Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supporting Information

Luminescent Color Tuning with Polymer Films Composed of Boron Diiminate Conjugated Copolymers by Changing Connection Points to Comonomers

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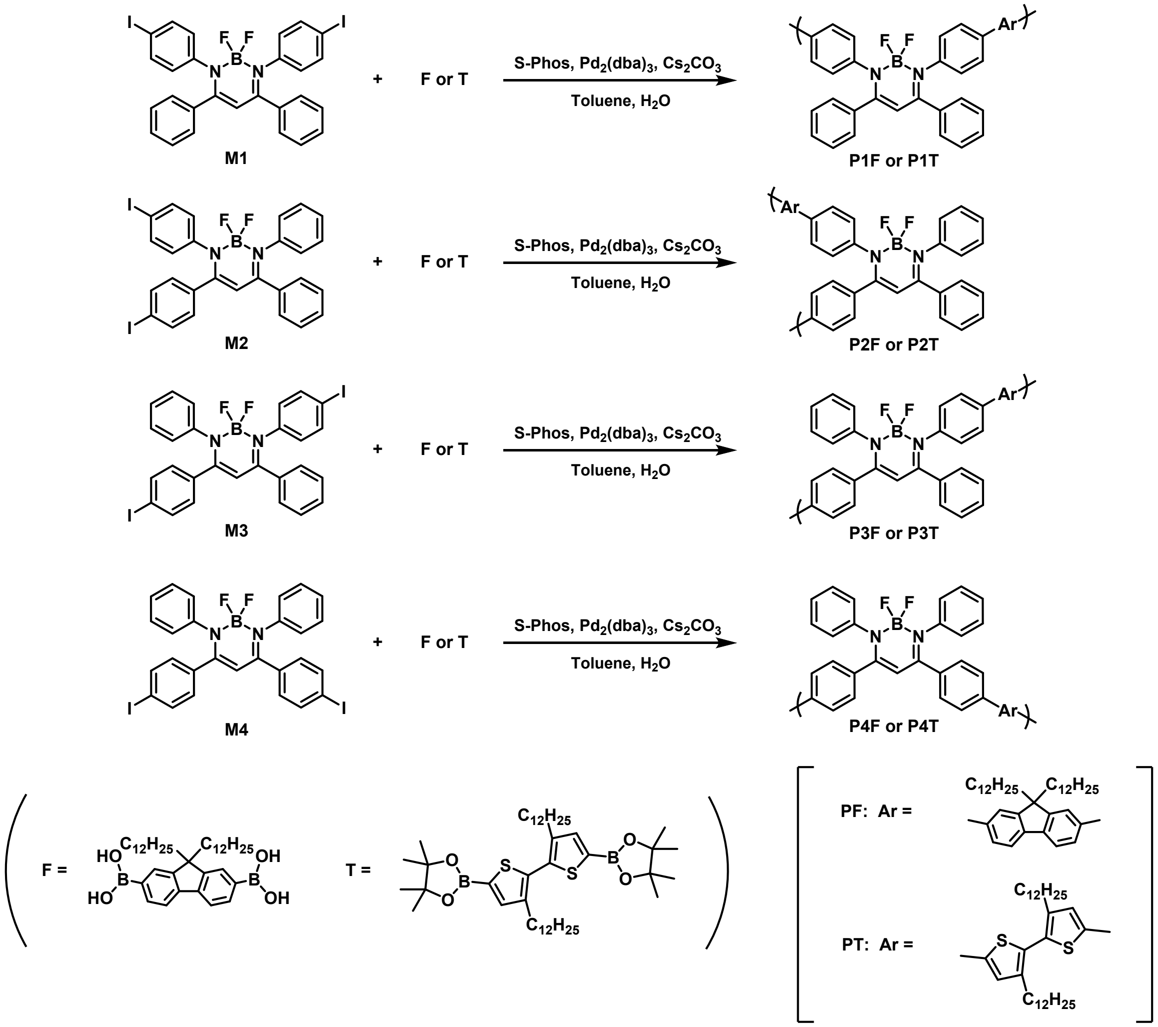
Experimental Section

Measurements: ^{1}H (400 MHz), ^{13}C (100 MHz), and ^{11}B (128 MHz) NMR spectra were recorded on JEOL JNM-EX400 spectrometers. In ^{1}H and ^{13}C spectra, tetramethylsilane (TMS) was used as an internal standard in $CDCl_3$, and ^{11}B NMR spectra were referenced externally to $BF_3{\cdot}OEt_2$ (sealed capillary). UV−vis spectra were recorded on a SHIMADZU UV-3600 spectrophotometer. Fluorescence emission spectra were measured with a HORIBA JOBIN YVON Fluoromax-4P spectrofluorometer. The number-average molecular weight (M_n) and the molecular weight distribution (weight-average molecular weight/number-average molecular weight (M_w/M_n)) values of all polymers were estimated by the size-exclusion chromatography (SEC) with a TOSOH G3000HXI system equipped with three consecutive polystyrene gel columns (TOSOH gels: α-4000, α-3000, and α-2500) and ultraviolet detector at 40 °C. The system was operated at a flow rate of 1.0 mL/min, with chloroform as an eluent. Polystyrene standards were employed for the calibration. Cyclic voltammetry (CV) was carried out on a BAS ALS-Electrochemical-Analyzer Model 600D with a glassy carbon working electrode, a Pt counter electrode, an Ag/Ag^+ reference electrode, and the ferrocene/ferrocenium external reference at a scan rate of 0.05 Vs^{-1} . All reactions were performed under argon.

Materials: 9,9-Didodecylfluorene-2,7-diboronicacid (Aldrich Chemical, Co.), 2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl (S-Phos, Aldrich Chemical, Co.) and tris(dibenzylideneacetone dipalladium(0)) ($Pd_2(dba)_3$, Tokyo Kasei Kogyo, Co.) were used as received. 4,4-Didodecyl-2,2'-bithiophene-5,5'-diboronic acid bis(pinacol) ester were synthesized according to the reported method.[1] **M1−M4** were synthesized according to our previous work (Scheme S1).[2]

Scheme S1. Synthesis of the polymers



Synthesis of P1F: Water (0.5 mL) was added to the solution of **M1** (50 mg, 0.074 mmol), 9,9-didodecylfluorene-2,7-diboronicacid **F** (44 mg, 0.074 mmol), $Pd_2(dba)_3$ (2.0 mg, 2.2 μmol), S-Phos (2.1 mg, 5.2 μmol) and cesium carbonate (241 mg, 74 mmol) in toluene (0.5 mL). The reaction mixture was stirred at 80 °C for 24 h under argon atmosphere, and then 1,4-dimethyl-2-iodobenzene (13 μL, 150 μmol) was added to the reaction mixture. The reaction mixture was stirred at 80 °C for 12 h, and poured into a large amount of methanol to collect the polymer by filtration. The precipitate was dissolved in a small amount of THF, and then the product was reprecipitated from ethanol. The polymer collected by filtration was dried in vacuum to give **P1F** as a yellow solid (52 mg, 77%). M_n = 8,500, M_w/M_n = 2.2. ^{1}H NMR ($CDCl_3$): δ = 7.69–7.11 (24H, Ar-*H*), 5.69 (1H, -C*H*=), 1.96 (4H, -CH_2-), 1.27–1.02 (36H, -C_7H_{15}), 0.87–0.83 (6H, -CH_3), 0.65 (4H, -CH_2-) ppm. ^{13}C NMR ($CDCl_3$): δ = 164.3, 151.7, 140.9, 140.0, 139.5, 139.2, 136.6, 129.5, 129.1, 128.2, 128.1, 126.9, 125.9, 121.3, 119.9, 100.0, 55.3, 40.4, 31.89, 30.1, 29.6, 29.5, 29.3, 29.3, 23.9, 22.7, 14.1 ppm. ^{11}B NMR ($CDCl_3$): δ = 1.76 (t, *J* = 31 Hz) ppm.

Synthesis of P1T Compound **P1T** was prepared from **M1** (50 mg, 0.074 mmol) and 4,4'-didodecyl-2,2'-bithiophene-5,5'-diboronicacid bis(pinacol) ester **T** (56 mg, 0.074 mmol) in 70% yield (48 mg, yellow solid) according to the same method with **P1F**. M_n = 6,900, M_w/M_n = 1.8. ^{1}H NMR ($CDCl_3$): δ = 7.41–6.96 (20H, Ar-*H*), 5.66 (1H, -C*H*=), 2.50–2.46 (4H, -CH_2-), 1.22 (40H, -$C_{10}H_{20}$-), 0.89−0.85 (6H, -CH_3) ppm. ^{13}C NMR ($CDCl_3$): δ = 164.3, 143.5, 143.0, 141.1, 136.4, 132.2, 129.6, 129.1, 128.3, 128.1, 125.4, 124.8, 100.0, 55.3, 31.9, 30.7, 29.7, 29.6, 29.6, 29.6, 29.5, 29.3, 29.1, 22.7, 14.1 ppm. ^{11}B NMR ($CDCl_3$): δ = 1.66 (t, *J* = 31 Hz) ppm.

Synthesis of P2F Compound **P2F** was prepared from **M2** (50 mg, 0.074 mmol) and 9,9-didodecylfluorene-2,7-diboronicacid **F** (44 mg, 0.074 mmol) in 63% yield (43 mg, yellow solid) according to the same method with **P1F**. M_n = 7,600, M_w/M_n = 1.7. ^{1}H NMR (CDCl$_3$): δ = 7.70–7.10 (24H, Ar-*H*), 5.72 (1H, -C*H*=), 1.96 (4H, -CH_2-), 1.16–0.99 (36H, -C_7H_{15}), 0.82 (6H, -CH_3), 0.62 (4H, -CH_2-) ppm. ^{13}C NMR (CDCl$_3$): δ = 164.5, 163.7, 151.9, 151.7, 142.8, 142.7, 141.8, 141.2, 141.1, 140.8, 140.5, 140.1, 139.8, 139.5, 139.4, 139.2, 138.9, 138.6, 136.5, 135.2, 129.8, 129.4, 129.1, 128.3, 128.1, 127.9, 127.1, 126.9, 126.3, 126.2, 126.0, 125.9, 121.3, 120.2, 120.0, 119.9, 100.0, 55.3, 40.4, 31.9, 30.0, 29.6, 29.5, 29.3, 29.2, 23.8, 22.6, 14.1 ppm. ^{11}B NMR (CDCl$_3$): δ = 1.76 (t, J = 31 Hz) ppm.

Synthesis of P2T Compound **P2T** was prepared from **M2** (50 mg, 0.074 mmol) and 4,4'-didodecyl-2,2'-bithiophene-5,5'-diboronicacid bis(pinacol) ester **T** (56 mg, 0.074 mmol) in 85% yield (58 mg, yellow solid) according to the same method with **P1F**. M_n = 4,500, M_w/M_n = 1.5. ^{1}H NMR (CDCl$_3$): δ = 7.52–6.94 (20H, Ar-*H*), 5.67 (1H, -C*H*=), 2.49–2.47 (4H, -CH_2-), 1.19 (40H, -$C_{10}H_{20}$-), 0.86−0.82 (6H, -CH$_3$) ppm. ^{13}C NMR (CDCl$_3$): δ = 164.6, 163.3, 143.9, 143.7, 143.6, 143.5, 143.2, 143.0, 142.5, 142.2, 141.7, 141.3, 141.2, 136.5, 135.5, 135.4, 135.3, 135.2, 132.3, 132.2, 129.8, 129.5, 129.07, 128.3, 128.1, 127.8, 126.3, 125.7, 125.5, 125.1, 124.8, 99.8, 31.9, 30.6, 29.6, 29.5, 29.4, 29.3, 22.7, 14.1 ppm. ^{11}B NMR (CDCl$_3$): δ = 1.76 (t, J = 31 Hz) ppm.

Synthesis of P3F Compound **P3F** was prepared from **M3** (50 mg, 0.074 mmol) and 9,9-didodecylfluorene-2,7-diboronicacid **F** (44 mg, 0.074 mmol) in 81% yield (55 mg, yellow solid) according to the same method with **P1F**. M_n = 13,500, M_w/M_n = 2.5. ^{1}H NMR (CDCl$_3$): δ = 7.73–7.07 (24H, Ar-*H*), 5.73 (1H, -C*H*=), 1.98 (4H, -CH_2-), 1.25–1.03 (36H, -C_7H_{15}), 0.88−0.84 (6H, -CH_3), 0.64

(4H, -CH_2-) ppm. ^{13}C NMR (CDCl3): δ = 164.1, 151.8, 151.7, 142.7, 142.6, 141.9, 140.9, 140.7, 140.5, 139.5, 136.6, 136.59, 135.0, 129.7, 129.2, 128.3, 128.0, 127.9, 127.0, 126.7, 126.0, 122.6, 122.4, 121.3, 120.0, 99.9, 55.3, 40.4, 31.9, 30.0, 29.6, 29.5, 29.3, 23.9, 22.7, 14.1 ppm.^{11}B NMR ($CDCl_3$): δ = 1.76 (t, J = 31 Hz) ppm.

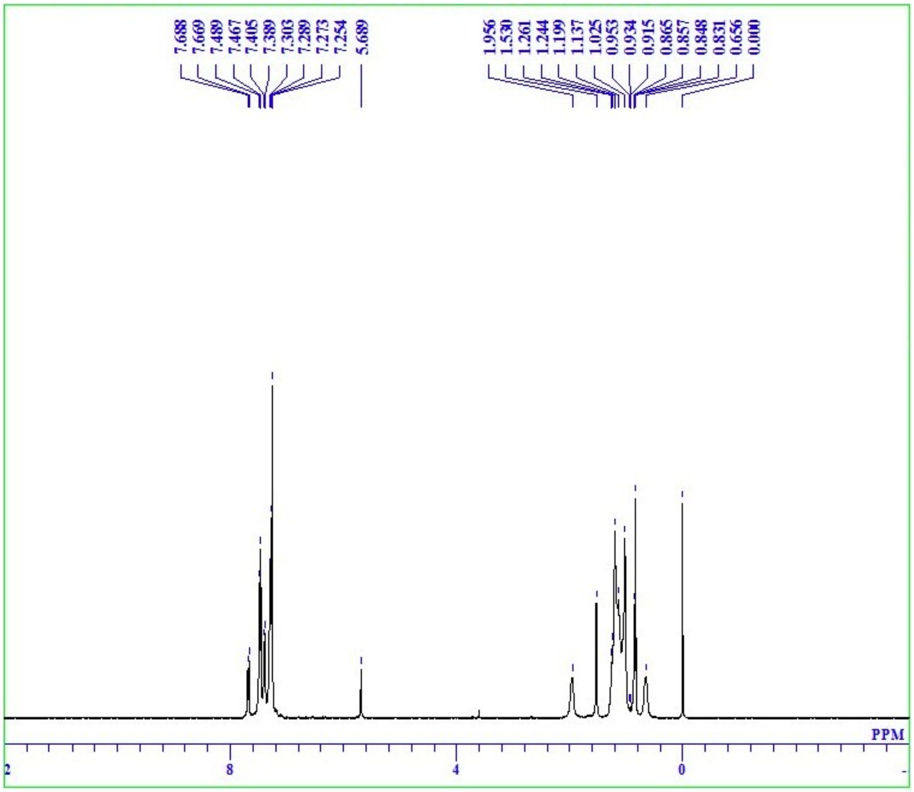
Synthesis of P3T Water (2 mL) was added to the solution of **M3** (107 mg, 0.160 mmol), 9,9-didodecylfluorene-2,7-diboronicacid **F** (120 mg, 0.160 mmol), $Pd_2(dba)_3$ (1.5 mg, 1.6 μmol), S-Phos (2.6 mg, 6.3 μmol) and cesium carbonate (519 mg, 1.6 mmol) in toluene (2.5 mL). The reaction mixture was stirred at 80 ˚C for 24 h under argon atmosphere, and then 1,4-dimethyl-2-iodobenzene (30 μL, 320 μmol) was added to the reaction mixture. The reaction mixture was stirred at 80 ˚C for 12 h, and poured into a large amount of methanol to collect the polymer by filtration. The precipitate was dissolved in a small amount of THF, and then the product was reprecipitated from ethanol. The polymer collected by filtration was dried in vacuum to give **P3T** as a yellow solid (133 mg, 91%). M_n = 8,500, M_w/M_n = 2.2. ^{1}H NMR ($CDCl_3$): δ = 7.46–6.92 (20H, Ar-H), 5.68 (1H, -CH=), 2.48 (4H, -CH_2-), 1.22 (40H, -$C_{10}H_{20}$-), 0.89−0.86 (6H, -CH_3) ppm. ^{13}C NMR ($CDCl_3$): δ = 164.1, 163.8, 143.8, 143.7, 143.6, 143.4, 143.2, 143.0, 142.5, 142.2, 141.8, 141.1, 136.4, 135.2, 132.1, 129.8, 129.6, 129.1, 128.4, 128.3, 128.1, 127.7, 126.4, 125.6, 125.3, 124.9, 99.7, 31.9, 30.7, 29.6, 26.6, 29.5, 29.5, 29.4, 29.3, 29.1, 22.7, 14.1 ppm.^{11}B NMR ($CDCl_3$): δ = 1.76 (t, J = 32 Hz) ppm.

Synthesis of P4F Compound **P4F** was prepared from **M4** (50 mg, 0.074 mmol) and 9,9-didodecylfluorene-2,7-diboronicacid **F** (44 mg, 0.074 mmol) in 80% yield (55 mg, yellow solid) according to the same method with **P1F**. M_n = 12,000, M_w/M_n = 1.9. ^{1}H NMR ($CDCl_3$): δ = 7.75–7.12

(24H, Ar-*H*), 5.76 (1H, -C*H*=), 1.99 (4H, -CH_2-), 1.26–1.03 (36H, -C_7H_{15}), 0.86-0.83 (6H, -CH_3), 0.64 (4H, -CH_2-) ppm. ^{13}C NMR ($CDCl_3$): δ = 164.0, 151.9, 142.6, 142.0, 140.6, 138.9, 135.3, 129.7, 128.4, 127.9, 126.7, 126.3, 126.2, 121.3, 120.2, 99.7, 55.4, 40.4, 31.9, 30.0, 29.6, 29.5, 29.5, 29.3, 29.2, 23.9, 22.9, 14.1 ppm. ^{11}B NMR ($CDCl_3$): δ = 1.76 (t, J = 31 Hz) ppm.

Synthesis of P4T Compound **P4T** was prepared from **M4** (50 mg, 0.074 mmol) and 4,4'-didodecyl-2,2'-bithiophene-5,5'-diboronic acid bis(pinacol) ester **T** (56 mg, 0.074 mmol) in 80% yield (56 mg, yellow solid) according to the same method with **P1F**. M_n = 7,200, M_w/M_n = 1.9. ^{1}H NMR ($CDCl_3$): δ = 7.47–6.97 (20H, Ar-*H*), 5.69 (1H, -C*H*=), 2.52–2.48 (4H, -CH_2-), 1.22 (40H, -$C_{10}H_{20}$-), 0.88-0.85 (6H, -CH_3) ppm. ^{13}C NMR ($CDCl_3$): δ = 163.8, 143.9, 142.6, 141.9, 135.4, 135.3, 129.9, 129.1, 128.4, 127.8, 126.4, 125.7, 125.6, 125.0, 99.5, 31.9, 30.7, 29.7, 29.7, 29.6, 29.5, 29.4, 29.4, 29.1, 22.7, 14.1 ppm. ^{11}B NMR ($CDCl_3$): δ = 1.66 (t, J = 31 Hz) ppm.

(a)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1.261
1.244
1.199
1.137
1.025
0.953
0.934
0.915
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0.857
0.848
0.831
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0.000
PPM
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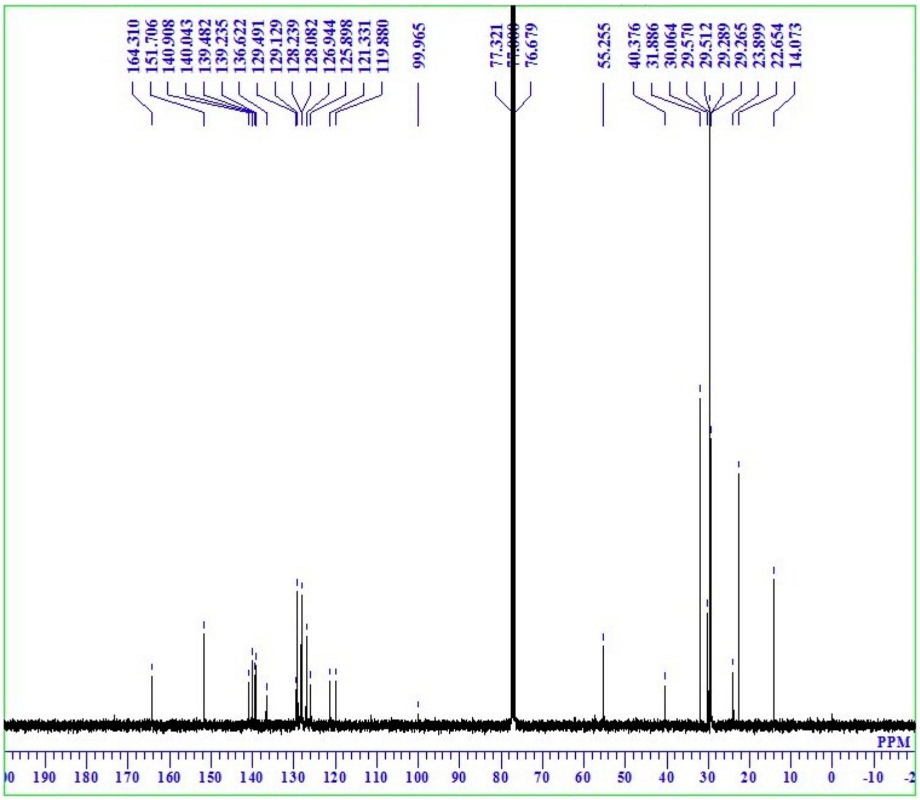
4
0

(b)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139.235
136.622
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129.129
128.239
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125.898
121.331
119.880
99.965
77.321
76.679
55.255
40.376
31.886
30.064
29.570
29.512
29.289
29.265
23.899
22.654
14.073
PPM
190
180
170
160
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80
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40
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20
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0
-10

(c)

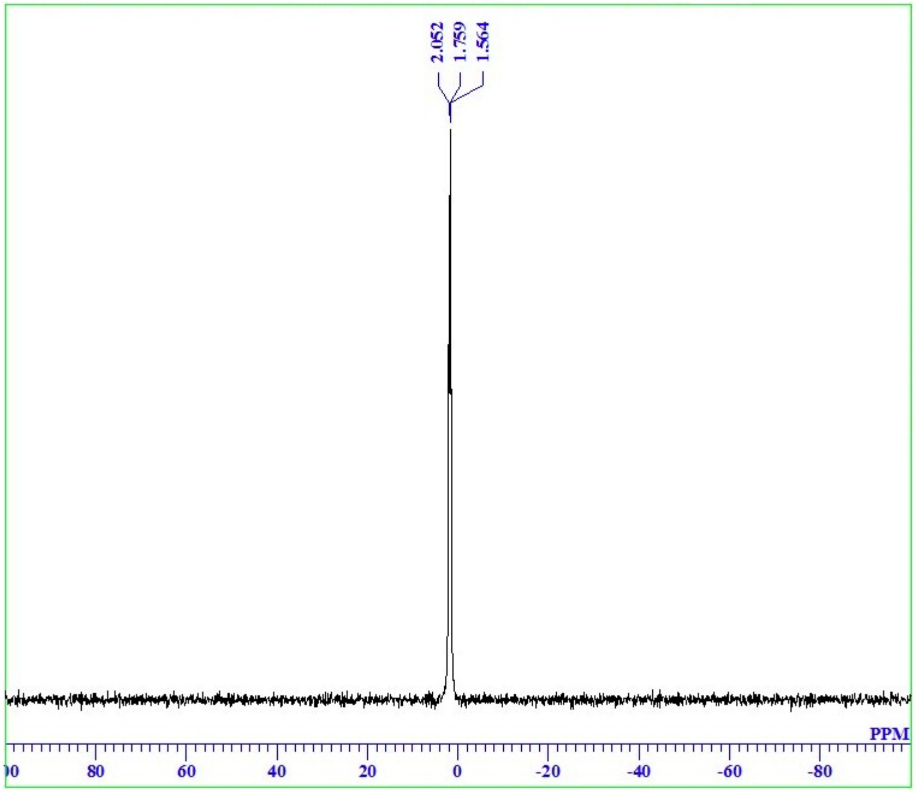
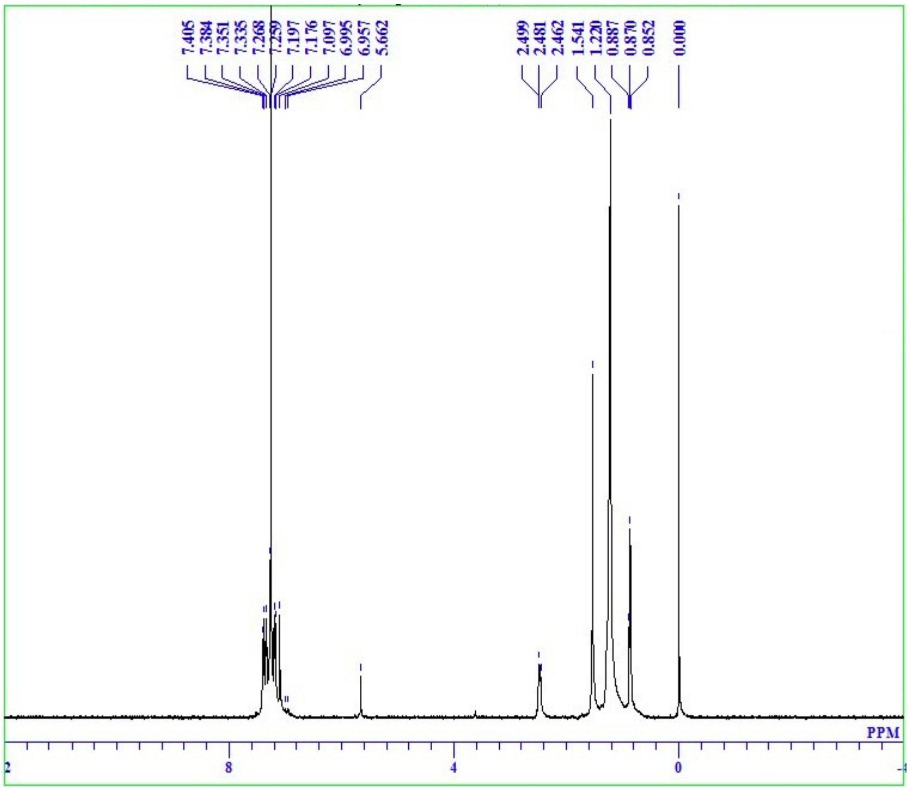


Figure S1. (a) ^{1}H, (b) ^{13}C, (c) ^{11}B NMR spectra of **P1F** in $CDCl_3$.

(a)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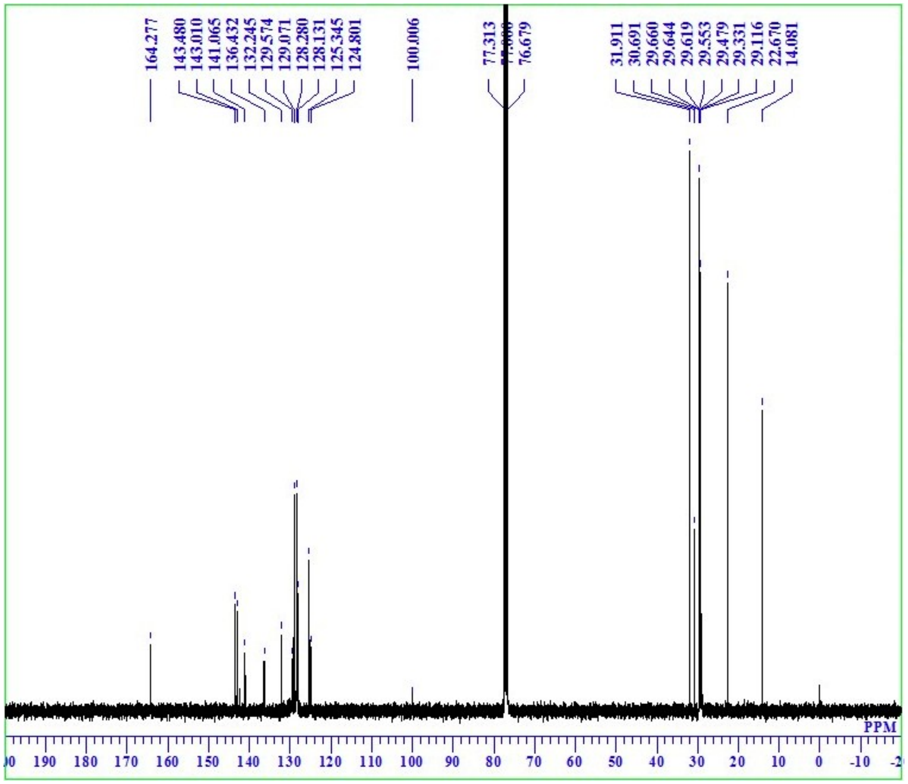
7.268
7.259
7.197
7.176
7.097
6.995
6.957
5.662
2.499
2.481
2.462
1.541
1.220
0.887
0.870
0.852
0.000
PPM
8
4
0

(b)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100.006
77.313
76.679
31.911
30.691
29.660
29.644
29.619
29.553
29.479
29.331
29.116
22.670
14.081
PPM
190
180
170
160
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-10

(c)

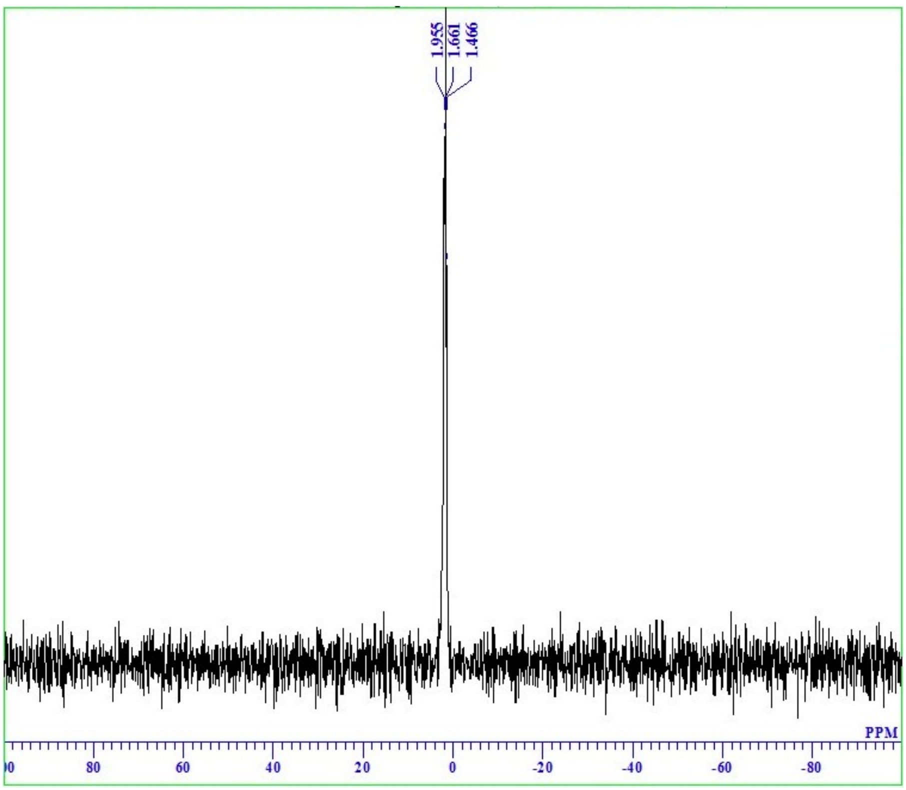
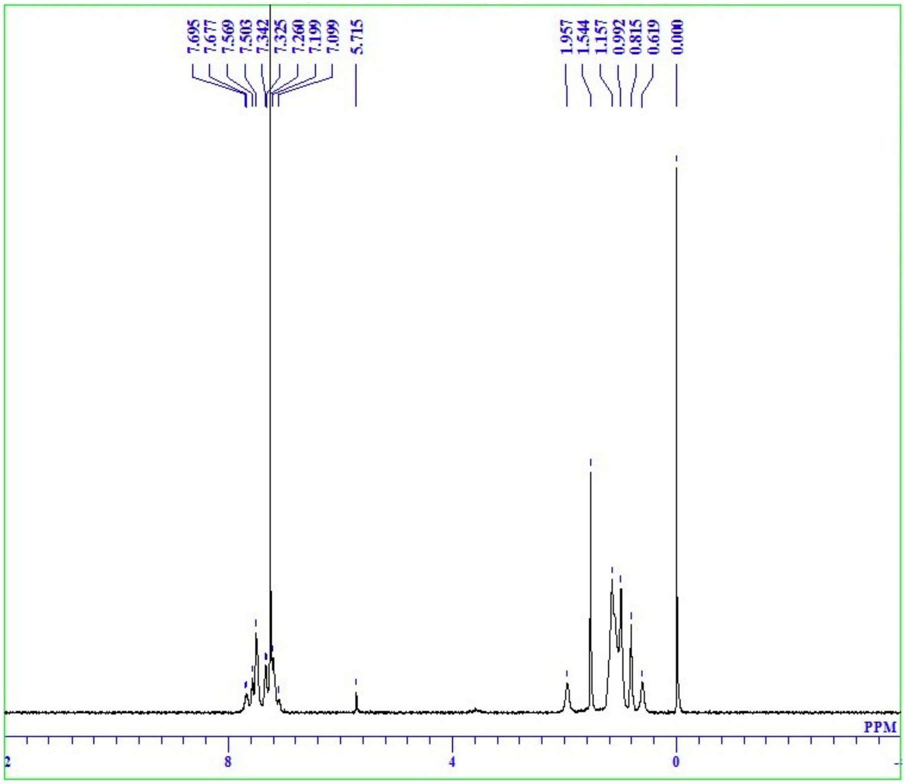


Figure S2. (a) ^{1}H, (b) ^{13}C, (c) ^{11}B NMR spectra of **P1T** in $CDCl_3$.

(a)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7.325
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0.619
0.000
PPM
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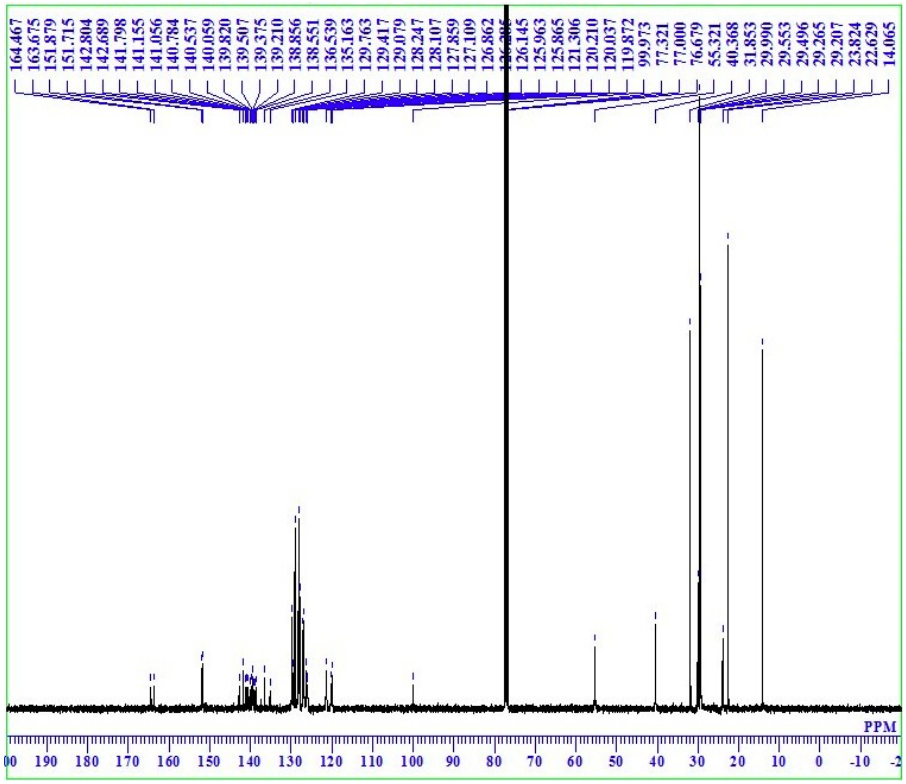
8
4
0
-

(b)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141.155
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140.784
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139.820
139.507
139.375
139.210
138.856
138.551
136.539
135.163
129.763
129.417
129.079
128.247
128.107
127.859
127.109
126.862
126.145
125.963
125.865
121.306
120.210
120.037
119.872
99.973
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77.000
76.679
55.321
40.368
31.853
29.990
29.553
29.496
29.265
29.207
23.824
22.629
14.065
PPM
00
190
180
170
160
150
140
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110
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10
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-10
-2

(c)

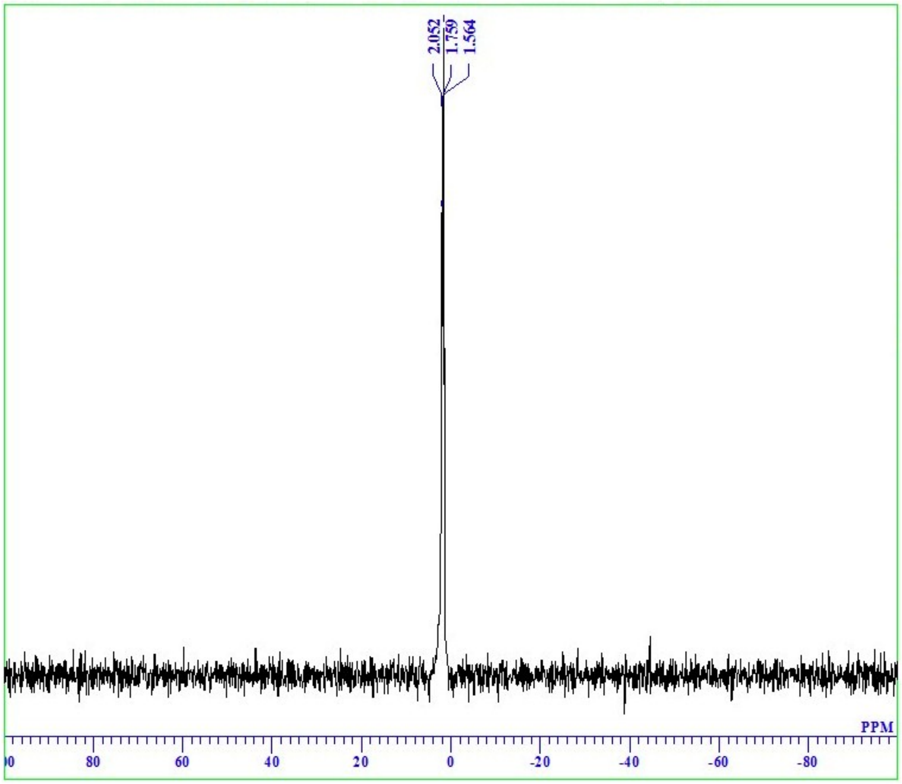
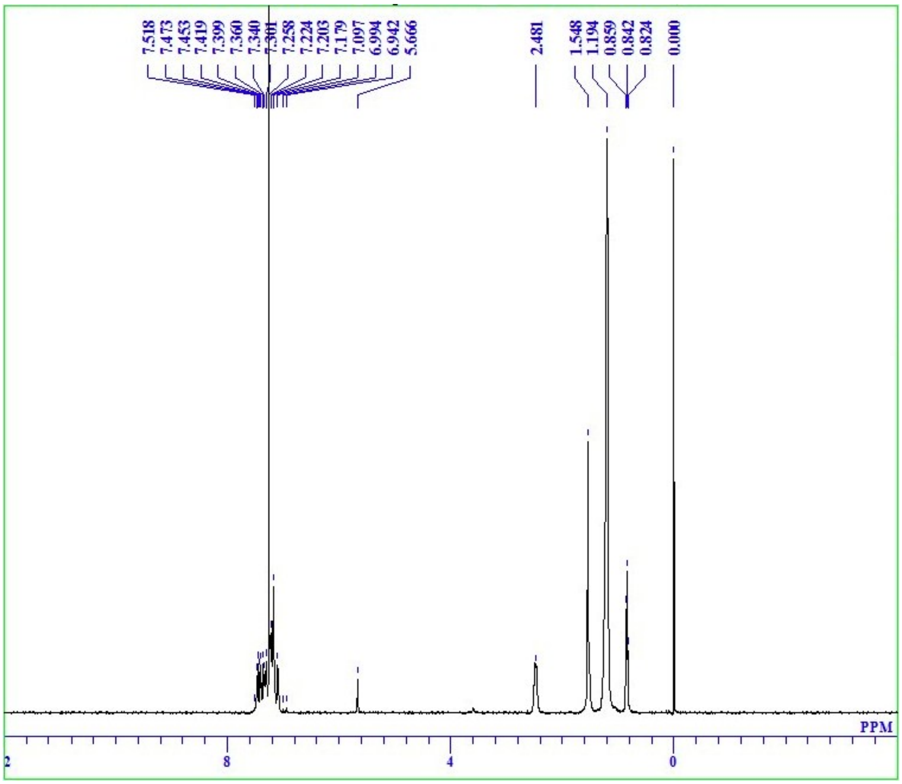


Figure S3. (a) ^{1}H, (b) ^{13}C, (c) ^{11}B NMR spectra of **P2F** in $CDCl_3$.

(a)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7.360
7.340
7.301
7.258
7.224
7.203
7.179
7.097
6.994
6.942
5.666
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1.194
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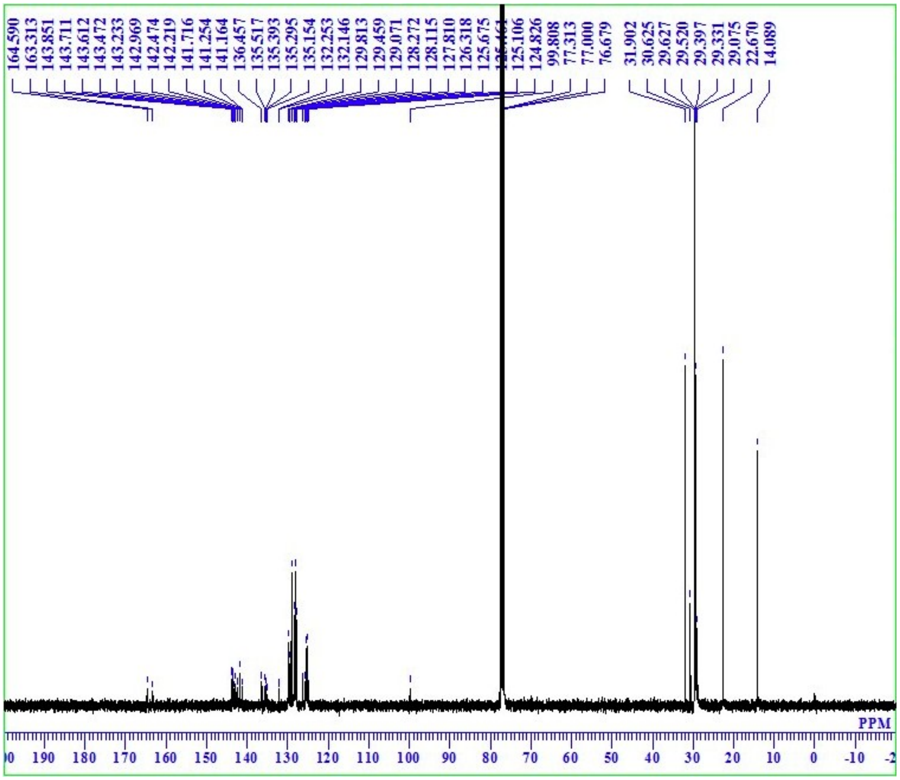
0.842
0.824
0.000
2
8
4
0
PPM

(b)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141.164
136.457
135.517
135.393
135.295
135.154
132.253
132.146
129.813
129.459
129.071
128.272
128.115
127.810
126.318
125.675
125.461
125.106
124.826
99.808
77.313
77.000
76.679
31.902
30.625
29.627
29.520
29.397
29.331
29.075
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14.089
00
190
180
170
160
150
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10
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-10
-2
PPM

(c)

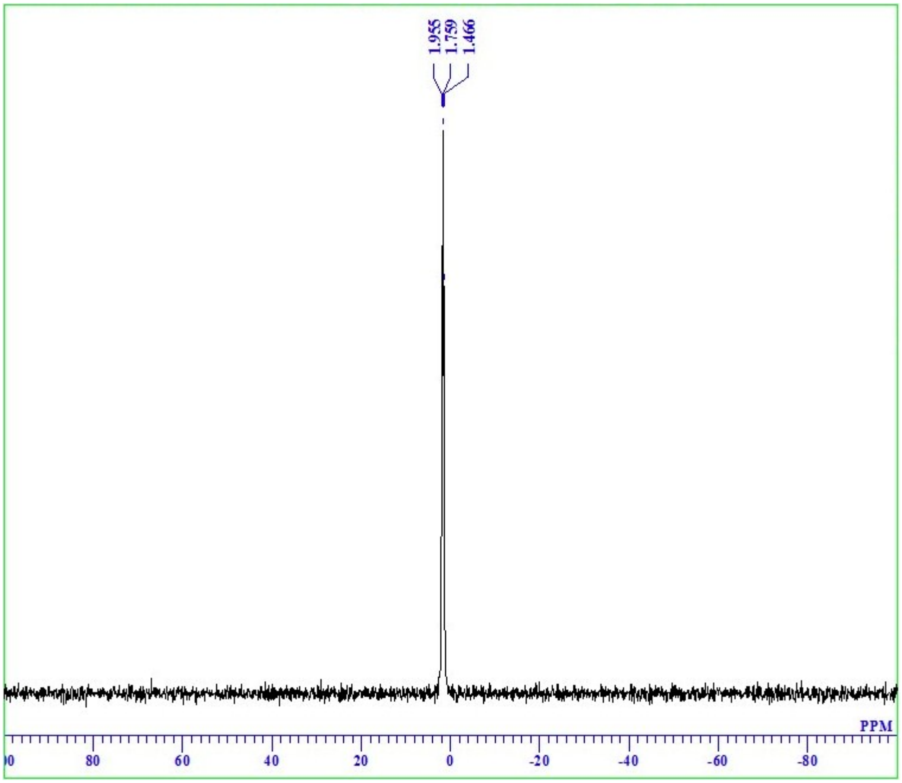
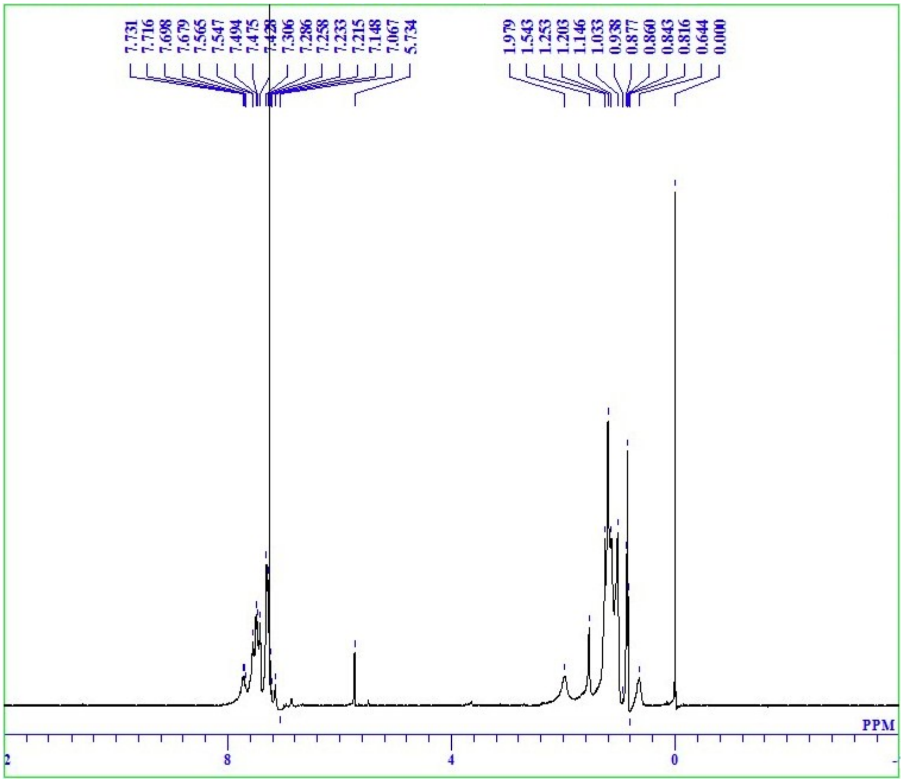


Figure S4. (a) ^{1}H, (b) ^{13}C, (c) ^{11}B NMR spectra of **P2T** in CDCl$_3$.

(a)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7.215
7.148
7.067
5.734
1.979
1.543
1.253
1.203
1.146
1.033
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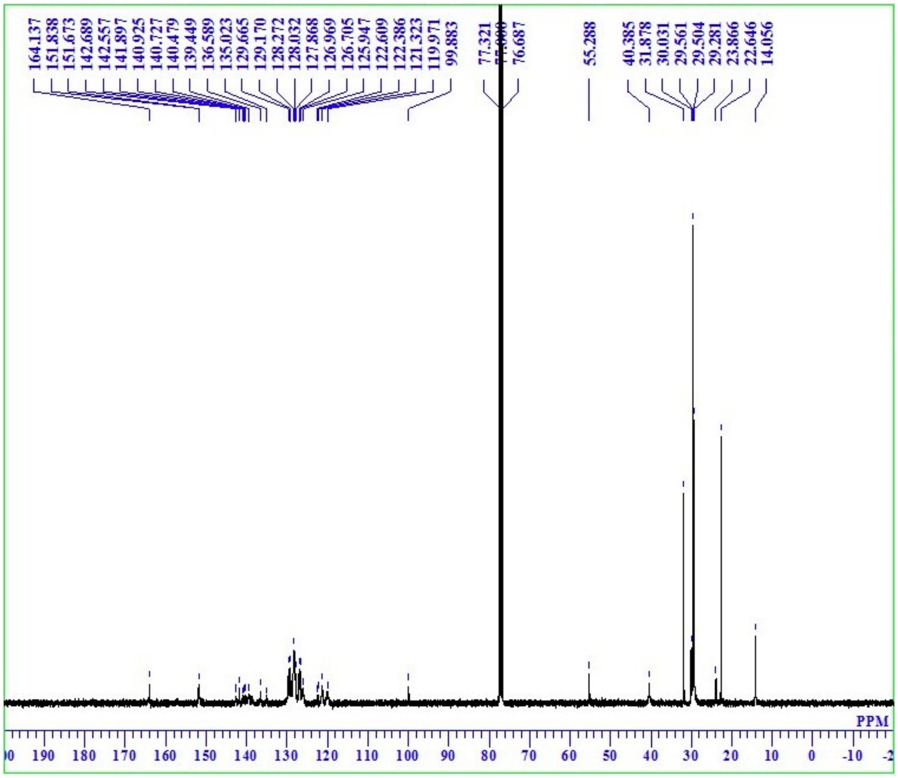
0.877
0.860
0.843
0.816
0.644
0.000
PPM
8
4
0

(b)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140.727
140.479
139.449
136.589
135.023
129.665
129.170
128.272
128.032
127.868
126.969
126.705
125.947
122.609
122.386
121.323
119.971
99.883
77.321
77.000
76.687
55.288
40.385
31.878
30.031
29.561
29.504
29.281
23.866
22.646
14.056
PPM
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

(c)

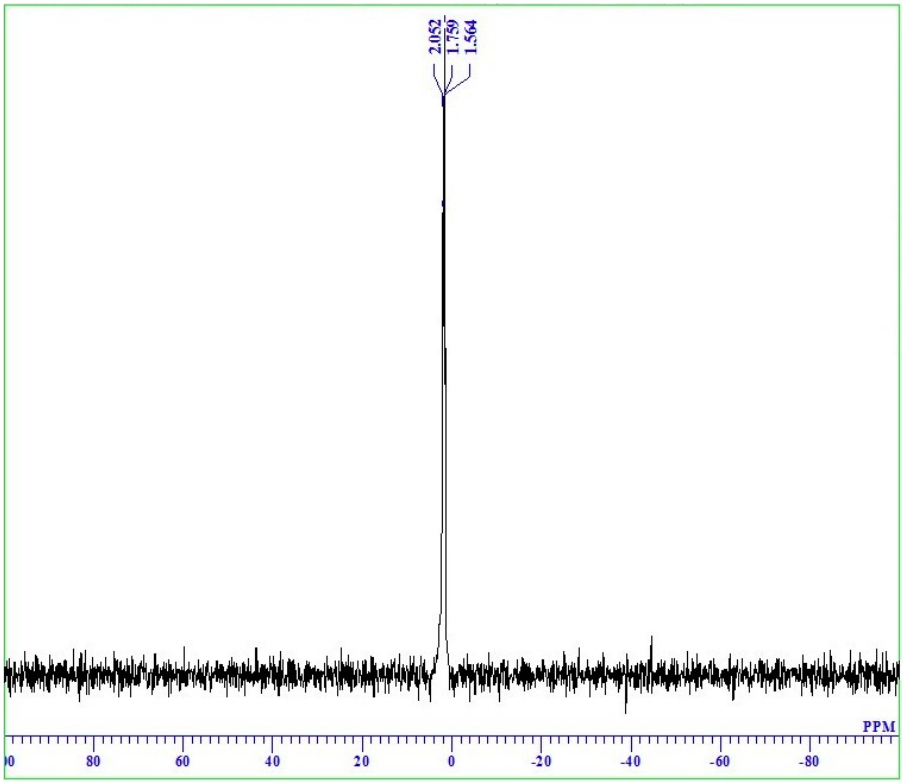
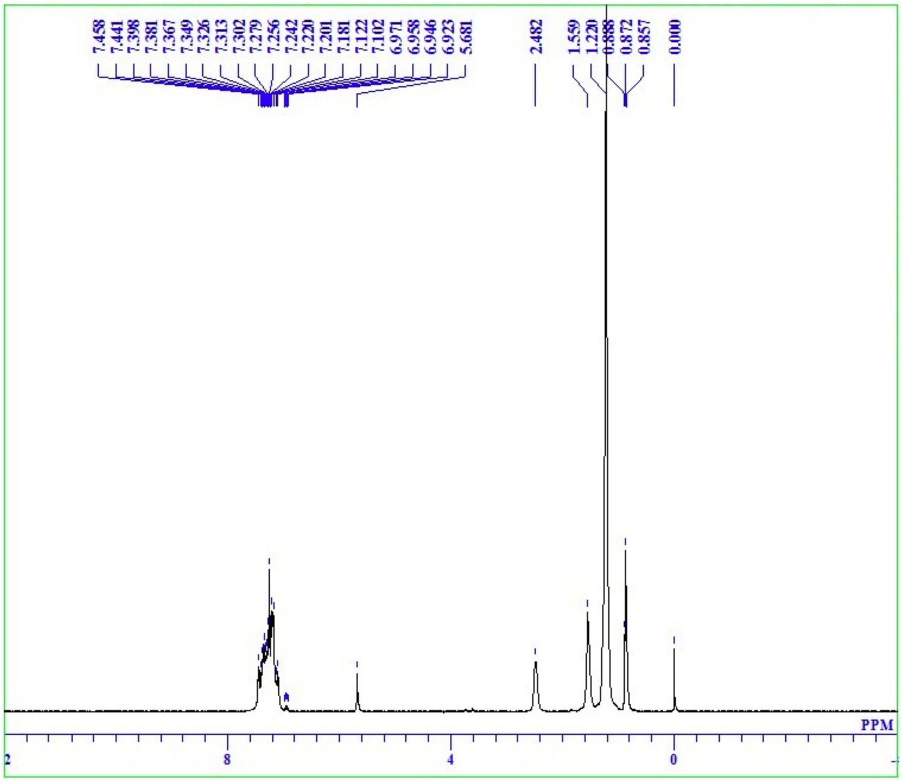


Figure S5. (a) ^{1}H, (b) ^{13}C, (c) ^{11}B NMR spectra of **P3F** in CDCl$_3$.

(a)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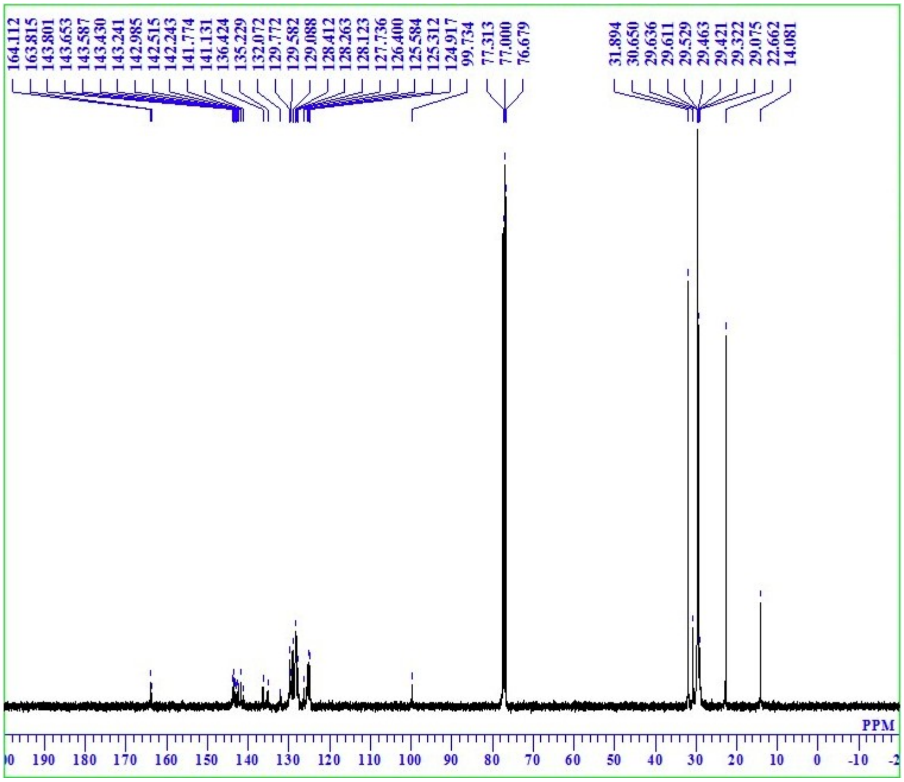
7.441
7.398
7.381
7.367
7.349
7.326
7.313
7.302
7.279
7.256
7.242
7.220
7.201
7.181
7.122
7.102
6.971
6.958
6.946
6.923
5.681
2.482
1.559
1.220
0.888
0.872
0.857
0.000
PPM
2
8
4
0

(b)


164.112
163.815
143.801
143.653
143.587
143.430
143.241
142.985
142.515
142.243
141.774
141.131
136.424
135.229
132.072
129.772
129.582
129.088
128.412
128.263
128.123
127.736
126.400
125.584
125.312
124.917
99.734
77.313
77.000
76.679
31.894
30.650
29.636
29.611
29.529
29.463
29.421
29.322
29.075
22.662
14.081
PPM
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

(c)

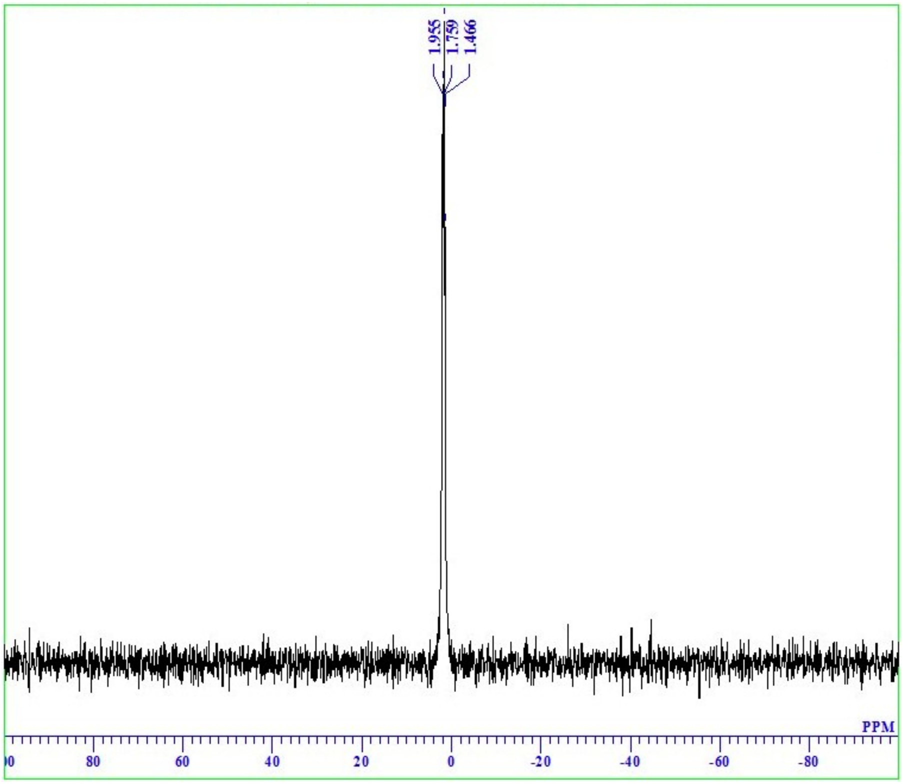
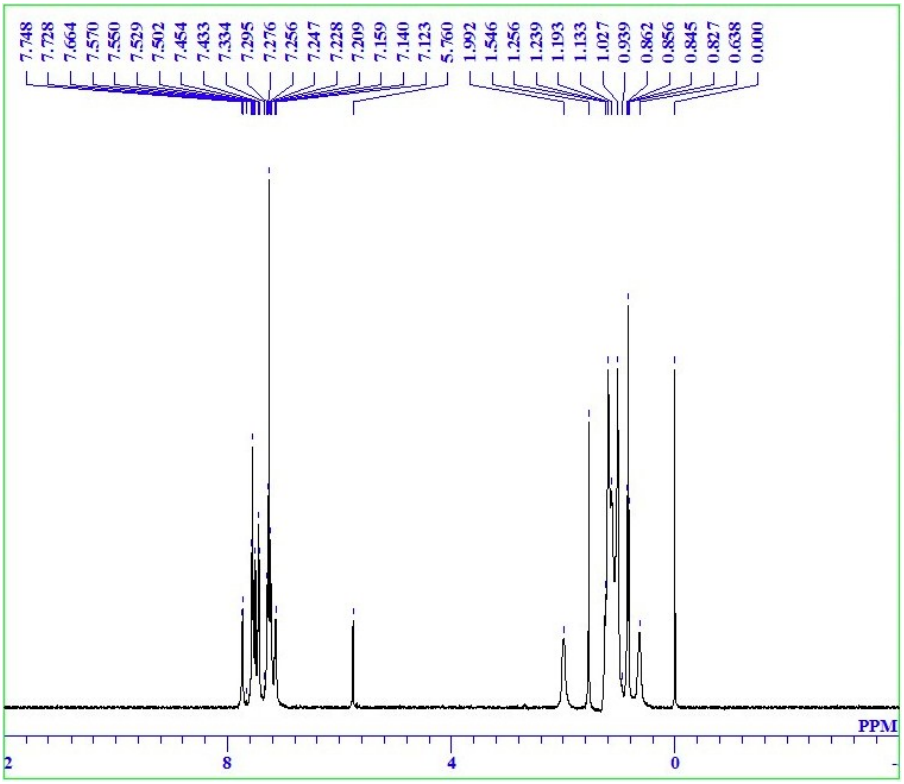


Figure S6. (a) ^{1}H, (b) ^{13}C, (c) ^{11}B NMR spectra of **P3T** in $CDCl_3$.

(a)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7.728
7.664
7.570
7.550
7.529
7.502
7.454
7.433
7.334
7.295
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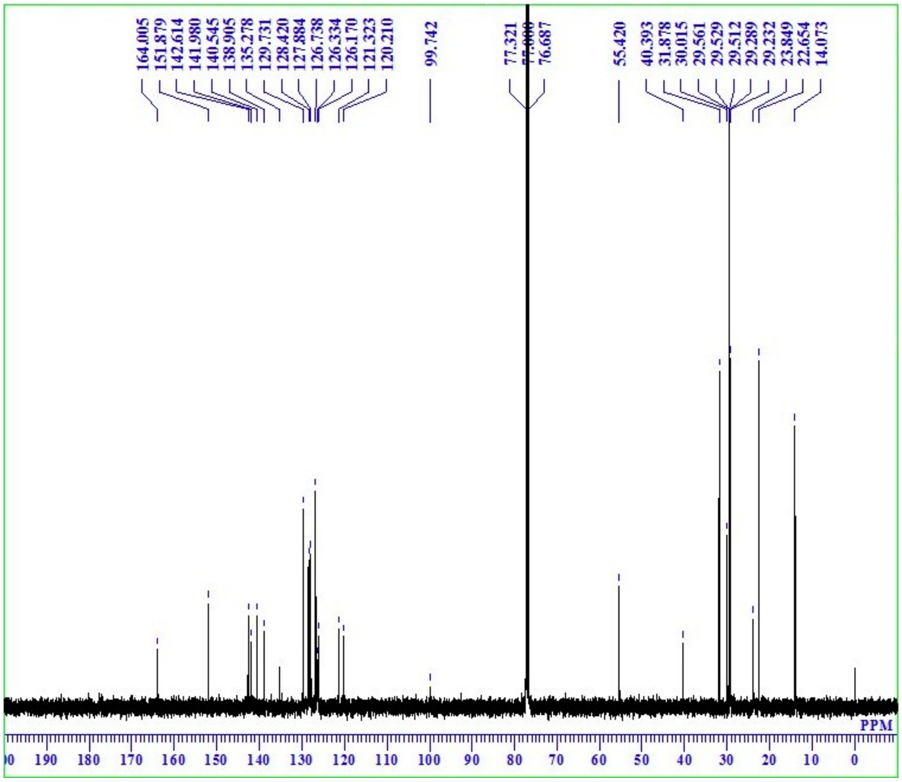
7.247
7.228
7.209
7.159
7.140
7.123
5.760
1.992
1.546
1.256
1.239
1.193
1.133
1.027
0.939
0.862
0.856
0.845
0.827
0.638
0.000
PPM
2
8
4
0

(b)


164.005
151.879
142.614
141.980
140.545
138.905
135.278
129.731
128.420
127.884
126.738
126.334
126.170
121.323
120.210
99.742
77.321
77.000
76.687
55.420
40.393
31.878
30.015
29.561
29.529
29.512
29.289
29.232
23.849
22.654
14.073
PPM
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

(c)

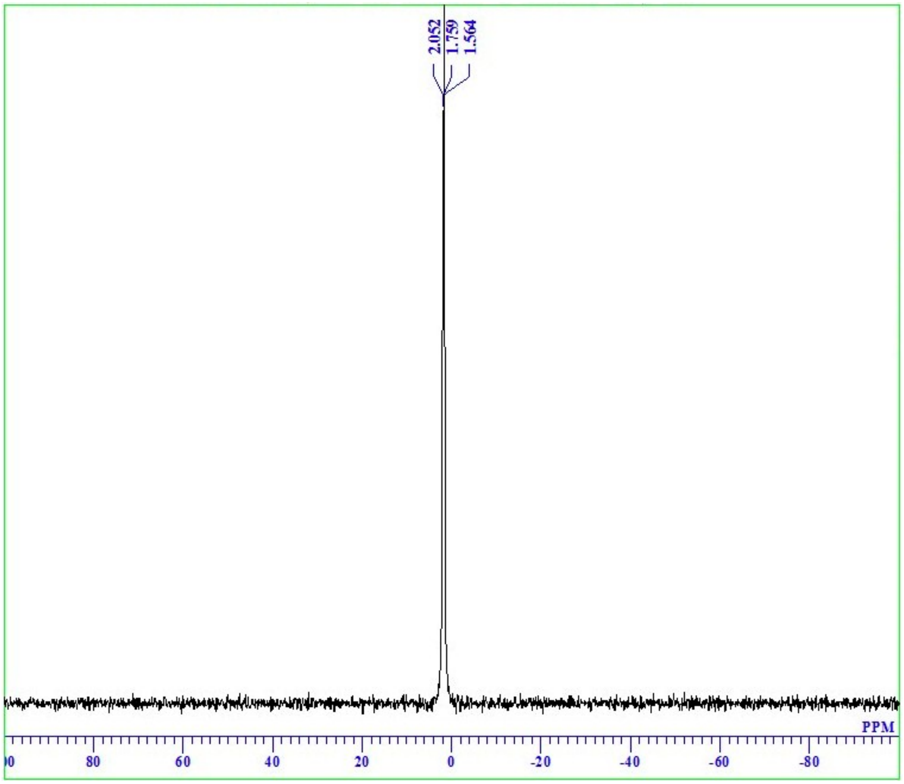
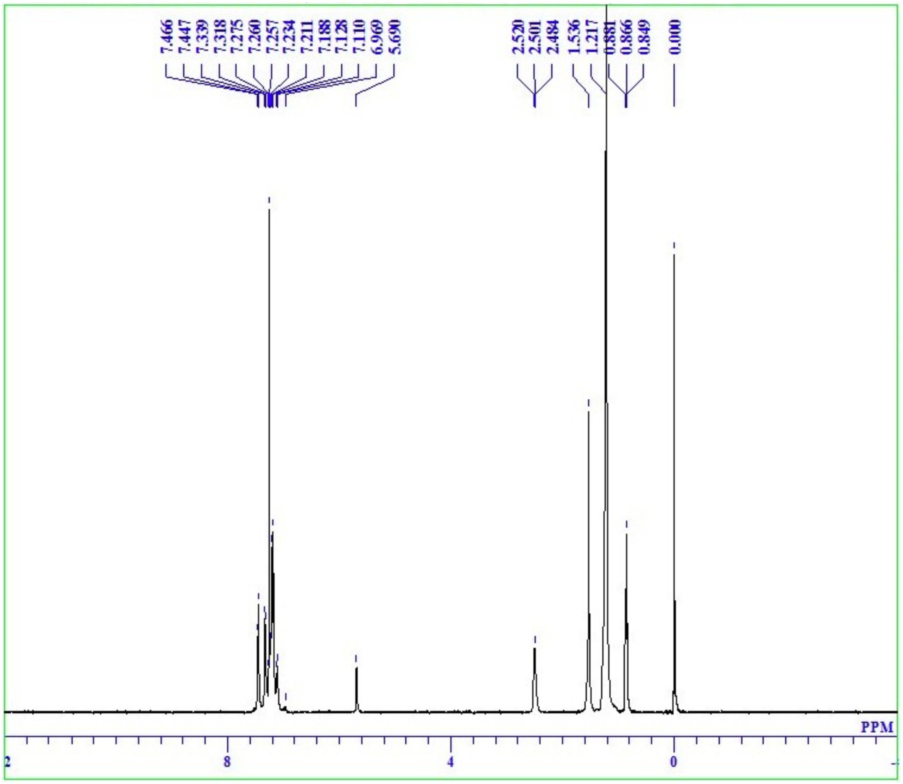


Figure S7. (a) ^{1}H, (b) ^{13}C, (c) ^{11}B NMR spectra of **P4F** in CDCl$_3$.

(a)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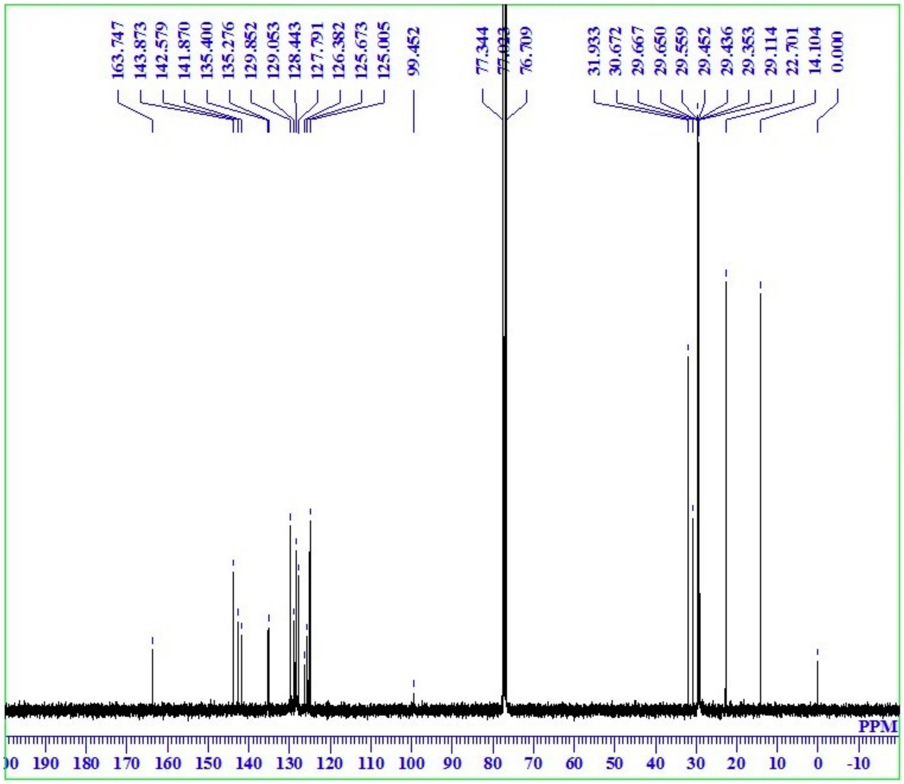
7.447
7.339
7.318
7.275
7.260
7.257
7.234
7.211
7.188
7.128
7.110
6.969
5.690
2.520
2.501
2.484
1.536
1.217
0.881
0.866
0.849
0.000
PPM
2
8
4
0

(b)


163.747
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142.579
141.870
135.400
135.276
129.852
129.053
128.443
127.791
126.382
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125.005
99.452
77.344
77.023
76.709
31.933
30.672
29.667
29.650
29.559
29.452
29.436
29.353
29.114
22.701
14.104
0.000
PPM
0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

(c)

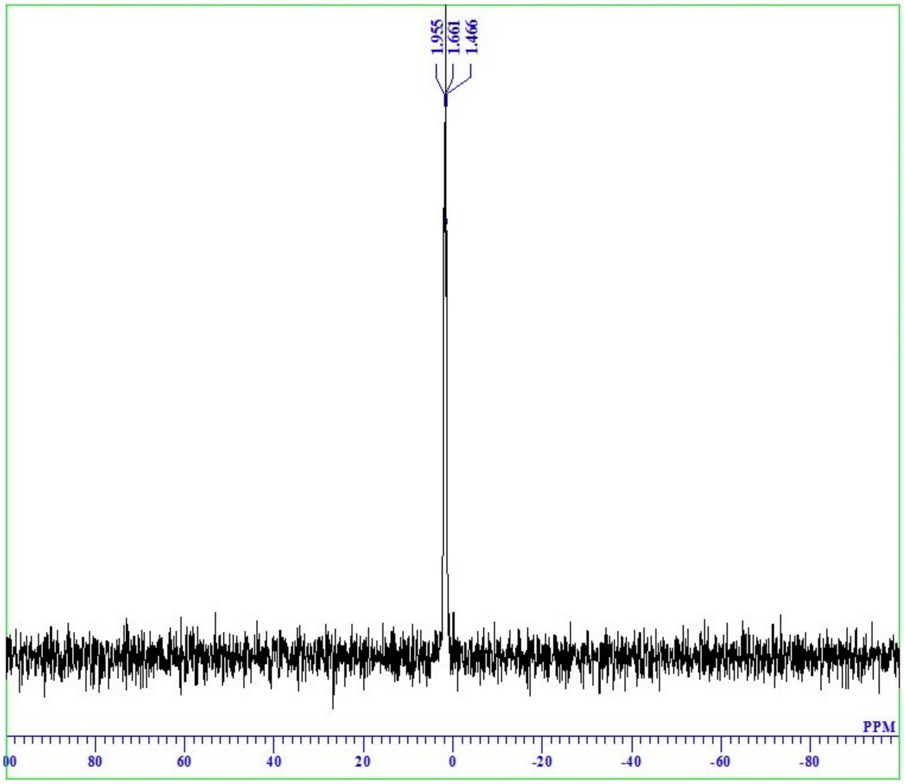

Figure S8. (a) ^{1}H, (b) ^{13}C, (c) ^{11}B NMR spectra of **P4T** in $CDCl_3$.

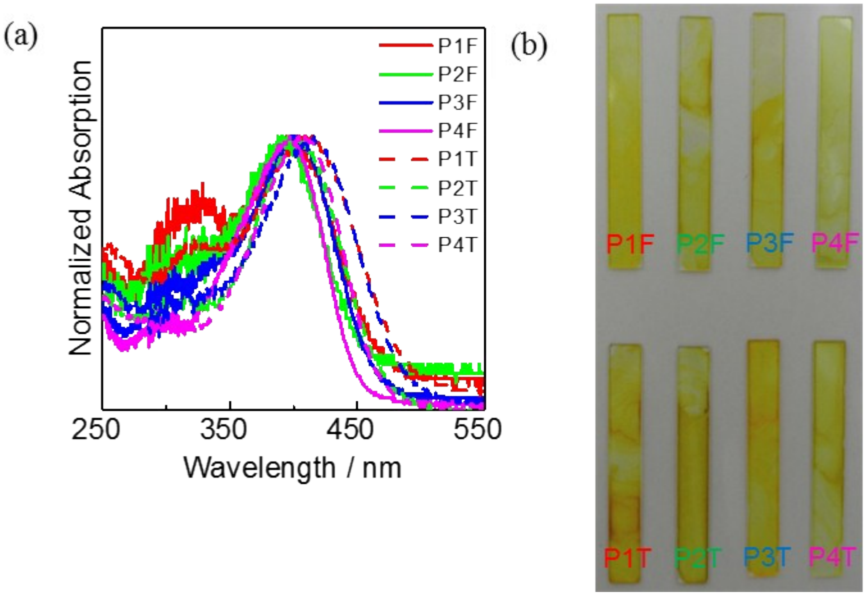

Figure S9. (a) UV−vis absorption spectra of each polymer in the film state. (b) Photograph of each polymer in the film state under visible irradiation.

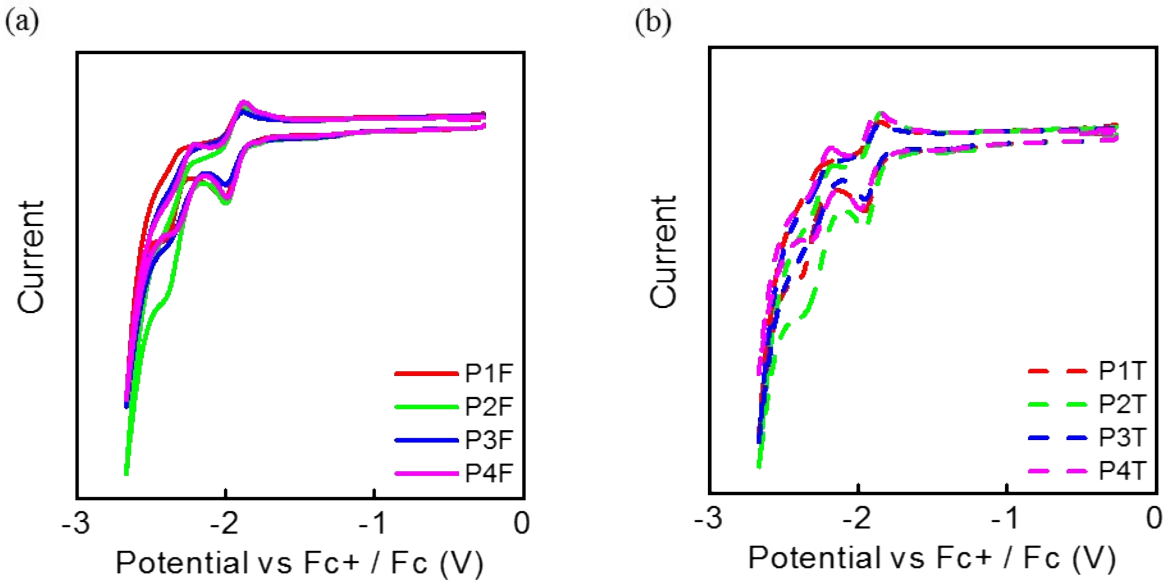

Figure S10. Cyclic voltammograms of (a) **P1F−P4F** and (b) **P1T−P4T** from 0 V to −2.4 V in CH_2Cl_2 (1×10^{-3} M) with 0.1 M Bu_4NPF_6 as a supporting electrolyte, AgCl/Ag as a reference electrode, Pt as working and counter electrodes, and scan rate at 100 mV/s.

Table S1. UV−vis absorption and electrochemical properties of the polymers

	$\lambda_{abs}{}^{a}$ (CHCl$_3$) [nm]	ε^{b} (CHCl$_3$) [M^{-1}cm^{-1}]	λ_{abs} (Film) [nm]	$E_g{}^{c}$ [eV]	$E_{red}{}^{d,e}$ [V]	HOMO[f] [eV]	LUMO[g] [eV]
P1F	397	50800	400	2.73	−1.85	-5.68	−2.95
P2F	388	53600	392	2.80	−1.84	-5.76	−2.96
P3F	397	56800	400	2.74	−1.83	-5.71	−2.97
P4F	392	50700	397	2.83	−1.84	-5.79	−2.96
P1T	402	34800	409	2.63	−1.81	-5.63	−2.99
P2T	396	31000	404	2.70	−1.81	-5.69	−2.99
P3T	404	40400	416	2.65	−1.81	-5.64	−2.99
P4T	401	37600	407	2.73	−1.82	-5.71	−2.98

[a] UV−vis spectra were measured in CHCl$_3$ (1.0 × 10^{-5} M).

[b] Molar absorption coefficients at the peak top wavelength.

[c] The optical band gap estimated from the onset wavelength of the UV−vis spectra in CHCl$_3$.

[d] CV was carried out in CH$_2$Cl$_2$ with 0.1 M Bu$_4$NPF$_6$ as supporting electrolyte.

[e] E_{red} is the onset potential of first reduction wave.

[f] Calculated from LUMO and optical band gap (E_g), HOMO = LUMO − E_g (eV).

[g] Calculated from the empirical formula, LUMO = −E_{red} − 4.80 (eV).[3]

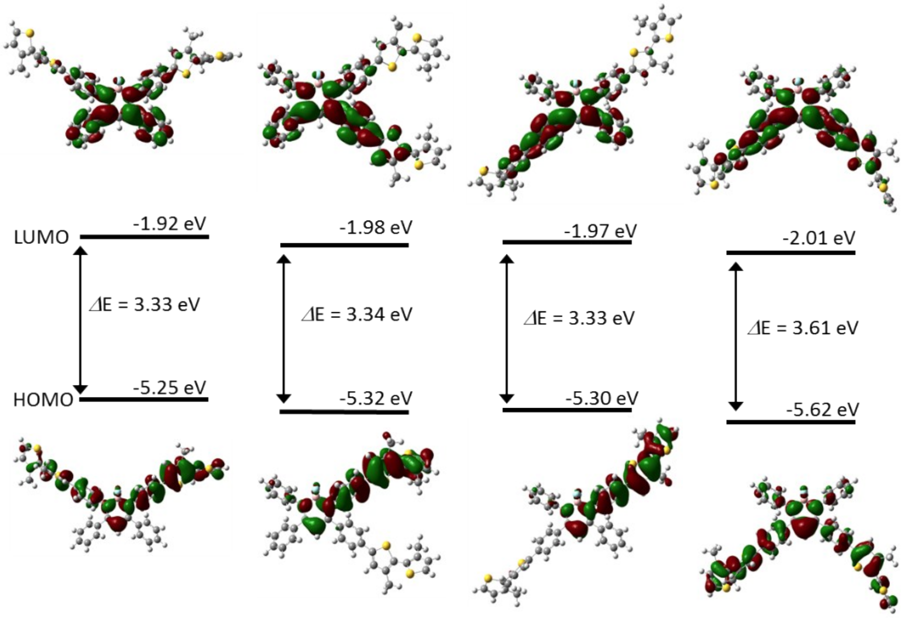

Figure S11. Structures and molecular orbital diagrams of the LUMO and HOMO of the model compounds with bithiophene obtained from the DFT calculations (B3LYP/6-31G (d)//B3LYP/6-31G (d)).[4]

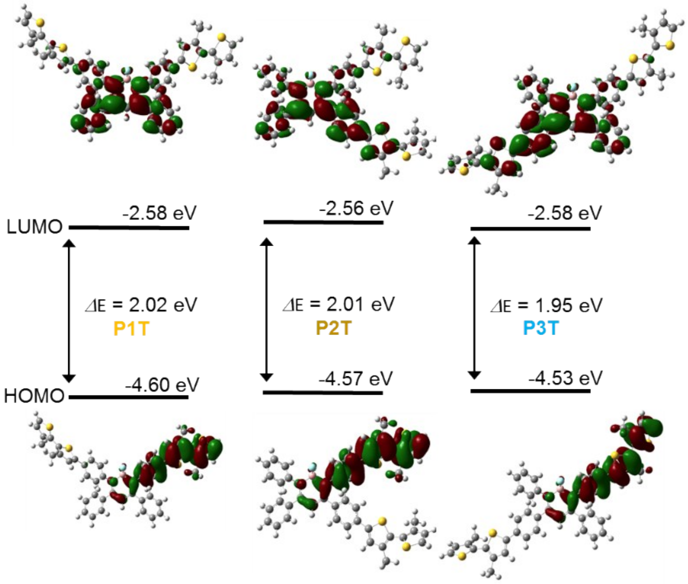

Figure S12. Structures and molecular orbital diagrams of the LUMO and HOMO of the model compounds with bithiophene obtained from the TD-DFT calculations (B3LYP/6-31G (d)//B3LYP/6-31G (d)).[4]

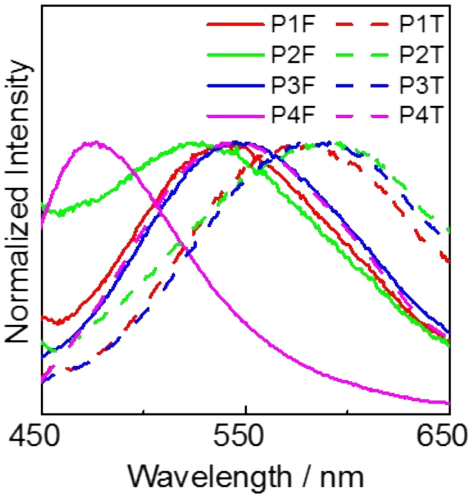

Figure S13. PL spectra of the polymers in $CHCl_3$ (1.0×10^{-5} M).

Lippert–Mataga Plots

Lippert–Mataga plots were conducted with the following formula.[5]

$$\Delta\nu = \nu_1 - \nu_0 = \frac{2(\mu_1 - \mu_0)^2}{hca^3}\Delta f + k \qquad (1)$$

$$\Delta f = \frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{n^2 - 1}{2(2n^2 + 1)} \qquad (2)$$

where $\Delta\nu$ is the Stokes shift, h is the Planck constant, c is the velocity of light, a is the Onsager radius of the chromophore, ε is the dielectric constant of the solvent, n is the refractive index of the solvent, and μ_1 and μ_0 are the dipole moments in the excited (1) and ground (0) states, respectively.

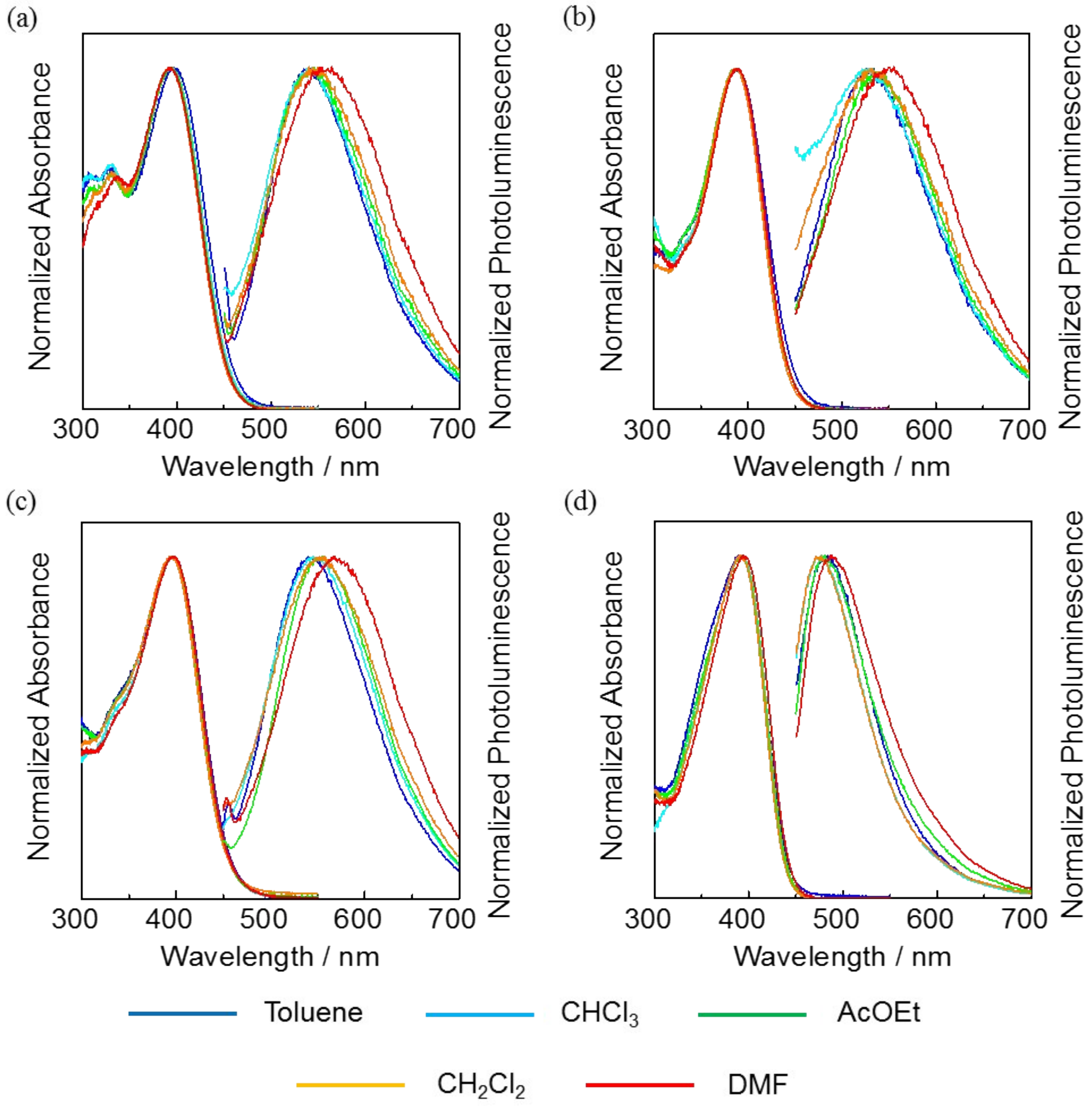

Figure S14. Normalized UV–vis absorption and photoluminescence spectra of (a) **P1F** (b) **P2F** (c) **P3F** (d) **P4F** in various solvents (1.0×10^{-5} M).

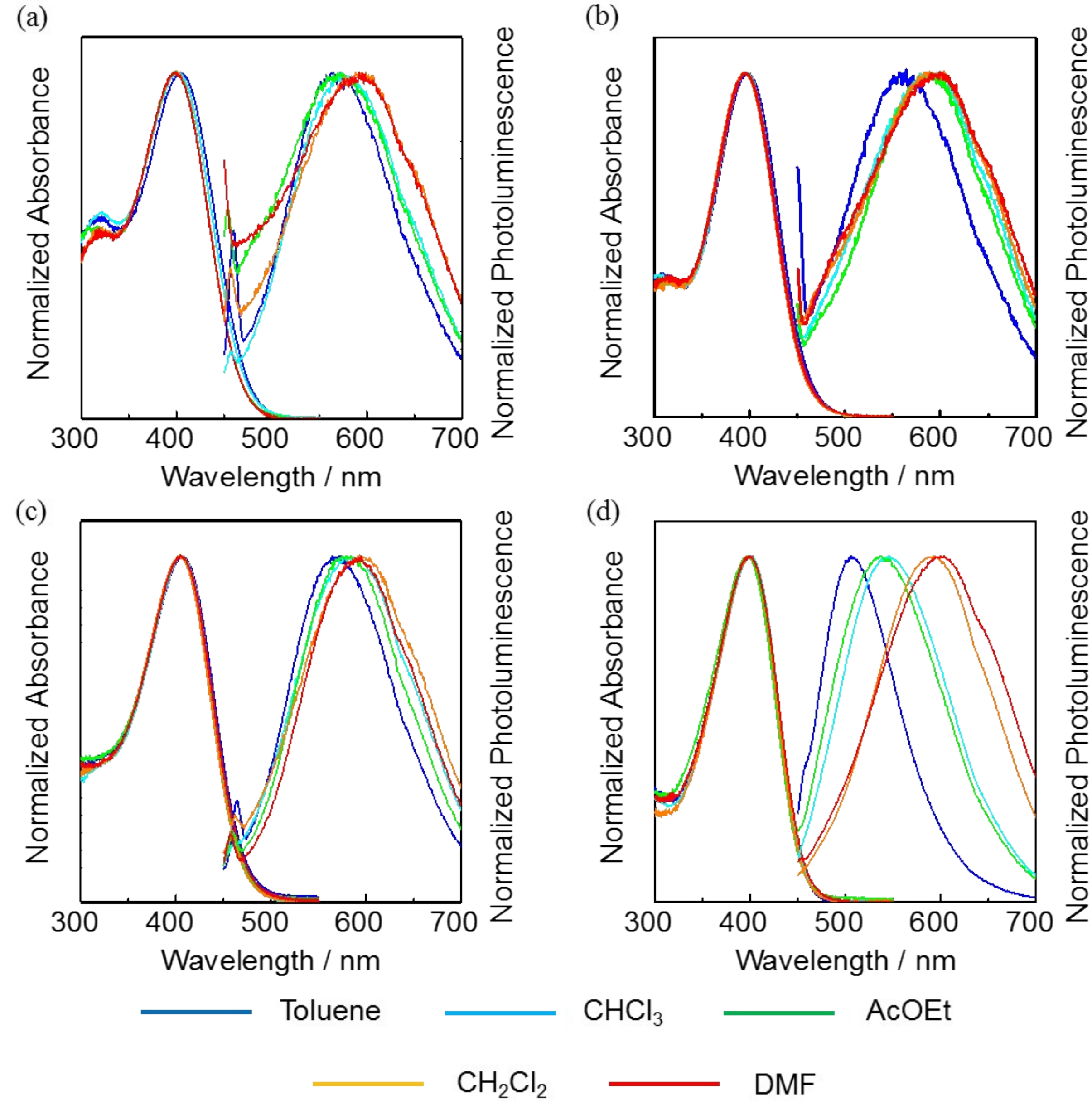

Figure S15. Normalized UV–vis absorption and photoluminescence spectra of (a) **P1T** (b) **P2T** (c) **P3T** (d) **P4T** in various solvents (1.0×10^{-5} M).

Table S2. Photophysical properties of **P1F** in various solvents (1.0×10^{-5} M)

Solvent	λ_{abs} [nm]	λ_{PL} [nm]	Stokes shift [cm^{-1}]
toluene	397	544	6807
$CHCl_3$	393	545	7097
AcOEt	394	547	7115
CH_2Cl_2	394	550	7215
DMF	393	552	7345

Table S3. Photophysical properties of **P2F** in various solvents (1.0×10^{-5} M)

Solvent	λ_{abs} [nm]	λ_{PL} [nm]	Stokes shift [cm^{-1}]
toluene	389	526	6696
$CHCl_3$	387	529	6952
AcOEt	386	533	7145
CH_2Cl_2	386	532	7126
DMF	389	545	7375

Table S4. Photophysical properties of **P3F** in various solvents (1.0×10^{-5} M)

Solvent	λ_{abs} [nm]	λ_{PL} [nm]	Stokes shift [cm^{-1}]
toluene	398	540	6639
$CHCl_3$	396	545	6936
AcOEt	396	555	7266
CH_2Cl_2	393	557	7492
DMF	397	568	7583

Table S5. Photophysical properties of **P4F** in various solvents (1.0×10^{-5} M)

Solvent	λ_{abs} [nm]	λ_{PL} [nm]	Stokes shift [cm^{-1}]
toluene	391	482	4840
$CHCl_3$	391	477	4644
AcOEt	391	481	4785
CH_2Cl_2	393	477	4459
DMF	395	489	4878

Table S6. Photophysical properties of **P1T** in various solvents (1.0×10^{-5} M)

Solvent	λ_{abs} [nm]	λ_{PL} [nm]	Stokes shift [cm^{-1}]
toluene	405	570	7163
$CHCl_3$	401	574	7532
AcOEt	399	573	7627
CH_2Cl_2	401	588	7962
DMF	399	592	8171

Table S7. Photophysical properties of **P2T** in various solvents (1.0×10^{-5} M)

Solvent	λ_{abs} [nm]	λ_{PL} [nm]	Stokes shift [cm^{-1}]
toluene	397	557	7236
$CHCl_3$	397	592	8283
AcOEt	395	585	8222
CH_2Cl_2	395	587	8298
DMF	396	600	8604

Table S8. Photophysical properties of **P3T** in various solvents (1.0×10^{-5} M)

Solvent	λ_{abs} [nm]	λ_{PL} [nm]	Stokes shift [cm^{-1}]
toluene	407	573	7118
$CHCl_3$	404	581	7541
AcOEt	405	594	7856
CH_2Cl_2	405	594	7856
DMF	405	600	8025

Table S9. Photophysical properties of **P4T** in various solvents (1.0×10^{-5} M)

Solvent	λ_{abs} [nm]	λ_{PL} [nm]	Stokes shift [cm^{-1}]
toluene	401	506	5175
$CHCl_3$	402	545	6541
AcOEt	396	538	6665
CH_2Cl_2	401	594	8134
DMF	399	600	8396

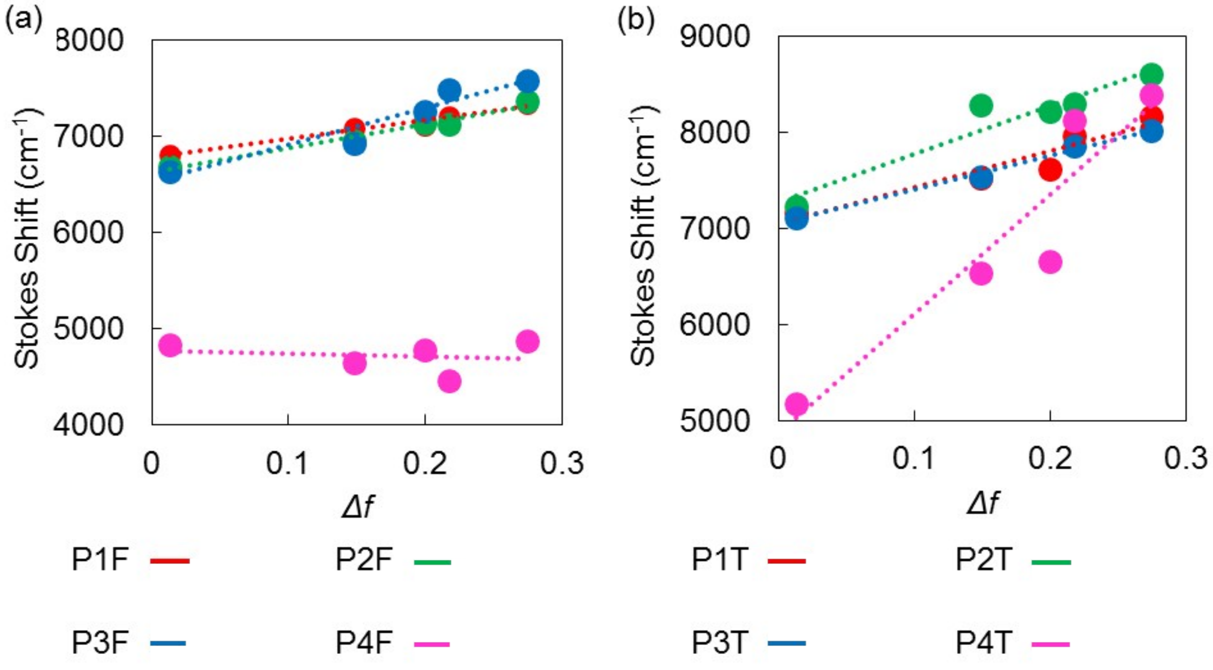

Figure S16. Lippert–Mataga plots for (**a**) **P1F−P4F** (**b**) **P1T−P4T**. Solvents and Δ*f*: toluene, 0.0132; chloroform, 0.148; ethyl acetate, 0.200; dichloromethane, 0.217; dimethylformamide, 0.274.

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2) Yamaguchi, M.; Ito, S.; Hirose, A.; Tanaka, K.; Chujo, Y. *J. Mater. Chem. C* **2016**, *3*, 5314.

3) Chen, C.-P.; Chan, S.-H.; Chao, T.-C.; Ting, C.; Ko, B.-T. *J. Am. Chem. Soc.* **2008**, *130*, 12828.

4) Frish, M. J. *et al*. GAUSSIAN 09 (Revision D.01), Gaussian, Inc., Wallingford CT, 2009.

5) (a) Valeur, B. Molecular Fluorescence: Principles and Applications, Wiley-VCH, Weinheim, 2002. (b) Kulkarni, P. A.; Wu, P. T.; Kwon, T. W.; Jenekhe, S. A. *J. Phys. Chem. B* **2005**, *109*, 19584. (c) Filarowski, A.; Kluba, M.; Cieślik-Boczula, K.; Koll, A.; Kochel, A.; Pandey, L.; De Borggraeve, W. M.; Auweraer, M. V. d.; Catalán, J.; Boens, N. *Photochem. Photobiol. Sci.*, **2010**, *9*, 996. (d) Pina, J.; de Melo, J. S.; Breusov, D.; Scherf, U. *Phys. Chem. Chem. Phys.* **2013**, *15*, 15204.