Supporting Information

Dithieno[3,2-*a*:3′,2′-*j*][5,6,11,12]chrysene Diimides: A Versatile Electron-Deficient Building Block for Polymeric Semiconductors

Xueqian Zhao,[a, §] Congwu Ge,[a, §] Xiaopeng Xu,[b] Jintao Huang,[a] Xiaodi Yang,[c] Qiang Peng,[b] Wei-Shi Li[a] and Xike Gao[a, *]

[a] Key Laboratory of Synthetic and Self-Assembly Chemistry for Organic Functional Molecules, Centre for Excellence in Molecular Synthesis, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai 200032, China

[b] Key Laboratory of Green Chemistry and Technology of Ministry of Education, College of Chemistry, State Key Laboratory of Polymer Materials Engineering, Sichuan University, Chengdu 610064, China

[c] Experiment Center for Science and Technology, Shanghai University of Traditional Chinese Medicine, Shanghai 201203, China

[§]X. Z. and C.G. contributed equally to this work

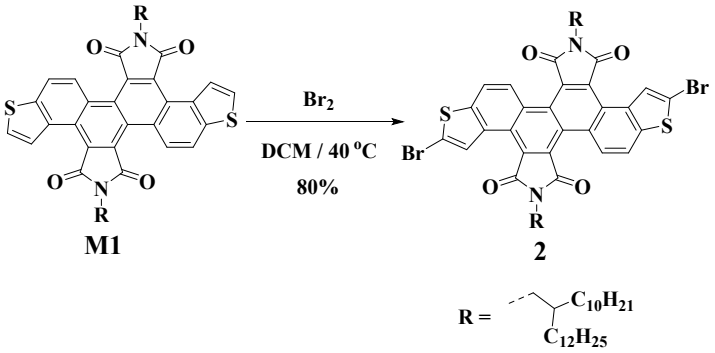
[*]E-mail: gaoxk@mail.sioc.ac.cn

Experimental Section

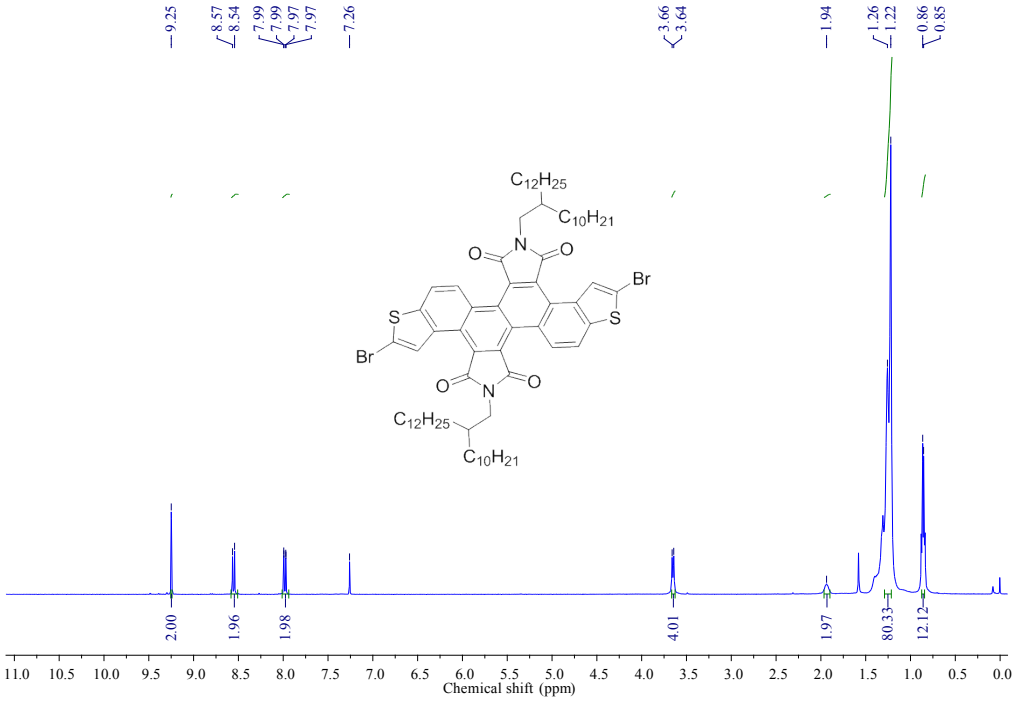
1. Materials and General Methods

Commercially available reagents and solvents were obtained and used as received unless otherwise mentioned. Compounds **M1** and **1** were synthesized according to the reported procedures.[1] ^{1}H NMR (300 MHz or 400 MHz) and ^{13}C NMR (100 MHz) spectra were measured on Varian Mercury (300 MHz and 400 MHz) or JEOL NMR (400 MHz) instruments. Elemental analyses were performed on an Elementar Vario EL III elemental analyzer. Mass spectra (EI, DART, ESI and MALDI-TOF) were carried out on Thermo Fisher Scientific LTQ FT Ultra Mass Spectrometer, Waters Micromass GCT premier or Agilent Technologies 5973N. Optical absorption spectra were measured on a U-3900 UV-vis spectrophotometer. Thermogravimetric analysis (TGA) measurements were conducted on a TGA Q500 instrument under a dry nitrogen flow at a heating rate of 10 ºC/min, heating from room temperature to 500 ºC. Differential scanning calorimetry (DSC) measurements were performed on a DSC Q2000 instrument under a dry nitrogen flow at a heating rate of 10 ºC/min, heating from room temperature to 350 ºC. Cyclic voltammetry (CV) was carried out on CHI610D instruments using Bu_4NPF_6 (0.1 M) as supporting electrolyte and ferrocene as an internal reference at a scan rate of 100 mV/s. The CV cell consisted of a platinum button working electrode, a platinum wire counter electrode, and an $Ag/AgNO_3$ reference electrode. Melting point was measured on SGW X-4 or WRS-1A microscopic melting point apparatus. X-ray diffraction (XRD) measurements were carried out in the reflection mode with Cu Kα radiation using a 2-kW Rigaku X-ray diffraction system. Atomic force microscopy (AFM) was recorded on a Bruker Inova atomic microscope in tapping mode with a silicon tip. Transmission electron microscopy (TEM) measurements were performed in a JEM-2100 instrument.

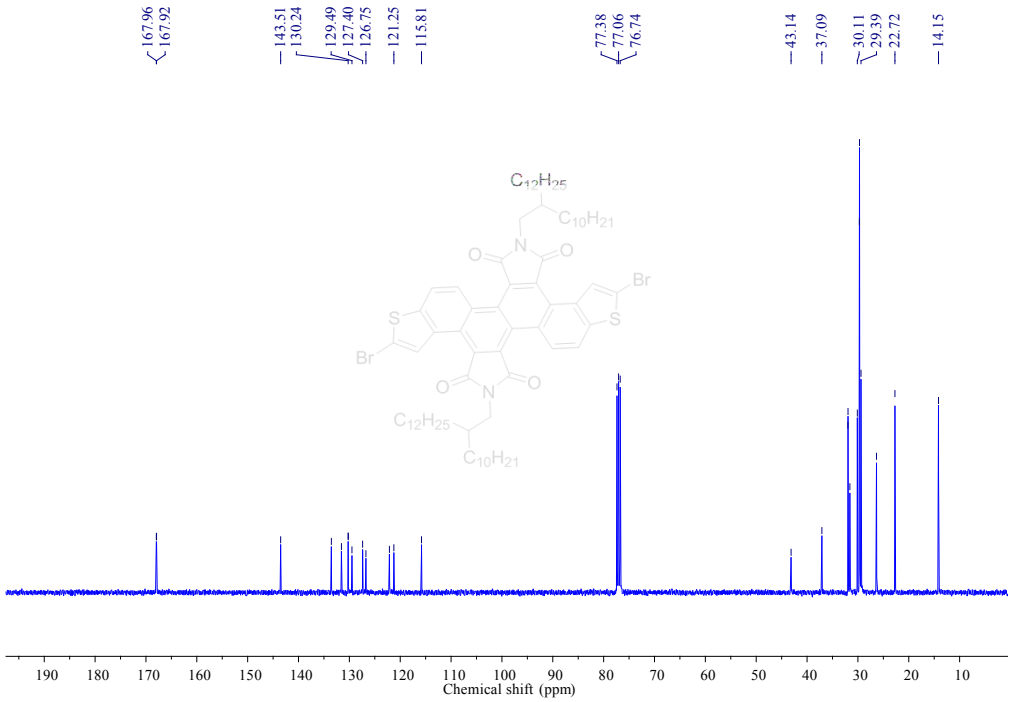
2. Synthesis and characterizations



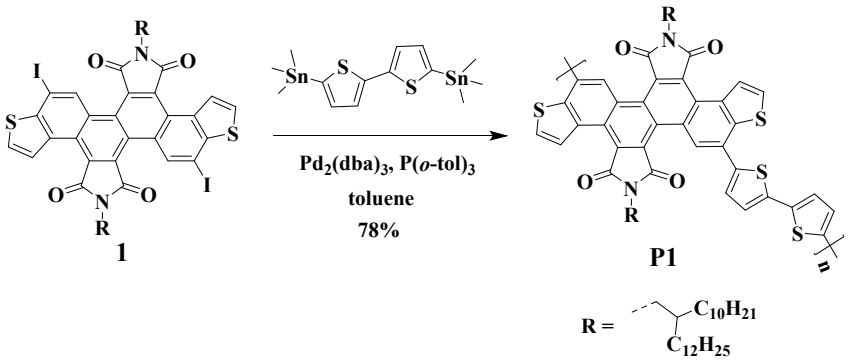
Compound 2: Compound **M1** (130 mg, 0.11 mmol) was dissolved in 20 mL DCM solution. Bromine (43 mg, 0.28 mmol) was then added to the solution and stirred at 40 ºC for 3 h. 20 mL Na_2SO_3 aqueous solution was added to quench the reaction. The aqueous phase was removed and the organic phase was dried by anhydrous Na_2SO_4. After removing the DCM solvent under reduced pressure, the crude product was purified by silica gel column chromatography, using the mixture of petroleum ether and dichloromethane (4:1) as the eluent. 118 mg red solid product was obtained (yield: 80%) Mp: 120-121 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.25 (s, 2H), 8.54-8.57 (d, J = 8.8 Hz, 2H), 7.97-7.99 (d, J = 8.8 Hz, 2H), 3.64-3.66 (d, J = 7.2 Hz, 4H), 1.94 (br, 2H), 1.22-1.26 (m, 80H), 0.85-0.86 (m, 12 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 167.9, 167.9, 143.5, 133.5, 131.5, 130.2, 130.2, 129.4, 127.4, 126.7, 122.1, 121.2, 115.8, 43.1, 37.0, 32.0, 31.9, 31.5, 30.1, 29.7, 29.6, 29.4, 26.3, 22.7, 14.1.



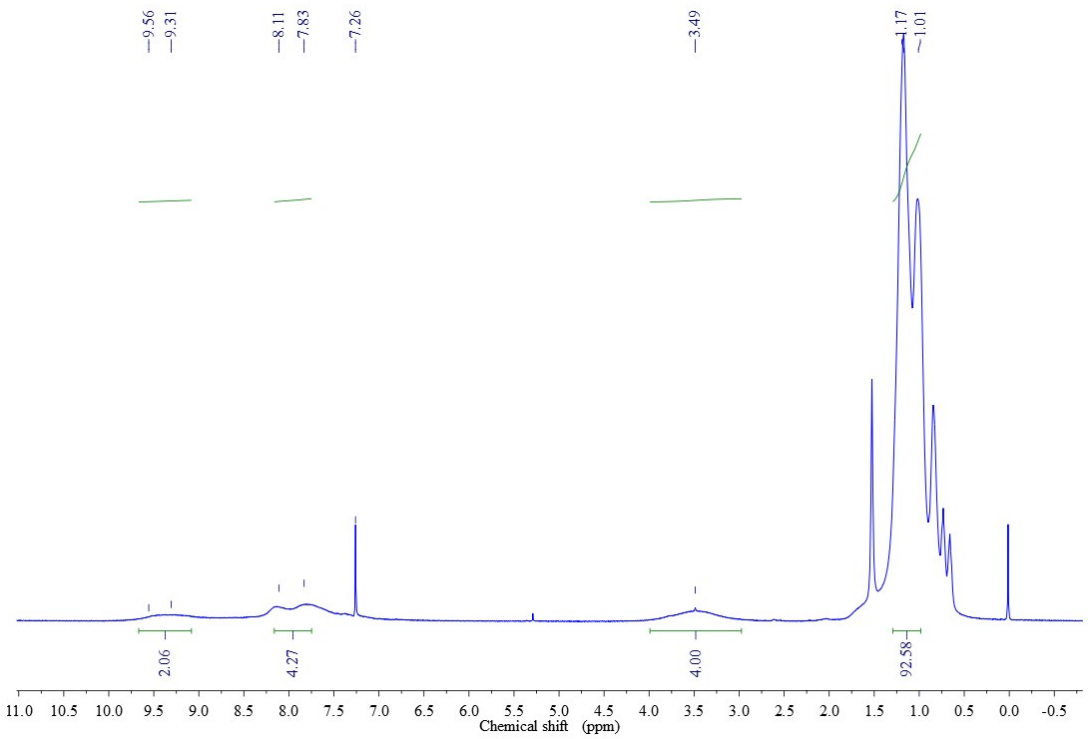
^{1}H NMR of compound **2**



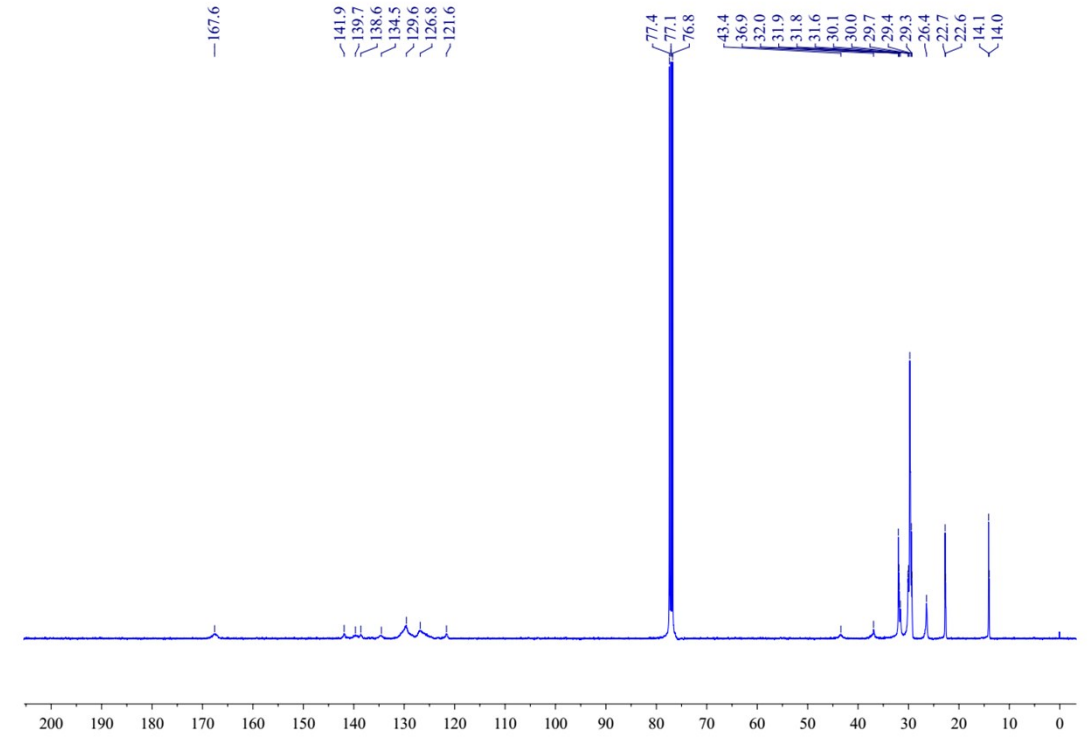
^{13}C NMR of compound **2**



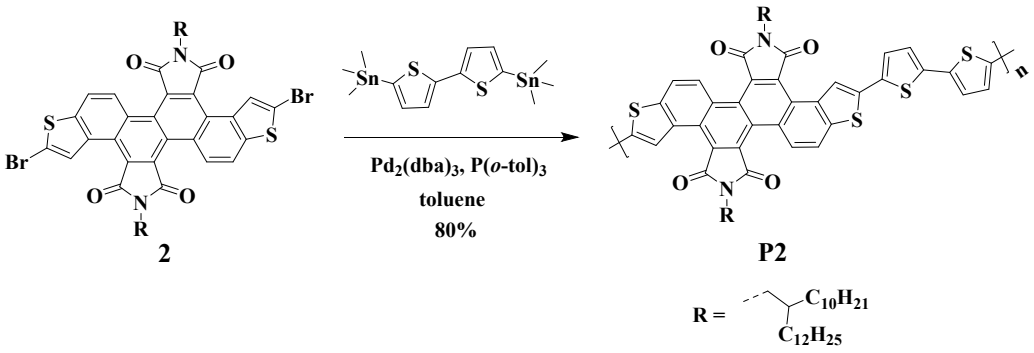
P1: To a mixture of compound **1** (192.7 mg, 0.14 mmol) and 5,5'-bis(trimethylstannyl)bithiophene (68 mg, 0.14 mmol) in 20 mL toluene solution, $Pd_2(dba)_3$ (3 mg, 2% mmol) and P(o-tol)$_3$ (3 mg, 4% mmol) was added under N_2 atmosphere. The mixture was stirred at 110 ºC for 36 h. 1 mL KF solution was added to quench the reaction. The mixture was dropped into 200 mL methanol solution to get a green precipitate. The precipitate was filtered and subjected to Soxhlet extraction successively with methanol, acetone, hexane and ethyl acetate to remove the oligomers and impurities. The residue was extracted by DCM to obtain 140 mg dark-green solid (yield: 78%). M_n = 24305, PDI = 1.65. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.85-9.76 (br, 2H), 7.42-8.29 (br, 4H), 3.02-3.99 (br, 4H), 0.46-1.47 (br, 92 H). Anal. Calcd for $C_{82}H_{110}N_2O_4S_4$: C, 74.84; H, 8.43; N, 2.13. Found: C, 74.51; H, 8.50; N, 1.76.



^{1}H NMR of polymer **P1**



^{13}C NMR of polymer **P1**



P2: To a mixture of compound **2** (107 mg, 0.081 mmol) and 5,5'-bis(trimethylstannyl)bithiophene (40 mg, 0.081 mmol) in the 5 mL toluene solution, $Pd_2(dba)_3$ (3 mg, 4% mmol)and P(o-tol)$_3$ (3 mg, 8% mmol) was added under N_2 atmosphere. The mixture was stirred at 100 ºC for 10 minutes. 1 mL KF solution was added to quench the reaction. The mixture was dropped into 200 mL methanol solution to get a green precipitate. The precipitate was filtered and subjected to Soxhlet extraction successively with methanol, acetone, hexane and ethyl acetate to remove the oligomers and impurities. The residue was extracted by dichlorobenzene to obtain 86 mg dark-green solid (yield: 80%). M_n = 65775, PDI = 3.13. Anal. Calcd for $C_{82}H_{110}N_2O_4S_4$: C, 74.84; H, 8.43; N, 2.13. Found: C, 74.11; H, 8.13; N, 1.96.

3. Fabrication and measurement of BGTC OFETs

The Si/SiO_2 substrates with a capacitance of 10 nF cm^{-2} was used as the gate electrode and dielectric layer. Thin films of **P1** and **P2** were deposited on octadecyltrichlorosilane (OTS)-treated Si/SiO_2 substrates by spin-coating their respectively chloroform or chlorobenzene solutions (5 mg mL^{-1}). Gold, used as source and drain electrode, were deposited on the top of the active layer through a shadow mask under high vacuum ($\sim 10^{-7}$ Torr), affording a bottom-gate top-contact (BGTC) device configuration. The channel length (L) and width (W) were 31 μm and 273 μm, respectively. The electric characteristics of the OFET devices were measured by using a Keithley 4200-SCS semiconductor parameter analyzer in a glovebox with a nitrogen atmosphere. The field-effect mobility was calculated in the saturation regime according to the equation $I_{DS} = (\mu WC_i/2L)(V_G - V_T)^2$, where I_{DS} is the drain-source current, V_G is the gate voltage, V_T is the threshold voltage, μ is the field-effect mobility, W is the channel width, L is the channel length, and C_i is the capacitance per unit area of the gate dielectric layer.

4. Fabrication and measurement of all-polymer solar cells

PTB7-Th and **P1** with a weight ratio of 1:1 were co-dissolved in chlorobenzene, the total material concentration was 18 mg mL^{-1}, different amounts of DIO was added as solvent additive for the blend films. The all-polymer solar cells were fabricated with a structure of ITO/ZnO/active layer/MoO_3/Ag. A thin layer (~30 nm) of ZnO sol-gel was spin-coated onto ITO glass and annealed at 180 ºC in ambient condition for 30 min then transferred into glovebox immediately. Active layers (the as prepared solutions) were then spin-coated in the glovebox. Finally, MoO_3 (~10 nm) and Ag (80 nm) anodes were thermal evaporated through a shadow mask in glovebox at a chamber pressure of ~2.0

$\times 10^{-6}$ mbar. The active area of the device was 4 mm^2. Current density–voltage (*J–V*) curves were detected on a Keithley 2400 source meter. Photocurrent was obtained upon irradiation using a solar simulator (XES-70S1, SAN-EI ELECTRIC CO., LTD.), with AM 1.5 G filter. Light intensity was calibrated to 100 mW cm^{-2} using a NREL-certified standard silicon cell (AK-200, Konica Minolta, INC.). External quantum efficiency (EQE) was recorded by a Newport quantum efficiency test model 77890 (Newport Co. Ltd.) with a Xe lamp.

5. Density functional theory (DFT) calculations

To investigate the relationship between the molecular structure and optoelectronic performance, the geometry optimization was performed using the Gaussian 16 package with the B3LYP hybrid density functional and the 6-31G(d,p) basis set. The long side chains were replaced by methyl groups, and the trimers were utilized to represent the polymeric backbone in order to simplify the calculations.[2]

The full optimization was carried out based on assumed planar conformation. Strong geometric twist taken place around the inter-ring C-C bonds. The non-planar structures at 298.15 K and 1 atm were estimated from the gas-phase studies. Harmonic vibration frequency calculations at the same level were performed to verify all stationary points as local minima (with no imaginary frequency).

Considering one of the most ideal molecular configuration, the structural planarization was very important factor to improve the charge transfer property. The planar structures were also optimized by constraining the molecules to planar conformations (thus, freezing out he torsional motions along the long polymer chains). All the optimized geometry and frontier molecular orbitals are listed in the Table S5-8 and Figure S8.

Peak No	Mp	Mn	Mw	Mz	Mz+1	PDI
1	32203	24305	40035	72315	121450	1.64718

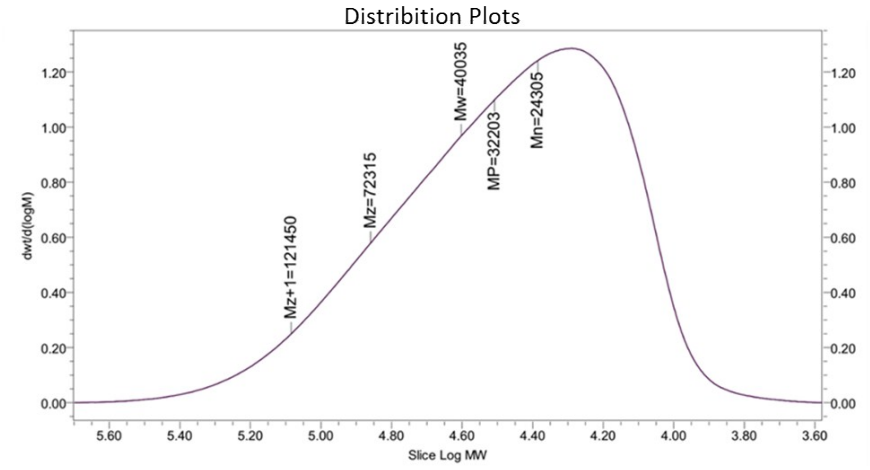


Figure S1 GPC distribution plots of polymer **P1** with tetrahydrofuran as eluent at room temperature.

MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	164776	65775	205910	421396	651893	177885	3.13052

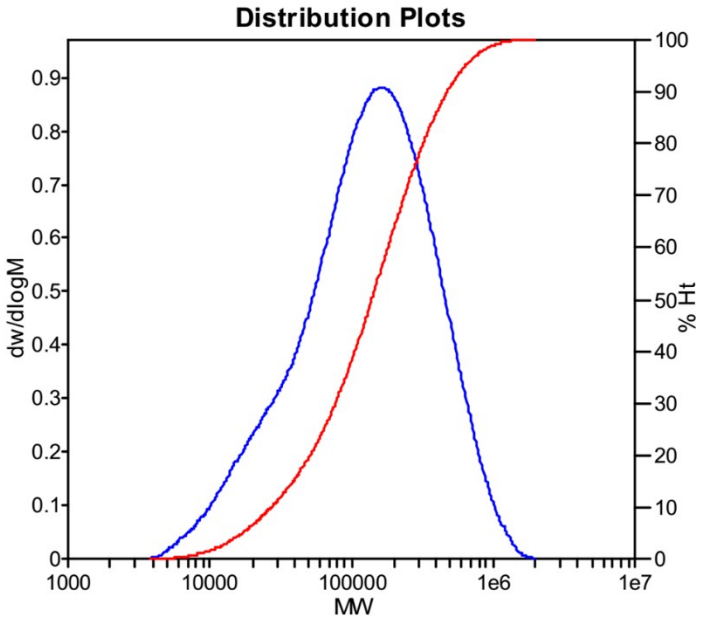


Figure S2 GPC distribution plots of polymer **P2** with 1,2,3-trichlorobenzene as eluent at 150 ºC.

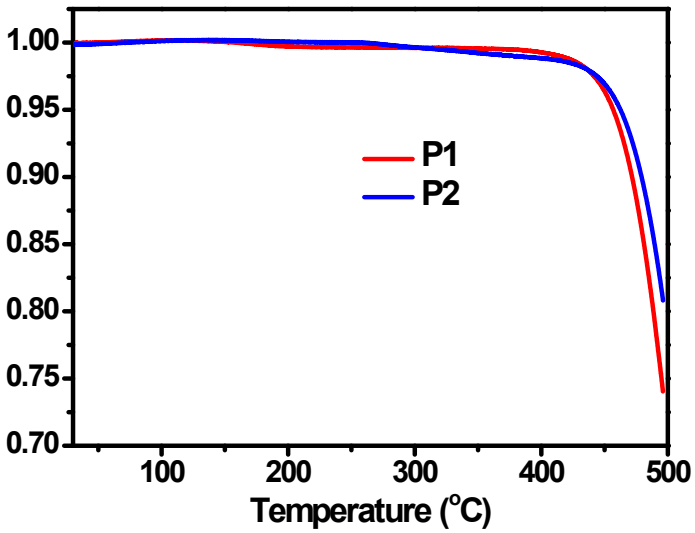


Figure S3 TGA plots of polymers **P1** and **P2** under a nitrogen flow with a heating rate of 10 ºC/min.

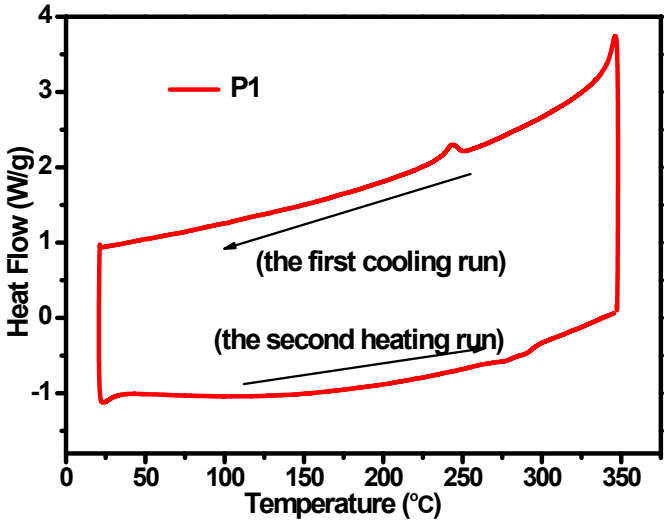


Figure S4 DSC plots of polymer **P1.**

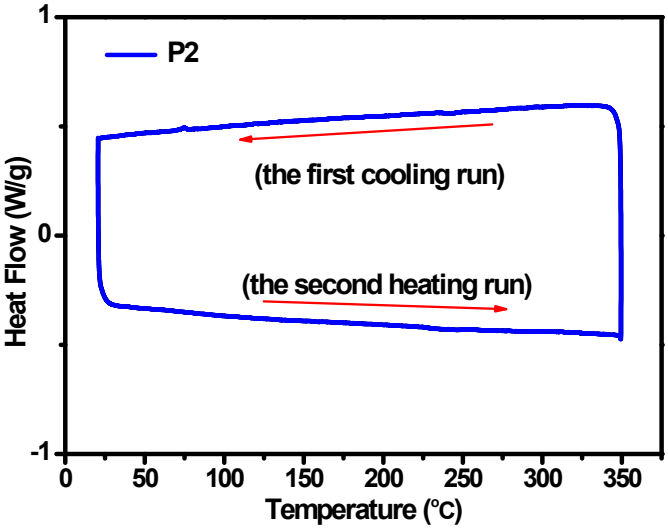


Figure S5 DSC plots of polymer **P2.**

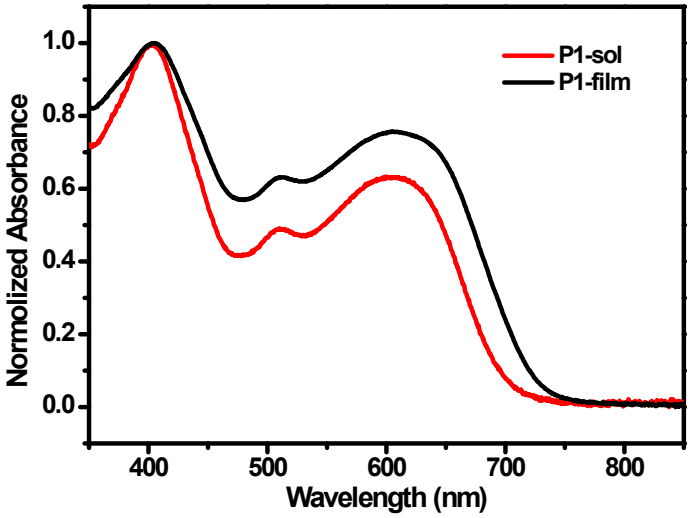


Figure S6 UV-vis absorption spectra of polymer **P1** in dichloromethane solution and in thin film.

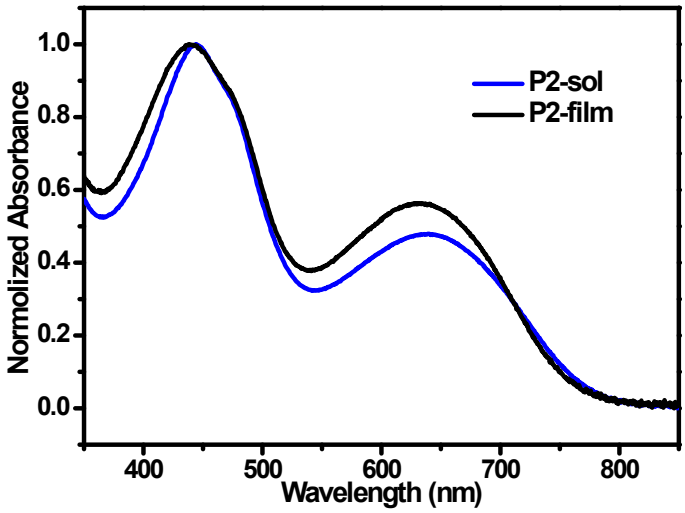


Figure S7 UV-vis absorption spectra of polymer **P2** in chlorobenzene solution and in thin films.

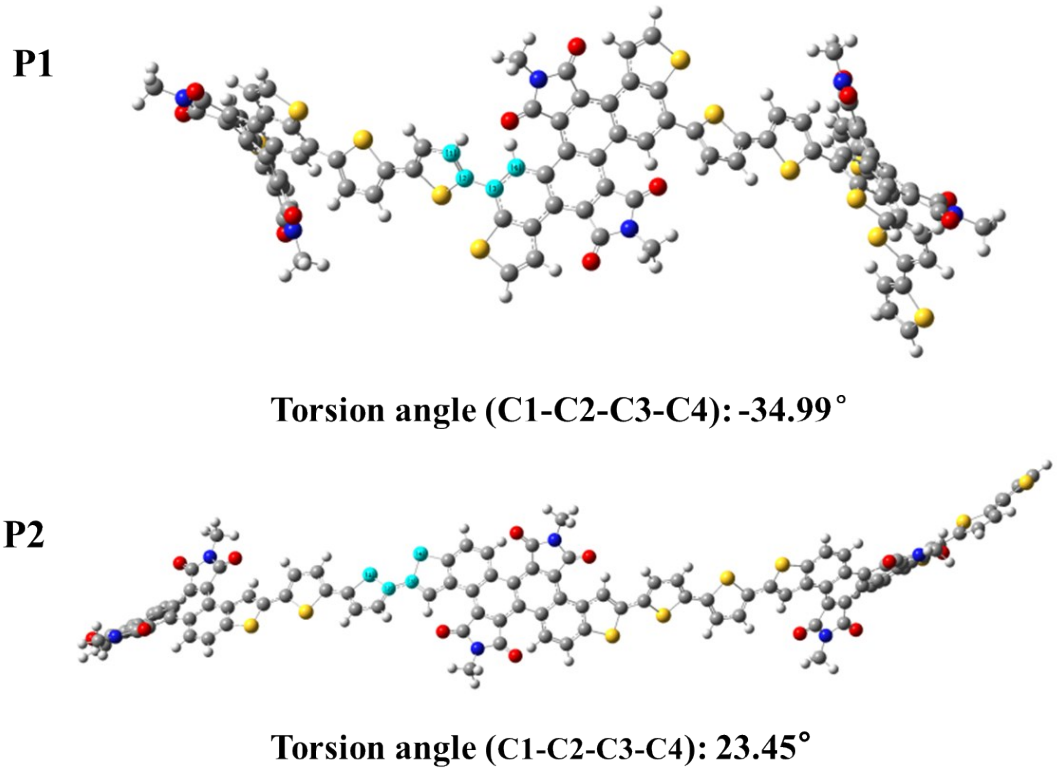


Figure S8 Molecular geometries and torsion angles of model molecules of **P1** and **P2** obtained by DFT calculations.

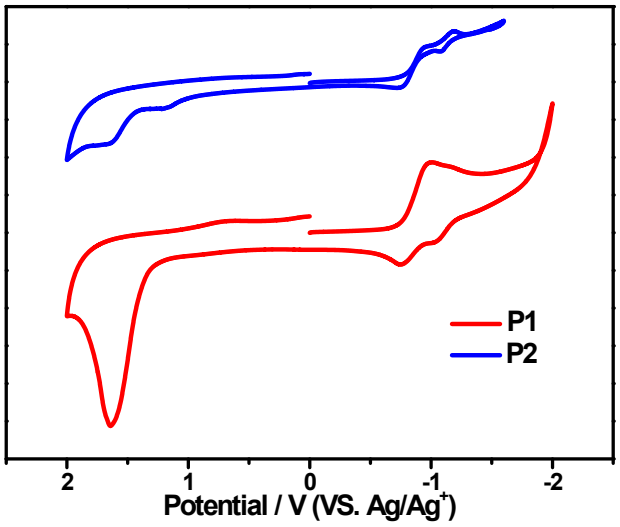


Figure S9 Cyclic voltammograms of thin films of **P1** and **P2** in 0.1 M $Bu_4N^+PF_6^-$ solution in acetonitrile at a scan rate 100 mV/s.

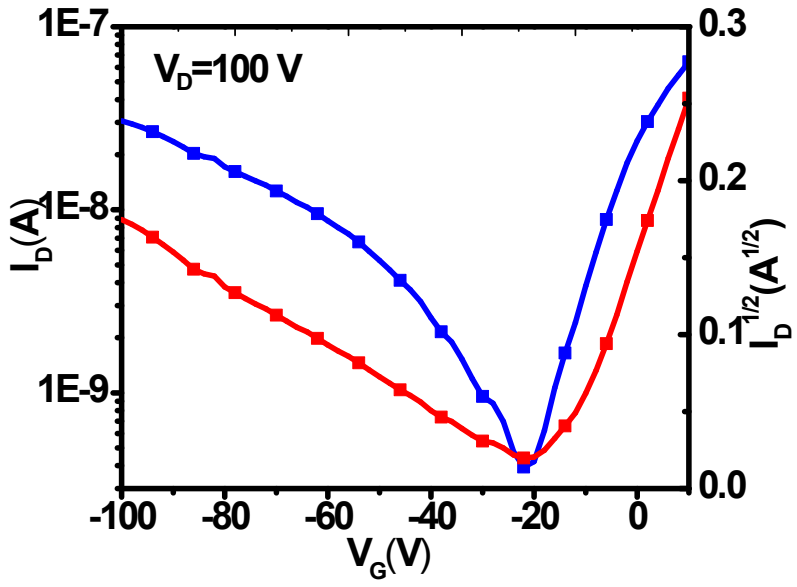


Figure S10 Typical transfer characteristics of OFETs based on **P2**.

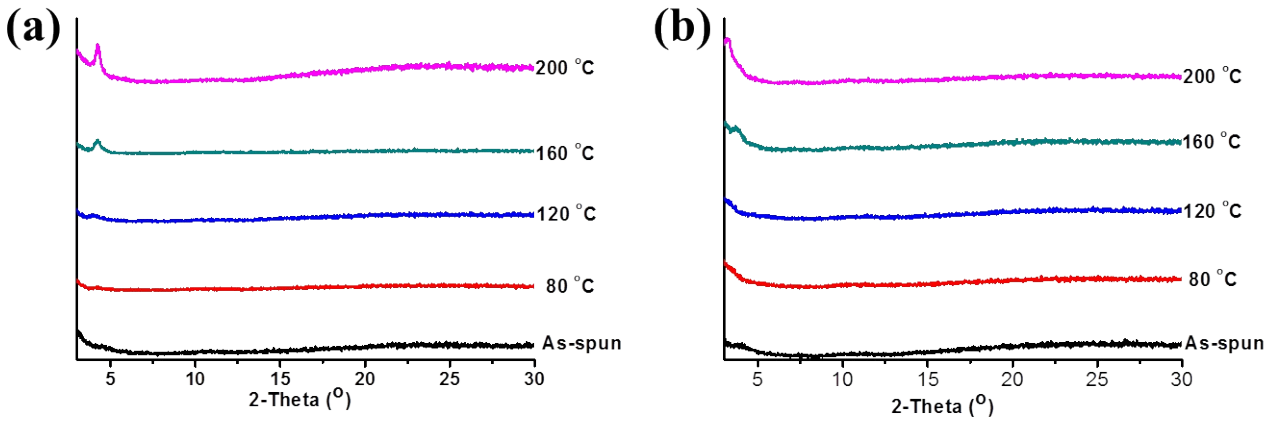


Figure S11 X-ray diffraction (XRD) patterns of as-spun and after thermal annealing at 80 ºC, 120 ºC, 160 ºC, 200 ºC thin films of **P1** (a) and **P2** (b).

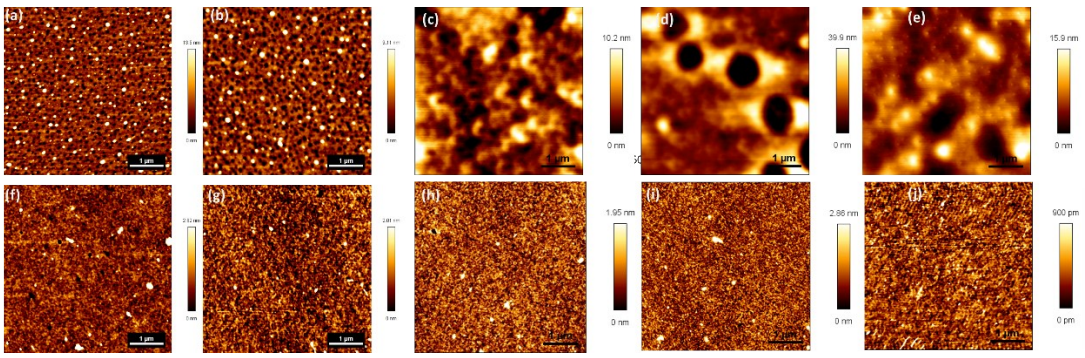
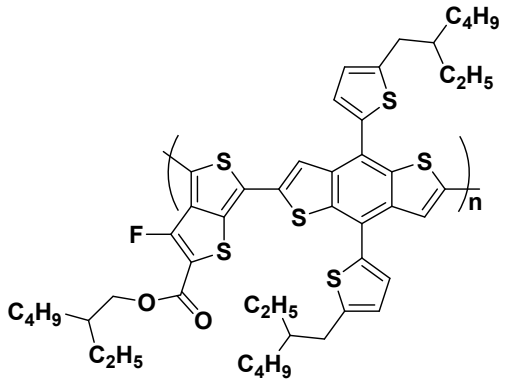


Figure S12 AFM images of thin films of **P1** (a-e) and **P2** (f-j), as-spun (a, f),after thermal annealing at 80 ºC (b, g), 120 ºC (c, h), 160 ºC (d, i), 200 ºC (e, j), respectively.



PTB7-Th

Figure S13 Chemical structure of **PTB7-Th**.

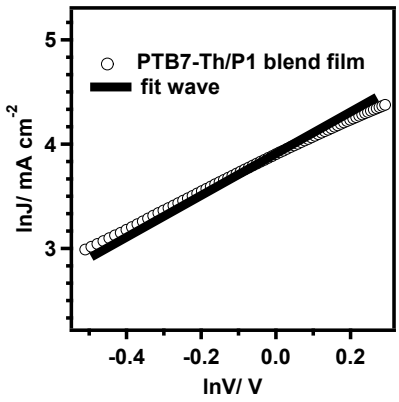


Figure S14 SCLC fittings of the hole-only device based on the PTB7-Th/**P1** blend films with 1% (v/v) DIO.

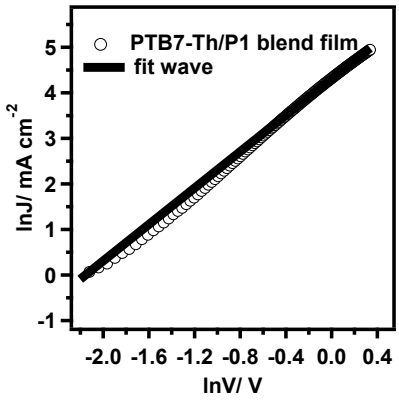


Figure S15 SCLC fittings of the electron-only device based on the PTB7-Th/**P1** blend films with 1% (v/v) DIO.

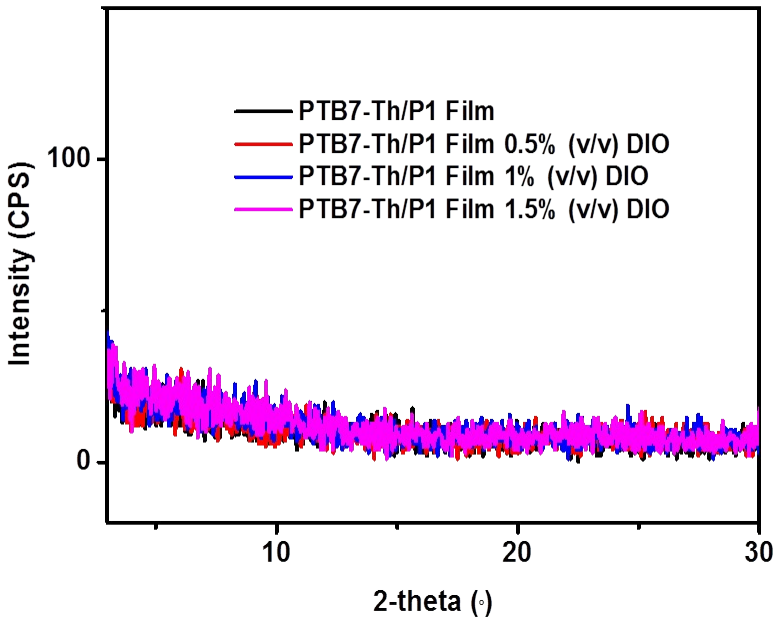


Figure S16 X-ray diffraction (XRD) patterns of PTB7-Th/**P1** as-cast, with 0.5% (v/v) DIO, with 1.0% (v/v) DIO, with 1.5% (v/v) DIO films.

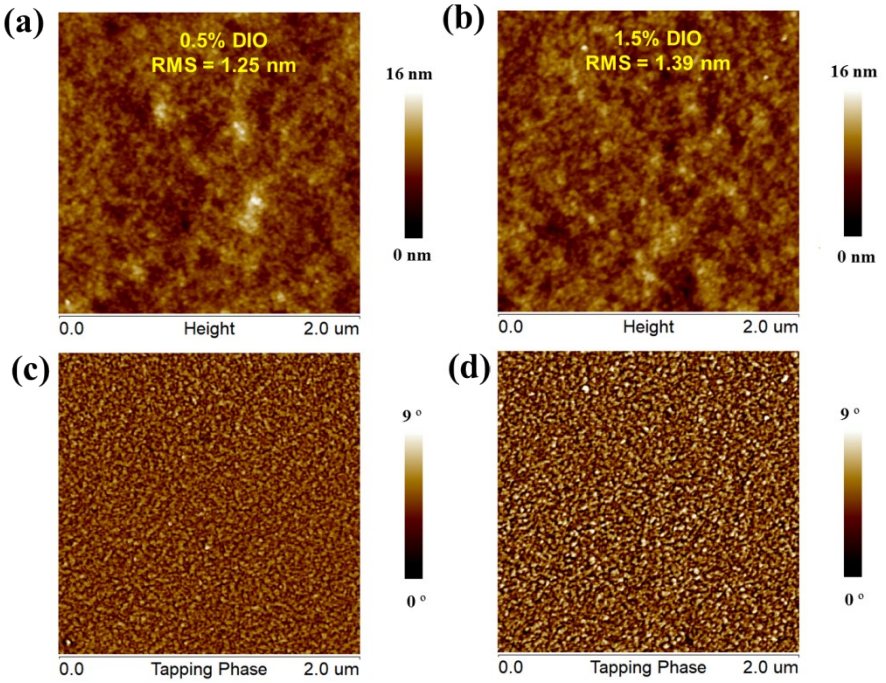


Figure S17 AFM height and phase images (2 × 2 μm^2) of PTB7-Th/**P1** blend films with 0.5% (v/v) DIO (a,c) and with 1.5% (v/v) DIO (b,d).

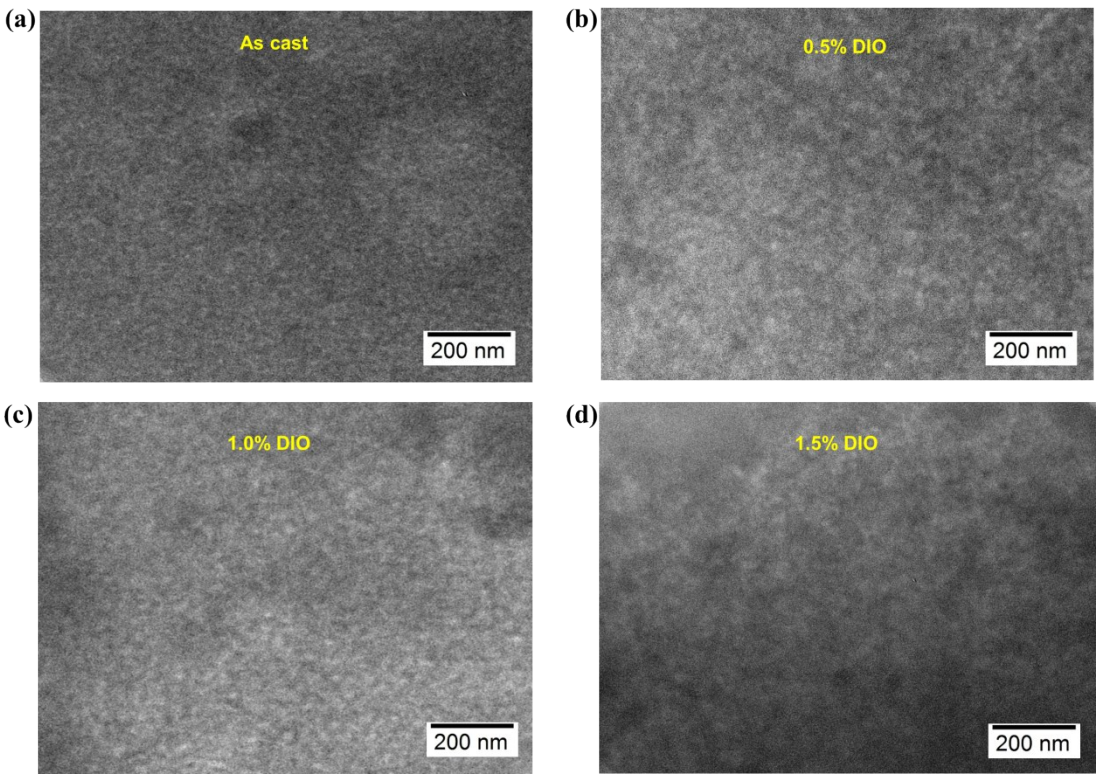


Figure S18 TEM images of PTB7-Th/**P1** as-cast (a), with 0.5% (v/v) DIO (b), with 1.0% (v/v) DIO (c) and with 1.5% (v/v) DIO (d) films, respectively.

Table S1. Summarize of experimental and calculated optoelectronic parameters of **P1** and **P2**.

Polymer	λ_{max} **(nm)** **soln/film**	$E_{LUMO}{}^{a}$ **(eV)**	$E_{HOMO}{}^{b}$ **(eV)**	$E_g{}^{opt\ c}$ **(eV)** **soln/film**	$E_g{}^{cv}$ **(eV)**
P1	607/610	− 4.01	− 6.05	1.76/1.71	2.04
P2	638/640	− 3.96	− 5.76	1.63/1.59	1.80

$^{a}E_{LUMO} = -(E_{onset,}{}^{red} - E_{1/2}(Fc/Fc^{+}) + 5.10)$ (eV).[2] $^{b}E_{HOMO} = -(E_{onset,}{}^{ox} - E_{1/2}(Fc/Fc^{+}) + 5.10)$ (eV).[3] ^{c}Obtained from the onset wavelength of solution/film absorption.

Table S2 Characteristics of OFET device based on **P1** at different annealing temperatures.

Polymer	Annealing Temperature (ºC)	V_T (V) (Ave.)	I_{on}/I_{off}	μ_e (cm²/V.s) Max. (Ave.)
P1	As-spun	31.6 (35.3)	10^4~10^5	1.8 (1.6) ×10^{-2}
	80	24.4 (27.8)	~10^5	2.9 (2.1) ×10^{-2}
	120	28.3 (29.7)	10^5~10^6	4.7 (4.6) ×10^{-2}
	160	23.8 (24.5)	10^5~10^6	6.4 (6.3) ×10^{-2}
	200	24.1 (25.0)	~10^6	0.11 (0.10)

Table S3 Characteristics of OFET device based on **P2** at different annealing temperatures.

Polymer	Annealing Temperature (ºC)	V_T (V) (Ave.)	I_{on}/I_{off}	μ_h(cm²/V.s) Max. (Ave.)	μ_e (cm²/V.s) Max. (Ave.)
P2	As-spun	−46.7 (−48.9)	~10^3	1.84 (1.66) ×10^{-4}	
		55.0 (57.8)	~10^3		3.59 (3.50) ×10^{-4}
	80	−46.2 (−48.0)	10^3~10^4	2.86 (2.71) ×10^{-4}	
		45.2 (56.0)	10^3~10^4		6.16 (5.92) ×10^{-4}
	120	−40.5 (−42.7)	10^3~10^4	4.81 (4.54) ×10^{-4}	
		42.5 (45.7)	10^3~10^4		9.82 (9.06) ×10^{-4}
	160	−38.7 (−41.9)	~10^4	6.25 (5.97) ×10^{-4}	
		39.9 (43.8)	~10^4		1.16 (1.15) ×10^{-3}
	200	−30.8 (−32.4)	~10^4	8.70 (8.28) ×10^{-4}	
		35.9 (40.1)	~10^4		1.79 (1.71) ×10^{-3}

Table S4. Characteristics of all-polymer solar cells based on PTB7-Th/**P1** blend films.

Active Layer (1:1)	DIO (v/v,%)	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	PCE (%)
PTB7-Th/P1	0	1.01	9.66	42.5	4.15
	0.5	1.00	11.18	49.5	5.53
	1	0.99	12.43	61.1	7.52
	1.5	0.98	12.00	43.3	5.09

Table S5. Optimized geometry and frontier molecular orbitals of **P1** (non-planar structure)

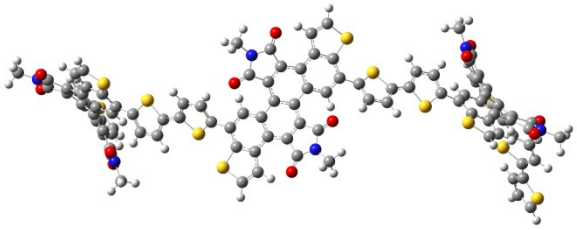
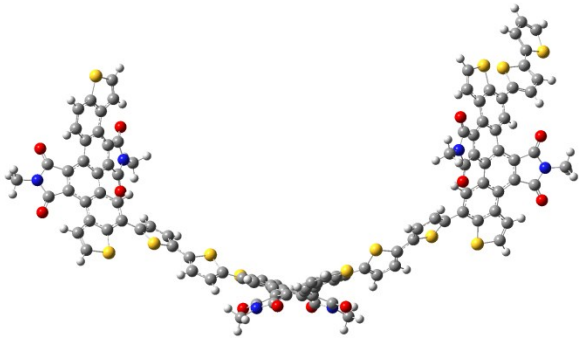
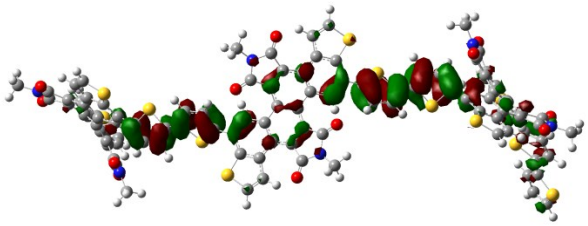
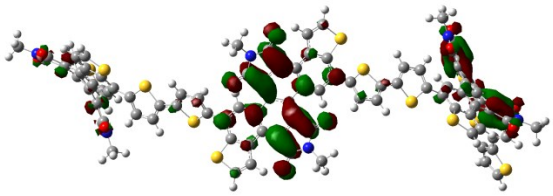
Optimized geometry	Top view  Side view 
HOMO -5.2761eV	
LUMO -3.2564eV	

Table S6. Optimized geometry and frontier molecular orbitals of P2 (non-planar structure)

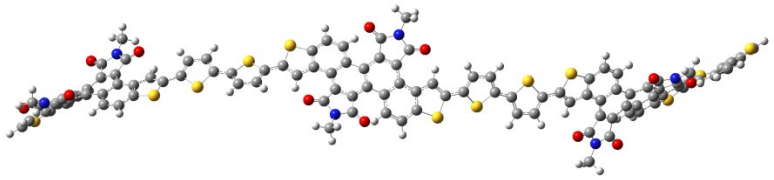
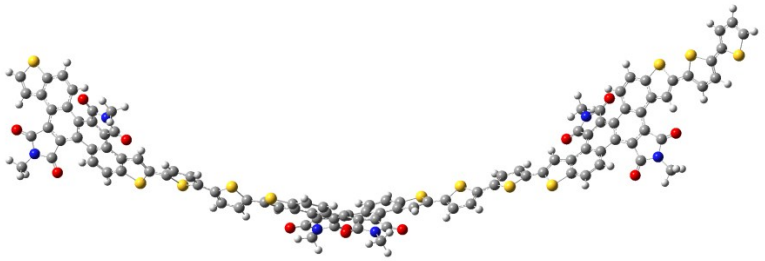
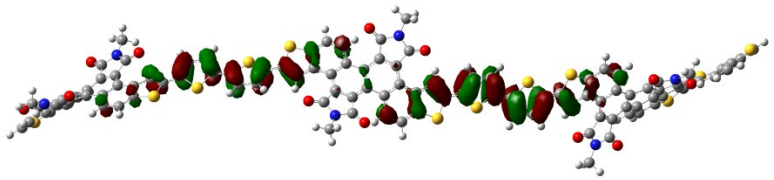
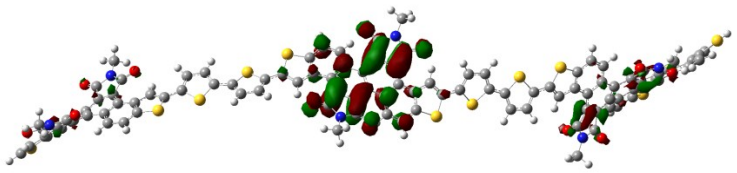
Optimized geometry	Top view  Side view 
HOMO -5.0695eV	
LUMO -3.2004eV	

Table S7. Optimized geometry and frontier molecular orbitals of **P1** (planar structure)

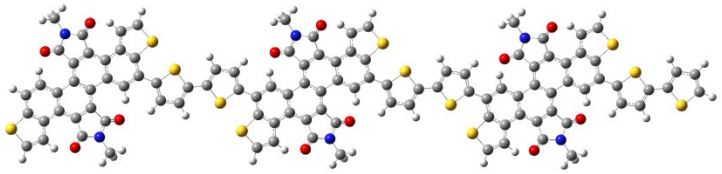
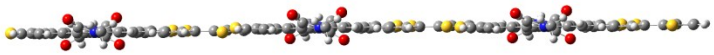
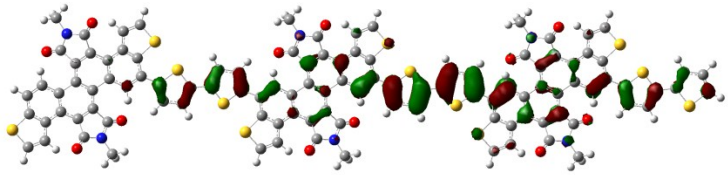
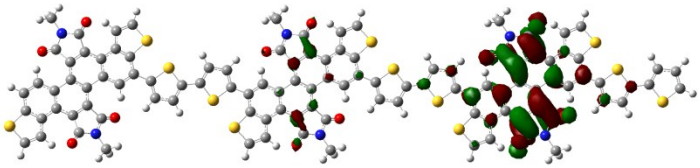
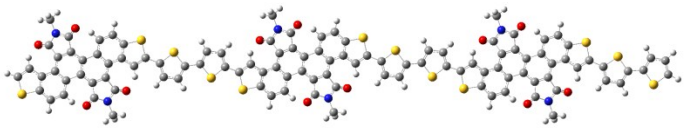
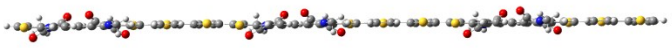
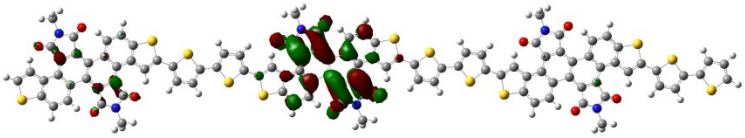
Optimized geometry	Top view  Side view 
HOMO - 5.0750eV	
LUMO - 3.1663eV	

Table S8. Optimized geometry and frontier molecular orbitals of **P2** (planar structure)

Optimized geometry	Top view  Side view 
HOMO -5.0595eV	
LUMO -3.0496eV	

Cartesian Coordinates (in Å)

P1 (non-planar structure)

C	15.975296	-0.377302	1.656441
C	15.331470	-0.379075	0.424261
C	16.032956	-0.211438	-0.809799
C	17.445566	-0.330875	-0.720201
C	15.413024	0.053546	-2.096028
C	16.136950	-0.157986	-3.319505
C	17.457263	-0.685915	-3.166730
C	18.099764	-0.706305	-1.934266
C	14.968817	-0.817782	2.690390
N	13.782936	-1.056111	2.005388
C	13.916108	-0.848446	0.634841
C	18.359127	-1.375909	-4.159480
N	19.495104	-1.760494	-3.450850
C	19.411495	-1.426686	-2.104223
O	20.262048	-1.741296	-1.290852
O	18.199241	-1.631682	-5.339057
O	15.075393	-1.003232	3.889273
O	13.026845	-1.072636	-0.166698
C	13.471379	0.964677	-3.311062
C	14.174984	0.730275	-4.519898
C	15.485617	0.197498	-4.552715
C	14.128335	0.634971	-2.134809
H	13.643110	0.885282	-1.206234
C	20.189901	0.552683	1.706409
C	19.464382	0.530739	2.924769
C	18.080976	0.239528	2.987509
C	17.368541	-0.080121	1.778421
C	18.110481	-0.086676	0.547370
C	19.477543	0.260903	0.552512
H	19.993362	0.354487	-0.388463
C	17.590115	0.345409	4.337441
C	15.981110	0.124979	-5.903286
C	15.082206	0.549400	-6.827554
C	18.556058	0.667714	5.235037
S	20.124047	0.869420	4.510923
S	13.576877	1.070015	-6.130056
H	16.566551	0.152965	4.614799
H	16.954172	-0.260109	-6.160422
H	15.209996	0.584272	-7.900760
C	12.582458	-1.567481	2.642345
H	12.800760	-2.499370	3.169473
H	12.192517	-0.842218	3.361255
H	11.847595	-1.745523	1.857631
C	20.593730	-2.519975	-4.020567
H	21.526065	-1.953149	-3.953155
H	20.718593	-3.464346	-3.485297
H	20.351404	-2.711364	-5.065564
H	18.444206	0.796335	6.302875

C	12.116231	1.513274	-3.215479
C	11.167431	1.154968	-2.278516
S	11.495970	2.792591	-4.246209
C	9.954705	1.873979	-2.390596
H	11.341739	0.366289	-1.555383
C	9.953658	2.802221	-3.413417
H	9.091596	1.695842	-1.759256
C	8.899775	3.702668	-3.824856
C	8.761022	4.394843	-5.012058
S	7.554684	4.050623	-2.756201
C	7.589977	5.185468	-5.074219
H	9.469979	4.308660	-5.827696
C	6.806422	5.110256	-3.939767
H	7.298346	5.773124	-5.937361
C	29.968513	9.288693	3.642147
C	29.879369	7.915399	3.464413
C	30.665165	7.215509	2.497403
C	31.742662	7.960340	1.946153
C	30.440507	5.845723	2.069785
C	31.466648	5.111420	1.382883
C	32.709519	5.801611	1.222731
C	32.819581	7.169360	1.435337
C	29.194791	9.635657	4.887895
N	28.685355	8.437600	5.378307
C	29.070862	7.347091	4.603567
C	34.093092	5.275925	0.925007
N	34.945658	6.374282	0.979165
C	34.272614	7.545224	1.315741
O	34.837948	8.605778	1.503182
O	34.485314	4.142559	0.713688
O	29.025538	10.698407	5.457296
O	28.805010	6.193367	4.888054
C	28.833861	3.994343	1.808452
C	29.854062	3.261283	1.150677
C	31.145710	3.789388	0.914841
C	29.159594	5.275874	2.227630
H	28.371861	5.876484	2.650822
C	32.412966	11.502633	0.907982
C	31.523535	12.197272	1.740876
C	30.683853	11.546795	2.671801
C	30.760006	10.113703	2.781364
C	31.692078	9.410654	1.939888
C	32.485977	10.135588	1.011927
H	33.142731	9.599335	0.346303
H	33.016304	12.030499	0.176723
C	29.820415	12.494915	3.330835
C	31.958388	2.858934	0.174063
C	31.321852	1.692015	-0.100409
C	30.020236	13.775609	2.922973
S	31.262259	13.923597	1.709233

S	29.695561	1.637992	0.513413
H	29.108452	12.225181	4.093985
H	32.981113	3.053168	-0.104739
H	31.716884	0.837236	-0.632039
C	27.932741	8.336759	6.615985
H	28.501890	8.770895	7.441483
H	26.981236	8.867955	6.529668
H	27.751868	7.278465	6.802643
C	36.387571	6.297197	0.826265
H	36.717411	6.940628	0.006780
H	36.885900	6.617858	1.744647
H	36.638335	5.259164	0.609465
H	29.509075	14.661814	3.272898
C	27.481461	3.500853	2.081583
C	26.730551	3.790516	3.203429
S	26.551811	2.508115	0.970817
C	25.439007	3.214190	3.190181
H	27.125723	4.377176	4.025002
C	25.173665	2.475814	2.053501
H	24.731333	3.310345	4.005810
C	23.975766	1.747190	1.699971
C	23.805246	0.764341	0.744587
S	22.461250	2.066335	2.522528
C	22.484518	0.263061	0.675915
H	24.619569	0.393883	0.132268
C	21.619570	0.846808	1.580184
H	22.169758	-0.531236	0.008504
C	2.067970	8.343952	-3.266224
C	2.195457	9.691666	-3.582524
C	3.385115	10.237647	-4.156635
C	4.311782	9.278914	-4.646405
C	3.685299	11.653791	-4.271795
C	4.701830	12.119185	-5.175163
C	5.332494	11.105659	-5.962579
C	5.193839	9.754728	-5.665462
C	0.620937	8.098738	-2.917255
N	-0.026172	9.321851	-3.049647
C	0.835359	10.329521	-3.476261
C	6.134664	11.209568	-7.235705
N	6.432189	9.902753	-7.615464
C	5.881485	8.966155	-6.748536
O	5.954666	7.765183	-6.939613
O	6.464768	12.179235	-7.893889
O	0.027794	7.079215	-2.613980
O	0.467353	11.461457	-3.734251
C	3.303538	13.929448	-3.404240
C	4.286561	14.392402	-4.315613
C	4.997356	13.527734	-5.181552
C	3.051990	12.565354	-3.401278
H	2.371250	12.186278	-2.657398

C	5.562297	5.849404	-3.710887
C	4.433650	5.353043	-3.010136
C	3.255391	6.113149	-2.819195
C	3.167279	7.436480	-3.378320
C	4.300111	7.928127	-4.113706
C	5.461237	7.134533	-4.222875
H	6.337801	7.557242	-4.684585
C	2.295877	5.390389	-2.024514
C	5.976146	14.254049	-5.949144
C	5.975290	15.587340	-5.694452
C	2.720316	4.151395	-1.667740
S	4.309719	3.774007	-2.263666
S	4.795498	16.056886	-4.506594
H	1.323451	5.778191	-1.768236
H	6.621789	13.793505	-6.678728
H	6.604692	16.342542	-6.144853
C	-1.456645	9.491691	-2.867774
H	-2.005444	8.805574	-3.517413
H	-1.736836	9.290426	-1.830513
H	-1.697745	10.522854	-3.124870
C	7.139226	9.548040	-8.833037
H	8.063325	9.013600	-8.597265
H	6.514527	8.907404	-9.460128
H	7.371030	10.474370	-9.357978
H	2.184214	3.416072	-1.083595
C	2.538647	14.776260	-2.485303
C	1.220871	14.584714	-2.122657
S	3.209582	16.150090	-1.620320
C	0.743062	15.531642	-1.185545
H	0.613013	13.798372	-2.555758
C	1.689091	16.462690	-0.807638
H	-0.277494	15.551110	-0.820272
C	1.560494	17.572092	0.114866
C	2.351710	18.694532	0.239272
S	0.262367	17.613086	1.297348
C	1.920180	19.583413	1.263178
H	3.205622	18.883740	-0.401324
C	0.802827	19.140612	1.916170
H	2.416482	20.517970	1.497338
H	0.262512	19.615252	2.723102

P2 (non-planar structure)

C	11.110521	13.807364	-10.628859
C	12.201976	13.416909	-9.867093
C	13.461127	13.069139	-10.449338
C	13.612436	13.444468	-11.812624
C	14.543103	12.390055	-9.759447
C	15.875335	12.398641	-10.303217
C	16.046757	13.170801	-11.495003

C	14.965970	13.617000	-12.240900
C	10.053375	14.315651	-9.679734
N	10.588880	14.203968	-8.403430
C	11.891133	13.703863	-8.421266
C	17.298164	13.734229	-12.121447
N	16.879110	14.491053	-13.211229
C	15.492690	14.503848	-13.339238
O	14.908838	15.168421	-14.173588
O	18.466192	13.636368	-11.789422
O	8.948516	14.785283	-9.888147
O	12.584823	13.598111	-7.428367
C	15.235947	10.889294	-7.960441
C	16.539945	10.911264	-8.469411
C	16.893969	11.632941	-9.632373
C	14.261819	11.615887	-8.603762
H	13.250868	11.567234	-8.232836
C	11.474853	13.631486	-14.893692
C	10.205913	13.802100	-14.327563
C	9.994982	13.866273	-12.931156
C	11.137105	13.778238	-12.058326
C	12.440497	13.627978	-12.649563
C	12.565433	13.543792	-14.060628
H	13.536898	13.376334	-14.496620
H	14.988944	10.291775	-7.089103
H	11.597559	13.545967	-15.968358
C	8.598376	13.944453	-12.626449
C	18.261930	11.398748	-9.984239
C	18.932734	10.573018	-9.117169
C	7.782663	13.976354	-13.729843
S	8.712176	13.895819	-15.226238
S	17.888280	10.021397	-7.807800
H	8.210997	13.982174	-11.621559
H	18.735635	11.832144	-10.849542
C	6.340984	14.092169	-13.732921
C	5.535420	14.578818	-12.721492
S	5.363507	13.577878	-15.096478
C	4.157340	14.554126	-13.033346
H	5.937892	14.971941	-11.795393
C	3.877962	14.055405	-14.292197
H	3.387131	14.922104	-12.364911
C	2.601116	13.897919	-14.945380
C	2.328484	13.653467	-16.278538
S	1.105694	14.000835	-14.031642
C	0.948907	13.573122	-16.574135
H	3.106096	13.566158	-17.028966
C	0.135115	13.746929	-15.471335
H	0.552799	13.425382	-17.571847
C	9.906947	14.660625	-7.205589
H	9.650502	15.719340	-7.293474
H	8.988137	14.089752	-7.048948

H	10.586484	14.510294	-6.366945
C	17.766586	15.271723	-14.054768
H	17.682718	14.949916	-15.095874
H	17.512026	16.332857	-13.995232
H	18.783116	15.111575	-13.696388
C	29.609717	2.729951	-7.763870
C	30.392547	1.589459	-7.862340
C	31.671516	1.587188	-8.502917
C	32.217083	2.876888	-8.750018
C	32.409174	0.399945	-8.894320
C	33.812092	0.478910	-9.202828
C	34.407411	1.767395	-9.015603
C	33.642319	2.913140	-8.860788
C	28.462244	2.413949	-6.836194
N	28.640130	1.098137	-6.429942
C	29.795422	0.532541	-6.970363
C	35.854084	2.157520	-8.846271
N	35.860322	3.528426	-8.602149
C	34.574688	4.058706	-8.558493
O	34.342600	5.218499	-8.275684
O	36.865662	1.480090	-8.859289
O	27.545338	3.106751	-6.431171
O	30.195374	-0.580253	-6.687874
C	32.349685	-1.952699	-9.545049
C	33.721354	-1.888141	-9.830625
C	34.476098	-0.703209	-9.684408
C	31.714884	-0.823578	-9.089851
H	30.652940	-0.863626	-8.908851
C	30.968494	6.273616	-9.751068
C	29.651653	6.223236	-9.278601
C	29.120755	5.092743	-8.616394
C	29.979511	3.957639	-8.397475
C	31.338694	4.027204	-8.864765
C	31.787834	5.188482	-9.545670
H	32.790075	5.215160	-9.941436
H	31.791684	-2.869521	-9.704668
H	31.333089	7.141554	-10.290550
C	27.729629	5.272478	-8.329881
C	35.833163	-0.903529	-10.128648
C	36.073936	-2.168321	-10.562792
C	27.228043	6.489798	-8.717560
S	28.465099	7.487671	-9.481523
S	34.674942	-3.203978	-10.470183
H	27.121690	4.525583	-7.846284
H	36.592799	-0.139589	-10.093393
H	37.008338	-2.567229	-10.932730
C	25.875869	6.965862	-8.525195
C	24.948251	6.512246	-7.607324
S	25.185635	8.245494	-9.507692
C	23.706943	7.184073	-7.677077

H	25.175834	5.737832	-6.884374
C	23.659178	8.171122	-8.643950
H	22.875628	6.973144	-7.013851
C	22.574112	9.059110	-8.984474
C	22.597444	10.209990	-9.750212
S	20.943102	8.743531	-8.417132
C	21.340542	10.845805	-9.864294
H	23.507063	10.601493	-10.191513
C	20.325537	10.190675	-9.194079
H	21.181151	11.777626	-10.393891
C	27.780786	0.433848	-5.466337
H	27.757950	0.991954	-4.526910
H	26.761519	0.358605	-5.853579
H	28.190065	-0.562006	-5.297597
C	37.054124	4.299882	-8.305167
H	37.168597	5.114739	-9.024385
H	36.992459	4.726244	-7.300685
H	37.905359	3.622671	-8.370540
C	-9.633165	12.210334	-16.977541
C	-8.523450	12.943355	-16.583761
C	-7.184940	12.505501	-16.833309
C	-7.069537	11.442880	-17.771377
C	-5.994150	13.060046	-16.215104
C	-4.693976	12.807073	-16.777191
C	-4.687264	12.056718	-17.994913
C	-5.804650	11.362153	-18.433789
C	-10.848964	13.078401	-16.765466
N	-10.382952	14.285866	-16.262015
C	-8.992471	14.307880	-16.151057
C	-3.623518	11.929368	-19.056832
N	-4.181129	11.160679	-20.073782
C	-5.498828	10.803805	-19.799505
O	-6.201648	10.201775	-20.588322
O	-2.501254	12.399539	-19.117649
O	-12.028195	12.875205	-16.994816
O	-8.360179	15.289218	-15.811084
C	-4.997907	14.233031	-14.317536
C	-3.730591	14.011309	-14.869691
C	-3.536727	13.299272	-16.075446
C	-6.102748	13.758232	-14.984229
H	-7.074470	13.896477	-14.538579
C	-8.976168	8.346110	-18.704952
C	-10.270092	8.698654	-18.303402
C	-10.574484	9.950107	-17.720566
C	-9.512758	10.909305	-17.558634
C	-8.190189	10.547708	-17.996148
C	-7.960949	9.260169	-18.546692
H	-6.959256	8.973433	-18.822871
H	-5.109034	14.747922	-13.368955
H	-8.769085	7.361948	-19.112214

C	-11.946601	10.007115	-17.315160
C	-2.142135	13.132176	-16.353422
C	-1.310448	13.717504	-15.431899
C	-12.666347	8.875324	-17.605053
S	-11.666863	7.655353	-18.394032
S	-2.221620	14.505666	-14.144178
H	-12.387856	10.861837	-16.829372
H	-1.766799	12.599480	-17.211539
C	-14.074420	8.659074	-17.351358
C	-15.050683	9.617381	-17.165058
S	-14.765492	7.051678	-17.214944
C	-16.337222	9.077540	-16.930922
H	-14.843998	10.679111	-17.230731
C	-16.373329	7.697265	-16.939693
H	-17.224135	9.685272	-16.791554
C	-17.503192	6.812150	-16.753665
C	-17.623056	5.476746	-17.077070
S	-18.989764	7.391573	-16.018280
C	-18.892532	4.924082	-16.749327
H	-16.828265	4.915387	-17.555210
C	-19.738523	5.835057	-16.179028
H	-19.166742	3.892773	-16.938454
H	-20.755243	5.690505	-15.841831
C	-11.240750	15.425859	-15.992158
H	-11.789851	15.711364	-16.892945
H	-11.960187	15.183711	-15.205778
H	-10.599755	16.246624	-15.670948
C	-3.515361	10.856015	-21.327745
H	-3.434019	9.774473	-21.462660
H	-4.077689	11.271748	-22.167556
H	-2.521814	11.301704	-21.287127

P1 (planar structure)

C	17.822953	5.311167	2.045826
C	16.926808	5.607662	1.043269
C	17.299060	5.736388	-0.297929
C	18.654585	5.553405	-0.624307
C	16.287598	6.069156	-1.420146
C	16.769370	6.172797	-2.739242
C	18.133610	5.968558	-2.968297
C	19.027705	5.674767	-1.964804
C	16.966997	4.860782	3.229538
N	15.736468	5.463937	3.045827
C	15.667128	6.060030	1.803913
C	18.809804	5.541717	-4.265783
N	20.167115	5.590541	-4.006050
C	20.399735	5.804432	-2.663949
O	21.514978	6.115314	-2.278209
O	18.357375	5.119973	-5.311429

O	17.172254	4.066307	4.126282
O	14.770237	6.843578	1.541180
C	14.035722	6.540950	-2.149528
C	14.644211	6.579096	-3.408588
C	15.869886	6.480727	-3.753089
C	14.914871	6.269058	-1.138351
H	14.550216	6.197649	-0.139915
C	21.921269	4.756532	1.213383
C	21.432212	4.618237	2.514718
C	20.097209	4.826229	2.830753
C	19.189131	5.116771	1.816678
C	19.668607	5.229695	0.496333
C	21.044087	5.055751	0.211305
H	21.422103	5.183718	-0.776553
C	19.806404	4.685278	4.216046
C	16.185745	6.704217	-5.118959
C	15.087846	7.011875	-5.878991
C	20.897121	4.370435	4.959195
S	22.308299	4.172445	3.995898
S	13.669551	6.955005	-4.910368
H	18.855685	4.854108	4.676053
H	17.172094	6.722613	-5.533502
H	15.040830	7.235290	-6.935032
C	14.663078	5.484681	4.022120
H	13.741634	5.094518	3.582956
H	14.969115	4.852901	4.855472
H	14.481298	6.505491	4.368380
C	21.212974	5.455667	-5.002984
H	21.750792	6.399637	-5.125435
H	21.925242	4.683501	-4.702847
H	20.733759	5.171739	-5.939575
H	20.951538	4.215362	6.027935
C	12.606020	6.766948	-1.923425
C	11.971584	6.737675	-0.701387
S	11.509083	7.105801	-3.228624
C	10.569771	7.000645	-0.830774
H	12.480047	6.569104	0.238794
C	10.214938	7.214696	-2.144137
H	9.876102	7.036534	0.000124
C	8.868096	7.507879	-2.625544
C	8.513442	7.721836	-3.938997
S	7.568999	7.598584	-1.545910
C	7.103118	7.986359	-4.072870
H	9.211774	7.700635	-4.766672
C	6.476955	7.954747	-2.846698
H	6.611862	8.243124	-5.001234
C	34.706103	1.998865	5.918666
C	33.811508	2.295335	4.914748
C	34.185692	2.423842	3.574078
C	35.541680	2.240666	3.249710

C	33.175922	2.756564	2.450340
C	33.659644	2.860005	1.131963
C	35.024182	2.655565	0.904862
C	35.916797	2.361849	1.909778
C	33.847421	1.544459	7.098316
N	32.613672	2.142761	6.912252
C	32.547639	2.744933	5.674697
C	35.734603	2.275717	-0.393440
N	37.084986	2.363214	-0.111942
C	37.287306	2.573555	1.239248
O	38.366711	2.951517	1.657085
O	35.309419	1.864684	-1.455029
O	34.051644	0.749978	7.995176
O	31.654476	3.531910	5.411450
C	30.925166	3.228497	1.717599
C	31.535503	3.266416	0.459426
C	32.761670	3.167877	0.116735
C	31.802804	2.956641	2.730098
H	31.436519	2.885225	3.727858
C	38.805594	1.443703	5.092289
C	38.314619	1.305640	6.392923
C	36.979174	1.513804	6.706980
C	36.072613	1.804312	5.691534
C	36.554036	1.917019	4.371881
C	37.929913	1.742891	4.088893
H	38.314573	1.830083	3.097501
H	39.859757	1.298528	4.877927
C	36.686327	1.373059	8.091859
C	33.079557	3.391158	-1.248701
C	31.982800	3.698833	-2.010374
C	37.775920	1.058207	8.836655
S	39.226922	0.913639	7.848678
S	30.563172	3.643266	-1.043670
H	35.732345	1.521432	8.552384
H	34.065746	3.398795	-1.663499
H	31.937097	3.919904	-3.066982
C	31.541537	2.164343	7.890115
H	30.612964	1.802838	7.442069
H	31.835298	1.508406	8.709108
H	31.379961	3.180395	8.260081
C	38.149081	2.299885	-1.096587
H	38.629416	3.275933	-1.207874
H	38.903849	1.572018	-0.790329
H	37.700495	1.992784	-2.041076
H	37.839701	0.898962	9.903742
C	29.495160	3.454685	1.941579
C	28.858928	3.425615	3.162689
S	28.401489	3.800650	0.635506
C	27.457332	3.688710	3.031214
H	29.365465	3.254599	4.103442

C	27.104450	3.902636	1.717302
H	26.761056	3.717290	3.860201
C	25.758349	4.195857	1.233877
C	25.405641	4.409738	-0.080119
S	24.472159	4.371359	2.320990
C	24.005588	4.671182	-0.210949
H	26.100325	4.364550	-0.909828
C	23.367529	4.642886	1.009186
H	23.500367	4.851962	-1.150555
C	0.970325	8.858221	-1.798229
C	0.082687	9.153608	-2.808909
C	0.466158	9.279312	-4.147187
C	1.823970	9.093800	-4.462154
C	-0.535718	9.611101	-5.278373
C	-0.042973	9.711929	-6.593610
C	1.322584	9.505098	-6.811004
C	2.208760	9.212484	-5.799798
C	0.140370	8.388855	-0.616004
N	-1.130462	9.035503	-0.848014
C	-1.185581	9.653468	-2.143225
C	2.004158	9.072323	-8.098095
N	3.408197	9.148219	-7.763475
C	3.606629	9.364389	-6.366314
O	4.652526	9.648034	-5.748285
O	1.478311	8.653970	-9.138426
O	0.463354	7.578757	0.269767
O	-2.025405	10.451628	-2.607238
C	-2.780928	10.084077	-6.027092
C	-2.162151	10.119164	-7.281326
C	-0.933863	10.018386	-7.615373
C	-1.910483	9.813237	-5.008028
H	-2.330726	9.568054	-4.070600
C	5.074483	8.296779	-2.596076
C	4.574783	8.161681	-1.298503
C	3.237519	8.372021	-0.993940
C	2.338067	8.661574	-2.016008
C	2.828518	8.771417	-3.332427
C	4.206123	8.595225	-3.606204
H	4.556913	8.406693	-4.581491
C	2.935051	8.234148	0.389322
C	-0.606351	10.239074	-8.979180
C	-1.697877	10.546397	-9.748377
C	4.019441	7.919415	1.141667
S	5.447559	7.756586	0.195946
S	-3.124749	10.491606	-8.792371
H	2.008758	8.464163	0.863931
H	0.382108	10.289661	-9.383354
H	-1.735318	10.769246	-10.804940
C	-2.217258	9.052993	0.116679
H	-1.935779	8.398330	0.943077

H	-2.388087	10.065433	0.494719
H	-3.142669	8.685055	-0.334913
C	4.477848	9.014865	-8.737998
H	4.986454	9.970692	-8.896787
H	5.212087	8.276803	-8.404501
H	4.030565	8.680529	-9.675473
H	4.066568	7.776283	2.212373
C	-4.212214	10.312418	-5.813053
C	-4.856618	10.286234	-4.596191
S	-5.299257	10.646013	-7.128296
C	-6.257028	10.550622	-4.737597
H	-4.352875	10.130724	-3.651432
C	-6.600795	10.762557	-6.054230
H	-6.958319	10.591480	-3.913322
C	-7.943314	11.056329	-6.547232
C	-8.286957	11.268211	-7.863953
S	-9.293079	11.170548	-5.465662
C	-9.687585	11.531173	-8.005608
H	-7.580250	11.238417	-8.683881
C	-10.332089	11.505628	-6.788800
H	-10.190059	11.727363	-8.944726
H	-11.385851	11.670653	-6.608214

P2 (planar structure)

C	10.556770	9.195237	-11.741020
C	11.690391	8.933100	-11.004925
C	12.963275	8.836314	-11.574643
C	13.076535	9.015575	-12.964774
C	14.233748	8.542164	-10.742475
C	15.467415	8.468929	-11.417234
C	15.482897	8.666619	-12.801468
C	14.348204	8.926262	-13.535263
C	9.477630	9.523046	-10.698632
N	9.880066	8.901177	-9.537437
C	11.151896	8.371883	-9.682512
C	16.651957	9.043021	-13.713937
N	16.162971	8.945114	-15.002417
C	14.803070	8.700969	-14.988826
O	14.231412	8.286354	-15.980005
O	17.772676	9.449797	-13.472533
O	8.487291	10.230883	-10.729150
O	11.589909	7.541562	-8.909544
C	15.306745	8.109873	-8.624143
C	16.530113	8.066205	-9.301191
C	16.613351	8.195689	-10.679531
C	14.167595	8.347246	-9.341983
H	13.246207	8.413733	-8.808426
C	10.746509	9.734724	-15.920666
C	9.530454	9.843217	-15.241544

C	9.424996	9.638992	-13.873132
C	10.571795	9.383234	-13.127053
C	11.807470	9.300709	-13.799694
C	11.877112	9.469756	-15.203265
H	12.802087	9.411625	-15.731225
H	15.261789	7.975866	-7.548021
H	10.797392	9.877354	-16.995541
C	8.096026	9.746155	-13.377342
C	17.921596	8.005246	-11.196765
C	18.846510	7.727471	-10.224616
C	7.188675	10.031596	-14.344970
S	7.947148	10.187768	-15.935597
S	18.108645	7.726502	-8.612580
H	7.800608	9.608185	-12.360250
H	18.190980	8.004041	-12.230563
C	5.709664	10.204711	-14.094611
C	5.084200	10.099381	-12.872135
S	4.624997	10.562081	-15.393601
C	3.673687	10.321128	-12.982827
H	5.606278	9.898407	-11.945859
C	3.303762	10.582111	-14.283480
H	2.980813	10.293970	-12.151095
C	1.898471	10.860848	-14.760538
C	1.528707	11.121836	-16.061271
S	0.572029	10.860074	-13.651576
C	0.117996	11.342130	-16.172314
H	2.226491	11.162253	-16.888509
C	-0.507531	11.237430	-14.949852
H	-0.398746	11.595826	-17.088333
C	9.064723	8.791669	-8.341672
H	9.007124	9.752573	-7.822384
H	8.053532	8.477064	-8.607928
H	9.529455	8.046956	-7.696000
C	16.972205	8.988135	-16.206533
H	17.046178	7.995022	-16.658721
H	16.526383	9.670555	-16.933234
H	17.961806	9.344342	-15.921615
C	31.265386	5.472257	-7.007918
C	32.385618	5.217232	-6.249159
C	33.668183	5.112812	-6.795305
C	33.806039	5.276412	-8.185154
C	34.923502	4.826724	-5.937720
C	36.168730	4.744770	-6.589839
C	36.208771	4.926894	-7.975731
C	35.087427	5.179578	-8.732141
C	30.168285	5.811742	-5.988000
N	30.549823	5.201934	-4.813453
C	31.823401	4.669849	-4.930991
C	37.390846	5.324653	-8.857775
N	36.935703	5.213139	-10.158962

C	35.578221	4.960516	-10.177717
O	35.031431	4.547626	-11.183755
O	38.491188	5.762036	-8.584156
O	29.179218	6.519812	-6.043401
O	32.246822	3.846506	-4.142595
C	35.958623	4.416993	-3.796185
C	37.193634	4.364553	-4.451106
C	37.301212	4.478556	-5.829131
C	34.832535	4.647476	-4.536526
H	33.901904	4.720013	-4.019963
C	31.529137	5.964927	-11.189336
C	30.301476	6.082197	-10.532934
C	30.171766	5.893352	-9.164398
C	31.304991	5.644794	-8.395483
C	32.552180	5.553543	-9.045350
C	32.646653	5.706848	-10.449277
H	33.580374	5.636152	-10.960492
H	35.894307	4.295171	-2.719593
H	31.598890	6.094192	-12.264857
C	28.834424	6.007357	-8.693257
C	38.618111	4.281079	-6.321141
C	39.525493	4.013270	-5.329864
C	27.944543	6.282894	-9.679795
S	28.730973	6.420675	-11.258467
S	38.769500	4.022271	-3.741302
H	28.521019	5.881098	-7.680030
H	38.916899	4.282293	-7.348749
H	40.585277	3.822442	-5.420043
C	26.461572	6.460265	-9.457401
C	25.814616	6.369197	-8.245007
S	25.400299	6.803625	-10.779103
C	24.406529	6.591102	-8.382924
H	26.320166	6.178213	-7.307510
C	24.059808	6.837934	-9.692701
H	23.699146	6.574212	-7.563234
C	22.663441	7.112736	-10.197448
C	22.316886	7.359572	-11.507301
S	21.322647	7.122781	-9.113658
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H	23.027488	7.390447	-12.323840
C	20.261591	7.489583	-10.433185
H	20.411954	7.832878	-12.572879
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H	29.648744	6.071018	-3.121922
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H	30.165394	4.365745	-2.970478
C	37.772439	5.272712	-11.343330
H	37.855266	4.285968	-11.807476
H	37.345707	5.966575	-12.070930
H	38.755611	5.622868	-11.029789

C	-10.290471	12.877308	-15.913369
C	-9.124107	12.611297	-15.231829
C	-7.876749	12.532830	-15.858020
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C	-6.569268	12.234216	-15.087009
C	-5.365826	12.180727	-15.816025
C	-5.412117	12.401015	-17.196154
C	-6.579428	12.664482	-17.875387
C	-11.324625	13.181735	-14.819720
N	-10.868736	12.542510	-13.687929
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C	-4.287143	12.803076	-18.151807
N	-4.830759	12.722252	-19.419548
C	-6.186872	12.466539	-19.350994
O	-6.798117	12.063189	-20.322979
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O	-12.318118	13.885191	-14.795070
O	-9.124356	11.185426	-13.157088
C	-5.401982	11.775163	-13.024913
C	-4.209118	11.751203	-13.755276
C	-4.187024	11.903672	-15.133602
C	-6.572907	12.016083	-13.688384
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C	-11.472901	13.574830	-19.354616
C	-11.517149	13.347633	-17.986478
C	-10.337229	13.087929	-17.295436
C	-9.131631	13.025129	-18.022577
C	-9.124475	13.217472	-19.424858
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H	-5.398573	11.623190	-11.950269
H	-10.284109	13.646458	-21.161388
C	-12.823840	13.437277	-17.431520
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C	-1.933171	11.443991	-14.784283
C	-13.774416	13.731965	-18.353817
S	-13.087151	13.919365	-19.973076
S	-2.611118	11.411213	-13.139951
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C	-15.242148	13.890477	-18.036391
C	-15.812903	13.760840	-16.789724
S	-16.385287	14.261848	-19.279922
C	-17.228294	13.974334	-16.835137
H	-15.249316	13.548229	-15.890710
C	-17.656366	14.253801	-18.113928
H	-17.885121	13.928025	-15.975587
C	-19.082915	14.530282	-18.524592
C	-19.510828	14.809744	-19.803473
S	-20.366264	14.518666	-17.364261

C	-20.926423	15.021797	-19.849249
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C	-21.497248	14.892761	-18.602586
H	-21.489837	15.255399	-20.744184
H	-22.543527	15.001359	-18.350381
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H	-11.665254	13.359841	-11.919712
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H	-11.136096	11.653212	-11.849125
C	-4.074898	12.791755	-20.656577
H	-4.014082	11.807075	-21.128750
H	-4.556232	13.483211	-21.351416
H	-3.076218	13.150261	-20.408577

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