An AIE-based self-assembled fluorescent probe for COX-2 imaging

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1. Absorption and Fluorescence emission spectra of TPI-IMC in different solvents.

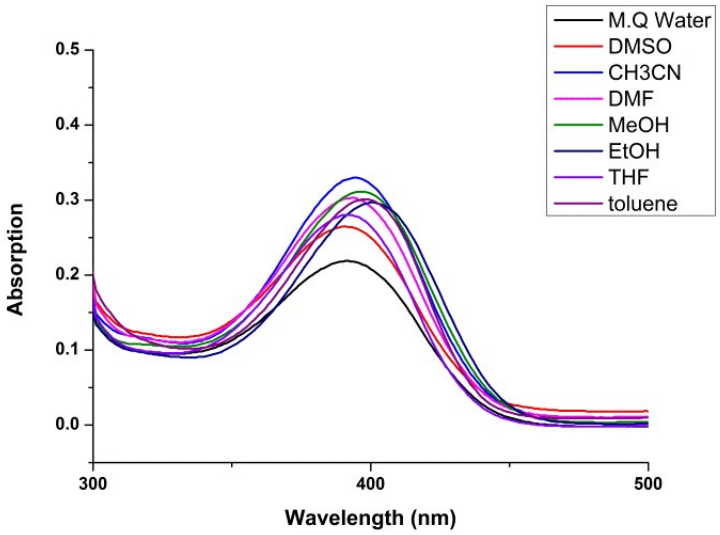

Figure S1. UV-Vis spectrum of TPI-IMC in different solution

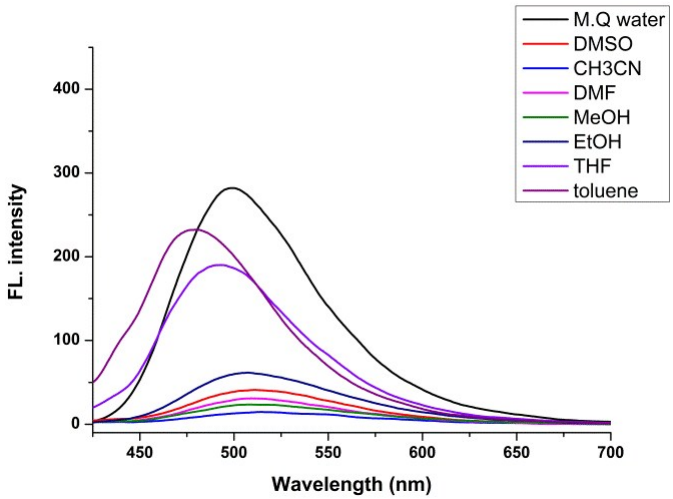

Figure S2. Fluorescent spectrum of TPI-IMC in different solution

2. Calculation of fluorescence quantum yield[1]

Fluorescence quantum yield was determined using optically matching solutions of quinine sulfate (Φ_f = 0.546 in 1N H_2SO_4) as the standard at an excitation wavelength of 350 nm and the quantum yield was calculated using the following equation:

$\Phi_s = \Phi_r$ (ArFs/AsFr) (ns^2/nr^2) [2]

where, s and r denote sample and reference, respectively, A is the absorbance, F is the relative integrated fluorescence intensity, and n is the refractive index of the solvent.

3. Fluorescent spectra of TPI-IMC upon addition with COX-2 enzyme (0.4 μg/mL)

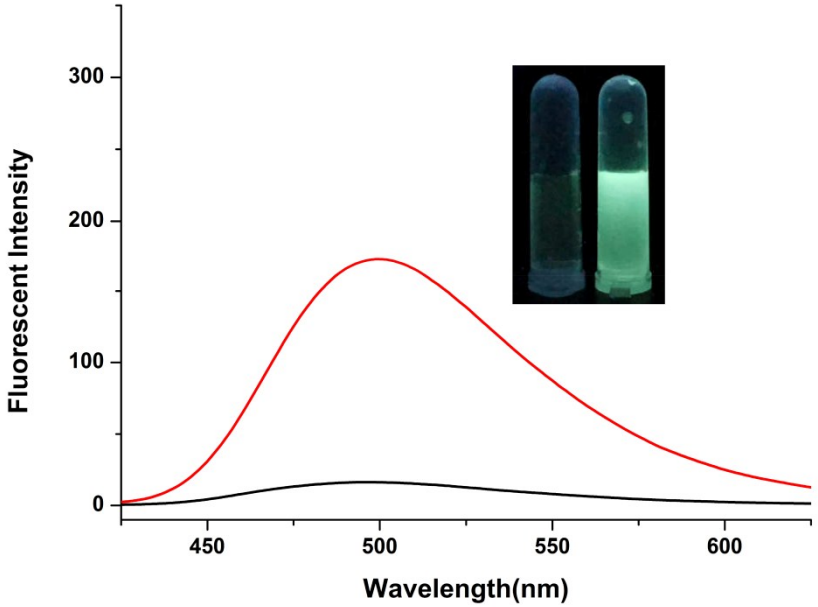

Figure S3. Fluorescence response of TPI-IMC (5 μM) to COX-2 (0.4 μg/mL), λex=380 nm. Inset: Fluorescence changes of TPI-IMC upon addition of COX-2 under excitation with UV light (365 nm).

4. Photostability in solution:

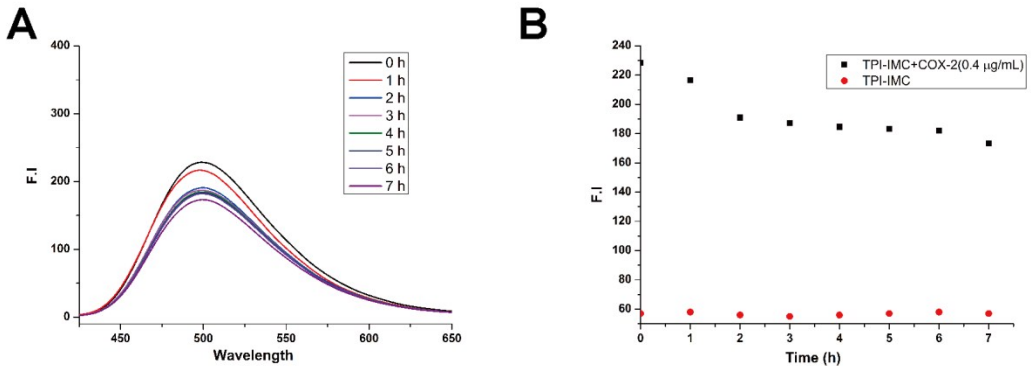

Figure S4 (A) Fluorescent spectra over time for TPI-IMC in presence of COX-2 subject to continuous illumination under 365nm with UV lamp. (B) Fluorescent emission intensity over time for TPI-IMC in absence and presence of COX-2 subject to continuous illumination under 365nm with UV lamp.

5. Competitive experiments

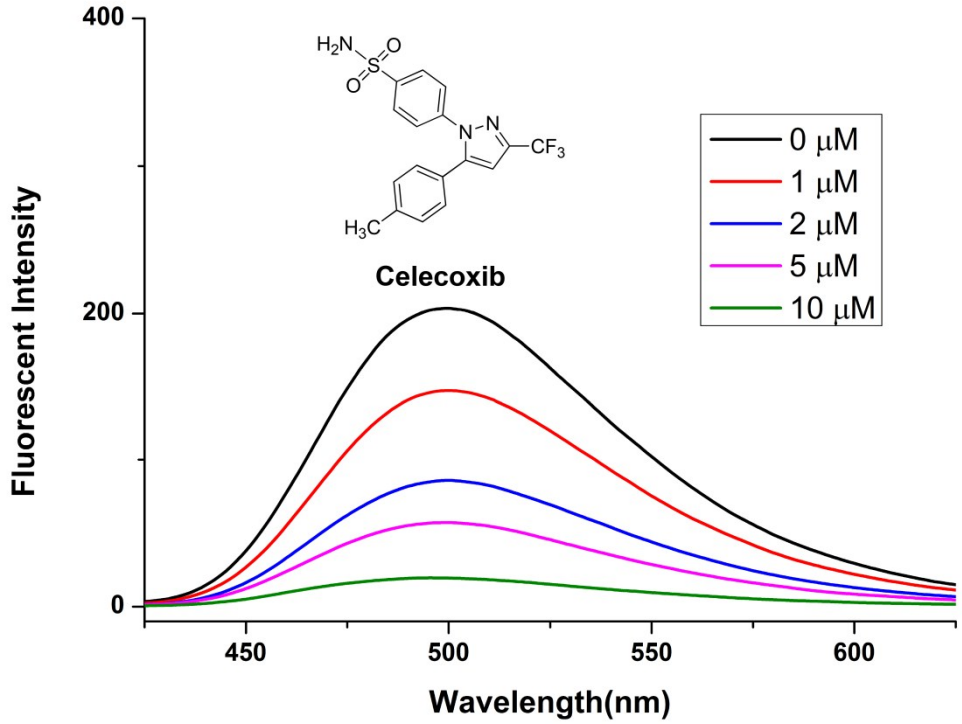

Figure S5. Competitive binding between TPI-IMC (5μM) and celecoxib.

6. Dynamic Light Scattering

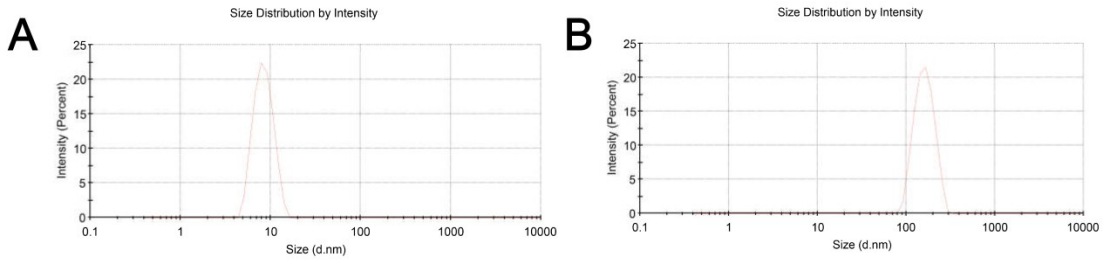

Figure S6. DLS results of TPI-IMC in absence (A) and presence (B) of COX-2 (0.4μg/mL)

7. Computational details

The molecule geometry, HOMO and LUMO energy levels were calculated by MOE (Molecular Operating Environment, 2014.10). Gaussian is the engine. The molecule geometry, HOMO and LUMO energy levels were calculated by MOE (Molecular Operating Environment, 2014.10). 6-31G(d)(B3LYP) was chosen as the basis set.

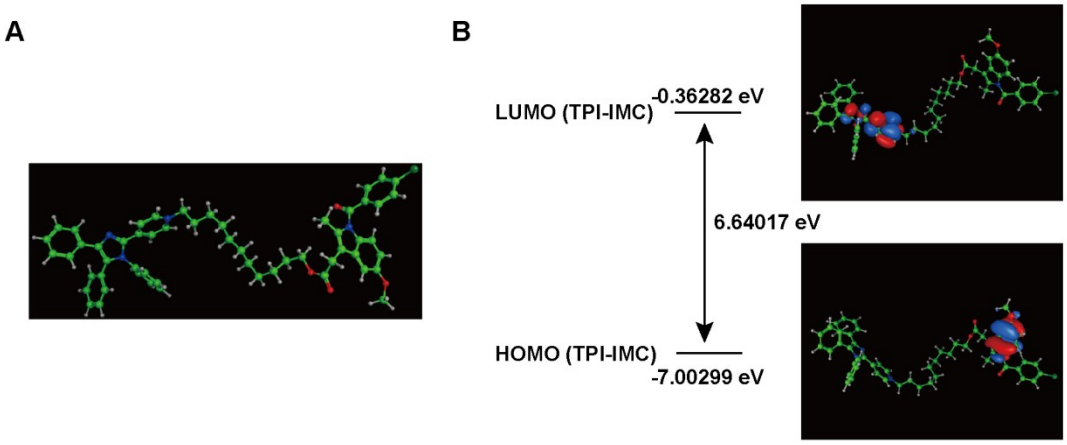

Figure S7. (A) Calculated optimal configuration of TPI-IMC; (B) calculated HOMO and LUMO electron cloud distribution of TPI-IMC.

8. Selectivity of TPI-IMC to different biospecies

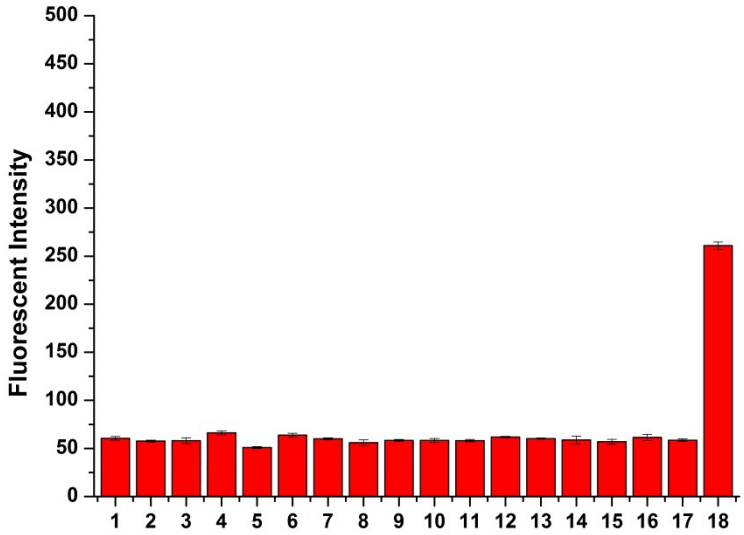

Figure S8. Fluorescence intensity of TPI-IMC(5μM) at 500 nm in the presence of different biospecies: 1.Cys, 2. Hcy, 3. GSH, 4. H_2O_2, 5. Na^+, 6. Mg^{2+}, 7. RNA, 8. DNA, 9. lysozyme, 10. proteinase, 11.collagen, 12. hemoglobin, 13. BSA, 14. trypsin, 15. HCO_3^-, 16. HPO_4^{2-}, 17. COX-1, 18. COX-2.

9. The influence of pH value on the fluorescent intensity in 500 nm of TPI-IMC

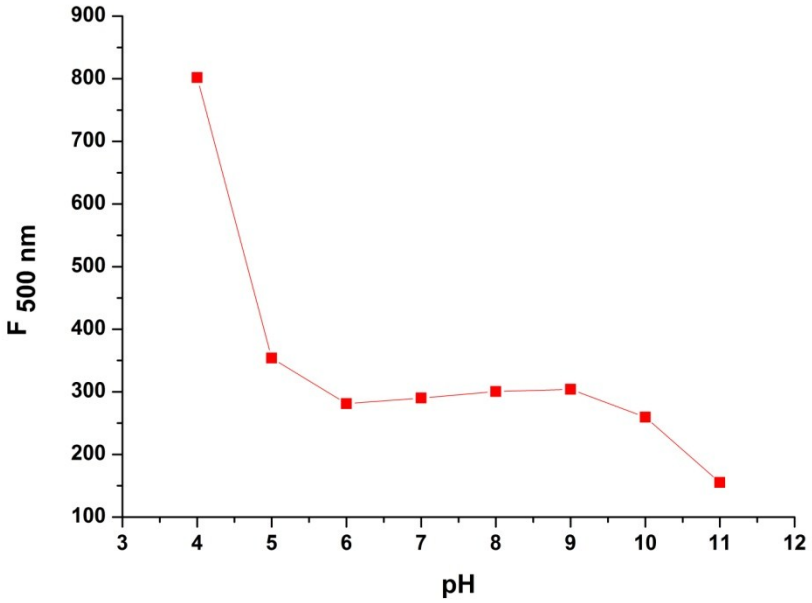

Figure S9 The influence of pH value on the fluorescent intensity in 500 nm **of TPI-IMC**

10. Cytotoxicity

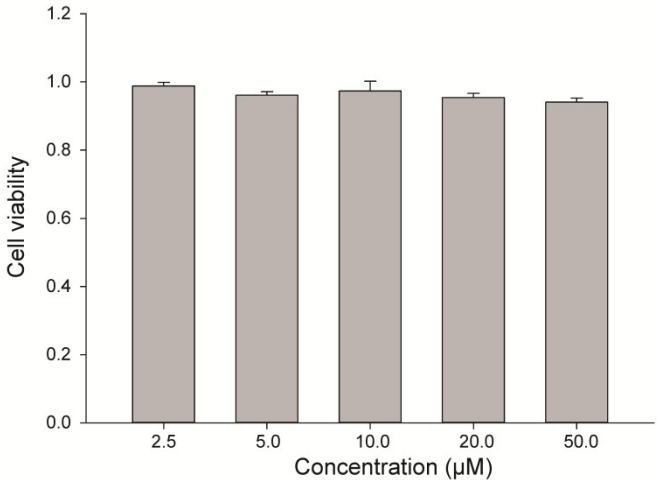

Figure S10. The cell viability of **TPI-IMC** of indicated concentration (2.5 μM, 5.0μM, 10.0μM, 20.0 μM, 50.0 μM)

11. Inhibition assay

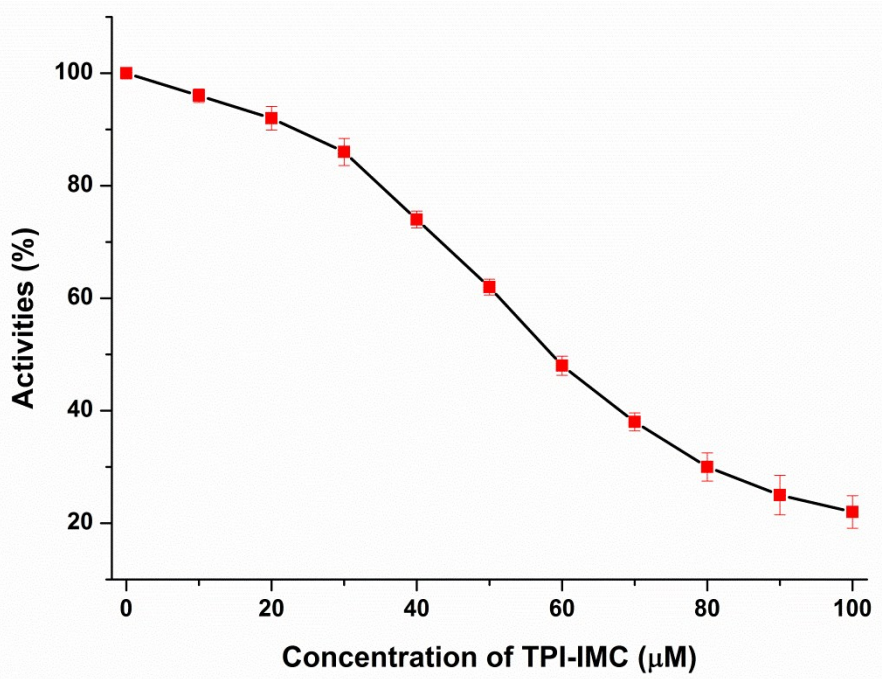

Fig.S11 Dose-inhibition curves of TPI-IMC (0-100.0 μM) with COX-2 (0.4 μg/mL) enzyme

11. ^{1}H-NMR, ^{13}C-NMR and MS characterization

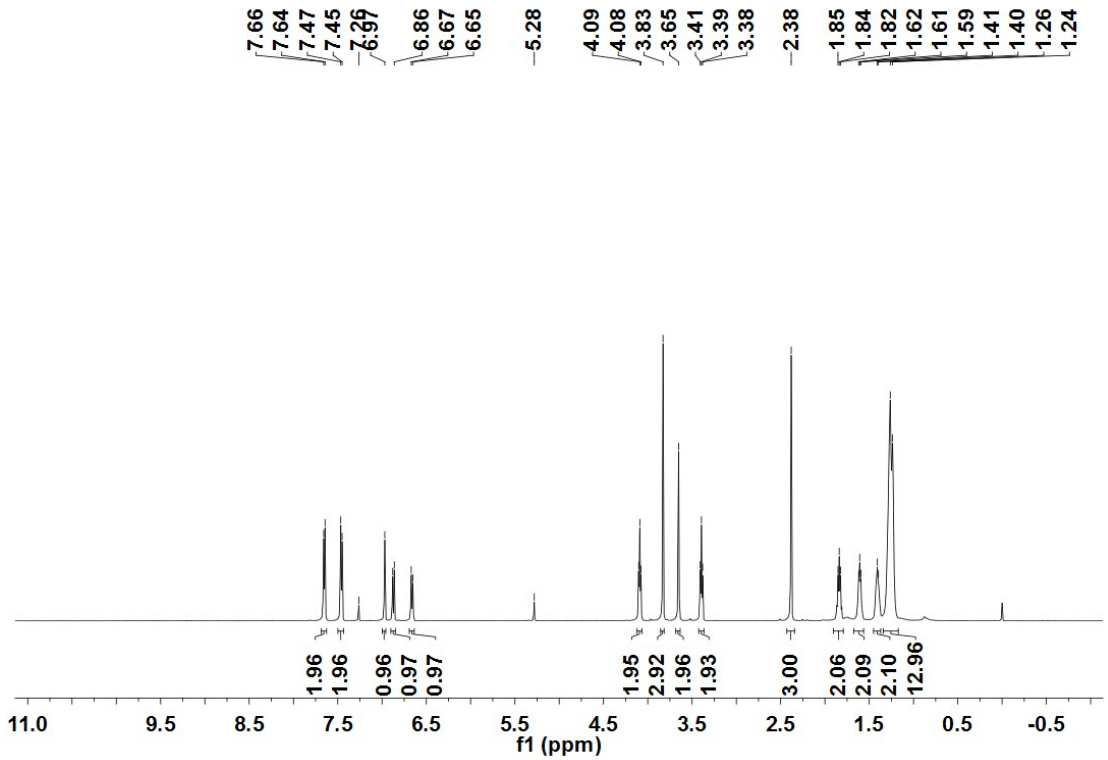

Figure S12. ^{1}H NMR spectrum of Compound 2

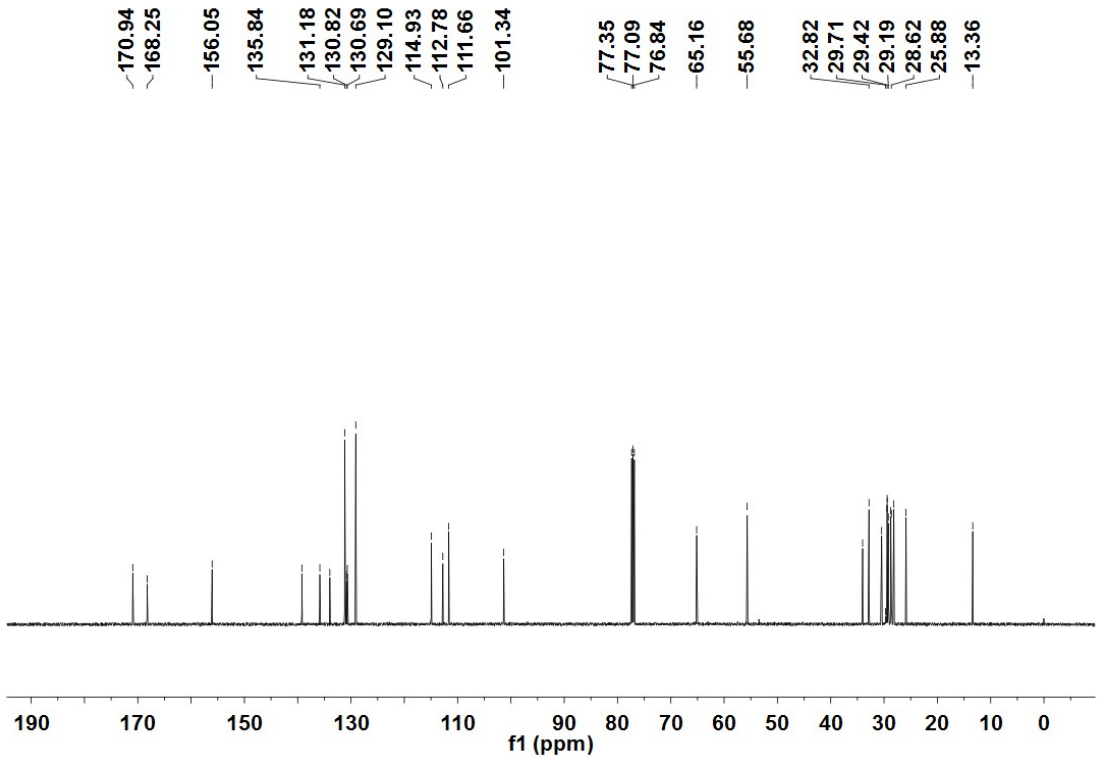

Figure S13. ^{13}C NMR spectrum of Compound 2

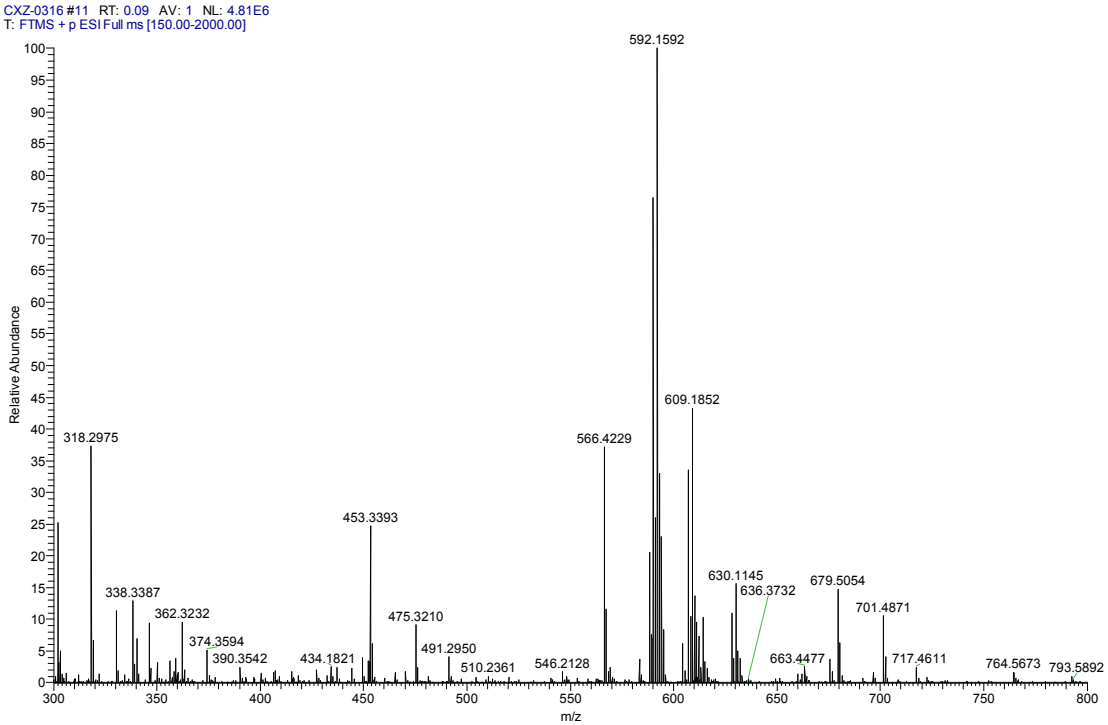

Figure S14 HRMS spectrum of Compound 2

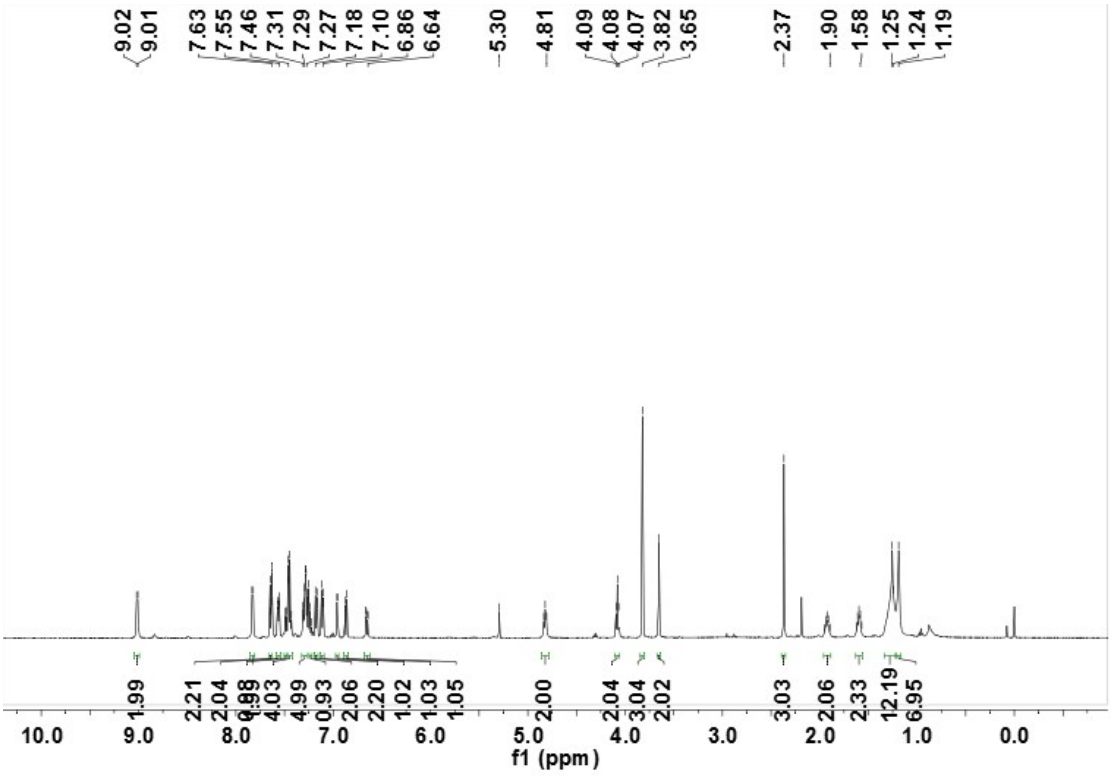

Fig.S15 ^{1}H NMR spectrum of TPI-IMC

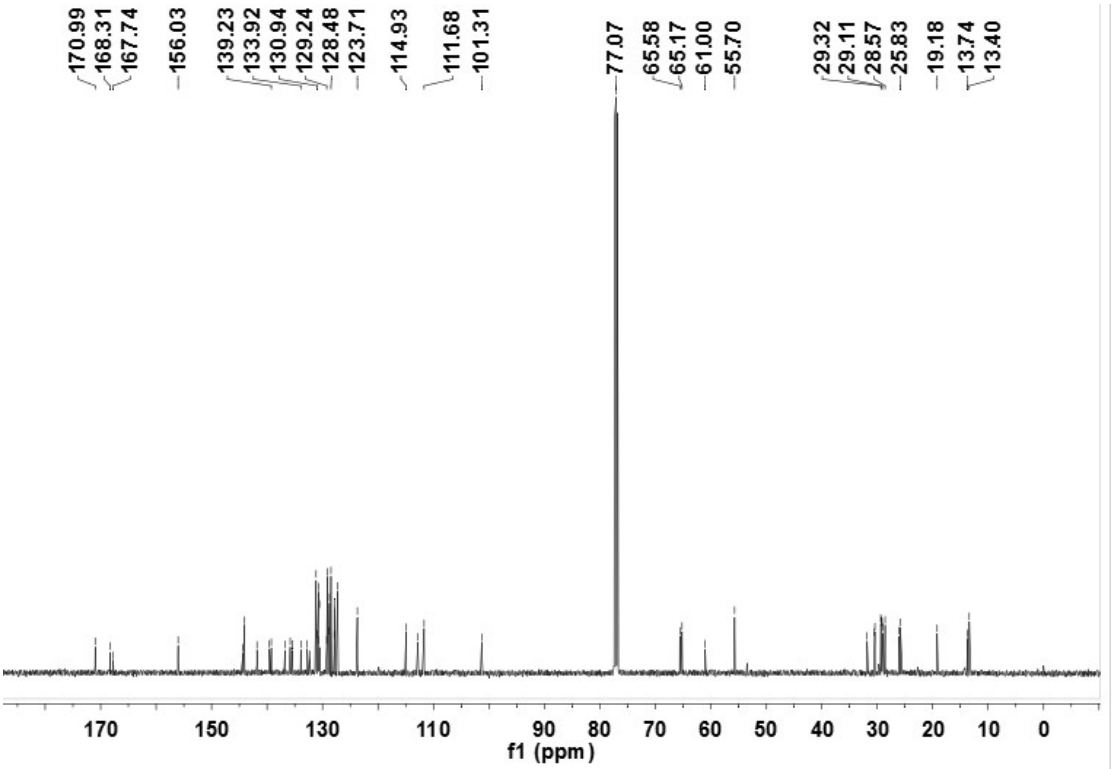

Fig.S16 ^{13}C NMR spectrum of TPI-IMC

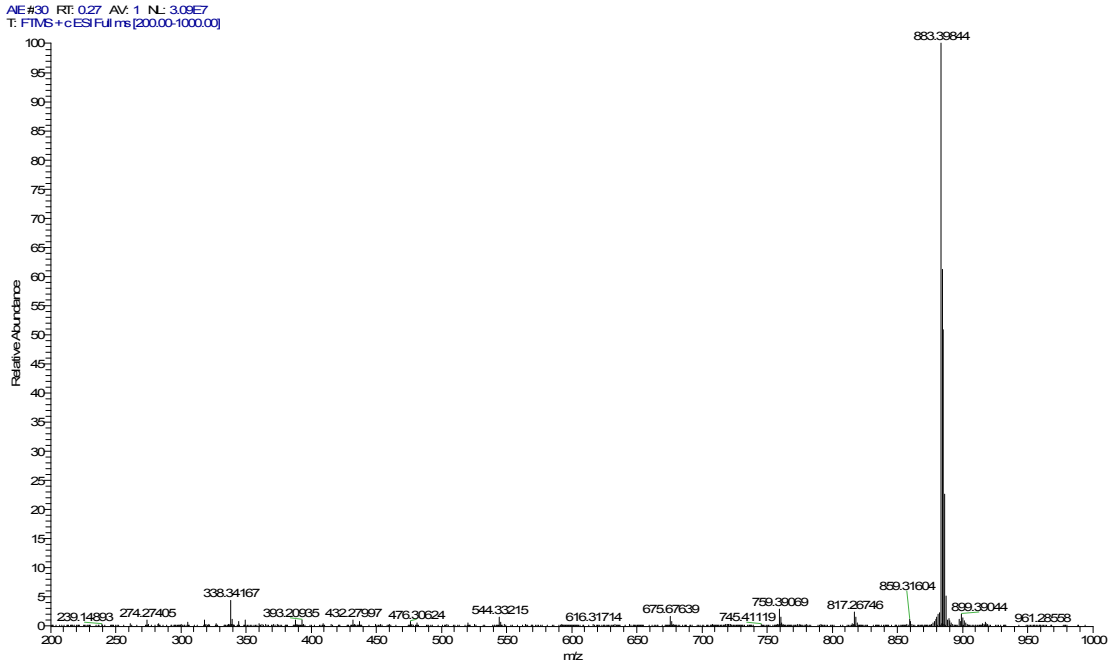

Figure S17. HRMS spectrum of TPI-IMC

Reference

1. D. Magde, G. E. Rojas and P. G. Seybold, *Photochemistry and Photobiology*, 1999, **70**, 737-744.