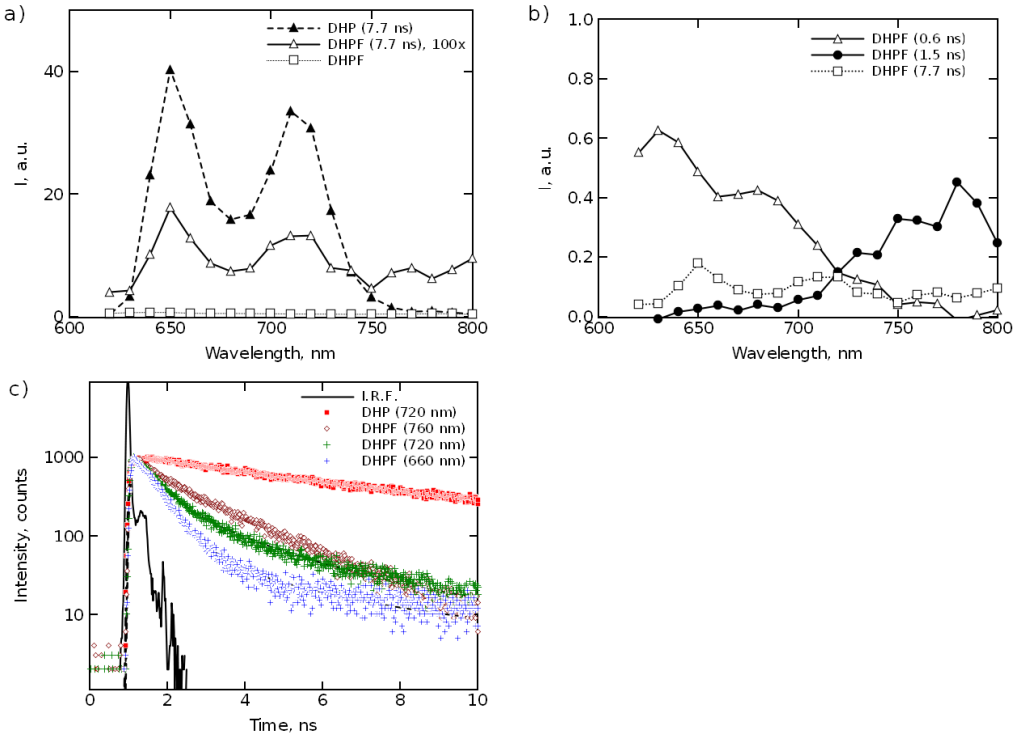
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Directed electron transfer in Langmuir-Schäfer layer of porphyrin-fullerene and phthalocyanine-fullerene dyads in inverted organic solar cells

A. Tolkki, K. Kaunisto, A. Efimov, H. Kivistö, L. Storbacka, R. Savikoski, K. Huttunen, S. Lehtimäki, H. Lemmetyinen

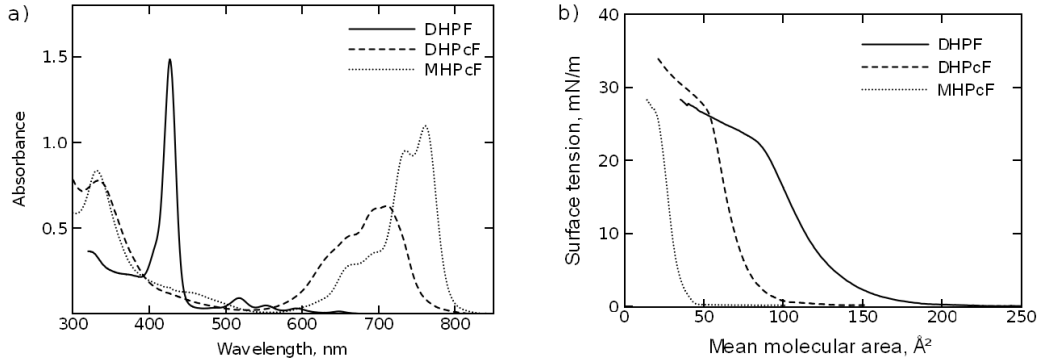
Department of Chemistry and Bioengineering, Tampere University of Technology, P.O. Box 541, FI-33101, Tampere, Finland

Supplementary Information, S1



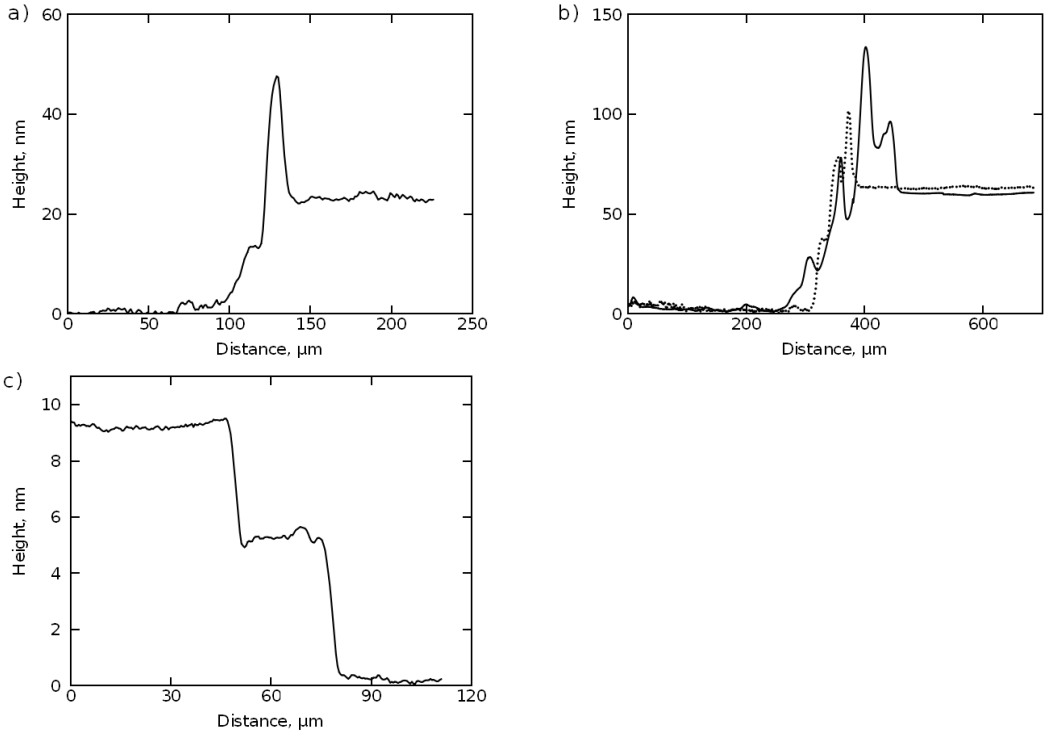
FigureS1. a) Decay associated fluorescence component spectra of DHP and the longest-living component of DHPF in $CHCl_3$. The signal of DHPF is multiplied with 100 for comparison to the spectrum of DHP. b) The three components of the DHPF fluorescence decay in $CHCl_3$. Intensities are expressed as a product of relative amplitude and the corresponding lifetime ($A\ \tau$), which were obtained from three-exponential global fit. c) Decay curves (colored markers) at different monitoring wavelengths and convoluted fits (dashed lines) (λ_{ex} = 405 nm, 2.5 MHz). Signals were accumulated to 1000 counts.

Supplementary Information, S2



FigureS2. a) Absorption spectra of dyads in solutions (0.3 mM in $CHCl_3$), from which the spreading of the molecules onto the Langmuir surface was performed. b) Langmuir surface pressure-area isotherms of complete compressions.

Supplementary Information, S3



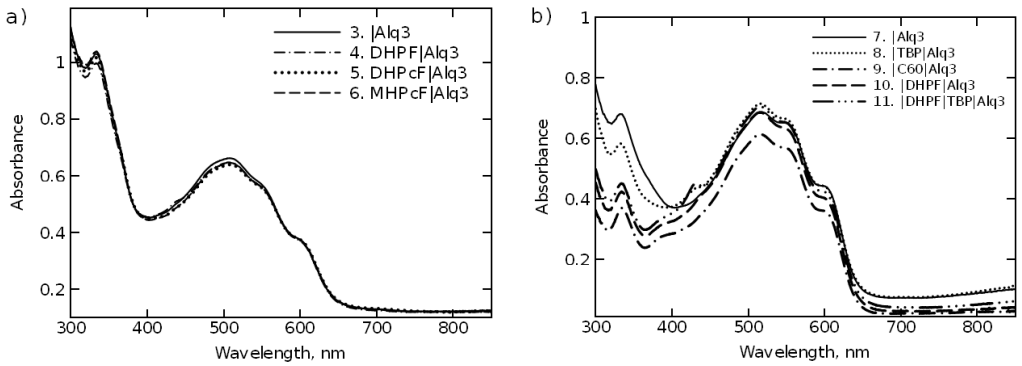
FigureS3. Data obtained with optical profilometer: Step profiles of a) Quartz|1xODA|7xDHPF, b) P3HT:PCBM|Alq_3 (solid) and P3HT:PCBM|1xDHPF|Alq_3 (dashed) deposited onto ITO|ZnO substrate, and c) Calibration measurement: Two LB deposited double-layers of octadecylamine (ODA) on stack (d_1≈2.5 nm). Phase shifting mode and 20× objective were used. Data is averaged from 50 µm width perpendicular to the step. For calibration measurement, the step was produced by adjusting the depth of vertical dipping. Otherwise the steps were post-produced by removing part of the film with $CHCl_3$.

Supplementary Information, S4

Table S4. Long term air stability of the OSCs presented in the main text: Indexes *i* and *f* indicate initial and final values obtained after 1 day and several months after preparation and storage in dark ambient atmosphere. The device with the highest initial performance was investigated.

Device (days in storage)	P_{in} *i/f* (mW/cm^2)	J_{sc} *i/f* (mA/cm^2)	V_{oc} *i/f* (V)	FF *i/f*	η_i (%)	η_f (%)	$\Delta\eta$ (%)
1. P3HT:PCBM|Alq_3 (390)	42.9 / 39.7	3.89 / 3.28	0.41 / 0.54	0.49 / 0.54	1.84	2.27	+52
2. P3HT:PCBM|DHPF|Alq_3 (390)	42.9 / 39.7	4.94 / 3.58	0.49 / 0.55	0.47 / 0.55	2.64	2.73	+7.6
3. P3HT:PCBM|Alq_3 (350)	41.1 / 39.7	3.54 / 3.35	0.47 / 0.52	0.54 / 0.59	2.19	2.49	+26
4. P3HT:PCBM|DHPF|Alq_3 (350)	41.1 / 39.7	4.80 / 3.01	0.51 / 0.54	0.54 / 0.60	3.21	2.79	-8.8
5. P3HT:PCBM|DHPcF|Alq_3 (350)	41.1 / 39.7	4.32 / 3.56	0.50 / 0.53	0.54 / 0.57	2.86	2.47	-9.9
6. P3HT:PCBM|MHPcF|Alq_3 (350)	41.1 / 39.7	4.76 / 3.31	0.46 / 0.53	0.55 / 0.61	2.92	3.11	+14
7. P3HT:PCBM|Alq_3 (30)	38.1 / -	4.56 / -	0.51 / -	0.60 / -	3.64	-	-
8. P3HT:PCBM|TBP|Alq_3 (30)	38.1 / -	4.82 / -	0.49 / -	0.56 / -	3.47	-	-
9. P3HT:PCBM|C60|Alq_3 (30)	38.1 / -	4.96 / -	0.51 / -	0.57 / -	3.82	-	-
10. P3HT:PCBM|DHPF|Alq_3 (30)	38.1 / 36.1	5.49 / 4.24	0.52 / 0.55	0.59 / 0.57	4.39	3.67	-16.4
11. P3HT:PCBM|DHPF|TBP|Alq_3 (30)	38.1 / 36.1	5.09 / 4.43	0.53 / 0.55	0.58 / 0.64	4.18	4.34	+3.8

Supplementary Information, S5



FigureS5. Absorption spectra of the OSC devices equipped with P3HT:PCBM layer and a) different dyad compounds (DHPF, DHPcF and MHPcF) as monolayers. b) Plain porphyrin (TBP), plain C_{60}, DHPF monolayer, and DHPF|TBP double-layer.