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Enhancement of ambipolar charge transport for quinoidal bithiophene-diazaisoindigo-based donor–acceptor copolymers *via* fluorine substitution strategies

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General procedures and requirements

All chemicals were purchased from Innochem and Aladdin and used as received unless otherwise stated. The water- or air-sensitive reactions were performed using the Schlenk technique under an argon atmosphere with anhydrous solvents. Anhydrous tetrahydrofuran (THF) was obtained by distillation with sodium.

Instruments

^{1}H and ^{13}C nuclear magnetic resonance (NMR) spectra of all monomers were measured on Bruker-400 NMR spectrometer at 400 and 101 MHz, respectively, in 1,1,2,2-tetrachloroethane-d$_2$ ($CDCl_2CDCl_2$) at room temperature. ^{1}H NMR spectra of all polymers were measured on Bruker-500 NMR spectrometer at 500 MHz in $CDCl_2CDCl_2$ at 120 °C. Matrix-assisted laser desorption ionization time of-flight (MALDI-TOF) mass spectra were acquired on a 9.4T Solarix FT-ICR mass spectrometer. High-temperature gel permeation chromatography (HT-GPC) analysis was conducted on a PL-GPC 220 system using polystyrenes as the standards and 1,2,4-trichlorobenzene as the eluent, respectively. The UV−vis−NIR absorption spectra of all polymers were collected on a Hitachi U-3010 spectrophotometer. The optical bandgaps were calculated from the absorption onset of thin films according to the equation: $E_g^{opt} = 1240/\lambda_{onset}\, eV$. Cyclic voltammetry (CV) of all polymers were obtained on a CHI660c electrochemical analyser with a three-electrode cell at a scan rate of 50 m V^{-1} s^{-1} under an argon atmosphere. In the measuring process, 0.1 M *n*-Bu_4NPF_6 in dry acetonitrile, platinum stick, platinum and Ag/AgCl wire were adopted as supporting electrolyte, working electrode, counter electrode and reference electrode, respectively. The HOMO and LUMO energy levels were estimated by the equations: $E_{HOMO} =- \left(4.40 + E_{onset}^{ox}\right) eV$, $E_{LUMO} =- \left(4.40 + E_{onset}^{re}\right) eV$, where in E_{onset}^{ox} which and E_{onset}^{re} represent the oxidation and reduction onset-potentials of polymers versus

Fc/Fc$^+$, respectively. $E_g = -(E_{HOMO} - E_{LUMO})\ eV$. Thermogravimetric analysis (TGA) was conducted on a PerkinElmer series 7 thermal analysis system at a heating rate of 20 ℃ min^{-1} under nitrogen, and differential scanning calorimetry (DSC) analyses were carried out on a Mettler Toledo Instrument DSC822 calorimeter at a heating/cooling rate of 10 °C min^{-1} under nitrogen atmosphere. Atomic force microscopy (AFM) measurements were tested in a Digital Instruments Nanoscope V atomic force microscope operated ScanAsyst mode under ambient conditions. 2D grazing-incidence wide-angle X-ray scattering (2D-GIWAXS) were obtained at beamline BL14B1 of Shanghai Synchrotron Radiation Facility. The film samples are the same as those used in device performance analysis.

Device fabrication and characterization

Polyethylene terephthalate (PET) was used as the substrates of a top-gated bottom-contact (TGBC) organic field−effect transistor (OFET) devices. The substrates were washed by an ultrasonic cleaner with acetone, deionized water, and ethanol, and then dried under a nitrogen flow and heated at 120 °C for 10 min. Au (50 nm, Ti was used as an adhesive layer) was deposited on the silicon substrate as source and drain electrodes with $W/L = 47$ ($W = 1400\ \mu$m, $L = 30\ \mu$m). The active polymer layer was deposited by spin-coating a polymer solution in *o*-dichlorobenzene (*o*-DCB) (3.0 mg/mL) at a speed of 1200 rpm for 60 s followed by thermal annealing on a hotplate at 140 °C for 10 min. Afterward, the dielectric was spin coated from CYTOP (1:3) at a speed of 1500 rpm for 60 s followed by thermal annealing on a hotplate at 100 °C for 3 min. The AlO_x layer was formed by evaporation of 5 nm Al and oxidation of 1 h in air. Therewith, Polyvinyl alcohol (PVA) was spin coated at a speed of 1000 rpm for 60 s, and then annealed at 100 °C for 30 min. Finally, Al (70 nm) was vacuum-evaporated as the gate electrode.

All the spin coating processes were conducted in a glovebox and the evaluations of these OFET devices were accomplished using a Keithley 4200 SCS semiconductor parameter analyzer on a probe stage. The carrier mobility, μ, was calculated from the data in the saturated regime according to the following equation: $I_{DS} = (W/2L)C_i\mu(V_{GS} - V_{TH})^2$, where I_{DS} denotes the saturation drain current, W/L means the channel width/channel length, C_{i} refers to the capacitance per unit area of gate dielectric layer, V_{GS} is the gate voltage, and V_{TH} is the threshold voltage.

Materials and synthetic procedures

*(3Z,3'Z)-3,3'-((E)-5H,5'H-[2,2'-bithiophenylidene]-5,5'-diylidene)bis(6-bromo-1-(2-decyltetradecyl)-1,3-dihydro-2H-pyrrolo[2,3-b]pyridin-2-one) (**5a**)*. 2,2'-bithiophene (0.33g, 2 mmol), TMEAD (0.51 g, 4.4 mmol) and anhydrous THF (20 mL) were added to a 100 mL Schlenk tube, then *n*-BuLi (2.5 M in hexane, 1.8 ml, 4.4 mmol) was added at −35 °C. After stirring at −35 °C for 1 h, the mixture was directly transferred to a solution of **2a** (2.48 g, 4.4 mmol) in anhydrous THF (50 mL) at −35°C. The mixture was stirred at −35 °C for 0.5 h, then warmed to room temperature and stirred overnight. Subsequently, quenched with NH_4Cl (aq.) and extracted with ethyl acetate. The combined organic phase was washed with water and then dried over with anhydrous $NaSO_4$. After the removal of the solvent, the residue was purified by silica gel chromatography eluting with ethyl acetate and petroleum ether (1:8) to give the

target compound **3a** as a black liquid. Becasue compound **3a** is unstable, the next step was taken immediately after purification. Then, a solution of **3a** (1.25 g, 1 mmol) in THF (7.5 mL) and AcOH (7.5 mL), and a solution of $SnCl_2$ (1.06 g, 5.6 mmol) in 0.75 mL saturated HCl were added to a 100 mL two-necked round-bottom flask. The resulting mixture was heated to 100 °C and stirred for 1 h under an argon atmosphere. After cooling to room temperature, the mixture was quenched with water and extracted with ethyl acetate. The combined organic phase was washed with water and then dried over with anhydrous $NaSO_4$. Removal of the solvent under reduced pressure to get the crude compound **4a**, which was directly used to the next step without purification. Thereafter, a solution of **4a** (1.0 g, 0.80 mmol) and DDQ (0.55 g, 2.40 mmol) in toluene (20 mL) was added to a 100 mL two-necked round-bottom flask. The mixture was stirred for 1 h at room temperature. After removing the toluene under reduced pressure, the residue was purified by silica gel chromatography eluting with dichloromethane and petroleum ether (1:1) to give monomer **5a** as a deep blue solid (0.82 g, 82%), which contains three isomers. ^1H NMR (400 MHz, $CDCl_2CDCl_2$) δ 8.56 (d, J = 5.7 Hz, 1H), 7.75 – 7.50 (m, 5H), 7.27 – 7.14 (m, 2H), 3.84 – 3.68 (m, 4H), 2.06 (s, 2H), 1.70 – 1.26 (m, 80H), 0.90 (t, J = 6.6 Hz, 12H). ^{13}C NMR (101 MHz, $CDCl_2CDCl_2$) δ 167.07, 165.39, 155.69, 154.91, 151.25, 150.03, 149.86, 142.72, 142.59, 141.33, 139.62, 138.82, 134.09, 120.82, 115.48, 114.69, 114.58, 113.37, 43.44, 36.33, 36.24, 31.99, 31.48, 30.06, 29.79, 29.77, 29.74, 29.71, 29.66, 29.43, 29.41, 26.24, 22.79, 14.31. HRMS (MALDI-TOF): Calcd for $C_{70}H_{106}Br_2N_4O_2S_2$: 1258.61. Found: 1259.61.

(3Z,3'Z)-3,3'-((E)-3,3'-difluoro-5H,5'H-[2,2'-bithiophenylidene]-5,5'-diylidene)bis(6-bromo-1-(2-decyltetradecyl)-1,3-dihydro-2H-pyrrolo[2,3-b]pyridin-2-one) ***(5b)****.* The similar synthetic procedure of **3a** was carried out using 3,3'-difluoro-2,2'-bithiophene (0.404 g, 2 mmol), TMEAD (0.51 g, 4.4 mmol), **2a** (2.48 g, 4.4 mmol) and anhydrous THF (70 mL) to give the target compound **3b** as a black liquid. Becasue compound **3b** is unstable, the next step was taken immediately after purification. Then, the similar synthetic procedure of **4a** was carried out using **3b** (1.33 g, 1 mmol), $SnCl_2$ (1.06 g, 5.6 mmol), saturated HCl (0.75 mL), THF (7.5 mL) and AcOH (7.5 mL). Therewith, the similar synthetic procedure of **5a** was carried out using **4b** (1.04 g, 0.80 mmol), DDQ (0.55 g, 2.40 mmol) and toluene (20 mL). After removing the toluene under reduced pressure, the residue was purified by silica gel chromatography eluting with dichloromethane and petroleum ether (1:1) to give monomer **5b** as a deep blue solid (0.81 g, 78%), which contains three isomers. ^{1}H NMR (400 MHz, $CDCl_2CDCl_2$) δ 8.37 (t, J = 2.0 Hz, 1H), 7.53 (dd, J = 8.2, 2.3 Hz, 1H), 7.47 (dd, J = 7.9, 3.6 Hz, 1H), 7.32 (s, 1H), 7.21 – 7.14 (m, 2H), 3.72 (dd, J = 20.6, 7.0 Hz, 4H), 2.03 (s, 2H), 1.71 – 1.16 (m, 80H), 0.90 (t, J = 6.7 Hz, 12H). ^{13}C NMR (101 MHz, $CDCl_2CDCl_2$) δ 166.61, 166.51, 165.11, 164.71, 163.75, 163.38, 162.32, 161.92, 155.56, 155.47, 155.12, 144.54, 144.44, 143.86, 143.77, 140.13, 140.05, 139.53, 130.91, 129.05, 127.27, 127.12, 127.01, 120.93, 115.16, 114.84, 114.71, 114.25, 114.18, 113.54, 113.44, 43.72, 43.38, 36.29, 36.19, 32.00, 31.48, 30.05, 29.81, 29.78, 29.76, 29.72, 29.67, 29.45, 29.42, 26.25, 26.23, 22.79, 14.30. HRMS (MALDI-TOF): Calcd for $C_{70}H_{104}Br_2F_2N_4O_2S_2$: 1294.59. Found: 1295.59.

*(3Z,3'Z)-3,3'-((E)-5H,5'H-[2,2'-bithiophenylidene]-5,5'-diylidene)bis(6-bromo-1-(4-decyltetradecyl)-1,3-dihydro-2H-pyrrolo[2,3-b]pyridin-2-one) (**5c**)*. The similar synthetic procedure of **3a** was carried out using 2,2'-bithiophene (0.33g, 2 mmol), TMEAD (0.51 g, 4.4 mmol), **2b** (2.48 g, 4.4 mmol) and anhydrous THF (70 mL) to give the target compound **3c** as a black liquid. Becasue compound **3c** is unstable, the next step was taken immediately after purification. Then, the similar synthetic procedure of **4a** was carried out using **3c** (1.25 g, 1 mmol), $SnCl_2$ (1.06 g, 5.6 mmol), saturated HCl (0.75 mL), THF (7.5 mL) and AcOH (7.5 mL). Therewith, the similar synthetic procedure of **5a** was carried out using **4c** (1.0 g, 0.80 mmol), DDQ (0.55 g, 2.40 mmol) and toluene (20 mL). After removing the toluene under reduced pressure, the residue was purified by silica gel chromatography eluting with dichloromethane and petroleum ether (1:1) to give monomer **5c** as a deep blue solid (0.84 g, 83%), which contains three isomers. ^1H NMR (400 MHz, $CDCl_2CDCl_2$) δ 8.57 (dd, J = 11.9, 5.7 Hz, 1H), 7.77 – 7.48 (m, 5H), 7.23 – 7.16 (m, 2H), 3.96 – 3.77 (m, 4H), 1.65 (s, 10H), 1.26 (d, J = 10.7 Hz, 72H), 0.93 – 0.87 (m, 12H). ^{13}C NMR (101 MHz, $CDCl_2CDCl_2$) δ 166.81, 165.11, 155.34, 154.52, 152.12, 150.41, 141.56, 141.36, 139.53, 139.01, 138.86, 136.86, 136.14, 135.22, 132.90, 132.62, 132.51, 131.08, 130.80, 129.04, 124.51, 123.55, 122.29, 121.76, 120.86, 117.26, 115.67, 115.14, 114.29, 113.37, 113.30, 111.52, 110.04, 39.68, 37.48, 37.06, 33.57, 32.78, 32.00, 30.69, 30.39, 30.22, 29.80, 29.76, 29.44, 27.17, 26.71, 24.96, 22.79, 19.86, 14.31. HRMS (MALDI-TOF): Calcd for $C_{70}H_{106}Br_2N_4O_2S_2$: 1259.61. Found: 1259.61.

(3Z,3'Z)-3,3'-((E)-3,3'-difluoro-5H,5'H-[2,2'-bithiophenylidene]-5,5'-diylidene)bis(6-bromo-1-(4-decyltetradecyl)-1,3-dihydro-2H-pyrrolo[2,3-b]pyridin-2-one) ***(5d)***. The similar synthetic procedure of **3a** was carried out using 3,3'-difluoro-2,2'-bithiophene (0.404 g, 2 mmol), TMEAD (0.51 g, 4.4 mmol), **2b** (2.48 g, 4.4 mmol) and anhydrous THF (70 mL) to give the target compound **3d** as a black liquid. Becasue compound **3d** is unstable, the next step was taken immediately after purification. Then, the similar synthetic procedure of **4a** was carried out using **3d** (1.33 g, 1 mmol), $SnCl_2$ (1.06 g, 5.6 mmol), saturated HCl (0.75 mL), THF (7.5 mL) and AcOH (7.5 mL). Therewith, the similar synthetic procedure of **5a** was carried out using **4a** (1.04 g, 0.80 mmol), DDQ (0.55 g, 2.40 mmol) and toluene (20 mL). After removing the toluene under reduced pressure, the residue was purified by silica gel chromatography eluting with dichloromethane and petroleum ether (1:1) to give monomer **5d** as a deep blue solid (0.83 g, 80%), which contains three isomers. ^{1}H NMR (400 MHz, $CDCl_2CDCl_2$) δ 8.39 (d, J = 2.3 Hz, 1H), 7.61 – 7.46 (m, 2H), 7.32 (d, J = 8.9 Hz, 1H), 7.26 – 7.15 (m, 2H), 3.93 – 3.73 (m, 4H), 1.65 (s, 10H), 1.26 (d, J = 13.0 Hz, 72H), 0.90 (t, J = 6.7 Hz, 12H). ^{13}C NMR (101 MHz, $CDCl_2CDCl_2$) δ 173.47, 170.85, 166.37, 164.89, 156.07, 154.77, 151.25, 147.06, 140.56, 140.14, 134.08, 133.97, 130.60, 130.51, 126.52, 126.41, 125.38, 125.15, 121.00, 120.13, 115.42, 114.91, 113.31, 112.49, 112.06, 109.98, 39.67, 37.00, 33.55, 32.00, 30.65, 30.22, 29.81, 29.76, 29.45, 26.71, 24.85, 22.79, 14.31. HRMS (MALDI-TOF): Calcd for $C_{70}H_{104}Br_2F_2N_4O_2S_2$: 1295.59. Found: 1295.59.

P1. Monomer **5a** (125.96 mg 0.10 mmol), 2,5-bis(trimethylstannyl)thiophene (40.98 mg, 0.10 mmol), $Pd_2(dba)_3$ (3.0 mg), P(*o*-tol)$_3$ (9 mg), and chlorobenzene (5 mL) were added to a 25 mL Schlenk tube. After the tube was conducted with a freeze−pump−thaw cycle three times under argon at −78 °C, the reaction mixture was heated to 120 °C, and stirred for 48 h under an argon atmosphere. The resulting sticky solution was cooled by ice water and then poured into 100 mL of methanol containing 6 M hydrochloric acid (5 mL) and stirred for 2 h. The formed black solid was collected by filtration and subjected to Soxhlet extraction for 72 h in methanol, acetone, and hexane for the removal of the low molecular weight fraction of the material and residual catalytic impurities. The final solid residue was collected with *o*-DCB. After removing the organic solvent under reduced pressure, the desired polymer material **P1** was obtained as a black film-like solid (108.9 mg, 92%). HT-GPC (1,2,4-trichlorobenzene, 150 °C): M_n = 53.6 kDa, M_w = 123.53 kDa, PDI = 2.30. Elemental Anal. Calcd for $C_{74}H_{110}N_4O_2S_3$: C 75.08, H 9.37, N 4.73, S 8.12. Found: C 75.03, H 9.11, N 4.64, S 8.24.

P1-2F. The similar synthetic procedure of **P1** was carried out using monomer **5b** (129.55 mg, 0.10 mmol), 2,5-bis(trimethylstannyl)thiophene (40.98 mg, 0.10 mmol), $Pd_2(dba)_3$ (3.0 mg), P(*o*-tol)$_3$ (9 mg), and chlorobenzene (5 mL) to give the desired polymer material **P1-2F** as a black film-like solid after removing the solvent (109.8 mg, 90%). HT-GPC (1,2,4-trichlorobenzene, 150 °C): M_n = 76.8 kDa, M_w = 160.8 kDa, PDI = 2.10. Elemental Anal. Calcd for $C_{74}H_{108}F_2N_4O_2S_3$: C 72.86, H 8.92, N 4.59, S 7.88. Found: C 72.60, H 8.64, N 4.52, S 7.95.

P2. The similar synthetic procedure of **P1** was carried out using monomer **5c** (125.96 mg, 0.10 mmol), 2,5-bis(trimethylstannyl)thiophene (40.98 mg, 0.10 mmol), $Pd_2(dba)_3$ (3.0 mg), P(*o*-tol)$_3$ (9 mg), and chlorobenzene (5 mL) to give the desired polymer material **P2** as a black film-like solid after removing the solvent (110.1 mg, 93%). HT-GPC (1,2,4-trichlorobenzene, 150 °C): $M_n = 46.9$ kDa, $M_w = 106.1$ kDa, PDI = 2.26. Elemental Anal. Calcd for $C_{74}H_{110}N_4O_2S_3$: C 75.08, H 9.37, N 4.73, S 8.12. Found: C 75.03, H 9.21, N 4.52, S 7.96.

P2-2F. The similar synthetic procedure of **P1** was carried out using monomer **5d** (129.55 mg, 0.10 mmol), 2,5-bis(trimethylstannyl)thiophene (40.98 mg, 0.10 mmol), $Pd_2(dba)_3$ (3.0 mg), P(*o*-tol)$_3$ (9 mg), and chlorobenzene (5 mL) to give the desired polymer material **P2-2F** as a black film-like solid after removing the solvent (111.0 mg, 91%). HT-GPC (1,2,4-trichlorobenzene, 150 °C): $M_n = 81.2$ kDa, $M_w = 205.0$ kDa, PDI = 2.52. Elemental Anal. Calcd for $C_{74}H_{108}F_2N_4O_2S_3$: C 72.86, H 8.92, N 4.59, S 7.88. Found: C 73.24, H 8.82, N 4.47, S 7.70.

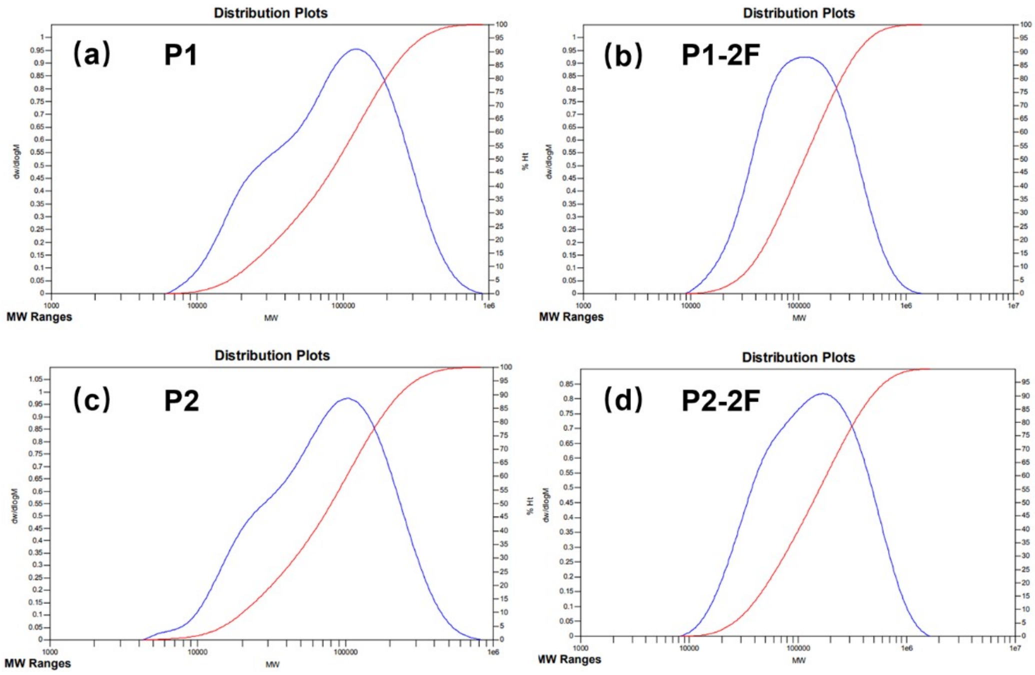


Figure S1. (a−d) GPC distribution plots of copolymers (a) **P1**, (b) **P1-2F**, (c) **P2** and (d) **P2-2F**.

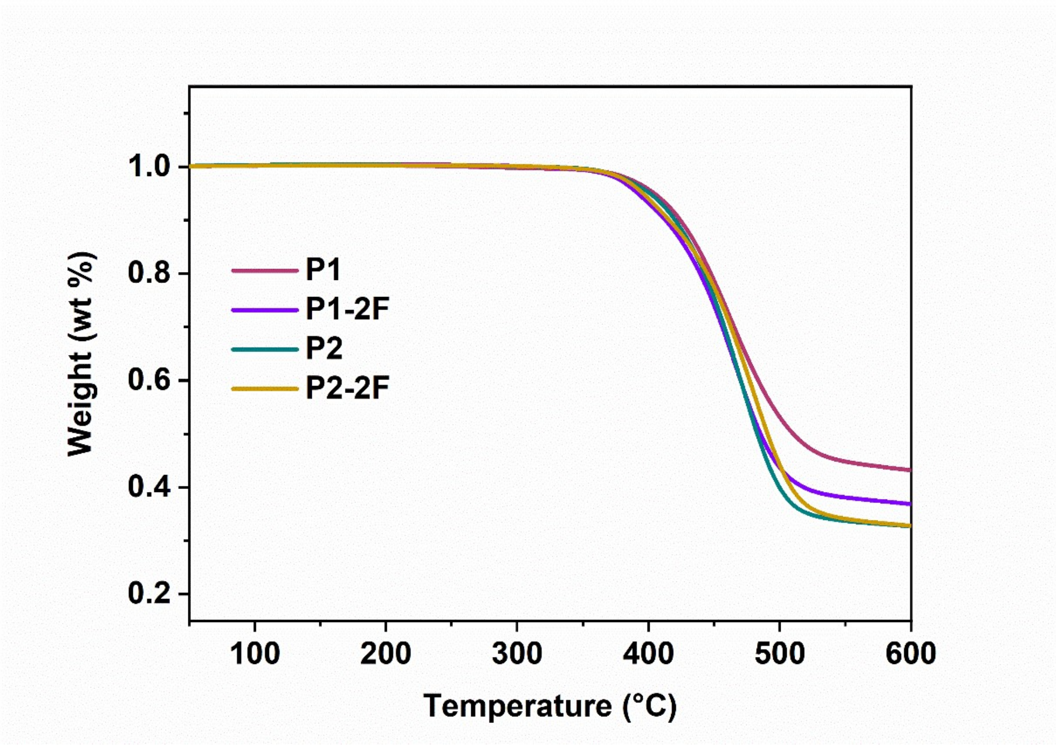


Figure S2. TGA traces of copolymers **P1**, **P1-2F**, **P2** and **P2-2F**.

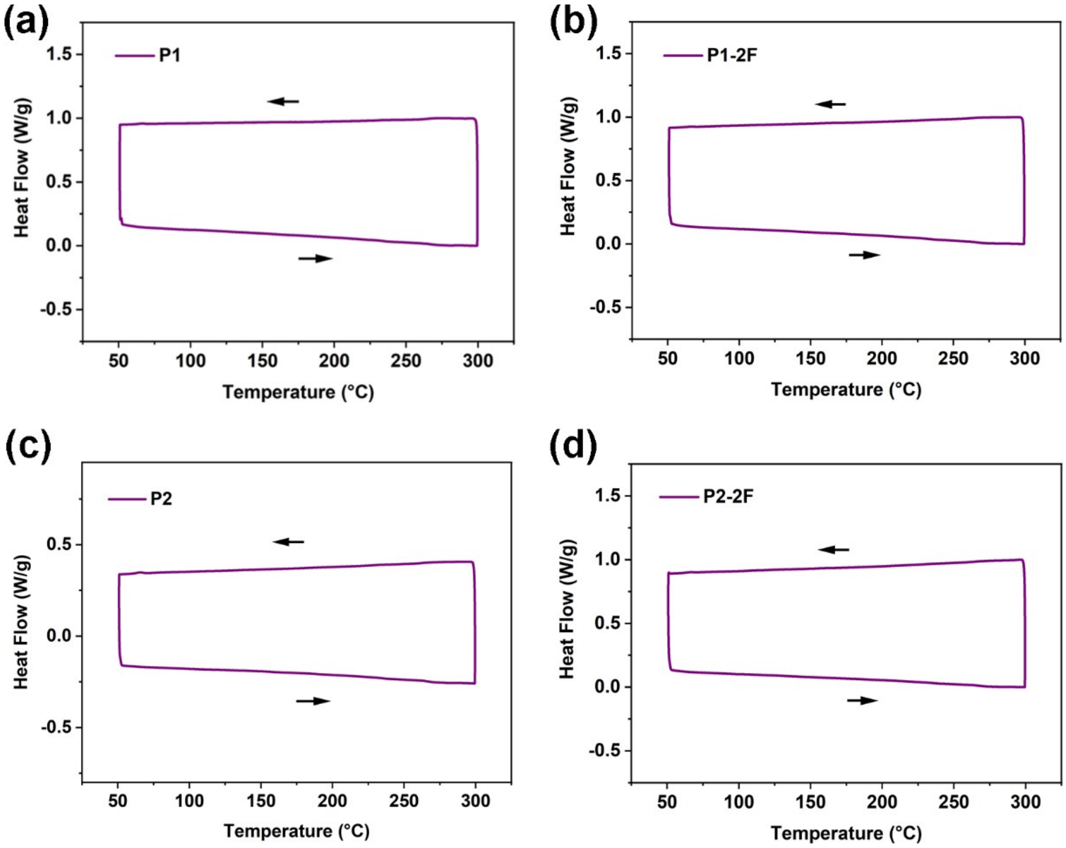


Figure S3. (a–d) DSC curves of copolymers (a) **P1**, (b) **P1-2F**, (c) **P2** and (d) **P2-2F**.

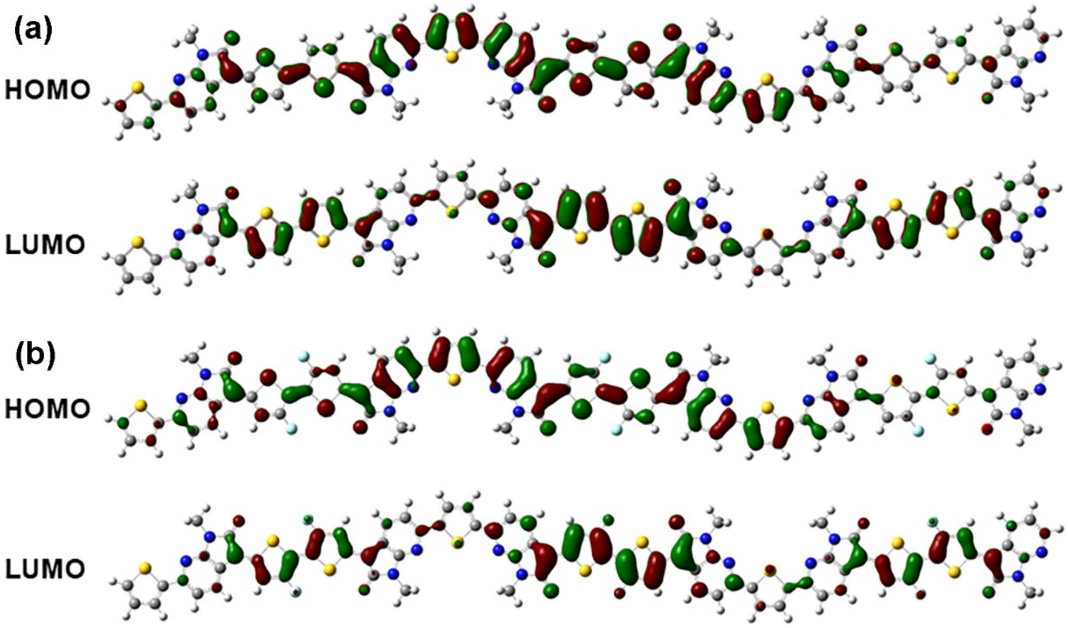


Figure S4. (a,b) The electron state density distributions in the HOMOs and LUMOs of copolymers (a) **P1**/**P2** and (b) **P1-2F**/**P2-2F**.

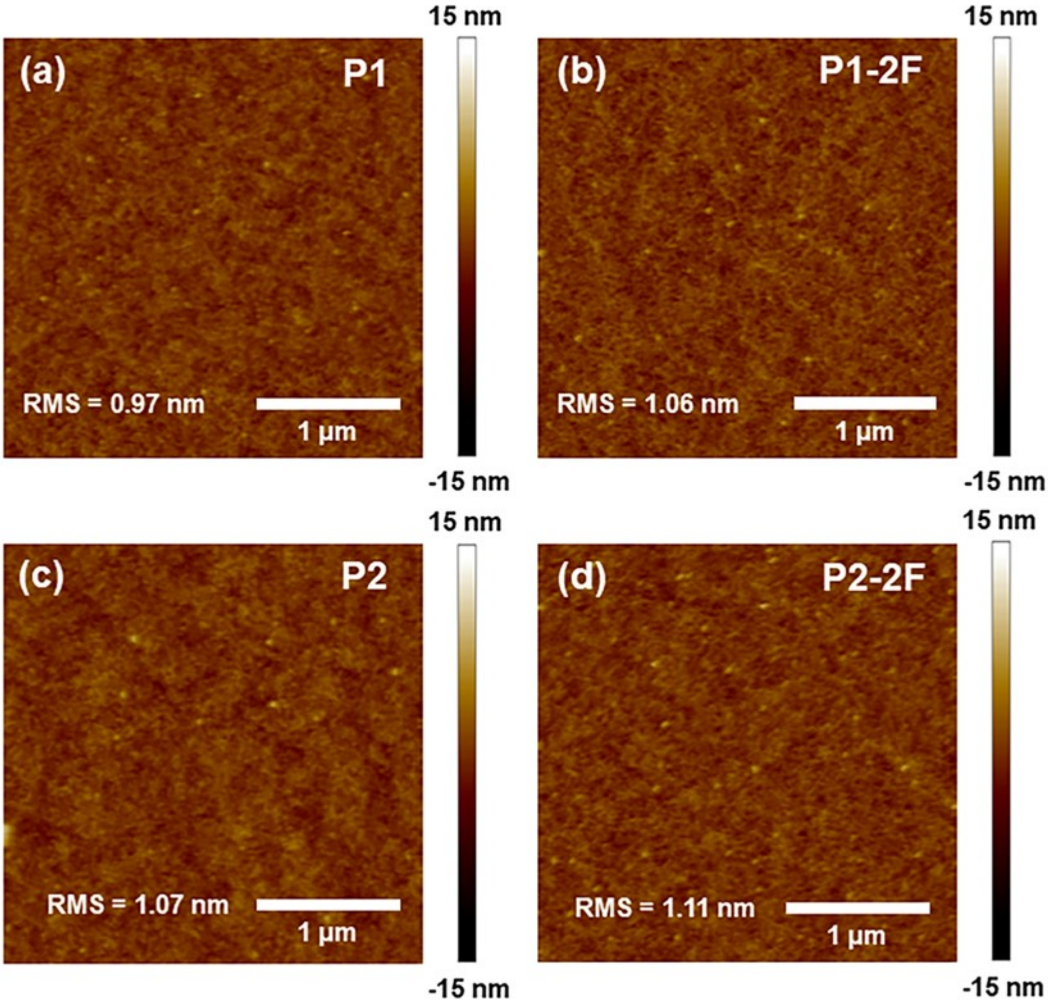


Figure S5. (a−d) Tapping-mode AFM height images of the pristine films of copolymers (a) **P1**, (b) **P1-2F**, (c) **P2** and (d) **P2-2F**.

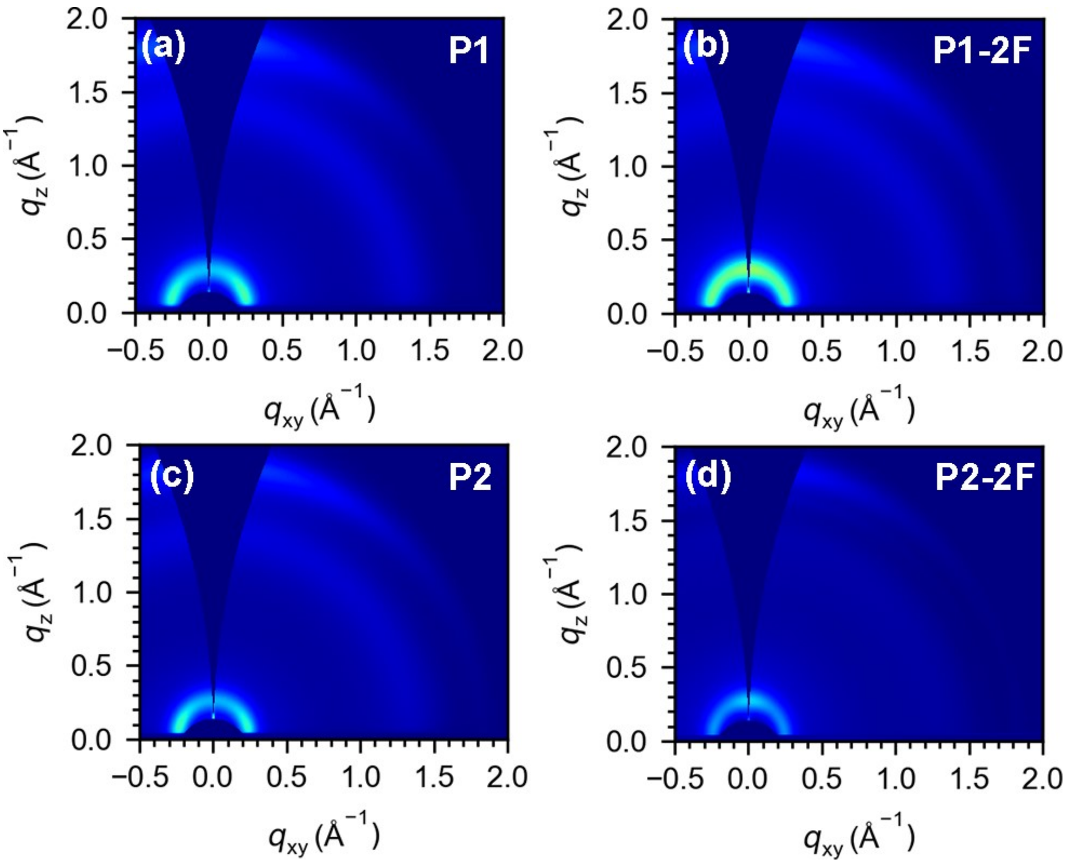
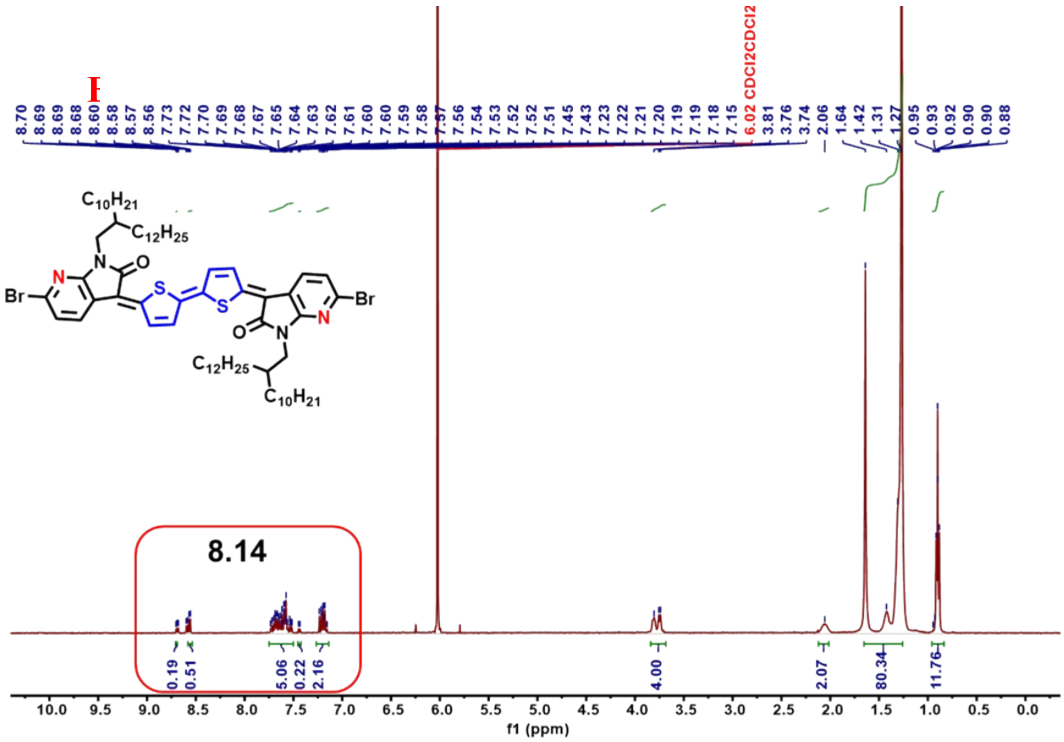
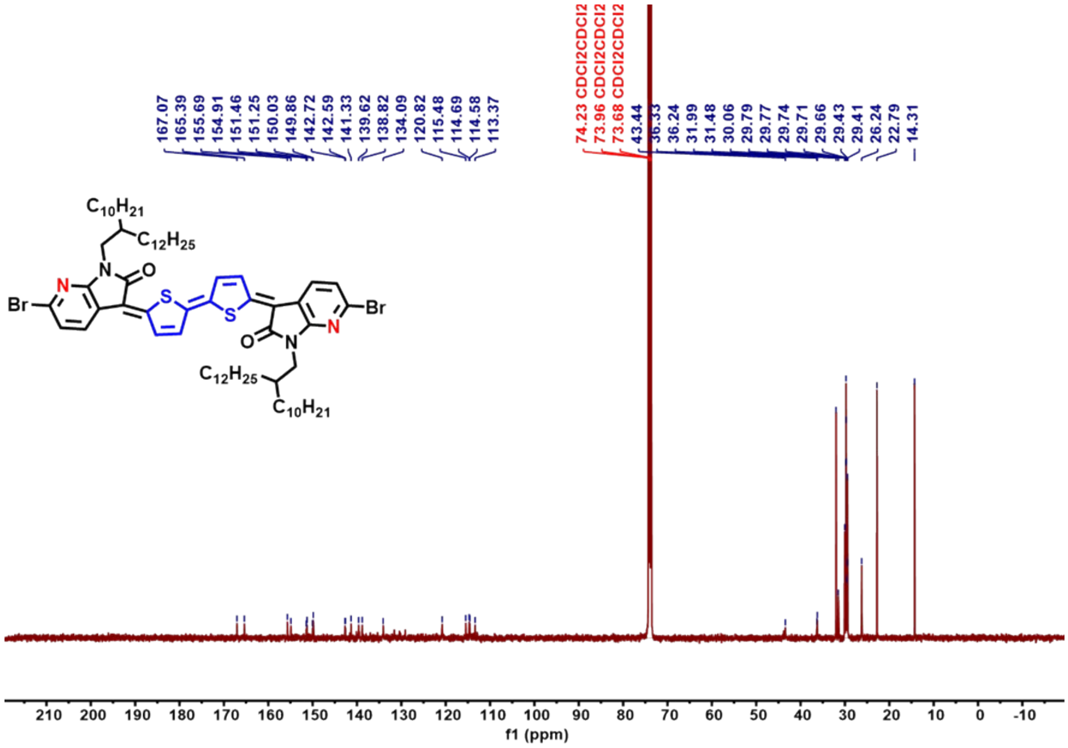
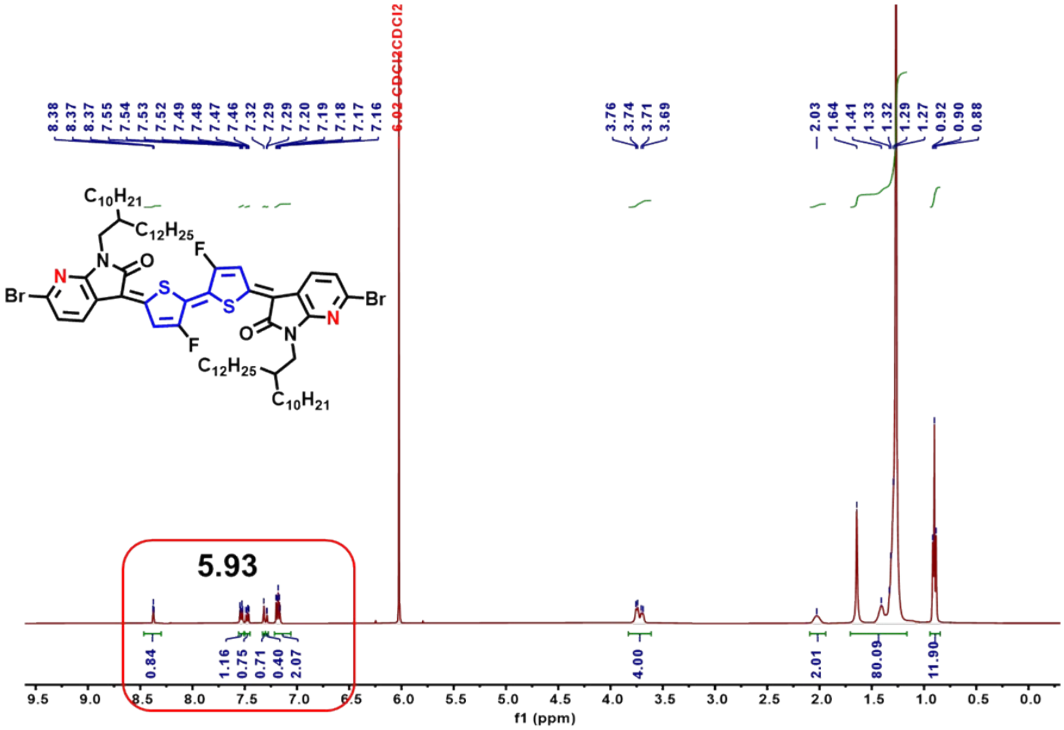


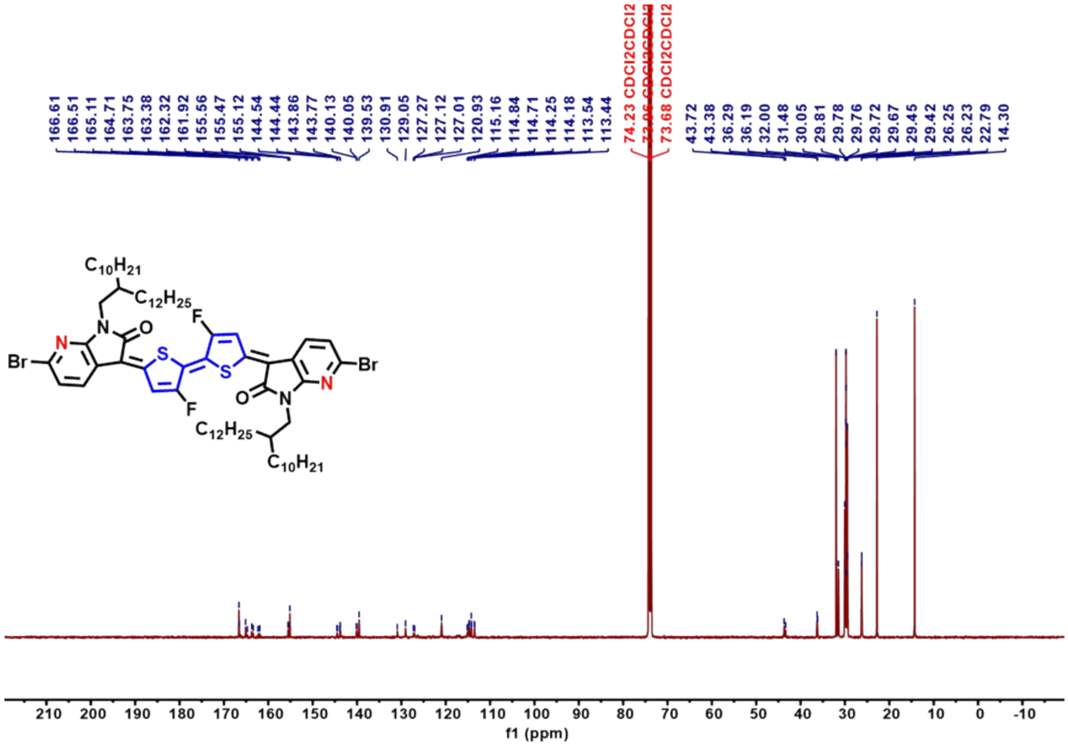
Figure S6. (a−d) 2D-GIWAXS diffraction patterns of the pristine (a) **P1**, (b) **P1-2F**, (c) **P2** and (d) **P2-2F** thin films deposited on corning glass.

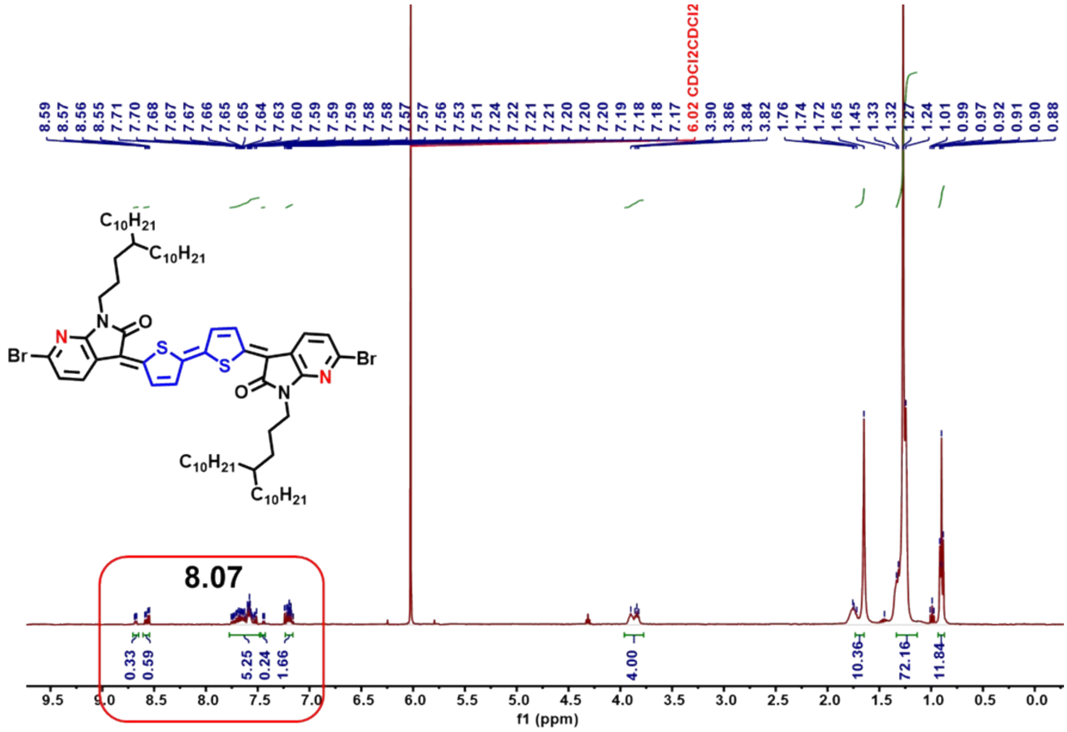
NMR of monomers and polymers.

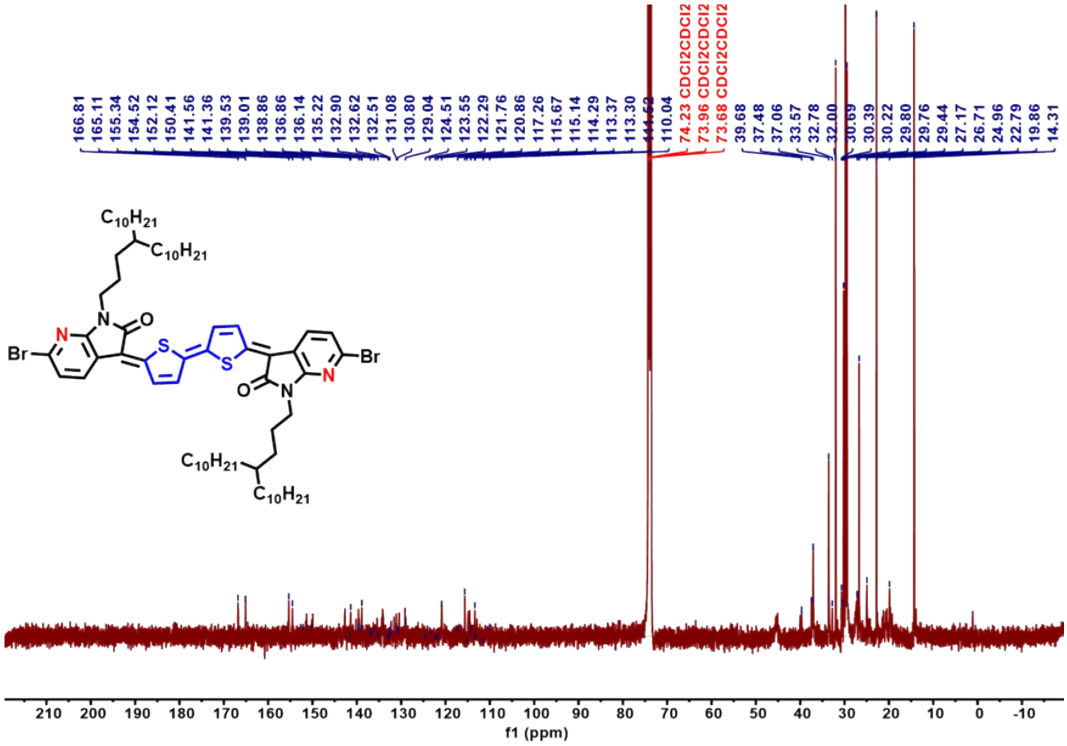





8.38 8.37 7.55 7.54 7.53 7.52 7.49 7.48 7.47 7.46 7.32 7.29 7.29 7.20 7.19 7.18 7.17 7.16
6.02 CDCl2CDCl2
3.76 3.74 3.71 3.69
2.03 1.64 1.41 1.33 1.32 1.29 1.27 0.92 0.90 0.88
5.93
0.84
1.16 0.75 0.71 0.40 2.07
4.00
2.01
80.09
11.90
$C_{10}H_{21}$
$C_{12}H_{25}$
N
O
F
S
Br
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


166.61 166.51 165.11 164.71 163.75 163.38 162.32 161.92 155.56 155.47 155.12 144.54 144.44 143.86 143.77 140.13 140.05 139.53 130.91 129.05 127.27 127.12 127.01 120.93 115.16 114.84 114.71 114.25 114.18 113.54 113.44
74.23 CDCl2CDCl2
73.96 CDCl2CDCl2
73.68 CDCl2CDCl2
43.72 43.38 36.29 36.19 32.00 31.48 30.05 29.81 29.78 29.76 29.72 29.67 29.45 29.42 26.25 26.23 22.79 14.30
$C_{10}H_{21}$
$C_{12}H_{25}$
N
O
F
S
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.59 8.57 8.56 8.55 7.71 7.70 7.68 7.67 7.67 7.66 7.65 7.65 7.64 7.63 7.60 7.59 7.59 7.59 7.58 7.58 7.57 7.57 7.56 7.53 7.51 7.24 7.22 7.21 7.21 7.20 7.20 7.20 7.19 7.18 7.18 7.17
6.02 CDCl2CDCl2
3.90 3.86 3.84 3.82 1.76 1.74 1.72 1.65 1.45 1.33 1.32 1.27 1.24 1.01 0.99 0.97 0.92 0.91 0.90 0.88
C10H21
C10H21
N
O
Br
N
S
S
Br
N
O
N
C10H21
C10H21
8.07
0.33
0.59
5.25
0.24
1.66
4.00
10.36
72.16
11.84
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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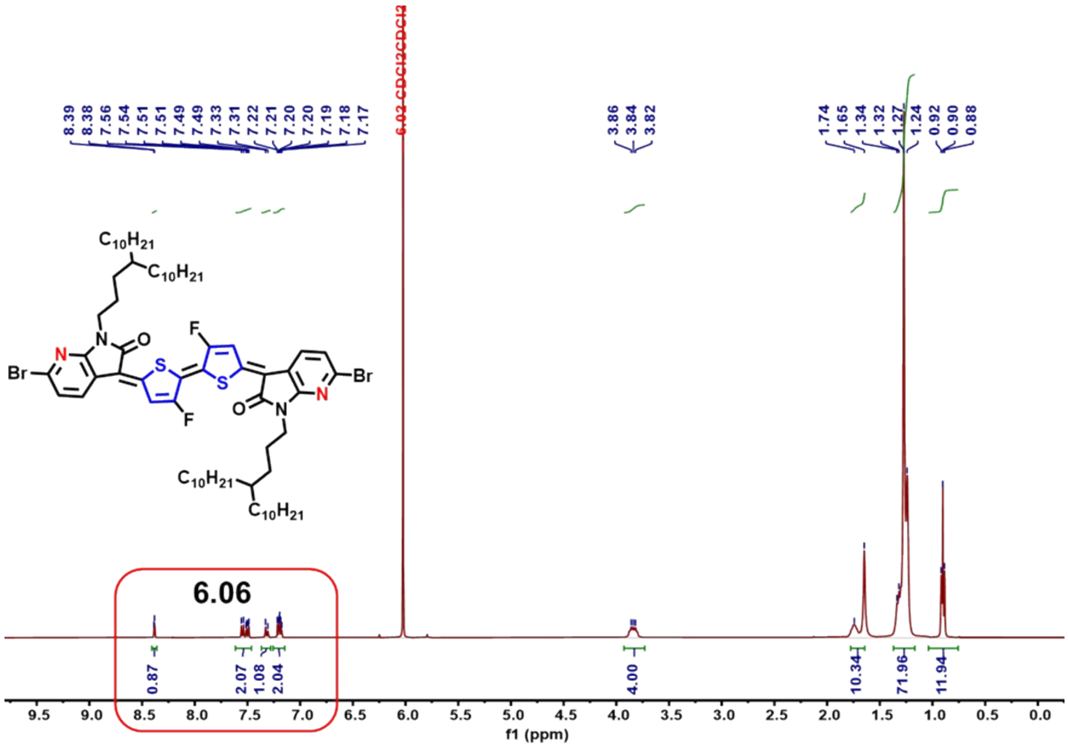
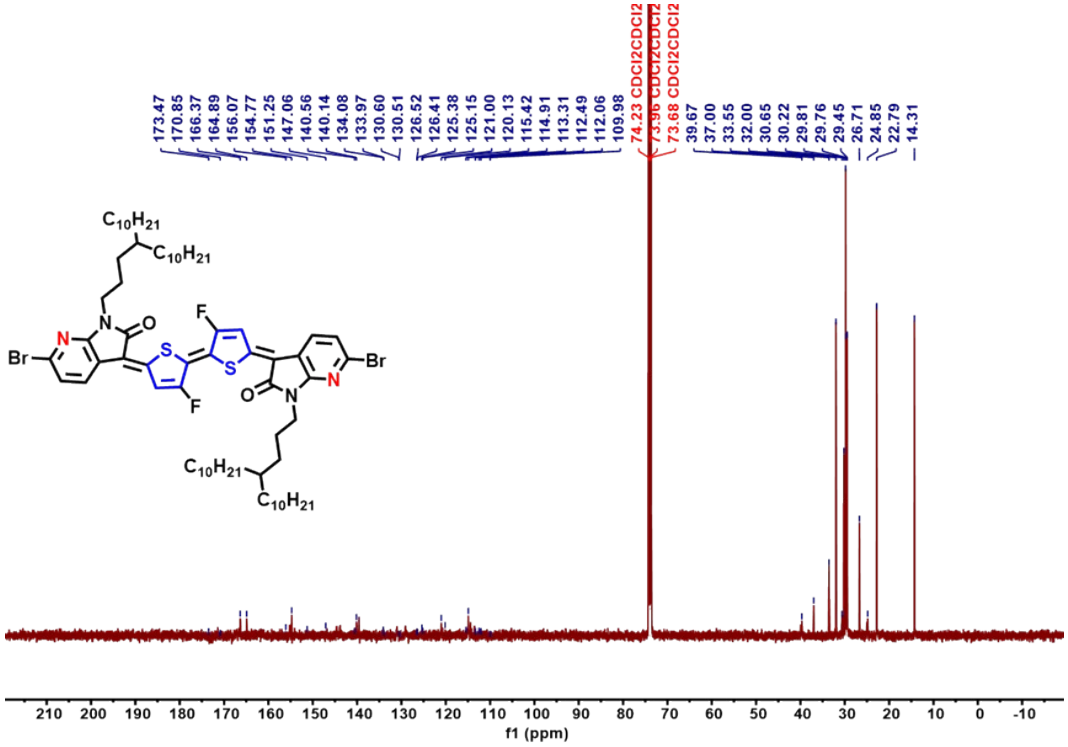
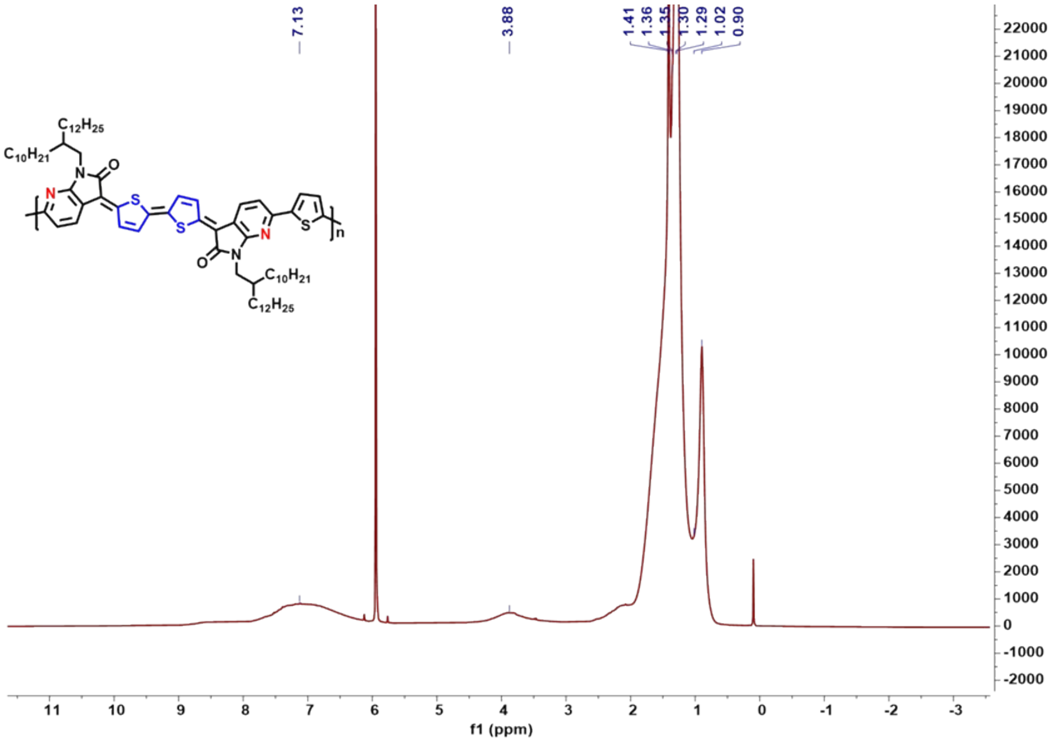
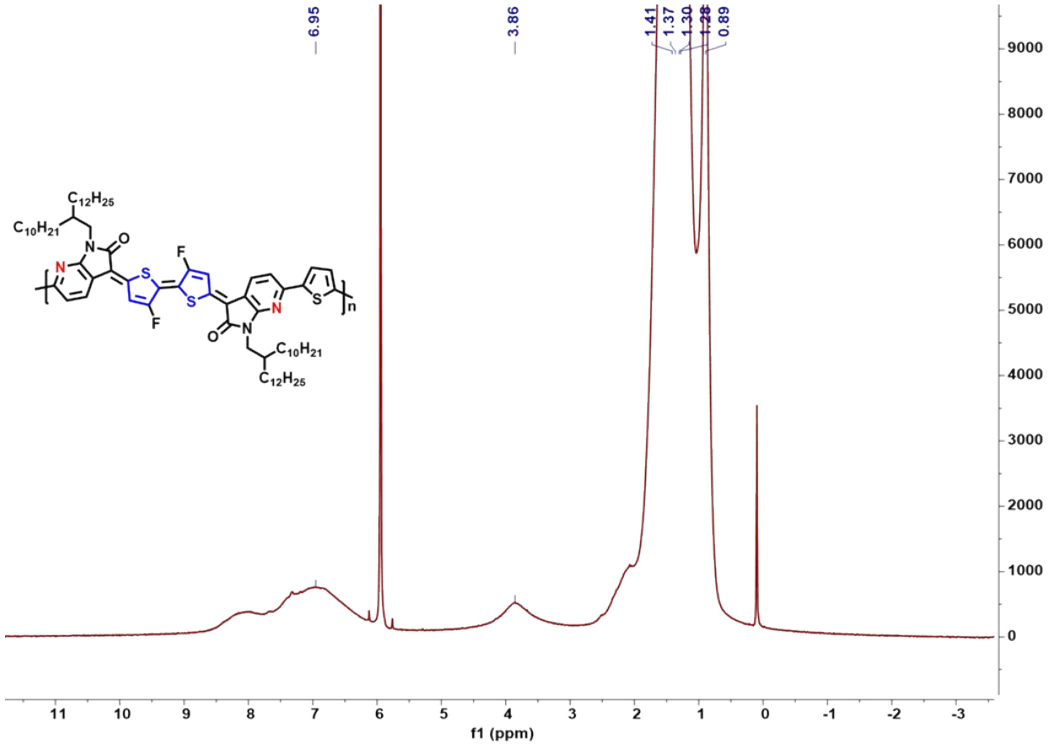
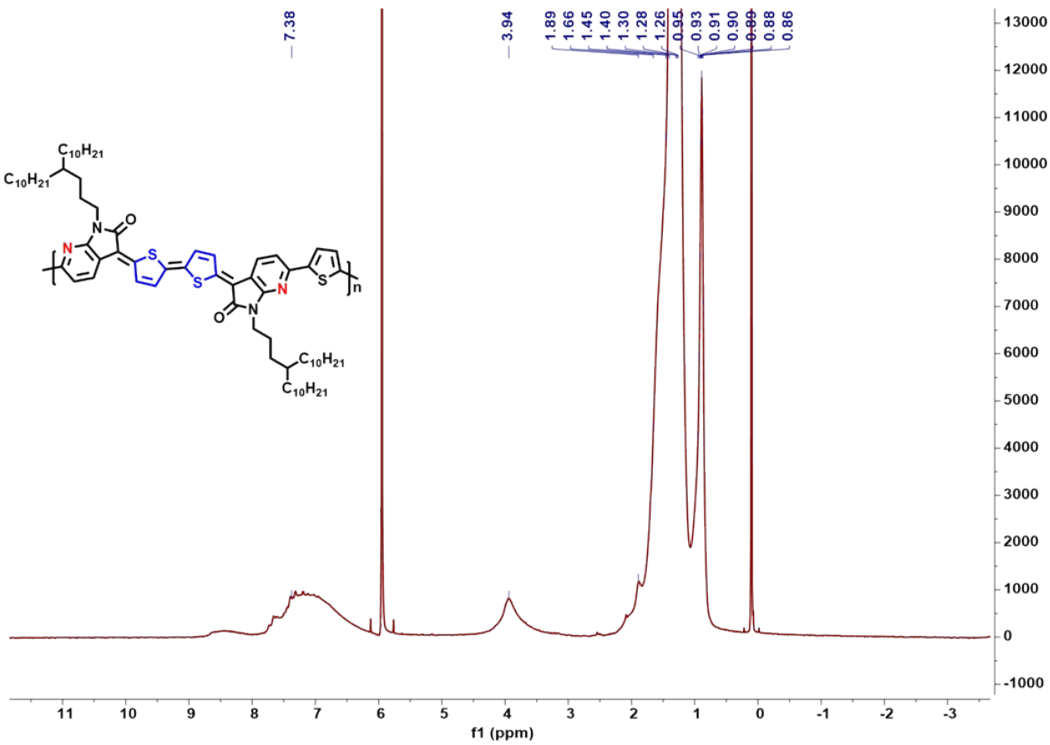
74.23 CDCl2CDCl2
73.96 CDCl2CDCl2
73.68 CDCl2CDCl2
39.68 37.48 37.06 33.57 32.78 32.00 30.69 30.39 30.22 29.80 29.76 29.44 27.17 26.71 24.96 22.79 19.86 14.31
C10H21
C10H21
N
O
Br
N
S
S
Br
N
O
N
C10H21
C10H21
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

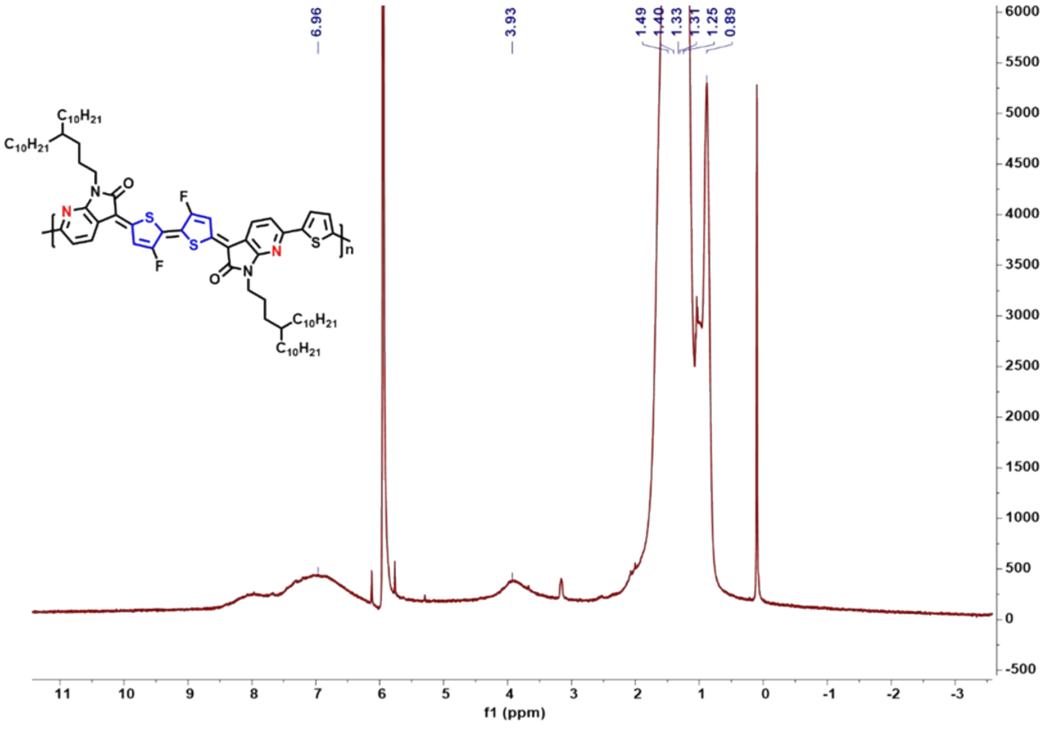

8.39
8.38
7.56
7.54
7.51
7.51
7.49
7.49
7.33
7.31
7.22
7.21
7.20
7.20
7.19
7.18
7.17
6.02 CDCl2CDCl2
3.86
3.84
3.82
1.74
1.65
1.34
1.32
1.27
1.24
0.92
0.90
0.88
C10H21
C10H21
Br
N
N
O
S
F
S
F
O
N
N
Br
C10H21
C10H21
6.06
0.87
2.07
1.08
2.04
4.00
10.34
71.96
11.94
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


173.47
170.85
166.37
164.89
156.07
154.77
151.25
147.06
140.56
140.14
134.08
133.97
130.60
130.51
126.52
126.41
125.38
125.15
121.00
120.13
115.42
114.91
113.31
112.49
112.06
109.98
74.23 CDCl2CDCl2
73.96 CDCl2CDCl2
73.68 CDCl2CDCl2
39.67
37.00
33.55
32.00
30.65
30.22
29.81
29.76
29.45
26.71
24.85
22.79
14.31
C10H21
C10H21
Br
N
N
O
S
F
S
F
O
N
N
Br
C10H21
C10H21
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.13
3.88
1.41
1.36
1.35
1.30
1.29
1.02
0.90
C12H25
C10H21
N
O
S
n
C10H21
C12H25
22000
21000
20000
19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)


6.95
3.86
1.41
1.37
1.30
1.28
0.89
C12H25
C10H21
N
O
S
F
n
C10H21
C12H25
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)


7.38
3.94
1.89
1.66
1.45
1.40
1.30
1.28
1.26
0.95
0.93
0.91
0.90
0.89
0.88
0.86
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)
$C_{10}H_{21}$
N
O
S
n


6.96
3.93
1.49
1.40
1.33
1.31
1.25
0.89
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)
$C_{10}H_{21}$
N
O
S
F
n