Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Supporting Information

Unravelling Fullerene-Perovskite Interactions Introduces Advanced Blend Films for Performance-Improved Solar Cells

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This Supporting Information contains additional NMR and FTIR spectra, supporting the ideas proposed in the main text as conclusion of the discussion of the obtained results about perovskite-fullerene interactions. Moreover, the synthetic details and characterization by ^{1}H- and ^{13}C-NMR, FTIR, UV-vis spectroscopies and cyclic voltammogram of the novel fullerene are included. Topography and phase AFM images of C_{70}- and **FU11**-containing perovksite layers are also available in this text. Finally, the statistics of every PV parameter in the three different configurations have been included.

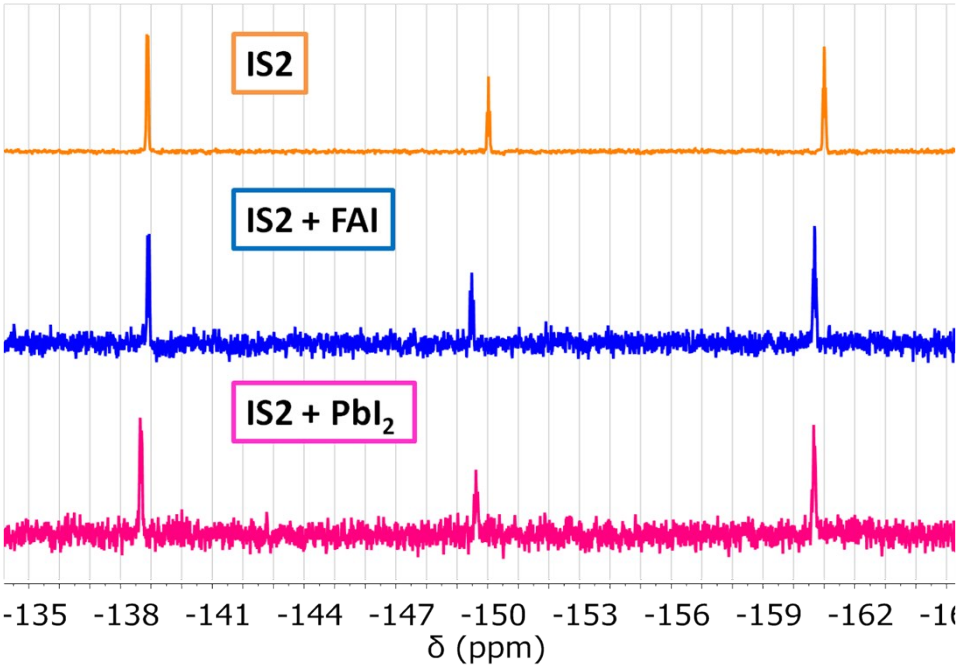
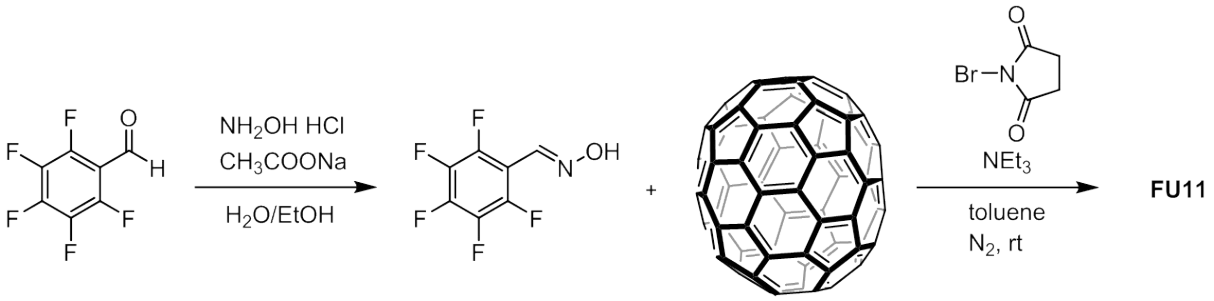
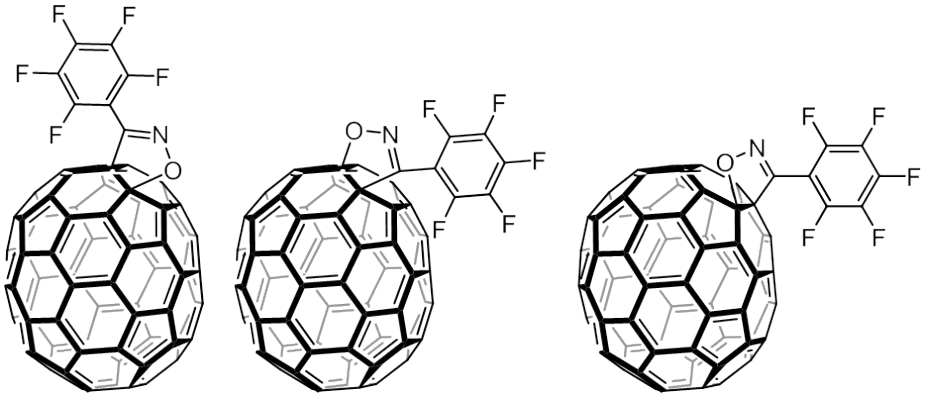


Figure S1. ^{19}F-NMR spectra of **IS2**-saturated DMF:DMSO (4:1) solution and in presence of FAI and PbI_2 separately.

*Synthesis of **FU11**:*



Scheme S1. Synthesis of **FU11**.



2,3,4,5,6-pentafluorobenzaldehyde oxime (89.0 mg, 420 µmol) and *N*-bromosuccinimide (75 mg, 420 µmol) were dissolved in anhydrous toluene under nitrogen atmosphere and stirred at r.t. for 30 min. C_{70} (118 mg, 140 µmol) and NEt_3 (60 µl, 420 µmol) were added and the mixture stirred at r.t. for 2 h. The solvent was removed under reduced pressure and the residue purified by column chromatography (eluent: CS_2). The product was precipitated from $CHCl_3$ to pentane to obtain 34 mg (32.4 µmol, 23%) of a brown solid.

3 isomers

^{19}F-NMR (376.4 MHz, $CDCl_3$):

δ [ppm] = –134.8 – –135.6 (2 F), –147.2 – –147.8 (1 F), –158.3 – –159.1 (2 F)

MALDI-TOF (high resolution): [$M^{\cdot+}$] calculated: 1048.9895 m/z; found: 1048.9942 m/z

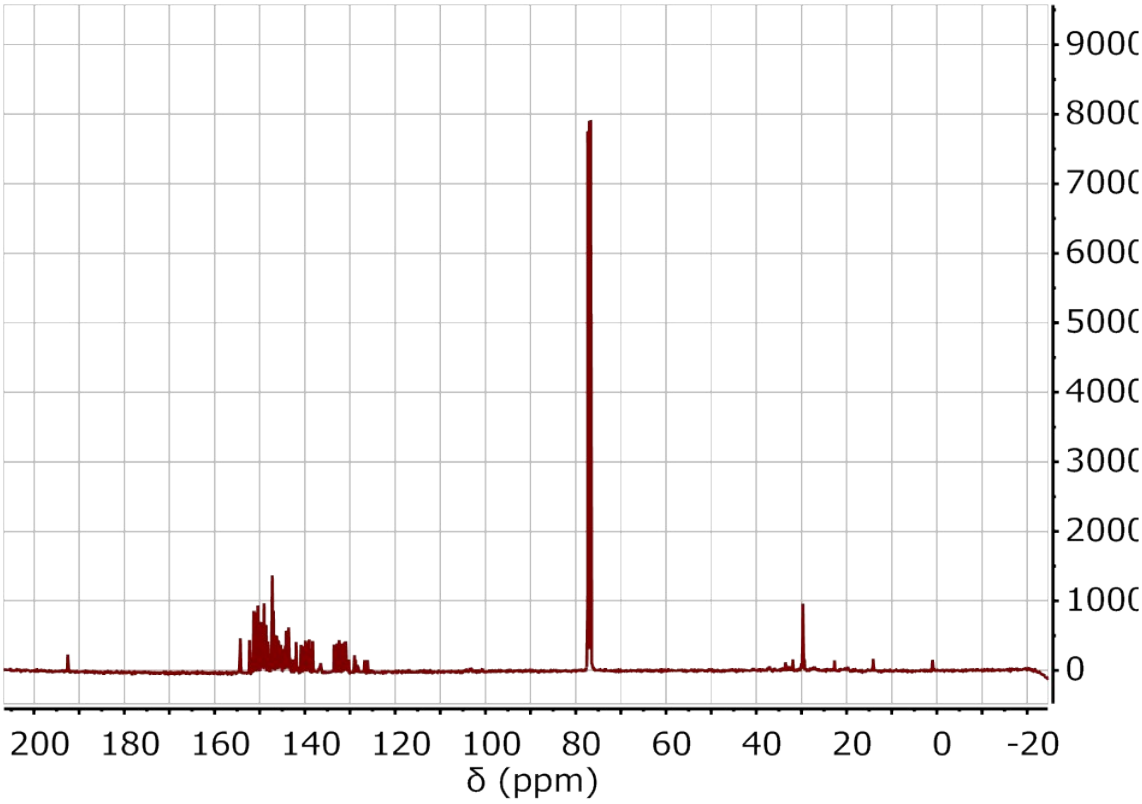


Figure S2. ^{13}C-NMR spectrum of **FU11**.

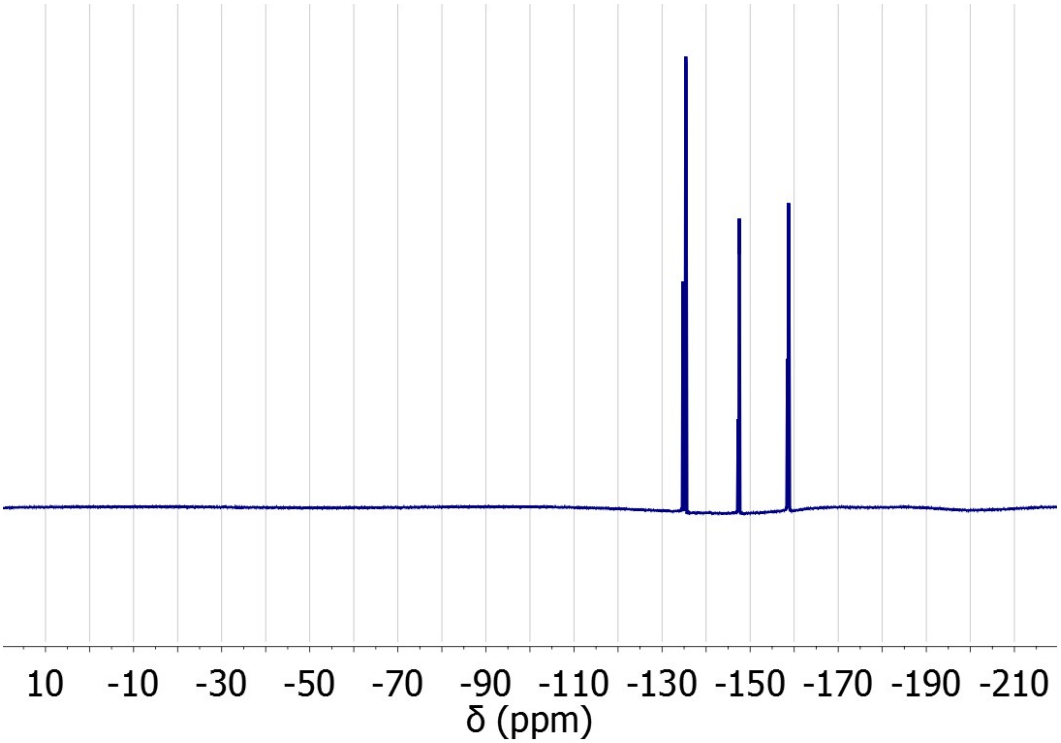


Figure S3. ^{19}F-NMR spectrum of **FU11**.

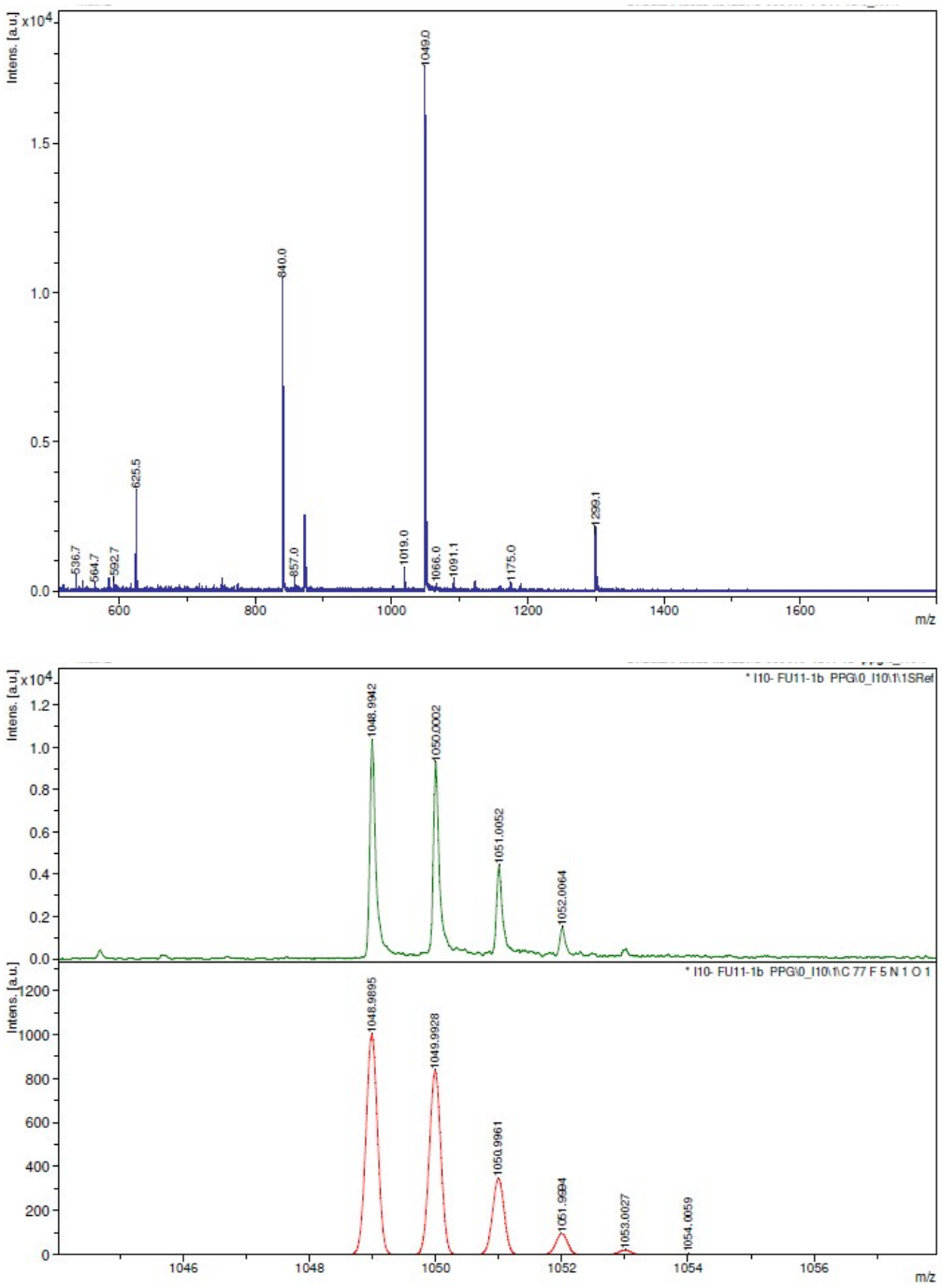


Figure S4. Mass spectra (high resolution below) of **FU11**.

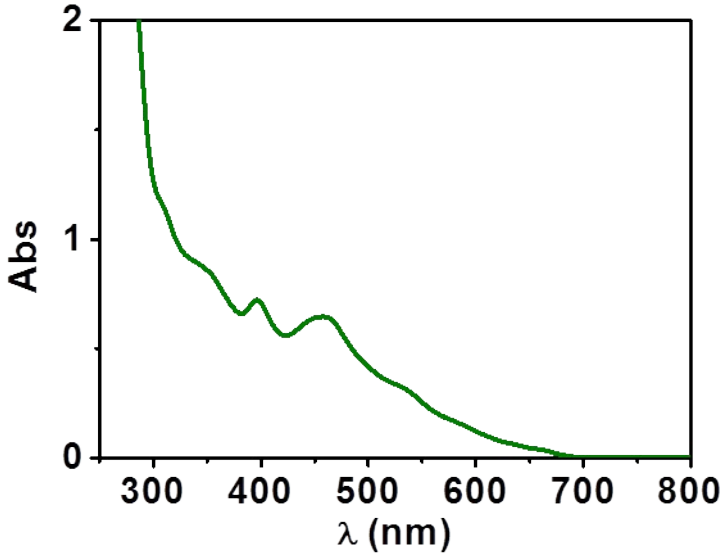


Figure S5. UV-vis spectrum of **FU11** in CH_2Cl_2. A bandgap value of 2.64 eV was extrapolated.

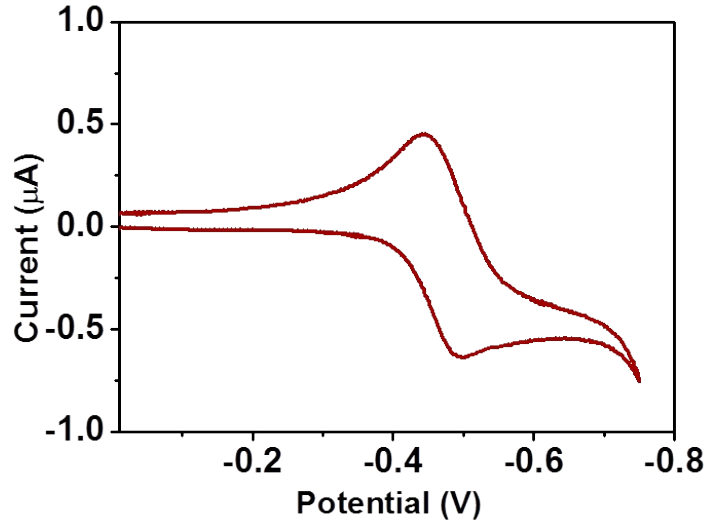


Figure S6. Cyclic voltammogram of **FU11** in DCM/TBAHFP (0.1M) vs. Fc/Fc^+ at a scanning rate of 250 mV s^{-1}. LUMO energy level was calculated using the formula: E(LUMO) = -4.8eV-($E_{1/2}$red) = -3.87 eV. HOMO level was calculated through the formula: E(LUMO) – bandgap = -6.51 eV .

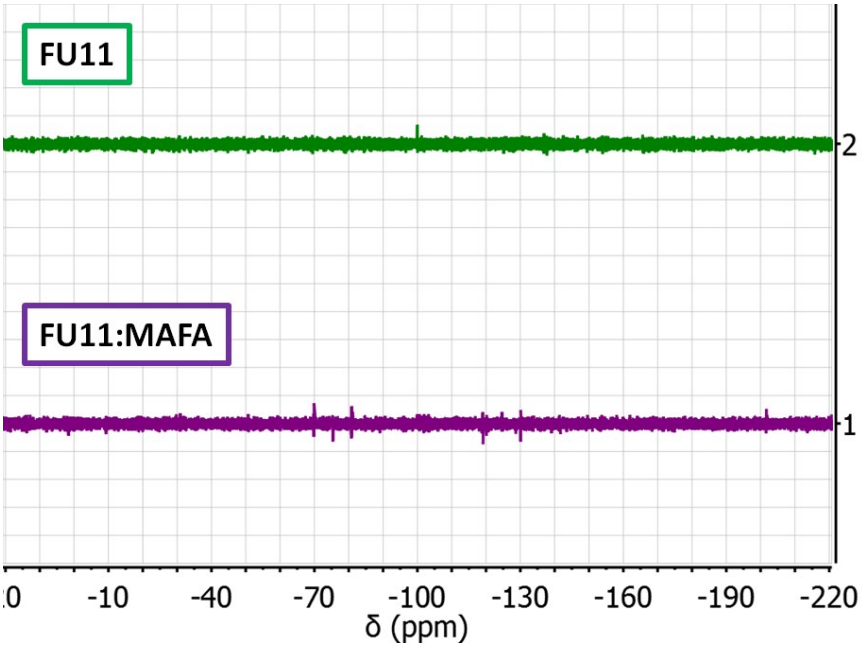


Figure S7. ^{19}F-NMR spectra of **FU11**-saturated solution in DMF:DMSO (4:1) with and without MAFA perovskite (1.2 M).

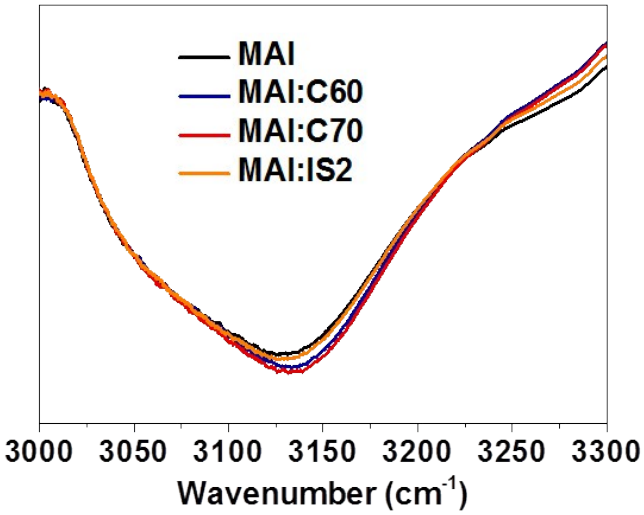


Figure S8. FTIR spectra of MAI solutions (1.5 M) in DMSO and in the presence of different fullerenes.

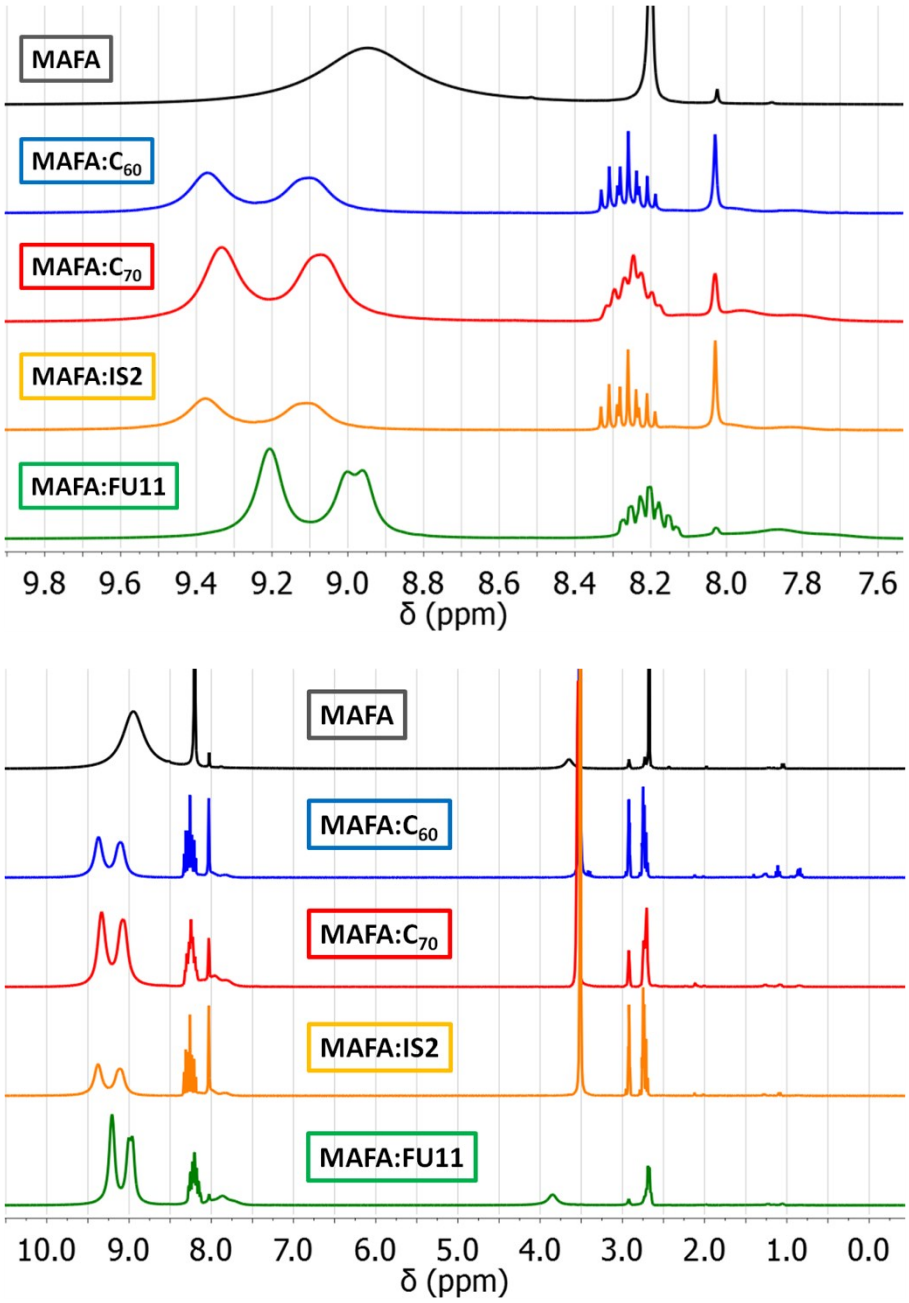


Figure S9. ^{1}H-NMR spectra of MAFA perovskite solutions (1.2 M) in DMF:DMSO (4:1) and in the presence of different fullerenes and **FU11** (full spectra below). The signal of FA protons at 8.95 ppm split and get shifted to higher chemical shift values in the presence of fullerenes.

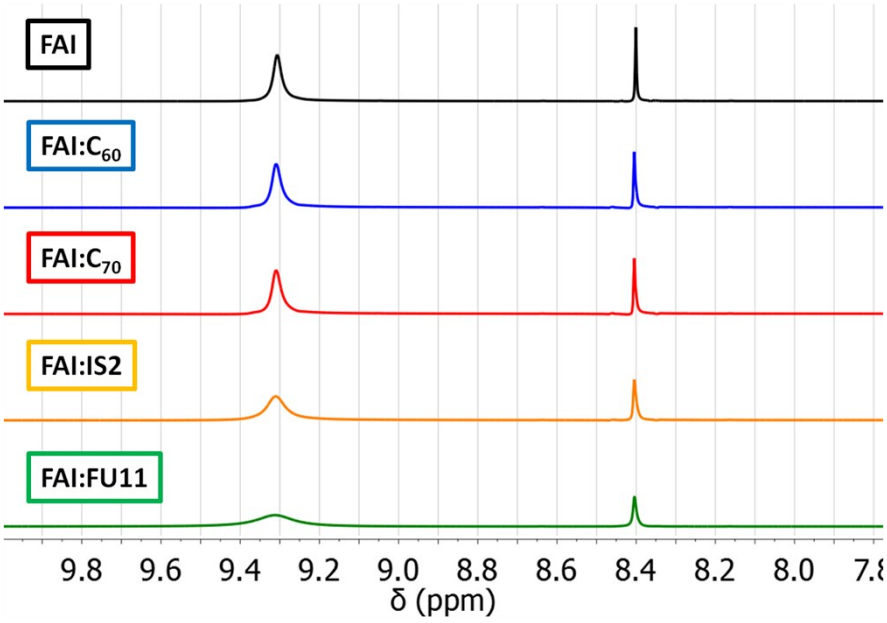


Figure S10. ^{1}H-NMR spectra of FAI solutions (1.5 M) in DMF:DMSO (4:1) and in the presence of different fullerenes and **FU11**.

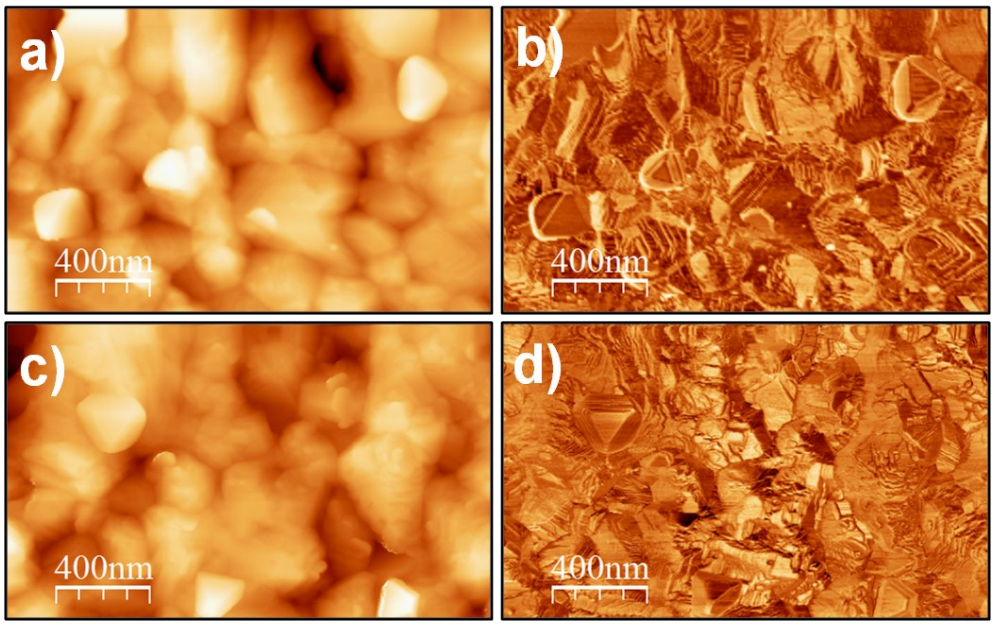


Figure S11. Topography (z = 170 nm) and phase AFM images for the a) and b) C_{70}-containing and c) and d) **FU11**-containing perovskite layers at the initial measurement stage. Both samples present a very similar topography and phase signal without any remarkable fullerene type related features.

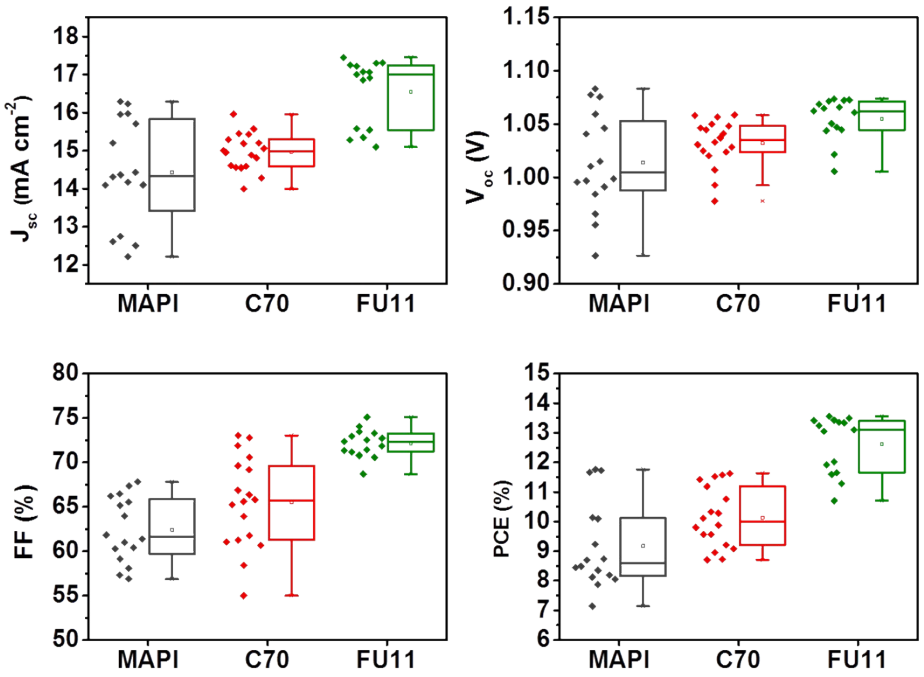


Figure S12. PV parameters of PSCs in ETL-free configuration.

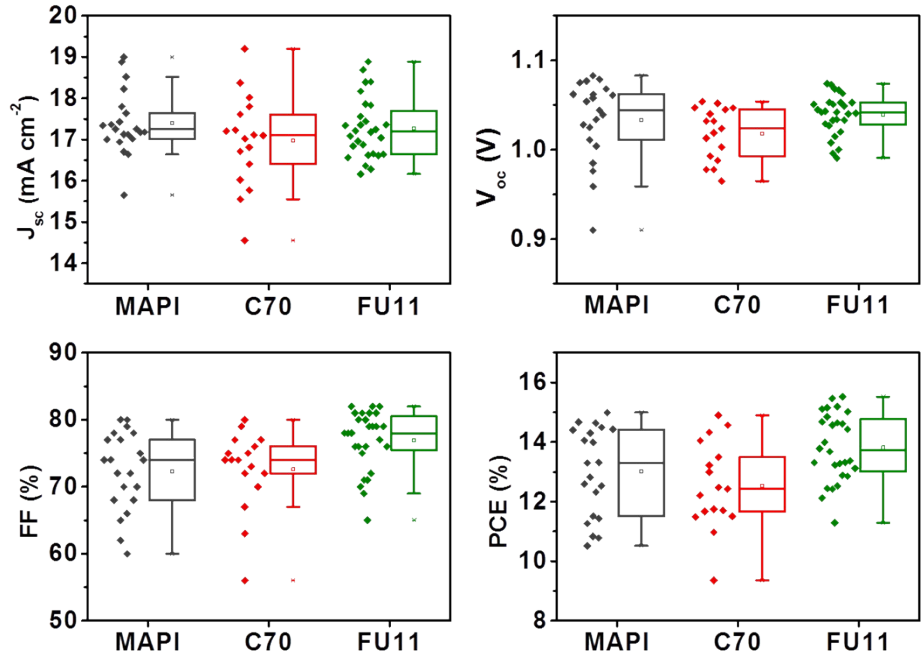


Figure S13. PV parameters of PSCs in n-i-p configuration.

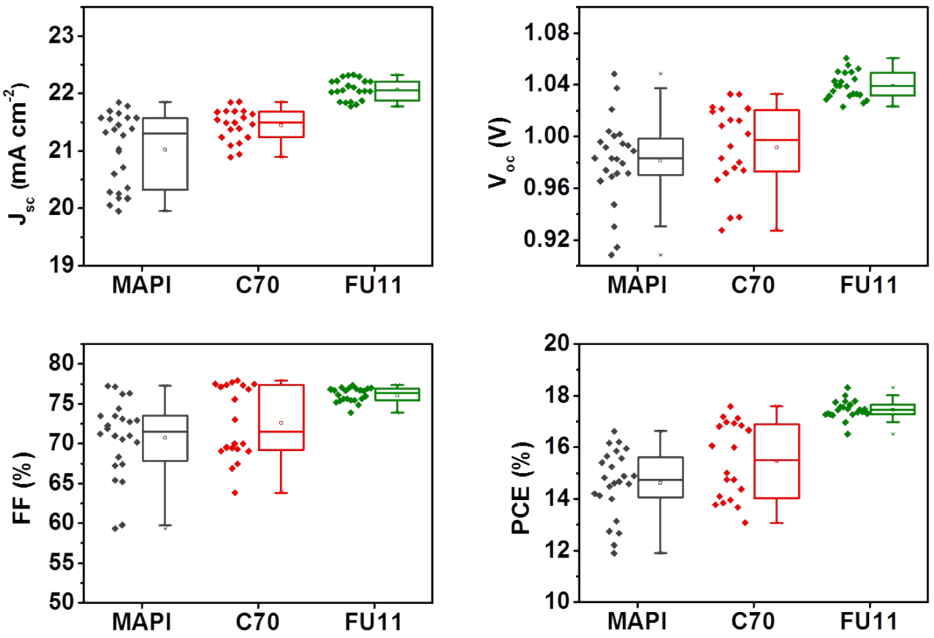


Figure S14. PV parameters of PSCs in p-i-n configuration.