Supporting Information

Orthogonal effect on Pyrene-Porphyrin conjugates towards the detection of Volatile Organic Compounds under UV and Visible light illumination through Surface Photovoltage

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Content

1. Structural Characterization

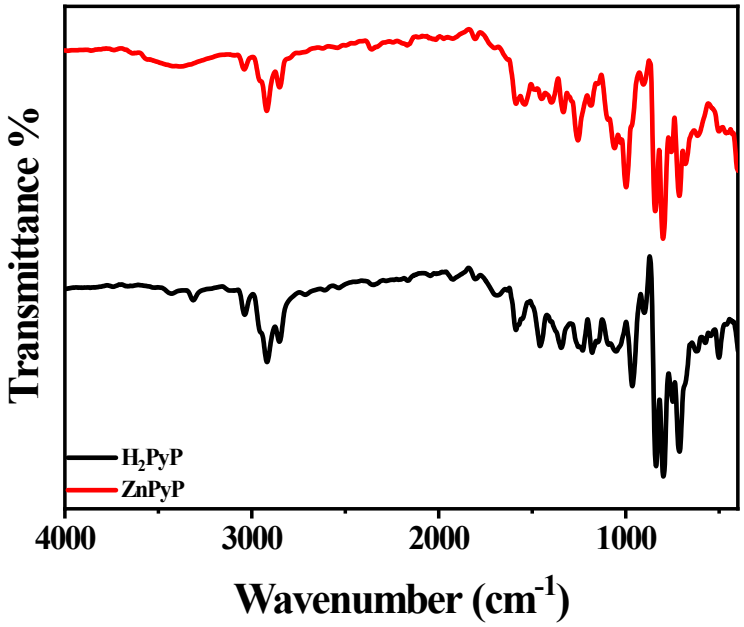


Fig. S1 Stacked FT-IR spectra of H_2PyP and ZnPyP.

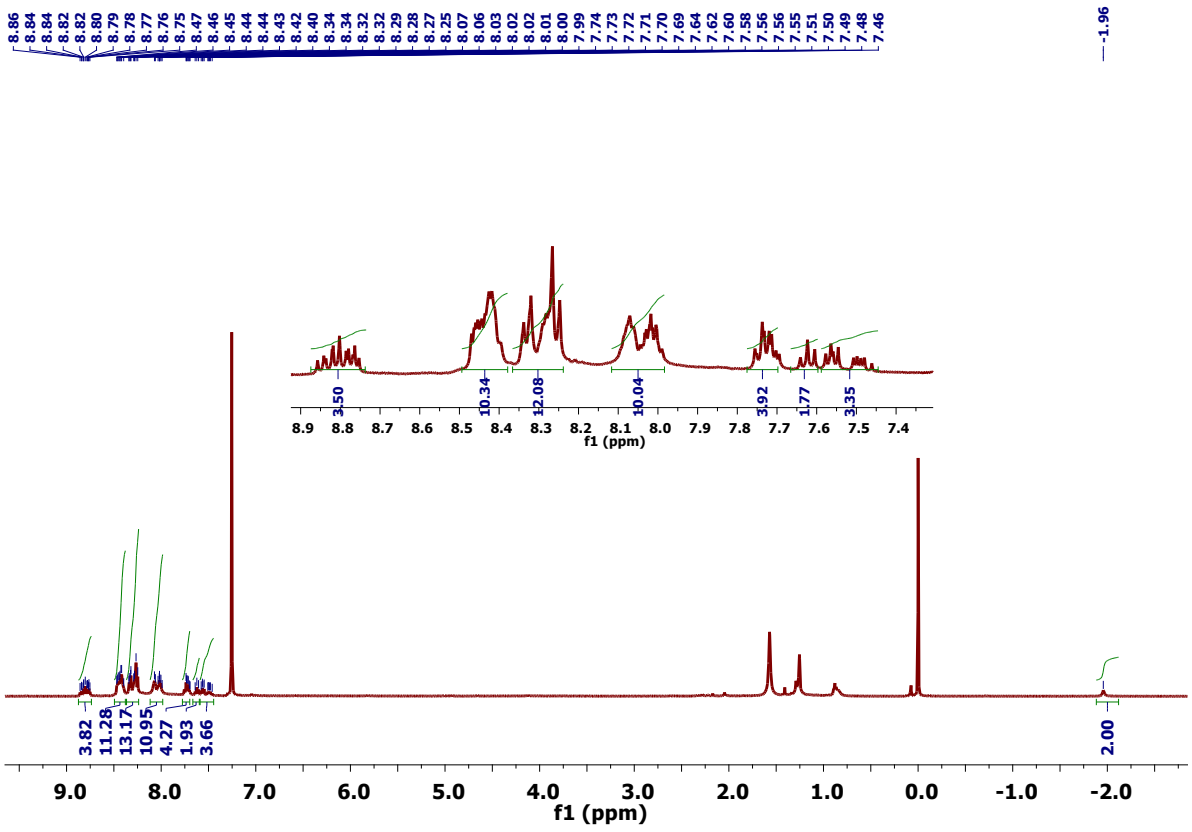


Fig. S2 ^1H NMR (300 MHz) of H_2PyP in $CDCl_3$.

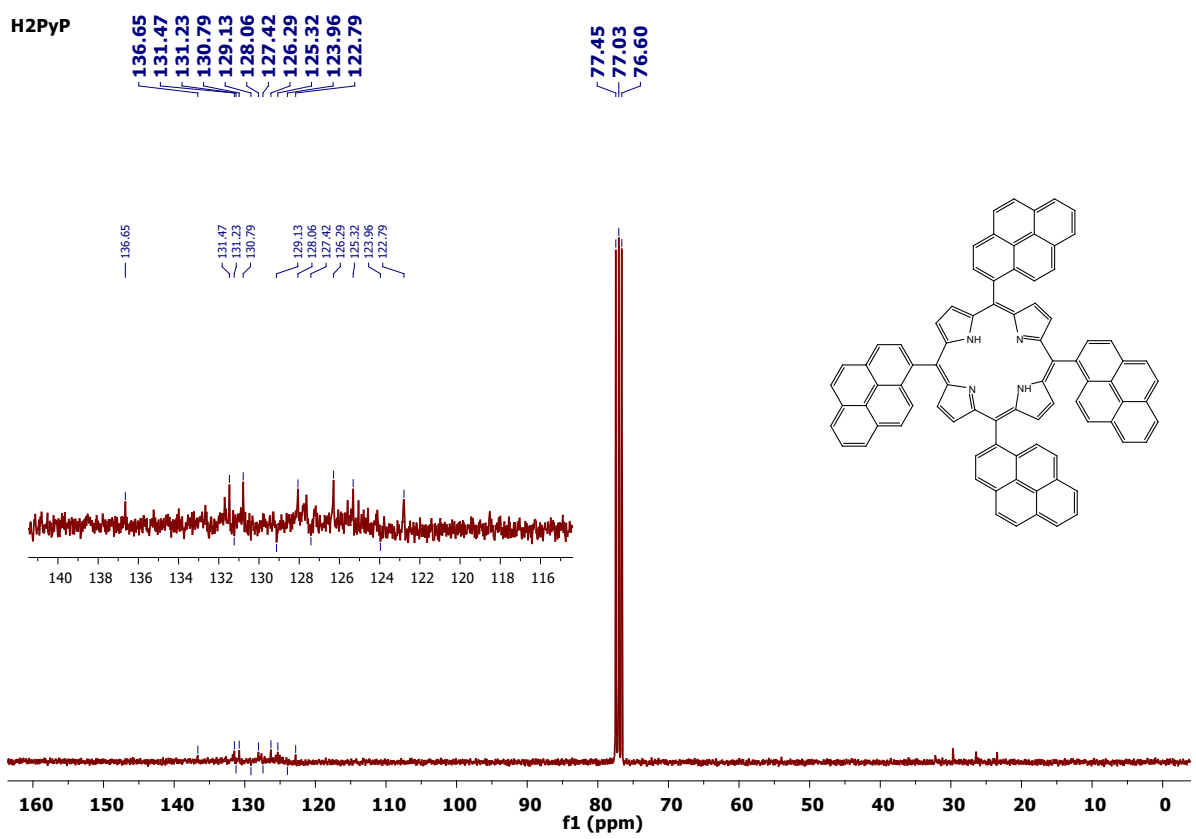


Fig. S3 ^{13}C NMR (75 MHz) of H_2PyP in $CDCl_3$.

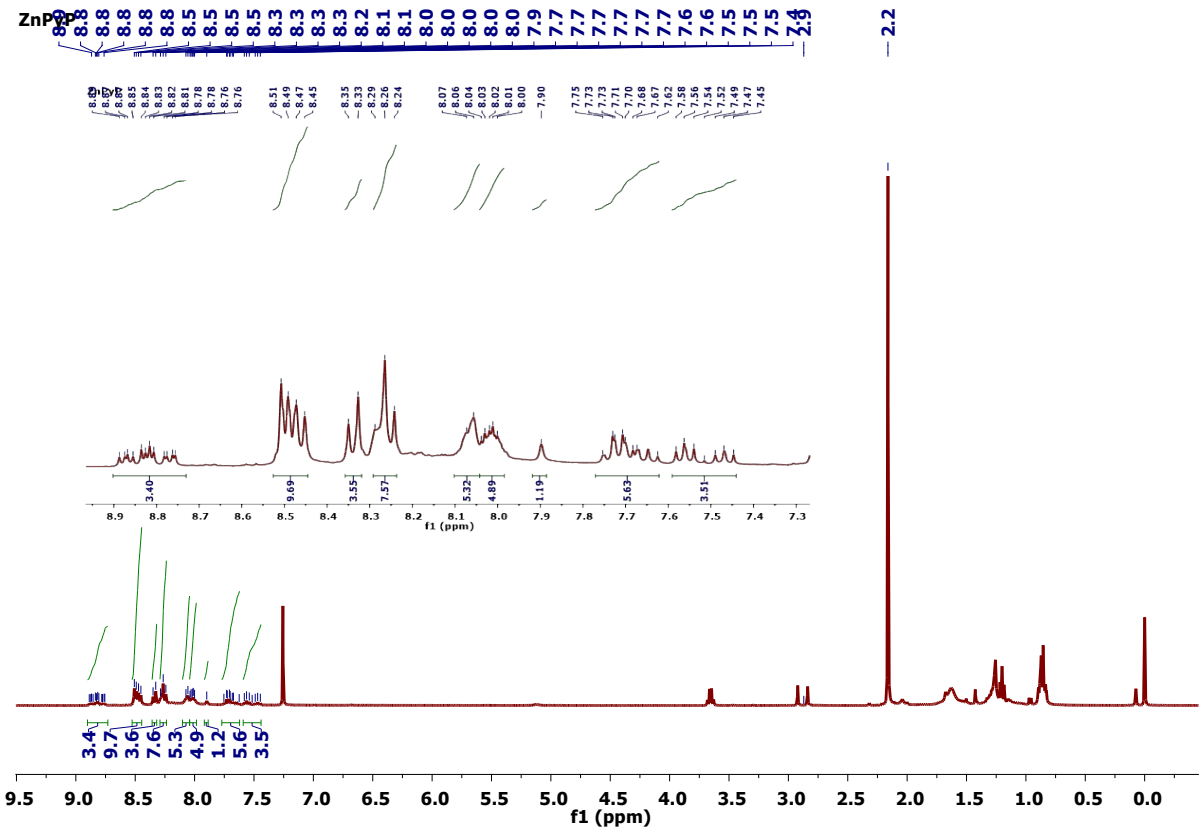


Fig. S4 ^{1}H NMR (300 MHz) of ZnPyP in $CDCl_3$.

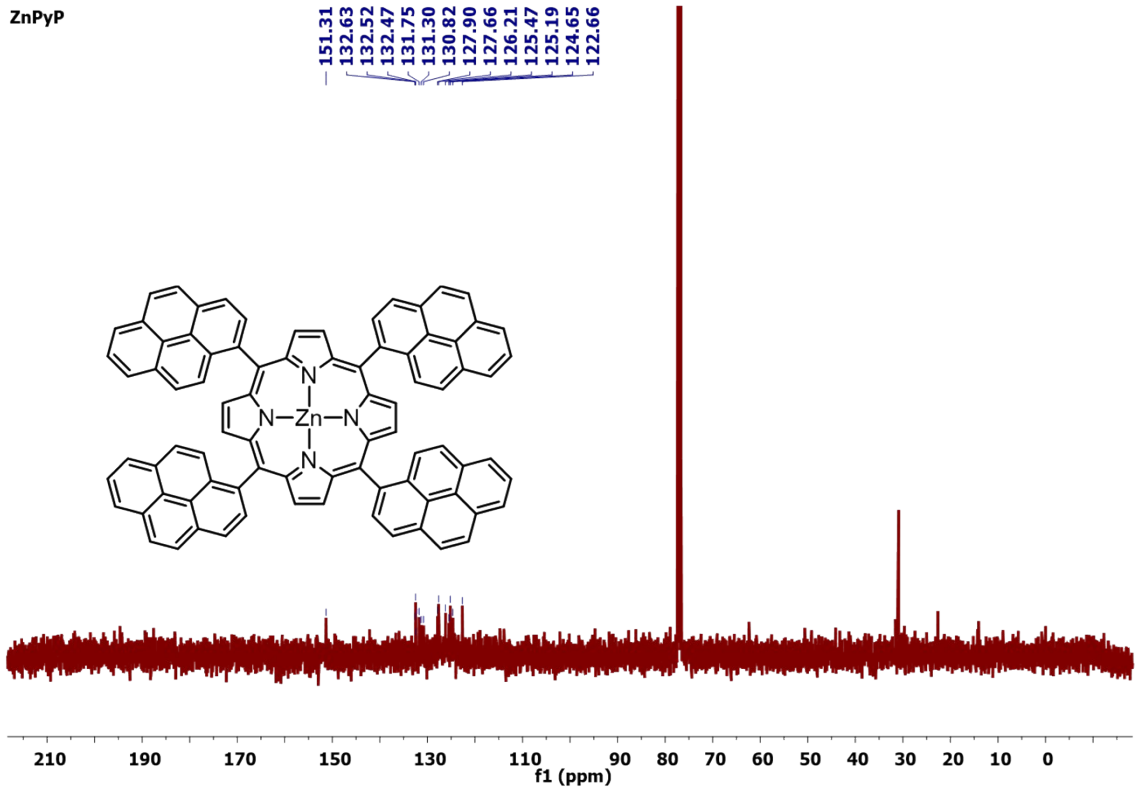


Fig. S5 ^{13}C NMR (75 MHz) of ZnPyP in $CDCl_3$.

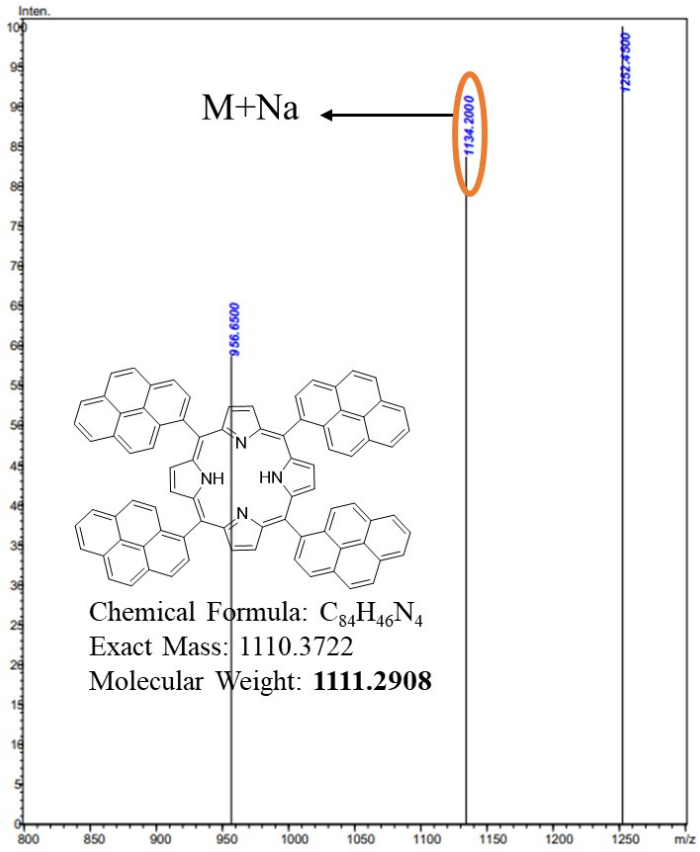


Fig. S6 The ESI-MS of H_2PyP.

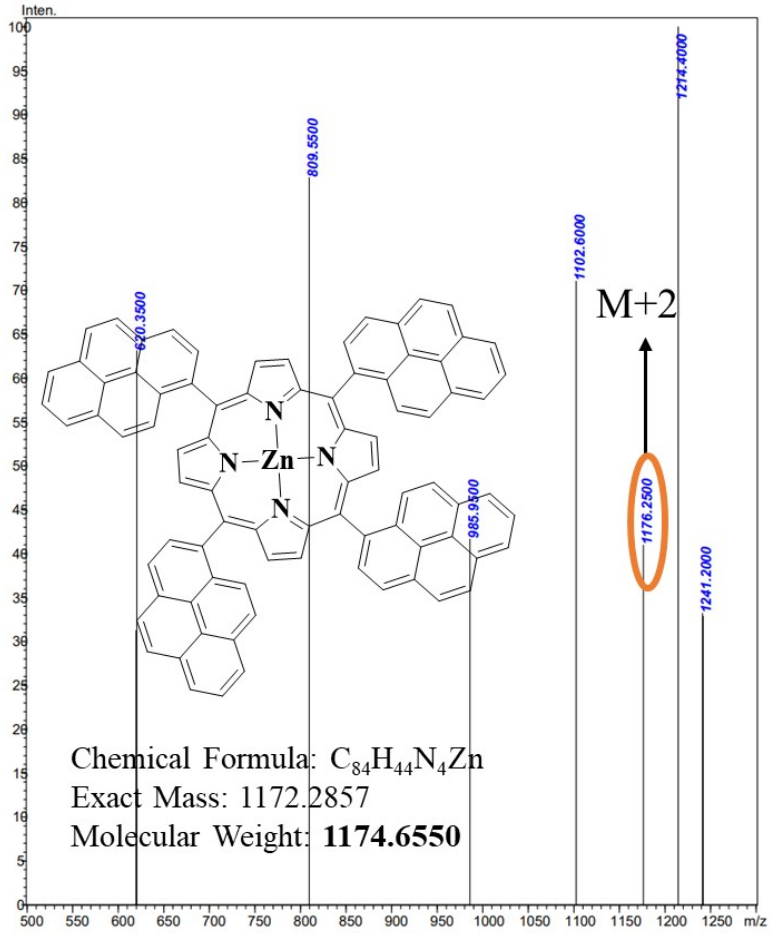
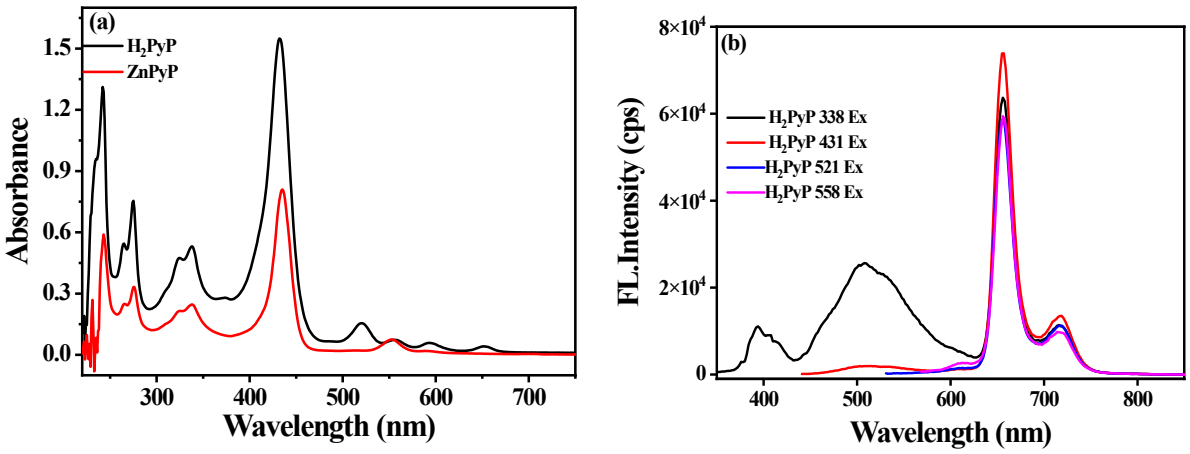


Fig. S7 The ESI-MS of ZnPyP.

2. Photophysical properties



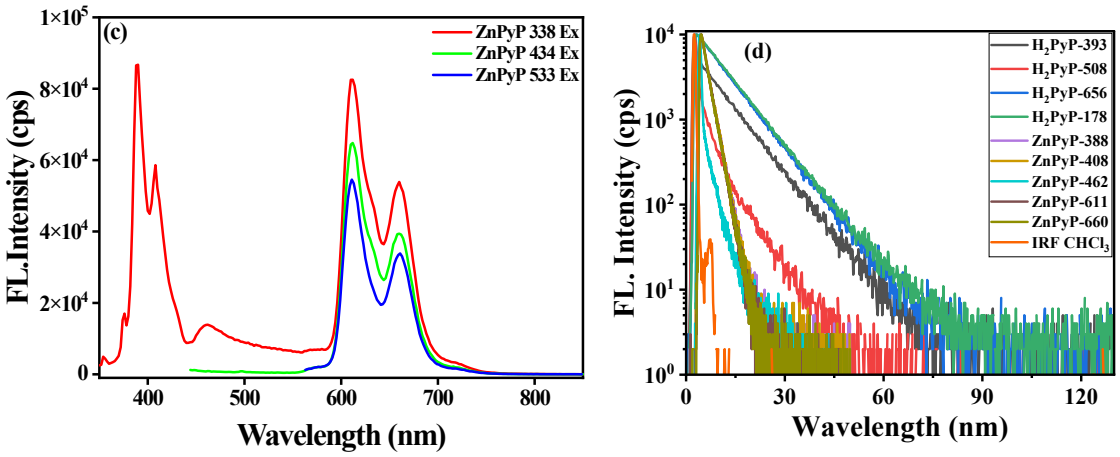


Fig. S8 Absorption spectra of H_2PyP and ZnPyP (a) in chloroform solution. Fluorescence Emission spectra of (b, c) H_2PyP and ZnPyP, lifetime decay profile of (d) H_2PyP and ZnPyP in solution.

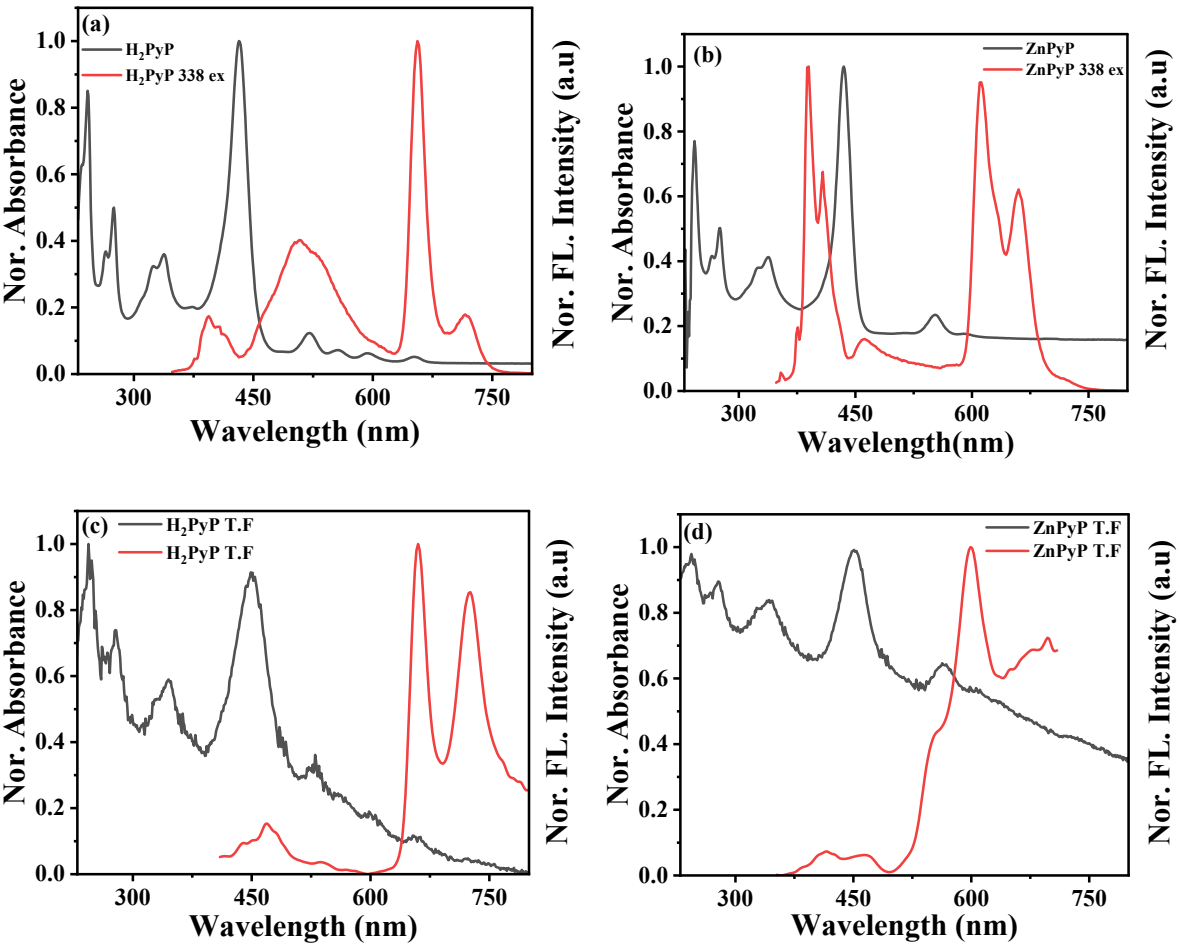


Fig. S9 UV-visible and emission spectrum of solution and thin film H_2PyP and ZnPyP comparison studies.

3. SKP Measurements

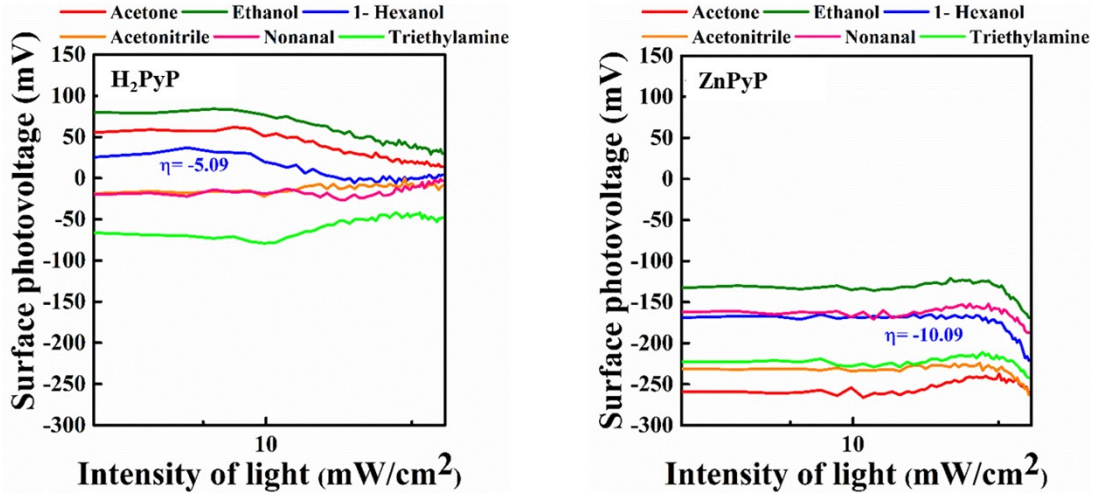


Fig. S10 Surface photovoltage changes of H_2PyP and ZnPyP under visible light illumination under various VOC media.

Table S1. The η values of H_2PyP and ZnPyP under visible light illumination for various VOC atmospheres

η	Acetone	Ethanol	1-hexanol	Acetonitrile	Nonanal	Triethylamine
ZnPyP	-7.218	-4.90663	-10.098	-2.60796	-8.935	-2.617
H_2PyP	-0.5246	-0.79701	-5.0918	-2.22788	-4.55	-1.67582

Table. S2 Various pyrene and porphyrin derivatives have been employed previously for VOC detection

Sl No.	**Material**	**VOCs**	**Reference**
1.	H_2TPPSH, CoTPPSH	Triethylamine	[1]
2.	Pyrene Tetratopic Ligands Layered on ZnO Nanorods	Ethanol (alcohol) and n-hexane (alkane)	[2]
3	Porphyrin-Functionalized ZnO Nanorods	Triethylamine	[3]
4	Pyrene Coated ZnO Nanorods	Triethylamine	http://dx.doi.org/10.5162/IMCS2018/P2NG.20
5	triphenylamine	Nonanal	[4]

	derivatives functionalized zinc oxide nanorods		
6	multi-walled carbon nanotubes coated with pyrene based organic molecules	Triethylamine	[5]
7	porphyrin functionalized boron doped diamond thin films	Triethylamine	[6]
8	Triphenylamine-porphyrin conjugates as antenna modular systems	1-hexanol	[7]
9	Porphyrinoid-Functionalized ZnO Nanoflowers	Benzylamine	[8]

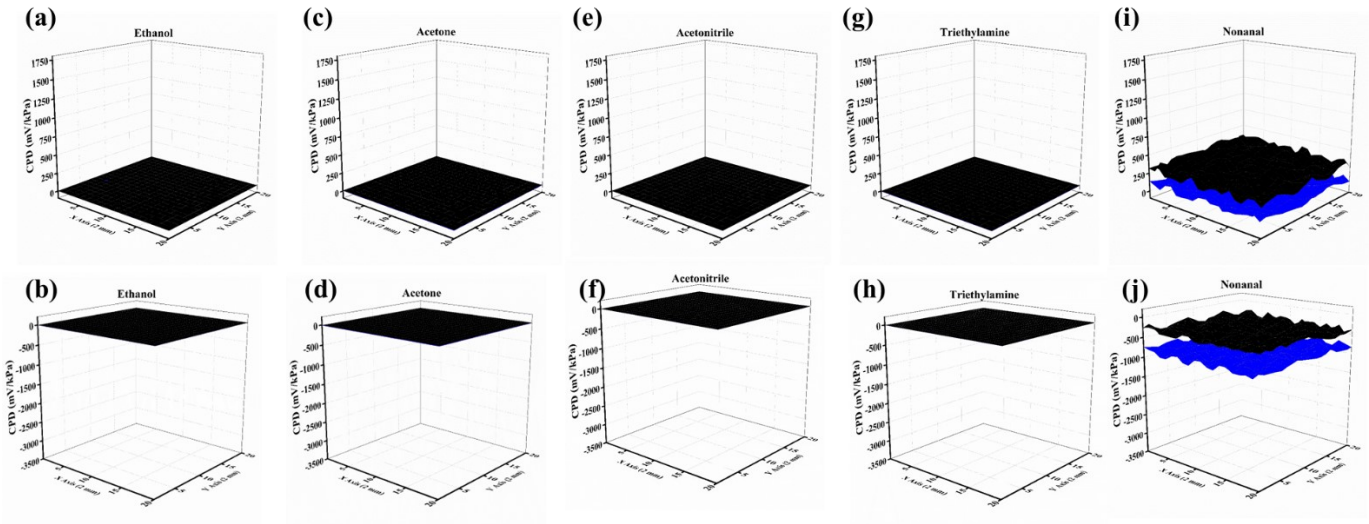


Fig. S11 Raster scan images on dark and UV light illumination of (a, c, e, g, i) H_2PyP and (b, d, f, h, j) ZnPyP under VOC exposure.

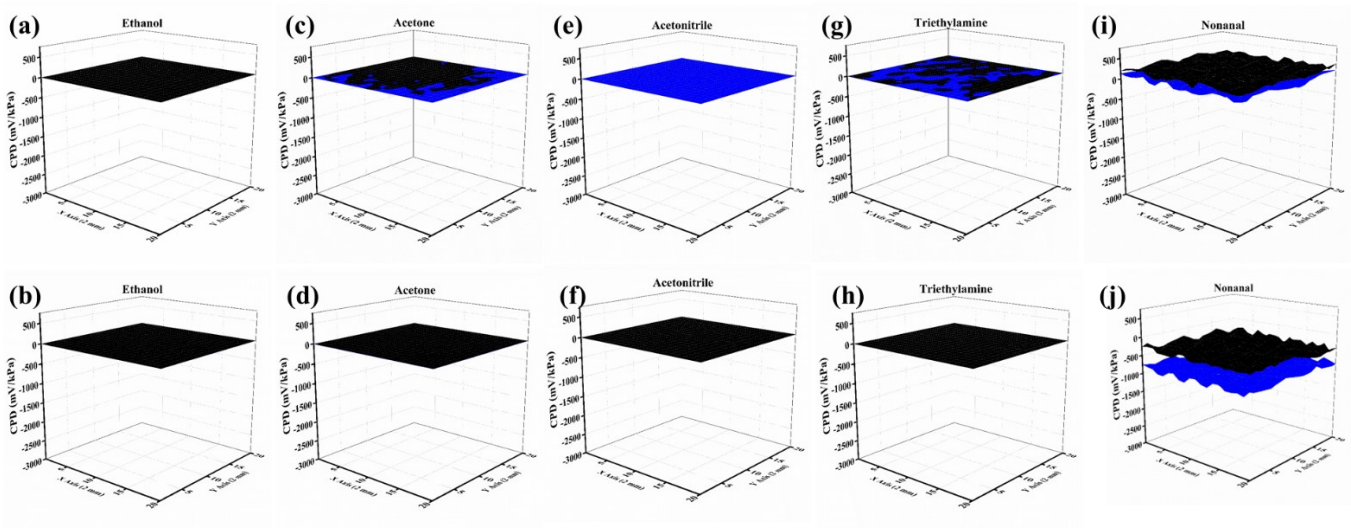


Fig. S12 Raster scan images on dark and Visible light illumination of (a, c, e, g, i) H_2PyP and (b, d, f, h, j) ZnPyP under VOC exposure.

4. DFT

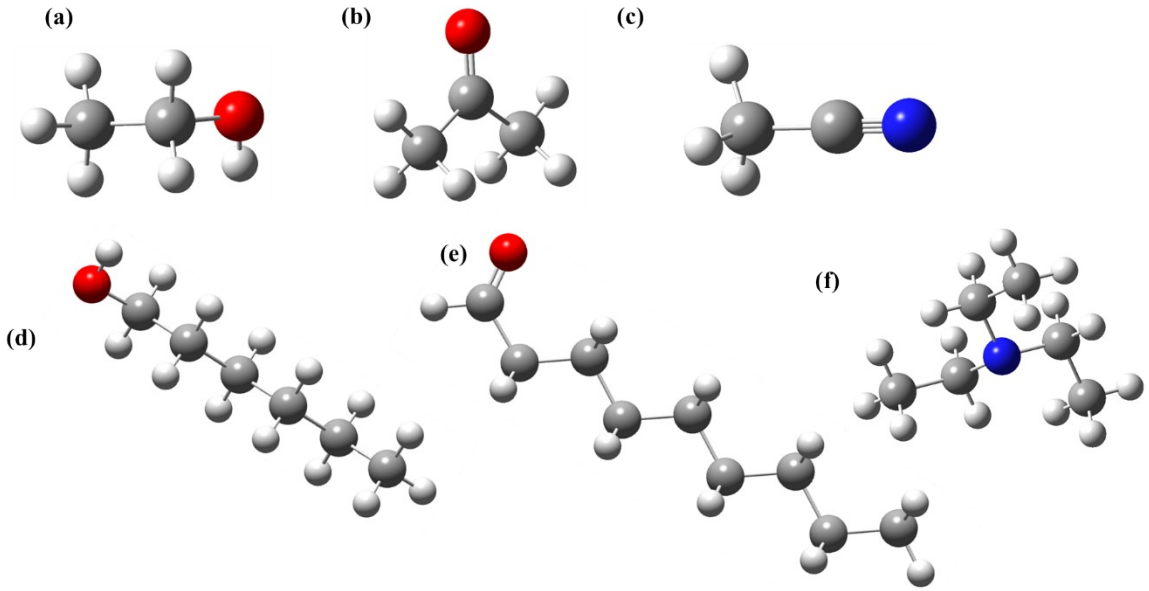


Fig. S13 Optimised structures of (a) EtOH, (b) Acetone, (c) ACN, (d) 1-Hexanol, (e) Nonanal, and (f) TEA

Table S3. details on the adsorption energy of VOCs with H_2PyP

Name of VOC	**Adsorption energy (eV)**
Ethanol	-0.21
Acetone	-0.08
Acetonitrile	-0.12
1-hexanol	-0.15
Nonanal	-0.11
Triethylamine	-0.02

Table S4. details on the adsorption energy of VOCs with ZnPyP

Name of VOC	**Adsorption energy (eV)**
Ethanol	-0.33
Acetone	-0.26
Acetonitrile	-0.23
1-hexanol	-0.34
Nonanal	-0.28
Triethylamine	-0.02

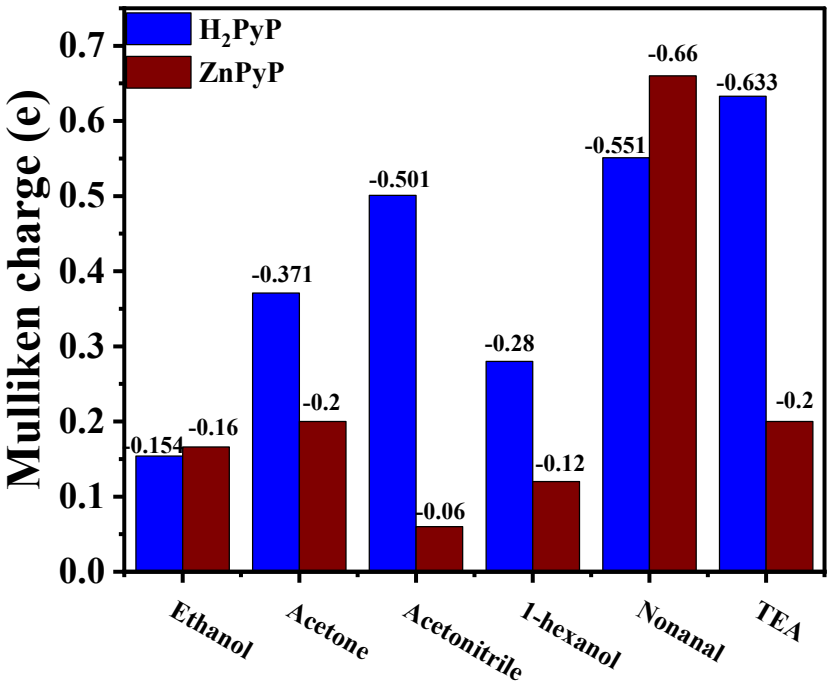


Fig. S14 Plot of Mulliken Charge analyses in VOCs adsorbed H_2PyP and ZnPyP.

Reference

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