Electronic Supplementary Material (ESI) for Polymer Chemistry.

Synthesis, Optoelectronic properties and Photovoltaic Performances of Wide Band-Gap Copolymers Based on Dibenzosilole and Quinoxaline units, Rivals to P3HT

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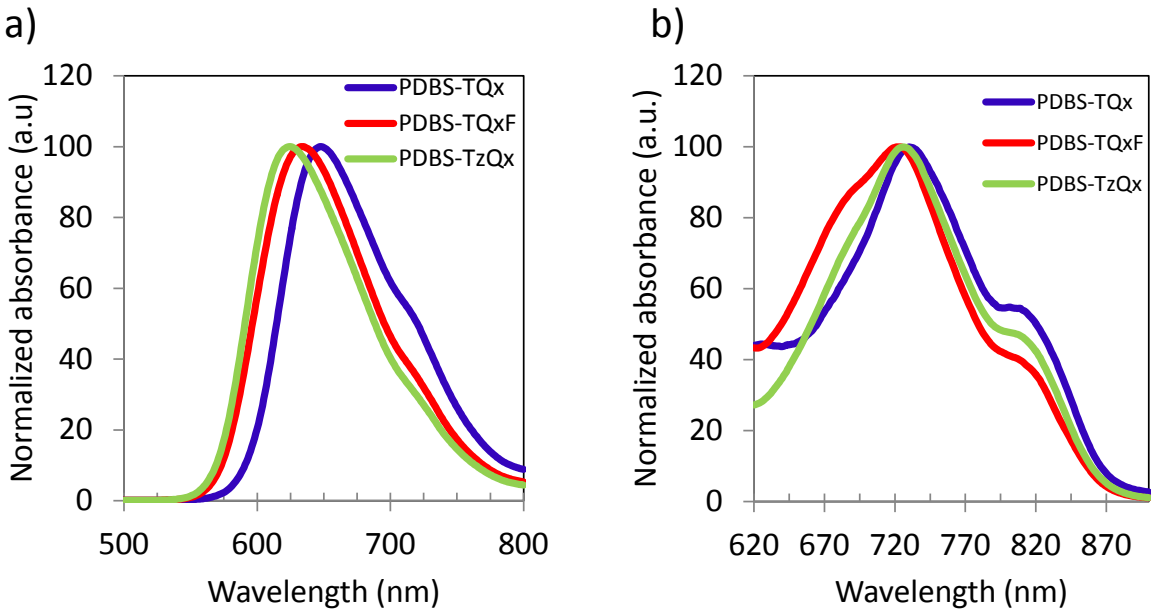

Figure S1. Emission spectra of PDBS-TQx, PDBS-TQxF and PDBS-TzQx (a) in solution in chloroform and (b) in thin film.

Table S1. Single crystal X-Ray diffraction table for monomers TQx, TQx-Br-TzQx-Br

	TQx	TQxF-Br	TzQx-Br
Empirical formula	$C_{40}H_{46}N_2S_4$	$C_{40}H_{42}Br_2F_2N_2S_4$	$C_{38}H_{42}Br_2N_4S_4$
crystal size (mm)	0.869 x 0.614 x 0.451	0.457 x 0.057 x 0.043	0.727 x 0.628 x 0.013
crystal system	Tetragonal	Triclinic	Triclinic
a (Å)	17.5664(3)	16.7687(11)	9.0551(6)
b (Å)	17.5664(3)	18.2589(12)	10.0299(7)
c (Å)	44.8654(11)	20.6070(12)	22.0044(12)
α (°)	90.00	112.675(6)	91.596(5)
β (°)	90.00	100.139(5)	97.865(5)
γ (°)	90.00	92.575(5)	105.823(6)
V ($Å^3$)	13844.4(5)	5686.5(7)	1900.2(2)
Z	16	6	2
Space group	$I4_1/a$	P-1	P-1
D_{calcd} (g cm^{-3})	1.311	1.536	1.473
μ (mm^{-1})	0.307	2.401	2.386
θ range (°)	3.180 - 30.506	3.215 - 26.372	3.230 - 30.508
Number of data collected	21885	38407	21348
Number of unique data	10530	22546	11488
R(int)	0.0423	0.0686	0.0821
R (all data)	0.1014	0.1857	0.2292
Rw (all data)	0.1373	0.1659	0.2507
R (I>2σ(I))	0.0556	0.0742	0.0870
R_w (I>2σ(I))	0.1151	0.1218	0.1758
F(000)	5824	2688	864
Peak/hole ((e.$Å^{-3}$)	0.379/-0.478	1.323/-0.828	0.785/-0.772
Temperature (K)	150(2)	150(2)	150(2)

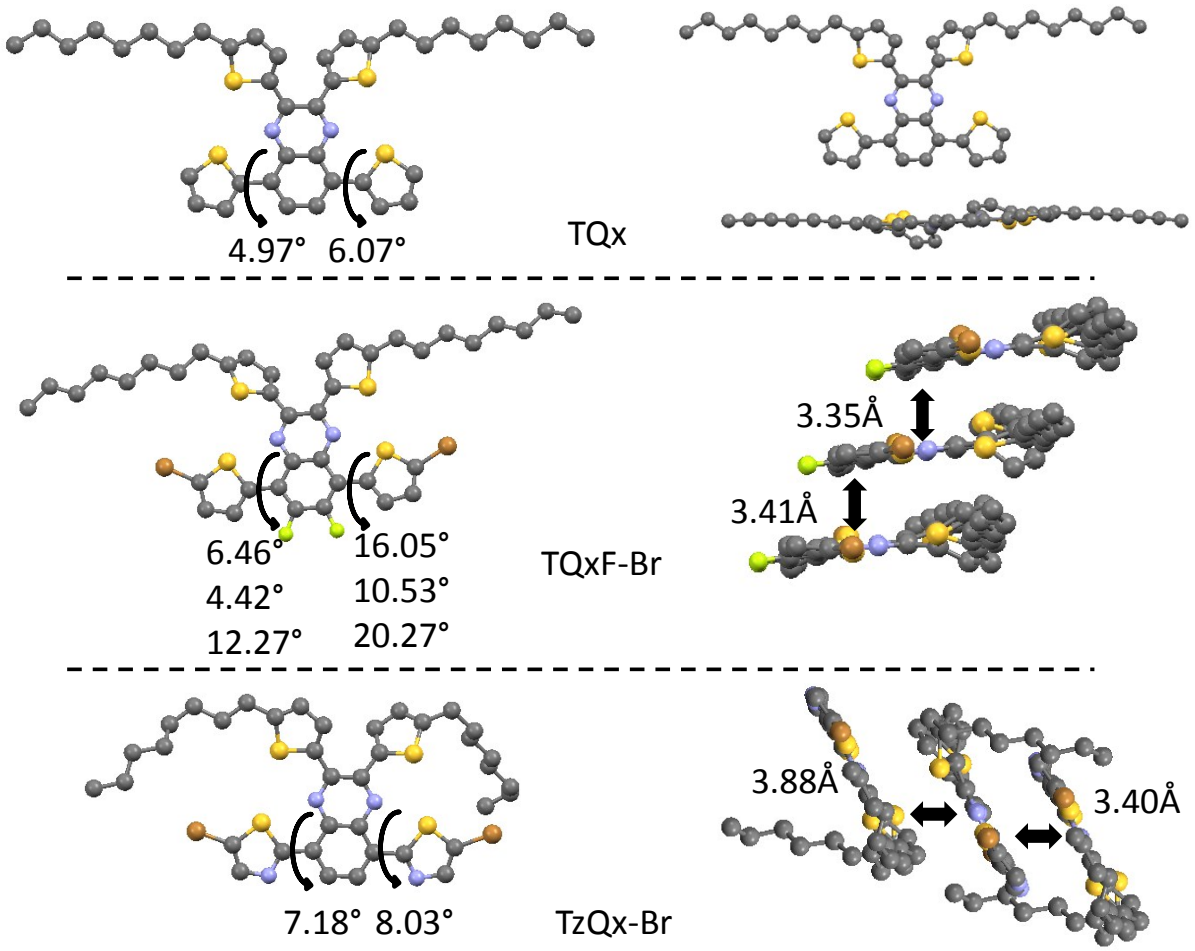

Figure S2. Chemical structure and stacking types in solid state of the molecules TQx, TQxF-Br and TzQx-Br determined by single crystal X-Ray diffraction measurements.

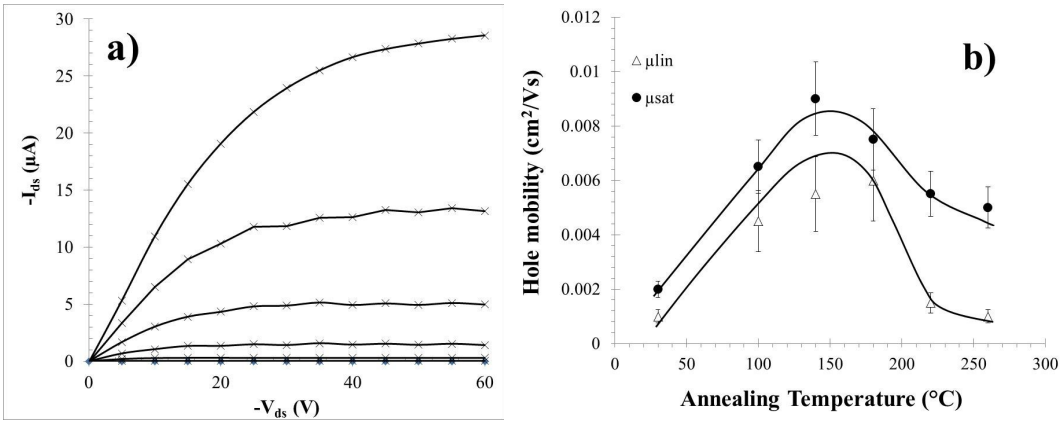

Figure S3. a) Output characteristic of a PDBS-TQxF OFET device annealed at 140°C for 10 minutes with a gate voltage ranging from 0 to -60 V by step of -10 V and b) Hole mobilities of

the polymer PDBS-TQxF in OFET devices in linear and saturated regimes as a function of the annealing temperature.

Table S2. Photovoltaic properties of the devices based on PDBS-TQx:$PC_{71}BM$ deposited in solution with various solvents and additives.

Active layer	Solvent	Additive	Thickness (nm)	V_{OC} (V)	J_{SC} ($mA.cm^{-2}$)	FF	η (%)
PDBS-TQx : $PC_{71}BM$ 1 : 2	o-DCB	3 % DIO	160	0.23	6.84	0.31	0.50
PDBS-TQx : $PC_{71}BM$ 1 : 2	CB	3 % DIO	50	0.85	9.72	0.62	5.14
PDBS-TQx : $PC_{71}BM$ 1 : 2	CB	10 % Anisole	50	0.82	4.55	0.43	1.60
PDBS-TQx : $PC_{71}BM$ 1 : 2	CB	10 % Anisole 3% DIO	50	0.83	8.14	0.58	3.87

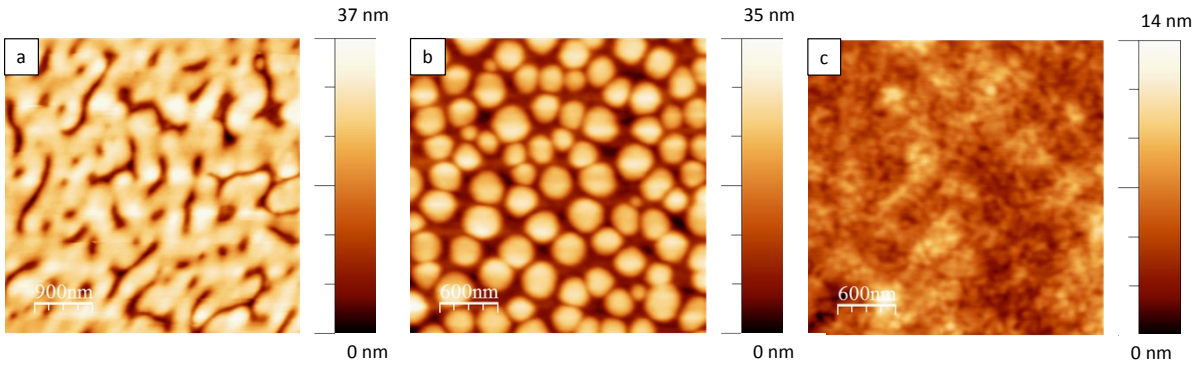

Figure S4. AFM images, topography, 3µm x 3 µm of active layer made of: PDBS-TQx : $PC_{70}BM$ 1:2 deposited in solution in chlorobenzene (a) and with additives such as 10 % anisole (b) and 3 % DIO (c).

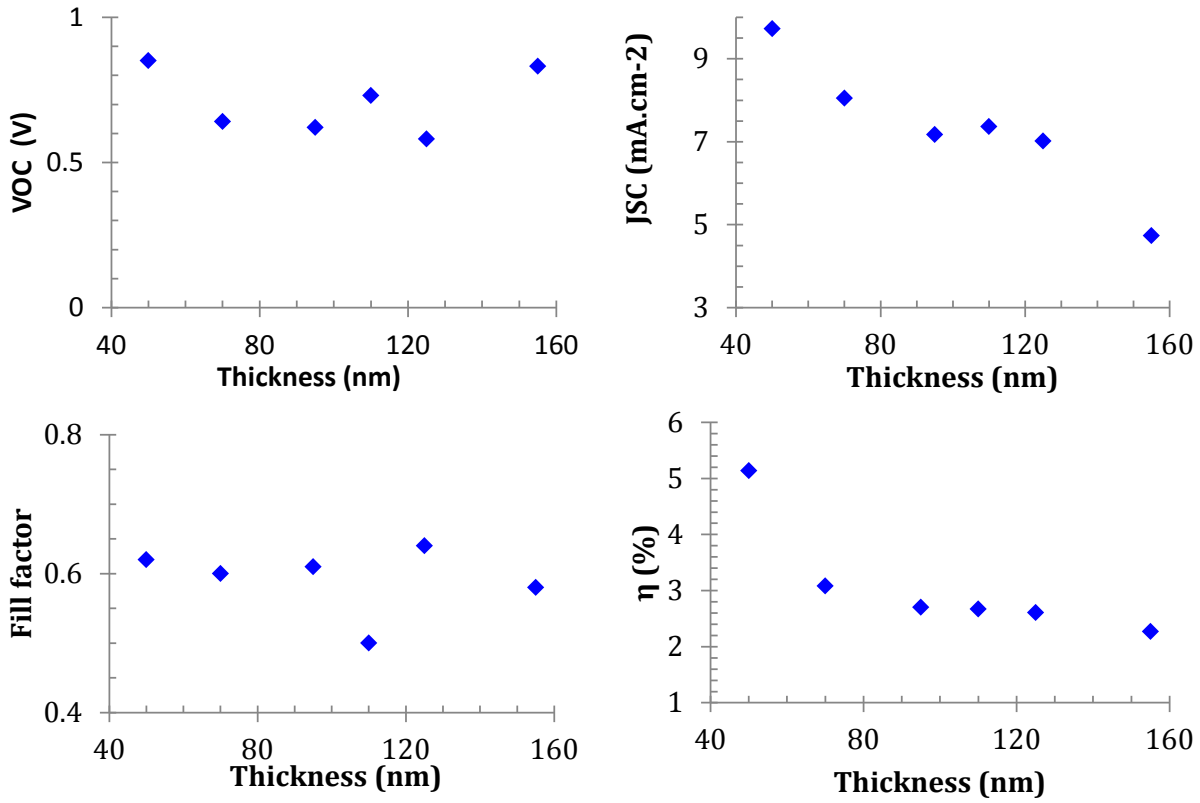

Figure S5. Photovoltaic characteristics obtained with the blend PDBS-TQx:$PC_{71}BM$ 1:2 according to the active layer thickness.

Table S3. Photovoltaic characteristics obtained with the blend PDBS-TQx:$PC_{71}BM$ 1:2. [a]PCE average on five devices.

Active layer	Solvent	Additive	Thickness (nm)	V_{OC} (V)	J_{SC} (mA.cm^{-2})	FF	η (%)
PDBS-TQx : $PC_{71}BM$ 1 : 2	CB	3 % DIO	155	0.83	4.73	0.58	2.27
PDBS-TQx : $PC_{71}BM$ 1 : 2	CB	3 % DIO	125	0.58	7.01	0.64	2.61
PDBS-TQx : $PC_{71}BM$ 1 : 2	CB	3 % DIO	110	0.73	7.36	0.50	2.67
PDBS-TQx : $PC_{71}BM$ 1 : 2	CB	3 % DIO	95	0.62	7.17	0.61	2.70
PDBS-TQx : $PC_{71}BM$ 1 : 2	CB	3 % DIO	70	0.64	8.04	0.60	3.08
PDBS-TQx : $PC_{71}BM$ 1 : 2	CB	3 % DIO	50	0.85	9.72	0.62	5.14 ([a]4.93)

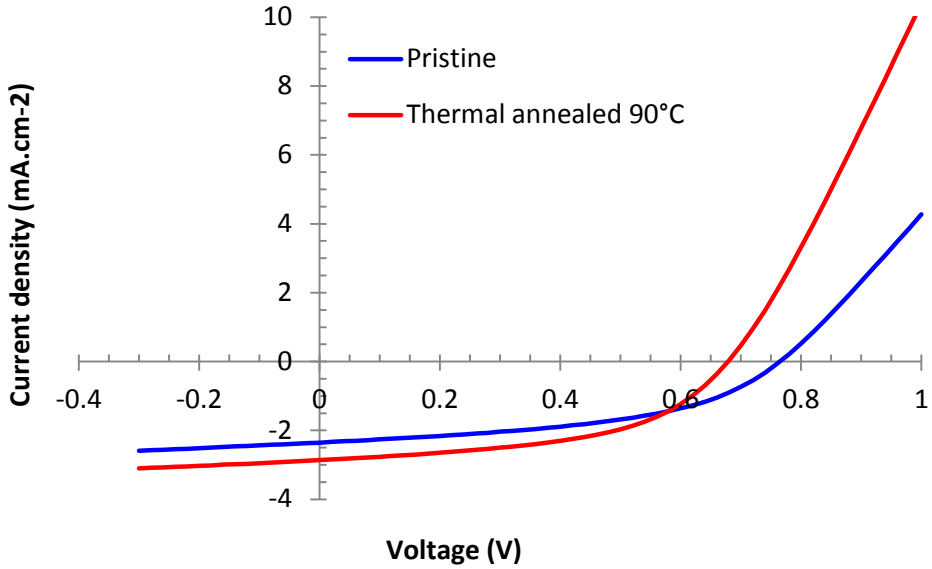

Figure S6. *J*-V curves of the devices from PDBS-TQxF with $PC_{71}BM$ deposited in solution in *p*-xylene.

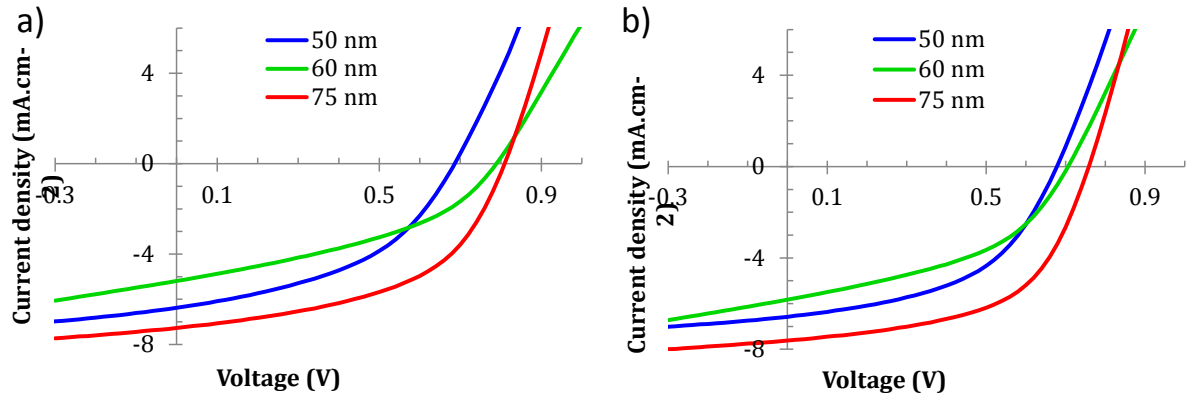

Figure S7. *J*-V curves of the devices from PDBS-TQxF with $PC_{71}BM$ deposited in solution in chlorobenzene (a) as cast and (b) after thermal annealing at 120 °C.

Table S4. Photovoltaic characteristics obtained with the blend PDBS-TQxF:$PC_{71}BM$ 1:2. [a]PCE average on five devices.

Active layer	Solvent	Thermal annealing (°C)	Thickness (nm)	V_{OC} (V)	J_{SC} ($mA.cm^{-2}$)	FF	η (%)
PDBS-TQxF : $PC_{71}BM$ 1 : 2	*p*-xylene + 3 % DIO	-	60	0.77	2.36	0.47	0.85
PDBS-TQxF : $PC_{71}BM$ 1 : 2	*p*-xylene + 3 % DIO	90	60	0.68	2.86	0.51	0.99
PDBS-TQxF : $PC_{71}BM$ 1 : 2	CB + 3 % DIO	-	50	0.69	6.38	0.45	1.96
PDBS-TQxF : $PC_{71}BM$ 1 : 2	CB + 3 % DIO	120	50	0.68	6.58	0.49	2.20
PDBS-TQxF : $PC_{71}BM$ 1 : 2	CB + 3 % DIO	-	60	0.79	5.20	0.40	1.64
PDBS-TQxF : $PC_{71}BM$ 1 : 2	CB + 3 % DIO	120	60	0.71	5.83	0.44	1.83
PDBS-TQxF : $PC_{71}BM$ 1 : 2	CB + 3 % DIO	-	75	0.81	7.27	0.51	2.98 ([a]2.78)
PDBS-TQxF : $PC_{71}BM$ 1 : 2	CB + 3 % DIO	120	75	0.76	7.61	0.55	3.19

Table S5. Photovoltaic characteristics obtained with the blend PDBS-TzQx:$PC_{71}BM$. [a]PCE average on five devices.

Active layer	Solvent	Additive	Thickness (nm)	V_{OC} (V)	J_{SC} ($mA.cm^{-2}$)	FF	η (%)
PDBS-TzQx : $PC_{71}BM$ 1 : 2	CB	3 % DIO	50	0.63	4.92	0.41	1.27 ([a]1.03)
PDBS-TzQx : $PC_{71}BM$ 1 : 2	CB	3 % DIO	100	0.54	4.09	0.40	0.89
PDBS-TzQx : $PC_{71}BM$ 1 : 3	CB	3 % DIO	85	0.54	2.93	0.43	0.67