Electronic Supplementary Information

Novel poly(triphenylamine-*alt*-fluorene) with asymmetric hexaphenylbenzene and pyrene moieties: synthesis, fluorescence, flexible near-infrared electrochromic devices and theoretical investigation

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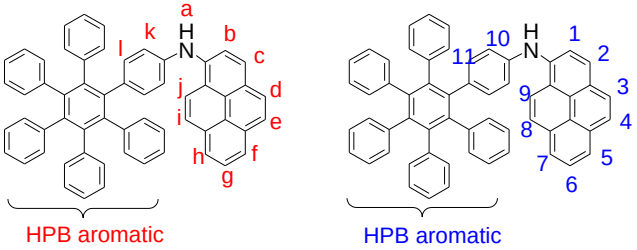
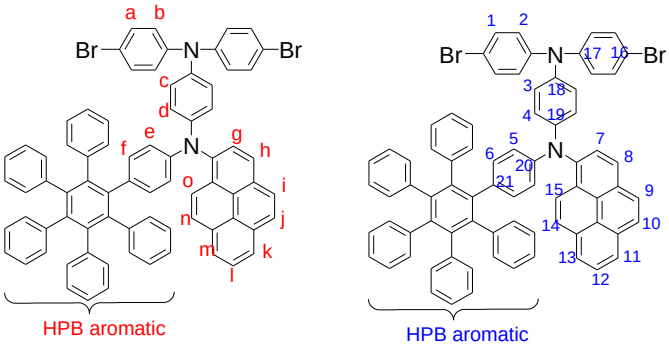
Characterization of HPBNHPY

IR (KBr): 3406 cm^{-1} (-NH stretch), 3028 cm^{-1} (Ar-H stretch), 1597 and 1516 cm^{-1} (C=C stretch in Ar), 1292 cm^{-1} (Ar-N stretch). ^{1}H NMR (600 MHz; CD_2Cl_2; Me_4Si), δ_H (ppm): 6.15 (s, broad, 1H, H_a), 6.66 (d, 2H, *J* = 8.4 Hz, H_k), 6.82 (d, 2H, *J* = 9 Hz, H_l), 6.88 - 6.96 (m, 15H, Ar-H of HPB), 6.98 - 7.03 (m, 10H. Ar-H of HPB), 7.59 (d, 1H, *J* = 7.8 Hz, H_b), 7.91 (d, 1H, *J* = 7.8 Hz, H_j), 7.91-7.98 (m, 4H, H_d, H_e, H_g, H_i), 8.01 (d, 1H, *J* = 8.4 Hz, H_c), 8.11 (m, 2H, H_h, H_f). ^{13}C NMR (150 MHz; CD_2Cl_2; Me_4Si), δ_C (ppm): 117.29 (C_{10}), 117.79 (C_1), 121.68 (C_3), 122.27 (C_4), 124.71 (C_7), 125.10 (C_5), 125.59 (C_9), 125.68, 125.77, 126.12 (C_2), 126.44, 126.68, 127.10 (C_6), 127.16, 127.21, 127.96 (C_8), 131.99, 132.10, 132.40, 132.96 (C_{11}), 134.50 (C_{13}), 138.22, 140.74, 140.79, 140.86, 141.17, 141.40, 141.43, 141.60, 141.94 (C_{12}). MS (ESI-TOF): m/z $[M]^+$ $C_{58}H_{39}N$: calcd.: 749.3083, found: 749.3077. T_m: >300 °C (by DSC at a heating rate of 10 °C /min).



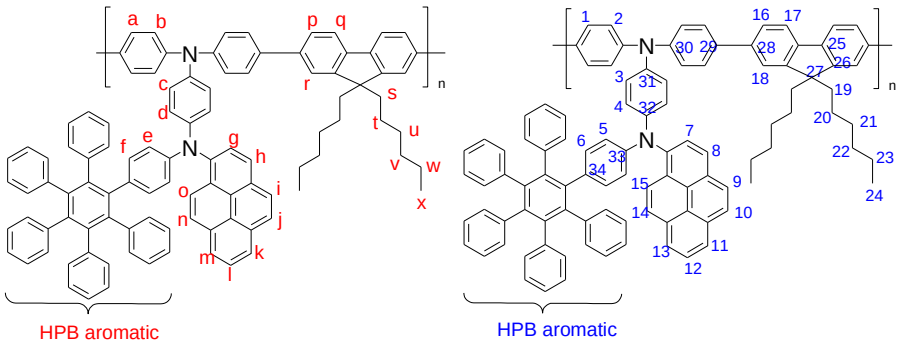
Characterization of DIBRHPBPY

IR (KBr): 3028 cm^{-1} (Ar-H stretch), 1600 and 1500 cm^{-1} (C=C stretch in Ar), 1261 cm^{-1} (Ar-N stretch), 1068 cm^{-1} (Ar-Br). ^{1}H NMR (600 MHz; CD_2Cl_2; Me_4Si), δ_H (ppm): 6.59 (d, 2H, J = 8.4 Hz H_e), 6.69 (d, 2H, J = 9.0 Hz, H_f), 6.76 (m, 2H, J = 1.8 Hz, H_d), 6.84-6.95 (m, 31H, H_b, H_c, Ar-H of HPB), 7.34 (d, 4H, J = 7.2 Hz, H_a), 7.63 (d, 1H, J = 8.4 Hz, H_g), 7.87-7.89 (m, 2H, H_n, H_o), 8.00-8.04 (m, 3H, H_i, H_j, H_l), 8.12 (d, 1H, J = 8.4 Hz, H_h), 8.16-8.18 (m, 2H, H_m, H_k). ^{13}C NMR (150 MHz; CD_2Cl_2; Me_4Si), δ (ppm): 114.78, 115.19 (C_{16}), 121.36 (C_5), 122.85, 123.53 (C_4), 123.55 (C_3), 123.93 (C_{15}), 125.23 (C_2), 125.51 (C_{13}), 125.73, 125.78, 125.86 (C_{11}), 125.96, 126.36 (C_8), 126.85 (C_{12}), 126.96, 127.08, 127.11, 127.17, 127.21, 127.43 (C_9), 127.74 (C_7), 127.83 (C_{10}), 128.07 (C_{14}), 129.85, 131.58, 131.79, 131.86, 131.98, 132.07, 132.09, 132.57 (C_6), 132.71, 132.78 (C_1),133.08, 135.53 (C_{21}), 137.05, 140.23 (C_{18}), 140.76, 140.81, 140.84, 140.93, 140.98, 141.05, 141.29, 141.36, 141.43, 145.12, 146.03 (C_{19}), 146.32 (C_{20}), 147.28 (C_{17}). MS (ESI-TOF): m/z $[M]^+$ $C_{76}H_{50}Br_2N_2$: calcd: 1148.2341, found: 1148.2335. T_g: 183 °C, T_m: >300 °C (by DSC at a heating rate of 10 °C /min).



Characterization of HPBPYFL6

IR (KBr): 3028 cm^{-1} (Ar-H stretch), 2954, 2927 and 2854 cm^{-1} (C-H stretch), 1597 and 1500 cm^{-1} (C=C stretch in Ar), 1261 cm^{-1} (Ar-N stretch). ^{1}H NMR (600 MHz; CD_2Cl_2; Me_4Si), δ_H (ppm): 0.77-0.79 (m, 10H, H_x, H_t), 1.07-1.16 (m, 12H, H_u, H_v, H_w), 2.08 (s, broad, 4H, H_s), 6.63 (d, 2H, J = 7.8 Hz, H_e), 6.72 (d, 2H, J = 8.4 Hz, H_f), 6.8-6.97 (m, 27H, H_d, Ar-H of HPB), 7.03 (d, 2H, J = 7.2 Hz, H_c), 7.23 (d, 4H, J = 7.2 Hz, H_b), 7.62-7.66 (m, 8H, H_a, H_p, H_r), 7.71 (d, 1H, J = 6.0 Hz, H_g), 7.78 (d, 2H, J = 7.8 Hz, H_q), 7.91-7.95 (m, 2H, H_n, H_o), 8.00 - 8.07 (m, 3H, H_i, H_j, H_l), 8.16-8.21 (m, 3H, H_h, H_k, H_m). ^{13}C NMR (150 MHz; CD_2Cl_2; Me_4Si), δ_C (ppm): 14.36 (C_{24}), 23.17 (C_{23}), 24.48 (C_{20}), 30.30 (C_{22}), 32.11 (C_{21}), 41.03 (C_{19}), 55.86 (C_{27}), 120.48 (C_{17}), 121.17 (C_5), 121.56 (C_{18}), 123.81 (C_4), 124.07 (C_2+C_{15}), 125.32 (C_{13}), 125.49 (C_{11}), 125.75, 125.78, 125.99 (C_{16}), 126.39 (C_8), 126.78 (C_3), 126.82 (C_{12}), 127.09, 127.11, 127.19, 127.38 (C_9), 127.59 (C_7), 127.67 (C_{10}), 127.78, 128.04 (C_{14}), 128.29 (C_1), 129.35, 129.80, 131.63, 131.90, 131.99, 132.11, 132.78 (C_6), 135.24 (C_{34}), 135.90 (C_{29}), 139.99 (C_{28}), 140.34 (C_{25}), 140.76, 140.80, 140.91, 141.09, 141.39, 141.45, 141.70, 141.90 (C_{31}), 141.45, 145.49 (C_{32}), 146.55 (C_{33}), 147.59 (C_{30}), 152.33 (C_{26}). T_g: 260 °C (by DSC at a heating rate of 10 °C/min).



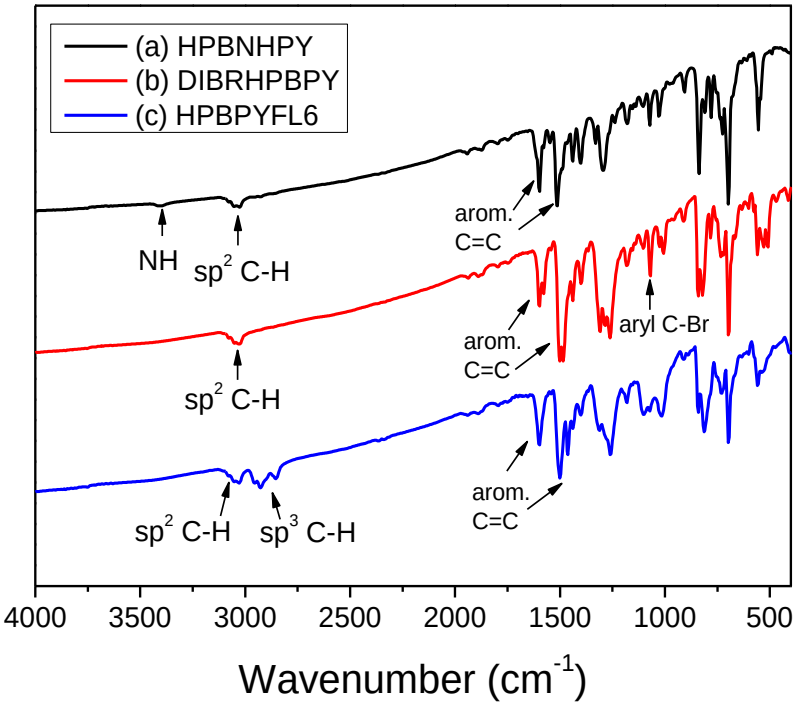
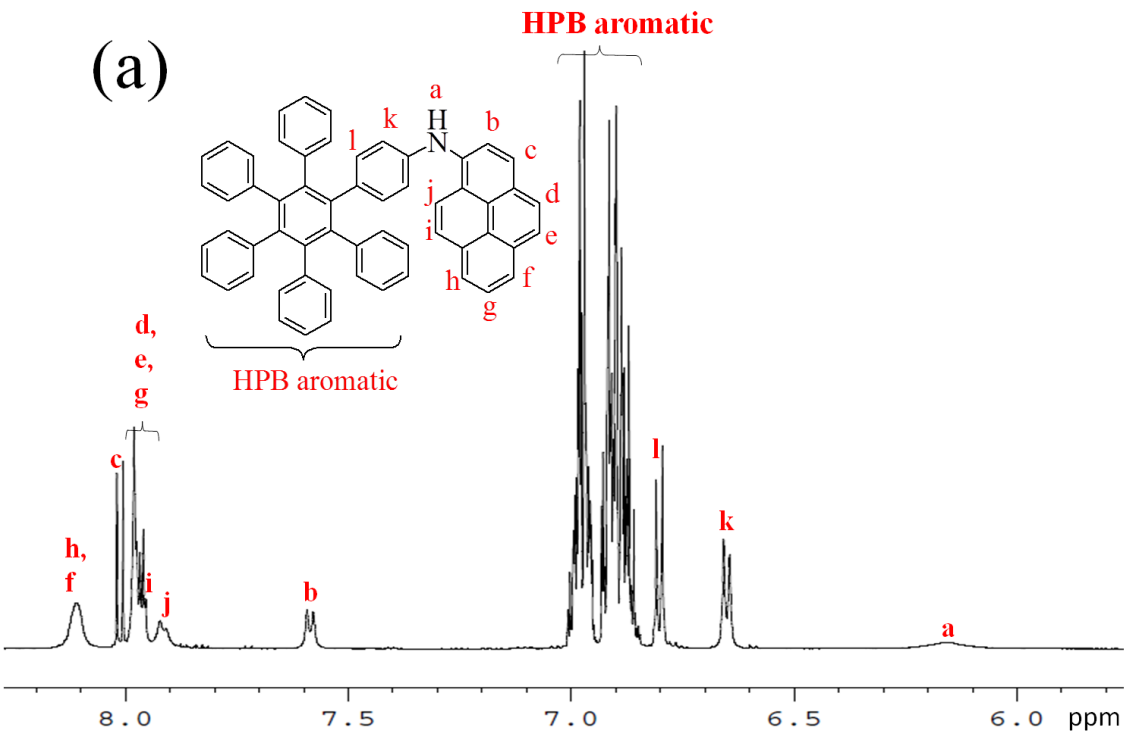
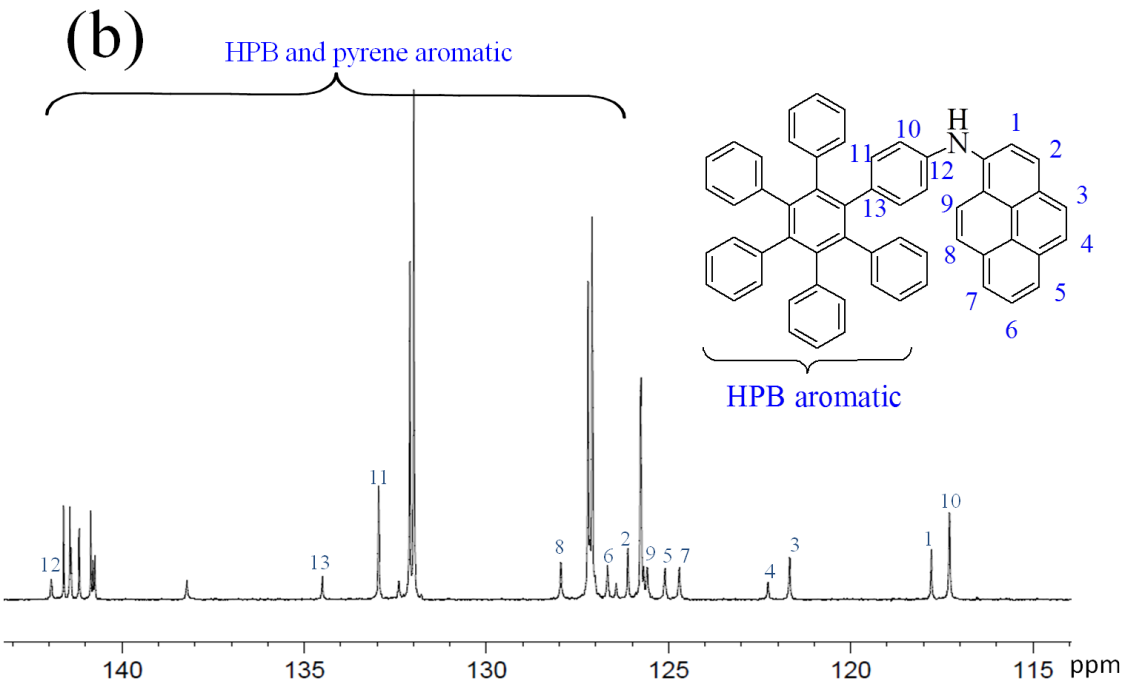


Fig. S1 FT-IR spectra of (a) **HPBNHPY**, (b) dibromo monomer **DIBRHPBPY** and (c) conjugated polymer **HPBPYFL6**.


(a)
HPB aromatic
a
k
H
N
b
l
c
j
d
i
e
h
f
g
HPB aromatic
d,
e,
g
c
h,
f
i
j
b
l
k
a
8.0
7.5
7.0
6.5
6.0
ppm


(b)
HPB and pyrene aromatic
10
H
N
1
11
2
12
3
9
13
4
8
5
7
6
HPB aromatic
12
13
11
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6
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4
3
1
10
140
135
130
125
120
115
ppm

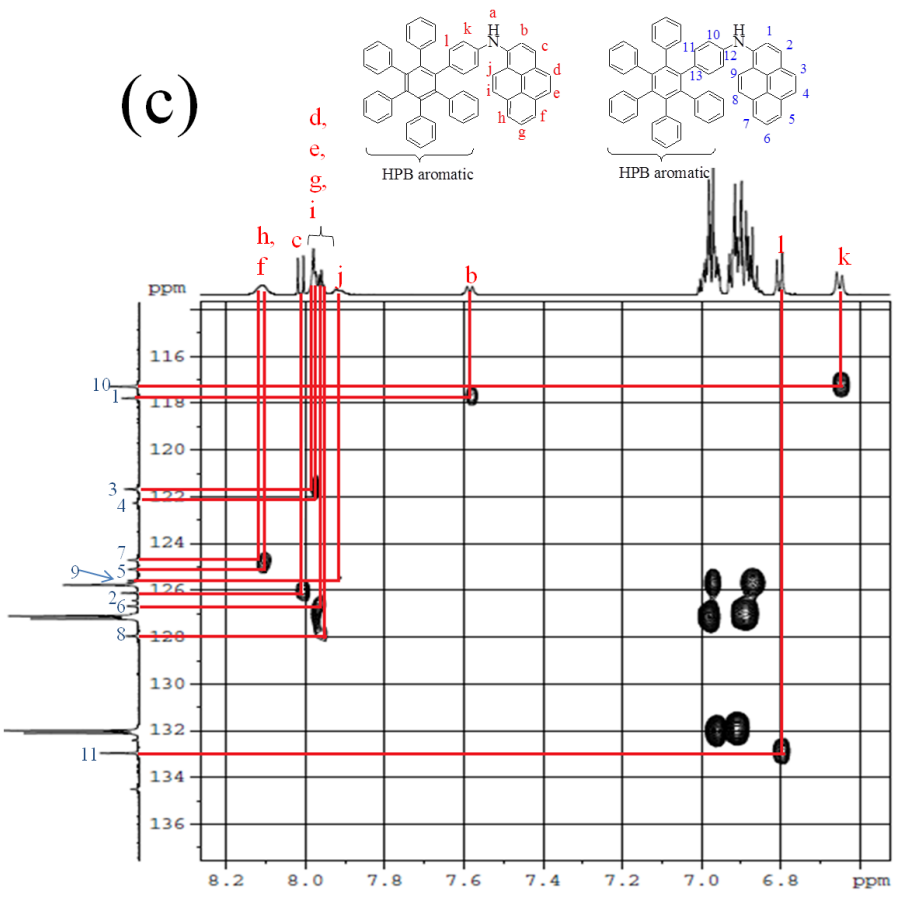
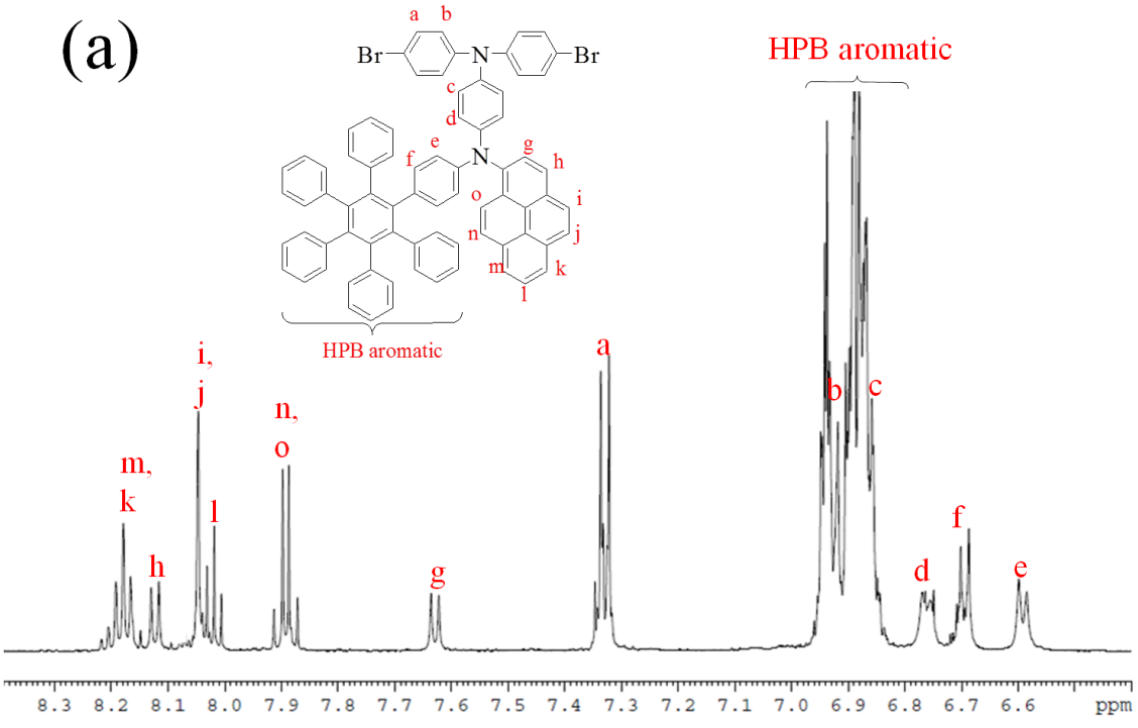


Fig. S2 (a) ^{1}H NMR spectra**,** (b) ^{13}C NMR spectra and (c) HSQC spectra of **HPBNHPY** in CD_2Cl_2.



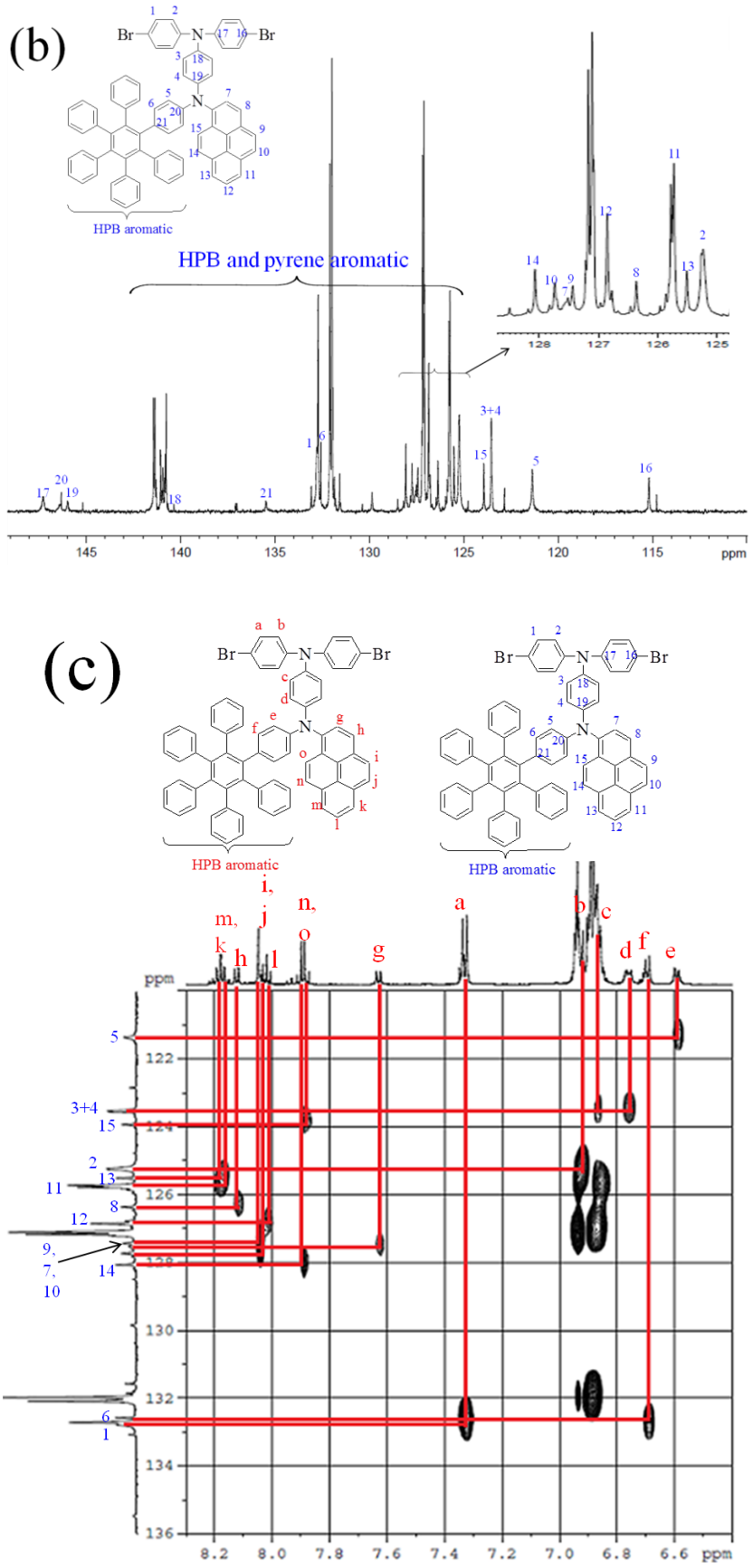
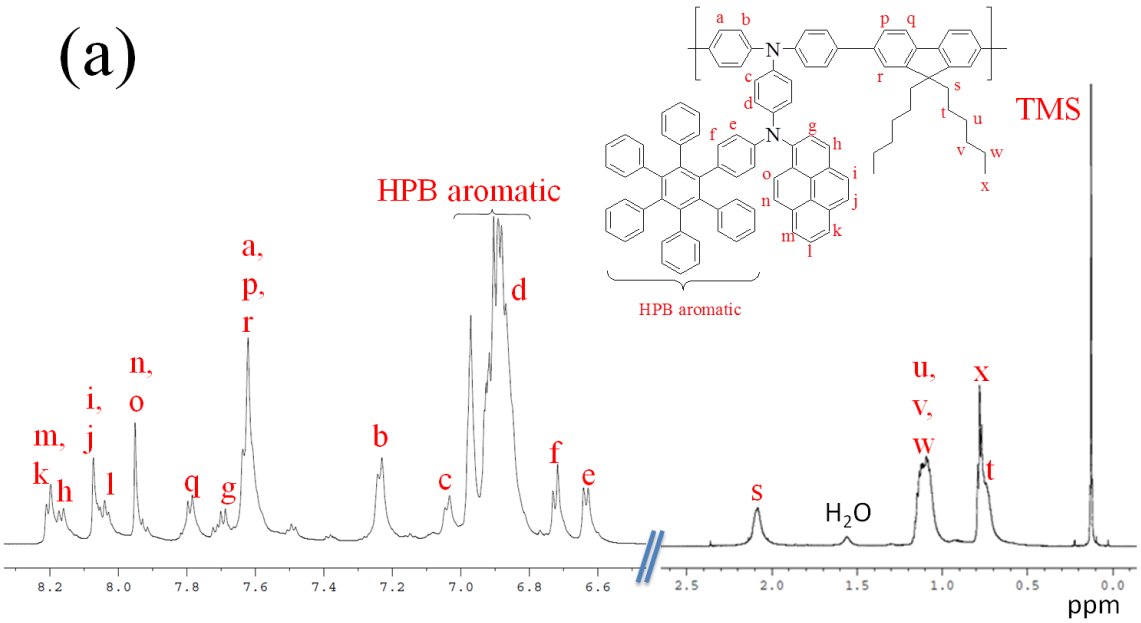
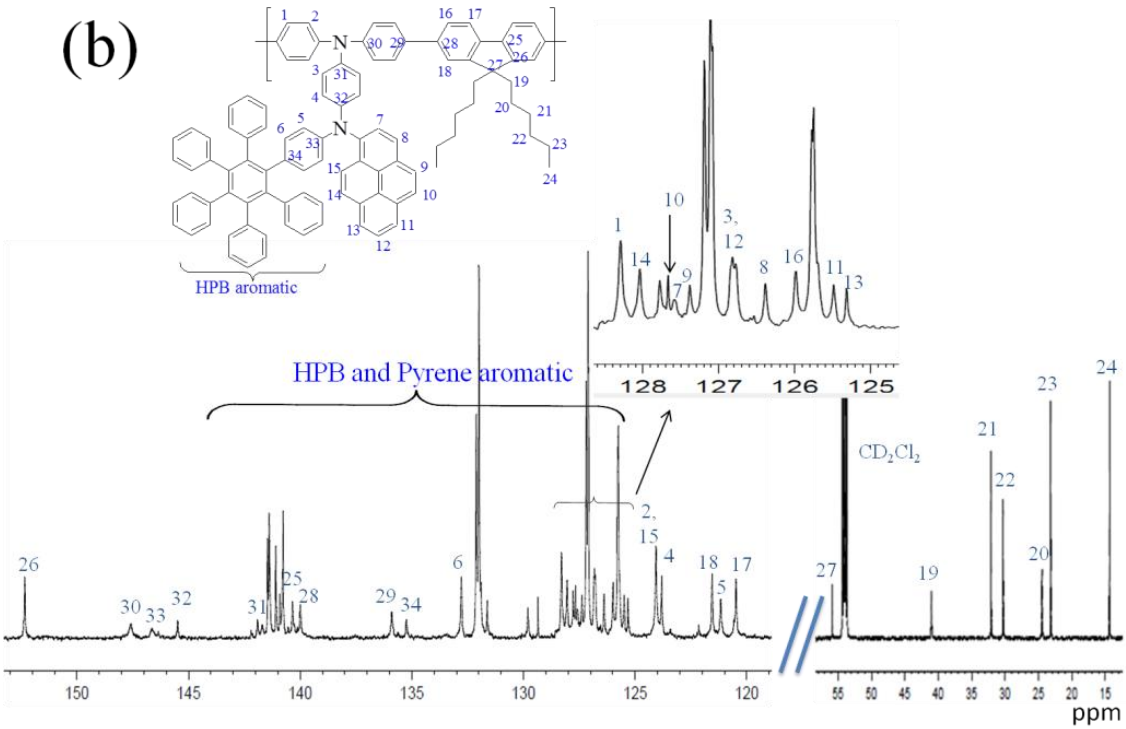


Fig. S3 (a) ^{1}H NMR spectra**,** (b) ^{13}C NMR spectra and (c) HSQC spectra of dibromo compound **DIBRHPBPY** in CD_2Cl_2.


(a)
HPB aromatic
TMS
H_2O
ppm


(b)
HPB aromatic
HPB and Pyrene aromatic
CD_2Cl_2
ppm

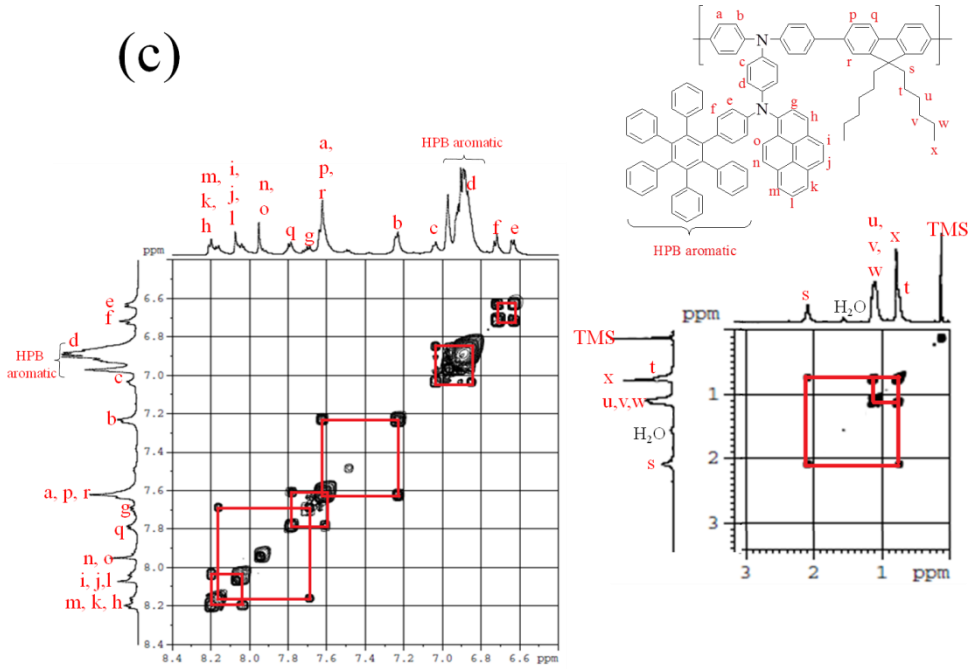


Fig. S4 (a) ^{1}H NMR spectra**,** (b) ^{13}C NMR spectra and (c) COSY spectra of conjugated polymer **HPBPYFL6** in CD_2Cl_2.

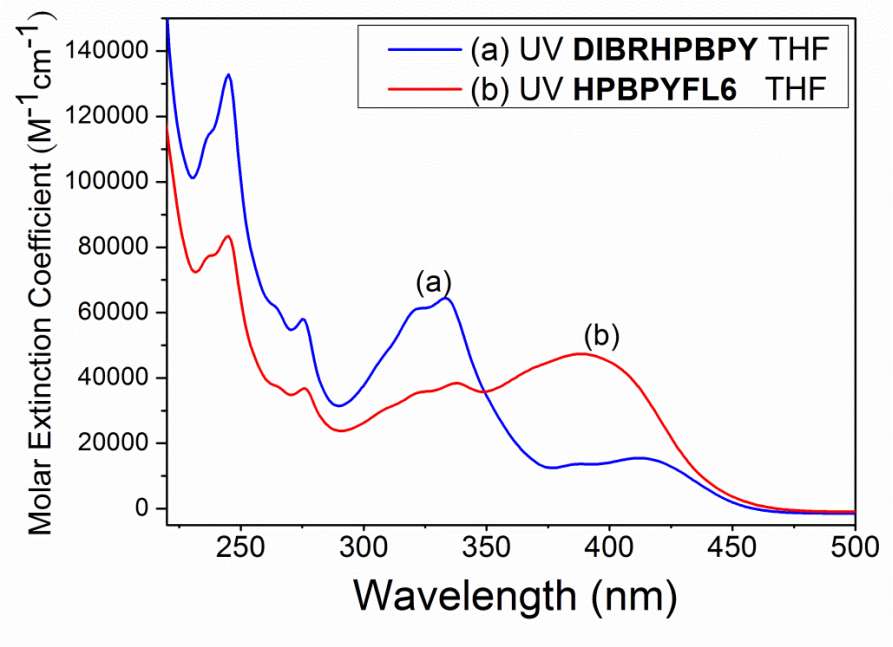


Fig. S5 Absorption spectra of (a) **DIBRHPBPY** and (b) **HPBPYFL6** in a THF solution (10^{-5} M).

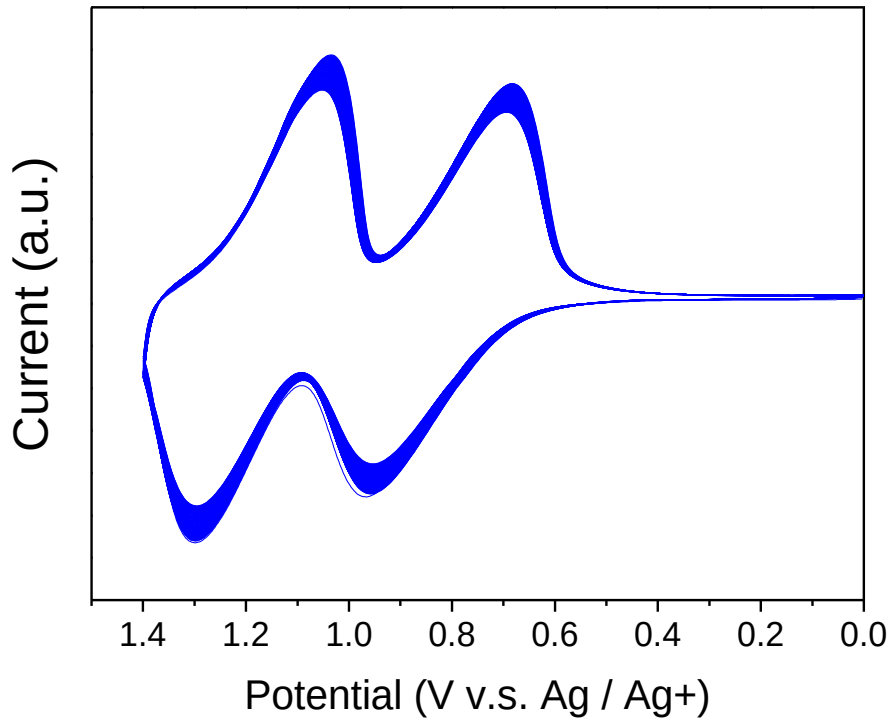


Fig. S6 Cyclic voltammograms of **HPBPYFL6** in CH_3CN containing 0.1 M TBAP with 100 cycles. The sweep rate is 100 mV/s

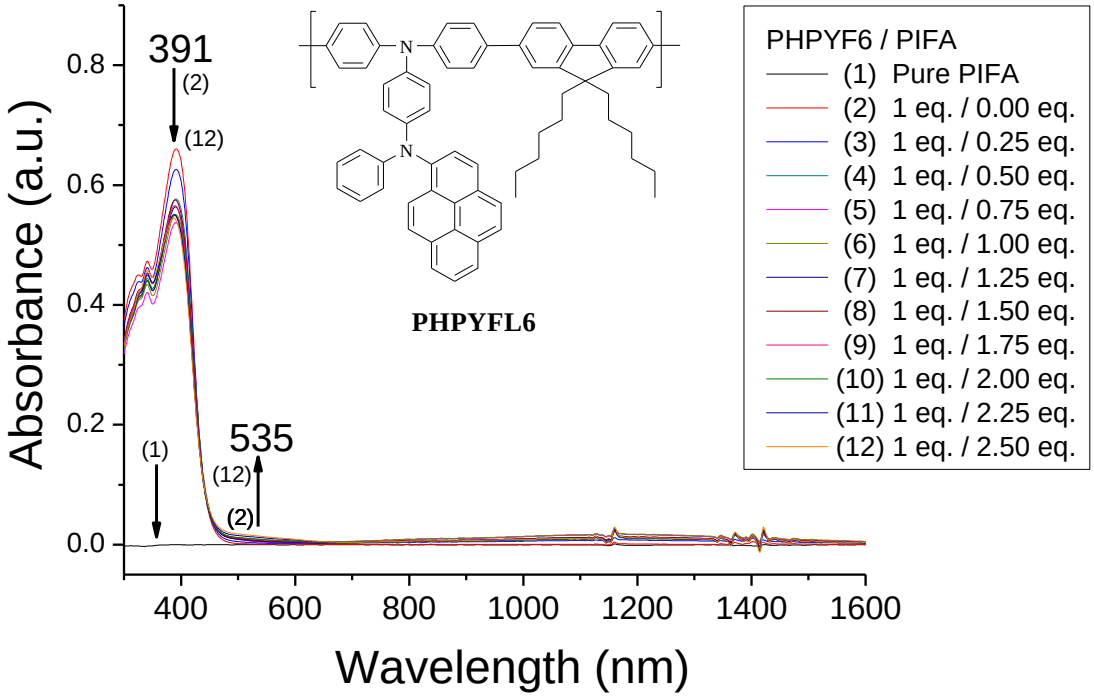


Fig. S7 UV/Vis/NIR spectra of **PHPYFL6** oxidized with various PIFA contents in CH_2Cl_2 recorded at room temperature.

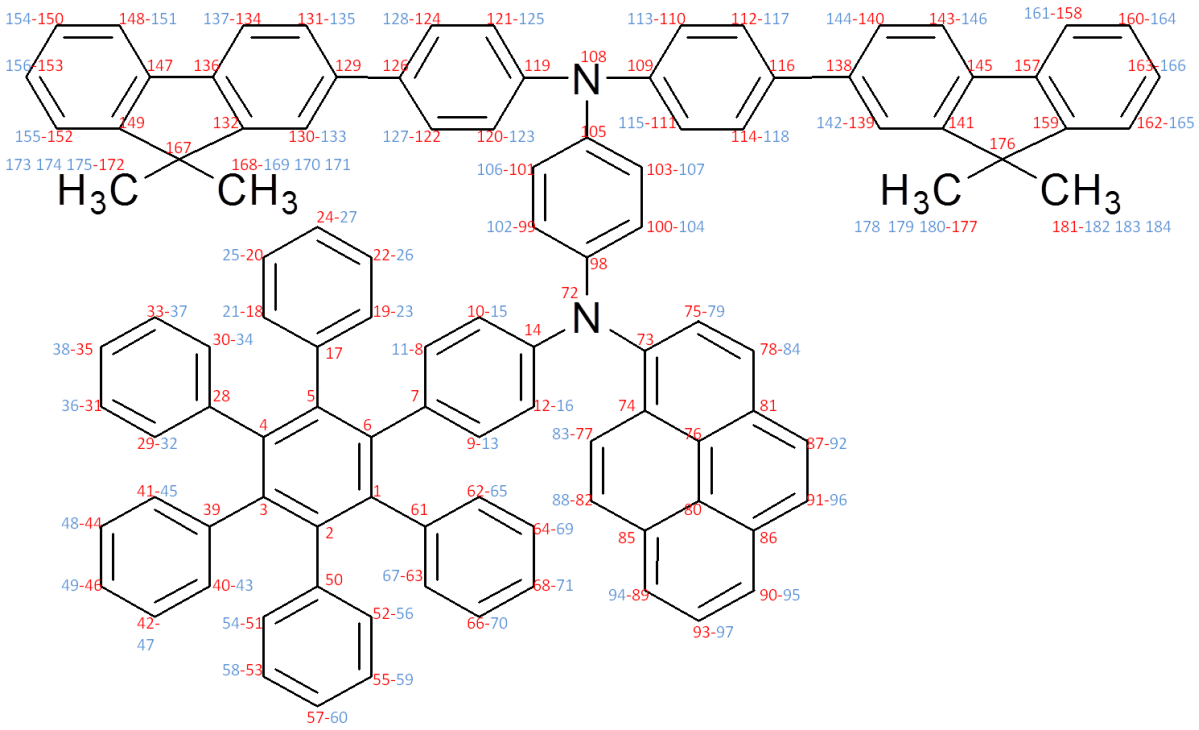


Fig. S8 Optimized structure of model compound **HPBPYFL** with labels. The carbon and nitrogen atoms are presented by red, and hydrogen atoms are presented by blue.

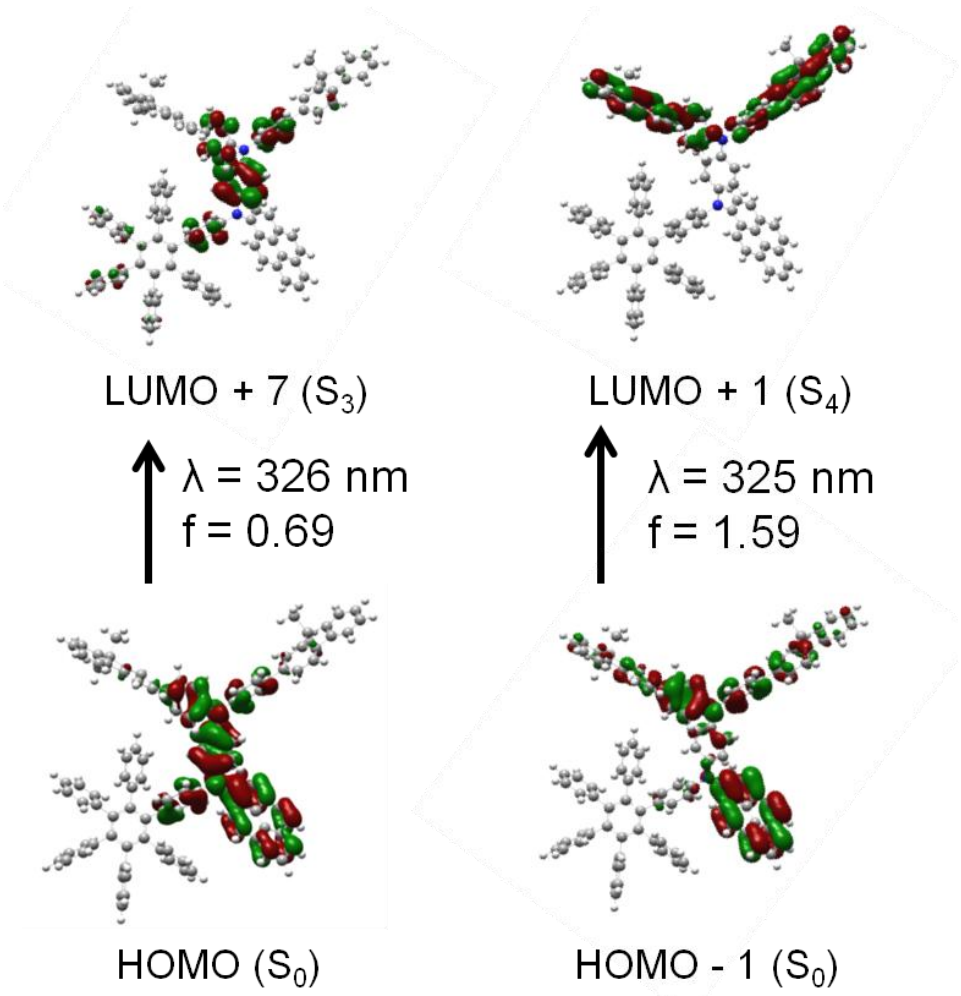


Fig. S9 Electronic distribution for the transitions of **HPBPYFL** in the natural state.

Table S1 Optical properties of the conjugated polymer, **HPBPYFL6**, in different solvents.

Solvent	ε^a	λ_{max}^{abs} (nm)^b	λ_{max}^{PL} (nm)^c	Φ_F (%)^d
Toluene	2.4	388	515	67.4
$CHCl_3$	4.8	388	530	65.7
THF	7.6	388	545	39.2
CH_2Cl_2	8.9	389	567	16.8
NMP	32.2	391	577	11.4

[a] Dielectric constants of the solvents. [b] Concentration of the polymer solutions = 1×10^{-5} M. [c] Excitation wavelength = absorption max of different solutions. [d] Fluorescence quantum yields (Φ_F) were measured in integrating sphere using 9,10-diphenylanthracene in cyclohexane (1×10^{-5} M) as a reference standard (Φ_F = 0.9).

Table S2 Atomic charge distribution of **HPBPYFL** atoms in natural state, first oxidation state, second oxidation state and charge difference of ΔQ1 and ΔQ2.

	(0,1)	(1,2)	(2,1)	Q1 (%)	Q2 (%)
C^1	-0.01311	-0.00701	-0.00509	0.61	0.19
C^2	-0.01314	-0.00484	0.00170	0.83	0.65
C^3	-0.01349	-0.00395	0.01483	0.95	1.88
C^4	-0.01363	-0.00670	-0.00362	0.69	0.31
C^5	-0.01399	-0.01284	-0.01937	0.12	-0.65
C^6	-0.01158	-0.01775	-0.05846	-0.62	-4.07
C^7	-0.08481	-0.05393	0.02951	3.09	8.34
C^8	-0.18695	-0.19342	-0.20183	-0.65	-0.84
C^9	-0.18451	-0.18901	-0.19551	-0.45	-0.65
C^{10}	-0.27374	-0.25141	-0.24059	2.23	1.08
H^{11}	0.24297	0.24690	0.26920	0.39	2.23
C^{12}	-0.27002	-0.23403	-0.20494	3.60	2.91
H^{13}	0.24338	0.25092	0.27309	0.75	2.22
C^{14}	0.20123	0.16954	0.10176	-3.17	-6.78
H^{15}	0.25117	0.24002	0.25451	-1.12	1.45
H^{16}	0.25337	0.24968	0.27085	-0.37	2.12
C^{17}	-0.05488	-0.05946	-0.05175	-0.46	0.77
C^{18}	-0.20949	-0.20514	-0.21684	0.44	-1.17
C^{19}	-0.20956	-0.20076	-0.20617	0.88	-0.54
C^{20}	-0.23786	-0.24456	-0.25305	-0.67	-0.85
H^{21}	0.24141	0.24066	0.24706	-0.08	0.64
C^{22}	-0.23367	-0.23319	-0.23362	0.05	-0.04
H^{23}	0.24165	0.24421	0.25326	0.26	0.91

C^{24}	-0.24217	-0.23913	-0.25952	0.30	-2.04
H^{25}	0.23818	0.23266	0.24188	-0.55	0.92
H^{26}	0.24018	0.23678	0.24684	-0.34	1.01
H^{27}	0.23802	0.23026	0.23744	-0.78	0.72
C^{28}	-0.05635	-0.06708	-0.07076	-1.07	-0.37
C^{29}	-0.20982	-0.20574	-0.21323	0.41	-0.75
C^{30}	-0.20958	-0.20426	-0.21161	0.53	-0.74
C^{31}	-0.23432	-0.23255	-0.23180	0.18	0.08
H^{32}	0.24081	0.23703	0.23863	-0.38	0.16
C^{33}	-0.23405	-0.23169	-0.23035	0.24	0.13
H^{34}	0.24106	0.24021	0.24284	-0.09	0.26
C^{35}	-0.23960	-0.23098	-0.23185	0.86	-0.09
H^{36}	0.23840	0.23563	0.24429	-0.28	0.87
H^{37}	0.23869	0.23726	0.24629	-0.14	0.90
H^{38}	0.23799	0.23594	0.24650	-0.21	1.06
C^{39}	-0.05625	-0.06784	-0.07357	-1.16	-0.57
C^{40}	-0.20948	-0.20418	-0.20991	0.53	-0.57
C^{41}	-0.20956	-0.20385	-0.20992	0.57	-0.61
C^{42}	-0.23424	-0.23171	-0.23028	0.25	0.14
H^{43}	0.24089	0.23788	0.23961	-0.30	0.17
C^{44}	-0.23424	-0.23163	-0.23025	0.26	0.14
H^{45}	0.24086	0.23847	0.24001	-0.24	0.15
C^{46}	-0.23961	-0.22988	-0.22932	0.97	0.06
H^{47}	0.23845	0.23664	0.24568	-0.18	0.90
H^{48}	0.23847	0.23687	0.24581	-0.16	0.89
H^{49}	0.23794	0.23631	0.24720	-0.16	1.09
C^{50}	-0.05607	-0.06780	-0.07240	-1.17	-0.46
C^{51}	-0.20942	-0.20367	-0.21033	0.58	-0.67
C^{52}	-0.20966	-0.20440	-0.21151	0.53	-0.71
C^{53}	-0.23410	-0.23147	-0.22991	0.26	0.16
H^{54}	0.24095	0.23906	0.24150	-0.19	0.24
C^{55}	-0.23428	-0.23189	-0.23098	0.24	0.09
H^{56}	0.24069	0.23719	0.23817	-0.35	0.10
C^{57}	-0.23963	-0.22983	-0.22991	0.98	-0.01
H^{58}	0.23851	0.23716	0.24644	-0.14	0.93
H^{59}	0.23834	0.23633	0.24492	-0.20	0.86
H^{60}	0.23792	0.23634	0.24724	-0.16	1.09

C^{61}	-0.05609	-0.06831	-0.06989	-1.22	-0.16
C^{62}	-0.21061	-0.20788	-0.21998	0.27	-1.21
C^{63}	-0.20986	-0.20491	-0.21269	0.50	-0.78
C^{64}	-0.23527	-0.23192	-0.23500	0.34	-0.31
H^{65}	0.23978	0.23514	0.23828	-0.46	0.31
C^{66}	-0.23201	-0.23146	-0.22864	0.06	0.28
H^{67}	0.24081	0.24128	0.24776	0.05	0.65
C^{68}	-0.23712	-0.22993	-0.23332	0.72	-0.34
H^{69}	0.23601	0.23582	0.24015	-0.02	0.43
H^{70}	0.23959	0.23793	0.24860	-0.17	1.07
H^{71}	0.23845	0.23716	0.24613	-0.13	0.90
N^{72}	-0.56546	-0.54626	-0.32082	1.92	22.54
C^{73}	0.19247	0.19890	0.09073	0.64	-10.82
C^{74}	-0.05735	-0.06265	-0.00877	-0.53	5.39
C^{75}	-0.23407	-0.23740	-0.22472	-0.33	1.27
C^{76}	-0.01244	-0.01222	-0.02541	0.02	-1.32
C^{77}	-0.19963	-0.19798	-0.26217	0.17	-6.42
C^{78}	-0.21111	-0.19080	-0.23101	2.03	-4.02
C^{79}	0.25372	0.24362	0.25606	-1.01	1.24
C^{80}	-0.01904	-0.01474	-0.00938	0.43	0.54
C^{81}	-0.05955	-0.06308	0.00836	-0.35	7.14
C^{82}	-0.20567	-0.18946	-0.12946	1.62	6.00
H^{83}	0.25839	0.24005	0.24560	-1.83	0.56
H^{84}	0.24099	0.23867	0.26382	-0.23	2.52
C^{85}	-0.05282	-0.06489	-0.08219	-1.21	-1.73
C^{86}	-0.05507	-0.06465	-0.07714	-0.96	-1.25
C^{87}	-0.20604	-0.19736	-0.24524	0.87	-4.79
H^{88}	0.23895	0.23590	0.25627	-0.31	2.04
C^{89}	-0.21488	-0.19129	-0.16878	2.36	2.25
C^{90}	-0.21553	-0.18992	-0.16261	2.56	2.73
C^{91}	-0.20507	-0.18960	-0.13905	1.55	5.06
H^{92}	0.23993	0.23648	0.25763	-0.35	2.12
C^{93}	-0.23277	-0.23041	-0.23204	0.24	-0.16
H^{94}	0.23862	0.23424	0.25434	-0.44	2.01
H^{95}	0.23883	0.23601	0.25812	-0.28	2.21
H^{96}	0.23994	0.23867	0.26046	-0.13	2.18
H^{97}	0.24245	0.24215	0.26430	-0.03	2.22

C^{98}	0.18259	0.24128	0.36095	5.87	11.97
C^{99}	-0.25981	-0.25879	-0.21564	0.10	4.32
C^{100}	-0.24989	-0.25500	-0.21271	-0.51	4.23
C^{101}	-0.23564	-0.21265	-0.23711	2.30	-2.45
H^{102}	0.26116	0.27991	0.31208	1.88	3.22
C^{103}	-0.23545	-0.21317	-0.23464	2.23	-2.15
H^{104}	0.25655	0.27392	0.30245	1.74	2.85
C^{105}	0.15624	0.12613	0.38122	-3.01	25.51
H^{106}	0.25433	0.26601	0.30054	1.17	3.45
H^{107}	0.25520	0.26645	0.30065	1.13	3.42
N^{108}	-0.55554	-0.21735	-0.33395	33.82	-11.66
C^{109}	0.19506	0.14560	0.08595	-4.95	-5.97
C^{110}	-0.26259	-0.22178	-0.20486	4.08	1.69
C^{111}	-0.26010	-0.22323	-0.23096	3.69	-0.77
C^{112}	-0.20627	-0.19722	-0.21491	0.91	-1.77
H^{113}	0.25441	0.26362	0.27038	0.92	0.68
C^{114}	-0.20664	-0.19825	-0.22418	0.84	-2.59
H^{115}	0.25364	0.26330	0.25703	0.97	-0.63
C^{116}	-0.07813	-0.02330	0.02594	5.48	4.92
H^{117}	0.24570	0.25745	0.27304	1.18	1.56
H^{118}	0.24467	0.25648	0.26916	1.18	1.27
C^{119}	0.19531	0.14607	0.08706	-4.92	-5.90
C^{120}	-0.25954	-0.22271	-0.22916	3.68	-0.65
C^{121}	-0.26261	-0.22180	-0.20449	4.08	1.73
C^{122}	-0.20624	-0.19815	-0.22516	0.81	-2.70
H^{123}	0.25397	0.26386	0.25734	0.99	-0.65
C^{124}	-0.20736	-0.19779	-0.21645	0.96	-1.87
$H^{12}5$	0.25413	0.26343	0.27038	0.93	0.70
C^{126}	-0.07833	-0.02371	0.02647	5.46	5.02
H^{127}	0.24515	0.25674	0.26902	1.16	1.23
H^{128}	0.24490	0.25694	0.27219	1.20	1.53
C^{129}	-0.04479	-0.06414	-0.10190	-1.94	-3.78
C^{130}	-0.21587	-0.20236	-0.20301	1.35	-0.07
C^{131}	-0.22732	-0.21008	-0.21200	1.72	-0.19
C^{132}	0.00450	0.01213	0.00652	0.76	-0.56
H^{133}	0.24170	0.23206	0.23972	-0.96	0.77
C^{134}	-0.20580	-0.19258	-0.20983	1.32	-1.73

H^{135}	0.24372	0.23327	0.24241	-1.05	0.91
C^{136}	-0.05371	-0.03902	-0.01218	1.47	2.68
H^{137}	0.23967	0.24189	0.25232	0.22	1.04
C^{138}	-0.04478	-0.06402	-0.10232	-1.92	-3.83
C^{139}	-0.21583	-0.20232	-0.20239	1.35	-0.01
C^{140}	-0.22696	-0.20980	-0.21169	1.72	-0.19
H^{141}	0.00434	0.01198	-0.00319	0.76	-1.52
H^{142}	0.24169	0.23182	0.24154	-0.99	0.97
C^{143}	-0.20566	-0.19239	-0.21033	1.33	-1.79
C^{144}	0.24397	0.23364	0.24184	-1.03	0.82
C^{145}	-0.05376	-0.03901	-0.01270	1.48	2.63
H^{146}	0.23974	0.24205	0.25231	0.23	1.03
C^{147}	-0.04965	-0.05865	-0.07255	-0.90	-1.39
C^{148}	-0.21298	-0.19759	-0.19988	1.54	-0.23
C^{149}	-0.00245	0.00188	0.00304	0.43	0.12
C^{150}	-0.24128	-0.23200	-0.23866	0.93	-0.67
H^{151}	0.23873	0.23436	0.24235	-0.44	0.80
C^{152}	-0.22915	-0.22220	-0.23069	0.70	-0.85
C^{153}	-0.23521	-0.21985	-0.21430	1.54	0.56
H^{154}	0.24008	0.24070	0.25044	0.06	0.97
H^{155}	0.23831	0.23709	0.24497	-0.12	0.79
H^{156}	0.23966	0.23989	0.25041	0.02	1.05
C^{157}	-0.04946	-0.05854	-0.07278	-0.91	-1.42
C^{158}	-0.21294	-0.19750	-0.20091	1.54	-0.34
C^{159}	-0.00251	0.00178	-0.00578	0.43	-0.76
C^{160}	-0.24128	-0.23197	-0.23779	0.93	-0.58
H^{161}	0.23881	0.23453	0.24234	-0.43	0.78
C^{162}	-0.22922	-0.22229	-0.22960	0.69	-0.73
C^{163}	-0.23536	-0.21993	-0.21533	1.54	0.46
H^{164}	0.24004	0.24072	0.25043	0.07	0.97
H^{165}	0.23817	0.23693	0.24631	-0.12	0.94
H^{166}	0.23956	0.23981	0.25061	0.03	1.08
C^{167}	-0.08635	-0.09653	-0.08808	-1.02	0.85
C^{168}	-0.63015	-0.63256	-0.63115	-0.24	0.14
H^{169}	0.22378	0.23069	0.23491	0.69	0.42
H^{170}	0.24036	0.24041	0.24117	0.01	0.08
H^{171}	0.22417	0.22027	0.21882	-0.39	-0.15

C^{172}	-0.63019	-0.63249	-0.63154	-0.23	0.10
H^{173}	0.22337	0.21907	0.21847	-0.43	-0.06
H^{174}	0.24027	0.24045	0.24335	0.02	0.29
H^{175}	0.22399	0.23097	0.23516	0.70	0.42
C^{176}	-0.08629	-0.09646	-0.27421	-1.02	-17.78
C^{177}	-0.63016	-0.63242	0.27570	-0.23	90.81
H^{178}	0.22324	0.21873	-0.64173	-0.45	-86.05
H^{179}	0.24014	0.24028	0.21945	0.01	-2.08
H^{180}	0.22383	0.23081	0.23984	0.70	0.90
C^{181}	-0.6302	-0.63256	0.23734	-0.24	86.99
H^{182}	0.24063	0.24074	0.228008	0.01	-1.27
H^{183}	0.22427	0.22019	0.194625	-0.41	-2.56
H^{184}	0.22354	0.23052	0.219705	0.70	-1.08