Electronic Supplementary Information

Influence of shape on crystal structure and optical properties of heterocyclic conjugated molecules

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General Experimental Information

Experimental

Unless otherwise specified, all reactants and solvents were purchased from commercial sources. Reactions were performed under air-free conditions, with procedures based on previous literature from the Thomas Lab, or from cited reference. Purification by flash column chromatography used silica gel (230-400 mesh) as the stationary phase, with the mobile phases listed in each methodology.

Nuclear Magnetic Resonance (NMR)

NMR spectra were acquired using a Bruker Advance III 500 MHz spectrometer in deuterated chloroform. TopSpin 3.6 was used to analyze and integrate spectra.

High Resolution Mass Spectrometry (HRMS)

For the compounds that do not have associated crystal structures, high resolution mass spectrometry data is provided. The HRMS data was acquired using a Waters Synapt G2-Si#UGA354 electrospray ionization time of flight spectrometer. The tolerance of this analysis is 5.0 ppm with DBE minimum of -1.5 and maximum of 100.0.

This data was collected in collaboration with Furong Sun and the Mass Spectrometry Lab at The University of Illinois – Urbana.

Optical Properties: Absorbance, Emission, and Excitation

Solution samples for optical data were prepared in quartz cuvettes and spectroscopy grade chloroform. Thin films used microscope slides and were deposited using spin cast deposition, and annealed in a 100°C oven for 10 minutes. Powder analysis was performed by either placing the powders in a Teflon holder or pressing onto glass plates. UV/Vis Absorption spectra were collected either using a Varian Cary-100 spectrophotometer (**TT-F5**, **TT-H5**, **DTT-F5**, **DTT-H5**) or a Varian Cary-Flexible (**BDT-F5**, **BDT-H5**, **mCPDT-F5**, **mCPDT-H5**). Emission and excitation spectra were collected using PTI Quantum Master 4 with a 90° angle detector and a 75W Xe lamp irradiation source. Quantum yield measurements for solution were collected using dilute chloroform solutions with their respective standard listed in the data table. QY for solid state used a PTI petite K-Sphere with the same fluorimeter. Fluorescence lifetimes in solution were calculated using a 403 nm pulsed LED light source for time correlated single photon counting (TCSPC). Ludox (2 drops in 100 mL deionized water) was used as the standard to determine the instrument response function. These results were analyzed using FelixGX with a 1 to 4 exponential lifetime analysis.

Differential Scanning Calorimetry (DSC)

DSC spectra were obtained using a TA Discover DSC 250 with a finned-air colling system (FACS). 1-2 mg of each powder was placed into a TZero pan and lid and heated at a rate of 10 °C/min, and cooled at 5 °C/min.

Single Crystal X-Ray Diffraction (SC-XRD)

Crystals were grown in a 1.0- or 1.5-dram vial by slow vapor diffusion of hexanes into chloroform or dichloromethane. For the analysis of BDT-F5 and TT-F5, single crystal data was obtained in collaboration with Peter Müller and the X-Ray Diffraction Facility at Massachisetts Institute of Technology using a Bruker-AXS X8 Kappa Duo four-circle diffractometer coupled to a Smart Apex2 CCD detector with Cu Kα radiation (λ = 1.54184 Å), from an IμS micro-source.

The single crystal analysis of DTT-F5, DTT-H5, mCPDT-F5, mCPDT-H5 used a low temperature single crystal XRD collected on a Bruker D8 quest diffractometer coupled with a Photon CMOS detector with Mo Kα radiation (λ = 0.71073 Å) from a fine-focused sealed tube source.

All structures were analyzed using φ and ω scans, and by using ShelXL and ShelXS to solve and refine the structure solutions against F2. G.M. Sheldrick (2015) "Crystal structure refinement with SHELXL", Acta Cryst., C71, 3-8 (Open Access)

Wide Angle X-Ray Scattering (WAXS)

The WAXS is performed with the XCalibur Instrument (Oxford) located at the Institute of Materials Science X-Ray lab (University of Connecticut at Storrs, CT). The instrument has a fine focus Copper X-ray tube and a high-speed Onyx CCD 2D detector to collect high-quality diffraction data. The 4-circle kappa goniometer allows easy crystal mounting and

alignment. Each powder sample was placed between two pieces of Kapton tape, and analyzed by Cu Kα radiation, λ = 1.542 Å. The 2D data then were converted to 1D data via circular average around the beam center.

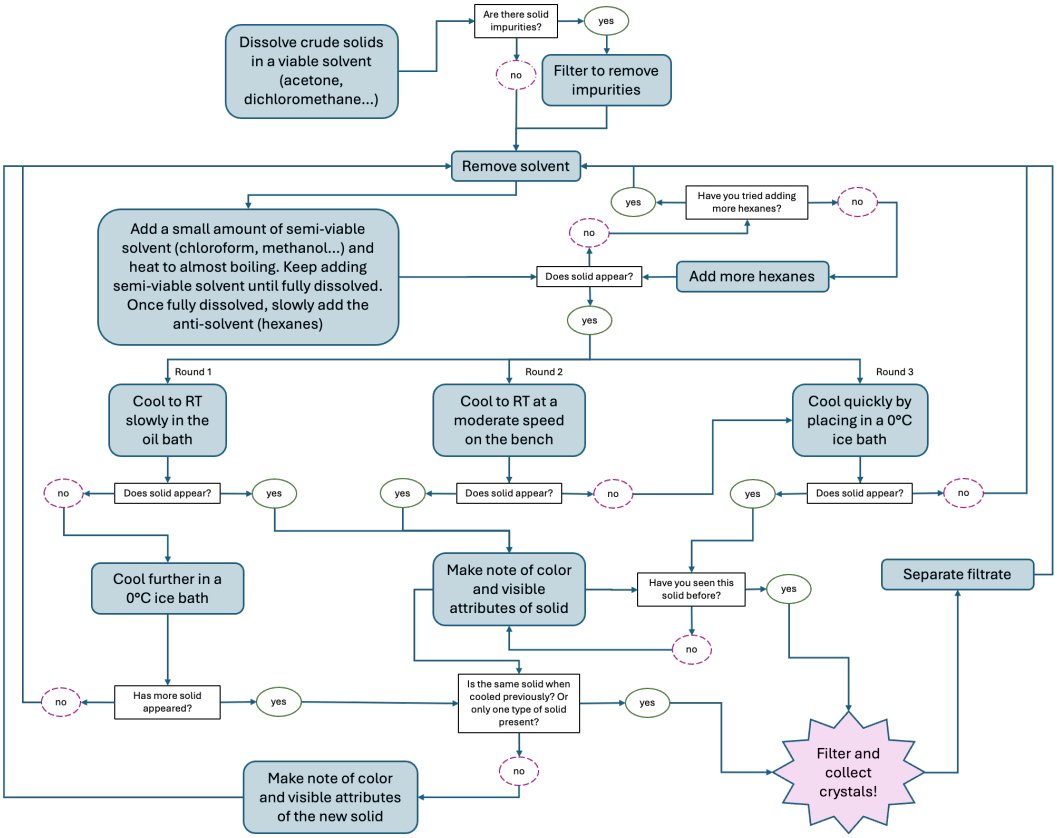
Density Functional Theory (DFT)

DFT calculations were performed using the Gaussian 16 software package with ultrafine integrations. Both optimized geometries and frontier molecular orbitals for solution state using chloroform as the solvent model were determined using the B3LYP/6-31G (d,p) basis set level of theory. All of the free energies are reported in a.u. and cartesian coordinates in angstroms. The timise dependent analysis for the HOMO and LUMO energy levels were performed on these optimized geometries for solution, and on the single crystal XRD coordinates where applicable, were calculated using the same basis set. Transitions where the oscillator strength is larger than 0.2 is listed for each compound.

Polymorph Separation

Each polymorph was separated using various techniques including different crystallization methods, with a standard procedure. Each isolated polymorph was analyzed by NMR to confirm purity. **TT-H5** was the first polymorph to be identified and collected. Upon slow recrystallization, both yellow and orange solids were observed once filtered. After a few attempts of collecting one type of solid, recrystallizing, and continuing to see both solids, the mixture was hand separated by using a spatula and forceps. This did not yield 100% separation, but the NMR spectra of the collected solids were identical to the original **TT-H5** solid. Photos of the separated polymorph can be seen in Figure 6 of the manuscript.

For other samples, a series of slow, fast, warm, cold, and various solvent combinations were used to separate each polymorph. NMRs spectra of each solid were obtained prior to isolating the solids to rule out collected solids being impurities. An example of polymorph separation includes completely dissolving a solid in a viable solvent (acetone, dichloromethane, etc..) and filtering the solution to remove insoluble impurities, then removing solvent by rotary evaporator. Warming solid in just enough semi-soluble solvent (chloroform, methanol…) fully dissolved the solid. Then, warm non-solvent was slowly added until solid began to form. The was cooled slowly in the oil bath to room temperature, then placed in an ice bath to obtain more solid. Crystals were collected by filtration and and rinsed with cold solvent, followed by collecting of filtrate to try and get a different polymorph. The process was repeated using a different cooling method, or a different solvent. See a flow chart below for the methods used to obtain different polymorphs:



Experimental Procedures

(2,3,4,5,6-Pentafluorophenyl)methyl 2-iodobenzoate (1)

2-Iodobenzoic acid (1.25 g, 5.0 mmol), dimethylaminopyridine (DMAP, 122 mg, 1.0 mmol), and dicyclohexylcarbodiimide (DCC, 1.1 g, 5.5 mmol) were added to a flame dried round bottom flask. A solution of pentafluorobenzyl alcohol (1.0 g, 5.25 mmol) in 60 mL anhydrous dichloromethane was then added. The mixture was stirred at room temperature overnight, followed by filtration over Celite. The filtrate was washed with water and brine, dried over magnesium sulfate, and concentrated by rotary evaporation. The crude product was then purified by flash column chromatography on silica, using pure dichloromethane as the eluent, to yield 2.0 g of **1** as a white solid (4.7 mmol, 93% yield).

^{1}H NMR: (500 MHz, $CDCl_3$): δ 8.03 (d, 1H), 7.81 (d, 1H), 7.43 (t, 1H), 7.19 (t, 1H), 5.48 (s, 2H).

The peaks are consistent with those reported in the literature.[1]

Phenylmethyl 2-iodobenzoate (2)

Following an identical procedure as **1**, using benzyl alcohol (0.54 mL, 5.3 mmol) in place of pentafluorobenzyl alcohol. The reaction afforded 1.6 g of **2** as a colorless oil (4.7 mmol, 94% yield).

^{1}H NMR: (500 MHz, $CDCl_3$): δ 8.02 (d, 1H), 8.01 (d, 1H), 7.50 (d ,2H), 7.44-7.40 (m, 4H), 7.18 (t, 1H), 5.40 (s, 2H).

The peaks are consistent with those reported in the literature.[1]

(2,3,4,5,6-Pentafluorophenyl)methyl 2-[2-(trimethylsilyl)ethynyl]benzoate (3)

Compound **1** (850 mg, 2.0 mmol) was dissolved in 15 mL of degassed THF/NEt_3 mixture (2:1, v:v). Trimethylsilyl acetylene (300 mg, 3.0 mmol), bis(triphenylphosphine)palladium(II) dichloride (70 mg, 0.1 mmol), and copper(I) iodide (20 mg, 0.1 mmol) were then added to the flask. The reaction was stirred overnight at 80 °C under an atmosphere of argon. After filtering over Celite, the solvent was removed by rotatory evaporation. The crude

product was purified by flash column chromatography on silica, using dichloromethane as an eluent, and 765 mg of compound **3** was collected as a brown oil (1.9 mmol, 96% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.90 (d, 1H), 7.60 (d, 1H), 7.47 (t, 2H), 7.39-7.37 (m, 1H), 5.47 (s, 2H), 0.28 (s, 9H).

The peaks are consistent with those reported in the literature.[1]

Phenylmethyl 2-[2-(trimethylsilyl)ethynyl]benzoate (**4**)

Compound **2** (490 mg, 1.5 mmol) was subjected to Sonogashira coupling and followed the same procedure for **3**. 451 mg of **4** as a dark oil was collected (1.45 mmol, 97% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.90 (d, 1H), 7.57 (d, 1H), 7.47-7.30 (m, 7H), 5.38 (s, 2H), 0.22 (s, 9H).

The peaks are consistent with those reported in the literature.[1]

(2,3,4,5,6-Pentafluorophenyl)methyl 2-ethynyl benzoate (5)

Compound **3** (750 mg, 1.8 mmol) was dissolved in 10 mL of tetrahydrofuran and cooled to 0°C. Tetra-*n*-butylammonium fluoride was added as a 1.0 M THF solution (2.0 mL, 2.0 mmol). The mixture was stirred for 10 minutes at 0°C, then quenched by adding cold water. The product was extracted twice by diethyl ether, washed with brine, dried over $MgSO_4$, and concentrated by rotary evaporation. The crude product was passed through a silica plug using 1:1 dichloromethane:hexanes as eluent to afford 540 mg of **5** as a dark oil (1.65 mmol, 92% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.93 (d, 1H), 7.64 (d, 1H), 7.52 (t, 2H), 7.43 (t, 1H), 5.48 (s, 2H), 3.38 (s, 1H).

The peaks are consistent with those reported in the literature.[1]

Phenylmethyl 2-ethynyl benzoate (6)

Compound **4** (450 mg 1.4 mmol) was dissolved in 10 mL of tetrahydrofuran and cooled to 0°C. Tetra-n-butylammonium fluoride (TBAF) was added as a 1.0 M THF solution (2 mL, 2 mmol). The mixture was stirred for 10 min in the ice bath, then quenched adding cold water. The product was extracted twice by diethyl ether, washed with brine, dried with $MgSO_4$, and concentrated by Rotary evaporator. The crude product was passed through a silica plug, using 1:1 dichloromethane:hexanes as the eluent. This produced 200 mg of **6** as a dark oil after purification mg, (60% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.99 (d, 1H), 7.65 (d, 1H), 7.52-7.36 (m, 7H), 5.41 (s, 2H), 3.38 (s, 1H).

The peaks are consistent with those reported in the literature.[1]

2,5-bis((trimethylsilyl)ethynyl)thieno[3,2-b]thiophene (7)

2,5-Dibromothieno[3,2-*b*]thiophene (120 mg, 0.4 mmol), copper(I) iodide (2 mg, 0.012 mmol), and bis(triphenylphosphine)palladium(II) dichloride (6 mg, 0.008 mmol) was added to a flame dried round bottom flask. Trimethylsilyl acetylene (91 mg, 0.93 mmol) was dissolved in 10 mL of degassed diisopropylamine and tetrahydrofuran (2:1, v:v) and added to the flask. After refluxing overnight under an argon atmosphere, the reaction mixture was filtered through Celite and purified by flash column chromatography on silica, using 1:2 dichloromethane:hexanes as the eluent producing 100 mg of **7** as a colorless solid (0.3 mmol, 75% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.31 (s, 1H), 0.29 (s, 9H).

2,5-diethynylthieno[3,2-b]thiophene (8)

Compound **7** (100 mg, 0.3 mmol) was dissolved in 10 mL of tetrahydrofuran and cooled to 0 °C. Tetra-*n*-butylammonium fluoride was added dropwise as a 1.0 M tetrahydrofuran solution (0.7 mL, 0.7 mmol) and stirred for 15 minutes at 0 °C. Then, the reaction was quenched by adding 10 mL of water. The product was extracted 3 times with diethyl ether, dried over magnesium sulfate, and concentrated by rotary evaporation to yield 90 mg of **8** as oily orange crystals, which was used without further purification.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.61 (s, 2H), 4.20 (s, 2H).
The peaks are consistent with those reported in the literature.[2]

Bis((perfluorophenyl)methyl) 2,2'-(thieno[3,2-b]thiophene-2,5-diylbis(ethyne-2,1-diyl))dibenzoate (TT-F5)
2,5-Dibromothieno[3,2-*b*]thiophene (55 mg, 0.19 mmol) was added to a flame dried round bottom flask containing compound **5** (125 mg, 0.39 mmol), copper (I) iodide (20 mg, 0.006 mmol), and tetrakis(triphenylphosphine)palladium(0) (40 mg, 0.009 mmol) in 8 mL of degassed tetrahydrofuran and triethylamine (1:1, v:v). The flask was heated to 60°C and stirred overnight under an argon atmosphere. Once cooled, the reaction mixture was filtered over Celite, and reduced with a rotary evaporator to a yellow oil. The crude product was then purified by flash column chromatography on silica, using 2:1 CH_2Cl_2:hexanes as the eluent. Recrystallization from chloroform and hexanes yielded 21 mg of **TT-F5** as a yellow powder (0.03 mmol, 14% yield).
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.03 (d, 1H), 7.69 (d, 1H), 7.57 (t, 1H), 7.44 (t, 1H), 7.40 (s, 1H), 5.52 (s, 2H).
^{13}C NMR (125 MHz, $CDCl_3$): δ 165.1, 139.7, 134.0, 132.4, 131.0, 130.3, 128.4, 126.5, 124.2, 123.4, 94.3, 88.3, 54.0

Dibenzyl 2,2'-(thieno[3,2-b]thiophene-2,5-diylbis(ethyne-2,1-diyl))dibenzoate (TT-H5)
Compound 8 (90 mg, 0.5 mmol) was added to a flame-dried round bottom flask with tetrakis(triphenylphosphine)palladium(0) (0.03 mg, 0.025 mmol), copper (I) iodide (0.03 mg, 0.015 mmol) and dissolved in argon sparged 2:1 THF:TEA (volume of solvent). Compound **2** (360 mg, 1.05 mmol) was added and the reaction was heated to 70 °C overnight under inert conditions. After filtration through Celite, the crude product was purified via flash column chromatography on silica with a gradient from 2:1 Hexanes:CH_2Cl_2 to 1:2 Hexanes:CH_2Cl_2. Recrystallization in chloroform and hexanes yielded **TT-H5** as two polymorphs: 55 mg of a yellow solid and 45 mg of an orange solid (total 0.16 mmol, 33% yield).
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.09 (d, 1H), 7.67 (d, 1H), 7.56-7.51 (m, 3H), 7.43 (t, 1H), 7.42-7.36 (m, 3H), 7.11 (s, 1H), 5.46 (s, 2H).
^{13}C NMR (125 MHz, $CDCl_3$): δ 165.9, 139.6, 135.8, 133.8, 131.9, 131.4, 130.9, 128.6, 128.4, 128.3, 128.3, 126.5, 124.4, 123.1, 94.7, 88.2, 67.2
HRMS (TOF, ESI) m/z calculated for $C_{38}H_{25}O_4S_2$ [M+1] is 609.1194, found 609.1188

Bis((perfluorophenyl)methyl) 2,2'-(dithieno[3,2-b:2',3'-d]thiophene-2,6-diylbis(ethyne-2,1-diyl)) dibenzoate (DTT-F5)
2,6-Dibromodithieno[3,2-*b*:2′,3′-*d*]thiophene (250 mg, 0.7 mmol) was added to a flame-dried round bottom flask and dissolved in 15 mL of degassed tetrahydrofuran and triethylamine mixture (1:2, v:v). Copper (I) iodide (4 mg, 0.02 mmol), tetrakis(triphenylphosphine)palladium(0) (40 mg, 0.04 mmol), and compound **5** (480 mg, 1.5 mmol) were added, and the reaction mixture was stirred at 65°C overnight under an argon atmosphere. After filtering over Celite, the crude product was purified by flash column chromatography on silica, using 1:1 hexanes:diethyl ether as the eluent. Recrystallization in chloroform and hexanes produced 260 mg of **DTT-F5** as a dark yellow solid (0.30 mmol, 44% yield).
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.03 (d, 1H), 7.68 (d, 1H), 7.56 (t, 1H), 7.48 (s, 1H), 7.43 (t, 1H), 5.52 (s, 2H)
^{13}C NMR (125 MHz, $CDCl_3$): δ 165.6, 124.1, 134.0, 132.4, 131.8, 131.0, 130.3, 128.4, 125.5, 124.1, 123.4, 93.8, 88.3, 54.0.

Dibenzyl 2,2'-(dithieno[3,2-b:2',3'-d]thiophene-2,6-diylbis(ethyne-2,1-diyl))dibenzoate (DTT-H5)
2,6-Dibromodithieno[3,2-*b*:2′,3′-*d*]thiophene (250 mg, 0.7 mmol) was added to a flame dried round bottom flask and dissolved in 15 mL of a degassed tetrahydrofuran and triethylamine mixture (1:2, v:v). Copper (I) iodide (4

mg, 0.02 mmol), tetrakis(triphenylphosphine)palladium(0) (40 mg, 0.04 mmol), and compound **6** (350 mg, 1.5 mmol) were added, and the reaction mixture was stirred at 65 °C for 16 hours under an argon atmosphere. After filtering over Celite, the crude product was purified by flash column chromatography on silica, using 1:1 hexanes:diethyl ether as the eluent. Recrystallization in chloroform and hexanes produced **DTT-H5** as two polymorphic solids: 74 mg of orange solid and 56 mg of red solid (0.20 mmol total, 28% yield)

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.09 (d, 1H), 7.68 (d, 1H), 7.57-7.52 (m, 3H), 7.44-7.37 (m, 4H), 7.19 (s, 1H) 5.47 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 166.0, 142.0, 135.9, 133.8, 131.9, 131.8, 131.4, 131.0, 128.7, 128.5, 128.3, 128.3, 125.7, 124.2, 94.3, 88.2, 67.2

Bis((perfluorophenyl)methyl) 2,2'-(benzo[1,2-b:4,5-b']dithiophene-2,6-diylbis(ethyne-2,1-diyl)) dibenzoate (BDT-F5)

2,6-Dibromobenzo[1,2-*b*:4′,5′-*b*]dithiophene (122 mg, 0.35 mmol) was added to a flame-dried round bottom flask and dissolved in 15 mL of a degassed tetrahydrofuran and triethylamine mixture (1:2, v:v). Copper(I) iodide (3 mg, 0.01 mmol), tetrakis(triphenylphosphine)palladium(0) (23 mg, 0.02 mmol), and compound **5** (260 mg, 0.8 mmol) were added, and the reaction mixture was stirred at 65 °C for 16 hours under inert conditions. After filtering over Celite and reducing by rotary evaporation, the crude product was purified by flash column chromatography on silica, using 1:1 dichloromethane:hexanes as the eluent. Recrystallization in chloroform and hexanes produced 30 mg of **BDT-F5** as a yellow solid (0.03 mmol, 10% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.19 (s, 1H), 8.06 (d, 1H), 7.71 (d, 1H), 7.58 (t, 1H), 7.52 (s, 1H), 7.47 (t, 1H) 5.53 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 165.2, 138.1, 137.8, 134.2, 132.4, 131.1, 130.6, 128.6, 128.1, 124.0, 123.2, 116.6, 94.2, 88.1, 54.1

Dibenzyl 2,2'-(benzo[1,2-b:4,5-b']dithiophene-2,6-diylbis(ethyne-2,1-diyl))dibenzoate (BDT-H5)

2,6-Dibromobenzo[1,2-*b*:4′,5′-*b*]dithiophene (175 mg, 0.5 mmol) was added to a flame-dried round bottom flask and dissolved in 15 mL of a degassed mixture of tetrahydrofuran and triethylamine (1:2, v:v). Copper (I) iodide (3 mg, 0.015 mmol), tetrakis(triphenylphosphine)palladium(0) (29 mg, 0.025 mmol), and compound **6** (260 mg, 1.1 mmol) were added, and the reaction mixture was stirred at 65 °C for 16 hours under an argon atmosphere. After filtering over Celite, the crude product was purified by flash column chromatography on silica, using 1:1 dichloromethane and hexanes as the eluent. Recrystallization in chloroform and hexanes produced 31 mg of **BDT-H5** as a yellow solid (0.05 mmol, 24% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.13 (s, 1H), 8.09 (d, 1H), 7.71 (d, 1H), 7.58-7.53 (m, 3H), 7.45 (t, 1H), 7.40-7.34 (m, 4H) 5.48 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$): *δ* 165.9, 138.1, 137.8, 135.9, 134.1, 131.9, 131.6, 130.9, 128.6, 128.5, 128.4, 128.3, 124.2, 123.0, 116.6, 94.7, 88.1, 67.2

HRMS (TOF, ESI): m/z calculated for $C_{41}H_{27}O_4S_2$ [M+1] is 659.1351, found 659.1343

4,4-dimethyl-4H-cyclopenta[2,1-b:3,4-b']dithiophene (9)

Following a previously reported procedure[3]. In a flame dried found bottom flask, cushed potassium hydroxide (1.6 g, 28 mmol) was dissolved in 20 mL of dimethylsulfoxide. 4H-cyclopenta[2,1-b:3,4-b']dithiophene (1g, 5.6 mmol) was then added and stirred for 1 hour at room temperature under an argon atmosphere. Methyl iodide (2.39 g, 16 mmol) was then added and the reaction stirred for 16 hours, before 20 mL of deionized water was added. The reaction mixture was extracted with dichloromethane (3 x 20 mL), dried over magnesium sulfate, and concentrated. Purification by flash column chromatography on silica using hexanes produced 1.08 g of **7** as a peach-colored solid (26.3 mmol , 94% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.19 (d, 2H), 7.02 (d, 2H), 1.49 (s, 6H).

2,6-dibromo-4,4-dimethyl-4H-cyclopenta[2,1-b:3,4-b']dithiophene (10)

Following a previously reported procedure[3]. Compound **9** (1.00 g, 4.85 mmol) was added to a flame-dried round bottom flask with 40 mL of degassed dimethylformamide. In small portions over 5 minutes, *N*-bromosuccinimide (1.80 g, 10.2 mmol) was added, and stirred under an argon atomsphere at room temperature for 1 hour. Then, the mixture was extracted with hexanes (4 x 60 mL), washed with brine, and dried over magnesium sulfate. The concentrated residue was purified by flash column chromatography on silica two times, using hexanes as the eluent. Recrystallization from boiling hexanes yielded 0.70 g of **8** as a yellow oil (2.0 mmol, 42% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.02 (s, 1H), 1.42 (s, 3H).

Dibenzyl 2,2'-((4,4-dimethyl-4H-cyclopenta[2,1-b:3,4-b']dithiophene-2,6-diyl)bis(ethyne-2,1-diyl)) dibenzoate (mCPDT-F5)

Compounds **10** (127 mg, 0.35 mmol) and **5** (250 mg, 0.8 mmol) were dissolved in 15 mL of a degassed mixture tetrahydrofuran and triethylamine (1:2, v:v) in a flame-dried round bottom flask. After 10 minutes, copper(I) iodide (2 mg, 0.01 mmol) and tetrakis(triphenylphosphine)palladium(0) (23 mg, 0.02 mmol) were added, and the reaction mixture was stirred at 70 °C for 16 hours under an argon atmosphere. After filtering through Celite, the crude product was purified twice by flash column chromatography on silica, using 1:1 dichloromethane/hexanes as the eluent, and then 5% ethyl acetate in hexanes. The product was then recrystallized twice from chloroform and hexanes. This produced 110 mg of **mCPDT-F5** as a brown/yellow solid (0.13 mmol, 37% yield)

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.01 (d, 1H), 7.65 (d, 1H), 7.54 (t, 1H), 7.41 (t, 1H), 7.22 (s, 1H), 5.52 (s, 2H), 1.51 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 165.2, 161.3, 137.5, 133.9, 132.3, 130.9, 130.0, 128.0, 136.0, 123.9, 123.7, 93.4, 89.4, 54.0, 45.6, 24.9.

Bis((perfluorophenyl)methyl) 2,2'-((4,4-dimethyl-4H-cyclopenta[2,1-b:3,4-b']dithiophene-2,6-diyl) bis(ethyne-2,1-diyl))dibenzoate (mCPDT-H5)

Compounds **8** (127 mg, 0.35 mmol) and **6** (190 mg, 0.8 mmol) were dissolved in 15 mL of a degassed mixture of tetrahydrofuran and triethylamine (1:2, v:v) in a flame-dried round bottom flask. After 10 minutes, copper(I) iodide (2 mg, 0.01 mmol) and tetrakis(triphenylphosphine)palladium(0) (23 mg, 0.02 mmol) were added, and the reaction mixture was stirred at 70 °C for 16 hours under an argon atmosphere. After filtering through Celite, and rinsing with ethyl acetate and hexanes (1:4, v:v) the filtrate was reduced to an orange solid. This crude product was purified by flash column chromatography on silica, using 1:4 ethyl acetate:hexanes as the eluent, followed by a second flash column on silica eluting with of 5% ethyl acetate in hexanes, and by recrystallization in chloroform and hexanes was required. This produced 100 mg of **mCPDT-H5** as a dark yellow iridescent solid (0.161 mmol, 46% yield)

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.07 (d, 1H), 7.65 (d, 1H), 7.54-7.52 (m, 3H), 7.42-7.36 (m, 4H), 7.04 (s, 1H), 5.47 (s, 2H), 1.47 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 166.0, 161.2, 137.4, 136.0, 133.6, 131.9, 131.0, 130.9, 128.6, 128.3, 128.2, 127.9, 126.1, 123.9, 123.7, 93.9, 98.2, 67.0, 45.4, 25.0

Synthesis References

1. W. J. Mullin, R. H. Pawle, S. A. Sharber, P. Müller and S. W. Thomas, *Journal of Materials Chemistry C*, 2019, **7**, 1198-1207.
2. P. Li, B. Ahrens, N. Feeder, P. R. Raithby, S. J. Teat and M. S. Khan, *Dalton Transactions,* 2005, 874-883.
3. N. Ferri, N. Algethami, A. Vezzoli, S. Sangtarash, M. McLaughlin, H. Sadeghi, C. J. Lambert, R. J. Nichols and S. J. Higgins, *Angewandte Chemie International Edition*, 2019, **58**, 16583-16589.

Nuclear Magnetic Resonance spectra

Figure S1: ^{1}H and ^{13}C NMR spectra of **TT-F5**

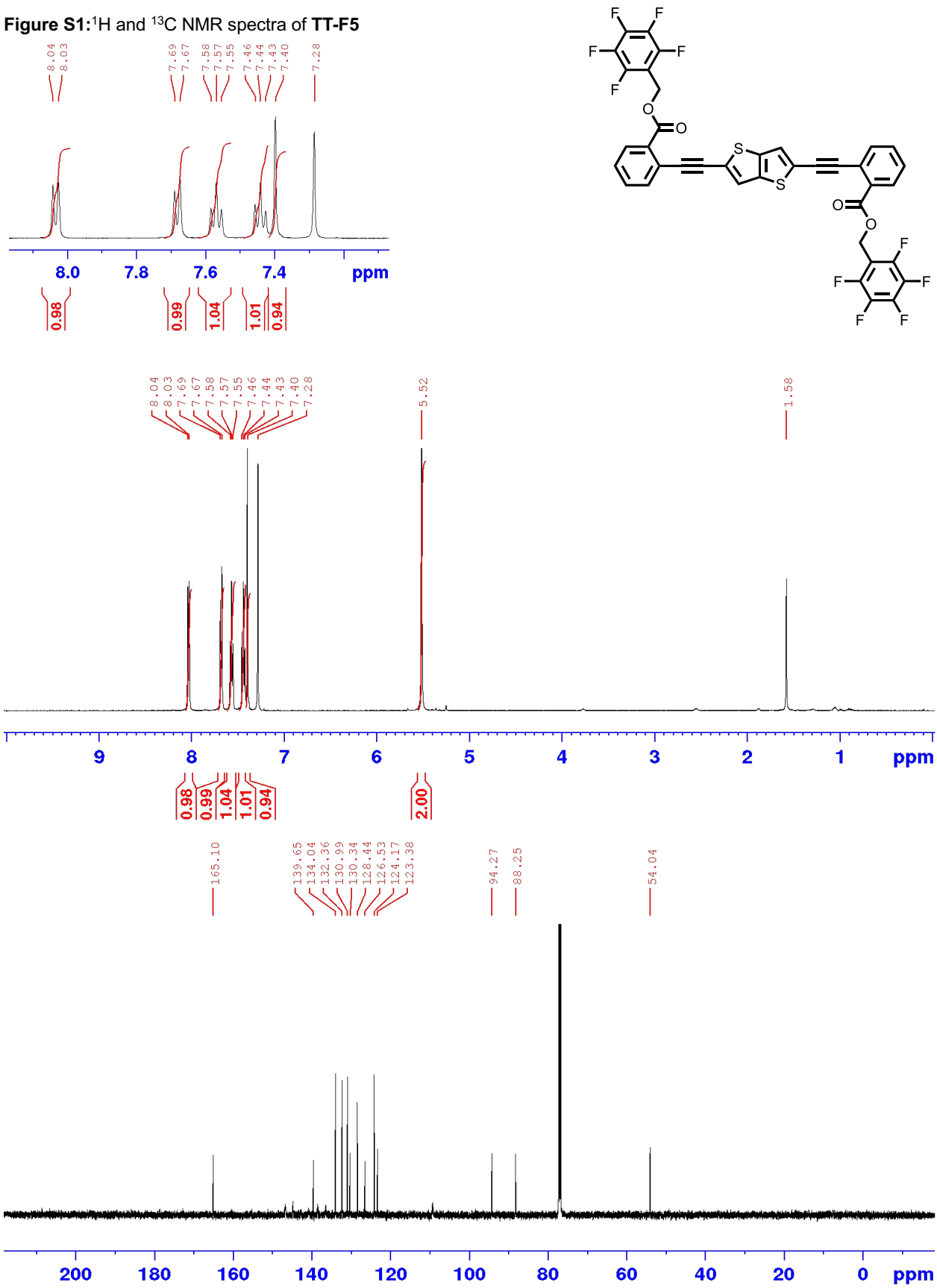


Figure S2: ^{1}H and ^{13}C NMR spectra of **TT-H5**

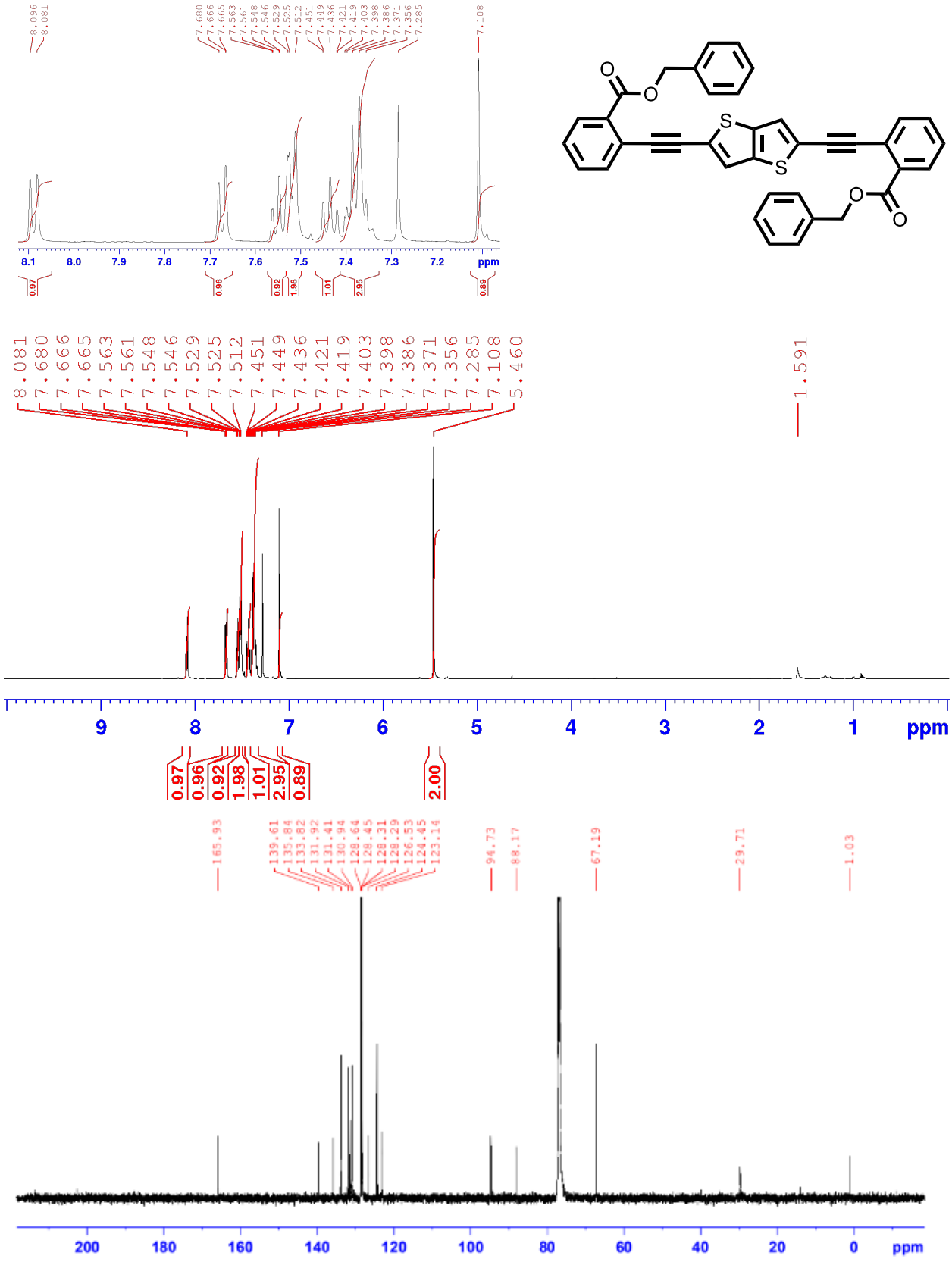


Figure S3: ^{1}H and ^{13}C NMR spectra of **DTT-F5**

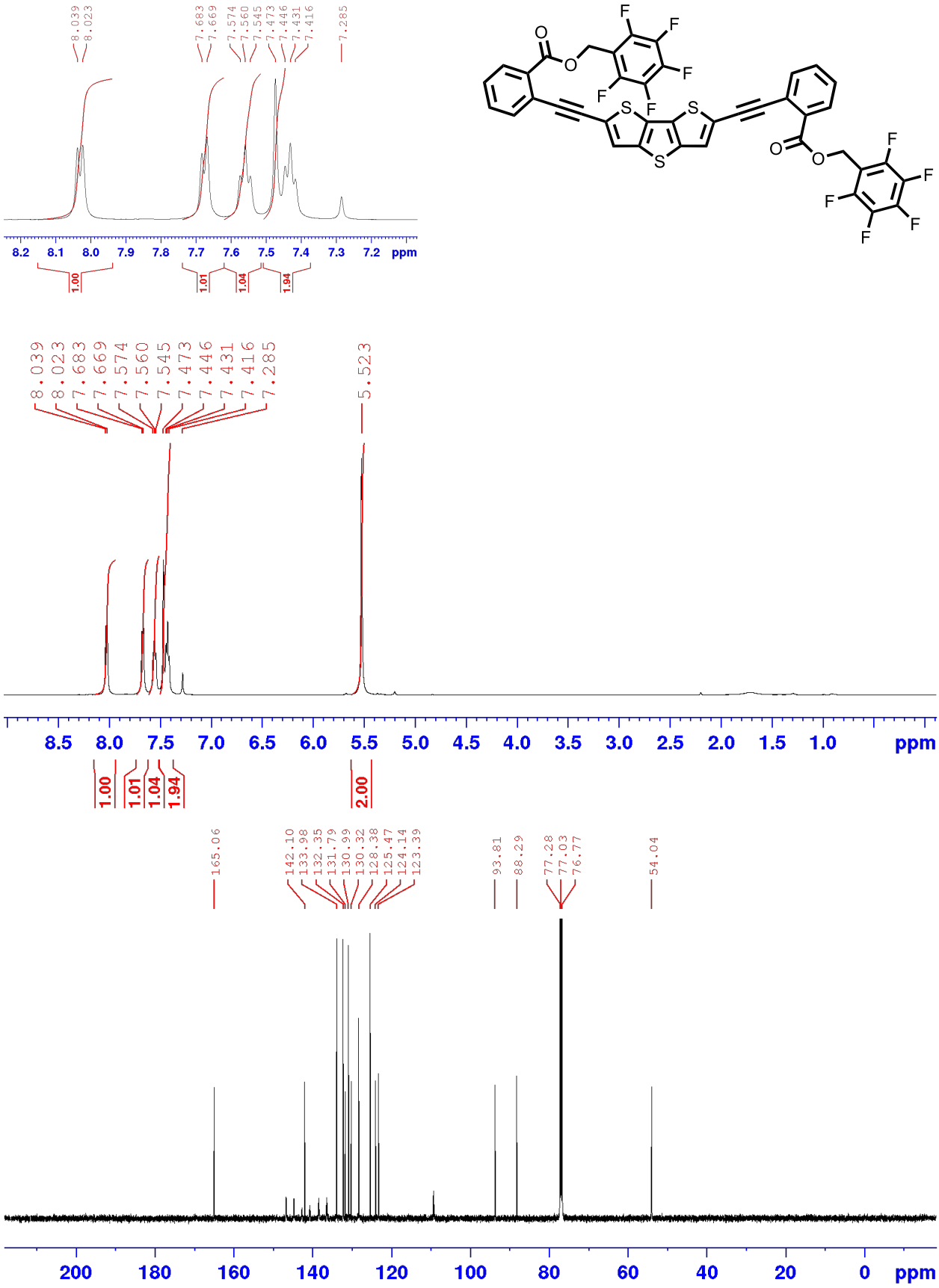


Figure S4:^{1}H and ^{13}C NMR spectra of **DTT-H5**

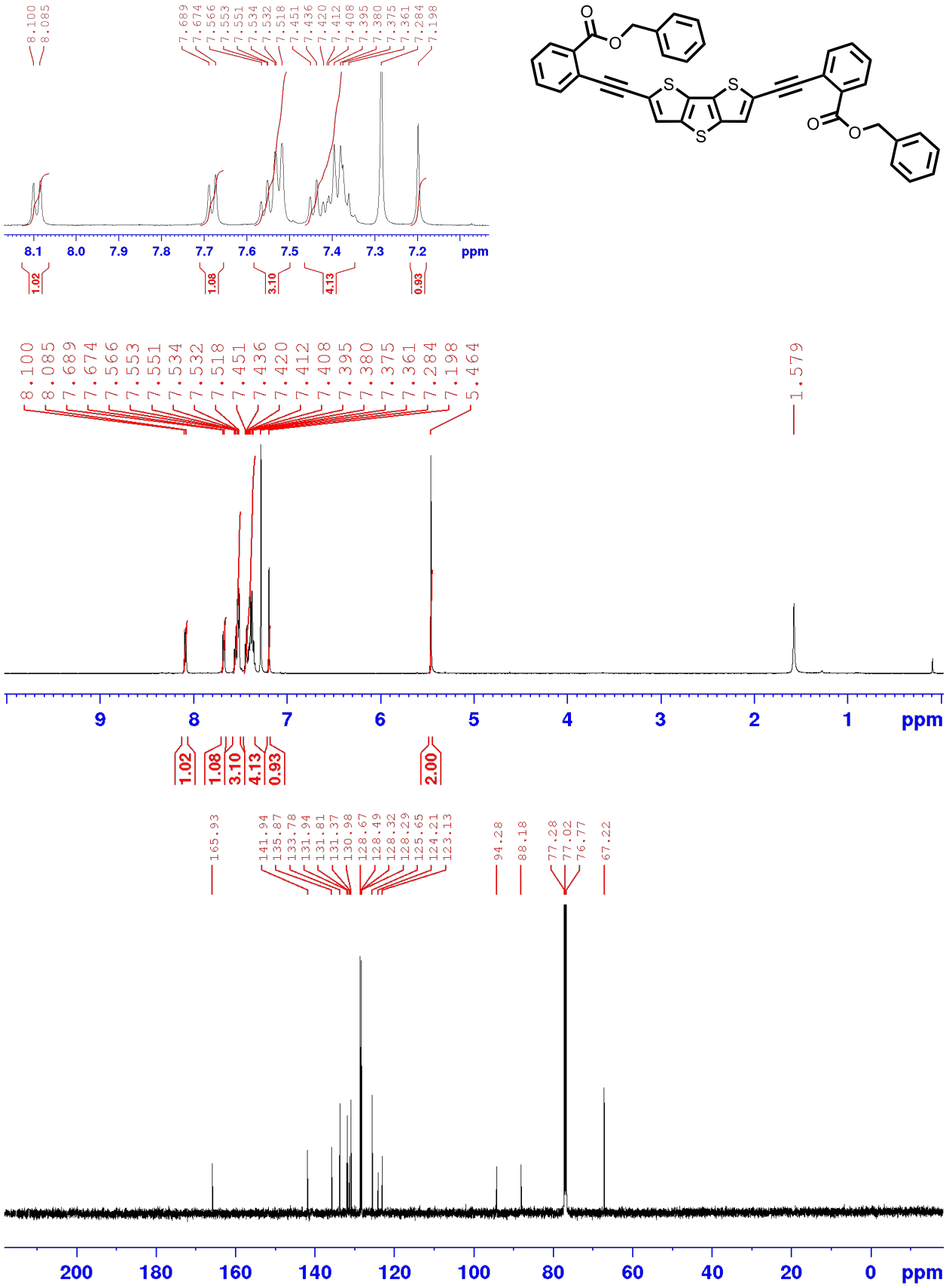


Figure S5: ^{1}H and ^{13}C NMR spectra of **BDT-F5**

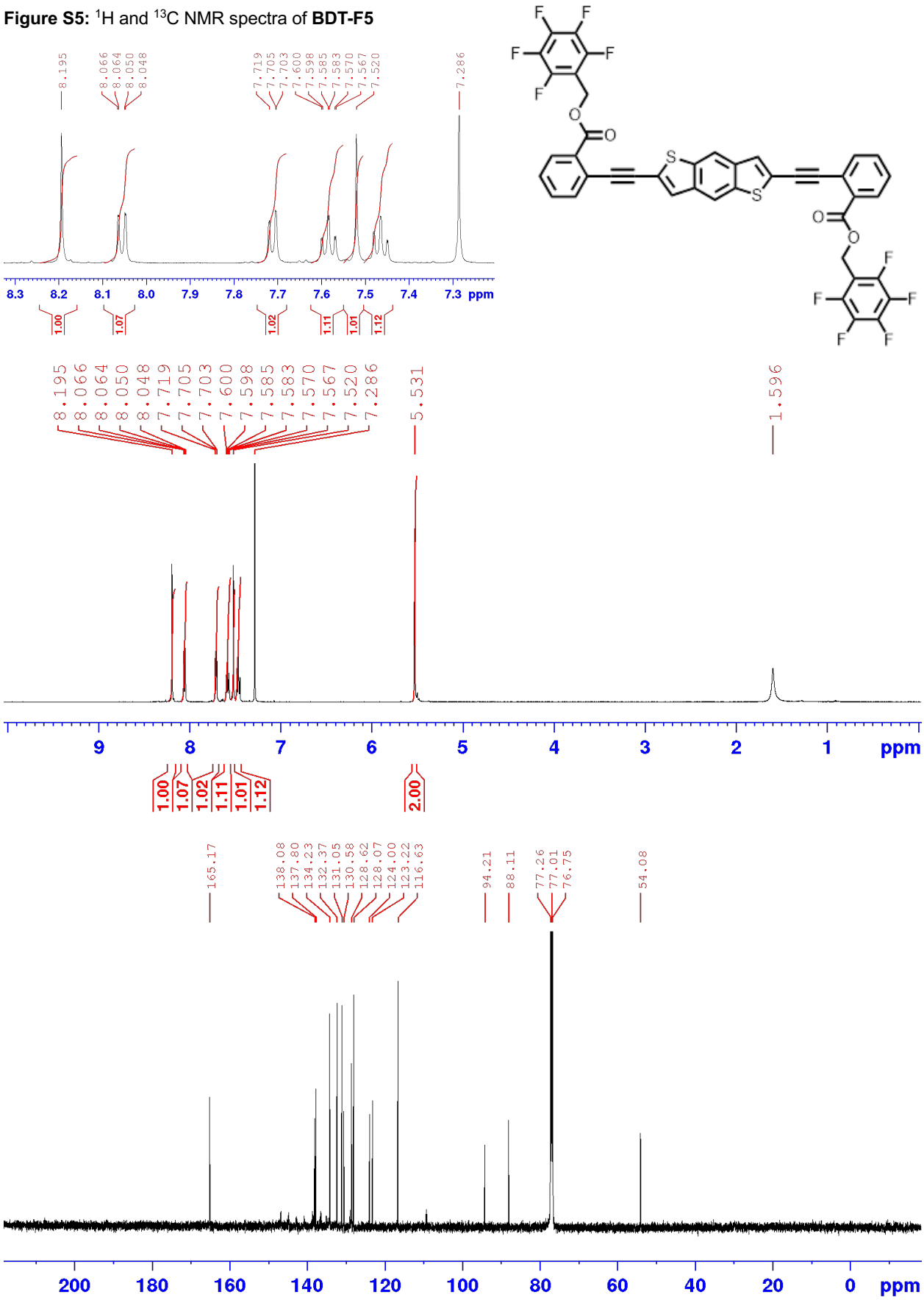


Figure S6: ^{1}H and ^{13}C NMR spectra of **BDT-H5**

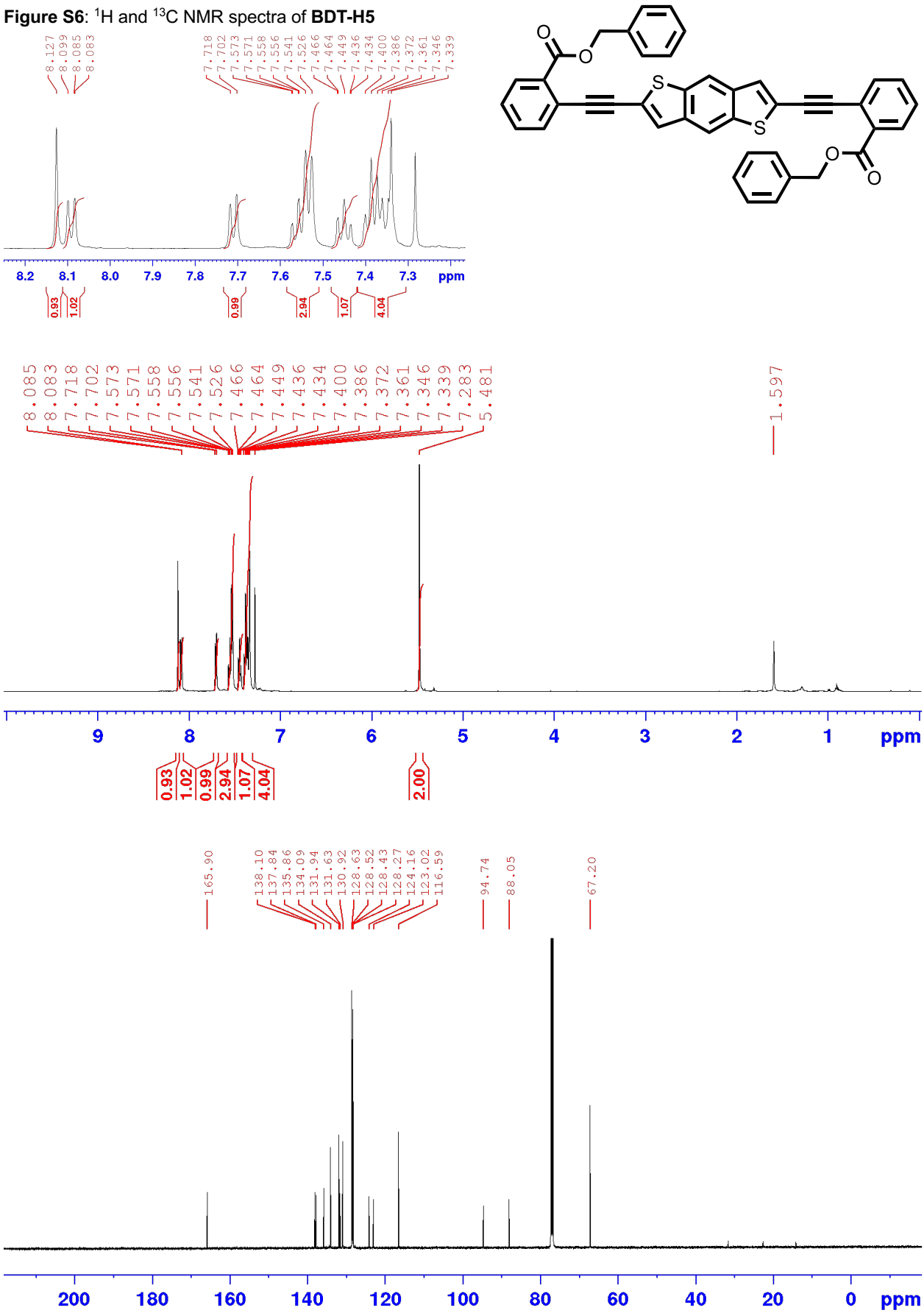


Figure S7: ^{1}H and ^{13}C NMR spectra of **mCPDT-F5**

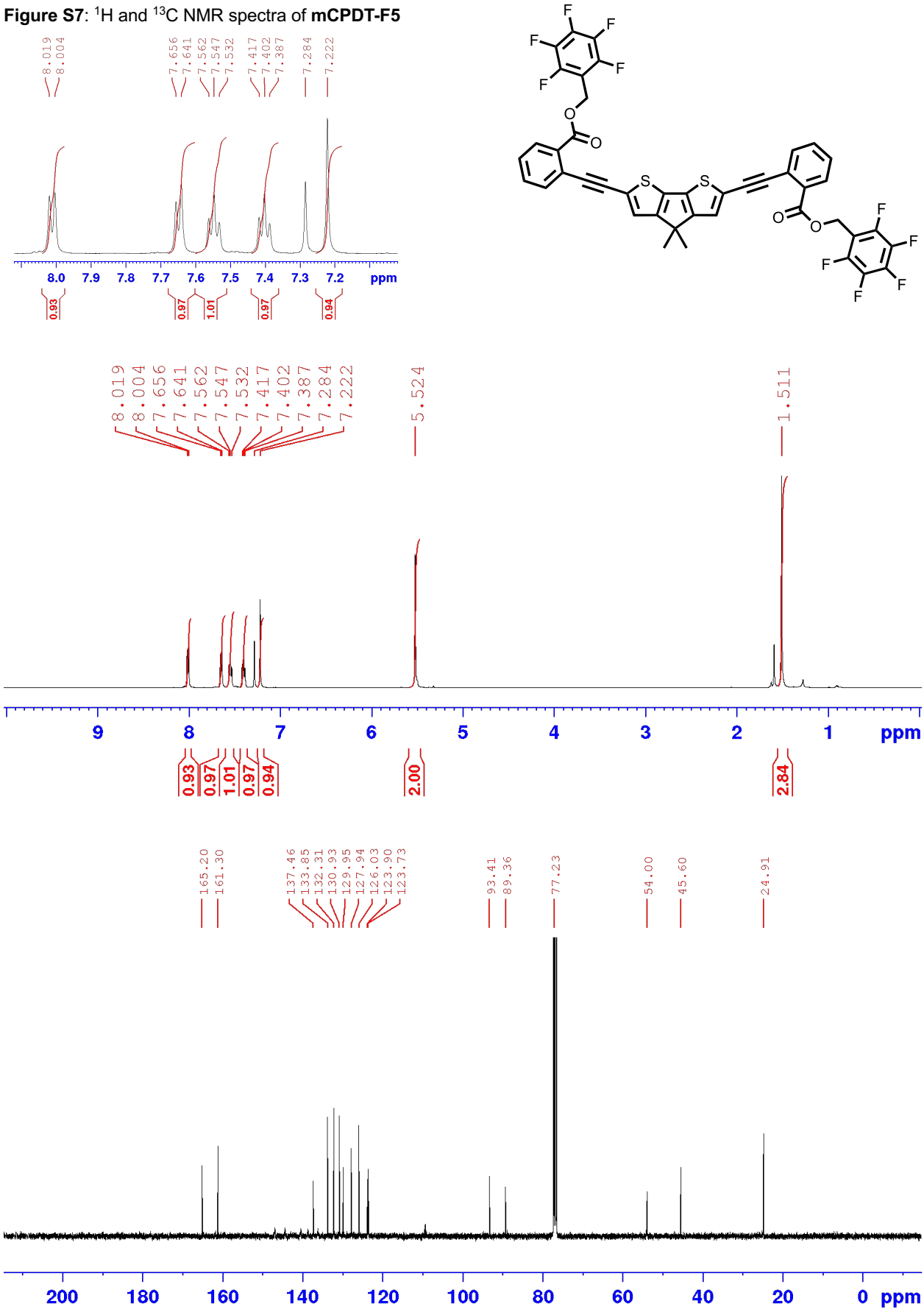
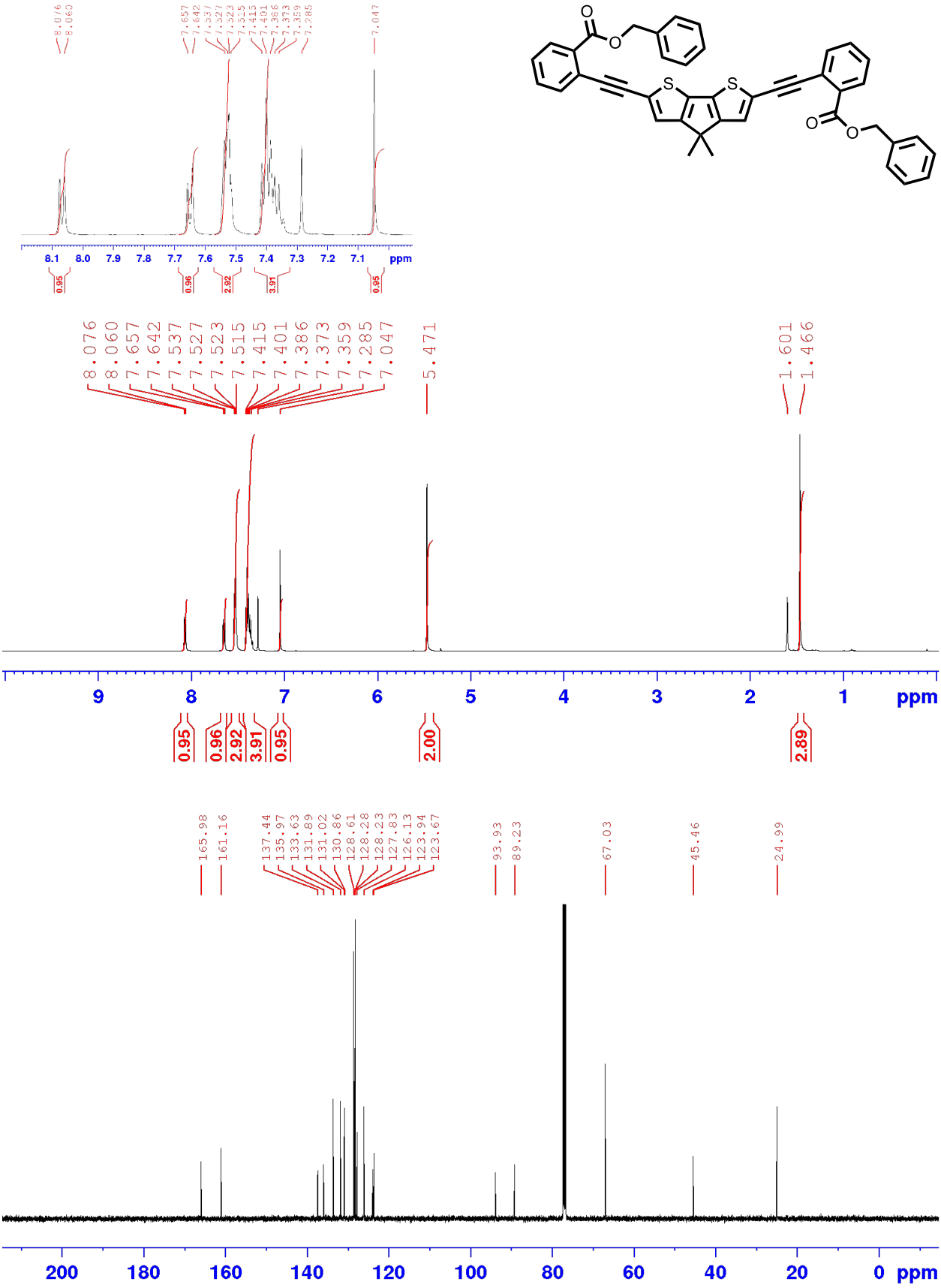


Figure S8: ^{1}H and ^{13}C NMR spectra of **mCPDT-H5**



High Resolution Mass Spectroscopy

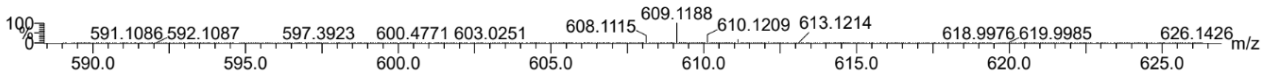
Figure S9: HRMS of **TT-H5**

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
48 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-90 H: 0-120 O: 0-6 S: 2-2

Order# 18850 Elisa Guzman TT-H5 MSL, SCS, UIUC SYNAPTG2-Si#UGA354
Synapt2_36579a 36 (0.724) Cm (31:38-4:8) 1: TOF MS ES+
3.24e+006



Minimum:				-1.5				
Maximum:		5.0	5.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
609.1188	609.1194	-0.6	-1.0	26.5	913.3	n/a	n/a	C38 H25 O4 S2

Order# 18850 Elisa Guzman TT-H5 MSL, SCS, UIUC SYNAPTG2-Si#UGA354
Synapt2_36579a 36 (0.724) Cm (31:38-4:8) 1: TOF MS ES+
3.24e6

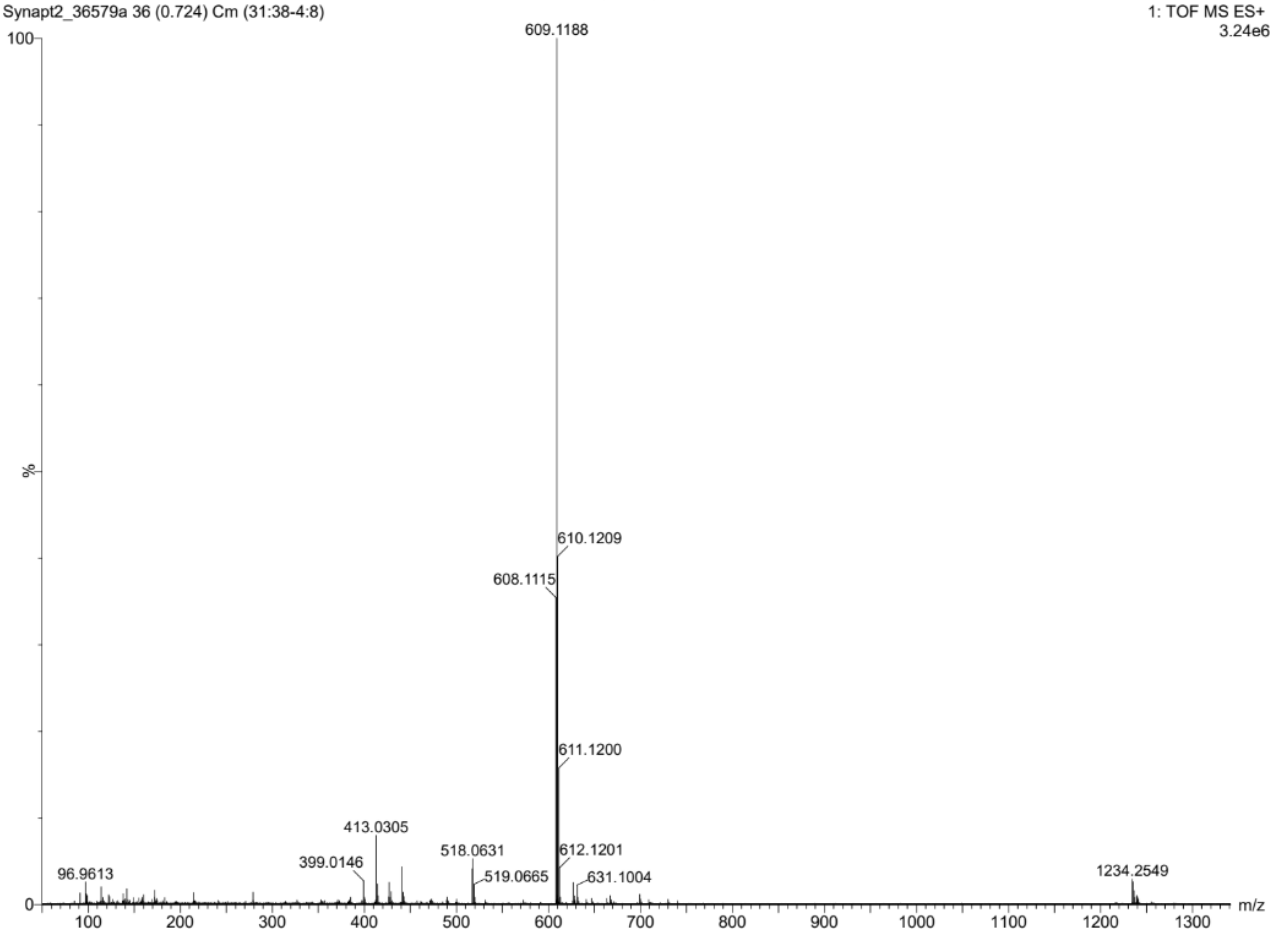


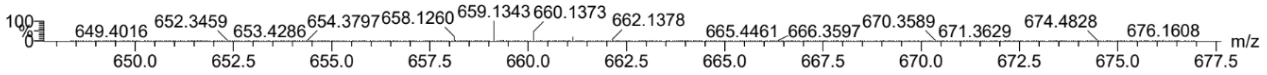
Figure S10: HRMS of **BDT-H5**

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

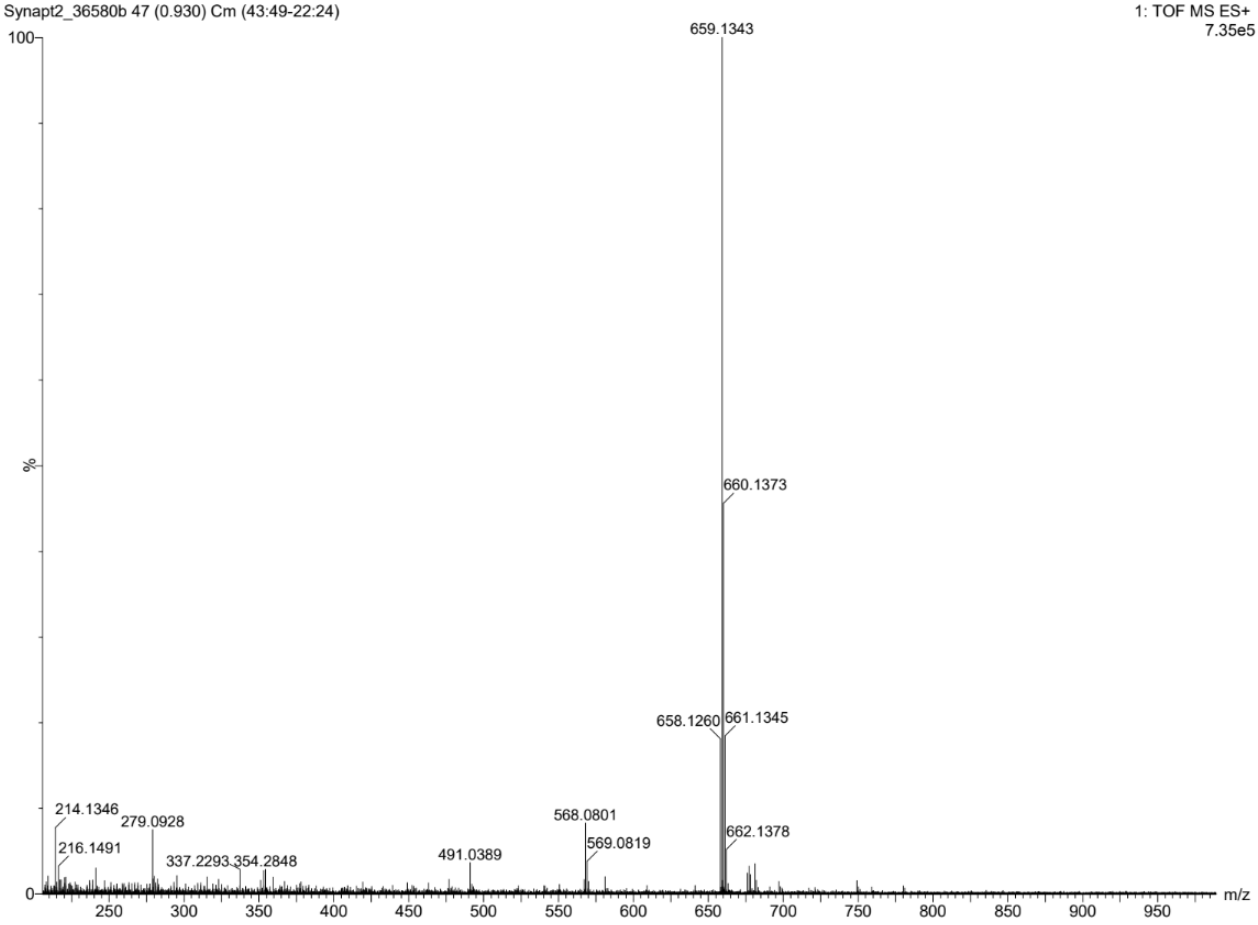
Monoisotopic Mass, Even Electron Ions
53 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-90 H: 0-120 O: 0-6 S: 2-2

Order# 18851 Elisa Guzman BDT-H5 MSL, SCS, UIUC SYNAPTG2-Si#UGA354
Synapt2_36580b 47 (0.930) Cm (43:49-22:24) 1: TOF MS ES+
7.35e+005



Minimum:				-1.5				
Maximum:		5.0	5.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
659.1343	659.1351	-0.8	-1.2	29.5	700.1	n/a	n/a	C42 H27 O4 S2

Order# 18851 Elisa Guzman BDT-H5 MSL, SCS, UIUC SYNAPTG2-Si#UGA354
Synapt2_36580b 47 (0.930) Cm (43:49-22:24) 1: TOF MS ES+
7.35e5



Optical Properties

Figure S11: Thienothiophene optical spectroscopy. A) Absorbance of TT-F5. B) Absorbance of TT-H5 C) Emission comparison between F5 and H5 molecules in solution (chloroform) and as a spin-cast solid film. D) Excitation and emission of polymorphs powder of H5

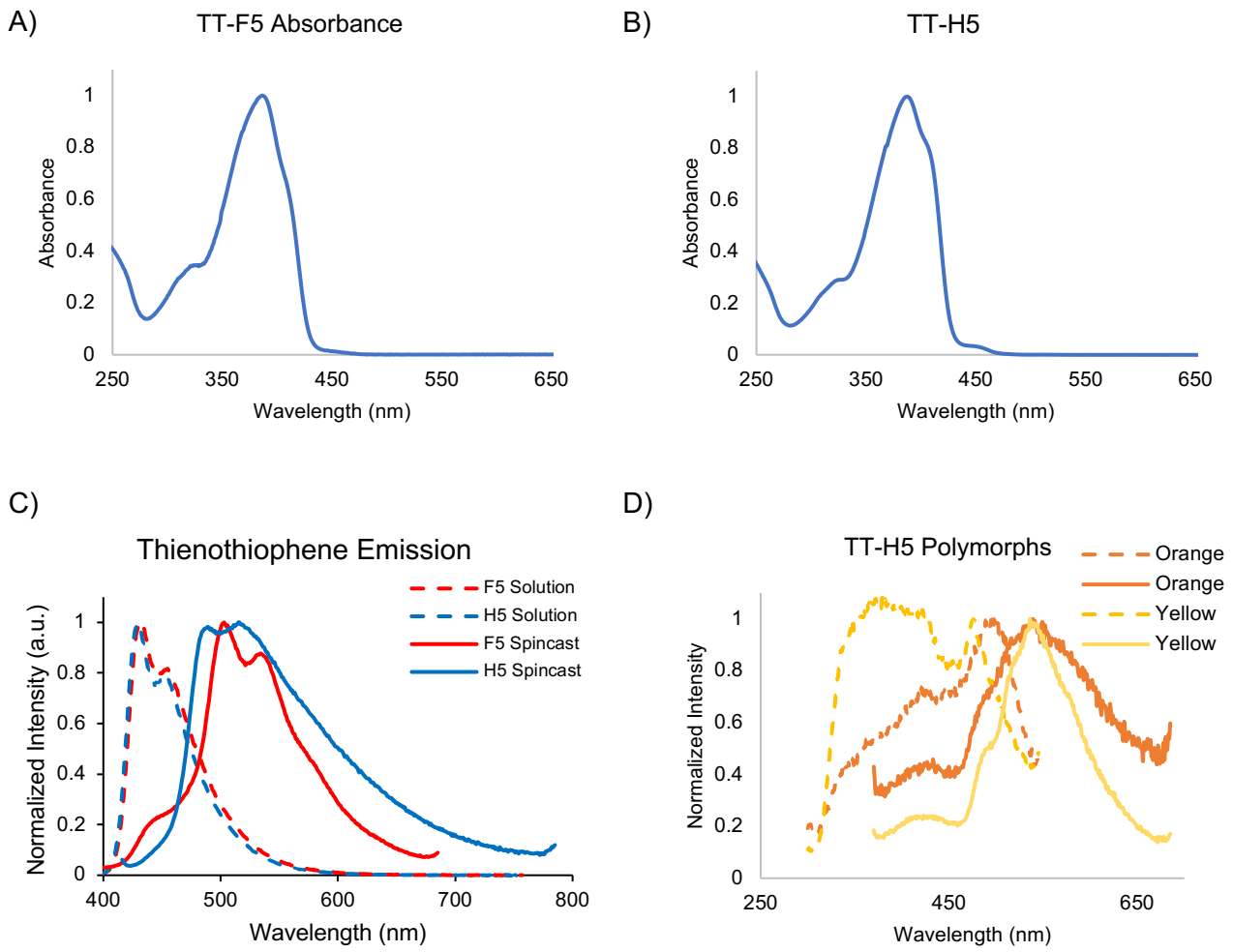


Figure S12: Dithienothiophene optical spectroscopy. A) Absorbance of DTT-F5. B) Absorbance of DTT-H5 C) Emission comparison between F5 and H5 molecules in solution (chloroform) and as a spin-cast solid film. D) Emission for the isolated powders F5. E) Excitation and emission comparison of DTT-H5 polymorphs.

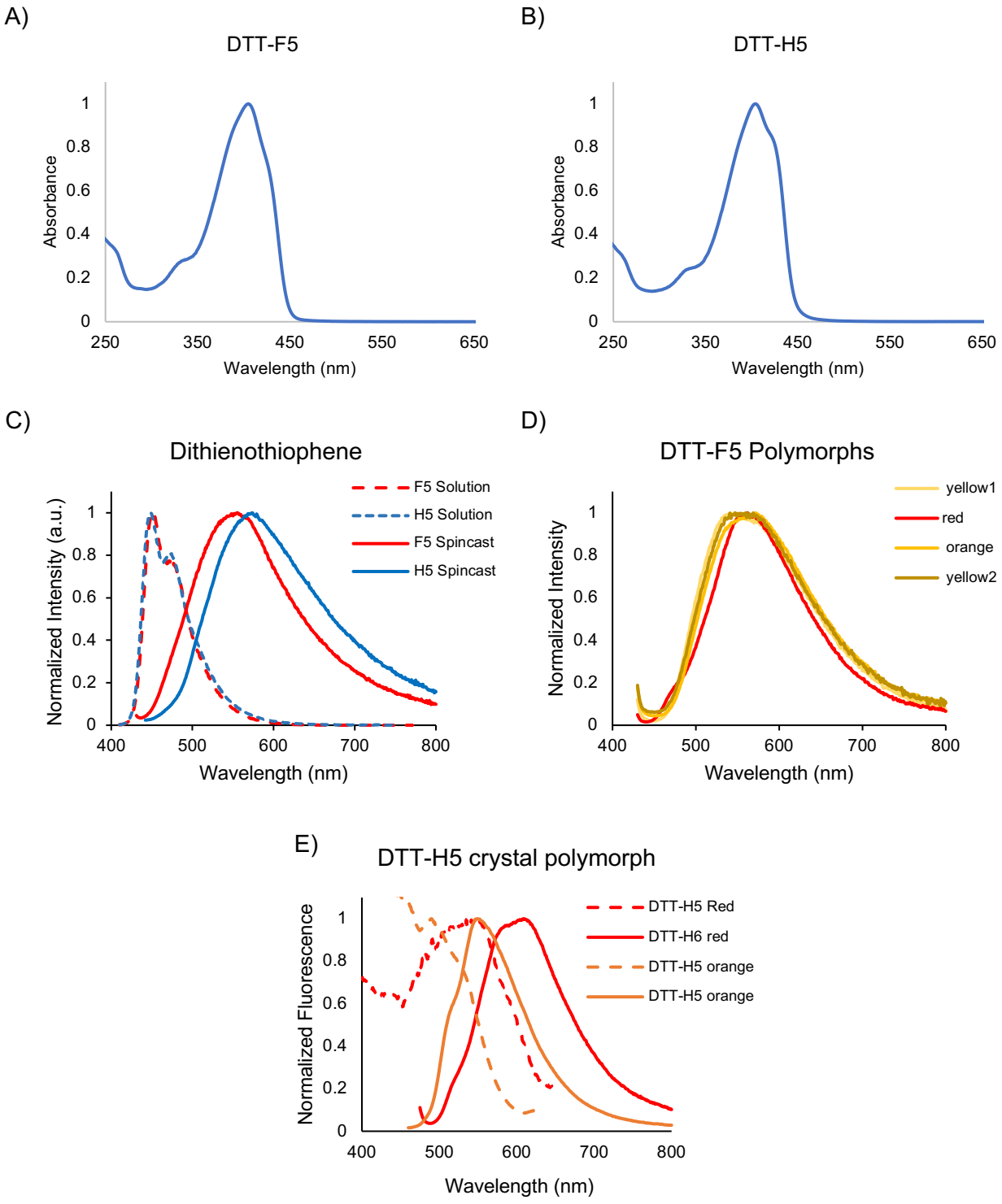


Figure S13: Benzodithiophene optical spectroscopy. A) Absorbance of BDT-F5. B) Absorbance of BDT-H5 C) Emission comparison between F5 and H5 molecules in solution (chloroform) and as a spin-cast solid film. D) Excitation and emission for the H5 yellow powder before and melting. E) Emission of BDT-F5 powders before and after melting.

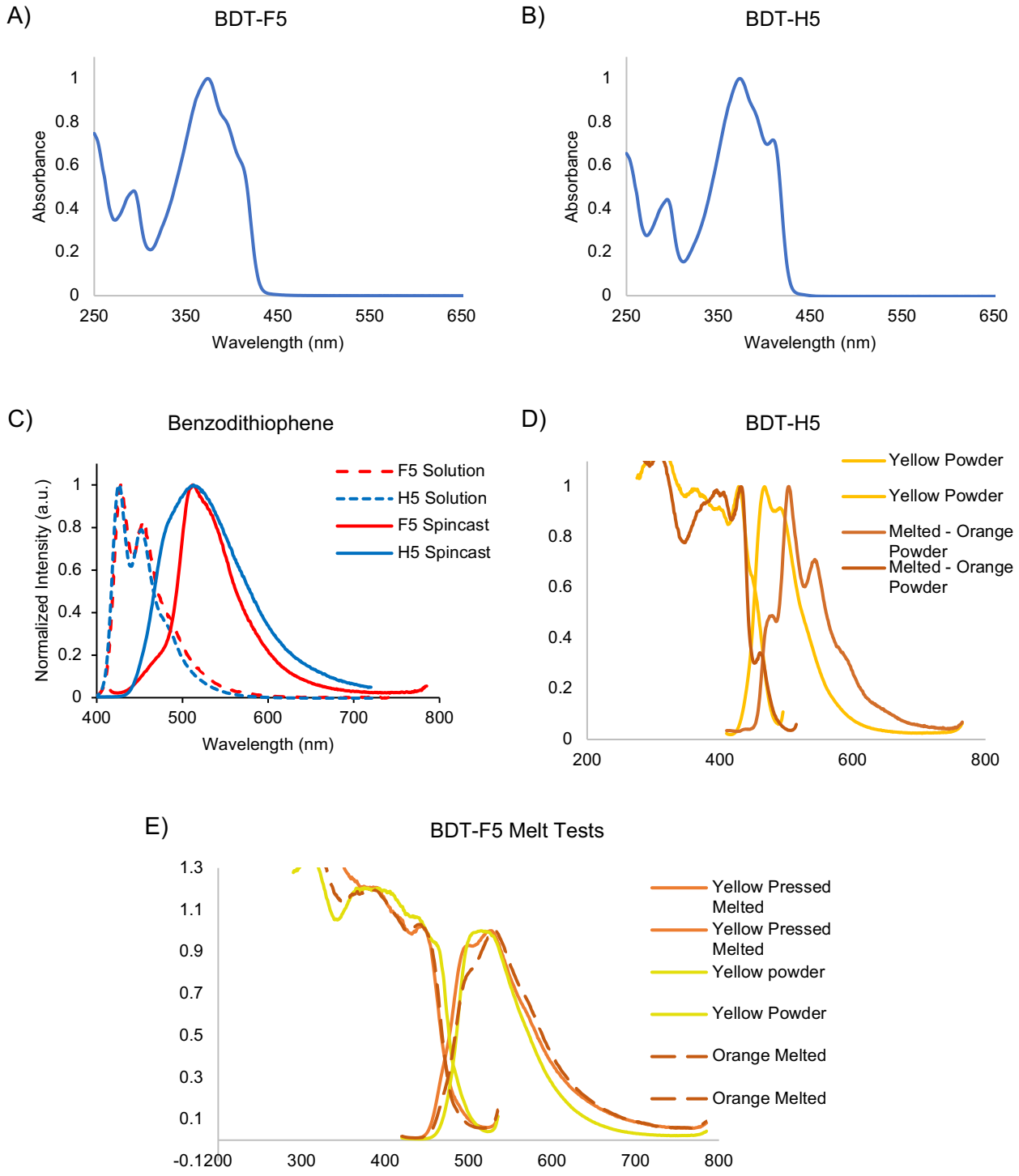


Figure S14: Images of each solid before and after melting and recrystallizing. A) BDT-H5 before, B) BDT-H5 After. C) BDT-F5 yellow before D) BDT-F5 yellow after. E) BDT-F5 orange before. F) BDT-F5 orange after.

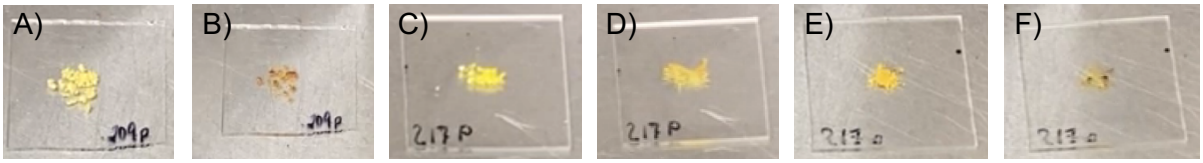


Figure S15: Methylated cyclopentadithiophene optical spectroscopy. A) Absorbance of mCPDT-F5. B) Absorbance of mCPDT-H5 C) Emission comparison between F5 and H5 molecules in solution (chloroform) and as a spin-cast solid film. D) Emission for the isolated powders F5. E) Emission comparison of isolated H5 polymorphs.

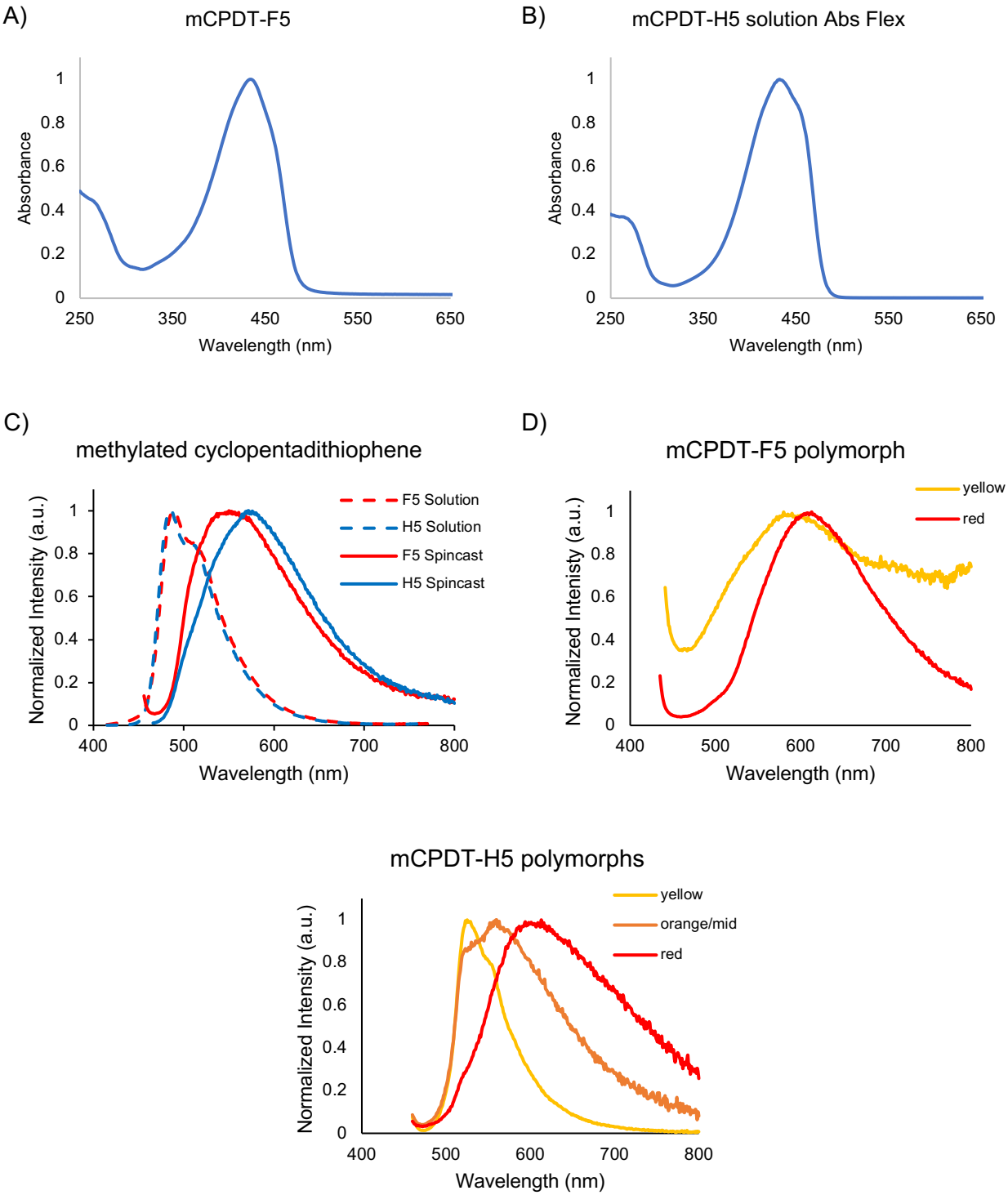


Table S1: Polymorph emission data for spun cast films from 2 mg/mL of chloroform solutions, and powders. Melting point data is based on the DSCs seen below. Each polymorph is denoted with a letter corresponding to the color of the solid, yellow (y), orange (o), red (r).

	$\lambda_{max,\ emis}$[3] (nm)	mp (°C)
TT-H5	513, 537 (y) (o)	140-143 (y), 153-156 (o)
TT-F5	506	182-183
BDT-H5	513 465 (y), 506 (o),	148-149 (o), 159-160 (y)
BDT-F5	505	205-209 (o), 215-216 (y)
DTT-H5	579, 548 (o), 606 (r)	43-146, 131-132 (o)
DTT-F5	553, 555 (o) (y) 559 (r)	144-160, 152-159 (y), 160-163(y), 178-181 (o)
mCPDT-H5	572	167-168 (y), 142-155 (o)
mCPDT-F5	546, 595 (y), 608 (r)	150-167 (r), 160-170 (o)

Differential Scanning Calorimetry

Figure S16: DSC of TT-F5 showing repeatable melting point at 183 °C.

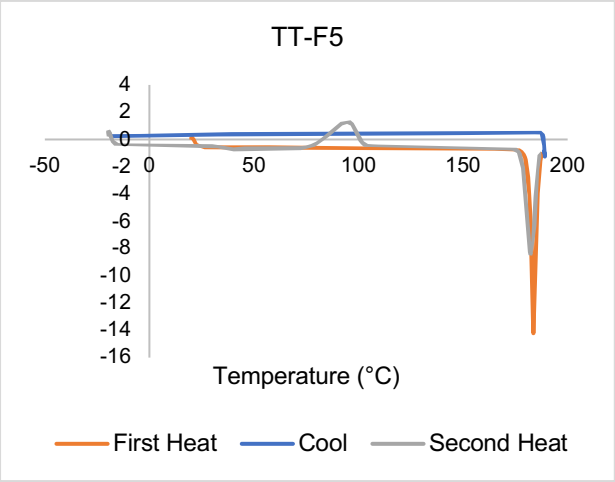
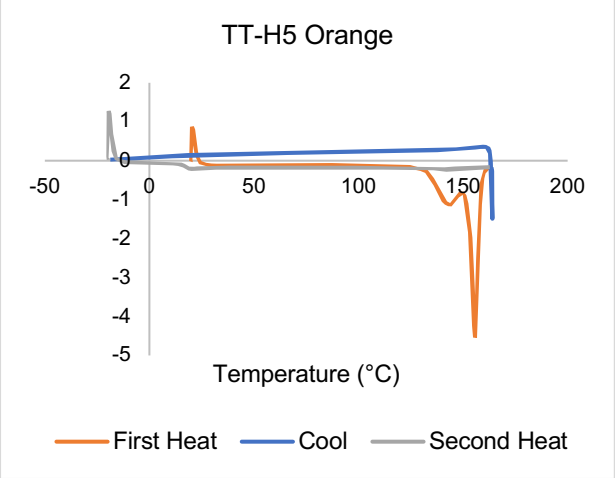


Figure S17: DSC of TT-H5 orange and yellow polymorphs. If mainly the orange polymorph is present, no reformation is seen. If mainly yellow polymorph is present, the sample recrystallizes into that crystal structure.



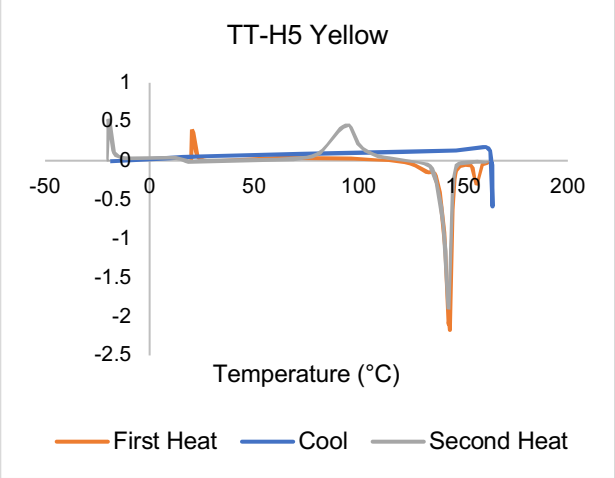


Figure S18: DSC of DTT-F5 of the mixed crystals and isolated yellow, orange, and red solid collected. Each sample melts at 162 °C, with some unknown polymorph spike at 180 °C seen in DTT-F5 orange. This completely disappears if fully melted, seen in DTT-F5 orange, but will persist if not allowed to melt the first pass, as seen in DTT-F5 yellow.

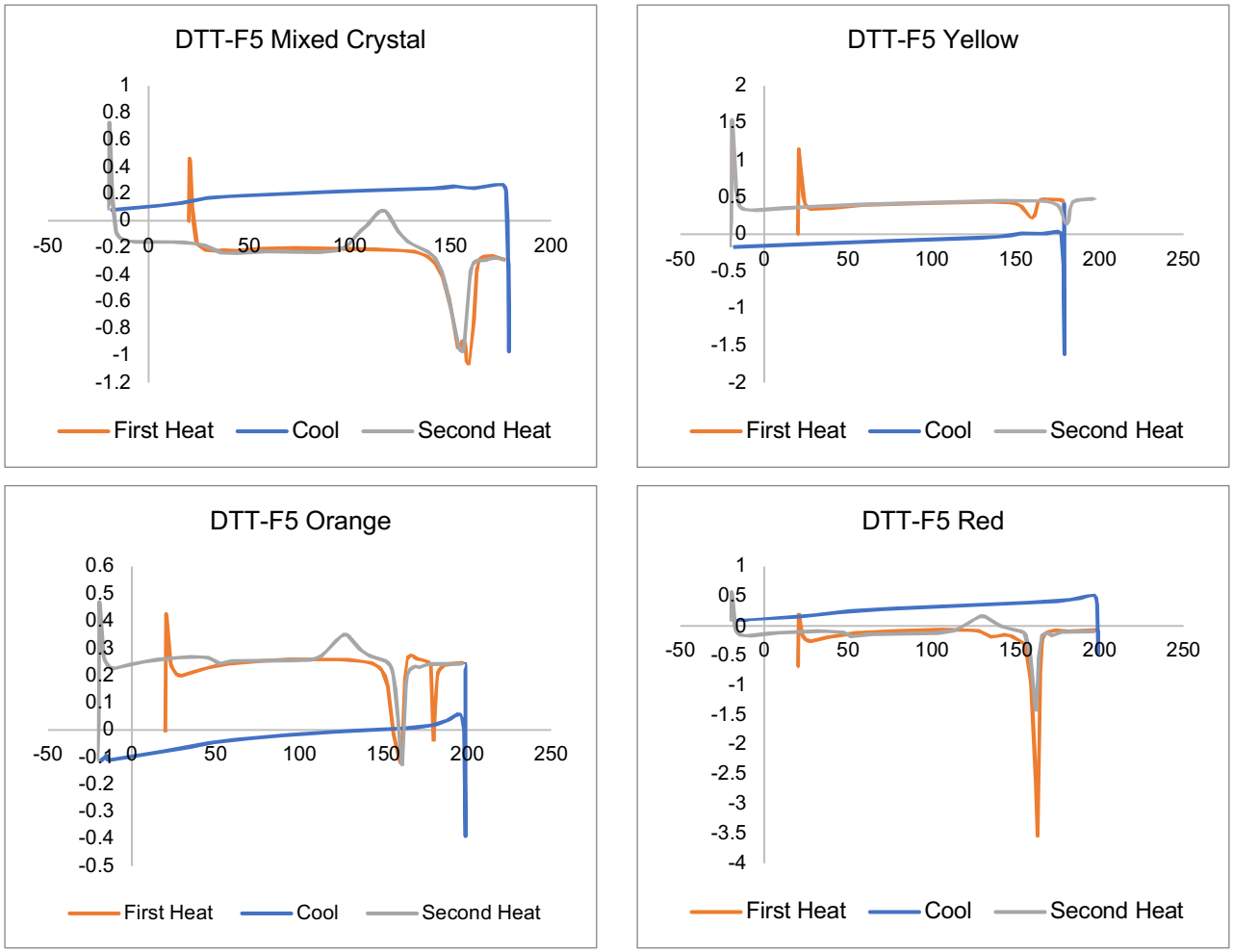


Figure S19: DTT-H5 DSC of the red polymorph with different upper temps each heat to show the different polymorph melting temperatures.

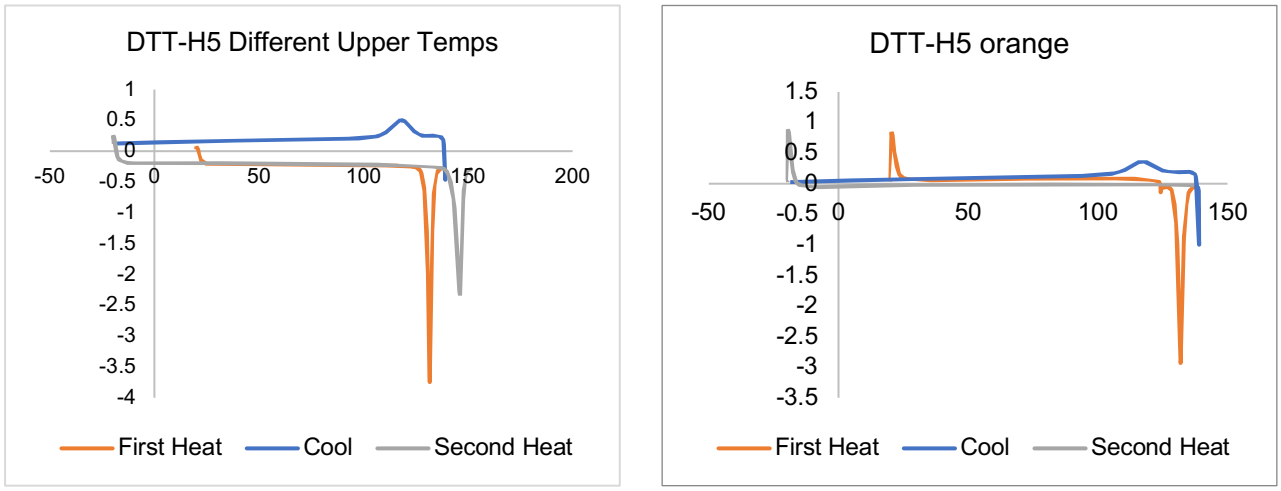
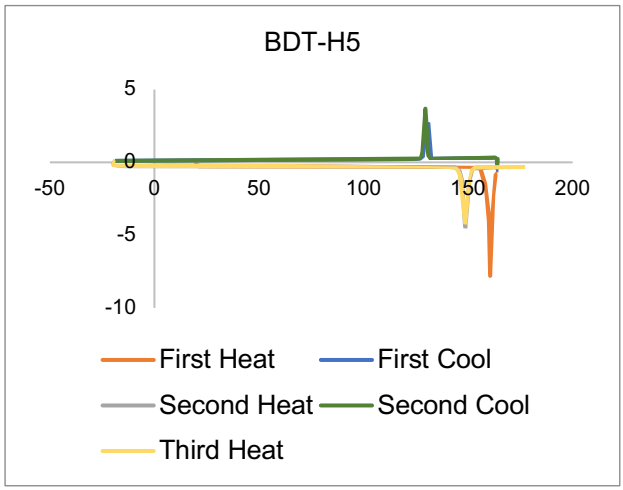


Figure S20: DSC results of BDT-H5 show yellow and orange polymorphs. The isolated yellow polymorph analysis, confirms the higher temperature melting point is for the yellow powder.



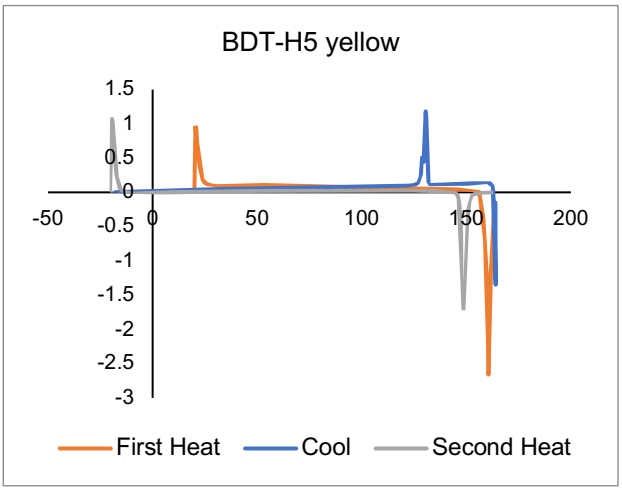
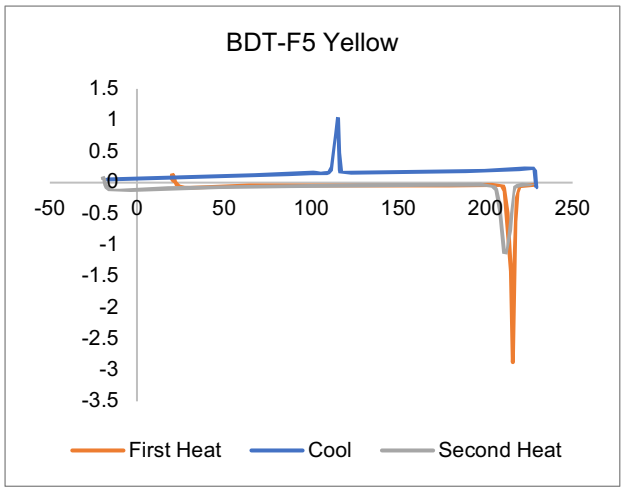


Figure S21: DSC results of BDT-F5 with yellow and orange polymorphs. The yellow polymorph having an initial melting point of 215°C, and reforming to have a melting point of 212°C. The orange polymorph requires three heating cycles to fully unify the crystal structure to the 210 °C melting point.



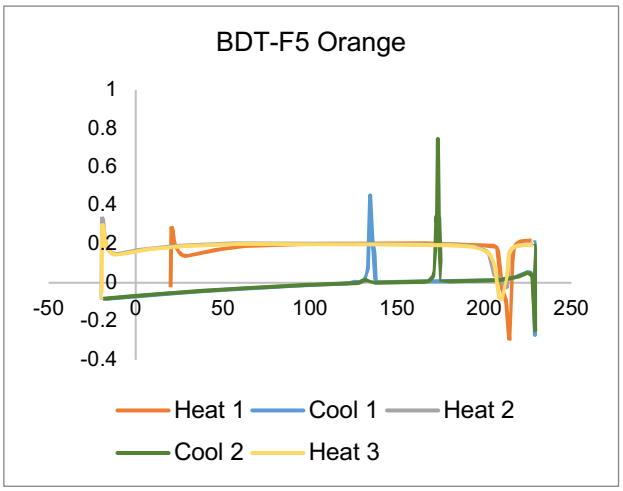


Figure S22: DSC on the mCPDT-F5 polymorphs. Each polymorph melts at the same temperature, and does not remelt.

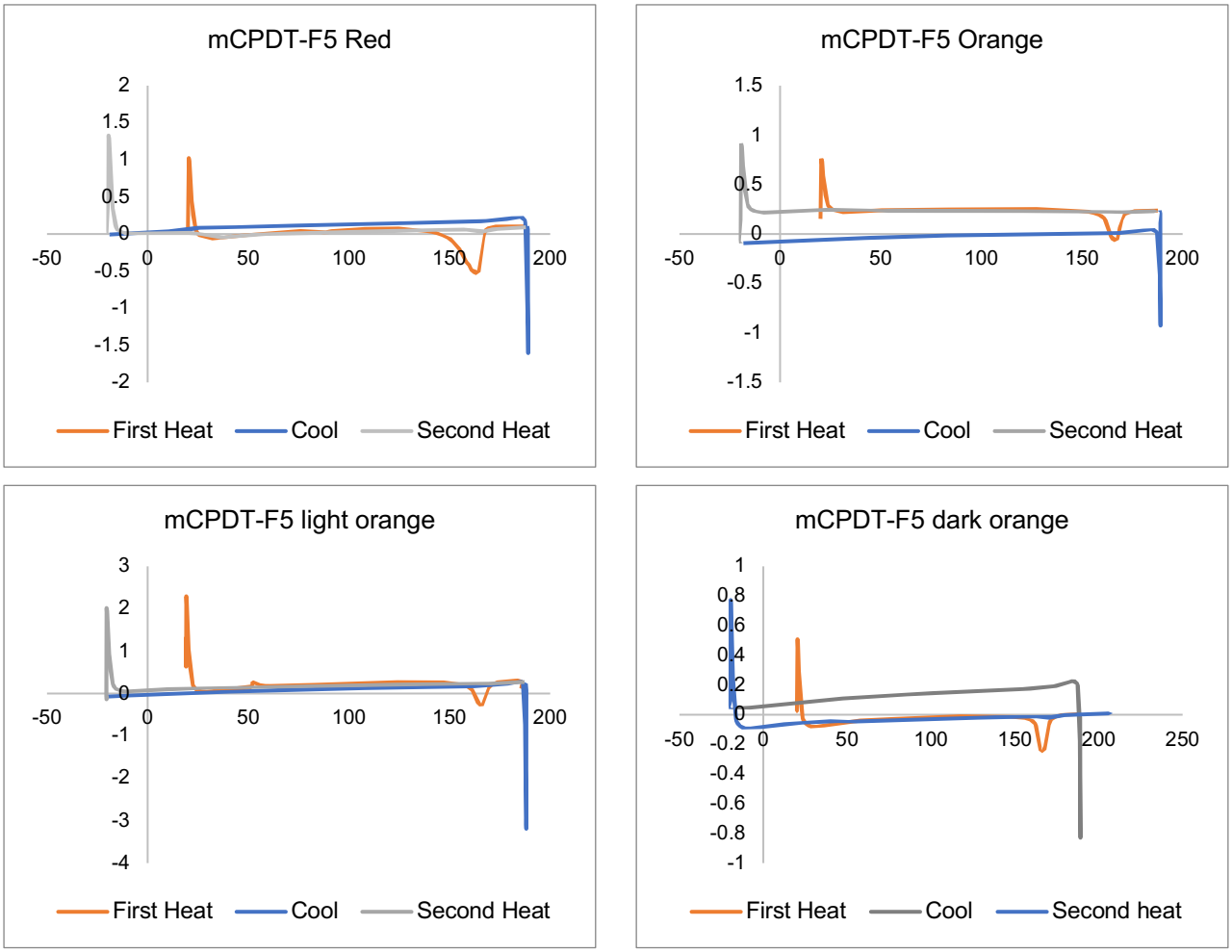
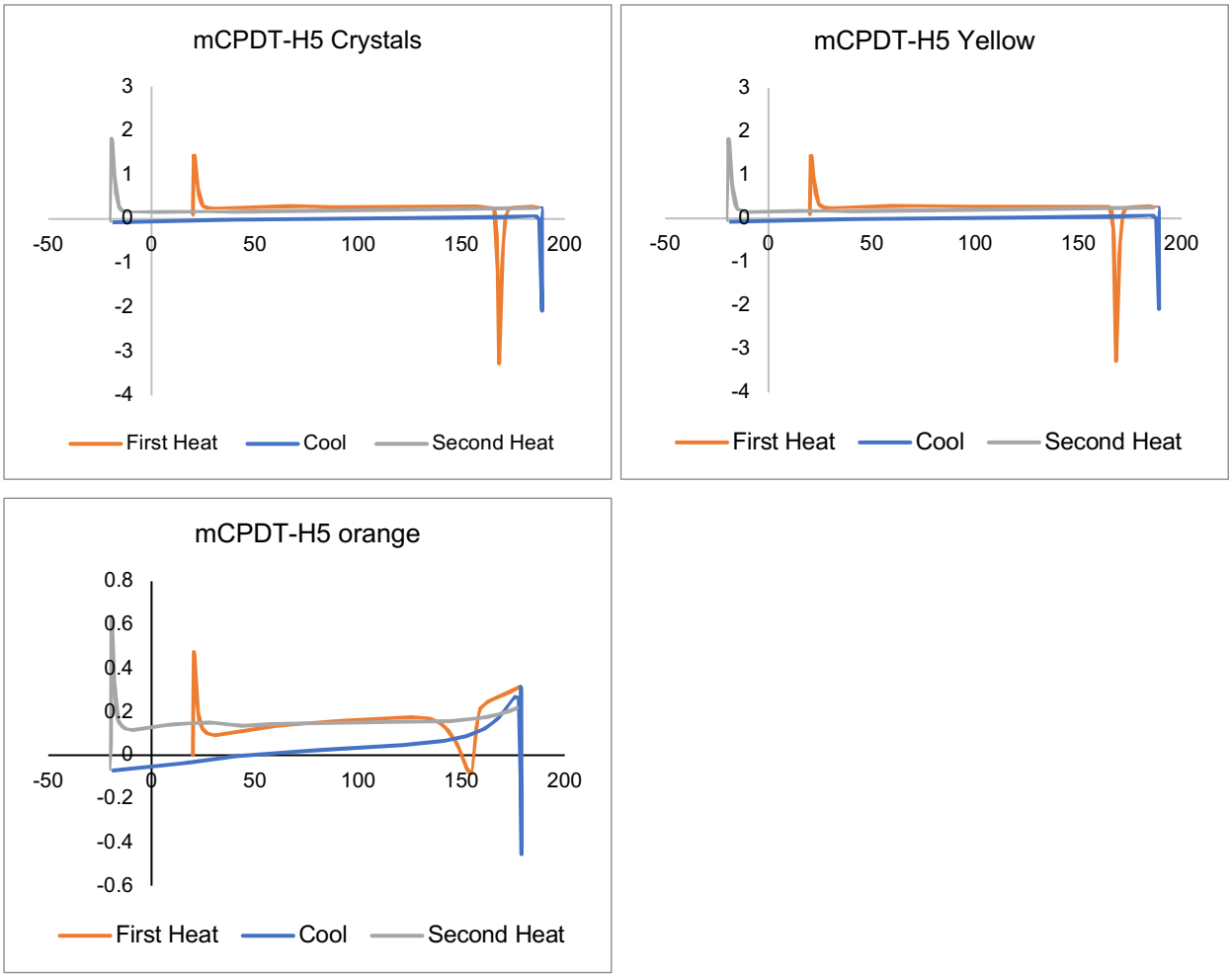


Figure S23: The DSC of mCDPT-H5 of crystals, and isolated yellow and orange powders.



Single Crystal X-Ray Diffraction

Table S2: Crystal data and structure refinement for **TT-F5**

Identification code	P22313_t5	
Empirical Formula	C38 H14 F10 O4 S2	
Formula Weight	788.61 g/mol	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal Size	0.115 x 0.110 x 0.060 mm^3	
Crystal system	Monoclinic	
Space group	$P2_{1/c}$	
Unit Cell dimensions	*a* = 29.4547(10) Å	α = 90°
	b = 6.6980(3) Å	β = 95.5699°
	c = 8.0253(3) Å	γ = 90°
Volume	1575.82(11)$Å^3$	
Z	2	
Density (calculated)	1.662 g/cm3	
Absorption coefficient	2.483 mm^{-1}	
F(000)	792	
Theta range for data collection	1.507 to 77.366°	
Index ranges	-37<=h<=37, 0<=k<=8, 0<=l<9	
Reflections Collected	4344	
Independent reflections	4344 [R(int) =0.1142]	
Completeness to theta = 67.679°	97.2 %	
Max and min transmission	0.427432 and 0.261926	
Structure solution technique		
Structure solution program		
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4344 / 426 / 264	
Goodness-of-fit on F^2	3.109	
Final *R* indices [*I*>2\σ(*I*)]	*R*1 = 0.1385, *wR*2 = 0.3844	
R indices (all data)	*R*1 = 0.1550, *wR*2 = 0.3927	
Largest diff. peak and hole	2.369 and -0.918 $eÅ^{-3}$	

Table S3: Crystal data and structure refinement for **DTT-F5.**

Identification code	EG1013010132021	
Empirical Formula	C40 H14 F10 O4 S3	
Formula Weight	844.72 g/mol	
Temperature	100.(2) K	
Wavelength	0.71073 Å	
Crystal Size	0.180 x 0.180 x 0.120 mm^3	
Crystal system	triclinic	
Space group	*P -1*	
Unit Cell dimensions	*a* = 8.5406(2) Å	α = 101.0600(10)°
	b = 11.0477(3) Å	β = 101.2360(10)°
	c = 18.4450(5) Å	γ = 91.4290(10) °
Volume	1671.78(8) $Å^3$	
Z	2	
Density (calculated)	1.678 g/cm3	
Absorption coefficient	0.324 mm^{-1}	
F(000)	848	
Theta range for data collection	2.6629 to 25.3262°	
Index ranges	-10<=*h*<= 10, -13<=*k*<=13, -22<=*l*<=22	
Reflections Collected	81693	
Independent reflections	6098 [R_{int} = 0.0340]	
Completeness to theta = 25.24	99.6 %	
Max and min transmission	0.96 and 0.93	
Structure solution technique	direct methods	
Structure solution program	SHELXT 2018/2 (Sheldrick, 2018)	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6098 / 0 / 514	
Goodness-of-fit on F^2	1.148	
Final *R* indices [*I*>2\σ(*I*)]	*R*1 = 0.0345, *wR*2 = 0.0741	
R indices (all data)	*R*1 = 0.0434, *wR*2 = 0.0830	
Largest diff. peak and hole	0.321 and -0.275 e.$Å^{-3}$	

Table S4: Crystal data and structure refinement for **DTT-H5**

Identification code	dtth5	
Empirical Formula	C40 H24 O4 S3	
Formula Weight	664.77 g/mol	
Temperature	293(2) K	
Wavelength	0.71073Å	
Crystal Size	0.300 x 0.200 x 0.020 mm^3	
Crystal system	orthorhombic	
Space group	Pnma	
Unit Cell dimensions	*a* = 8.3626(3) Å	α = 90°
	b = 40.8701(18) Å	β = 90°
	c = 9.6924 (4) Å	γ = 90°
Volume	3312.7(2)$Å^3$	
Z	4	
Density (calculated)	1.333 g/cm3	
Absorption coefficient	0.266 mm^{-1}	
F(000)	1376	
Theta range for data collection	2.579 to 26.013°	
Index ranges	-10<=h<=10, -50<=k<=48, -11<=l<=11	
Reflections Collected	62864	
Independent reflections	3200 [R(int) = 0.0838]	
Completeness to theta = 25.242	98.4 %	
Max and min transmission	0.7147 and 0.7019	
Refinement method	Full-matric least-squares on F^2	
Data / restraints / parameters	3200 / 688 / 305	
Goodness-of-fit on F^2	1.589	
Final *R* indices [*I*>2\σ(*I*)]	*R*1 = 0.1583, *wR*2 = 0.1832	
R indices (all data)	*R*1 = 0.2060, *wR*2 = 0.1964	
Largest diff. peak and hole	0.298 and -0.307 $eÅ^{-3}$	

Table S5: Crystal data and structure refinement for **BDT-F5.**

Identification code	g23053	
Empirical Formula	C42H16F10O4S2	
Formula Weight	838.67 g/mol	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal Size	0.015 x 0.200 x 0.310 mmmm^3	
Crystal system	triclinic	
Space group	*P -1*	
Unit Cell dimensions	*a* = _ 3.9311(3) Å	α = 93.740(3)°
	b = _ 6.7913(5)Å	β = 91.628(3)°
	c = 31.150(2)Å	γ = 93.783(3) °
Volume	827.59(11)Å^3	
Z	1	
Density (calculated)	1.683 g/cm3Mg/m^3	
Absorption coefficient	2.407mm^{-1}	
F(000)	422	
Theta range for data collection	2.85 to 77.49°	
Index ranges	-4<=h<=4, -8<=k<=8, -39<=l<=39	
Reflections Collected	36817	
Independent reflections	3472 [R(int) = 0.0490]	
Completeness to theta = 67.68	99.9%	
Max and min transmission	0.9650 and 0.5220	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3472 / 306 / 281	
Goodness-of-fit on F^2	1.031	
Final *R* indices [*I*>2\σ(*I*)]	*R*1 = 0.0321, *wR*2 = 0.0848	
R indices (all data)	*R*1 = 0.0335, *wR*2 = 0.0858	
Largest diff. peak and hole	0.461 and -0.285 eÅ-3	

Table S6: Crystal data and structure refinement for **mCPDT-F5.**

Identification code	EG1011498082023	
Empirical Formula	$C_{43}H_{20}F_{10}O_4S_2$	
Formula Weight	854.71 g/mol	
Temperature	273(2) K	
Wavelength	0.71073 Å	
Crystal Size	0.100 x 0.150 x 0.200 mm^3	
Crystal system	triclinic	
Space group	P -1	
Unit Cell dimensions	*a* = 11.6355(7) Å	α = 101.821(3)°
	b = 12.2032(7) Å	β = 104.702(3)°
	c = 14.9256(10) Å	γ = 113.286(3)°
Volume	1768.36(19) $Å^3$	
Z	2	
Density (calculated)	1.605 g/cm^3	
Absorption coefficient	0.251 mm^{-1}	
F(000)	864	
Theta range for data collection	2.48 to 28.37°	
Index ranges	-15<=h<=15, -16<=k<=16, -19<=l<=19	
Reflections Collected	105002	
Independent reflections	8821 [R(int) = 0.1063]	
Completeness to theta = 25.24	99.9 %	
Max and min transmission	0.9750 and 0.9520	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	8821 / 0 / 534	
Goodness-of-fit on F^2	1.077	
Final *R* indices [*I*>2\σ(*I*)]	*R*1 = 0.0819, *wR*2 = 0.2042	
R indices (all data)	*R*1 = 0.1586, *wR*2 = 0.2847	
Largest diff. peak and hole	1.162 and -0.667 eÅ-3	

Table S7: Crystal data and structure refinement for **mCPDT-H5.**

Identification code	EG101156_1	
Empirical Formula	C43H30O4S2	
Formula Weight	674.79 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal Size	0.155 x 0.320 x 0.330 mm^3	
Crystal system	orthorhombic	
Space group	P n m a	
Unit Cell dimensions	*a* = 8.1998(7) Å	α = 90°
	b = 40.439(3) Å	β = 90°
	c = 10.0135(8) Å	γ = 90°
Volume	3320.4(5) $Å^3$	
Z	4	
Density (calculated)	1.350 g/cm3	
Absorption coefficient	0.206 mm^{-1}	
F(000)	1408	
Theta range for data collection	1.01 to 32.03°	
Index ranges	-12<=h<=12, -59<=k<=59, -14<=l<=10	
Reflections Collected	46590	
Independent reflections	5796 [R(int) = 0.0417]	
Completeness to theta = 25.24	99.1 %	
Max and min transmission	0.9700 and 0.9000	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	5796 / 0 / 264	
Goodness-of-fit on F^2	1.073	
Final *R* indices [*I*>2\σ(*I*)]	*R*1 = 0.0385, *wR*2 = 0.0988	
R indices (all data)	*R*1 = 0.0469, *wR*2 = 0.1037	
Largest diff. peak and hole	0.541 and -0.381 eÅ-3	

Wide Angle X-Ray Scan

Figure S24: WAXS results of thienothiophene H5 of both the yellow and orange polymorphs.

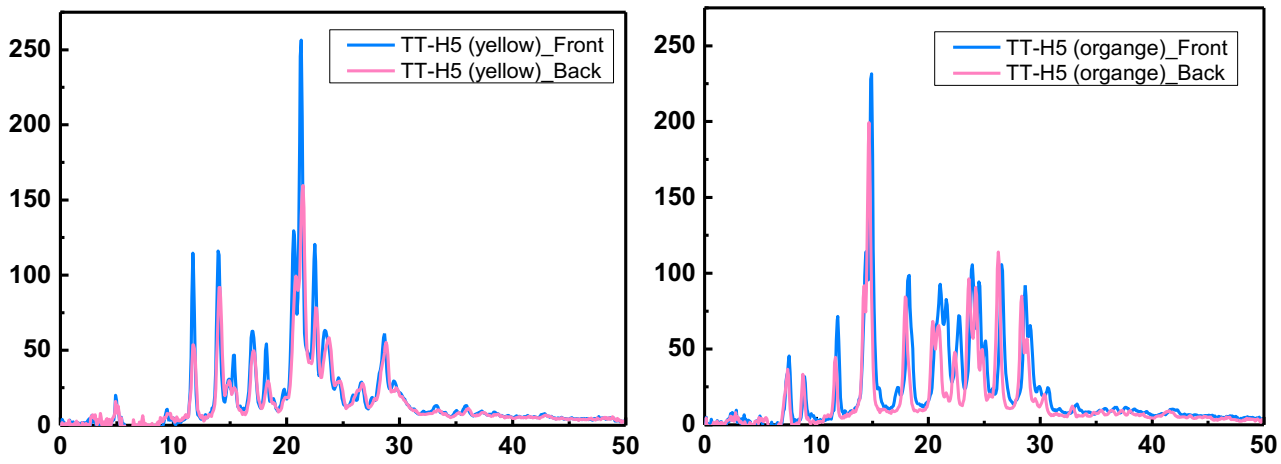


Figure S25: WAXS of dithienothiophene F5 powder, as well as isolated yellow and orange powders.

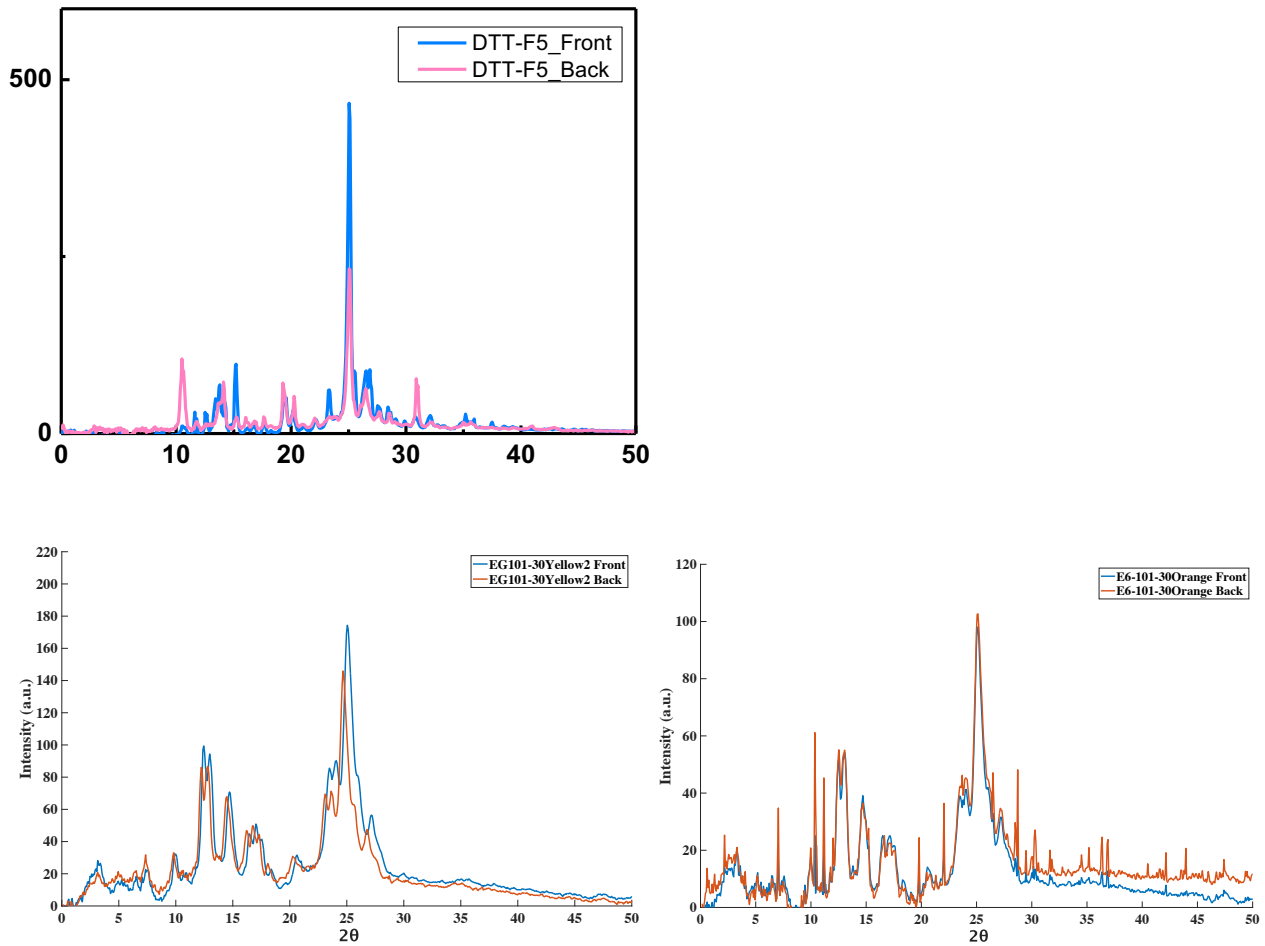


Figure S26: WAXS dithienothiophene H5 both orange and red polymorphs.

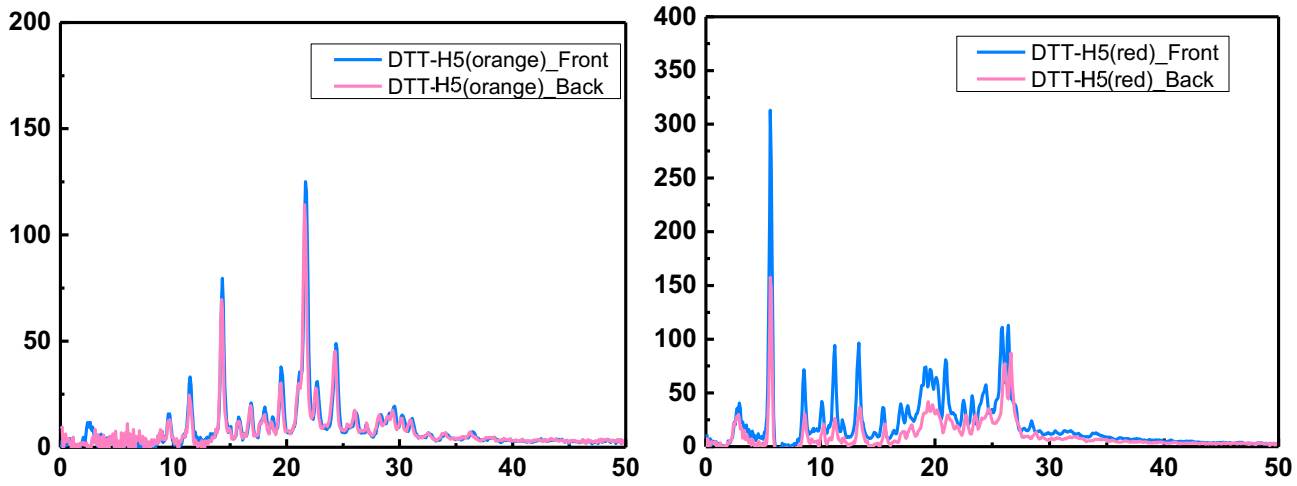


Figure S27: WAXS of BDT-F5 yellow solid

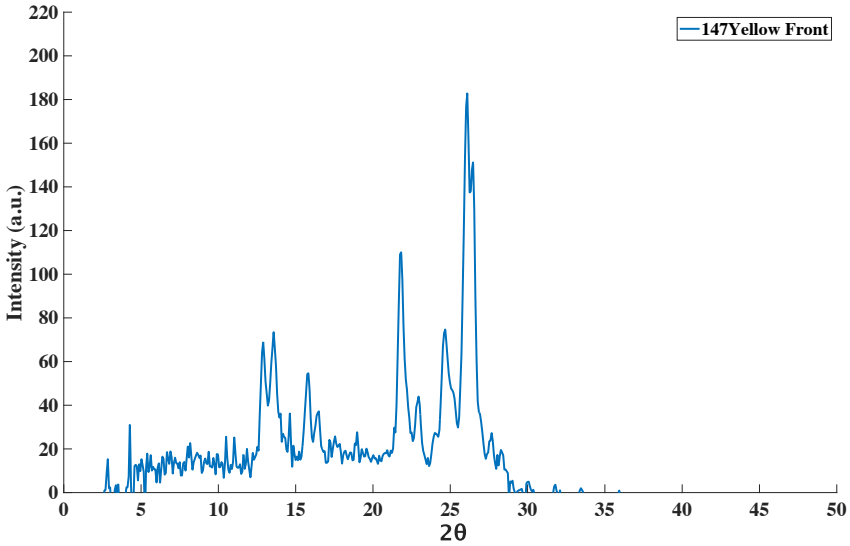


Figure S28: WAXS of BDT-H5 red and orange polymorphs

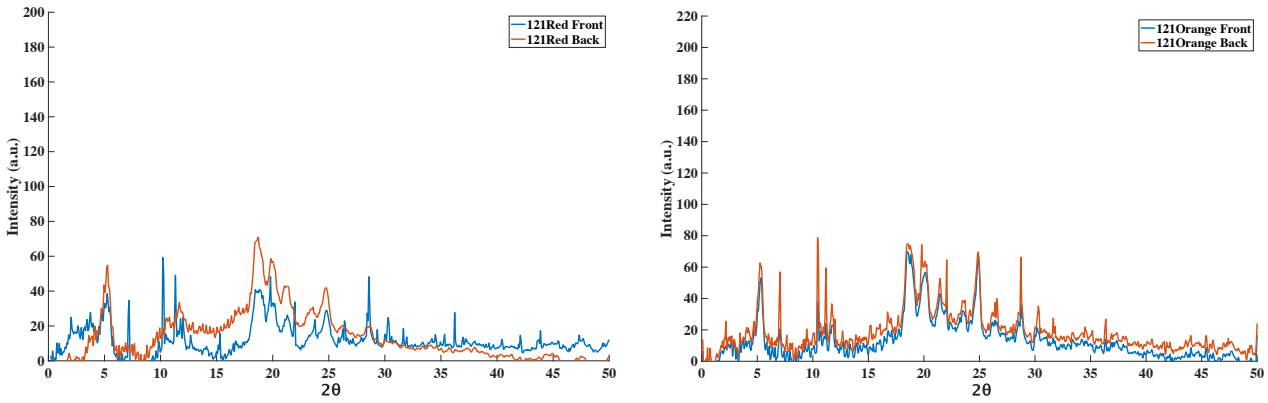


Figure S29: WAXS of mCPDT-F5 dark red and orange powders.

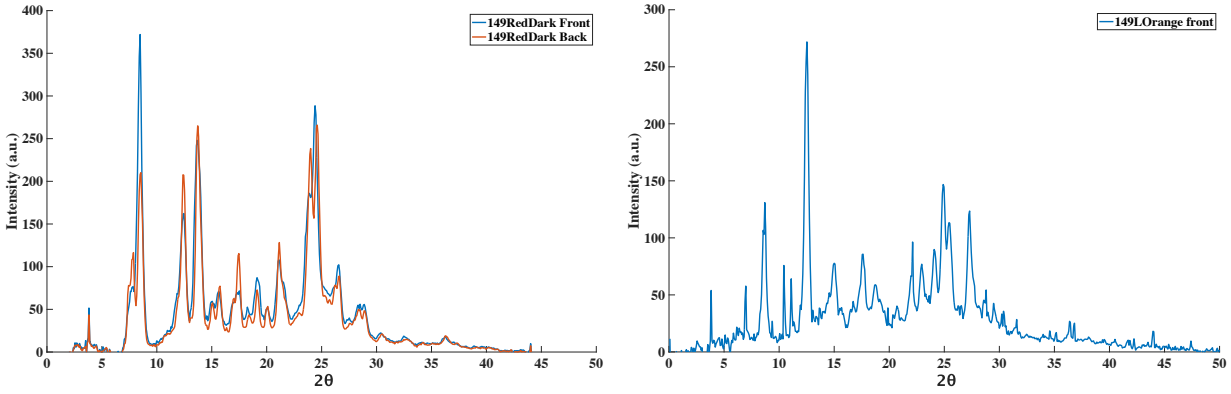
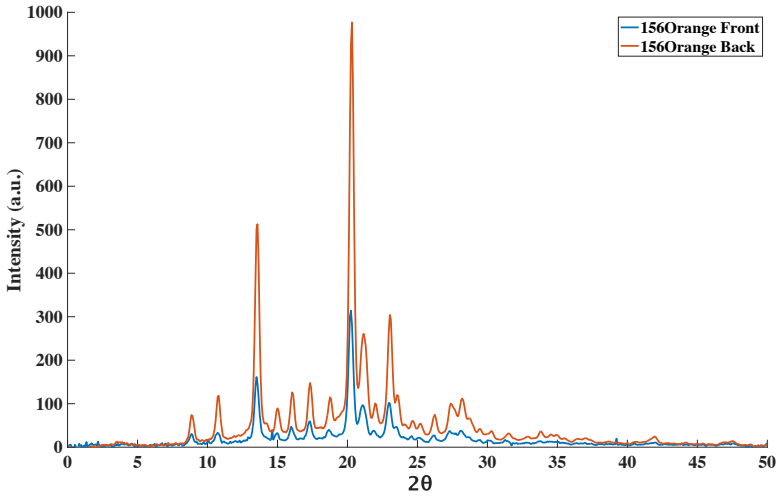


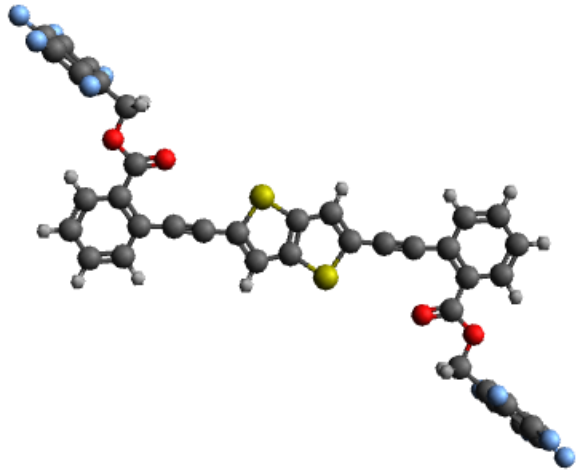
Figure S30: WAXS of mCPDT-H5 orange polymorph



Density Functional Theory Calculations

TT-F5

Solution Optimization



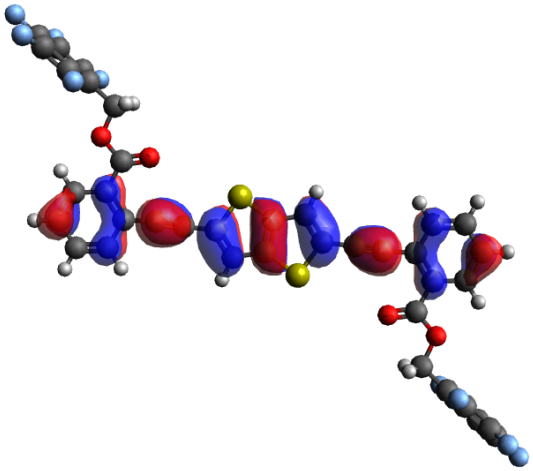
Energy: -3551.98 a.u

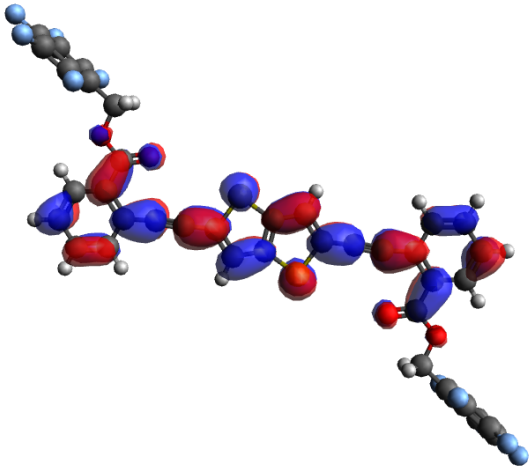
Cartesian Coordinates:

C	11.0505790000	-11.6536830000	-0.0341120000
C	10.3621480000	-12.9711370000	-0.1125250000
C	11.1161450000	-14.1755070000	-0.1706570000
C	10.4205020000	-15.4024760000	-0.2399410000
C	9.0319690000	-15.4421980000	-0.2526530000
C	8.2957350000	-14.2554990000	-0.1964390000
C	8.9612400000	-13.0357900000	-0.1269130000
O	12.2546150000	-11.4820820000	-0.0155340000
O	10.1704560000	-10.6212600000	0.0184360000
C	12.5354030000	-14.2307330000	-0.1638750000
C	10.7725190000	-9.3076660000	0.1045550000
C	9.6614480000	-8.3011510000	0.1787210000
C	9.1417720000	-7.7026250000	-0.9700710000
C	7.5605500000	-6.4330850000	0.3205310000
C	8.0529730000	-7.0165680000	1.4854380000
C	9.0879740000	-7.9425150000	1.3998620000
C	13.7389450000	-14.4275450000	-0.1666950000
C	8.1076570000	-6.7728520000	-0.9141400000
C	19.7314720000	-15.0053700000	-0.1705910000
C	18.9850380000	-13.8386730000	-0.1715190000
C	17.5972760000	-14.1027640000	-0.1691560000
C	17.2669920000	-15.4632810000	-0.1682970000
S	18.6998190000	-16.4556500000	-0.1674660000
S	16.1644480000	-13.1103950000	-0.1673140000
C	15.1327940000	-14.5606790000	-0.1677130000
C	15.8792300000	-15.7273760000	-0.1685450000
C	23.8135950000	-17.9124210000	-0.0384880000
C	24.5020500000	-16.5951350000	-0.1194800000

C	23.7480930000	-15.3907770000	-0.1783810000
C	24.4437620000	-14.1639700000	-0.2502140000
C	25.8322830000	-14.1243970000	-0.2646990000
C	26.5684760000	-15.3110840000	-0.2077290000
C	25.9029460000	-16.5306320000	-0.1356520000
O	22.6095550000	-18.0839600000	-0.0195920000
C	22.3288500000	-15.3354180000	-0.1698280000
C	21.1253170000	-15.1385350000	-0.1712690000
O	24.6937010000	-18.9447570000	0.0160710000
C	24.0916090000	-20.2581860000	0.1044830000
C	25.2026460000	-21.2645120000	0.1816380000
C	25.7234870000	-21.8651700000	-0.9655140000
C	27.3034340000	-23.1322700000	0.3290390000
C	26.8098230000	-22.5466330000	1.4923600000
C	25.7748960000	-21.6208620000	1.4040190000
C	26.7575630000	-22.7948140000	-0.9068130000
F	9.6510630000	-8.0109710000	-2.1726710000
F	6.5662760000	-5.5442520000	0.3882930000
F	7.5278350000	-6.6873140000	2.6714520000
F	9.5459380000	-8.4885760000	2.5366860000
F	25.2153880000	-21.5590790000	-2.1691950000
F	28.2976530000	-24.0209600000	0.3994530000
F	27.3337670000	-22.8736730000	2.6795150000
F	25.3157780000	-21.0726980000	2.5393640000
F	7.6352620000	-6.2098400000	-2.0324900000
F	27.2310930000	-23.3599000000	-2.0236360000
H	10.9952420000	-16.3210680000	-0.2839820000
H	8.5235600000	-16.3998210000	-0.3067600000
H	7.2110580000	-14.2808830000	-0.2063430000
H	8.3970950000	-12.1127130000	-0.0822530000
H	11.4045690000	-9.2598300000	0.9926930000
H	11.3959260000	-9.1379340000	-0.7744620000
H	19.4379060000	-12.8556110000	-0.1730140000
H	15.4263620000	-16.7104390000	-0.1685260000
H	23.8690530000	-13.2453860000	-0.2948030000
H	26.3407120000	-13.1668980000	-0.3207810000
H	27.6531420000	-15.2858170000	-0.2190260000
H	26.4670630000	-17.4536960000	-0.0904010000
H	23.4588690000	-20.3041770000	0.9922200000
H	23.4688990000	-20.4297810000	-0.7746710000

Solution Time Dependent Calculations

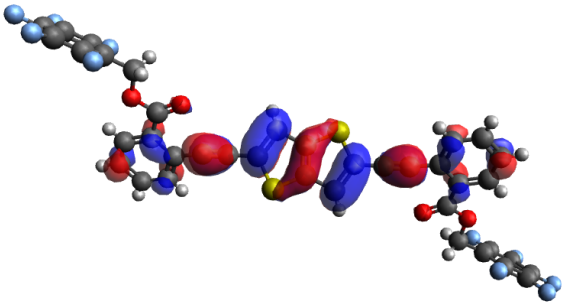


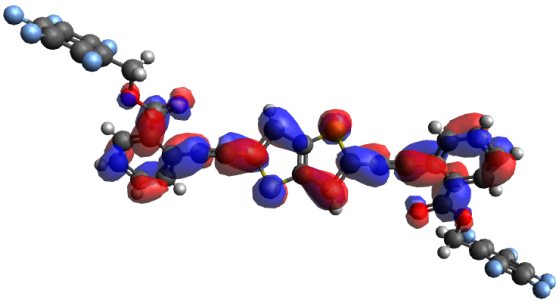


HOMO: -5.415 LUMO: -2.393

	Transition Orbitals	Transition Energy	Wavelength	Oscillator Strength (f)
Solution	HOMO → LUMO	2.7644 eV	448.50 nm	2.5048
	HOMO → LUMO+2	3.7958 eV	326.64 nm	0.227

Single Crystal Time Dependent Calculations

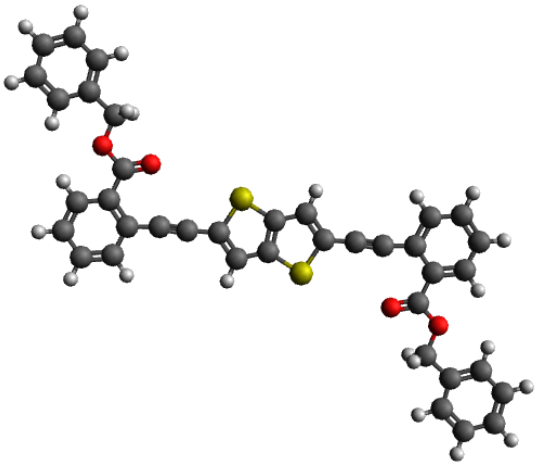




HOMO: -5.252 LUMO: -2.146

	Transition Orbitals	Transition Energy	Wavelength	Oscillator Strength (f)
Crystal	HOMO → LUMO HOMO → LUMO+4	2.8674 eV	432.40 nm	1.4837
	HOMO-1 → LUMO HOMO → LUMO+2 HOMO → LUMO+4	3.6775 eV	337.14 nm	0.3526

TT-H5



Energy: -2559.73 a.u

Cartesian Coordinates:

C	9.2595980000	-9.5115030000	0.0026770000
C	8.5741930000	-10.8341450000	0.0010280000
C	9.3329480000	-12.0370280000	-0.0001660000
C	8.6432030000	-13.2693920000	-0.0017480000
C	7.2549410000	-13.3168840000	-0.0020730000
C	6.5135850000	-12.1322100000	-0.0008310000
C	7.1739980000	-10.9076420000	0.0006770000
O	10.4650380000	-9.3455880000	0.0044170000
O	8.3839240000	-8.4779290000	0.0019990000
C	10.7526470000	-12.0879150000	0.0000430000
C	8.9760800000	-7.1659860000	0.0035040000
C	7.8968070000	-6.1088490000	0.0009660000
C	6.5324130000	-6.4117110000	-0.0037300000
C	5.9825090000	-4.0518430000	-0.0037110000
C	7.3456300000	-3.7428150000	0.0009490000
C	8.2939170000	-4.7639100000	0.0032950000
C	11.9559690000	-12.2864770000	0.0000500000
C	5.5813800000	-5.3872490000	-0.0060330000
C	17.9482360000	-12.8729730000	0.0008210000
C	17.2033510000	-11.7052730000	0.0023900000
C	15.8151300000	-11.9671860000	0.0016180000
C	15.4827580000	-13.3271370000	-0.0005350000
S	16.9141400000	-14.3216900000	-0.0016500000
S	14.3837460000	-10.9726340000	0.0027370000
C	13.3496460000	-12.4213610000	0.0002350000
C	14.0945390000	-13.5890550000	-0.0013240000
C	22.0382020000	-15.7828960000	-0.0016120000
C	22.7236510000	-14.4602770000	-0.0000050000
C	21.9649360000	-13.2573660000	0.0012100000
C	22.6547230000	-12.0250270000	0.0027730000

C	24.0429850000	-11.9775830000	0.0030870000
C	24.7843020000	-13.1622820000	0.0018450000
C	24.1238500000	-14.3868270000	0.0003310000
O	20.8327560000	-15.9487710000	-0.0027290000
C	20.5452380000	-13.2064370000	0.0010030000
C	19.3419170000	-13.0078630000	0.0009880000
O	22.9138370000	-16.8165040000	-0.0017180000
C	22.3216290000	-18.1284210000	-0.0031550000
C	23.4008620000	-19.1856010000	-0.0017750000
C	24.7652710000	-18.8827930000	0.0015590000
C	25.3150830000	-21.2426830000	0.0007470000
C	23.9519450000	-21.5516570000	-0.0025590000
C	23.0036960000	-20.5305240000	-0.0038280000
C	25.7162660000	-19.9072930000	0.0027940000
H	9.2226260000	-14.1861190000	-0.0026980000
H	6.7510590000	-14.2784300000	-0.0032760000
H	5.4289500000	-12.1627100000	-0.0010350000
H	6.6037550000	-9.9875600000	0.0017100000
H	9.6239290000	-7.0693860000	-0.8746650000
H	9.6196480000	-7.0694610000	0.8848300000
H	6.2123020000	-7.4469170000	-0.0056510000
H	5.2420950000	-3.2574910000	-0.0055090000
H	7.6702540000	-2.7063940000	0.0027920000
H	9.3526850000	-4.5155800000	0.0069530000
H	4.5245310000	-5.6381530000	-0.0096640000
H	17.6577050000	-10.7228890000	0.0040040000
H	13.6401940000	-14.5714440000	-0.0029450000
H	22.0753300000	-11.1082810000	0.0037200000
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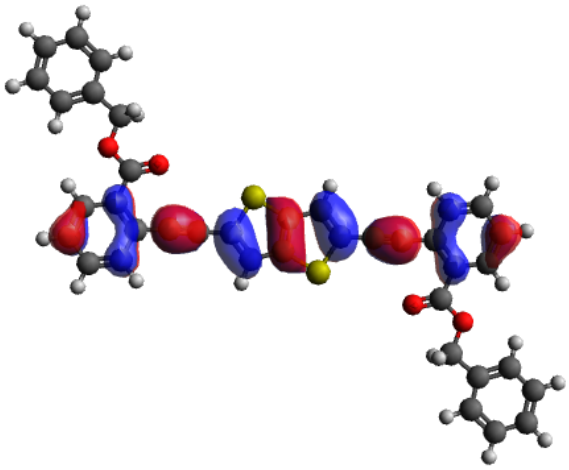
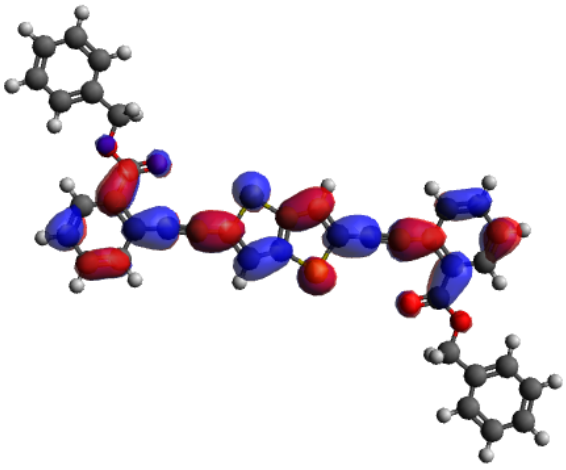
H	25.8689380000	-13.1318160000	0.0020560000
H	24.6940620000	-15.3069290000	-0.0006800000
H	21.6744660000	-18.2252660000	0.8754920000
H	21.6773660000	-18.2246550000	-0.8840050000
H	25.0854240000	-17.8476000000	0.0032290000
H	26.0554660000	-22.0370640000	0.0017150000
H	23.6272790000	-22.5880650000	-0.0041740000
H	21.9449140000	-20.7788130000	-0.0064240000
H	26.7731280000	-19.6564310000	0.0053750000

Solution Time Dependent Calculations





HOMO: -5.388

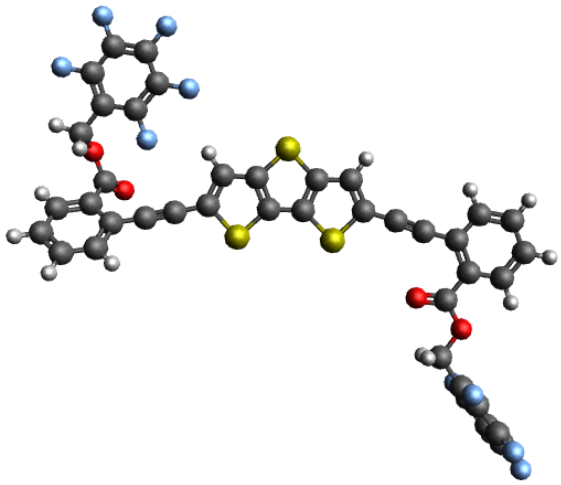
LUMO: -2.316

	Transition Orbitals	Transition Energy	Wavelength	Oscillator Strength (f)
Solution	HOMO → LUMO	2.7730 eV	447.12 nm	2.4989
	HOMO → LUMO+2	3.8088 eV	325.52 nm	0.2046

Single Cystal Time Dependent Calculations

No data obtained

DTT-F5



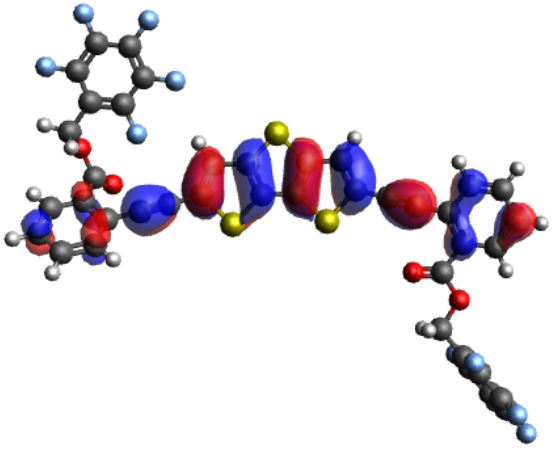
Energy: -4026.37 a.u

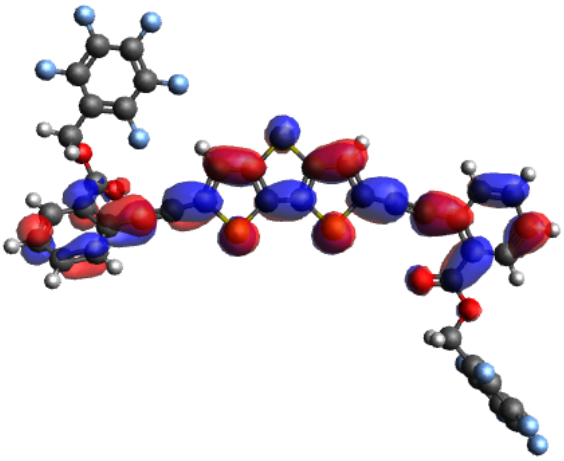
Cartesian Coordinates:

C	9.4236540000	-12.0453280000	0.4972410000
C	8.6172120000	-13.2342790000	0.8863080000
C	9.2407280000	-14.5001310000	1.0643170000
C	8.4359960000	-15.6011840000	1.4308560000
C	7.0665400000	-15.4605450000	1.6165230000
C	6.4588680000	-14.2140580000	1.4412820000
C	7.2330870000	-13.1163840000	1.0793800000
O	10.6257550000	-12.0331310000	0.3115090000
O	8.6586880000	-10.9316220000	0.3631220000
C	10.6311840000	-14.7343670000	0.8960290000
C	9.3812750000	-9.7366790000	-0.0182570000
C	8.3902510000	-8.6131130000	-0.1101800000
C	8.0919600000	-7.8139010000	0.9946090000
C	6.5173700000	-6.5184360000	-0.2779660000
C	6.7882590000	-7.3012290000	-1.3975530000
C	7.7120650000	-8.3372190000	-1.2986200000
C	11.7973180000	-15.0741870000	0.7854080000
C	7.1730470000	-6.7712210000	0.9243950000
C	17.6453870000	-16.3545230000	0.1375790000
C	17.0211050000	-15.1092970000	0.0099120000
C	15.6234400000	-15.1759690000	0.2297220000
C	15.1903080000	-16.4730590000	0.5275440000
S	16.5096800000	-17.6385080000	0.5375750000
S	14.2970220000	-14.0524130000	0.2267400000
C	13.1589640000	-15.3603340000	0.6335780000
C	13.8012590000	-16.5812160000	0.7566500000
C	23.7872450000	-16.0835480000	-2.3500470000
C	24.2572860000	-14.8511860000	-1.6343480000
C	23.3344050000	-13.9717720000	-1.0128860000
C	23.8083050000	-12.7483980000	-0.4996270000

C	25.1523800000	-12.4029110000	-0.6053990000
C	26.0582320000	-13.2784880000	-1.2077320000
C	25.6091630000	-14.4989900000	-1.7112020000
O	22.9402960000	-16.0574140000	-3.2125780000
C	21.9674510000	-14.3267340000	-0.8397620000
C	20.8138720000	-14.6529550000	-0.6238090000
O	24.4294470000	-17.2607850000	-2.1010540000
C	24.9907500000	-17.5616870000	-0.8028990000
C	24.2373890000	-18.7254520000	-0.2105680000
C	22.8971330000	-18.5923540000	0.1534690000
C	22.7620850000	-20.8949910000	0.8164450000
C	24.0999780000	-21.0615800000	0.4695270000
C	24.8165390000	-19.9828690000	-0.0451010000
C	22.1533120000	-19.6514850000	0.6563160000
C	19.0418310000	-16.3299100000	-0.0750890000
C	19.4941660000	-15.0549210000	-0.3687030000
S	18.1721120000	-13.8659740000	-0.3815230000
F	7.9562270000	-9.0749730000	-2.3924300000
F	6.1589910000	-7.0558890000	-2.5528240000
F	5.6315940000	-5.5223520000	-0.3584730000
F	6.9135540000	-6.0168220000	1.9988550000
F	8.7109340000	-8.0347440000	2.1645220000
F	26.1017560000	-20.1811760000	-0.3783910000
F	20.8643280000	-19.4852680000	0.9829050000
F	22.0639160000	-21.9231440000	1.3033390000
F	22.2929330000	-17.3993130000	0.0073520000
F	24.6859940000	-22.2542810000	0.6235750000
H	8.9108600000	-16.5667570000	1.5661570000
H	6.4724320000	-16.3242860000	1.8984500000
H	5.3896330000	-14.0989880000	1.5853830000
H	6.7690200000	-12.1479170000	0.9412540000
H	10.1458340000	-9.5237250000	0.7302660000
H	9.8726320000	-9.9043200000	-0.9779050000
H	13.2748630000	-17.4952730000	0.9998450000
H	23.1066930000	-12.0797180000	-0.0128730000
H	25.4941320000	-11.4520150000	-0.2090910000
H	27.1070900000	-13.0128870000	-1.2893320000
H	26.3078490000	-15.1757900000	-2.1933740000
H	24.9307880000	-16.6897040000	-0.1491850000
H	26.0384790000	-17.8257880000	-0.9450250000
H	19.7045270000	-17.1823020000	-0.0041360000

Solution Time Dependent Calculations

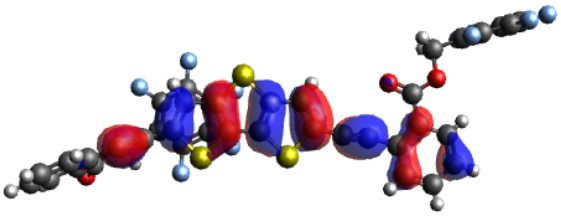


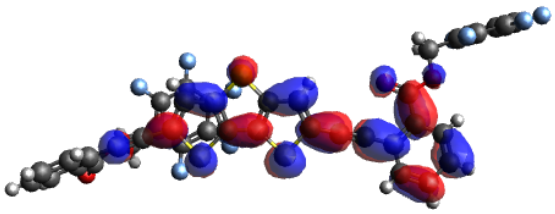


HOMO: -5.335 LUMO: -2.325

	Transition Orbitals	Transition Energy	Wavelength	Oscillator Strength (f)
Solution	HOMO → LUMO	2.7418 eV	452.20 nm	2.4112
	HOMO-3 → LUMO HOMO-2 → LUMO HOMO → LUMO+2	3.7240 eV	332.93 nm	0.2093

Single Cystal Time Dependent Calculations

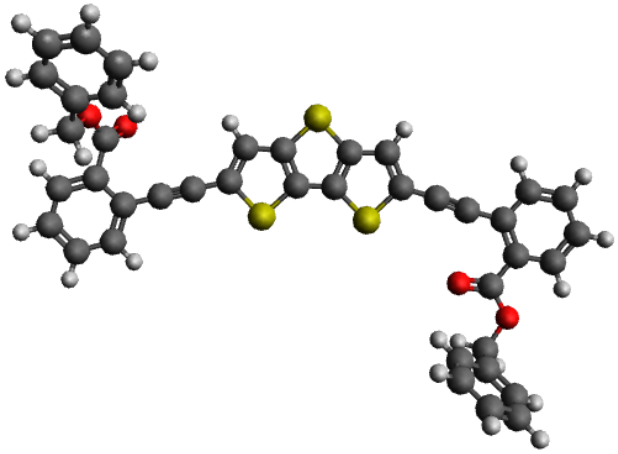




HOMO: -5.355 LUMO: -2.047

	Transition Orbitals	Transition Energy	Wavelength	Oscillator Strength (f)
Crystal	HOMO-2 → LUMO+1 HOMO → LUMO HOMO → LUMO+1	3.1111 eV	398.52 nm	0.7337
	HOMO → LUMO HOMO → LUMO+1	3.1465 eV	394.04 nm	1.0369
	HOMO-2 → LUMO HOMO → LUMO HOMO → LUMO+2	3.7130 eV	333.92 nm	0.4584

DTT-H5



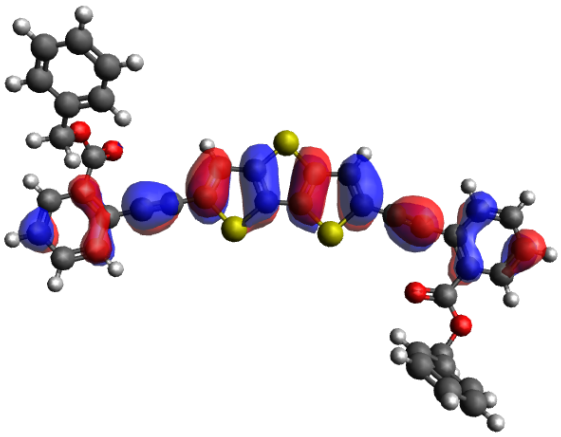
Energy: -3034.12 a.u

Cartesian Coordinates:

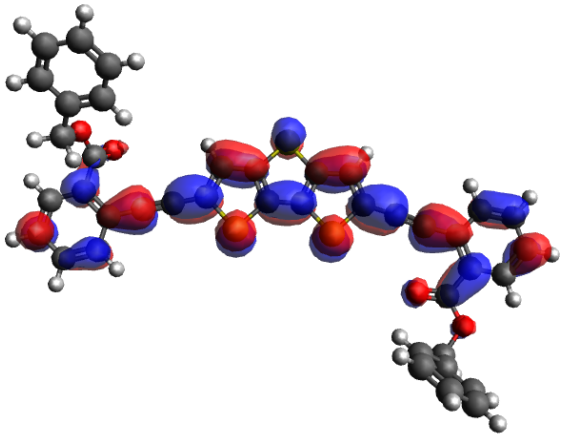
C	8.3650260000	-10.7416760000	-0.3283200000
C	7.5122530000	-11.9389810000	-0.0769490000
C	8.0862400000	-13.2395330000	-0.0438580000
C	7.2404680000	-14.3445770000	0.1966170000
C	5.8768510000	-14.1749590000	0.4005510000
C	5.3175760000	-12.8945100000	0.3697230000
C	6.1334040000	-11.7927150000	0.1318390000
O	9.5745580000	-10.7669830000	-0.4704470000
O	7.6326210000	-9.6062700000	-0.3893350000
C	9.4672690000	-13.5061570000	-0.2416740000
C	8.3562600000	-8.3608500000	-0.6136400000
C	8.7257460000	-7.6917780000	0.6867160000
C	9.9533960000	-7.9620170000	1.3072440000
C	9.3905640000	-6.4593450000	3.1184150000
C	8.1655080000	-6.1841330000	2.5069630000
C	7.8369200000	-6.7976770000	1.2975130000
C	10.6190900000	-13.8766230000	-0.3948790000
C	10.2836810000	-7.3487390000	2.5162240000
C	16.4193180000	-15.2789090000	-1.2049370000
C	15.8371420000	-14.0065480000	-1.1984410000
C	14.4389290000	-14.0487320000	-0.9776970000
C	13.9622320000	-15.3546550000	-0.8164680000
S	15.2408780000	-16.5587890000	-0.9365820000
S	13.1513770000	-12.8870300000	-0.8542360000
C	11.9697600000	-14.1918380000	-0.5832850000
C	12.5704470000	-15.4396710000	-0.5937260000
C	22.9765530000	-15.2291860000	-2.0488820000
C	23.2170790000	-13.7567190000	-2.2222090000
C	22.1266180000	-12.8504170000	-2.2629280000
C	22.3883370000	-11.4877360000	-2.5138580000

C	23.6855310000	-11.0414400000	-2.7440320000
C	24.7533460000	-11.9414300000	-2.7188760000
C	24.5151640000	-13.2886530000	-2.4491640000
O	22.2462520000	-15.8589760000	-2.7839730000
C	20.7899270000	-13.2719230000	-2.0268380000
C	19.6367480000	-13.6079810000	-1.8207720000
O	23.6408470000	-15.8884070000	-1.0704380000
C	24.2581300000	-15.1946470000	0.0536740000
C	24.1653270000	-16.0865670000	1.2633900000
C	22.9403440000	-16.2569520000	1.9231380000
C	23.9826020000	-17.7547350000	3.5100880000
C	25.2062160000	-17.5895040000	2.8601270000
C	25.2947530000	-16.7606060000	1.7395820000
C	22.8482040000	-17.0873850000	3.0386330000
C	17.8145940000	-15.2778740000	-1.4239110000
C	18.3104710000	-13.9953960000	-1.5867380000
S	17.0280110000	-12.7682900000	-1.4672400000
H	7.6787560000	-15.3363420000	0.2200060000
H	5.2501780000	-15.0421650000	0.5843920000
H	4.2533560000	-12.7560260000	0.5300630000
H	5.7078880000	-10.7974670000	0.1074790000
H	9.2376310000	-8.5770920000	-1.2183530000
H	7.6574780000	-7.7486480000	-1.1861360000
H	10.6413650000	-8.6598480000	0.8404100000
H	9.6494400000	-5.9804840000	4.0582420000
H	7.4691770000	-5.4904020000	2.9688540000
H	6.8849870000	-6.5785610000	0.8204470000
H	11.2385970000	-7.5632440000	2.9870210000
H	12.0136330000	-16.3561450000	-0.4464420000
H	21.5573710000	-10.7908520000	-2.5299870000
H	23.8628750000	-9.9896340000	-2.9448960000
H	25.7653040000	-11.5980320000	-2.9070000000
H	25.3438470000	-13.9898400000	-2.4356300000
H	23.7411590000	-14.2466220000	0.2200080000
H	25.3014140000	-14.9829480000	-0.1942060000
H	22.0577860000	-15.7377610000	1.5588750000
H	23.9114390000	-18.3989500000	4.3814470000
H	26.0904940000	-18.1053750000	3.2222050000
H	26.2478000000	-16.6353320000	1.2323590000
H	21.8946470000	-17.2115660000	3.5431320000
H	18.4456810000	-16.1561290000	-1.4683940000

Solution Time Dependent Calculations



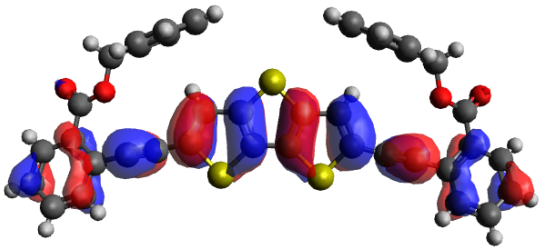
HOMO: -5.305



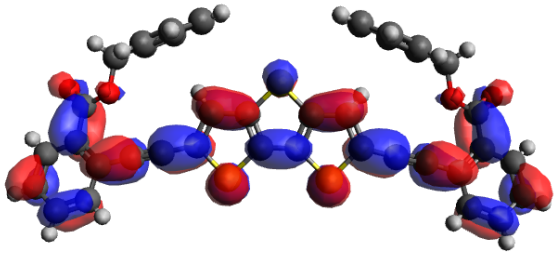
LUMO: -2.330

	Transition Orbitals	Transition Energy	Wavelength	Oscillator Strength (f)
Solution	HOMO → LUMO	2.7218 eV	455.52 nm	2.5496
	HOMO-2 → LUMO	3.7317 eV	332.25 nm	0.1913
	HOMO → LUMO+1			
	HOMO → LUMO+2			
	HOMO → LUMO+3			

Single Cystal Time Dependent Calculations



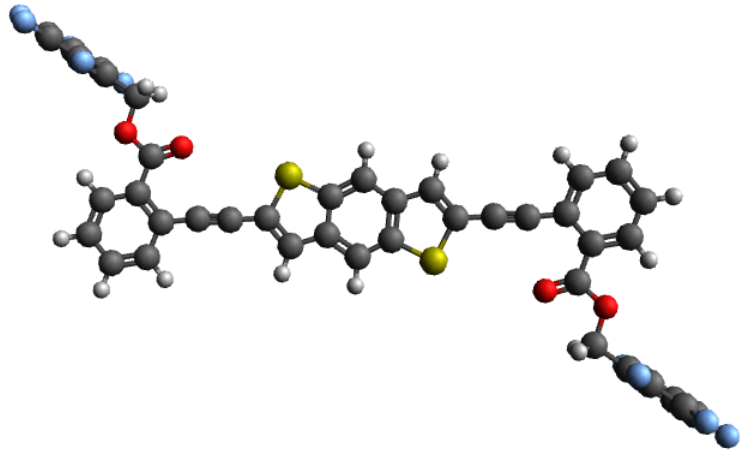
HOMO: -5.238



LUMO: -1.953

	Transition Orbitals	Transition Energy	Wavelength	Oscillator Strength (f)
Crystal	HOMO → LUMO	3.0693 eV	403.95 nm	1.9584
	HOMO → LUMO+2	3.8960 eV	318.24 nm	0.247

BDT-F5



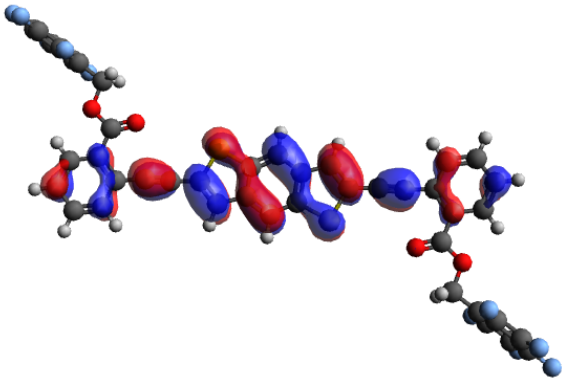
Energy: -3705.64 a.u.

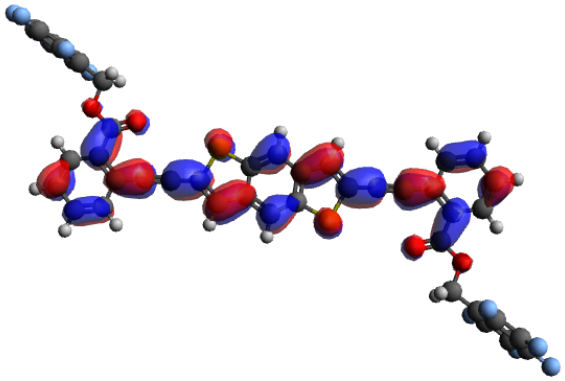
Cartesian Coordinates:

C	10.4500510000	-13.8850980000	0.0339330000
C	9.7943370000	-15.2211370000	-0.0196150000
C	10.5770110000	-16.4078660000	-0.0479770000
C	9.9124270000	-17.6523110000	-0.0962850000
C	8.5250850000	-17.7264020000	-0.1152820000
C	7.7605040000	-16.5570890000	-0.0872740000
C	8.3957150000	-15.3200120000	-0.0404250000
O	9.5449640000	-12.8733730000	0.0210630000
C	11.9980650000	-16.4272470000	-0.0337500000
C	13.2057880000	-16.5903620000	-0.0282250000
C	17.0716560000	-16.1408430000	0.0194840000
C	16.7902170000	-17.5427860000	-0.0268300000
S	15.5879630000	-15.1952020000	0.0366000000
C	14.6057640000	-16.6800400000	-0.0185660000
C	15.3847350000	-17.8098770000	-0.0473270000
C	25.7679160000	-20.2282980000	-0.0341600000
C	26.4235360000	-18.8922030000	0.0190930000
C	25.6407730000	-17.7055270000	0.0472180000
C	26.3052670000	-16.4610240000	0.0952560000
C	27.6926060000	-16.3868280000	0.1142150000
C	28.4572710000	-17.5560890000	0.0864380000
C	27.8221490000	-18.7932230000	0.0398600000
O	26.6730760000	-21.2399560000	-0.0210200000
C	24.2197170000	-17.6862460000	0.0330010000
C	23.0119820000	-17.5232080000	0.0274360000
O	24.5696000000	-20.4293370000	-0.0846260000
S	20.6298030000	-18.9184110000	-0.0374090000
C	21.6120070000	-17.4335620000	0.0177580000
C	20.8330280000	-16.3037310000	0.0465190000
C	17.8493090000	-18.4660070000	-0.0467800000

C	19.1461100000	-17.9727660000	-0.0203170000
C	19.4275480000	-16.5708230000	0.0260000000
C	18.3684580000	-15.6476010000	0.0459480000
C	10.1132780000	-11.5429170000	0.0746030000
C	8.9791060000	-10.5607800000	0.0308010000
C	8.4811390000	-10.0791950000	-1.1810380000
C	7.4259450000	-9.1737870000	-1.2374620000
C	6.8352790000	-8.7386340000	-0.0536620000
C	7.3052090000	-9.2041380000	1.1718840000
C	8.3618150000	-10.1093640000	1.1984710000
O	11.6483840000	-13.6841550000	0.0844110000
C	26.1048650000	-22.5704620000	-0.0742350000
C	27.2390960000	-23.5525090000	-0.0299230000
C	27.8566230000	-24.0042620000	-1.1973370000
C	28.9132840000	-24.9094090000	-1.1702610000
C	29.3830320000	-25.3744770000	0.0555210000
C	28.7921320000	-24.9389720000	1.2390740000
C	27.7368830000	-24.0336590000	1.1821610000
F	9.0334570000	-10.4811860000	-2.3359000000
F	6.9748260000	-8.7239090000	-2.4142880000
F	5.8205840000	-7.8714670000	-0.0935820000
F	6.7380670000	-8.7836570000	2.3087090000
F	8.7958730000	-10.5413490000	2.3924160000
F	27.4227490000	-23.5726980000	-2.3915000000
F	29.4806580000	-25.3302300000	-2.3068460000
F	30.3977760000	-26.2415650000	0.0959010000
F	27.1843230000	-23.6313230000	2.3367880000
F	29.2430740000	-25.3884310000	2.4161280000
H	10.5097980000	-18.5571380000	-0.1186080000
H	8.0402260000	-18.6969410000	-0.1520570000
H	6.6768030000	-16.6089130000	-0.1017610000
H	7.8089330000	-14.4103510000	-0.0184450000
H	14.9625610000	-18.8071000000	-0.0823700000
H	25.7078330000	-15.5562340000	0.1174000000
H	28.1773910000	-15.4162430000	0.1507780000
H	29.5409690000	-17.5041860000	0.1008940000
H	28.4089970000	-19.7028460000	0.0180610000
H	21.2551970000	-15.3065060000	0.0815670000
H	17.6471950000	-19.5317160000	-0.0819190000
H	18.5705720000	-14.5818920000	0.0810870000
H	10.6897450000	-11.4342320000	0.9945380000
H	10.7846260000	-11.4039450000	-0.7740390000
H	25.4333740000	-22.7092110000	0.7743300000
H	25.5285750000	-22.6794880000	-0.9942410000

Solution Time Dependent Calculations

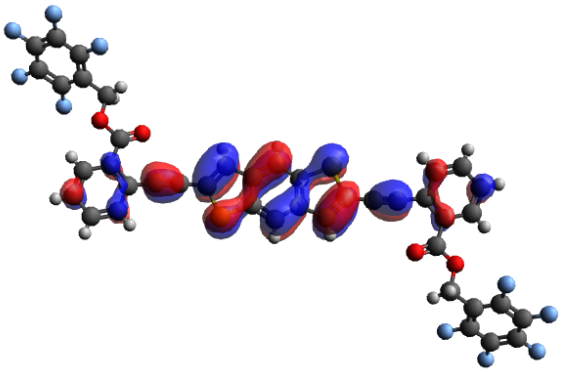


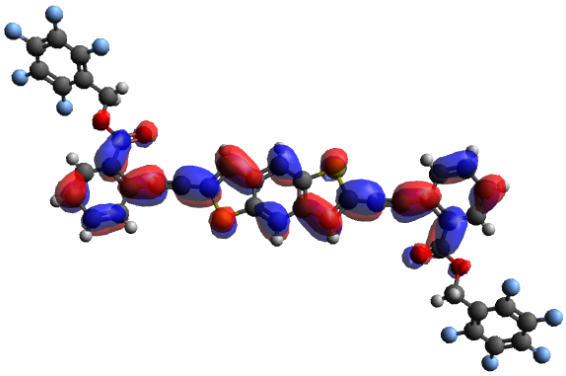


HOMO: -5.425 LUMO: -2.386

	Transition Orbitals	Transition Energy	Wavelength	Oscillator Strength (f)
Solution	HOMO → LUMO	2.7748 eV	446.82 nm	2.4741
	HOMO-10 → LUMO HOMO → LUMO+2	3.7911 eV	327.04 nm	0.1979
	HOMO-10 → LUMO HOMO-2 → LUMO+1 HOMO-1 → LUMO+2 HOMO →> LUMO+9	4.1808 eV	296.56 nm	0.2332

Single Cystal Time Dependent Calculations

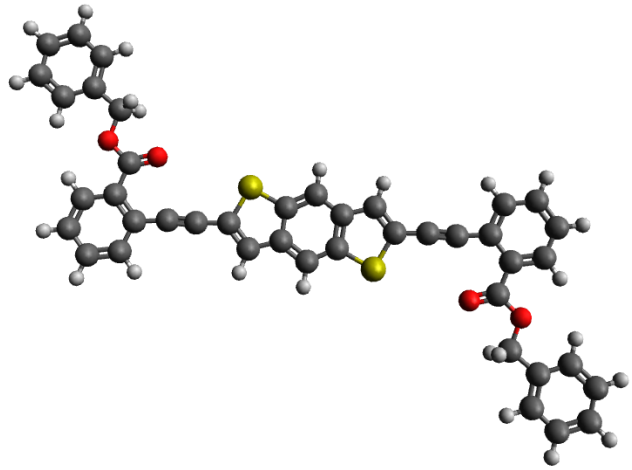




HOMO: -5.337 HOMO: -2.174

	Transition Orbitals	Transition Energy	Wavelength	Oscillator Strength (f)
Crystal	HOMO → LUMO	2.9683 eV	417.70 nm	1.7263
	HOMO → LUMO+2	3.8069 eV	325.69 nm	0.2437
	HOM-10 → LUMO HOMO-2 → LUMO+1 HOMO-1 →LUMO+2 HOMO →LUMO+9	4.2319 eV	292.97 nm	0.2354
	HOMO-8 →LUMO HOMO-1 → LUMO+2 HOMO → LUMO+9	4.5947 eV	269.84 nm	0.2195

BDT-H5



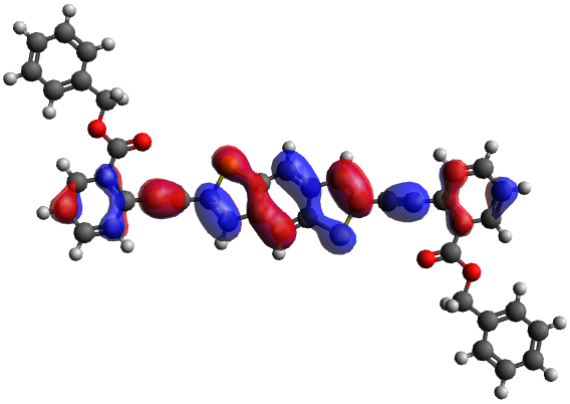
Energy: -2713.39 a.u

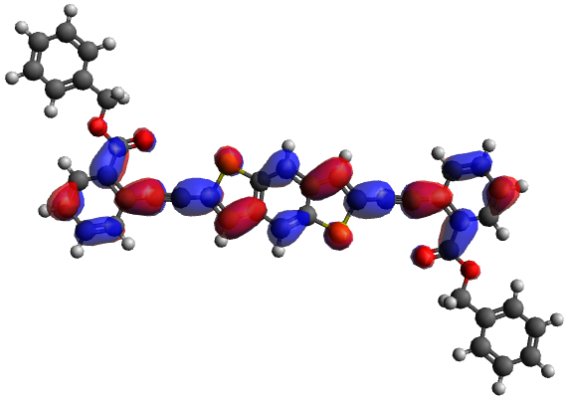
Cartesian Coordinates:

C	8.3606310000	-9.7465950000	0.0009610000
C	7.7087140000	-11.0868190000	-0.0009450000
C	8.4968150000	-12.2704230000	-0.0025690000
C	7.8389210000	-13.5194710000	-0.0043550000
C	6.4520180000	-13.6021100000	-0.0045230000
C	5.6816870000	-12.4364090000	-0.0029030000
C	6.3109950000	-11.1953290000	-0.0011430000
O	7.4587570000	-8.7359500000	0.0018330000
C	9.9182790000	-12.2845580000	-0.0025400000
C	11.1259630000	-12.4485830000	-0.0026650000
C	14.9919130000	-11.9952400000	-0.0015930000
C	14.7113940000	-13.3981150000	-0.0030580000
S	13.5074810000	-11.0505660000	-0.0009020000
C	12.5260450000	-12.5371080000	-0.0025690000
C	13.3059930000	-13.6666360000	-0.0035880000
C	23.6991240000	-16.0746240000	-0.0007210000
C	24.3510080000	-14.7343830000	-0.0007300000
C	23.5628750000	-13.5507990000	-0.0009190000
C	24.2207360000	-12.3017320000	-0.0008190000
C	25.6076370000	-12.2190570000	-0.0005740000
C	26.3779990000	-13.3847380000	-0.0004270000
C	25.7487240000	-14.6258370000	-0.0005010000
O	24.6010230000	-17.0852470000	-0.0003170000
C	22.1414110000	-13.5367050000	-0.0012120000
C	20.9337230000	-13.3727150000	-0.0014850000
O	22.4985190000	-16.2711380000	-0.0009800000
S	18.5522050000	-14.7707300000	-0.0035240000
C	19.5336410000	-13.2841880000	-0.0018170000
C	18.7536930000	-12.1546600000	-0.0009300000
C	15.7712170000	-14.3207200000	-0.0037590000

C	17.0677730000	-13.8260560000	-0.0029730000
C	17.3482930000	-12.4231810000	-0.0015270000
C	16.2884700000	-11.5005760000	-0.0008390000
C	8.0177510000	-7.4093570000	0.0035570000
C	6.9125830000	-6.3793730000	0.0032470000
C	5.5560700000	-6.7157210000	0.0009120000
C	4.5801030000	-5.7149650000	0.0006860000
C	4.9482490000	-4.3700940000	0.0027550000
C	6.3033500000	-4.0276100000	0.0050680000
C	7.2764800000	-5.0250430000	0.0053230000
O	9.5612410000	-9.5501120000	0.0016780000
C	24.0420630000	-18.4118560000	-0.0001690000
C	25.1472740000	-19.4417930000	0.0014370000
C	26.5037720000	-19.1053850000	0.0033740000
C	27.4797810000	-20.1060990000	0.0048860000
C	27.1116920000	-21.4509870000	0.0044980000
C	25.7566040000	-21.7935300000	0.0025810000
C	24.7834330000	-20.7961390000	0.0010480000
H	8.4414710000	-14.4211590000	-0.0056040000
H	5.9722920000	-14.5758980000	-0.0059130000
H	4.5981320000	-12.4939240000	-0.0030090000
H	5.7175680000	-10.2900630000	0.0001560000
H	12.8845300000	-14.6647880000	-0.0046570000
H	23.6181620000	-11.4000600000	-0.0009530000
H	26.0873370000	-11.2452550000	-0.0005080000
H	27.4615520000	-13.3271940000	-0.0002520000
H	26.3421740000	-15.5310880000	-0.0004030000
H	19.1751570000	-11.1565080000	0.0001600000
H	15.5698610000	-15.3871610000	-0.0048560000
H	16.4898250000	-10.4341350000	0.0002770000
H	8.6618420000	-7.2960750000	-0.8753640000
H	8.6599390000	-7.2975520000	0.8840660000
H	5.2615050000	-7.7584830000	-0.0007550000
H	3.5297460000	-5.9918010000	-0.0011270000
H	4.1885200000	-3.5941970000	0.0025700000
H	6.6023510000	-2.9835070000	0.0066880000
H	8.3288120000	-4.7507180000	0.0071400000
H	23.3980540000	-18.5239590000	0.8789630000
H	23.3998030000	-18.5248830000	-0.8804690000
H	26.7982940000	-18.0626090000	0.0037300000
H	28.5301270000	-19.8292170000	0.0063740000
H	27.8714530000	-22.2268510000	0.0056750000
H	25.4576470000	-22.8376470000	0.0022590000
H	23.7311130000	-21.0705100000	-0.0004570000

Solution Time Dependent Calculations





HOMO: -5.403

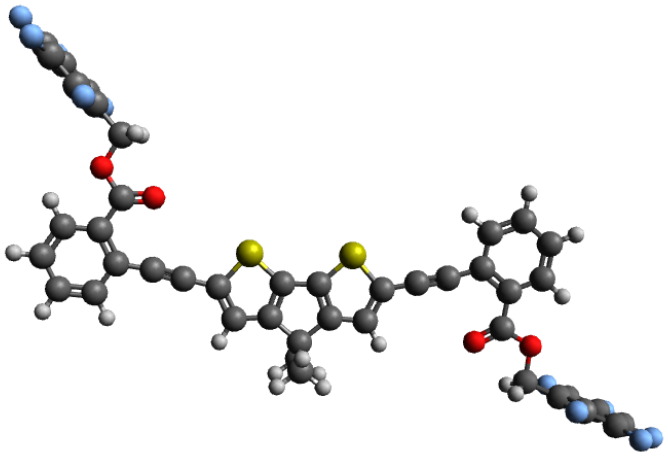
LUMO: -2.356

	Transition Orbitals	Transition Energy	Wavelength	Oscillator Strength (f)
Solution	HOMO → LUMO	2.7843 eV	445.30 nm	2.4813
	HOMO-1 → LUMO	3.2409 eV	382.56 nm	0.3726
	HOMO-12 → LUMO HOMO-2 → LUMO+1 HOMO-1 → LUMO+2 HOMO → LUMO+5	4.1967 eV	295.43 nm	0.2394

Single Cystal Time Dependent Calculations

No data obtained

mCPDT-F5



Energy: -3746.13 a.u

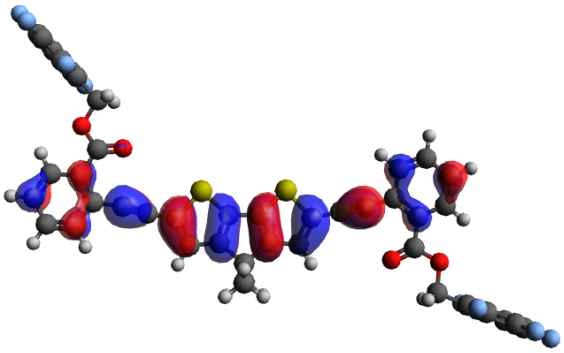
Cartesian Coordinates:

C	9.2554870000	-13.4250110000	-0.0149730000
C	8.3739220000	-14.6189540000	-0.1153370000
C	8.9350810000	-15.9246660000	-0.1829530000
C	8.0573860000	-17.0282610000	-0.2756250000
C	6.6800730000	-16.8527470000	-0.3001010000
C	6.1343040000	-15.5671950000	-0.2333270000
C	6.9795620000	-14.4665130000	-0.1424350000
O	8.5456690000	-12.2669700000	0.0126650000
O	10.4707450000	-13.4415120000	0.0385740000
C	10.3273580000	-16.1982560000	-0.1648400000
C	11.4874160000	-16.5782160000	-0.1583480000
C	17.1601530000	-18.2583760000	-0.0996490000
C	16.7600410000	-16.9264500000	-0.0392120000
C	15.3270240000	-16.8646990000	-0.0734780000
C	14.8195590000	-18.1582080000	-0.1567190000
C	15.9491610000	-19.1871260000	-0.1814600000
S	14.0880110000	-15.6618300000	-0.0415010000
C	12.8410320000	-16.9271920000	-0.1432100000
C	13.4141750000	-18.1949950000	-0.1965570000
C	23.9939940000	-18.8581050000	0.0463830000
C	24.2679220000	-17.3981890000	0.1216700000
C	23.1958430000	-16.4628100000	0.1362530000
C	23.5079050000	-15.0861700000	0.2065810000
C	24.8243820000	-14.6476190000	0.2595650000
C	25.8736950000	-15.5715240000	0.2447720000
C	25.5898670000	-16.9312230000	0.1769160000
O	22.8942310000	-19.3717790000	-0.0340330000
C	21.8214710000	-16.8137320000	0.0872750000
C	20.6118910000	-16.9735300000	0.0525800000
O	25.1358520000	-19.5941500000	0.0769580000

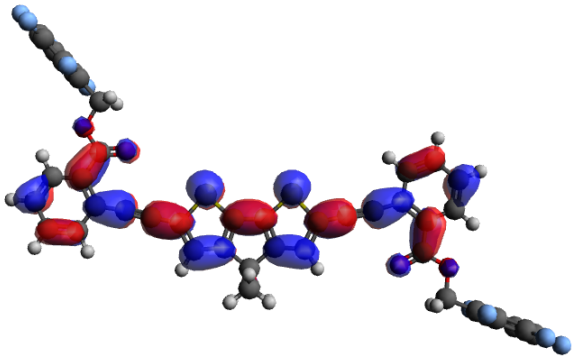
C	24.9423320000	-21.0259610000	0.0015320000
C	26.2955620000	-21.6728200000	0.0628280000
C	27.0430660000	-21.9055660000	-1.0927580000
C	28.1260570000	-22.6391370000	1.3512100000
C	26.8699630000	-22.0444220000	1.2794460000
C	28.3013230000	-22.4982960000	-1.0508310000
C	18.5576550000	-18.4151790000	-0.0726110000
C	19.2329760000	-17.2002070000	0.0083480000
S	18.0945400000	-15.8340300000	0.0522530000
C	15.8779060000	-20.1355210000	1.0364460000
C	15.9468260000	-20.0004630000	-1.4953020000
C	9.3438450000	-11.0637020000	0.1091260000
C	8.4046640000	-9.8927360000	0.1166580000
C	7.9019590000	-9.3699260000	1.3091690000
C	7.0260620000	-8.2886290000	1.3294200000
C	6.6241870000	-7.7124260000	0.1270220000
C	7.1033130000	-8.2140450000	-1.0806750000
C	7.9783910000	-9.2958790000	-1.0710190000
F	8.4267720000	-9.7588030000	-2.2479110000
F	8.2739460000	-9.9052210000	2.4820820000
F	5.7823820000	-6.6757430000	0.1320180000
F	6.5664540000	-7.8043990000	2.4892920000
F	6.7179760000	-7.6579430000	-2.2353250000
F	28.6476300000	-22.9918230000	2.5320670000
F	26.1989610000	-21.8418800000	2.4237320000
F	28.9913430000	-22.7155660000	-2.1766910000
F	26.5422300000	-21.5657540000	-2.2903620000
C	28.8439090000	-22.8627530000	0.1789880000
F	30.0511810000	-23.4308760000	0.2337640000
H	8.4835870000	-18.0241680000	-0.3277450000
H	6.0306680000	-17.7198340000	-0.3714320000
H	5.0588130000	-15.4249110000	-0.2519580000
H	6.5646190000	-13.4677660000	-0.0901400000
H	12.8091250000	-19.0916180000	-0.2612190000
H	22.6920270000	-14.3717400000	0.2184350000
H	25.0328220000	-13.5834790000	0.3123850000
H	26.9040690000	-15.2339800000	0.2856320000
H	26.3970040000	-17.6528800000	0.1648370000
H	24.3163150000	-21.3500360000	0.8341810000
H	24.4329960000	-21.2724290000	-0.9315530000
H	19.0898340000	-19.3582150000	-0.1092230000
H	15.8816750000	-19.5740690000	1.9745430000
H	16.7333580000	-20.8182760000	1.0392780000
H	14.9643520000	-20.7372660000	0.9981420000
H	16.8054020000	-20.6785850000	-1.5258190000
H	15.0362470000	-20.6033440000	-1.5690690000

H	15.9962010000	-19.3423810000	-2.3669430000
H	9.9362250000	-11.0957130000	1.0247260000
H	10.0243630000	-11.0141990000	-0.7423020000

Solution Time Dependent Calculations



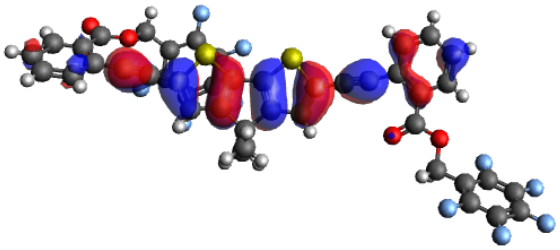
HOMO: -5.068



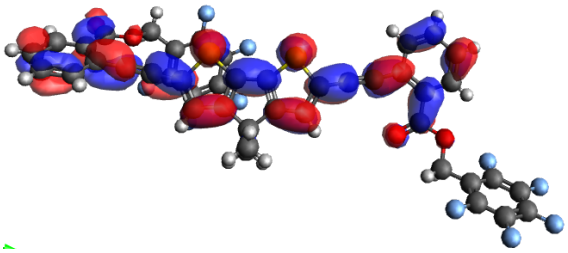
LUMO: -2.360

	Transition Orbitals	Transition Energy	Wavelength	Oscillator Strength (f)
Solution	HOMO → LUMO	2.4812 eV	499.69 nm	2.6351
	HOMO → LUMO+2	3.4760 eV	356.68 nm	0.1919

Single Cystal Time Dependent Calculations



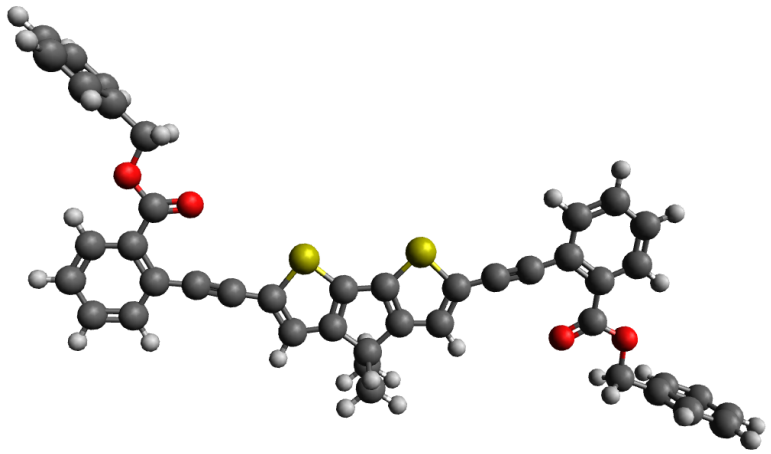
HOMO: -5.058



LUMO: -2.061

	Transition Orbitals	Transition Energy	Wavelength	Oscillator Strength (f)
Crystal	HOMO → LUMO HOMO → LUMO+1 HOMO →LUMO+2	2.7993 eV	442.91 nm	1.6682
	HOMO → LUMO HOMO → LUMO+1	3.1150 eV	398.02 nm	0.2583
	HOMO-1 → LUMO HOMO → LUMO HOMO → LUMO+2	3.5235 eV	351.87 nm	0.3426

mCPDT-H5



Energy: -2753.89 a.u

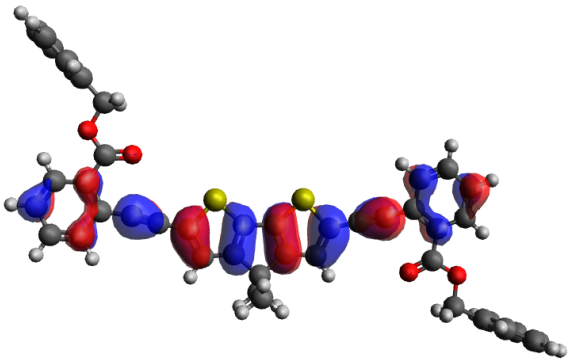
Cartesian Coordinates:

C	9.13630000	-8.34700000	-0.05480000
C	8.27210000	-9.54900000	-0.22710000
C	8.84980000	-10.84350000	-0.34460000
C	7.98840000	-11.95170000	-0.50930000
C	6.60980000	-11.79120000	-0.55620000
C	6.04730000	-10.51660000	-0.43950000
C	6.87700000	-9.41190000	-0.27670000
O	8.41020000	-7.21110000	0.05460000
O	10.35350000	-8.35560000	-0.01430000
C	10.24490000	-11.10330000	-0.30590000
C	11.40760000	-11.47490000	-0.28880000
C	17.09460000	-13.10510000	-0.18410000
C	16.67900000	-11.78490000	-0.03700000
C	15.24680000	-11.73270000	-0.11080000
C	14.75590000	-13.02080000	-0.30390000
C	15.89660000	-14.03530000	-0.37080000
S	13.99390000	-10.54650000	-0.02740000
C	12.76400000	-11.81200000	-0.25760000
C	13.35260000	-13.06710000	-0.38660000
C	23.89510000	-13.72350000	0.07600000
C	24.17520000	-12.27890000	0.31330000
C	23.11130000	-11.33780000	0.39200000
C	23.43070000	-9.97920000	0.61470000
C	24.74800000	-9.56250000	0.75460000
C	25.78960000	-10.49170000	0.67710000
C	25.49770000	-11.83410000	0.45870000
O	22.79020000	-14.20970000	-0.08560000
C	21.73640000	-11.66770000	0.26440000
C	20.52800000	-11.81460000	0.17670000
O	25.02770000	-14.46330000	0.05680000

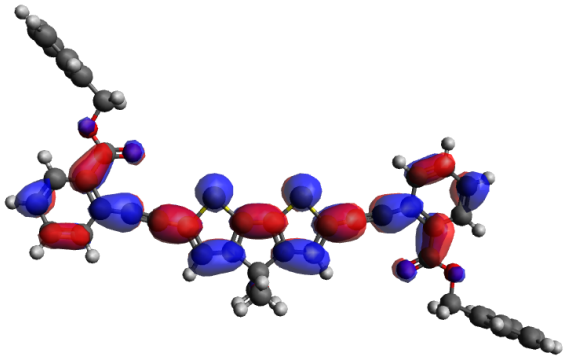
C	24.84600000	-15.88760000	-0.17540000
C	26.20110000	-16.53840000	-0.13480000
C	26.72640000	-17.00960000	1.07510000
C	28.74470000	-17.71930000	-0.05140000
C	28.22890000	-17.25330000	-1.26280000
C	26.96370000	-16.66620000	-1.30250000
C	27.99120000	-17.59700000	1.11830000
C	18.49210000	-13.25260000	-0.12510000
C	19.15260000	-12.04240000	0.06850000
S	17.99950000	-10.69210000	0.17840000
C	15.94180000	-14.74930000	-1.74040000
C	15.80070000	-15.07210000	0.77080000
C	9.17770000	-5.98700000	0.22430000
C	8.20590000	-4.84440000	0.33150000
C	7.69630000	-4.45990000	1.57820000
C	6.78050000	-3.41190000	1.67750000
C	6.36480000	-2.73640000	0.52780000
C	6.86800000	-3.11210000	-0.71970000
C	7.78350000	-4.16080000	-0.81560000
H	8.42820000	-12.93900000	-0.59870000
H	5.97290000	-12.66120000	-0.68380000
H	4.97070000	-10.38550000	-0.47530000
H	6.45000000	-8.42100000	-0.18560000
H	12.75950000	-13.96190000	-0.53410000
H	22.62000000	-9.26120000	0.67520000
H	24.96260000	-8.51190000	0.92450000
H	26.82080000	-10.17190000	0.78580000
H	26.29850000	-12.56030000	0.39700000
H	24.35790000	-16.02130000	-1.14460000
H	24.18010000	-16.28250000	0.59640000
H	26.13980000	-16.91730000	1.98550000
H	29.72780000	-18.17980000	-0.01970000
H	28.80950000	-17.35000000	-2.17540000
H	26.56220000	-16.30630000	-2.24620000
H	28.38660000	-17.96170000	2.06170000
H	19.03460000	-14.18610000	-0.21510000
H	16.80840000	-15.41570000	-1.79480000
H	15.04050000	-15.35330000	-1.88570000
H	16.00930000	-14.02820000	-2.55940000
H	15.76890000	-14.58200000	1.74750000
H	16.66470000	-15.74380000	0.74960000
H	14.89670000	-15.67920000	0.65950000
H	9.79280000	-6.08560000	1.12270000
H	9.84650000	-5.87530000	-0.63320000
H	8.02140000	-4.98290000	2.47380000
H	6.39510000	-3.12050000	2.65000000

H	5.65510000	-1.91790000	0.60430000
H	6.55090000	-2.58710000	-1.61580000
H	8.17680000	-4.45040000	-1.78660000

Solution Time Dependent Calculations



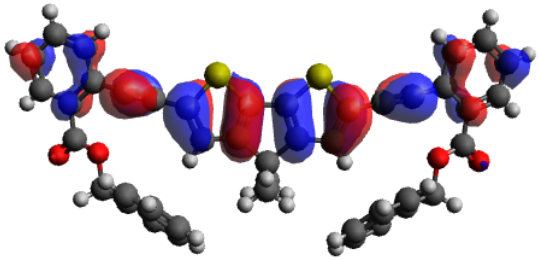
HOMO: -5.025



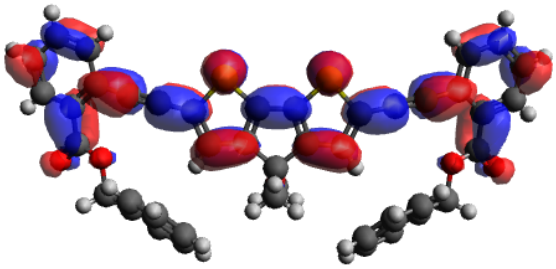
LUMO: -2.300

	Transition Orbitals	Transition Energy	Wavelength	Oscillator Strength (f)
Solution	HOMO → LUMO	2.5017 eV	495.59 nm	2.667

Single Cystal Time Dependent Calculations



HOMO: -4.912



LUMO: -1.988

	Transition Orbitals	Transition Energy	Wavelength	Oscillator Strength (f)
Crystal	HOMO → LUMO	2.7853 eV	445.14 nm	2.1071