Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting info

Dimers of Diethynyl-Conjugated Zinc-Phthalocyanine as Hole Selective Layers for Perovskites solar cells Fabrication

Meenakshi Pegu,[a,†] Desiré Molina,[b,†] Maria J. Álvaro-Martins,[b] María Castillo,[b] Lydia Ferrer,[b] Peng Huang,[a] Samrana Kazim,[a,c] Ángela Sastre-Santos,[b] Shahzada Ahmad [a,c*]*

[a]BCMaterials, Basque Center for Materials, Applications, and Nanostructures, UPV/EHU Science Park, 48940 Leioa, Spain,

Tel: +34 946128811 E-mail: shahzada.ahmad@bcmaterials.net

[b]Área de Química Orgánica, Instituto de Bioingeniería Universidad Miguel Hernández Avda. de la Universidad, s/n, Elche 03202, Spain, E-mail: asastre@umh.es

[c]IKERBASQUE, Basque Foundation for Science, Bilbao, 48009, Spain

† MP and DM contributed equally to this work

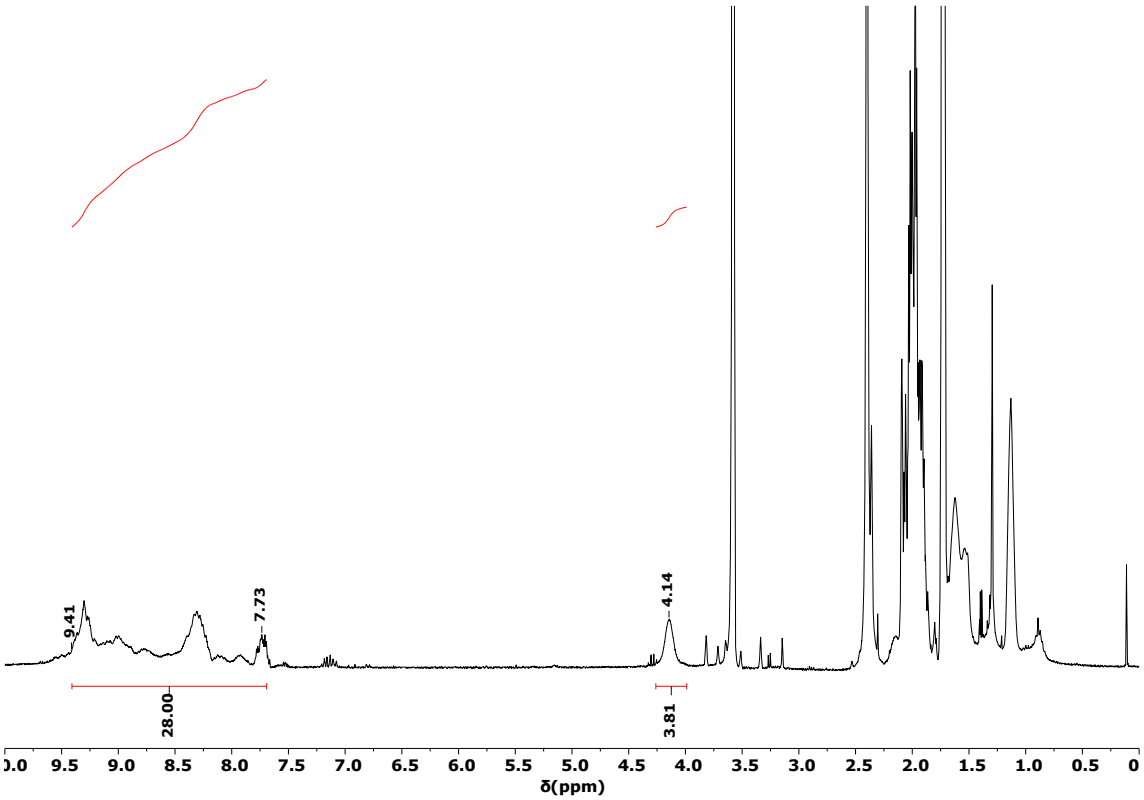

Figure S1. ^{1}H NMR (400 MHz) spectrum of **ZnPc 1** in THF-d_8 at 25°C.

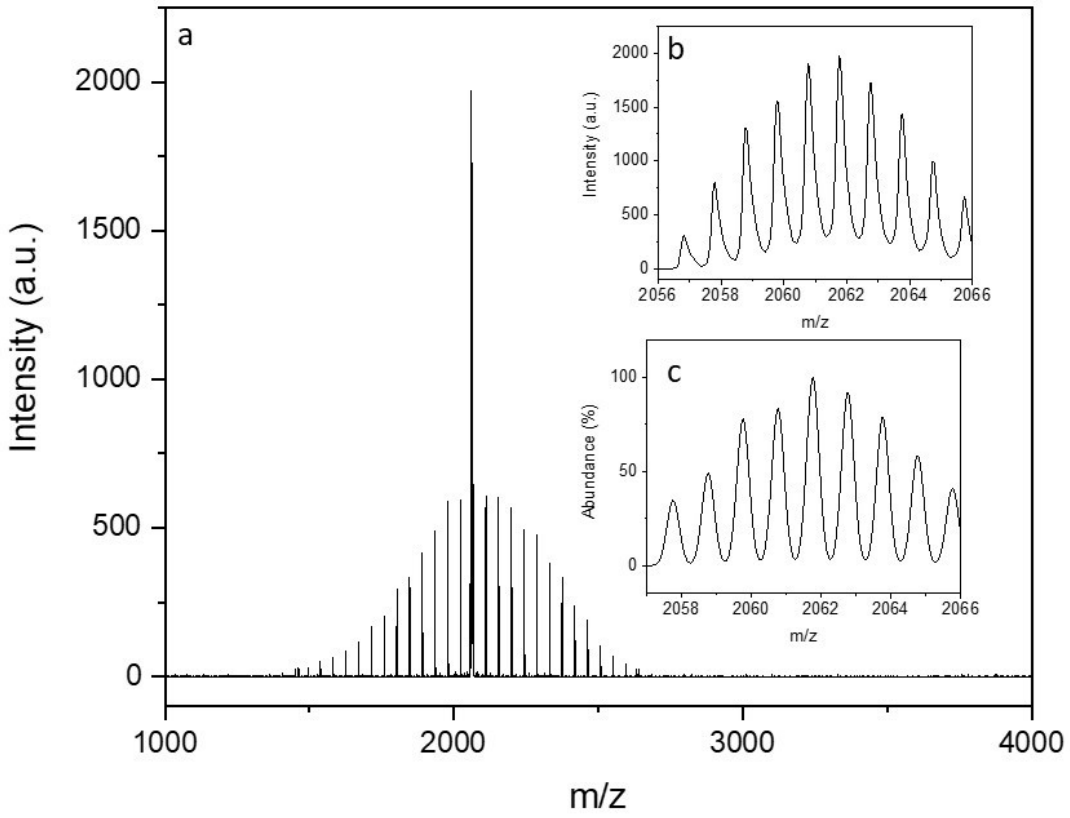

Figure S2. (a) MALDI-TOF spectrum of **ZnPc 1** (dithranol peaks can be observed), (b) experimental, and (c) theoretical isotopic patterns.

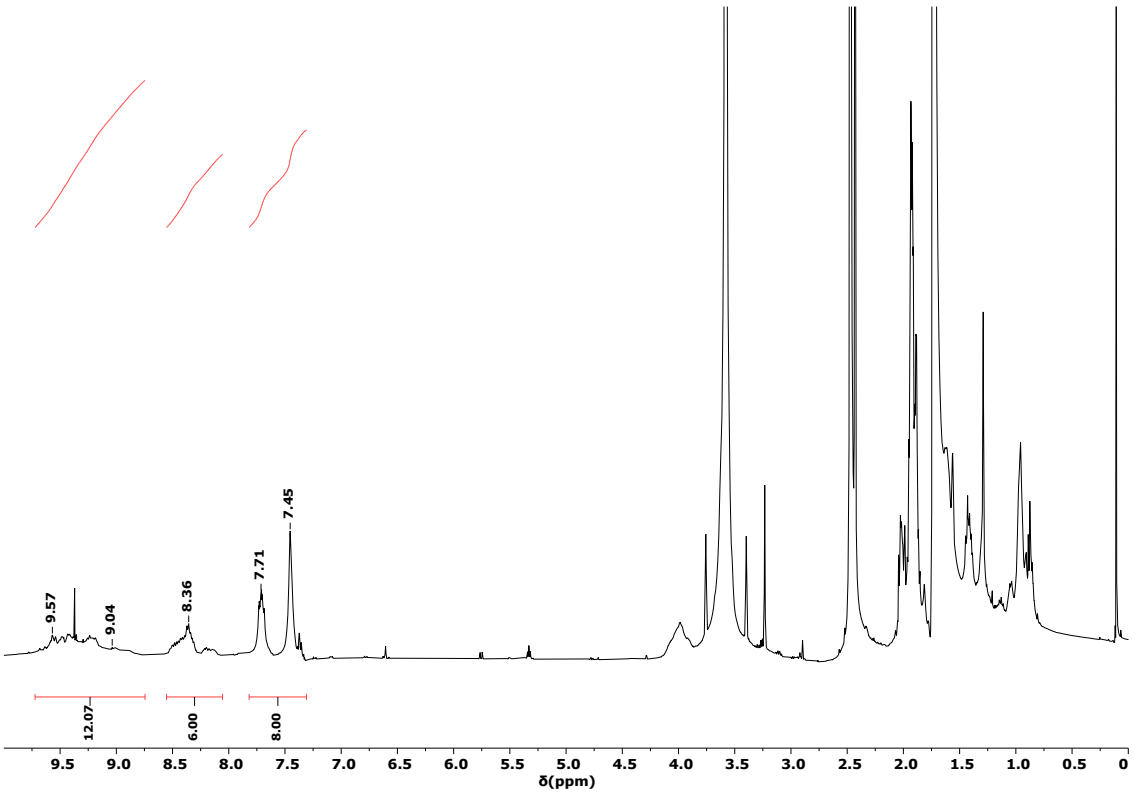

Figure S3. ^{1}H NMR (400 MHz) spectrum of **ZnPc 2** in THF-d_8 at 25°C.

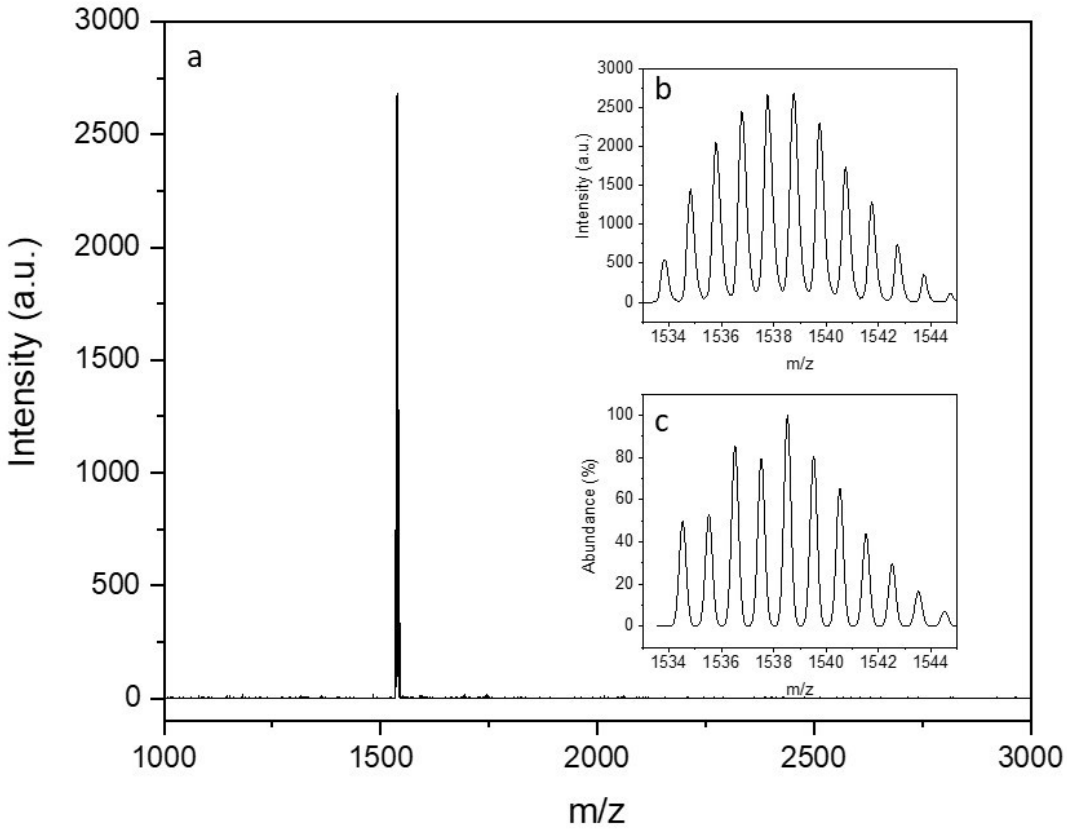

Figure S4. (a) MALDI-TOF spectrum of **ZnPc 2**, (b) experimental, and (c) theoretical isotopic patterns.

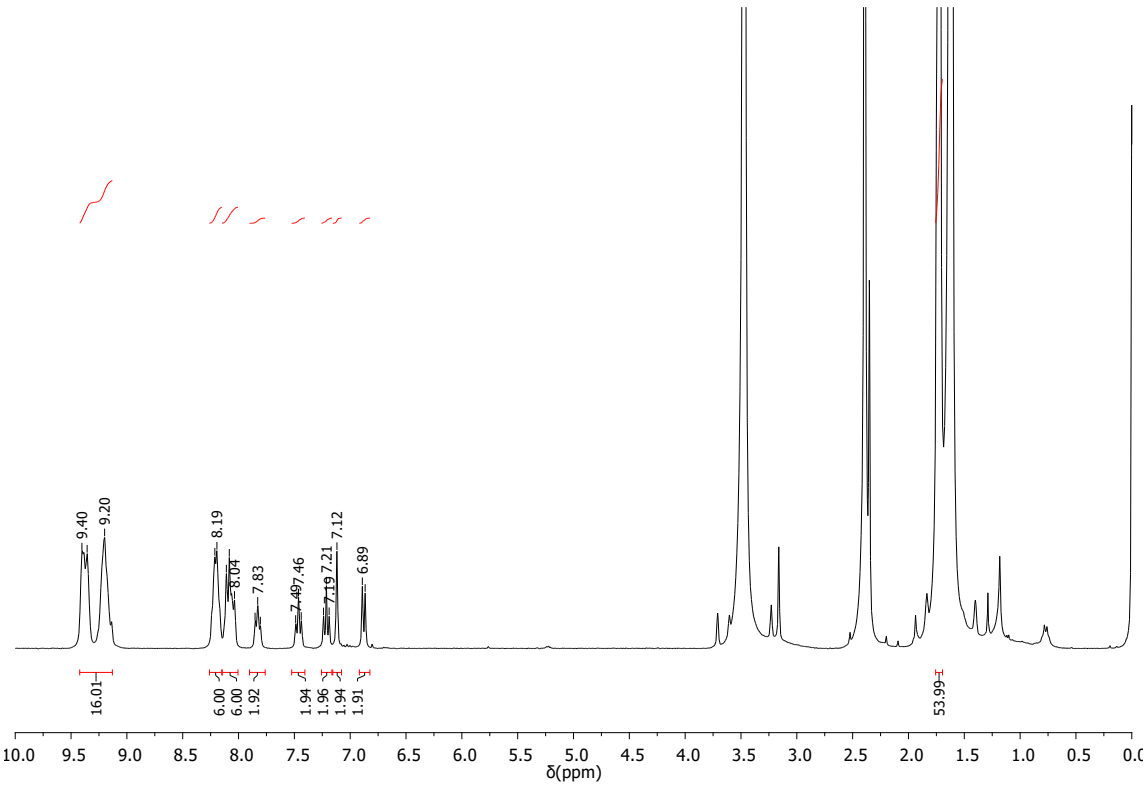

Figure S5. ^{1}H NMR (400 MHz) spectrum of **ZnPc 3** in THF-d_8 at 25°C.

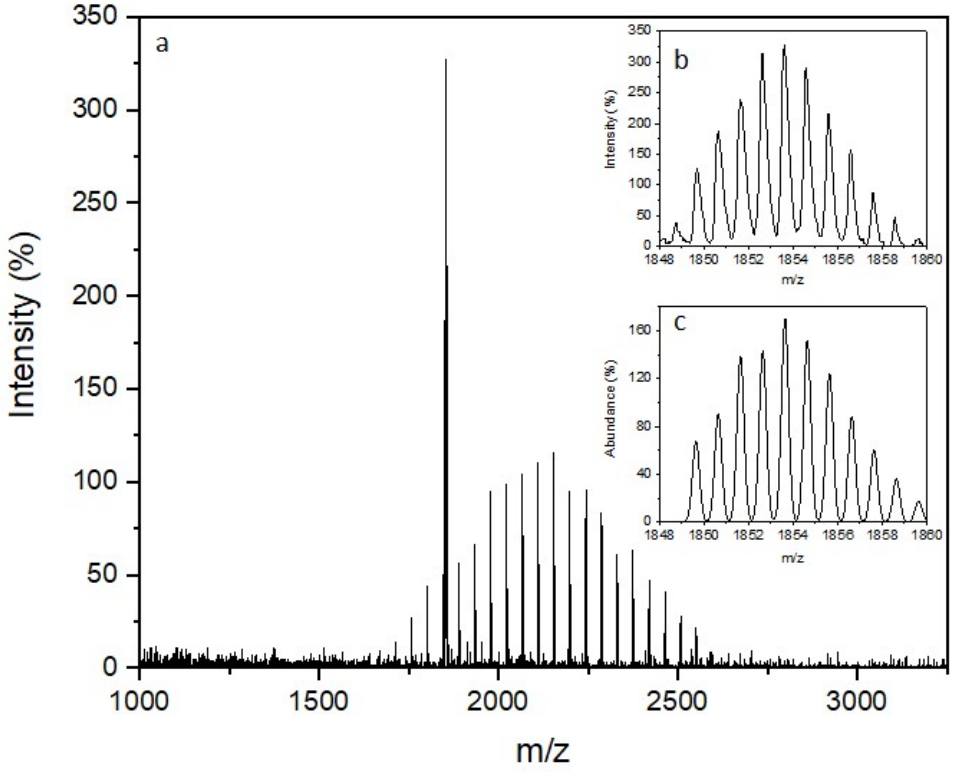

Figure S6. (a) MALDI-TOF spectrum of **ZnPc 3** (dithranol peaks can be observed), (b) experimental, and (c) theoretical isotopic patterns.

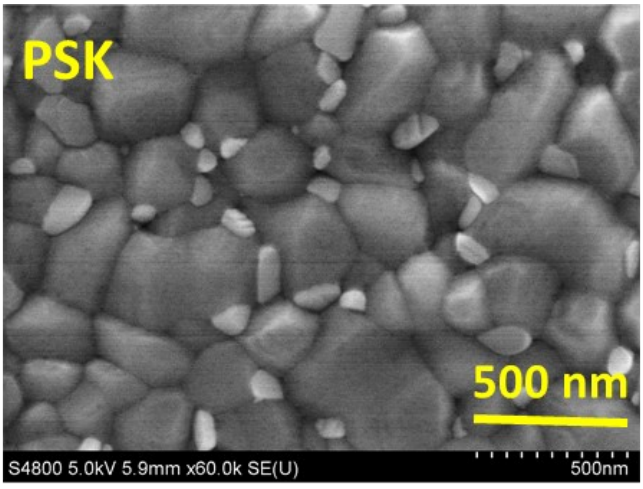

Figure S7: Top surface SEM image of the perovskite layer.

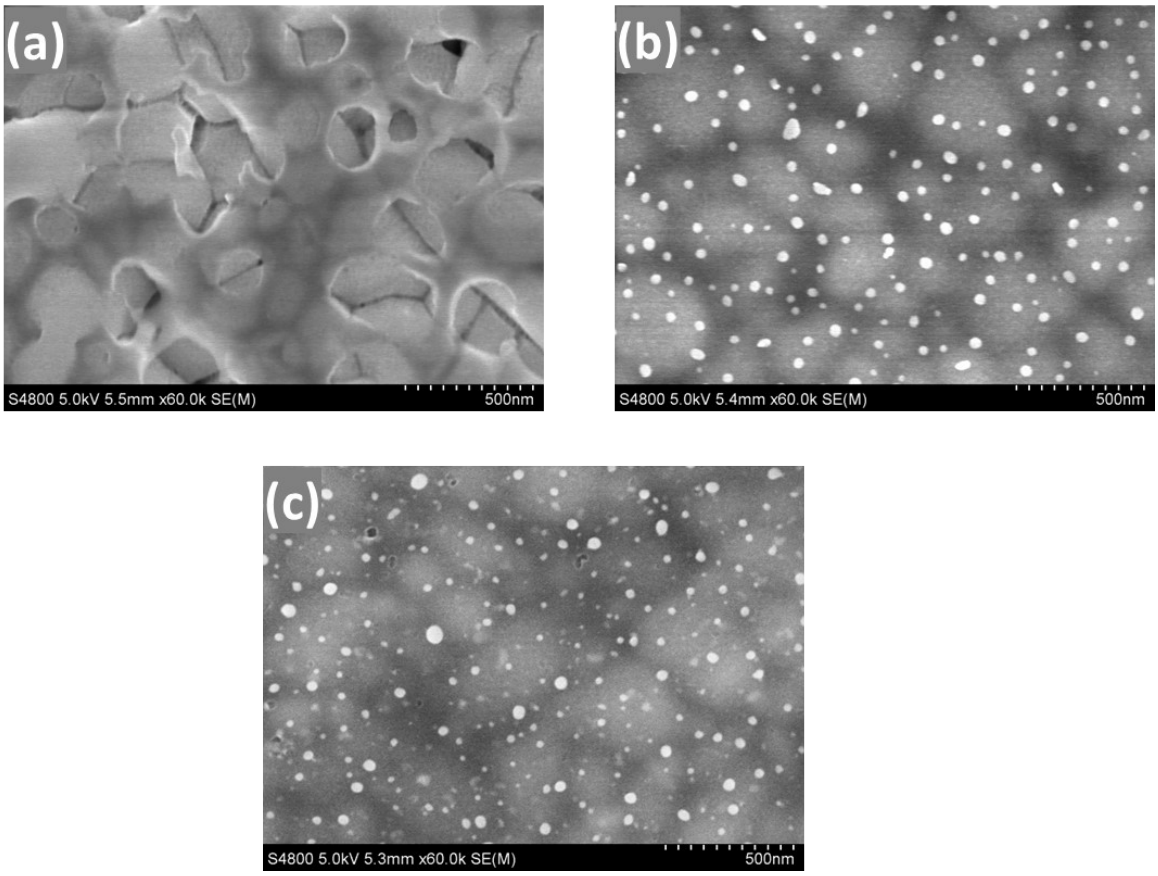

Figure S8: Surface SEM images of Pc dimers. Doped condition of ZnPcs (a) **ZnPc 1**, (b) **ZnPc 2**, and (c) **ZnPc 3**.

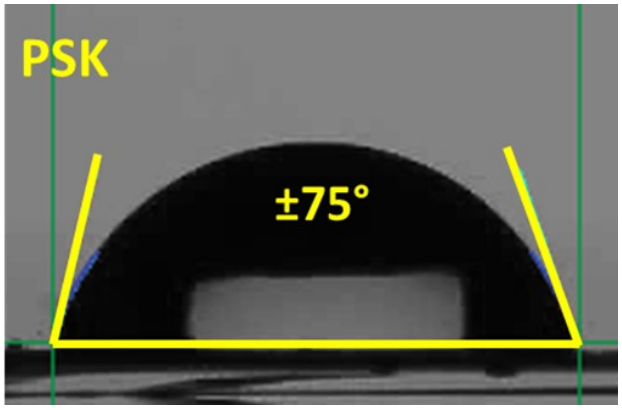

Figure S9: Contact angle measurement of the perovskite layer thin film.

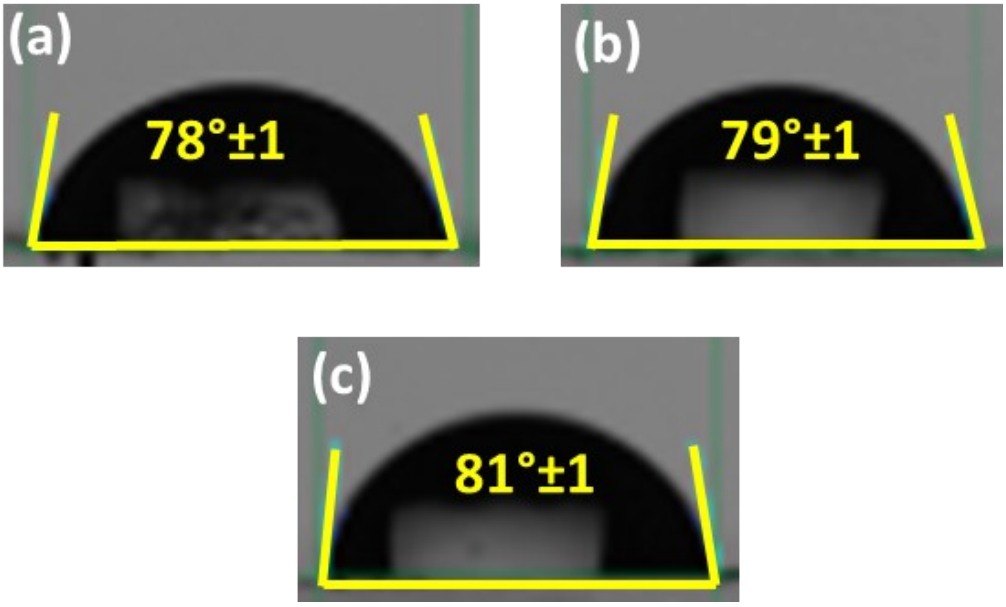

Figure S10: Contact angle measurement of of Pc dimers. Doped condition of ZnPcs (a) **ZnPc 1**, (b) **ZnPc 2**, and (c) **ZnPc 3.**

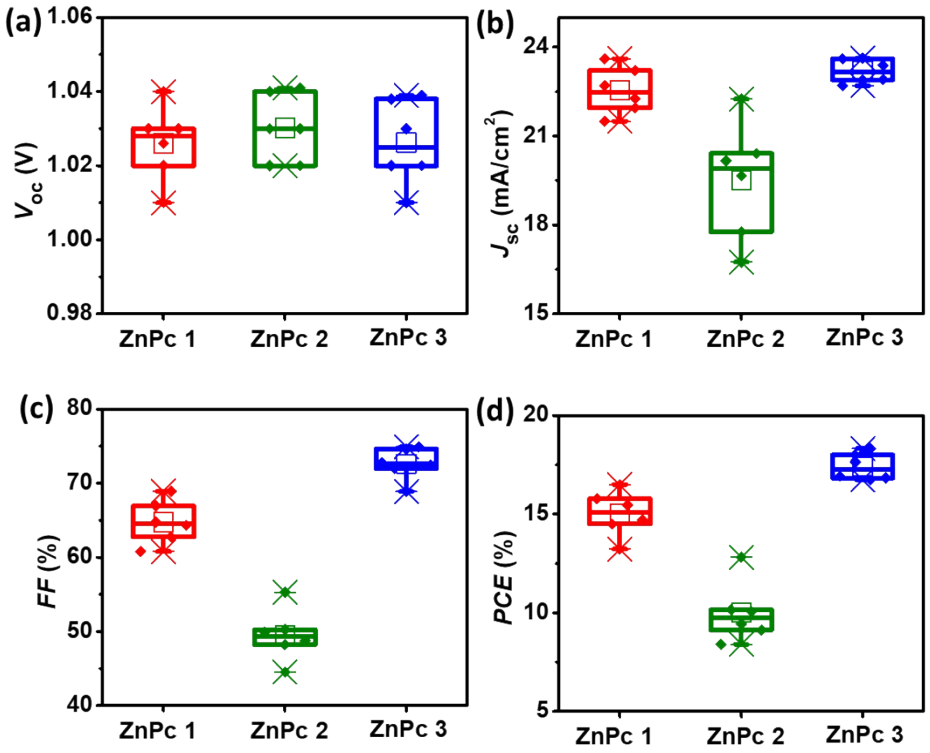

Figure S11: Device statistics of doped ZnPc dimers as HTMs (a) V_{oc}, (b) J_{sc}, (c) *FF,* and (d) *PCE*.

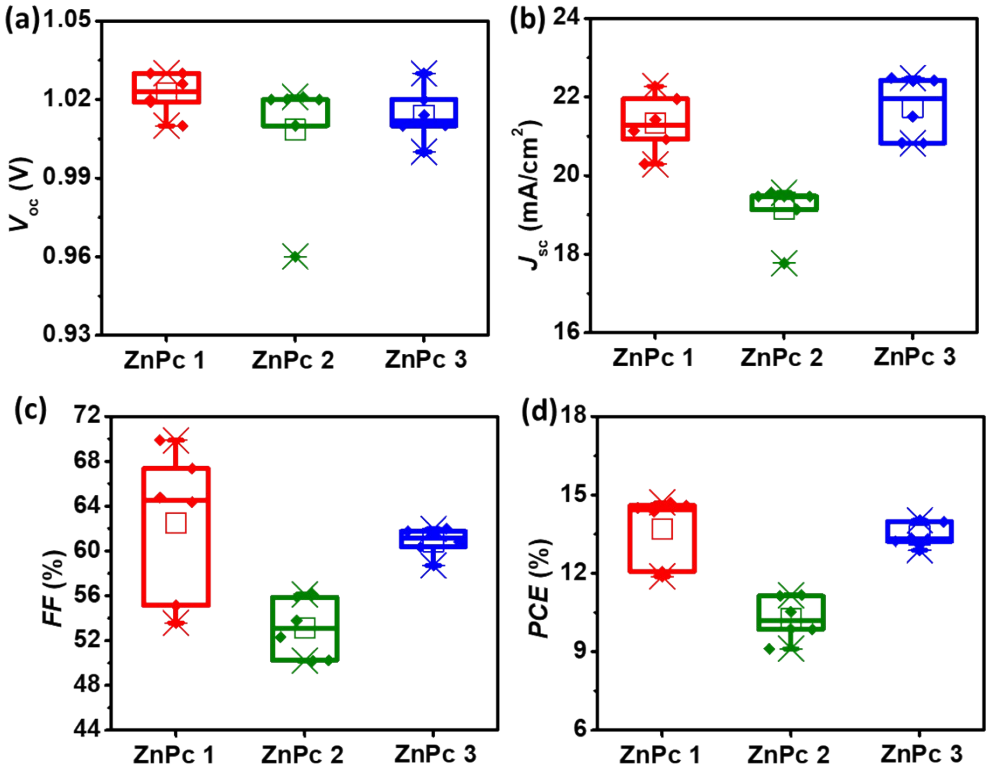

Figure S12: Device statistics of undoped ZnPc dimers as HTMs (a) V_{oc}, (b) J_{sc}, (c) *FF,* and (d) *PCE*.

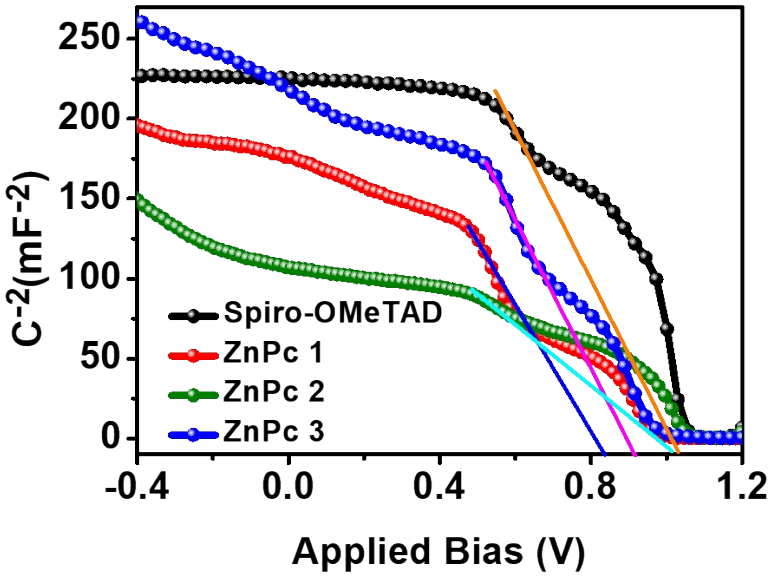

Figure S13: Mott- Schottky plots for PSCs based on Spiro-OMeTAD and ZnPc dimers (**ZnPc 1, ZnPc 2,** and **ZnPc 3).**

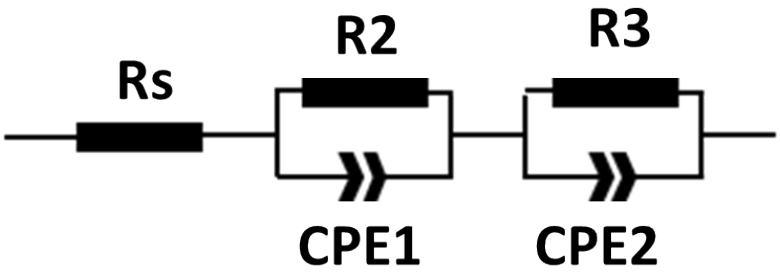

Figure S14: Electrical equivalent circuit used for impedance spectra.