Electronic Supplementary Information

for

Preparing Polythiophene Derivative with Alternating Alkyl and Thioalkyl Side Chains via Kumada Coupling for Efficient Organic Solar Cells

*Ziyi Xie, Qingyun Wei, Tong Shan, Xiaoyang Zheng, Yi Zhang and Hongliang Zhong**

School of Chemistry and Chemical Engineering, Shanghai Key Lab of Electrical Insulation and Thermal Aging, Shanghai Jiao Tong University, Shanghai 200240, China

E-mail: hlzhong@sjtu.edu.cn

General procedure

All reactions were carried out under argon atmosphere, the solvents and reagents were used as commercially supplied. ^{1}H NMR spectra were collected on a Bruker AV-400 (400 MHz) spectrometers. The number-average (M_n) and weight-average (M_w) molecular weights were determined by Shimadzu-20A GPC running in chlorobenzene at 80 ℃, using one PL mixed B column which is calibrated against narrow polydispersity polystyrene standards. The theoretical calculation was performed by density functional theory (DFT) at B3LYP/6-31G level. The absorption spectra were measured by a PerkinElmer Lambda 750S recording spectrophotometer. Cyclic voltammetry (CV) measurements of these products were conducted on a CHI660D voltammetry analyzer in acetonitrile solution with 0.1 M tetrabutylammonium hexafluorophosphate (n-Bu_4NPF_6) as supporting electrolyte at room temperature via conventional three-electrode configuration, consisting of a ITO glass (coated with polymers) as working electrode, an Ag/AgCl wire as reference electrode and a platinum sheet as counter electrode. The ferrocene (HOMO: -4.8 eV) was used as in internal reference. Grazing-incidence wide-angle x-ray scattering (GIWAXS) characterizations were carried out at the beamline 14B1 of Shanghai Synchrotron Radiation Facility (SSRF).

Device Fabrication

The Indium tin oxide (ITO)-coated glass substrates were pre-cleaned by sequential ultra-sonication in deionized water, acetone and isopropanol for 30 min each. After 20 min of ultraviolet-ozone treatment, a thin layer of 15 nm thick PEDOT-PSS was spin-coated onto the substrates as the anode interlayer and annealed at 150 °C for 15 min.

Subsequently, the substrates were transferred into the nitrogen-filled glove box. Then the active layer solutions with donor/acceptor (D/A) weight ratio of 1:1 in chlorobenzene at a concentration of 8 mg·mL^{-1} were spin-coated on the PEDOT-PSS layer to form around 100 nm thick active layer, followed with thermal annealing at 110 °C for 10 min. Then PDINO solution in methanol (1 mg·mL^{-1}) was spin-coated on the active layer to give a 5 nm thick cathode interlayer. Finally, about 80 nm thick of Ag was deposited onto the active layer under high vacuum, giving an effective cell area of 3.68 mm^2.

OSC device characterization

The device *J-V* characteristics were recorded by a Keithley 2420 Source Meter unit in forward direction under AM 1.5G 1 sun irradiance (100 mW·cm^{-2}) as generated by a 300W Xe lamp solar simulator (Enlitech SS-F5-3A) at room temperature. Standard Si diode with KG-5 filter was used to calibrate the light intensity. Enlitech EQE system (Enlitech QE-M110) with a Si diode as reference cell was used to characterize the EQE spectra. Monochromatic light was generated from an Enlitech lamp source with a monochromator.

Charge carrier mobility measurement.

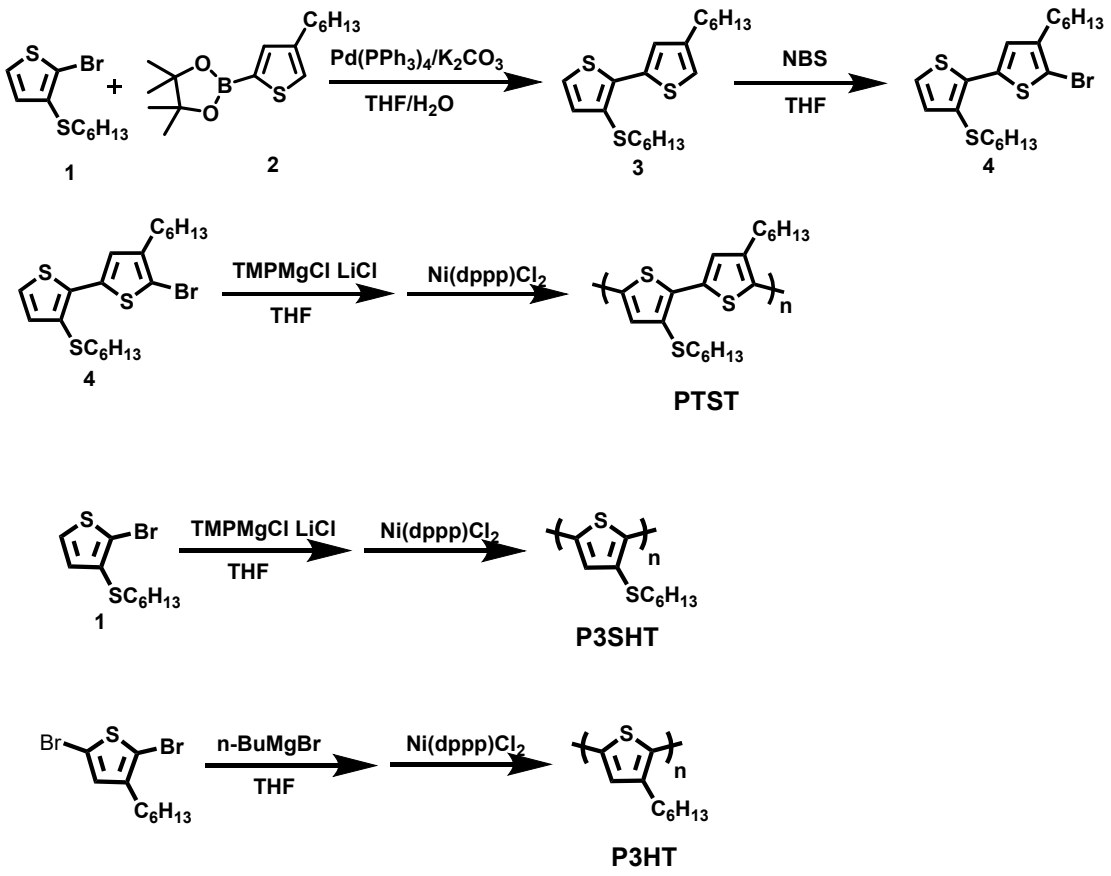
Hole-only diode configuration: ITO/PEDOT-PSS/active layers/MoO_3/Ag. Electron-only diode configuration: ITO/ZnO/active layers/PDINO/Ag. PEDOT-PSS, MoO_3, ZnO and Ag were deposited by the same route as OSCs devices. The thickness was 104, 101 and 109 nm for P3HT, P3SHT and PTST based blend films, respectively. The mobility in active layers were determined by fitting the dark current hole/electron-only diodes to the space-charge limited current (SCLC) model. The mobility was determined by the equation:

$$J = \frac{9\varepsilon_0\varepsilon_r\mu_0 V^2}{8L^3}$$

where J was current density, μ_0 was the hole or electron mobility, ε_r was the dielectric permittivity of the active layer (generally taken to be about 3 for organic materials), ε_0 was the dielectric permittivity of free space (ε_0 = 8.854187817×10^{-12} F/m), L was the film thickness, and V was the voltage, which was defined as $V = V_{appl}$-V_{bi}, where V_{appl} was the applied voltage, V_{bi} was the built-in voltage.

Synthesis

All chemicals and reagents were used as received from commercial sources without further purification. Solvents for chemical synthesis were purified according to standard procedures. The compounds **1** and **2** were prepared according to reported methods in literatures[1, 2].



Scheme S1. The synthetic routes of PTST, P3SHT and P3HT.

The synthesis of compound **3**

In a dry flask, compound **1** (268 mg, 0.96 mmol) and compound **2** (282 mg, 0.96 mmol) were added, then Pd $(PPh_3)_4$ (55 mg, 5% mol) and K_2CO_3 (663 mg, 4.80 mmol) were added under argon, followed by the addition of THF (20 mL) and H_2O (5 mL). After being stirred at 80 °C overnight, the mixture was cooled to room temperature and extracted by hexane. The organic phase was dried over Na_2SO_4 and then the solvent was removed with rotary evaporator. The crude product was purified by column chromatography on silica gel with hexane as eluent to afford the product (285 mg, 0.78 mmol, 81% yield) as colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.20 (s, 1H), 7.15 (d, 1H), 7.02 (d, 1H), 6.90 (s, 1H), 2.87 - 2.80 (t, 2H), 2.63 - 2.55 (t, 2H), 1.69 - 1.54 (m, 4H), 1.45 - 1.20 (m, 12H), 0.94 - 0.82 (m, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 143.16, 135.98, 135.13, 131.99, 127.60, 127.58, 122.87, 120.68, 36.02, 31.71, 31.38, 30.45, 30.42, 29.56, 29.03, 28.42, 22.65, 22.55, 14.13, 14.04.

The synthesis of compound **4**

Compound **3** (285mg, 0.78mmol) was dissolved in anhydrous THF (10 mL) in a three-neck flask and stirred under argon. After cooling the solution to -20 °C, N-bromosuccinimide (139 mg, 0.78 mol) was added dropwise. Then the mixture was allowed to be back to room temperature slowly and kept stirring for 10 h. The mixture was quenched by Na_2SO_3 aqueous solution and extracted by hexane, then washed two

times each with brine, and dried over Na_2SO_4. The solvent was evaporated, and the product was purified by column chromatography on silica gel with hexane as eluent to afford the product (287 mg, 0.65 mmol, 83% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.15 (d, 1H), 7.02 (s, 1H), 7.00 (d, 1H), 2.87 - 2.68 (t, 2H), 2.59 - 2.49 (t, 2H), 1.65 - 1.53 (m, 4H), 1.45 - 1.19 (m, 12H), 0.92-0.82 (m, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 141.66, 136.04, 135.06, 132.38, 127.83, 126.63, 123.03, 110.23, 36.32, 31.64, 31.36, 29.67, 29.57, 29.47, 28.93, 28.40, 22.62, 22.55, 14.12, 14.03.

The synthesis of polymer **PTST**

Compound **4** (253 mg, 0.57 mmol) was dissolved in anhydrous THF (10 mL) in a dry flask and stirred under argon. After cooling to 0 °C, 12,2,6,6-tetramethylpiperidinylmagnesium chloride - lithium chloride complex solution (0.60 mL, 1 M in THF) was added dropwise, and the mixture was stirred for 1 h. The solution was then heated up to 35 °C followed by the addition of Ni(dppp)Cl_2 catalyst (8.13 mg, 0.015 mmol). The combined mixture was stirred at 50 °C for 5 h. The deep red solution was then cooled to room temperature, quenched with 1 mL HCl (5 M), and precipitated into methanol. The product was purified by Soxhlet extraction using methanol, THF and chloroform. The fraction in chloroform was precipitated in methanol and recovered as dark purple solid (46 mg, 19%). PTST can be completely dissolved in chlorobenzene and chloroform when heated to 60 ℃. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.24 (s, 1H), 7.10 (s, 1H), 2.97 - 2.87 (m, 2H), 2.85 - 2.74 (m, 2H), 1.76 - 1.62 (m, 4H), 1.48 - 1.15 (m, 12H), 0.95 - 0.83 (m, 6H). GPC (PTST): M_n = 17.5 kg·mol^{-1}, M_w = 30.6 kg·mol^{-1}, Đ = 1.75.

The synthesis of polymer **P3SHT**

The polymer **P3SHT** was prepared following the similar method for **PTST**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (m, 1H), 2.94 (m, 2H), 1.76 – 1.15 (m, 8H), 0.99 - 0.84 (m, 3H). GPC (P3SHT): M_n = 16.2 kg·mol^{-1}, M_w = 32.4 kg·mol^{-1}, Đ = 2.01.

The synthesis of **P3HT**

The 2,5-dibromo-3-hexyl thiophene (489 mg, 1.5 mmol) was dissolved in 8 mL THF under argon. To this solution, buthylmagnesium bromide (1.5 mL, 1.0 M in THF) was added dropwise at 0 ℃ and then the solution was kept stirring for 1 h. The mixture was heated to reflux, followed by the addition of Ni(dppp)Cl_2 (8 mg, 0.015 mmol). After keeping reflux for 4 hours, the mixture was poured into 100 mL methanol. The solid was collected and Soxhlet extracted by methanol, THF and chloroform. The fraction in chloroform solution was recovered as purple solid (169 mg, 1.0 mmol, yield: 67%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.98 (br, 1H), 2.89 – 2.71 (m, 2H), 1.77 – 1.21 (m, 8H), 0.98 - 0.83 (m, 3H). GPC (P3HT): M_n = 16.5 kg·mol^{-1}, M_w = 23.6 kg·mol^{-1}, Đ = 1.43.

Supplementary Figures and Tables

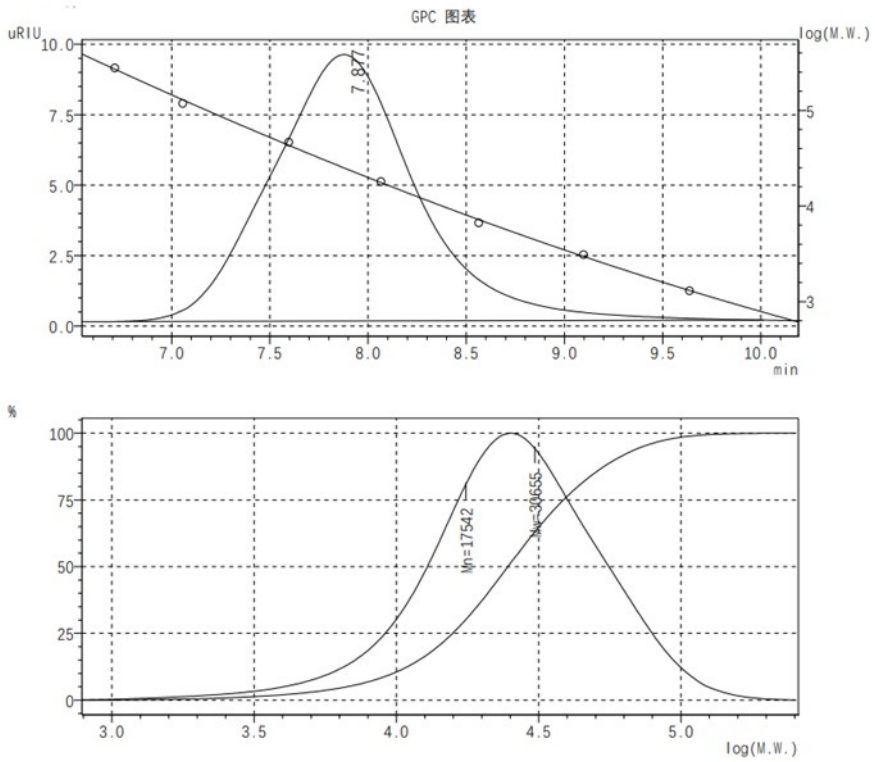


Figure S1. GPC spectra of polymer PTST.

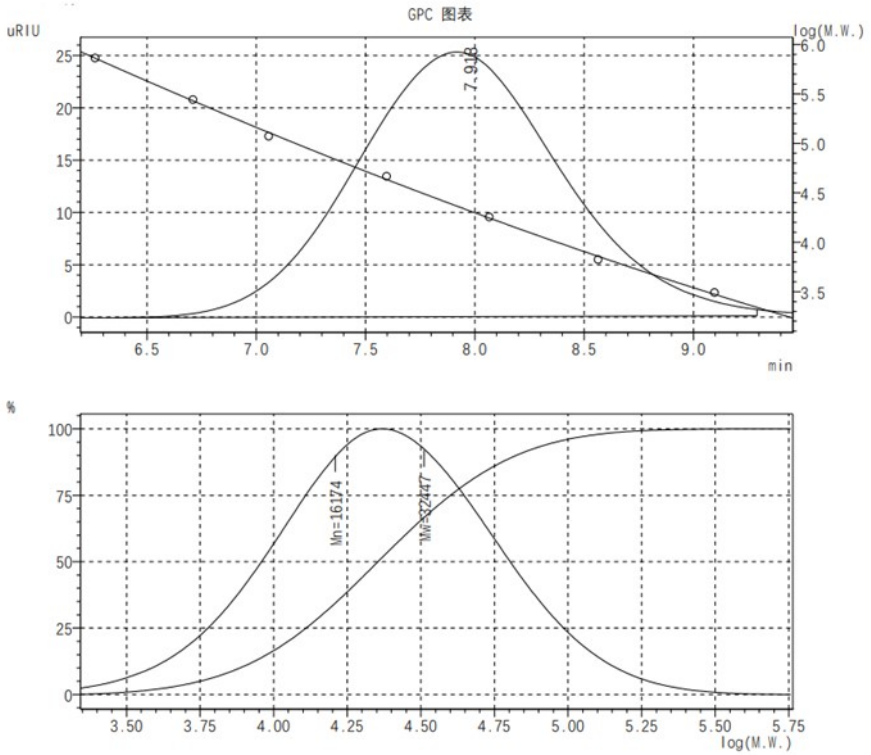


Figure S2. GPC spectra of polymer P3SHT.

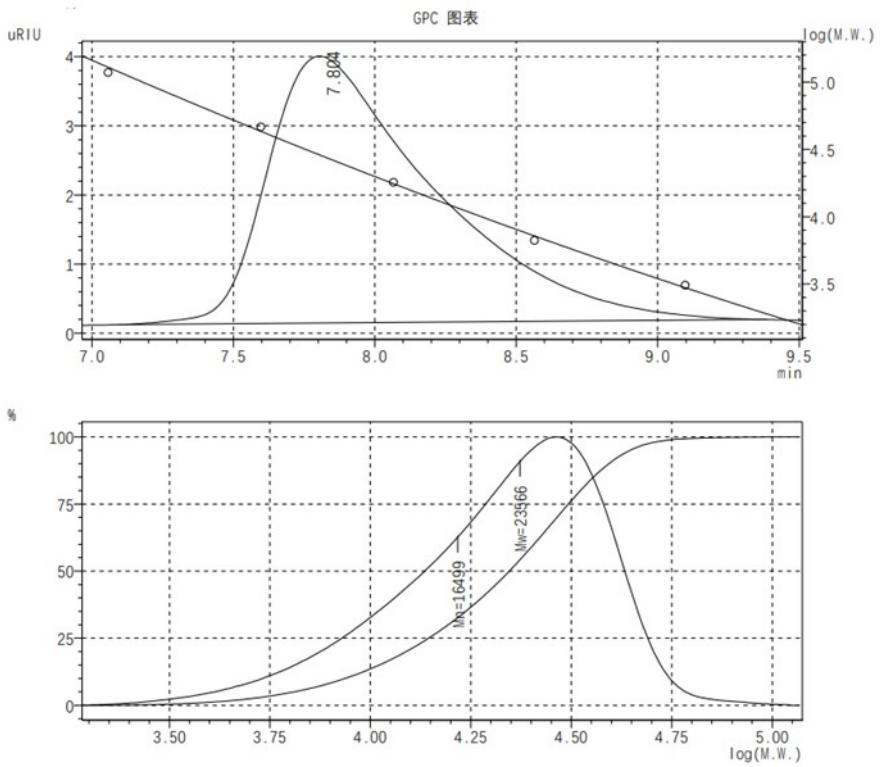


Figure S3. GPC spectra of polymer P3HT.

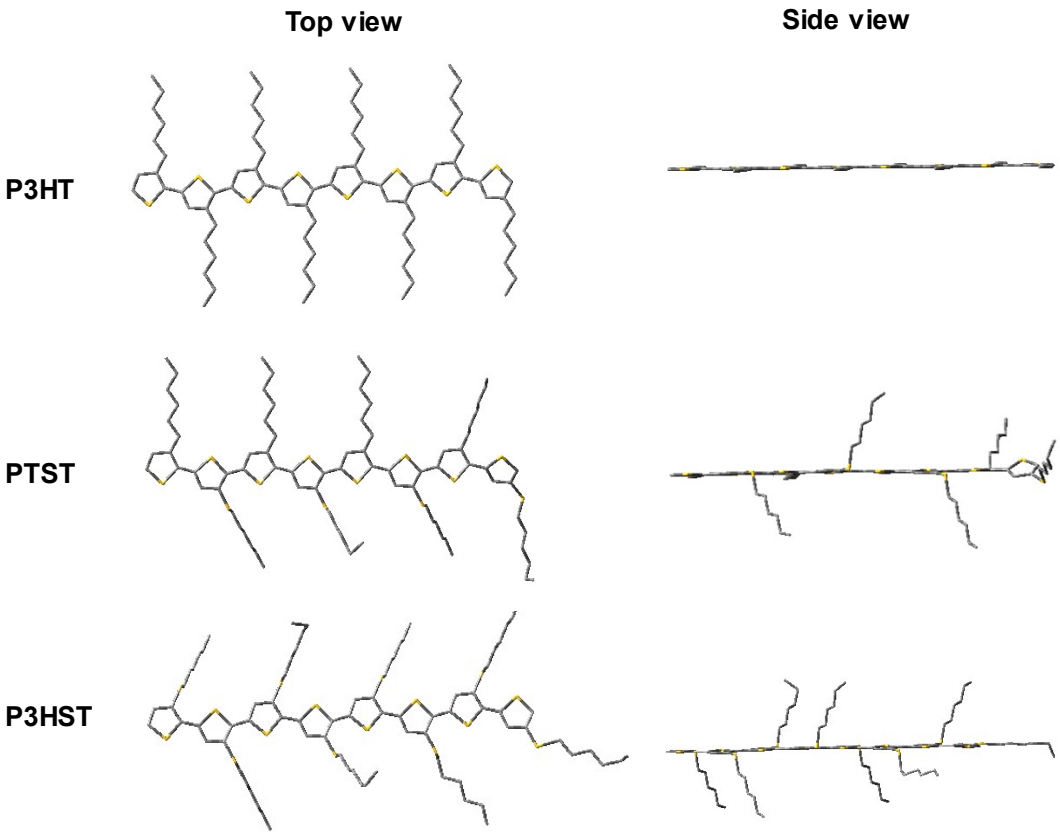


Figure S4. The optimized geometries of P3HT, PTST and P3HST based on density functional theory (DFT) at B3LYP/6-31G level. The hydrogen atoms are omitted for clarification.

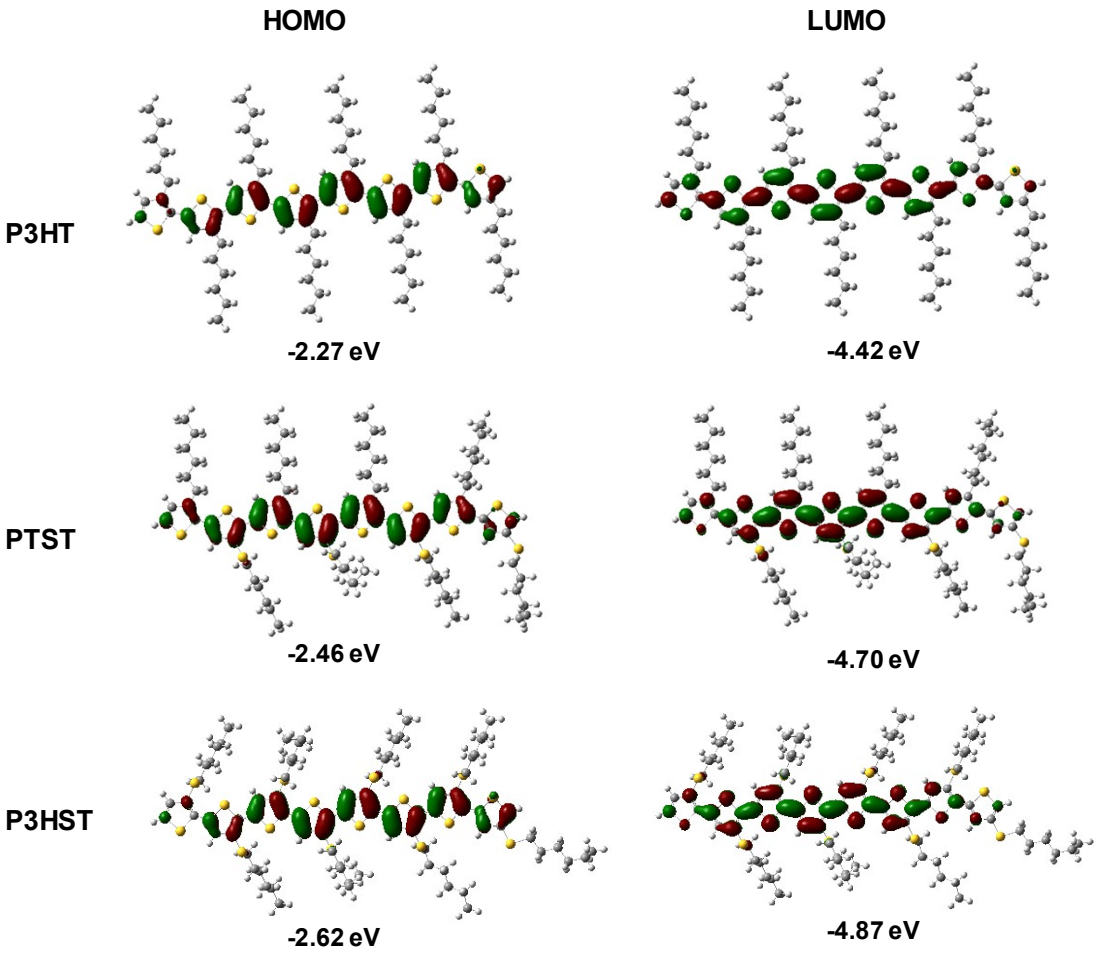


Figure S5. The calculated HOMO and LUMO of P3HT, PTST and P3HST based on density functional theory (DFT) at B3LYP/6-31G level.

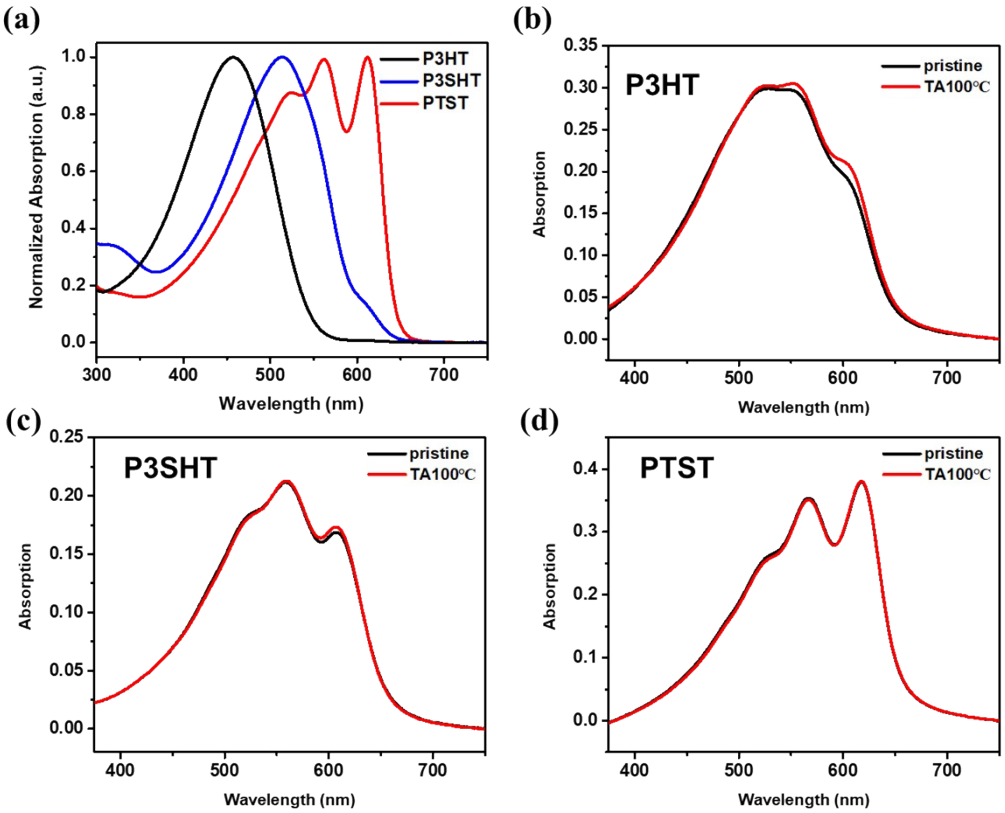


Figure S6. (a) Normalized UV-vis absorption spectra of P3HT, P3SHT and PTST in chlorobenzene solution. UV-vis absorption spectra of (b) P3HT, (c) P3SHT and (d) PTST films with or without thermal annealing at 100℃ for 5 minutes.

Figure S7. Photos of P3HT, P3SHT and PTST in chlorobenzene solution.

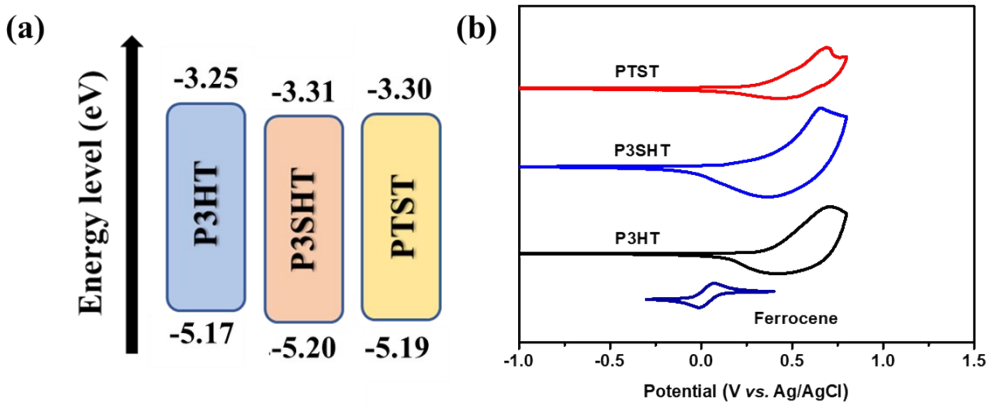


Figure S8. (a) Energy levels diagram and (b) cyclic voltammetry curves of P3HT, P3SHT and PTST.

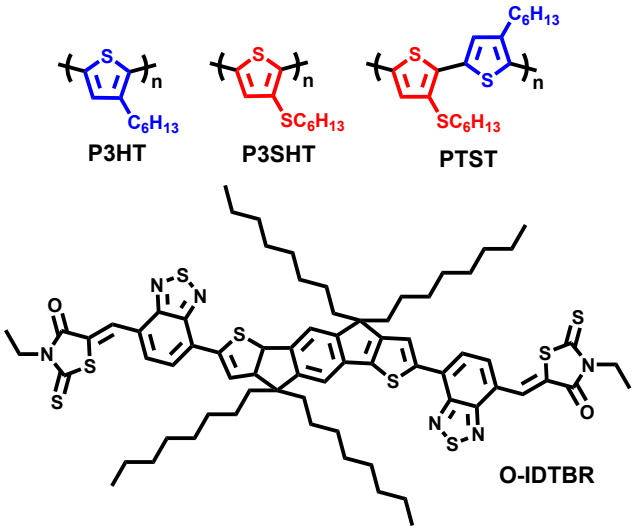


Figure S9. Chemical structures of P3HT, P3SHT, PTST and O-IDTBR.

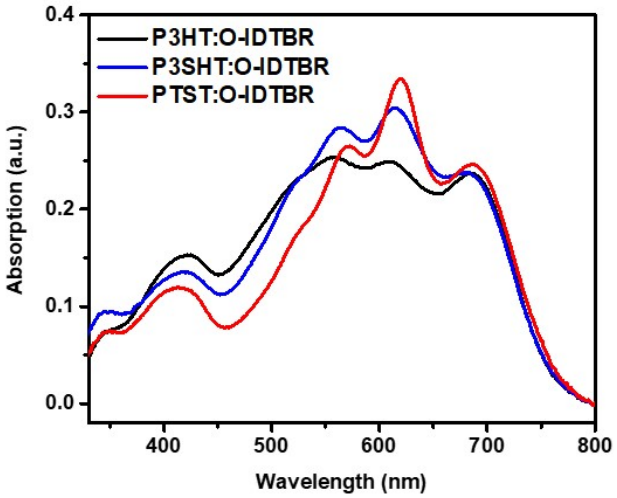


Figure S10. The UV-Vis absorption spectra of the optimal donor:O-IDTBR devices.

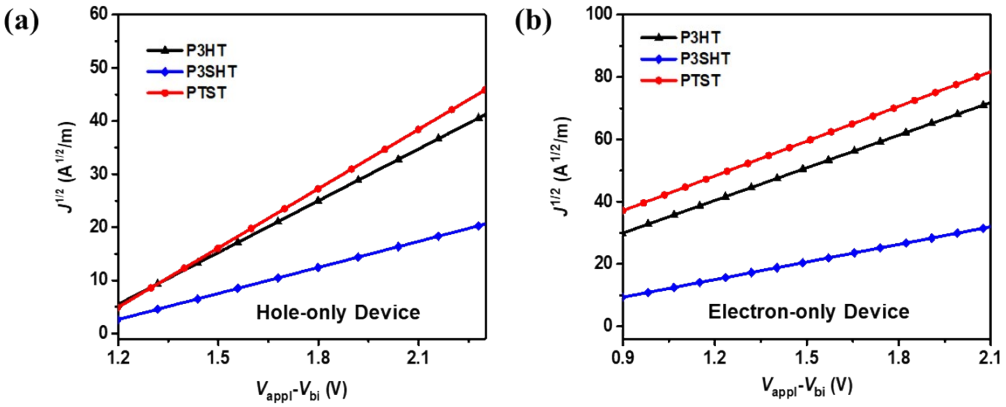


Figure S11. $J^{1/2}$-V plots of (a) hole-only and (b) electron-only devices based on donor:O-IDTBR blend film under the optimized conditions.

NMR Characterization

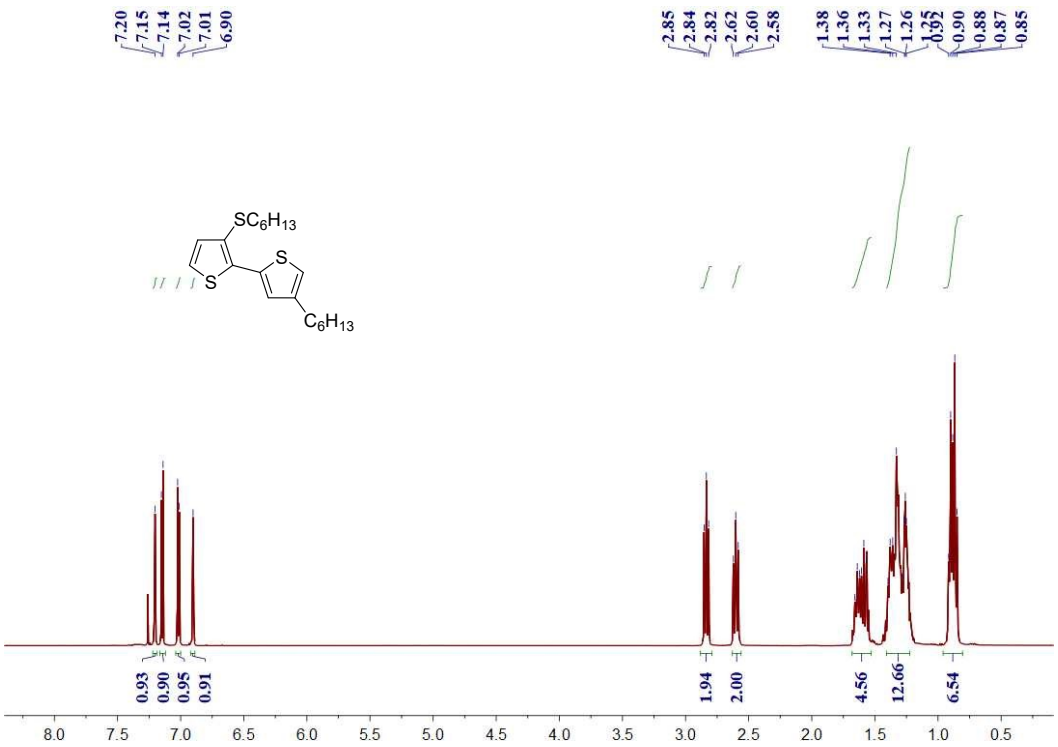


Figure S12. ^{1}H NMR spectra of compound **3**.

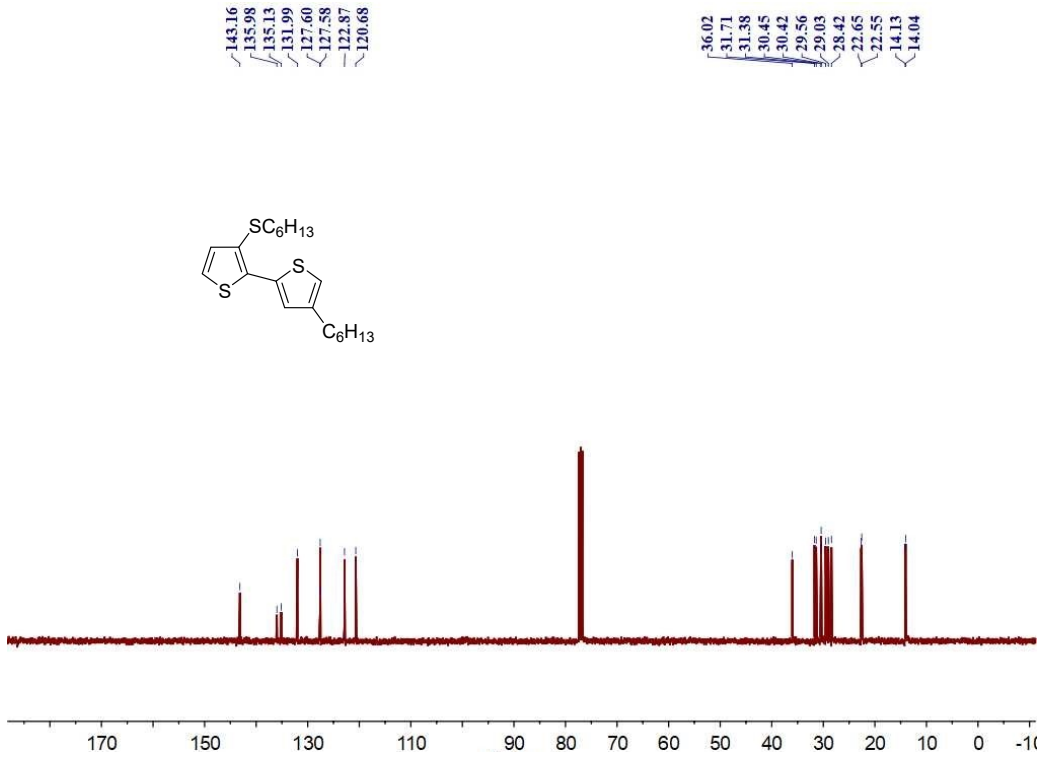


Figure S13. ^{13}C NMR spectra of compound **3**.

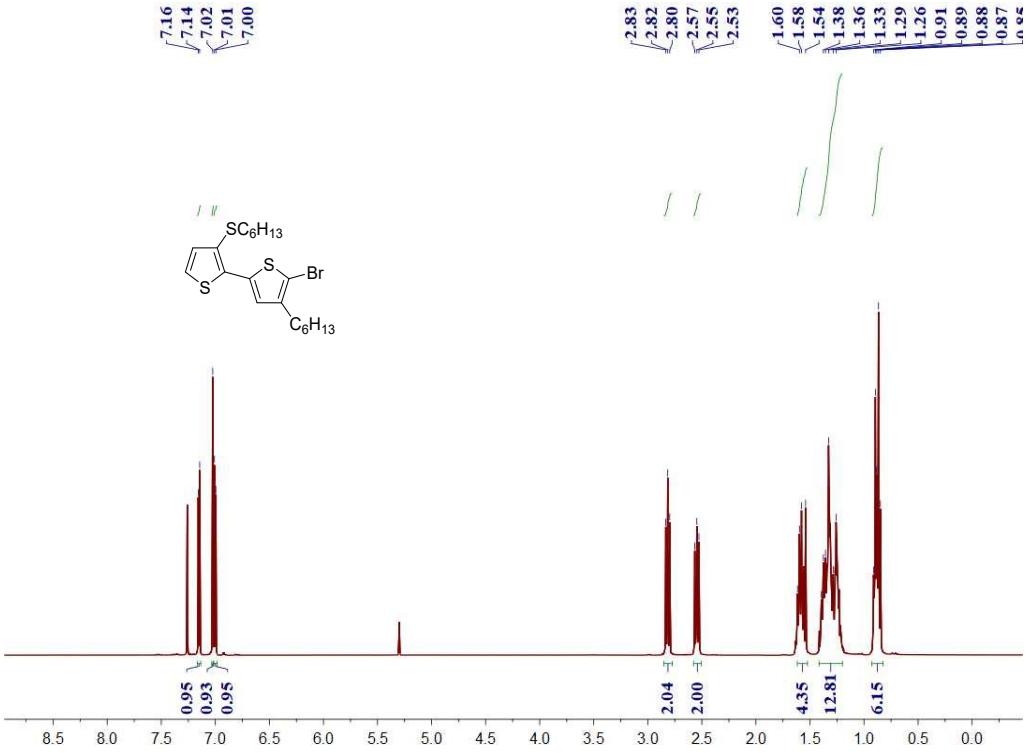


Figure S14. [1]H NMR spectra of compound **4**.

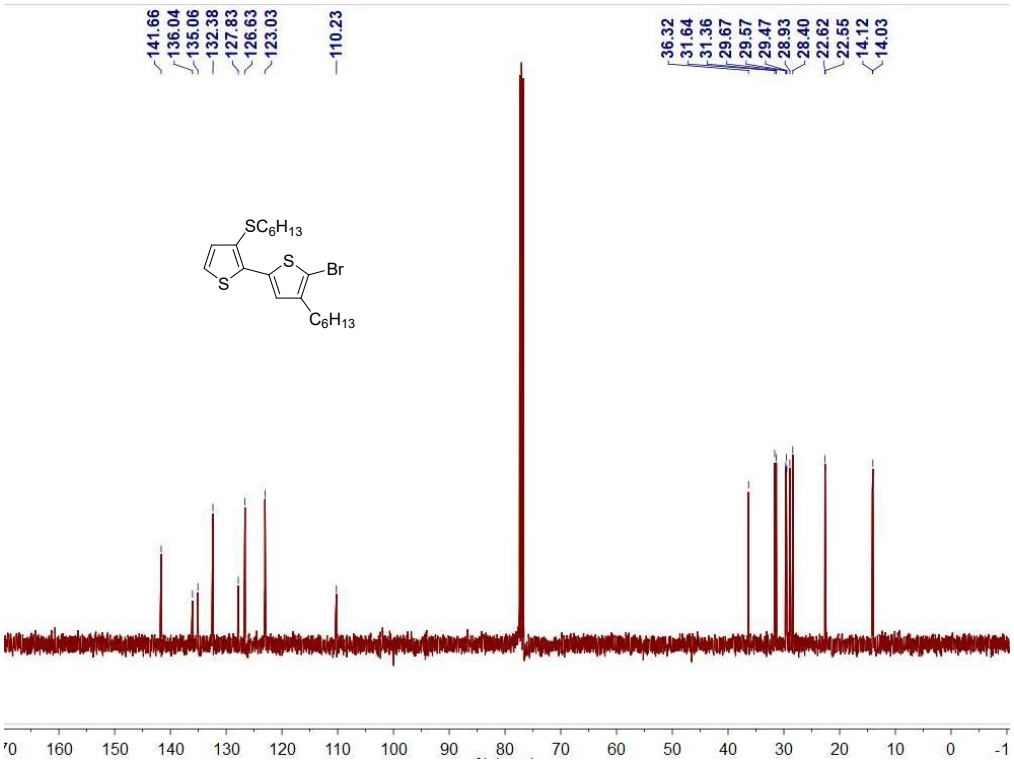


Figure S15. [13]C NMR spectra of compound **4**.

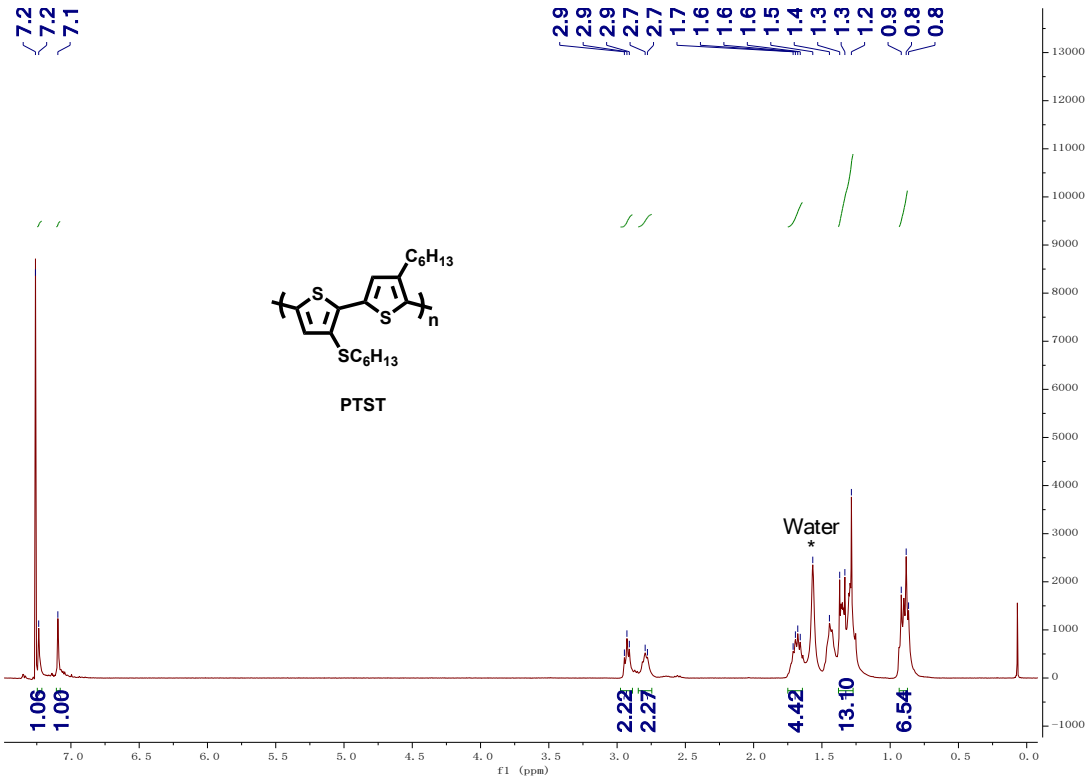


Figure S16. [1]H NMR spectra of polymer PTST.

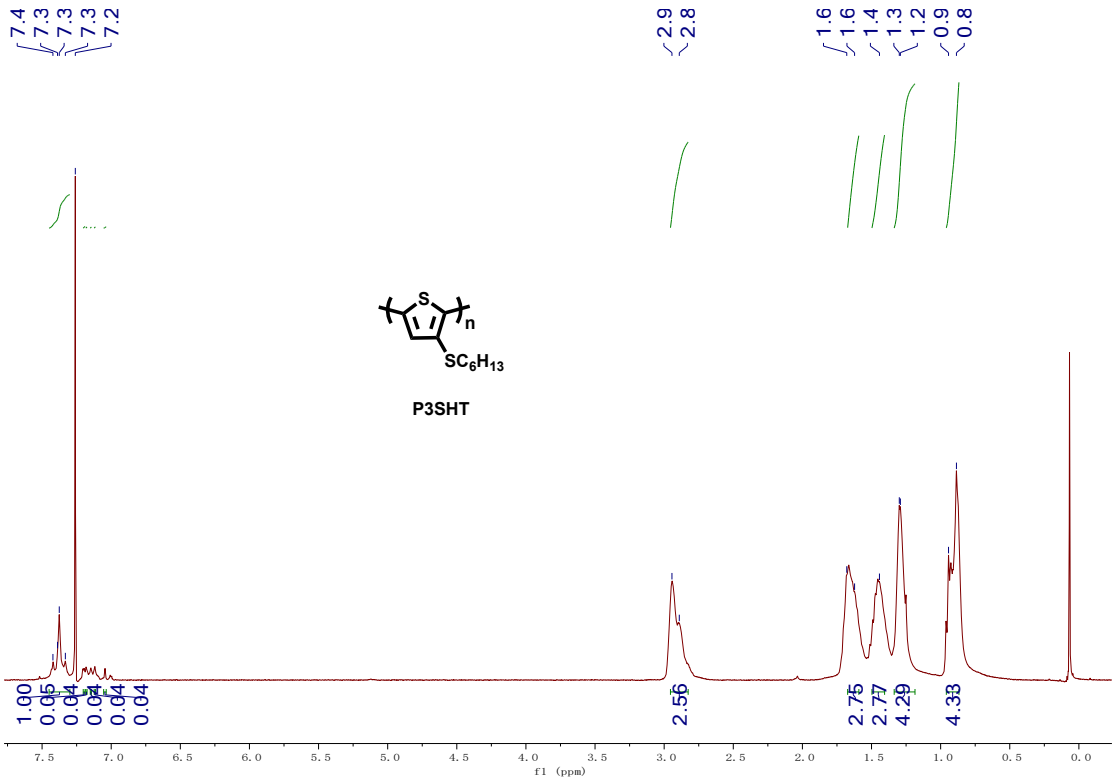


Figure S17. [1]H NMR spectra of polymer P3SHT.

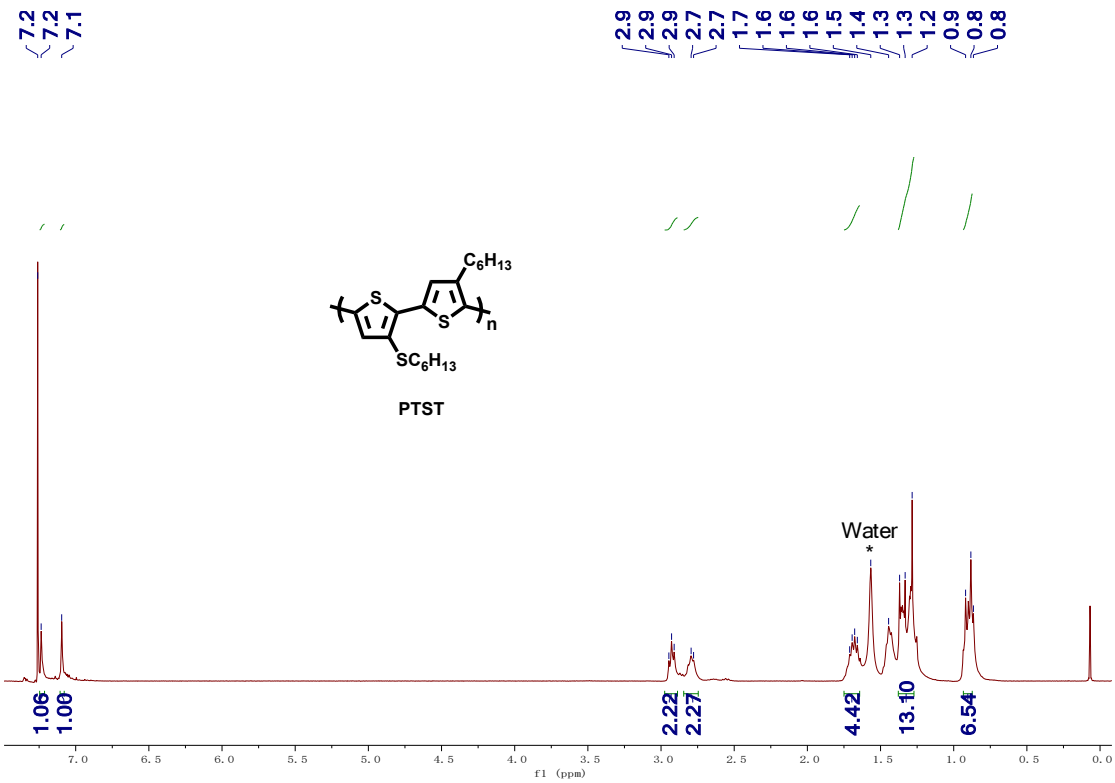


Figure S18. ^{1}H NMR spectra of polymer P3HT.

Table S1. Characteristic length scale of packing phenomenon for neat films of donors.

Neat	Lamellar			
	q [Å^{-1}]	(100) distance [Å]	FWHM [Å^{-1}]	CCL [Å]
P3SHT	0.38	16.5	0.40	15.7
PTST	0.37	17.0	0.063	99.7

Optimized Geometry Coordinates Data based on DFT Calculation

Optimized Geometry Coordinates for 8 units P3HT

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.079649	0.184198	-0.000026
2	6	0	0.340693	1.501586	-0.000010
3	6	0	1.654944	1.763175	0.000028
4	6	0	2.326683	0.594470	0.000015
5	16	0	1.365166	-0.518275	0.000012
6	6	0	3.656880	0.345413	0.000015
7	6	0	4.254995	-0.857112	0.000017
8	6	0	5.591861	-0.764981	0.000043
9	6	0	5.933192	0.538933	0.000021
10	16	0	4.713025	1.360233	0.000013
11	6	0	2.228698	3.163541	0.000034
12	6	0	1.217695	4.323223	0.000068
13	6	0	1.922834	5.691214	-0.000002
14	6	0	0.919186	6.855866	0.000019
15	6	0	1.624103	8.221779	0.000023
16	6	0	0.619594	9.381733	0.000047
17	6	0	6.512581	-1.966114	-0.000038
18	6	0	5.837780	-3.348826	0.000077
19	6	0	6.871565	-4.488705	0.000033
20	6	0	6.200128	-5.871877	0.000073
21	6	0	7.230942	-7.012016	0.000016
22	6	0	6.556476	-8.390314	0.000080
23	6	0	7.151150	1.128749	0.000055
24	6	0	7.409860	2.446266	-0.000058
25	6	0	8.723263	2.712198	0.000010
26	6	0	9.399327	1.545699	-0.000067
27	16	0	8.438762	0.430881	-0.000003
28	6	0	10.730615	1.296376	-0.000064
29	6	0	11.309338	0.078626	-0.000036
30	6	0	12.644709	0.161806	-0.000113
31	6	0	12.961092	1.460159	-0.000085
32	16	0	11.785150	2.326524	-0.000040
33	6	0	9.285959	4.117419	-0.000011
34	6	0	8.260449	5.264799	0.000036
35	6	0	8.940452	6.645004	0.000032
36	6	0	7.912265	7.788398	0.000011
37	6	0	8.585819	9.169800	0.000036

38	6	0	7.554931	10.306403	0.000040
39	6	0	13.645737	-0.962964	-0.000092
40	6	0	13.043357	-2.376414	0.000005
41	6	0	14.131274	-3.463573	-0.000074
42	6	0	13.528472	-4.878004	0.000013
43	6	0	14.613627	-5.966451	-0.000068
44	6	0	14.007711	-7.376277	0.000054
45	6	0	-6.989654	-0.790978	0.000038
46	6	0	-6.738585	0.528331	-0.000021
47	6	0	-5.426302	0.800466	0.000020
48	6	0	-4.745328	-0.362742	0.000004
49	16	0	-5.698573	-1.482365	0.000018
50	6	0	-3.413727	-0.604083	0.000029
51	6	0	-2.812935	-1.805221	-0.000021
52	6	0	-1.476453	-1.710599	-0.000019
53	6	0	-1.138317	-0.405687	0.000013
54	16	0	-2.360104	0.413895	-0.000007
55	6	0	-4.862863	2.205011	-0.000013
56	6	0	-5.884433	3.355386	-0.000012
57	6	0	-5.194097	4.730813	0.000007
58	6	0	-6.211317	5.883760	0.000019
59	6	0	-5.523157	7.258085	0.000000
60	6	0	-6.542163	8.405438	0.000030
61	6	0	-0.555256	-2.911653	0.000027
62	6	0	-1.229622	-4.294581	-0.000017
63	6	0	-0.196058	-5.434835	-0.000026
64	6	0	-0.868587	-6.817372	-0.000053
65	6	0	0.160904	-7.958655	-0.000096
66	6	0	-0.515704	-9.335917	-0.000108
67	6	0	-14.011233	-1.759104	-0.000091
68	6	0	-13.800549	-0.442173	-0.000117
69	6	0	-12.482641	-0.196916	-0.000011
70	6	0	-11.811453	-1.371677	-0.000036
71	16	0	-12.759097	-2.505869	-0.000003
72	6	0	-10.477965	-1.609455	-0.000015
73	6	0	-9.866132	-2.805509	0.000012
74	6	0	-8.530336	-2.699332	0.000008
75	6	0	-8.202236	-1.392033	-0.000014
76	16	0	-9.430827	-0.584412	0.000027
77	6	0	-11.908564	1.203495	-0.000066
78	6	0	-12.924109	2.359330	-0.000030
79	6	0	-12.224069	3.730026	-0.000011
80	6	0	-13.232165	4.890802	-0.000007
81	6	0	-12.533242	6.259696	-0.000025

82	6	0	-13.543074	7.415080	-0.000081
83	6	0	-7.595054	-3.889065	0.000030
84	6	0	-8.244311	-5.283677	0.000007
85	6	0	-7.183113	-6.398671	0.000031
86	6	0	-7.816268	-7.799415	0.000056
87	6	0	-6.753087	-8.909543	0.000083
88	6	0	-7.387335	-10.306684	0.000098
89	1	0	-0.422329	2.290930	0.000065
90	1	0	3.725657	-1.818951	0.000027
91	1	0	2.863476	3.279179	0.910737
92	1	0	2.863437	3.279188	-0.910663
93	1	0	0.567532	4.257600	-0.905080
94	1	0	0.567535	4.257670	0.905168
95	1	0	2.579192	5.770527	0.899186
96	1	0	2.579246	5.770624	-0.899117
97	1	0	0.262954	6.779396	-0.899355
98	1	0	0.262927	6.779456	0.899379
99	1	0	2.280341	8.304253	0.899439
100	1	0	2.280368	8.304193	-0.899294
101	1	0	1.144442	10.364913	0.000081
102	1	0	-0.034467	9.346843	-0.901031
103	1	0	-0.034461	9.346884	0.901152
104	1	0	7.155651	-1.911759	-0.910479
105	1	0	7.155703	-1.911791	0.910486
106	1	0	5.192794	-3.454016	0.905228
107	1	0	5.192799	-3.454017	-0.905093
108	1	0	7.526180	-4.396507	-0.899141
109	1	0	7.526160	-4.396537	0.899229
110	1	0	5.546143	-5.966194	0.899375
111	1	0	5.546102	-5.966227	-0.899201
112	1	0	7.886250	-6.923825	-0.899440
113	1	0	7.886242	-6.923837	0.899504
114	1	0	7.315188	-9.206551	0.000094
115	1	0	5.915184	-8.523874	0.901172
116	1	0	5.915177	-8.523915	-0.901011
117	1	0	6.643852	3.232613	0.000027
118	1	0	10.783737	-0.885862	-0.000070
119	1	0	13.988612	1.847996	-0.000114
120	1	0	9.919192	4.239545	0.910751
121	1	0	9.919126	4.239558	-0.910788
122	1	0	7.611277	5.190337	-0.905255
123	1	0	7.611325	5.190333	0.905343
124	1	0	9.594853	6.736795	0.899402
125	1	0	9.594794	6.736834	-0.899385

126	1	0	7.257537	7.697828	-0.899201
127	1	0	7.257543	7.697794	0.899308
128	1	0	9.239829	9.266980	0.899512
129	1	0	9.239743	9.267022	-0.899413
130	1	0	8.056925	11.301304	0.000055
131	1	0	6.901781	10.256628	-0.900993
132	1	0	6.901753	10.256602	0.901123
133	1	0	14.294160	-0.841217	-0.900036
134	1	0	14.294252	-0.841149	0.899827
135	1	0	12.401397	-2.508855	0.903478
136	1	0	12.401314	-2.508843	-0.903513
137	1	0	14.779894	-3.338531	-0.899489
138	1	0	14.779894	-3.338473	0.899383
139	1	0	12.879797	-5.004215	0.899415
140	1	0	12.879737	-5.004176	-0.899372
141	1	0	15.263787	-5.846263	-0.899510
142	1	0	15.263779	-5.846274	0.899435
143	1	0	14.805792	-8.154239	0.000055
144	1	0	13.373889	-7.541295	0.901203
145	1	0	13.373797	-7.541237	-0.901033
146	1	0	-7.508412	1.311123	0.000004
147	1	0	-3.339340	-2.768568	-0.000025
148	1	0	-4.228631	2.325477	0.910383
149	1	0	-4.228572	2.325407	-0.910389
150	1	0	-6.534123	3.283469	-0.905011
151	1	0	-6.534087	3.283446	0.905013
152	1	0	-4.538751	4.817334	0.899167
153	1	0	-4.538739	4.817296	-0.899131
154	1	0	-6.866706	5.799543	-0.899305
155	1	0	-6.866673	5.799507	0.899344
156	1	0	-4.868087	7.348630	0.899362
157	1	0	-4.868061	7.348570	-0.899371
158	1	0	-6.029774	9.395096	0.000047
159	1	0	-7.195762	8.362323	-0.901078
160	1	0	-7.195790	8.362297	0.901038
161	1	0	0.087601	-2.857764	-0.910742
162	1	0	0.087632	-2.857843	0.910730
163	1	0	-1.874471	-4.400034	0.905174
164	1	0	-1.874493	-4.400033	-0.905285
165	1	0	0.458481	-5.342838	-0.899262
166	1	0	0.458487	-5.342871	0.899248
167	1	0	-1.522727	-6.911195	0.899287
168	1	0	-1.522760	-6.911159	-0.899361
169	1	0	0.816402	-7.871261	-0.899459

170	1	0	0.816368	-7.871270	0.899346
171	1	0	0.241642	-10.153433	-0.000073
172	1	0	-1.157297	-9.468420	0.900990
173	1	0	-1.157269	-9.468394	-0.901126
174	1	0	-15.000242	-2.237000	-0.000002
175	1	0	-14.608658	0.300375	-0.000036
176	1	0	-10.382260	-3.774434	-0.000044
177	1	0	-11.275416	1.321896	0.911433
178	1	0	-11.275439	1.321843	-0.911411
179	1	0	-13.574302	2.290464	-0.904947
180	1	0	-13.574319	2.290446	0.904799
181	1	0	-11.568188	3.811860	0.899173
182	1	0	-11.568168	3.811891	-0.899198
183	1	0	-13.887997	4.811611	-0.899437
184	1	0	-13.888031	4.811602	0.899368
185	1	0	-11.877491	6.344989	0.899394
186	1	0	-11.877457	6.344998	-0.899411
187	1	0	-13.022993	8.400711	-0.000026
188	1	0	-14.196955	7.377093	-0.901180
189	1	0	-14.197050	7.377095	0.901093
190	1	0	-6.953297	-3.825430	-0.910990
191	1	0	-6.953280	-3.825486	0.910917
192	1	0	-8.887151	-5.401772	0.905004
193	1	0	-8.887094	-5.401779	-0.905038
194	1	0	-6.530792	-6.290036	-0.898965
195	1	0	-6.530857	-6.289993	0.899055
196	1	0	-8.467195	-7.911654	0.899510
197	1	0	-8.467188	-7.911642	-0.899435
198	1	0	-6.100311	-8.802619	-0.899249
199	1	0	-6.100270	-8.802586	0.899327
200	1	0	-6.605408	-11.100735	0.000066
201	1	0	-8.024454	-10.458594	0.901193
202	1	0	-8.024460	-10.458635	-0.900990

Optimized Geometry Coordinates for 8 units of P3SHT

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.114005	-0.063768	0.281603
2	6	0	-0.680735	1.246697	0.261559
3	6	0	0.724725	1.433557	0.151963
4	6	0	1.461662	0.261656	0.089230

5	16	0	0.327686	-1.182293	0.156609
6	6	0	2.864604	-0.010820	-0.016517
7	6	0	3.469827	-1.247775	-0.110410
8	6	0	4.888395	-1.237907	-0.214282
9	6	0	5.460022	0.023815	-0.206367
10	16	0	4.144259	1.295304	-0.044273
11	16	0	1.430593	3.131798	0.143648
12	6	0	1.467835	3.483165	-1.744543
13	6	0	1.929525	4.921680	-1.979310
14	6	0	1.985965	5.275531	-3.479821
15	6	0	2.449243	6.721316	-3.736231
16	6	0	2.507294	7.087903	-5.230655
17	16	0	5.815192	-2.822586	-0.315604
18	6	0	5.932591	-3.017824	-2.228680
19	6	0	6.403108	-4.426721	-2.594523
20	6	0	7.831986	-4.768687	-2.132496
21	6	0	8.296977	-6.157431	-2.605957
22	6	0	9.720581	-6.514120	-2.139860
23	6	0	6.813520	0.488963	-0.292955
24	6	0	7.240738	1.796827	-0.389085
25	6	0	8.650598	1.985877	-0.449752
26	6	0	9.392203	0.818551	-0.405312
27	16	0	8.263777	-0.623916	-0.278141
28	6	0	10.804220	0.544903	-0.438608
29	6	0	11.416353	-0.675138	-0.247114
30	6	0	12.844298	-0.660025	-0.356888
31	6	0	13.361089	0.573308	-0.632434
32	16	0	12.070187	1.825701	-0.781130
33	16	0	9.337878	3.684628	-0.614356
34	6	0	9.678386	4.102103	1.228703
35	6	0	10.090780	5.569645	1.346036
36	6	0	10.396575	5.969836	2.804221
37	6	0	10.789523	7.451425	2.948934
38	6	0	11.101471	7.860973	4.400198
39	16	0	13.776103	-2.222850	-0.121634
40	6	0	15.563220	-1.636764	-0.394962
41	6	0	16.515887	-2.826060	-0.248769
42	6	0	17.987910	-2.415696	-0.457967
43	6	0	18.959023	-3.603562	-0.314717
44	6	0	20.448926	-3.226910	-0.454308
45	6	0	-9.050917	-0.618800	0.679399
46	6	0	-8.626666	0.678895	0.478782
47	6	0	-7.219860	0.862884	0.381080
48	6	0	-6.473964	-0.297665	0.510113

49	16	0	-7.599361	-1.727472	0.764390
50	6	0	-5.066857	-0.567776	0.474026
51	6	0	-4.451966	-1.802708	0.523746
52	6	0	-3.030930	-1.790252	0.472716
53	6	0	-2.466404	-0.528411	0.373768
54	16	0	-3.794470	0.740685	0.355653
55	16	0	-6.312884	2.434916	0.082877
56	6	0	-6.126421	3.068358	1.886747
57	6	0	-5.334039	4.375771	1.886345
58	6	0	-5.149212	4.937369	3.311844
59	6	0	-4.358435	6.259654	3.330356
60	6	0	-4.098326	6.823642	4.743193
61	16	0	-2.094927	-3.372958	0.489047
62	6	0	-1.686926	-3.529422	2.360163
63	6	0	-0.922795	-4.832340	2.595687
64	6	0	-0.562917	-5.034182	4.082817
65	6	0	0.213163	-6.342544	4.327638
66	6	0	0.537410	-6.622000	5.810292
67	6	0	-16.969617	-1.195910	0.883828
68	6	0	-16.588522	0.074755	0.580834
69	6	0	-15.165103	0.267534	0.519364
70	6	0	-14.417860	-0.866308	0.782219
71	16	0	-15.550555	-2.273003	1.126193
72	6	0	-13.004432	-1.128513	0.830892
73	6	0	-12.387008	-2.337632	1.065952
74	6	0	-10.963224	-2.320147	1.052899
75	6	0	-10.403529	-1.080355	0.795964
76	16	0	-11.737917	0.162291	0.569794
77	16	0	-14.469358	1.929489	0.161689
78	6	0	-14.317020	1.847322	-1.752077
79	6	0	-13.777040	3.181070	-2.268591
80	6	0	-13.628817	3.191166	-3.804335
81	6	0	-13.072771	4.522383	-4.341931
82	6	0	-12.917901	4.545428	-5.873936
83	16	0	-9.816171	-3.722114	1.368530
84	6	0	-9.630121	-4.423817	-0.410433
85	6	0	-8.596721	-5.550379	-0.401851
86	6	0	-8.390922	-6.157371	-1.805192
87	6	0	-7.348355	-7.290259	-1.819757
88	6	0	-7.130516	-7.901105	-3.216360
89	6	0	-12.358465	5.876305	-6.401249
90	6	0	-6.086110	-9.028680	-3.223089
91	6	0	-5.367524	7.271592	5.488305
92	6	0	1.512854	-5.615672	6.444412

93	6	0	10.183136	-7.898491	-2.621168
94	6	0	11.484118	9.343241	4.537767
95	6	0	20.848500	-2.736595	-1.856702
96	6	0	2.969267	8.532787	-5.478159
97	1	0	-1.357168	2.088339	0.338255
98	1	0	2.911560	-2.175191	-0.105349
99	1	0	2.152683	2.759990	-2.194337
100	1	0	0.456699	3.312416	-2.123245
101	1	0	1.249654	5.615179	-1.465755
102	1	0	2.923582	5.065665	-1.534318
103	1	0	2.665040	4.579125	-3.993830
104	1	0	0.991610	5.127217	-3.927494
105	1	0	1.771818	7.417550	-3.218476
106	1	0	3.443797	6.868839	-3.288450
107	1	0	3.184739	6.392070	-5.747117
108	1	0	1.513490	6.938276	-5.678268
109	1	0	4.932167	-2.814262	-2.617203
110	1	0	6.627202	-2.252963	-2.585783
111	1	0	5.696073	-5.165993	-2.193402
112	1	0	6.351583	-4.511434	-3.691188
113	1	0	8.526436	-4.002322	-2.508242
114	1	0	7.886242	-4.722375	-1.035843
115	1	0	7.594378	-6.922067	-2.239756
116	1	0	8.254310	-6.201913	-3.705454
117	1	0	10.421311	-5.746680	-2.499953
118	1	0	9.760580	-6.474244	-1.041505
119	1	0	6.557531	2.635504	-0.427877
120	1	0	10.861971	-1.577916	-0.022300
121	1	0	14.386293	0.877405	-0.763973
122	1	0	10.469216	3.430150	1.571172
123	1	0	8.757716	3.893163	1.779571
124	1	0	9.289217	6.209083	0.951891
125	1	0	10.977689	5.754440	0.724424
126	1	0	9.515696	5.764813	3.431047
127	1	0	11.208478	5.337625	3.193553
128	1	0	11.666864	7.659110	2.317311
129	1	0	9.974978	8.082453	2.561623
130	1	0	10.226484	7.647268	5.031628
131	1	0	11.918600	7.233166	4.785074
132	1	0	15.620443	-1.201869	-1.397309
133	1	0	15.777168	-0.862693	0.348091
134	1	0	16.398767	-3.270857	0.748548
135	1	0	16.246633	-3.603716	-0.976115
136	1	0	18.096765	-1.960547	-1.452216

137	1	0	18.257984	-1.638437	0.273160
138	1	0	18.800970	-4.070918	0.668344
139	1	0	18.707938	-4.369152	-1.064793
140	1	0	21.057217	-4.105288	-0.197312
141	1	0	20.696444	-2.454877	0.289483
142	1	0	-9.310785	1.514738	0.407505
143	1	0	-5.005569	-2.731093	0.582366
144	1	0	-7.134926	3.207693	2.283765
145	1	0	-5.616955	2.283920	2.452568
146	1	0	-4.349570	4.211862	1.427047
147	1	0	-5.852610	5.119597	1.266264
148	1	0	-6.136808	5.084716	3.770216
149	1	0	-4.625006	4.194037	3.931782
150	1	0	-3.393323	6.100559	2.827255
151	1	0	-4.896928	7.012457	2.734234
152	1	0	-3.413935	7.679267	4.658102
153	1	0	-3.569399	6.066637	5.341139
154	1	0	-1.090306	-2.656111	2.634498
155	1	0	-2.636502	-3.508653	2.901160
156	1	0	-1.525428	-5.682485	2.247463
157	1	0	-0.002317	-4.829999	1.996174
158	1	0	0.028870	-4.175828	4.429316
159	1	0	-1.484706	-5.042144	4.684409
160	1	0	-0.375758	-7.181444	3.928219
161	1	0	1.150304	-6.320704	3.750586
162	1	0	0.964446	-7.631522	5.890129
163	1	0	-0.399490	-6.639424	6.386926
164	1	0	-17.961313	-1.605642	0.993485
165	1	0	-17.284947	0.884724	0.406927
166	1	0	-12.936880	-3.253649	1.240397
167	1	0	-13.642600	1.019910	-1.985891
168	1	0	-15.312491	1.629687	-2.147957
169	1	0	-14.447646	3.995261	-1.961367
170	1	0	-12.801024	3.384316	-1.807460
171	1	0	-12.965730	2.368887	-4.112087
172	1	0	-14.606801	2.991430	-4.267483
173	1	0	-13.735161	5.345183	-4.032390
174	1	0	-12.095628	4.722192	-3.876094
175	1	0	-12.258133	3.721138	-6.182655
176	1	0	-13.894864	4.347408	-6.338933
177	1	0	-10.615316	-4.779687	-0.721866
178	1	0	-9.322723	-3.593829	-1.051938
179	1	0	-7.638030	-5.168104	-0.025515
180	1	0	-8.917650	-6.338767	0.292702

181	1	0	-9.350994	-6.540536	-2.181913
182	1	0	-8.077378	-5.365899	-2.502444
183	1	0	-6.389496	-6.906742	-1.438731
184	1	0	-7.661951	-8.082365	-1.122623
185	1	0	-8.088742	-8.285059	-3.596290
186	1	0	-6.819586	-7.108356	-3.912728
187	1	0	-12.257322	5.863221	-7.492546
188	1	0	-13.016244	6.713502	-6.135900
189	1	0	-11.368613	6.083975	-5.975491
190	1	0	-5.952138	-9.443400	-4.228787
191	1	0	-5.110182	-8.664229	-2.878383
192	1	0	-6.387264	-9.849460	-2.559919
193	1	0	-5.117668	7.709483	6.461702
194	1	0	-6.051126	6.434401	5.669993
195	1	0	-5.913602	8.029351	4.911754
196	1	0	1.749393	-5.895812	7.477499
197	1	0	1.096773	-4.601836	6.465634
198	1	0	2.455808	-5.577666	5.884183
199	1	0	11.197541	-8.124172	-2.272531
200	1	0	9.517922	-8.688310	-2.249626
201	1	0	10.185632	-7.954633	-3.717168
202	1	0	11.700372	9.605459	5.579840
203	1	0	12.375135	9.577483	3.941638
204	1	0	10.671527	9.993687	4.190425
205	1	0	21.924544	-2.534309	-1.910129
206	1	0	20.326371	-1.812480	-2.130134
207	1	0	20.612480	-3.491381	-2.617808
208	1	0	2.998235	8.765062	-6.548987
209	1	0	2.292795	9.250945	-4.997813
210	1	0	3.974726	8.700373	-5.072165

Optimized Geometry Coordinates for 4 repeat units (8 thiophene rings) of PTST

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.565370	0.296247	0.269772
2	6	0	-0.231204	1.607638	-0.012727
3	6	0	1.157579	1.920747	-0.048782
4	6	0	1.967144	0.820260	0.219398
5	16	0	0.953712	-0.677960	0.515293
6	6	0	3.389283	0.664487	0.293874

7	6	0	4.105600	-0.485743	0.558833
8	6	0	5.520751	-0.344657	0.582919
9	6	0	5.988142	0.934992	0.328194
10	16	0	4.560282	2.049871	0.043637
11	6	0	1.680535	3.312940	-0.352321
12	6	0	0.605052	4.372957	-0.657056
13	6	0	1.214855	5.750819	-0.972021
14	6	0	0.156919	6.826113	-1.278834
15	6	0	0.761658	8.205603	-1.598478
16	6	0	-0.301756	9.273449	-1.901214
17	16	0	6.767229	-1.650059	0.938646
18	6	0	6.945368	-2.440935	-0.802030
19	6	0	7.968351	-3.575459	-0.738063
20	6	0	8.166325	-4.251342	-2.110500
21	6	0	9.177653	-5.411685	-2.067729
22	6	0	9.383933	-6.090027	-3.434590
23	6	0	7.300355	1.510145	0.250377
24	6	0	7.621811	2.841406	0.077358
25	6	0	9.012103	3.161116	0.007604
26	6	0	9.828584	2.049522	0.133683
27	16	0	8.833617	0.527536	0.355118
28	6	0	11.260449	1.886817	0.100243
29	6	0	11.974795	0.772222	-0.274017
30	6	0	13.398321	0.893220	-0.139319
31	6	0	13.811718	2.101887	0.342445
32	16	0	12.412630	3.190502	0.677777
33	6	0	9.471613	4.588807	-0.191384
34	6	0	9.513640	5.414551	1.118767
35	6	0	9.954911	6.870291	0.887212
36	6	0	10.005168	7.703775	2.180498
37	6	0	10.450797	9.159965	1.952542
38	6	0	10.504786	9.984572	3.248541
39	16	0	14.751012	-0.295303	-0.486314
40	6	0	13.786401	-1.766699	-1.205406
41	6	0	14.770944	-2.865085	-1.614869
42	6	0	14.053304	-4.092445	-2.212609
43	6	0	15.034569	-5.205104	-2.629249
44	6	0	14.366976	-6.425202	-3.297218
45	6	0	-8.442031	-0.829441	0.304890
46	6	0	-8.092959	0.470003	-0.010420
47	6	0	-6.700566	0.767589	-0.048183
48	6	0	-5.904123	-0.334136	0.251975
49	16	0	-6.935148	-1.813121	0.583271
50	6	0	-4.484388	-0.502542	0.337729

51	6	0	-3.781005	-1.651427	0.641873
52	6	0	-2.365036	-1.526159	0.663497
53	6	0	-1.881795	-0.260195	0.366822
54	16	0	-3.297770	0.861065	0.045157
55	6	0	-6.161851	2.146519	-0.383048
56	6	0	-7.225609	3.214114	-0.702424
57	6	0	-6.600324	4.578934	-1.042757
58	6	0	-7.646414	5.662538	-1.360906
59	6	0	-7.026136	7.029151	-1.705088
60	6	0	-8.077690	8.105865	-2.017720
61	16	0	-1.319299	-2.994892	1.025728
62	6	0	-1.080861	-2.795145	2.920744
63	6	0	-0.226925	-3.951387	3.442021
64	6	0	-0.013005	-3.873167	4.968072
65	6	0	0.861436	-5.024949	5.500856
66	6	0	1.041787	-5.029975	7.033306
67	6	0	-16.306116	-1.862675	0.269892
68	6	0	-15.977584	-0.590217	-0.088840
69	6	0	-14.565722	-0.305052	-0.110011
70	6	0	-13.789544	-1.400367	0.245091
71	16	0	-14.852780	-2.848109	0.623184
72	6	0	-12.368520	-1.585712	0.360343
73	6	0	-11.684060	-2.727297	0.717823
74	6	0	-10.264787	-2.617085	0.749384
75	6	0	-9.765779	-1.369853	0.408965
76	16	0	-11.165992	-0.248043	0.027452
77	6	0	-14.005811	1.055101	-0.485073
78	6	0	-15.055242	2.125632	-0.841092
79	6	0	-14.412253	3.474225	-1.211574
80	6	0	-15.443845	4.561349	-1.563440
81	6	0	-14.805711	5.911909	-1.937096
82	6	0	-15.842835	6.992556	-2.282645
83	16	0	-9.054315	-3.915050	1.228704
84	6	0	-8.796772	-4.798855	-0.457096
85	6	0	-7.819943	-5.959691	-0.267183
86	6	0	-7.546456	-6.710519	-1.586622
87	6	0	-6.588247	-7.902621	-1.407930
88	6	0	-6.301160	-8.657517	-2.718844
89	6	0	-5.352826	-9.852227	-2.529077
90	6	0	1.829884	-3.827432	7.580448
91	6	0	10.389024	-7.251881	-3.384380
92	6	0	13.448597	-7.234078	-2.364848
93	1	0	-0.991929	2.354207	-0.196204
94	1	0	3.631297	-1.442875	0.732744

95	1	0	2.287412	3.666834	0.494349
96	1	0	2.368683	3.261729	-1.208791
97	1	0	-0.005508	4.045885	-1.510816
98	1	0	-0.076338	4.468788	0.200534
99	1	0	1.830882	6.079872	-0.121207
100	1	0	1.898094	5.658492	-1.829942
101	1	0	-0.460926	6.496368	-2.128282
102	1	0	-0.525647	6.920523	-0.420155
103	1	0	1.380812	8.533721	-0.750464
104	1	0	1.442425	8.111043	-2.457276
105	1	0	0.157186	10.243626	-2.123947
106	1	0	-0.913609	8.986186	-2.765610
107	1	0	-0.976667	9.410406	-1.046883
108	1	0	7.257292	-1.647781	-1.485784
109	1	0	5.956908	-2.806824	-1.091673
110	1	0	8.931443	-3.186299	-0.379977
111	1	0	7.637571	-4.325208	-0.006717
112	1	0	7.198288	-4.626795	-2.474306
113	1	0	8.503411	-3.501212	-2.841798
114	1	0	10.145168	-5.038604	-1.698364
115	1	0	8.838089	-6.162499	-1.338192
116	1	0	8.415517	-6.457885	-3.804564
117	1	0	9.725659	-5.339305	-4.162556
118	1	0	6.860989	3.608320	-0.014438
119	1	0	11.496781	-0.119334	-0.660520
120	1	0	14.806880	2.473522	0.520250
121	1	0	10.461359	4.609172	-0.660460
122	1	0	8.784707	5.082039	-0.893347
123	1	0	8.519102	5.399237	1.587687
124	1	0	10.198109	4.931264	1.829281
125	1	0	10.948192	6.876557	0.412968
126	1	0	9.268819	7.349951	0.171810
127	1	0	9.012229	7.698970	2.656155
128	1	0	10.690525	7.223303	2.895480
129	1	0	11.441375	9.163004	1.473992
130	1	0	9.764380	9.640339	1.239558
131	1	0	10.827241	11.014225	3.054800
132	1	0	9.519861	10.027305	3.730475
133	1	0	11.207027	9.543374	3.967140
134	1	0	13.093504	-2.121136	-0.436356
135	1	0	13.216885	-1.400675	-2.064968
136	1	0	15.482914	-2.464587	-2.348894
137	1	0	15.358817	-3.175700	-0.740554
138	1	0	13.334084	-4.482298	-1.478863

139	1	0	13.466835	-3.780967	-3.090548
140	1	0	15.773870	-4.779933	-3.323835
141	1	0	15.598441	-5.540296	-1.745201
142	1	0	15.154933	-7.087152	-3.682664
143	1	0	13.794718	-6.087668	-4.174195
144	1	0	-8.844834	1.219890	-0.215512
145	1	0	-4.266638	-2.597419	0.843452
146	1	0	-5.545817	2.509562	0.453004
147	1	0	-5.479339	2.069677	-1.242181
148	1	0	-7.843246	2.880217	-1.548420
149	1	0	-7.902573	3.332620	0.155821
150	1	0	-5.975634	4.913683	-0.200531
151	1	0	-5.922954	4.464491	-1.902676
152	1	0	-8.272983	5.327520	-2.201862
153	1	0	-8.323009	5.778765	-0.500205
154	1	0	-6.397706	7.362092	-0.865828
155	1	0	-6.351854	6.912895	-2.566339
156	1	0	-7.607755	9.066593	-2.257765
157	1	0	-8.698375	7.813562	-2.874095
158	1	0	-8.745607	8.264320	-1.161623
159	1	0	-0.595793	-1.829703	3.084454
160	1	0	-2.075990	-2.786019	3.373044
161	1	0	-0.705426	-4.907733	3.189744
162	1	0	0.748015	-3.942664	2.935855
163	1	0	0.445776	-2.906549	5.218274
164	1	0	-0.989730	-3.896103	5.475166
165	1	0	0.411729	-5.980218	5.192428
166	1	0	1.850749	-4.980335	5.020214
167	1	0	1.558001	-5.956162	7.322187
168	1	0	0.051950	-5.068795	7.512258
169	1	0	-17.281687	-2.314335	0.357764
170	1	0	-16.726801	0.148246	-0.339862
171	1	0	-12.182358	-3.658591	0.953993
172	1	0	-13.389554	1.436797	0.342423
173	1	0	-13.320343	0.944830	-1.338408
174	1	0	-15.670226	1.777024	-1.683095
175	1	0	-15.737266	2.273556	0.008467
176	1	0	-13.789142	3.822846	-0.373831
177	1	0	-13.730713	3.330683	-2.063835
178	1	0	-16.068983	4.212904	-2.400005
179	1	0	-16.124439	4.706502	-0.710330
180	1	0	-14.178446	6.258037	-1.102317
181	1	0	-14.127729	5.766792	-2.791050
182	1	0	-15.360271	7.941361	-2.544056

183	1	0	-16.462237	6.686032	-3.134948
184	1	0	-16.513534	7.180413	-1.434735
185	1	0	-9.777388	-5.147635	-0.790077
186	1	0	-8.414898	-4.053766	-1.159845
187	1	0	-6.872026	-5.582536	0.140711
188	1	0	-8.226624	-6.660877	0.474159
189	1	0	-8.498202	-7.069021	-2.006529
190	1	0	-7.124890	-6.011571	-2.324541
191	1	0	-5.638975	-7.545796	-0.980027
192	1	0	-7.013485	-8.602436	-0.672358
193	1	0	-7.250928	-9.007218	-3.149939
194	1	0	-5.870345	-7.958992	-3.451323
195	1	0	-5.165792	-10.369010	-3.477462
196	1	0	-4.384483	-9.527385	-2.128174
197	1	0	-5.774666	-10.582504	-1.827090
198	1	0	1.970259	-3.909640	8.664569
199	1	0	1.314305	-2.879938	7.386134
200	1	0	2.823811	-3.767453	7.118564
201	1	0	10.516667	-7.713202	-4.370527
202	1	0	11.374180	-6.906897	-3.046013
203	1	0	10.054044	-8.032768	-2.690215
204	1	0	13.046188	-8.115180	-2.878063
205	1	0	12.596600	-6.639862	-2.014868
206	1	0	13.997337	-7.584091	-1.481118

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