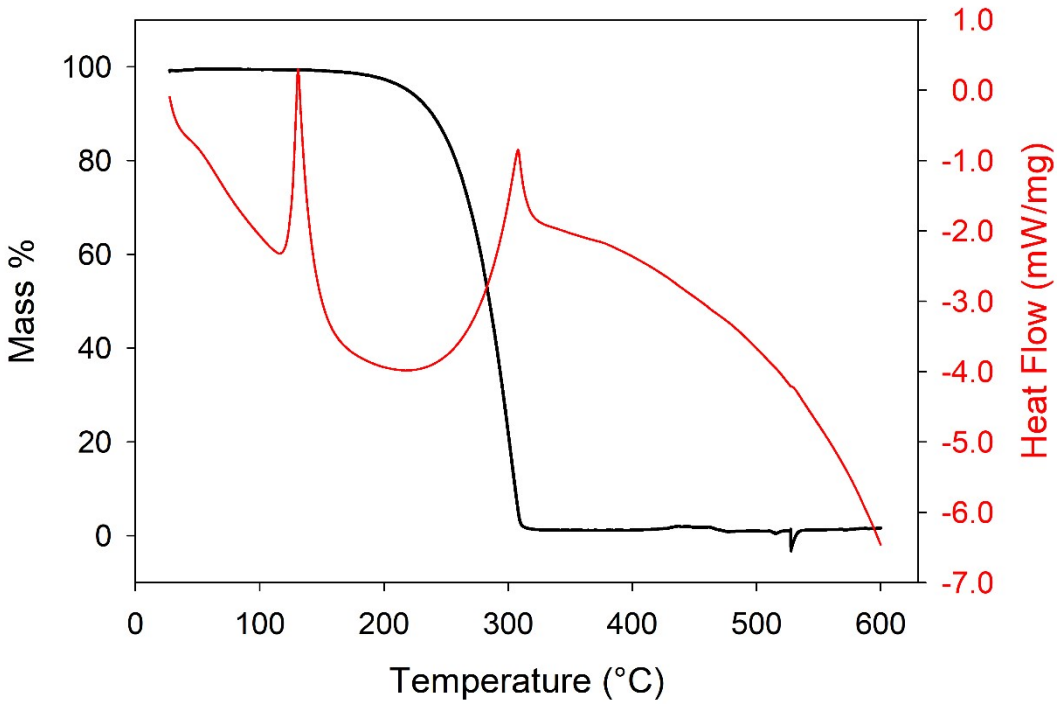


Figure S6. Thermogravimetric analysis and differential scanning calorimetry traces (20 K/min heating rate) of 3,5-dithiophene-2-yl-1,2,4-oxadiazole.

Small Molecule Model Degradation

Products of $LiAlH_4$ Degradation

Anhydrous tetrahydrofuran (8 mL) was added via syringe to a 3-neck round-bottom flask with T-ODA-T (35.0 mg; 0.149 mmol) under argon. The resulting solution was cooled in an ice bath. Lithium aluminum hydride (33 mg; 0.87 mmol) was added through a side arm in one portion. The mixture was removed from the ice bath after the bubbling ceased and was allowed to slowly warm to room temperature. After bubbling was no longer observed, the reaction mixture was heated to a reflux for 10 hours. After this heating period, the reaction mixture was cooled in an ice bath and 20 mL of DI water was added dropwise. The resulting mixture was extracted with chloroform (25 mL). The chloroform fraction was dried over $MgSO_4$, filtered, and concentrated under vacuum to yield 30.3 mg of viscous yellow oil. The crude products were run through a silica column using 2:1 hexanes:ethylacetate as the mobile phase. The eluent was concentrated under vacuum to yield N-(thiophen-2-ylmethyl)thiophene-2-amidoxime as 9.1 mg of yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (dd, J = 5.1, 1.1 Hz, 1H), 7.29 (dd, J = 3.6, 1.1 Hz, 1H), 7.23 (dd, J = 5.0, 1.2 Hz, 1H), 7.07 (dd, J = 5.1, 3.7 Hz, 1H), 6.95 (dd, J = 5.0, 3.5 Hz, 1H), 6.93 – 6.90 (m, 1H), 5.80 – 5.76 (NH, m, 1H), 4.60 (CH_2, d, J = 5.6 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.85, 132.02, 128.41, 127.49, 127.37, 127.09, 124.97, 124.95, 43.17. HRMS (DART-TOF): [M+H$^+$] Calculated for $C_{10}H_{11}N_2OS_2$: 239.0307, found: 239.0306.

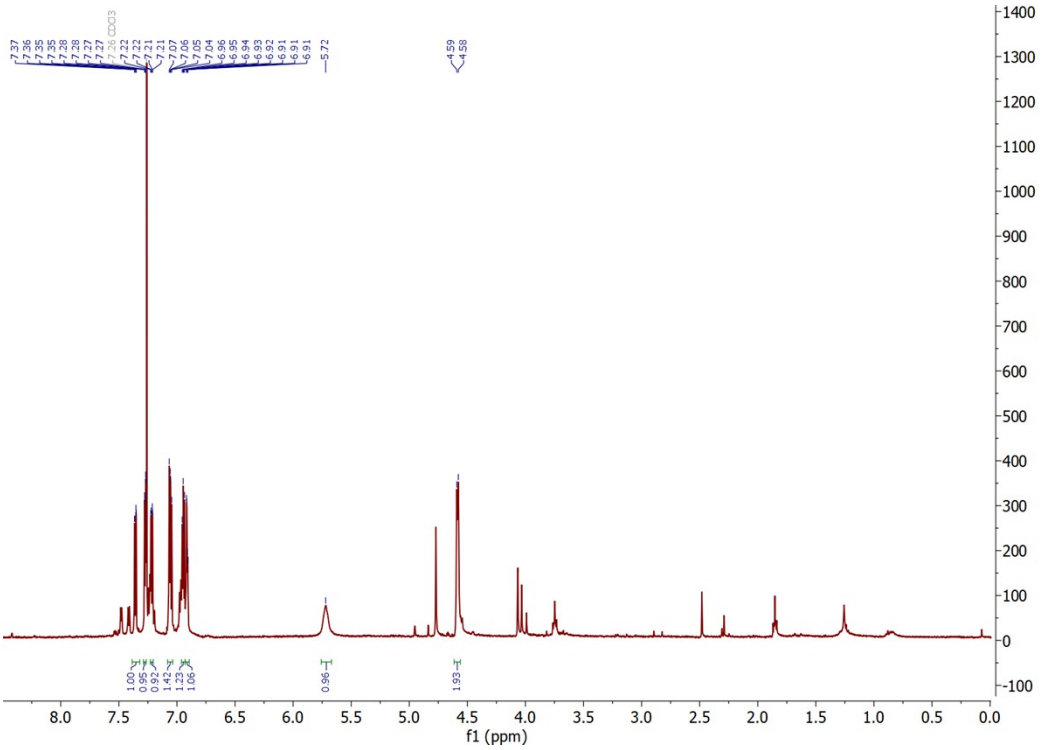


Figure S7. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of crude decomposition products from the treatment of T-ODA-T with $LiAlH_4$. The peak positions and integrations are shown for the major product.

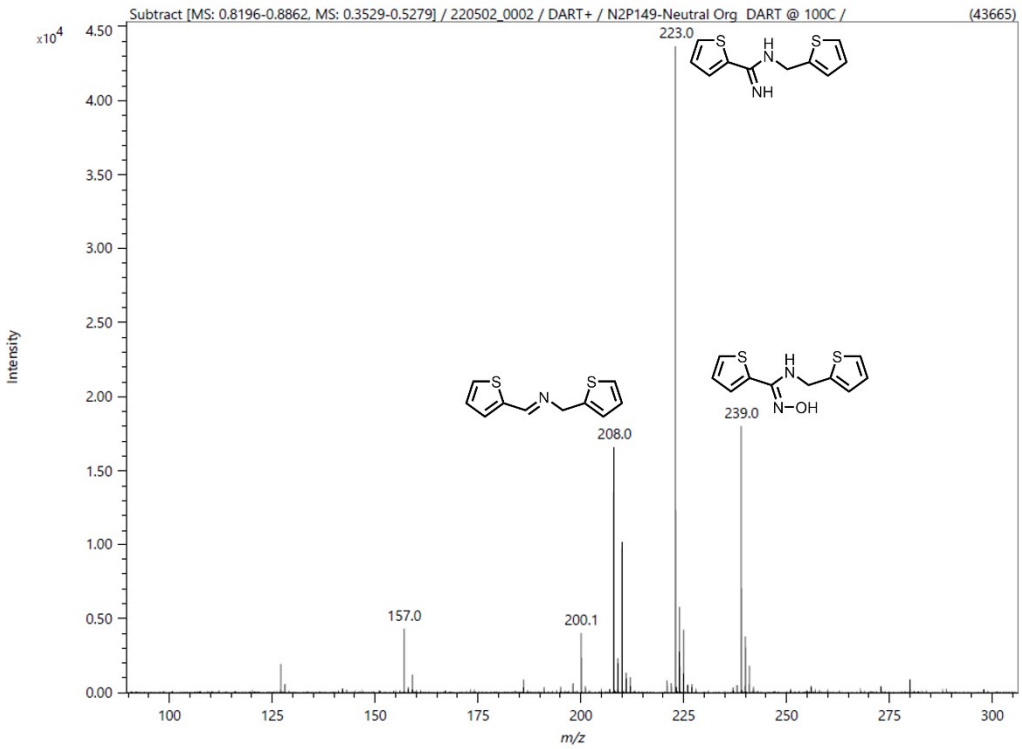


Figure S8. Mass Spectrum (DART, positive mode) of the crude decomposition products from the treatment of T-ODA-T with $LiAlH_4$.

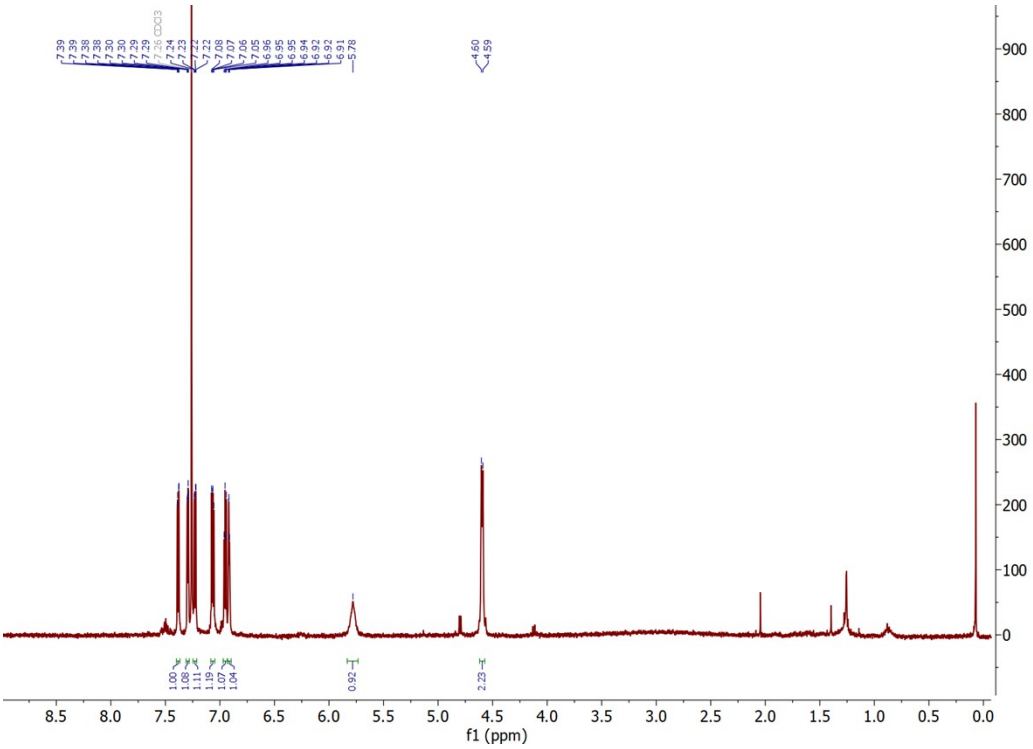


Figure S9. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of column-purified degradation product (amidoxime) from the treatment of T-ODA-T with $LiAlH_4$.

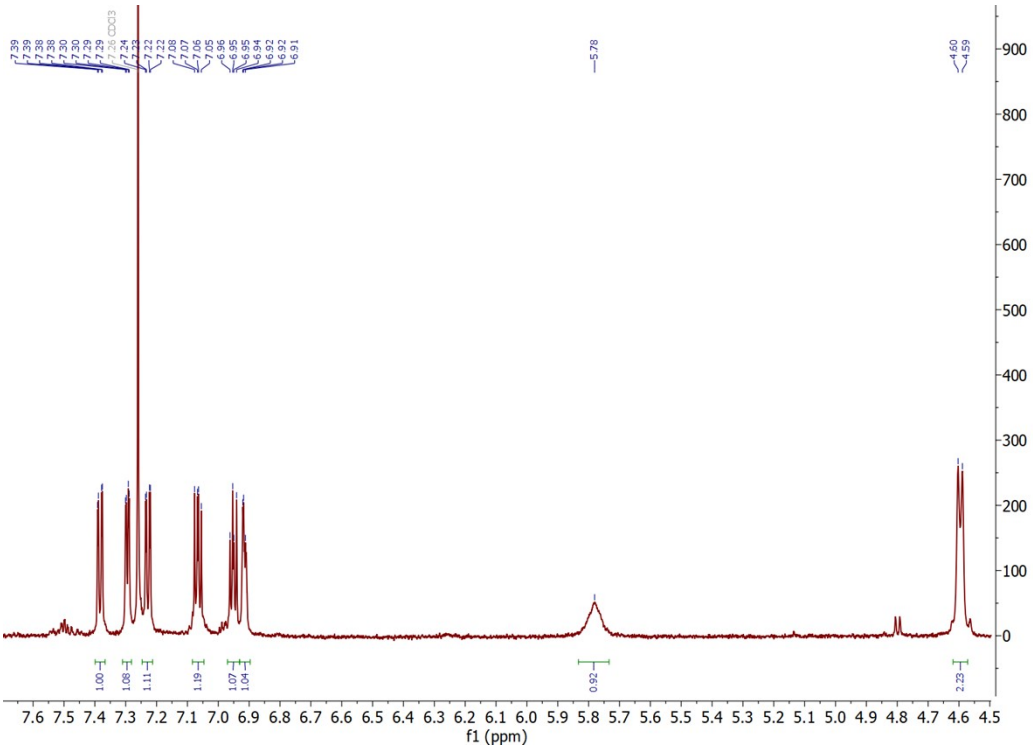


Figure S10. Close up of product peaks in ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of column-purified degradation product (amidoxime) from the treatment of T-ODA-T with $LiAlH_4$.

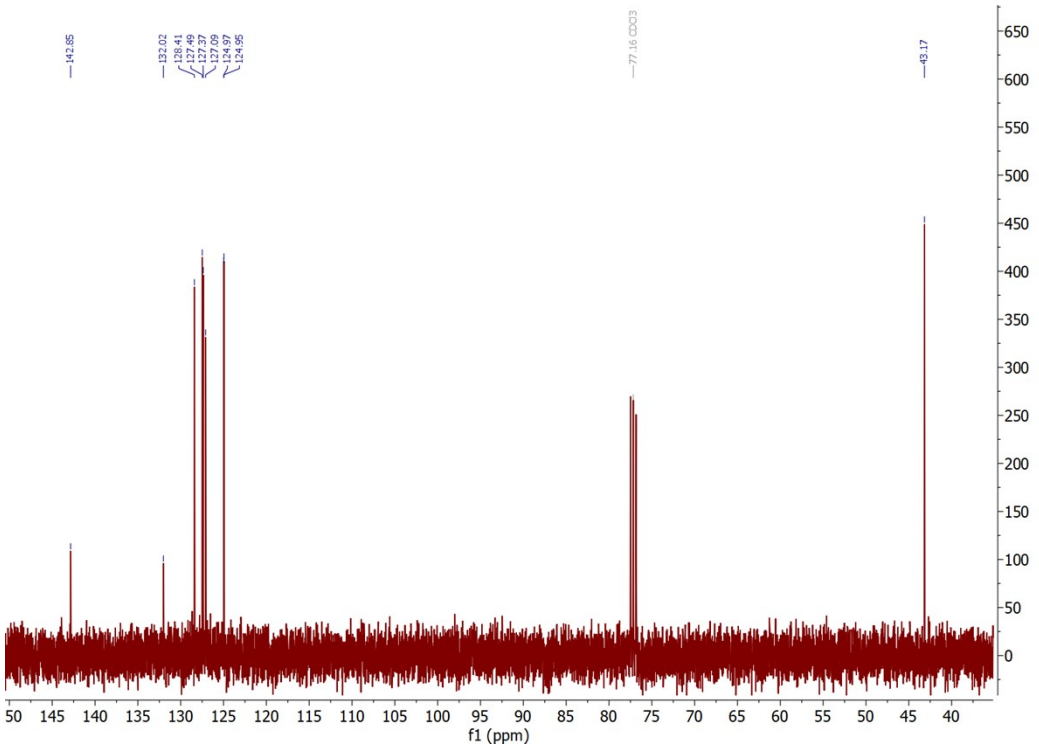


Figure S11. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of column-purified degradation product (amidoxime) from the treatment of T-ODA-T with $LiAlH_4$.

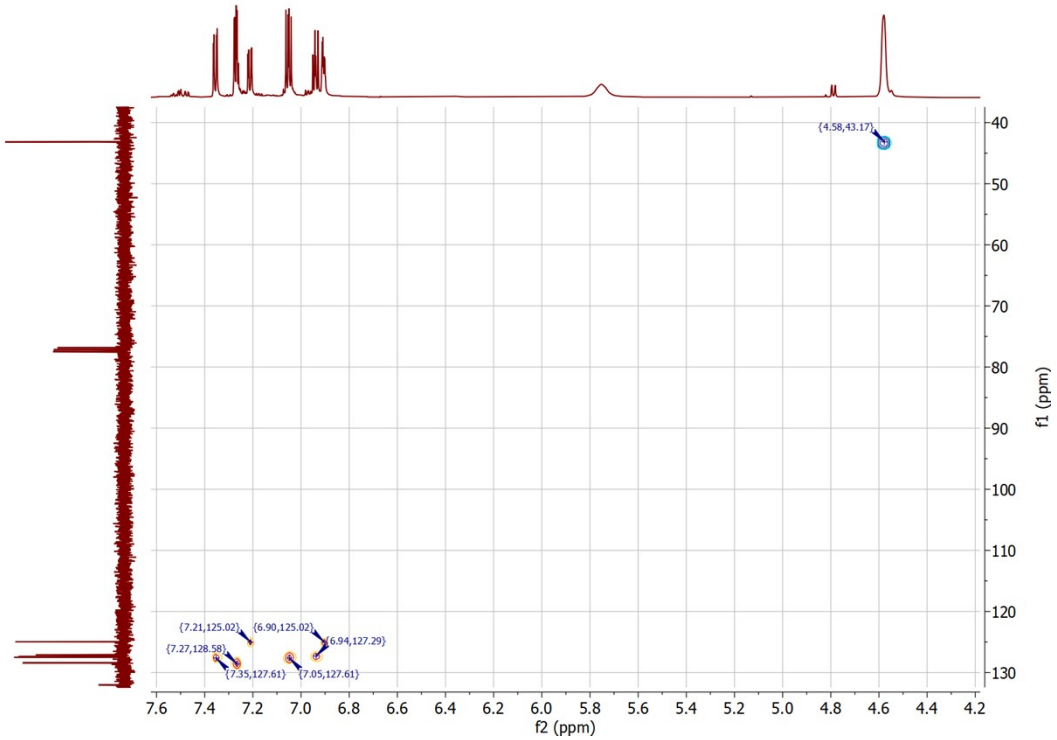


Figure S12. HSQC 2D NMR spectrum (400 MHz, $CDCl_3$) of column-purified degradation product (amidoxime) from the treatment of T-ODA-T with $LiAlH_4$.

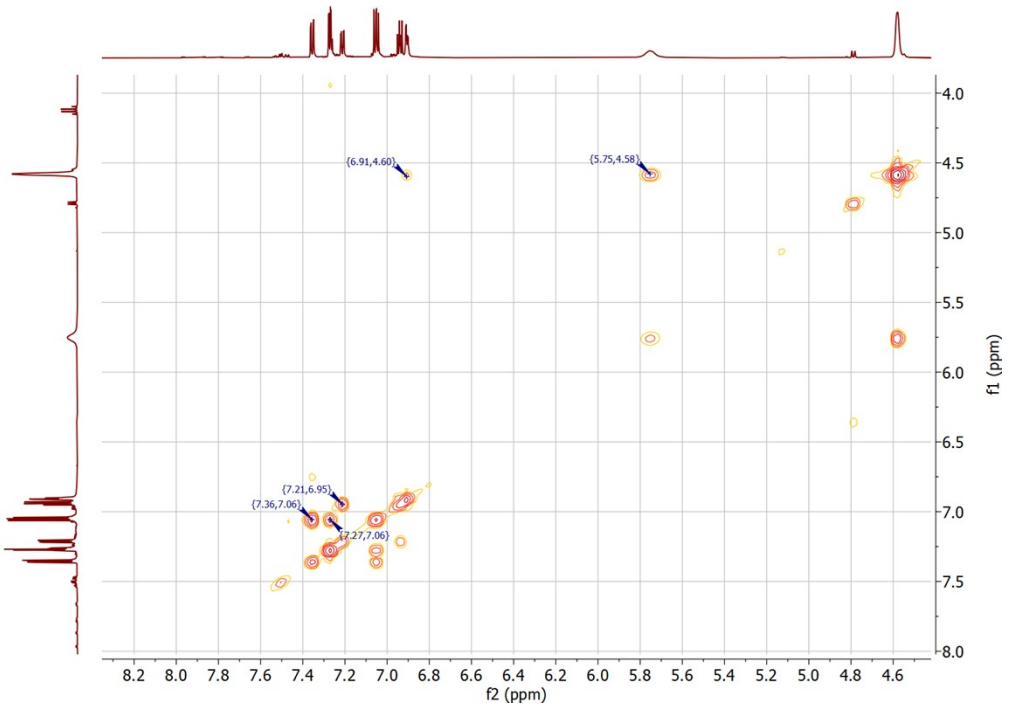


Figure S13. gCOSY 2D NMR spectrum (400 MHz, $CDCl_3$) of column-purified degradation product (amidoxime) from the treatment of T-ODA-T with $LiAlH_4$.

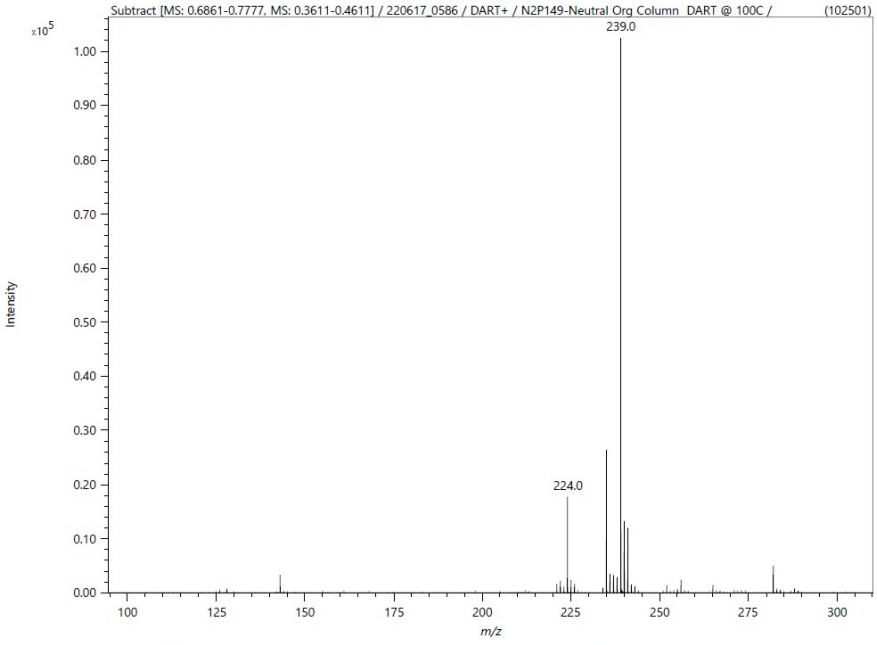


Figure S14. Mass spectrum (DART, positive mode) of column-purified degradation product (amidoxime) from the treatment of T-ODA-T with $LiAlH_4$.

Products of $LiAlH_4$ Degradation Followed by Acid-Catalyzed Hydrolysis

Anhydrous tetrahydrofuran (8 mL) was added via syringe to a 3-neck round-bottom flask with T-ODA-T (30.2 mg; 0.129 mmol) under argon. The resulting solution was cooled in an ice bath. Lithium aluminum hydride (16 mg; 0.42 mmol) was added through a side arm in one portion. The mixture was removed from the ice bath after the bubbling ceased and was allowed to slowly warm to room temperature. After bubbling was no longer observed, the reaction mixture was heated to a reflux for 10 hours. After this heating period, the reaction mixture was cooled in an ice bath and 20 mL of DI water was added dropwise. The resulting mixture was extracted with dichloromethane (3x 15 mL). The dichloromethane fraction was dried over $MgSO_4$, filtered, and concentrated under vacuum to yield 17.6 mg of yellow solid as the crude product.

The crude product was dissolved in ethanol/water (50:50; 5 mL) and two drops of 12 M HCl were added. The resulting solution was refluxed for 15 hours. After cooling to room temperature, the resulting solution was neutralized with saturated sodium bicarbonate solution and extracted with diethyl ether (3x 15 mL). The ether layer was dried over $MgSO_4$, filtered, and concentrated under vacuum to yield a viscous yellow oil (22 mg).

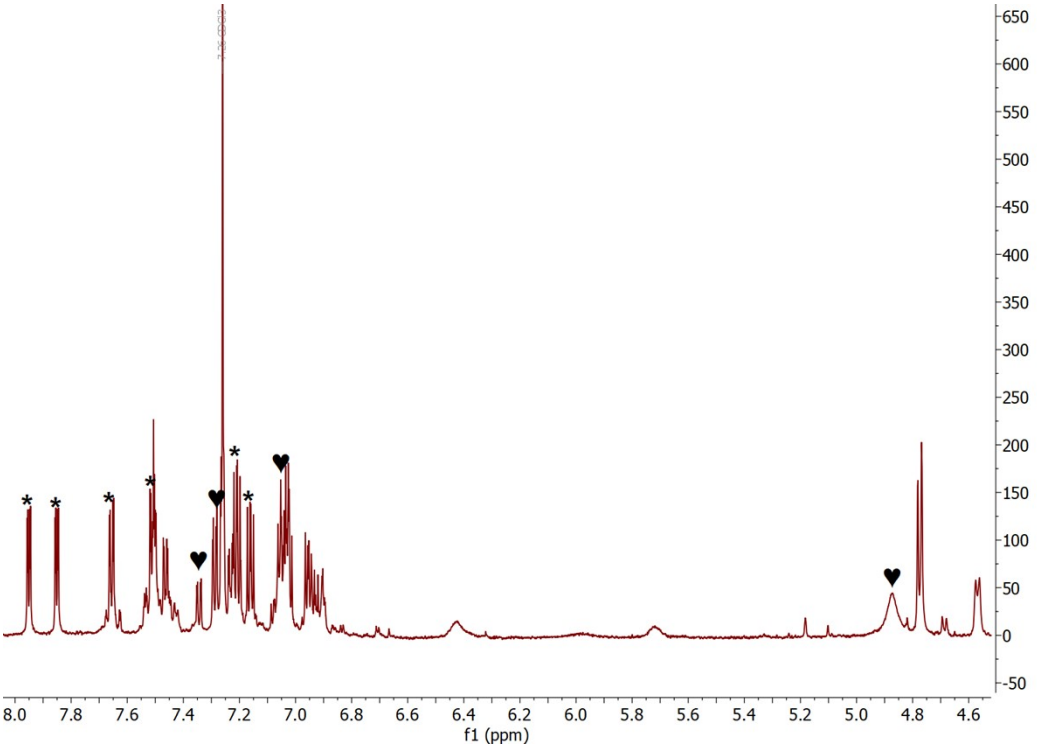


Figure S15. ^1H NMR spectrum (400 MHz, $CDCl_3$) of the degradation products of T-ODA-T after treatment with $LiAlH_4$ and subsequent acid-catalyzed hydrolysis. The asterisk (*) marks peaks from unreacted T-ODA-T and the heart (♥) marks peaks from thiophene-2-amidoxime from comparison with spectrum in Figure S1.

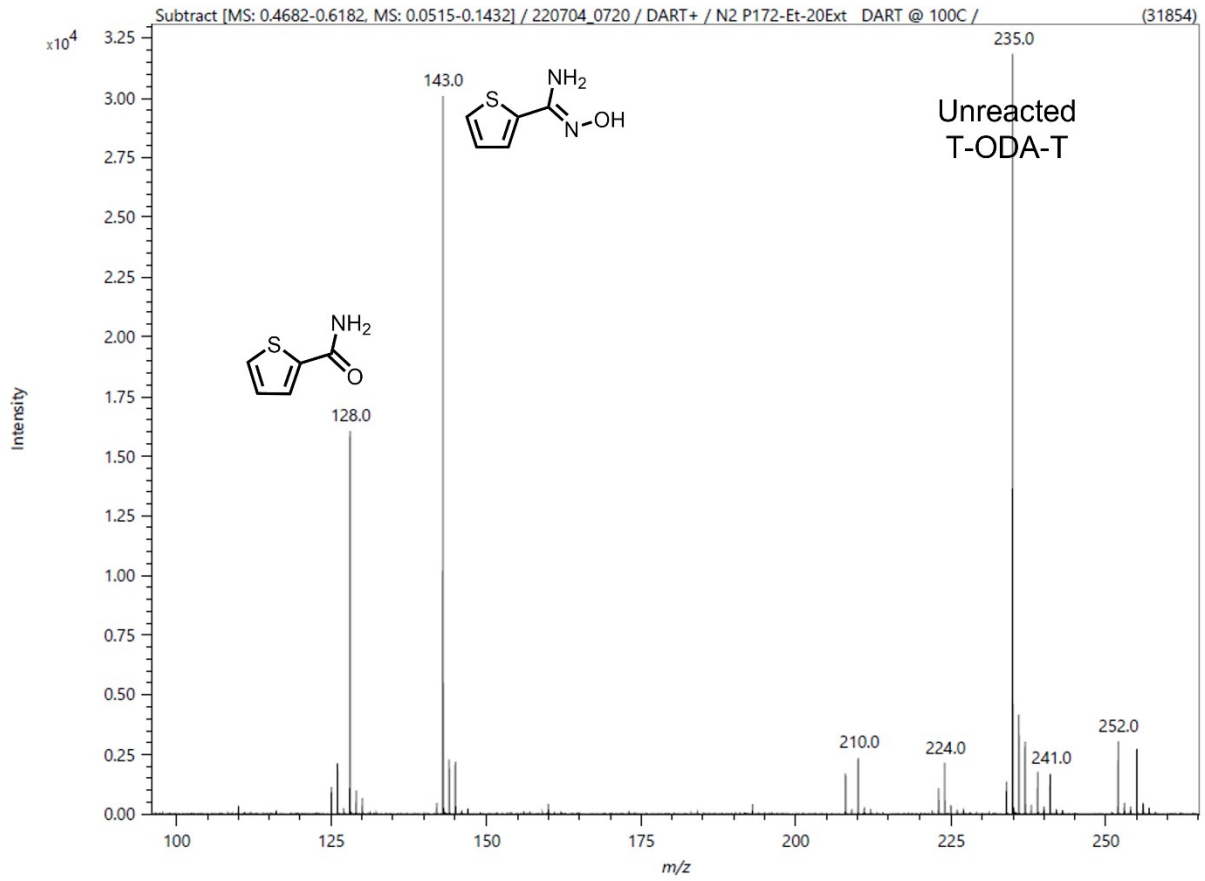
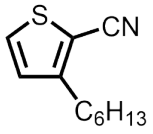


Figure S16. Mass spectrum (DART, positive mode) of the degradation products of T-ODA-T after treatment with $LiAlH_4$ and subsequent acid-catalyzed hydrolysis.

Monomer Synthesis

Synthesis of 3-hexylthiophene-2-carbonitrile



2-bromo-3-hexylthiophene (4.9367 g; 19.971 mmol) was dissolved in anhydrous dimethylformamide (20 mL) in a 3-neck flask under an atmosphere of $Ar_{(g)}$. CuCN (9.5 g; 110 mmol) was added in one portion through a side-arm. The resulting suspension was refluxed for 18 hours. After the reaction mixture was cooled to room temperature, DI water (50 mL) was added, and the resulting suspension was stirred for 10 minutes. The precipitate was removed by gravity filtration, and the filtrate was extracted with toluene (50 mL) and washed with DI water (3 x 30 mL). The organic layer was dried over $MgSO_4$, and the solvent was removed under vacuum. The crude product was purified by column chromatography (silica) using 5:1 hexanes:dichloromethane as the mobile phase to afford an orange oil (3.0154 g; 78%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.47 (d, J= 5.1 Hz, 1H), 6.96 (d, 5.1 Hz, 1H), 2.79 (t, J = 7.6 Hz, 2H), 1.71 – 1.59 (m, 2H), 1.40 – 1.24 (m, 2H), 0.88 (t, J = 6.8 Hz, 3H). ^{13}C NMR ($CDCl_3$, 126 MHz): δ 154.96, 131.79, 128.86, 114.47, 105.57, 31.60, 30.28, 29.99, 28.91, 22.65, 14.16.

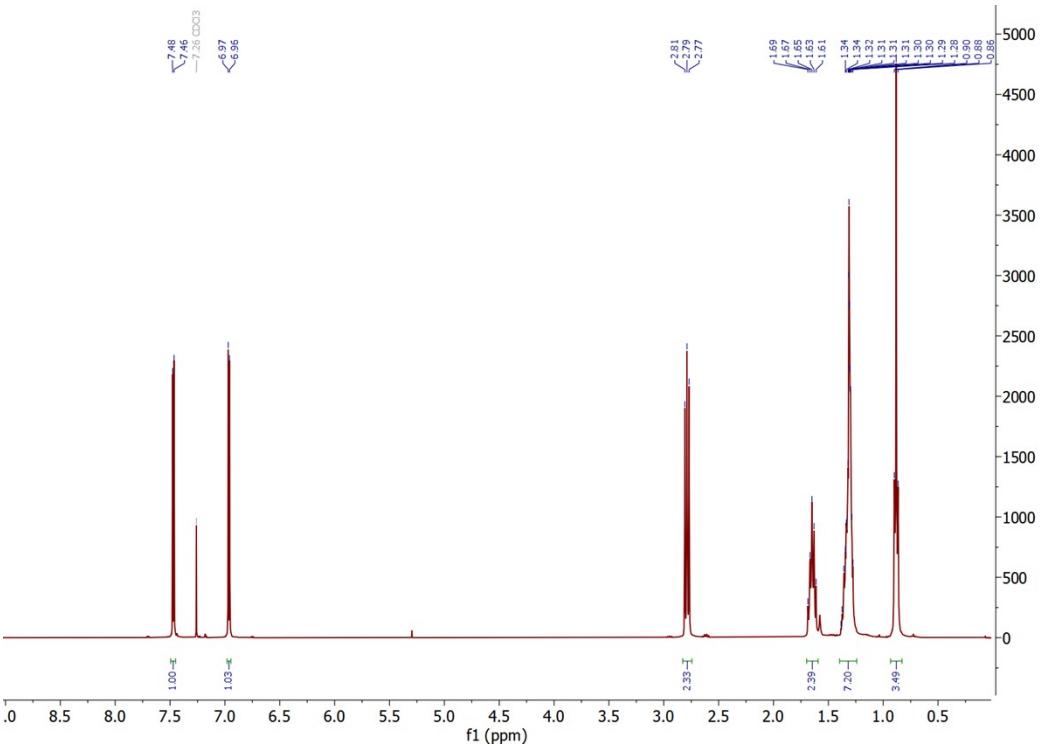


Figure S17. ^{1}H NMR spectrum (400 MHz) of 3-hexylthiophene-2-carbonitrile in $CDCl_3$.

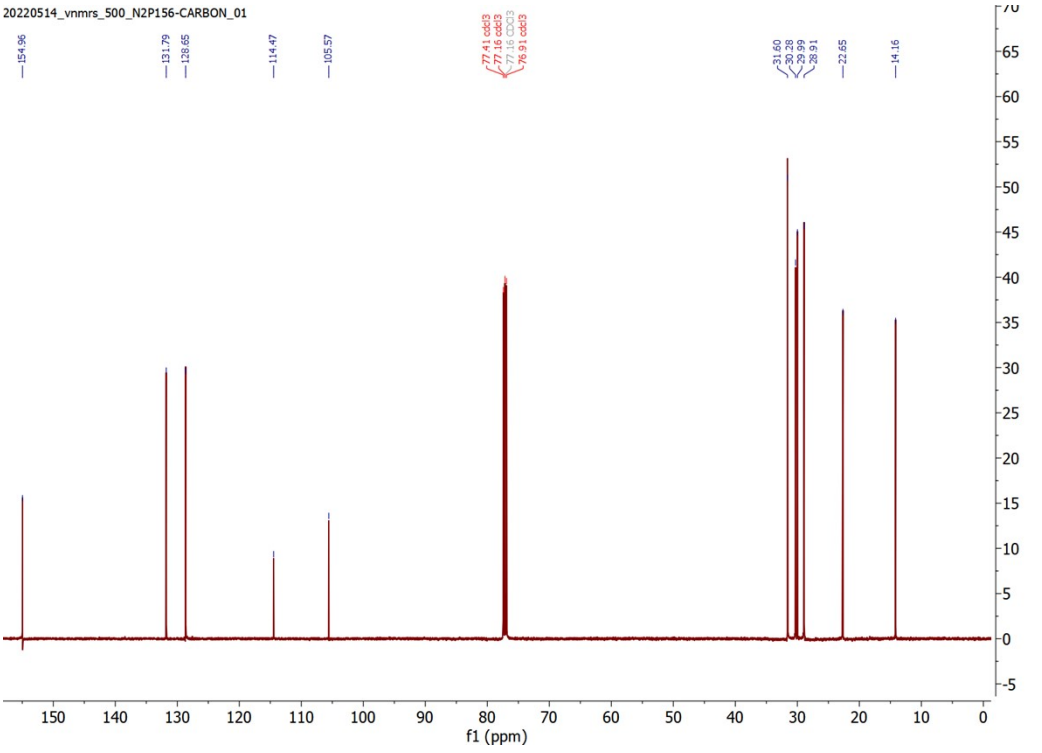
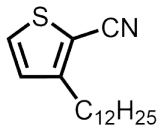


Figure S18. ^{13}C NMR spectrum (126 MHz) of 3-hexylthiophene-2-carbonitrile in $CDCl_3$.

Synthesis of 3-dodecylthiophene-2-carbonitrile



2-bromo-3-dodecylthiophene (4.52 g; 13.6 mmol) was dissolved in anhydrous dimethylformamide (20 mL) in a 3-neck flask under an atmosphere of $Ar_{(g)}$. CuCN (6.3823 g; 71.26 mmol) was added in one portion through a side-arm. The resulting suspension was refluxed for 24 hours under $Ar_{(g)}$. After the reaction mixture was cooled to room temperature, DI water (20 mL) and toluene (20 mL) were added, and the resulting mixture was stirred overnight. The precipitate was removed by gravity filtration, and the organic layer was separated and washed with DI water (25 mL) and then brine (25 mL). The organic layer was dried over $MgSO_4$, and the solvent was removed under vacuum. The crude product was purified by column chromatography (silica) using 5:1 hexanes:dichloromethane as the mobile phase to afford a yellow oil (3.4475 g; 91%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.47 (d, J = 5.1 Hz, 1H), 6.96 (d, J = 5.0 Hz, 1H), 2.79 (t, J = 7.7 Hz, 2H), 1.70 – 1.59 (m, 2H), 1.38 – 1.26 (m, 18H), 0.88 (t, J = 6.8 Hz, 3H).

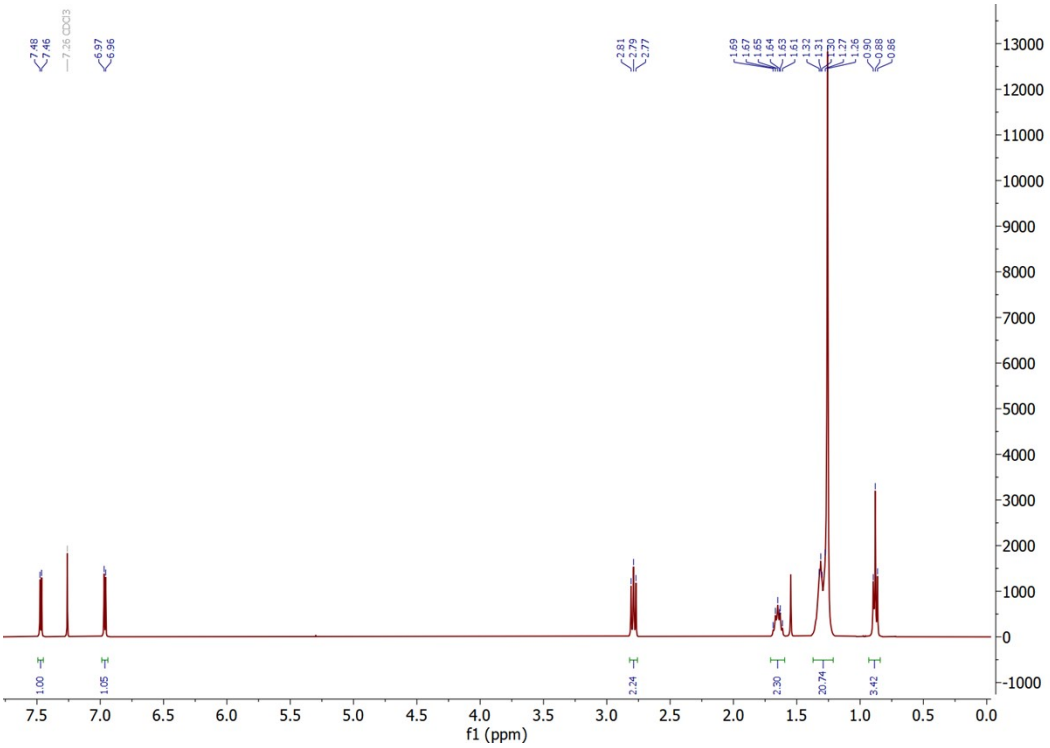
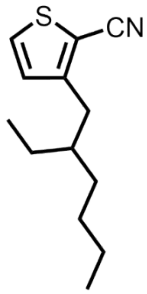


Figure S19. ^{1}H NMR spectrum (400 MHz) of 3-dodecylthiophene-2-carbonitrile in $CDCl_3$.

Synthesis of 3-(2-ethylhexyl)thiophene-2-carbonitrile (N2P160)



2-bromo-3-(2-ethylhexyl)thiophene (0.94 g; 3.4 mmol) was dissolved in anhydrous dimethylformamide (10 mL) in a 3-neck flask under an atmosphere of $Ar_{(g)}$. CuCN (2.0304 g; 22.67 mmol) was added in one portion through a side-arm. The resulting suspension was refluxed for 24 hours under $Ar_{(g)}$. After the reaction mixture was cooled to room temperature, DI water (10 mL) and toluene (10 mL) were added, and the resulting suspension was stirred overnight. The precipitate was removed by gravity filtration, and the organic layer was separated and washed with DI water (25 mL) and then brine (25 mL). The

organic layer was dried over $MgSO_4$, and the solvent was removed under vacuum. The crude product was purified by column chromatography (silica) using 9:1 hexanes:chloroform as the mobile phase to afford a yellow oil (0.6791 g; 91%). ^{1}H NMR ($CDCl_3$, 400 MHz): 7.47 (d, J = 5.1 Hz, 1H), 6.94 (d, J = 5.1 Hz, 1H), 2.73 (d, J = 7.2 Hz, 2H), 1.70 – 1.60 (m, 1H), 1.36 – 1.19 (m, 8H), 0.93 – 0.83 (m, 6H).

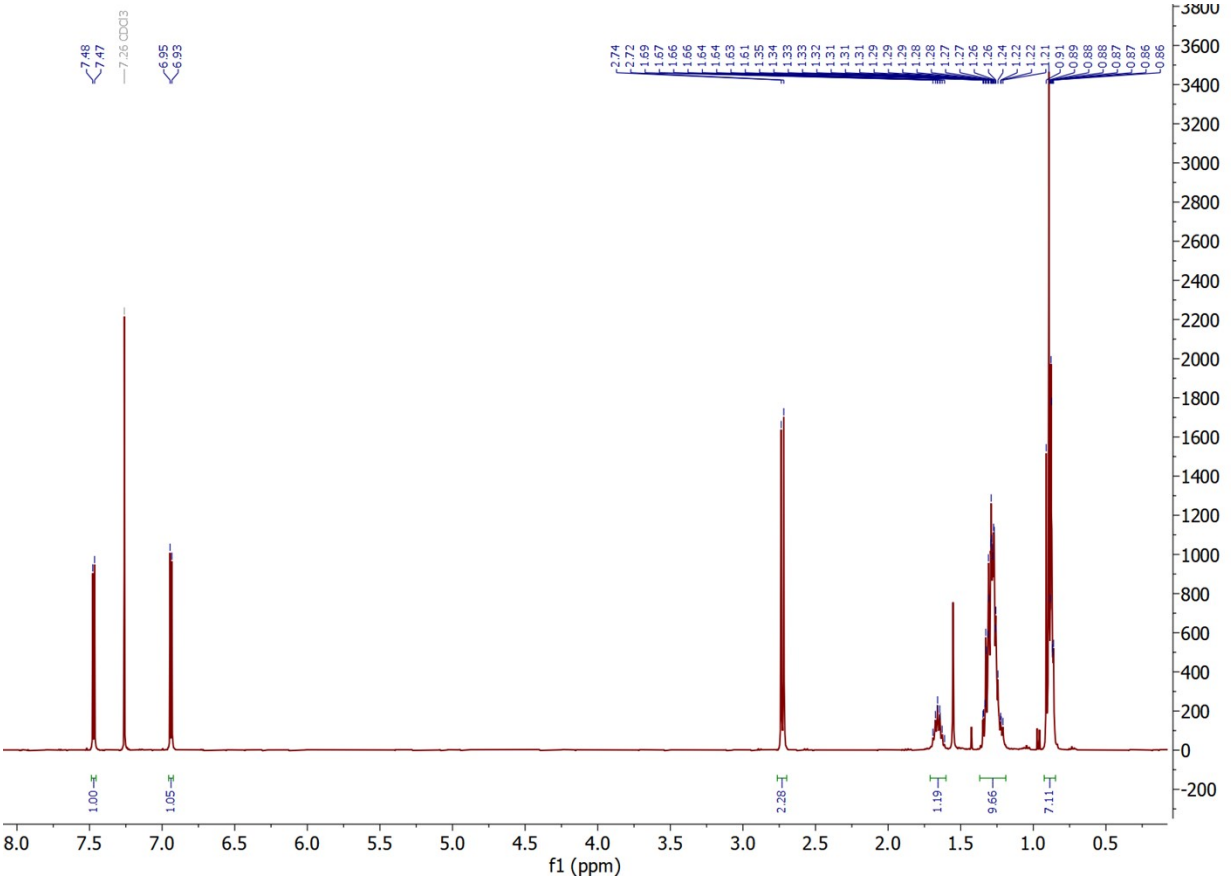
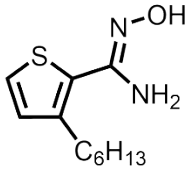


Figure S20. ^{1}H NMR spectrum (400 MHz) of 3-(2-ethylhexyl)thiophene-2-carbonitrile in $CDCl_3$.

Synthesis of 3-hexylthiophene-2-amidoxime



Hydroxylamine (1.12 mL; 50 wt% aqueous solution) was added to a stirring solution of 3-hexylthiophene-2-carbonitrile (1.0043 g; 5.17 mmol) in ethanol (7 mL). The reaction mixture was refluxed for 2 hours. After cooling, the solution was concentrated under vacuum and redissolved in ethyl acetate. The solution was washed with DI water (3 x 15 mL), dried over $MgSO_4$, filtered, and concentrated under vacuum to afford the product as a pale yellow oil (1.1898 g) with a < 10% starting material impurity by ^{1}H NMR. This product was used without further purification. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.22 (d, J = 5.1 Hz, 1H), 6.91 (d, J = 5.1 Hz, 1H), 4.87 (s, 2H), 2.82 – 2.74 (m, 2H), 1.66 – 1.55 (m, 2H), 1.39 – 1.28 (m, 6H), 0.90 – 0.84 (m, 3H). ^{13}C NMR ($CDCl_3$, 126 MHz): δ 148.75, 143.08, 129.86, 127.65, 125.53, 31.80, 30.98, 29.39, 29.32, 22.74, 14.23. HRMS (DART-TOF): [M+H$^+$] Calculated for $C_{11}H_{19}N_2OS$ = 227.12, found = 227.12.

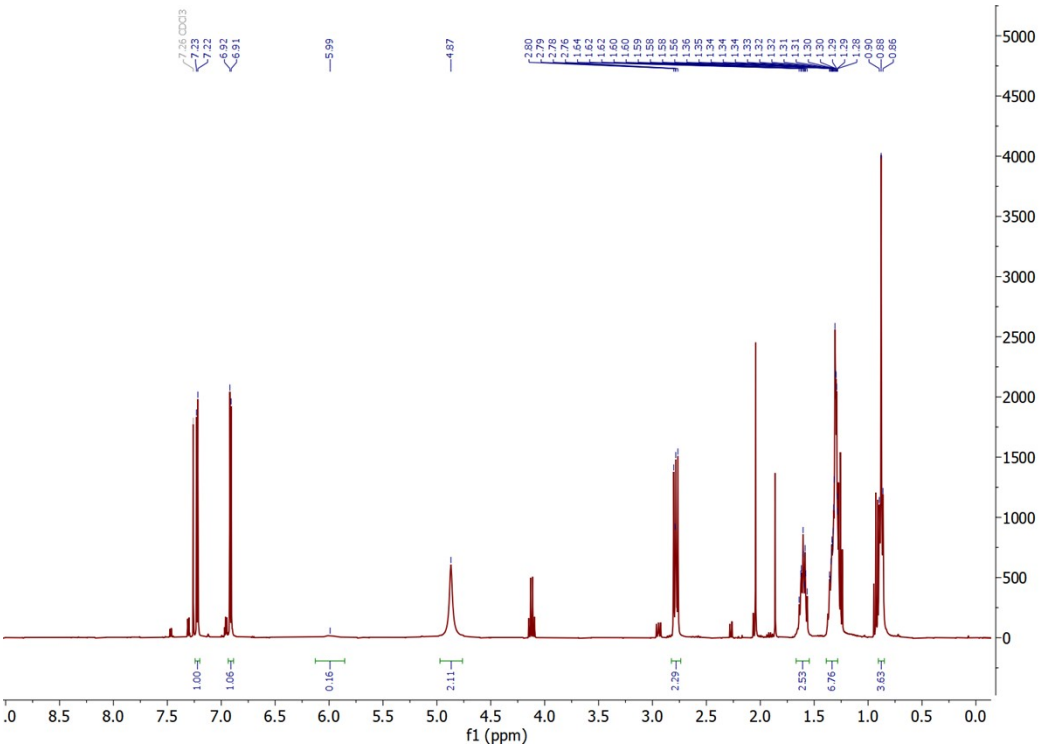


Figure S21. ^{1}H NMR spectrum (400 MHz) of 3-hexylthiophene-2-amidoxime in $CDCl_3$.

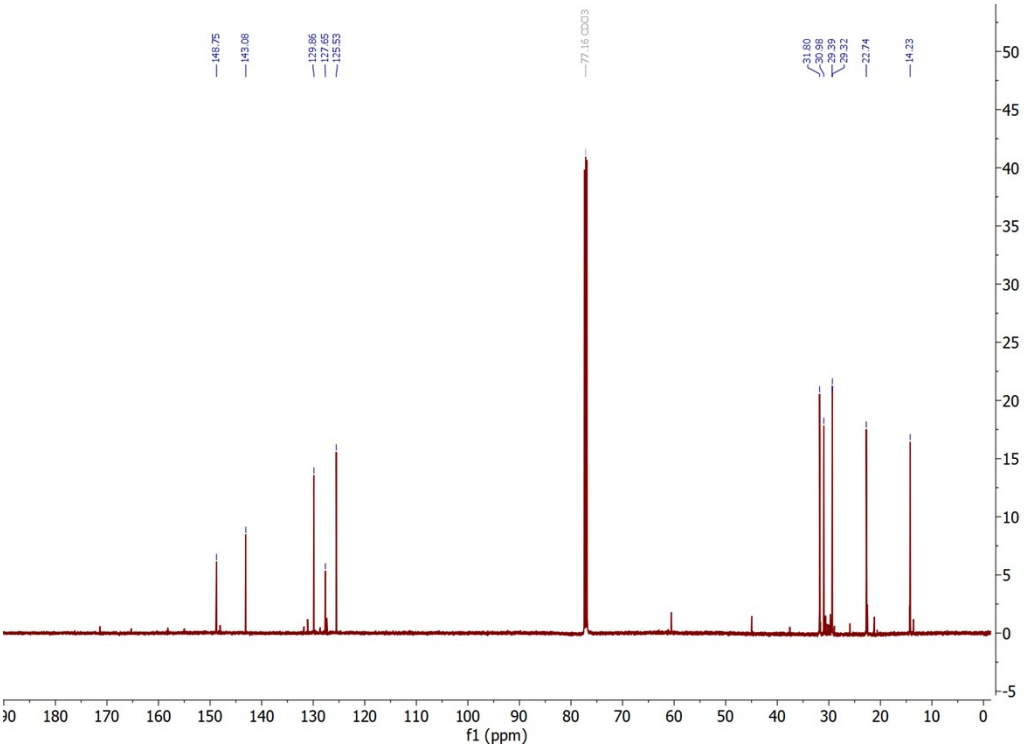


Figure S22. ^{13}C NMR spectrum (126 MHz) of 3-hexylthiophene-2-amidoxime in $CDCl_3$.

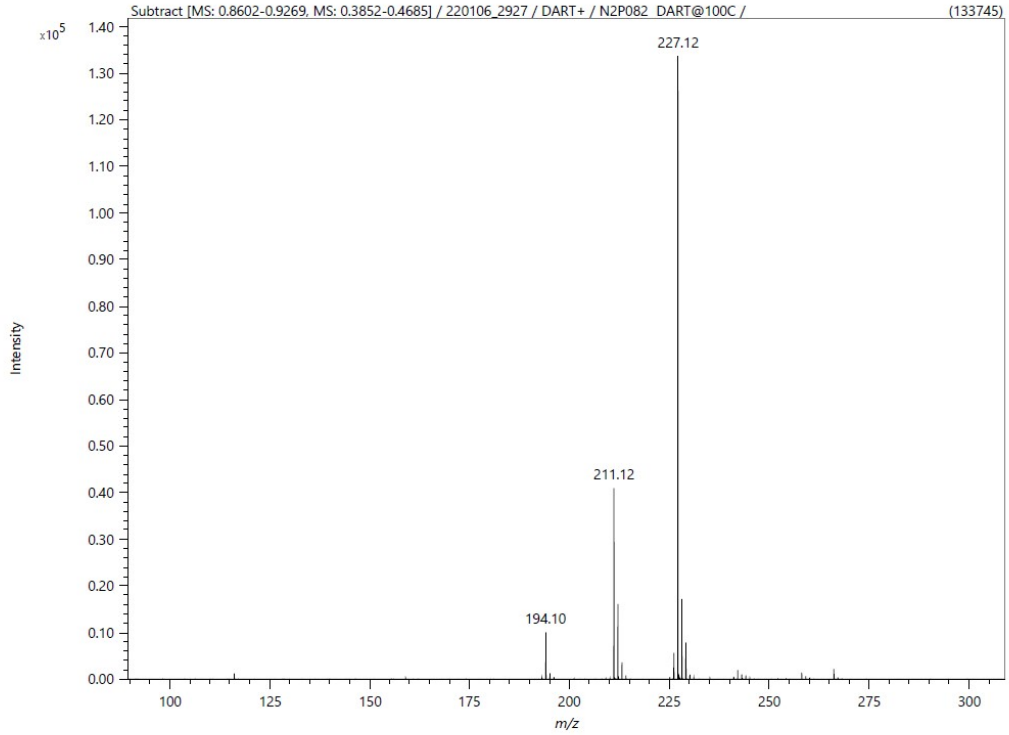
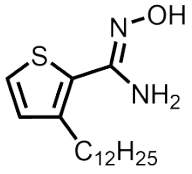


Figure S23. Mass spectrum (DART, positive mode) of 3-hexylthiophene-2-amidoxime.

Synthesis of 2-amidoxime-3-dodecylthiophene



Hydroxylamine (1.2 mL; 50 wt% aqueous solution) was added to a stirring solution of 3-dodecylthiophene-2-carbonitrile (1.2050 g; 4.3428 mmol) in ethanol (9 mL). The reaction mixture was refluxed for 2 hours. After cooling, the solution was concentrated under vacuum and redissolved in ethyl acetate. The solution was washed with DI water (3 x 15 mL), dried over $MgSO_4$, filtered, and concentrated under vacuum to afford the product as a white crystalline powder (1.2366 g) with a < 10% starting material impurity by ^{1}H NMR. This product was used without further purification. ^{1}H NMR (DMSO, 400 MHz): δ 9.58 (s, 1H), 7.38 (d, J = 5.1 Hz, 1H), 6.93 (d, J = 5.1 Hz, 1H), 5.65 (s, 2H), 2.72 (t, J = 7.7 Hz, 2H), 1.57 – 1.47 (m, 2H), 1.30 – 1.21 (m, 18H), 0.89 – 0.81 (m, 3H).

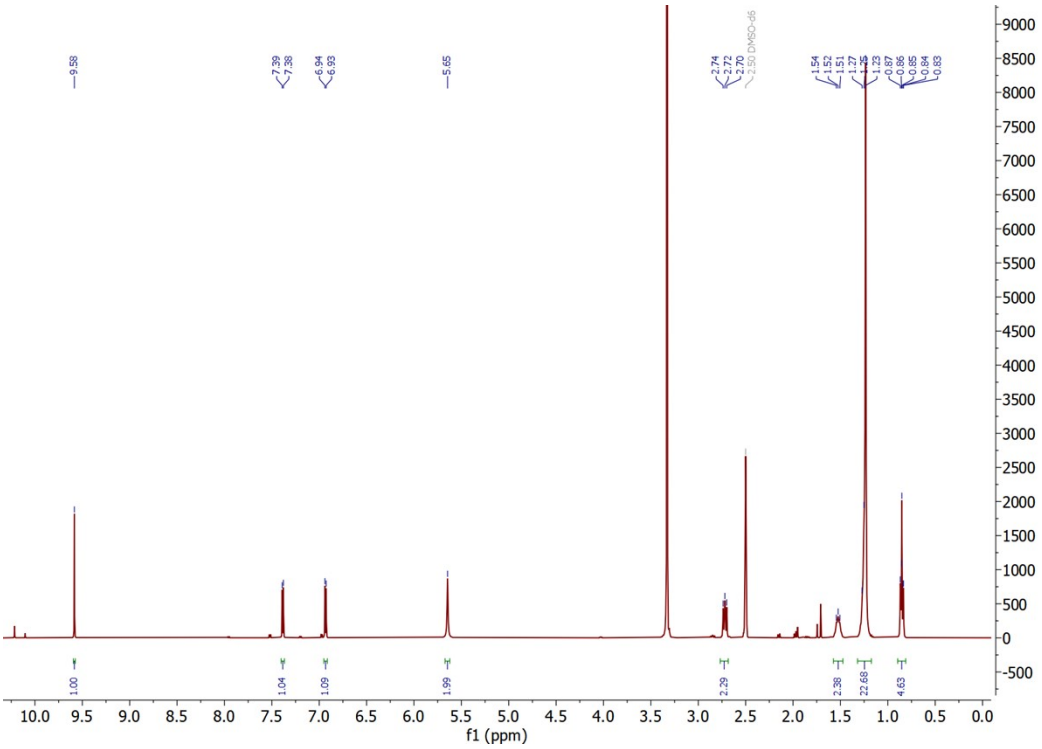
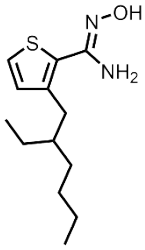


Figure S24. ^{1}H NMR spectrum (400 MHz) of 3-dodecylthiophene-2-amidoxime in DMSO.

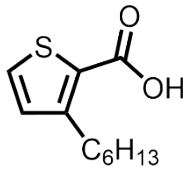
Synthesis of 2-amidoxime-3-(2-ethylhexyl)thiophene (N2P064)



Hydroxylamine (0.65 mL; 50 wt% aqueous solution) was added to a stirring solution of 3-hexylthiophene-2-carbonitrile (631.6 mg; 2.853 mmol) in ethanol (3 mL). The reaction mixture was refluxed for 1 hour. After cooling, the solution was concentrated under vacuum and redissolved in ethyl acetate. The solution was washed with DI water (3 x 10 mL), dried over $MgSO_4$, filtered, and concentrated under vacuum to afford the product as a yellow oil (686.2 mg) with a < 10% starting material impurity by ^{1}H NMR. This product was used without further purification. ^{1}H NMR ($CDCl_3$, 400 MHz): 9.55 (s, 1H), 7.39 (d, J = 5.1 Hz, 1H), 6.89 (d, J = 5.1 Hz, 1H), 5.65 (s, 2H), 2.69 (d, J = 7.2 Hz, 2H), 1.63 – 1.55 (m, 1H), 1.29 – 1.12 (m, 8H), 0.89 – 0.76 (m, 6H).

Figure S25. ^{1}H NMR spectrum (400 MHz) of 3-(2-ethylhexyl)thiophene-2-amidoxime in DMSO.

Synthesis of 3-hexylthiophene-2-carboxylic acid



Added 3-hexylthiophene-2-carbonitrile (1.0089 g; 5.219 mmol) to a stirring solution of NaOH (3 M) in water/EtOH (50:50 vol/vol; 5 mL). Refluxed reaction mixture for 17 hours. After cooling, the reaction mixture was concentrated under vacuum and redissolved in diethyl ether (10 mL) and DI water (10 mL). The aqueous layer was collected, acidified with a few drops of concentrated HCl, and extracted with diethyl ether (3 x 15 mL). The organic layer was dried over $MgSO_4$, filtered, and concentrated under vacuum to afford the product as a colorless oil that eventually formed colorless crystals (1.108 g; 84%). ^{1}H NMR ($CDCl_3$, 400 MHz): 7.49 (d, J = 5.0 Hz, 1H), 6.99 (d, J = 5.0 Hz, 1H), 3.02 (t, J = 7.7 Hz, 2H), 1.68 – 1.57 (m, 2H), 1.42 – 1.25 (m, 6H), 0.89 (t, J = 6.8 Hz, 3H). δ ^{13}C NMR ($CDCl_3$, 126 MHz): 154.95, 131.79, 128.65, 114.47, 105.56, 31.59, 30.27, 29.98, 28.90, 22.64, 14.15.

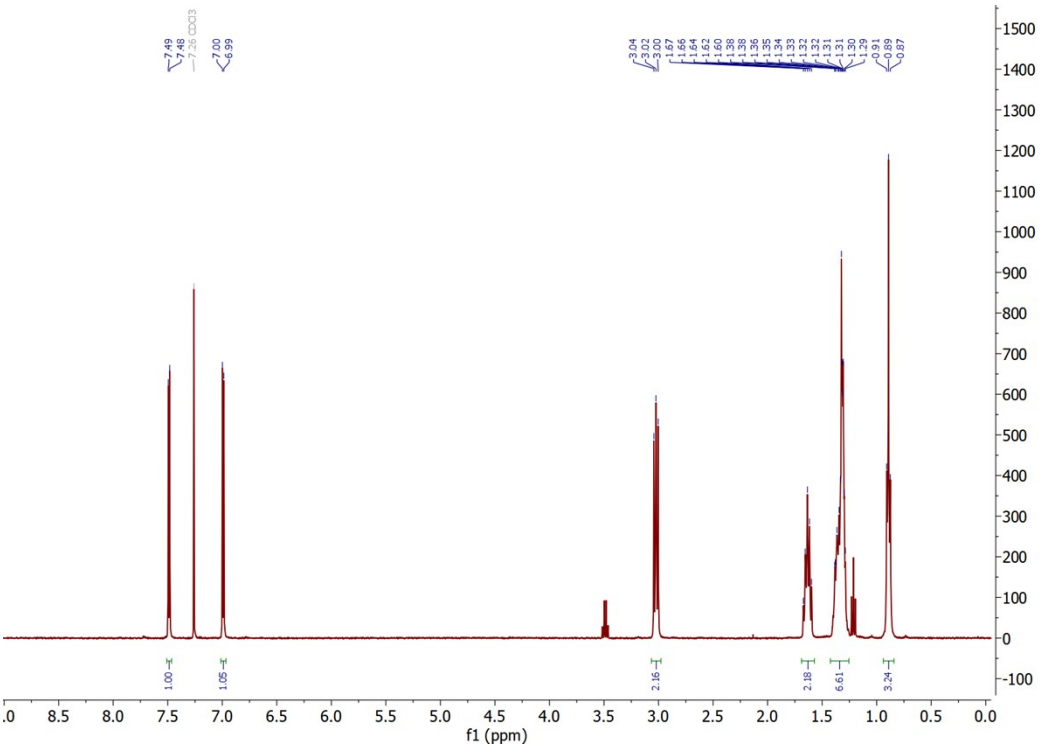


Figure S26. ^{1}H NMR spectrum (400 MHz) of 3-hexylthiophene-2-carboxylic acid in $CDCl_3$.

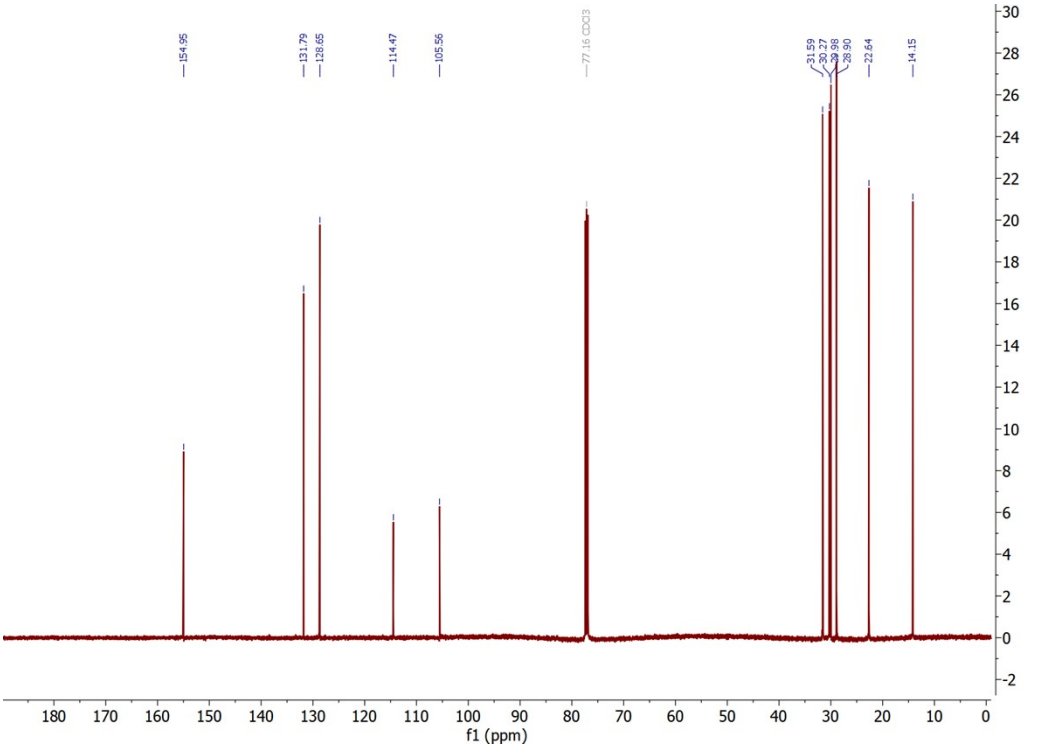
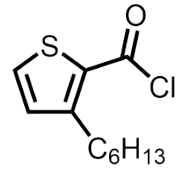
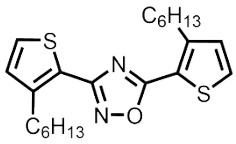


Figure S27. ^{13}C NMR spectrum (126 MHz) of 3-hexylthiophene-2-carboxylic acid in $CDCl_3$.

Synthesis of 3,5-bis(3-hexylthiophen-2-yl)-1,2,4-oxadiazole (N2P162 + N2P164)



Thionyl chloride (2.5 mL; 34 mmol) was added dropwise to stirring, neat 3-hexylthiophene-2-carboxylic acid (930.6 mg; 4.383 mmol) under an atmosphere of $Ar_{(g)}$ and cooled in an ice bath. The resulting mixture was allowed to slowly warm to room temperature and was then heated to reflux for 1 hour. The thionyl chloride was removed under vacuum, leaving the product as a red-brown oil stored under $Ar_{(g)}$. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.64 (d, J = 5.1 Hz, 1H), 7.05 (d, J = 5.1 Hz, 1H), 2.93 (t, J = 7.6 Hz, 2H), 1.60 (tt, J = 7.7, 6.4 Hz, 2H), 1.41 – 1.23 (m, 6H), 0.88 (t, J = 6.7 Hz, 3H).



The oil was redissolved in toluene (7.5 mL) and cooled in an ice bath. Anhydrous pyridine (0.53 mL; 6.57 mmol) was added dropwise, followed by the addition of 3-hexylthiophene-2-amidoxime (1.18 mg; 4.74 mmol accounting for starting material impurity). Left stirring in ice bath for 2 hours. After this period, the reaction mixture was heated to reflux for 24 hours. The reaction mixture was filtered while still hot and the filtrate was concentrated under vacuum. The crude product was redissolved in diethyl ether (25 mL) and was washed with DI water (2 x 40 mL) followed by brine (25 mL). The organic layer was dried over $MgSO_4$, filtered, and concentrated under vacuum. The resulting crude product was purified by column chromatography (silica) using 3:1 hexanes:dichloromethane as the mobile phase to afford the product as a pink oil (1.0334 g; 59%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.51 (d, J = 5.0 Hz, 1H), 7.40 (d, J = 5.1 Hz, 1H), 7.05 (d, J = 5.1 Hz, 1H), 7.02 (d, J = 5.1 Hz, 1H), 3.14 (t, J = 7.8 Hz, 2H), 3.09 (t, J = 7.7 Hz, 2H), 1.74 – 1.64 (m, 4H), 1.47 – 1.26 (m, 12H), 0.92 – 0.85 (m, 6H). ^{13}C NMR ($CDCl_3$, 126 MHz): δ 171.25, 165.08, 149.81, 146.60, 130.95, 130.68, 130.66, 128.12, 122.67, 119.90, 31.90, 31.82, 30.50, 30.42, 30.03, 29.94, 29.34, 29.32, 22.79, 22.77, 14.25, 14.23. HRMS (DART-TOF): [M+H$^+$] calculated for $C_{22}H_{31}N_2OS_2$: 403.19, found: 403.2.

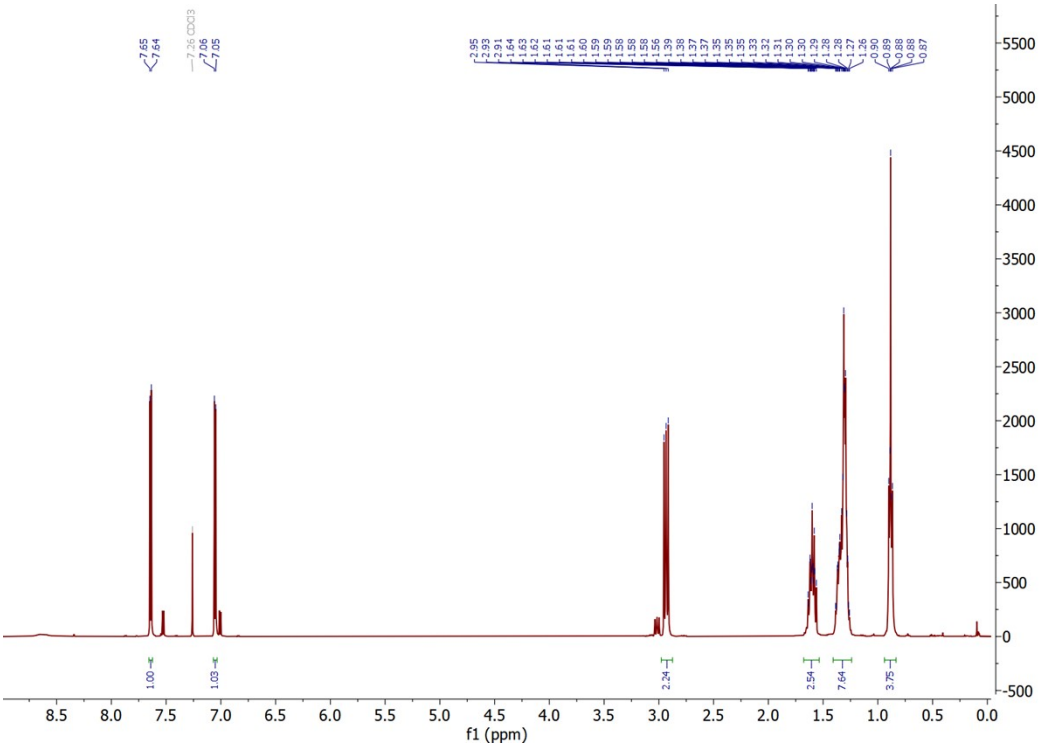


Figure S28. ^{1}H NMR spectrum (400 MHz) of 3-hexylthiophene-2-carbonyl chloride in $CDCl_3$.

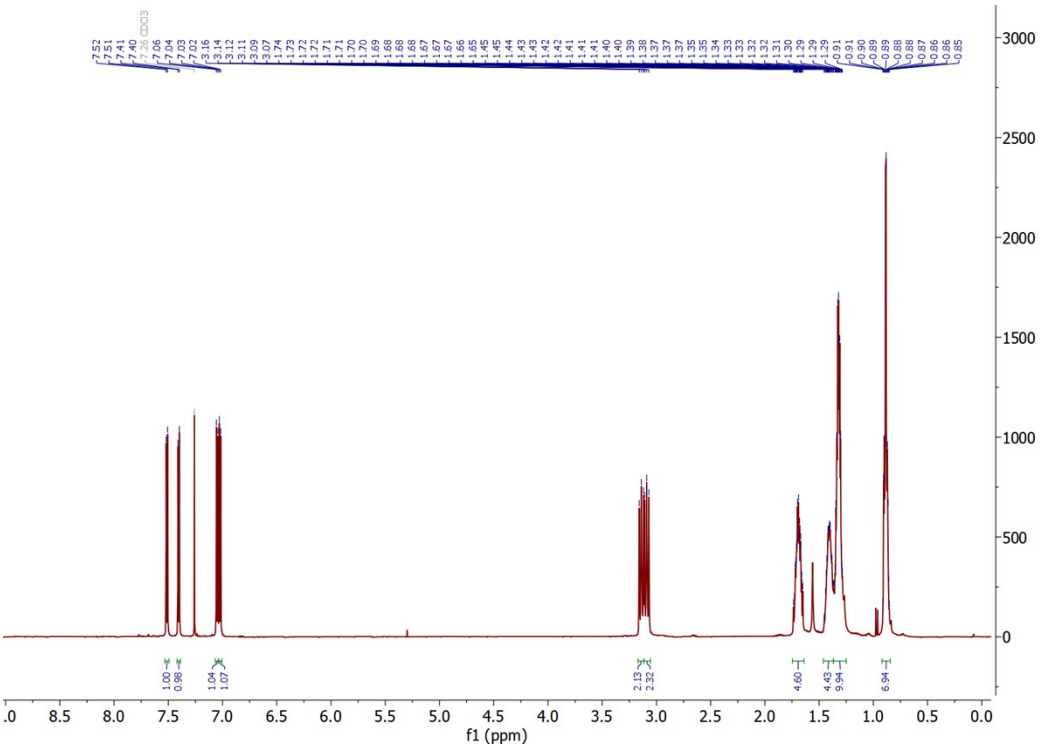


Figure S29. ^{1}H NMR spectrum (400 MHz) of 3,5-bis(3-hexylthiophen-2-yl)-1,2,4-oxadiazole in $CDCl_3$.

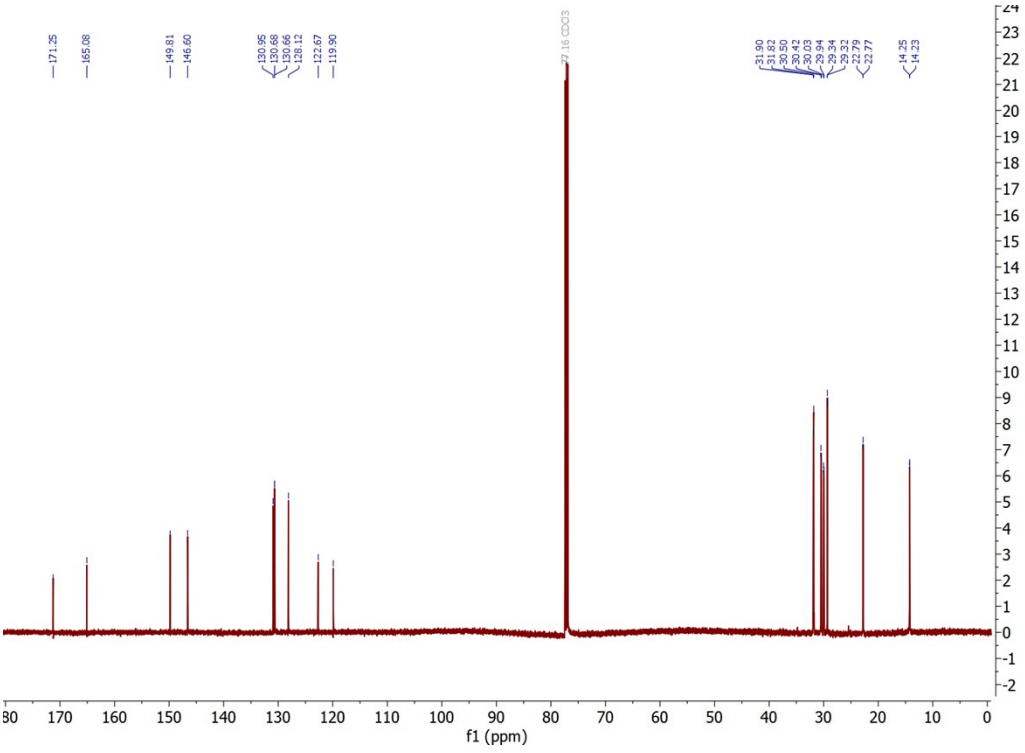
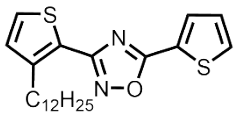


Figure S30. ^{13}C NMR spectrum (126 MHz) of 3,5-bis(3-hexylthiophen-2-yl)-1,2,4-oxadiazole in $CDCl_3$.

Synthesis of 3-(3-dodecylthiophen-2-yl)-5-(thiophen-2-yl)-1,2,4-oxadiazole



Thiophene-2-carbonyl chloride (0.74 mL; 5.7 mmol) was added to a stirring solution of 3-dodecylthiophene-2-amidoxime (1.6269 g; 5.2396 mmol) and pyridine (0.55 mL; 6.8 mmol) in toluene (25 mL) cooled in an ice bath. The mixture was left stirring in an ice bath for 2 hours. Following this period, the solution was heated to reflux for 24 hours. The reaction mixture was filtered while hot and the filtrate was concentrated under vacuum. The crude product was redissolved in ethyl acetate (80 mL) and was washed with saturated $NaHCO_3$ solution (20 mL), DI water (20 mL), and finally brine (20 mL). The organic layer was dried over $MgSO_4$, filtered, and concentrated under vacuum. The crude product was purified by column chromatography (silica) using 3:1 hexanes:dichloromethane as the mobile phase to afford the product as a viscous yellow oil that slowly became an off-white crystalline solid (891.5 mg; 40%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.95 (dd, J = 3.8, 1.2 Hz, 1H), 7.65 (dd, J = 5.0, 1.2 Hz, 1H), 7.42 (d, J = 5.1 Hz, 1H), 7.21 (dd, J = 5.0, 3.7 Hz, 1H), 7.03 (d, J = 5.1 Hz, 1H), 3.07 (t, J = 7.8 Hz, 2H), 1.74 – 1.62 (m, 2H), 1.44 – 1.19 (m, 18H), 0.92 – 0.81 (m, 3H). HRMS (DART-TOF): [M+H$^+$] Calculated for $C_{22}H_{31}N_2OS_2$: 403.1872, found: 403.1879.

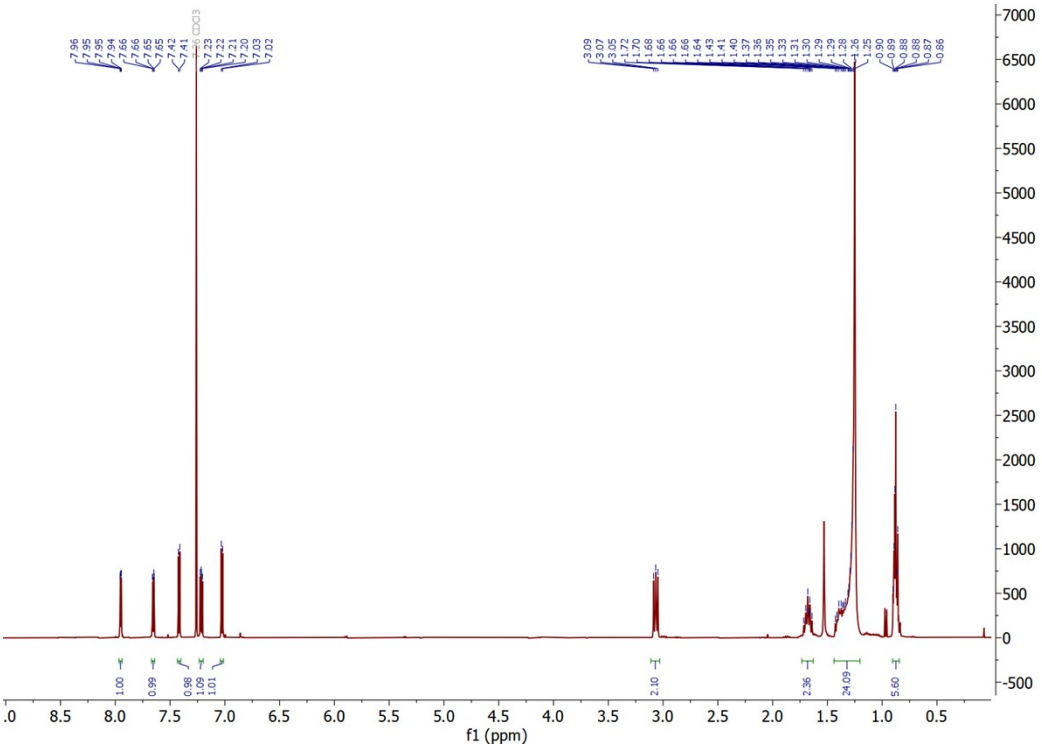


Figure S31. ^{1}H NMR spectrum (400 MHz) of 3-(3-dodecylthiophen-2-yl)-5-(thiophen-2-yl)-1,2,4-oxadiazole in $CDCl_3$.

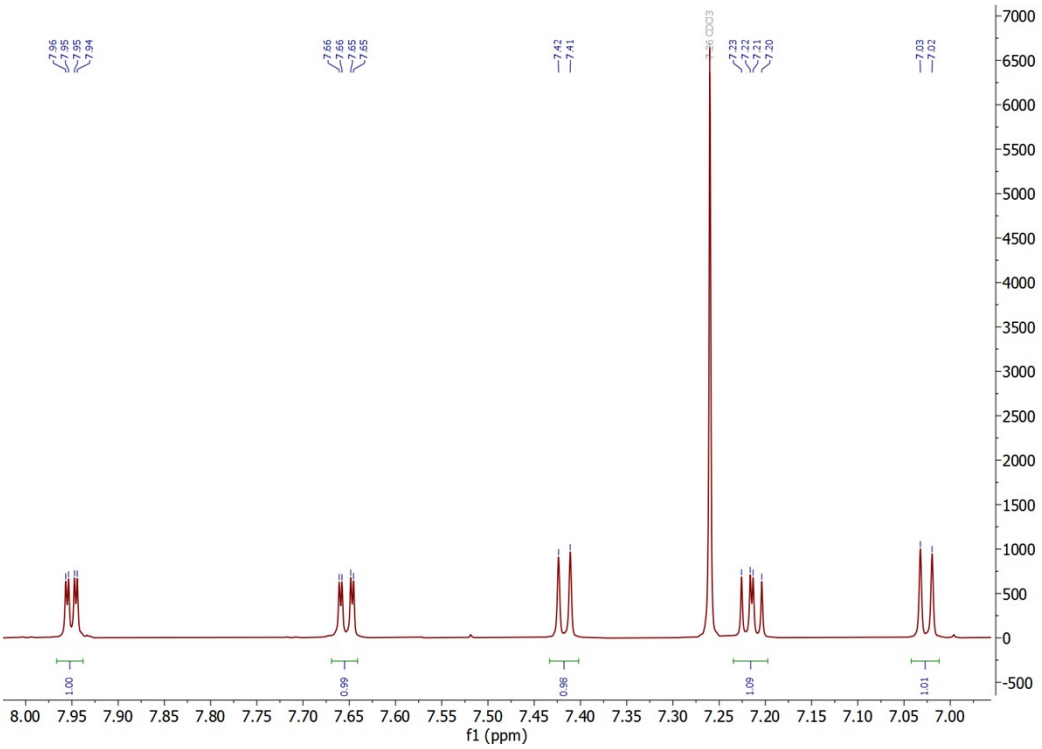


Figure S32. Aromatic region of ^{1}H NMR spectrum (400 MHz) of 3-(3-dodecylthiophen-2-yl)-5-(thiophen-2-yl)-1,2,4-oxadiazole in $CDCl_3$.

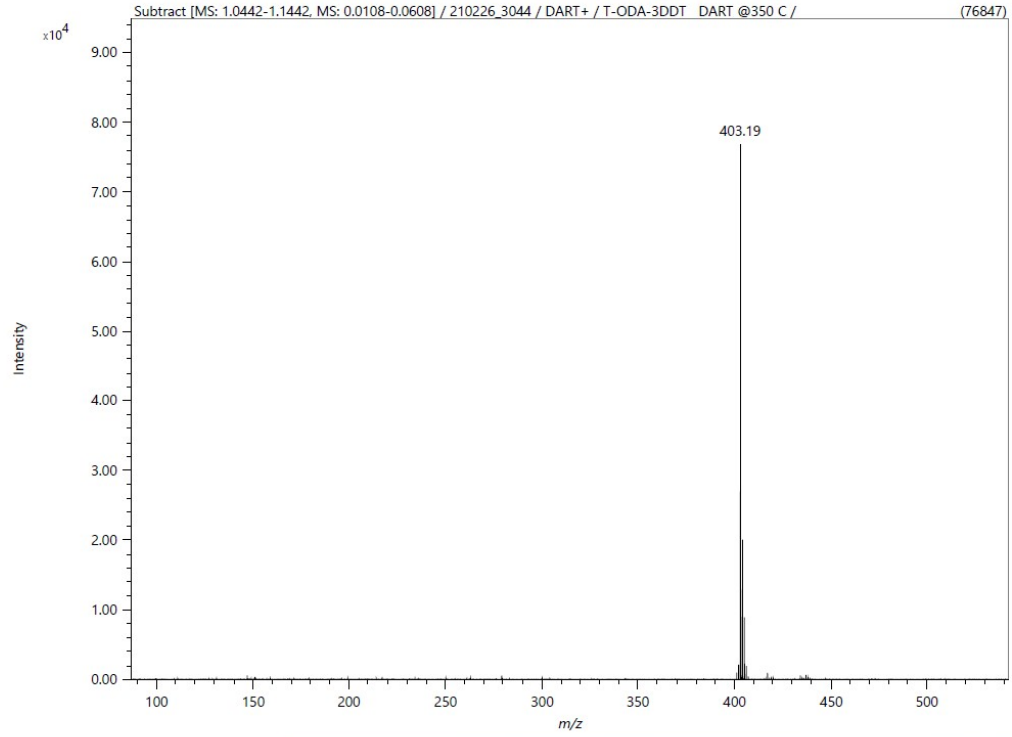
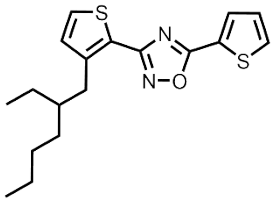


Figure S33. Mass spectrum (DART, positive mode) of 3-(3-dodecylthiophen-2-yl)-5-(thiophen-2-yl)-1,2,4-oxadiazole.

Synthesis of 3-(3-(2-ethylhexyl)thiophen-2-yl)-5-(thiophen-2-yl)-1,2,4-oxadiazole



Thiophene-2-carbonyl chloride (0.42 mL; 3.21 mmol) was added to a stirring solution of 3-(2-ethylhexyl)thiophene-2-amidoxime (679.8 mg; 2.672 mmol) and pyridine (0.32 mL; 4.0 mmol) in toluene (6 mL) cooled in an ice bath. The mixture was left stirring in an ice bath for 2 hours. Following this period, the solution was heated to reflux for 21 hours. The reaction mixture was filtered while hot and the filtrate was concentrated under vacuum. The crude product was redissolved in ethyl acetate (80 mL) and was washed DI water (2 x 20 mL), and finally brine (20 mL). The organic layer was dried over $MgSO_4$, filtered, and concentrated under vacuum. The crude product was purified by column chromatography (silica) using 4:1 hexanes:chloroform as the mobile phase to afford the product as a viscous yellow oil that slowly became an off-white crystalline solid (891.5 mg; 40%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.95 (dd, J = 3.7, 1.2 Hz, 1H), 7.65 (dd, J = 5.0, 1.2 Hz, 1H), 7.41 (d, J = 5.1 Hz, 1H), 7.21 (dd, J = 5.0, 3.8 Hz, 1H), 7.00 (d, J = 5.1 Hz, 1H), 3.03 (dd, J = 7.2, 1.7 Hz, 2H), 1.77 – 1.68 (m, 1H), 1.39 – 1.22 (m, 8H), 0.92 – 0.82 (m, 6H).

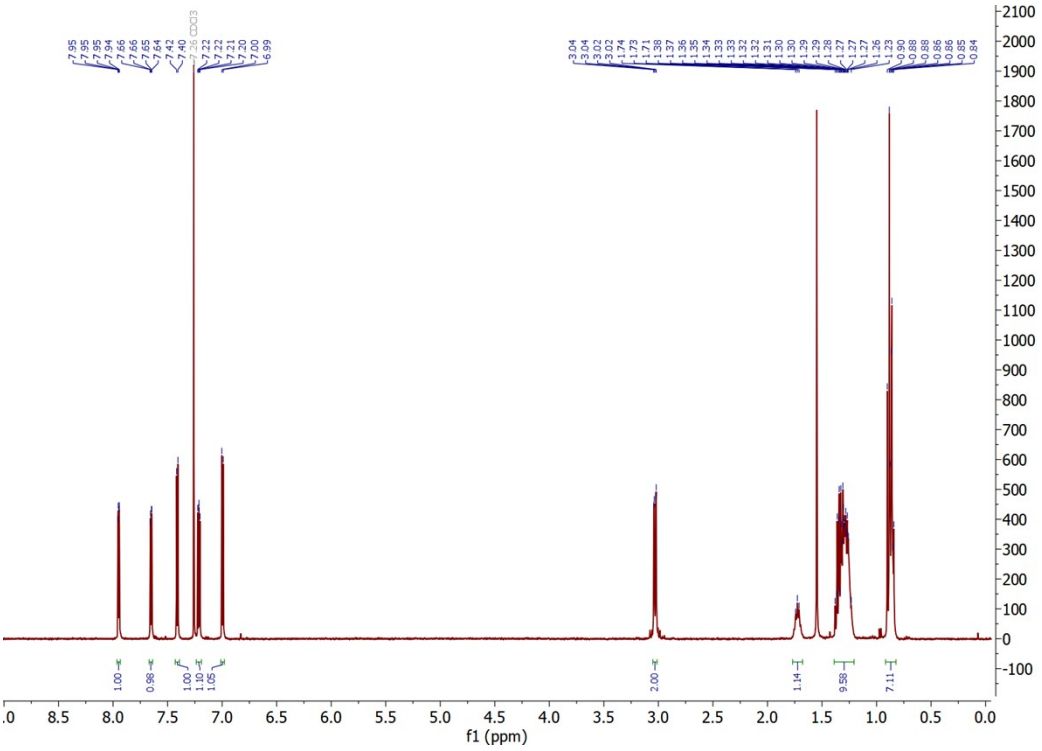
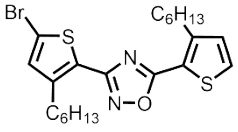


Figure S34. ^{1}H NMR spectrum (400 MHz) of 3-(3-(2-ethylhexyl)thiophen-2-yl)-5-(thiophen-2-yl)-1,2,4-oxadiazole in $CDCl_3$.

Synthesis of 3-(5-bromo-3-hexylthiophen-2-yl)-5-(3-hexylthiophen-2-yl)-1,2,4-oxadiazole



A solution of N-bromosuccinimide (996.5 mg; 5.5989 mmol) in anhydrous dimethylformamide (5mL) was added to an ice bath-cooled Schlenk flask containing 3,5-bis(3-hexylthiophen-2-yl)-1,2,4-oxadiazole (1.0304 g; 2.5592 mmol) dissolved in anhydrous dimethylformamide (5 mL). The reaction mixture was covered from light

and left to stir at room temperature for 20 hours. Following this period, the reaction mixture was heated to 50 °C for 2 hours. After cooling the reaction mixture back to room temperature, 25 mL of DI water was added. The solution was extracted with 40 mL diethyl ether, and the organic layer was washed with saturated $NaHCO_3$ solution (30 mL), DI water (30 mL), and finally brine (30 mL). The organic layer was dried over $MgSO_4$, filtered, and concentrated under vacuum. The crude product was purified by column chromatography (silica) using 15:1 hexanes:dichloromethane as the mobile phase to afford the product as a pale yellow oil (757.0 mg; 61%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.52 (d, J = 5.0 Hz, 1H), 7.05 (d, J = 5.1 Hz, 1H), 6.99 (s, 1H), 3.12 (t, J = 7.7 Hz, 2H), 3.03 (t, J = 7.7 Hz, 2H), 1.73 – 1.61 (m, 4H), 1.44 – 1.26 (m, 12H), 0.92 – 0.86 (m, 6H). ^{13}C NMR ($CDCl_3$, 126 MHz): δ 171.31, 164.19, 150.04, 147.06, 133.39, 130.99, 130.88, 124.29, 119.67, 115.95, 31.83, 31.82, 30.46, 30.22, 30.13, 29.94, 29.32, 29.25, 22.78, 22.75, 14.24, 14.23. HRMS (DART-TOF): [M+H$^+$] calculated for $C_{22}H_{30}BrN_2OS$: 481.1, found: 481.1.

The position of the bromine atom was determined using 2D NMR (HSQC, HMBC). First, the proton in the position next to the bromine was identified as the aromatic singlet at 6.99 ppm and HSQC was used to identify the carbon it is bound to at 133.39 ppm (**Figure S40**). The protons on the nearest methylene group were identified by HMBC, along with the other atoms in the brominated thiophene ring (**Figure S41**). The peak with low intensity in the HMBC (**Figure S41**) is expected to be the carbon that is four bonds away from the methylene protons, and is therefore bound to the bromine atom.

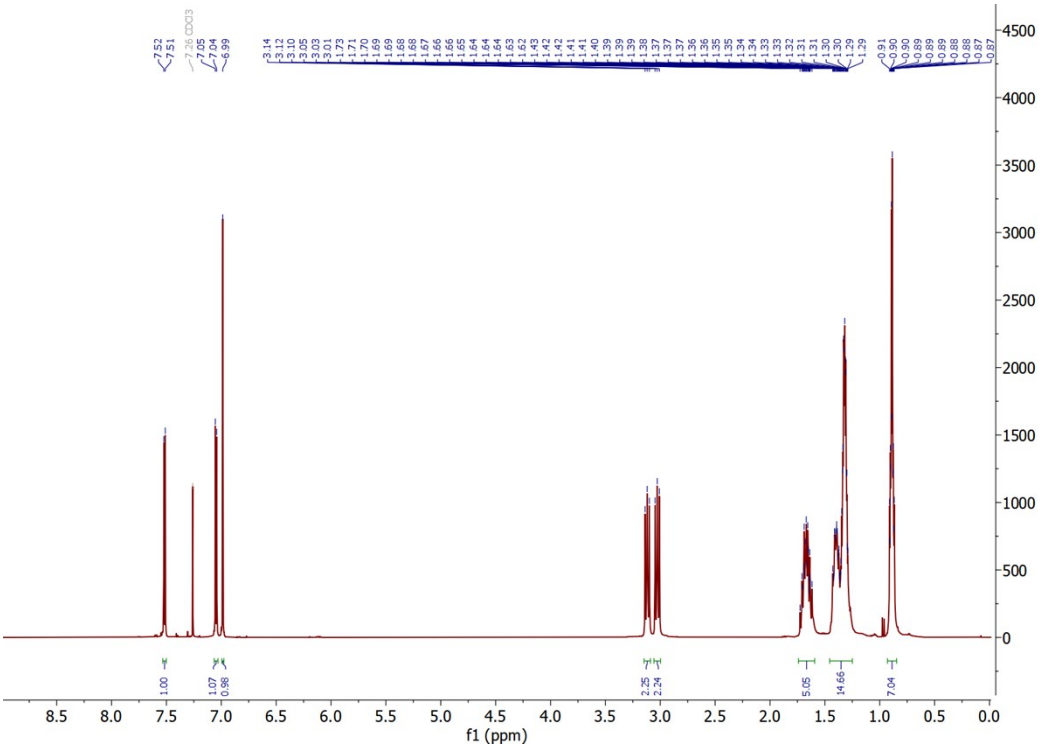


Figure S35. ^{1}H NMR spectrum (400 MHz) of 3-(5-bromo-3-hexylthiophen-2-yl)-5-(3-hexylthiophen-2-yl)-1,2,4-oxadiazole in $CDCl_3$.

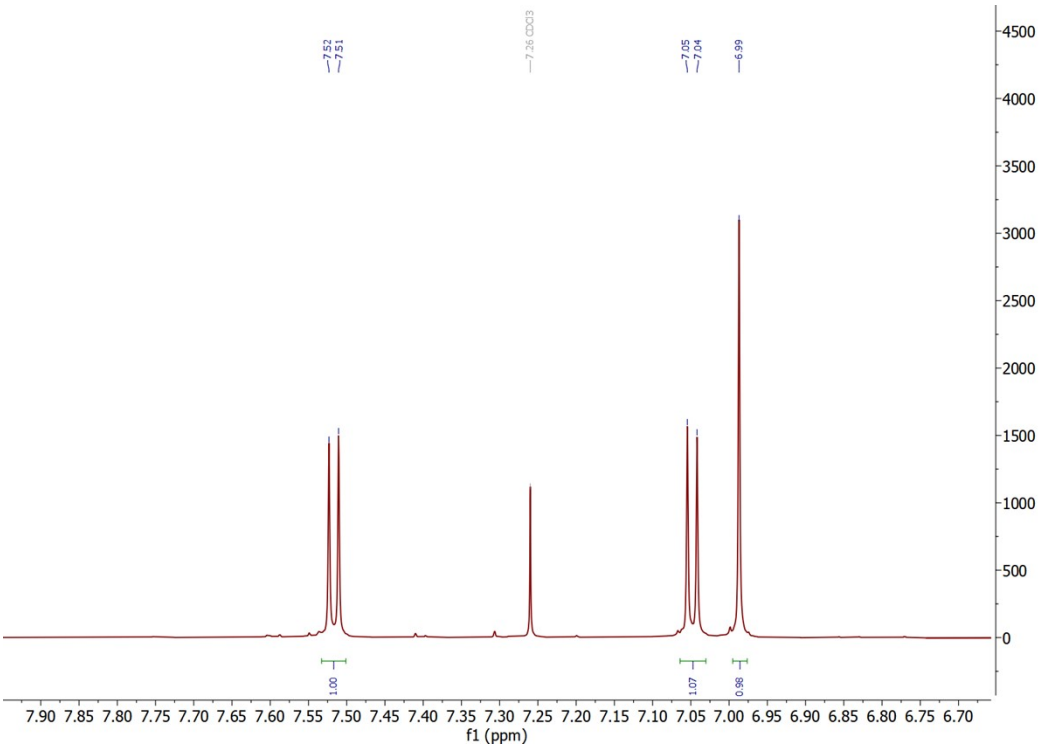


Figure S36. Aromatic region of ^{1}H NMR spectrum (400 MHz) of 3-(5-bromo-3-hexylthiophen-2-yl)-5-(3-hexylthiophen-2-yl)-1,2,4-oxadiazole in $CDCl_3$.

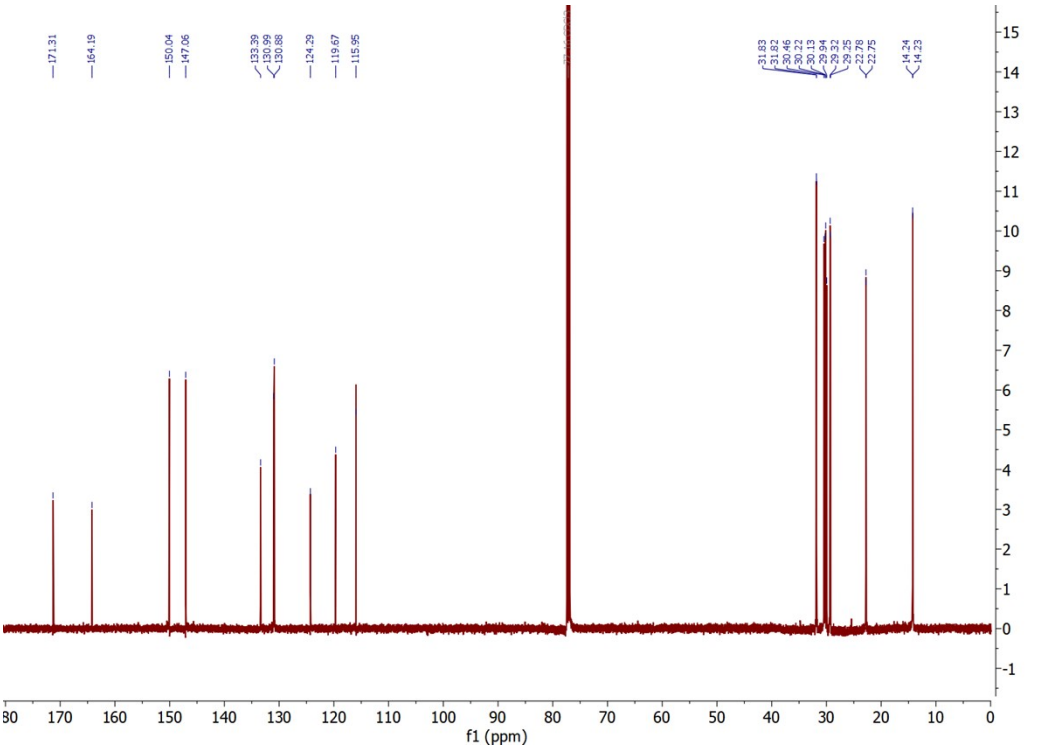


Figure S37. ^{13}C NMR spectrum (126 MHz) of 3-(5-bromo-3-hexylthiophen-2-yl)-5-(3-hexylthiophen-2-yl)-1,2,4-oxadiazole in $CDCl_3$.

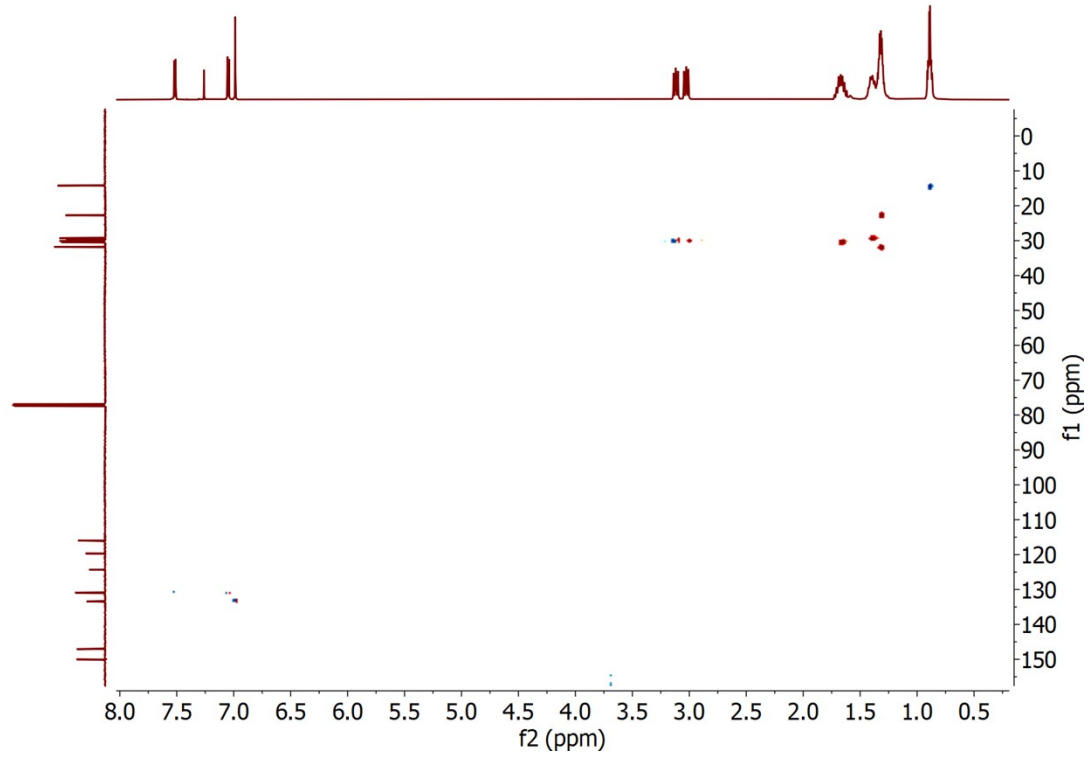


Figure S38. HSQC 2D NMR spectrum of 3HT-ODA-3HT-Br.

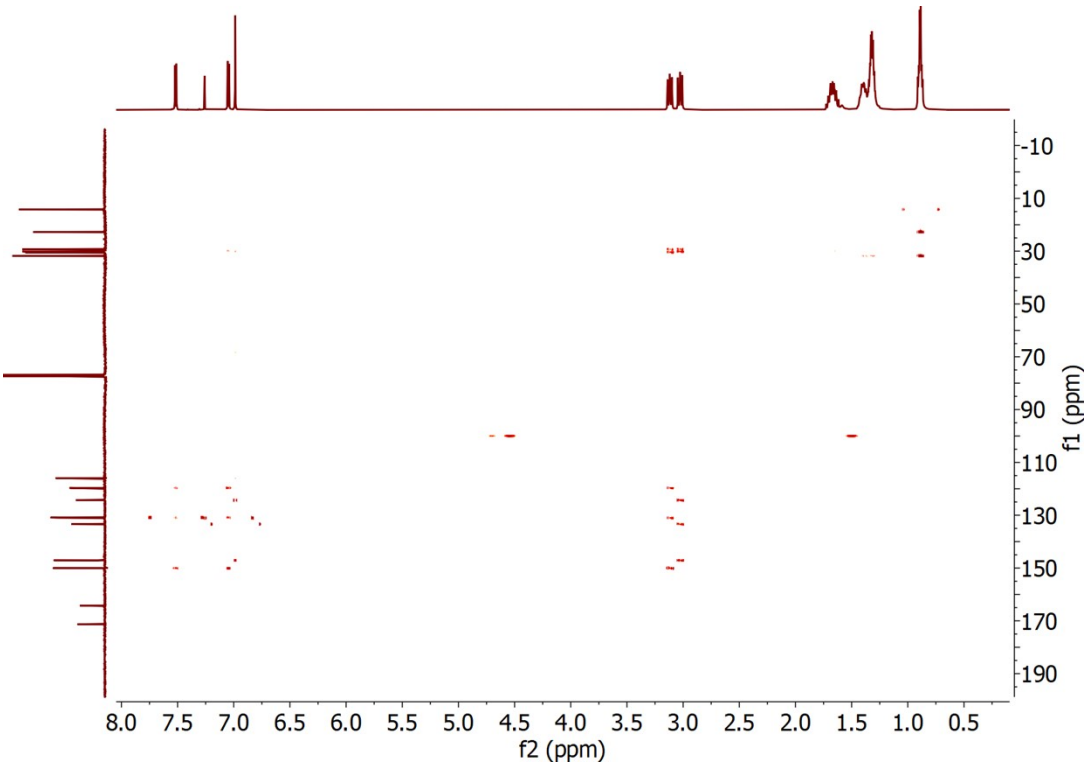


Figure S39. HMBC 2D NMR spectrum of 3HT-ODA-3HT-Br.

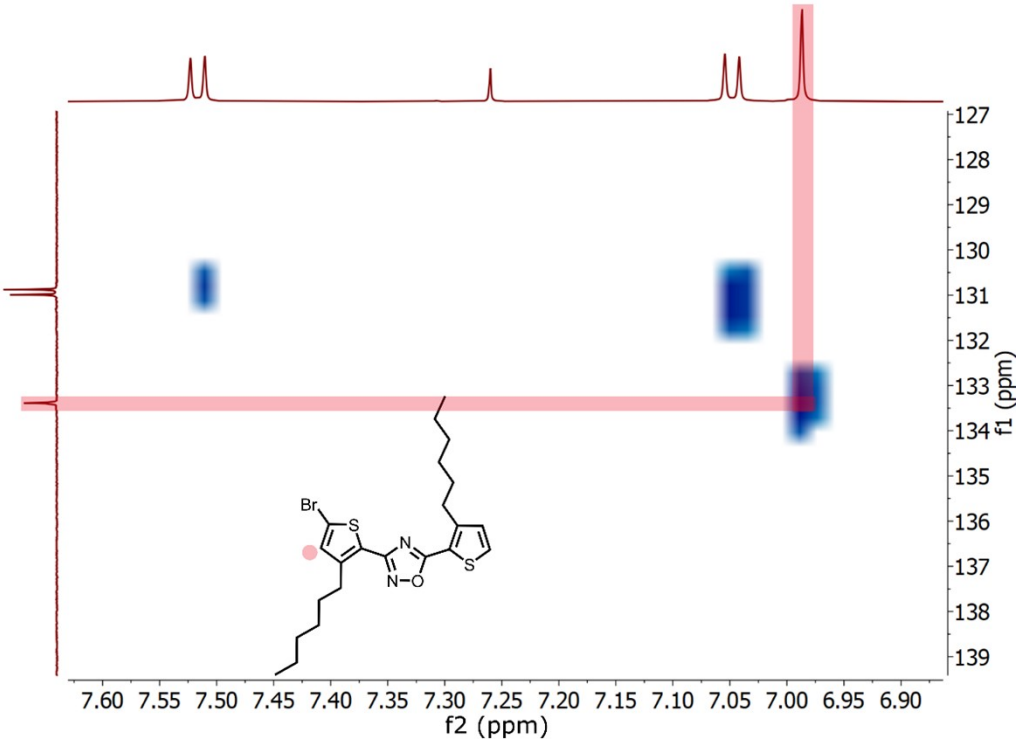


Figure S40. The aromatic region of the HSQC 2D NMR spectrum of 3HT-ODA-3HT-Br.

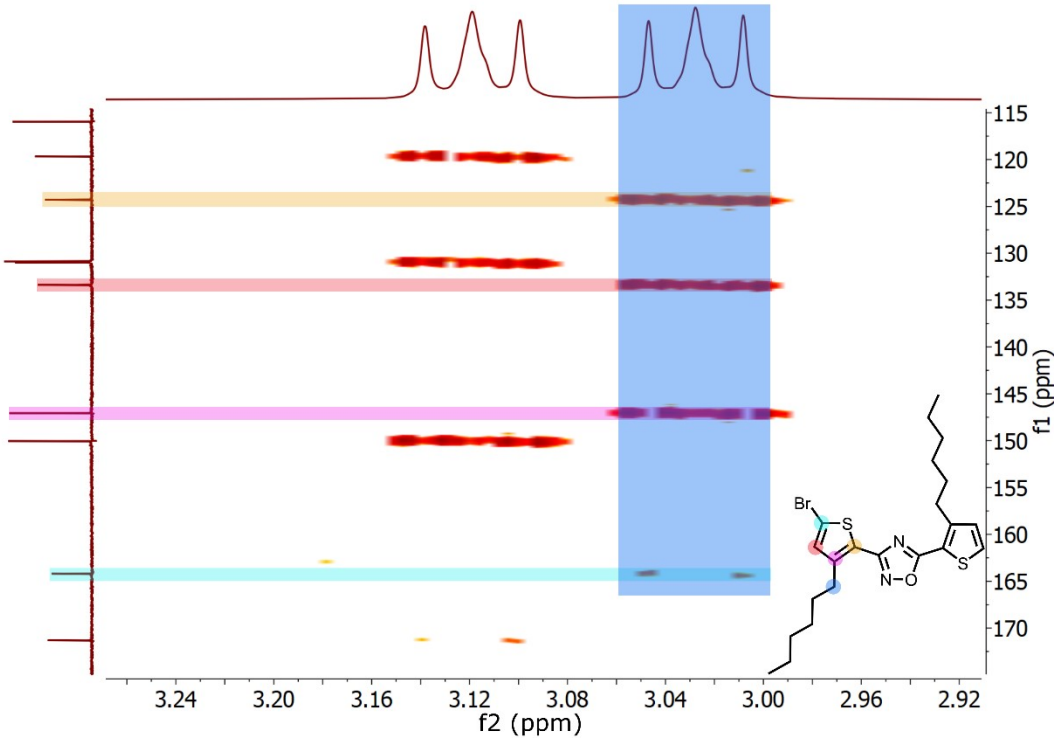


Figure S41. HMBC 2D NMR spectrum of 3HT-ODA-3HT-Br depicting the correlations between the carbon atoms in the brominated thiophene ring and the protons on the nearest methylene group.

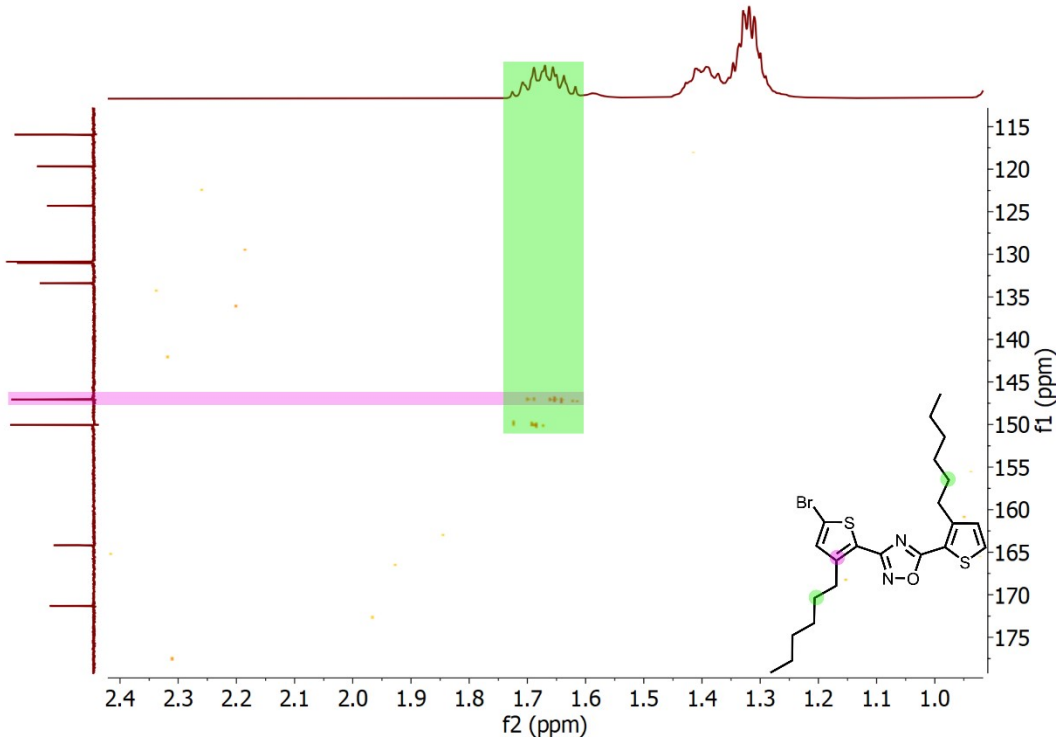


Figure S42. HMBC 2D NMR spectrum of 3HT-ODA-3HT-Br showing the correlation between the protons on the second methylene group in the hexyl chain and the nearest carbon atom on the brominated thiophene ring.

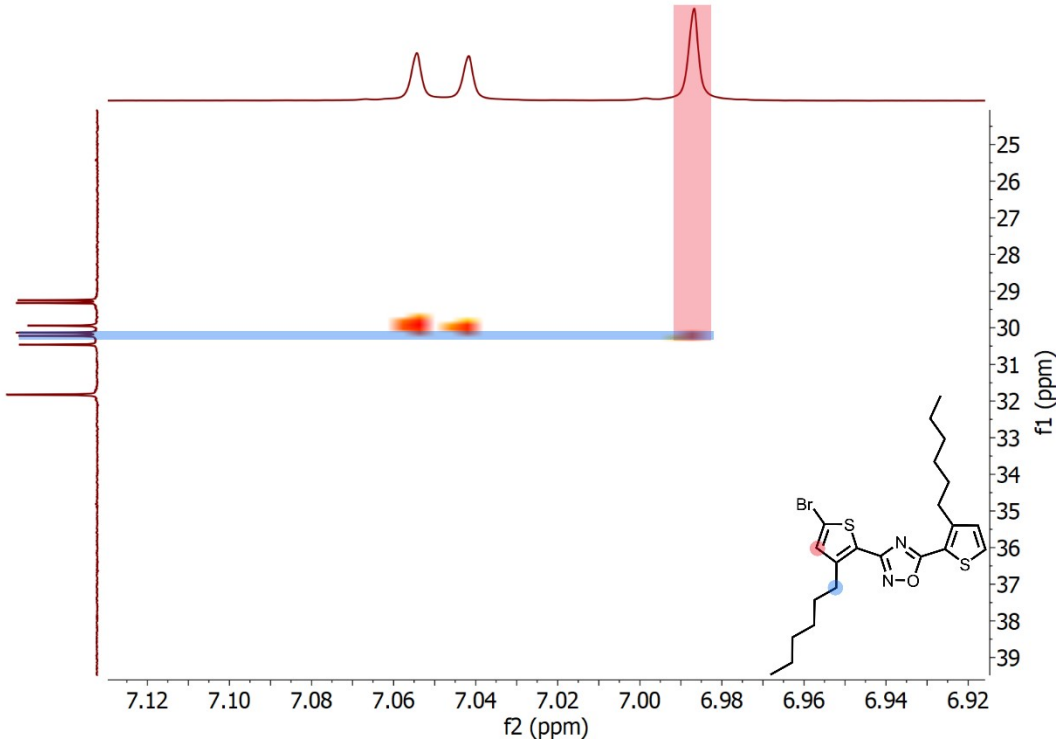


Figure S43. HMBC 2D NMR Spectrum of T-ODA-3DDT-Br showing the correlation between the aryl proton on the brominated thiophene ring and the first carbon atom in the hexyl chain.

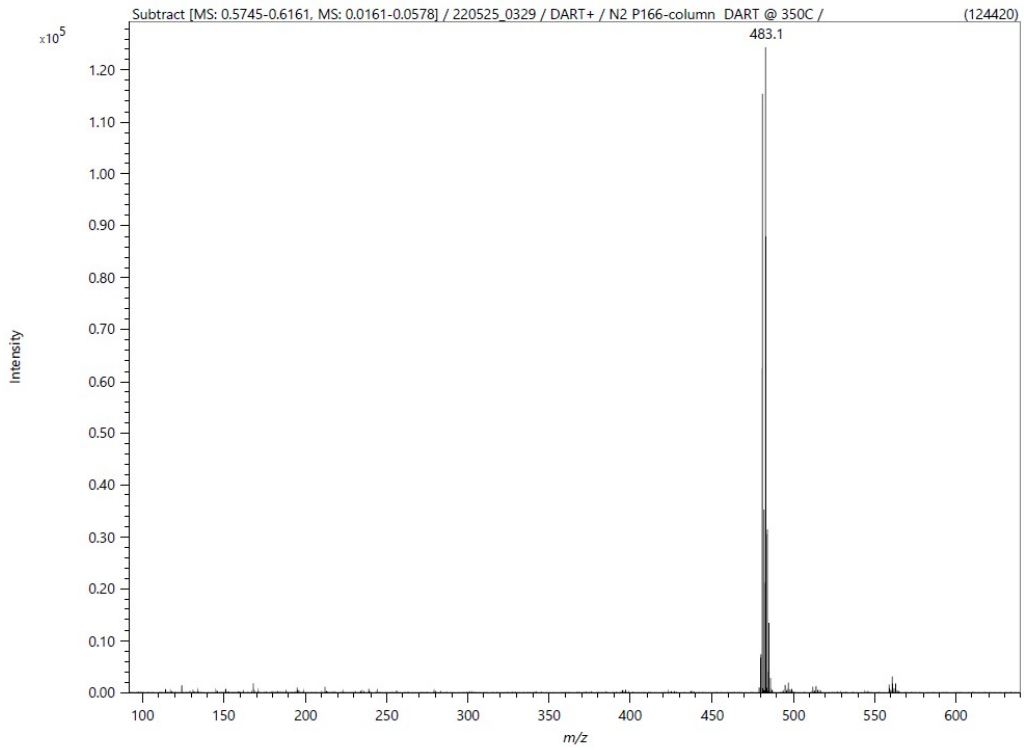


Figure S44. Mass spectrum (DART, positive mode) of 3-(5-bromo-3-hexylthiophen-2-yl)-5-(3-hexylthiophen-2-yl)-1,2,4-oxadiazole.

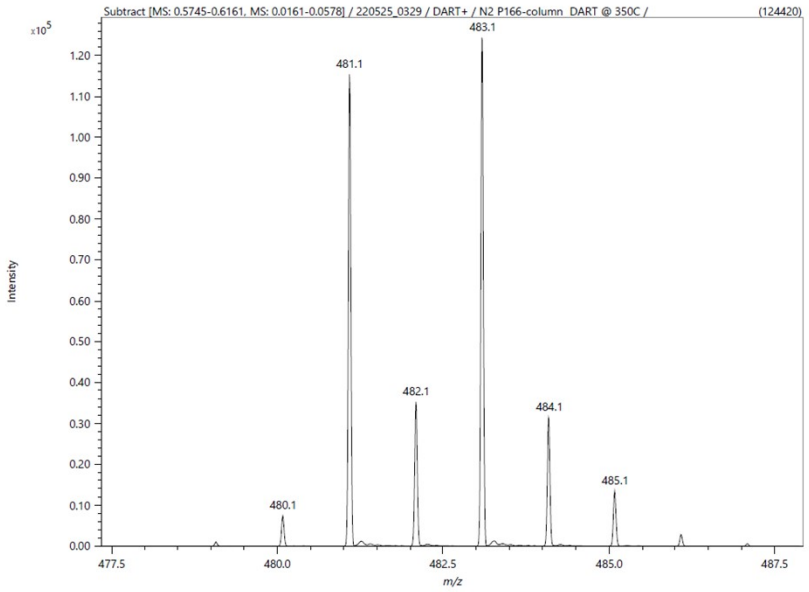
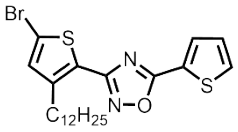


Figure S45. Isotopic splitting pattern in mass spectrum (DART, positive mode) of 3-(5-bromo-3-hexylthiophen-2-yl)-5-(3-hexylthiophen-2-yl)-1,2,4-oxadiazole.

Synthesis of 3-(5-bromo-3-dodecylthiophen-2-yl)-5-(thiophen-2-yl)-1,2,4-oxadiazole (N2P055)



N-bromosuccinimide (711.6 mg; 3.998 mmol) was added in one portion to a solution of 3-(3-dodecylthiophen-2-yl)-5-(thiophen-2-yl)-1,2,4-oxadiazole (852.2 mg; 1.997 mmol) dissolved in tetrahydrofuran (4.5 mL). The reaction mixture was covered from light and left to stir at room temperature for 20 hours. Following this period, the reaction mixture was heated to 50 °C for 2 hours. After cooling the reaction mixture back to room temperature, 25 mL of DI water was added. The solution was extracted with 40 mL diethyl ether, and the organic layer was washed with saturated $NaHCO_3$ solution (30 mL), DI water (30 mL), and finally brine (30 mL). The organic layer was dried over $MgSO_4$, filtered, and concentrated under vacuum. The crude product was purified by column chromatography (silica) using 15:1 hexanes:dichloromethane as the mobile phase to afford the product as a pale yellow oil that slowly formed colorless crystals (757.0 mg; 61%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.94 (dd, J = 3.8, 1.2 Hz, 1H), 7.66 (dd, J = 5.0, 1.2 Hz, 1H), 7.21 (dd, J = 5.0, 3.8 Hz, 1H), 6.99 (s, 1H), 3.01 (t, J = 7.7 Hz, 2H), 1.71 – 1.59 (m, 2H), 1.43 – 1.19 (m, 18H), 0.88 (t, J = 6.9 Hz, 3H). HRMS (DART-TOF): [M+H$^+$] calculated for $C_{22}H_{30}BrN_2OS_2$: 481.0977, found: 481.0973.

The position of the bromine was assigned using 2D NMR (HMBC and HSQC) following a similar method to 3HT-ODA-3HT-Br.

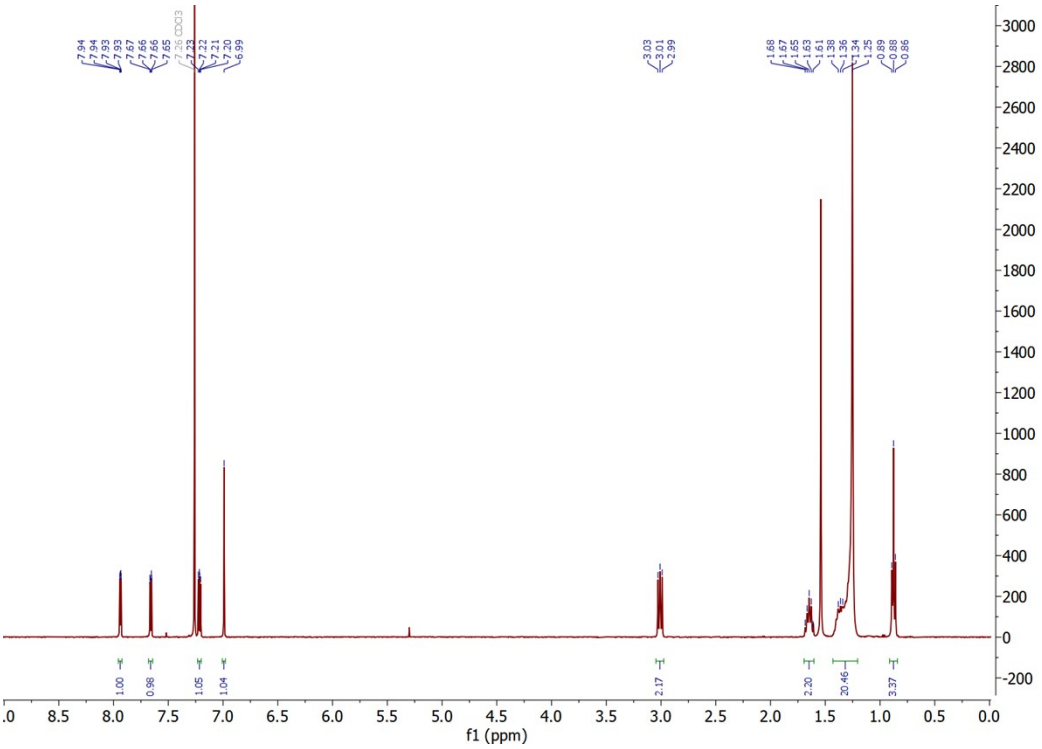


Figure S46. ^{1}H NMR spectrum (400 MHz) of 3-(5-bromo-3-dodecylthiophen-2-yl)-5-(thiophen-2-yl)-1,2,4-oxadiazole in $CDCl_3$.

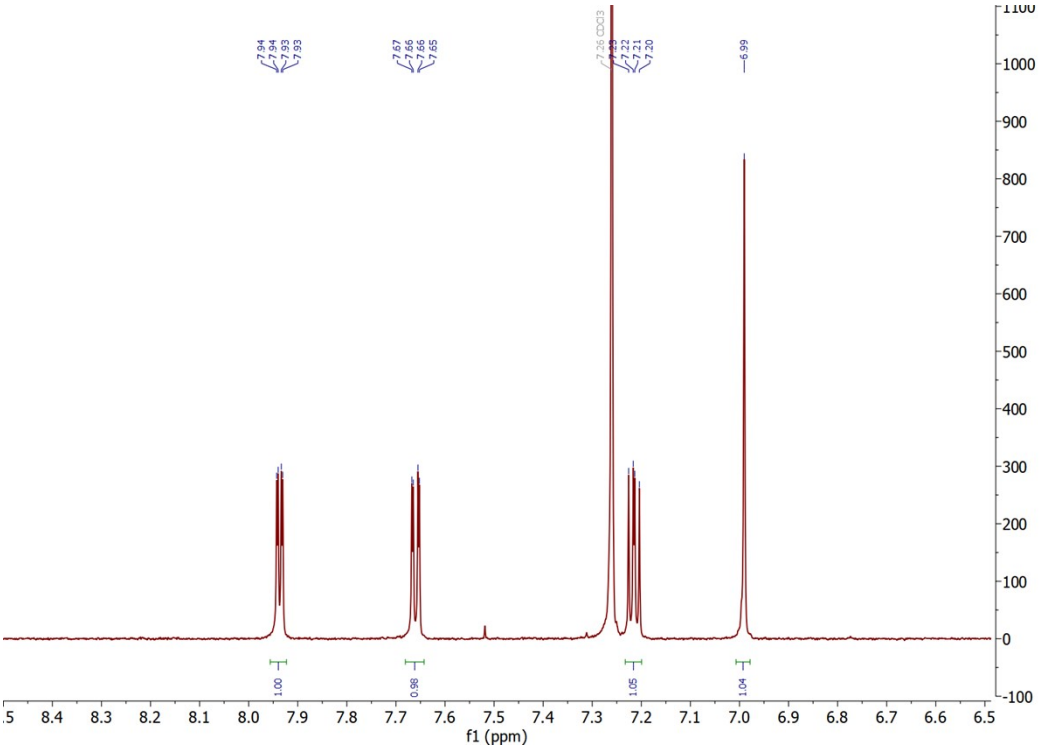


Figure S47. Aromatic region ^{1}H NMR spectrum (400 MHz) of 3-(5-bromo-3-dodecylthiophen-2-yl)-5-(thiophen-2-yl)-1,2,4-oxadiazole in $CDCl_3$.

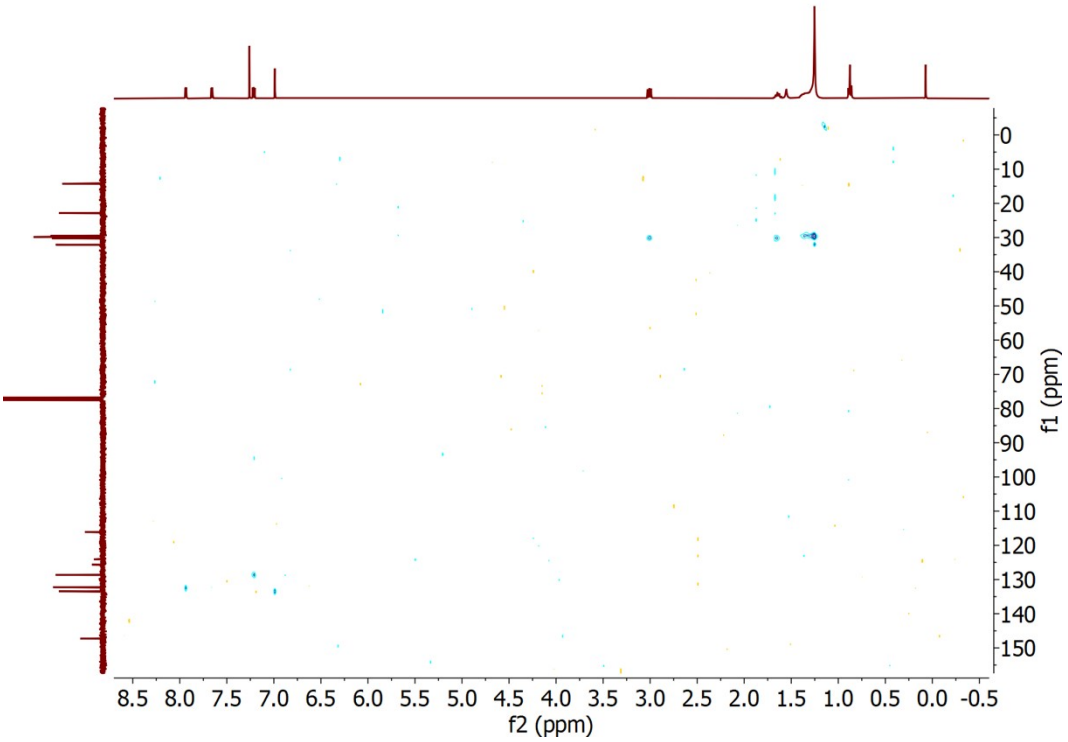


Figure S48**.** HSQC 2D NMR spectrum of T-ODA-3DDT-Br.

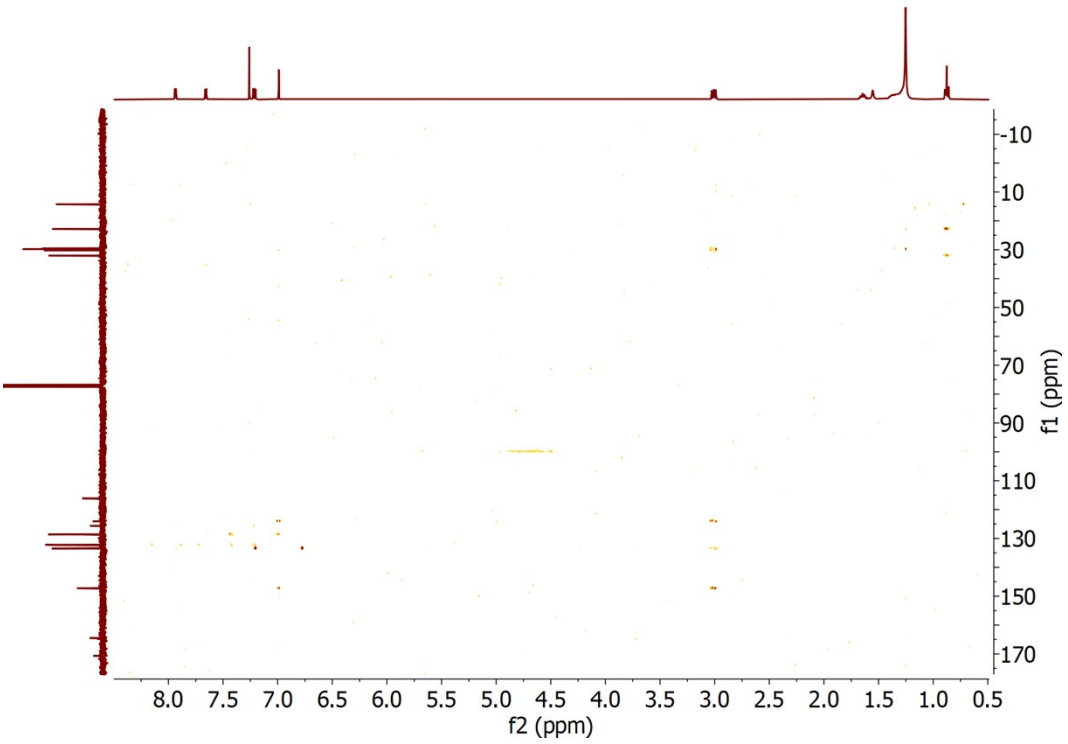


Figure S49**.** HMBC 2D NMR spectrum of T-ODA-3DDT-Br.

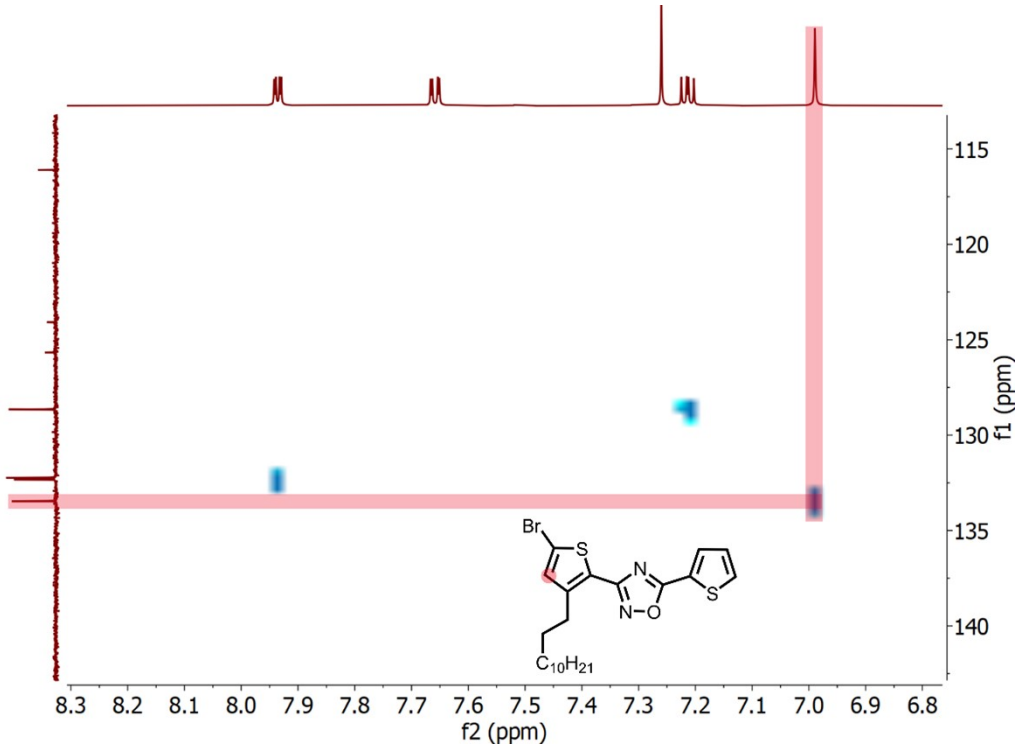


Figure S50. HSQC 2D NMR spectrum of T-ODA-3DDT-Br showing the correlation between the proton on the brominated thiophene ring and the carbon it is bound to.

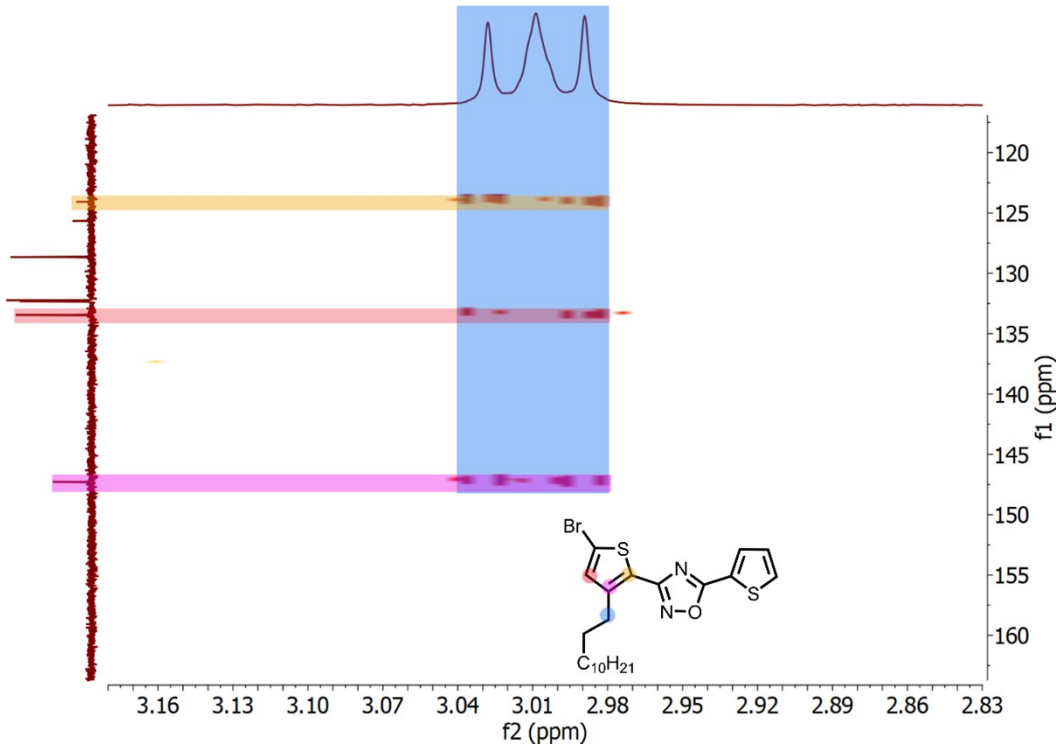


Figure S51. HMBC 2D NMR spectrum of T-ODA-3DDT-Br showing correlations between the carbons in the brominated thiophene ring and the protons on the nearest methylene group.

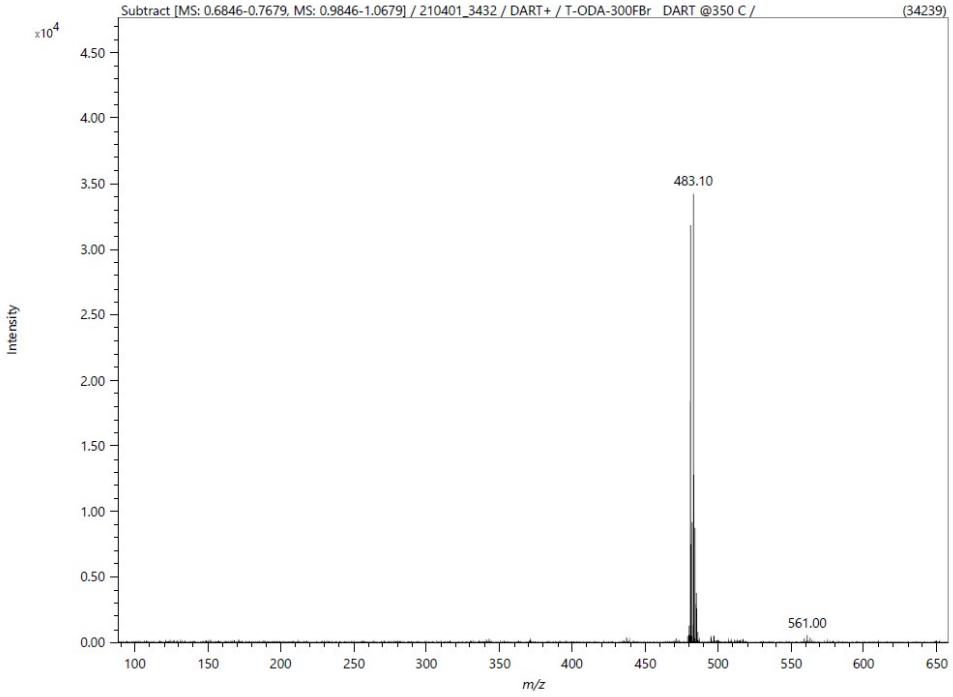


Figure S52. Mass spectrum (DART, positive mode) of 3-(5-bromo-3-dodecylthiophen-2-yl)-5-(thiophen-2-yl)-1,2,4-oxadiazole.

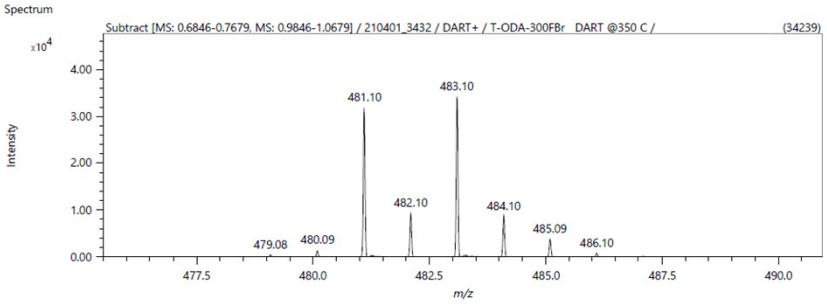
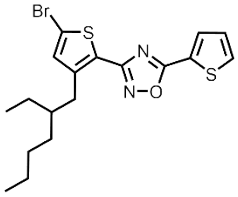


Figure S53. Isotopic splitting pattern in mass spectrum (DART, positive mode) of 3-(5-bromo-3-dodecylthiophen-2-yl)-5-(thiophen-2-yl)-1,2,4-oxadiazole.

Synthesis of 3-(5-bromo-3-(2-ethylhexyl)thiophen-2-yl)-5-(thiophen-2-yl)-1,2,4-oxadiazole



N-bromosuccinimide (286 mg; 0.825 mmol) was added in one portion to a solution of 3-(3-(2-ethylhexyl)thiophen-2-yl)-5-(thiophen-2-yl)-1,2,4-oxadiazole (286 mg; 0.825 mmol) dissolved in tetrahydrofuran (4.5 mL). The reaction mixture was covered from light and left to stir at room temperature for 20 hours. Following this period, the reaction mixture was heated to 50 °C for 2 hours. After cooling the reaction mixture back to room temperature, 25 mL of DI water was added. The solution was extracted with 40 mL diethyl ether, and the organic layer was washed with saturated $NaHCO_3$ solution (30 mL), DI water (30 mL), and finally brine (30 mL). The organic layer was dried over $MgSO_4$, filtered, and concentrated under vacuum. The crude product was purified by column chromatography (silica) using 15:1 hexanes:dichloromethane as the mobile phase to afford the product as a pale yellow oil (757.0 mg; 61%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.93 (dd, J = 3.8, 1.1 Hz, 1H), 7.66 (dd, J = 5.0, 1.1 Hz, 1H), 7.21 (dd, J = 5.0, 3.8 Hz, 1H), 6.96 (s, 1H), 2.97 (d, J = 7.2 Hz, 2H), 1.74 – 1.63 (m, 1H), 1.40 – 1.22 (m, 8H), 0.94 – 0.81 (m, 6H). HRMS (DART-TOF): [M+H$^+$] calculated for $C_{18}H_{22}BrN_2OS_2$: 425.04, found: 425.03.

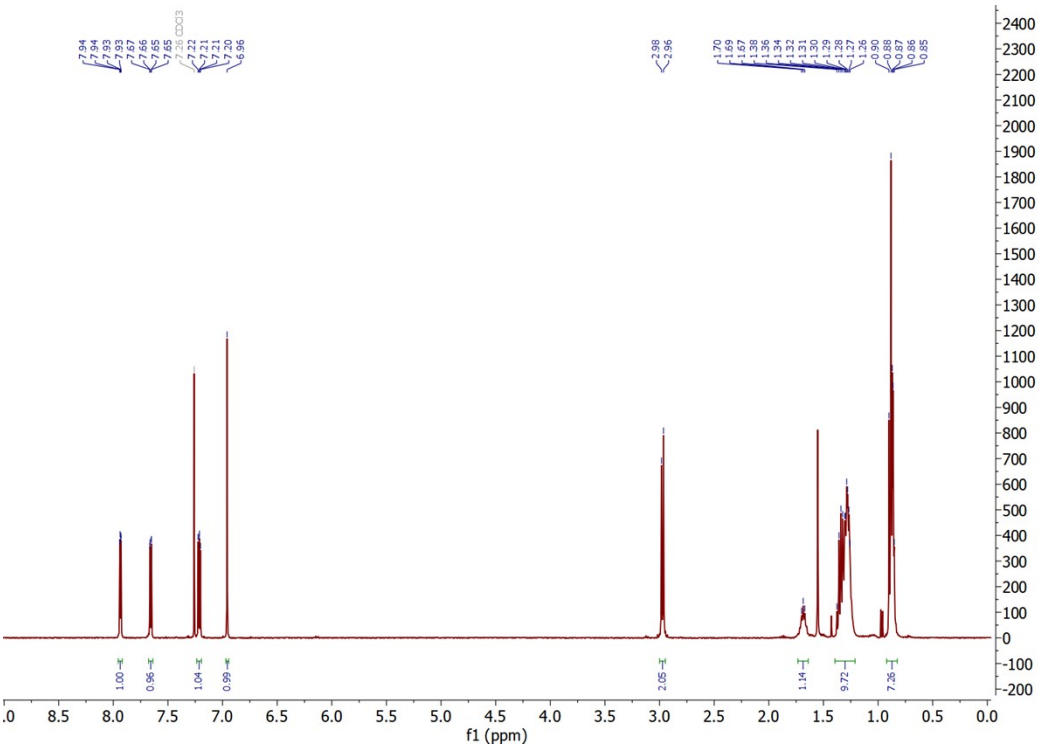


Figure S54. ^{1}H NMR spectrum (400 MHz) of 3-(5-bromo-3-(2-ethylhexyl)thiophen-2-yl)-5-(thiophen-2-yl)-1,2,4-oxadiazole in $CDCl_3$.

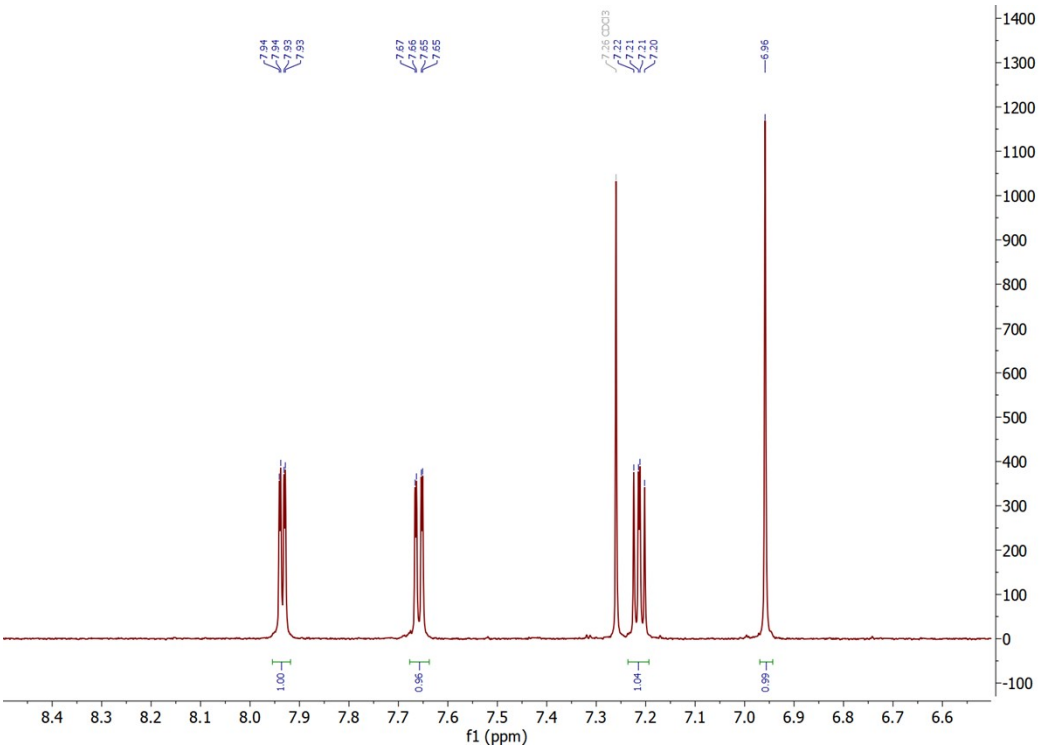


Figure S55. Aromatic region of ^{1}H NMR spectrum (400 MHz) of 3-(5-bromo-3-(2-ethylhexyl)thiophen-2-yl)-5-(thiophen-2-yl)-1,2,4-oxadiazole in $CDCl_3$.

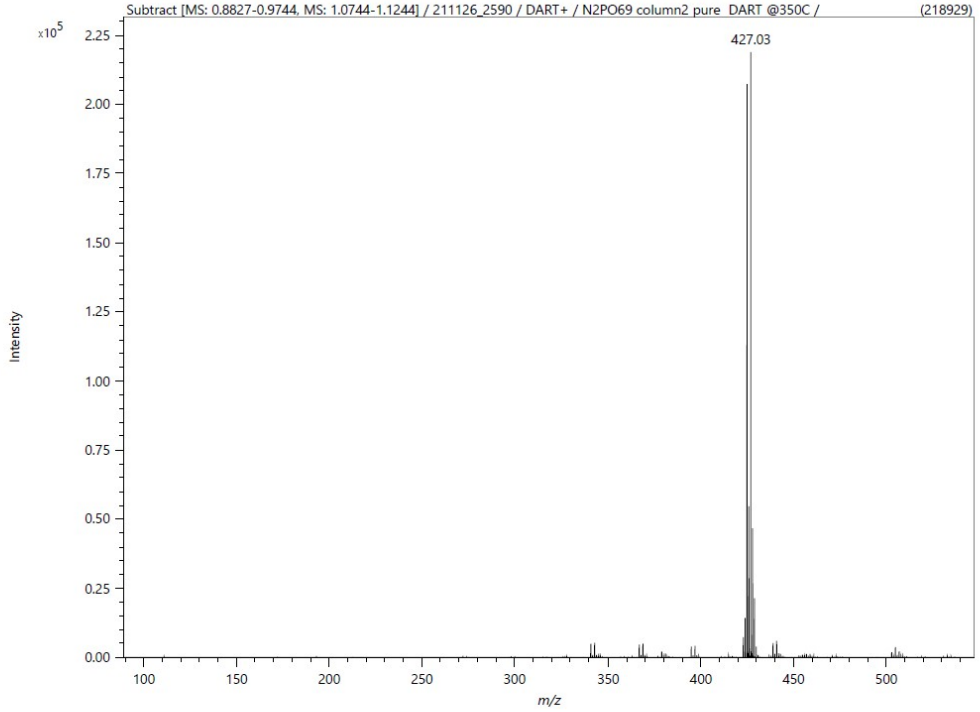


Figure S56. Mass spectrum (DART, positive mode) of 3-(5-bromo-3-(2-ethylhexyl)thiophen-2-yl)-5-(thiophen-2-yl)-1,2,4-oxadiazole.

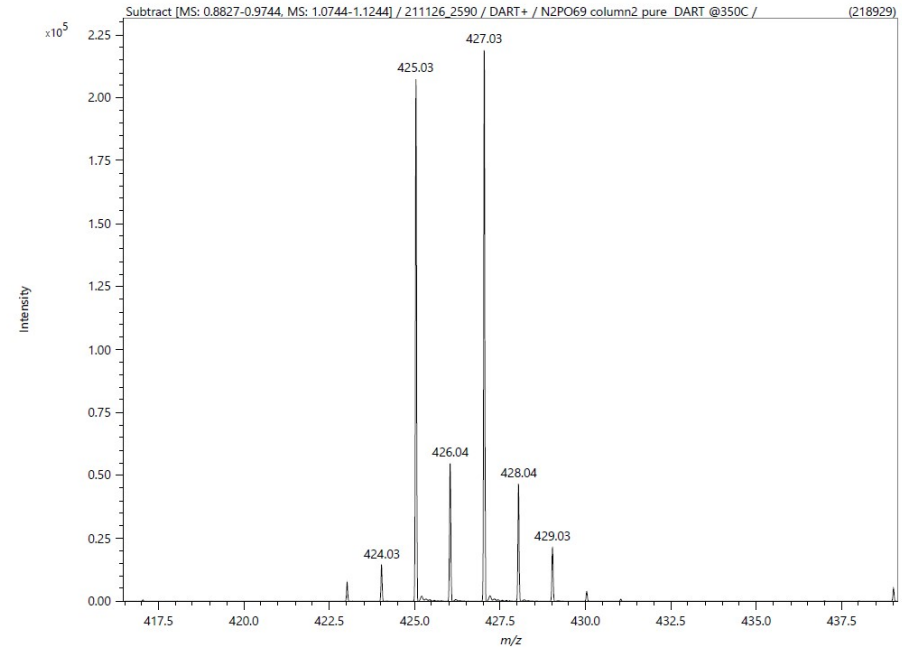


Figure S57. Isotopic splitting pattern in mass spectrum (DART, positive mode) of 3-(5-bromo-3-(2-ethylhexyl)thiophen-2-yl)-5-(thiophen-2-yl)-1,2,4-oxadiazole.

A Note on the Bromination of the Monomers

Several sets of conditions were tested for brominating 3HT-ODA-3HT (**Figure S58**). The reaction is slow at room temperature, but biproducts are not observed by TLC. The approach of holding the reaction at room temperature for a long period followed by a short period of heating is believed to slightly lower the amount of biproducts generated while still allowing the reaction to be completed in a timely manner. The other biproducts observed are regioisomers of the mono/dibrominated products.

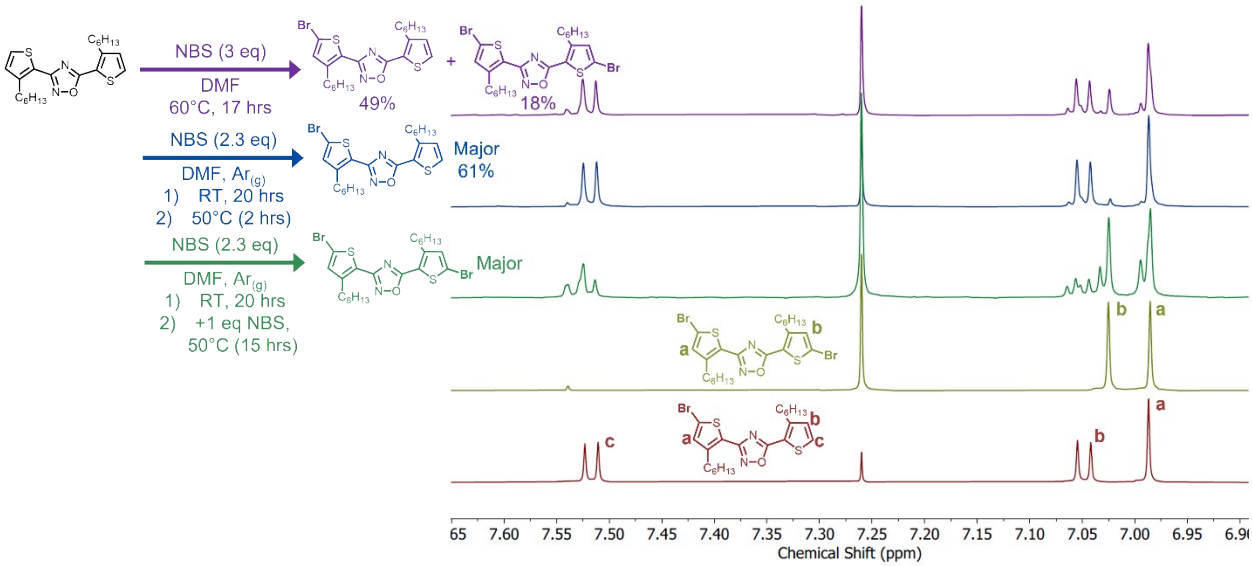
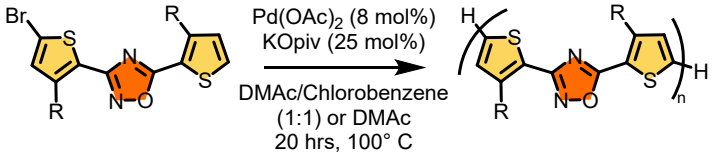


Figure S58. ^{1}H NMR spectra ($CHCl_3$; 500 MHz) of the crude products from bromination attempts using several sets of bromination conditions. The yellow and red spectra are of the isolated dibrominated and isolated monobrominated products respectively.

Polymer Synthesis

Phosphine-Free DHAP



Phosphine-Free DHAP of T-ODA-3DDT-Br

A 2 mL microwave vial was loaded with T-ODA-3DDT-Br (96.4 mg; 0.200 mmol), PivOK (43.7 mg; 0.312 mmol), $Pd(OAc)_2$ (3.7 mg; 0.016 mmol), anhydrous N,N-dimethylacetamide (1 mL) and chlorobenzene (1 mL). The vial was sealed and sparged with stirring for 30 minutes. The vial was lowered into a 100 °C

preheated oil bath and was heated for 22 hours. After cooling to room temperature, the vial was unsealed and a few mL of tetrahydrofuran were added. The reaction mixture was precipitated into stirring methanol (100 mL). The resulting suspension was centrifuged and the pellets were collected by filtration, rinsing with additional methanol. The polymer was purified by Soxhlet extractions with acetone, methanol, hexanes, and finally chloroform to collect the polymer. The chloroform fraction was concentrated under vacuum, precipitated into stirring acetone, and then filtered to afford the polymer as a yellow solid (20.6 mg; 26%). TCB GPC (140 °C): M_W = 7200, M_N = 3800, Đ = 1.9.

A further Soxhlet extraction with chlorobenzene yielded an additional 16.3 mg (20%) of brown solid.

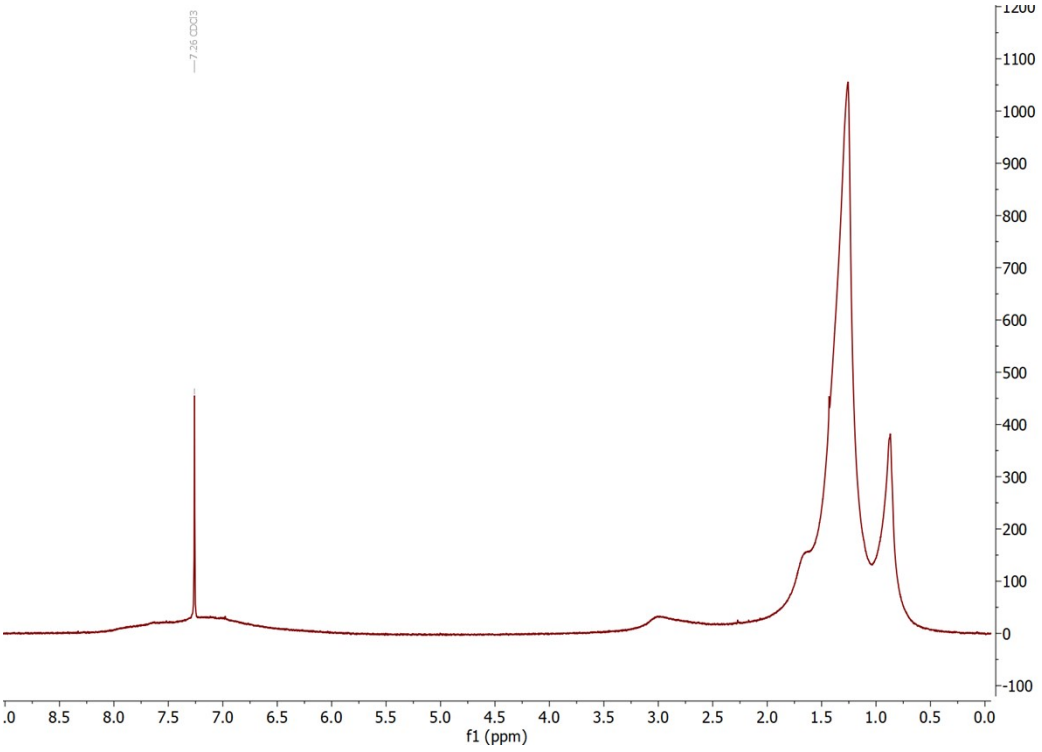


Figure S59. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of P(T-ODA-3DDT) synthesized by phosphine-free DHAP conditions.

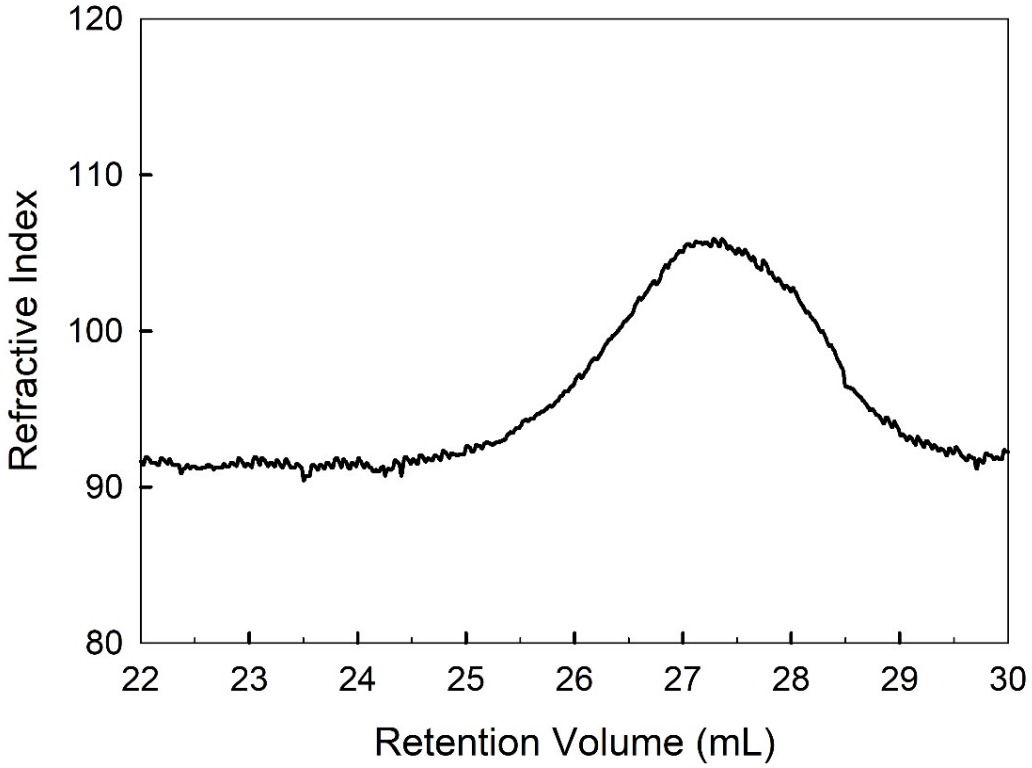


Figure S60. GPC trace (1,2,4-trichlorobenzene, 140 °C) of P(T-ODA-3DDT) synthesized by phosphine-free DHAP conditions.

Phosphine-Free DHAP of T-ODA-3EHT-Br

T-ODA-3EHT-Br was synthesized using a similar method as the phosphine-free DHAP of T-ODA-3DDT-Br, starting with 69.2 mg (0.163 mmol) of monomer. The chloroform Soxhlet extraction yielded 0.3 mg of yellow solid, and the chlorobenzene Soxhlet extraction yielded 0.6 mg of yellow solid (1.6% yield combined). A large amount of light brown solid remained in the Soxhlet thimble after the final chlorobenzene extraction.

Phosphine-Free DHAP of 3HT-ODA-3HT-Br

A 2 mL microwave vial was loaded with 3HT-ODA-3HT-Br (96.4 mg; 0.200 mmol), PivOK (43.9 mg; 0.313 mmol), $Pd(OAc)_2$ (3.6 mg; 0.016 mmol). The vial was sealed and the contents were put under an atmosphere of argon. Anhydrous N,N-dimethylacetamide (2 mL) was added by syringe, and the reaction mixture was stirred at room temperature for 30 minutes. After this period, the vial was submerged in a 100°C preheated oil bath for 22 hours. After cooling to room temperature, the vial was unsealed and a few mL of chloroform were added to redissolve the contents. The reaction mixture was precipitated into stirring methanol (200 mL) acidified with a few drops of concentrated HCl. The resulting precipitate was collected by filtration and was purified by Soxhlet extractions with acetone, methanol, hexanes, and finally

chloroform to collect the polymer. The chloroform fraction was concentrated under vacuum, precipitated into stirring MeOH, and then filtered to afford the polymer as a brown solid (30.6 mg; 38%). THF GPC (40 °C): M_W = 9600, M_N = 5200, Đ = 1.8.

A further Soxhlet extraction with chlorobenzene yielded an additional 21.7 mg (27%) of dark orange-brown solid.

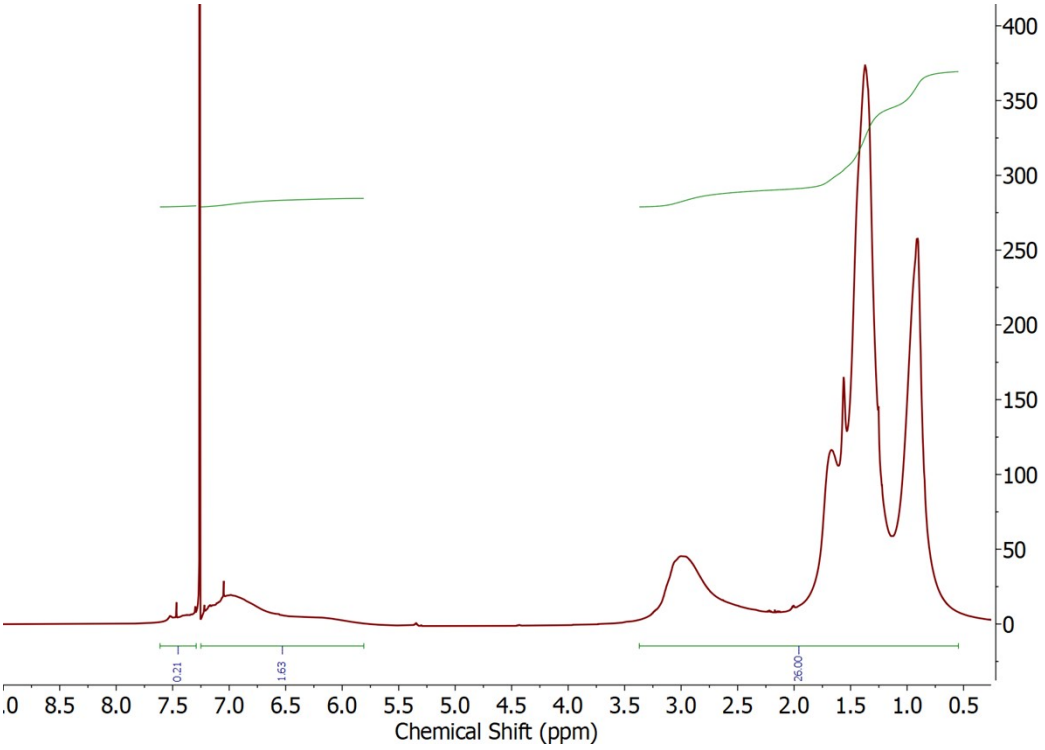


Figure S61. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of P(3HT-ODA-3HT) synthesized by phosphine-free DHAP conditions.

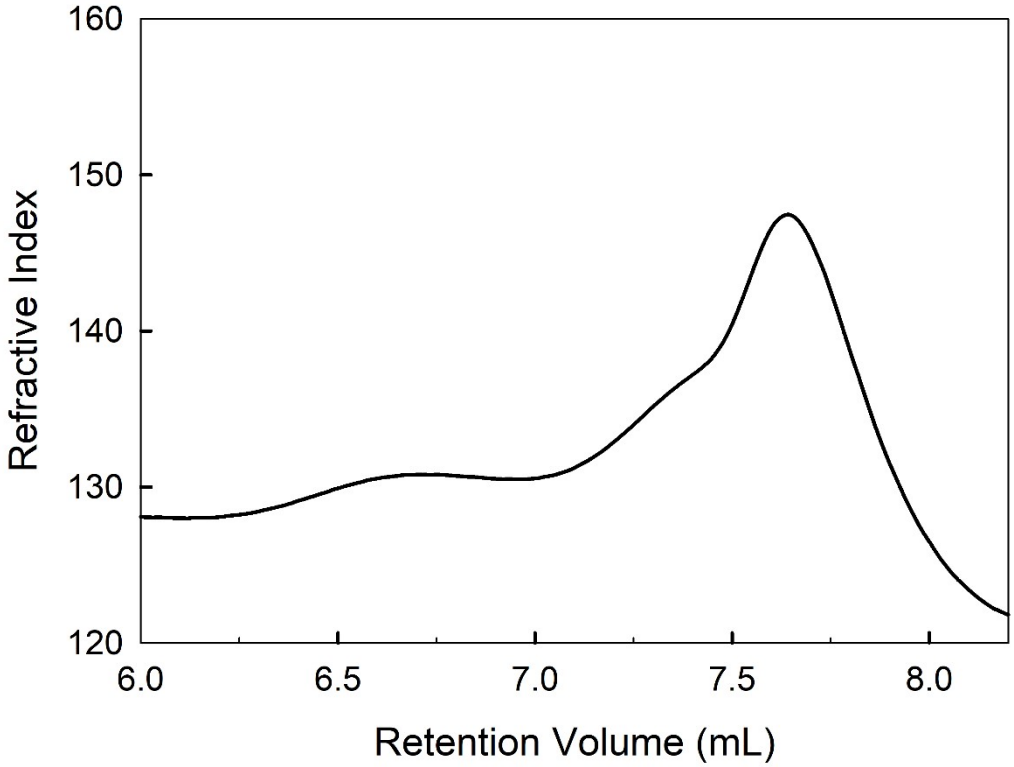
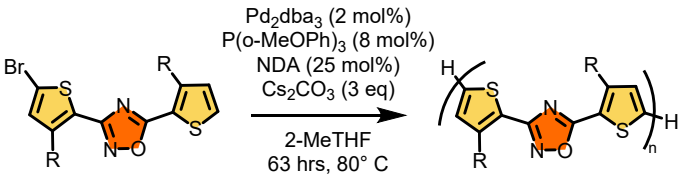


Figure S62. GPC trace (THF, 40 °C) of P(3HT-ODA-3HT) synthesized by phosphine-free DHAP conditions.

Branching-Suppressing DHAP



Branching-Suppressing DHAP of T-ODA-3DDT-Br

A 2 mL microwave vial was loaded with a stir bar, T-ODA-3DDT-Br (48.3 mg; 0.100 mmol), $Pd_2(dba)_3$ (1.8 mg, 0.0020 mmol), P(o-MeOPh)$_3$ (2.8 mg, 0.0079 mmol), and Cs_2CO_3 (98.0 mg; 0.301 mmol). The vial was sealed and vacuum/argon cycled 3 times. Neo-decanoic acid (0.005 mL; 0.03 mmol), and anhydrous 2-methyltetrahydrofuran (2.0 mL) were added to the vial by syringe. The vial was lowered into an 85 °C pre-heated oil bath and was left heating for 63 hours. After cooling to room temperature, the vial was unsealed and the reaction mixture was poured into a beaker with tetrahydrofuran (15 mL). The resulting solution was precipitated into a solution of MeOH (120 mL) and dilute HCl (5%, 20 mL). The precipitate was collected by filtration and was purified by Soxhlet extraction with methanol, hexanes, and finally collected with chloroform. The chloroform fraction was concentrated under vacuum to afford the product as a yellow solid (6.5 mg; 16%). THF GPC (40 °C): M_W = 4500, M_N = 3800, Đ = 1.2.

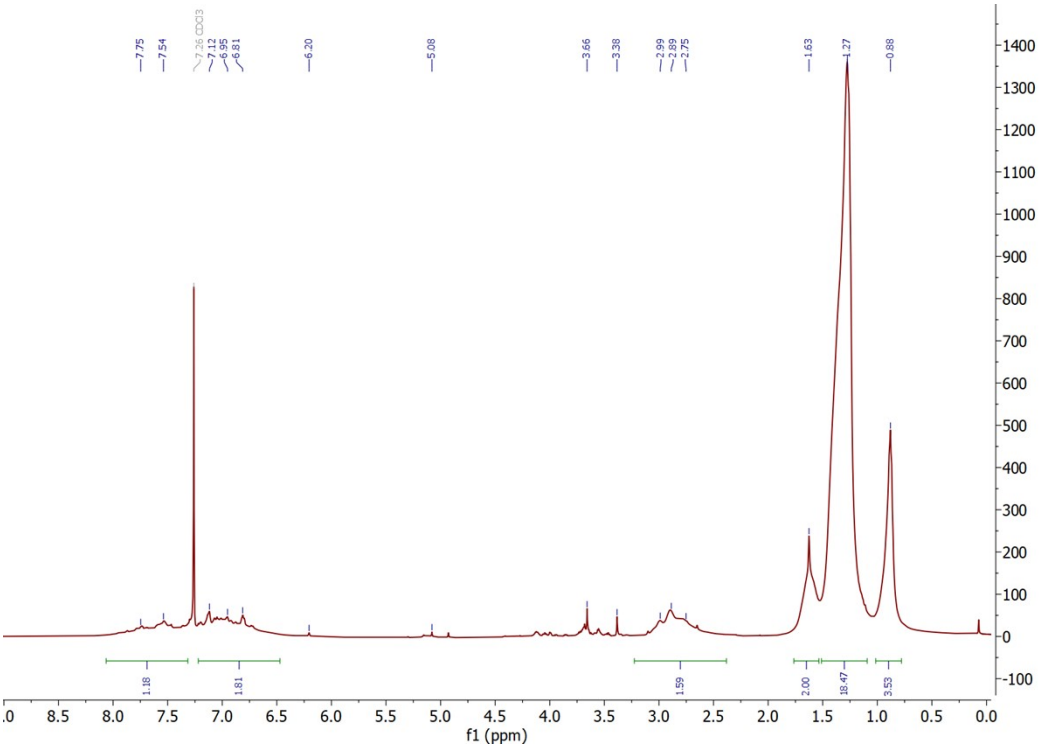


Figure S63. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of P(T-ODA-3DDT) synthesized by branching-suppressing DHAP conditions.

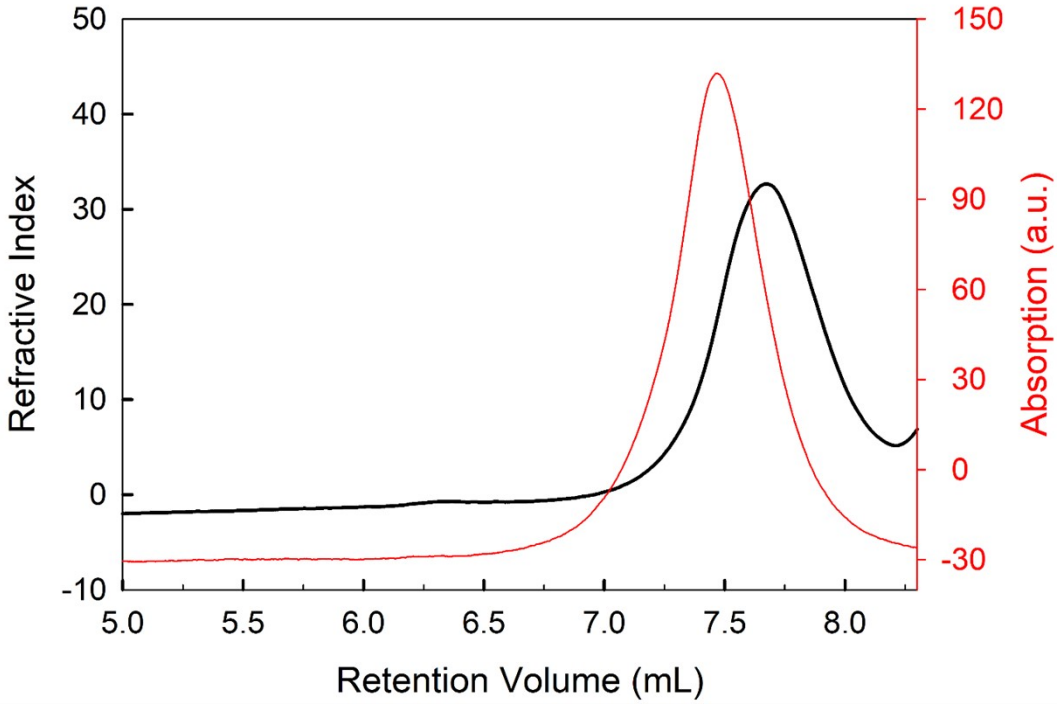


Figure S64. GPC trace (tetrahydrofuran, 40 °C) of P(T-ODA-3DDT) synthesized by branching suppressing DHAP.

Branching-Suppressing DHAP of 3HT-ODA-3HT-Br

Identical conditions to the branching-suppressing DHAP of T-ODA-3DDT-Br were used to polymerize T-ODA-3DDT-Br (48.1 mg; 0.0999 mmol). The product was obtained as a yellow solid (8.7 mg; 22%) from the chloroform extract. THF GPC (40 °C): M_W = 4500, M_N = 3700, Đ = 1.2.

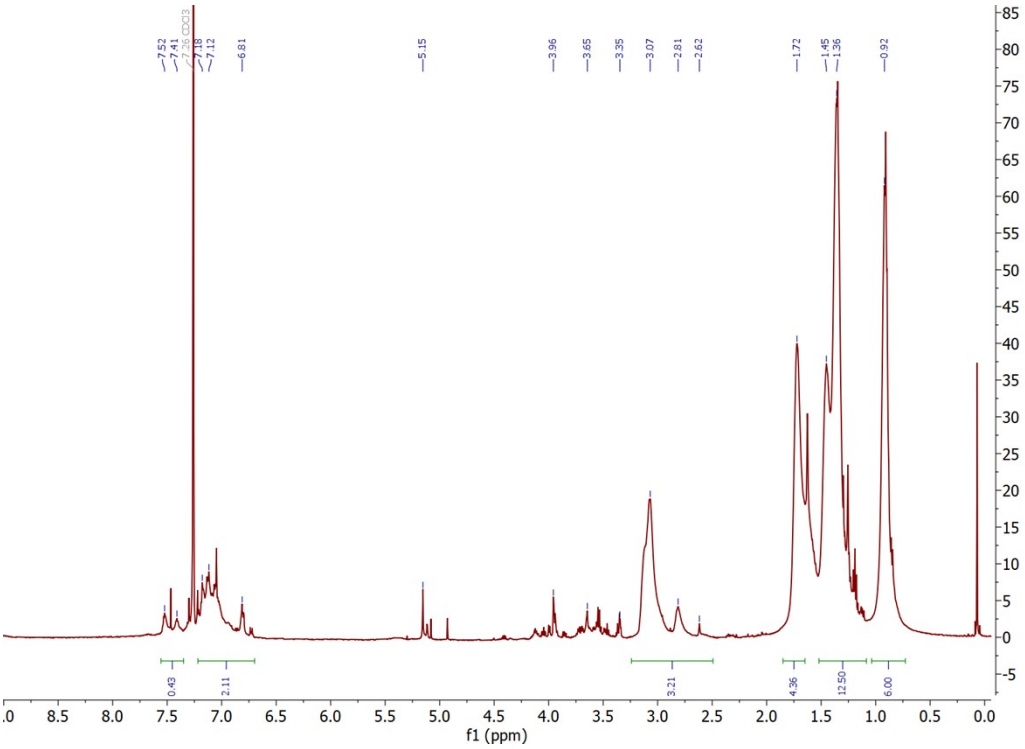


Figure S65. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of P(3HT-ODA-3HT) synthesized by branching-suppressing DHAP.

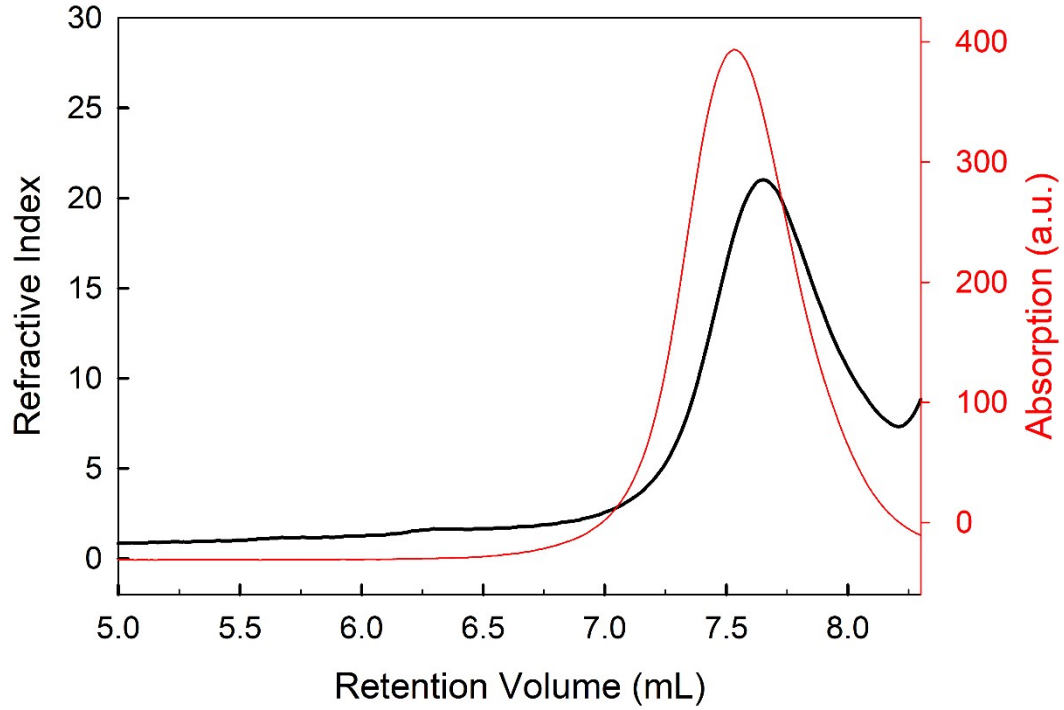


Figure S66. GPC trace (tetrahydrofuran, 40 °C) of P(3HT-ODA-3HT) synthesized by branching-suppressing DHAP.

MALDI-TOF of P(T-ODA-3DDT) Using a Dithranol Matrix

A MALDI-TOF spectrum of the hexanes Soxhlet extract of **P(T-ODA-3DDT)** was collected using the same conditions described above, except dithranol was used as the matrix instead of DCTB. The laser intensity required to get a spectrum was much higher for the dithranol sample than for the DCTB sample, so the additional low intensity peaks observed in the spectrum of the dithranol sample are likely due to additional degradation/fragmentation.

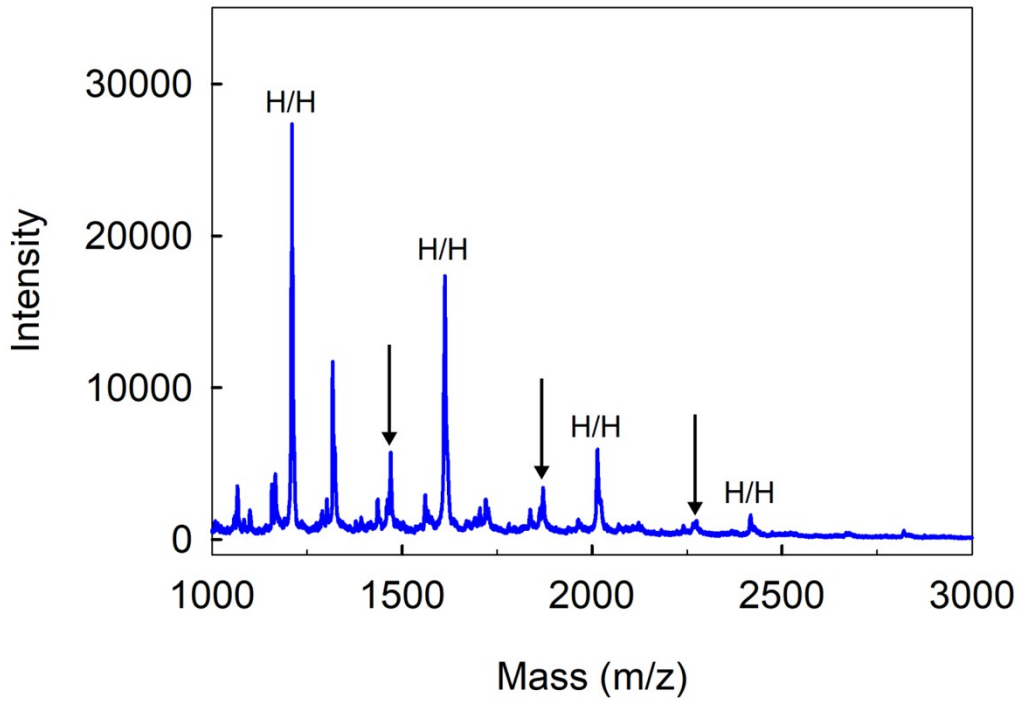


Figure S67. MALDI-TOF mass spectrum of the hexanes Soxhlet fraction of P(T-ODA-3DDT) using a dithranol matrix. The arrows indicate the positions of peaks corresponding to H/H + 250 (mass of polymer with H/H end groups plus 250).

Relative Quantum Yield Calculations for Polymers

Quantum yields were calculated using the relative method.[2] Quinine sulfate in 0.5 M H_2SO_4 was used as the reference (Φ = 0.546).[3]

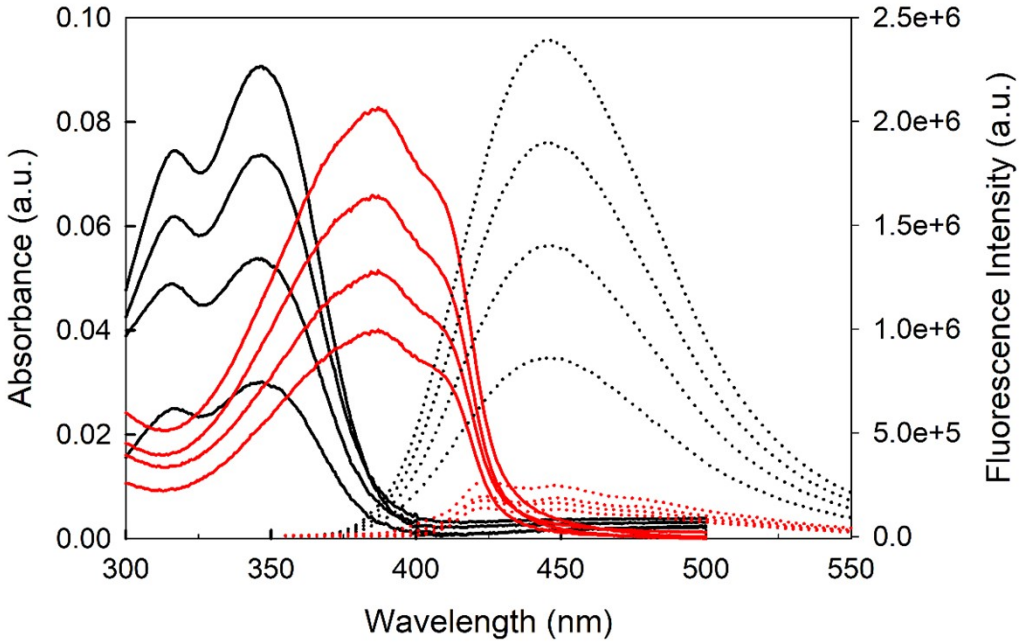


Figure S68. Absorption (solid lines) and photoluminescence (dotted lines) spectra of P(T-ODA-3DDT) in chloroform (red) and quinine sulfate in 0.5 M H_2SO_4 (black) used for the determination of the quantum yield. Excitation at 340 nm.

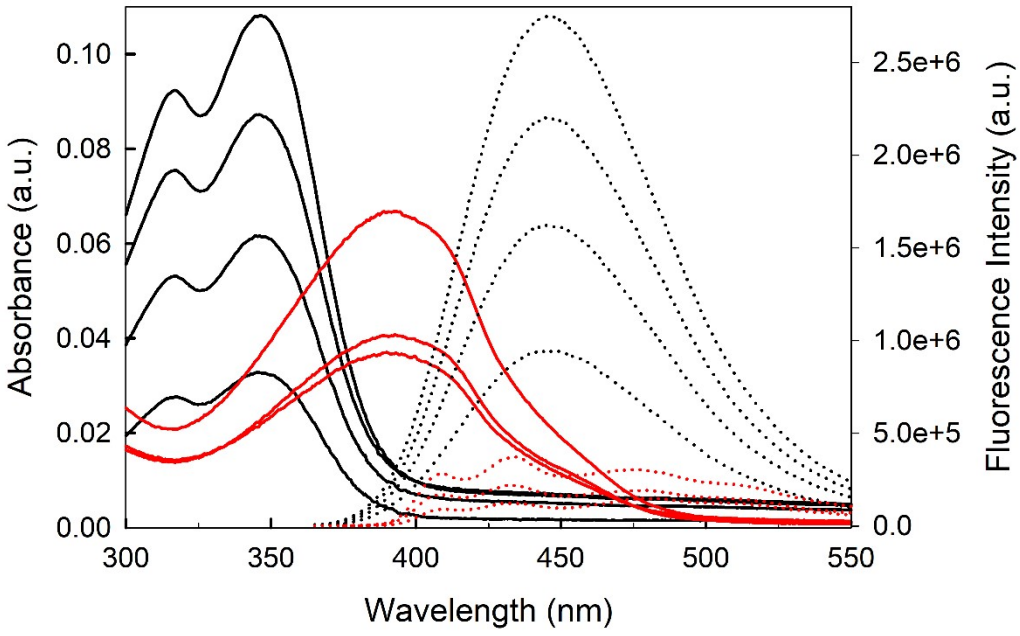


Figure S69. Absorption (solid lines) and photoluminescence (dotted lines) spectra of P(3HT-ODA-3HT) in chloroform (red) and quinine sulfate in 0.5 M H_2SO_4 (black) used for the determination of the quantum yield. Excitation at 350 nm.

Polymer Degradation Study

A solution of **P(3HT-ODA-3HT)** (10 mg; 0.025 mmol; synthesized from phosphine-free DHAP conditions) in THF (10 mL) under an atmosphere of argon was cooled in an ice bath and $LiAlH_4$ (4 mg; 0.1 mmol) was added. The reaction mixture was allowed to warm to room temperature and was then heated to a reflux for 17 hours. After this period, the reaction mixture was cooled in an ice bath and 5 mL of water was added dropwise. The resulting mixture was removed from the ice bath and stirred at room temperature for 20 minutes. The reaction mixture was then concentrated under vacuum, redissolved in 25 mL of chloroform, and washed 3x with 20 mL of water. The chloroform fraction was dried over $MgSO_4$, filtered, and concentrated under vacuum to yield a yellow sticky solid (12 mg).

The crude product from the above reduction (9.8 mg) was dissolved into a minimal amount of chloroform and the resulting solution was rapidly precipitated into a stirring 5 mL solution of water/ethanol (1:1), acidified with a few drops of concentrated HCl. A few drops of THF were added and the resulting mixture was refluxed for 17 hours. After cooling to room temperature, the reaction mixture was neutralized with $NaHCO_3$ and extracted with 25 mL $CHCl_3$. The extract was washed with water (3 x 20 mL), dried over $MgSO_4$, filtered, and concentrated under vacuum to yield a yellow solid (7.9 mg).

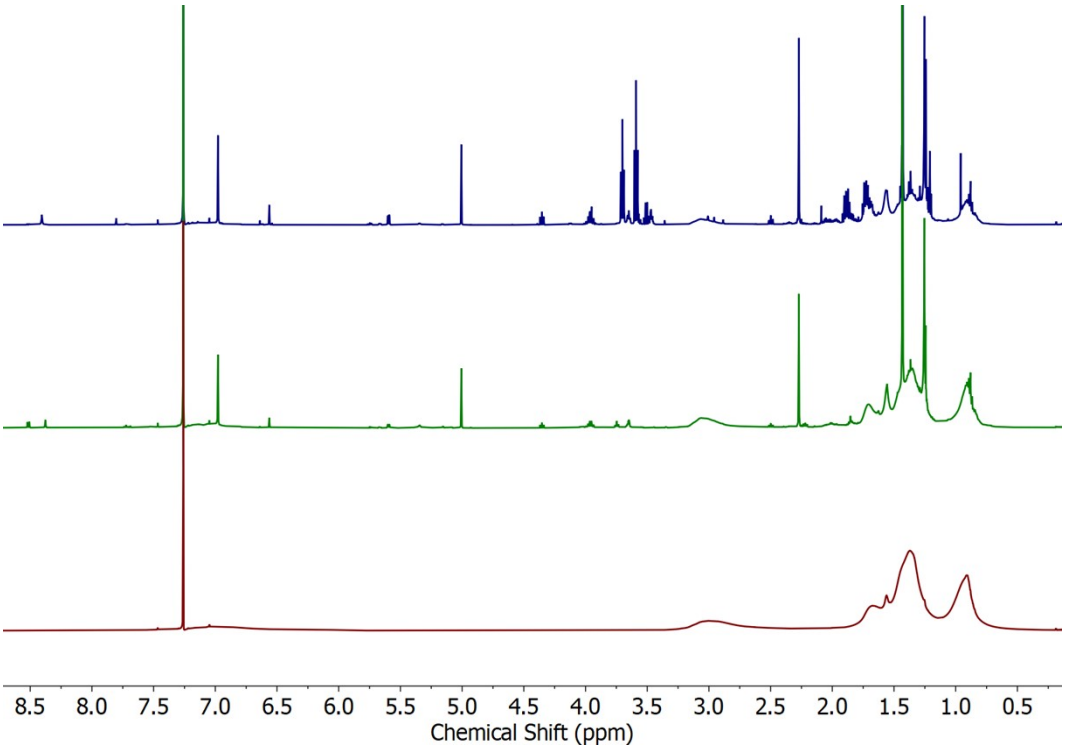


Figure S70. ^1H NMR spectra (500 MHz, $CDCl_3$) of P(3HT-ODA-3HT) (red), after reduction with $LiAlH_4$ (green) and after subsequent acid treatment (blue).

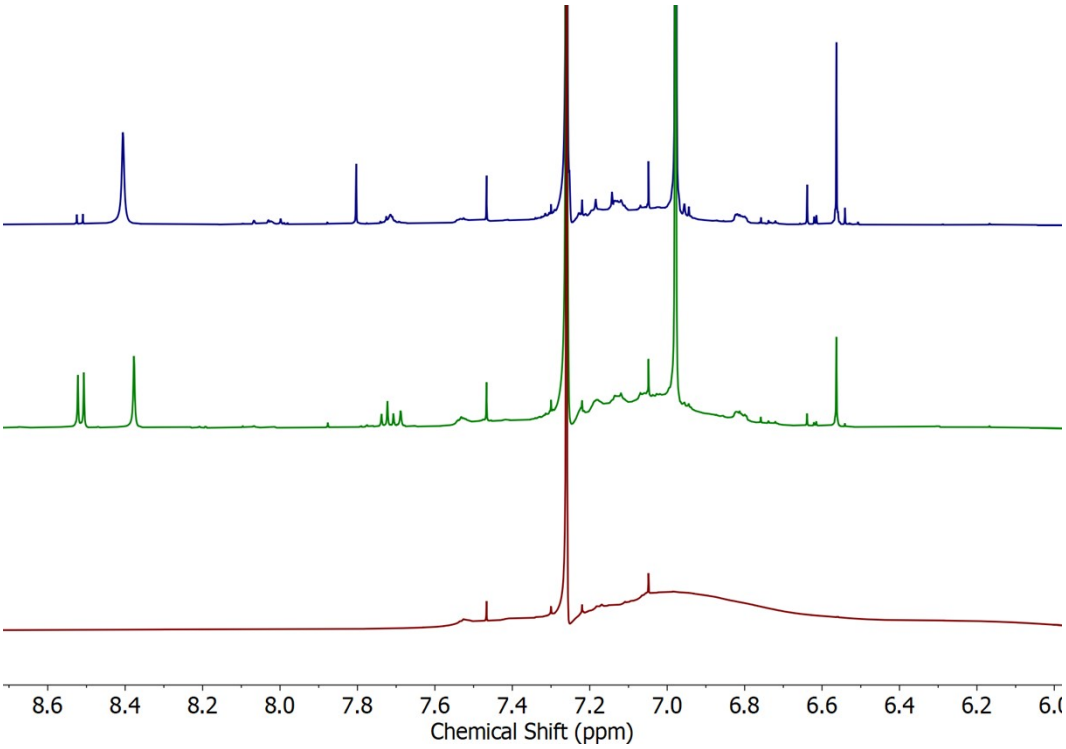


Figure S71. Aromatic regions of ^{1}H NMR spectra (500 MHz, $CDCl_3$) of P(3HT-ODA-3HT) (red), after reduction with $LiAlH_4$ (green) and after subsequent acid treatment (blue).

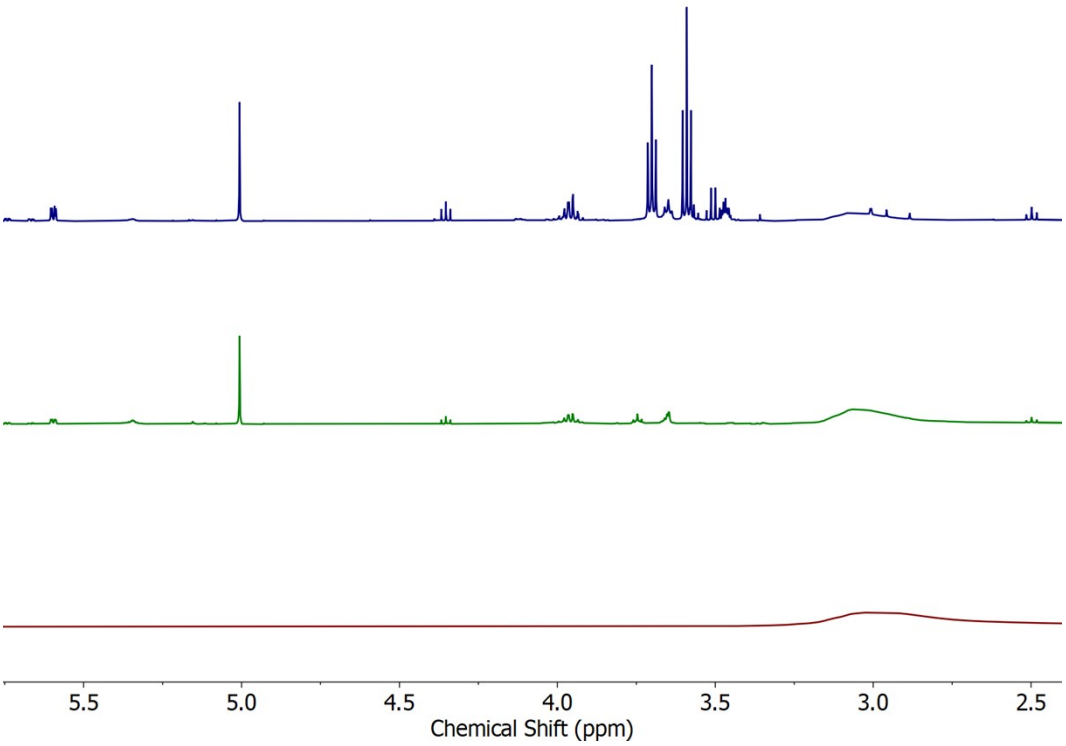


Figure S72. Methylene regions of ^{1}H NMR spectra (500 MHz, $CDCl_3$) of P(3HT-ODA-3HT) (red), after reduction with $LiAlH_4$ (green) and after subsequent acid treatment (blue).

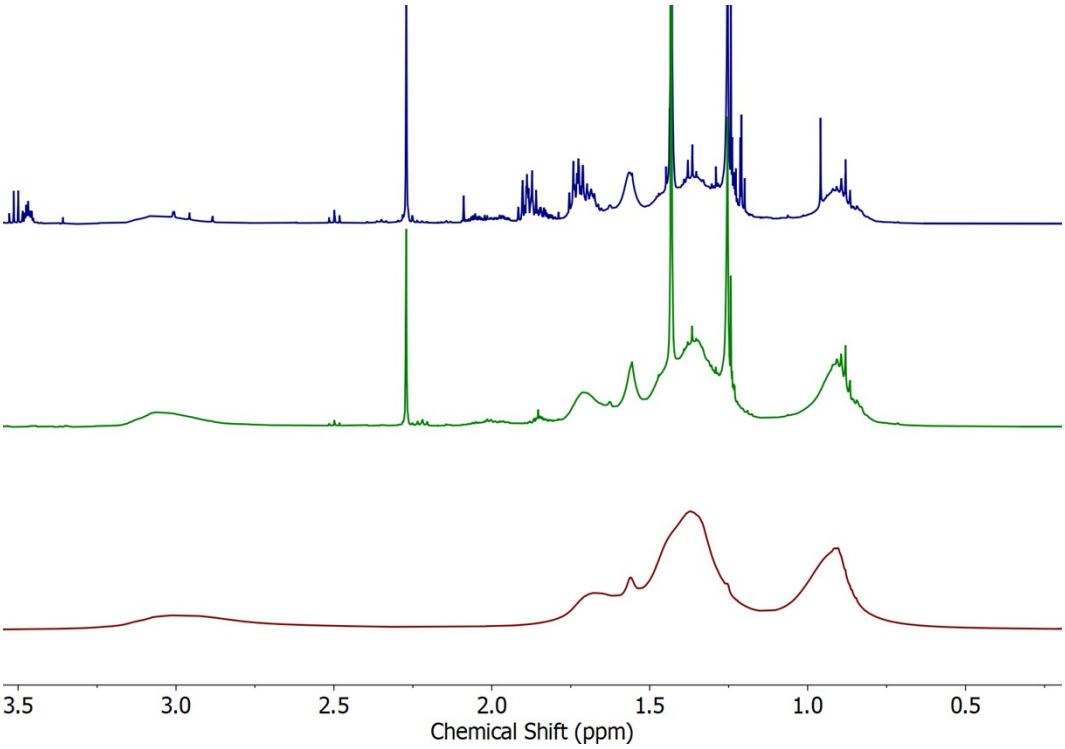


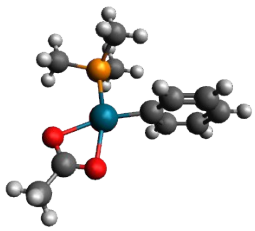
Figure S73. The methylene and methyl regions of ^{1}H NMR spectra (500 MHz, $CDCl_3$) of P(3HT-ODA-3HT) (red), after reduction with $LiAlH_4$ (green) and after subsequent acid treatment (blue).

DFT Information

All calculations were performed using Gaussian 16.[4] The B3LYP[5,6] functional was used in combination with the DGDZVP[7] basis set for Pd atoms and the TZVP[8] basis set for all other atoms. The active catalyst species was modelled by [Pd(C_5H_6)(PMe_3)(OAc)]. Monomer alkyl chains were appended to methyl groups to decrease computational time. Free energies were calculated at 298 K and 1 atm on single molecules in vacuum. The transition states were confirmed by frequency calculations, exhibiting a single imaginary frequency.

Cartesian Coordinates for Optimized Geometries

Catalyst

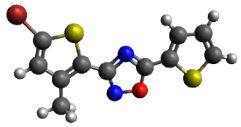


Pd	0.60067	-0.16445	0.00347
P	-0.10870	2.01589	-0.00219

C	-1.34962	-0.71750	0.00009
C	-3.27912	-1.54867	-1.20378
H	-3.76681	-1.76965	-2.14655
C	-2.00389	-0.98964	1.20199
H	-1.51619	-0.79222	2.14980
C	-1.99928	-0.99383	-1.20331
H	-1.50796	-0.79957	-2.14992
C	-3.28373	-1.54443	1.19943
H	-3.77505	-1.76212	2.14107
C	-3.92589	-1.82258	-0.00293
H	-4.91960	-2.25386	-0.00408
O	2.82743	-0.12487	0.00953
O	1.76951	-2.06067	0.01120
C	2.84848	-1.39637	0.00995
C	4.16760	-2.12605	-0.01379
H	4.98412	-1.45449	0.24484
H	4.13784	-2.97332	0.67129
H	4.33636	-2.52021	-1.01871
C	-1.09568	2.58059	-1.45314
H	-2.02877	2.02028	-1.49446
H	-1.31225	3.64827	-1.38154
H	-0.53534	2.38748	-2.36793
C	-1.09927	2.58598	1.44414
H	-1.31550	3.65340	1.36791
H	-2.03253	2.02593	1.48536
H	-0.54119	2.39633	2.36104
C	1.35854	3.13399	-0.00245
H	1.05427	4.18264	-0.00330
H	1.96689	2.92692	0.87746
H	1.96725	2.92576	-0.88188

Monomers

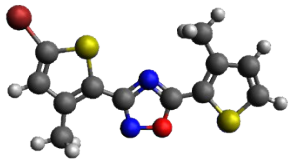
CM1



C	-3.26396	-0.07864	0.00001
C	-3.22189	1.28288	-0.00012
C	-1.89425	1.79933	-0.00018
C	-0.95172	0.79374	-0.00010
S	-1.68710	-0.80291	-0.00001
Br	-4.81798	-1.15439	0.00010
H	-4.10438	1.90623	-0.00017
C	-1.59174	3.26949	-0.00026

C	0.49135	0.88465	0.00001
N	1.29044	-0.23796	-0.00017
N	1.15295	2.02123	0.00014
O	2.50091	1.60704	0.00025
C	2.49087	0.26156	-0.00001
C	3.74450	-0.44596	-0.00003
C	3.91053	-1.80870	-0.00024
C	5.27151	-2.19756	-0.00023
C	6.12558	-1.13113	-0.00003
H	5.60419	-3.22563	-0.00039
S	5.28676	0.38320	0.00025
H	7.20395	-1.14094	0.00000
H	-2.51494	3.84896	-0.00108
H	-1.00127	3.55256	-0.87380
H	-1.00262	3.55292	0.87407
H	3.07386	-2.49221	-0.00042

CM2

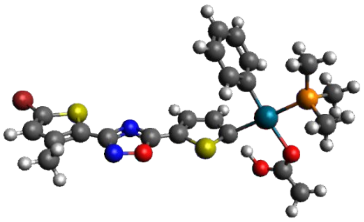


C	3.40096	-0.04245	0.00007
C	3.39274	1.31952	-0.00092
C	2.07820	1.86917	-0.00107
C	1.11063	0.88792	-0.00015
S	1.80597	-0.72657	0.00082
Br	4.92740	-1.15722	0.00053
H	4.29048	1.92072	-0.00157
C	1.81267	3.34646	-0.00190
C	-0.33010	1.01473	0.00007
N	-1.15632	-0.08838	-0.00026
N	-0.96226	2.16663	0.00055
O	-2.31939	1.78777	0.00046
C	-2.34773	0.43913	0.00007
C	-3.62546	-0.21789	-0.00005
C	-3.87688	-1.57753	-0.00117
C	-5.27422	-1.84455	-0.00067
C	-6.05024	-0.72301	0.00074
H	-5.68059	-2.84661	-0.00138
C	-2.83477	-2.65639	-0.00249
S	-5.10754	0.72383	0.00145

H	-7.12681	-0.65940	0.00132
H	2.75008	3.90268	-0.00580
H	1.23315	3.64532	0.87374
H	1.22683	3.64332	-0.87394
H	-2.18648	-2.58335	0.87238
H	-2.18298	-2.57806	-0.87422
H	-3.30719	-3.63865	-0.00628

Monomer CMD Transition States

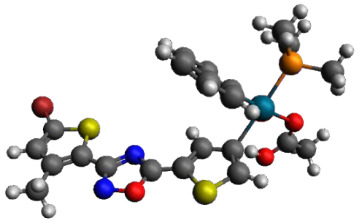
CM1_TSα



Pd	3.90516	-0.08741	-0.17955
P	5.89260	0.91642	0.60305
C	2.96818	1.71415	-0.06195
C	2.41517	3.85261	-1.06054
H	2.48968	4.53817	-1.89734
C	2.22678	2.07068	1.06392
H	2.12904	1.38476	1.89674
C	3.05904	2.61663	-1.12267
H	3.62172	2.36225	-2.01412
C	1.58432	3.30769	1.12561
H	1.00577	3.56577	2.00550
C	1.67761	4.20355	0.06567
H	1.17580	5.16230	0.11395
O	5.10267	-1.97178	-0.34116
O	3.51058	-2.98075	-1.54459
C	4.66713	-2.94244	-1.00593
C	5.53160	-4.16735	-1.18845
H	6.54531	-3.98066	-0.84218
H	5.09924	-4.99235	-0.61848
H	5.53593	-4.46433	-2.23732
C	7.19737	0.97865	-0.70228
H	6.87843	1.64373	-1.50489
H	8.14555	1.33577	-0.29499
H	7.33048	-0.02201	-1.11233
C	5.89584	2.62028	1.30318
H	6.90132	2.90246	1.62110
H	5.53517	3.32423	0.55441

H	5.21834	2.66354	2.15534
C	6.66502	-0.10722	1.92973
H	7.65546	0.27022	2.19211
H	6.02853	-0.09269	2.81468
H	6.73891	-1.13390	1.57367
C	-7.45929	0.14973	-0.11723
C	-7.54621	-0.38353	1.13301
C	-6.28567	-0.80284	1.64831
C	-5.26212	-0.57009	0.75570
S	-5.83659	0.16842	-0.73223
Br	-8.89085	0.82268	-1.15315
H	-8.47473	-0.47895	1.67722
C	-6.12559	-1.42133	3.00670
C	-3.84714	-0.84336	0.88340
N	-2.95680	-0.54979	-0.12356
N	-3.30129	-1.38600	1.95005
O	-1.93625	-1.45300	1.61215
C	-1.81712	-0.93964	0.37196
C	-0.51552	-0.87715	-0.23689
C	-0.23043	-0.36264	-1.48413
C	1.13730	-0.44244	-1.80055
C	1.94623	-1.00907	-0.82476
H	1.53768	-0.09408	-2.74378
H	-0.99403	0.04856	-2.12926
S	0.93239	-1.46769	0.53281
H	2.84395	-1.99936	-1.21270
H	-7.09152	-1.50152	3.50561
H	-5.45632	-0.83020	3.63487
H	-5.68335	-2.41710	2.93922

CM1_TSβ

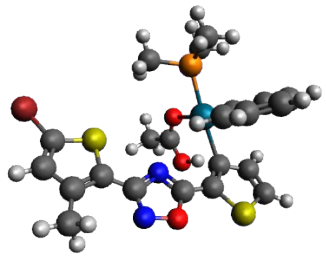


Pd	3.52803	-0.13463	0.22057
P	5.13946	-1.74703	-0.39711
C	2.51627	-0.50218	-1.50520
C	2.04529	0.00516	-3.82699
H	2.23184	0.61415	-4.70450
C	1.57228	-1.52832	-1.56121

H	1.36311	-2.13159	-0.68488
C	2.74737	0.26174	-2.64918
H	3.46689	1.07199	-2.63191
C	0.86904	-1.78337	-2.73883
H	0.13166	-2.57786	-2.76038
C	1.10571	-1.01955	-3.87697
H	0.55790	-1.21541	-4.79068
O	3.05076	1.22717	3.06860
O	4.72107	0.10197	2.10100
C	4.20109	0.67240	3.08872
C	4.95062	0.73496	4.39777
H	4.32765	0.32608	5.19433
H	5.88668	0.18560	4.33423
H	5.15076	1.77845	4.64732
C	6.85244	-1.08713	-0.20214
H	6.94587	-0.65966	0.79536
H	7.59680	-1.87376	-0.34175
H	7.02243	-0.29800	-0.93490
C	5.11761	-3.20621	0.73486
H	5.93904	-3.89047	0.51232
H	5.20451	-2.85361	1.76212
H	4.17066	-3.73552	0.62830
C	5.15029	-2.50343	-2.07701
H	5.97051	-3.21760	-2.17153
H	4.20136	-3.00714	-2.25659
H	5.25887	-1.72104	-2.82736
C	-6.52870	-0.96081	0.43556
C	-7.11374	0.10012	-0.18638
C	-6.18514	1.12489	-0.53065
C	-4.90023	0.80316	-0.15178
S	-4.81557	-0.76653	0.63455
Br	-7.40060	-2.52135	1.05325
H	-8.17194	0.15883	-0.39666
C	-6.59082	2.39323	-1.22356
C	-3.67465	1.55580	-0.31190
N	-2.46486	1.07404	0.13198
N	-3.61456	2.73859	-0.88277
O	-2.24388	3.05940	-0.80603
C	-1.63611	2.02427	-0.19373
C	-0.21519	2.07632	0.02176
C	0.55839	1.11150	0.61112
C	1.95253	1.42360	0.69265
C	2.17970	2.66675	0.14181
H	2.59106	1.21650	1.93883

H	0.12170	0.19415	0.98137
S	0.76005	3.44972	-0.47167
H	3.11807	3.19797	0.07406
H	-7.66441	2.39812	-1.41280
H	-6.06769	2.50993	-2.17461
H	-6.33767	3.27020	-0.62467

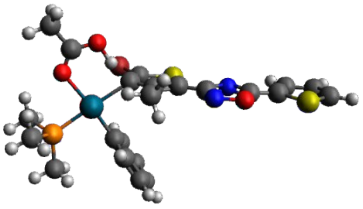
CM1_TSγ



Pd	1.78953	-0.93134	0.40549
P	1.32411	-3.01337	-0.58182
C	2.71957	-0.34803	-1.30765
C	4.70934	-0.16774	-2.68047
H	5.77092	-0.34632	-2.81148
C	1.99371	0.28669	-2.31624
H	0.93447	0.47857	-2.18845
C	4.08251	-0.57426	-1.50214
H	4.67336	-1.05907	-0.73344
C	2.62094	0.69461	-3.49365
H	2.04246	1.19401	-4.26288
C	3.98032	0.46561	-3.68171
H	4.46717	0.78235	-4.59615
O	1.06962	0.13619	3.32905
O	0.73006	-1.75423	2.18809
C	0.59039	-1.03863	3.20891
C	-0.20756	-1.56432	4.37873
H	-1.18593	-1.07845	4.37729
H	-0.34551	-2.64017	4.29873
H	0.28547	-1.30878	5.31599
C	2.06683	-4.39252	0.39512
H	1.76611	-4.27894	1.43601
H	1.73660	-5.36336	0.01963
H	3.15394	-4.33578	0.33811
C	-0.48236	-3.38239	-0.53241
H	-0.68475	-4.40098	-0.87012

H	-0.83142	-3.25482	0.49145
H	-1.01577	-2.67703	-1.16935
C	1.80544	-3.39837	-2.31767
H	1.50333	-4.41363	-2.58181
H	1.33059	-2.68780	-2.99308
H	2.88396	-3.29481	-2.42988
C	-4.76056	0.12820	-0.39527
C	-5.13086	1.38824	-0.75319
C	-4.05790	2.32500	-0.68647
C	-2.88422	1.73514	-0.27243
S	-3.08435	0.01742	0.04467
Br	-5.87270	-1.40097	-0.34680
H	-6.13389	1.65163	-1.05655
C	-4.22191	3.77687	-1.03065
C	-1.57583	2.32090	-0.07191
N	-0.49577	1.56834	0.32541
N	-1.31412	3.59593	-0.25603
O	0.05409	3.68792	0.05718
C	0.46520	2.44763	0.39382
C	1.83918	2.25093	0.77084
C	3.78175	1.31501	1.58296
C	4.23858	2.56179	1.27575
H	1.65569	0.47824	2.28725
S	2.99051	3.56823	0.62077
H	5.23453	2.96028	1.39459
H	-5.24319	3.97966	-1.35340
H	-3.53712	4.07574	-1.82634
H	-3.99353	4.41438	-0.17424
C	2.39714	1.09695	1.29462
H	4.41915	0.55812	2.02065

CM1_TSβBr



Pd	-2.55880	0.13567	-0.33434
P	-4.56879	1.36854	-0.36884
C	-1.58616	1.75488	0.42169
C	-0.40694	3.84738	0.09075
H	-0.00599	4.59447	-0.58518

C	-1.42909	1.90958	1.79921
H	-1.80780	1.15805	2.48213
C	-1.07206	2.73567	-0.42750
H	-1.17412	2.64038	-1.50247
C	-0.76580	3.02224	2.31679
H	-0.64528	3.12114	3.38985
C	-0.25463	3.99642	1.46521
H	0.26293	4.85864	1.86799
O	-1.97298	-2.81388	-1.46908
O	-3.78123	-1.52867	-1.20053
C	-3.22493	-2.58865	-1.57242
C	-4.05684	-3.69729	-2.17226
H	-4.07829	-4.53809	-1.47588
H	-5.07245	-3.35872	-2.36275
H	-3.59419	-4.05033	-3.09405
C	-5.24057	1.54299	-2.08011
H	-5.29453	0.55413	-2.53420
H	-6.23356	1.99735	-2.06979
H	-4.56850	2.16241	-2.67422
C	-5.90850	0.46151	0.51972
H	-6.87312	0.95698	0.39115
H	-5.95718	-0.55307	0.12625
H	-5.66848	0.41034	1.58184
C	-4.67013	3.07643	0.31470
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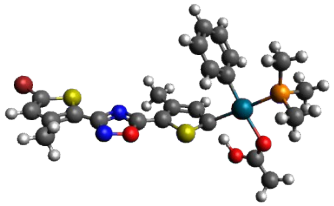
H	-4.37838	3.06500	1.36430
H	-3.97416	3.72451	-0.21639
C	-0.18989	-1.39765	1.04150
C	-0.58507	-0.98901	-0.20724
C	0.56964	-0.54330	-0.95381
C	1.74985	-0.62024	-0.25203
S	1.50433	-1.25804	1.37087
Br	-1.31289	-2.12010	2.39679
H	-1.41230	-1.89056	-0.88409
C	0.47116	-0.06891	-2.37445
C	3.09401	-0.26832	-0.65244
N	4.17164	-0.43791	0.19297
N	3.40556	0.23210	-1.82901
O	4.80500	0.40266	-1.74620
C	5.17092	-0.01644	-0.52209
C	6.56149	0.04262	-0.15032
C	7.10070	-0.34345	1.05112
C	8.50382	-0.16228	1.10937
C	9.01790	0.35810	-0.04430

H	9.10732	-0.40793	1.97146
H	6.49585	-0.74131	1.85302
S	7.79589	0.64196	-1.23810
H	10.04582	0.59410	-0.26926
H	-0.55314	-0.16493	-2.73317
H	1.13178	-0.63921	-3.03055
H	0.77677	0.97603	-2.46327

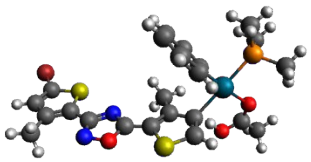
CM2_TS



Pd	3.93886	-0.09687	-0.12287
P	5.92040	0.87585	0.71331
C	3.01836	1.71332	-0.00742
C	2.51453	3.87034	-0.99284
H	2.61782	4.56516	-1.81892
C	2.25353	2.06524	1.10425
H	2.12676	1.37008	1.92535
C	3.14529	2.62756	-1.05442
H	3.72662	2.37727	-1.93501
C	1.62424	3.30904	1.16559
H	1.02766	3.56345	2.03447
C	1.75386	4.21662	0.11943
H	1.26283	5.18098	0.16766
O	5.11774	-1.99361	-0.27861
O	3.54326	-2.96502	-1.53496
C	4.68643	-2.94930	-0.96717
C	5.53885	-4.18344	-1.14420
H	6.54852	-4.01193	-0.77874
H	5.08658	-5.00673	-0.58727
H	5.55770	-4.47332	-2.19484
C	7.25454	0.93847	-0.56216
H	6.96039	1.61561	-1.36417
H	8.19726	1.28089	-0.13029
H	7.38617	-0.05900	-0.98039
C	5.92694	2.57179	1.43269
H	6.92807	2.83932	1.77602
H	5.59070	3.28800	0.68415
H	5.23108	2.61311	2.27003

C	6.65329	-0.17044	2.04489
H	7.64224	0.19271	2.33195
H	5.99859	-0.15791	2.91650
H	6.72294	-1.19415	1.67952
C	-7.44589	0.12573	0.01362
C	-7.49583	-0.42936	1.25619
C	-6.21863	-0.84528	1.73232
C	-5.22016	-0.58791	0.81853
S	-5.83920	0.17027	-0.64139
Br	-8.90929	0.80255	-0.97436
H	-8.40924	-0.54282	1.82212
C	-6.01853	-1.48509	3.07545
C	-3.79963	-0.84965	0.90562
N	-2.93784	-0.52683	-0.11749
N	-3.22297	-1.40736	1.94664
O	-1.86706	-1.45438	1.57543
C	-1.77904	-0.91491	0.34005
C	-0.48712	-0.83670	-0.28218
C	-0.18384	-0.30444	-1.52848
C	1.20010	-0.40464	-1.79715
C	1.98432	-0.98822	-0.81568
H	1.62300	-0.04839	-2.72859
C	-1.17039	0.30089	-2.48318
S	0.94281	-1.45118	0.51261
H	2.88118	-1.98250	-1.20272
H	-6.96995	-1.57776	3.59948
H	-5.33426	-0.90148	3.69435
H	-5.57434	-2.47768	2.97937
H	-1.94659	-0.41378	-2.76229
H	-0.66164	0.63560	-3.38738
H	-1.68332	1.15425	-2.03604

CM2_TSβ



Pd	-3.56797	-0.13987	-0.21601
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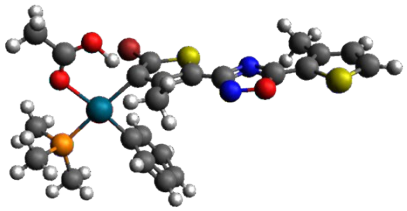
C	-2.29611	0.33911	3.87802
H	-2.48540	1.05173	4.67301
C	-1.81488	-1.46110	1.82064
H	-1.60736	-2.17289	1.02977

C	-2.90595	0.51575	2.63616
H	-3.55734	1.36901	2.48823
C	-1.20246	-1.63615	3.06217
H	-0.53406	-2.47599	3.21570
C	-1.44338	-0.73819	4.09653
H	-0.96650	-0.87221	5.05982
O	-2.96474	1.06864	-3.12656
O	-4.65852	-0.03174	-2.17157
C	-4.10749	0.49745	-3.16430
C	-4.80459	0.48825	-4.50330
H	-4.14378	0.05647	-5.25601
H	-5.73321	-0.07480	-4.45175
H	-5.01226	1.51597	-4.80659
C	-6.95582	-0.88432	0.12557
H	-6.98484	-0.54048	-0.90760
H	-7.74864	-1.61538	0.29689
H	-7.11048	-0.02702	0.78106
C	-5.30758	-3.16250	-0.55565
H	-6.17786	-3.77856	-0.31989
H	-5.32690	-2.89186	-1.61089
H	-4.40008	-3.73396	-0.36020
C	-5.41946	-2.22702	2.18592
H	-6.28475	-2.88280	2.29961
H	-4.51151	-2.76734	2.45056
H	-5.51158	-1.37947	2.86432
C	6.67045	-0.94748	-0.31110
C	7.21974	0.16525	0.24967
C	6.25954	1.18171	0.52579
C	4.98740	0.80121	0.15881
S	4.95396	-0.81461	-0.53213
Br	7.59115	-2.51662	-0.82819
H	8.27408	0.26702	0.46297
C	6.62329	2.50030	1.14415
C	3.73952	1.52660	0.26546
N	2.54770	0.98417	-0.15800
N	3.64119	2.73720	0.76581
O	2.26431	3.01467	0.66103
C	1.68551	1.92763	0.10482
C	0.26682	1.94674	-0.11454
C	-0.52408	0.95949	-0.66816
C	-1.91772	1.31989	-0.73228
C	-2.11337	2.58585	-0.22773
H	-2.54197	1.09778	-1.98972
C	-0.00168	-0.34879	-1.18287

S	-0.67789	3.35914	0.33967
H	-3.04271	3.13378	-0.16840
H	7.69513	2.54858	1.33728
H	6.09120	2.65702	2.08443
H	6.34751	3.33245	0.49356
H	-0.81283	-0.92335	-1.62894
H	0.44644	-0.93798	-0.38036
H	0.78099	-0.19969	-1.92864

CM2_TSβBr

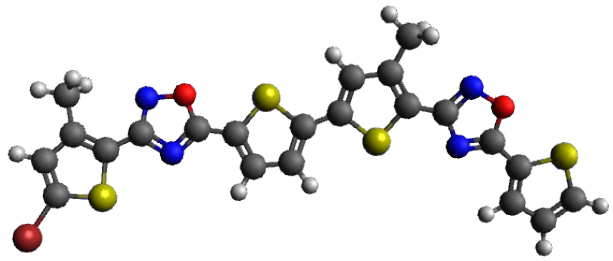


Pd	-2.72029	0.14473	-0.32723
P	-4.74438	1.35411	-0.28003
C	-1.75694	1.73499	0.49895
C	-0.59805	3.85133	0.26115
H	-0.20727	4.63293	-0.38085
C	-1.59398	1.82624	1.88145
H	-1.96235	1.04000	2.53008
C	-1.25614	2.75930	-0.30560
H	-1.36335	2.71395	-1.38332
C	-0.93783	2.91932	2.44764
H	-0.81279	2.96887	3.52360
C	-0.43973	3.93701	1.64034
H	0.07224	4.78408	2.08067
O	-2.12237	-2.75118	-1.58953
O	-3.93608	-1.48807	-1.26044
C	-3.37590	-2.52885	-1.67796
C	-4.20454	-3.61625	-2.31980
H	-4.21180	-4.48850	-1.66299
H	-5.22473	-3.27822	-2.48510
H	-3.74811	-3.92222	-3.26136
C	-5.45180	1.57648	-1.97123
H	-5.49980	0.60274	-2.45747
H	-6.45087	2.01515	-1.92672
H	-4.80032	2.22579	-2.55631
C	-6.05529	0.40107	0.60349
H	-7.02724	0.89096	0.51490
H	-6.10370	-0.59863	0.17352
H	-5.79093	0.31277	1.65735
C	-4.85272	3.03689	0.46211

H	-5.87317	3.41969	0.39929
H	-4.54075	2.99443	1.50506
H	-4.17478	3.71082	-0.06007
C	-0.30985	-1.41779	0.94464
C	-0.73367	-0.96242	-0.27808
C	0.40165	-0.47397	-1.02828
C	1.59641	-0.56698	-0.35399
S	1.38949	-1.27365	1.24558
Br	-1.39769	-2.20897	2.29019
H	-1.56269	-1.84622	-0.97503
C	0.27008	0.05766	-2.42583
C	2.92925	-0.18476	-0.76579
N	4.02538	-0.38268	0.04952
N	3.21123	0.37047	-1.92375
O	4.60964	0.55005	-1.86352
C	5.01003	0.07979	-0.66548
C	6.40885	0.14305	-0.33831
C	7.02496	-0.27978	0.82436
C	8.42895	-0.05194	0.77829
C	8.85691	0.52370	-0.38146
H	9.09293	-0.31298	1.59096
C	6.33191	-0.90224	2.00019
S	7.55797	0.81787	-1.48163
H	9.86358	0.79445	-0.65773
H	-0.75786	-0.04421	-2.77244
H	0.93151	-0.46997	-3.11578
H	0.55299	1.11165	-2.47469
H	7.05279	-1.13679	2.78355
H	5.81308	-1.81918	1.71560
H	5.57141	-0.23632	2.41127

Dimers

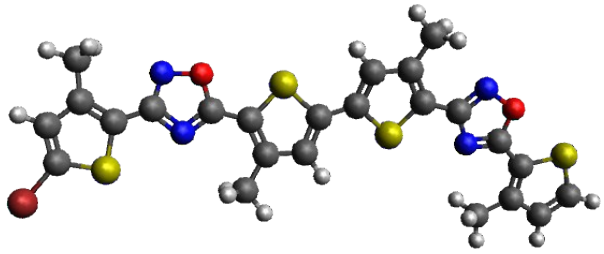
CM1-dimer



C	-8.40507	-0.98817	-0.00545
C	-8.74869	0.29689	-0.29867
C	-7.62309	1.16293	-0.41070
C	-6.43719	0.49481	-0.19467

S	-6.69104	-1.21021	0.14950
Br	-9.58962	-2.44255	0.22697
H	-9.76937	0.62503	-0.43245
C	-7.74811	2.62471	-0.72775
C	-5.08086	0.99598	-0.21559
N	-4.00004	0.17691	0.02410
N	-4.76855	2.25029	-0.45991
O	-3.36093	2.25273	-0.37244
C	-2.99039	0.99091	-0.08397
C	-1.59349	0.69124	0.06485
C	-1.04891	-0.53305	0.36846
C	0.35564	-0.50815	0.45673
C	0.90368	0.73466	0.21831
H	0.95323	-1.37307	0.70835
S	-0.35081	1.90816	-0.13715
H	-8.79539	2.89972	-0.85301
H	-7.20866	2.87945	-1.64204
H	-7.31805	3.24034	0.06465
H	-1.65835	-1.41040	0.53029
H	5.68996	3.66637	1.36440
S	10.52976	-1.27813	-0.16012
C	10.81409	-2.97375	-0.36091
C	9.65291	-3.69065	-0.42832
C	8.79918	-1.54520	-0.16756
O	8.31362	0.78937	0.10828
C	7.85420	-0.46841	-0.02991
H	11.82711	-3.33928	-0.41722
C	8.50029	-2.87669	-0.31811
N	7.18352	1.62270	0.22059
C	6.17899	0.77723	0.13799
C	5.02573	3.70423	0.49895
N	6.55588	-0.53878	-0.01874
C	4.79027	1.17332	0.20113
C	4.24320	2.43203	0.35496
H	9.62307	-4.76360	-0.55265
S	3.56103	-0.06682	0.06274
C	2.82770	2.38572	0.37289
H	7.48347	-3.24060	-0.34678
H	4.35304	4.55434	0.61246
C	2.29239	1.12626	0.23303
H	2.21857	3.26982	0.50748
H	5.66328	3.87768	-0.37007

CM2-dimer



C	-8.58529	-0.88534	-0.04361
C	-8.90264	0.40704	-0.33343
C	-7.76021	1.25268	-0.43374
C	-6.58840	0.56214	-0.21253
S	-6.87645	-1.13932	0.12220
Br	-9.79795	-2.31884	0.17423
H	-9.91604	0.75480	-0.47288
C	-7.85595	2.71791	-0.74503
C	-5.22250	1.03809	-0.22151
N	-4.15923	0.19711	0.02235
N	-4.88595	2.28650	-0.45744
O	-3.48029	2.26371	-0.36014
C	-3.12980	0.99195	-0.07425
C	-1.73724	0.68630	0.07864
C	-1.16508	-0.53762	0.37926
C	0.24430	-0.44680	0.45689
C	0.75669	0.80873	0.21995
H	0.86925	-1.29430	0.70434
S	-0.52882	1.94341	-0.12617
H	-8.89705	3.01292	-0.87625
H	-7.30535	2.96659	-1.65432
H	-7.41988	3.32187	0.05304
C	-1.91804	-1.81387	0.61222
H	5.46298	3.87452	1.34413
S	10.43861	-0.85166	-0.14283
C	10.84729	-2.51835	-0.33456
C	9.74313	-3.31595	-0.40430
C	8.72818	-1.24868	-0.15776
O	8.16310	1.06216	0.10501
C	7.74132	-0.21293	-0.02678
H	11.88378	-2.81202	-0.38470
C	8.51401	-2.60681	-0.30483
N	7.01083	1.86340	0.21315
C	6.03060	0.99100	0.13558
C	4.79878	3.88796	0.47792
N	6.44251	-0.31576	-0.01426
C	4.63152	1.34989	0.19746

C	4.05060	2.59423	0.34325
H	9.79391	-4.38938	-0.52432
S	3.43534	0.07662	0.06842
C	2.63674	2.51026	0.36230
C	7.17292	-3.27669	-0.35674
H	4.10349	4.72067	0.58418
C	2.13469	1.23637	0.23104
H	2.00401	3.37860	0.49055
H	5.43257	4.07141	-0.39178
H	-1.22654	-2.62594	0.83631
H	-2.51012	-2.08888	-0.26216
H	-2.62175	-1.71376	1.44016
H	7.29230	-4.35330	-0.47788
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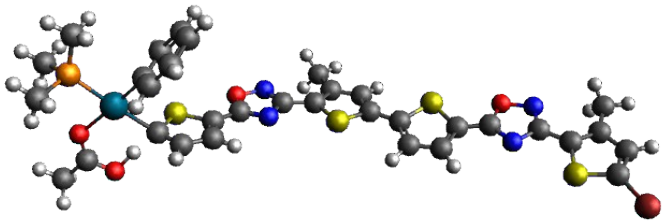
H	6.59958	-3.08809	0.55248

Dimer CMD Transition States

CM1-dimer_TSα



C	12.87592	-1.82645	-0.36569
C	13.39403	-0.84860	0.42847
C	12.41738	0.09496	0.85931
C	11.16423	-0.20228	0.36897
S	11.17011	-1.64856	-0.63004
Br	13.82675	-3.26307	-1.14369
H	14.43761	-0.79439	0.70300
C	12.74694	1.26326	1.74221
C	9.91028	0.49162	0.56383
N	8.73874	0.04834	-0.00756
N	9.78380	1.58279	1.28749
O	8.40928	1.88008	1.18050
C	7.86765	0.92592	0.39962
C	6.46117	0.97364	0.11453
C	5.75607	0.09101	-0.66766
C	4.38883	0.40915	-0.76828
C	4.02881	1.53756	-0.06154
H	3.68533	-0.16037	-1.35920
S	5.41790	2.22204	0.76301

H	13.80870	1.26753	1.98886
H	12.17304	1.23290	2.67040
H	12.49747	2.20910	1.25744
H	6.22774	-0.74934	-1.15626
H	-0.08813	5.51981	-0.02831
S	-5.78486	1.35637	-0.83083
C	-6.39774	-0.21455	-1.31665
C	-5.31906	-1.07530	-1.46916
C	-4.13040	0.80808	-0.83243
O	-3.24902	2.92660	-0.12118
C	-3.01617	1.65291	-0.49711
H	-7.33778	-0.15793	-2.33868
C	-4.05603	-0.51875	-1.20110
N	-1.99631	3.50733	0.14522
C	-1.15375	2.52621	-0.09697
C	0.48500	5.08705	0.79377
N	-1.74855	1.35322	-0.50019
C	0.28070	2.64995	0.04077
C	1.03538	3.74024	0.42618
H	-5.44762	-2.10335	-1.78207
S	1.27457	1.25120	-0.30868
C	2.42005	3.44176	0.42504
H	-3.11652	-1.04860	-1.27131
H	1.29331	5.77070	1.05379
C	2.72954	2.15415	0.05259
H	3.17357	4.17646	0.67677
H	-0.19945	5.01741	1.64135
H	-10.13995	1.43649	-4.34642
C	-10.28353	0.39310	-4.05802
H	-10.09485	-0.21702	-4.94147
H	-11.30363	0.25151	-3.70916
C	-9.29157	0.04582	-2.97342
O	-8.06526	-0.00585	-3.32306
O	-9.69986	-0.15847	-1.80482
H	-11.55587	0.36590	0.03177
H	-11.35061	-2.48022	-0.77247
C	-11.39713	0.03922	1.05862
C	-11.15387	-2.73676	0.26800
H	-12.34685	-0.25957	1.50702
Pd	-8.27569	-0.80963	-0.20604
H	-12.09913	-2.90315	0.78881
H	-10.97742	0.87026	1.62576
P	-10.19736	-1.36253	1.04649
H	-10.56333	-3.65261	0.29475

C	-7.10847	-1.51519	1.30313
C	-10.08195	-1.85928	2.81644
H	-6.80825	0.40085	2.24549
H	-11.07449	-2.06264	3.22283
C	-6.59757	-0.66124	2.27993
H	-7.18084	-3.56130	0.62017
C	-6.80375	-2.87547	1.37077
H	-9.61046	-1.06030	3.38770
H	-9.45788	-2.74727	2.90741
C	-5.79245	-1.15957	3.30477
C	-5.99742	-3.37242	2.39494
H	-5.39779	-0.48044	4.05214
C	-5.49122	-2.51606	3.36754
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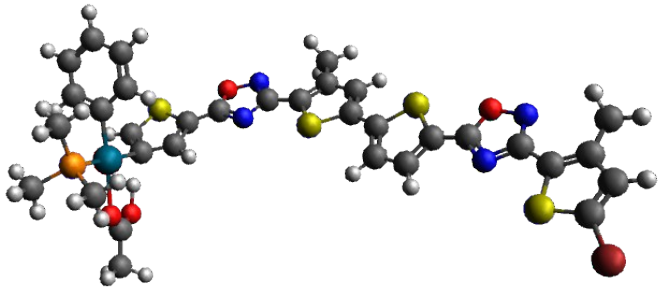
H	-4.86389	-2.90093	4.16230

CM1-dimer_TSa



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S	9.98207	-1.92095	-0.23479
Br	12.43156	-3.89559	-0.40583
H	13.35242	-1.18931	0.90035
C	11.92318	1.21335	1.49751
C	8.99334	0.54459	0.49788
N	7.76844	0.13161	0.02398
N	9.00360	1.76509	0.98834
O	7.66885	2.18855	0.82051
C	7.00873	1.16545	0.24515
C	5.61073	1.31400	-0.04658
C	4.79701	0.38056	-0.64211
C	3.47141	0.82407	-0.80561
C	3.25210	2.10166	-0.33417
H	2.69768	0.23322	-1.27539

S	4.72450	2.77366	0.34286
H	12.98542	1.14979	1.73364
H	11.37420	1.43277	2.41530
H	11.76354	2.06463	0.83297
H	5.16350	-0.58613	-0.95613
H	-0.40868	6.44383	-1.09049
S	-6.54371	2.88836	-0.94282
C	-7.27338	1.33273	-1.15606
C	-6.37925	0.28581	-1.21352
C	-4.95360	2.14721	-0.92437
O	-3.83112	4.25319	-0.65251
C	-3.74714	2.91262	-0.76849
H	-8.34984	1.28614	-1.22863
C	-5.04537	0.78843	-1.08480
N	-2.51486	4.73301	-0.51057
C	-1.79175	3.63557	-0.55745
C	0.13758	6.12317	-0.20153
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C	0.52905	4.67740	-0.29322
H	-6.60089	-0.63670	-2.25776
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C	1.87263	4.23196	-0.23674
H	-4.15906	0.16882	-1.11891
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H	2.70754	4.91332	-0.13852
H	-0.52646	6.30063	0.64658
H	-7.25095	-3.25982	-4.91449
C	-6.43541	-3.46193	-4.21948
H	-5.50170	-3.25791	-4.74719
H	-6.45641	-4.50239	-3.90465
C	-6.53951	-2.53862	-3.02970
O	-6.65876	-1.29322	-3.28740
O	-6.49693	-3.01222	-1.86981
H	-8.55426	-4.72677	-0.45752
H	-5.60610	-4.93987	-0.23206
C	-8.60119	-4.56687	0.61923
C	-5.72558	-4.81530	0.84340
H	-8.65973	-5.53053	1.12955
Pd	-6.80298	-1.65166	-0.11926
H	-5.93038	-5.78088	1.31031
H	-9.49548	-3.98619	0.84583
P	-7.10260	-3.62405	1.14521

H	-4.79939	-4.40886	1.25021
C	-7.16796	-0.53929	1.54485
C	-7.24396	-3.57450	2.98140
H	-9.31336	-0.58514	1.31369
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H	-8.09731	-2.96043	3.26608
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C	-6.38300	0.69805	3.47439
H	-9.76571	0.75892	3.31815
C	-7.69248	0.99552	3.83757
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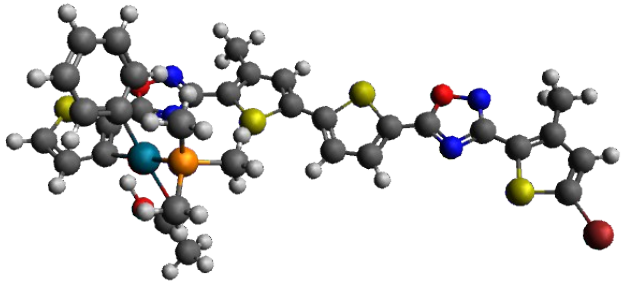
CM1-dimer_TSb



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S	8.96387	-1.11531	-0.38945
Br	11.65265	-2.73081	-0.68501
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C	7.65002	1.11503	0.55540
N	6.49690	0.59855	0.00776
N	7.49245	2.27008	1.16485
O	6.11644	2.53317	1.00149
C	5.60543	1.49802	0.30861
C	4.20424	1.49359	-0.00637
C	3.53062	0.53026	-0.71770
C	2.16031	0.81231	-0.87297
C	1.76681	1.99360	-0.27961
H	1.47907	0.18079	-1.42569

S	3.12676	2.77618	0.50492
H	11.50900	2.09935	1.95847
H	9.86410	2.10264	2.61793
H	10.19276	2.93664	1.11749
H	4.02732	-0.34105	-1.11966
H	-2.39441	5.87748	-0.76937
S	-8.04096	1.61289	-0.78293
C	-8.65046	0.04027	-1.17533
C	-7.64819	-0.86069	-1.37909
C	-6.39492	1.01204	-0.89875
O	-5.53538	3.22243	-0.53235
C	-5.28655	1.90548	-0.69580
H	-9.71667	-0.11670	-1.23369
C	-6.32756	-0.33381	-1.21742
N	-4.29386	3.85680	-0.36089
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C	-1.85302	5.54735	0.11934
N	-4.01282	1.62955	-0.64332
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H	-7.84332	-1.88921	-1.65272
S	-0.98079	1.62159	-0.49435
C	0.11677	3.90897	-0.03563
H	-5.41388	-0.67126	-2.20464
H	-1.06304	6.26731	0.33360
C	0.45483	2.59288	-0.24530
H	0.85385	4.68511	0.12344
H	-2.57303	5.56253	0.93937
H	-7.20611	-2.89288	1.31940
H	-8.40547	-2.43106	3.41202
H	-3.37103	-2.39436	3.35162
C	-6.87340	-2.07506	1.94817
C	-7.55866	-1.81291	3.13496
C	-3.48340	-3.34682	2.83520
H	-4.47457	-3.73554	3.06542
H	-3.52702	-2.19078	-5.10862
H	-1.40361	-1.61287	1.26581
Pd	-4.77487	-1.65301	-0.16009
H	-2.72258	-4.04659	3.18621
C	-5.78608	-1.28829	1.56747
C	-7.16244	-0.76404	3.95830
O	-4.78153	-0.86182	-3.25543
C	-3.80062	-1.65003	-3.05279
O	-3.53542	-2.17269	-1.94379

H	-7.69537	-0.55977	4.87903
C	-2.91539	-1.93956	-4.24214
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H	-0.88993	-3.31765	1.22876
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C	-5.39249	-0.23863	2.39823
H	-2.35403	-1.03617	-4.48972
H	-1.37516	-2.48307	-0.27392
C	-3.37446	-4.79375	0.32311
H	-5.76459	0.84997	4.21251
H	-4.55332	0.39011	2.12332
H	-4.35382	-5.23592	0.50635
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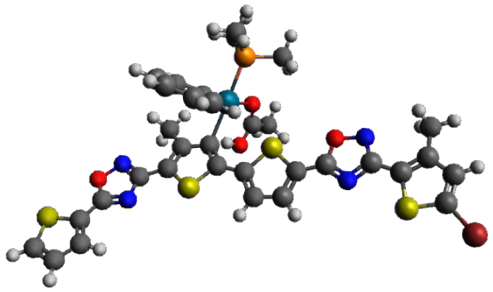
CM1-dimer_TSc



C	9.15751	-2.10101	0.17940
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S	7.45626	-2.43269	0.09576
Br	10.40937	-3.51174	0.30656
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C	8.33116	1.54391	-0.01351
C	5.74338	-0.28260	-0.08685
N	4.70625	-1.18599	-0.11994
N	5.37157	0.97762	-0.15085
O	3.96526	0.89157	-0.23309
C	3.65537	-0.42096	-0.20912
C	2.27704	-0.81102	-0.27130
C	1.78718	-2.09587	-0.24184
C	0.38597	-2.15332	-0.32125
C	-0.22378	-0.91511	-0.41008

H	-0.17086	-3.07956	-0.33471
S	0.98010	0.36263	-0.39006
H	9.36494	1.88847	0.01507
H	7.79101	1.99218	0.82280
H	7.86099	1.92410	-0.92239
H	2.43300	-2.95960	-0.17366
H	-5.18850	1.21573	-2.28753
S	-9.59543	-3.79291	-0.11846
C	-9.72451	-5.45255	0.35831
C	-8.50507	-6.01794	0.60227
C	-7.85104	-3.86638	0.01566
O	-7.58131	-1.57212	-0.63695
C	-7.00957	-2.73096	-0.26223
H	-10.69806	-5.91091	0.42933
C	-7.43325	-5.11368	0.40714
N	-6.53216	-0.65128	-0.83785
C	-5.45536	-1.35740	-0.56440
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C	-3.66762	0.42243	-0.98524
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S	-2.78308	-1.89442	-0.20259
C	-2.24063	0.57112	-0.91660
H	-6.38929	-5.35503	0.54521
H	-3.99867	2.40409	-1.71914
C	-1.62925	-0.61641	-0.52504
H	-1.68472	1.14403	-2.06632
H	-5.27925	1.80946	-0.64724
H	-0.38766	0.99679	2.32402
H	-1.28606	0.40617	4.52956
H	1.75051	4.04548	0.87504
C	-1.38908	1.31636	2.58712
C	-1.89810	0.97832	3.84123
C	1.16598	4.80599	0.35736
H	1.30337	4.67513	-0.71521
H	0.66774	2.56077	-4.72943
H	-0.19415	4.18639	3.11144
Pd	-1.43775	2.55967	-0.15411
H	1.51488	5.79617	0.65767
C	-2.16042	2.04284	1.68002
C	-3.18207	1.36770	4.20822
O	-1.29136	1.47974	-3.18235
C	-0.75248	2.63664	-3.14413

O	-0.65282	3.33019	-2.10498
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P	-0.62298	4.58489	0.75015
C	-0.72869	4.95305	2.55181
H	0.09651	4.20229	-4.35029
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C	-3.95592	2.09412	3.30928
C	-3.44708	2.43253	2.05507
H	-0.94344	3.04873	-5.23727
H	-1.77058	4.93144	2.86894
C	-1.41853	6.04931	-0.04445
H	-4.96106	2.39876	3.57871
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H	-1.33079	5.94723	-1.12557
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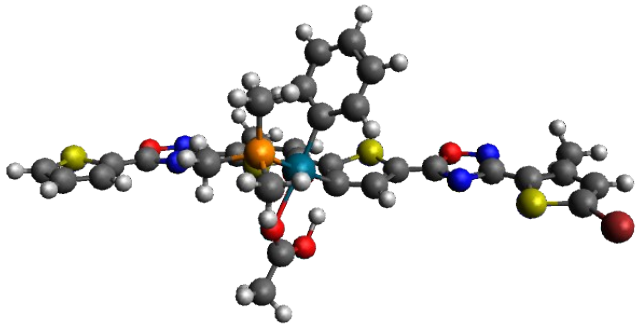
CM1-dimer_TSd



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S	7.19770	-0.42507	-0.65644
Br	10.05058	-1.72946	-0.96562
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C	8.41062	3.27089	0.55078
C	5.67368	1.77895	-0.01516
N	4.56145	1.01946	-0.29391
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O	4.00398	3.06253	0.33037
C	3.58017	1.84695	-0.06847
C	2.17050	1.60400	-0.19321
C	1.57552	0.44161	-0.60823

C	0.15131	0.45992	-0.63100
C	-0.32355	1.70804	-0.23320
H	-0.41863	-0.05083	-1.80141
S	0.97171	2.82051	0.19535
H	9.47022	3.50177	0.66181
H	7.91205	3.44977	1.50536
H	7.97261	3.97375	-0.16051
H	2.16946	-0.41219	-0.90560
H	-4.86787	5.15182	-0.76809
S	-10.09171	0.39530	-0.41680
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C	-9.41482	-2.06738	-0.78513
C	-8.38832	-0.00252	-0.49403
O	-7.72127	2.28464	-0.21602
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C	-8.19936	-1.34731	-0.69371
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H	-9.47279	-3.13490	-0.94244
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H	-7.21523	-1.78568	-0.77322
H	-3.49301	5.75246	0.17548
C	-1.68385	2.18091	-0.17360
H	-1.46445	4.32363	0.03172
H	-4.87522	4.97989	0.97093
H	-2.03048	0.05488	2.51738
H	-1.27048	0.63238	4.77966
H	-4.09632	-2.81244	1.02893
C	-1.04328	-0.25718	2.83779
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H	-3.64458	-3.43811	-0.56275
H	-2.72599	-1.32711	-4.56921
H	-2.20724	-3.09319	3.30412
Pd	-0.82742	-1.46097	0.09453
H	-3.93918	-4.57023	0.78678
C	-0.21005	-0.96479	1.97153
C	0.65269	-0.30372	4.56012

O	-0.79396	-0.35725	-2.93107
C	-1.38366	-1.48896	-2.92300
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C	-1.69611	-3.87009	2.73698
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C	1.05882	-1.34002	2.41469
H	-1.12573	-1.90959	-5.00656
H	-0.66029	-3.90022	3.07291
C	-1.00378	-4.93944	0.13016
H	2.48059	-1.30187	4.02415
H	1.73275	-1.88170	1.76112
H	-1.06144	-4.80734	-0.94966
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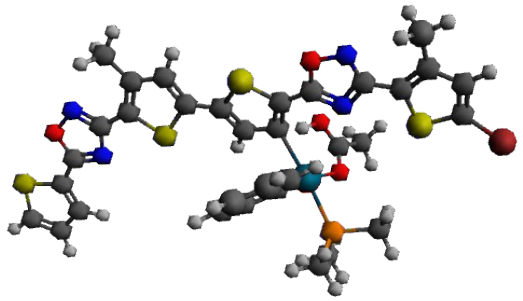
CM1-dimer_TSe



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S	-5.98057	-0.26053	-0.44717
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O	-2.38323	-3.40355	0.26670
C	-2.10713	-2.12775	-0.07671
C	-0.73496	-1.73461	-0.23618

C	-0.27130	-0.52790	-0.73328
C	1.15020	-0.53836	-0.78756
C	1.75649	-1.68752	-0.33531
H	-0.92426	-0.04874	-1.85772
S	0.55211	-2.85062	0.18595
H	-7.74407	-4.46463	0.78992
H	-6.15721	-4.27763	1.55792
H	-6.25078	-4.73495	-0.12575
H	6.71054	-4.52577	-0.83835
S	11.26416	0.87199	-0.29684
C	11.45967	2.58568	-0.44695
C	10.26285	3.23793	-0.53996
C	9.52264	1.04227	-0.36132
O	9.16198	-1.32217	-0.16273
C	8.63589	-0.08980	-0.28391
H	12.45173	3.00834	-0.45757
C	9.15473	2.35822	-0.49126
N	8.07661	-2.22103	-0.11231
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C	6.03248	-4.42744	0.01159
N	7.33682	-0.09132	-0.31774
C	5.66323	-1.90402	-0.20029
C	5.18357	-3.19560	-0.10603
H	10.17661	4.31042	-0.64012
S	4.36667	-0.73046	-0.32126
C	3.76812	-3.23104	-0.14375
H	8.12042	2.66489	-0.54871
H	5.40588	-5.31794	0.06262
C	3.16411	-2.00068	-0.26181
H	3.20782	-4.15560	-0.10183
H	6.66136	-4.39210	0.90334
H	1.30740	1.85164	1.58976
H	2.05244	1.29665	3.86215
H	-0.45775	4.99441	-0.01870
C	0.62472	1.33906	2.25749
C	1.05149	1.02300	3.54776
C	-1.52274	4.87829	-0.22023
H	-1.65617	4.67177	-1.28140
H	-1.93117	1.46860	-5.16287
H	-0.93575	4.03927	2.74547
Pd	-1.29113	1.42162	-0.05565
H	-2.04264	5.80102	0.04593
C	-0.65429	0.98606	1.82712
C	0.20244	0.35665	4.42528

O	-1.36729	0.17935	-2.99588
C	-1.97794	1.29761	-3.02495
O	-2.08962	2.06373	-2.03757
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C	-1.99365	3.97039	2.49501
H	-2.88865	2.73718	-4.33912
H	-2.47355	4.93749	2.65689
C	-1.07456	0.00249	4.00171
C	-1.50212	0.31893	2.71194
H	-3.50836	1.07935	-4.48564
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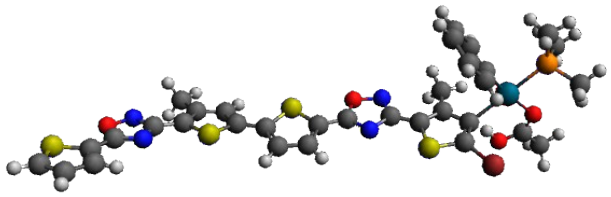
CM1-dimer_TSf



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C	-3.75024	-1.14389	-0.26769
C	-2.52633	-0.64485	-0.64768
S	-2.68905	0.67776	-1.79876
Br	-5.47421	1.64871	-2.81458
H	-5.83160	-1.32240	-1.44639
C	-3.92634	-2.29596	0.67822
C	-1.19486	-1.04366	-0.24850
N	-0.06974	-0.42996	-0.75887
N	-0.94097	-2.00391	0.61538
O	0.47009	-2.02049	0.67352
C	0.89983	-1.06124	-0.16608
C	2.31362	-0.84303	-0.31124
C	2.91731	0.07967	-1.13001
C	4.32337	0.04614	-1.06089
C	4.81245	-0.90027	-0.18595

H	4.96524	0.68479	-1.65145
S	3.49793	-1.76995	0.58488
H	-4.98068	-2.55832	0.75989
H	-3.54896	-2.04982	1.67337
H	-3.36720	-3.17263	0.34546
H	2.34912	0.74587	-1.76296
H	9.60932	-3.89803	0.73064
S	14.40973	1.26678	0.06679
C	14.71834	2.84525	-0.57349
C	13.57530	3.47219	-0.98225
C	12.69402	1.45957	-0.22547
O	12.17565	-0.71591	0.64681
C	11.73834	0.43312	0.09897
H	15.73061	3.21542	-0.60894
C	12.41737	2.68252	-0.78443
N	11.03919	-1.52278	0.85455
C	10.05390	-0.77226	0.41046
C	8.86216	-3.52212	1.43214
N	10.44960	0.45742	-0.07008
C	8.66759	-1.18035	0.41870
C	8.10388	-2.36349	0.85396
H	13.56187	4.46441	-1.40994
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C	6.69817	-2.36619	0.67964
H	11.41236	2.98737	-1.03777
H	8.18113	-4.33472	1.68512
C	6.18546	-1.21516	0.12784
H	6.08114	-3.21585	0.94059
H	9.40598	-3.23001	2.33259
H	-5.65995	2.90731	0.24501
H	-4.25450	4.29664	1.70240
H	-9.61223	2.26630	0.06000
C	-5.27862	2.48613	1.16792
C	-4.47735	3.27593	1.99262
C	-9.95116	1.32217	0.48664
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H	-8.13472	2.80236	2.56911
Pd	-6.74233	0.01332	0.31756
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C	-3.95983	2.75893	3.17600
O	-6.51929	-2.12255	-2.07417
C	-7.75046	-2.00506	-1.75881

O	-8.17704	-1.23326	-0.86802
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C	-8.72467	-2.85541	-2.53901
P	-8.63313	0.63576	1.58151
C	-8.52316	1.86003	2.95385
H	-9.71938	-2.80247	-2.10298
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H	-3.84175	1.02495	4.44209
H	-5.25356	-0.36931	2.99708
H	-9.62764	-1.57484	1.59314
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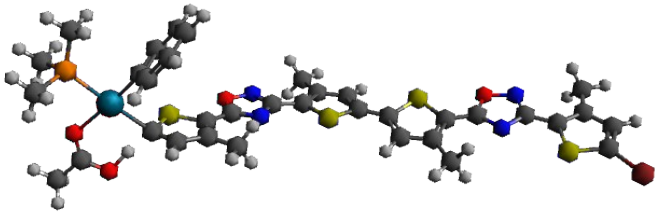
CM2-dimer_TSα



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S	-11.22835	-1.52471	0.56328
Br	-13.95720	-3.03014	1.02988
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C	-9.85694	0.54948	-0.62467
N	-8.71846	0.06914	-0.01688
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O	-8.29006	1.87011	-1.22179
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C	-6.39991	0.92093	-0.10590
C	-5.69944	0.04361	0.70389
C	-4.32846	0.38349	0.77453
C	-3.96813	1.49015	0.03897
H	-3.62161	-0.17118	1.37678
S	-5.35599	2.15429	-0.79369
H	-13.68707	1.45665	-2.15452

H	-12.03906	1.34720	-2.79749
H	-12.35554	2.35505	-1.40531
C	-6.29318	-1.12205	1.43784
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C	6.52621	-0.12840	1.28588
C	5.48731	-1.01436	1.51978
C	4.20591	0.77339	0.81963
O	3.31565	2.85242	0.03026
C	3.08266	1.59252	0.46065
H	7.49487	0.01824	2.27626
C	4.17991	-0.54109	1.26707
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C	-0.21501	2.58505	-0.10376
C	-0.96686	3.66405	-0.52469
H	5.66492	-2.01851	1.88520
S	-1.21379	1.20282	0.29479
C	-2.35264	3.37066	-0.51166
C	2.94639	-1.37170	1.46628
H	-1.21934	5.67532	-1.21337
C	-2.66658	2.09759	-0.09585
H	-3.10412	4.09863	-0.78789
H	0.26344	4.89502	-1.79093
H	10.28330	1.84420	4.09071
C	10.46245	0.79165	3.86143
H	10.32593	0.22990	4.78557
H	11.47693	0.67071	3.48915
C	9.45475	0.33888	2.83165
O	8.24346	0.25240	3.22487
O	9.83547	0.08702	1.66323
H	11.59386	0.60318	-0.29660
H	11.56921	-2.17691	0.72532
C	11.41488	0.19332	-1.28977
C	11.35386	-2.52212	-0.28539
H	12.36243	-0.08768	-1.75401
Pd	8.39065	-0.71701	0.15455
H	12.28956	-2.67590	-0.82696
H	10.92915	0.95695	-1.89751
P	10.29543	-1.26452	-1.12675
H	10.81588	-3.46809	-0.22256
C	7.20532	-1.55634	-1.26951

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C	6.13603	-3.51691	-2.21297
H	5.36889	-0.75423	-4.01538
C	5.56543	-2.74029	-3.21647
H	5.94517	-4.58371	-2.17592
H	4.92999	-3.19586	-3.96619
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H	2.38990	-1.48565	0.53425
H	2.26280	-0.90728	2.17912
H	-5.52453	-1.63925	2.01188
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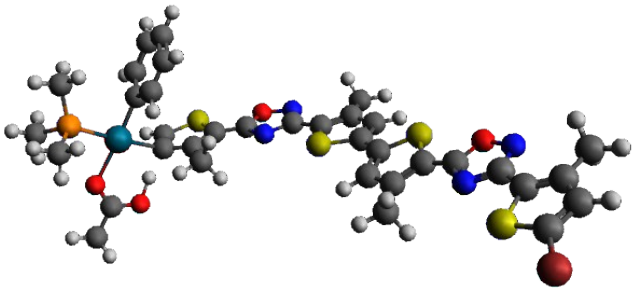
H	-7.08365	-0.80160	2.11835

CM2-dimer_TSa



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S	10.18421	-1.97119	-0.29719
Br	12.69011	-3.87378	-0.47587
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C	12.03355	1.21248	1.44432
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N	7.91146	0.01392	-0.03173
N	9.09848	1.67931	0.93854
O	7.75315	2.06481	0.77312
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C	5.71792	1.15162	-0.08863
C	4.88491	0.22286	-0.68844

C	3.56281	0.71050	-0.80720
C	3.36764	1.98015	-0.31145
H	2.77070	0.13839	-1.27114
S	4.85781	2.62033	0.34445
H	13.09757	1.17969	1.67885
H	11.47944	1.41217	2.36354
H	11.84750	2.06104	0.78320
C	5.30454	-1.13293	-1.17404
H	-0.25863	6.37803	-0.90297
S	-6.39747	2.99685	-0.77737
C	-7.22953	1.50218	-1.01016
C	-6.40986	0.39840	-1.08338
C	-4.85866	2.14500	-0.78366
O	-3.69533	4.21413	-0.47021
C	-3.63151	2.87237	-0.62436
H	-8.30610	1.52891	-1.09803
C	-5.02791	0.78544	-0.95687
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C	0.67314	4.58197	-0.16694
H	-6.69768	-0.46457	-2.17450
S	0.59022	1.99363	-0.45528
C	2.01241	4.12099	-0.14095
C	-3.90052	-0.20039	-1.03731
H	1.19152	6.64425	0.08170
C	2.15466	2.76048	-0.28552
H	2.85622	4.79033	-0.03620
H	-0.34932	6.19118	0.83149
H	4.45770	-1.65388	-1.62054
H	5.69878	-1.74054	-0.35772
H	6.10224	-1.05989	-1.91493
H	-4.29181	-1.19665	-1.24069
H	-3.33426	-0.22897	-0.10426
H	-3.19016	0.06997	-1.82046
H	-8.25437	0.63618	2.01382
H	-7.42165	1.53620	4.13974
H	-10.54622	-2.73536	0.95966
C	-7.30769	0.27927	2.40194
C	-6.83568	0.79401	3.60924
C	-9.92837	-3.56747	0.62144
H	-9.97707	-3.61583	-0.46563

H	-8.73646	-2.13479	-4.87302
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Pd	-7.25432	-1.43587	-0.05965
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C	-5.34706	-1.09460	2.22283
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H	-3.91917	-0.91434	3.81837
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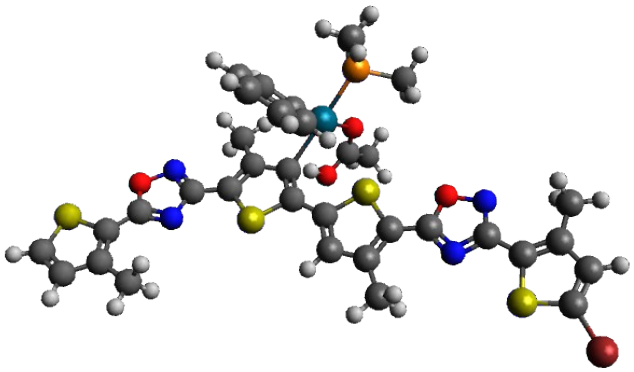
CM2-dimer_TSb



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Br	10.45933	-3.47176	0.28589
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N	4.73822	-1.18669	-0.11758
N	5.38590	0.98250	-0.11729
O	3.98149	0.88740	-0.20374
C	3.67717	-0.43023	-0.19875
C	2.29933	-0.81091	-0.27185
C	1.76847	-2.09066	-0.25838
C	0.35997	-2.06655	-0.34426
C	-0.20179	-0.80779	-0.42019
H	-0.23431	-2.96972	-0.37262
S	1.04737	0.41816	-0.38107
H	9.37095	1.92426	0.08531
H	7.78812	2.00215	0.87881
H	7.87599	1.96203	-0.86634
C	2.56346	-3.36013	-0.17643
H	-5.07453	1.51365	-2.30735
S	-9.68772	-3.24560	-0.19618
C	-9.95961	-4.88504	0.27494
C	-8.79595	-5.54402	0.54199
C	-7.95361	-3.46235	-0.02600
O	-7.57854	-1.18874	-0.67365
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H	-10.96700	-5.26647	0.32688
C	-7.63041	-4.74490	0.37532
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C	-5.44737	-1.05479	-0.59132
C	-4.46078	1.79712	-1.44990
N	-5.75532	-2.35042	-0.22857
C	-4.08178	-0.58164	-0.65086
C	-3.59252	0.65828	-0.99975
H	-8.75862	-6.57923	0.85238
S	-2.79729	-1.69243	-0.22368
C	-2.16105	0.75354	-0.92589
C	-6.24119	-5.25853	0.61305
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C	-1.59510	-0.45706	-0.53735
H	-1.57987	1.30790	-2.07249
H	-5.15639	2.09957	-0.66404
H	1.89856	-4.22375	-0.17421
H	3.17590	-3.38659	0.72636
H	3.25271	-3.45095	-1.01772
H	-6.27229	-6.30186	0.92739
H	-5.72839	-4.67610	1.38029
H	-5.63024	-5.18202	-0.28799

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C	-1.28804	1.45645	2.58341
C	-1.81152	1.13514	3.83595
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H	1.52965	4.72791	-0.71163
H	0.87499	2.65137	-4.68962
H	0.02484	4.26705	3.11605
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H	1.78563	5.82940	0.66971
C	-2.03062	2.21205	1.67598
C	-3.08128	1.57019	4.20124
O	-1.16874	1.63036	-3.18587
C	-0.58089	2.76293	-3.14076
O	-0.45956	3.44971	-2.09952
H	-3.48752	1.31919	5.17359
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P	-0.39449	4.69592	0.75844
C	-0.48293	5.05614	2.56270
H	0.31492	4.30312	-4.34556
H	-0.01628	6.01771	2.78481
C	-3.82653	2.32549	3.30193
C	-3.30321	2.64716	2.04926
H	-0.71793	3.15101	-5.24402
H	-1.52428	5.06997	2.88201
C	-1.13819	6.19380	-0.02416
H	-4.82055	2.66589	3.56984
H	-3.90634	3.23364	1.36590
H	-1.05720	6.09600	-1.10622
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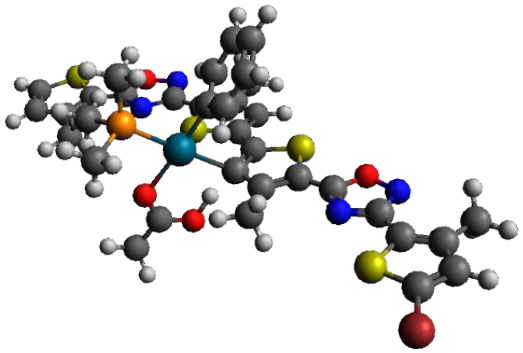
CM2-dimer_TSc

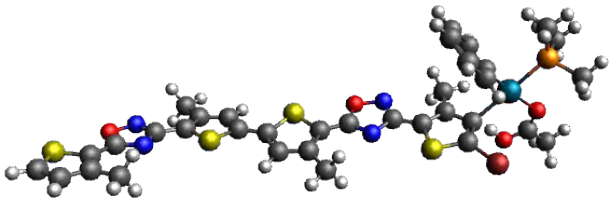


C	9.11223	-0.18420	-0.66632

C	9.46777	1.08093	-0.30953
C	8.34687	1.92931	-0.07423
C	7.15291	1.26875	-0.26357
S	7.39221	-0.40773	-0.73445
Br	10.28696	-1.61178	-1.06480
H	10.49329	1.40776	-0.21486
C	8.48463	3.36821	0.33068
C	5.79658	1.75590	-0.12957
N	4.70943	0.94458	-0.35895
N	5.49604	2.98774	0.21493
O	4.08766	2.98583	0.21095
C	3.69742	1.73978	-0.13858
C	2.29284	1.46216	-0.21476
C	1.67354	0.27710	-0.55933
C	0.24084	0.34629	-0.52085
C	-0.19651	1.61936	-0.16489
H	-0.36206	-0.19773	-1.67073
S	1.12903	2.72115	0.15745
H	9.53647	3.64217	0.41433
H	7.99642	3.55875	1.28832
H	8.00751	4.03096	-0.39385
C	2.41547	-0.96254	-0.96653
H	-4.66951	5.22162	-0.34760
S	-10.01022	0.78570	-0.52176
C	-10.57213	-0.75771	-1.05493
C	-9.54642	-1.59529	-1.38105
C	-8.34371	0.27922	-0.74367
O	-7.57503	2.45360	-0.11174
C	-7.26611	1.18766	-0.45883
H	-11.63142	-0.95564	-1.09717
C	-8.25694	-1.01877	-1.21053
N	-6.35616	3.12488	0.10429
C	-5.45386	2.19942	-0.14070
C	-3.99427	4.94003	0.46228
N	-5.98198	0.97270	-0.49056
C	-4.03052	2.43020	-0.05164
C	-3.35341	3.60815	0.20281
H	-9.69631	-2.60448	-1.73946
S	-2.93540	1.08432	-0.30469
C	-1.95348	3.41504	0.18798
C	-6.98329	-1.75251	-1.50934
H	-3.23355	5.71344	0.56907
C	-1.54419	2.12351	-0.06789
H	-1.25743	4.22639	0.35465

H	-4.59846	4.91881	1.37166
H	1.71306	-1.75171	-1.23176
H	3.05905	-1.32134	-0.16084
H	3.07191	-0.77022	-1.81707
H	-7.20158	-2.72402	-1.95313
H	-6.39514	-1.90818	-0.60284
H	-6.34793	-1.18711	-2.19209
H	-1.88745	0.28599	2.61930
H	-1.08070	0.94599	4.84225
H	-4.16280	-2.63679	1.30961
C	-0.92961	-0.08536	2.96445
C	-0.47194	0.29302	4.22681
C	-3.63471	-3.46930	0.84472
H	-3.72981	-3.37942	-0.23669
H	-2.72104	-1.47768	-4.37255
H	-2.29994	-2.83013	3.60702
Pd	-0.82642	-1.48110	0.31042
H	-4.07517	-4.41071	1.17979
C	-0.15934	-0.91572	2.15021
C	0.75801	-0.15864	4.69412
O	-0.75274	-0.54460	-2.77529
C	-1.40599	-1.64008	-2.70357
O	-1.60727	-2.26925	-1.63907
H	1.11377	0.13735	5.67353
C	-1.96169	-2.16992	-4.00366
P	-1.84374	-3.37798	1.28091
C	-1.82059	-3.66670	3.09998
H	-2.40166	-3.15419	-3.86278
H	-2.34098	-4.59368	3.34822
C	1.53043	-0.98727	3.88708
C	1.07334	-1.36600	2.62434
H	-1.17033	-2.21268	-4.75252
H	-0.78964	-3.71946	3.44767
C	-1.15805	-4.94307	0.58088
H	2.49489	-1.34014	4.23485
H	1.69684	-2.00840	2.01333
H	-1.20814	-4.88848	-0.50610
H	-1.71921	-5.81157	0.93210
H	-0.11384	-5.04732	0.87598

CM2-dimer_TSd



C	-4.67411	0.85289	-1.56448
C	-5.11921	-0.28778	-0.94592
C	-3.98521	-1.06468	-0.49798
C	-2.76907	-0.48680	-0.77690
S	-2.95413	1.04784	-1.62040
Br	-5.75794	2.18829	-2.37795
H	-6.08066	-1.00597	-1.66549
C	-4.14278	-2.39240	0.18438
C	-1.43032	-0.94989	-0.48443
N	-0.31505	-0.23180	-0.86425
N	-1.16159	-2.06807	0.15370
O	0.24893	-2.08561	0.19466
C	0.66898	-0.96522	-0.42742
C	2.08117	-0.72691	-0.52441
C	2.72174	0.34018	-1.12852
C	4.12865	0.22510	-1.02950
C	4.57156	-0.89560	-0.36488
H	4.80360	0.95166	-1.46164
S	3.21915	-1.86213	0.18079
H	-5.19546	-2.66978	0.23020
H	-3.74347	-2.36343	1.20070
H	-3.59190	-3.17612	-0.33946
C	2.03911	1.48321	-1.81965
H	9.25756	-4.17071	0.00350
S	14.22286	0.77287	0.47827
C	14.66691	2.41682	0.19128
C	13.58864	3.19907	-0.10111
C	12.53352	1.15843	0.19406
O	11.91883	-1.11970	0.59545
C	11.52969	0.13441	0.28508
H	15.70283	2.70966	0.25582
C	12.35186	2.49607	-0.10494
N	10.75562	-1.91304	0.61838
C	9.80272	-1.05715	0.32183
C	8.51059	-3.91472	0.75730
N	10.24304	0.23141	0.10601
C	8.40520	-1.41362	0.22725
C	7.79829	-2.64048	0.40989

H	13.66340	4.25717	-0.31120
S	7.24619	-0.15959	-0.16594
C	6.39691	-2.56306	0.21805
C	11.03539	3.15176	-0.39981
H	7.80060	-4.73782	0.83864
C	5.92852	-1.30972	-0.10088
H	5.75009	-3.42690	0.29665
H	9.04816	-3.82293	1.70303
H	2.77687	2.17738	-2.22211
H	1.38462	2.02491	-1.13479
H	1.40485	1.13220	-2.63510
H	11.17797	4.21389	-0.59888
H	10.34122	3.04201	0.43505
H	10.54965	2.69570	-1.26415
H	-5.96926	2.78638	0.86514
H	-4.56004	3.88945	2.54629
H	-9.88586	2.10682	0.65081
C	-5.54977	2.19605	1.67144
C	-4.74610	2.82397	2.62317
C	-10.19858	1.08584	0.87012
H	-10.38179	0.56966	-0.07150
H	-9.03787	-1.76897	-3.93099
H	-8.35788	2.11899	3.18788
Pd	-6.97176	-0.09107	0.35948
H	-11.11387	1.10858	1.46531
C	-5.79430	0.82448	1.74331
C	-4.17976	2.09048	3.66084
O	-6.77151	-1.66230	-2.43922
C	-7.99517	-1.64770	-2.07676
O	-8.41147	-1.09848	-1.02974
H	-3.55341	2.57839	4.39782
C	-8.97396	-2.33467	-2.99927
P	-8.84292	0.20749	1.76335
C	-8.72072	1.10737	3.36627
H	-9.95891	-2.39450	-2.54252
H	-9.69375	1.14780	3.85959
C	-4.41869	0.72239	3.73717
C	-5.22422	0.09414	2.78679
H	-8.60964	-3.33145	-3.24880
H	-8.00159	0.60584	4.01267
C	-9.61661	-1.40441	2.22494
H	-3.97655	0.13668	4.53543
H	-5.39170	-0.97391	2.86580
H	-9.79626	-1.97528	1.31459

H	-10.55852	-1.25265	2.75629
H	-8.93303	-1.96823	2.85993

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