Supplementary Information

Modulating Carrier Transfer Ability—Linker Effect on Thieno[3,4-c]pyrrole-4,6-dione Based Conjugated Polymers.

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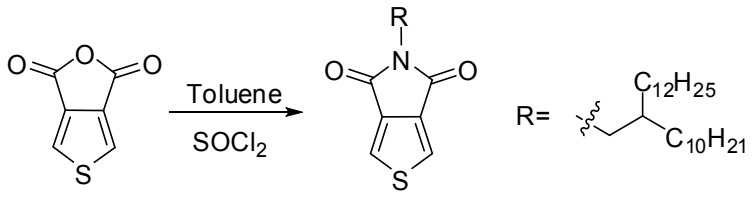
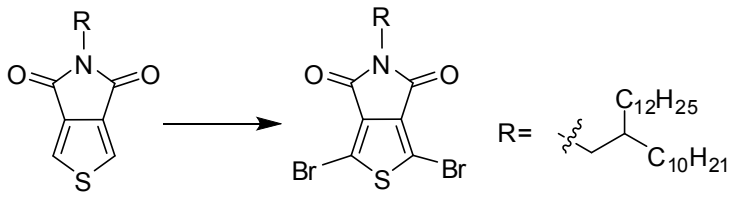
Contents

1. ***Synthesis of compounds 3,4,6 and 7***



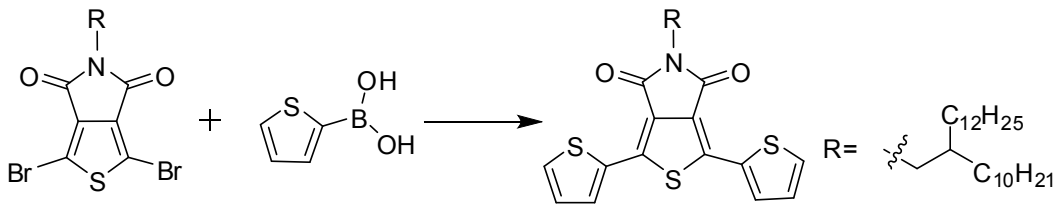
1 **3**

Synthesis of compound 3[1]: To the solution of compound **2** (16.4 g, 0.0465 mol) in toluene (40 mL),compound **1** (4.77 g, 0.031 mol) was added, and then the mixture was refluxed over 24h. After removal of the toluene, prepared $SOCl_2$ (35 mL) was added, the solution then was warmed 85℃ and refluxed 24h. The reaction mixture was extracted with ethyl acetate three times, and dried over anhydrous Na_2SO_4. After the solvent had been removed, the residue was passed through a silica gel column using CH_2Cl_2/hexane (1:3) as an eluent. Then solvent was removed under reduced pressure, Recrystallization of the crude product from hexane provided a pale yellow solid. Yield: 4.2g (27.7%). ^{1}H NMR (400MHz, $CDCl_3$, ppm): δ = 7.80 (s, 2H), 3.51 (d, *J* = 7.2 Hz, 2H), 1.85 (m, 1H), 1.24 (m, 40H), 0.89-0.87 (t, *J* = 7.0 Hz, 6H). 13C NMR (400 MHz, $CDCl_3$, ppm): δ 162.91, 136.69, 125.33, 77.21, 77.00, 76.79, 42.79, 36.90, 31.91, 31.50, 29.96, 29.67, 29.62,29.59, 29.35, 29.32, 26.28, 22.67, 14.08. Elemental analysis: Calcd. For [$C_{30}H_{51}NO_2S$]: C 73.57, H 10.50, N 2.86, S 6.55. Found: C 73.55, H 10.48, N 2.83, S 6.52; MS (MALDI-TOF): 489.36 (M^+).



3 **4**

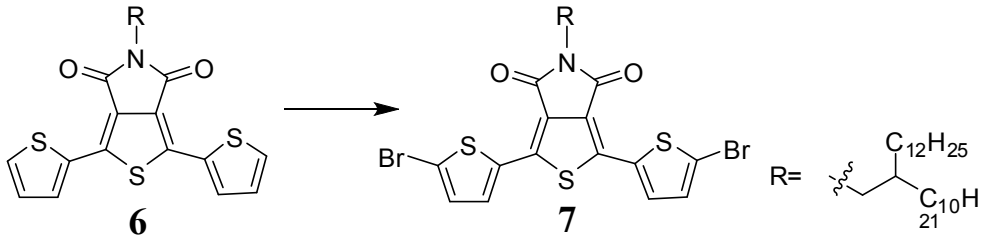
Synthesis of compound 4[1]**:** Concentrated sulfuric acid (12 mL) and trifluoro acetic acid (40 mL) were added to a flask of compound **3** (4.2 g, 8.48 mmol), then N-bromobutanimide (NBS 4.23 g, 0.024 mol) was added in three portions, the reaction mixture was stired at 55℃ and kept in the dark for 12h. The reaction mixture was cooled to room temperature, poured into 200mL ice water, adjusted pH using $NaHCO_3$, extracted with CH_2Cl_2 in several times, washed with brine, combined the organic phase, dried over anhydrous Na_2SO_4, then removed the solvent under vacuum pressure, the crude product was purified through column chromatography using CH_2Cl_2/hexane (1:3) as an eluent, After removal solvent, afforded the product as yellow solid. Yield: 5.0g (90.1%).^{1}H NMR (400MHz, $CDCl_3$, ppm): δ=3.48 (d, *J* = 7.2 Hz, 2H), 1.81 (m, 1H), 1.36-1.20 (m, 40H), 0.89-0.87(t, *J* = 7.0 Hz, 6H). 13C NMR (400 MHz, $CDCl_3$, ppm): δ 160.62, 134.78, 112.86, 77.21, 77.00, 76.79, 43.14, 31.92, 31.51, 29.90, 29.68, 29.65, 29.62, 29.59, 29.35, 26.31, 22.68, 14.09. Elemental analysis: Calcd. For [$C_{30}H_{49}Br_2NO_2S$]: C 55.64, H 7.63, N 2.16, S 4.95. Found: C 55.62, H 7.62, N 2.14, S 4.93; MS (MALDI-TOF): 647.18 (M^+).



4 **5** **6**

Compound **6** and **7** were synthesized via reported method with only N-alkyl chain differences.[2] The H-NMR, MS and elementary analysis were carried out and the products were used in next reactions without further purifications.

Synthesis of compound 6: compound **4** (1.5 g, 2.32 mmol) and compound **5** (0.652 g, 5.1 mmol) were dissolved in a mixture of THF (40 mL) and H_2O (3 mL), $NaHCO_3$ (5.85 g, 0.0696 mol) was used as base and tetrakis(triphenylphosphine)palladium (0.134 g, 5% mol) was used as catalyst, the reaction mixture was refluxed at 70℃ and kept in the dark overnight. The reaction mixture was diluted with H_2O, then extracted with CH_2Cl_2 two times, combined the organic phase, dried over anhydrous Na_2SO_4, filtered the product solution, then removed the solvent under reduced pressure, the crude product was purified by column chromatography using CH_2Cl_2/hexane (1:2) as an eluent afford 1.024 g of the product as a sodium orange solid. (Yield = 80%).^{1}H NMR (400MHz, $CDCl_3$, ppm): δ = 8.026 (d, *J* = 3.9 Hz, 2H), 7.428 (d, *J* = 3.8 Hz, 2H), 7.125-7.108 (t, *J* = 4.2 Hz, 2H), 3.552(d, *J* = 7.2 Hz, 2H), 1.889 (m, 1H), 1.364-1.232 (m, 40H), 0.887-0.853 (m, 6H). Elemental analysis: Calcd. For [$C_{38}H_{55}NO_2S_3$]: C 69.78, H 8.48, N 2.14, S 14.71. Found: C 69.72, H 8.46, N 2.12, S 14.74; MS (MALDI-TOF): 653.34 (M^+).



Synthesis of compound 7: compound **6** (0.90 g, 1.38 mmol) was dissolved in a mixture of AcOH(25 mL) and $CHCl_3$ (25 mL), the mixture solution was cooled to 0℃and kept in the dark, then N-bromobutanimide(440 mg, 2.47 mmol) was added in several times, the solution was stired about 3h, cooling bath was removed, the crude product then was poured into ice water and adjusted PH to neutral with $NaHCO_3$, extracted with CH_2Cl_2, washed organic phase with brine then combined the organic phase, dried over anhydrous Na_2SO_4, the solvent was removed under reduced pressure, the crude product was purified by a silica gel column using CH_2Cl_2/hexane(1:3) as an eluent, thus afforded the product as orange solid. Yield: 1.045 g, (93.2%).^{1}H NMR (400MHz, $CDCl_3$, ppm): δ = 7.601 (d, *J* = 4.0 Hz 2H), 7.006 (d, *J* = 3.9 Hz, 2H), 3.475 (d, *J* = 7.2 Hz, 2H), 1.838 (m, 1H), 1.350-1.230 (m, 40H), 0.880-0.853 (m, 6H). Elemental analysis: Calcd. For [$C_{38}H_{53}Br_2NO_2S_3$]: C 56.22, H 6.58, N 1.73, S 11.85. Found: C 56.18, H 6.56, N 1.71, S 11.81; MS (MALDI-TOF): 811.16 (M^+).

2. *TGA analysis of Q1,Q2 and Q3*

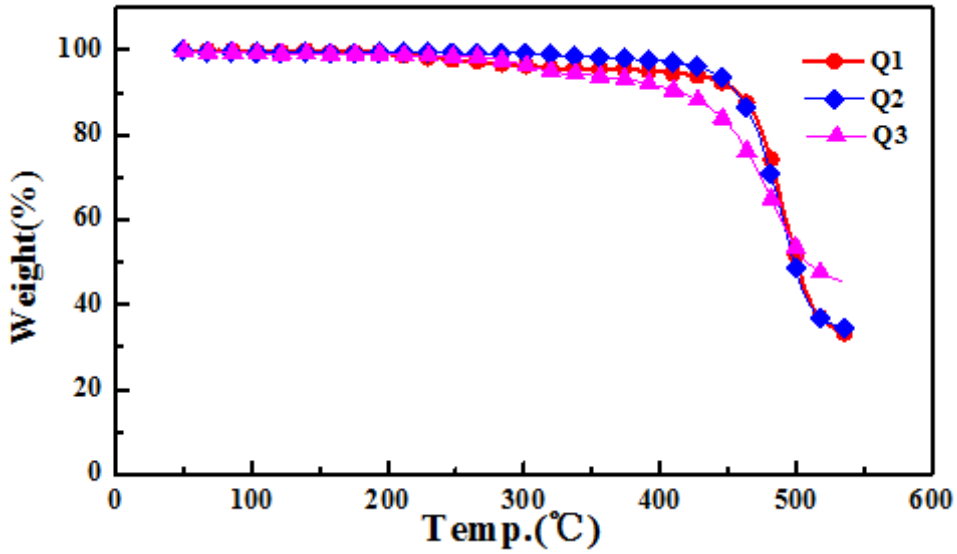


Figure S1. TGA analysis of polymer **Q1**,**Q2** and **Q3**.

3. *Theoretical calculations for Q1,Q2and Q3*

Geometries optimization and frequency analysis were performed at the level of B3LYP /6-31G* by using Gaussian09 (revision A.02)[3]. The coordinates and energies at the optimized geometries for 4 repeated units of **Q1, Q2** and **Q3** are listed below and there were no any imaginary frequencies. Then the molecular orbitals were analyzed, the energy gaps between HOMO and LUMO were obtained.

Q1:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.524609	-2.010011	0.000211
2	6	0	-5.103592	-1.956089	-0.000994
3	6	0	-6.936421	-3.430089	0.004103
4	7	0	-5.732097	-4.158588	0.005097
5	6	0	-4.588689	-3.342708	0.002121
6	6	0	-4.566256	-0.686547	-0.004566
7	16	0	-5.907517	0.475802	-0.006296
8	6	0	-7.156896	-0.784491	-0.002303
9	8	0	-3.445698	-3.766581	0.002294
10	8	0	-8.048190	-3.930306	0.006124
11	6	0	-5.669647	-5.608751	0.008720

12	6	0	-8.542537	-0.400375	-0.002183
13	6	0	-3.213271	-0.199351	-0.006798
14	6	0	-9.044540	0.894149	-0.004797
15	6	0	-10.448512	0.962447	-0.003855
16	6	0	-11.057245	-0.283029	-0.000505
17	16	0	-9.861786	-1.563720	0.001482
18	16	0	-1.811364	-1.261235	-0.003686
19	6	0	-0.714603	0.105266	-0.008966
20	6	0	-1.414542	1.301828	-0.012558
21	6	0	-2.809546	1.129061	-0.011328
22	6	0	5.106206	1.961295	-0.001384
23	6	0	6.527352	2.011875	-0.000309
24	6	0	4.591999	3.347822	0.001780
25	7	0	5.739820	4.162295	0.004488
26	6	0	6.939855	3.432078	0.003511
27	6	0	7.156472	0.785166	-0.002930
28	16	0	5.904376	-0.472473	-0.006777
29	6	0	4.565618	0.692713	-0.004955
30	8	0	8.049029	3.938047	0.005536
31	8	0	3.446823	3.765721	0.002170
32	6	0	5.696082	5.613178	0.008394
33	6	0	3.212058	0.207106	-0.007168
34	6	0	8.541627	0.399341	-0.002947
35	6	0	2.807807	-1.121242	-0.012049
36	6	0	1.412865	-1.293761	-0.013140
37	6	0	0.713185	-0.097026	-0.009089
38	16	0	1.810208	1.269163	-0.003556
39	16	0	9.861114	1.562363	0.001052
40	6	0	11.056163	0.281161	-0.001271
41	6	0	10.446992	-0.964073	-0.004981
42	6	0	9.042953	-0.895339	-0.005917
43	6	0	16.994917	-1.144277	-0.001815
44	6	0	18.417325	-1.092232	0.000305
45	6	0	16.580810	-2.563466	-0.008669
46	7	0	17.783446	-3.293897	-0.010423
47	6	0	18.929441	-2.480553	-0.005216
48	6	0	18.955867	0.174782	0.006462
49	16	0	17.617728	1.338672	0.009659
50	6	0	16.365498	0.081634	0.002580
51	8	0	20.070541	-2.907750	-0.005498
52	8	0	15.467834	-3.061467	-0.012155
53	6	0	17.843452	-4.744120	-0.017238
54	6	0	14.979629	0.468603	0.002372
55	6	0	20.313564	0.663366	0.010465

56	6	0	14.479488	1.763493	0.006225
57	6	0	13.075185	1.833498	0.005306
58	6	0	12.465235	0.588952	0.000739
59	16	0	13.659548	-0.693082	-0.002671
60	16	0	21.718175	-0.396602	0.007336
61	6	0	22.788832	0.959123	0.015026
62	6	0	22.121701	2.157066	0.019760
63	6	0	20.715794	1.989138	0.017177
64	6	0	-18.418625	1.088677	0.000175
65	6	0	-16.996240	1.140985	-0.001645
66	6	0	-18.930990	2.476911	-0.005290
67	7	0	-17.785130	3.290470	-0.010130
68	6	0	-16.582385	2.560267	-0.008251
69	6	0	-16.366596	-0.084799	0.002755
70	16	0	-17.618558	-1.342077	0.009445
71	6	0	-18.956927	-0.178451	0.006093
72	8	0	-15.469476	3.058420	-0.011539
73	8	0	-20.072157	2.903902	-0.005835
74	6	0	-17.845412	4.740690	-0.016732
75	6	0	-20.314525	-0.667289	0.009744
76	6	0	-14.980624	-0.471462	0.002777
77	6	0	-20.716511	-1.993140	0.016256
78	6	0	-22.122383	-2.161323	0.018502
79	6	0	-22.789727	-0.963495	0.013711
80	16	0	-21.719329	0.392421	0.006377
81	16	0	-13.660839	0.690519	-0.002225
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95	1	0	3.507678	-1.949270	-0.015083
96	1	0	0.929877	-2.264170	-0.017365
97	1	0	11.000667	-1.895959	-0.006884
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103	1	0	12.522397	2.765949	0.007956
104	1	0	23.857538	0.792720	0.015639
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106	1	0	20.015929	2.817382	0.020198
107	1	0	-16.819986	5.110585	-0.014714
108	1	0	-18.368850	5.096911	-0.907950
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110	1	0	-20.016498	-2.821258	0.019373
111	1	0	-22.615703	-3.125963	0.023468
112	1	0	-23.858464	-0.797288	0.014086
113	1	0	-12.522884	-2.768236	0.008829
114	1	0	-15.117332	-2.643478	0.010189

Nuclear repulsive energy:13840.6134360380 Hartrees

Q2:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-20.091832	0.867291	0.000799
2	6	0	-21.515243	0.851195	0.000996
3	6	0	-19.645705	2.277461	0.001232
4	7	0	-20.828299	3.036120	0.001677
5	6	0	-21.995920	2.250311	0.001562
6	6	0	-22.086697	-0.401697	0.000657
7	16	0	-20.779202	-1.599325	0.000082
8	6	0	-19.494241	-0.374825	0.000317
9	8	0	-23.130047	2.696199	0.001841
10	8	0	-18.525625	2.758647	0.001197
11	6	0	-20.836824	4.487471	0.002283
12	6	0	-18.119758	-0.798023	0.000017
13	6	0	-23.456209	-0.856325	0.000702
14	6	0	-17.654518	-2.106614	-0.000402
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16	6	0	-15.607449	-0.981291	-0.000330
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25	6	0	20.091838	-0.867272	0.000880
26	6	0	21.995939	-2.250273	0.001892
27	7	0	20.828326	-3.036093	0.002102
28	6	0	19.645726	-2.277447	0.001504
29	6	0	19.494233	0.374837	0.000238
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31	6	0	22.086689	0.401737	0.000584
32	8	0	18.525649	-2.758641	0.001518
33	8	0	23.130069	-2.696152	0.002264
34	6	0	20.836871	-4.487444	0.002942
35	6	0	23.456197	0.856378	0.000586
36	6	0	18.119747	0.798024	-0.000119
37	6	0	23.890167	2.172239	0.000147
38	6	0	25.299599	2.306848	0.000269
39	6	0	25.938143	1.093432	0.000799
40	16	0	24.835558	-0.236495	0.001135
41	16	0	16.769168	-0.330880	0.000115
42	6	0	15.607438	0.981276	-0.000505
43	6	0	16.252960	2.209916	-0.000848
44	6	0	17.654499	2.106613	-0.000629
45	6	0	7.626087	1.219840	-0.000696
46	6	0	6.204057	1.200371	-0.000745
47	6	0	8.072085	2.630040	-0.000608
48	7	0	6.885469	3.387013	-0.000591
49	6	0	5.722524	2.599230	-0.000666
50	6	0	5.635581	-0.056358	-0.000796
51	16	0	6.948747	-1.250684	-0.000811
52	6	0	8.228954	-0.021230	-0.000684
53	8	0	4.590742	3.052062	-0.000688
54	8	0	9.194788	3.104945	-0.000551
55	6	0	6.857832	4.838053	-0.000491
56	6	0	9.603654	-0.440538	-0.000599
57	6	0	4.272337	-0.511657	-0.000826
58	6	0	10.070633	-1.749069	-0.000566
59	6	0	11.471754	-1.851237	-0.000477
60	6	0	12.116466	-0.621849	-0.000481
61	16	0	10.953986	0.689379	-0.000530

62	6	0	13.539117	-0.417713	-0.000388
63	6	0	14.184674	0.777417	-0.000627
64	16	0	2.893913	0.583643	-0.000786
65	6	0	1.765169	-0.756930	-0.000851
66	6	0	2.441027	-1.969478	-0.000911
67	6	0	3.839134	-1.831691	-0.000903
68	6	0	-6.204052	-1.200395	-0.000718
69	6	0	-7.626082	-1.219869	-0.000697
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71	7	0	-6.885454	-3.387038	-0.000932
72	6	0	-8.072072	-2.630073	-0.000893
73	6	0	-8.228959	0.021196	-0.000517
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82	6	0	-2.441030	1.969460	-0.000494
83	6	0	-1.765173	0.756911	-0.000679
84	16	0	-2.893920	-0.583660	-0.000828
85	6	0	-0.337925	0.589206	-0.000704
86	6	0	0.337920	-0.589226	-0.000834
87	16	0	-10.953994	-0.689412	-0.000551
88	6	0	-12.116471	0.621819	-0.000312
89	6	0	-11.471756	1.851205	-0.000175
90	6	0	-10.070636	1.749034	-0.000229
91	1	0	-20.330729	4.871881	0.891828
92	1	0	-20.325005	4.872303	-0.883752
93	1	0	-21.878717	4.808120	-0.000835
94	1	0	-18.315667	-2.966004	-0.000548
95	1	0	-15.715211	-3.151363	-0.000937
96	1	0	-13.600318	-1.696500	-0.000606
97	1	0	-14.123541	1.336687	-0.000066
98	1	0	-27.002614	-0.901625	0.001132
99	1	0	-25.815807	-3.259406	0.000423
100	1	0	-23.210359	-3.016932	0.000168
101	1	0	21.878766	-4.808088	-0.000046
102	1	0	20.330712	-4.871716	0.892511
103	1	0	20.325124	-4.872424	-0.883070
104	1	0	23.210325	3.016982	-0.000239
105	1	0	25.815771	3.259483	-0.000017

106	1	0	27.002602	0.901714	0.001003
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108	1	0	18.315643	2.966007	-0.000826
109	1	0	6.339723	5.209904	0.887464
110	1	0	6.339290	5.209992	-0.888152
111	1	0	7.891414	5.184529	-0.000708
112	1	0	9.410388	-2.609150	-0.000584
113	1	0	12.010341	-2.792184	-0.000403
114	1	0	14.123539	-1.336711	-0.000100
115	1	0	13.600303	1.696474	-0.000968
116	1	0	1.926596	-2.923840	-0.000966
117	1	0	4.521304	-2.674479	-0.000957
118	1	0	-7.891374	-5.184553	-0.002038
119	1	0	-6.338618	-5.209826	-0.888417
120	1	0	-6.340312	-5.210115	0.887195
121	1	0	-4.521307	2.674463	-0.000311
122	1	0	-1.926598	2.923821	-0.000357
123	1	0	0.222949	1.522779	-0.000589
124	1	0	-0.222953	-1.522799	-0.000922
125	1	0	-12.010341	2.792153	-0.000023
126	1	0	-9.410390	2.609113	-0.000121

Nuclear repulsive energy: 14484.7839564163 Hartrees

Q3:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-20.756585	1.054984	0.000273
2	6	0	-22.179263	1.029093	0.000574
3	6	0	-20.318755	2.467619	-0.001229
4	7	0	-21.504872	3.219064	-0.001802
5	6	0	-22.668253	2.425644	-0.000763
6	6	0	-22.740735	-0.228599	0.001952
7	16	0	-21.423775	-1.415919	0.002852
8	6	0	-20.149514	-0.181262	0.001387
9	8	0	-23.804686	2.864779	-0.000987
10	8	0	-19.199874	2.951435	-0.001879
11	6	0	-21.522389	4.670598	-0.003328

12	6	0	-18.768715	-0.589334	0.001491
13	6	0	-24.106680	-0.693621	0.002730
14	6	0	-18.293807	-1.895637	0.002504
15	6	0	-16.892697	-1.996132	0.002362
16	6	0	-16.262513	-0.758776	0.001235
17	16	0	-17.431756	0.550821	0.000319
18	16	0	-25.493551	0.389495	0.001643
19	6	0	-26.586513	-0.948121	0.003391
20	6	0	-25.939475	-2.157123	0.004746
21	6	0	-24.531122	-2.012599	0.004371
22	6	0	-14.889575	-0.489702	0.000806
23	6	0	-13.697057	-0.226197	0.000422
24	6	0	22.183949	-1.015197	0.000882
25	6	0	20.761419	-1.048931	-0.000114
26	6	0	22.677999	-2.410272	-0.001048
27	7	0	21.521484	-3.208821	-0.003219
28	6	0	20.328708	-2.462842	-0.002705
29	6	0	20.147298	0.184252	0.001464
30	16	0	21.414997	1.425607	0.004286
31	6	0	22.738259	0.245257	0.003252
32	8	0	19.208862	-2.944420	-0.004047
33	8	0	23.813512	-2.851845	-0.000822
34	6	0	21.562433	-4.659854	-0.005812
35	6	0	24.102094	0.716357	0.004882
36	6	0	18.764779	0.586472	0.001197
37	6	0	24.521523	2.036837	0.007024
38	6	0	25.929425	2.186438	0.008267
39	6	0	26.580877	0.979828	0.007071
40	16	0	25.492754	-0.361844	0.004398
41	16	0	17.431342	-0.557871	-0.000729
42	6	0	16.257910	0.747852	0.000309
43	6	0	16.884109	1.987263	0.001974
44	6	0	18.285432	1.891244	0.002473
45	6	0	7.819109	1.728913	-0.001898
46	6	0	6.398233	1.696389	-0.001982
47	6	0	8.249674	3.144203	-0.001381
48	7	0	7.059125	3.889679	-0.001210
49	6	0	5.901362	3.089702	-0.001541
50	6	0	5.841514	0.435041	-0.002349
51	16	0	7.165019	-0.746975	-0.002638
52	6	0	8.432709	0.494573	-0.002221
53	8	0	4.761107	3.519809	-0.001527
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56	6	0	9.814592	0.093767	-0.002199
57	6	0	4.479955	-0.030685	-0.002466
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59	6	0	11.696986	-1.304520	-0.002441
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64	6	0	2.667502	-1.518638	-0.002707
65	6	0	4.062322	-1.356890	-0.002725
66	6	0	13.693538	0.210022	-0.001077
67	6	0	14.885708	0.475098	-0.000463
68	6	0	-6.397355	-1.703643	-0.000370
69	6	0	-7.818138	-1.740138	-0.000111
70	6	0	-5.899139	-3.096792	0.000177
71	7	0	-7.052186	-3.898778	0.000704
72	6	0	-8.247355	-3.155518	0.000625
73	6	0	-8.435420	-0.507200	-0.000511
74	16	0	-7.170934	0.737565	-0.001242
75	6	0	-5.844391	-0.441070	-0.000957
76	8	0	-9.365579	-3.640111	0.001137
77	8	0	-4.760886	-3.532219	0.000232
78	6	0	-7.007516	-5.349841	0.001407
79	6	0	-4.483605	0.026910	-0.001341
80	6	0	-9.817922	-0.108531	-0.000431
81	6	0	-4.067248	1.353418	-0.001798
82	6	0	-2.672465	1.516217	-0.002133
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84	16	0	-3.096839	-1.052582	-0.001314
85	16	0	-11.149654	-1.255582	0.000435
86	6	0	-12.325207	0.047822	-0.000006
87	6	0	-11.701214	1.288761	-0.000787
88	6	0	-10.300134	1.195538	-0.001019
89	6	0	-0.603882	0.102274	-0.002137
90	6	0	0.600005	-0.103290	-0.002291
91	1	0	-22.566227	4.984802	-0.002235
92	1	0	-21.017044	5.057207	-0.892273
93	1	0	-21.014551	5.058982	0.883403
94	1	0	-18.949787	-2.758919	0.003319
95	1	0	-16.345460	-2.930506	0.003053
96	1	0	-27.652301	-0.763925	0.003340
97	1	0	-26.448999	-3.113300	0.005976
98	1	0	-23.845346	-2.852544	0.005299
99	1	0	20.532188	-5.016037	0.001419

100	1	0	22.077377	-5.025622	-0.898104
101	1	0	22.091193	-5.027532	0.877457
102	1	0	23.832582	2.874200	0.007669
103	1	0	26.435497	3.144452	0.009967
104	1	0	27.647331	0.799539	0.007607
105	1	0	16.333860	2.919861	0.002809
106	1	0	18.938520	2.756703	0.003731
107	1	0	5.988278	5.649949	-0.005044
108	1	0	7.534139	5.731089	0.889738
109	1	0	7.542238	5.731538	-0.886018
110	1	0	9.644057	-2.077043	-0.003290
111	1	0	12.248699	-2.236219	-0.002746
112	1	0	2.161577	-2.475974	-0.002875
113	1	0	4.755420	-2.190648	-0.002911
114	1	0	-8.036901	-5.708536	0.004431
115	1	0	-6.482385	-5.714521	0.888092
116	1	0	-6.487366	-5.715811	-0.887713
117	1	0	-4.761108	2.186554	-0.001882
118	1	0	-2.167280	2.473949	-0.002497
119	1	0	-12.253454	2.220142	-0.001164
120	1	0	-9.648929	2.062454	-0.001605

Nuclear repulsive energy:14011.3988700235 Hartrees

4. *AFM image of the films of polymer Q3*

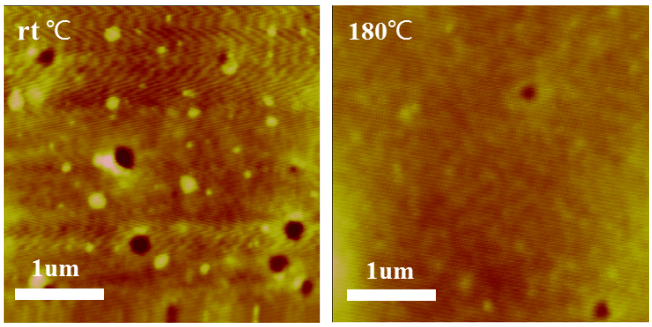

Figure S2. AFM image of the films of polymer **Q3**

5. *XRD of the films of polymer Q1, Q2 and Q3*

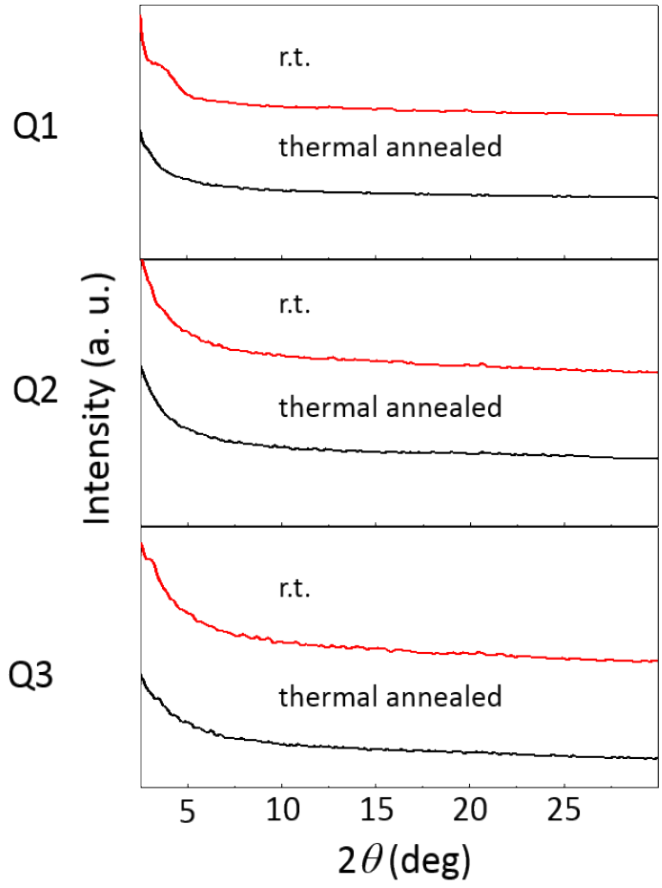

Figure S3. 5. XRD of the films of polymer Q1, Q2 and Q3

6. *[1]HNMR &[13]CNMR of compounds3,4, 6,7,Q1,Q2 andQ3*

Compound 3

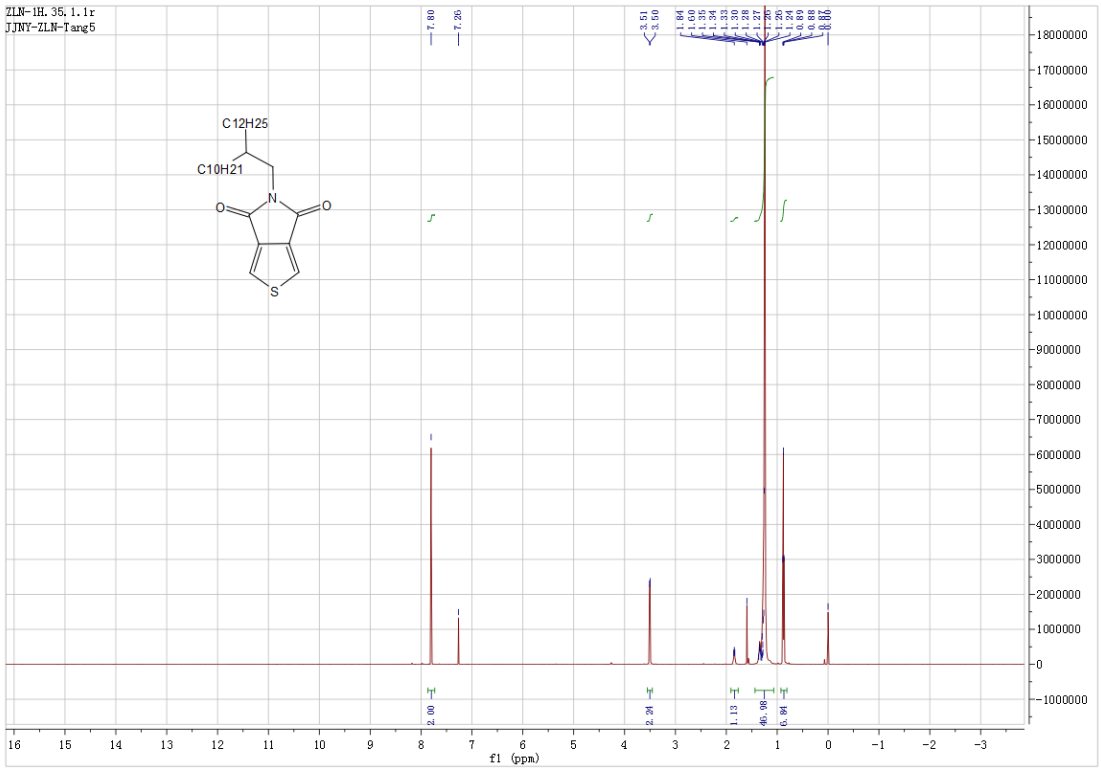

Figure S4. [1]H NMR spectrum of **3** (400 MHz, r. t., in $CDCl_3$).

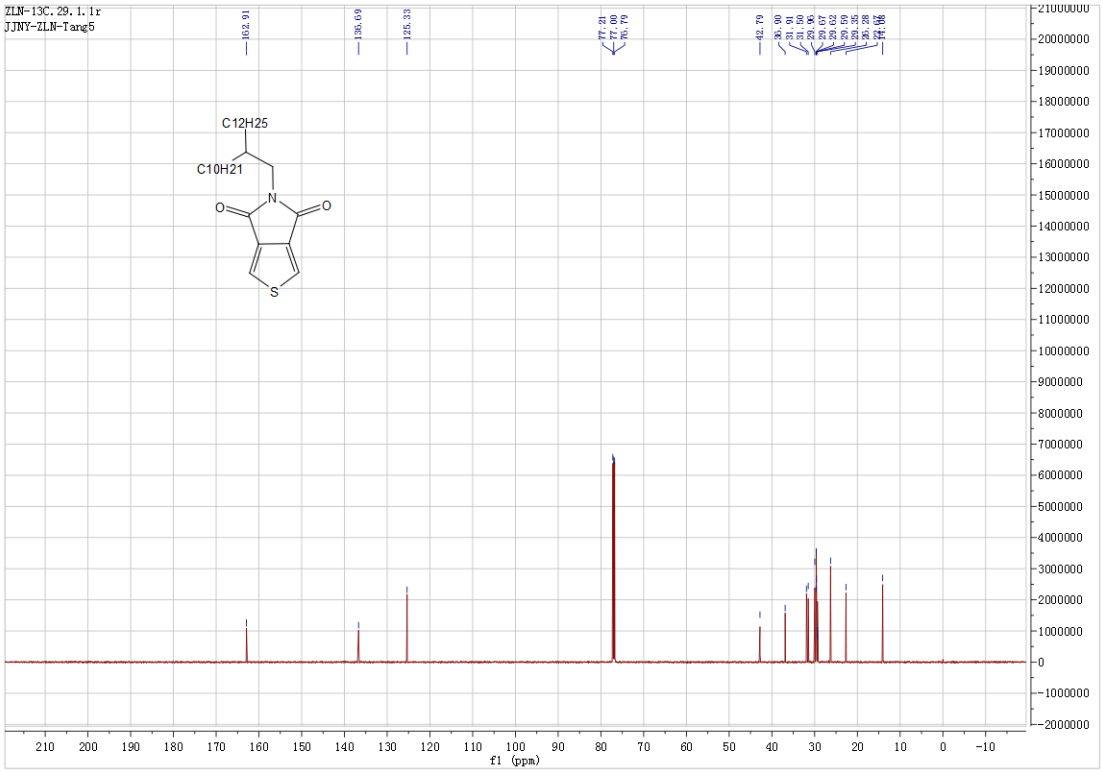

Figure S5.[13]C NMR spectrum of **3** (400 MHz, r. t., in $CDCl_3$).

Compound 4

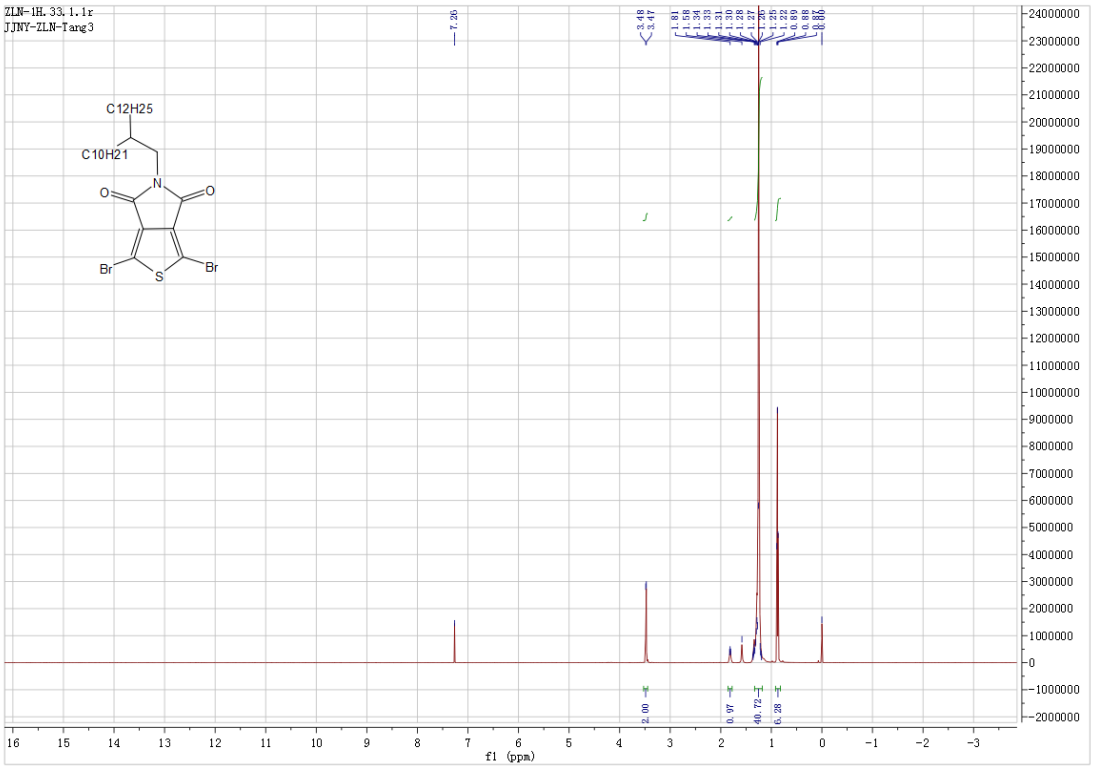

Figure S6. ^{1}H NMR spectrum of **4** (400 MHz, r. t., in $CDCl_3$).

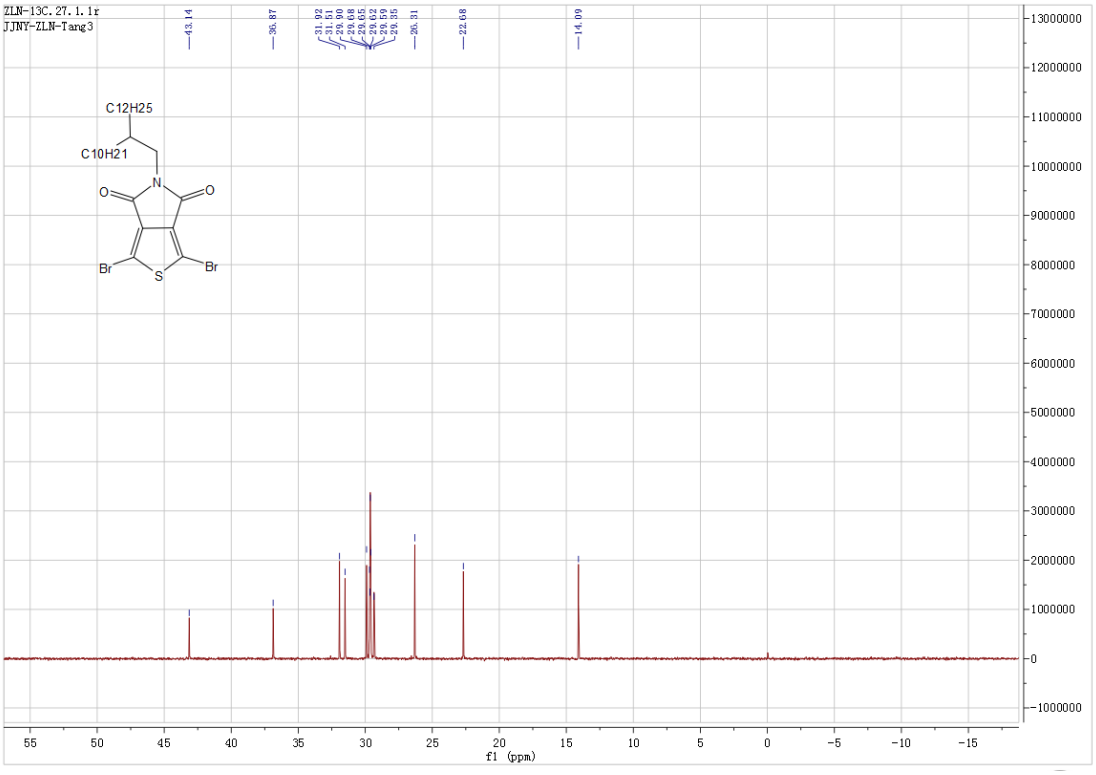

Figure S7. ^{13}C NMR spectrum of **4** (400 MHz, r. t., in $CDCl_3$).

Compound 6

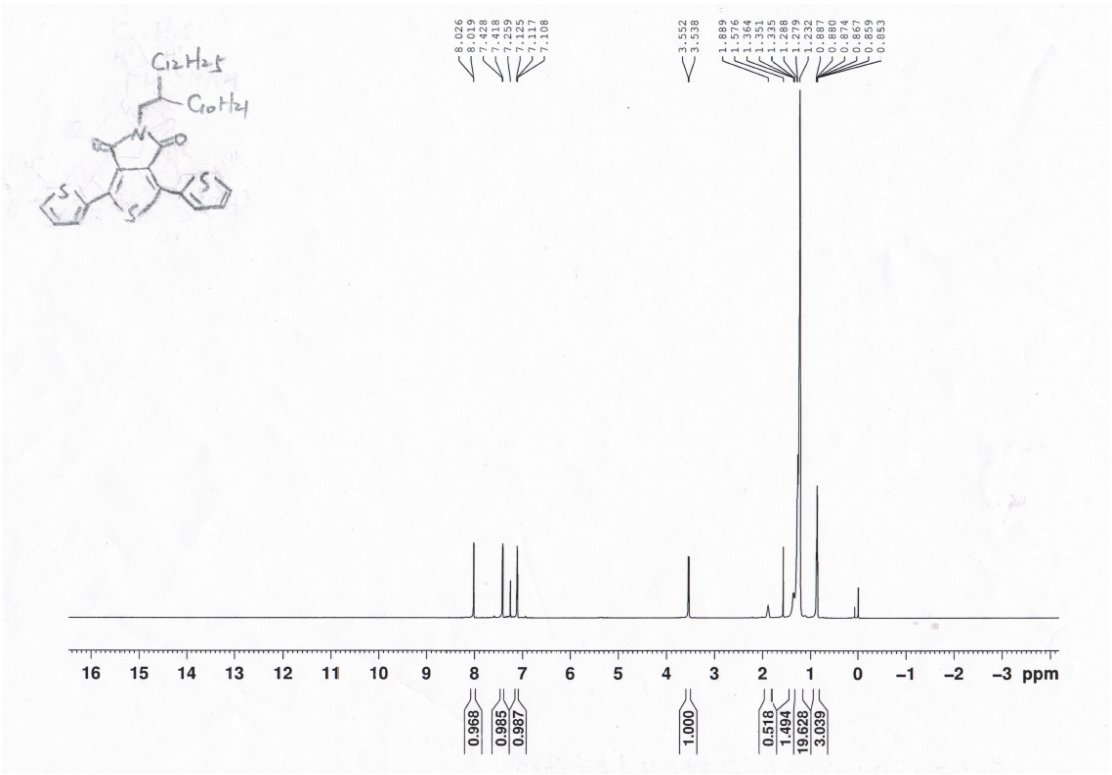

Figure S8.[1]H NMR spectrum of **6** (400 MHz, r. t., in $CDCl_3$).

Compound 7

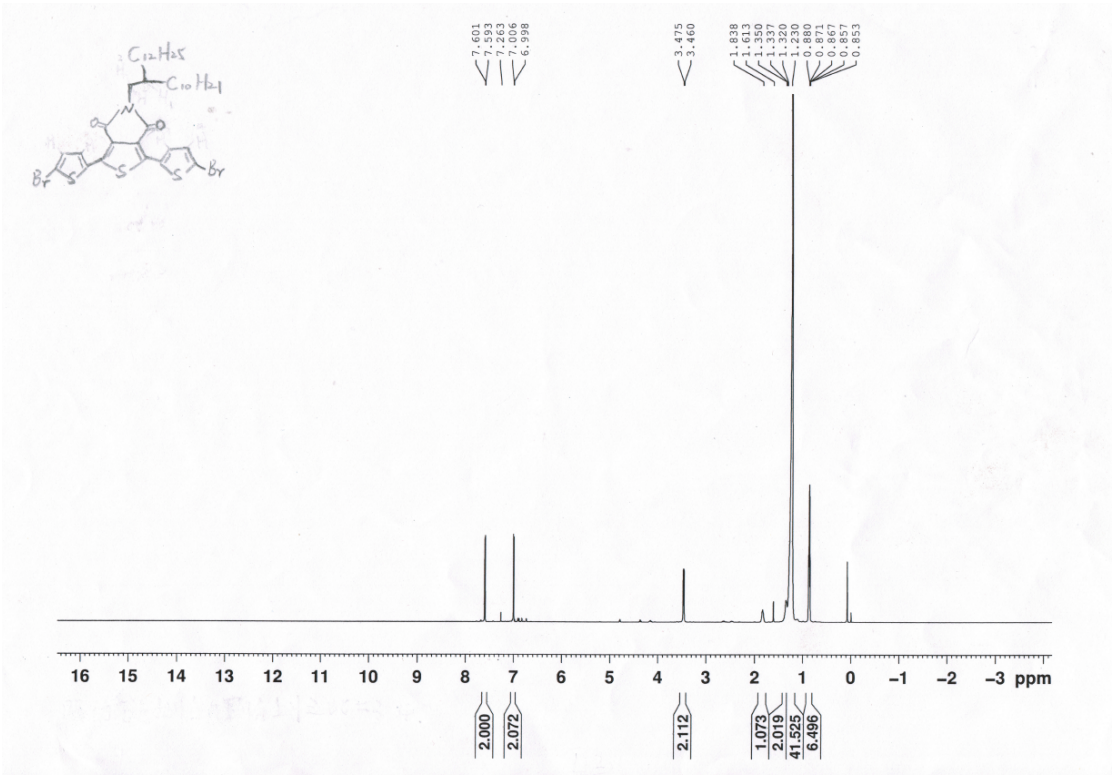

Figure S9.[1]H NMR spectrum of **7**(400 MHz, r. t., in $CDCl_3$).

Polymer Q1

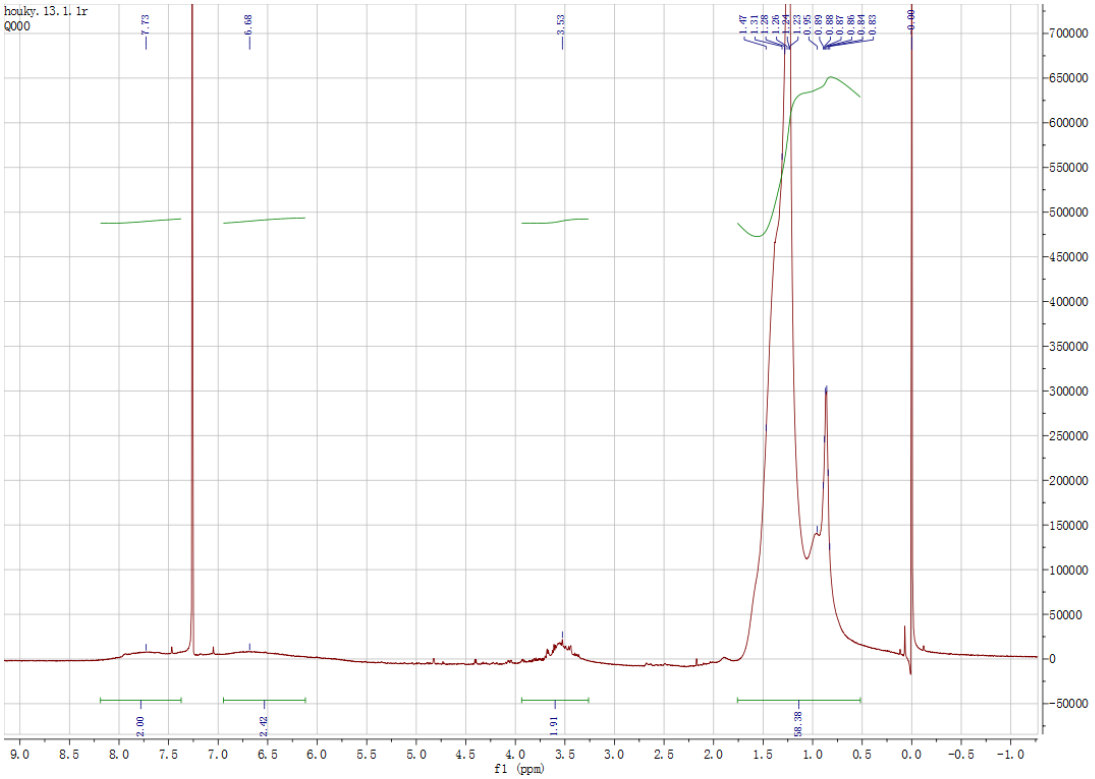

Figure S10.^{1}H NMR spectrum of polymer **Q1**(400 MHz, r. t., in $CDCl_3$).

Polymer Q2

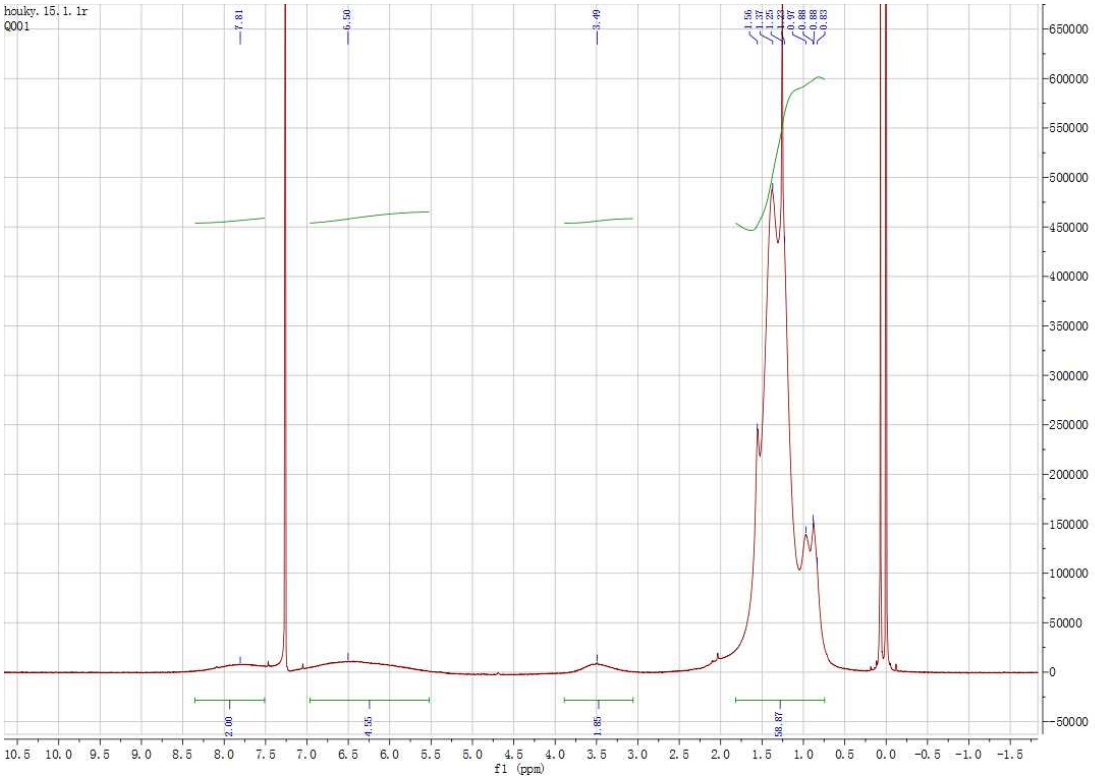

Figure S11.^{1}H NMR spectrum of polymer **Q2** (400 MHz, r. t., in $CDCl_3$).

Polymer Q3

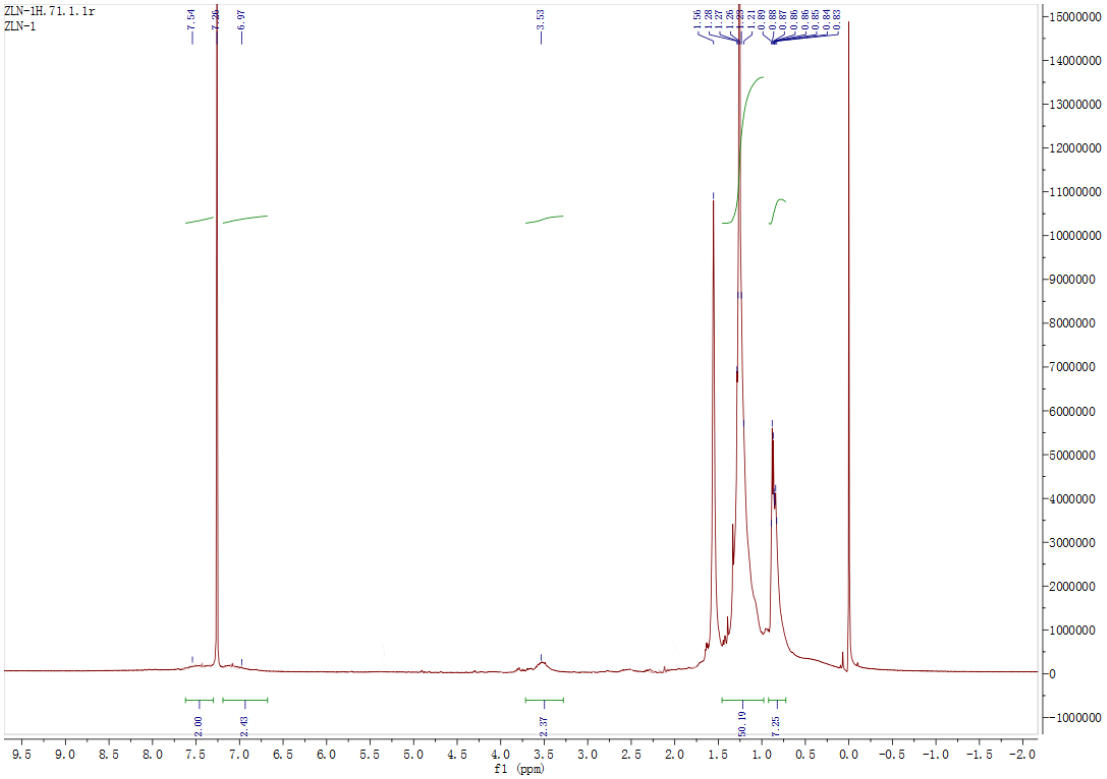

Figure S12. ^{1}H NMR spectrum of polymer **Q3** (400 MHz, r. t., in $CDCl_3$).

7. Reference

(1) Nielsen, C. B.; Bjørnholm, T. *Org. Lett.,* 2004, **6**, 3381.

(2) Guo, X.; Ortiz, R. P.; Zheng, Y.; Kim, M.-G.; Zhang, S.; Hu, Y.;Lu, G.; Facchetti, A.; Marks, T. J. *J. Am. Chem. Soc.*, 2011, **133**, 13685.

(3) M. J.Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G.Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T.Vreven, J. A. Montgomery, J. E. PeraltaJr., F. Ogliaro M., Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B.Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev,A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V.G.Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B.Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, *Gaussian, Inc., Wallingford CT*, 2009.