

# SUPPORTING INFORMATION

## **A solution-processed tetra-alkoxylated Zinc phthalocyanine as hole transporting material for emerging photovoltaic technologies**

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Figure S1\_a (*n*-BuO)<sub>4</sub>ZnPc <sup>1</sup>H NMR in THF-d<sub>8</sub>. Solvent peaks are labeled for sake of clarity

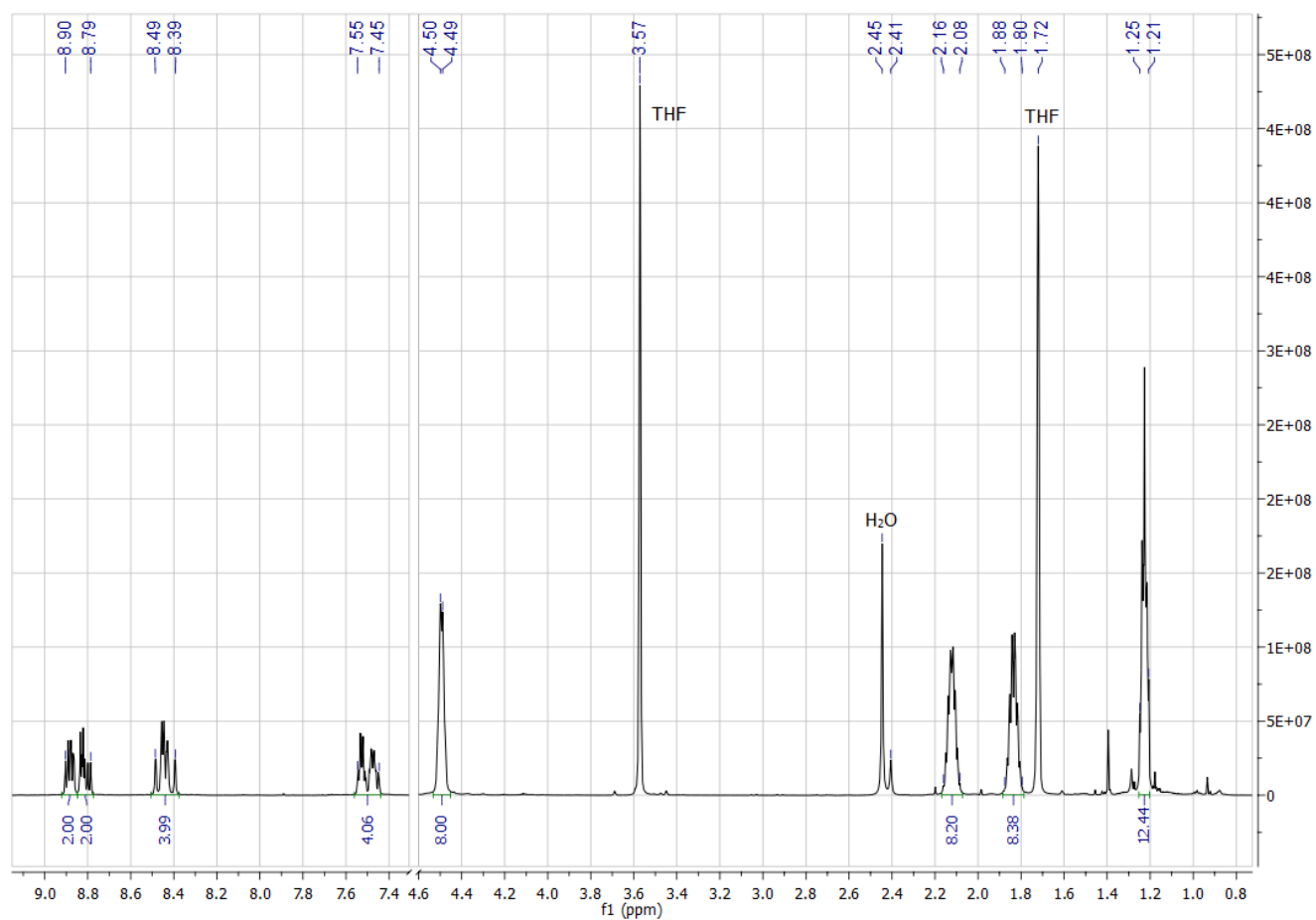


Figure S1\_b: aromatic portion of the NMR spectrum

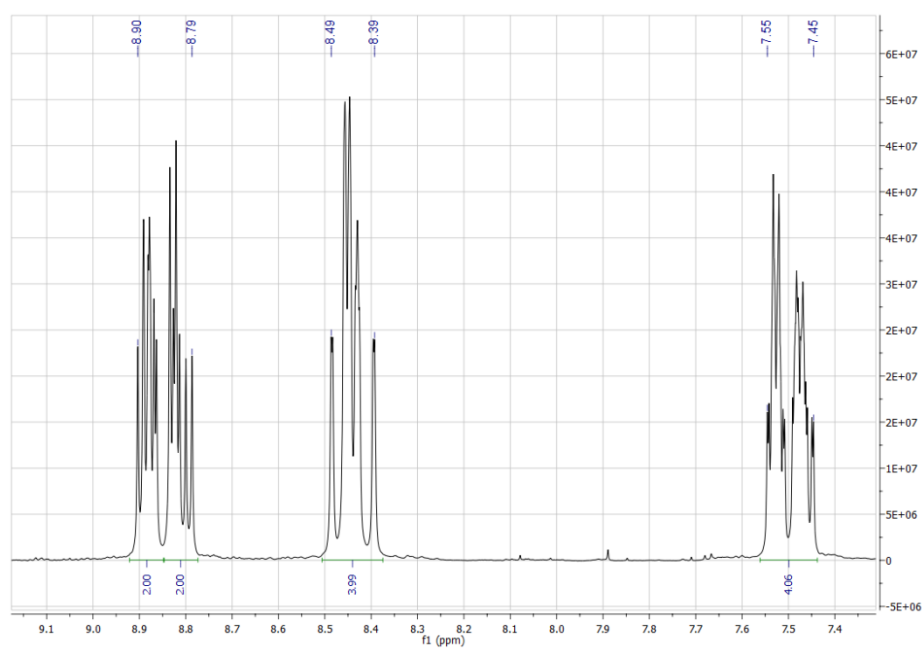


Figure S2: **(*n*-BuO)<sub>4</sub>ZnPc** MALDI-TOF spectrum

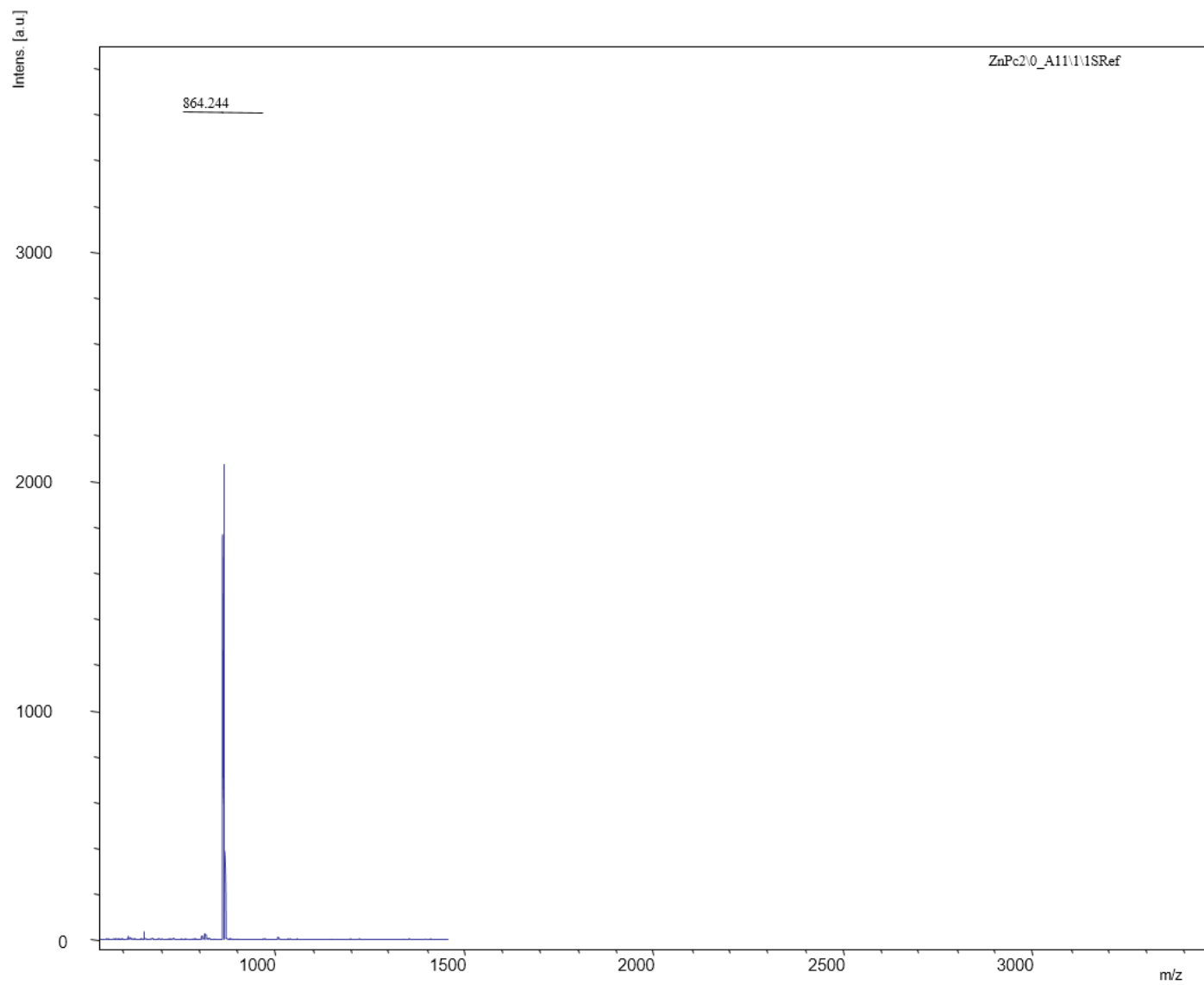
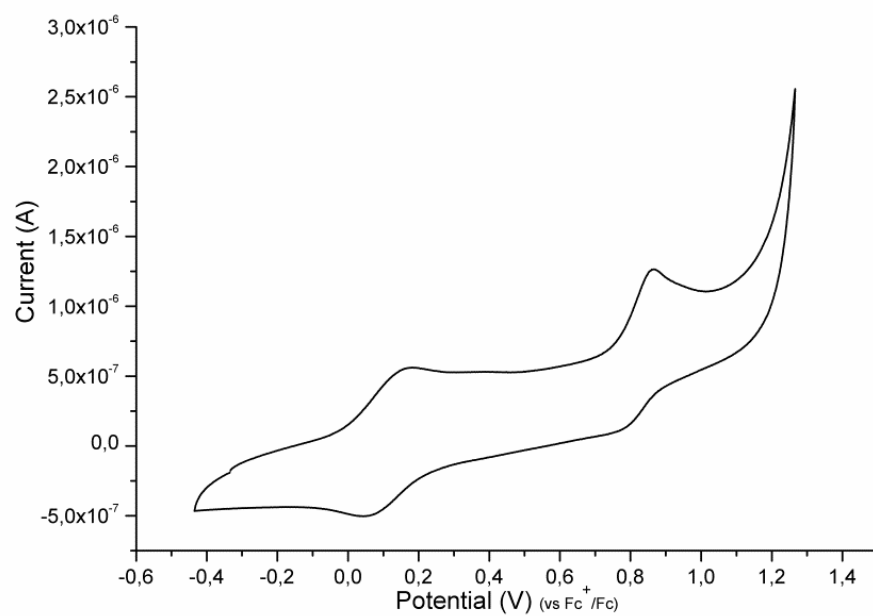


Figure S2 (*n*-BuO)<sub>4</sub>ZnPc anodic scan 0.02 V/s



$$E_{\text{ox}}^1 = 0.111 \text{ V vs Fc}^+/\text{Fc}$$

$$E_{\text{ox}}^2 = 0.818 \text{ V vs Fc}^+/\text{Fc}$$

**Table I** Overview of the quoted materials. Values are given for the bulkiest batch purchasable on <https://www.sigmaaldrich.com/italy.html> and on <https://www.tcichemicals.com/en/eu/>

Chemicals	batch	€/batch	€/g	required amount per 1g product (g)	(€)/g product
4-butoxyphthalonitrile	5.0 g	212.00	42.40	1.75	74.20
ZnCl <sub>2</sub>	1.0 kg	88.90	0.09	0.298	0.03
DMAE	2.0 l	77.50	0.04	4.45	0.18
DBU	2.5 kg	888.00	0.35	0.00155	0.01 (approx)
DCM	4x4.0 l	215.00	0.01	93.0	0.93
THF reagent grade, ≥99.0%, w/250 ppm BHT	2.5 l	78.60	0.03	44.4	1.33
Silica gel (60 Å, 130-270 mesh)	1.0 kg	175.00	0.18	50.0	9.00

Reagents, solvents and Silica gel have been quoted from Sigma-Aldrich.  
4-*n*-butoxyphthalonitrile has been quoted from TCI chemicals.

**Table II** Comparison of **Spiro-OMeTAD** quotations from different suppliers

	batch (g)	original quotation	quotation (€)*	price/g (€)
Sigma-Aldrich	5	1212.00 €	1212.00	242.40
Ossila (unsublimed >99.5%)	1	237.00 £	263.91	263.91
Ossila (sublimed >99.5%)	1	363.00 £	404.21	404.21
Solaronix	5	2200.00 CHF	1935.71	387.14

\*Currency conversion has been made on Aug, 20<sup>th</sup> 2018

**Figure S3:** flowchart for the synthesis of 1 kg of  $(n\text{-BuO})_4\text{ZnPc}$ . Reagents quantities are highlighted in red, solvent is highlighted in green and workup/purification materials are highlighted in blue

