Supporting Information

Impact of thienothiophene isomeric structures on the optoelectronic properties and photovoltaic performance in quinoxaline based donor-acceptor copolymers

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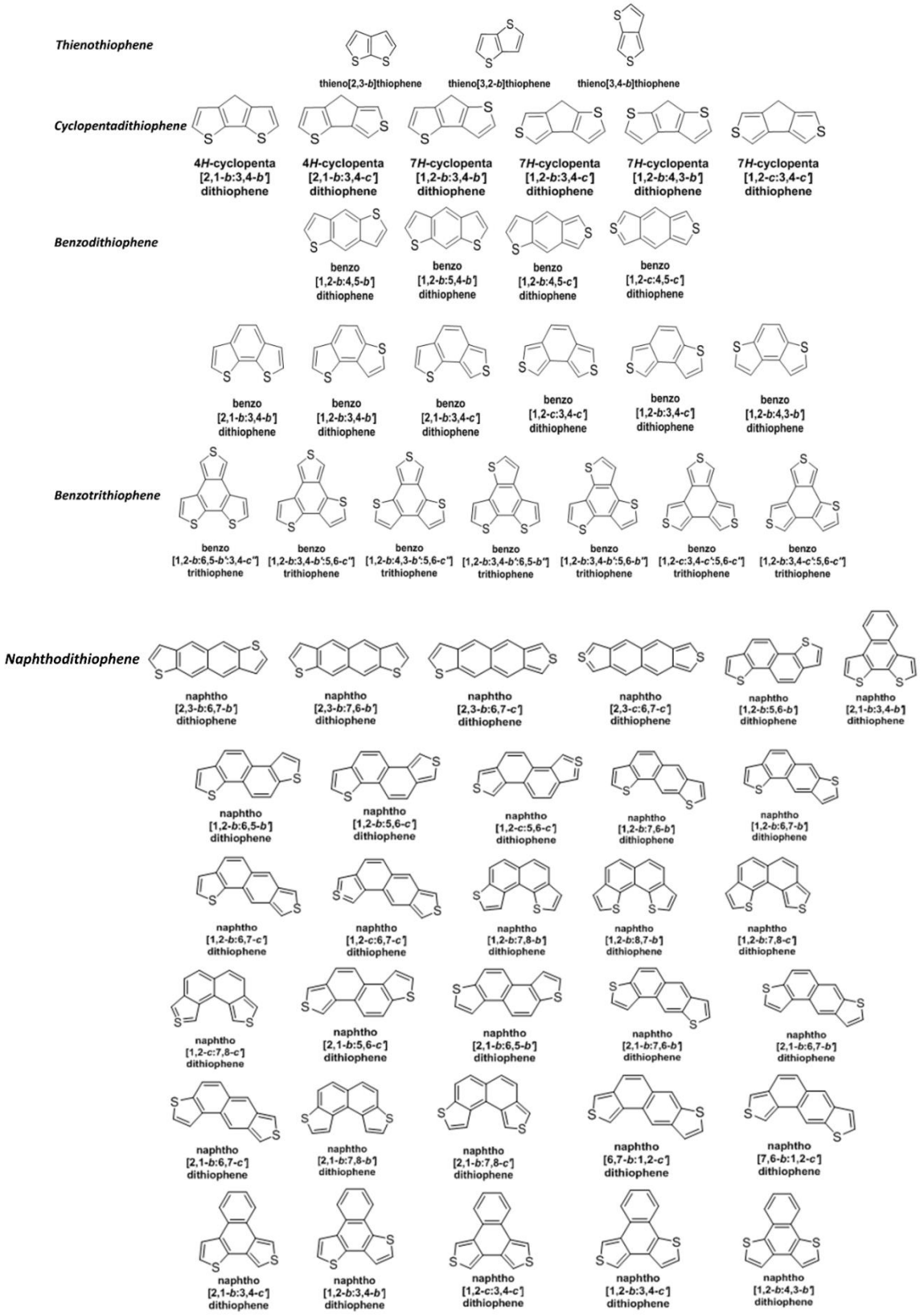


Figure S1. Isomeric structures of the most common electron rich building blocks for the synthesis of D-A conjugated polymers.

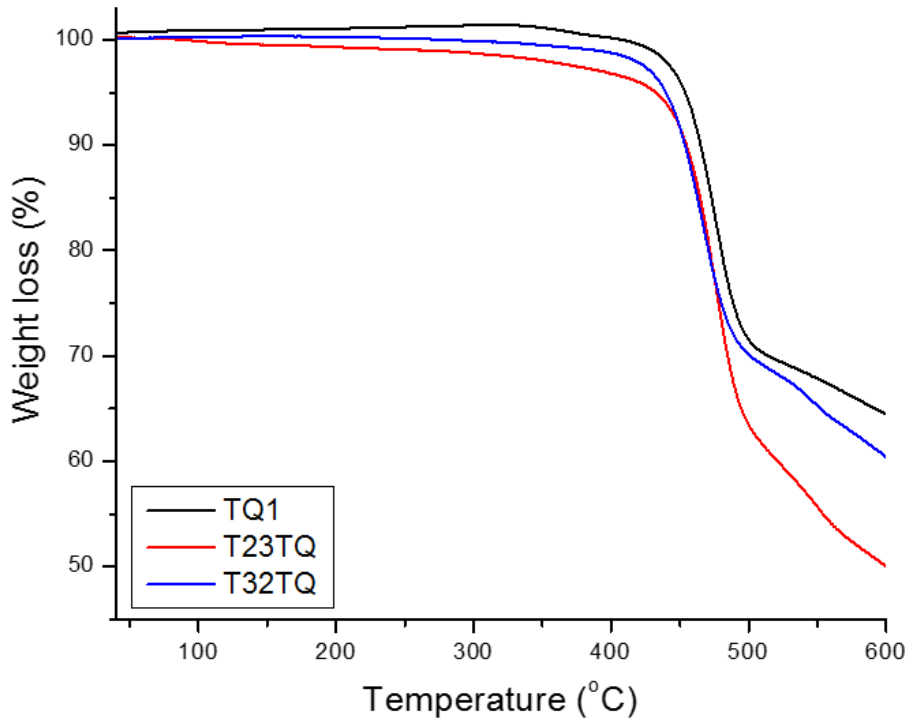
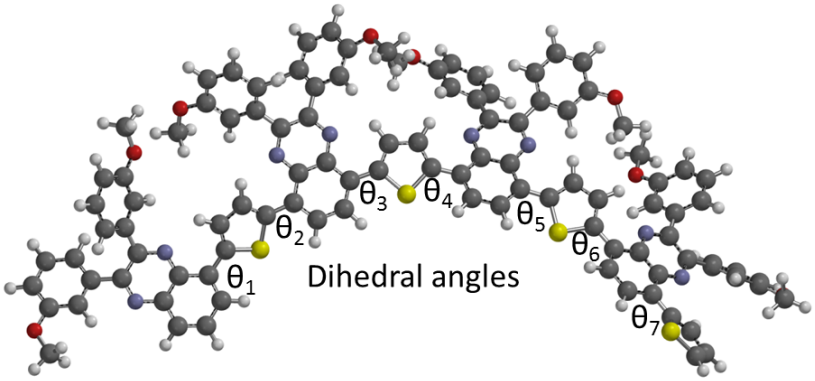
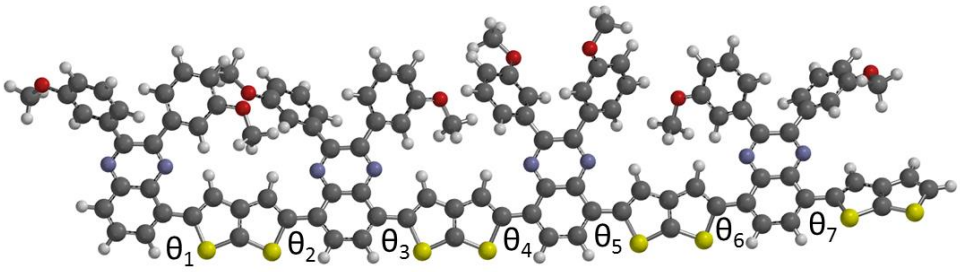


Figure S2. Thermogravimetric analysis graphs of the TQ1, T23TQ and T32TQ under a nitrogen atmosphere.

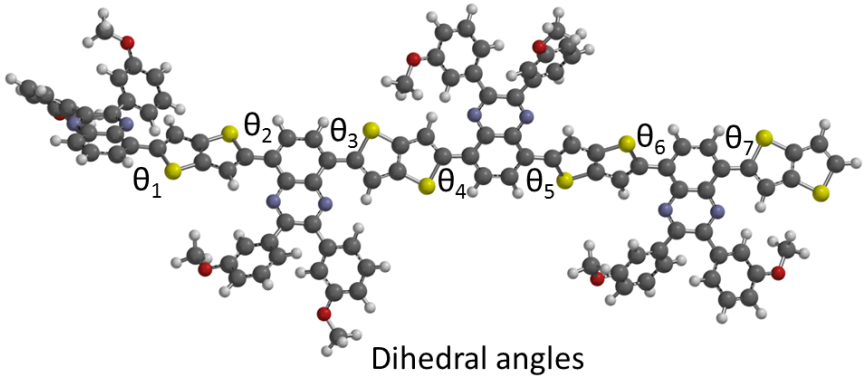


θ1	θ2	θ3	θ4	θ5	θ6	θ7
15.30°	23.03°	6.78°	24.76°	15.87°	31.20°	25.27°



Dihedral angles

θ1	θ2	θ3	θ4	θ5	θ6	θ7
28.56°	13.63°	22.38°	4.18°	10.72°	29.87°	26.12°



Dihedral angles

θ1	θ2	θ3	θ4	θ5	θ6	θ7
21.14°	22.50°	20.02°	23.48°	16.73°	22.93°	22.76°

Figure S3. Calculated dihedral angles for the tetramer model compounds of TQ1 (up), T23TQ (middle) and T32TQ (bottom).

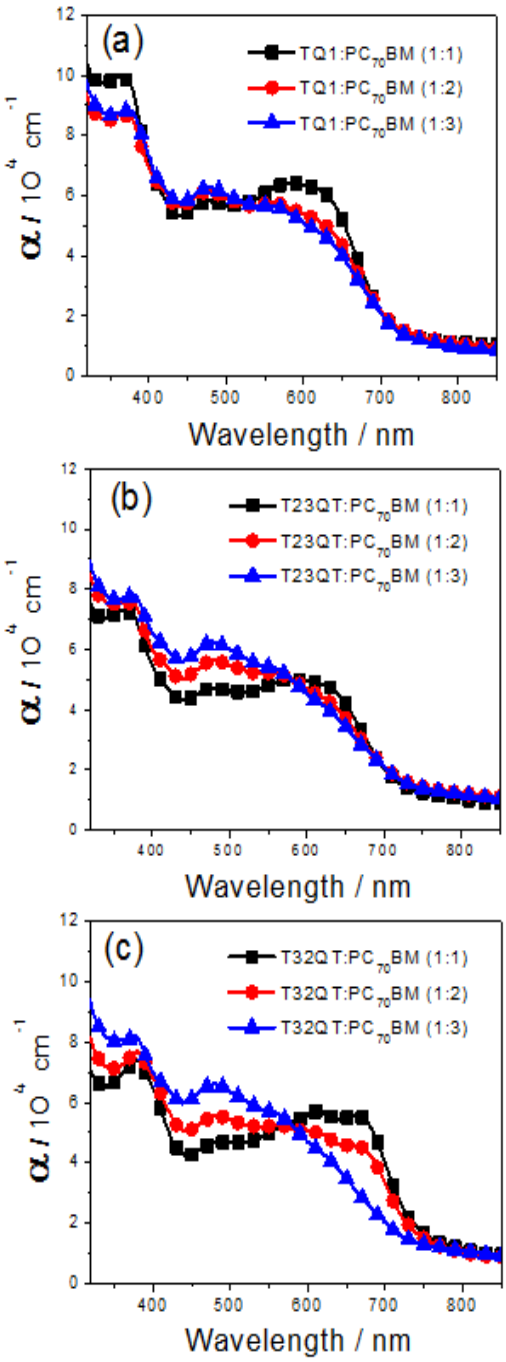
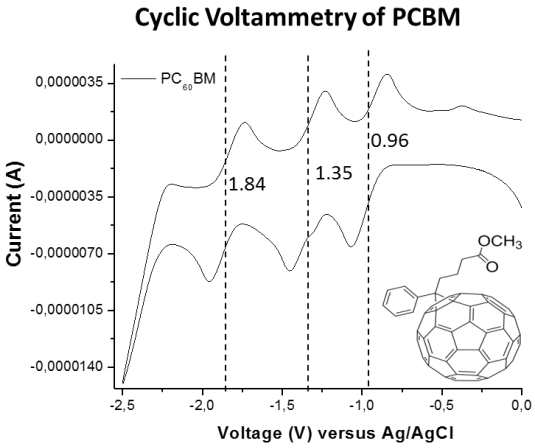


Figure S4. Thin film absorption spectra of (a) TQ1:$PC_{70}BM$, (b) T23TQ:$PC_{70}BM$ and (c) T32TQ:$PC_{70}BM$ in three different composition ratio (1:1, 1:2 and 1:3).



$E_{ox}^{Fc/Fc+} = 0.24$ V

E_{red}^{PCBM} (vs Fc/Fc^{+}) = E_{red}^{PCBM} (vs Ag/AgCl) - $E_{ox}^{Fc/Fc+}$ = -0.96 – 0.24 V = -1.20 V

E_{LUMO}^{PCBM} = - (5.10 – 1.20) eV = -3.90 eV

Figure S5. Cyclic voltamograph of $PC_{60}BM$ in ortho-dichlorobenzene solution and estimation of the E_{LUMO} of $PC_{60}BM$ from the corresponding first reduction potential.

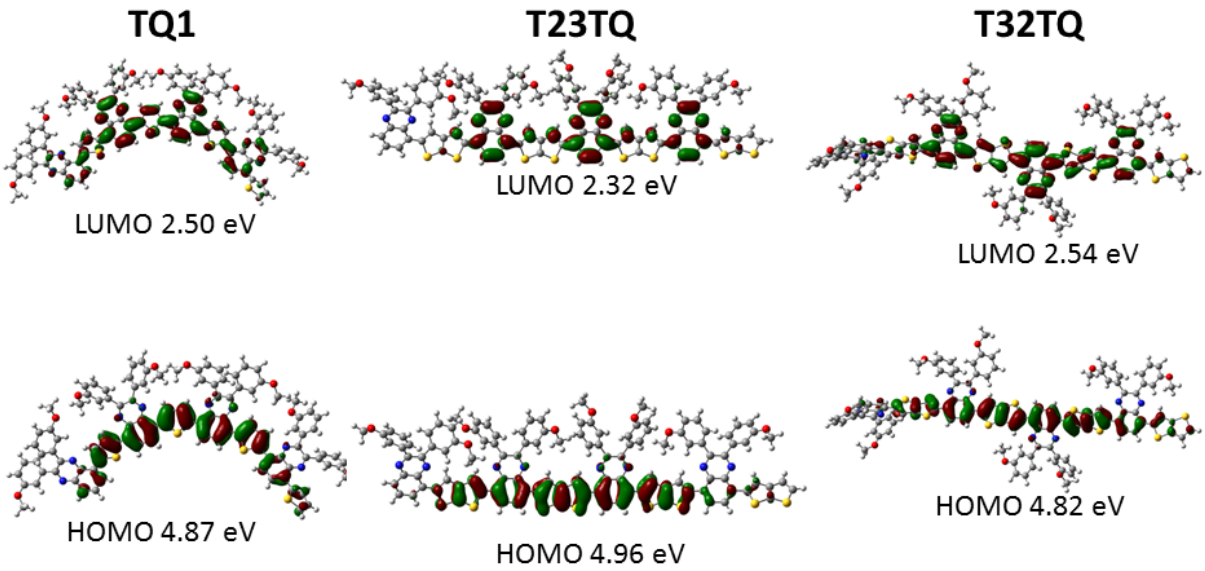


Figure S6. DFT [B3LYP/6-31G(d,p)] calculated frontier molecular orbitals of the HOMO (bottom) and LUMO (top) for the tetramers of TQ1, T23TQ and T32TQ.

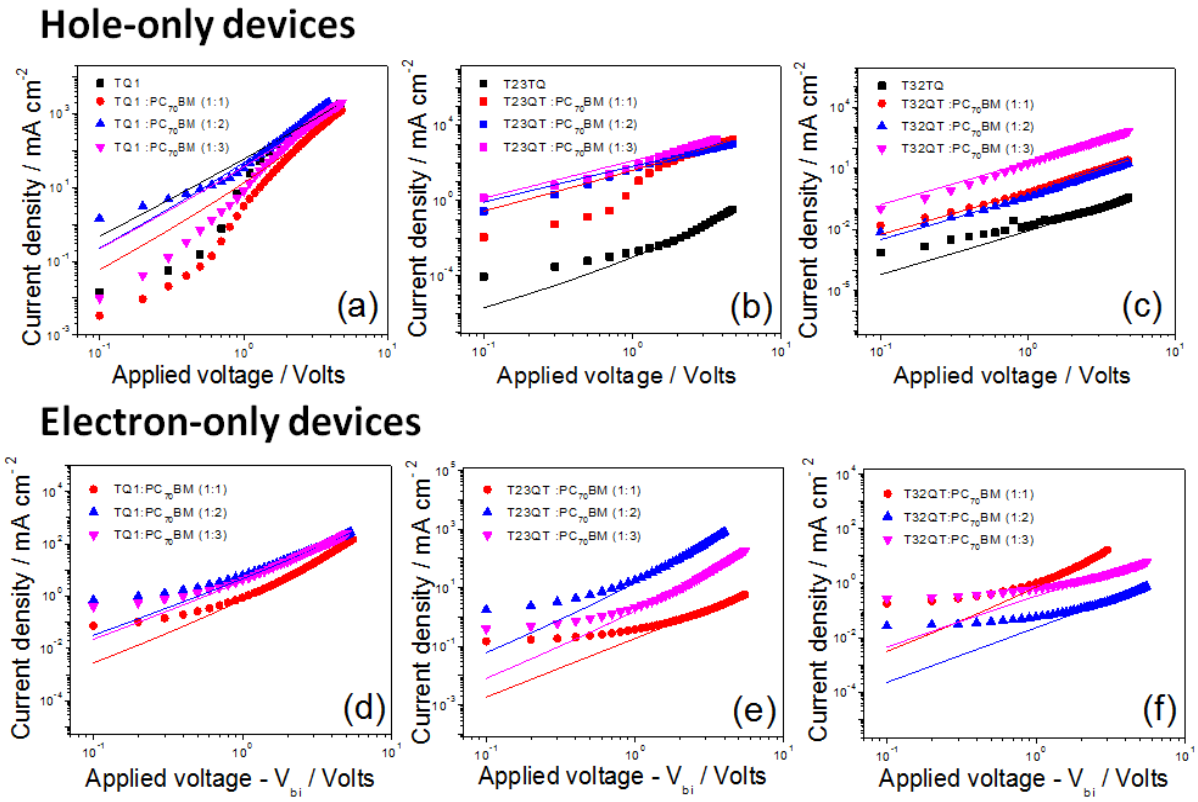


Figure S7. Dark J-V curves of hole-only devices (a-c) and electron-only devices (d-f) for pristine TQ1 (black square), TQ1:$PC_{70}BM$ 1:1 (red circle), 1:2 (blue up-triangle), 1:3 (pink down-triangle) composition ratio, pristine T23TQ (black square), T23TQ:$PC_{70}BM$ 1:1 (red circle), 1:2 (blue up-triangle), 1:3 (pink down-triangle) composition ratio, and pristine T32TQ (black square), T32TQ:$PC_{70}BM$ 1:1 (red circle), 1:2 (blue up-triangle) and 1:3 (pink down-triangle) composition ratio.

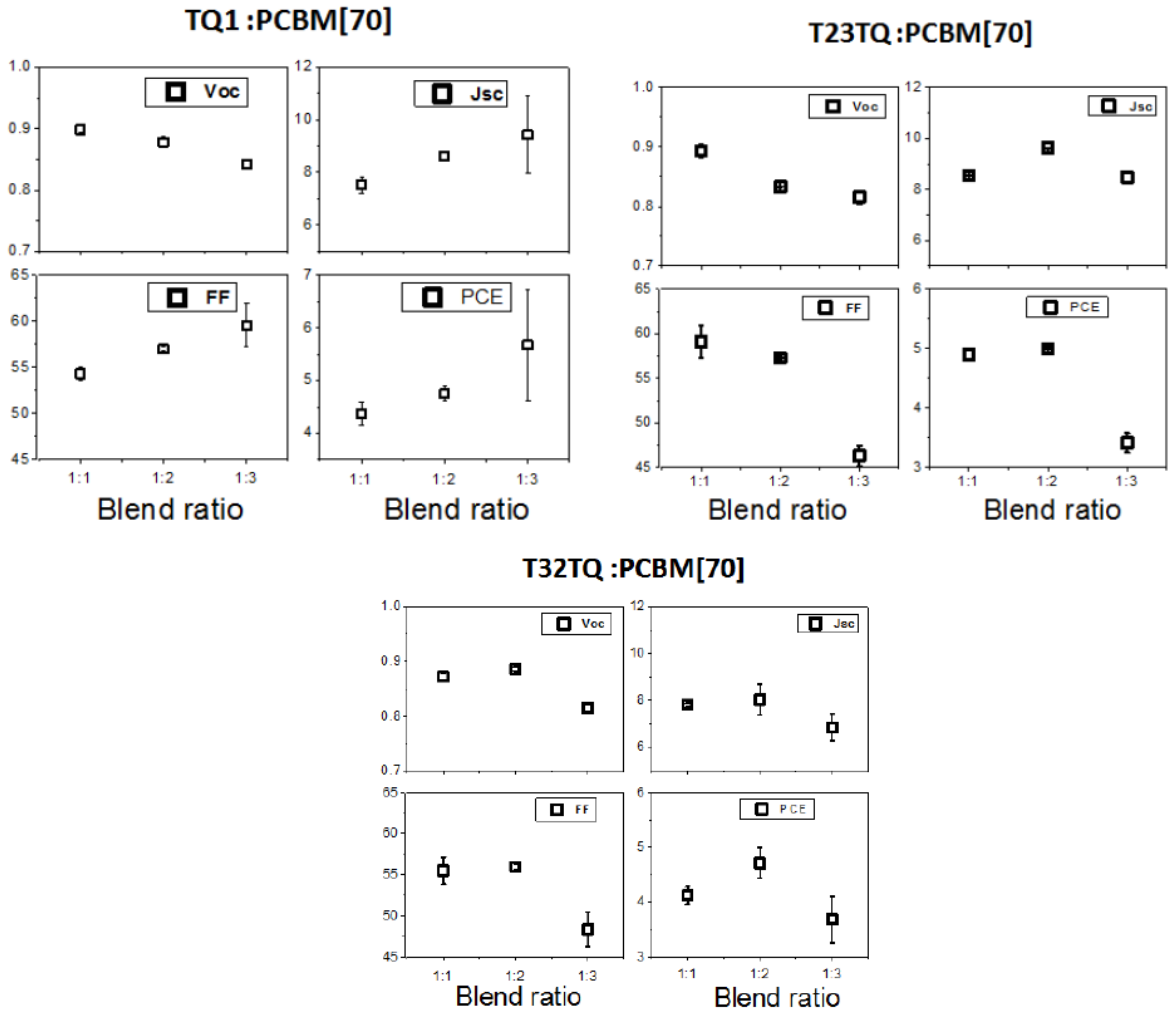
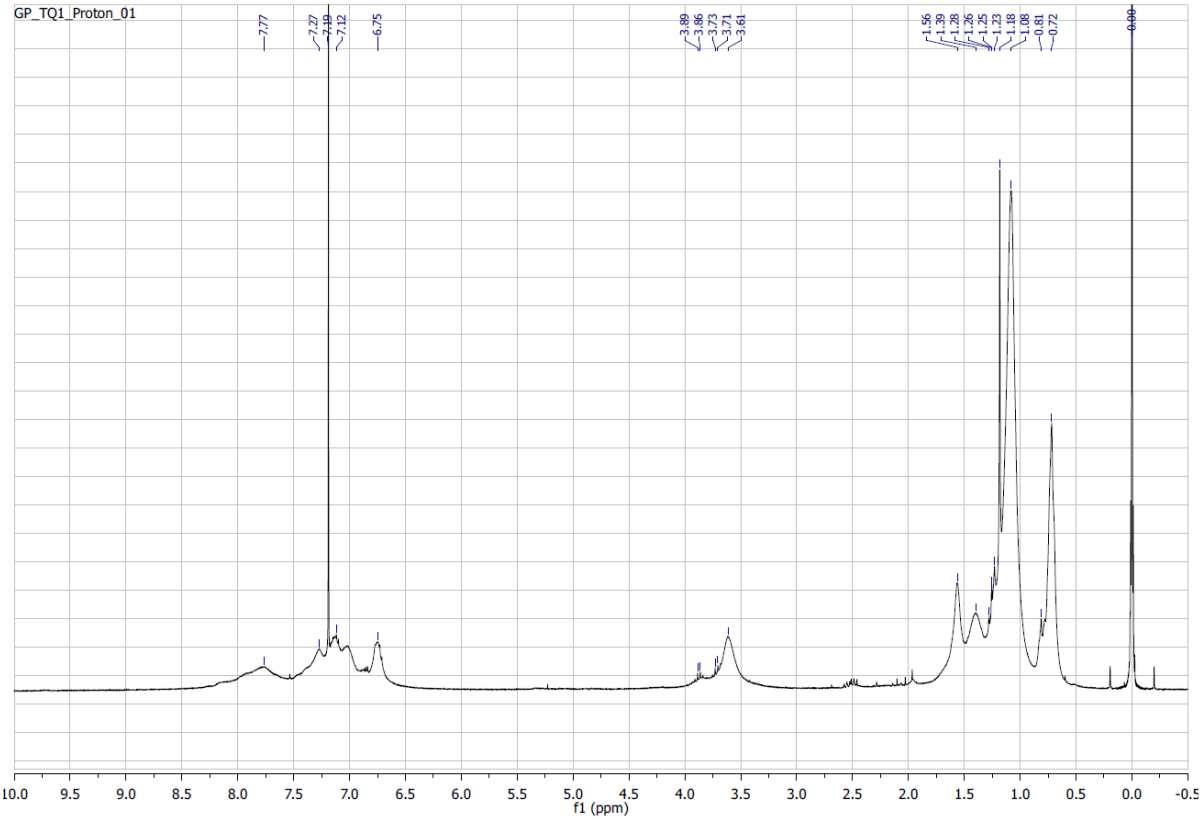
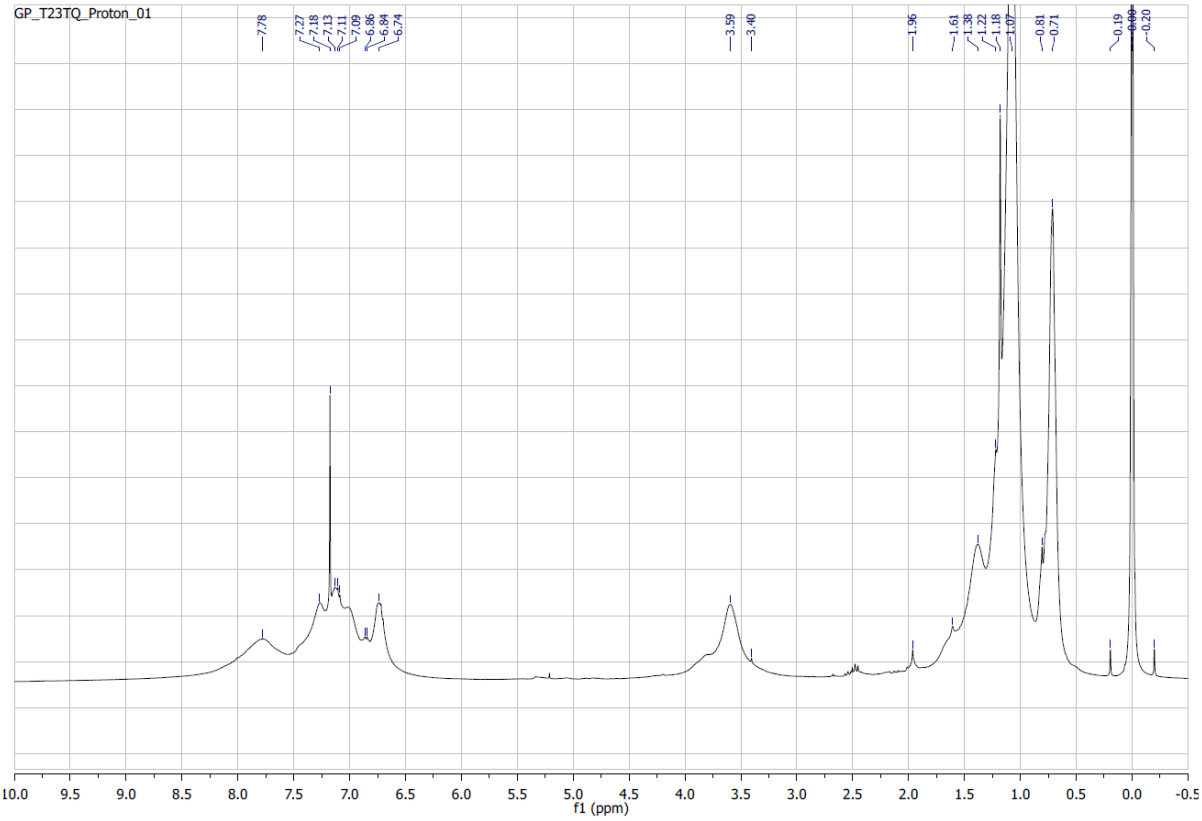


Figure S8. The basic figures of merit (V_{oc}, Jsc, FF and PCE) for the polymer:$PC_{70}BM$ OPV devices as a function of the polymer:$PC_{70}BM$ composition ratio (1:1, 1:2 and 1:3).


GP_TQ1_Proton_01
7.77
7.27
7.19
7.12
6.75
3.89
3.86
3.73
3.71
3.61
1.56
1.39
1.28
1.26
1.25
1.23
1.18
1.08
0.81
0.72
0.00
f1 (ppm)


GP_T23TQ_Proton_01
7.78
7.27
7.18
7.13
7.11
7.09
6.86
6.84
6.74
3.59
3.40
1.96
1.61
1.38
1.22
1.18
1.07
0.81
0.71
0.19
0.00
0.20
f1 (ppm)

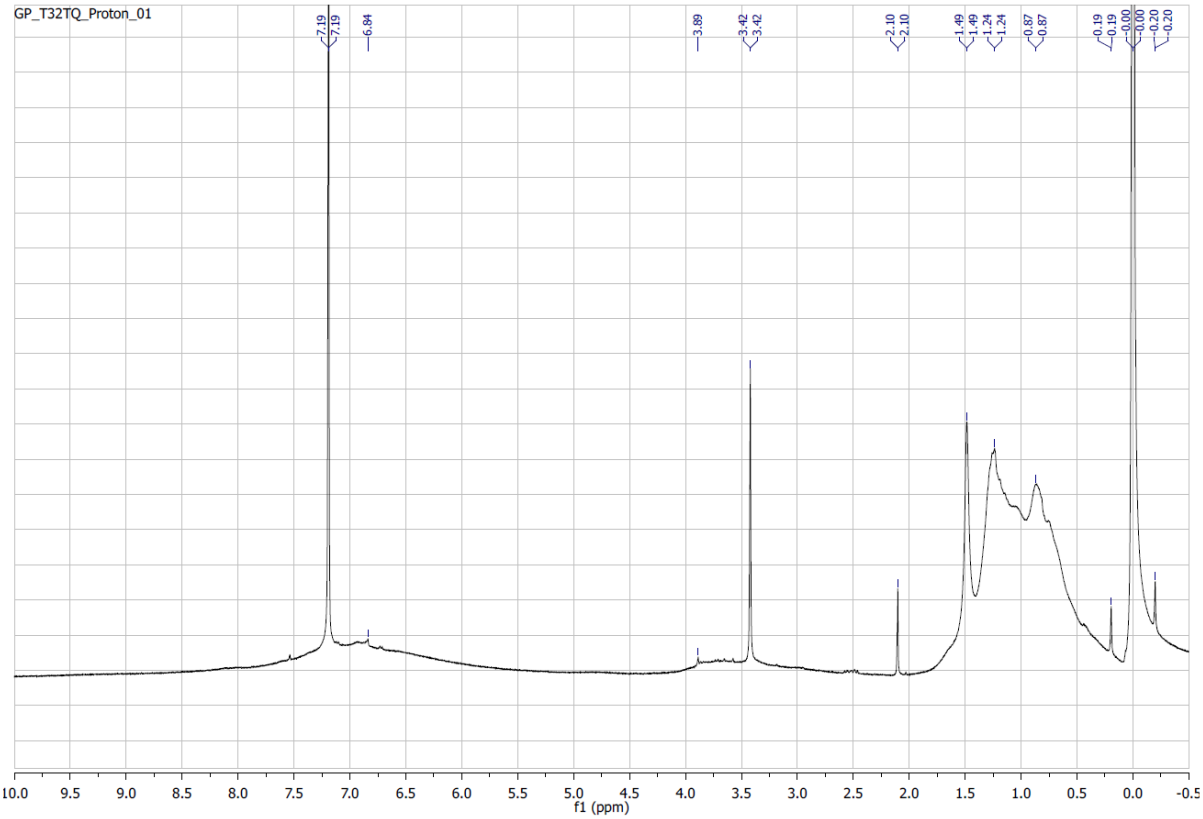


Figure S9. ^{1}H-NMR spectra (400 MHz) of TQ1, T23TQ and T32TQ in $CDCl_3$.

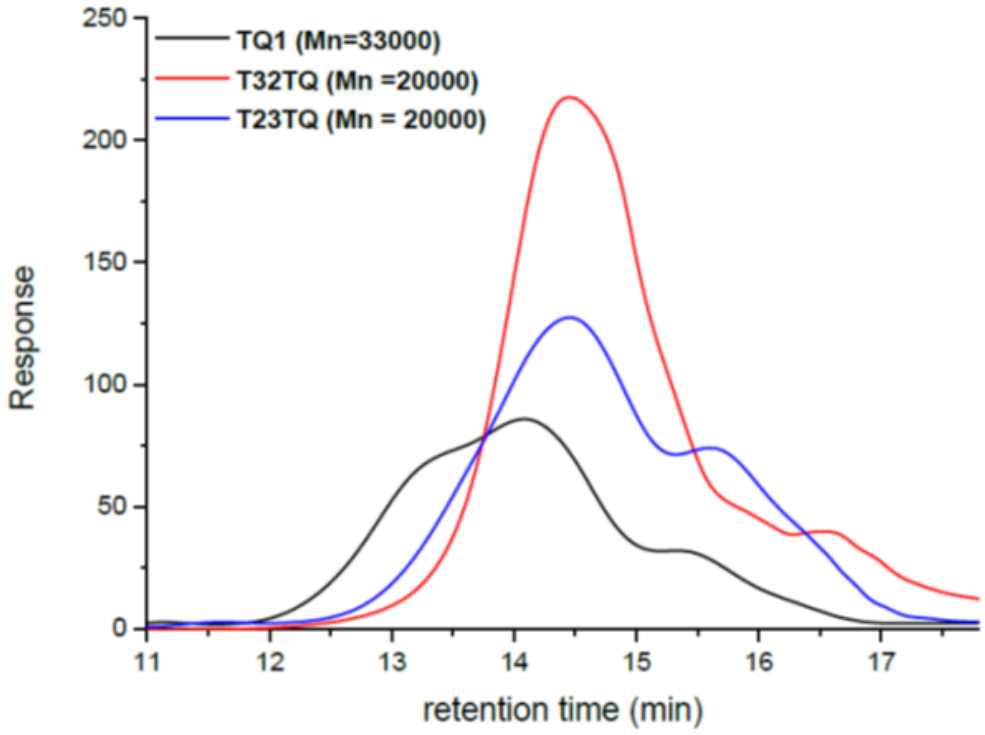


Figure S10. GPC chromatographs of TQ1, T23TQ and T32TQ.

Table S1. The obtained current densities and the calculated current densities from EQE of all the systems are presented.

Blend System	J_{sc} (mA/cm^2)	J_{sc} (mA/cm^2) calculated from EQE spectrum	Sun used
TQ1:$PC_{70}BM$ (1:1)	7.5 ± 0.32	6.8 ±0.24	0.98
TQ1:$PC_{70}BM$ (1:2)	8.6 ± 0.19	7.3 ±0.15	0.98
TQ1:$PC_{70}BM$ (1:3)	9.4 ± 1.45	7.8 ±0.51	0.98
T23TQ:$PC_{70}BM$ (1:1)	8.5 ± 0.02	6.6 ±0.17	0.98
T23TQ:$PC_{70}BM$ (1:2)	9.6 ± 0.02	6.9 ± 0.06	0.98
T23TQ:$PC_{70}BM$ (1:3)	8.5 ± 0.17	5.5 ±0.18	0.98
T32TQ:$PC_{70}BM$ (1:1)	7.8 ± 0.06	6.8 ± 0.03	0.98
T32TQ:$PC_{70}BM$ (1:2)	8.1 ± 0.65	7.1 ±0.20	0.98
T32TQ:$PC_{70}BM$ (1:3)	6.9 ± 0.58	5.7 ± 0.05	0.98