

Quinoxaline-functionlized C₆₀ derivatives as electron acceptors in organic solar cells

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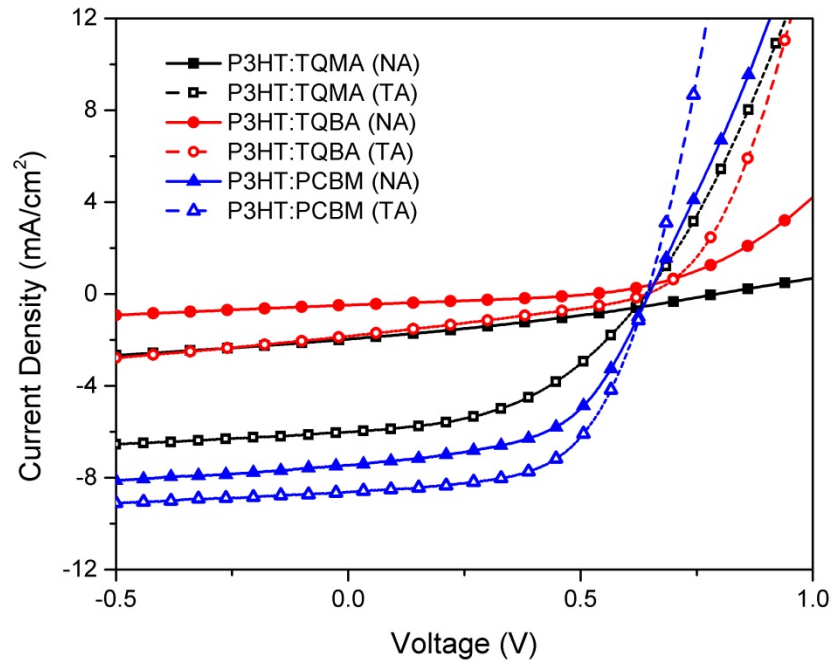


Fig. S1 J - V characteristics of as-cast (NA) and thermally annealed (TA) P3HT BHJ-OSCs devices with various acceptors under AM 1.5G (100 mW cm^{-2}) illumination. The device configuration is ITO/PEDOT:PSS/BHJ/Al.

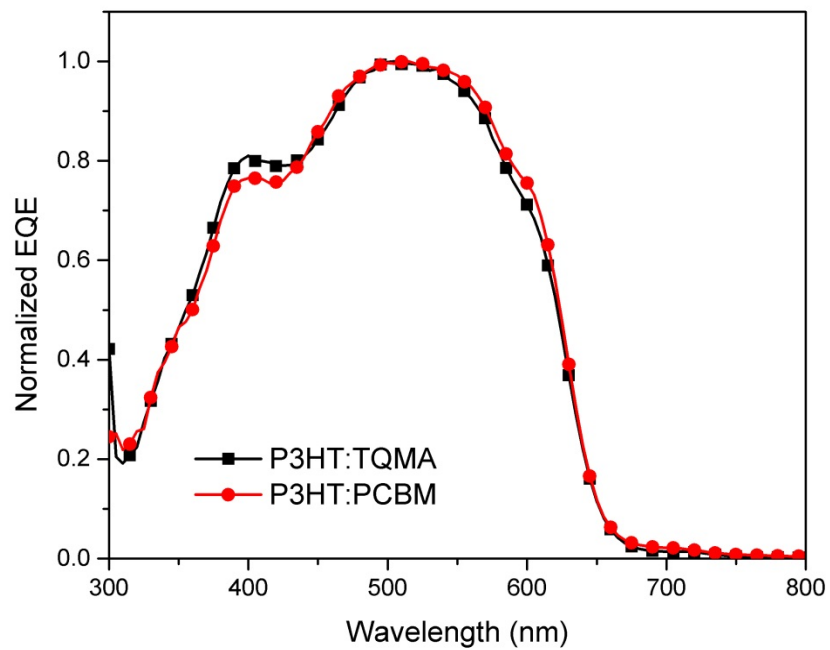


Fig. S2 EQE spectra of P3HT:TQMA and P3HT:PCBM BHJ-OSCs devices. Both spectra are normalized to their respective EQE_{max} .

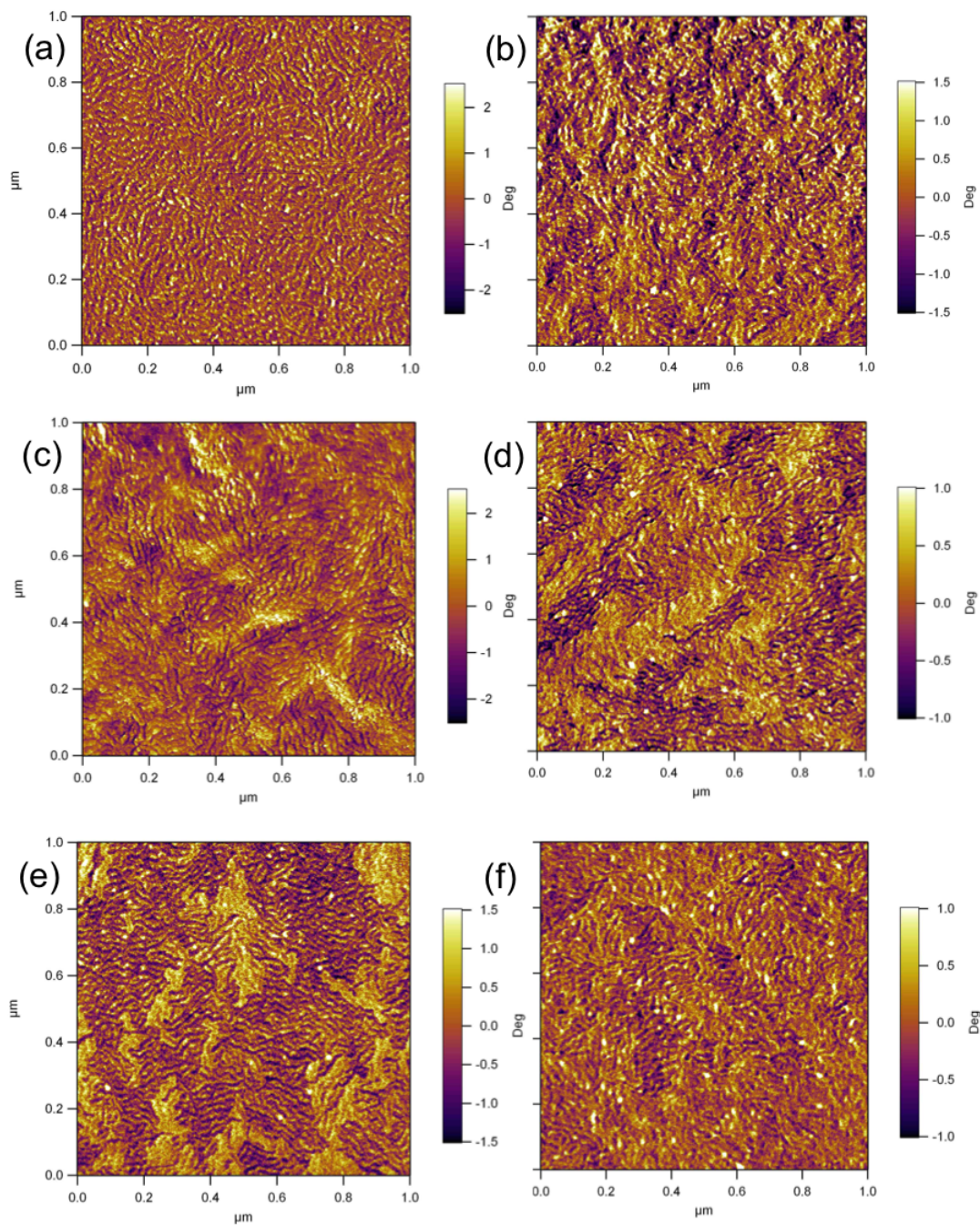


Fig. S3. Tapping-mode AFM phase images of (a,b) P3HT:TQMA, (c,d) P3HT:TQBA and (e,f) P3HT:PC₆₁BM. The left images are those of the as-cast (NA) blends, while the right ones correspond to the thermally-annealed (TA) blends. The scan size is $1 \times 1 \mu\text{m}^2$.

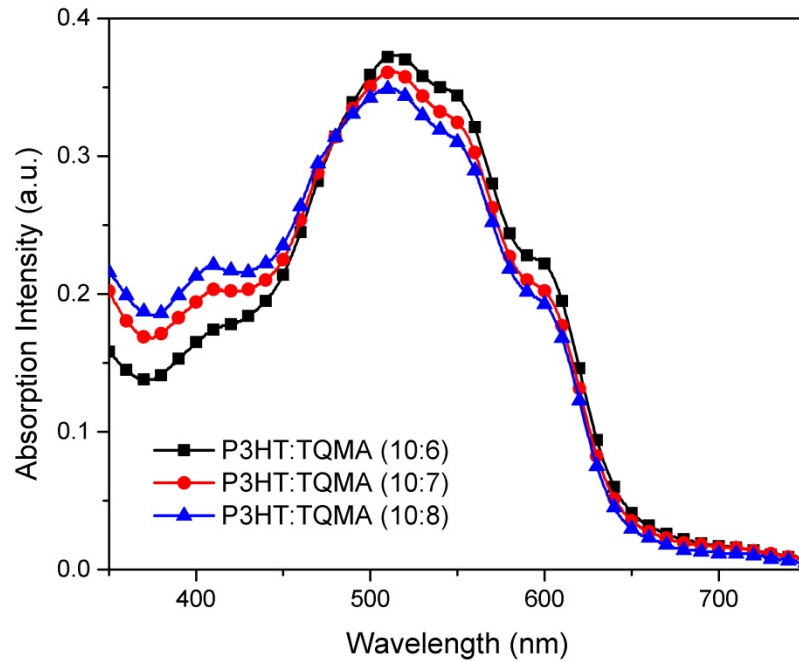


Fig. S4. UV-Vis absorption spectra of thermally annealed P3HT:TQMA blend films with different D:A ratios.

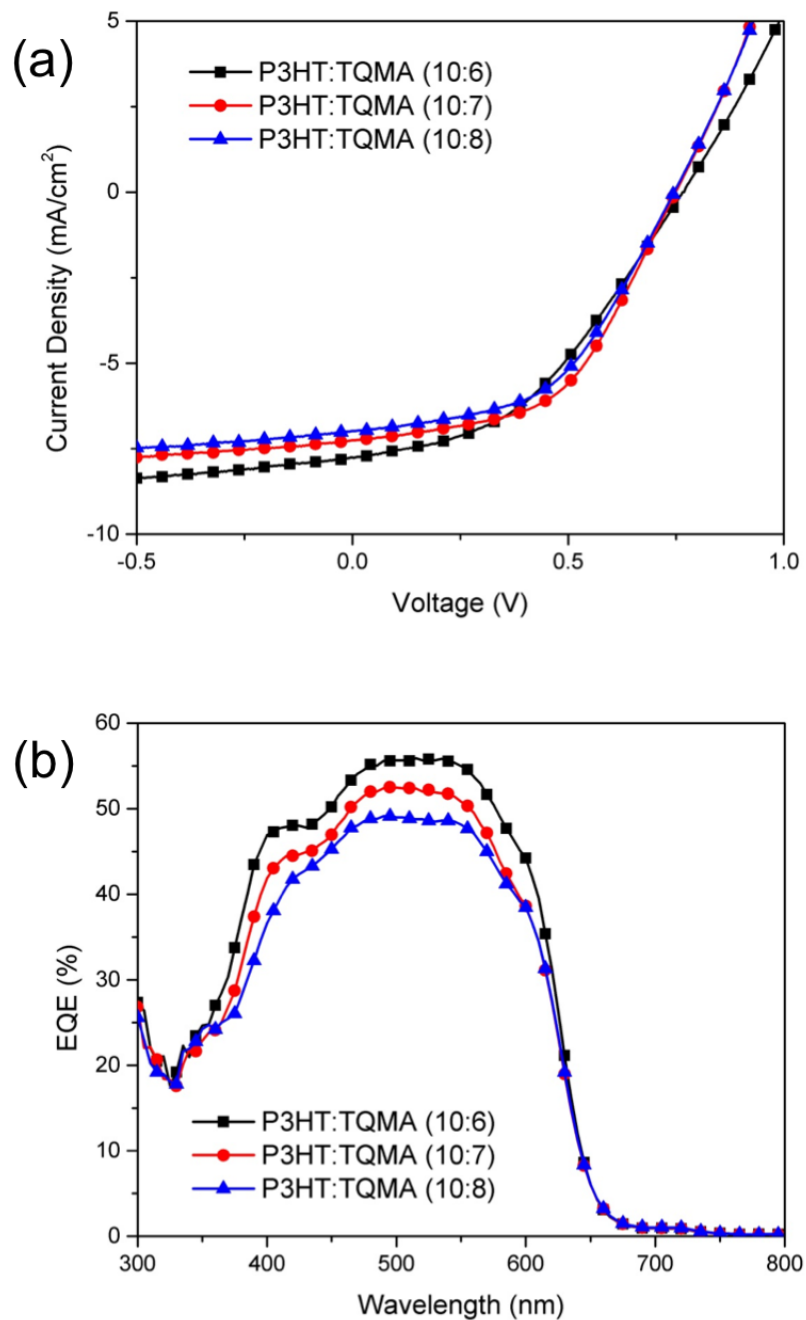
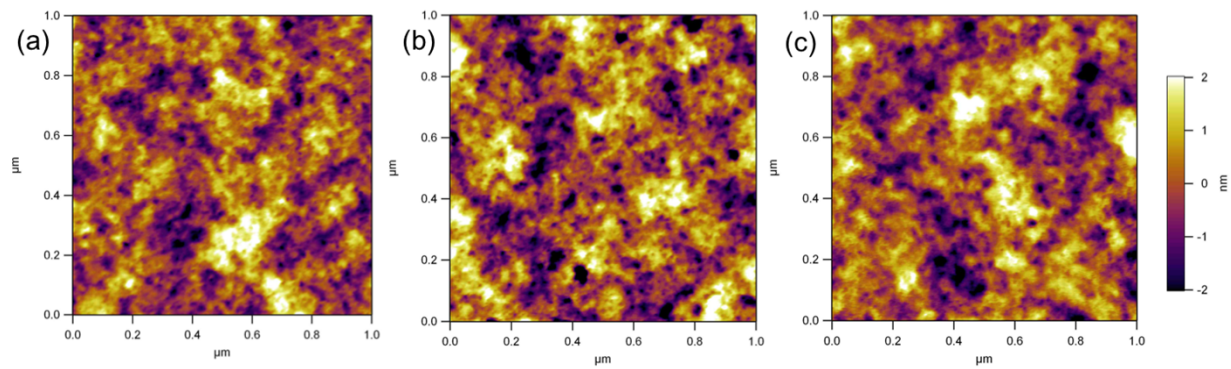


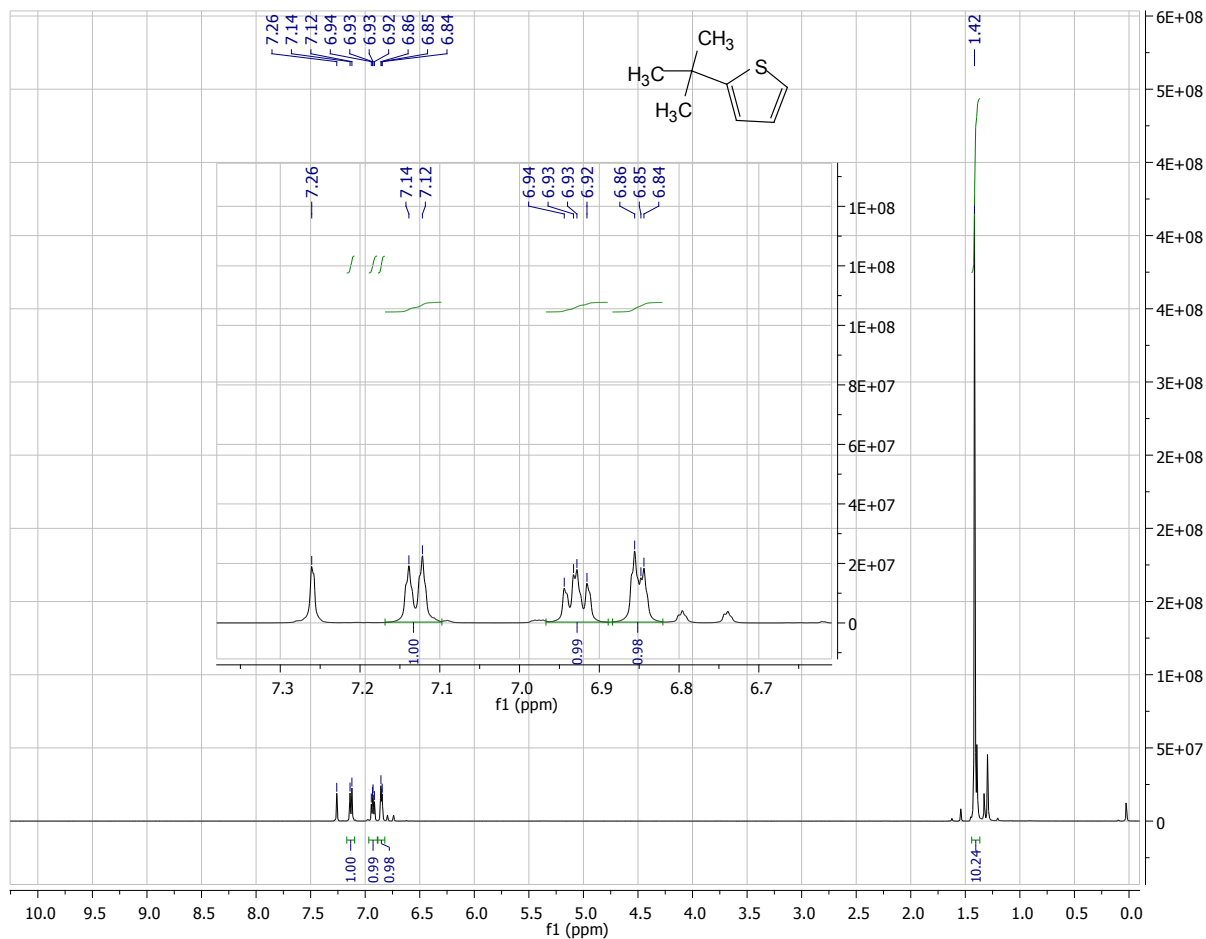
Fig. S5 (a) $J-V$ characteristics and (b) EQE spectra of P3HT:TQMA BHJ-OSCs devices with different D:A ratios. The device configuration is ITO/PEDOT:PSS/BHJ/TiO_x/Al. The $J-V$ characteristics were measured under AM 1.5G (100 mW cm^{-2}) illumination.

Fig. S6 Tapping-mode AFM height images of P3HT:TQMA with different D:A ratios: (a) 10:6, (b) 10:7 and (c) 10:8. The scan size is $1 \times 1 \mu\text{m}^2$.



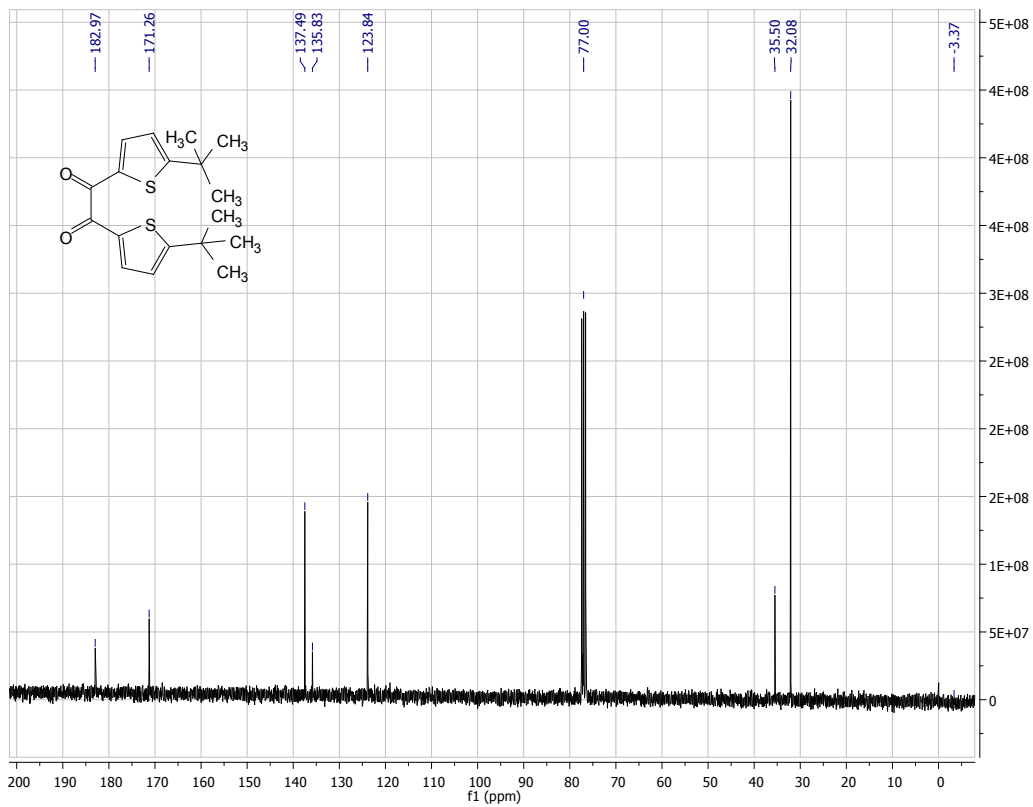
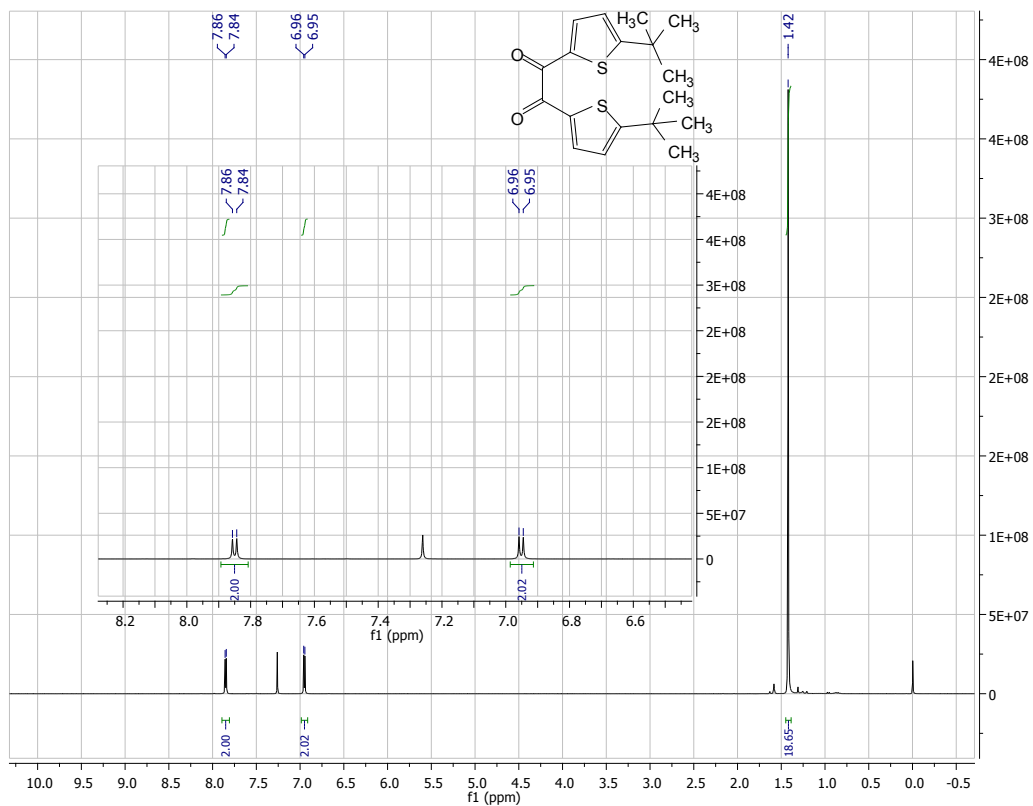
7. NMR and HRMS spectra for the compounds

2-*tert*-butylthiophene(R1): Synthesized according to the literature, colorless liquid. ¹H NMR (300 MHz, CDCl₃) δ: 7.14–7.12 (m, 1H), 6.94–6.92 (m, 1H), 6.86–6.84 (m, 1H), 1.39 (s, 9H).



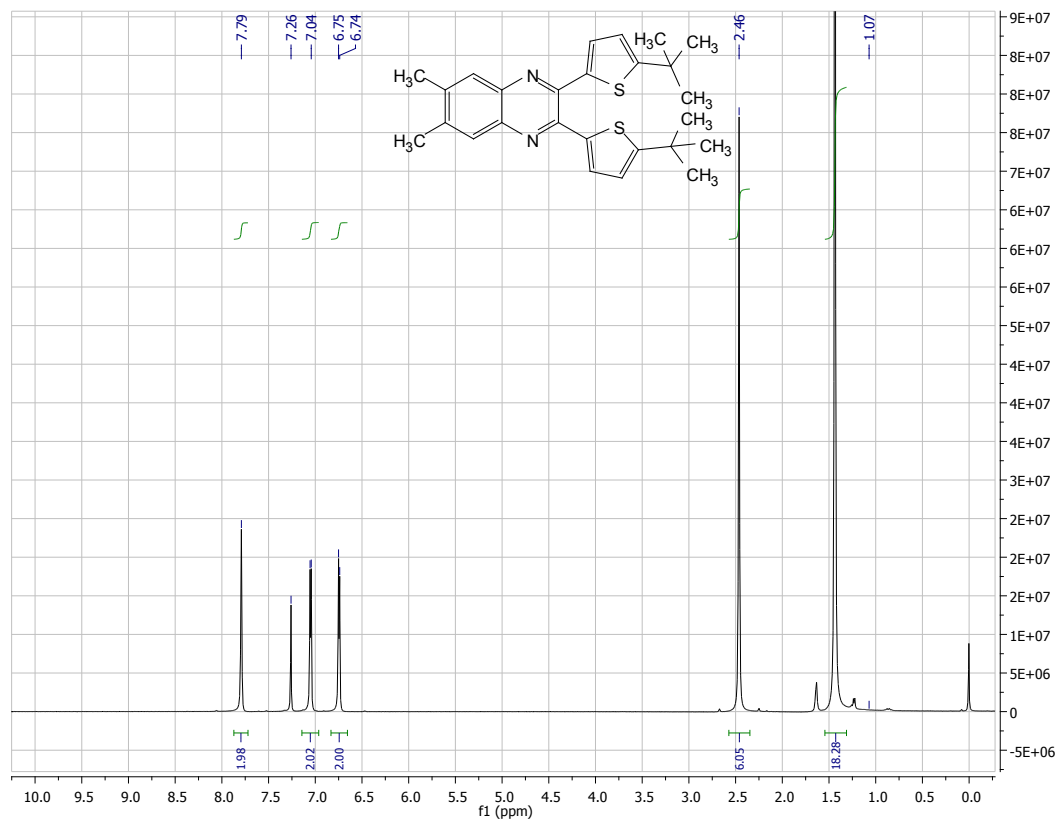
1,2-bis(5-*tert*-butylthiophen-2-yl)ethane-1,2-dione(R2):

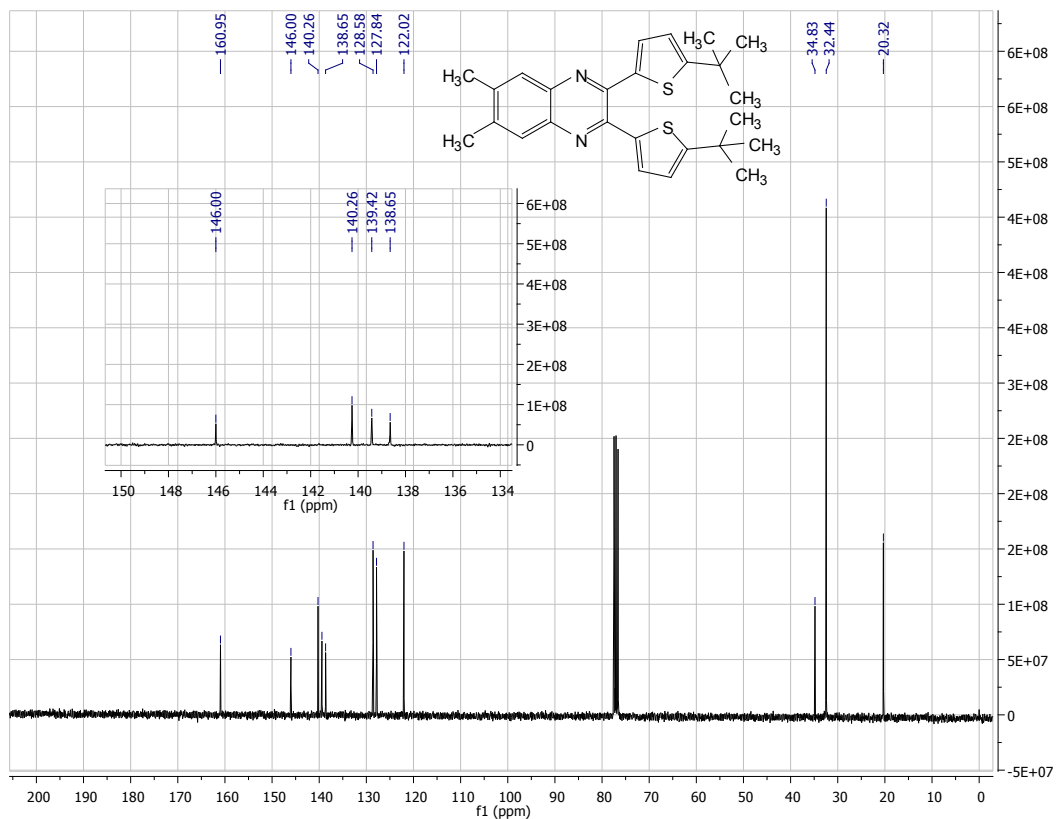
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
335.1143	335.1139	0.4	1.2	7.5	22.2	0.0	C ₁₈ H ₂₃ O ₂ S ₂



2,3-bis(5-*tert*-butylthiophen-2-yl)-6,7-dimethylquinoxaline(R3):

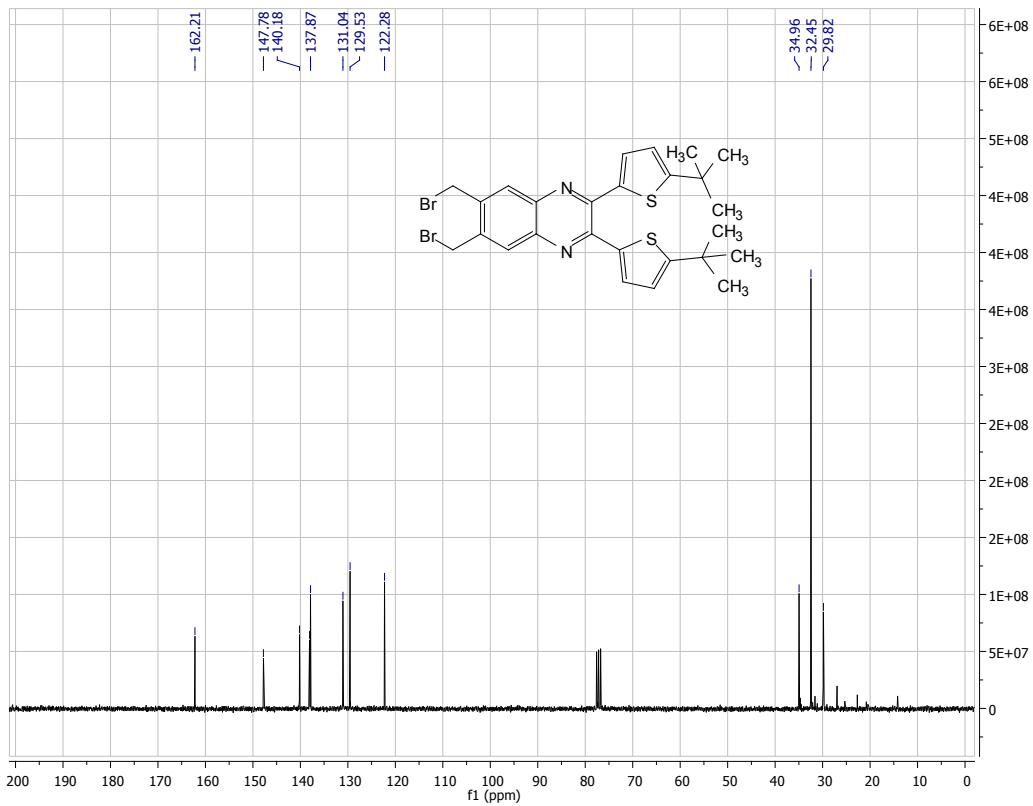
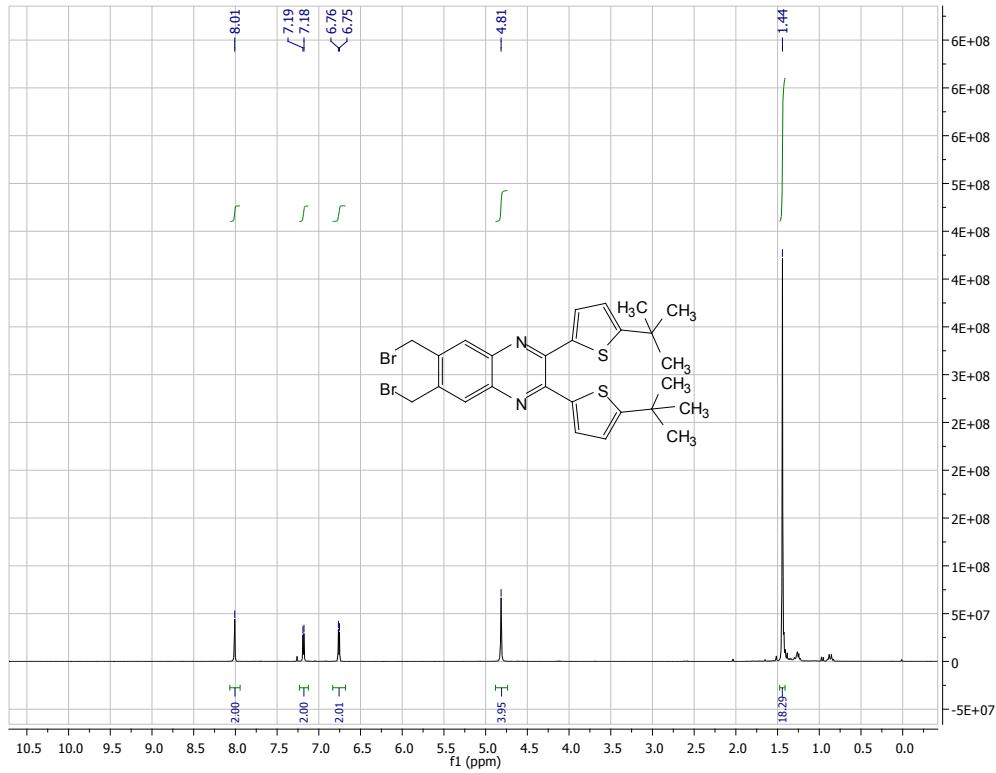
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
435.1919	435.1929	-1.0	-2.3	12.5	29.4	0.0	C ₂₆ H ₃₁ N ₂ S ₂





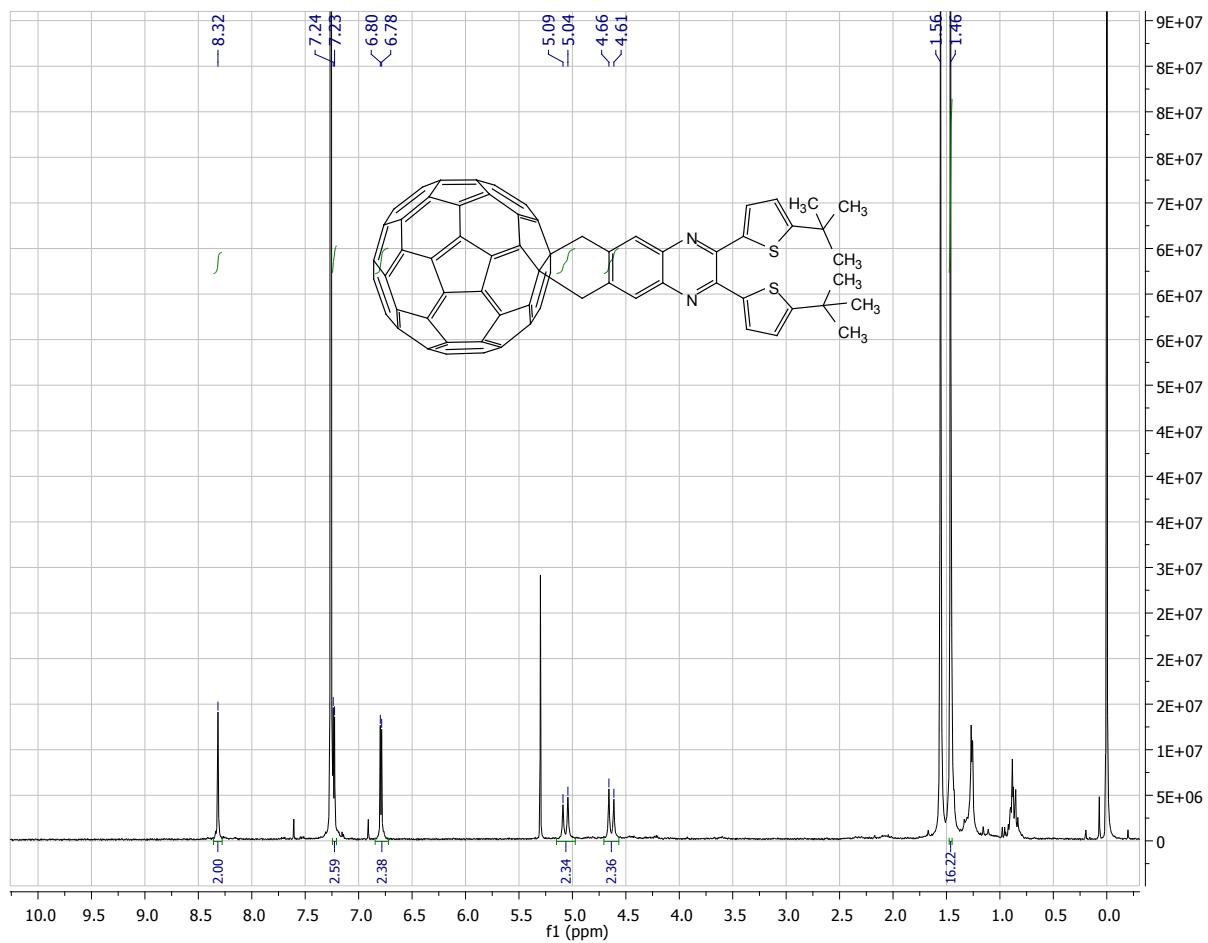
6,7-bis(bromomethyl)-2,3-bis(5-tert-butylthiophen-2-yl)quinoxaline(R4):

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
592.9991	593.0118	-12.7	-21.4	12.5	10.9	0.0	C26 H29 N2 S2 79Br 81Br

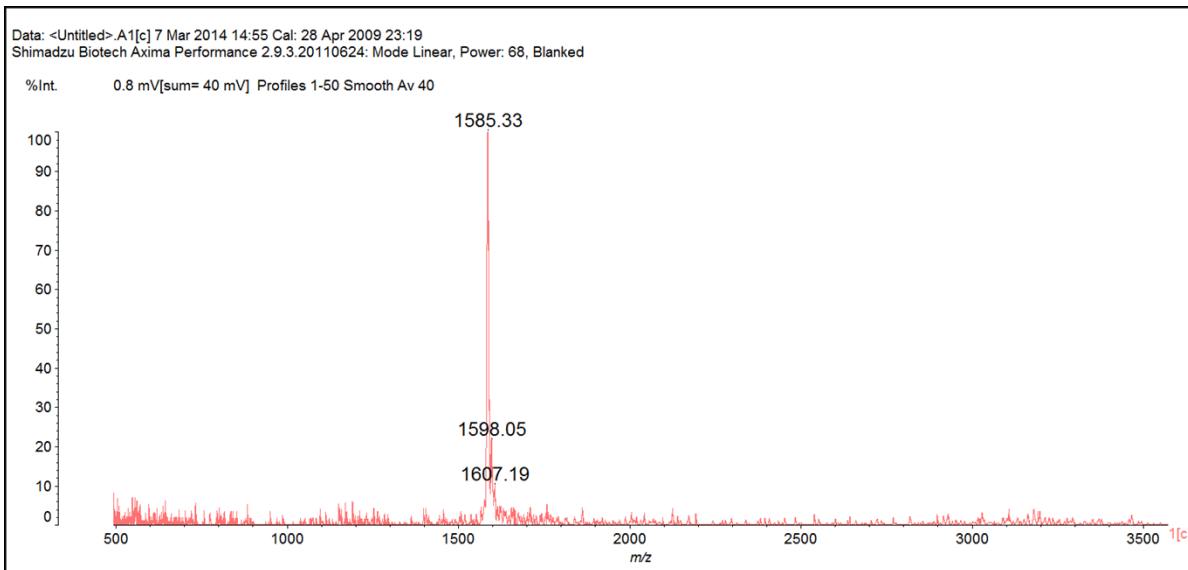
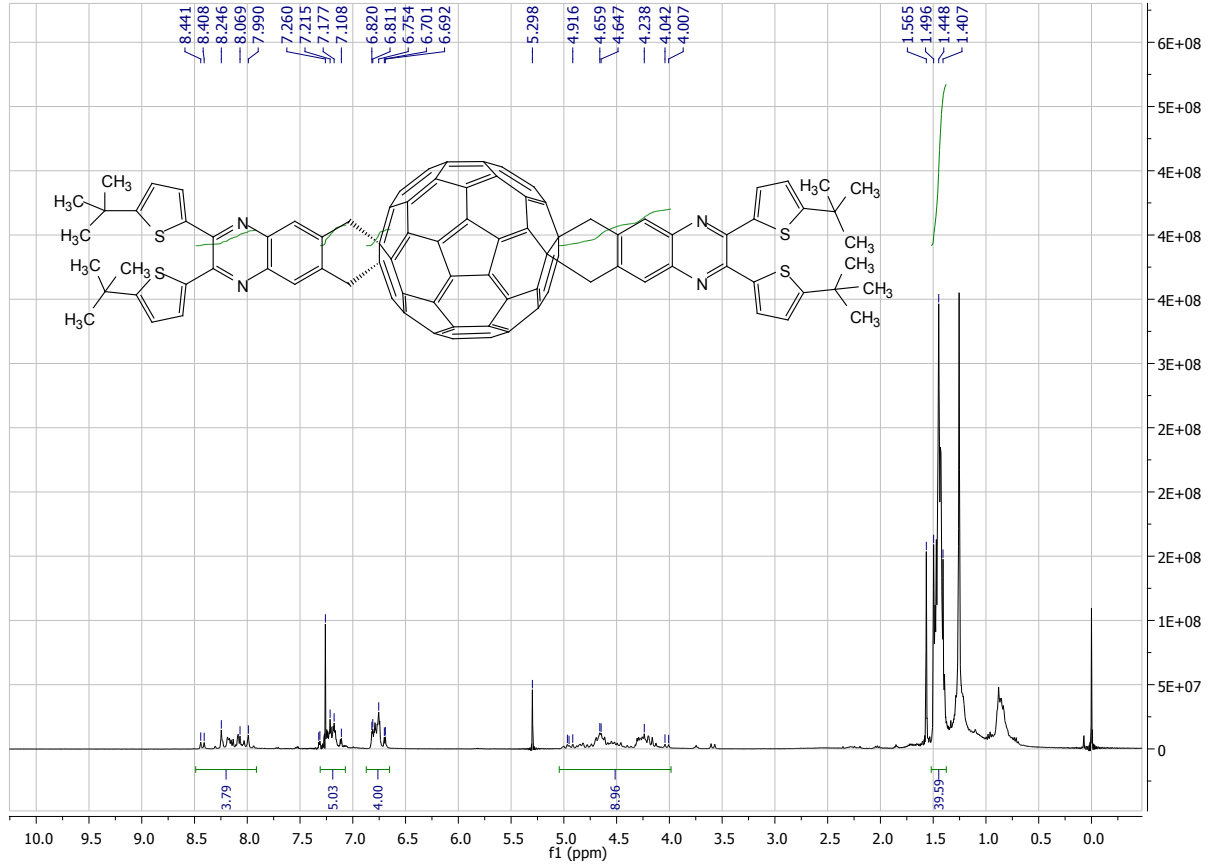


TQMA:

Minimum:				-1.5				
Maximum:		5.0	200.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula	
1153.0865	1153.1772	-90.7	-78.7	73.5	11.5	0.0	C86 H29 N2 S2	



TQBA:



Data: <Untitled> A2[c] 7 Mar 2014 15:05 Cal: 28 Apr 2009 23:19
Shimadzu Biotech Axima Performance 2.9.3.20110624: Mode Linear_neg, Power: 75, Blanked

%Int. 111 mV[sum= 5564 mV] Profiles 1-50 Smooth Av 40

