Supplementary Information

Novel bis-C₆₀ derivative compared to other fullerene bis-adducts in high efficiency polymer photovoltaic cells

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High-pressure liquid chromatography (HPLC) of purified mono- and bis-oQDMC₆₀

High-pressure liquid chromatography (HPLC) was conducted on an Agilent 1100 Series instrument. <u>Column</u>: Nacalai Tesque COSMOSIL 2-(1-pyrenyl)ethylsilica stationary phase (BuckyPrep column), 250 × 4.6 mm), <u>mobile phase</u>: toluene, 1 mL min⁻¹; <u>detection</u>: 330 nm. The analysis report for mono-oQDMC₆₀ and bis-oQDMC₆₀ are presented below.



Figure S1 and Table S1: Chromatogram and corresponding automatic peak fitting results for mono-oQDMC $_{60}$



Peak #	Ret.Time (min)	Туре	Width (min)	Area (mAU*s)	Height (mAU)	Area (%)	
 1	4.409	MM R	0.2456	1.68360e4	1142.52832	99.1679	-
2	4.927	MM T	0.1957	63.54811	6.27805	0.3743	
3	5.699	MM T	0.1581	66.19418	6.97937	0.3899	
4	8.115	MM	0.2420	11.52285	7.93747e-1	0.0679	

Figure S2 and Table S2: Chromatogram and corresponding automatic peak fitting results for bisoQDMC60. The peak at a retention time of 4.927 min is thought to correspond to an isomer of bisoQDMC₆₀.



Figure S3: Cyclic voltammetry measurement of PCBM, mono- and bis-oQDMC₆₀, bis-PCBM and ICBA.



Figure S4: Absorption spectra of the various fullerenes in ~25 nm thick solid films.



Figure S5: Impact of the polymer:fullerene ratio on photovoltaic device parameters (a) and on the optical absorption properties of the blend (b).



Figure S6: (a) Current density vs. voltage characteristics under 100 mW/cm² AM1.5G simulated solar illumination of devices blends of P3HT :bis-oQDMC₆₀ dried either fast or slow. (b) EQE of corresponding devices.

	processing	Position(°)	Position (Å)	Peak height (counts)	Width (°)	Area (counts)	Crystal size (nm)
Bis-oQDMC ₆₀	Fast drying	5.29	16.69	127.4	0.25	34.1	32
	Slow drying	5.27	16.75	48.7	0.34	17.9	23
Bis-oQDMC ₆₀	Fast drying	5.24	16.84	45.7	0.3	14.8	27
with additives	Slow drying	5.16	17.11	48.2	0.34	17.4	23
P3HT:PCBM	Slow drying	5.21	16.94	85.2	0.48	34.1	17
P3HT	Slow drying	5.38	16.41	176.9	0.4	76.1	20
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Table S3: Crystallographic parameters for P3HT:bis-oQDMC₆₀, P3HT:PCBM blends and P3HT layers processed in varying conditions. The here tabulated values are extracted from XRR measurements presented in Fig.4 (b).



Figure S7: Normalized UV-visible spectra of P3HT:bis-oQDMC₆₀ layers annealed as varying temperature for 10 min after the solvent annealing.