Supporting information

A triazatruxene-based molecular dyad for single-component organic solar cells

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NMR Spectra:

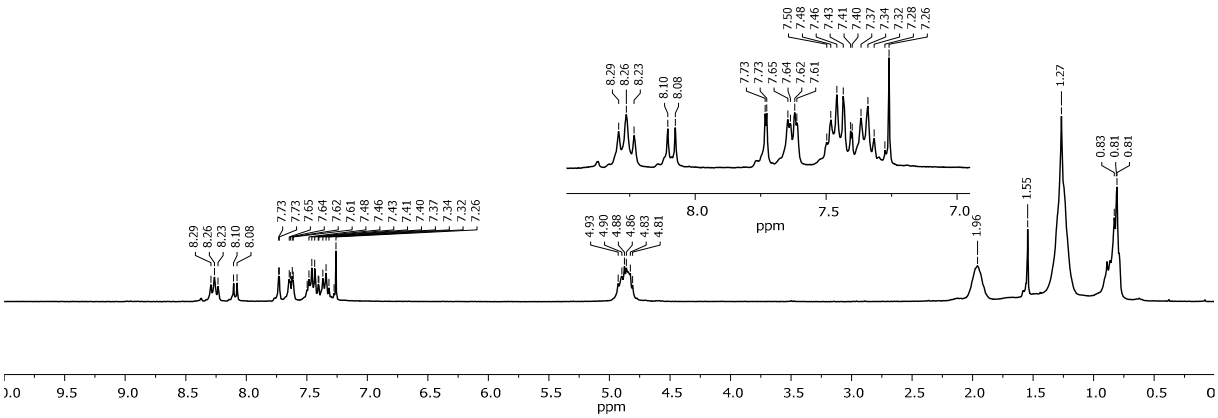

Figure S1: ^{1}H NMR (300 MHz) of **TAT-Br** in $CDCl_3$ at 20 °C.

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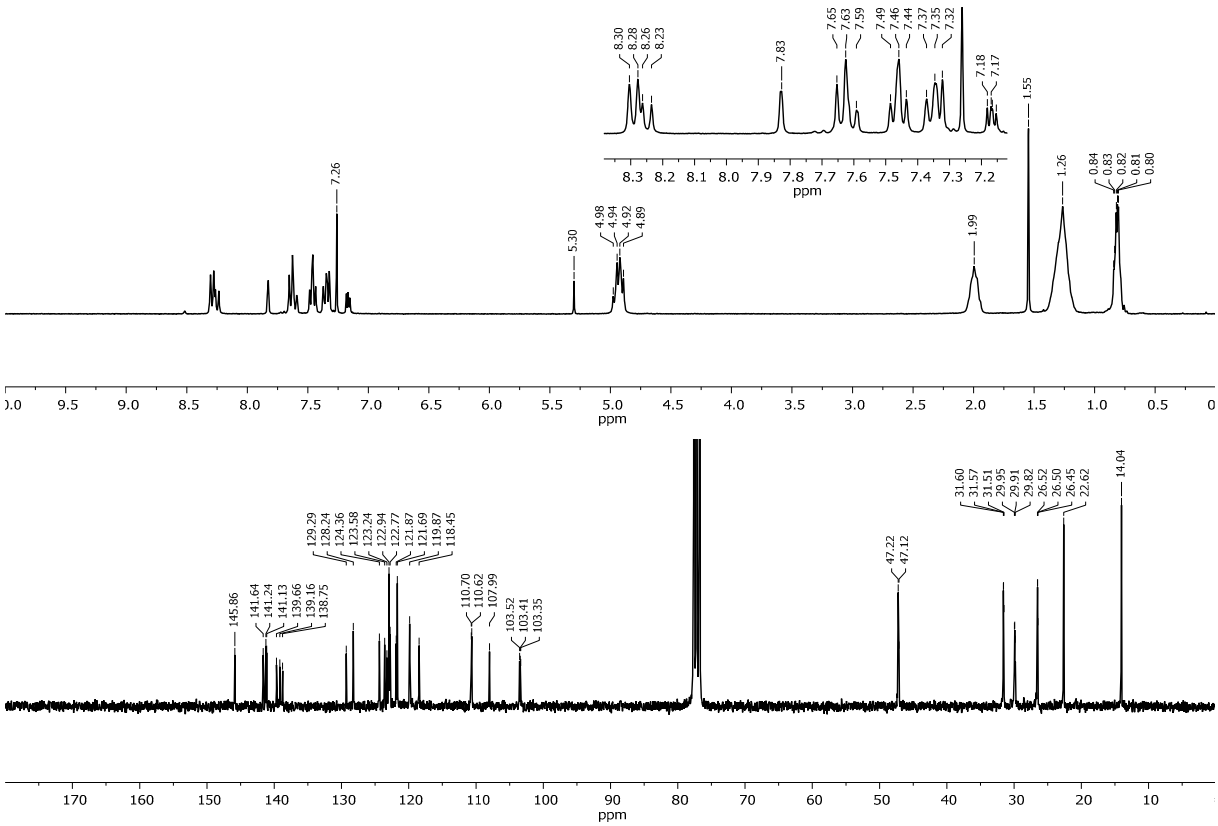


Figure S2 : ^{1}H NMR (300 MHz) (top) and ^{13}C NMR (76MHz) (bottom) of **TAT-T** in $CDCl_3$ at 20 °C.

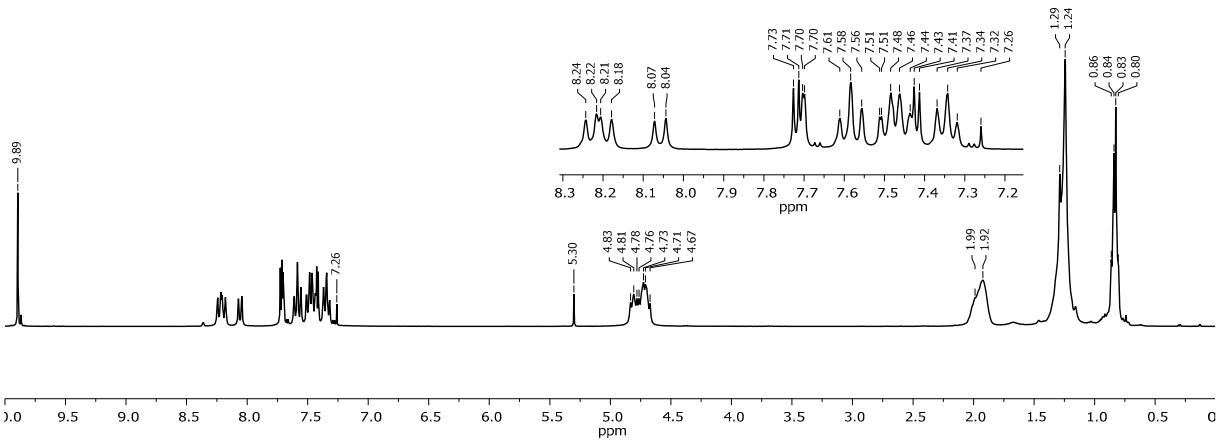


Figure S3 : ^{1}H NMR (300 MHz) of **TAT-T-CHO** in $CDCl_3$ at 20 °C.

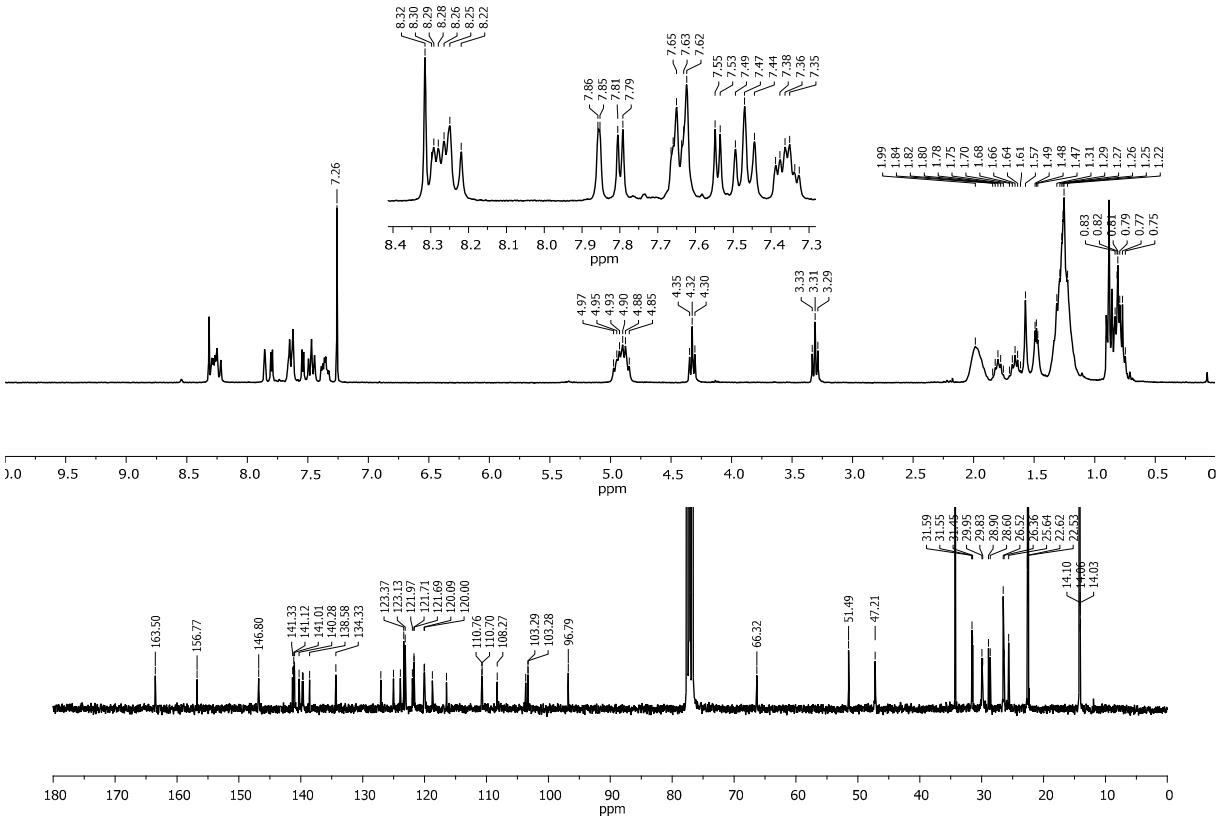


Figure S4 : ^{1}H NMR (300 MHz) (top) and ^{13}C NMR (76MHz) (bottom) of **TAT-σ-N$_3$** in $CDCl_3$ at 20 °C.

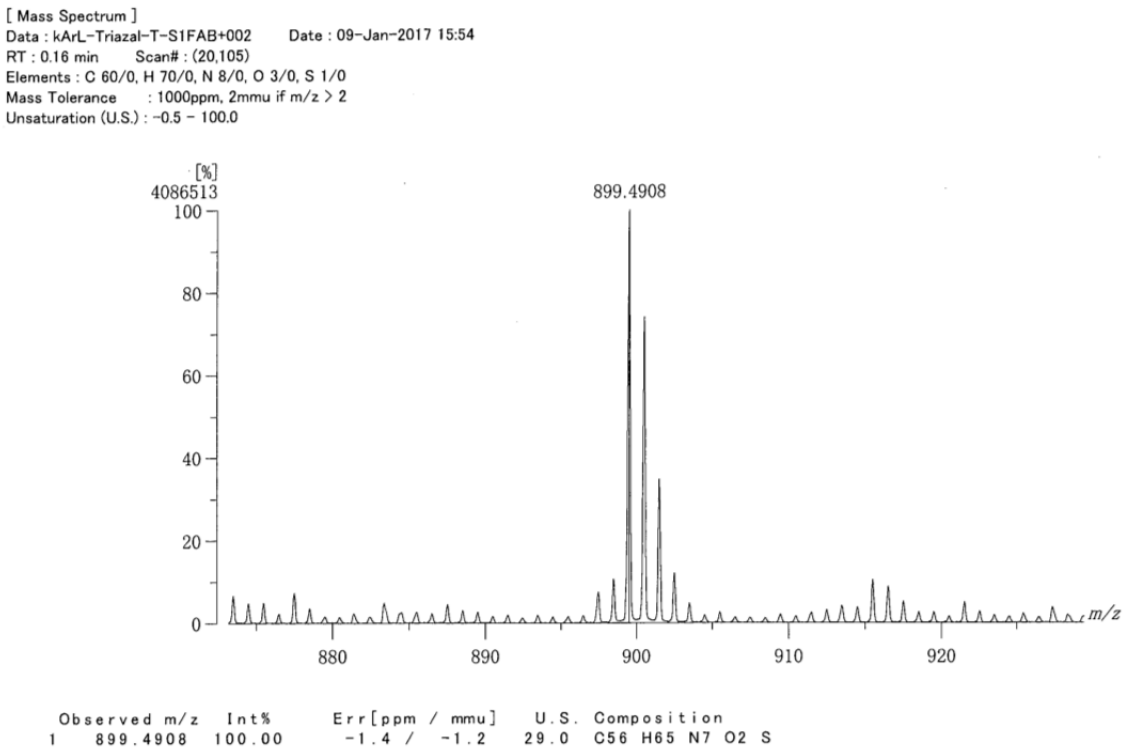


Figure S5 : HRMS of **TAT-σ-N_3**

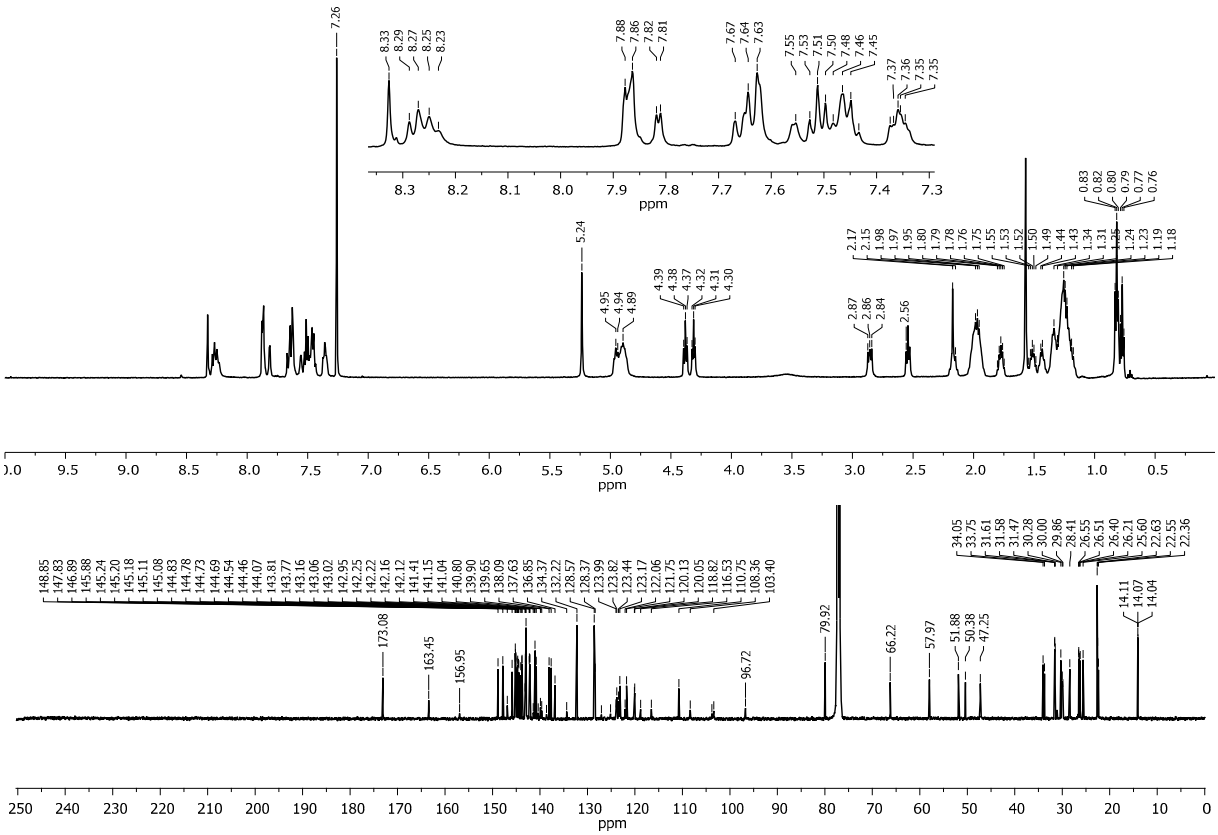


Figure S6 : ^{1}H NMR (300 MHz) (top) and ^{13}C NMR (76MHz) (bottom) of **TAT-σ-C$_{60}$** in $CDCl_3$ at 20 °C.

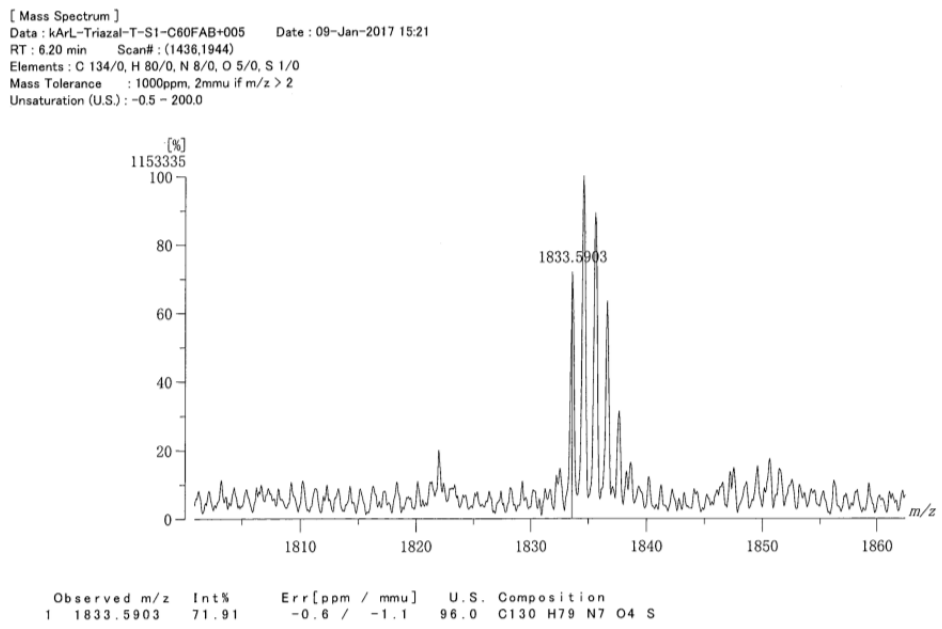


Figure S7: HRMS of **TAT-σ-C$_{60}$**.

Computational Chemistry

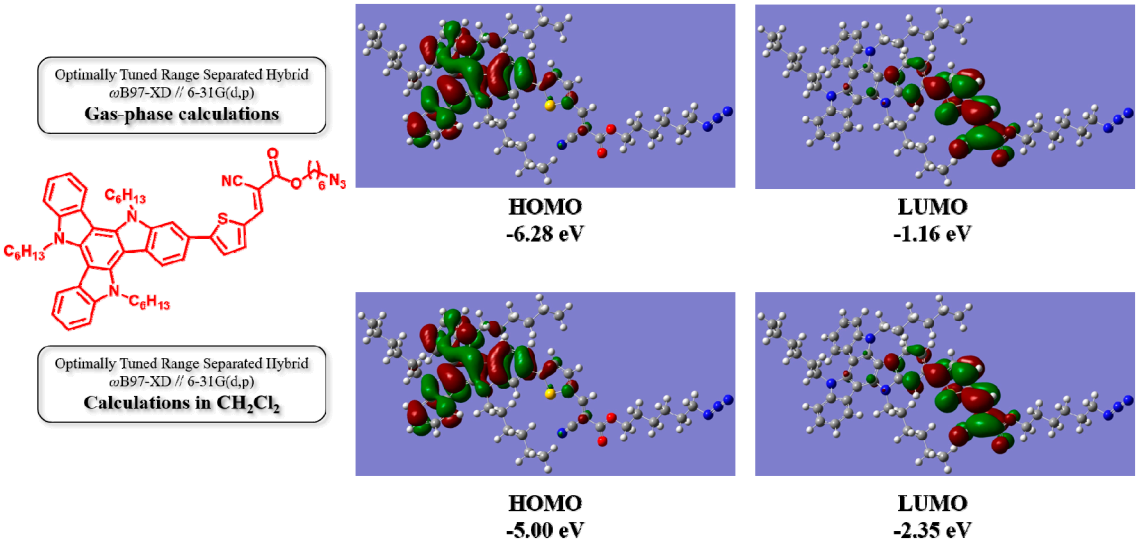


Figure S8: TAT-σ-N_3 HOMO and LUMO and their corresponding energies calculated in vacuum (top) and including dichloromethane molecules as a polarizable continuum (bottom).

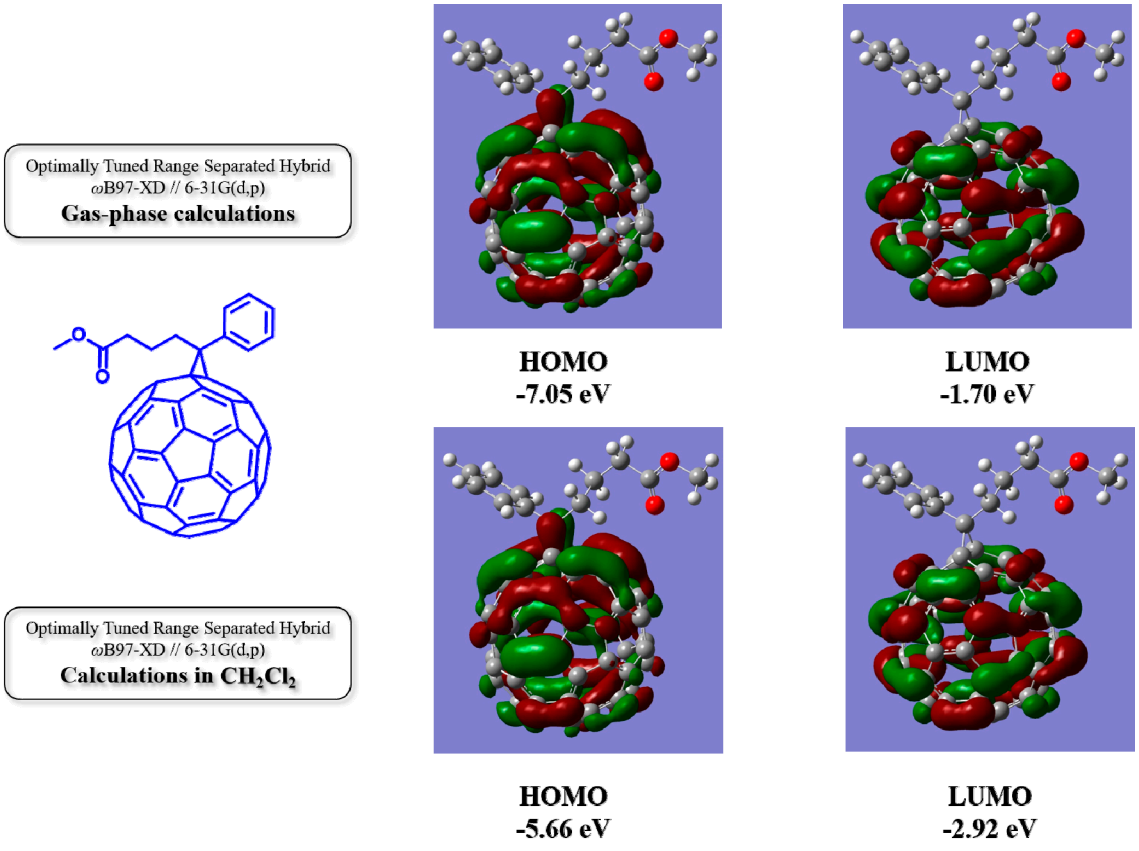
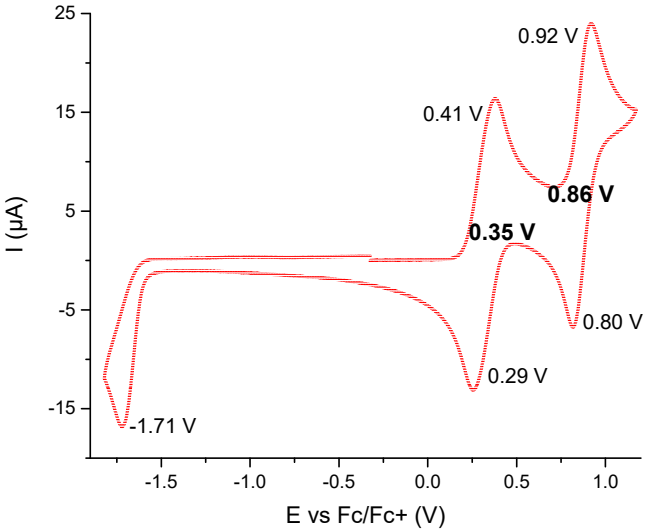
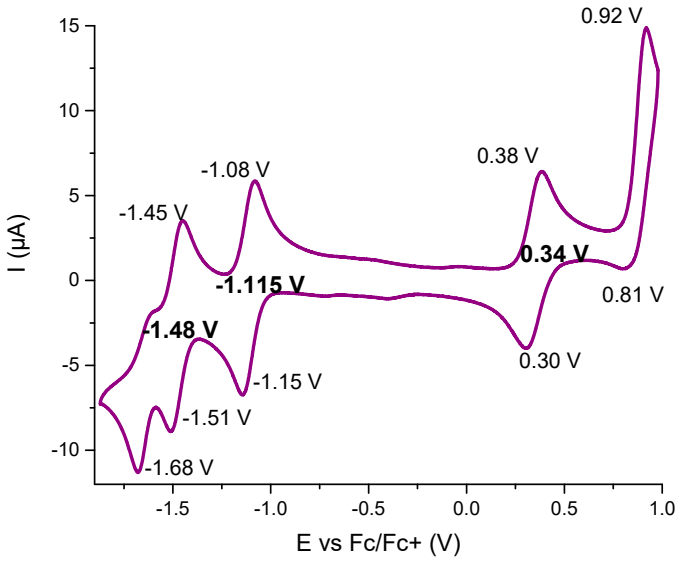


Figure S9: $PC_{61}BM$ HOMO and LUMO and their corresponding energies calculated in vacuum (top) and including dichloromethane molecules as a polarizable continuum (bottom).

Electrochemical data:





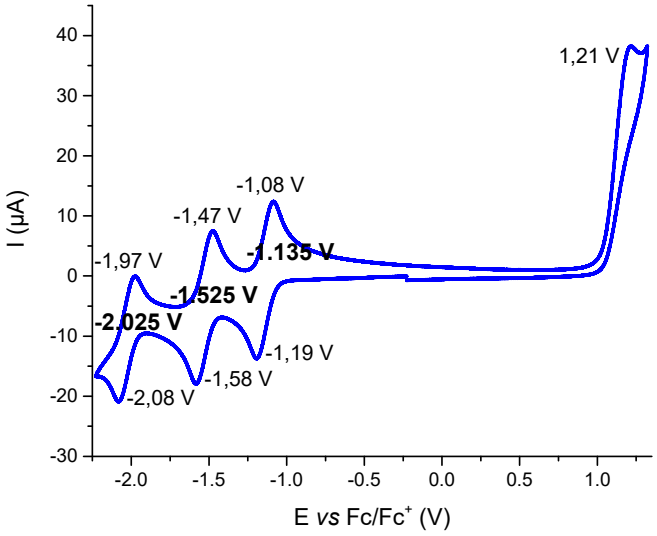


Figure S10. Cyclic voltammograms of **TAT-σ-N_3** (red), **TAT-σ-C_{60}** (purple), and the **$PC_{61}BM$** (blue) in 0.1 M Bu_4NPF_6/CH_2Cl_2, scan rate 100 mV s^{-1}, Pt working and counter electrode

Photovoltaic data:

Table S1. Photovoltaic data obtained from active layers processed with different solvents

Processing solvent	Voc (V)	Jsc ($mA.cm^{-1}$)	FF (%)	PCE (%)
CB	0.41	1.77	31.3	0.22
CF	0.81	1.80	28.6	0.41
MeTHF	0.04	1.40	24.5	0.01

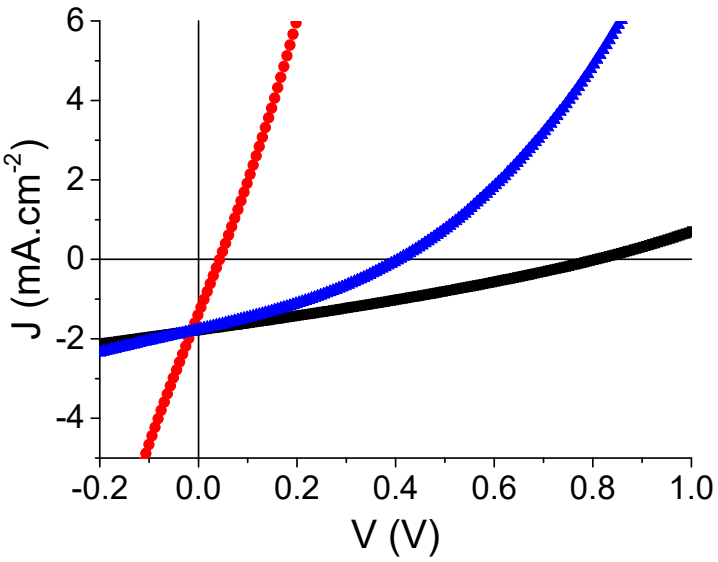
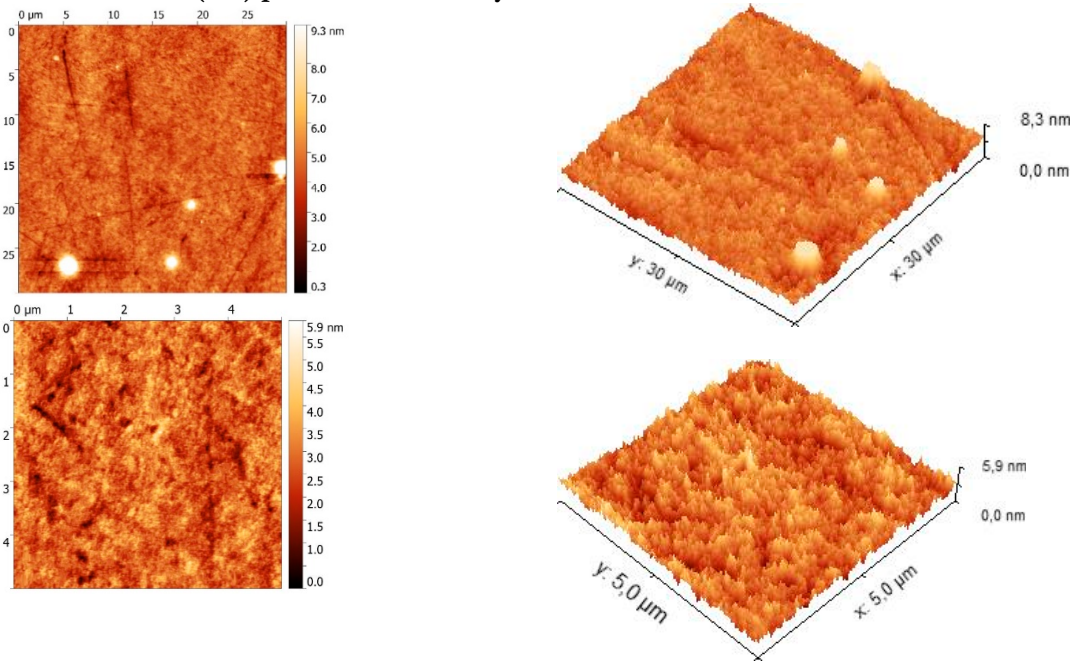


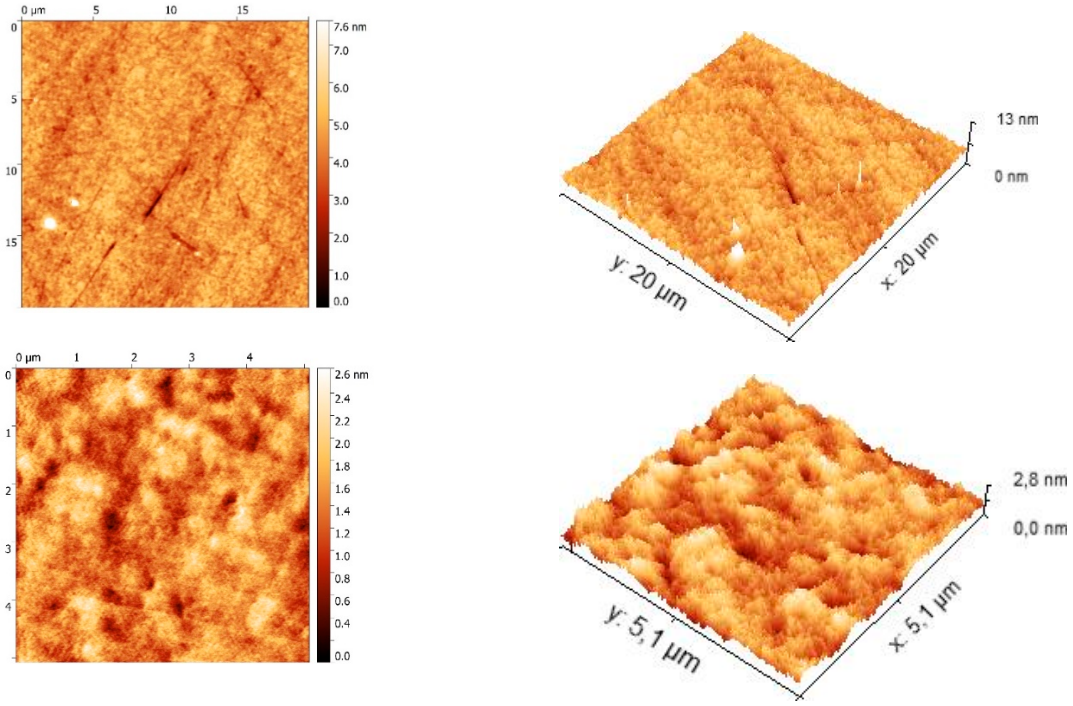
Figure S11. J−V characteristics measured under AM 1.5 simulated solar light under illumination (100 mW.cm^{-2}) of the best devices processed with CB (bleu), CF (black) and MeTHF (red)

Atomic Force Microscopy:

Chlorobenzene (CB) processed active layers: RMS = 0.65 nm



Chloroform (CB) processed active layers: RMS = 0.65 nm



2-methyltetrahydrofuran (MeTHF) processed active layers: RMS = 21 nm

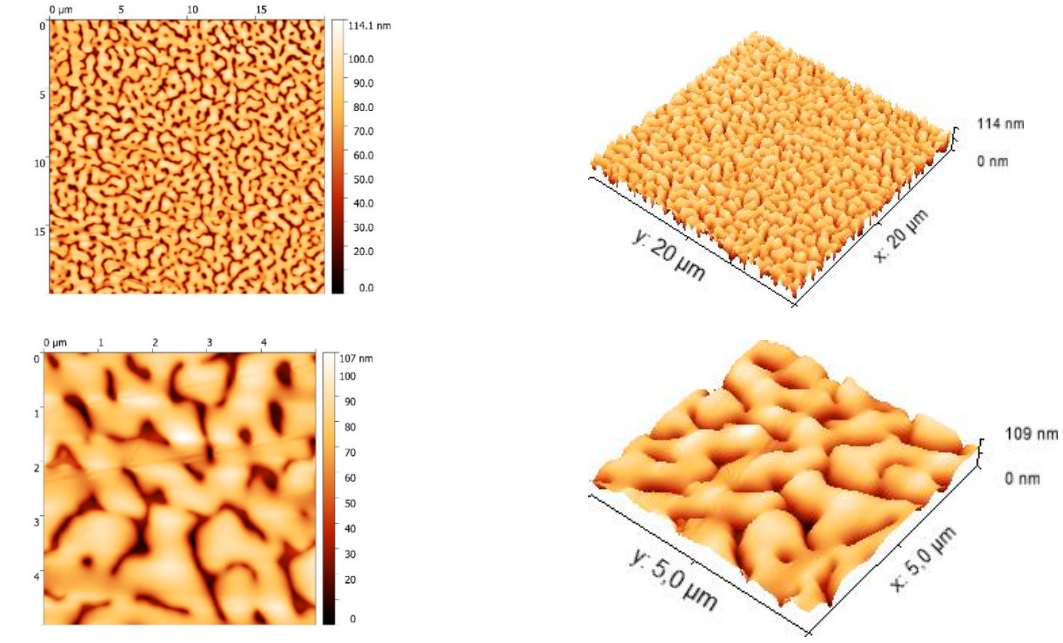


Figure S12. 2D and 3D surface topography images of the different active layers probed by atomic force microscopy