

Supporting Information

Synthesis and Characterization of n-Doped Poly(benzodifurandione) (n-PBDF) Derivatives via Aromatic Substitution

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General Considerations

All reactions were performed under nitrogen atmosphere in oven-dried glassware following standard Schlenk techniques. Commercial chemicals were purchased from suppliers including Sigma-Aldrich, TCI, Alfa Aesar, Fisher Scientific, Combi-Block and others and were used directly without further purification unless otherwise noted. Compounds synthesized following literature procedures matched the analytical data reported (by ^1H and ^{13}C NMR). Automated preparative chromatography was performed with a Yamazen Smart Flash AI-580S-Premium chromatography system. ^1H NMR, ^{19}F NMR, and ^{13}C NMR were recorded on Bruker NEO300, Bruker AV-III-400, and Bruker Avance-III-800 instruments with chemical shifts reported relative to residual solvent. HRMS data were obtained on a Thermo LTQ-Orbitrap mass spectrometer with a FTMS analyzer. Ultraviolet-Visible Light (UV-Vis) spectra were measured with an Agilent Technologies Cary 6000i UV-Vis-NIR Spectrophotometer using a 1-cm, two-window quartz cuvette. Solutions were prepared in dichloromethane (DCM) or dimethylformamide (DMF) at a concentration of 1.5×10^{-4} mM. Electrochemical measurements, cyclic voltammetry (CV), were carried out on a Biologic SP-150 potentiostat in a three-electrode cell at a scan rate of 40 mV/s, at 1.5×10^{-4} mM with 0.1 M TBAPF₆ in DCM as the supportive electrolyte, a platinum button working electrode, a platinum wire as the counter electrode, and a leakless Ag/AgCl electrode as reference electrode inside a nitrogen-filled glovebox. The voltammograms are reported in IUPAC convention, at 1mM analyte concentration with 0.1 M TBAPF₆ in DCM as the supportive electrolyte, a platinum button working electrode, a platinum wire as the counter electrode, and a leakless Ag/AgCl electrode as reference electrode. The voltage was scanned from -1.0 to 1.0 V vs Ag/AgCl. The spectroelectrochemical experiments were measured using a Biologic SP-150 potentiostat in combination with the Agilent Technologies Cary 6000i UV-Vis-NIR Spectrophotometer. Electron paramagnetic resonance (EPR) measurements were performed on a Bruker EMX EPR Spectrometer at room temperature (RT) in DCM. A Filmetrics R50 Sheet Resistance Mapper was used to measure the thin films sheet resistance using a four-probe configuration. The four-probe configuration, the sheet resistance then was measured using following equation based on previous reported literature¹:

$$R_s = \frac{w}{l} \times \frac{\Delta V}{I} = 10 \frac{\Delta V}{I} \quad (\text{Eq. S1})$$

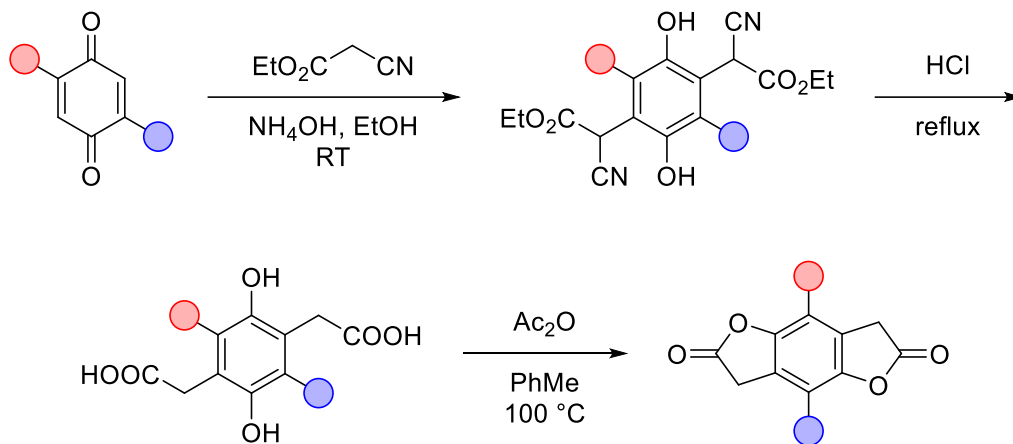
The conductivity were then calculated using the following equation:

$$\sigma = \frac{1}{R_s t} \quad (\text{Eq. S2})$$

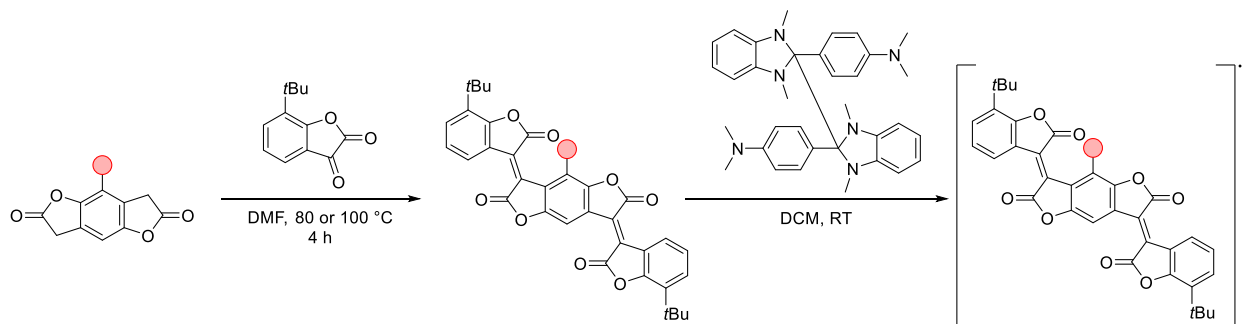
where t (film thickness) was measured by profilometer.

Synthetic Procedures

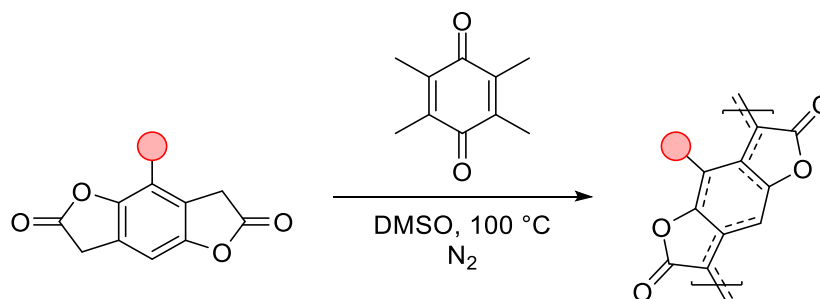
General BDF Monomer Synthesis Pathway:



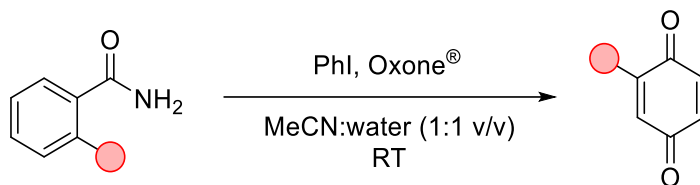
General Oligomer Synthesis:



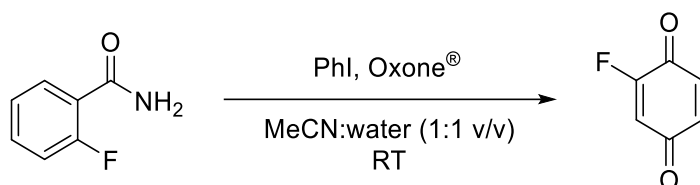
General Polymerization:



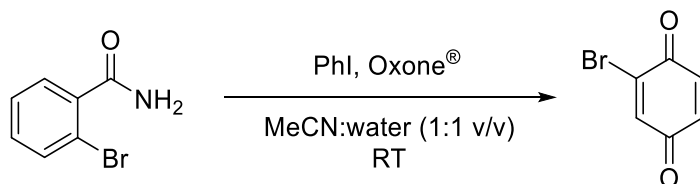
General Procedure A: Synthesis of 2-substituted benzoquinone derivatives



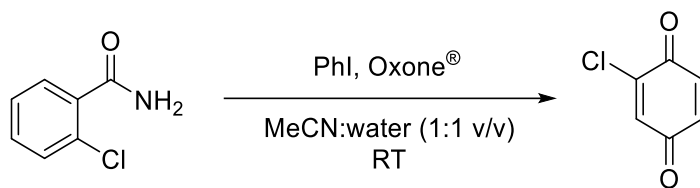
Oxidation of benzamides were performed via previously reported literature²: In a 500 mL, single neck round bottom flask, 2-substituted benzamide (1.0 eq.), iodobenzene (1.0 eq.), and Oxone® (2.0 eq.) were mixed in solution of MeCN:water (1:1 v/v, 0.17 M) for 14 h. The reaction was then diluted with water, extracted with dichloromethane (DCM), dried over Na₂SO₄, and evaporated via rotary evaporation. The solids were then purified with a short silica plug to afford a microcrystalline solid.



2-fluoro-1,4-benzoquinone (1b) was synthesized using General Procedure A; 2-fluorobenzamide (15 g, 107.8 mmol, 1.0 eq.), iodobenzene (22.0 g, 107.8 mmol, 1 eq.), and Oxone® (132.6 g, 215.6 mmol, 2 eq.) were suspended in a solution of MeCN:water (1:1 v/v, 650 mL). The resulting solids were purified using a short silica plug (9:1 Hex:DCM) to yield an orange microcrystalline solid (6.2 g, 46%). ¹H NMR (300 MHz, CDCl₃): δ (ppm) 6.88-6.75 (m, 2H), 6.50-6.40 (m, 1H); ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) -111.3; ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 187.3, 187.1, 179.6, 179.2, 161.8, 157.9, 137.1, 134.6, 115.5, 115.3; Analytical data matches previously reported literature.³

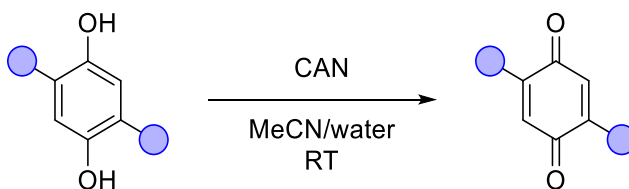


2-bromo-1,4-benzoquinone (4a) was synthesized using General Procedure A; 2-bromobenzamide (10 g, 50.0 mmol, 1.0 eq.), iodobenzene (10.2 g, 50.0 mmol, 1 eq.), and Oxone® (61.5 g, 100 mmol, 2 eq.) were suspended in a solution of MeCN:water (1:1 v/v, 300 mL). The resulting solids were purified using a short silica plug (9:1 Hex:DCM) to yield an orange microcrystalline solid (5.1 g, 54%). ¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.30 (d, *J* = 2.5 Hz, 1H), 6.96 (d, *J* = 10.1 Hz, 1H), 6.82 (dd, *J* = 2.2 Hz, 10.1 Hz, 1H); ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 184.7, 179.3, 138.3, 137.7, 136.8, 136.0; Analytical data matches previously reported literature.⁴

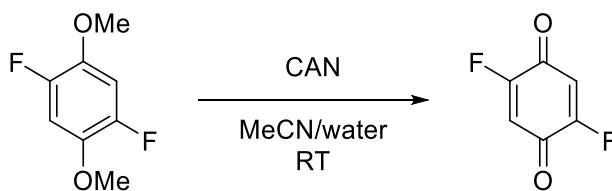


2-chloro-1,4-benzoquinone (5a) was synthesized using General Procedure A; 2-chlorobenzamide (15 g, 96.4 mmol, 1.0 eq.), iodobenzene (19.7 g, 96.4 mmol, 1 eq.), and Oxone[®] (118.5 g, 192.8 mmol, 2 eq.) were suspended in a solution of MeCN:water (1:1 v/v, 580 mL). The resulting solids were purified using a short silica plug (9:1 Hex:DCM) to yield an orange microcrystalline solid (7.88 g, 57%). ¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.01 (d, *J* = 2.4 Hz, 1H), 6.92 (d, *J* = 10.2 Hz, 1H), 6.81 (dd, *J* = 2.4 Hz, 10.2 Hz, 1H); ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 185.1, 179.4, 144.3, 137.0, 136.2, 133.9; Analytical data matches previously reported literature.²

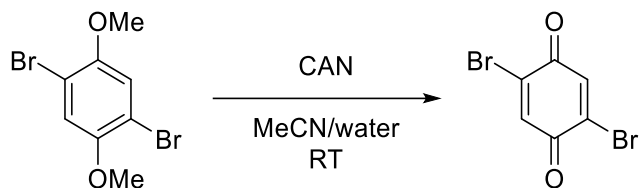
General Procedure B: Synthesis of 2,5-substituted benzoquinone derivatives



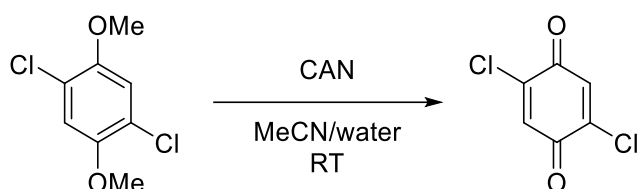
Oxidation of 2,5-substituted 1,4-dimethoxybenzenes were performed via previously reported literature⁵: In a 500 mL, single neck round bottom flask, 2,5-substituted 1,4-dimethoxybenzene (1.0 eq.) was dissolved in acetonitrile (MeCN, 0.34 M) and heated in an oil bath to dissolve (50 or 100 °C). A solution of cerium ammonium nitrate (CAN, 2.7 eq.) in water (0.47 M) was added via pressure equalizing dropping funnel into the reaction. After completion of the addition, the reacting mixture was cooled to room temperature (RT) and stirred for 1 h at RT. The precipitate that formed was filtered, washed with water, and dried.



2,5-difluoro-1,4-benzoquinone (6a) was synthesized using General Procedure B: 2,5-fluoro-1,4-dimethoxybenzene (1.0 g, 5.74 mmol, 1.0 eq.) was dissolved into MeCN (17 mL) and heated at 50 °C. Next a solution CAN (8.5 g, 15.5 mmol, 2.7 eq.) in water (33 mL) was added. The resulting precipitate was filtered, washed with water, to yield a yellow solid (0.18 g, 22%). ¹H NMR (300 MHz, CDCl₃): δ (ppm) 6.45-6.44 (m, 2H); ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) -109.0; ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 179.1, 162.0, 158.1, 113.6, 113.6, 113.5, 113.4; Analytical data matches previously reported literature.⁶

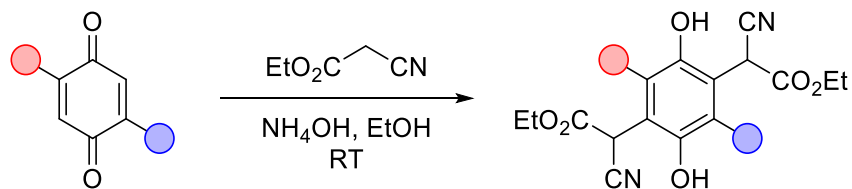


2,5-dibromo-1,4-benzoquinone (8a) was synthesized using General Procedure B: 2,5-dibromo-1,4-dimethoxybenzene (5.0 g, 16.9 mmol, 1.0 eq.) was dissolved into MeCN (50 mL) and heated at 100 °C. Next a solution CAN (25.0 g, 45.6 mmol, 2.7 eq.) in water (100 mL) was added. The resulting precipitate was filtered, washed with water, to yield a yellow solid (4.0 g, 89%). ¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.48 (s, 2H); ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 177.1, 137.9, 137.2; Analytical data matches previously reported literature.⁵

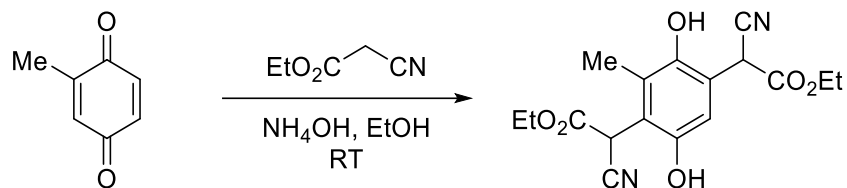


2,5-dichloro-1,4-benzoquinone (9a) was synthesized using General Procedure B: 2,5-difluoro-1,4-dimethoxybenzene (8.0 g, 38.64 mmol, 1.0 eq.) was dissolved into MeCN (114 mL) and heated at 50 °C. Next a solution CAN (57.2 g, 104.3 mmol, 2.7 eq.) in water (229 mL) was added. The resulting precipitate was filtered, washed with water, to yield a yellow solid (5.5 g, 80%). ¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.15 (s, 2H); ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 177.4, 144.8, 133.2; Analytical data matches previously reported literature.⁵

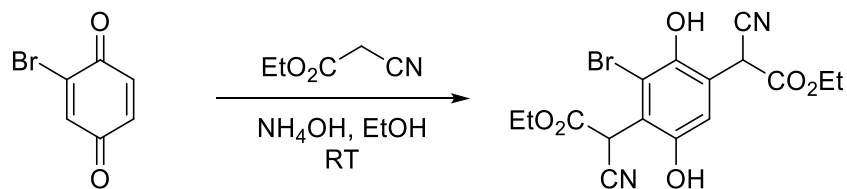
General Procedure C: Synthesis of substituted diethyl α,α'-dicyano-1,4-dihydroxy-*p*-benzenediacetate



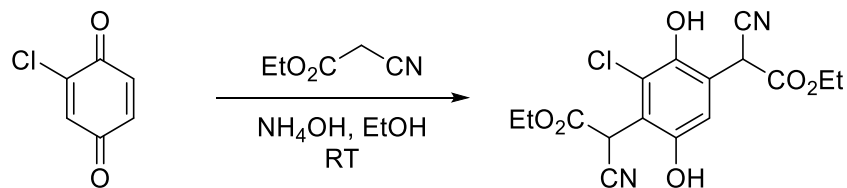
Michael addition of ethyl cyanoacetate and substituted benzoquinone was performed via previously reported literature⁷: In a 500 mL, three neck round bottom flask fitted with two pressure equalizing funnels, a mixture of ethyl cyanoacetate (0.56 eq.) and ethanol (2.8 M) was added. Substituted benzoquinone (1.0 eq.) was heated to 40 °C with ethanol (1.0 M). After dissolution, ethyl cyanoacetate (1.0 eq.) was added and mixed. This premix was then added to one of the dropping funnels. Next, concentrated ammonium hydroxide (1.28 eq.) was added into the reactor. A solution of concentrated ammonium hydroxide (5.14 eq.) in water was placed in the other dropping funnel. Addition of the two premixes is added simultaneously over 1 h. After complete addition, stirring is continued for an additional 0.5 h. Next, stirring is stopped and solids settled. The solids were filtered, washed with ethanol, and dried.



Diethyl 2,2'-(2-methyl-3,6-dihydroxy-5-methyl-1,4-phenylene)bis(2-cyanoacetate) (3b) was synthesized using General Procedure C: ethyl cyanoacetate (5.19 g, 45.9 mmol, 0.56 eq.) and ethanol (16.4 mL) was added into the reactor. 2-methyl-1,4-benzoquinone (10.0 g, 81.9 mmol, 1.0 eq.) was heated to 40 °C with ethanol (81.9 mL). After dissolution, ethyl cyanoacetate (8.7 mL, 81.9 mmol, 1.0 eq.) was added and mixed. This premix was then added to one of the dropping funnels. Next, concentrated ammonium hydroxide (4.1 mL, 104.8 mmol, 1.28 eq.) was added into the reactor. A solution of concentrated ammonium hydroxide (16.4 mL, 420.9 mmol, 5.14 eq.) in water (24.6 mL) is placed in the other dropping funnel. The solids were filtered, washed with ethanol, and dried as an orange/peach solid (1.6 g, 5.7%). ¹H NMR (300 MHz, DMSO-*d*₆): δ (ppm) 7.69-7.53 (m, 4H), 7.16 (s, 1H), 4.30-4.19 (m, 4H), 2.66 (s, 3H), 1.38-1.25 (m, 6H); ¹³C NMR (101 MHz, DMSO-*d*₆): δ (ppm) 165.5, 164.8, 164.5, 164.2, 146.0, 145.0, 120.9, 119.2, 110.5, 97.0, 82.9, 81.98, 58.9, 58.7, 14.5, 14.5, 13.3.

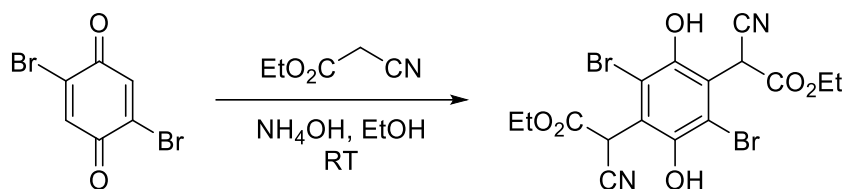


Diethyl 2,2'-(2-bromo-3,6-dihydroxy-5-methyl-1,4-phenylene)bis(2-cyanoacetate) (4b) was synthesized using General Procedure C: ethyl cyanoacetate (2.4 g, 21.0 mmol, 0.56 eq.) and ethanol (7.5 mL) was added into the reactor. 2-bromo-1,4-benzoquinone (7 g, 37.4 mmol, 1.0 eq.) was heated to 40 °C with ethanol (37 mL). After dissolution, ethyl cyanoacetate (4.0 mL, 37.4 mmol, 1.0 eq.) was added and mixed. This premix was then added to one of the dropping funnels. Next, concentrated ammonium hydroxide (1.9 mL, 47.9 mmol, 1.28 eq.) was added into the reactor. A solution of concentrated ammonium hydroxide (7.5 mL, 192.4 mmol, 5.14 eq.) in water (11.2 mL) is placed in the other dropping funnel. The solids were filtered, washed with ethanol, and dried as a pink solid (0.60 g, 4.0%). ¹H NMR (300 MHz, DMSO-*d*₆): δ (ppm) 7.89-7.74 (m, 3H), 7.63 (s, 1H), 7.32 (d, *J* = 1.6 Hz, 1H), 4.31-4.20 (m, 4H), 1.33 (t, *J* = 6.9 Hz, 6H); ¹³C NMR (75 MHz, DMSO-*d*₆): δ (ppm) 165.8, 164.7, 146.4, 145.7, 143.7, 121.6, 119.8, 99.4, 98.8, 91.7, 82.2, 81.8, 59.0, 58.7, 14.6, 14.5.

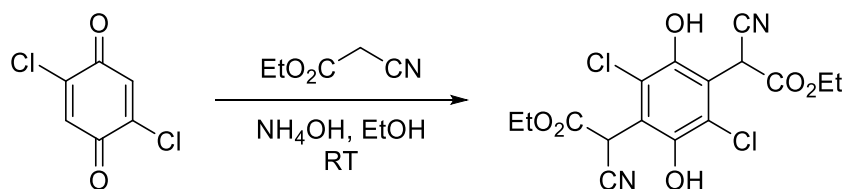


Diethyl 2,2'-(2-chloro-3,6-dihydroxy-5-methyl-1,4-phenylene)bis(2-cyanoacetate) (5b) was synthesized using General Procedure C: ethyl cyanoacetate (3.1 g, 27.5 mmol, 0.56 eq.) and etha-

nol (9.8 mL) was added into the reactor. 2-chloro-1,4-benzoquinone (7.0 g, 49.1 mmol, 1.0 eq.) was heated to 40 °C with ethanol (49.1 mL). After dissolution, ethyl cyanoacetate (5.2 mL, 49.1 mmol, 1.0 eq.) was added and mixed. This premix was then added to one of the dropping funnels. Next, concentrated ammonium hydroxide (2.4 mL, 62.9 mmol, 1.28 eq.) was added into the reactor. A solution of concentrated ammonium hydroxide (9.8 mL, 252.4 mmol, 5.14 eq.) in water (14.7 mL) is placed in the other dropping funnel. The solids were filtered, washed with ethanol, and dried as a pink solid (0.88 g, 4.9%). ¹H NMR (300 MHz, DMSO-d₆): δ (ppm) 8.01-7.63 (m, 4H), 7.30 (d, *J* = 11.6 Hz, 1H), 4.31-4.19 (m, 4H), 1.38-1.26 (m, 6H); ¹³C NMR (75 MHz, DMSO-d₆): δ (ppm) 165.8, 164.1, 146.4, 145.7, 122.0, 121.2, 118.2, 104.5, 99.4, 98.3, 82.1, 81.8, 59.0, 58.7, 14.6, 14.5.

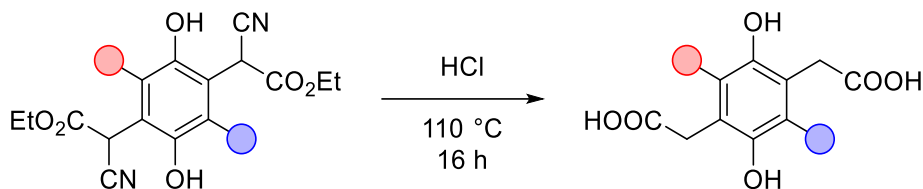


Diethyl 2,2'-(2,5-dibromo-3,6-dihydroxy-1,4-phenylene)bis(2-cyanoacetate) (8b) was synthesized using General Procedure C: ethyl cyanoacetate (3.6 g, 31.6 mmol, 0.56 eq.) and ethanol (11.2 mL) was added into the reactor. 2,5-dibromo-1,4-benzoquinone (15.0 g, 56.4 mmol, 1.0 eq.) was heated to 40 °C with ethanol (56.4 mL). After dissolution, ethyl cyanoacetate (6.4 g, 56.4 mmol, 1.0 eq.) was added and mixed. This premix was then added to one of the dropping funnels. Next, concentrated ammonium hydroxide (2.8 mL, 72.2 mmol, 1.28 eq.) was added into the reactor. A solution of concentrated ammonium hydroxide (11.3 mL, 290.0 mmol, 5.14 eq.) in water (17.0 mL) is placed in the other dropping funnel. The solids were filtered, washed with ethanol, and dried as a grey solid (6.12 g, 22%). ¹H NMR (400 MHz, DMSO-d₆): δ (ppm) 8.05-7.95 (m, 4H), 4.26 (q, *J* = 7.0 Hz, 4H), 1.33 (t, *J* = 7.1 Hz, 6H); ¹³C NMR (101 MHz, DMSO-d₆): 165.5, 163.5, 144.2, 120.4, 91.6, 82.8, 59.2, 14.6; HRMS (ESI+) [*M*]⁺ calcd. for C₁₆H₁₄Br₂N₂O₆: *m/z* = 488.929685, Found: *m/z* = 488.92866.

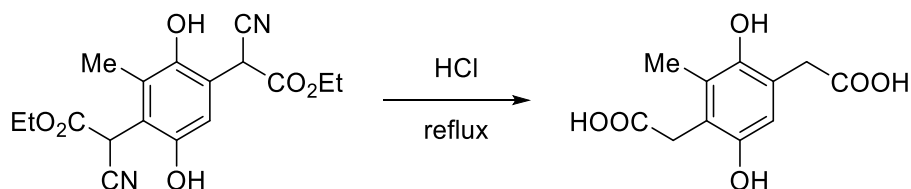


Diethyl 2,2'-(2,5-dichloro-3,6-dihydroxy-1,4-phenylene)bis(2-cyanoacetate) (9b) was synthesized using General Procedure C: ethyl cyanoacetate (3.6 g, 31.6 mmol, 0.56 eq.) and ethanol (11.3 mL) was added into the reactor. 2,5-dichloro-1,4-benzoquinone (10.0 g, 56.5 mmol, 1.0 eq.) was heated to 40 °C with ethanol (56.5 mL). After dissolution, ethyl cyanoacetate (6.0 mL, 56.5 mmol, 1.0 eq.) was added and mixed. This premix was then added to one of the dropping funnels. Next, concentrated ammonium hydroxide (2.8 mL, 72.3 mmol, 1.28 eq.) was added into the reactor. A solution of concentrated ammonium hydroxide (11.3 mL, 290.4 mmol, 5.14 eq) in water (17.0 mL) is placed in the other dropping funnel. The solids were filtered, washed with ethanol, and dried as a grey solid (10.0 g, 44%). ¹H NMR (400 MHz, DMSO-d₆): δ (ppm) 8.11-7.93 (m, 4H), 4.25 (q, *J* = 7.1 Hz, 4H), 1.31 (t, *J* = 7.0 Hz, 6H); ¹³C NMR (75 MHz, DMSO-d₆): δ (ppm) 165.6, 163.4, 142.9, 119.0, 103.7, 82.2, 59.2, 14.4.

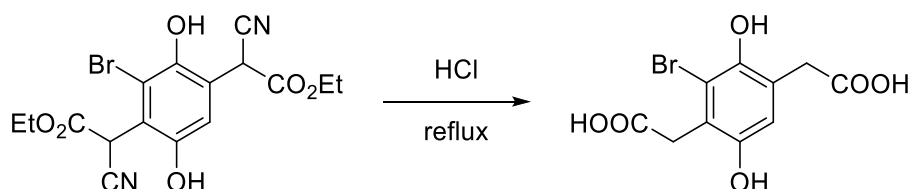
General Procedure D: Synthesis of substituted 1,4-dihydroxy-*p*-benzenediacetic acid



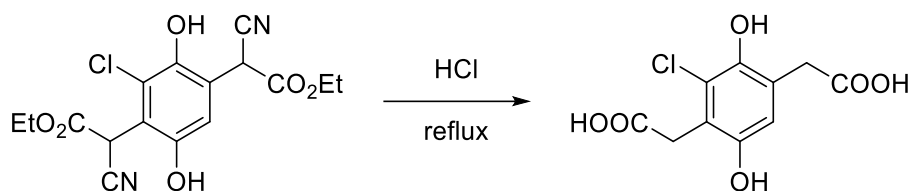
Acid hydrolysis was performed via previously reported literature⁷: Substituted diethyl α,α' -dicyano-1,4-dihydroxy-*p*-benzenediacetate (1.0 eq.) was transferred to a 500 mL, single neck round bottom flask equipped with a reflux condenser. Concentrated hydrochloric acid (HCl, 0.5 M) was added and the reaction was heated to 80 °C for 2 h, then refluxed for 14 h. Next, the reactor was cooled to RT. The solids formed were filtered, washed with water, and dried.



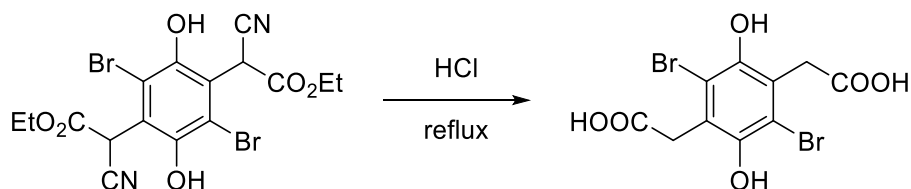
2,2'-(2,5-dihydroxy-3-methyl-1,4-phenylene)diacetic acid (3c) was synthesized using General Procedure D: Diethyl 2,2'-(2-chloro-3,6-dihydroxy-5-methyl-1,4-phenylene)bis(2-cyanoacetate) (0.5 g, 1.4 mmol, 1.0 eq.) was refluxed with concentrated hydrochloric acid (3 mL). The solids formed were filtered, washed with water, and dried as a tan solid (0.22 g, 62%). ¹H NMR (300 MHz, DMSO-*d*₆): δ (ppm) 7.06 (s, 1H), 3.94 (d, J = 8.3 Hz, 4H), 2.19 (s, 3H); ¹³C NMR (75 MHz, DMSO-*d*₆): δ (ppm) 174.4, 174.2, 149.6, 148.6, 123.4, 123.2, 117.2, 104.6, 33.7, 32.2, 12.2.



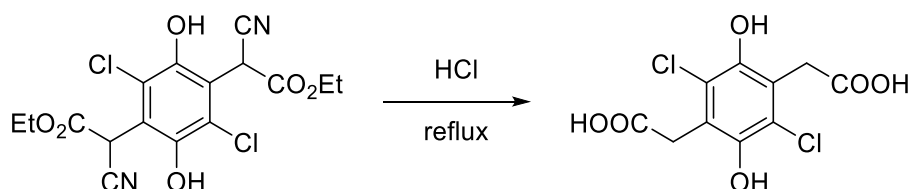
2,2'-(3-bromo-2,5-dihydroxy-1,4-phenylene)diacetic acid (4c) was synthesized using General Procedure D: Diethyl 2,2'-(2-chloro-3,6-dihydroxy-5-methyl-1,4-phenylene)bis(2-cyanoacetate) (0.5 g, 1.2 mmol, 1.0 eq.) was refluxed with concentrated hydrochloric acid (2.5 mL). The solids formed were filtered, washed with water, and dried as a light brown solid (0.18 g, 48%). ¹H NMR (300 MHz, DMSO-*d*₆): δ (ppm) 7.62-7.00 (m, 4H), 6.67-6.49 (m, 1H), 3.77-3.29 (m, 4H); ¹³C NMR (75 MHz, DMSO-*d*₆): δ (ppm) 172.8, 172.4, 149.0, 147.4, 123.5, 120.5, 117.1, 116.3, 35.9, 35.1.



2,2'-(3-chloro-2,5-dihydroxy-1,4-phenylene)diacetic acid (5c) was synthesized using General Procedure D: Diethyl 2,2'-(2-chloro-3,6-dihydroxy-5-methyl-1,4-phenylene)bis(2-cyanoacetate) (0.5 g, 1.4 mmol, 1.0 eq.) was refluxed with concentrated hydrochloric acid (2.7 mL). The solids formed were filtered, washed with water, and dried as a light brown solid (0.21 g, 58%). ^1H NMR (300 MHz, DMSO-d_6): δ (ppm) 7.68-7.10 (m, 4H), 6.72-6.47 (m, 1H), 3.76-3.23 (m, 4H); ^{13}C NMR (75 MHz, DMSO-d_6): δ (ppm) 172.4, 171.6, 148.7, 143.3, 123.5, 120.5, 119.2, 115.7, 36.0, 32.7.

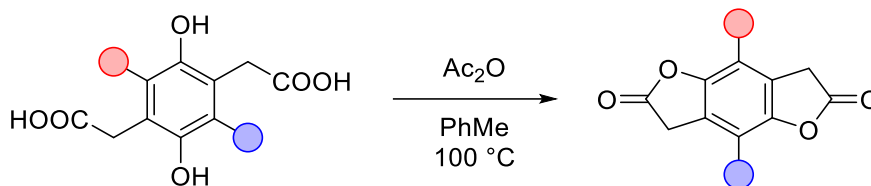


2,2'-(2,5-dibromo-3,6-dihydroxy-1,4-phenylene)diacetic acid (8c) was synthesized using General Procedure D: Diethyl 2,2'-(2,5-dibromo-3,6-dihydroxy-1,4-phenylene)bis(2-cyanoacetate) (4 g, 8.2 mmol, 1.0 eq) was refluxed with concentrated hydrochloric acid (16 mL). The solids formed were filtered, washed with water, and dried as a beige solid (2.0 g, 65%). ^1H NMR (400 MHz, DMSO-d_6): δ (ppm) 8.96 (s, 2H), 3.78 (s, 4H); ^{13}C NMR (101 MHz, DMSO-d_6): 171.2, 146.0, 124.2, 115.5, 36.9.

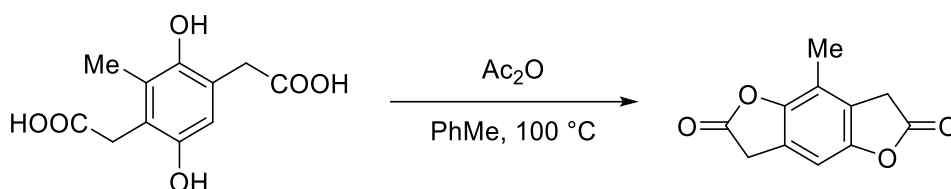


2,2'-(2,5-dichloro-3,6-dihydroxy-1,4-phenylene)diacetic acid (9c) was synthesized using General Procedure D: Diethyl 2,2'-(2,5-dichloro-3,6-dihydroxy-1,4-phenylene)bis(2-cyanoacetate) (1.0 g, 2.5 mmol, 1.0 eq.) was refluxed with concentrated hydrochloric acid (5.0 mL). The solids formed were filtered, washed with water, and dried as a beige solid (0.42 g, 57%). ^1H NMR (300 MHz, DMSO-d_6): δ (ppm) 9.05 (s, 2H), 3.71 (s, 4H); ^{13}C NMR (75 MHz, DMSO-d_6): δ (ppm) 171.2, 144.7, 122.2, 121.7, 33.8.

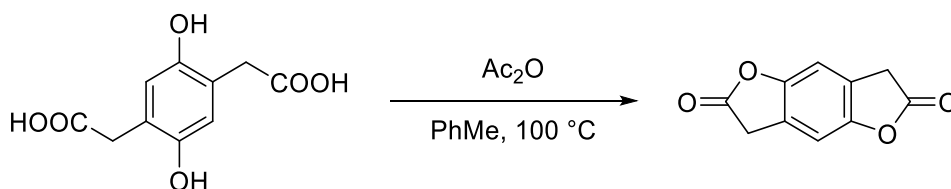
General Procedure E: Synthesis of substituted 3,7-dihydrobenzo[1,2-*b*:4,5-*b'*]difuran-2,6-dione (BDF)



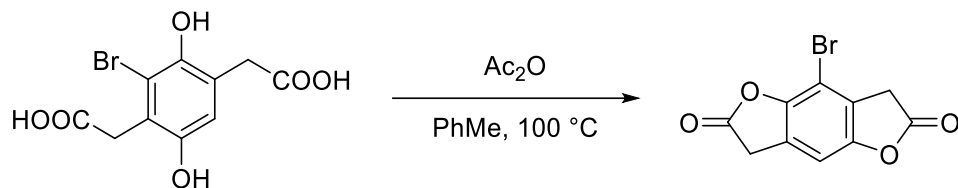
Acid catalyzed, intramolecular cyclization was performed via previously reported literature⁸. In a 250 mL round bottom flask equipped with a reflux condenser, substituted 1,4-dihydroxy-*p*-benzenediacetic acid (1.0 eq.) was suspended in anhydrous toluene (88 mM) and acetic anhydride (Ac₂O, 24.0 eq.). The reaction was heated at 100 °C for 5 h and then the solvent was removed via rotary evaporation. The residue was purified by silica gel chromatography (DCM) and recrystallized from boiling toluene.



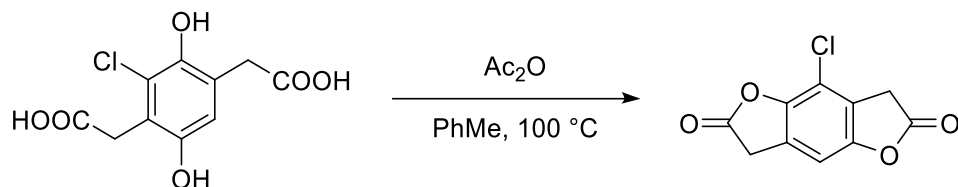
4-methyl-3,7-dihydrobenzo[1,2-*b*:4,5-*b'*]difuran-2,6-dione (BDF-Me) was synthesized using General Procedure E: 2,2'-(2,5-dihydroxy-3-methyl-1,4-phenylene)diacetic acid (0.2 g, 0.80 mmol, 1.0 eq.) was suspended in anhydrous toluene (9.5 mL) and acetic anhydride (Ac₂O, 1.9 mL, 24.0 eq.). The reaction was heated at 100 °C for 5 h and then the solvent was removed via rotary evaporation. The residue was purified by silica gel chromatography (DCM) and recrystallized from boiling toluene to yield white crystals (0.15 g, 89%). ¹H NMR (300 MHz, CDCl₃): δ (ppm) 6.90 (s, 1H), 3.78 (s, 2H), 3.68 (s, 2H) 2.27 (s, 3H); ¹³C NMR (101 MHz, DMSO-*d*₆): 173.6, 150.6, 149.6, 123.0, 122.6, 118.6, 107.2, 105.0, 34.1, 32.6, 12.8; HRMS (ESI-) [M-H]⁻ calcd. for [C₁₁H₇O₄]⁻: m/z = 203.0350, Found: m/z = 203.0347



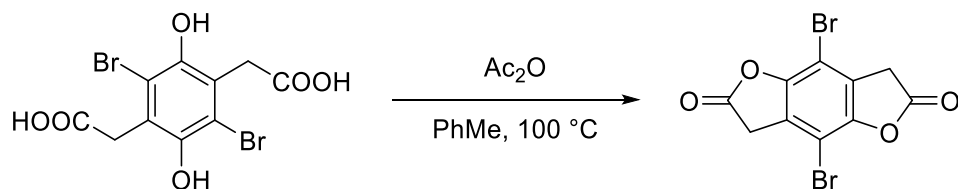
3,7-dihydrobenzo[1,2-*b*:4,5-*b'*]difuran-2,6-dione (BDF) was synthesized using General Procedure E: 2,2'-(2,5-dihydroxy-1,4-phenylene)diacetic acid (0.2 g, 0.88 mmol, 1.0 eq.) was suspended in anhydrous toluene (10.0 mL) and acetic anhydride (Ac₂O, 2.0 mL, 24.0 eq.). The reaction was heated at 100 °C for 5 h and then the solvent was removed via rotary evaporation. The residue was purified by silica gel chromatography (DCM) and recrystallized from boiling toluene to yield white crystals (0.15 g, 90%). ¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.07 (s, 2H), 3.79 (s, 4H): Analytical data matches previously reported literature.⁸



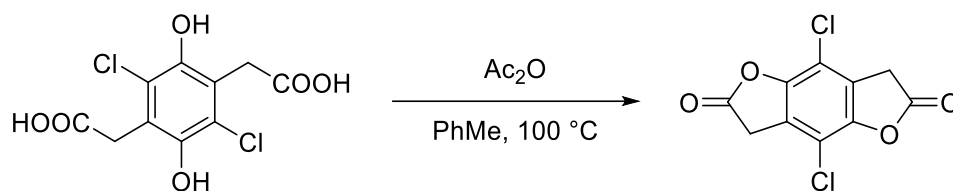
4-bromo-3,7-dihydrobenzo[1,2-*b*:4,5-*b'*]difuran-2,6-dione (BDF-Br) was synthesized using General Procedure E: 2,2'-(3-bromo-2,5-dihydroxy-1,4-phenylene)diacetic acid (0.2 g, 0.66 mmol, 1.0 eq.) was suspended in anhydrous toluene (7.4 mL) and acetic anhydride (Ac_2O , 1.5 mL, 24.0 eq.). The reaction was heated at 100 °C for 5 h and then the solvent was removed via rotary evaporation. The residue was purified by silica gel chromatography (DCM) and recrystallized from boiling toluene to yield white crystals (0.11 g, 60%). ^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ (ppm) 7.26 (s, 1H), 4.13–3.93 (m, 4H); ^{13}C NMR (101 MHz, $\text{DMSO}-d_6$): δ (ppm) 178.1, 173.0, 149.9, 146.3, 125.4, 123.0, 106.6, 106.2, 34.2, 32.9.



4-chloro-3,7-dihydrobenzo[1,2-*b*:4,5-*b'*]difuran-2,6-dione (BDF-Cl) was synthesized using General Procedure E: 2,2'-(3-chloro-2,5-dihydroxy-1,4-phenylene)diacetic acid (0.2 g, 0.77 mmol, 1.0 eq.) was suspended in anhydrous toluene (8.7 mL) and acetic anhydride (Ac_2O , 1.7 mL, 24.0 eq.). The reaction was heated at 100 °C for 5 h and then the solvent was removed via rotary evaporation. The residue was purified by silica gel chromatography (DCM) and recrystallized from boiling toluene to yield white crystals (0.12 g, 71%). ^1H NMR (300 MHz, $\text{DMSO}-d_6$): δ (ppm) 7.26 (s, 1H), 4.05 (d, $J = 7.2$ Hz, 4H); ^{13}C NMR (101 MHz, $\text{DMSO}-d_6$): δ (ppm) 173.4, 172.0, 150.3, 146.6, 125.8, 124.6, 123.3, 106.6, 34.5, 33.3; HRMS (ESI-) $[\text{M}-\text{H}]^-$ calcd. for $[\text{C}_{10}\text{H}_4\text{ClO}_4]^-$: $m/z = 222.9804$, Found: $m/z = 222.9807$.



4,8-dibromo-3,7-dihydrobenzo[1,2-*b*:4,5-*b'*]difuran-2,6-dione (BDF-Br₂) was synthesized using General Procedure E: 2,2'-(2,5-dibromo-3,6-dihydroxy-1,4-phenylene)diacetic acid (0.1 g, 0.26 mmol, 1.0 eq.) was suspended in anhydrous toluene (3.0 mL) and acetic anhydride (Ac_2O , 0.59 mL, 24.0 eq.). The reaction was heated at 100 °C for 5 h and then the solvent was removed via rotary evaporation. The residue was purified by silica gel chromatography (DCM) and recrystallized from boiling toluene to yield beige crystals (67.9 mg, 75%). ^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ (ppm) 4.09 (s, 4H); ^{13}C NMR (101 MHz, $\text{DMSO}-d_6$): δ (ppm) 171.4, 147.6, 126.0, 98.2, 35.6; HRMS (ESI-) $[\text{M}-\text{H}]^-$ calcd. for $[\text{C}_{10}\text{H}_3\text{Br}_2\text{O}_4]^-$: $m/z = 344.8404$, Found: $m/z = 344.8415$.



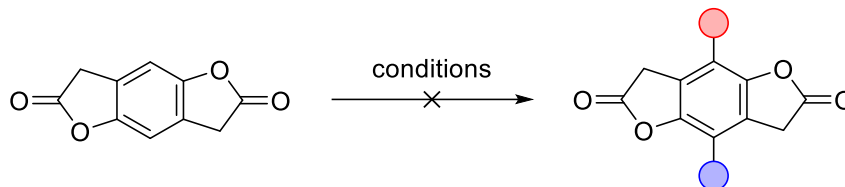
4,8-dichloro-3,7-dihydrobenzo[1,2-*b*:4,5-*b'*]difuran-2,6-dione (BDF-Cl₂) was synthesized using General Procedure E: 2,2'-(2,5-dichloro-3,6-dihydroxy-1,4-phenylene)diacetic acid (0.1 g, 0.34 mmol, 1.0 eq.) was suspended in anhydrous toluene (3.8 mL) and acetic anhydride (Ac₂O, 0.8 mL, 24.0 eq.). The reaction was heated at 100 °C for 5 h and then the solvent was removed via rotary evaporation. The residue was purified by silica gel chromatography (DCM) and recrystallized from boiling toluene to yield beige crystal (52.7 mg g, 60%). ¹H NMR (400 MHz, DMSO-*d*₆): δ (ppm) 4.13 (s, 4H); ¹³C NMR (101 MHz, DMSO-*d*₆): δ (ppm) 171.7, 146.1, 124.3, 109.7, 33.9; HRMS (ESI-) [M-H]⁻ calcd. for [C₉H₇Cl₂O₄]⁻: *m/z* = 256.9408, Found: *m/z* = 256.9419.

Unsuccessful halogenation reactions

Unsuccessful halogenation of BDF:

General procedure: BDF (1.0 eq.) and additive (3.0 eq.) were dissolved into the desired solvent. Next, the halogenating agent (2.2 eq.) was added to the reaction and mixed at the set temperature. The reaction progress was monitored via thin-layer chromatography (TLC) and/or crude ^1H NMR.

Table S1. Attempted direct halogenation of BDF.



Target compound	Halogenating agent	Additive	Solvent	Temperature (°C)	Result
BDF-Br ₂	HBr	DMSO	EtOAc	60	no reaction
BDF-Br ₂	Br ₂	FeCl ₃	CCl ₄	RT	no reaction
BDF-Br ₂	Br ₂	FeCl ₃	CCl ₄	reflux	no reaction
BDF-Br ₂	Br ₂	FeCl ₃	DMF	RT	no reaction
BDF-Br ₂	Br ₂	FeCl ₃	DMF	100	no reaction
BDF-Br ₂	Br ₂	FeCl ₃	AcOH	RT	no reaction
BDF-Br ₂	Br ₂	FeCl ₃	AcOH	reflux	no reaction
BDF-Br ₂	NBS	-	CCl ₄	RT	no reaction
BDF-Br ₂	NBS	-	CCl ₄	reflux	no reaction
BDF-Br ₂	NBS	-	DMF	RT	no reaction
BDF-Br ₂	NBS	-	DMF	100	no reaction
BDF-Br ₂	NBS	-	MeCN	RT	no reaction
BDF-Br ₂	NBS	-	MeCN	reflux	no reaction
BDF-Cl ₂	SO ₂ Cl ₂	-	CCl ₄	RT	no reaction
BDF-Cl ₂	SO ₂ Cl ₂	-	CCl ₄	reflux	no reaction
BDF-Cl ₂	SO ₂ Cl ₂	-	DMF	RT	no reaction
BDF-Cl ₂	SO ₂ Cl ₂	-	DMF	100	no reaction
BDF-Cl ₂	SO ₂ Cl ₂	-	AcOH	RT	no reaction
BDF-Cl ₂	SO ₂ Cl ₂	-	AcOH	reflux	no reaction
BDF-Cl ₂	NCS	-	CCl ₄	RT	no reaction
BDF-Cl ₂	NCS	-	CCl ₄	reflux	no reaction
BDF-Cl ₂	NCS	-	DMF	RT	no reaction
BDF-Cl ₂	NCS	-	DMF	100	no reaction
BDF-Cl ₂	NCS	-	MeCN	RT	no reaction
BDF-Cl ₂	NCS	-	MeCN	reflux	no reaction

Unsuccessful bromination of 1,4-dihydroxy-*p*-benzenediacetic acid:

General procedure: 1,4-dihydroxy-*p*-benzenediacetic acid (1.0 eq.) and additive (3.0 eq.) were dissolved into the desired solvent. Next, the brominating agent (2.2 eq.) was added to the reaction and mixed at the set temperature. The reaction progress was monitored via thin-layer chromatography (TLC) and/or crude ^1H NMR.

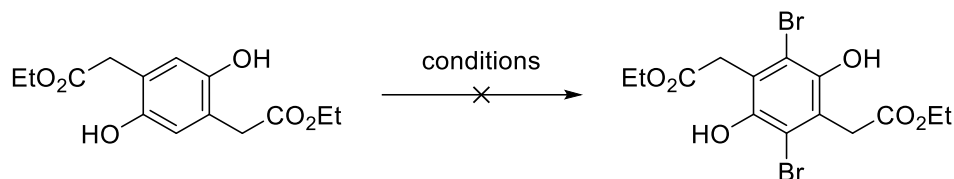
Table S2. Attempted direct bromination of 1,4-dihydroxy-*p*-benzenediacetic acid.

Halogenating agent	Additive	Solvent	Temperature (°C)	Result
HBr	DMSO	EtOAc	60	no reaction
Br ₂	FeCl ₃	CCl ₄	RT	no reaction
Br ₂	FeCl ₃	CCl ₄	reflux	no reaction
Br ₂	FeCl ₃	DMF	RT	no reaction
Br ₂	FeCl ₃	DMF	100	no reaction
Br ₂	FeCl ₃	AcOH	RT	no reaction
Br ₂	FeCl ₃	AcOH	reflux	no reaction
NBS	-	CCl ₄	RT	no reaction
NBS	-	CCl ₄	reflux	no reaction
NBS	-	DMF	RT	no reaction
NBS	-	DMF	100	no reaction
NBS	-	MeCN	RT	no reaction
NBS	-	MeCN	reflux	no reaction
NBS	NaHCO ₃	Water	RT	no reaction
NBS	NaHCO ₃	Water	RT	no reaction

Unsuccessful bromination of 1,4-diethyl 2,2'-(2,5-dihydroxy-1,4-phenylene)diacetate:

General procedure: 1,4-diethyl 2,2'-(2,5-dihydroxy-1,4-phenylene)diacetate (1.0 eq.) and additive (3.0 eq.) were dissolved into the desired solvent. Next, the brominating agent (2.2 eq.) was added to the reaction and mixed at the set temperature. The reaction progress was monitored via thin-layer chromatography (TLC) and/or crude ^1H NMR.

Table S3. Attempted direct bromination of 1,4-diethyl 2,2'-(2,5-dihydroxy-1,4-phenylene)diacetate.



Halogenating agent	Additive	Solvent	Temperature (°C)	Result
NBS	NH ₄ OAc	DCM	RT	no reaction
NBS	Diisopropanolamine	DCM	RT	no reaction
NBS	NH ₄ OAc	DCM	reflux	no reaction
NBS	Diisopropanolamine	DCM	reflux	no reaction
NBS	NH ₄ OAc	MeCN	RT	no reaction
NBS	Diisopropanolamine	MeCN	RT	no reaction
NBS	NH ₄ OAc	MeCN	reflux	no reaction
NBS	Diisopropanolamine	MeCN	reflux	no reaction
Br ₂	FeCl ₃	MeCN	RT	no reaction
Br ₂	FeCl ₃	AcOH	RT	no reaction
Br ₂	FeCl ₃	MeCN	reflux	no reaction
Br ₂	FeCl ₃	AcOH	reflux	no reaction
Br ₂	NaHCO ₃	water	RT	no reaction

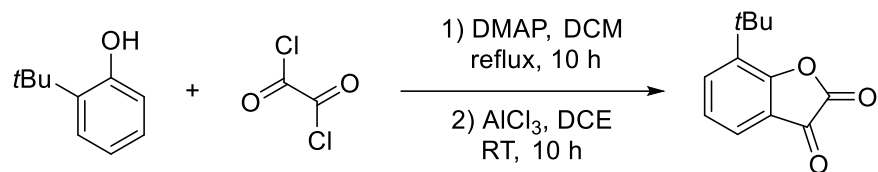
Unsuccessful halogenation of diethyl α,α' -dicyano-1,4-dihydroxy-*p*-benzenediacetate:

General procedure: diethyl α,α' -dicyano-1,4-dihydroxy-*p*-benzenediacetate (1.0 eq.) and additive (3.0 eq.) were dissolved into the desired solvent. Next, the brominating agent (2.2 eq.) was added to the reaction and mixed at the set temperature. The reaction progress was monitored via thin-layer chromatography (TLC) and/or crude ^1H NMR.

Table S4. Attempted direct bromination of diethyl α,α' -dicyano-1,4-dihydroxy-*p*-benzenediacetate.

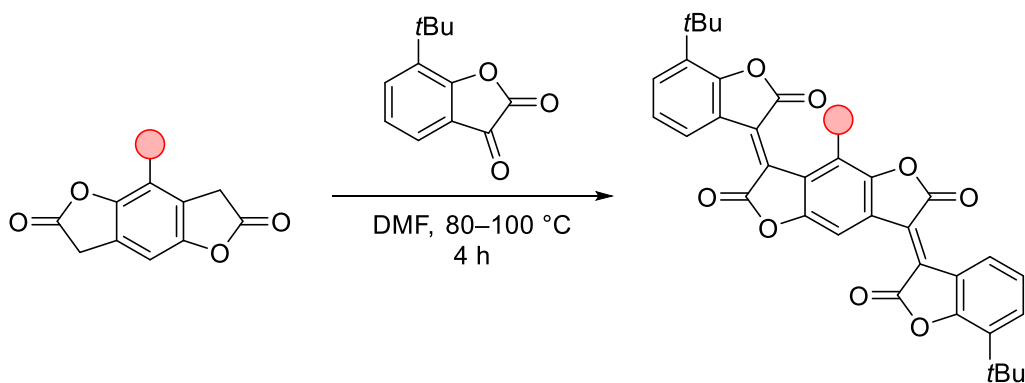
Halogenating agent	Additive	Solvent	Temperature (°C)	Result
HBr	DMSO	EtOAc	60	no reaction
Br ₂	FeCl ₃	DMF	RT	no reaction
Br ₂	FeCl ₃	DMF	100	no reaction
NBS	-	DMF	RT	no reaction
NBS	-	DMF	100	no reaction

General Procedure F: Synthesis of 7-*tert*-butylbenzofuran-2,3-dione

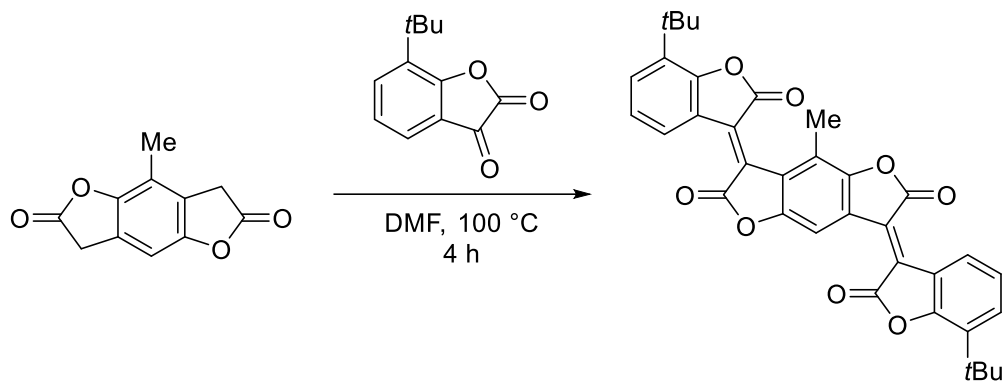


Friedel-Crafts acylation of 2-*tert*-butylphenol was performed via previously reported literature⁹: In a 250 mL, single neck round bottom flask, 2-*tert*-butylphenol (5.0 g, 32.3 mmol, 1.0 eq.) and 4-(dimethylamino)pyridine (DMAP, 0.17 g, 1.4 mmol, 0.06 eq.) are dissolved in dichloromethane (100 mL). To the reaction, oxalyl chloride (6.3 mL, 73.2 mmol, 2.2 eq.) was added dropwise via a pressure equalizing dropping funnel. The reaction was then heated to 40°C for 10 h. After refluxing, the solvent was removed via rotary evaporation and the residue was redissolved into 1,2-dichloroethane (30 mL). To this solution, aluminum chloride (13.3 g, 99.8 mmol, 3.0 eq.) was added in three equal portions. The reaction was mixed at room temperature for 10 h. Next, the reaction was quenched with water (30 mL), extracted with dichloromethane, dried over Na₂SO₄, and evaporated via rotary evaporation. The residue was recrystallized in hot hexanes to give pure product as a yellow/orange crystalline solid (4.6 g, 67%). ¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.72 (dd, *J* = 1.0 Hz, 7.9 Hz, 1H), 7.58 (dd, *J* = 1.1 Hz, 7.5 Hz, 1H), 7.26 (t, *J* = 7.92, 1H), 1.44 (s, 9H); ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 178.0, 162.3, 156.0, 137.9, 136.9, 125.6, 123.3, 119.5, 34.6, 29.5; Analytical data matches previously reported literature.⁹

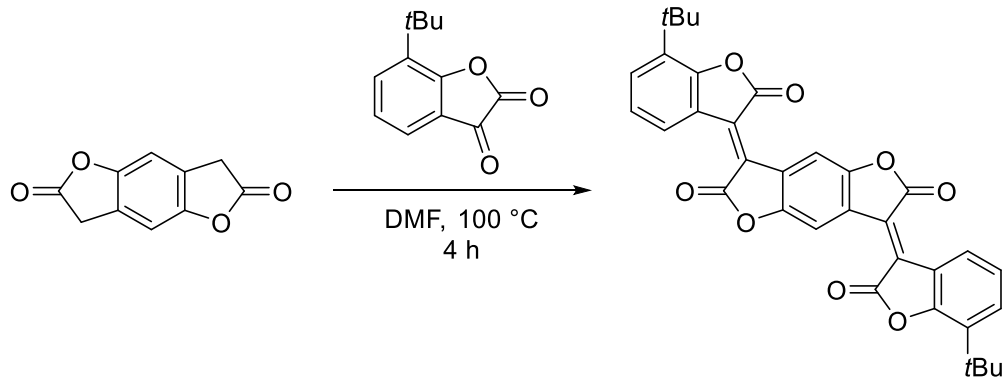
General Procedure G: Synthesis of Neutral Oligomers



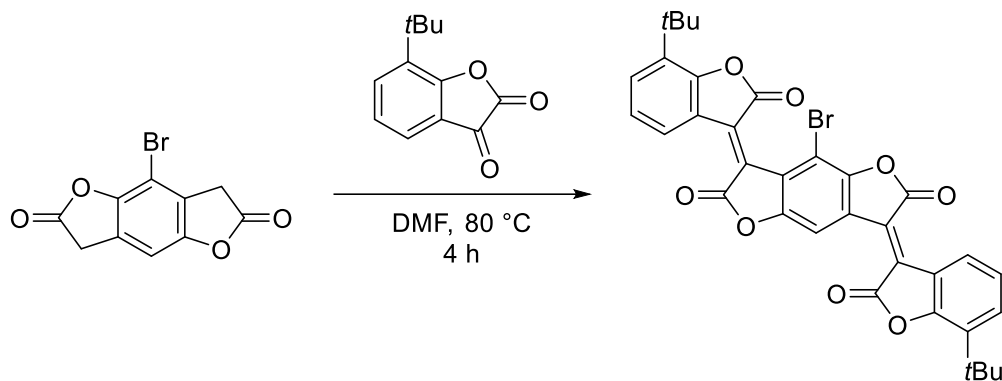
Condensation reaction between **BDF** derivatives and 7-(*tert*-butyl)benzofuran-2,3-dione was performed based on previous literature¹⁰: In a 50-mL Schlenk tube, substituted **BDF** (1.0 eq.) and 7-(*tert*-butyl)benzofuran-2,3-dione (2.0 eq.) were added and placed under an inert atmosphere by purging with N₂. To the reactor, anhydrous dimethylformamide (DMF, 21 mM) was added under positive pressure. The reaction was heated at 80 or 100 °C for 4. The reaction was then slightly cooled, and the solvent was removed via rotary evaporation. The residue was dissolved into a minimum amount of dichloromethane and precipitated into hexanes. The solids were isolated by filtration, washed with hexanes, and collected. The solids were then passed through a short silica plug and concentrated. The residue was recrystallized in hot hexanes to afford the pure product.



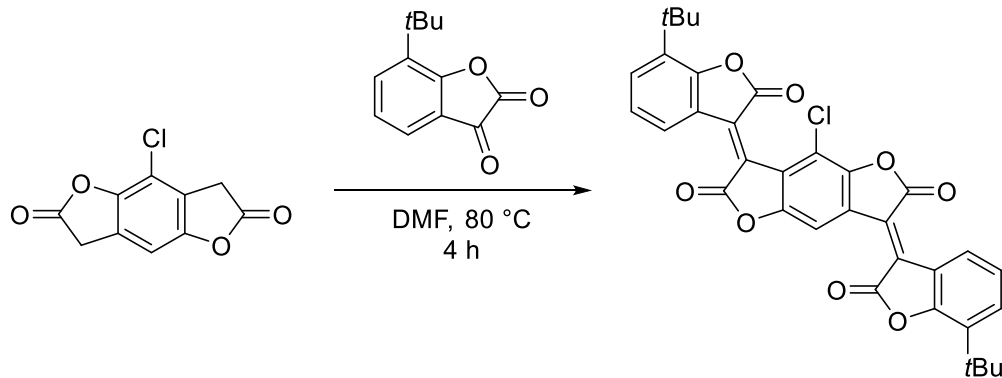
3,7-bis((E)-7-tert-butyl-2-oxobenzofuran-3(2H)-ylidene)-4-methyl-3,7-dihydrobenzo[1,2-b:4,5-b']difuran-2,6-dione (BFD-Me) was synthesized using General Procedure G: 4-methyl-3,7-dihydrobenzo[1,2-b:4,5-b']difuran-2,6-dione (0.1 g, 0.49 mmol, 1.0 eq.) and 7-(tert-butyl)benzofuran-2,3-dione (0.2 g, 0.98 mmol, 2.0 eq.) were dissolved into DMF (23 mL) and heated at 100 °C for 4 h under an inert atmosphere. After heating, the solvent was removed via rotary evaporation. The residue was dissolved into a minimum amount of dichloromethane and precipitated into hexanes. The solids were then passed through a short silica plug (2:1 DCM:hexanes) and concentrated. The residue was recrystallized in hot hexanes dried to yield a purple solid (40 mg, 14%). ¹H NMR (400 MHz, CDCl₃): δ (ppm) 8.98 (d, *J* = 8.03 Hz, 1H), 8.74 (s, 1H), 8.61 (d, *J* = 8.13 Hz, 1H), 7.54 (d, *J* = 7.83 Hz, 2H), 7.23-7.20 (m, 2H), 2.34 (s, 3H), 1.46 (s, 18H); ¹³C NMR (101 MHz, CDCl₃): 166.5, 166.2, 165.0, 154.8, 154.7, 152.4, 151.7, 134.4, 134.2, 133.6, 133.5, 132.7, 131.7, 131.3, 127.8, 125.7, 124.7, 124.0, 123.2, 123.0, 108.7, 107.9, 34.5, 29.7, 29.7, 17.3; HRMS (ESI-) [*M*]⁻ calcd. or [C₃₅H₂₇O₈]: *m/z* = 576.1784, Found: *m/z* = 576.1824.



3,7-bis((E)-7-tert-butyl-2-oxobenzofuran-3(2H)-ylidene)-3,7-dihydrobenzo[1,2-b:4,5-b']difuran-2,6-dione (BFD) was synthesized using General Procedure G: 3,7-dihydrobenzo[1,2-b:4,5-b']difuran-2,6-dione (0.1 g, 0.53 mmol, 1.0 eq.) and 7-(tert-butyl)benzofuran-2,3-dione (0.2 g, 1.0 mmol, 2.0 eq.) were dissolved into DMF (25 mL) and heated at 100 °C for 4 h under an inert atmosphere. After heating, the solvent was removed via rotary evaporation. The residue was dissolved into a minimum amount of dichloromethane and precipitated into hexanes. The solids were then passed through a short silica plug (2:1 DCM:hexanes) and concentrated. The residue was recrystallized in hot hexanes yield a purple solid (92 mg, 31%). ¹H NMR (400 MHz, CDCl₃): δ (ppm) 8.89 (d, *J* = 7.51 Hz, 2H), 8.92 (s, 2H), 7.54 (d, *J* = 8.01 Hz, 2H), 7.22 (t, *J* = 7.70 Hz, 2H), 1.46 (s, 18H); ¹³C NMR (101 MHz, CDCl₃): 166.6, 166.4, 154.9, 152.3, 134.2, 133.7, 131.92, 128.0, 127.6, 127.0, 124.8, 123.1, 110.9, 34.53, 29.7; HRMS (ESI-) [*M*]⁻ calcd. or [C₃₄H₂₇O₈]: *m/z* = 562.1628, Found: *m/z* = 562.1671.

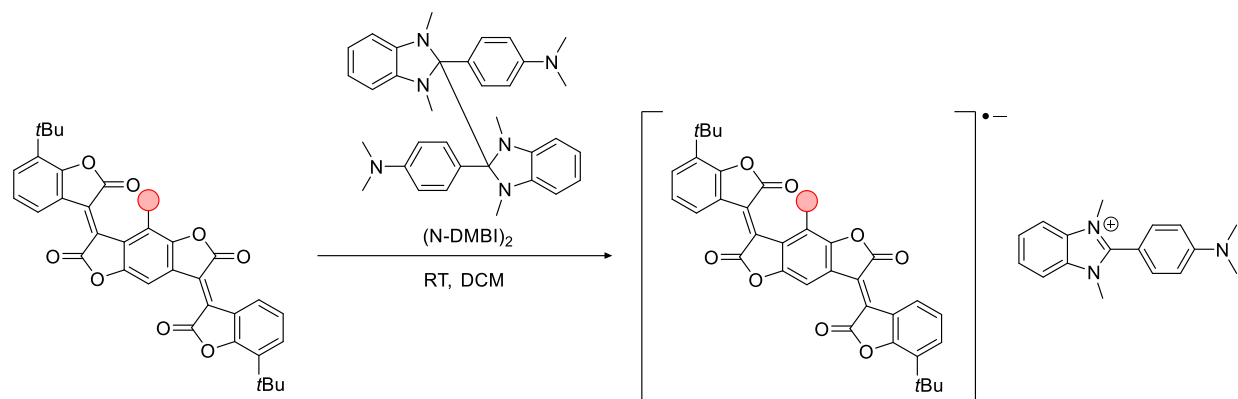


4-bromo-3,7-bis((E)-7-tert-butyl-2-oxobenzofuran-3(2H)-ylidene)-3,7-dihydrobenzo[1,2-b:4,5-b']difuran-2,6-dione (BFD-Br) was synthesized using General Procedure G: 4-bromo-3,7-dihydrobenzo[1,2-b:4,5-b']difuran-2,6-dione (25 mg, 92.9 μmol , 1.0 eq.) and 7-(tert-butyl)benzofuran-2,3-dione (38.3 mg, 187.7 μmol , 2.0 eq.) were dissolved into DMF (4.4 mL) and heated at 80 °C for 4 h under an inert atmosphere. After heating, the solvent was removed via rotary evaporation. The residue was dissolved into a minimum amount of dichloromethane and precipitated into hexanes. The solids were then passed through a short silica plug (2:1 DCM:hexanes) and concentrated. The residue was recrystallized in hot hexanes yield a purple solid (5.1 mg, 8.6%). ^1H NMR (800 MHz, CDCl_3): δ (ppm) 8.87 (d, J = 8.18 Hz, 1H), 8.85 (s, 1H), 8.60 (d, J = 9.09, 1H), 7.57 (d, J = 8.33 Hz, 2H), 7.25-7.23 (m, 2H), 1.46 (d, J = 3.82 Hz, 18H); ^{13}C NMR (201 MHz, CDCl_3): δ 166.5, 165.1, 164.6, 155.4, 155.3, 152.5, 150.1, 134.9, 134.8, 134.6, 134.4, 133.2, 128.3, 128.2, 127.3, 126.4, 125.1, 125.0, 124.8, 124.2, 123.3, 109.0, 30.0, 29.8; HRMS (ESI-) $[\text{M}+\text{H}]^-$ calcd. or $[\text{C}_{34}\text{H}_{26}\text{BrO}_8]^-$: m/z = 641.0811, Found: m/z = 641.0812.

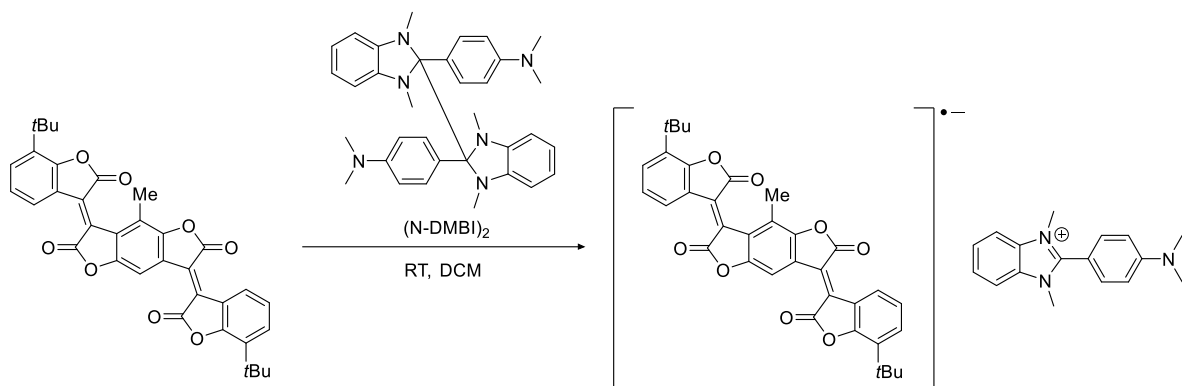


4-chloro-3,7-bis((E)-7-tert-butyl-2-oxobenzofuran-3(2H)-ylidene)-3,7-dihydrobenzo[1,2-b:4,5-b']difuran-2,6-dione (BFD-Cl) was synthesized using General Procedure G: 4-chloro-3,7-dihydrobenzo[1,2-b:4,5-b']difuran-2,6-dione (0.1 g, 0.45 mmol, 1.0 eq.) and 7-(tert-butyl)benzofuran-2,3-dione (0.18 g, 0.89 mmol, 2.0 eq.) were dissolved into DMF (21 mL) and heated at 80 °C for 4 h under an inert atmosphere. After heating, the solvent was removed via rotary evaporation. The residue was dissolved into a minimum amount of dichloromethane and precipitated into hexanes. The solids were collected by filtration, washed with hexanes, collected, and dried to yield a purple solid (24 mg, 9.1%). ^1H NMR (800 MHz, CDCl_3): δ (ppm) 8.97 (d, J = 8.29 Hz, 1H), 8.85 (s, 1H), 8.60 (d, J = 8.60 Hz, 1H), 7.57 (d, J = 7.94, 2H), 7.25-7.22 (m, 2H), 1.46 (d, J = 3.85 Hz, 18H); ^{13}C NMR (201 MHz, CDCl_3): δ 166.4, 165.4, 165.2, 164.5, 158.1, 155.3, 155.1, 152.3, 149.9, 134.7, 134.6, 134.4, 134.2, 133.1, 132.99, 128.1, 128.0, 127.1, 126.3, 126.2, 124.9, 124.8, 124.6, 124.1, 123.1, 118.1, 116.3, 108.8, 34.6, 34.6, 29.7; HRMS (ESI-) $[\text{M}+\text{H}]^-$ calcd. or $[\text{C}_{34}\text{H}_{26}\text{ClO}_8]^-$: m/z = 597.1316, Found: m/z = 597.1333.

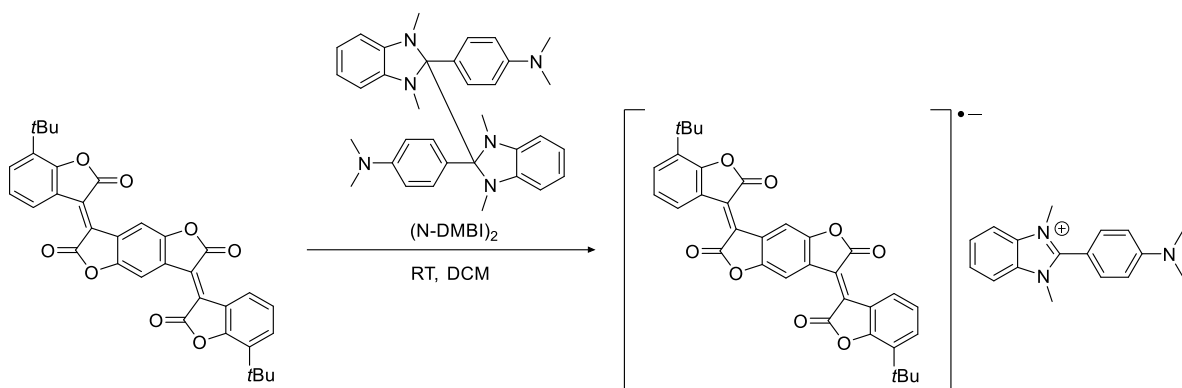
General Procedure H: Synthesis of Doped Oligomers



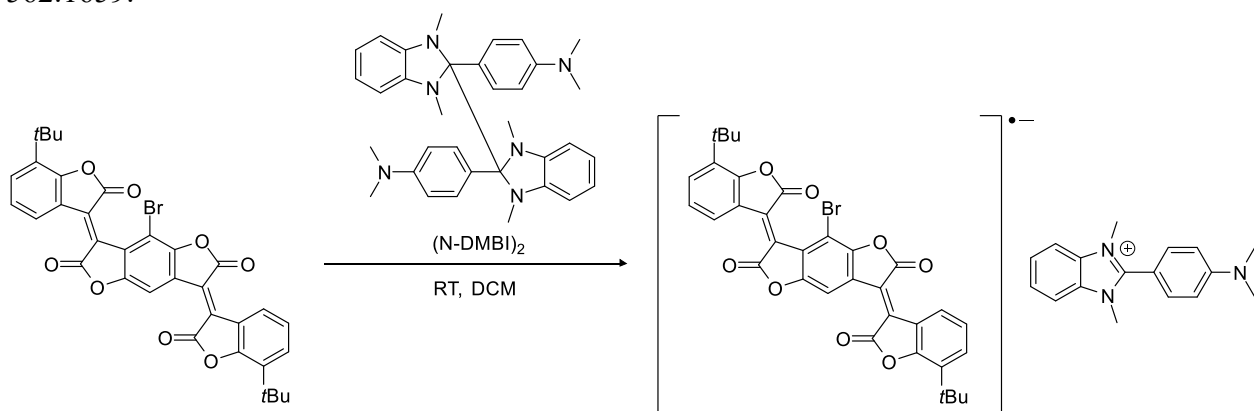
One electron reduction reaction between **BFD-X** derivatives and (N-DMBI)₂: In a 20-mL vial, substituted **BFD-X** (1.0 eq.) was dissolved into dichloromethane. (N-DMBI)₂¹¹ (0.5 eq.) was dissolved in dichloromethane and added dropwise to the **BFD-X** solution. The reaction was stirred at room temperature for 2 minutes and the consumption of **BFD-X** was monitored by UV-Vis absorption spectroscopy. After the reaction, 15 mL hexane was added, cooled down in a $-20\text{ }^{\circ}\text{C}$ freezer for 1 h, and filtered. The solids were washed with hexanes and dried to yield teal solids.



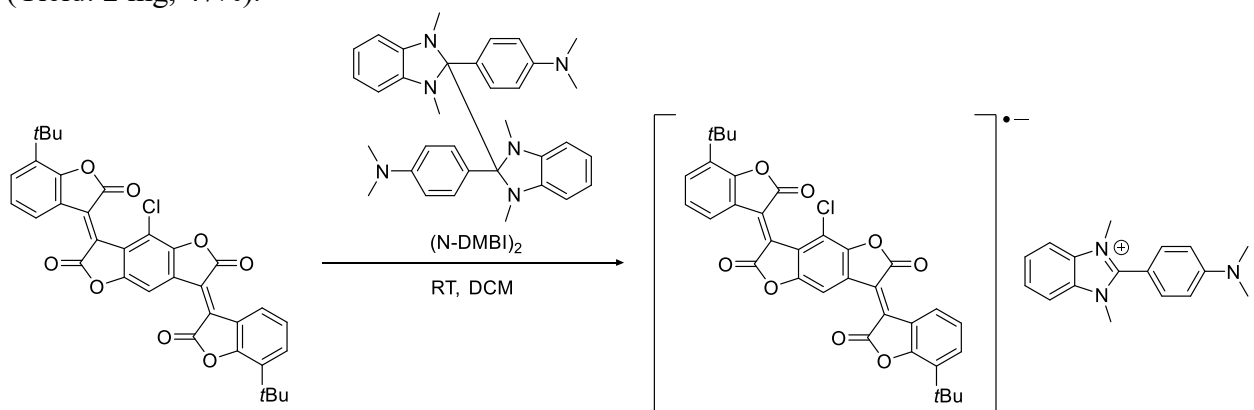
BFD-Me^{•-} was synthesized following General Procedure H: **BFD-Me** (10 mg, 1.0 eq) was dissolved in 4mL dichloromethane and (N-DMBI)₂ (4.6 mg, 0.5 eq) was dissolved in 1mL dichloromethane. (Yield: 9 mg, 63%). HRMS (ESI-) [M]⁻ calcd. for [C₃₅H₂₈O₈]⁻: m/z = 576.1790, Found: m/z = 576.1818.



BFD^{•-} was synthesized following General Procedure H: **BFD** (10 mg, 1.0 eq) was dissolved in 4mL dichloromethane and (N-DMBI)₂ (4.7 mg, 0.5 eq) was dissolved in 1mL dichloromethane. (Yield: 12 mg, 82%). HRMS (ESI-) [M]⁻ calcd. for [C₃₄H₂₆O₈]⁻: m/z = 562.1633, Found: m/z = 562.1659.

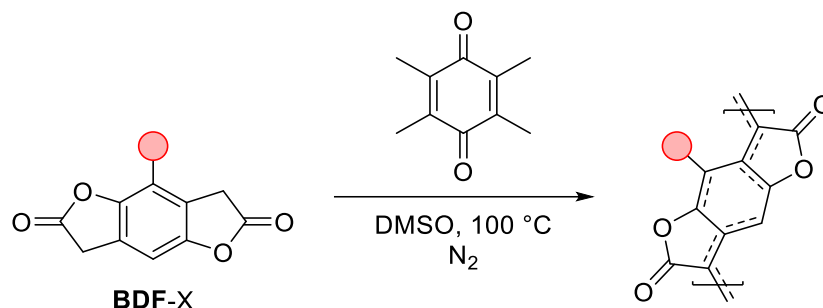


BFD-Br^{•-} was synthesized following General Procedure H: **BFD-Br** (3 mg, 1.0 eq) was dissolved in 4mL dichloromethane and (N-DMBI)₂ (1.2 mg, 0.5 eq) was dissolved in 1mL dichloromethane. (Yield: 2 mg, 47%).

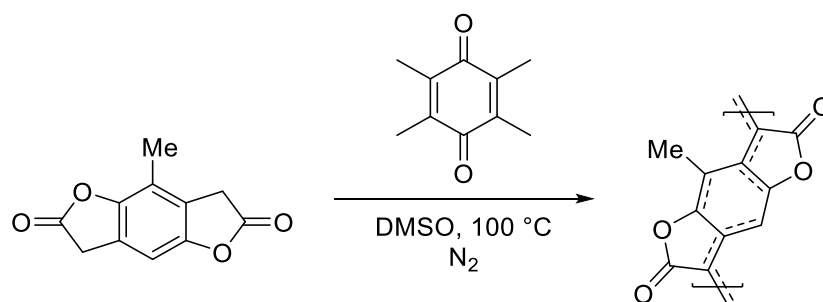


BFD-Cl^{•-} was synthesized following General Procedure H: **BFD-Cl** (5 mg, 1.0 eq) was dissolved in 4mL dichloromethane and (N-DMBI)₂ (2.2 mg, 0.5 eq) was dissolved in 1mL dichloromethane. (Yield: 5 mg, 70%). HRMS (ESI-) [M]⁻ calcd. for [C₃₄H₂₅ClO₈]⁻: m/z = 596.1243, Found: m/z = 596.1282.

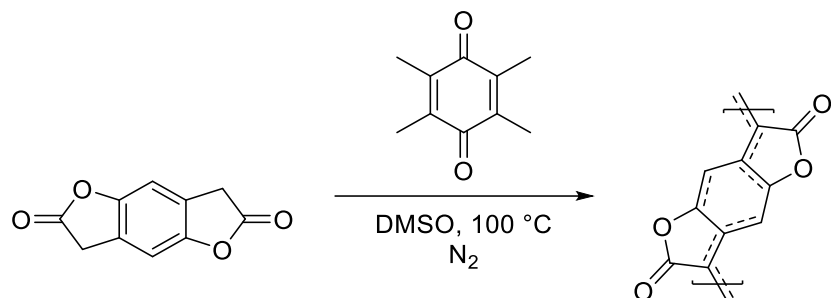
General Procedure I: Synthesis of n-PBDF-X



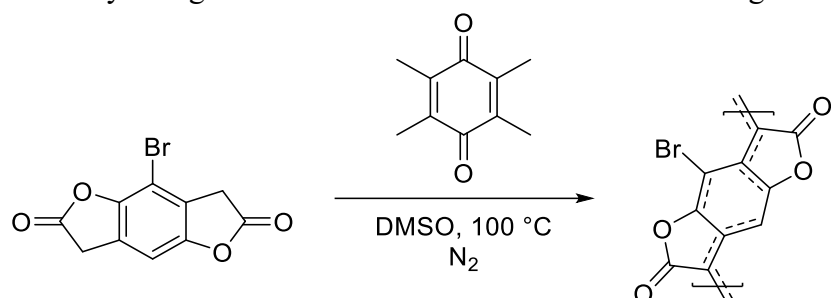
Oxidative Polymerization & *in situ* doping of substituted BDF were performed via previously reported literature¹²: substituted BDF (1.0 eq.) & tetramethylbenzoquinone (TMQ, 1.0 eq) were added to a 10-mL Schlenk tube. The reactor was evacuated and backfilled with N₂ three times. Under positive pressure, anhydrous dimethylsulfoxide (DMSO, 10 mg/mL) was added via syringe. The reactor was sealed and heated in an oil bath at 80 or 100 °C. After the polymerization was completed, the reaction was cooled, the polymer was transferred to a dialysis bag (cut-off molecular weight of 10 kDa, Viskase, USA), and dialyzed against DMSO to remove low molecular weight fractions & TMQ.



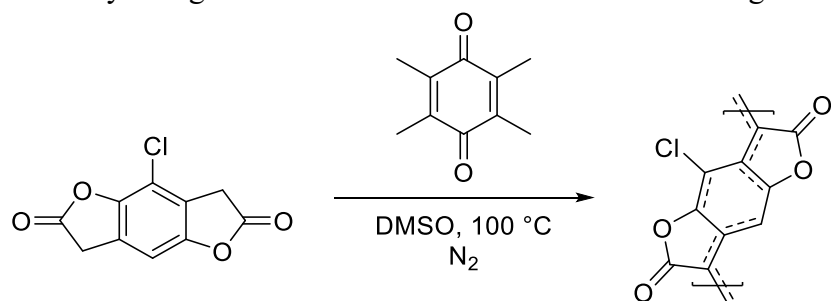
n-PBDF-Me was synthesized using General Procedure I: BDF-Me (20 mg, 98 μmol, 1.0 eq.) & TMQ (16.1 mg, 98 μmol, 1.0 eq.) were added to a 10-mL Schlenk tube. The reactor was evacuated and backfilled with N₂ three times. Under positive pressure, anhydrous dimethylsulfoxide (DMSO, 10 mg/mL) was added via syringe. The reactor was sealed and heated in an oil bath at 100 °C until the solution becomes viscous (approx. 1 h). After the polymerization was completed, the reaction was cooled, the polymer was transferred to a dialysis bag (cut-off molecular weight of 10 kDa, Viskase, USA), and dialyzed against DMSO to remove low molecular weight fractions & TMQ.



n-PBDF was synthesized using General Procedure I: BDF (20 mg, 105 μmol , 1.0 eq.) & TMQ (17.3 mg, 105 μmol , 1.0 eq.) were added to a 10-mL Schlenk tube. The reactor was evacuated and backfilled with N_2 three times. Under positive pressure, anhydrous dimethylsulfoxide (DMSO, 10 mg/mL) was added via syringe. The reactor was sealed and heated in an oil bath at 100 $^\circ\text{C}$ until the solution becomes viscous (approx. 1 h). After the polymerization was completed, the reaction was cooled, the polymer was transferred to a dialysis bag (cut-off molecular weight of 10 kDa, Viskase, USA), and dialyzed against DMSO to remove low molecular weight fractions & TMQ.



n-PBDF-Br was synthesized using General Procedure I: BDF-Br (20 mg, 74 μmol , 1.0 eq.) & TMQ (12.2 mg, 74 μmol , 1.0 eq.) were added to a 10-mL Schlenk tube. The reactor was evacuated and backfilled with N_2 three times. Under positive pressure, anhydrous dimethylsulfoxide (DMSO, 10 mg/mL) was added via syringe. The reactor was sealed and heated in an oil bath at 100 $^\circ\text{C}$ until the solution becomes viscous (approx. 1 h). After the polymerization was completed, the reaction was cooled, the polymer was transferred to a dialysis bag (cut-off molecular weight of 10 kDa, Viskase, USA), and dialyzed against DMSO to remove low molecular weight fractions & TMQ.



n-PBDF-Cl was synthesized using General Procedure I: BDF-Cl (20 mg, 89 μmol , 1.0 eq.) & TMQ (14.6 mg, 89 μmol , 1.0 eq.) were added to a 10-mL Schlenk tube. The reactor was evacuated and backfilled with N_2 three times. Under positive pressure, anhydrous dimethylsulfoxide (DMSO, 10 mg/mL) was added via syringe. The reactor was sealed and heated in an oil bath at 100 $^\circ\text{C}$ until the solution becomes viscous (approx. 1 h). After the polymerization was completed, the reaction was cooled, the polymer was transferred to a dialysis bag (cut-off molecular weight of 10 kDa, Viskase, USA), and dialyzed against DMSO to remove low molecular weight fractions & TMQ.

Neutral Oligomer Characterization

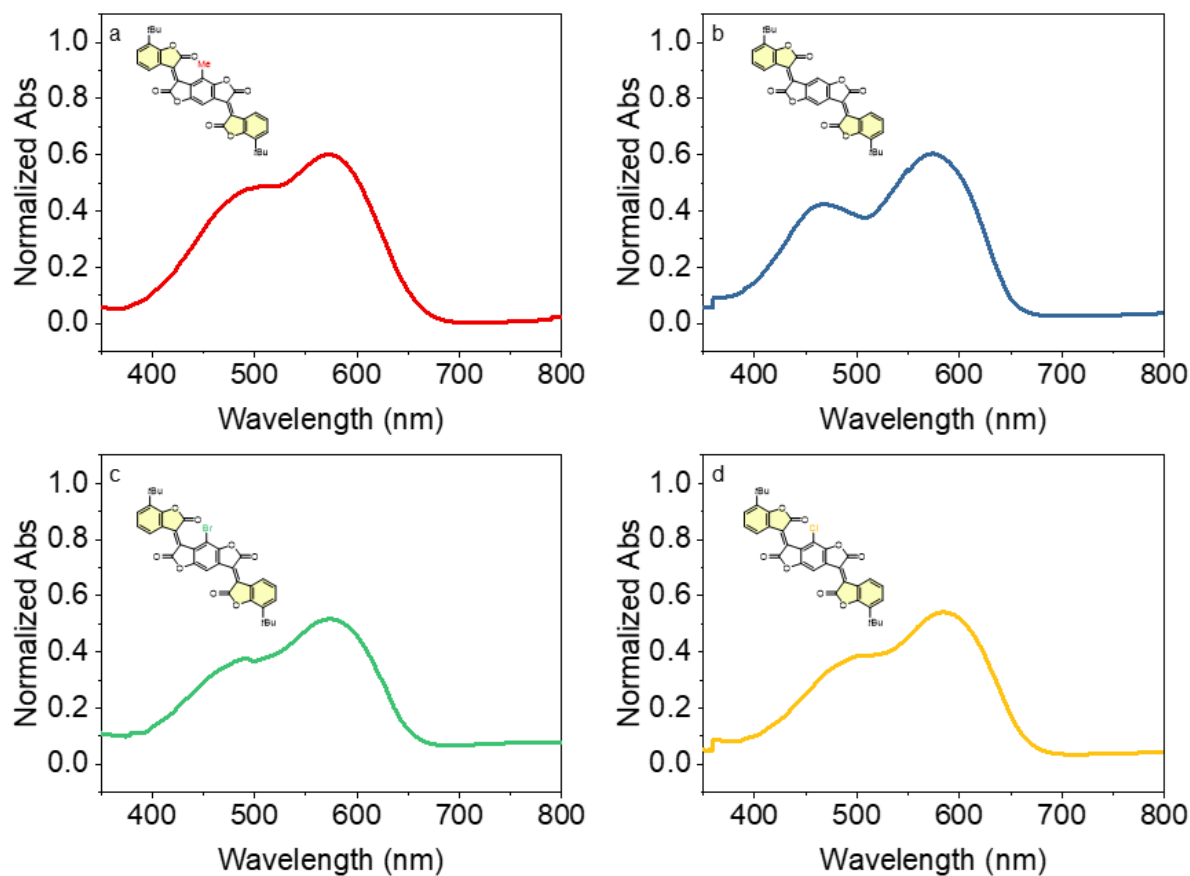


Figure S1. Solution UV-Vis absorption of neutral oligomers; (a) **BFD-Me**, (b) **BFD**, (c) **BFD-Br**, and (d) **BFD-Cl**.

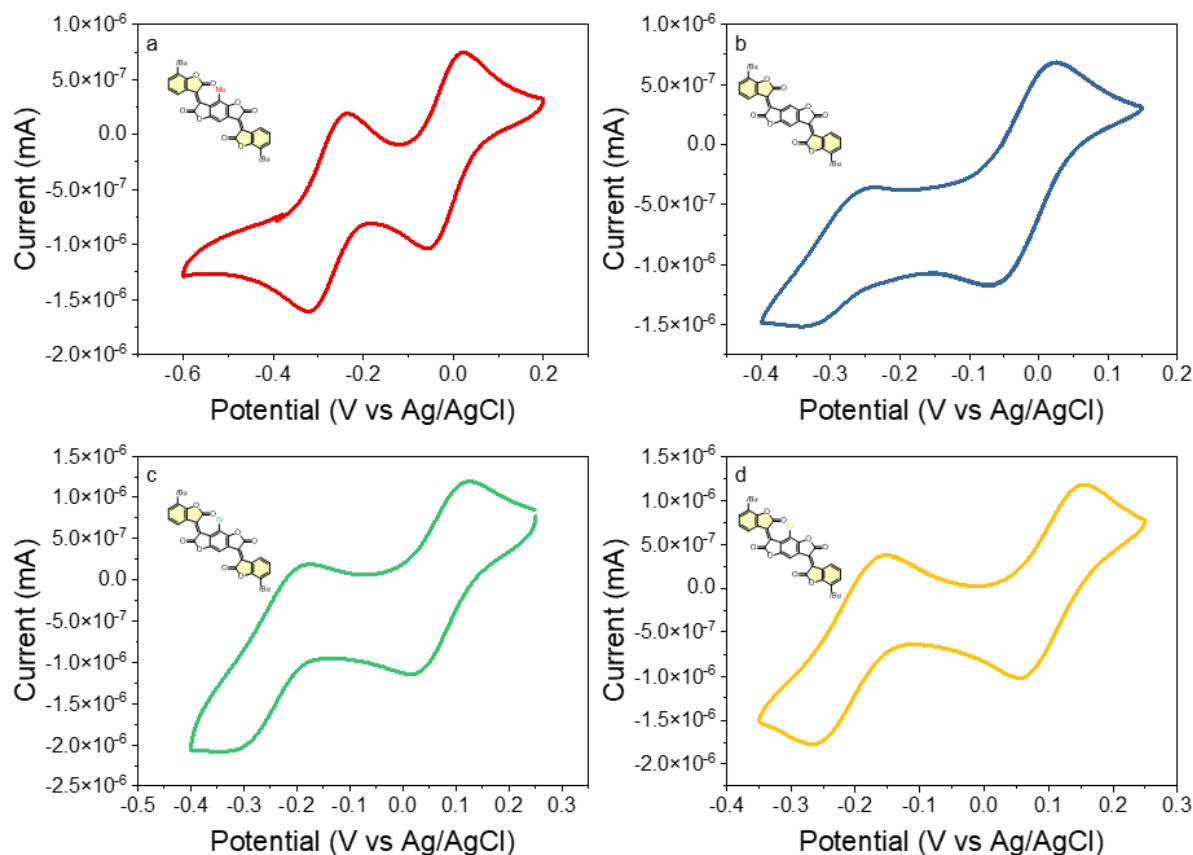


Figure S2. Solution cyclic voltammetry of neutral oligomers; (a) BFD-Me, (b) BFD, (c) BFD-Br, and (d) BFD-Cl.

Table S5. Energy level summary of neutral oligomers.

Solution	Calculated			Experimental		
	E_{HOMO} (eV)	E_{LUMO} (eV)	E_g (eV)	E_{HOMO} (eV)	E_{LUMO} (eV) ^a	E_g (eV) ^b
BFD-Me	-6.01	-3.75	-2.26	-6.33	-4.46	-1.87
BFD	-6.09	-3.77	-2.32	-6.35	-4.46	-1.89
BFD-Br	-6.11	-3.84	-2.27	-6.44	-4.53	-1.91
BFD-Cl	-6.13	-3.84	-2.29	-6.48	-4.58	-1.90

(a) $LUMO = -e(4.8 + E_{red}^{onset} - E_{Fc/Fc^+})$, ferrocene = 0.388 eV, $HOMO = LUMO - E_g$. (b) E_g is optical bandgap obtained from absorption threshold, $E_g = 1240/\lambda_{cut-off}$.

Temperature Effect & In Situ Doping Study:

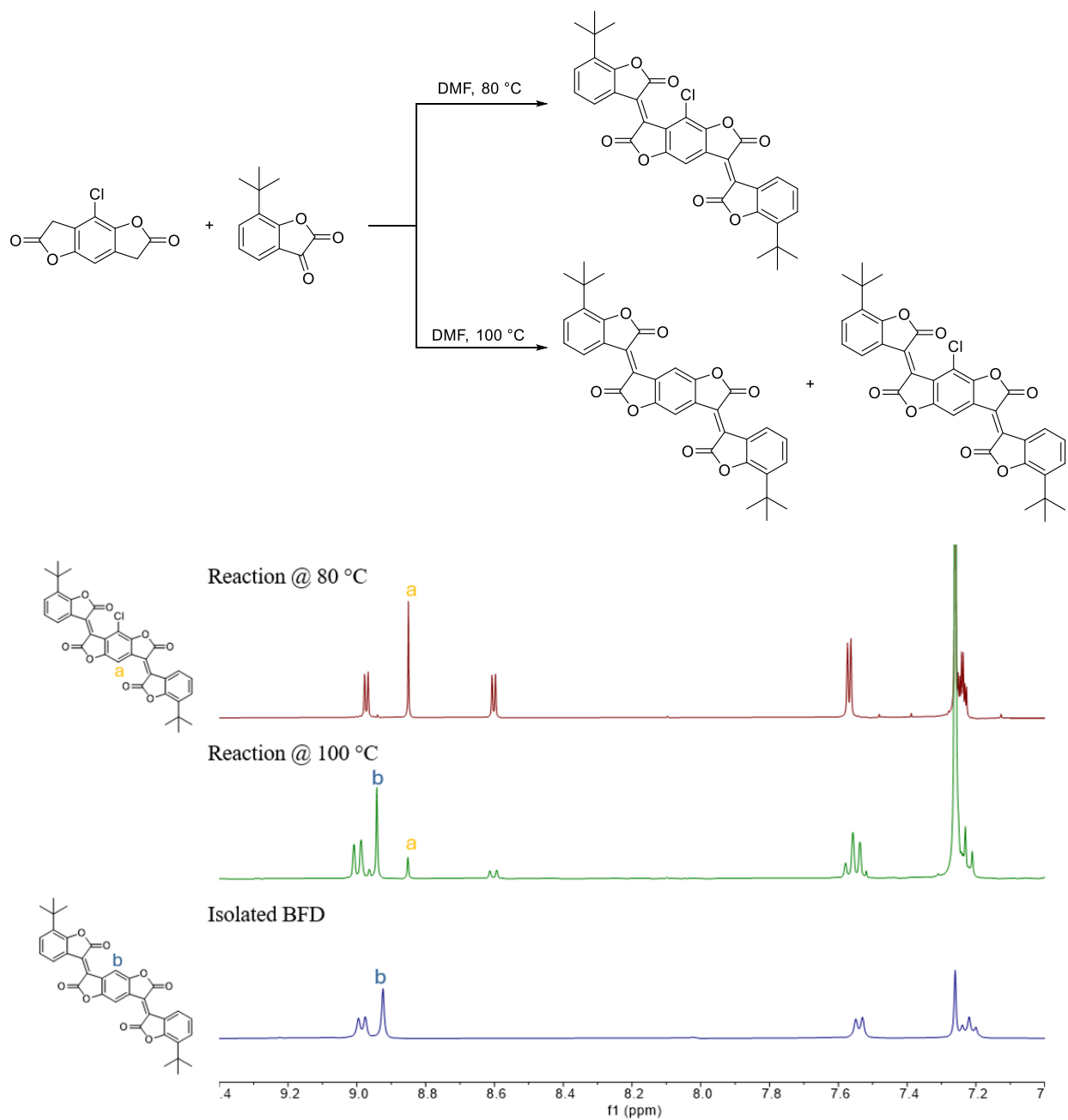


Figure S3. Temperature effect of **BFD-Cl** synthesis. Top: synthesis route to **BDF-Cl** at 80 and 100 °C; bottom: ^1H NMR comparison between reaction temperatures.

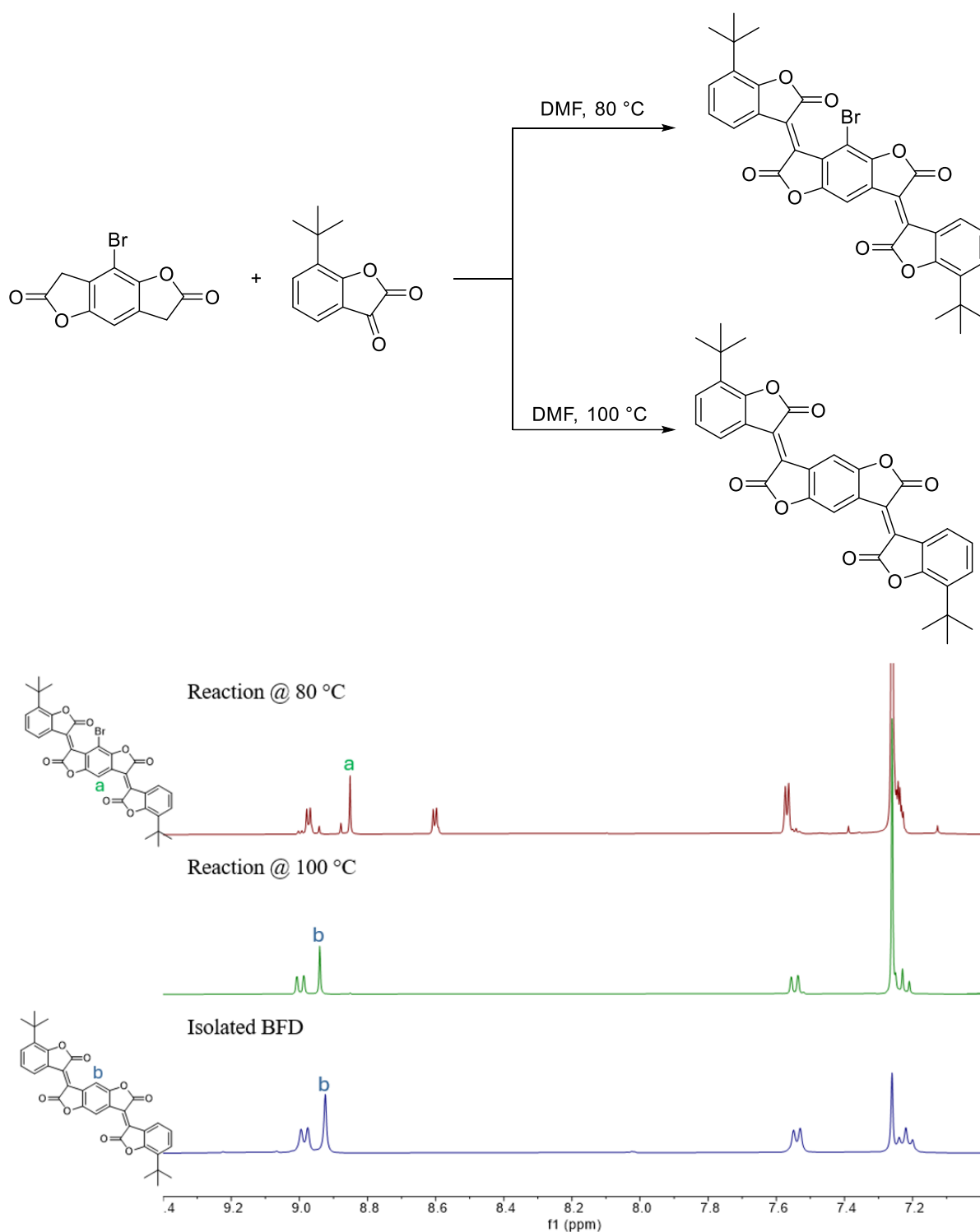


Figure S4. Temperature effect of **BFD-Br** synthesis. Top: synthesis route to **BDF-Br** at 80 and 100 °C; bottom: ¹H NMR comparison between reaction temperatures.

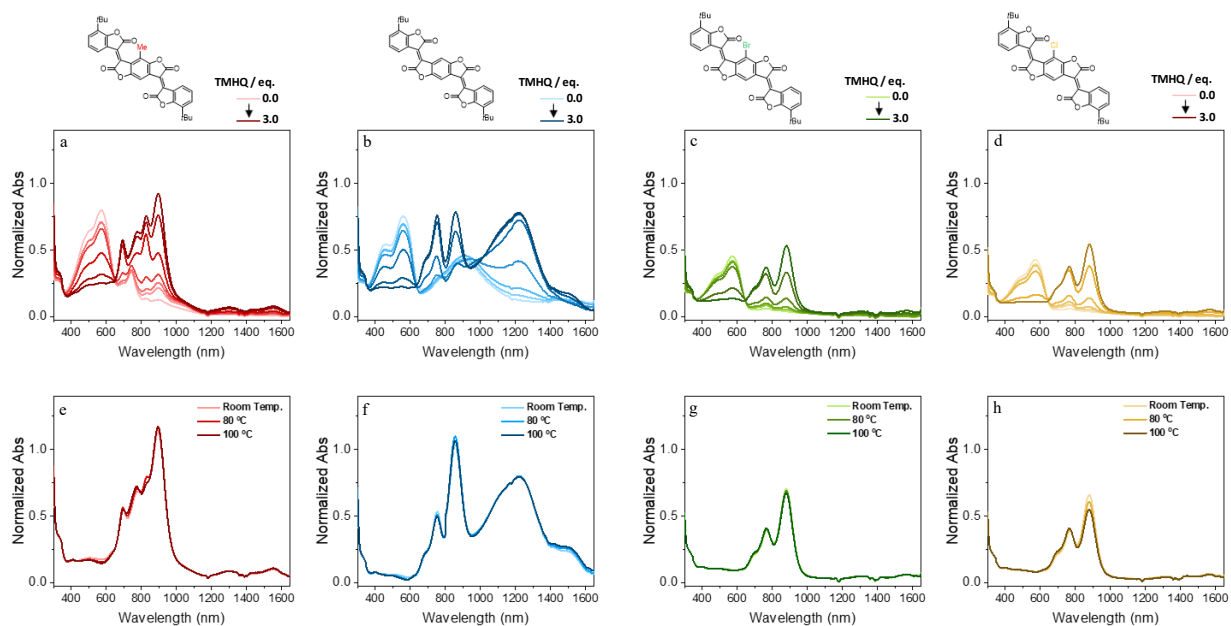


Figure S5. UV-Vis *in situ* doping experiments: (a–d) UV-Vis absorbance of oligomers doping titration experiment; (e–h) UV-Vis absorbance of doped oligomers at room temperature, 80 °C, and 100 °C.

Table S6. Summary of $\lambda_{\max}^{\text{abs}}$ from UV-Vis doping experiments.

	BDF-Me	BDF	BDF-Br	BDF-Cl
$\lambda_{\max}^{\text{abs}}$ (nm)	695, 780, 895, 1302, 1554	754, 857, 1222	768, 880, 1318, 1566	770, 880, 1313, 1559

Doped Oligomer Characterization

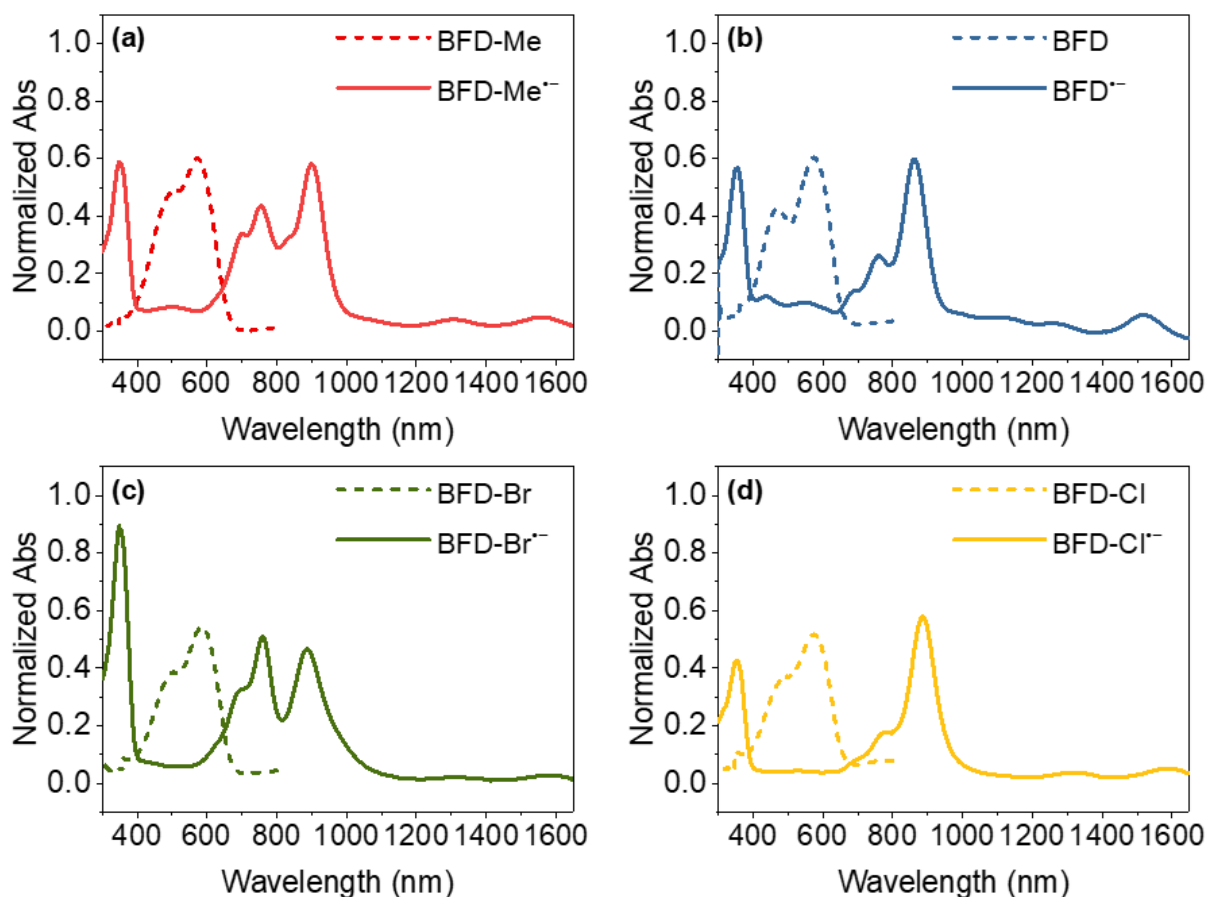


Figure S6. Solution UV-Vis absorption of doped and neutral oligomers; (a) **BFD-Me^{•-}** (solid) and **BFD-Me** (dashed), (b) **BFD^{•-}** (solid) and **BFD** (dashed) (c) **BFD-Br^{•-}** (solid) and **BFD-Br** (dashed), and (d) **BFD-Cl^{•-}** (solid) and **BFD-Cl** (dashed).

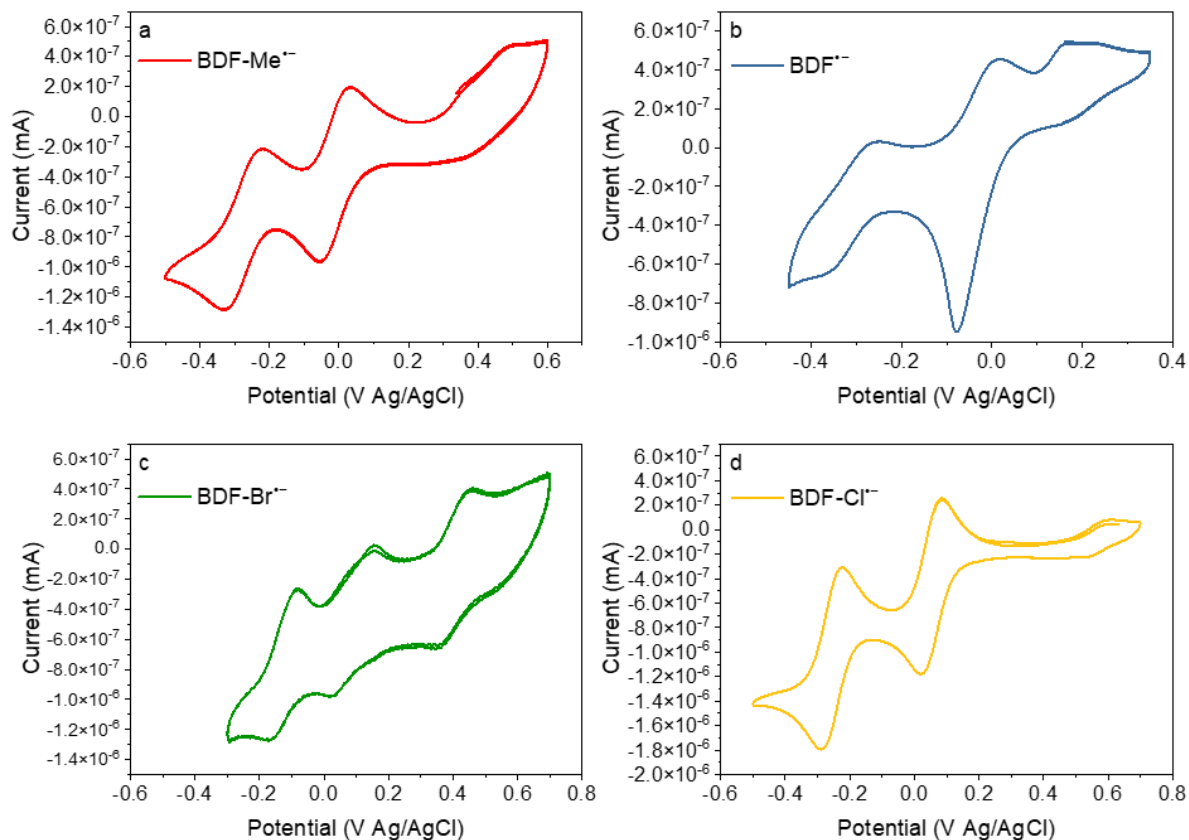


Figure S7. Solution cyclic voltammetry of doped oligomers; (a) **BFD-Me^{•-}**, (b) **BFD^{•-}**, (c) **BFD-Br^{•-}**, and (d) **BFD-Cl^{•-}**.

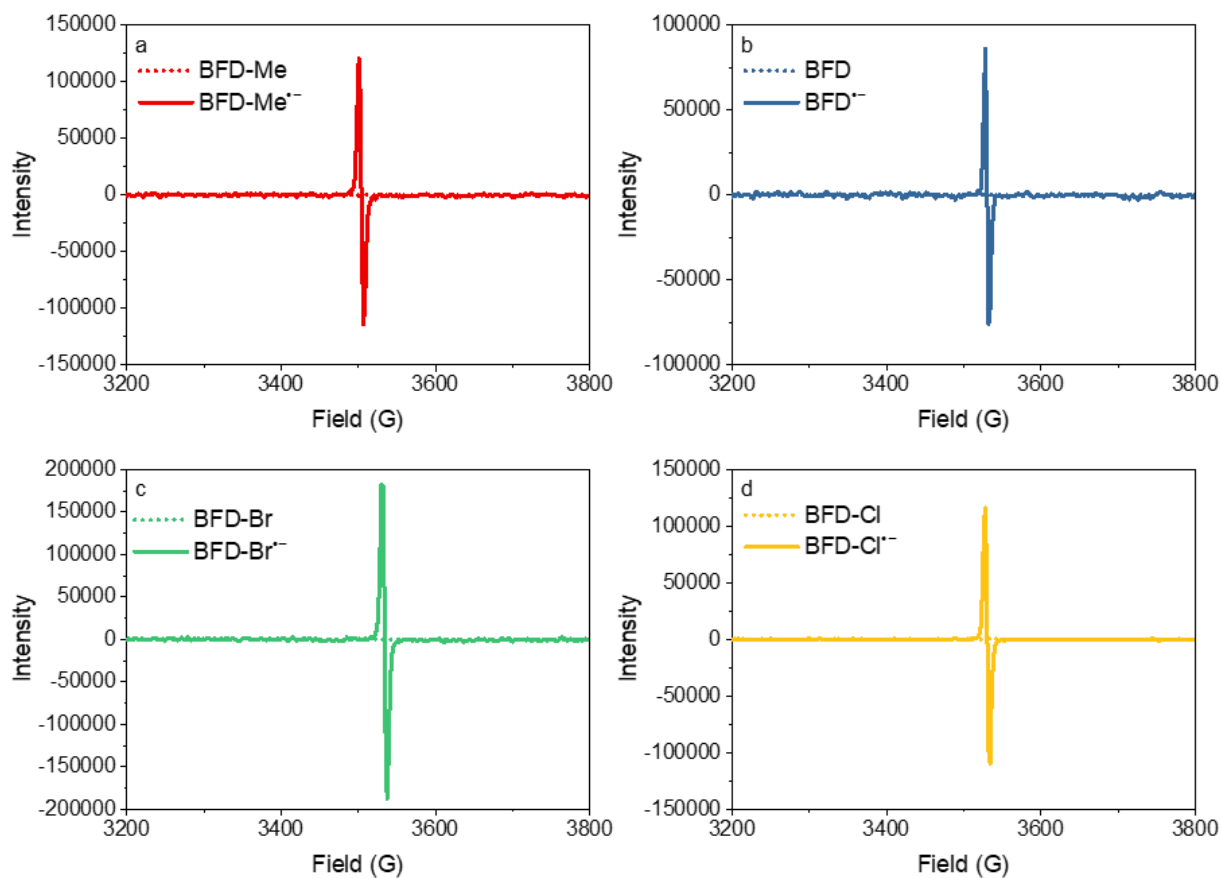


Figure S8. Room temperature electron paramagnetic resonance (RT-EPR) spectroscopy of doped oligomers (solid) and neutral oligomers (dashed).

Polymer Characterization

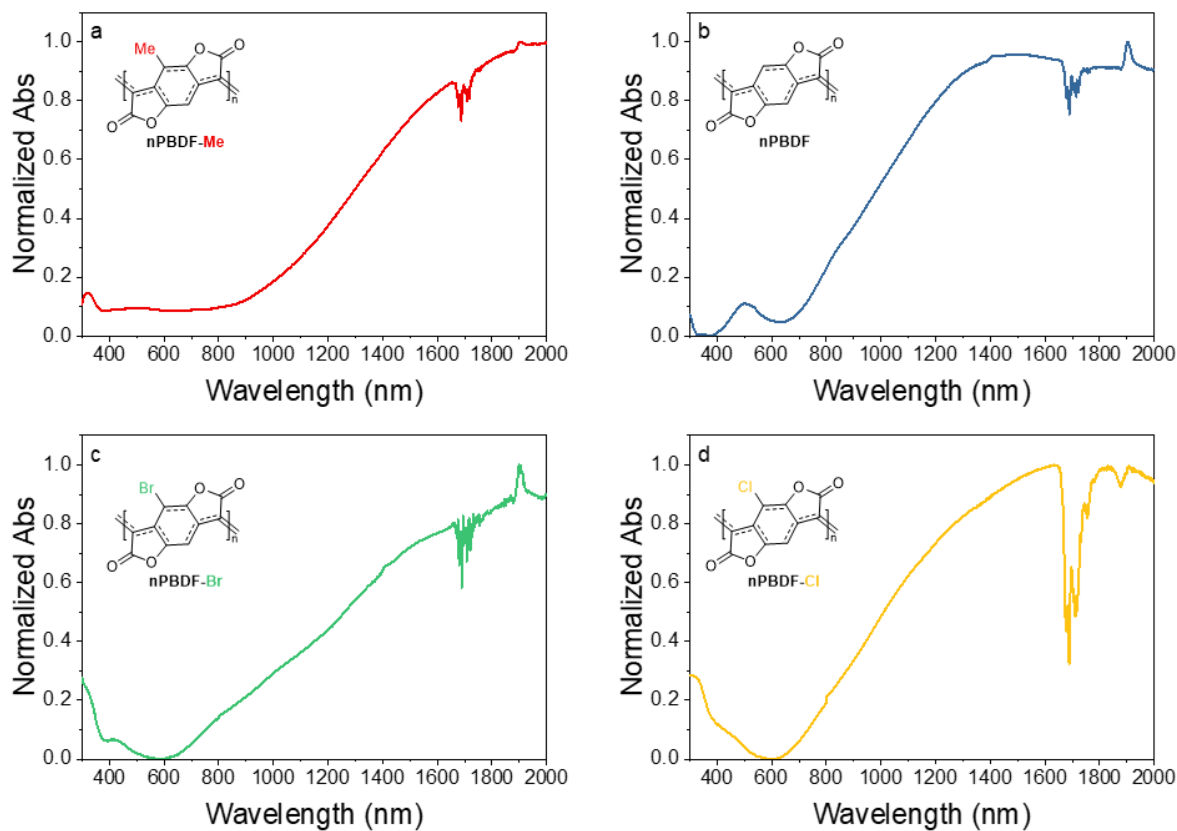


Figure S9. Film UV-Vis-NIR absorption of pristine polymer; (a) **n-PBDF-Me**, (b) **n-PBDF**, (c) **n-PBDF-Br**, and (d) **n-PBDF-Cl**.

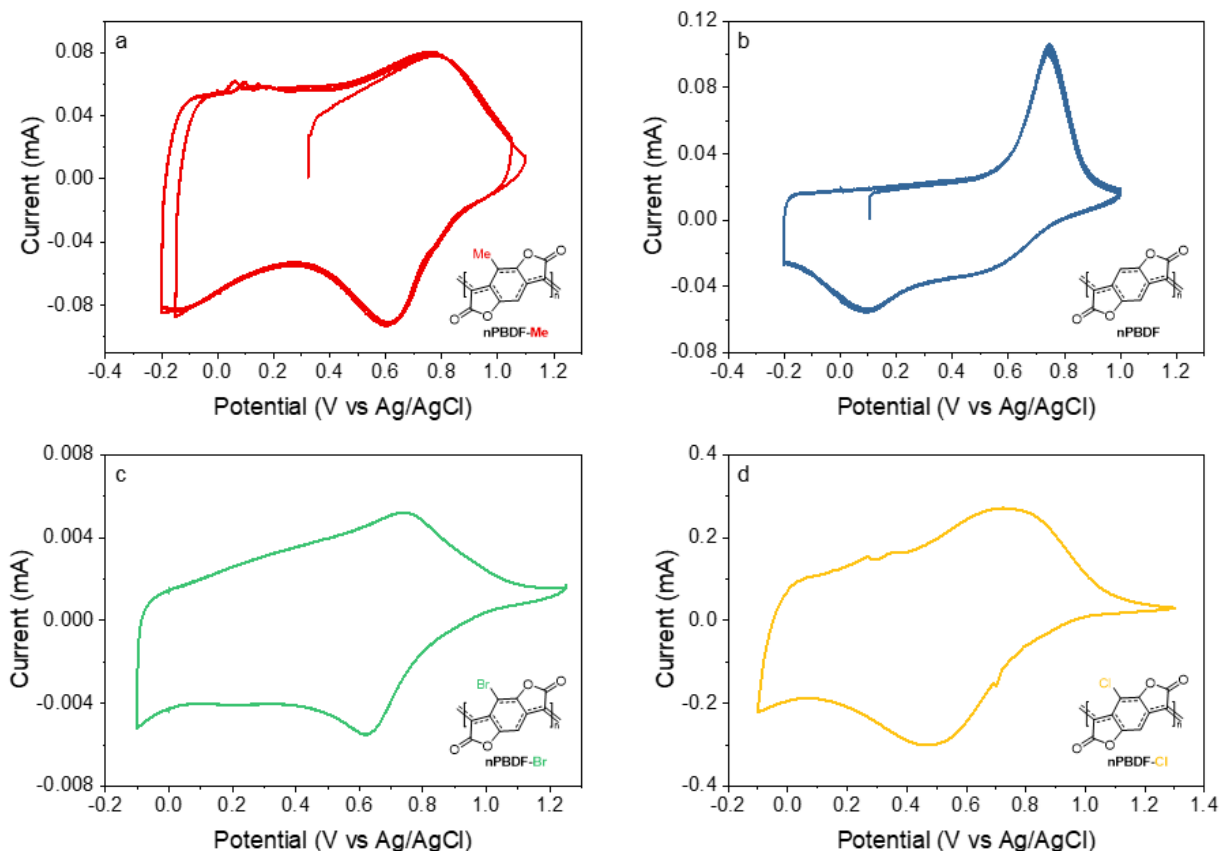


Figure S10. Film cyclic voltammetry of pristine polymer; (a) n-PBDF-Me, (b) n-PBDF, (c) n-PBDF-Br, and (d) n-PBDF-Cl.

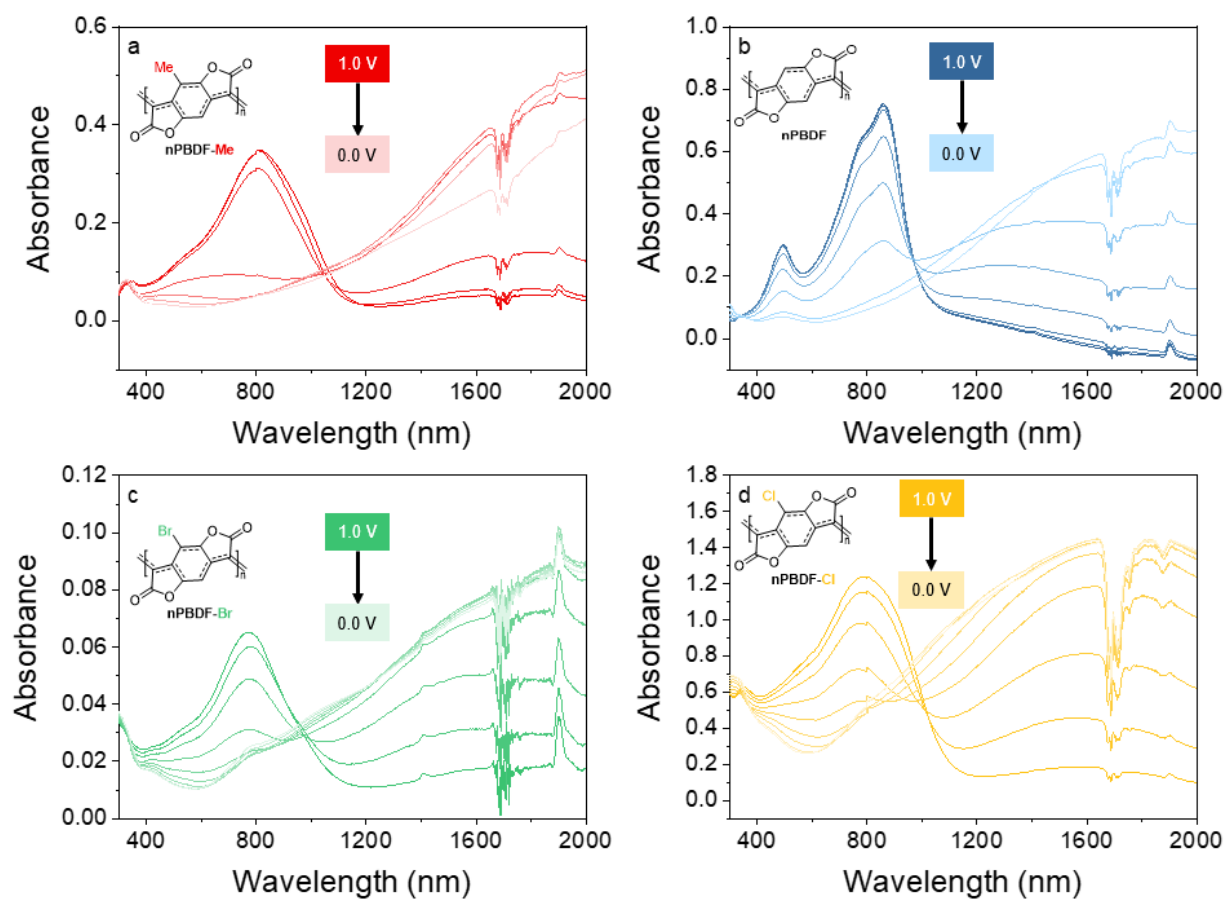


Figure S11. Film spectroelectrochemical analysis of polymer; (a) **n-PBDF-Me**, (b) **n-PBDF**, (c) **n-PBDF-Br**, and (d) **n-PBDF-Cl**.

Table S7. Summary of HOMO and LUMO energies n-PBDF derivatives.

Compound	$\lambda_{\max}^{\text{abs}}$ (nm) ^a	$E_{\text{red}}^{\text{onset}}$ (V) ^b	HOMO (eV) ^c	LUMO (eV) ^c	E_g (eV) ^d
n-PBDF-Me	810	0.80	-6.30	-5.20	1.10
n-PBDF	500, 860	0.81	-6.45	-5.15	1.30
n-PBDF-Br	774	0.87	-6.58	-5.27	1.31
n-PBDF-Cl	790	0.88	-6.48	-5.28	1.20

a) Measured as film. b) Cyclic voltammograms measured as film on ITO. c) $\text{LUMO} = -e(4.8 + E_{\text{red}}^{\text{onset}} - E_{\text{Fc/Fc}^+})$, ferrocene = 0.388 eV, $\text{HOMO} = \text{LUMO} - E_g$. d) E_g is optical bandgap obtained from absorption threshold, $E_g = 1240/\lambda_{\text{cut-off}}$.

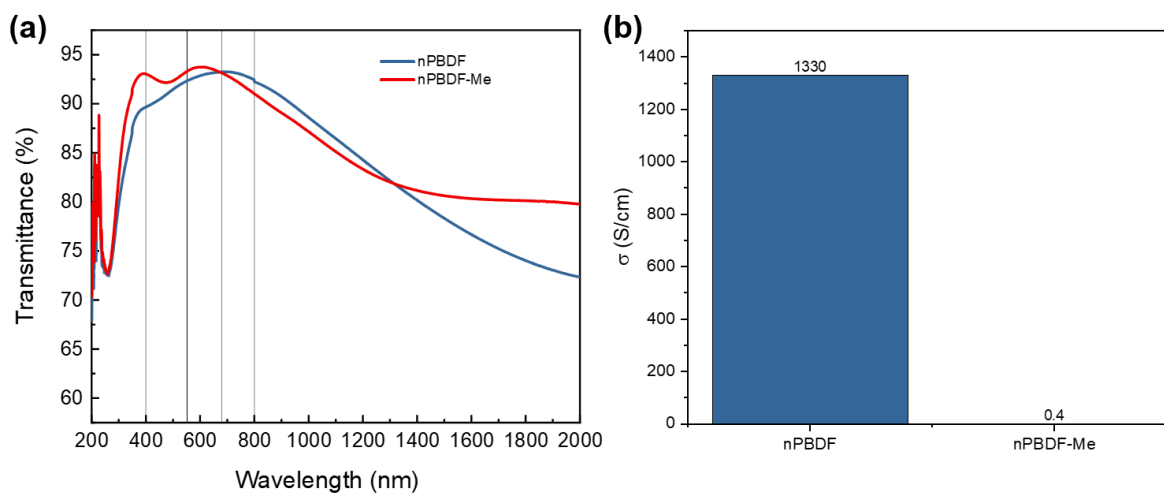


Figure S12. n-PBDF and n-PBDF-Me comparison for (a) UV–Vis–NIR transmittance and (b) conductivity calculated from sheet resistance measured by four-probe contact.

DFT Simulated Data

Density Functional Theory calculation were carried out using the Gaussian16¹³ program suite with the hybrid functional B3LYP (the Becke three parameter exchange functional¹⁴ and Lee–Yang–Parr correlation functional¹⁵) with all electron 6-31+G(d,p) basis set. The optimized geometry of the molecules with no imaginary frequency confirmed the global minima in the potential energy surface. Vertical excitation energies were computed using Time-Dependent DFT (TD-DFT)¹⁶ calculations using the same functional and basis set used to compute the optimized geometries. All calculations were carried out considering an isolated molecule in dichloromethane solvent and the solvation model used was IEFPCM.¹⁷

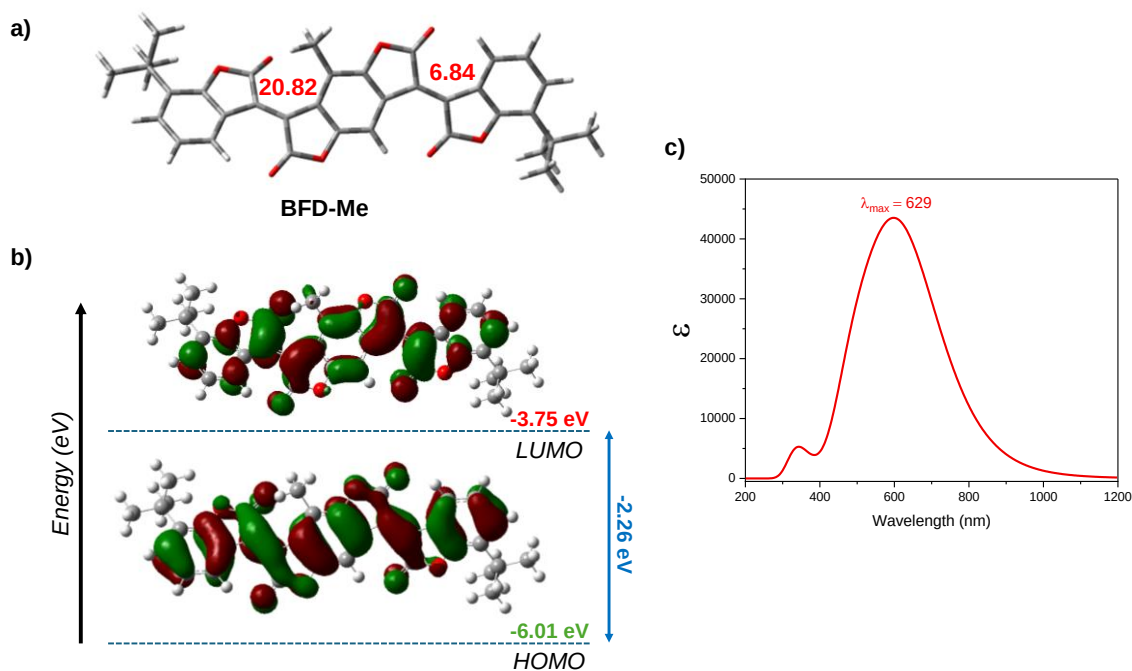


Figure S13. DFT calculated (a) molecular geometry & torsion angle (b) HOMO & LUMO energy levels and (c) simulated UV-Vis absorption of **BFD-Me**.

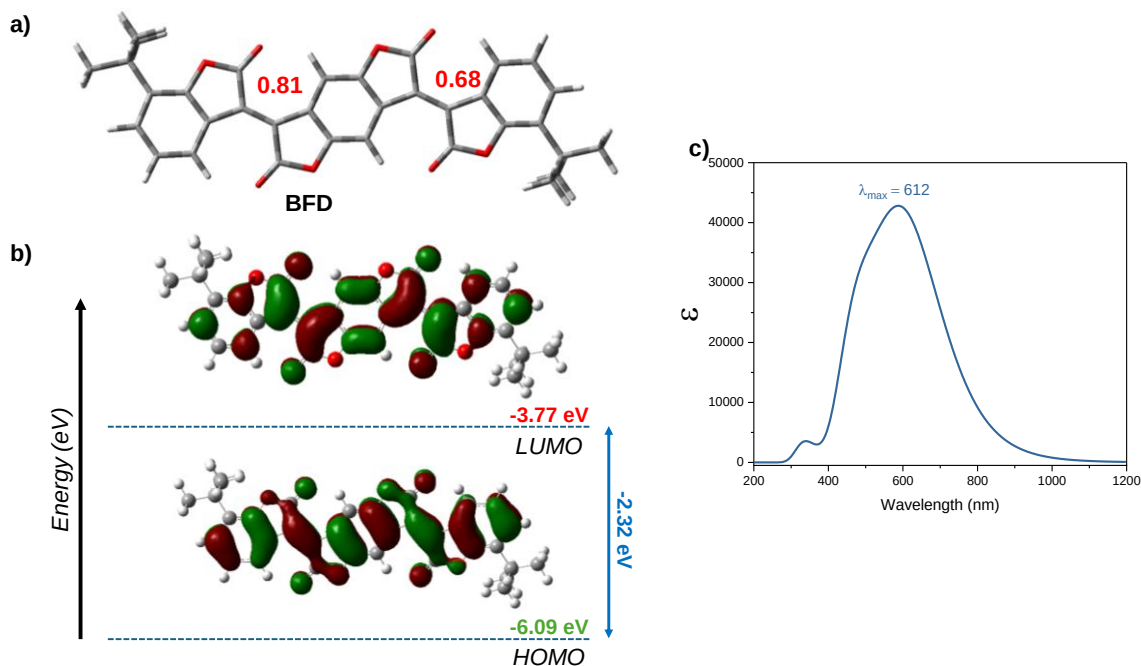


Figure S14. DFT calculated (a) molecular geometry & torsion angle (b) HOMO & LUMO energy levels and (c) simulated UV-Vis absorption of **BFD**.

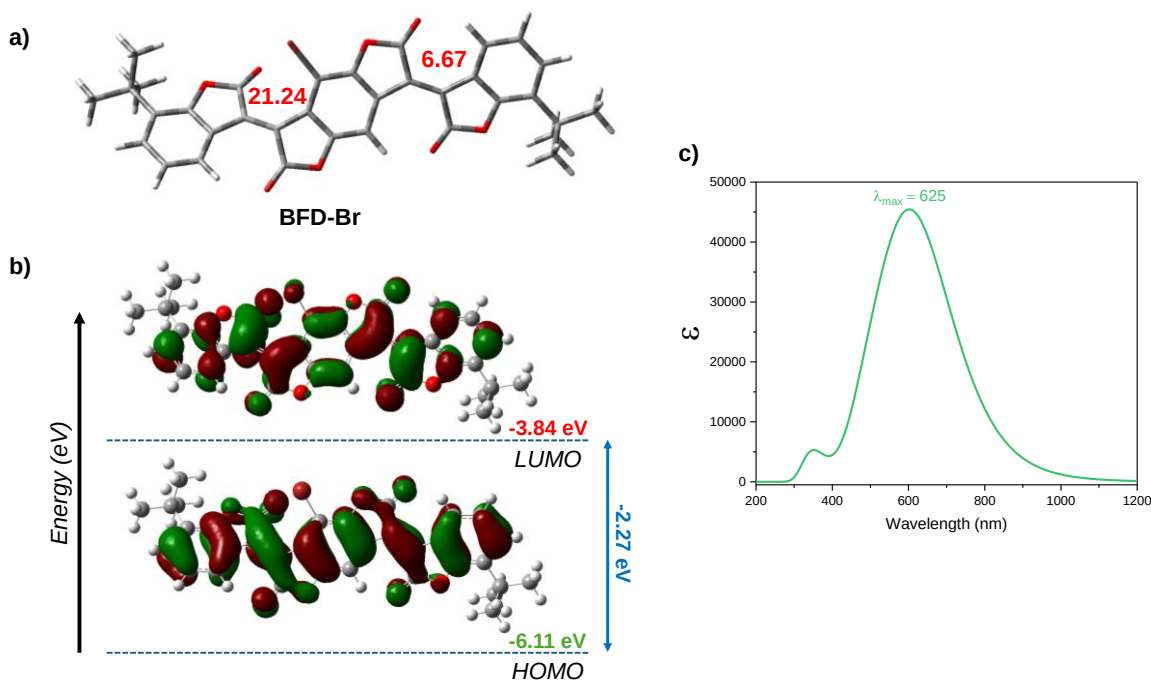


Figure S15. DFT calculated (a) molecular geometry & torsion angle (b) HOMO & LUMO energy levels and (c) simulated UV-Vis absorption of **BFD-Br**.

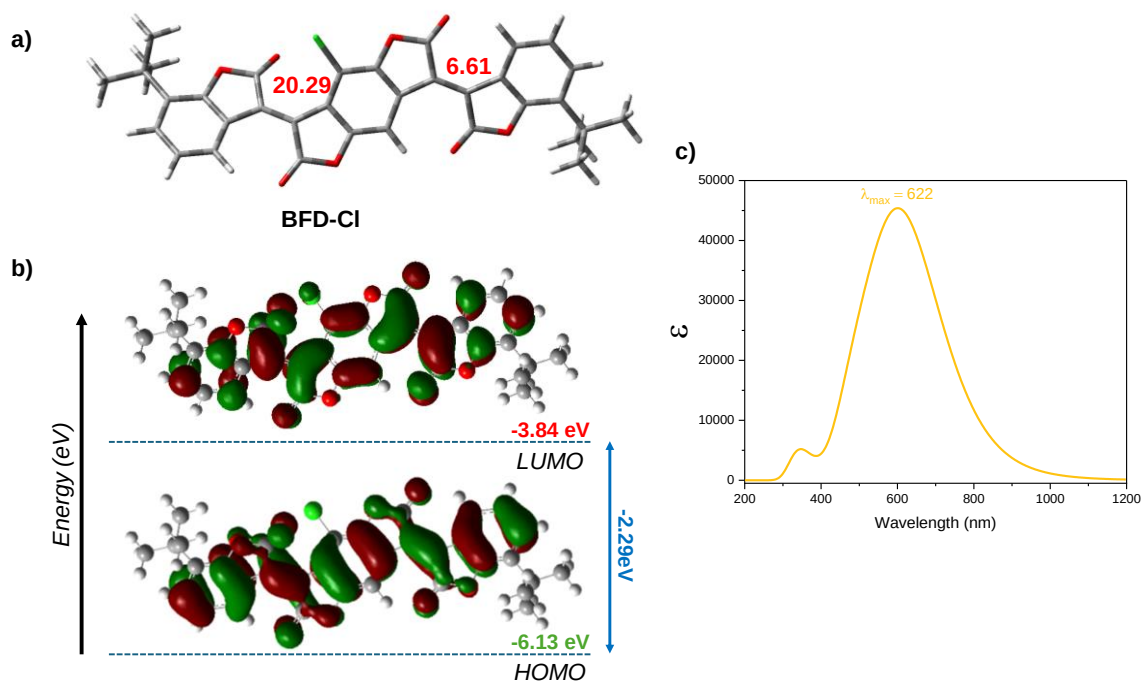


Figure S16. DFT calculated (a) molecular geometry & torsion angle (b) HOMO & LUMO energy levels and (c) simulated UV-Vis absorption of **BFD-Cl**.

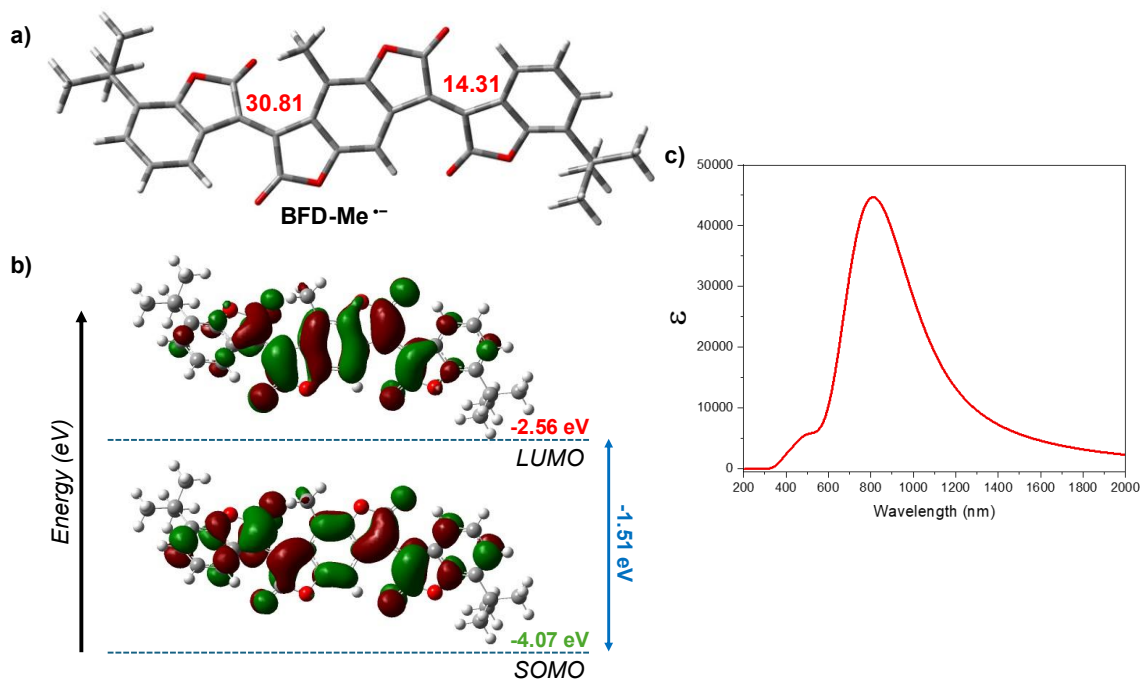


Figure S17. DFT calculated (a) molecular geometry & torsion angle (b) SOMO & LUMO energy levels and (c) simulated UV-Vis absorption of **BFD-Me^{•-}**.

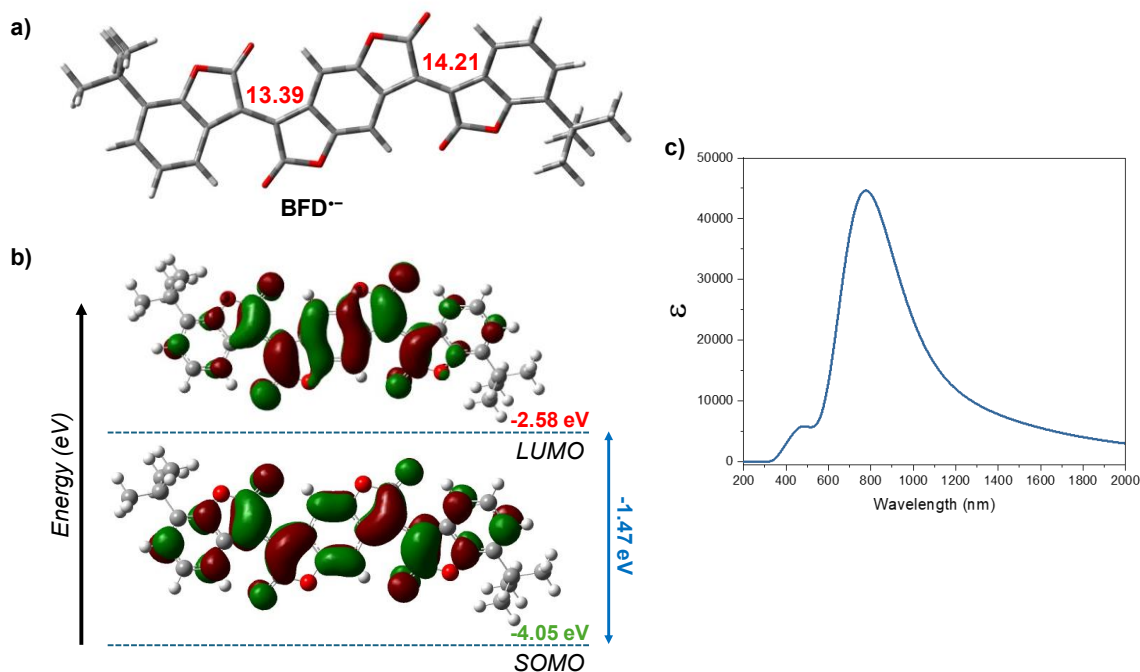


Figure S18. DFT calculated (a) molecular geometry & torsion angle (b) SOMO & LUMO energy levels and (c) simulated UV-Vis absorption of **BFD^{•-}**.

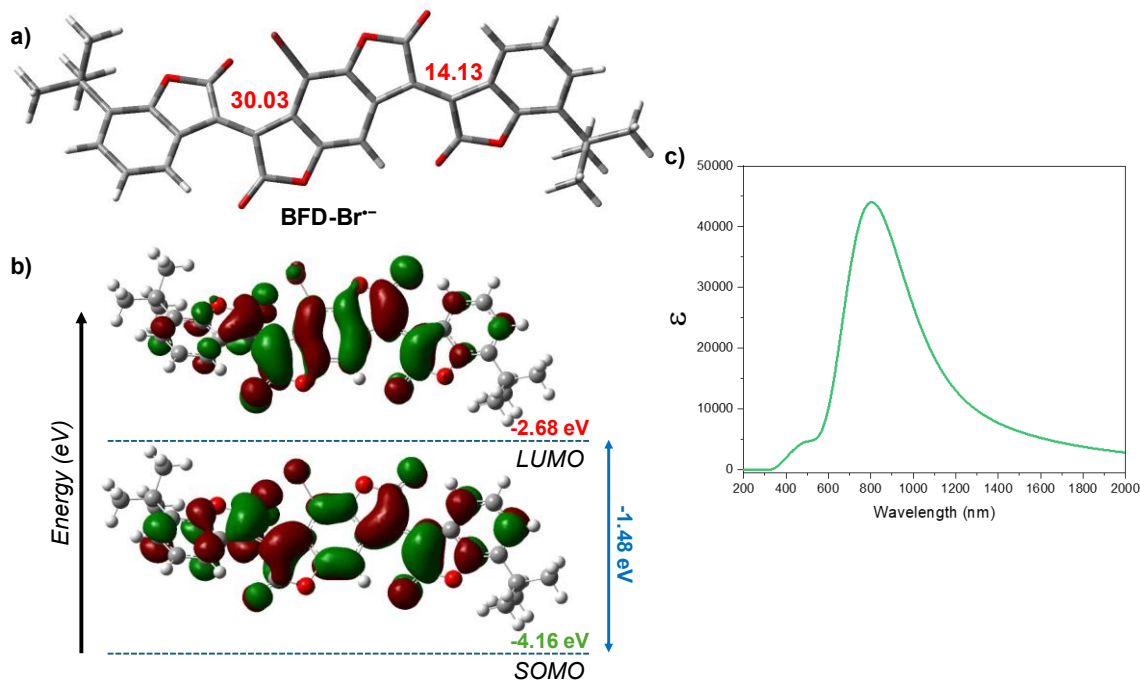


Figure S19. DFT calculated (a) molecular geometry & torsion angle (b) SOMO & LUMO energy levels and (c) simulated UV-Vis absorption of **BFD-Br^{•-}**.

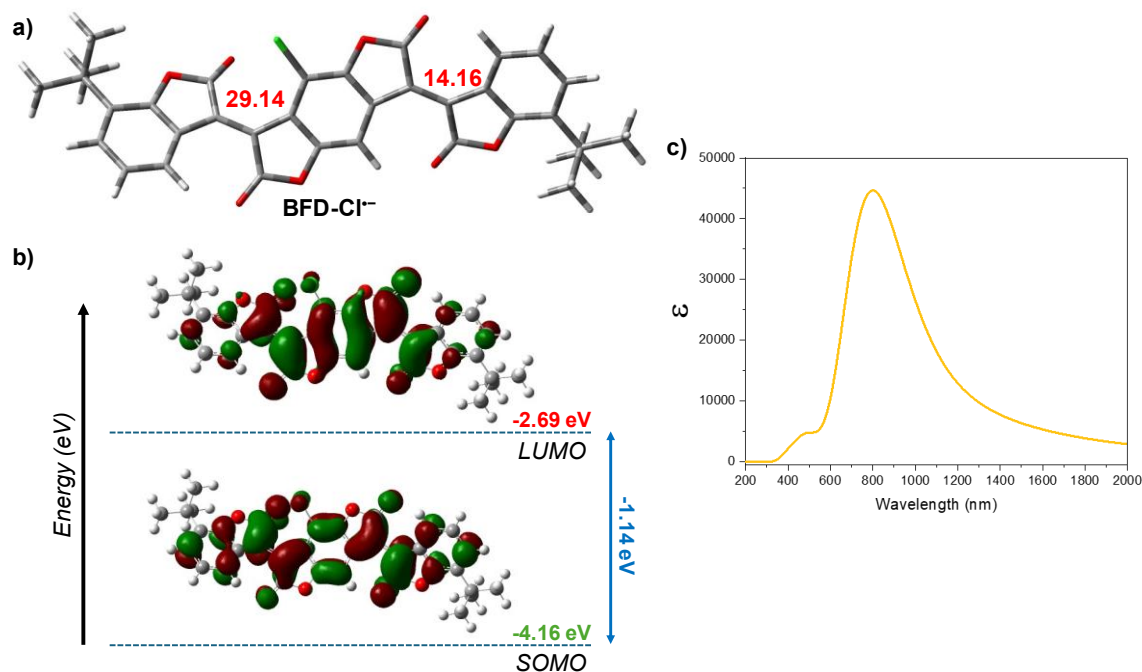


Figure S20. DFT calculated (a) molecular geometry & torsion angle (b) SOMO & LUMO energy levels and (c) simulated UV-Vis absorption of **BFD-Cl⁻**.

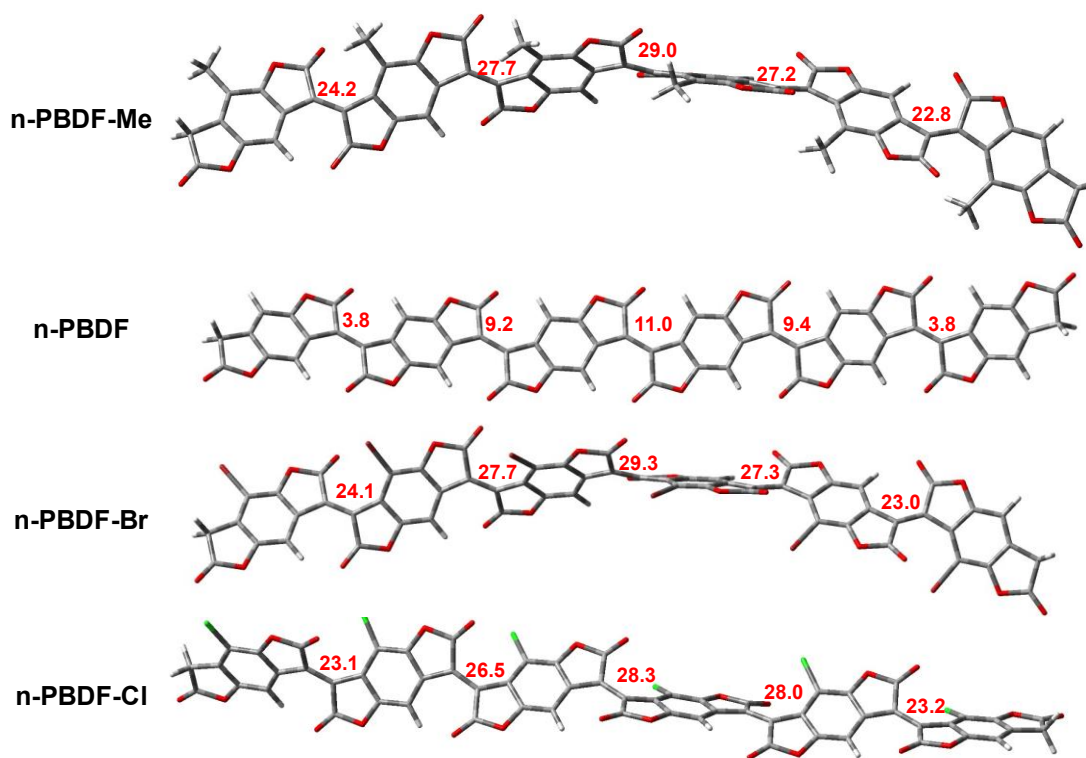


Figure S21. HOMO and LUMO frontier molecular orbitals of the **n-PBDF** derivatives with 6 repeating unit.

NMR Spectra

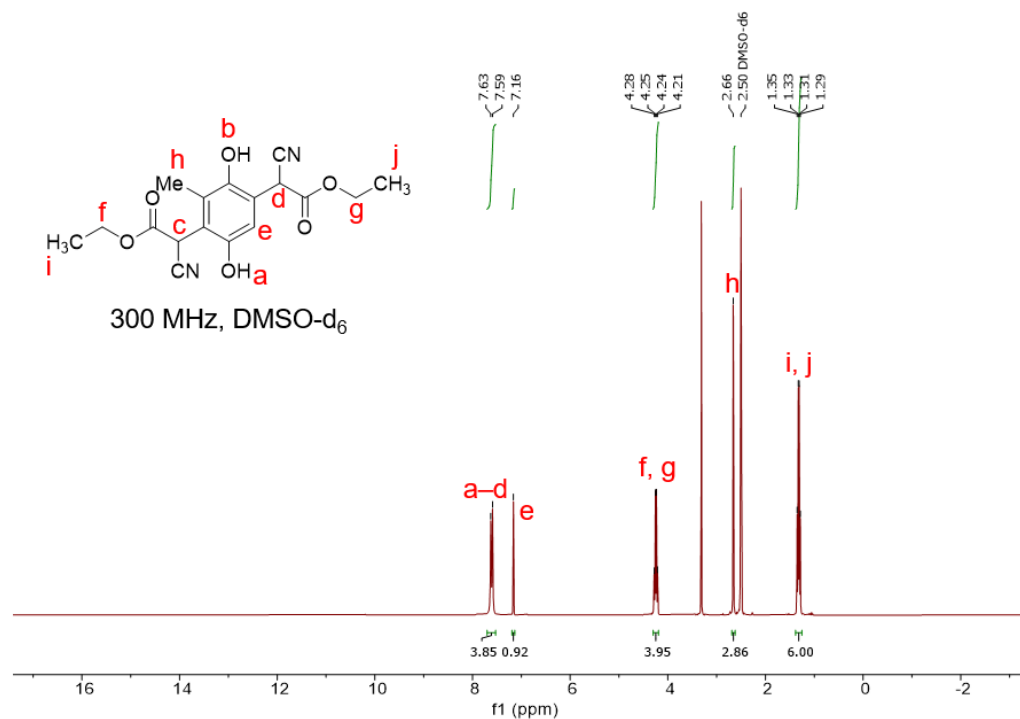


Figure S22. ¹H NMR of Diethyl 2,2'-(2-methyl-3,6-dihydroxy-5-methyl-1,4-phenylene)bis(2-cyanoacetate).

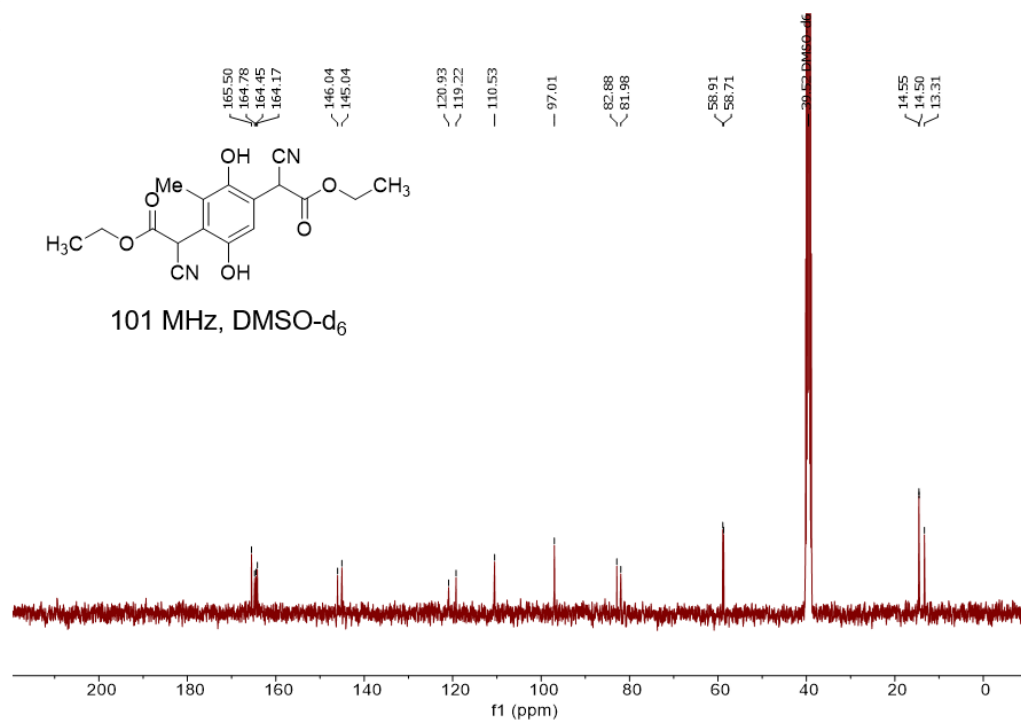


Figure S23. ¹³C NMR of Diethyl 2,2'-(2-methyl-3,6-dihydroxy-5-methyl-1,4-phenylene)bis(2-cyanoacetate).

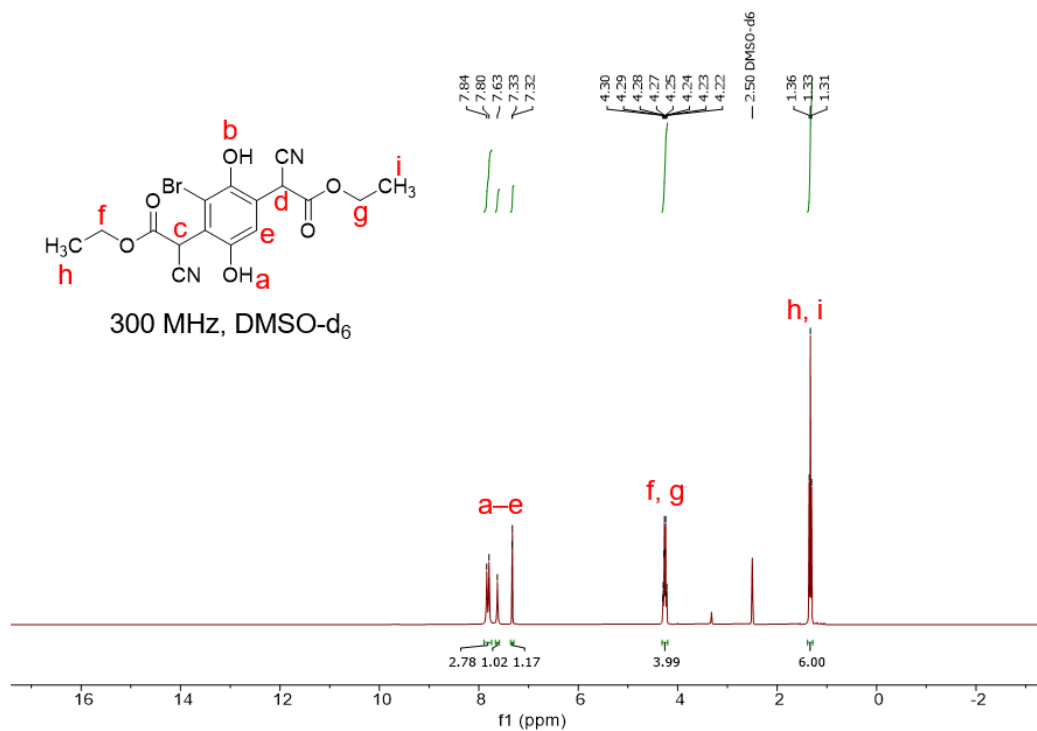


Figure S24. ¹H NMR of Diethyl 2,2'-(2-bromo-3,6-dihydroxy-5-methyl-1,4-phenylene)bis(2-cyanoacetate).

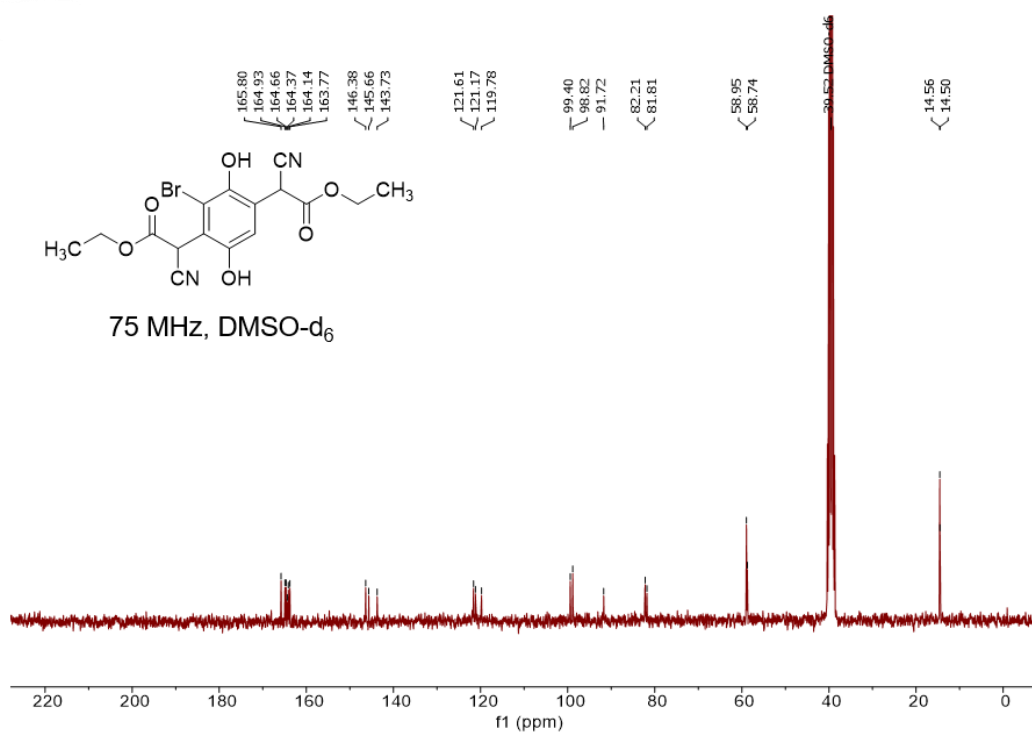


Figure S25. ¹³C NMR of Diethyl 2,2'-(2-bromo-3,6-dihydroxy-5-methyl-1,4-phenylene)bis(2-cyanoacetate).

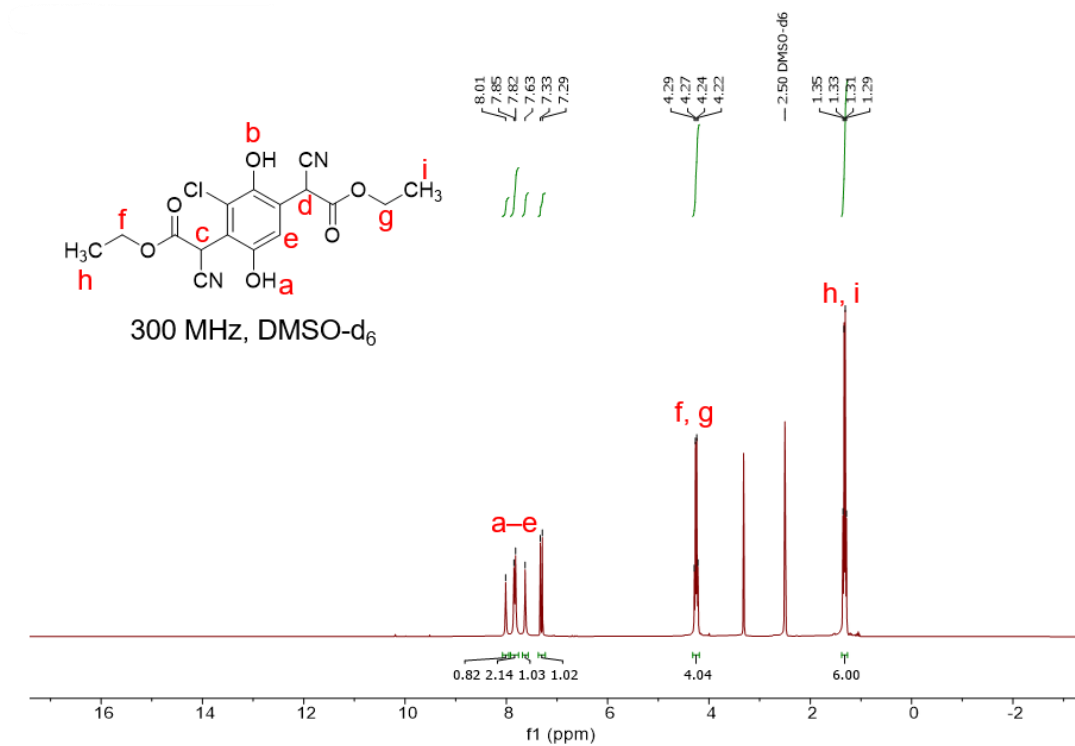


Figure S26. ¹H NMR of Diethyl 2,2'-(2-chloro-3,6-dihydroxy-5-methyl-1,4-phenylene)bis(2-cyanoacetate).

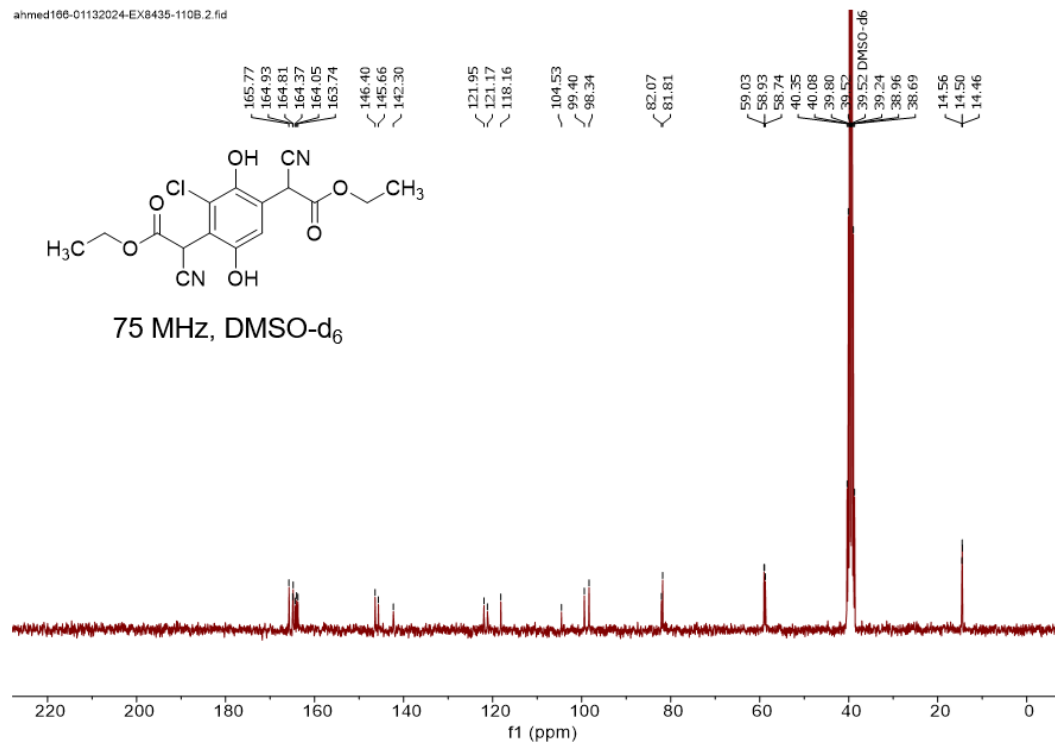


Figure S27. ¹³C NMR of Diethyl 2,2'-(2-chloro-3,6-dihydroxy-5-methyl-1,4-phenylene)bis(2-cyanoacetate).

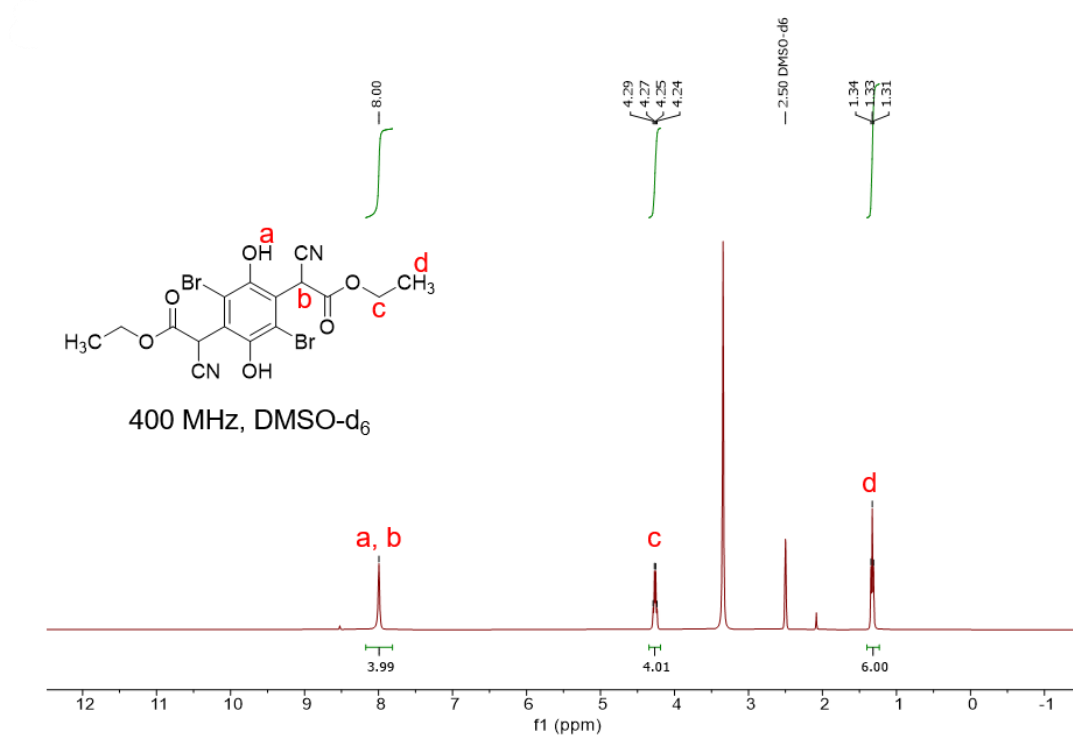


Figure S28. ¹H NMR of Diethyl 2,2'-(2,5-dibromo-3,6-dihydroxy-1,4-phenylene)bis(2-cyanoacetate).

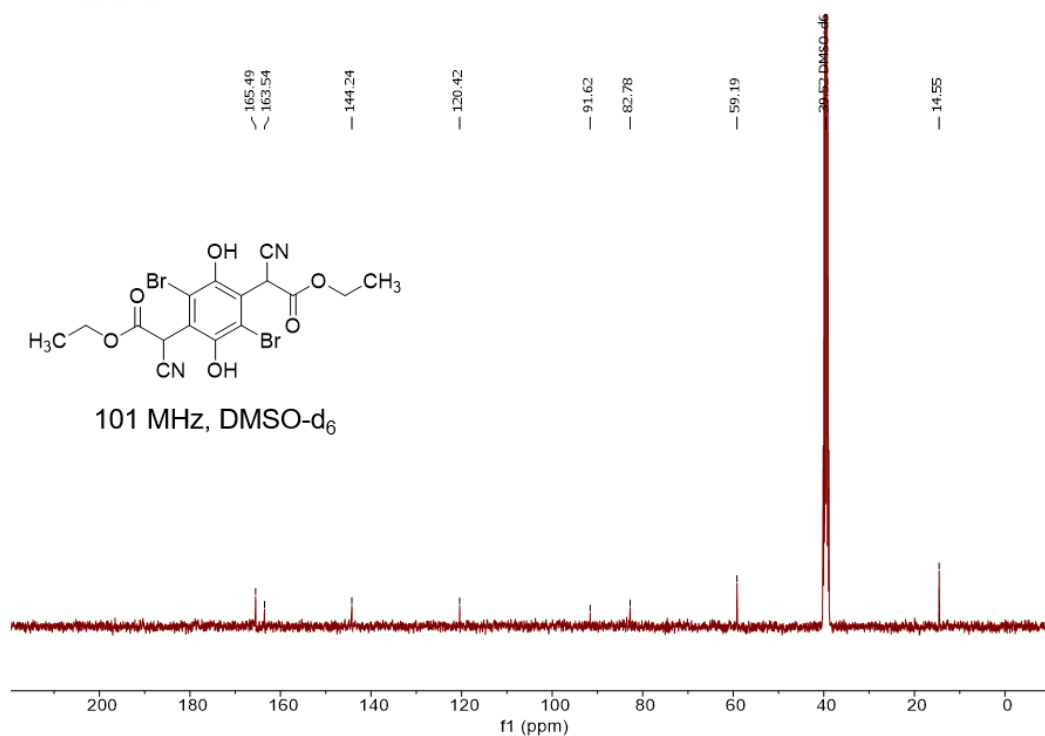


Figure S29. ¹³C NMR of Diethyl 2,2'-(2,5-dibromo-3,6-dihydroxy-1,4-phenylene)bis(2-cyanoacetate).

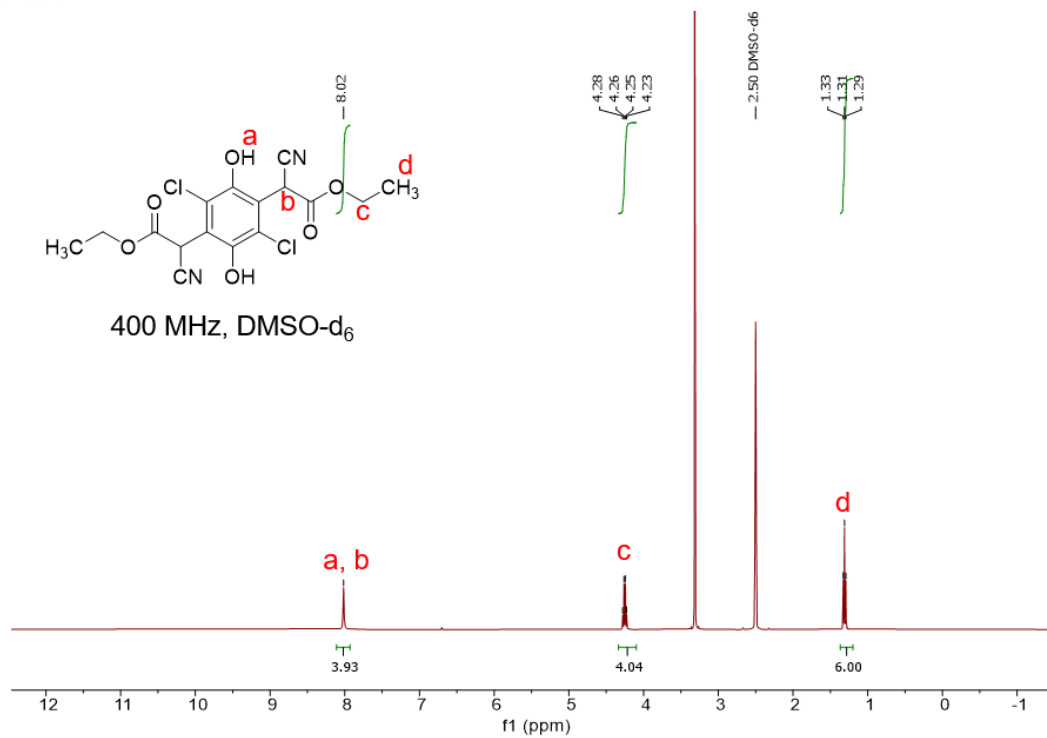


Figure S30. ¹H NMR of Diethyl 2,2'-(2,5-dichloro-3,6-dihydroxy-1,4-phenylene)bis(2-cyanoacetate).

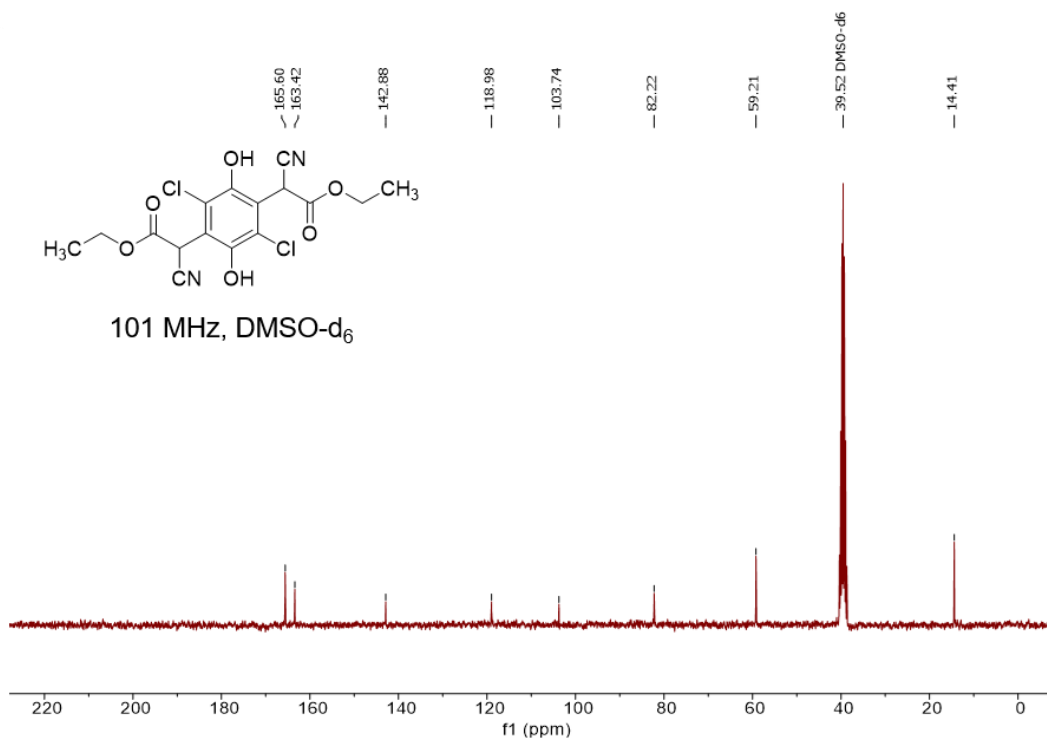


Figure S31. ¹³C NMR of Diethyl 2,2'-(2,5-dichloro-3,6-dihydroxy-1,4-phenylene)bis(2-cyanoacetate).

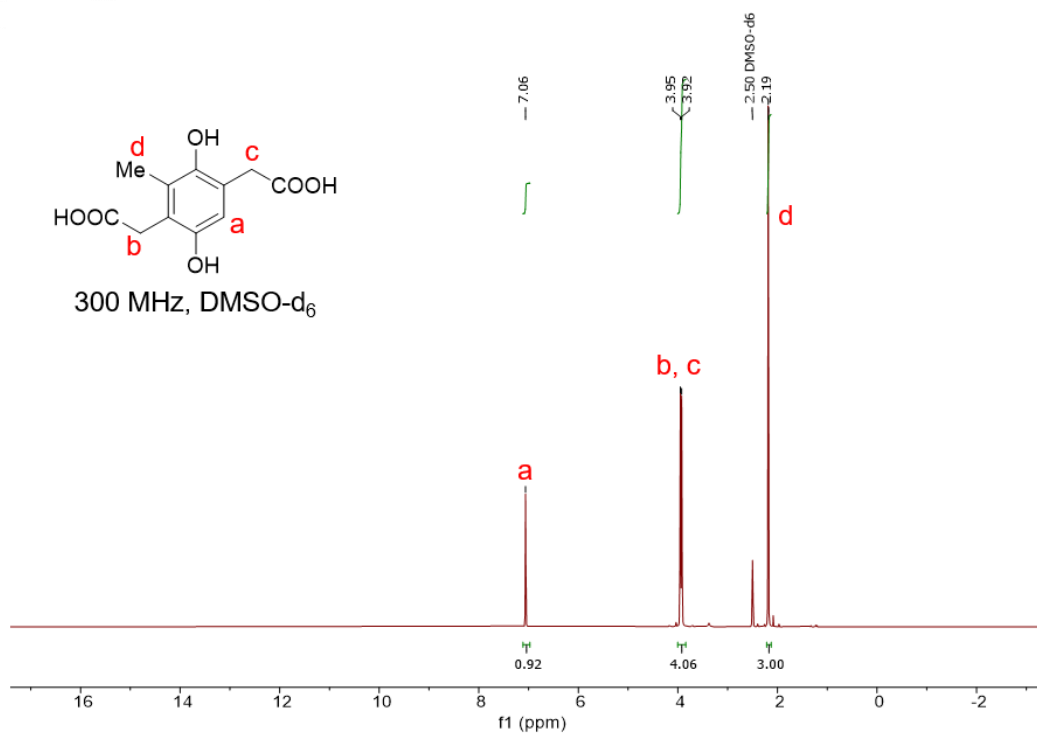


Figure S32. ¹H NMR of 2,2'-(2,5-dihydroxy-3-methyl-1,4-phenylene)diacetic acid.

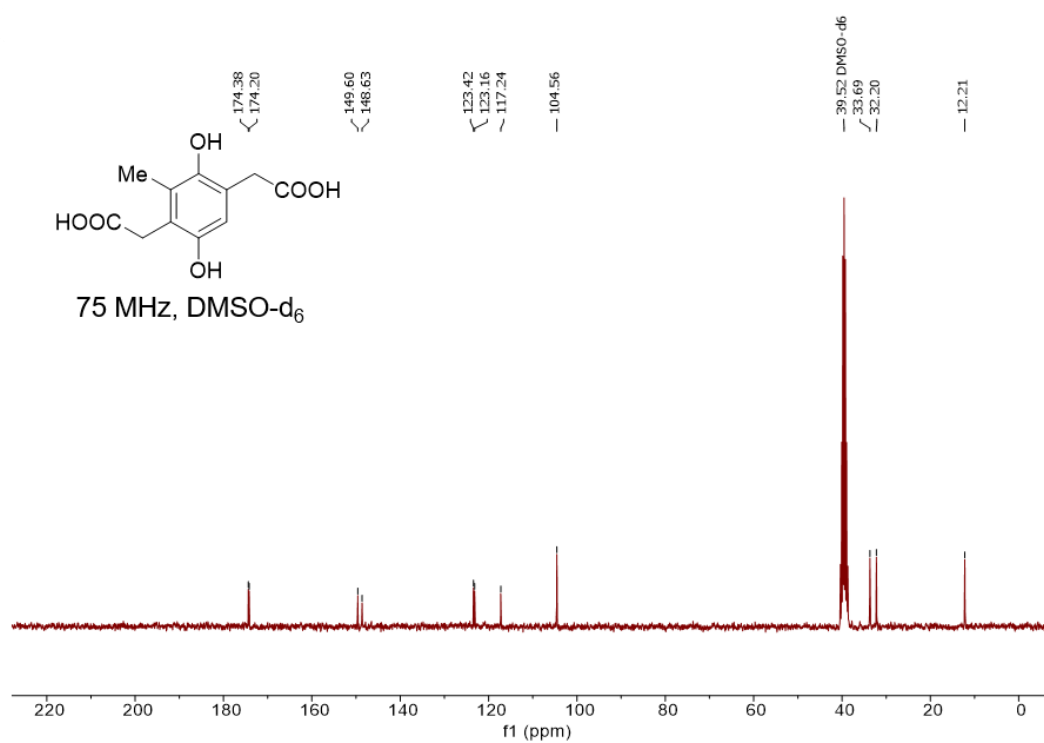


Figure S33. ¹³C NMR of 2,2'-(2,5-dihydroxy-3-methyl-1,4-phenylene)diacetic acid.

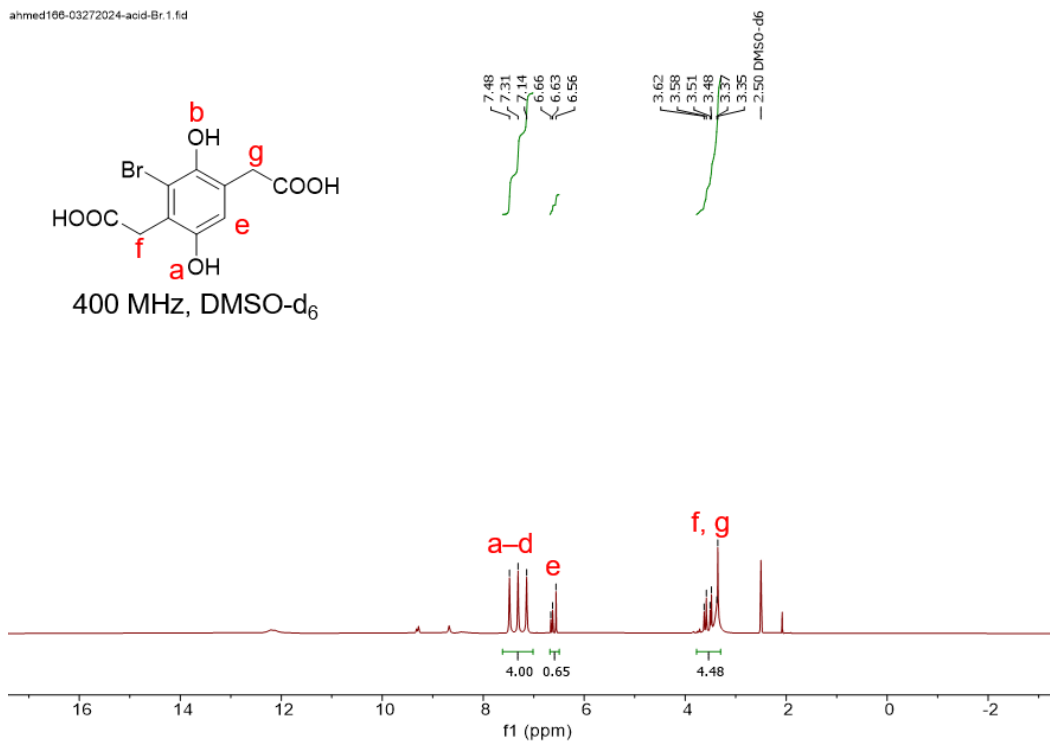


Figure S34. ¹H NMR of 2,2'-(3-bromo-2,5-dihydroxy-1,4-phenylene)diacetic acid,

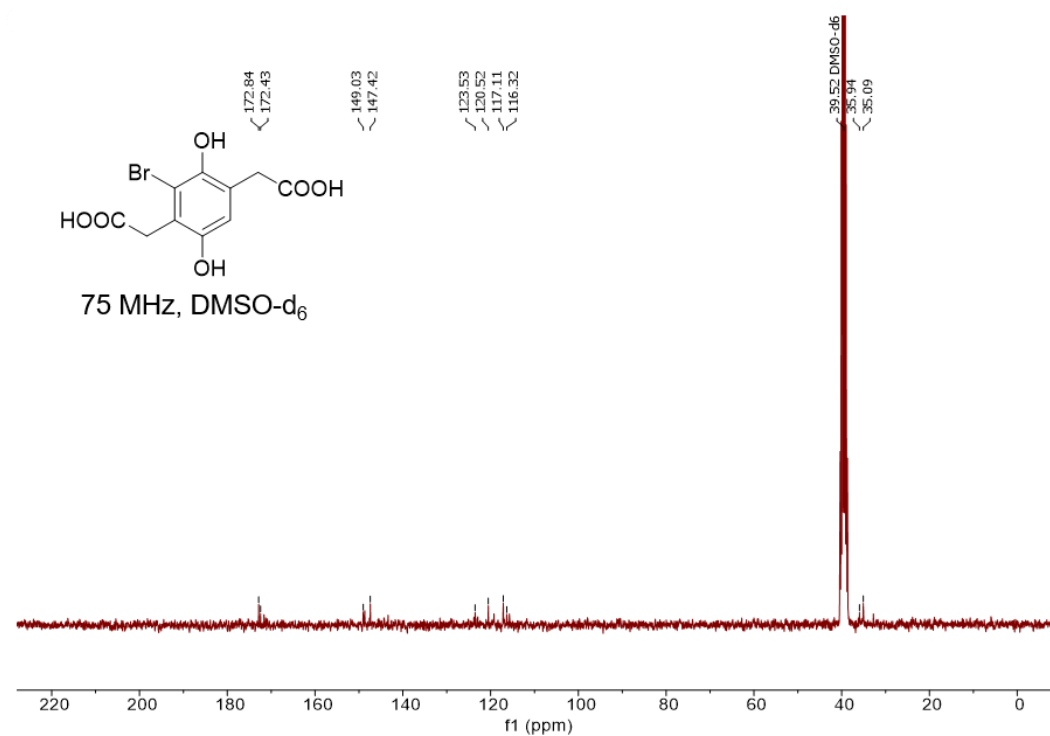


Figure S35. ¹³C NMR of 2,2'-(3-bromo-2,5-dihydroxy-1,4-phenylene)diacetic acid.

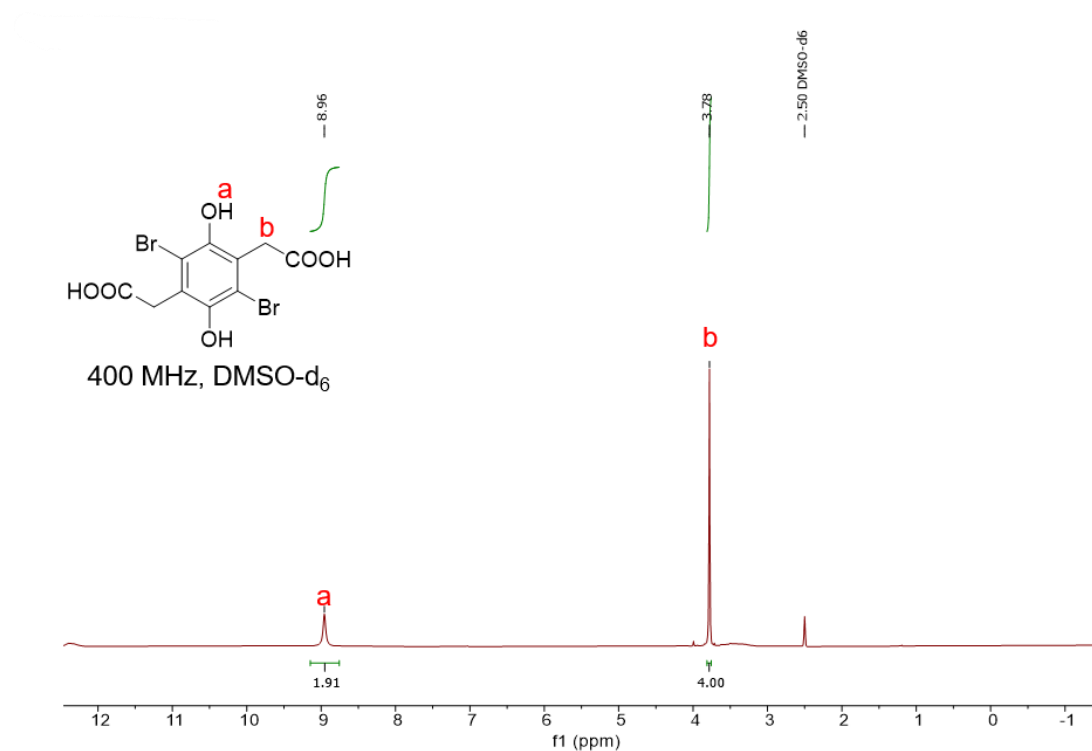


Figure S38. ¹H NMR of 2,2'-(2,5-dibromo-3,6-dihydroxy-1,4-phenylene)diacetic acid.

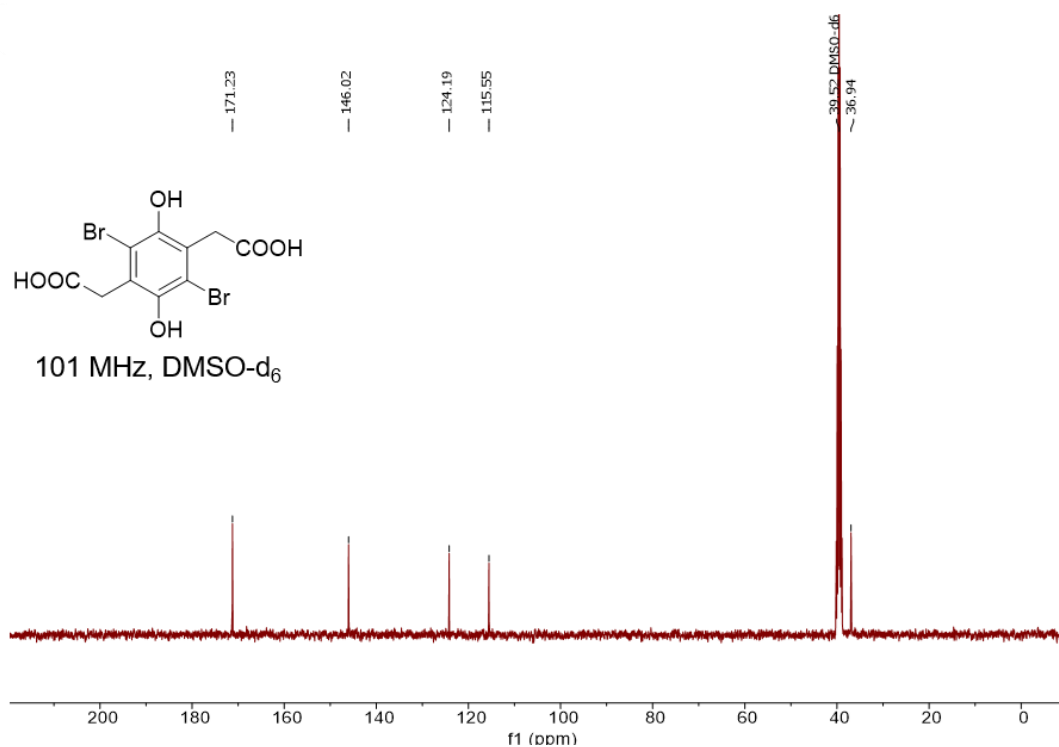


Figure S39. ¹³C NMR of 2,2'-(2,5-dibromo-3,6-dihydroxy-1,4-phenylene)diacetic acid.

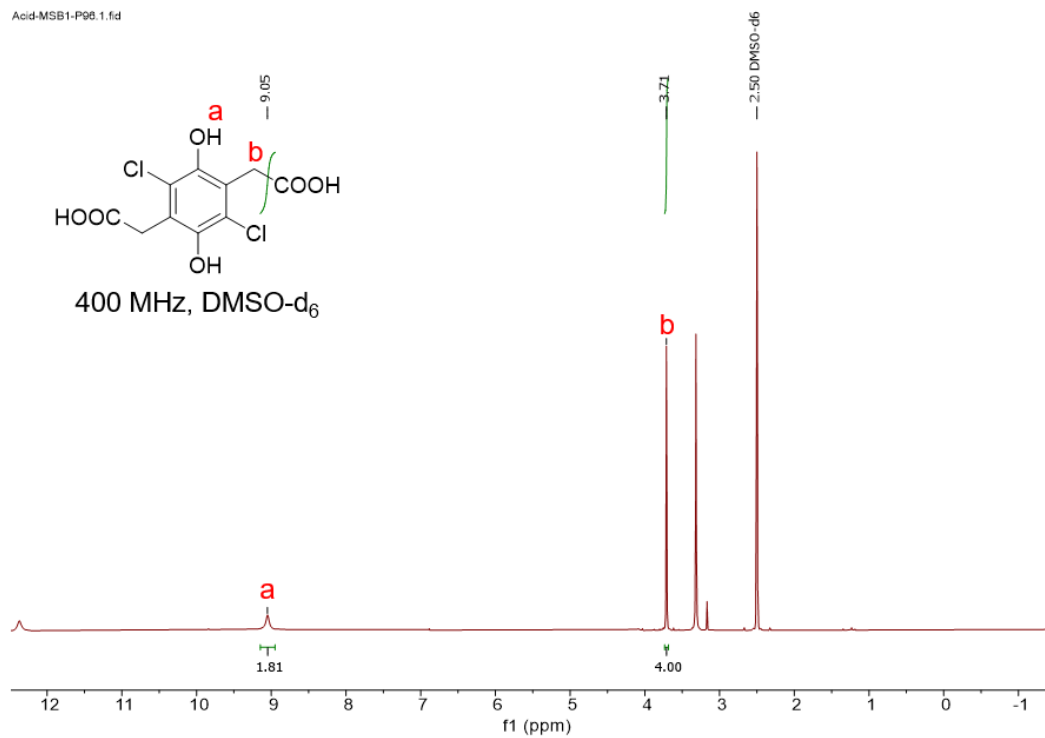


Figure S40. ¹H NMR of 2,2'-(2,5-dichloro-3,6-dihydroxy-1,4-phenylene)diacetic acid.

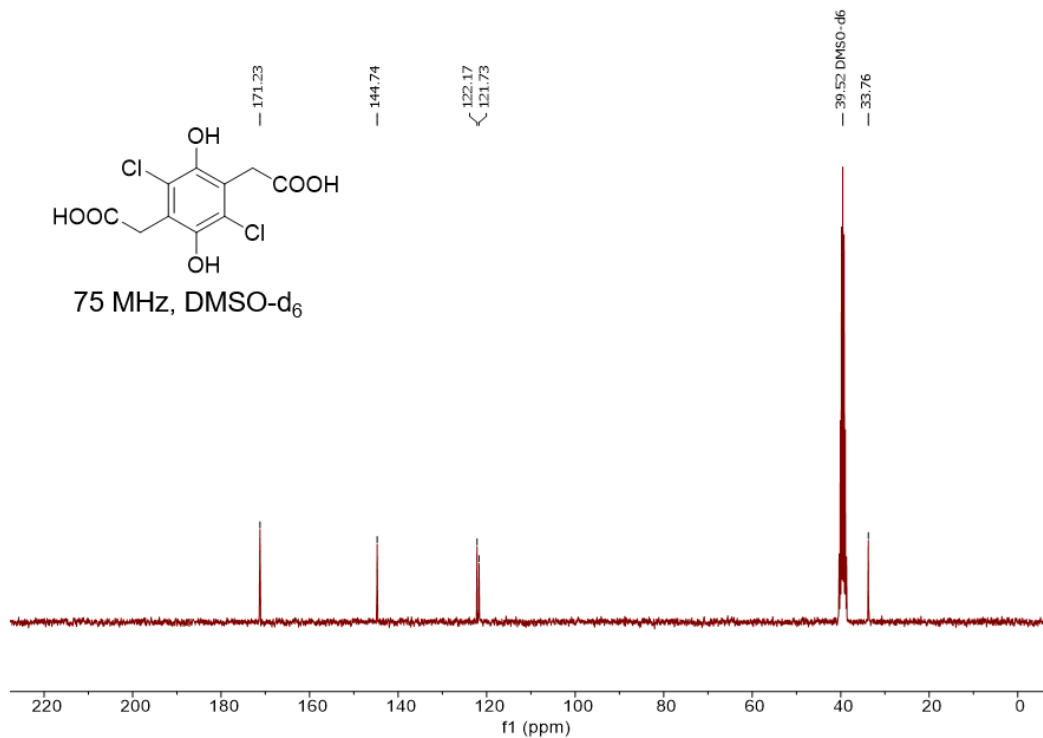


Figure S41. ¹³C NMR of 2,2'-(2,5-dichloro-3,6-dihydroxy-1,4-phenylene)diacetic acid.

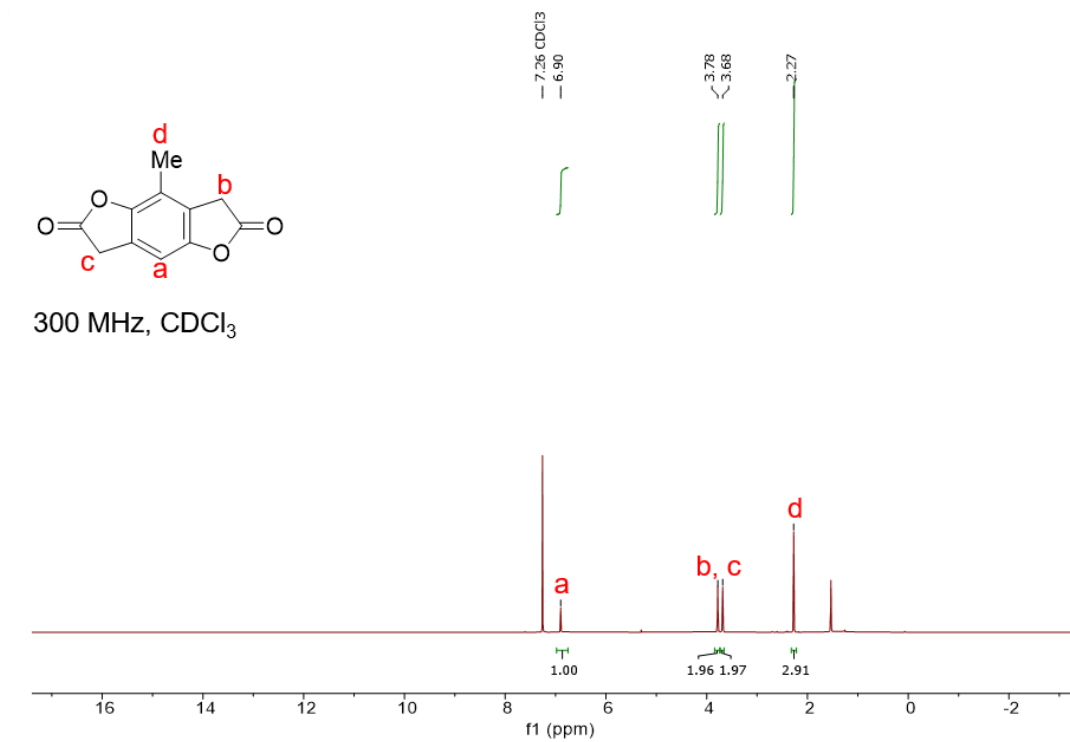


Figure S42. ¹H NMR of BDF-Me.

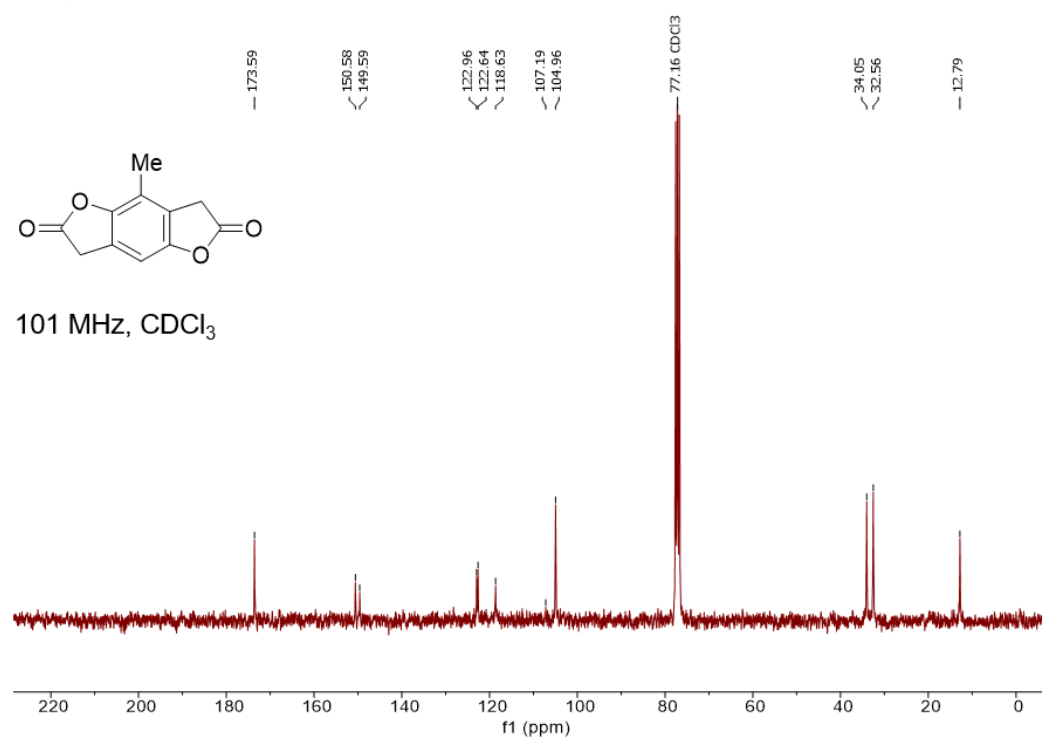


Figure S43. ¹³C NMR of BDF-Me.

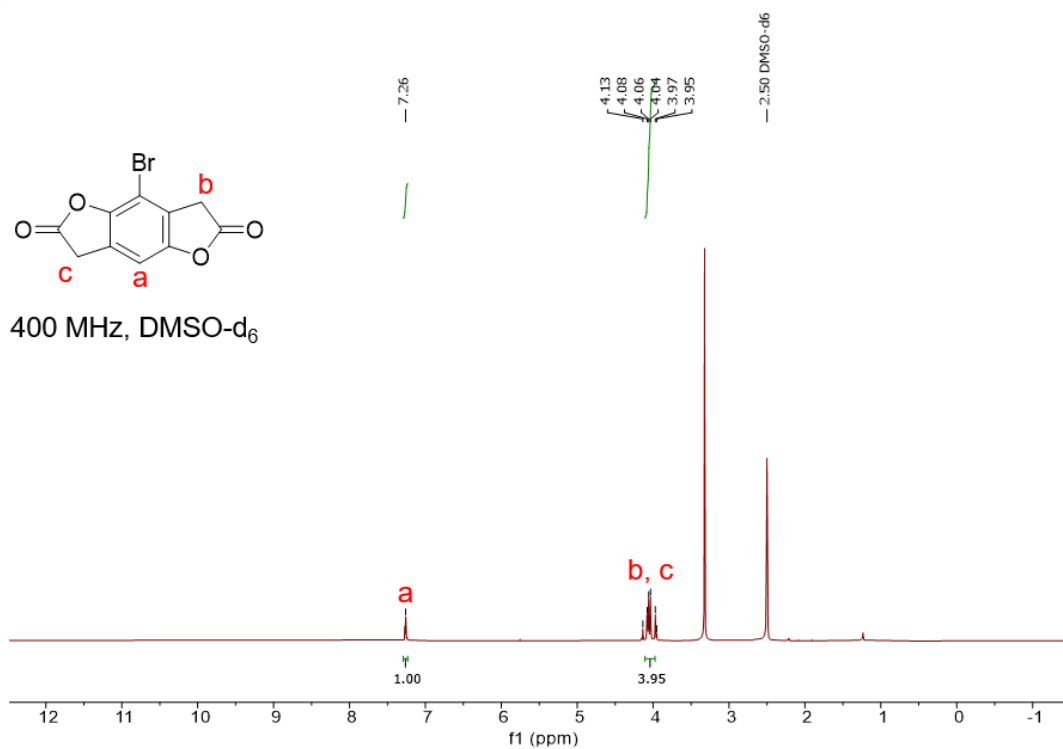


Figure S44. ¹H NMR of BDF-Br.

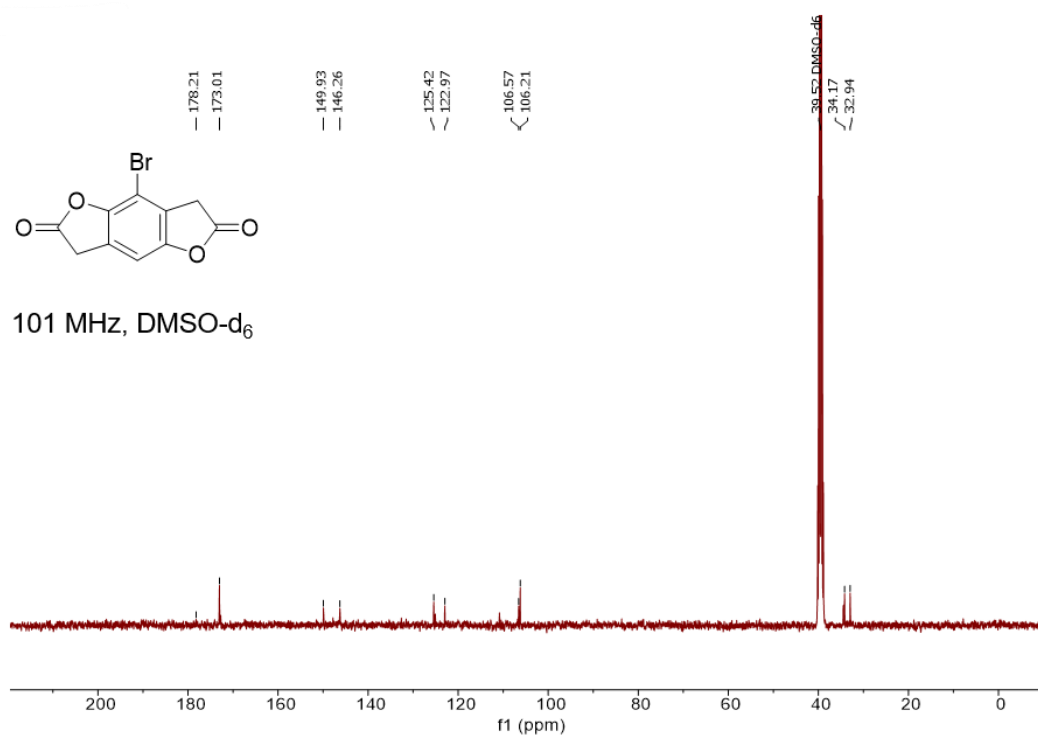


Figure S45. ¹³C NMR of BDF-Br.

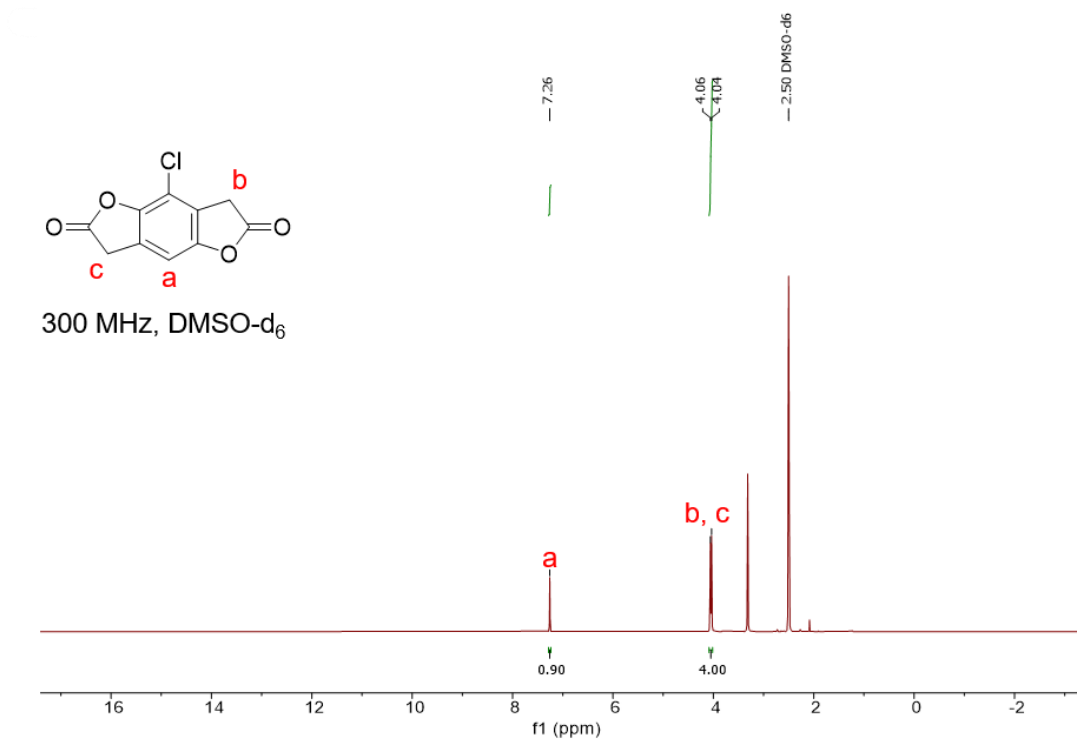


Figure S46. ¹H NMR of BDF-Cl.

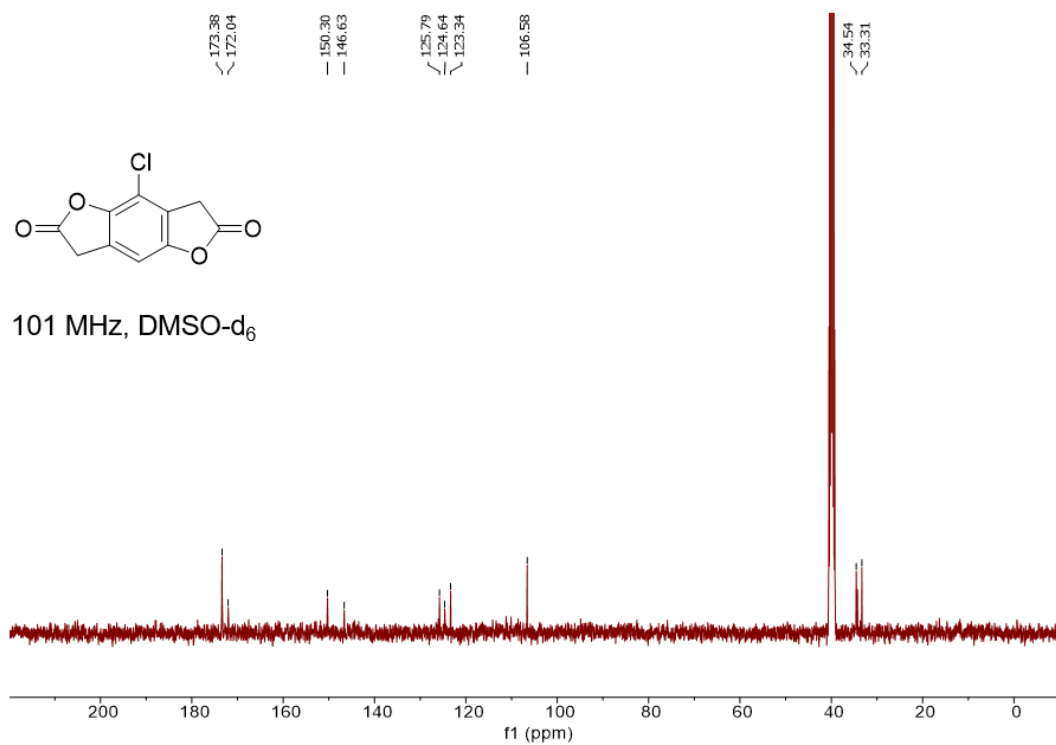


Figure S47. ¹³C NMR of BDF-Cl.

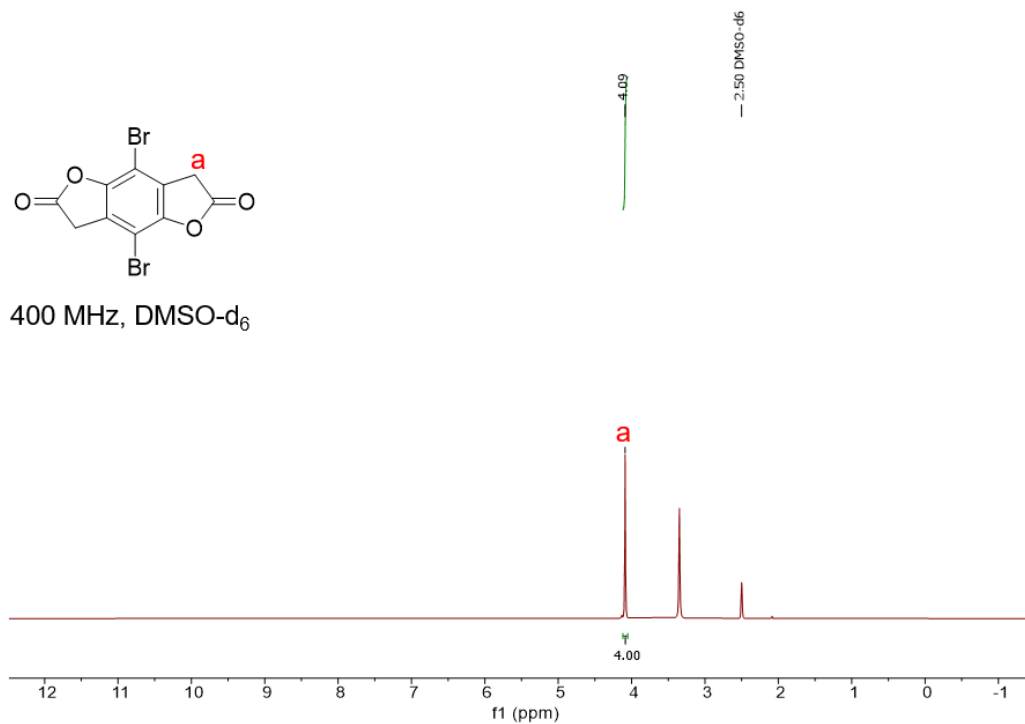


Figure S48. ¹H NMR of BDF-Br₂.

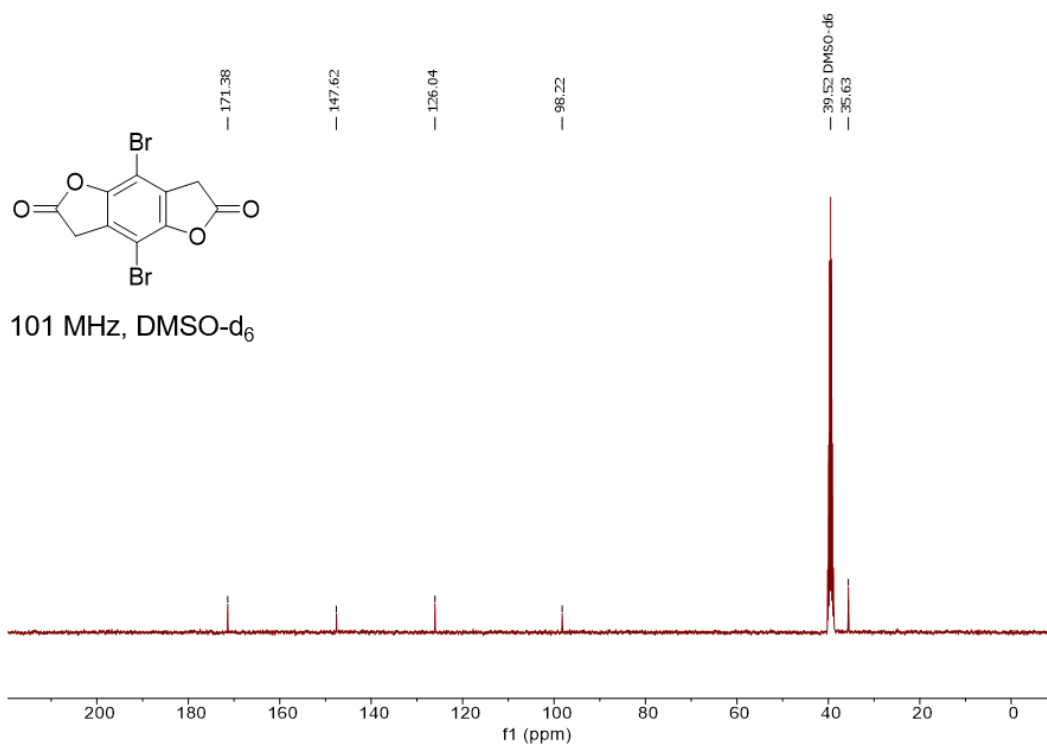


Figure S49. ¹³C NMR of BDF-Br₂.

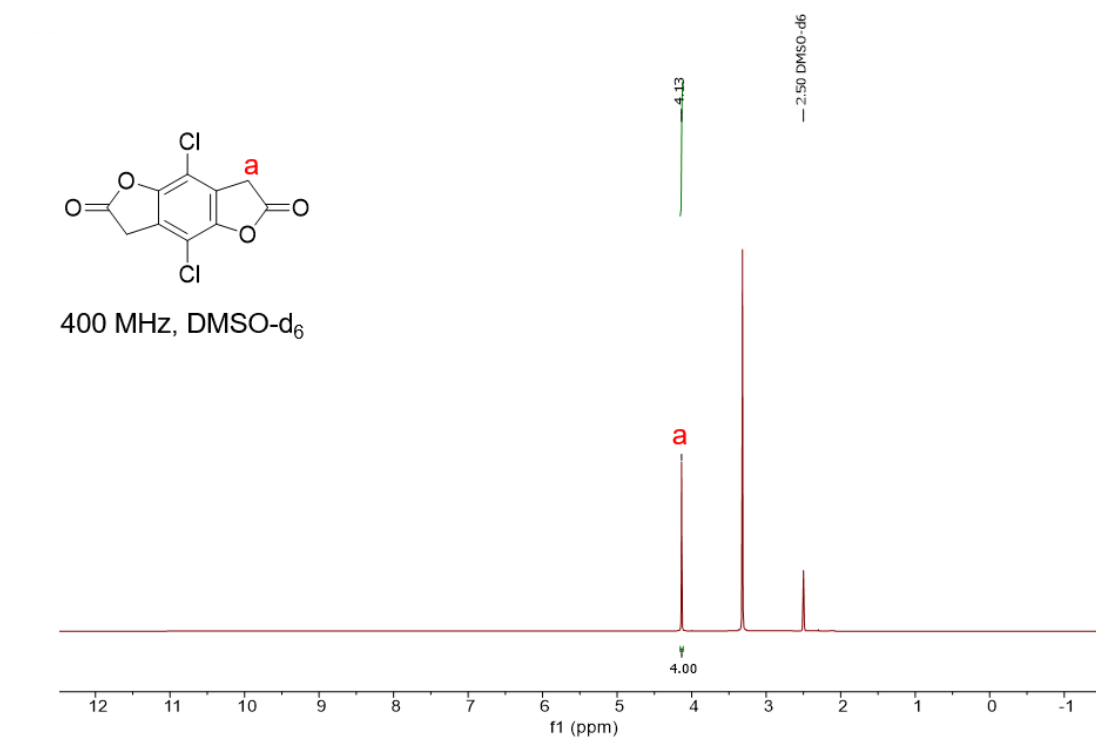


Figure S50. ¹H NMR of BDF-Cl₂.

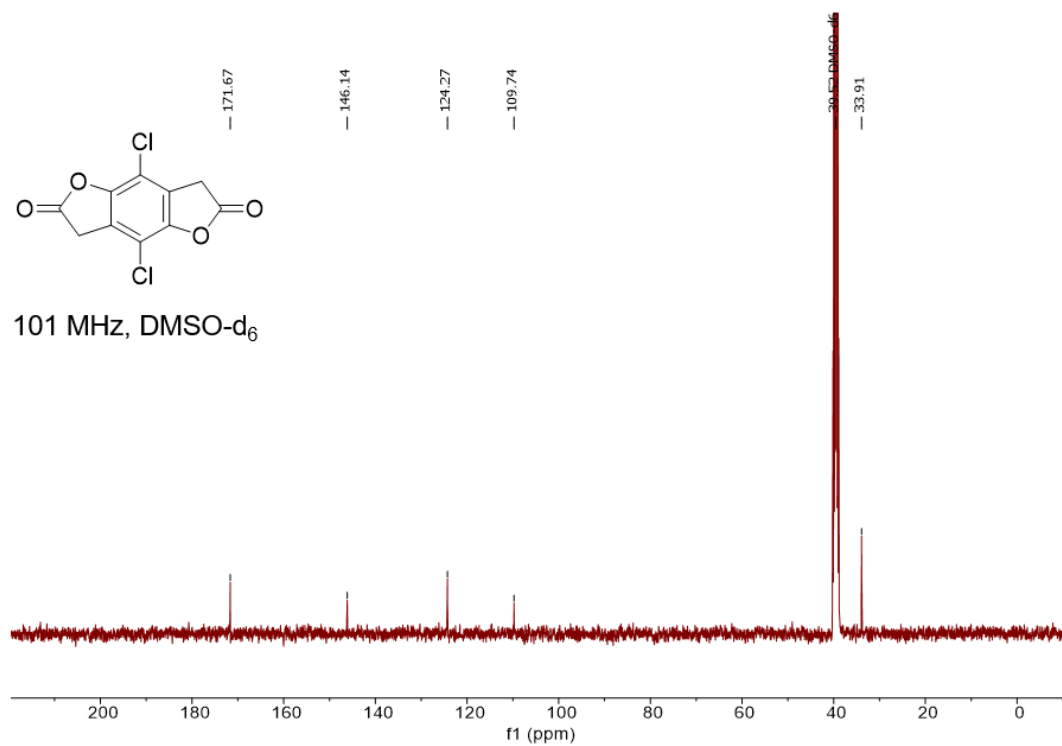


Figure S51. ¹³C NMR of BDF-Cl₂.

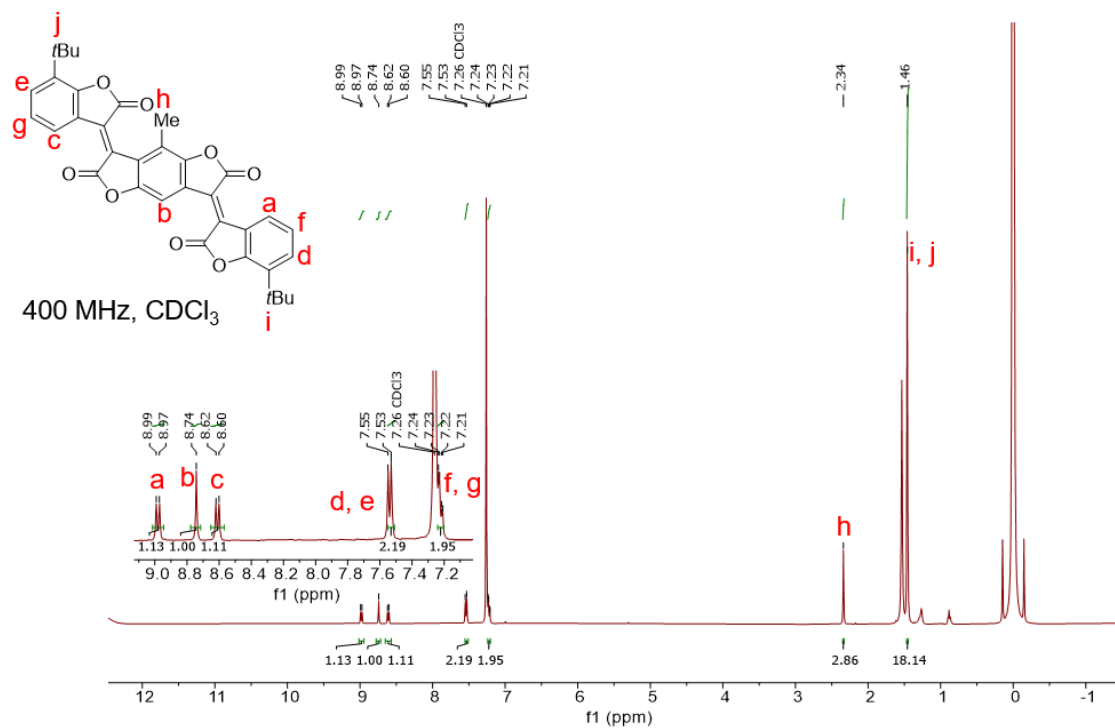


Figure S52. ¹H NMR of BFD-Me.

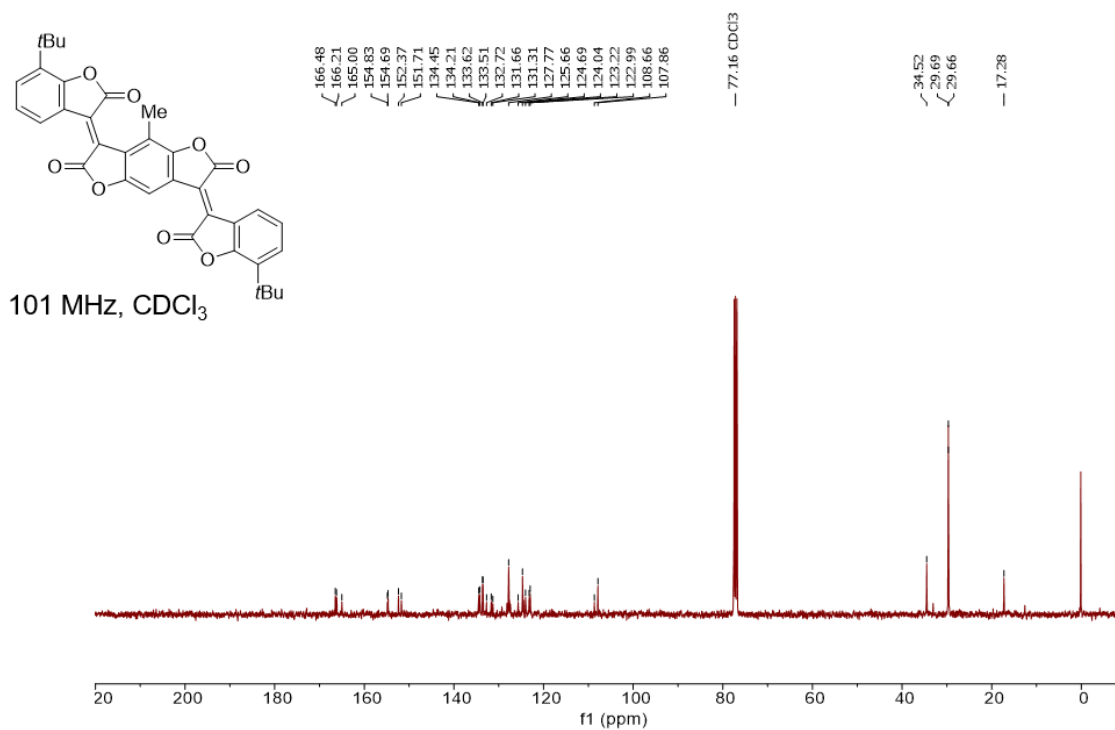


Figure S53. ¹³C NMR of BFD-Me.

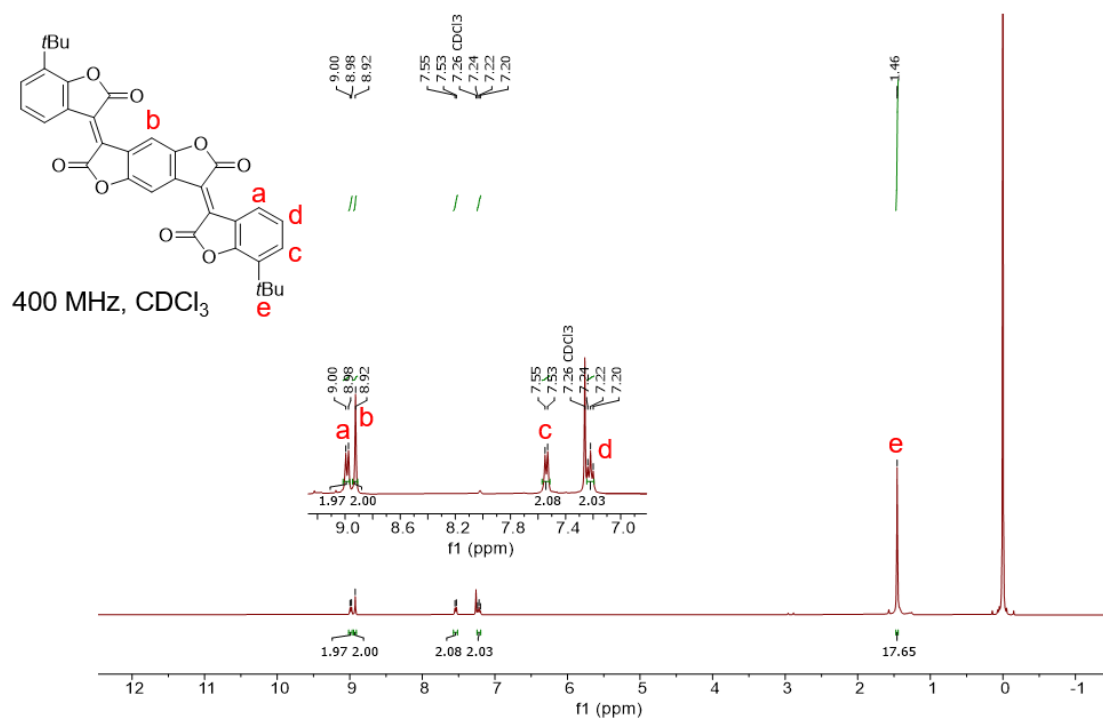


Figure S54. ¹H NMR of BFD.

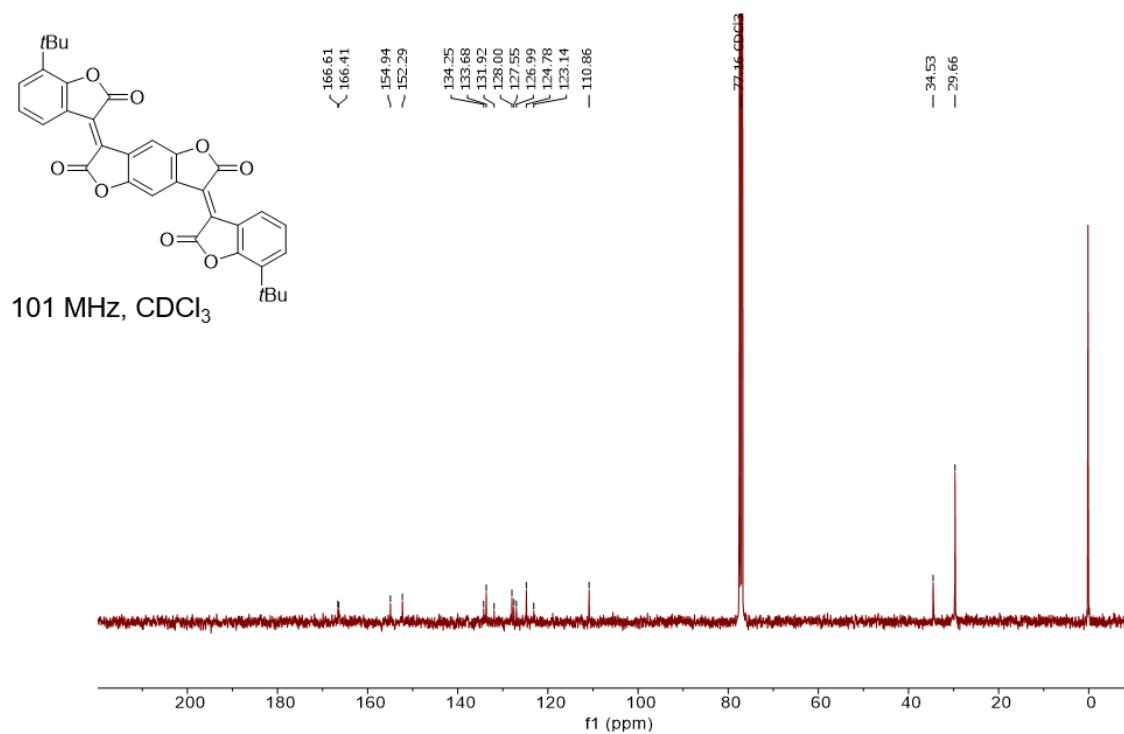


Figure S55. ¹³C NMR of BFD.

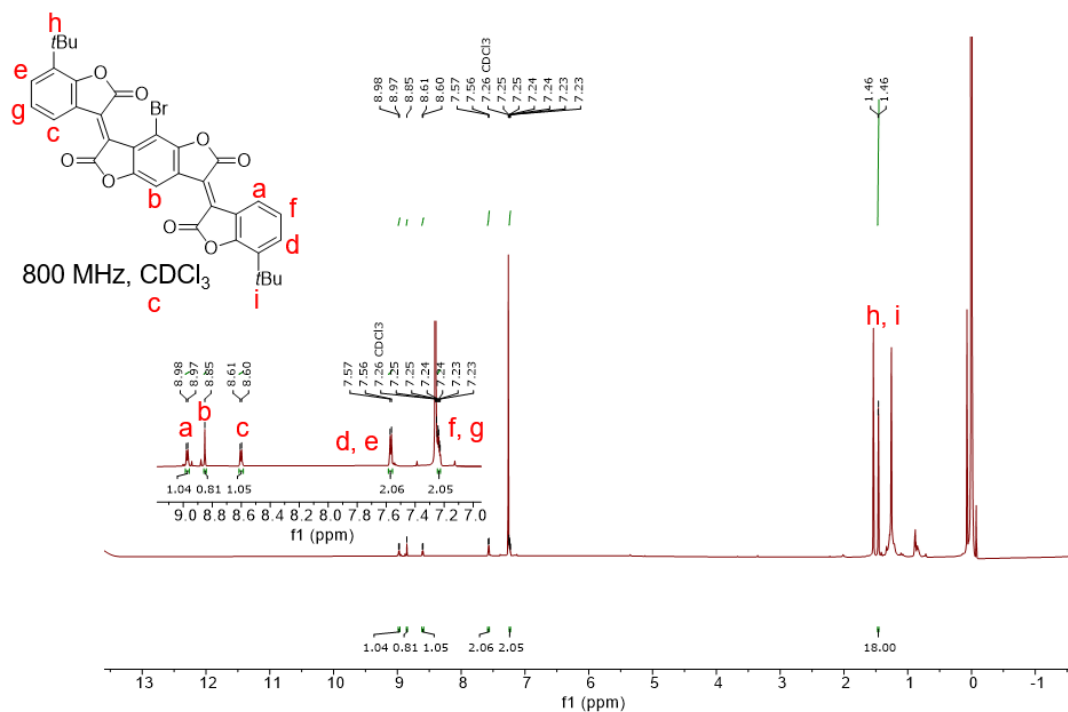


Figure S56. ¹H NMR of BFD-Br.

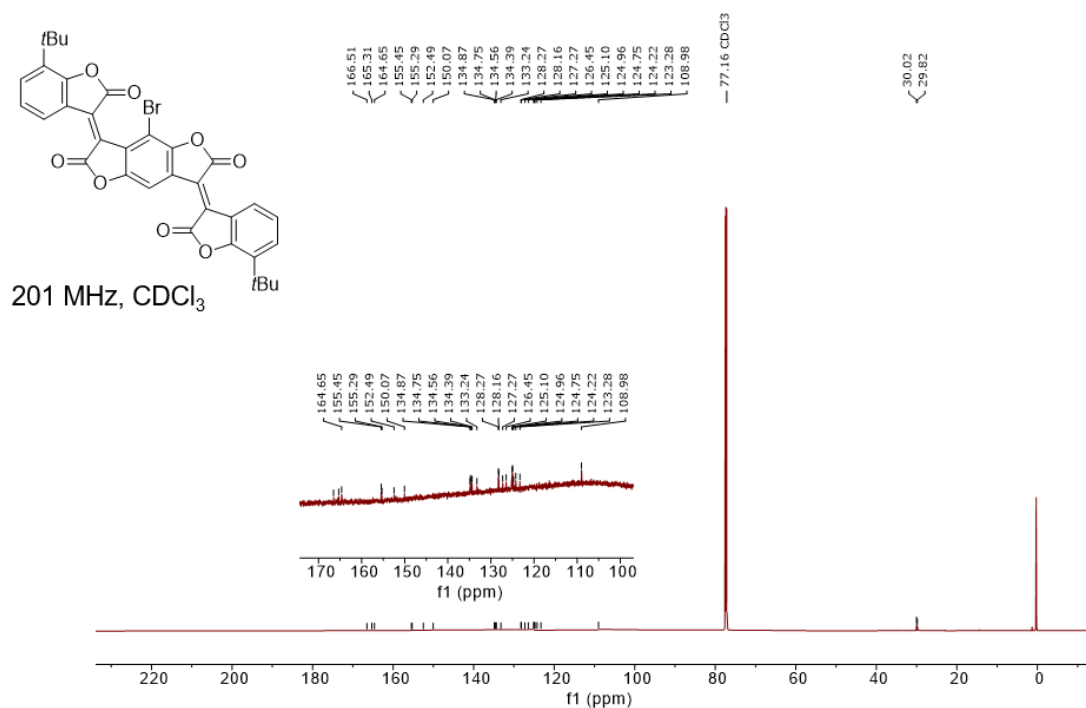
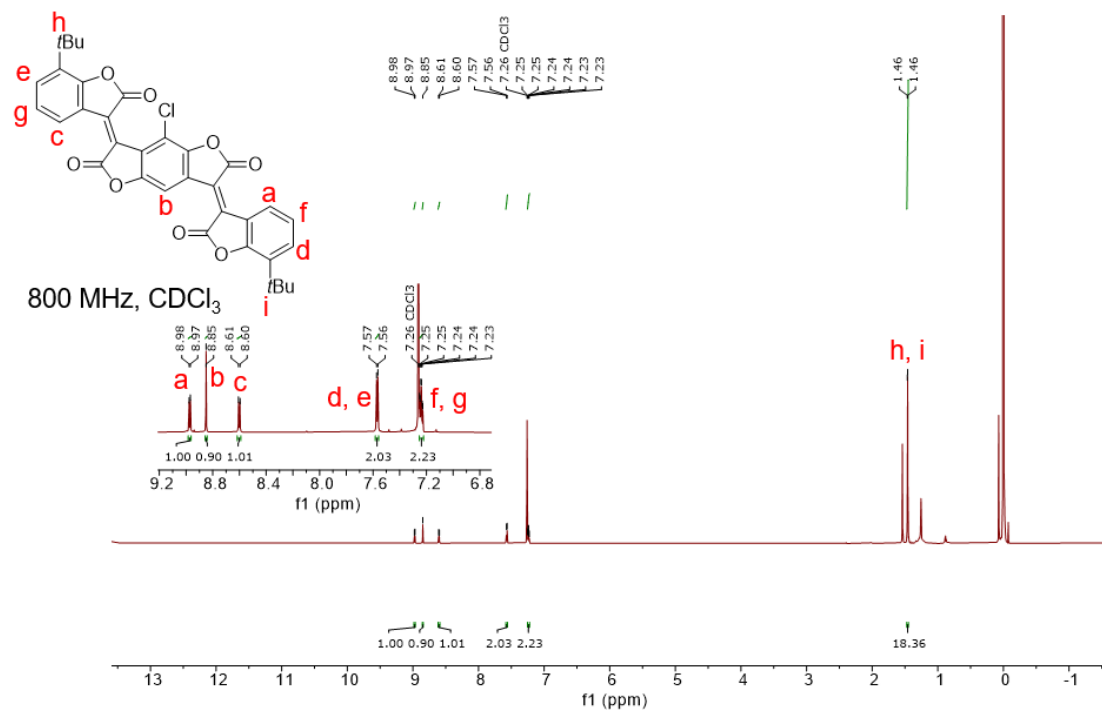
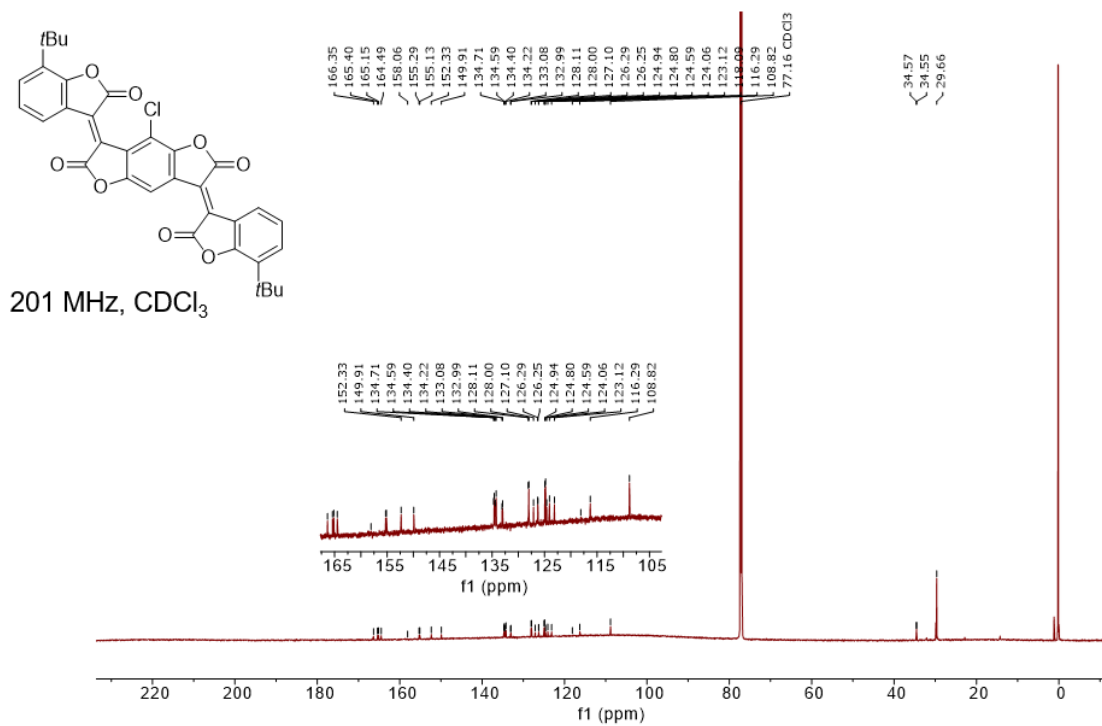


Figure S57. ¹³C NMR of BFD-Br.

Figure S58. ¹H NMR of BFD-Cl.Figure S59. ¹³C NMR of BFD-Cl.

X-Ray Diffraction Data

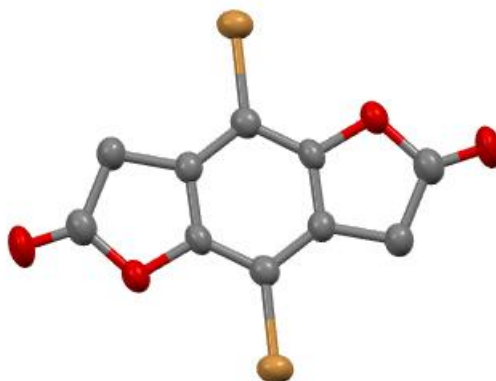


Figure S60. Displacement ellipsoid view of **BDF-Br₂**; hydrogen atoms omitted for clarity.

Table S8. Crystal Data for **BDF-Br₂**.

Crystal Data	
Chemical Formula	C ₁₀ H ₄ Br ₂ O ₄
Moiety Formula	C ₁₀ H ₄ Br ₂ O ₄
<i>M_r</i>	347.93
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ /c
Temperature (K)	265
<i>a</i> , <i>b</i> , <i>c</i> (Å)	10.8332(5), 5.5820(2), 17.3581(7)
α , β , γ (°)	90, 102.776(3), 90
<i>V</i> (Å ³)	1023.67(7)
<i>Z</i>	4
Radiation Type	Cu <i>K</i> α
μ (mm ⁻¹)	10.049
Crystal Size (mm)	0.123 × 0.095 × 0.007
Data Collection	
Diffractometer	Bruker AXS D8 Quest three circle diffractometer
Absorption Correction	multi-scan
<i>T_{min}</i> , <i>T_{max}</i>	0.507, 0.754
No. of measured, independent, and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	9857, 2003, 1688
<i>R_{int}</i>	0.0532
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.0451, 0.0960, 1.053
No. of reflections	2003
No. of parameters	145
No. of restraints	0
H-atom treatment	H-atom parameters constrained
	$w = 1/[\sigma^2(F_o^2) + (0.0418P)^2 + 1.893P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.676, -0.772
CCDC	2362078

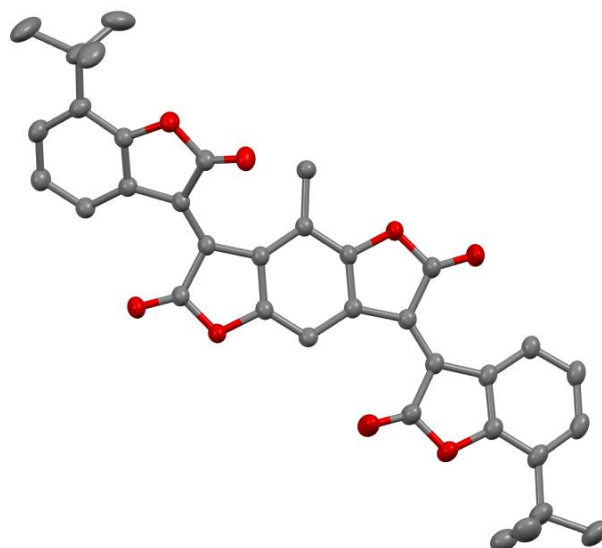


Figure S61. Displacement ellipsoid view of **BFD-Me**; hydrogen atoms omitted for clarity.

Table S9. Crystal Data for **BFD-Me**.

Crystal Data	
Chemical Formula	C ₃₅ H ₂₈ O ₈
Moiety Formula	C ₃₅ H ₂₈ O ₈
<i>M</i> _r	606.39
Crystal system, space group	Triclinic, <i>P</i> -1
Temperature (K)	150
<i>a</i> , <i>b</i> , <i>c</i> (Å)	10.1103(4), 14.9468(5), 30.9309(11)
α , β , γ (°)	96.8940(18), 91.0606(19), 98.8939(18)
<i>V</i> (Å ³)	4581.3(3)
<i>Z</i>	6
Radiation Type	Cu <i>K</i> α
μ (mm ⁻¹)	0.829
Crystal Size (mm)	0.23 × 0.18 × 0.04
Data Collection	
Diffractometer	Bruker AXS D8 Quest three circle diffractometer
Absorption Correction	multi-scan
<i>T</i> _{min} , <i>T</i> _{max}	0.6013, 0.7543
No. of measured, independent, and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	152538, 19841, 16442
<i>R</i> _{int}	0.0588
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.0581, 0.1369, 1.037
No. of reflections	19841
No. of parameters	1790
No. of restraints	2443
H-atom treatment	H-atom parameters constrained
	$w = 1/[\sigma^2(F_o^2) + (0.0698P)^2 + 1.5962P]$ where $P = (F_o^2 + 2F_c^2)/3$
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.449, -0.404
CCDC	2362079

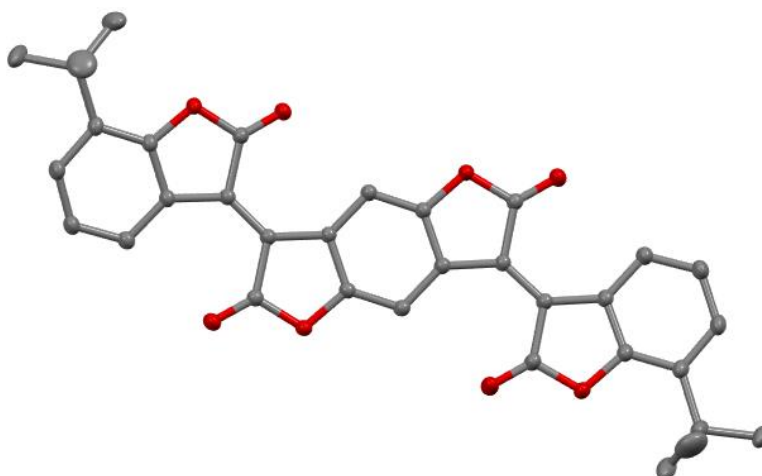


Figure S62. Displacement ellipsoid view of **BFD**; hydrogen atoms omitted for clarity.

Table S10. Crystal Data for **BFD**.

Crystal Data	
Chemical Formula	C ₃₄ H ₂₆ O ₈
Moiety Formula	C ₃₄ H ₂₆ O ₈
<i>M</i> _r	562.55
Crystal system, space group	Triclinic, <i>P</i> -1
Temperature (K)	150
<i>a</i> , <i>b</i> , <i>c</i> (Å)	5.9928(4), 10.6896(7), 21.0327(13)
α , β , γ (°)	77.706(2), 86.317(2), 85.385(2)
<i>V</i> (Å ³)	1310.67(15)
<i>Z</i>	2
Radiation Type	Mo <i>K</i> α
μ (mm ⁻¹)	0.102
Crystal Size (mm)	0.43 × 0.26 × 0.04
Data Collection	
Diffractometer	Bruker AXS D8 Quest three circle diffractometer
Absorption Correction	multi-scan
<i>T</i> _{min} , <i>T</i> _{max}	0.6879, 0.7645
No. of measured, independent, and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	43233, 10062, 7543
<i>R</i> _{int}	0.0342
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.0671, 0.1360, 1.017
No. of reflections	10062
No. of parameters	385
No. of restraints	0
H-atom treatment	H-atom parameters constrained
	$w = 1/[\sigma^2(F_o^2) + (0.0669P)^2 + 0.3499P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.498, -0.285
CCDC	2362080

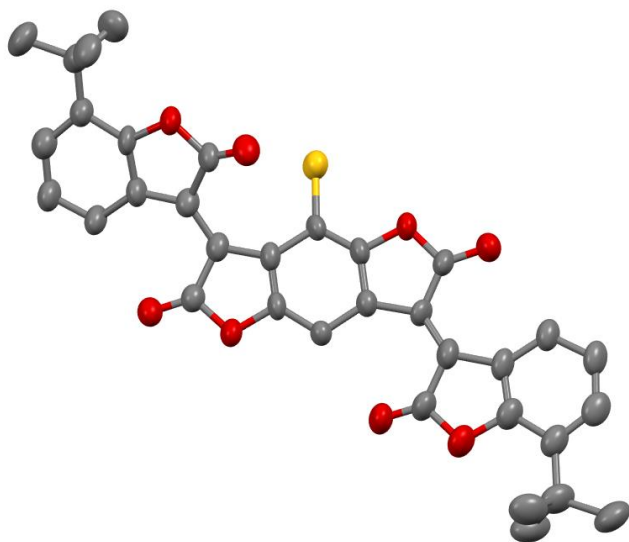


Figure S63. Displacement ellipsoid view of **BFD-Cl**; hydrogen atoms omitted for clarity.

Table S11. Crystal Data for **BFD-Cl**.

Crystal Data	
Chemical Formula	C ₃₄ H ₂₅ ClO ₈
Moiety Formula	C ₃₄ H ₂₅ ClO ₈
<i>M</i> _r	596.99
Crystal system, space group	triclinic, <i>P</i> 1
Temperature (K)	150
<i>a</i> , <i>b</i> , <i>c</i> (Å)	10.1307 (17), 14.987 (2), 15.937 (4)
α , β , γ (°)	98.998 (13), 93.872 (15), 96.733 (11)
<i>V</i> (Å ³)	2364.3 (8)
<i>Z</i>	3
Radiation Type	Cu <i>K</i> α
μ (mm ⁻¹)	1.490
Crystal Size (mm)	0.14 × 0.07 × 0.008
Data Collection	
Diffractometer	Bruker AXS D8 Quest three circle diffractometer
Absorption Correction	multi-scan
<i>T</i> _{min} , <i>T</i> _{max}	0.4462, 0.7533
No. of measured, independent, and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	39080, 16993, 6825
<i>R</i> _{int}	0.1797
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.2102, 0.3816, 0.987
No. of reflections	4991
No. of parameters	1181
No. of restraints	885
H-atom treatment	H-atom parameters constrained
	$w = 1/[\sigma^2(F_o^2) + (0.0822P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	1.019, -0.453
CCDC	2362081

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