Electronic Supplementary Information

Three-dimensional π-conjugated compounds as non-fullerene acceptors in organic photovoltaics: the influence of acceptor unit orientation at phase interfaces on photocurrent generation efficiency

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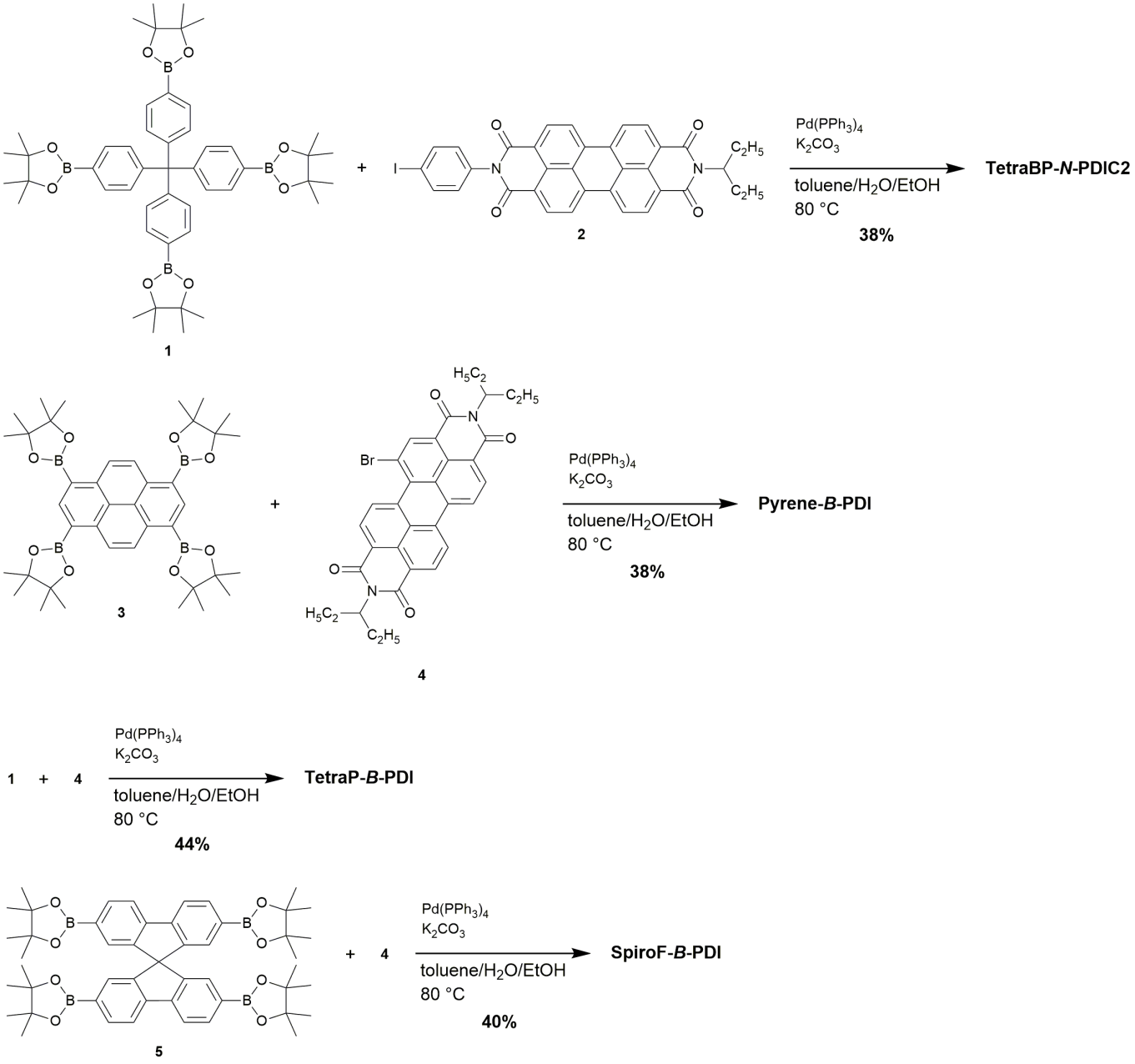
Schemes, Figures, and Tables



Scheme S1 Synthesis of PDI-based non-fullerene acceptors.

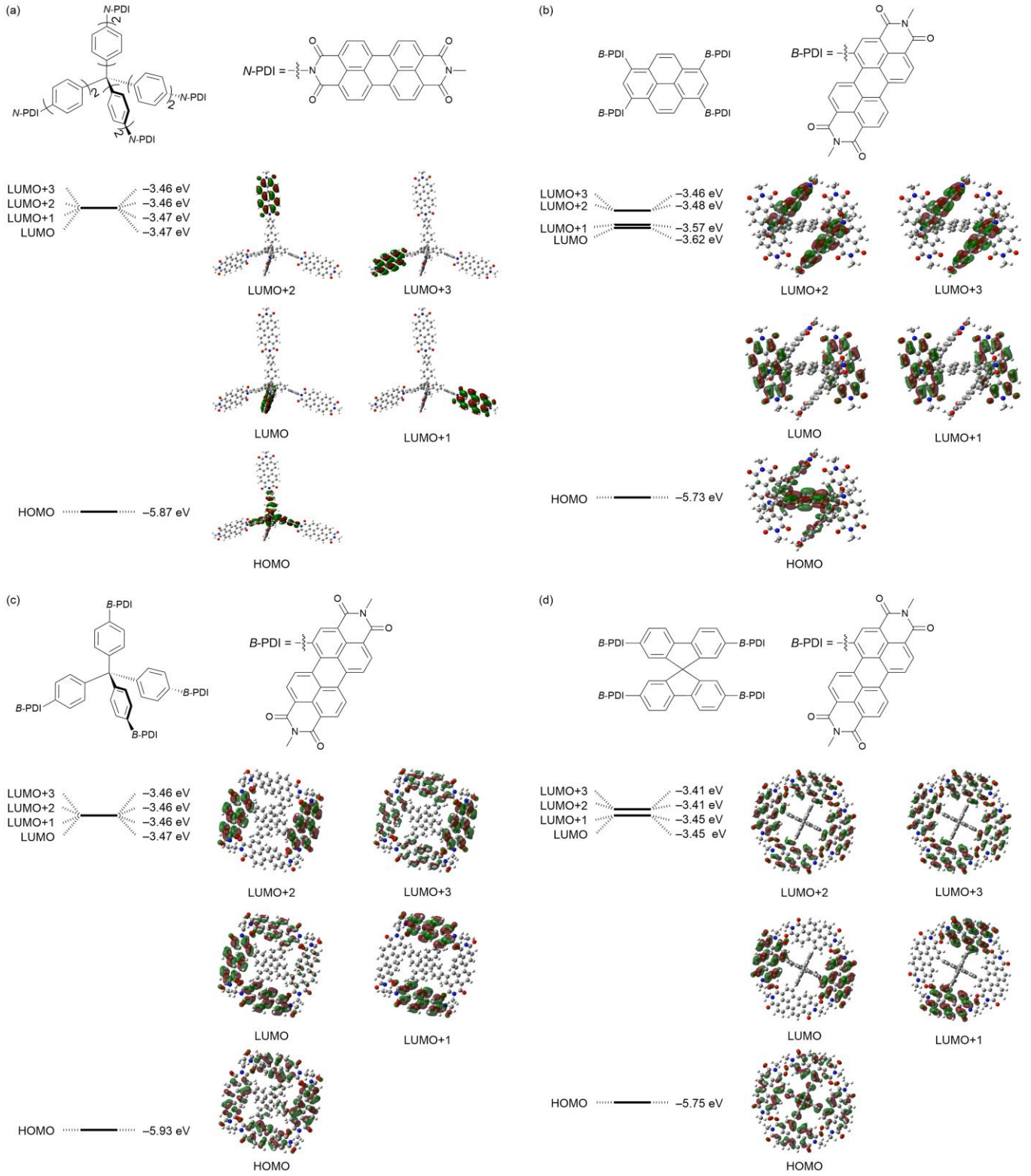


Fig. S1 Calculated structures and molecular orbitals of model compounds for (a) **TetraBP-*N*-PDIC9** and **TetraBP-*N*-PDIC2**, (b) **Pyrene-*B*-PDI**, (c) **TetraP-*B*-PDI**, and (d) **SpiroF-*B*-PDI**. All alkyl groups were replaced with methyl groups to ease the calculation.

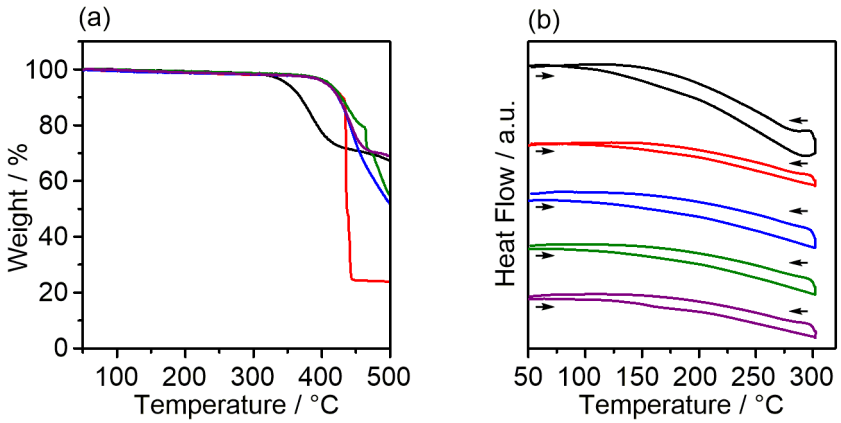


Fig. S2 (a) TGA and (b) DSC curves of **TetraBP-*N*-PDIC9** (black), **TetraBP-*N*-PDIC2** (red), **Pyrene-*B*-PDI** (blue), **TetraP-*B*-PDI** (green), and **SpiroF-*B*-PDI** (purple) with a scanning rate of 10 °C min^{-1} under N_2.

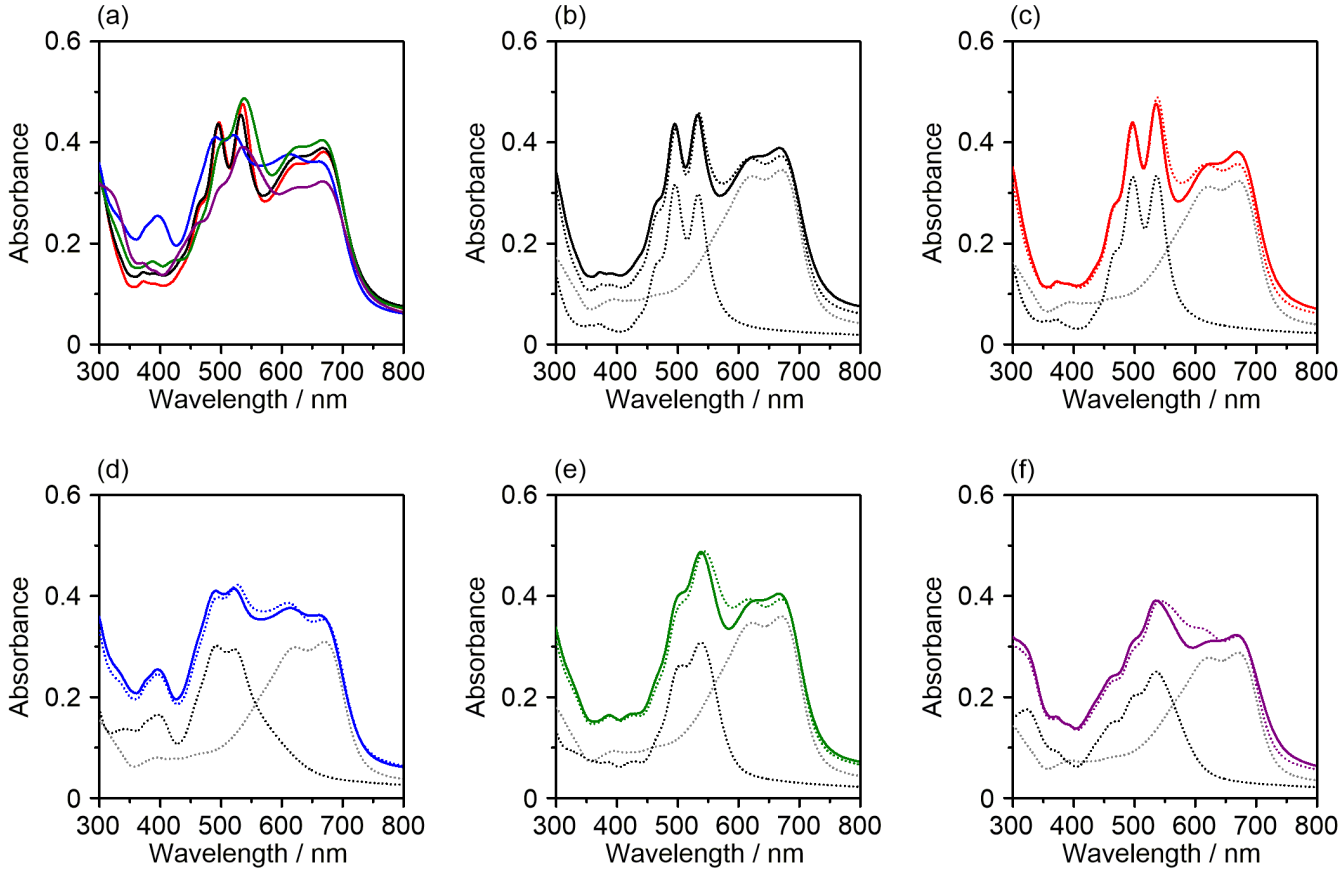


Fig. S3 (a) UV-vis absorption spectra of **PTB7**/**TetraBP-*N*-PDIC9** (black), **PTB7**/**TetraBP-*N*-PDIC2** (red), **PTB7**/**Pyrene-*B*-PDI** (blue), **PTB7**/**TetraP-*B*-PDI** (green), and **PTB7**/**SpiroF-*B*-PDI** (purple) blended films. (b–f) UV-vis absorption spectra of **PTB7**/acceptor blended films (solid line), **PTB7** (gray dotted line), acceptor (black dotted line), and summed spectra of **PTB7** and acceptor (colored dotted line).

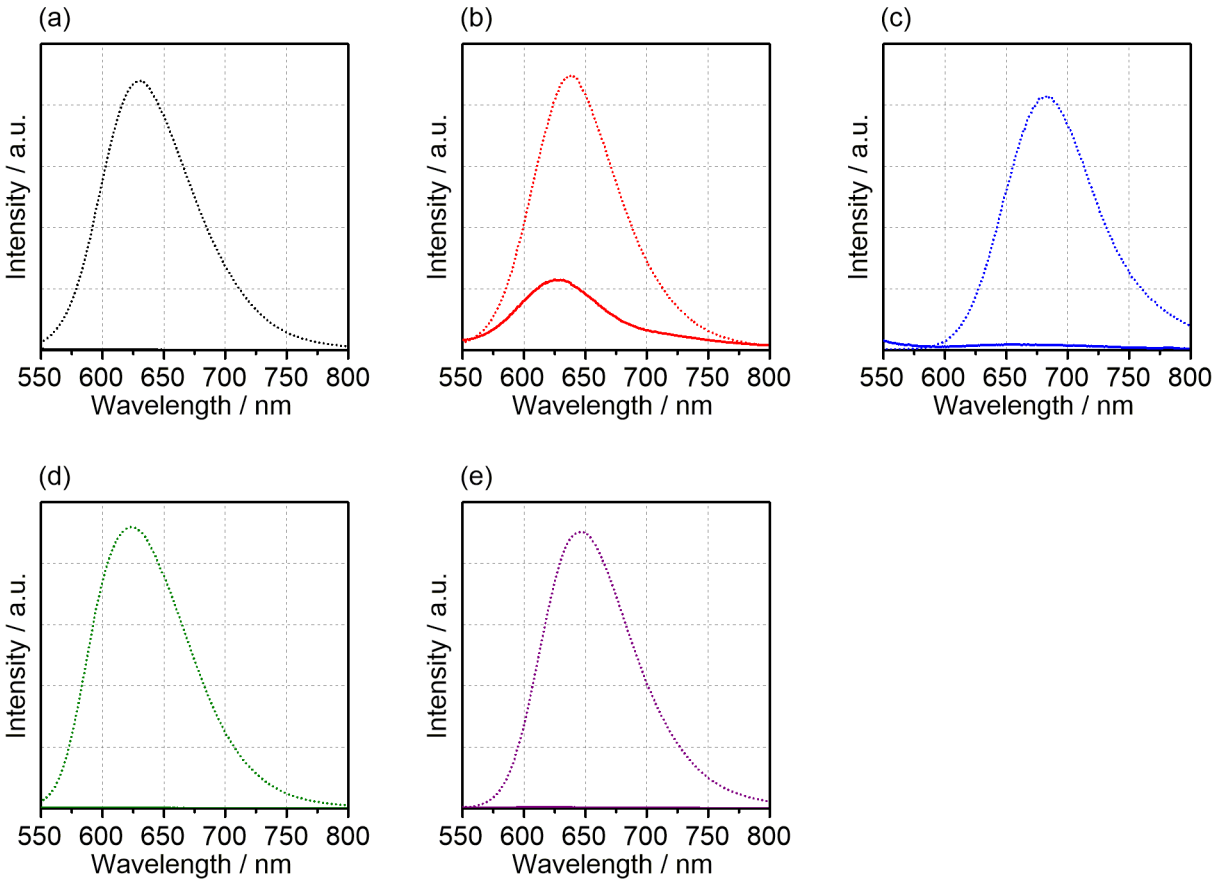


Fig. S4 Photoluminescence spectra of the **PTB7**/acceptor blended films (solid line) and acceptor pristine films (dotted line) for (a) **TetraBP-*N*-PDIC9**, (b) **TetraBP-*N*-PDIC2**, (c) **Pyrene-*B*-PDI**, (d) **TetraP-*B*-PDI**, and (e) **SpiroF-*B*-PDI**.

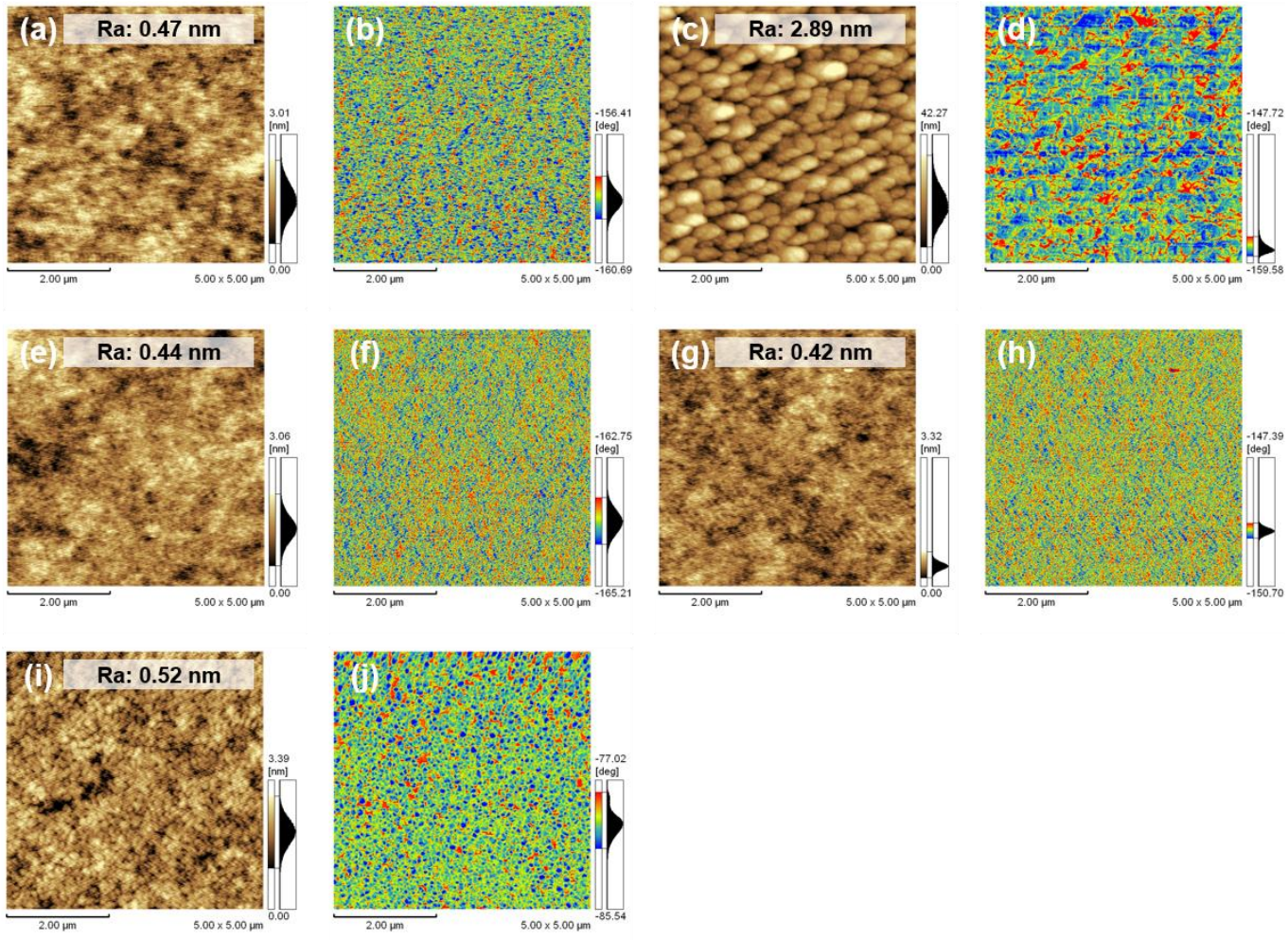


Fig. S5 AFM height and phase images of (a, b) **PTB7**/**TetraBP-*N*-PDIC9**, (c, d) **PTB7**/**TetraBP-*N*-PDIC2**, (e, f) **PTB7**/**Pyrene-*B*-PDI**, (g, h) **PTB7**/**TetraP-*B*-PDI**, and (i, j) **PTB7**/**SpiroF-*B*-PDI** blended films.

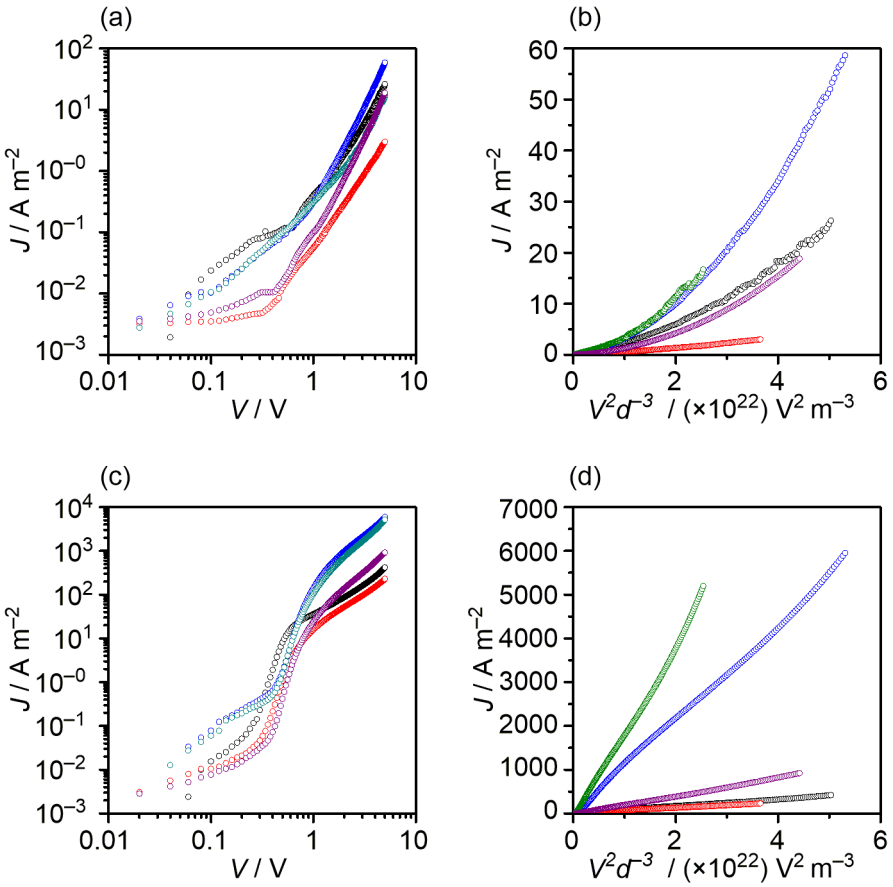


Fig. S6 (a) *J*–*V* and (b) *J*–V^2 d^{-3} characteristics of electron-only devices and (c) *J*–*V* and (d) *J*–V^2 d^{-3} characteristics of hole-only devices for **PTB7**/**TetraBP-*N*-PDIC9** (black), **PTB7**/**TetraBP-*N*-PDIC2** (red), **PTB7**/**Pyrene-*B*-PDI** (blue), **PTB7**/**TetraP-*B*-PDI** (green), and **PTB7**/**SpiroF-*B*-PDI** (purple) blended films.

Table S1 OPV characteristics of **PTB7**/**TetraBP-*N*-PDIC9** based devices.

Run	J_{SC} / mA cm^{-2}	V_{OC} / V	FF	PCE / %
1	0.14	0.39	0.29	0.02
2	0.12	0.38	0.32	0.01
3	0.12	0.38	0.31	0.01
4	0.13	0.36	0.32	0.01
average	0.13 ± 0.00	0.38 ± 0.01	0.31 ± 0.01	0.01 ± 0.00

Table S2 OPV characteristics of **PTB7**/**TetraBP-*N*-PDIC2** based devices.

Run	J_{SC} / mA cm^{-2}	V_{OC} / V	FF	PCE / %
1	0.74	0.65	0.27	0.13
2	0.74	0.61	0.26	0.12
3	0.68	0.56	0.26	0.10
4	0.65	0.55	0.25	0.09
average	0.70 ± 0.02	0.59 ± 0.02	0.26 ± 0.00	0.11 ± 0.01

Table S3 OPV characteristics of **PTB7**/**Pyrene-*B*-PDI** based devices.

Run	J_{SC} / mA cm^{-2}	V_{OC} / V	FF	PCE / %
1	7.65	0.72	0.37	2.02
2	7.49	0.72	0.37	1.97
3	7.44	0.72	0.37	1.96
4	6.61	0.72	0.36	1.72
average	7.30 ± 0.23	0.72 ± 0.02	0.37 ± 0.02	1.92 ± 0.07

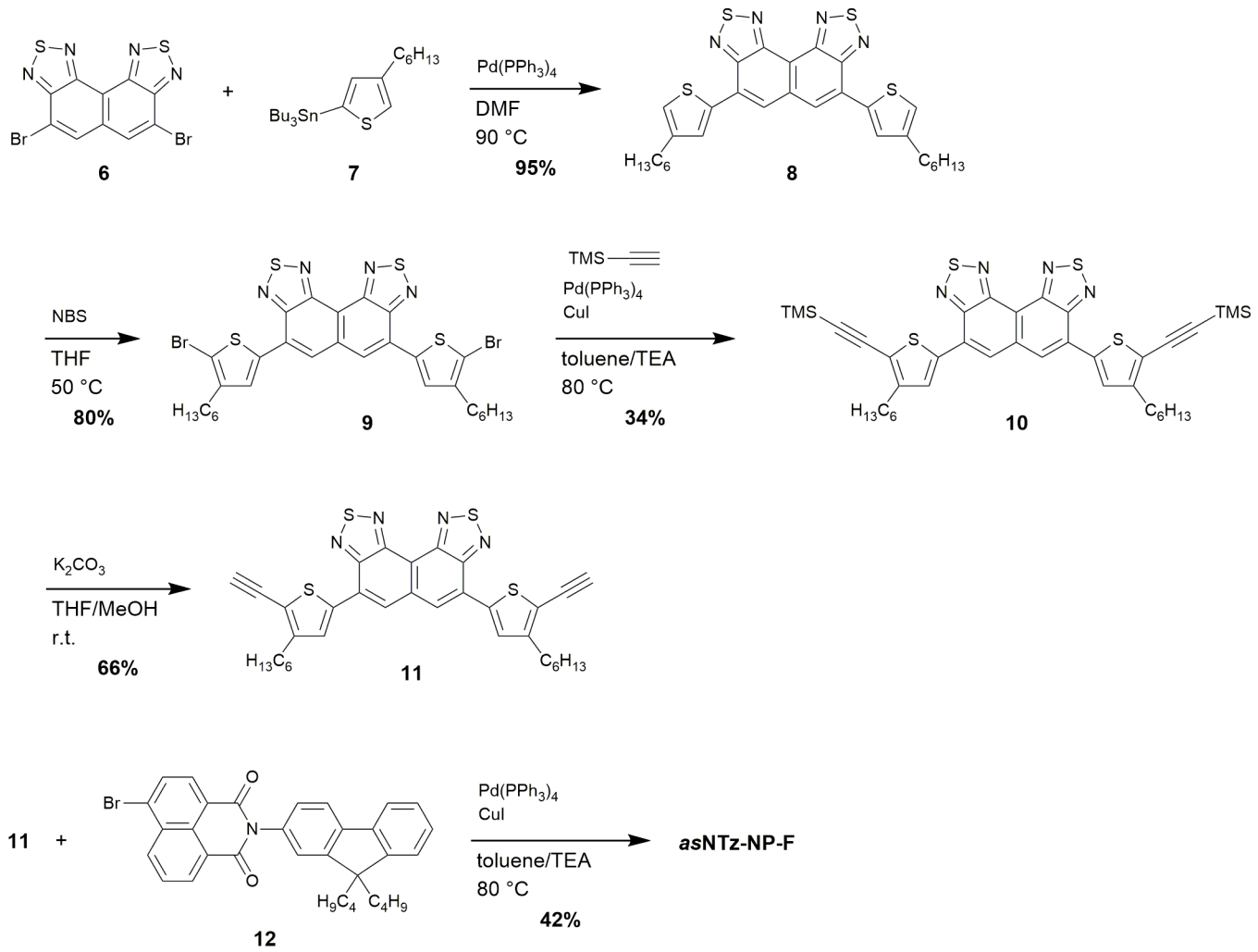
Table S4 OPV characteristics of **PTB7**/**TetraP-*B*-PDI** based devices.

Run	J_{SC} / mA cm^{-2}	V_{OC} / V	FF	PCE / %
1	2.94	0.74	0.30	0.65
2	2.95	0.75	0.29	0.64
3	2.96	0.74	0.30	0.64
4	2.73	0.74	0.30	0.60
average	2.90 ± 0.06	0.74 ± 0.00	0.30 ± 0.00	0.63 ± 0.01

Table S5 OPV characteristics of **PTB7**/**SpiroF-*B*-PDI** based devices.

Run	J_{SC} / mA cm^{-2}	V_{OC} / V	FF	PCE / %
1	5.90	0.75	0.36	1.57
2	6.07	0.74	0.35	1.56
3	5.83	0.75	0.35	1.56
4	5.96	0.75	0.34	1.54
average	5.94 ± 0.05	0.75 ± 0.00	0.35 ± 0.00	1.56 ± 0.01

Summarized Results for *as*NTz-NP-F



Scheme S2 Synthesis of ***as*NTz-NP-F**.

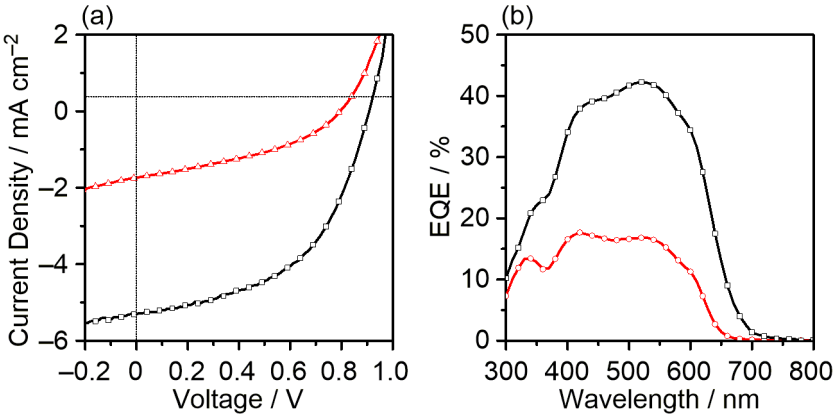


Fig. S7 (a) *J*–*V* curves and (b) EQE spectra for **P3HT/*as*NTz-NP-F** (red), and **P3HT/*s*NTz-NP-F** (black) OPV devices.

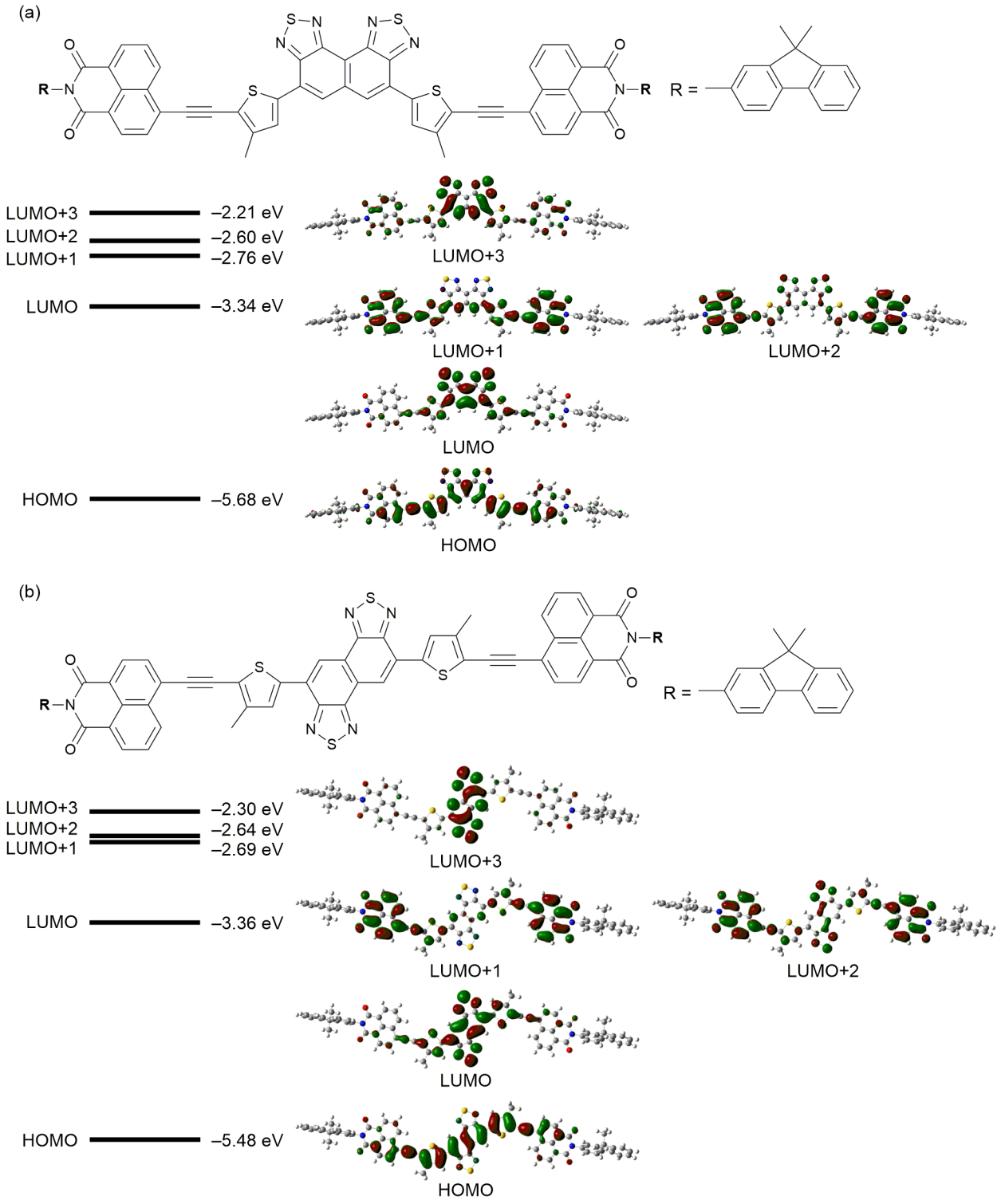


Fig. S8 Energy levels and molecular orbitals of (a) **as**NTz-NP-F and (b) ***s*NTz-NP-F** calculated by DFT at B3LYP/6-31 G(d,p) level. All the alkyl groups were replaced with methyl groups to facilitate the calculation.

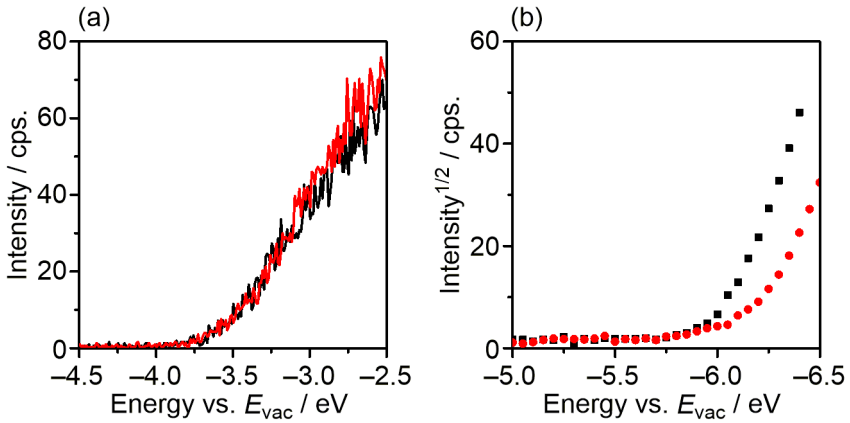


Fig. S9 (a) LEIPS and (b) PYS of ***as*NTz-NP-F** (red) and ***s*NTz-NP-F** (black).

Table S6 OPV characteristics and surface free energy data of ***as*NTz-NP-F** and ***s*NTz-NP-F**.

Compounds	J_{SC}/mA cm^{-2}	V_{OC}/V	FF	PCE/%	γ^{d}/mJ cm^{-2}	γ^{p}/mJ cm^{-2}	SFE/mJ cm^{-2}
***as*NTz-NP-F**	1.73	0.79	0.39	0.54	27.9	2.8	30.7
***s*NTz-NP-F**	5.31	0.90	0.52	2.48	28.1	2.8	30.9

Experimental Procedures

General Information of Synthesis. Column chromatography was performed on silica gel, KANTO Chemical silica gel 60N (40–50 μm). Thin-layer chromatography plates were visualized with UV light. Preparative gel-permeation chromatography (GPC) was performed on a Japan Analytical Industry LC-918 equipped with JAI-GEL 1H/2H. ^{1}H and ^{13}C NMR spectra were recorded on a JEOL ECS-400 spectrometer. Data are reported as follows: chemical shift in ppm (δ), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, br = broad), coupling constant (Hz). Mass spectra were obtained on a Shimadzu GCMS-QP-5050 or Shimadzu AXIMA-TOF. High-resolution mass spectrum (HRMS) was obtained using a Brucker ultraflex III (MALDI-TOF) or Brucker microTOF II (ESI-TOF). Elemental analyses were performed on Perkin Elmer LS-50B by the Elemental Analysis Section of CAC, ISIR, Osaka University.

Preparation of Materials. All reactions were carried out under a nitrogen atmosphere. Solvents of the highest purity grade were used as received. All reagents were purchased from commercial sources and used without purification. **1**,[1] **2**,[2] **3**,[3] **4**,[4] **5**,[5] **6**,[6] **7**,[7] and **12**[8] was prepared by our previously reported procedure and ^{1}H NMR data of these compounds were in agreement with those previously reported.

Synthesis

Synthesis of ***TetraBP-N-PDIC2***: **1** (50 mg, 0.061 mmol), **2** (241 mg, 0.364 mmol), $Pd(PPh_3)_4$ (14 mg, 0.012 mmol), and K_2CO_3 (168 mg, 1.21 mmol) were placed in a test tube with screw cap and dissolved with toluene (10 mL), H_2O (2 mL), and EtOH (1mL). The reaction mixture was stirred at 85 °C for 12 h. After being cooled to room temperature and addition of water, the resulting mixture was extracted with $CHCl_3$ and the organic layer was washed with water. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel ($CHCl_3$), followed by purification with preparative GPC ($CHCl_3$) to give **TetraBP-*N*-PDIC2** (57 mg, 38%). Deep red solid; ^{1}H NMR (400 MHz, 1,1,2,2-tetrachloroethane-d_2, 100 °C, δ): 8.76-8.59 (m, 32H), 7.92-7.83 (m, 8H), 7.75-7.68 (m, 8H), 7.58-7.51 (m, 8H), 7.50-7.43 (m, 8H), 5.08-5.00 (m, 4H), 2.30-2.21 (m, 8H), 2.03-1.95 (m, 8H), 1.55-1.44 (m, 12H), 0.99-0.95 (m, 12H); MS (MALDI-TOF, 1,8,9-trihydroxyanthracene matrix) *m/z* 2456.75 (M^-); HRMS (MALDI-TOF) *m*/*z* calcd for $C_{165}H_{108}N_8O_{16}$ (M^-): 2457.7917, found: 2457.7913.

Synthesis of ***Pyrene-B-PDI***: **3** (40 mg, 0.057 mmol), **4** (207 mg, 0.400 mmol), $Pd(PPh_3)_4$ (13 mg, 0.011 mmol), and K_2CO_3 (157 mg, 1.13 mmol) were placed in a test tube with screw cap and dissolved with toluene (10 mL), H_2O (2 mL), and EtOH (1mL). The reaction mixture was stirred at 80 °C for 24 h. After being cooled to room temperature and addition of water, the resulting mixture was extracted with $CHCl_3$ and the organic layer was washed with water. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel ($CHCl_3$), followed by purification with preparative GPC ($CHCl_3$) to give **Pyrene-*B*-PDI** (50 mg, 38%). Deep red solid; ^{1}H NMR (400 MHz, 1,1,2,2-tetrachloroethane-d_2, 140 °C, δ): 8.77-8.52 (m, 20H), 8.34-8.31 (m, 2H), 8.28-7.96 (m, 10H), 7.73-7.62 (m, 1H), 7.29-7.27 (s, 1H), 5.06-4.84 (m, 8H), 2.23-2.13 (m, 8H), 2.00-1.85 (m, 12H), 1.49-1.34 (m, 12H), 0.97-0.66 (m, 48H); MS (MALDI-TOF, 1,8,9-trihydroxyanthracene matrix) *m/z* 2315.36 (M^-); Anal. calcd for $C_{152}H_{122}N_8O_{16}$: C 78.81, H 5.31, N 4.84; found: C 78.58, H 5.45, N 4.71.

Synthesis of ***TetraP-B-PDI***: **1** (40 mg, 0.049 mmol), **4** (177 mg, 0.291 mmol), $Pd(PPh_3)_4$ (11 mg, 0.010 mmol), and K_2CO_3 (134 mg, 0.97 mmol) were placed in a test tube with screw cap and dissolved with toluene (10 mL), H_2O (2 mL), and EtOH (1mL). The reaction mixture was stirred at 80 °C for 24 h. After being cooled to room temperature and addition of water, the resulting mixture was extracted with $CHCl_3$ and the organic layer was washed with water. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel ($CHCl_3$), followed by purification with preparative GPC ($CHCl_3$) to give **TetraP-*B*-PDI** (52 mg, 44%). Deep red solid; ^{1}H NMR (400 MHz, $CDCl_3$, 50 °C, TMS, δ): 8.73–8.59 (m, 20H), 8.00–7.96 (m, 8H), 7.72–7.65 (m, 16H), 5.10–5.02 (m, 4H), 4.77–4.67 (m, 4H), 2.31–2.20 (m, 8H), 1.96–1.85 (m, 16H), 1.68–1.58 (m, 8H), 0.93 (t, J = 7.4 Hz, 24H),

0.65 (t, J = 6.0 Hz, 24H); ^{13}C NMR (100 MHz, $CDCl_3$, 50 °C, δ): 164.38, 164.33, 164.14, 164.06, 146.57, 141.61, 141.13, 135.97, 135.93, 134.97, 134.92, 134.58, 133.15, 132.89, 131.16, 131.03, 129.95, 129.73, 129.70, 129.63, 129.61, 129.28, 128.82, 128.63, 128.24, 127.77, 123.52, 122.70, 65.00, 57.85, 57.46, 25.12, 24.85, 11.29, 11.15; MS (MALDI-TOF, 1,8,9-trihydroxyanthracene matrix) *m/z* 2344.33 (M^-); HRMS (MALDI-TOF) *m/z* calcd for $C_{161}H_{132}N_8O_{16}$ (M^-): 2433.9795, found: 2433.9800.

Synthesis of ***SpiroF-B-PDI***: **5** (40 mg, 0.049 mmol), **4** (178 mg, 0.293 mmol), $Pd(PPh_3)_4$ (11 mg, 0.010 mmol), and K_2CO_3 (135 mg, 0.98 mmol) were placed in a test tube with screw cap and dissolved with toluene (10 mL), H_2O (2 mL), and EtOH (1mL). The reaction mixture was stirred at 80 °C for 24 h. After being cooled to room temperature and addition of water, the resulting mixture was extracted with $CHCl_3$ and the organic layer was washed with water. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel ($CHCl_3$), followed by purification with preparative GPC ($CHCl_3$) to give **SpiroF-*B*-PDI** (48 mg, 40%). Deep red solid; ^{1}H NMR (400 MHz, 1,1,2,2-tetrachloroethane-d_2, 140 °C, δ): 8.68-8.44 (m, 20H), 7.99-7.96 (m, 4H), 7.80-7.65 (m, 6H), 7.50 (s, 4H), 7.44-7.25 (m, 6H), 5.05-4.96 (m, 4H), 4.69-4.61 (m, 4H), 2.26-2.16 (m, 8H), 1.98-1.72 (m, 16H), 1.47-1.39 (m, 8H), 0.98-0.91 (m, 24H), 0.80-0.74 (m, 24H); MS (MALDI-TOF, 1,8,9-trihydroxyanthracene matrix) *m/z* 2429.19 (M^-); MS MALDI-TOF (1,8,9-trihydroxyanthracene matrix) *m/z* 2429.19 (M^-); HRMS (ESI-TOF) *m/z* calcd for $C_{161}H_{128}N_8O_{16}$ (M^-): 2429.9482, found: 2429.9490.

Synthesis of ***8***: **6** (300 mg, 0.75 mmol), 7 (819 mg, 1.79 mmol), and $Pd(PPh_3)_4$ (172 mg, 0.15 mmol) were placed in a round-bottomed flask and dissolved with DMF (100 mL). The reaction mixture was stirred at 90 °C for 12 h. After being cooled to room temperature, the solvent was evaporated under reduced pressure. The residue was purified by column chromatography on silica gel (hexane/$CHCl_3$ = 2/1) to give **8** (407 mg, 95%). Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, δ): 8.29 (s, 2H), 8.19 (s, 2H), 7.16 (s, 2H), 2.75 (t, J = 8.0 Hz, 4H), 1.75 (m, 4H), 1.45-1.34 (br, 12H), 0.92 (t, J = 7.3 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, δ): 152.23, 151.84, 144.63, 138.11, 134.75, 130.46, 128.55, 126.32, 122.63, 114.69, 31.73, 30.67, 30.49, 29.09, 22.67, 14.16; MS (EI) *m/z* 577 (M^+); HRMS (ESI-TOF) *m/z* calcd for $C_{30}H_{33}N_4S_4$ ($[M+H]^+$): 577.1588, found: 577.1578.

Synthesis of ***9***: To a stirred solution of **8** (407 mg, 0.71 mmol) in THF (140 mL) was added NBS (276 mg, 1.55 mmol), and the resulting mixture was stirred at 50 °C for 6 h. After being cooled to room temperature, the reaction was quenched by the addition of $NaHCO_3$ aq., and the resulting mixture was extracted with CH_2Cl_2 and the organic layer was washed with water. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (hexane/$CHCl_3$ = 1/1) to give **9** (416 mg, 80%). Orange solid; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, δ): 8.15 (s, 2H), 7.96 (s, 2H),

2.69 (t, *J* = 7.3 Hz, 4H), 1.72 (m, 4H), 1.44-1.35 (br, 12H), 0.92 (t, *J* = 6.9 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, *δ*): 151.53, 151.30, 143.27, 137.41, 134.15, 129.27, 127.24, 125.04, 114.38, 112.92, 31.68, 29.76, 29.71, 29.07, 22.68, 14.18; MS (EI) *m/z* 732 (M^+); Anal. calcd for $C_{30}H_{30}BrN_4O_4$: C 49.05, H 4.12, N 7.63; found: C 49.08, H 4.13, N 7.79.

*Synthesis of **10***: **9** (416 mg, 0.57 mmol), trimethylsilylacetylene (167 mg, 0.1.70 mmol), CuI (22 mg, 0.11 mmol), and $Pd(PPh_3)_4$ (131 mg, 0.11 mmol) were placed in a test tube with screw cap and dissolved with toluene (10 mL) and triethylamine (5 mL). The reaction mixure was stirred at 80 °C for 6 h. After being cooled to room temperature, the reaction mixture was concentrated under reduced pressure and then purified by column chromatography on silica gel (hexane/$CHCl_3$ = 1/1) to give **10** (150 mg, 34%). Orange solid; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, *δ*): 8.25 (s, 2H), 8.08 (s, 2H), 2.80 (t, *J* = 7.6 Hz, 4H), 1.75 (m, 4H), 1.41-1.35 (br, 12H), 0.92 (t, *J* = 6.9 Hz, 6H), 0.30 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$, *δ*): 152.09, 151.67, 149.85, 137.80, 134.41, 129.82, 127.76, 126.30, 121.11, 114.98, 103.72, 97.33, 31.73, 30.22, 29.83, 29.11, 22.75, 14.26, 0.07; MS (EI) *m/z* 768 (M^+); Anal. calcd for $C_{40}H_{48}N_4S_4Si_2$: C 62.45, H 6.29, N 7.28; found: C 62.45, H 6.35, N 7.17.

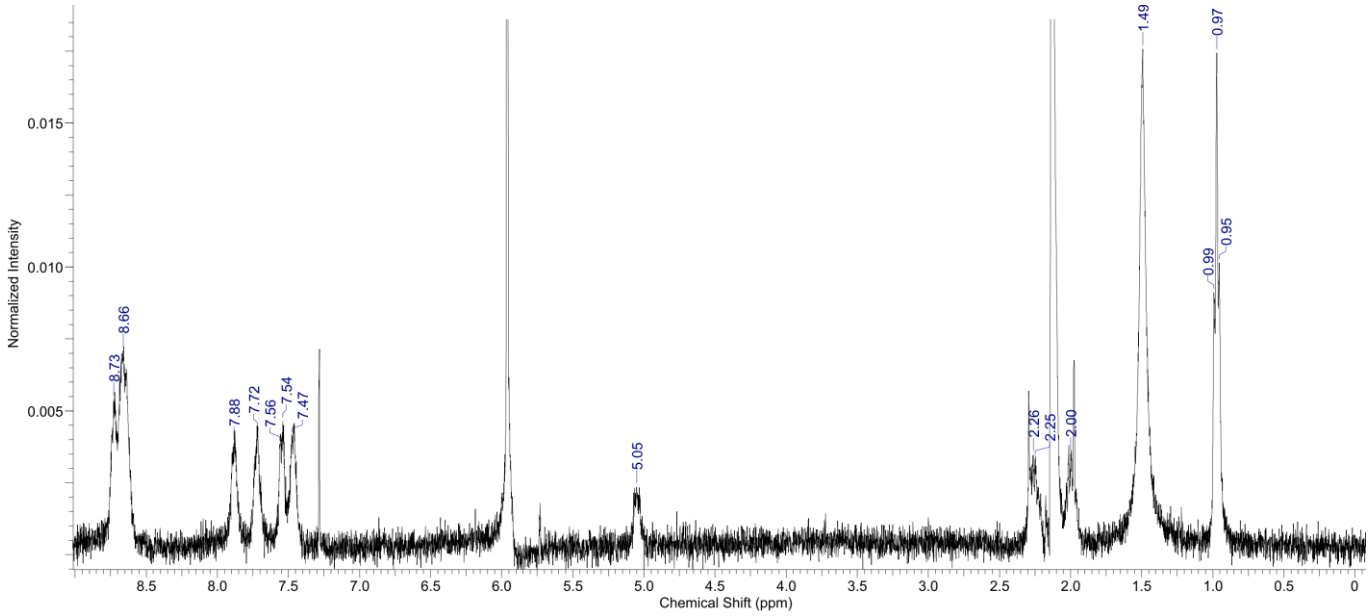
*Synthesis of **11***: **10** (150 mg, 0.20 mmol), K_2CO_3 (108 g, 0.78 mmol), THF (6 mL), and MeOH (3 mL) were placed in a test tube and the resulting slurry was stirred for 1 h. After filtration using celite and extraction with CH_2Cl_2, the filtrate was condensed under reduced pressure. The residue was purified by column chromatography on silica gel (hexane/$CHCl_3$ = 1/1) to give **11** (80 g, 66%). Orange solid; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, *δ*): 8.25 (s, 2H), 8.09 (s, 2H), 3.63 (s, 2H), 2.82 (t, *J* = 7.8 Hz, 4H), 1.75 (m, 4H), 1.44-1.35 (br, 12H), 0.92 (t, *J* = 5.5 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, *δ*): 151.73, 151.39, 150.04, 137.98, 134.08, 129.58, 127.39, 126.10, 119.62, 114.90, 85.47, 76.53, 31.66, 30.21, 29.70, 29.09, 22.68, 14.16; MS (MALDI-TOF, 1,8,9-trihydroxyanthracene matrix) *m/z* 624.02 (M^-). This compound was used for next step without further purification.

*Synthesis of **asNTz-NP-F***: **11** (80 mg, 0.13 mmol), 12 (170 mg, 0.38 mmol), CuI (5 mg, 0.03 mmol), and $Pd(PPh_3)_4$ (30 mg, 0.03 mmol) were placed in a test tube with screw cap and dissolved with toluene (5 mL) and triethylamine (2.5 mL). The reaction mixure was stirred at 110 °C for 6 h. After being cooled to room temperature, the reaction mixture was concentrated under reduced pressure and then purified by column chromatography on silica gel ($CHCl_3$), followed by purification with preparative GPC ($CHCl_3$) to give ***as*NTz-NP-F** (84 mg, 42%). Red solid; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, *δ*): 8.76 (d, *J* = 7.3 Hz, 2H), 8.71 (d, *J* = 7.0 Hz, 2H), 8.62 (d, *J* = 7.3 Hz, 2H), 8.32 (s, 2H), 8.19 (s, 2H), 7.98 (d, *J* = 7.0 Hz, 2H), 7.89 (t, *J* = 7.3 Hz, 2H), 7.86 (d, *J* = 8.2 Hz, 2H), 7.75 (dd, *J* = 7.8, 1.8 Hz, 2H), 7.40-7.35 (m, 3H), 7.31-7.29 (m, 2H), 3.03 (t, *J* = 7.8 Hz, 4H), 2.00 (t, *J* = 8.0 Hz, 8H), 1.91 (m, 4H), 1.47-1.38 (m, 8H), 1.15-

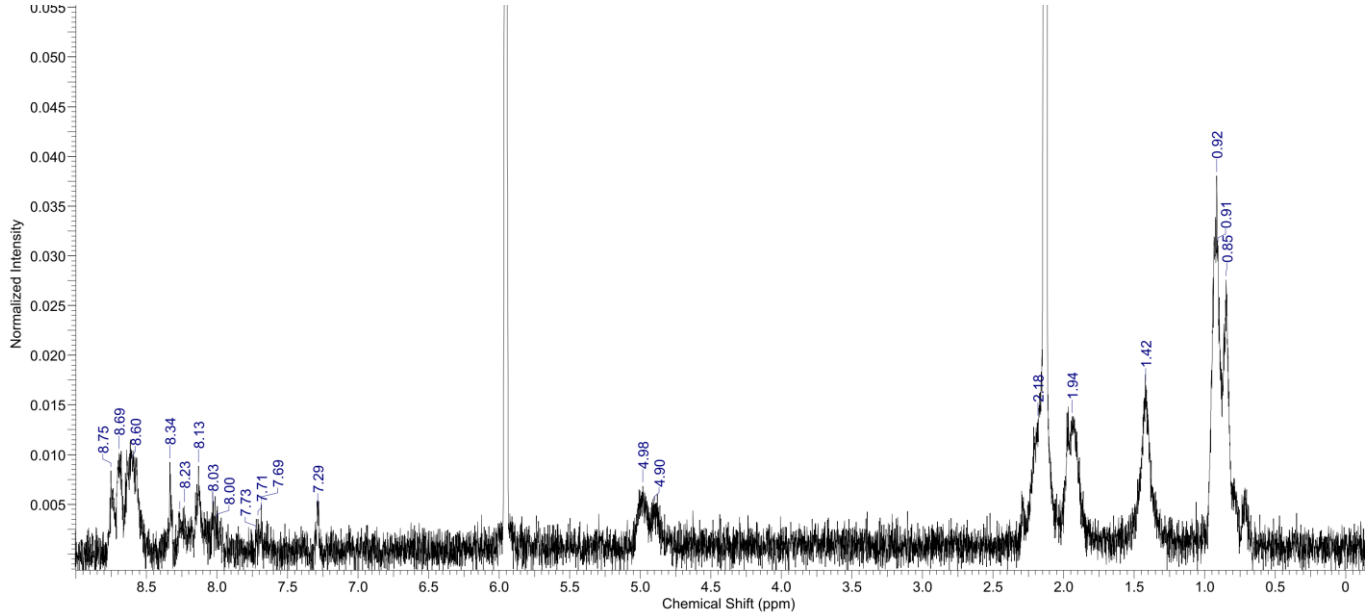
1.09 (m, 8H), 0.93 (t, J = 8.2 Hz, 6H), 0.87-0.81 (m, 4H), 0.72 (t, J = 8.0 Hz, 12H), 0.74-0.67 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$, δ): 163.86, 163.61, 151.66, 151.59, 151.23, 151.18, 150.44, 141.31, 140.46, 139.66, 133.87, 131.85, 131.66, 130.85, 130.36, 130.07, 129.81, 128.16, 127.36, 127.30, 127.15, 127.10, 126.86, 126.03, 126.01, 123.50, 123.20, 122.97, 122.14, 120.30, 120.08, 120.02, 114.97, 99.91, 95.20, 92.36, 55.21, 39.98, 31.76, 30.48, 30.34, 29.41, 26.02, 23.09, 22.78, 14.24, 13.87; MS (MALDI-TOF, 1,8,9-trihydroxyanthracene matrix) *m/z* 1566.40 (M^-); Anal. calcd for $C_{100}H_{90}N_6O_4S_6$: C 76.60, H 5.79, N 5.36; found: C 76.34, H 5.88, N 5.24.

NMR Spectra

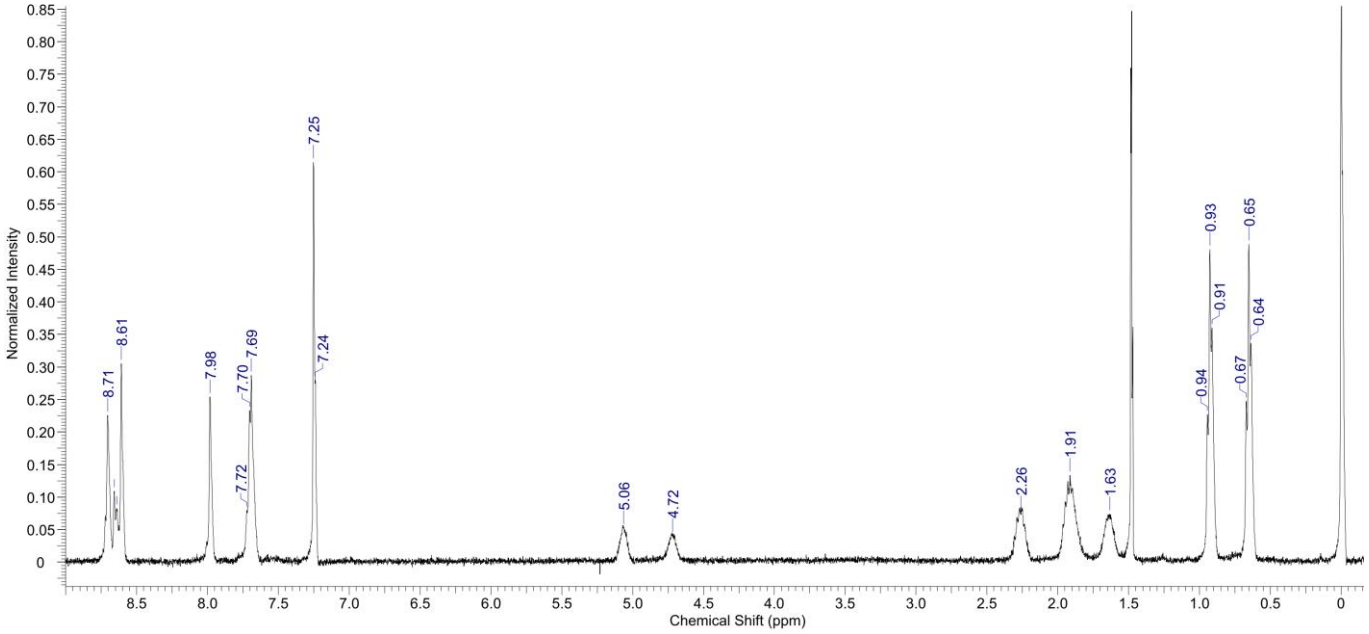
^{1}H NMR spectrum of **TetraBP-*N*-PDIC2**.



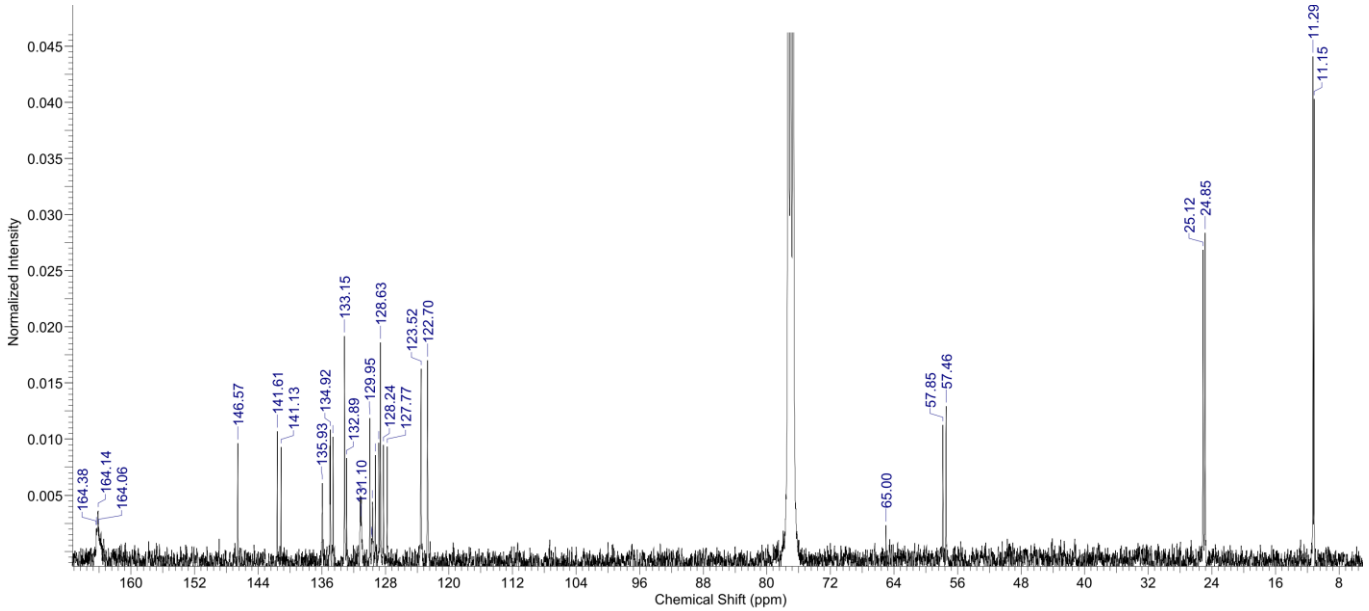
^{1}H NMR spectrum of **Pyrene-*B*-PDI**.



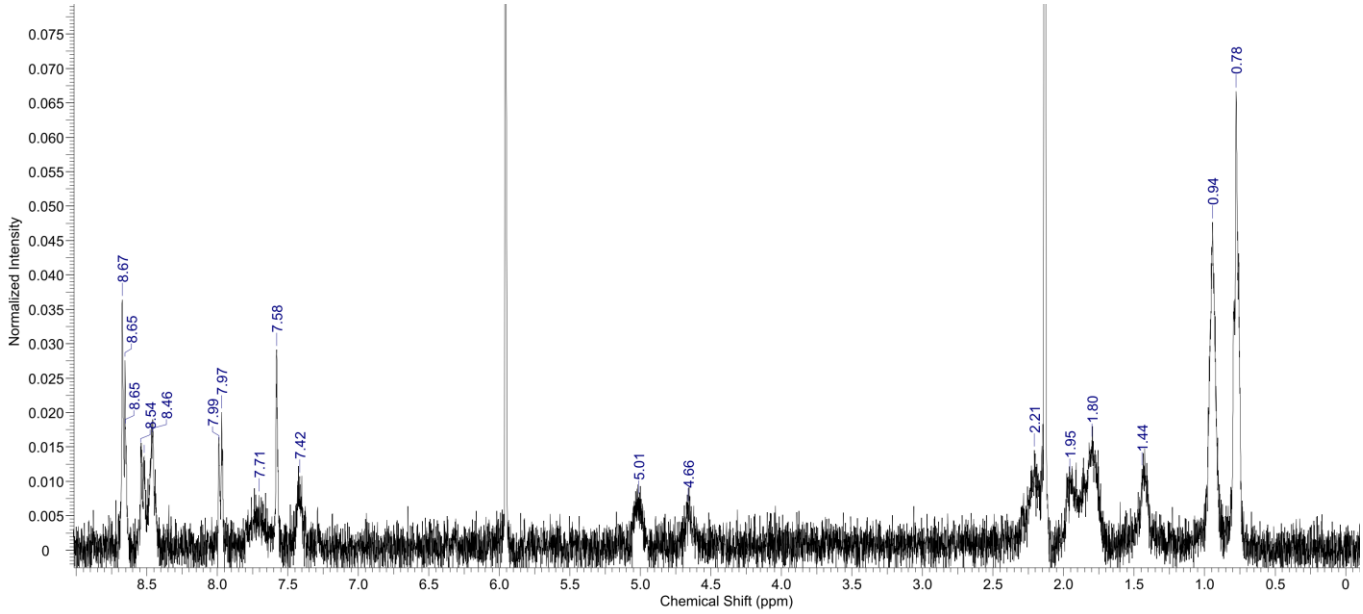
^{1}H NMR spectrum of **TetraP-*B*-PDI**.



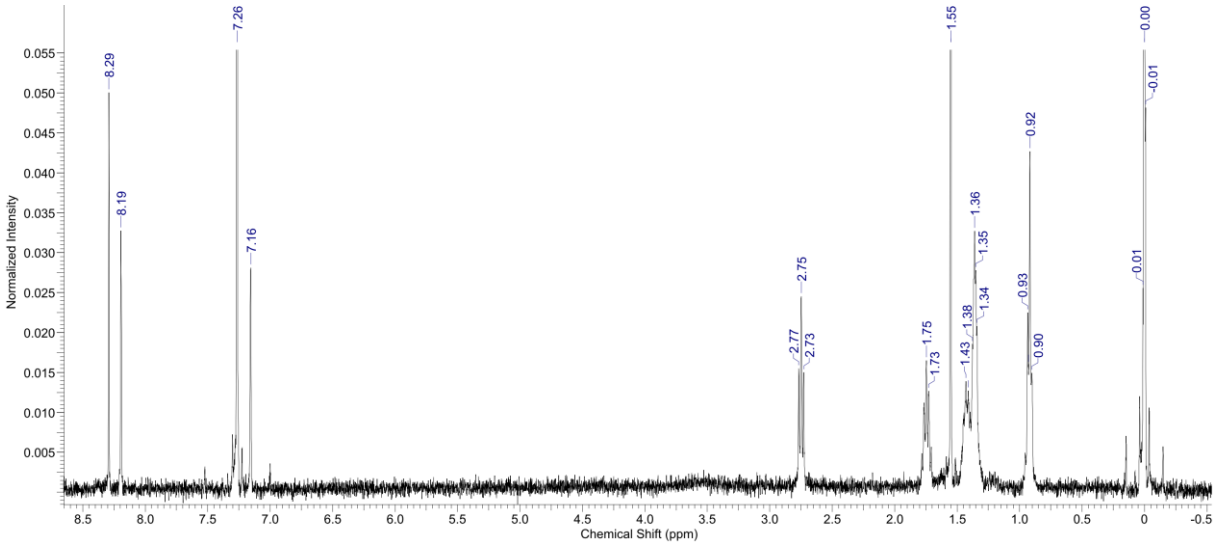
^{13}C NMR spectrum of **TetraP-*B*-PDI**.



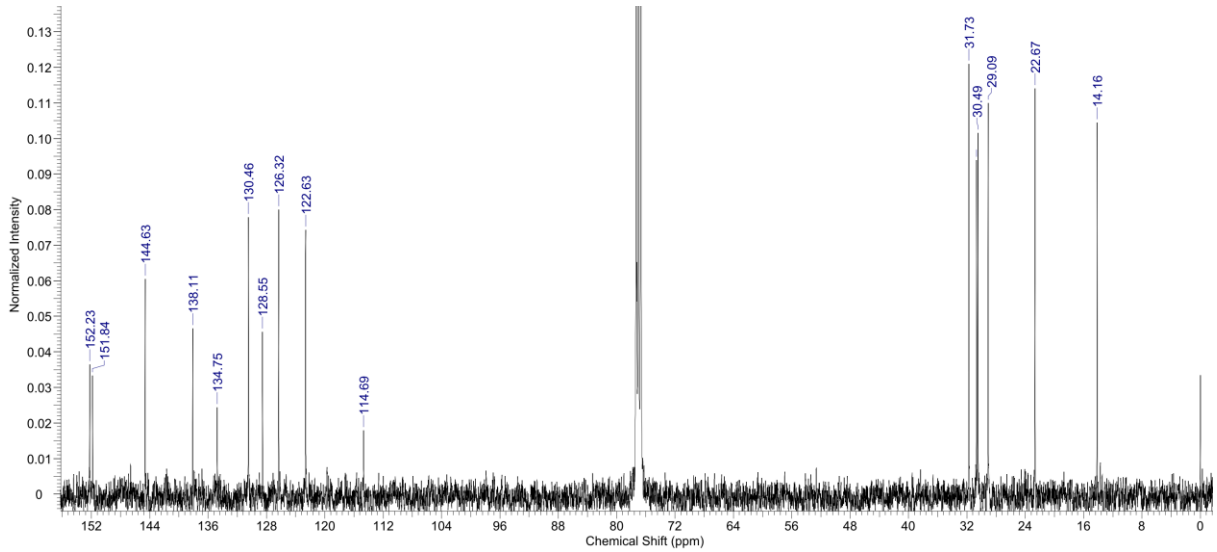
^{1}H NMR spectrum of **SpiroF-*B*-PDI**.



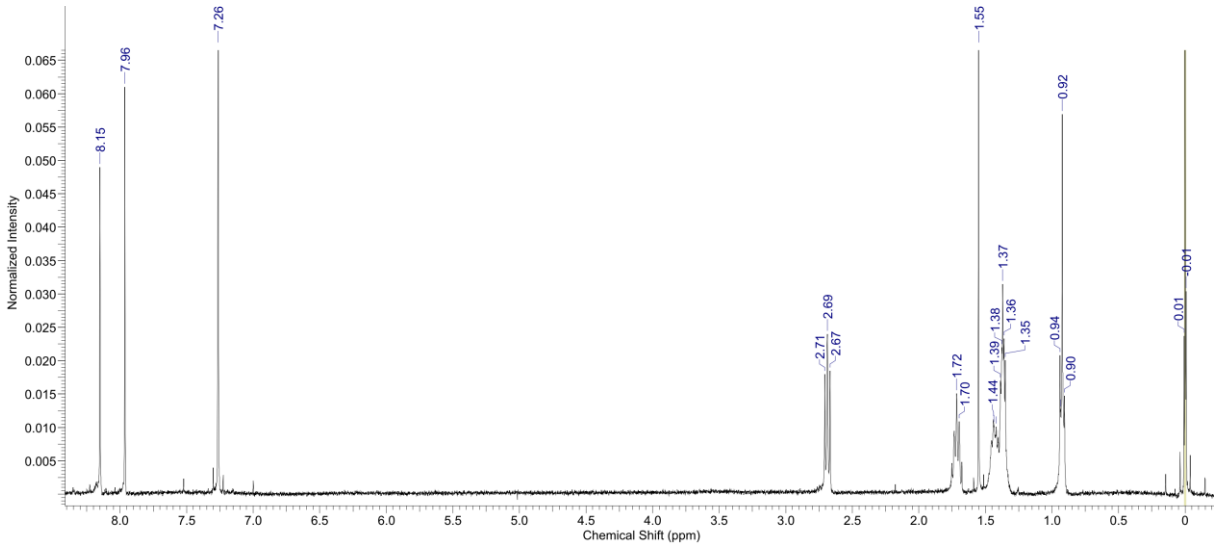
^{1}H NMR spectrum of **8**.



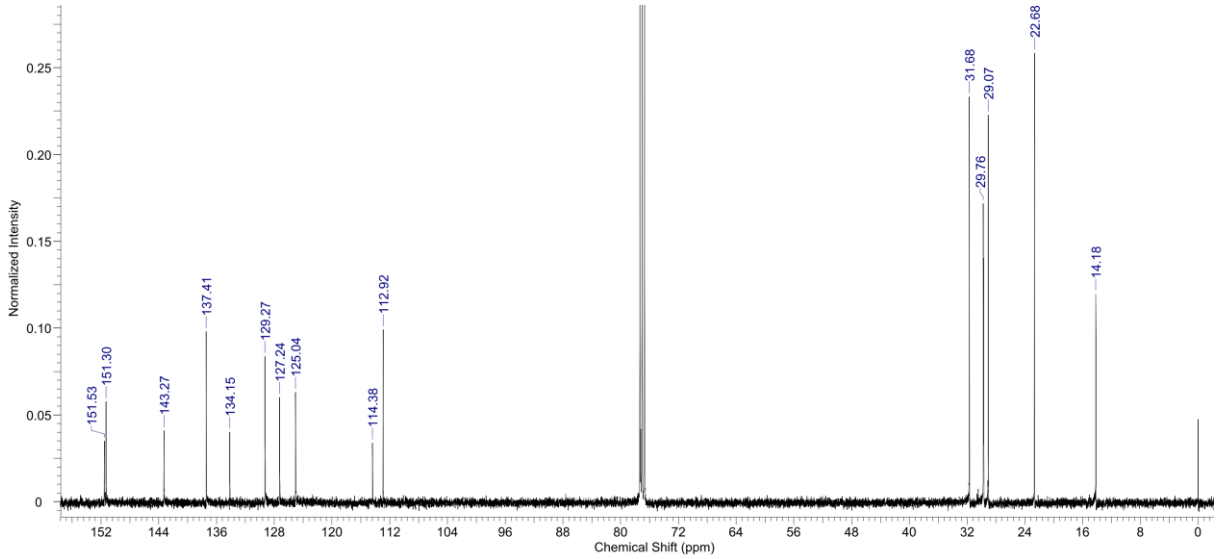
^{13}C NMR spectrum of **8**.



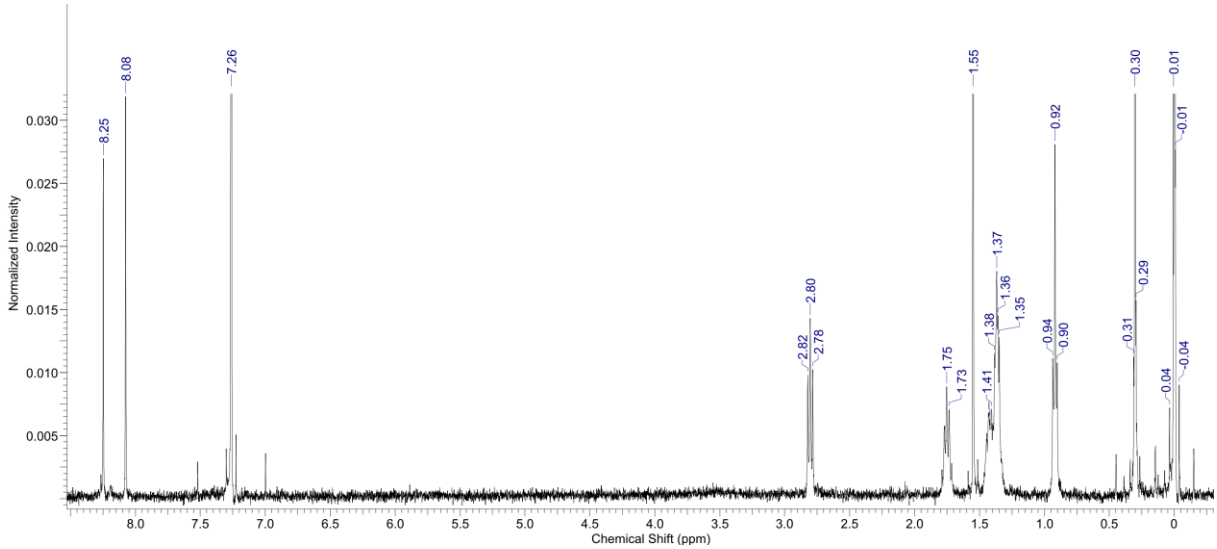
^{1}H NMR spectrum of **9**.



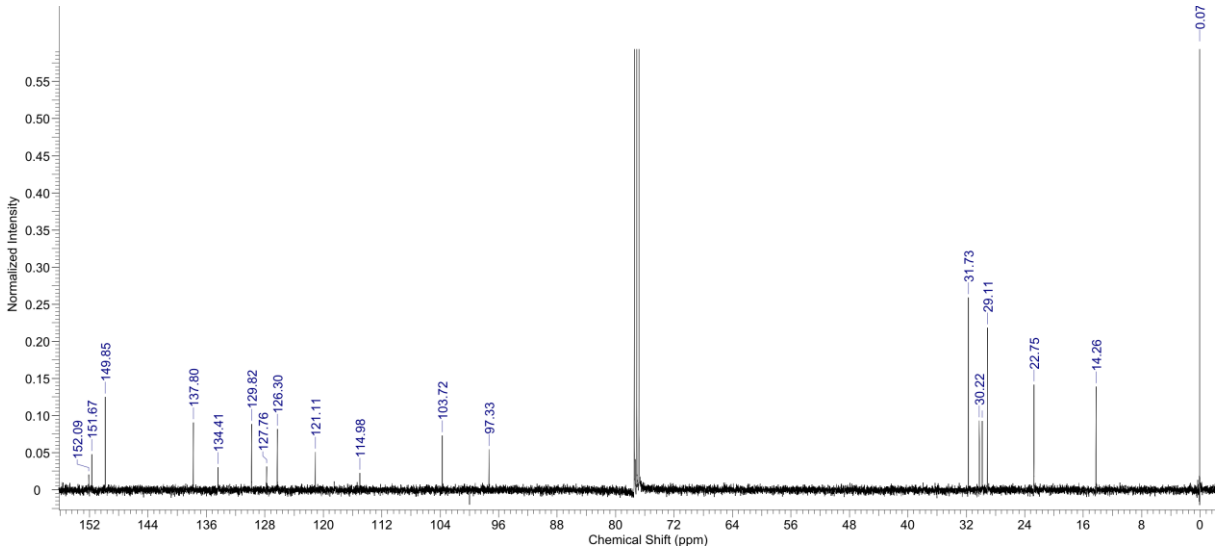
^{13}C NMR spectrum of **9**.



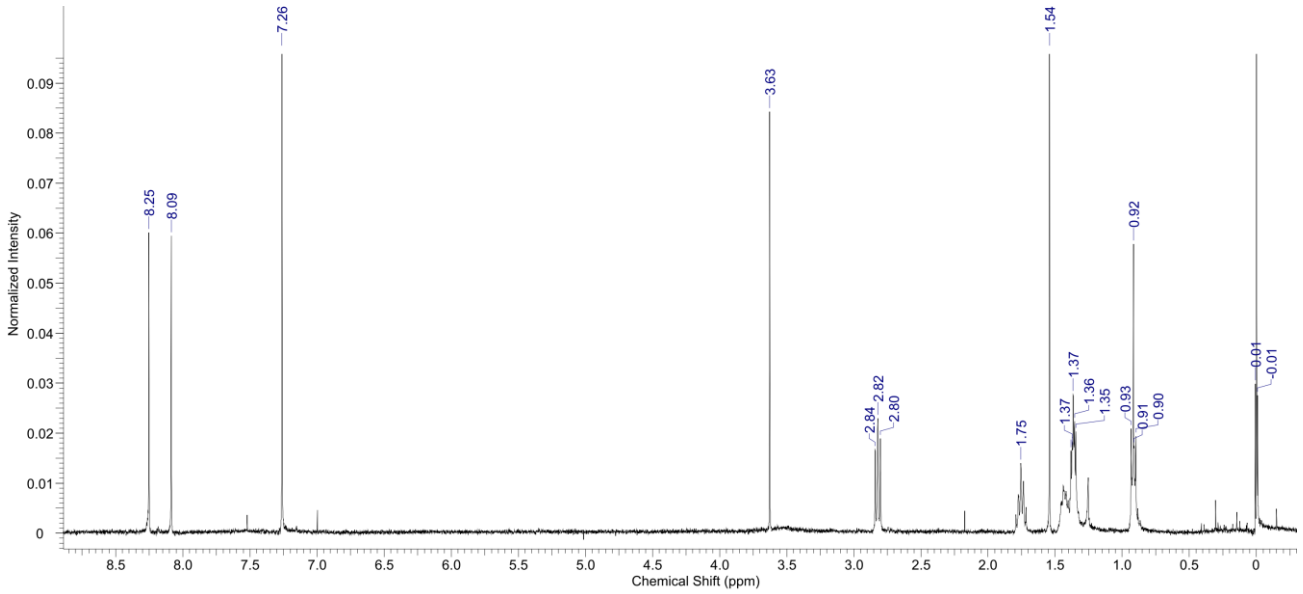
^{1}H NMR spectrum of **10**.



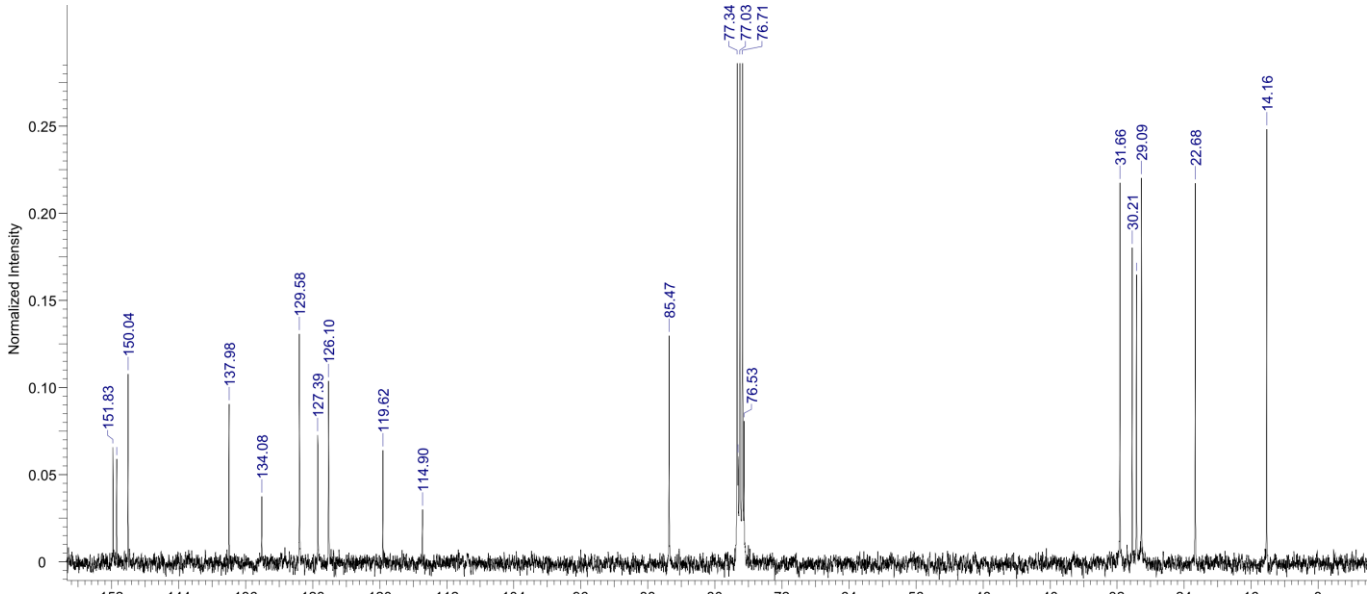
^{13}C NMR spectrum of **10**.



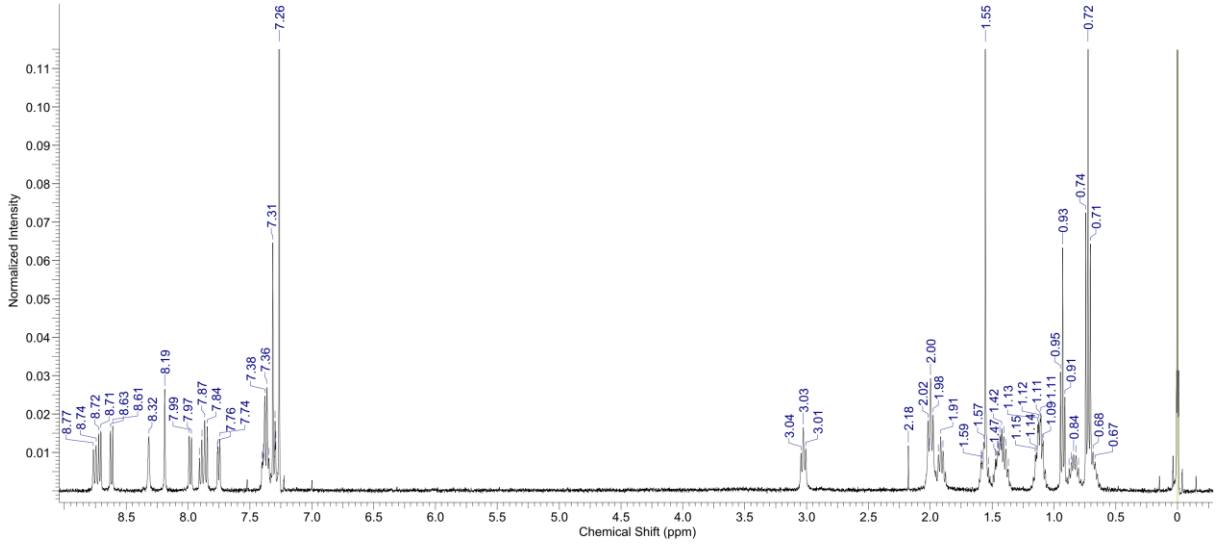
^{1}H NMR spectrum of **11**.



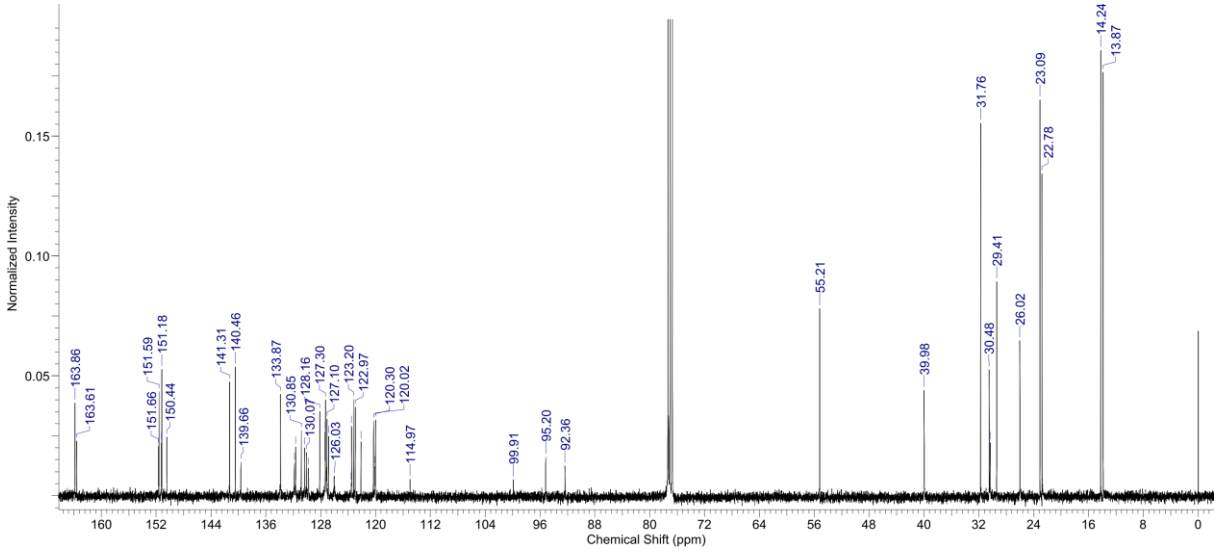
^{13}C NMR spectrum of **11**.



^{1}H NMR spectrum of ***as*NTz-NP-F**.



^{13}C NMR spectrum of ***as*NTz-NP-F**.



LEIPS Measurements

Experimental setup for the LEIPS is described elsewhere.[9] Sample films were incident to an electron beam with the kinetic energy in the range between 0 and 4 eV and the emitted photons were detected with an optical bandpass filter and a photomultiplier to obtain the LEIPS sepctrum. The electron affinities (EA) were determined as the onset energy of LEIPS spectrum with reference to the vaccuum level. EA were measured at two photon energies by changing the bandpass filter with the center wavelength of 260 and 285 nm.[10]

SCLC Measurements

Hole-only and electron-only devices were prepared with a structure of ITO/PEDOT:PSS/active layer/Au and ITO/TiO_x/active layer/Ca/Au, respectively.[11] The active layers were prepared from 10 mg mL^{-1} solution of materials in chloroform. The carrier mobilities of these devices were calculated by the following equation:

$$J = \frac{9}{8}\varepsilon\varepsilon_0\mu\frac{V^2}{d^3}$$

where ε, ε_0, μ, and d are the dielectric constant of the active layer, the permittivity of free space, the carrier mobility, and the measured thickness of active layer, respectively. We used the values of $\varepsilon = 3$, $\varepsilon_0 = 8.8 \times 10^{-12}$.

PLQE Estimation

Acceptor pristine films and PTB7/acceptor blended films were prepared on the quartz substrate by spin-coating using 10 mg mL^{-1} $CHCl_3$ solution, and the UV-vis absorption spectra and emission spectra were recorded, respectively. PLQE of blended films were calculated using following equation:

$$\text{PLQE} = 1 - \frac{\phi_{p:n}}{\phi_p}$$

where Φ_p and $\Phi_{p:n}$ are the normalized photoluminescence intensities of pristine films using absorbed photons at λ_{max} and the normalized photoluminescence intensities of blended films against relative ratio of acceptor component, respectively.

References

1 P. K. Iyer, S. Wang, *Tetrahedron Lett.*, 2006, **47**, 437.

2 A. M. Ramos, S. C. J. Meskers, E. H. A. Beckers, R. B. Prince, L. Brunsveld, R. A. J. Janssen, *J. Am. Chem. Soc.*, 2004, **126**, 9630.

3 B. A. G. Hammer, M. Baumgarten, K. Müllen, *Chem. Commun.*, 2014, **50**, 2034.

4 P. Rajasingh, R. Cohen, E. Shirman, L. J. Shimon, B. Rybtchinski, *J. Org. Chem.*, 2007, **72**, 5973.

5 X.-F. Wu, W.-F. Fu, Z. Xu, M. Shi, F. Liu, H.-Z. Chen, J.-H. Wan, T. P. Russell, *Adv. Funct. Mater.*, 2015, **25**, 5954.

6 S. Mataka, K. Takahashi, Y. Ikezaki, T. Hatta, A. Tori-i, M. Tashiro, *Bull. Chem. Soc. Japan*, 1991, **64**, 68.

7 F. P. V. Koch, P. Smith, M. Heeney, *J. Am. Chem. Soc.*, 2013, **135**, 13695.

8 S. Chatterjee, Y. Ie, M. Karakawa, Y. Aso, *Adv. Funct. Mater.*, 2016, **26**, 1161.

9 H. Yoshida, *Rev. Sci. Instrum.*, 2014, **85**, 016101.

10 H. Yoshida, *Chem. Phys. Lett.*, 2012, **539-540**, 180.

11 S. D. Dimitrov, J. R. Durrant, *Chem. Mater.*, 2014, **26**, 616; G. G. Malliaras, J. R. Salem, P. J. Brock, C. Scott, *Phys. Rev. B*, 1998, **58**, 13411; C. Goh, R. J. Kline, M. D. McGehee, E. N. Kadnikova, J. M. J. Fréchet, *Appl. Phys. Lett.*, 2005, **86**, 122110.

Computational Details

All calculations were conducted using Gaussian 09 program. The geometry was optimized with the restricted Becke Hybrid (B3LYP) at 6-31G(d, p) level.

Optimized structure of model compound for **TetraBP-N-PDIC9**/C2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-9.153634	-8.562356	-4.556408
2	6	0	-10.163357	-9.510211	-4.944549
3	6	0	-11.423260	-9.517497	-4.288497
4	6	0	-11.620038	-8.563189	-3.263596
5	6	0	-10.639325	-7.644744	-2.899554
6	6	0	-9.406660	-7.643020	-3.545912
7	6	0	-7.914963	-8.554392	-5.187529
8	6	0	-11.690741	-13.263484	-7.764327
9	6	0	-8.628674	-10.380734	-6.596150
10	6	0	-9.902766	-10.441604	-5.984207
11	6	0	-8.399769	-6.628927	-3.153178
12	7	0	-7.139329	-6.688387	-3.767502
13	6	0	-6.840583	-7.616525	-4.775822
14	8	0	-5.747570	-7.760941	-5.322665
15	8	0	-8.770217	-5.774160	-2.348532
16	6	0	-6.120654	-5.741364	-3.355182
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18	6	0	-12.168223	-11.393869	-5.713391
19	6	0	-10.908400	-11.388554	-6.370379
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21	6	0	-7.654990	-9.462986	-6.209146
22	6	0	-12.920595	-13.259045	-7.118111
23	6	0	-14.412772	-12.350050	-5.454118
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46	6	0	5.004850	-4.891186	12.660476
47	6	0	3.920883	-3.982750	12.679527
48	6	0	3.264194	-3.577344	11.520587
49	6	0	3.668883	-4.063122	10.280908

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51	6	0	8.928167	-8.033061	13.625792
52	6	0	6.834010	-6.769471	10.013277
53	6	0	6.485909	-6.309154	11.304493
54	6	0	2.938875	-3.618701	9.069887
55	7	0	3.423342	-4.044936	7.824430
56	6	0	4.482809	-4.957078	7.704983
57	8	0	4.972236	-5.364625	6.651985
58	8	0	1.927679	-2.941634	9.254621
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61	6	0	6.771985	-6.225966	13.757989
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63	6	0	8.260764	-7.635488	12.470327
64	6	0	6.173640	-6.342705	8.863894
65	6	0	8.528628	-7.536636	14.860161
66	6	0	7.073866	-6.145997	16.191308
67	6	0	6.017144	-5.249707	16.289768
68	6	0	5.343232	-4.844594	15.140745
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72	6	0	7.775120	-6.559527	17.429752
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76	6	0	2.314525	-2.204935	6.575889
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79	6	0	2.164087	-3.736420	4.269075
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83	6	0	-0.480525	-0.515017	1.764760
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85	6	0	1.478051	-1.280570	0.613144
86	6	0	1.921738	-1.902991	1.786256
87	6	0	10.585960	2.138419	-7.719593
88	6	0	11.899553	2.204205	-8.301158
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92	6	0	9.662713	1.203795	-8.171617
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106	6	0	15.125198	4.166417	-7.996729
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112	6	0	13.585021	1.349449	-9.896381
113	6	0	18.127137	3.376609	-10.108143
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115	6	0	17.568388	1.494833	-11.585371
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117	8	0	18.931746	4.180128	-9.643486
118	6	0	19.761704	2.539430	-11.699560
119	6	0	6.110736	0.515253	-5.745698
120	6	0	4.929055	0.319546	-5.014904
121	6	0	4.322992	1.374263	-4.324178
122	6	0	4.910266	2.639420	-4.427522
123	6	0	6.088603	2.834656	-5.163750
124	6	0	3.154672	1.141189	-3.465030
125	6	0	3.222121	1.417640	-2.094761
126	6	0	2.147961	1.129440	-1.248947
127	6	0	0.967052	0.524282	-1.730447
128	6	0	0.874655	0.335794	-3.120840
129	6	0	1.957499	0.617117	-3.968426
130	6	0	-6.289451	11.494988	1.786207
131	6	0	-7.082123	12.651032	2.107551
132	6	0	-7.253696	13.042546	3.462093
133	6	0	-6.607873	12.257448	4.445256
134	6	0	-5.833603	11.146063	4.124127
135	6	0	-5.675272	10.763834	2.795291
136	6	0	-6.128549	11.095783	0.464378
137	6	0	-9.918603	16.446823	0.724396
138	6	0	-7.485892	12.958412	-0.255367
139	6	0	-7.697958	13.401341	1.071396
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142	6	0	-5.370845	9.868852	0.111097
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144	8	0	-4.196697	9.108070	3.432169
145	6	0	-4.053346	7.927030	0.858376
146	6	0	-9.473674	16.082117	3.069164
147	6	0	-8.670934	14.936352	2.747175
148	6	0	-8.495755	14.549315	1.391432
149	6	0	-9.139908	15.337209	0.406225
150	6	0	-6.723364	11.832167	-0.555972
151	6	0	-10.084209	16.817563	2.053081
152	6	0	-9.652203	16.460837	4.400069
153	6	0	-9.054147	15.733643	5.421362
154	6	0	-8.272245	14.623287	5.114773
155	6	0	-8.053907	14.187507	3.784719
156	6	0	-10.918752	18.002338	2.364139
157	7	0	-11.009901	18.372139	3.700323
158	6	0	-10.479536	17.638435	4.754164
159	8	0	-10.668499	17.907125	5.937803
160	8	0	-11.492431	18.590643	1.451156
161	6	0	-11.830205	19.524148	4.026979
162	6	0	-4.028098	6.864648	1.774640
163	6	0	-3.358858	5.666614	1.491419
164	6	0	-2.686076	5.477555	0.277862
165	6	0	-2.703927	6.533426	-0.639934
166	6	0	-3.374399	7.734623	-0.354578
167	6	0	-2.008086	4.204302	-0.012057

168	6	0	-1.089824	3.654753	0.892286
169	6	0	-0.502316	2.404462	0.663969
170	6	0	-0.839039	1.631475	-0.461840
171	6	0	-1.685763	2.235117	-1.414688
172	6	0	-2.271998	3.486840	-1.185285
173	6	0	-0.213346	0.202670	-0.730063
174	1	0	-12.555260	-8.500320	-2.713783
175	1	0	-10.853929	-6.927288	-2.108300
176	1	0	-11.483673	-13.978222	-8.559355
177	1	0	-8.349157	-11.057648	-7.399088
178	1	0	-9.774233	-12.407292	-7.943750
179	1	0	-6.688706	-9.472905	-6.712121
180	1	0	-15.639821	-11.446908	-3.925112
181	1	0	-13.980499	-9.846636	-3.252547
182	1	0	-17.202593	-14.718137	-7.129349
183	1	0	-16.095341	-15.410255	-8.337815
184	1	0	-16.080442	-16.019972	-6.664497
185	1	0	-6.717179	-5.664289	-1.263786
186	1	0	-5.060460	-4.041127	-0.586305
187	1	0	-3.512915	-3.911507	-4.601451
188	1	0	-5.183372	-5.515586	-5.306339
189	1	0	-1.431107	-3.869682	-2.866056
190	1	0	0.188264	-2.209399	-2.119249
191	1	0	-3.029079	0.126591	-0.420761
192	1	0	-4.624674	-1.516435	-1.194168
193	1	0	3.547914	-3.558945	13.608062
194	1	0	2.432394	-2.878380	11.599929
195	1	0	9.760430	-8.731304	13.550781
196	1	0	7.644973	-7.476009	9.858775
197	1	0	8.628074	-8.062845	11.541057
198	1	0	6.498523	-6.721924	7.895662
199	1	0	5.709014	-4.858374	17.258054
200	1	0	4.528430	-4.141780	15.293277
201	1	0	8.826303	-7.901836	19.360719
202	1	0	9.909217	-8.916537	18.379376
203	1	0	10.311239	-7.205696	18.667241
204	1	0	2.379247	-1.546351	7.438626
205	1	0	1.433418	-0.630986	5.412678
206	1	0	2.110087	-4.367581	3.383869
207	1	0	3.034718	-5.311579	5.410837
208	1	0	-0.662580	-1.090371	3.825691
209	1	0	-1.448030	-0.016597	1.787153
210	1	0	2.085758	-1.404830	-0.280623
211	1	0	2.868119	-2.440468	1.762562
212	1	0	11.486728	-0.355615	-10.534761
213	1	0	9.299384	-0.415034	-9.556520
214	1	0	17.116569	4.950571	-8.186009
215	1	0	13.053971	4.814398	-6.412366
216	1	0	14.918315	4.898665	-7.220792
217	1	0	10.867036	4.653428	-5.450750
218	1	0	15.585559	-0.192687	-12.230507
219	1	0	13.366524	-0.303624	-11.317302
220	1	0	19.771093	2.171446	-12.729798
221	1	0	20.157617	3.559304	-11.685688
222	1	0	20.407642	1.900772	-11.088503
223	1	0	6.554759	-0.363381	-6.206907
224	1	0	4.510928	-0.683736	-4.955124
225	1	0	4.461620	3.492176	-3.920882
226	1	0	6.478235	3.848271	-5.210002

227	1	0	4.127450	1.842784	-1.664942
228	1	0	2.254968	1.369578	-0.192309
229	1	0	-0.039360	-0.036468	-3.577941
230	1	0	1.853436	0.426665	-5.035031
231	1	0	-6.684406	12.491536	5.503755
232	1	0	-5.354612	10.584948	4.925609
233	1	0	-10.392624	17.015550	-0.074193
234	1	0	-7.920392	13.477211	-1.105852
235	1	0	-9.055291	15.105951	-0.652255
236	1	0	-6.610057	11.532548	-1.597196
237	1	0	-9.189879	16.022598	6.462557
238	1	0	-7.836715	14.102747	5.963381
239	1	0	-11.485716	20.001208	4.949277
240	1	0	-11.809488	20.261836	3.219339
241	1	0	-12.860358	19.181833	4.168530
242	1	0	-4.557918	6.921962	2.722358
243	1	0	-3.388897	4.867928	2.230402
244	1	0	-2.183298	6.439578	-1.591283
245	1	0	-3.320154	8.521069	-1.103113
246	1	0	-0.817822	4.202500	1.793055
247	1	0	0.222799	2.050154	1.392959
248	1	0	-1.919590	1.722612	-2.346676
249	1	0	-2.960795	3.885273	-1.927726

Optimized structure of model compound for **Pyrene-B-PDI**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.677079	0.191630	0.508481
2	6	0	1.408697	1.384697	0.761952
3	6	0	2.570753	1.344447	1.576946
4	6	0	2.905075	0.146428	2.226977
5	6	0	2.158745	-1.030785	2.052971
6	6	0	1.068987	-1.023198	1.138278
7	6	0	-0.454862	0.217957	-0.372500
8	6	0	-0.895015	1.446486	-0.938843
9	6	0	-0.164594	2.608462	-0.644549
10	6	0	0.963127	2.576250	0.170237
11	6	0	0.340567	-2.184319	0.832727
12	6	0	-0.705446	-2.174316	-0.086635
13	6	0	-1.134032	-0.987507	-0.698292
14	6	0	-2.219844	-0.969600	-1.614475
15	6	0	-2.669593	0.262871	-2.113202
16	6	0	-2.042688	1.473594	-1.777515
17	6	0	4.823940	4.786565	2.768875
18	6	0	5.216943	4.153209	1.531693
19	6	0	6.328141	4.699625	0.821617
20	6	0	6.990681	5.818730	1.384143
21	6	0	6.600988	6.407225	2.577779
22	6	0	5.515392	5.894918	3.265854
23	6	0	3.747276	4.301832	3.495641
24	6	0	3.057673	3.190674	3.045809
25	6	0	3.411977	2.533755	1.852156
26	6	0	4.513688	3.007769	1.027179
27	6	0	4.966225	2.448398	-0.255758
28	6	0	6.060372	3.028042	-0.966818

29	6	0	6.749641	4.137472	-0.421457
30	6	0	6.481660	2.502687	-2.246437
31	6	0	7.565250	3.057903	-2.928081
32	6	0	8.253263	4.128395	-2.381922
33	6	0	7.847511	4.652420	-1.160361
34	6	0	4.376771	1.329366	-0.897064
35	6	0	4.761478	0.839070	-2.143969
36	6	0	5.809762	1.430726	-2.821128
37	6	0	5.120887	6.558829	4.532242
38	7	0	3.987854	6.073146	5.164414
39	6	0	3.302357	4.939133	4.758648
40	6	0	6.182654	0.900650	-4.152907
41	7	0	7.257139	1.504505	-4.790088
42	6	0	8.015359	2.525076	-4.237382
43	8	0	2.369430	4.446261	5.386712
44	8	0	5.800546	7.485572	4.965520
45	8	0	5.540256	-0.028847	-4.632958
46	8	0	9.019950	2.996760	-4.763726
47	6	0	3.577234	6.704172	6.405378
48	6	0	7.654614	0.964838	-6.077591
49	6	0	2.508028	-4.214681	4.903114
50	6	0	2.993366	-4.479253	3.572430
51	6	0	3.045340	-3.441689	2.584112
52	6	0	2.450115	-2.176802	2.956568
53	6	0	1.993021	-1.961677	4.273070
54	6	0	2.045241	-2.952617	5.238215
55	6	0	2.489074	-5.215617	5.877959
56	6	0	2.923370	-6.494619	5.572394
57	6	0	3.367760	-6.776954	4.288034
58	6	0	3.414744	-5.803745	3.259143
59	6	0	3.870300	-6.125850	1.946026
60	6	0	4.032554	-5.098564	0.985523
61	6	0	3.672146	-3.757934	1.307293
62	6	0	4.576538	-5.425335	-0.306957
63	6	0	4.827299	-4.419504	-1.234863
64	6	0	4.551406	-3.100682	-0.914366
65	6	0	3.992339	-2.789665	0.324035
66	6	0	4.192093	-7.449659	1.550633
67	6	0	4.676009	-7.761199	0.285722
68	6	0	4.876217	-6.747558	-0.638344
69	6	0	1.559640	-2.634275	6.602248
70	7	0	1.507301	-3.681631	7.508894
71	6	0	2.002732	-4.951279	7.254443
72	6	0	5.407904	-7.104475	-1.974553
73	7	0	5.587621	-6.064109	-2.875335
74	6	0	5.426070	-4.723600	-2.556109
75	8	0	2.066071	-5.842138	8.097606
76	8	0	1.245770	-1.478901	6.874746
77	8	0	5.676343	-8.277069	-2.224078
78	8	0	5.767257	-3.798912	-3.287447
79	6	0	1.036373	-3.390342	8.850782
80	6	0	6.139349	-6.399646	-4.174891
81	6	0	-3.165073	5.039598	-3.872336
82	6	0	-3.624806	4.915433	-2.510153
83	6	0	-4.347157	6.006472	-1.941703
84	6	0	-4.591632	7.138530	-2.758044
85	6	0	-4.150730	7.233042	-4.069811
86	6	0	-3.434741	6.186354	-4.624224
87	6	0	-2.441221	4.015938	-4.464584

88	6	0	-2.132505	2.880117	-3.736991
89	6	0	-2.552822	2.719123	-2.403005
90	6	0	-3.359916	3.731976	-1.743572
91	6	0	-3.910262	3.668493	-0.386005
92	6	0	-4.592920	4.785328	0.182014
93	6	0	-4.803376	5.953130	-0.589935
94	6	0	-5.083909	4.744308	1.539399
95	6	0	-5.745395	5.840523	2.093932
96	6	0	-5.940509	6.987453	1.342462
97	6	0	-5.478423	7.035592	0.032699
98	6	0	-3.831573	2.530502	0.455944
99	6	0	-4.296808	2.491735	1.768866
100	6	0	-4.912077	3.602876	2.313752
101	6	0	-2.965436	6.329254	-6.023913
102	7	0	-2.191530	5.297724	-6.531463
103	6	0	-1.957352	4.106410	-5.863449
104	6	0	-5.389088	3.534612	3.714361
105	7	0	-5.991841	4.673808	4.227717
106	6	0	-6.261928	5.812185	3.483444
107	8	0	-1.392090	3.140467	-6.368517
108	8	0	-3.280262	7.326563	-6.668143
109	8	0	-5.244068	2.493755	4.348917
110	8	0	-6.904015	6.770430	3.906022
111	6	0	-1.727972	5.411374	-7.902256
112	6	0	-6.491507	4.615068	5.588857
113	6	0	-3.653803	-4.341680	-3.829699
114	6	0	-4.384675	-4.005498	-2.630395
115	6	0	-3.956046	-2.936444	-1.770794
116	6	0	-2.790918	-2.199000	-2.219364
117	6	0	-2.096859	-2.580400	-3.386779
118	6	0	-2.513512	-3.636442	-4.175613
119	6	0	-4.075647	-5.373875	-4.672418
120	6	0	-5.216611	-6.096170	-4.372655
121	6	0	-5.931140	-5.794411	-3.223074
122	6	0	-5.551830	-4.766236	-2.324170
123	6	0	-6.305032	-4.499953	-1.141996
124	6	0	-5.879393	-3.491217	-0.244064
125	6	0	-4.721995	-2.708749	-0.542718
126	6	0	-6.626684	-3.279835	0.973048
127	6	0	-6.210423	-2.325530	1.893374
128	6	0	-5.089378	-1.560256	1.629246
129	6	0	-4.383265	-1.747042	0.441686
130	6	0	-7.479326	-5.223776	-0.805916
131	6	0	-8.198557	-5.000987	0.361578
132	6	0	-7.766699	-4.034806	1.254697
133	6	0	-1.724974	-3.960994	-5.388758
134	7	0	-2.157338	-5.036608	-6.147796
135	6	0	-3.331939	-5.729996	-5.905589
136	6	0	-8.542862	-3.831666	2.501863
137	7	0	-8.101658	-2.833088	3.357085
138	6	0	-6.931629	-2.112194	3.169697
139	8	0	-3.778890	-6.598530	-6.650195
140	8	0	-0.746811	-3.275762	-5.673381
141	8	0	-9.514129	-4.547858	2.730891
142	8	0	-6.467657	-1.336604	4.000121
143	6	0	-1.409113	-5.361675	-7.348556
144	6	0	-8.824517	-2.636487	4.600209
145	1	0	3.752632	0.137780	2.914513
146	1	0	-0.451161	3.573174	-1.058416

147	1	0	1.485834	3.516494	0.336669
148	1	0	0.588141	-3.140728	1.287027
149	1	0	-1.202577	-3.120987	-0.290291
150	1	0	-3.504243	0.275899	-2.816000
151	1	0	7.846727	6.283975	0.903563
152	1	0	7.150177	7.267693	2.956579
153	1	0	2.217762	2.813830	3.634122
154	1	0	9.104170	4.568296	-2.899591
155	1	0	8.434839	5.494596	-0.805955
156	1	0	3.563777	0.774796	-0.457794
157	1	0	4.226887	-0.005760	-2.576378
158	1	0	2.496354	6.614464	6.548846
159	1	0	4.087380	6.198525	7.231297
160	1	0	3.847785	7.763997	6.415611
161	1	0	8.208704	0.036602	-5.904736
162	1	0	6.770340	0.736174	-6.680909
163	1	0	8.289124	1.662036	-6.631417
164	1	0	1.558795	-0.994677	4.538408
165	1	0	2.916758	-7.282460	6.324180
166	1	0	3.699890	-7.798981	4.126627
167	1	0	4.772291	-2.303068	-1.621285
168	1	0	3.852658	-1.731512	0.502549
169	1	0	4.062342	-8.295126	2.220865
170	1	0	4.902506	-8.796525	0.036139
171	1	0	0.624207	-4.285282	9.325804
172	1	0	1.885754	-3.033146	9.441749
173	1	0	0.266033	-2.613471	8.832861
174	1	0	6.009176	-5.585942	-4.893599
175	1	0	7.207861	-6.605041	-4.053747
176	1	0	5.652686	-7.298992	-4.565801
177	1	0	-5.148718	7.998974	-2.397860
178	1	0	-4.369137	8.130584	-4.646180
179	1	0	-1.529384	2.099436	-4.206221
180	1	0	-6.453361	7.850612	1.763544
181	1	0	-5.666886	7.970591	-0.487146
182	1	0	-3.409676	1.595563	0.119906
183	1	0	-4.171644	1.583841	2.355667
184	1	0	-0.824427	4.815815	-8.062726
185	1	0	-2.519347	5.043162	-8.562778
186	1	0	-1.512834	6.454055	-8.154609
187	1	0	-7.495316	4.178996	5.565760
188	1	0	-5.848171	3.987807	6.213071
189	1	0	-6.548672	5.613677	6.031540
190	1	0	-1.212974	-2.013644	-3.690810
191	1	0	-5.558806	-6.899603	-5.022958
192	1	0	-6.808256	-6.412991	-3.055042
193	1	0	-4.746833	-0.815906	2.346488
194	1	0	-3.524369	-1.100876	0.343273
195	1	0	-7.880184	-6.001169	-1.450223
196	1	0	-9.089159	-5.593163	0.565268
197	1	0	-1.537709	-6.413737	-7.619188
198	1	0	-1.783474	-4.736126	-8.165034
199	1	0	-0.342732	-5.160556	-7.208777
200	1	0	-8.697852	-1.615134	4.971398
201	1	0	-9.892264	-2.833554	4.465423
202	1	0	-8.426397	-3.335803	5.342285

Optimized structure of model compound for **TetraP-B-PDI**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.325835	-4.819981	4.960153
2	6	0	5.521493	-4.835953	3.534966
3	6	0	4.851365	-3.892388	2.697788
4	6	0	3.856984	-3.054217	3.338233
5	6	0	3.707719	-3.055632	4.735014
6	6	0	4.450543	-3.908458	5.537254
7	6	0	6.007544	-5.719517	5.783624
8	6	0	7.557109	-6.954398	-0.442630
9	6	0	7.046935	-6.703437	3.858310
10	6	0	6.390526	-5.815603	2.971581
11	6	0	4.245269	-3.853718	7.004503
12	7	0	4.904043	-4.808429	7.765684
13	6	0	5.828639	-5.707436	7.255342
14	8	0	6.497904	-6.468050	7.950119
15	8	0	3.529569	-2.976785	7.480780
16	6	0	4.721020	-4.771210	9.204865
17	6	0	6.287371	-4.919705	-0.693856
18	6	0	6.022966	-4.890613	0.721684
19	6	0	6.583199	-5.886701	1.556837
20	6	0	7.337681	-6.912114	0.930720
21	6	0	6.869752	-6.656607	5.235127
22	6	0	7.038318	-5.954124	-1.252322
23	6	0	5.809445	-3.903571	-1.517608
24	6	0	5.113521	-2.840327	-0.968463
25	6	0	4.846146	-2.825036	0.397955
26	6	0	5.217299	-3.864257	1.287510
27	6	0	7.303729	-6.010234	-2.709685
28	7	0	6.734693	-5.011924	-3.489783
29	6	0	6.056994	-3.913533	-2.978199
30	8	0	5.667799	-2.969569	-3.660813
31	8	0	8.009057	-6.909553	-3.159589
32	6	0	6.992254	-5.043385	-4.917659
33	6	0	2.856631	-2.248791	2.607730
34	6	0	1.878771	-2.875731	1.822280
35	6	0	0.955950	-2.126593	1.084983
36	6	0	0.986936	-0.719924	1.089320
37	6	0	1.906280	-0.102190	1.964740
38	6	0	2.830290	-0.850786	2.702185
39	6	0	-3.592143	-3.434549	-6.802491
40	6	0	-3.884372	-4.124223	-5.572116
41	6	0	-3.203861	-3.781664	-4.361717
42	6	0	-2.329824	-2.626581	-4.425187
43	6	0	-2.057372	-1.991838	-5.649161
44	6	0	-2.662328	-2.403450	-6.825259
45	6	0	-4.245534	-3.777899	-7.988702
46	6	0	-6.547293	-7.526792	-3.160407
47	6	0	-5.504770	-5.447612	-6.816099
48	6	0	-4.874595	-5.150721	-5.582737
49	6	0	-2.325367	-1.687319	-8.079062
50	7	0	-2.953643	-2.121027	-9.237315
51	6	0	-3.951712	-3.082812	-9.265273
52	8	0	-4.595133	-3.371954	-10.270665
53	8	0	-1.527293	-0.754551	-8.046925
54	6	0	-2.649054	-1.419080	-10.470347

55	6	0	-4.777084	-6.364375	-2.008311
56	6	0	-4.480523	-5.600439	-3.194833
57	6	0	-5.210676	-5.849454	-4.381820
58	6	0	-6.248388	-6.815487	-4.317782
59	6	0	-5.199773	-4.782921	-7.996259
60	6	0	-5.806243	-7.306309	-2.009365
61	6	0	-4.026401	-6.182600	-0.850261
62	6	0	-2.974378	-5.284295	-0.845862
63	6	0	-2.700767	-4.537332	-1.989263
64	6	0	-3.455222	-4.612212	-3.186949
65	6	0	-6.131007	-8.093777	-0.795911
66	7	0	-5.393150	-7.817145	0.347266
67	6	0	-4.306222	-6.954669	0.383102
68	8	0	-3.577406	-6.811590	1.361170
69	8	0	-7.010665	-8.949293	-0.850106
70	6	0	-5.684803	-8.589475	1.540585
71	6	0	-1.754426	-1.943601	-3.251020
72	6	0	-0.380688	-1.988969	-2.979313
73	6	0	0.146532	-1.341581	-1.856458
74	6	0	-0.677074	-0.624554	-0.960326
75	6	0	-2.039196	-0.512925	-1.298401
76	6	0	-2.570653	-1.173981	-2.411052
77	6	0	3.741378	6.333480	-4.505055
78	6	0	4.237610	6.235527	-3.159114
79	6	0	3.536470	5.468582	-2.178600
80	6	0	2.430589	4.665583	-2.656432
81	6	0	1.964122	4.804816	-3.975096
82	6	0	2.591919	5.649449	-4.878163
83	6	0	4.413618	7.100846	-5.459726
84	6	0	7.750390	7.291665	0.153110
85	6	0	6.089248	7.660870	-3.837036
86	6	0	5.449471	6.906407	-2.823341
87	6	0	2.040206	5.752699	-6.250249
88	7	0	2.709134	6.587247	-7.134471
89	6	0	3.908976	7.221339	-6.848853
90	8	0	4.562199	7.854611	-7.673812
91	8	0	1.038215	5.108665	-6.548498
92	6	0	2.191190	6.684134	-8.486518
93	6	0	5.747651	6.148726	0.860985
94	6	0	5.242885	6.165749	-0.486793
95	6	0	5.988898	6.809131	-1.503601
96	6	0	7.249707	7.349771	-1.143653
97	6	0	5.584592	7.764512	-5.126787
98	6	0	6.994367	6.701202	1.155758
99	6	0	4.991051	5.584423	1.885293
100	6	0	3.733186	5.071808	1.613945
101	6	0	3.254673	5.076195	0.306193
102	6	0	3.999467	5.551586	-0.801798
103	6	0	7.538818	6.675273	2.534260
104	7	0	6.716682	6.150491	3.522679
105	6	0	5.490038	5.546238	3.279586
106	8	0	4.822031	4.982596	4.142614
107	8	0	8.672547	7.100062	2.740918
108	6	0	7.227008	6.111183	4.880471
109	6	0	1.808637	3.561287	-1.892304
110	6	0	0.439140	3.551166	-1.592832
111	6	0	-0.137991	2.481506	-0.896370
112	6	0	0.635489	1.393847	-0.439512
113	6	0	1.996624	1.387079	-0.802984

114	6	0	2.571054	2.448831	-1.509701
115	6	0	-5.747021	2.276743	6.484544
116	6	0	-5.989085	2.853644	5.187207
117	6	0	-5.228663	2.439867	4.048554
118	6	0	-4.129166	1.529546	4.309963
119	6	0	-3.934531	0.979580	5.588456
120	6	0	-4.745410	1.330288	6.655687
121	6	0	-6.511350	2.656040	7.591030
122	6	0	-8.465375	6.110875	2.405684
123	6	0	-7.737966	4.194514	6.221662
124	6	0	-7.002092	3.849893	5.061553
125	6	0	-4.485810	0.702179	7.973490
126	7	0	-5.235828	1.162172	9.045659
127	6	0	-6.284491	2.061757	8.930352
128	8	0	-7.023169	2.373073	9.861242
129	8	0	-3.647709	-0.191040	8.061276
130	6	0	-5.002222	0.558084	10.344350
131	6	0	-6.917092	4.587156	1.359986
132	6	0	-6.592893	4.007530	2.640050
133	6	0	-7.259510	4.469714	3.799937
134	6	0	-8.182743	5.535868	3.640235
135	6	0	-7.507585	3.610434	7.459876
136	6	0	-7.838489	5.630676	1.265939
137	6	0	-6.326239	4.098739	0.198256
138	6	0	-5.447216	3.032823	0.268963
139	6	0	-5.125352	2.486016	1.509091
140	6	0	-5.624538	2.968716	2.744978
141	6	0	-8.174175	6.246197	-0.040441
142	7	0	-7.497761	5.764514	-1.152892
143	6	0	-6.640313	4.673366	-1.130614
144	8	0	-6.148632	4.167876	-2.136330
145	8	0	-9.027046	7.129224	-0.088997
146	6	0	-7.822963	6.343164	-2.443412
147	6	0	-3.082792	1.175299	3.331768
148	6	0	-2.114745	2.114059	2.948708
149	6	0	-1.139743	1.797185	1.994546
150	6	0	-1.117582	0.541479	1.361229
151	6	0	-2.032542	-0.426444	1.833102
152	6	0	-2.999493	-0.115798	2.794723
153	6	0	-0.044483	0.151132	0.268235
154	1	0	2.964836	-2.402874	5.197390
155	1	0	8.141953	-7.768008	-0.868617
156	1	0	7.742862	-7.457923	3.501327
157	1	0	4.856757	-5.765334	9.641247
158	1	0	5.469227	-4.093289	9.627672
159	1	0	3.723361	-4.405153	9.464794
160	1	0	7.773396	-7.728685	1.500911
161	1	0	7.406902	-7.359638	5.869917
162	1	0	4.775156	-2.012864	-1.589478
163	1	0	4.352267	-1.928297	0.753838
164	1	0	6.197389	-4.535310	-5.471418
165	1	0	7.940656	-4.530379	-5.105867
166	1	0	7.069688	-6.073845	-5.276829
167	1	0	1.833234	-3.962456	1.772660
168	1	0	0.210439	-2.672278	0.511029
169	1	0	1.919265	0.981077	2.076373
170	1	0	3.541600	-0.329582	3.340530
171	1	0	-1.383170	-1.132687	-5.669349
172	1	0	-7.355021	-8.256840	-3.171768

173	1	0	-6.255604	-6.228062	-6.903217
174	1	0	-2.852311	-2.045831	-11.343429
175	1	0	-3.278376	-0.524764	-10.519655
176	1	0	-1.598610	-1.112924	-10.492257
177	1	0	-6.871561	-7.043175	-5.178633
178	1	0	-5.714565	-5.057376	-8.915732
179	1	0	-2.351564	-5.156699	0.037689
180	1	0	-1.826404	-3.904885	-1.908023
181	1	0	-5.402302	-8.040049	2.443366
182	1	0	-6.749582	-8.834967	1.595215
183	1	0	-5.109069	-9.519424	1.495464
184	1	0	0.291009	-2.536120	-3.638392
185	1	0	1.221906	-1.396779	-1.695412
186	1	0	-2.717232	0.104047	-0.713461
187	1	0	-3.632897	-1.071704	-2.627238
188	1	0	1.118420	4.202835	-4.313661
189	1	0	8.726857	7.721054	0.371548
190	1	0	7.004484	8.214537	-3.646438
191	1	0	2.522717	7.605074	-8.974551
192	1	0	2.560082	5.825658	-9.056612
193	1	0	1.097178	6.660849	-8.482269
194	1	0	7.895571	7.827870	-1.875776
195	1	0	6.115388	8.364003	-5.864716
196	1	0	3.110139	4.669644	2.410804
197	1	0	2.239183	4.712823	0.188098
198	1	0	6.409878	6.198721	5.602903
199	1	0	7.729349	5.150112	5.030114
200	1	0	7.943208	6.918415	5.058405
201	1	0	-0.198015	4.373685	-1.913664
202	1	0	-1.214055	2.502646	-0.731235
203	1	0	2.637069	0.538916	-0.570921
204	1	0	3.626540	2.393682	-1.772062
205	1	0	-3.108855	0.284231	5.753379
206	1	0	-9.183273	6.927156	2.344733
207	1	0	-8.540480	4.926637	6.195003
208	1	0	-5.256393	1.253375	11.149918
209	1	0	-5.637422	-0.329427	10.428392
210	1	0	-3.956141	0.257247	10.454697
211	1	0	-8.712101	5.965122	4.486824
212	1	0	-8.110534	3.910000	8.315726
213	1	0	-5.007043	2.610442	-0.632650
214	1	0	-4.477805	1.620561	1.458235
215	1	0	-8.687195	5.808813	-2.850410
216	1	0	-8.076763	7.402556	-2.342649
217	1	0	-6.984817	6.245385	-3.139400
218	1	0	-2.114576	3.108126	3.392763
219	1	0	-0.398690	2.558688	1.763231
220	1	0	-2.008375	-1.443915	1.445328
221	1	0	-3.701193	-0.886919	3.107432

Optimized structure of model compound for **SpiroF-B-PDI**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.412241	5.909158	-2.783230
2	6	0	-3.189621	4.892160	-3.240605

3	6	0	-2.906335	3.605852	-2.927887
4	6	0	-1.734730	3.338697	-2.302302
5	6	0	-0.994928	4.355850	-1.824883
6	6	0	-1.321225	5.639707	-2.040194
7	6	0	-2.720804	7.190165	-3.071459
8	6	0	-6.957388	3.382547	-5.629073
9	6	0	-4.524133	6.432017	-4.320654
10	6	0	-4.268447	5.144635	-4.017526
11	6	0	-0.500121	6.622555	-1.569684
12	7	0	-0.929356	7.916821	-1.792268
13	6	0	-1.998686	8.245112	-2.601595
14	8	0	-2.248130	9.403888	-2.858835
15	8	0	0.545067	6.417001	-0.990841
16	6	0	-0.151367	9.017140	-1.204342
17	6	0	-5.838561	1.925650	-4.222274
18	6	0	-4.921389	2.894795	-3.955685
19	6	0	-5.076639	4.144842	-4.443215
20	6	0	-6.091060	4.347386	-5.305646
21	6	0	-3.779177	7.438464	-3.855461
22	6	0	-6.858032	2.167038	-5.071402
23	6	0	-5.756890	0.726636	-3.610462
24	6	0	-4.748668	0.514358	-2.753107
25	6	0	-3.828382	1.461054	-2.547318
26	6	0	-3.848319	2.657034	-3.168423
27	6	0	-7.792999	1.226040	-5.381941
28	7	0	-7.649427	0.006784	-4.745989
29	6	0	-6.680741	-0.257589	-3.795505
30	8	0	-6.675913	-1.302729	-3.182656
31	8	0	-8.714699	1.421596	-6.146009
32	6	0	-8.635859	-1.040859	-5.045692
33	6	0	0.222092	-0.228219	-2.213720
34	6	0	0.058699	0.496051	-1.098310
35	6	0	0.566347	-0.231487	0.115320
36	6	0	1.256419	-1.337374	-0.614039
37	6	0	0.978732	-1.301514	-1.927099
38	6	0	-0.635826	-0.633245	0.921016
39	6	0	-0.724848	0.060673	2.061192
40	6	0	0.366902	0.832466	2.193567
41	6	0	1.191593	0.644107	1.150226
42	6	0	-0.328056	0.200339	-3.357072
43	6	0	-1.023790	1.352770	-3.354389
44	6	0	-1.116203	2.134578	-2.255525
45	6	0	-0.553738	1.686559	-1.116273
46	6	0	1.992495	-2.317001	-0.076510
47	6	0	2.532131	-3.276624	-0.858631
48	6	0	2.234194	-3.220968	-2.178709
49	6	0	1.466648	-2.259954	-2.721909
50	6	0	0.711593	1.693444	3.157382
51	6	0	1.864099	2.372860	3.028178
52	6	0	2.702079	2.200072	1.979845
53	6	0	2.358015	1.290046	1.045664
54	6	0	-1.576811	-1.509993	0.552376
55	6	0	-2.676660	-1.730567	1.304057
56	6	0	-2.764693	-0.966758	2.421204
57	6	0	-1.811844	-0.104286	2.822786
58	6	0	6.308579	3.979315	2.202887
59	6	0	5.203516	4.715871	2.490638
60	6	0	5.314537	5.951983	3.030393
61	6	0	6.558635	6.395982	3.294752

62	6	0	7.650813	5.679408	3.013594
63	6	0	7.540743	4.466881	2.452063
64	6	0	6.175583	2.752939	1.661737
65	6	0	0.667841	5.591924	1.751312
66	6	0	3.841280	2.928134	1.882470
67	6	0	3.966053	4.230572	2.238575
68	6	0	8.677664	3.774003	2.163853
69	7	0	8.488884	2.552639	1.545063
70	6	0	7.248975	1.981418	1.325255
71	8	0	7.159352	0.861881	0.866058
72	8	0	9.792841	4.179796	2.414933
73	6	0	9.680125	1.782726	1.157366
74	6	0	1.925334	7.140403	2.916611
75	6	0	3.005641	6.317092	2.832893
76	6	0	2.912097	5.086465	2.282090
77	6	0	1.737919	4.796163	1.688127
78	6	0	4.942011	2.240892	1.532127
79	6	0	0.746720	6.776215	2.371810
80	6	0	2.030541	8.341872	3.519166
81	6	0	3.220343	8.707180	4.018963
82	6	0	4.286544	7.912348	3.882912
83	6	0	4.220790	6.715778	3.268004
84	6	0	-0.353436	7.578754	2.383327
85	7	0	-0.215450	8.759860	3.088350
86	6	0	0.976593	9.197545	3.636749
87	8	0	1.053563	10.284934	4.168789
88	8	0	-1.392240	7.307946	1.818255
89	6	0	-1.388509	9.639402	3.192962
90	6	0	-5.919678	-3.745979	-0.087009
91	6	0	-5.741110	-3.627533	1.253392
92	6	0	-4.568146	-3.177007	1.758436
93	6	0	-3.666868	-2.589398	0.928036
94	6	0	-3.846567	-2.789145	-0.392304
95	6	0	-4.919948	-3.399702	-0.916957
96	6	0	-7.071771	-4.227701	-0.594600
97	6	0	-7.327202	-4.138253	5.654900
98	6	0	-7.886369	-4.411385	1.573584
99	6	0	-6.729779	-3.975532	2.109360
100	6	0	-5.005103	-3.556065	-2.269745
101	7	0	-6.205501	-4.054246	-2.742096
102	6	0	-7.272217	-4.397655	-1.932038
103	8	0	-8.301422	-4.838210	-2.398340
104	8	0	-4.105121	-3.290466	-3.039287
105	6	0	-6.325682	-4.267091	-4.192964
106	6	0	-5.073864	-3.764053	5.286520
107	6	0	-5.317165	-3.683193	3.951442
108	6	0	-6.550044	-3.908260	3.449832
109	6	0	-7.542814	-4.115888	4.335561
110	6	0	-8.059368	-4.545551	0.255047
111	6	0	-6.089250	-3.979119	6.147242
112	6	0	-3.814405	-3.649496	5.754845
113	6	0	-2.812670	-3.516457	4.872787
114	6	0	-3.075596	-3.411291	3.566861
115	6	0	-4.330657	-3.389954	3.077419
116	6	0	-5.902408	-4.048500	7.495118
117	7	0	-4.601738	-3.866408	7.929109
118	6	0	-3.517860	-3.720194	7.082598
119	8	0	-2.388937	-3.656423	7.521629
120	8	0	-6.798611	-4.259905	8.284761

121	6	0	-4.346701	-3.896236	9.376721
122	6	0	4.149497	-6.713869	0.516582
123	6	0	4.627754	-6.186183	-0.639874
124	6	0	5.463516	-6.899862	-1.429676
125	6	0	5.784065	-8.143669	-1.024216
126	6	0	5.326343	-8.664747	0.117831
127	6	0	4.509139	-7.953223	0.907356
128	6	0	3.305480	-5.993179	1.278736
129	6	0	5.595065	-2.427908	-3.239853
130	6	0	3.275859	-4.302150	-0.366358
131	6	0	4.276214	-4.938113	-1.028025
132	6	0	4.068068	-8.515186	2.067337
133	7	0	3.258884	-7.710627	2.846968
134	6	0	2.809482	-6.461308	2.460348
135	8	0	2.020036	-5.851401	3.150923
136	8	0	4.353123	-9.640659	2.418465
137	6	0	2.790418	-8.242042	4.135464
138	6	0	6.395674	-4.486069	-3.921004
139	6	0	5.783212	-5.067828	-2.855089
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141	6	0	4.985986	-3.021207	-2.209356
142	6	0	2.866710	-4.815317	0.808104
143	6	0	6.278161	-3.159457	-4.132155
144	6	0	7.126209	-5.232361	-4.773989
145	6	0	7.253038	-6.545750	-4.532542
146	6	0	6.695223	-7.093783	-3.448175
147	6	0	5.965945	-6.375593	-2.572999
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149	7	0	7.630482	-3.331593	-6.012554
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153	6	0	8.315681	-2.699006	-7.149337
154	1	0	-0.037650	4.130320	-1.326725
155	1	0	-7.760651	3.646051	-6.337992
156	1	0	-5.379533	6.766635	-4.924259
157	1	0	0.617706	9.371709	-1.927877
158	1	0	-0.795683	9.874320	-0.906756
159	1	0	0.354497	8.733631	-0.255462
160	1	0	-6.293784	5.306616	-5.802888
161	1	0	-4.085399	8.461405	-4.133332
162	1	0	-4.644904	-0.422692	-2.180519
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164	1	0	-8.928513	-1.047302	-6.119233
165	1	0	-8.248859	-2.067944	-4.874626
166	1	0	-9.546189	-0.896908	-4.420004
167	1	0	-0.216519	-0.377410	-4.288350
168	1	0	-1.457317	1.689191	-4.312319
169	1	0	-0.659624	2.240266	-0.169265
170	1	0	2.159421	-2.258016	1.010350
171	1	0	2.577167	-4.010653	-2.869790
172	1	0	1.244726	-2.268034	-3.801061
173	1	0	0.061431	1.858617	4.031220
174	1	0	2.120527	3.074599	3.841366
175	1	0	2.943942	1.129810	0.126323
176	1	0	-1.363453	-2.040611	-0.385839
177	1	0	-3.669019	-0.991019	3.052964
178	1	0	-1.943172	0.481130	3.746945
179	1	0	6.783477	7.383641	3.721252

180	1	0	8.626711	6.138189	3.247114
181	1	0	-0.250619	5.243324	1.249316
182	1	0	10.541367	2.429717	0.880707
183	1	0	9.987586	1.111363	1.991417
184	1	0	9.513579	1.170726	0.243395
185	1	0	1.576827	3.906541	1.062834
186	1	0	4.840436	1.185589	1.234113
187	1	0	3.376071	9.672206	4.530599
188	1	0	5.207184	8.333994	4.310598
189	1	0	-1.397714	10.234416	4.132572
190	1	0	-1.419732	10.335237	2.323317
191	1	0	-2.344776	9.072558	3.234587
192	1	0	-3.149578	-2.351220	-1.117286
193	1	0	-8.203072	-4.314565	6.302280
194	1	0	-8.753702	-4.735251	2.166396
195	1	0	-5.892333	-3.423831	-4.775886
196	1	0	-5.801756	-5.207640	-4.478912
197	1	0	-7.372477	-4.335391	-4.556826
198	1	0	-8.592586	-4.277418	4.051400
199	1	0	-9.031838	-4.939230	-0.086408
200	1	0	-1.752106	-3.490347	5.174913
201	1	0	-2.186745	-3.360417	2.917381
202	1	0	-4.143765	-4.940979	9.705801
203	1	0	-3.490348	-3.251982	9.674618
204	1	0	-5.194749	-3.489962	9.970773
205	1	0	6.465577	-8.812585	-1.568546
206	1	0	5.660226	-9.684555	0.374419
207	1	0	5.517160	-1.329385	-3.305464
208	1	0	2.664108	-7.447193	4.903479
209	1	0	1.819506	-8.770999	3.998559
210	1	0	3.516745	-8.941097	4.604915
211	1	0	4.511577	-2.323344	-1.502487
212	1	0	2.055159	-4.319090	1.360017
213	1	0	7.833670	-7.215072	-5.189831
214	1	0	6.886222	-8.171834	-3.349026
215	1	0	7.645036	-2.688066	-8.038792
216	1	0	8.640084	-1.657896	-6.930610
217	1	0	9.264037	-3.213027	-7.420131
