

Supplementary Material

Exploring improved strategies for therapeutic studies and biological activities of novel zinc and indium phthalocyanines

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1. Photochemical Studies

1.1 Singlet oxygen quantum yields (Φ_{Δ})

Singlet oxygen efficiency was determined in air (no oxygen bubbled) using their relative method (Eq. 1) with unsubstituted ZnPc (in organic solvent) as reference and 1,3-Diphenylisobenzofuran (DPBF) (in organic solvent) as chemical quenchers for singlet oxygen,

$$\Phi_{\Delta} = \Phi_{\Delta}^{\text{Std}} \frac{R \cdot I_{\text{abs}}^{\text{Std}}}{R^{\text{Std}} \cdot I_{\text{abs}}} \quad (1)$$

where is the singlet oxygen quantum yield for the Standard ZnPc ($\Phi_{\Delta}=0.67$ in DMSO) [6,37]. R and R_{Std} are the DPBF photo bleaching rates in the presence of the respective samples and standard, respectively. I_{abs} and $I_{\text{abs}}^{\text{Std}}$ are the rates of light absorption by the sample and standard, respectively. The samples containing DPBF were prepared in the dark and irradiated at the Q band region. The absorption band of the DPBF reduced by light irradiation (The light intensity of 7.05×10^{15} photons $\text{s}^{-1} \text{cm}^{-2}$). The degradation of DPBF was monitored using UV-Vis spectroscopy after each 5 s light irradiation at 417 nm for PDT.

1.2 Photodegradation quantum yields (Φ_{d})

Photodegradation quantum yields were determined using Eq. 2 [6],

$$\Phi_{\text{d}} = \frac{(C_0 - C_t) \cdot V \cdot N_A}{I_{\text{abs}} \cdot S \cdot t} \quad (2)$$

where “ C_0 ” and “ C_t ” are the sample concentrations before and after irradiation respectively, “ V ” is the reaction volume, “ N_A ” is the Avogadro’s constant, “ S ” is the irradiated cell area, “ t ” is the irradiation time, “ I_{abs} ” is the overlap integral of the radiations of light intensity and the absorption of the sample. A light intensity of 2.42×10^{16} photons $s^{-1} cm^{-2}$ was employed to determinate the photodegradation. The degradation of max. Q band was monitored after each 5 minute irradiation.

2. Confirmation of Structure

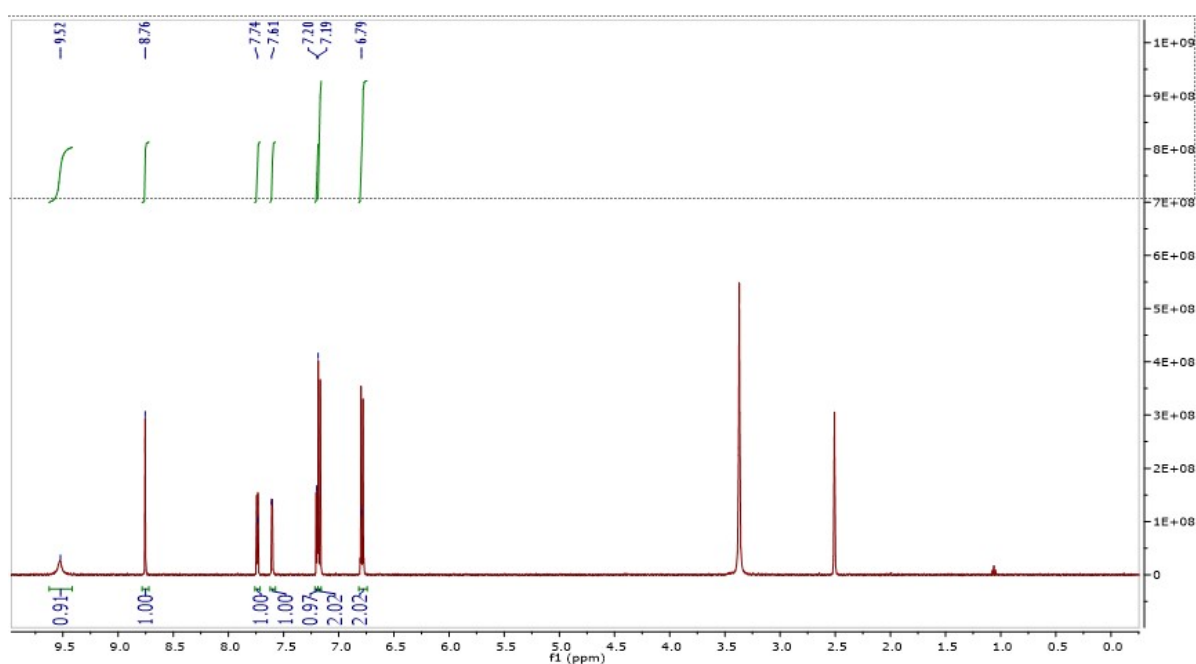


Figure S1. 1H -NMR spectra of compound D1

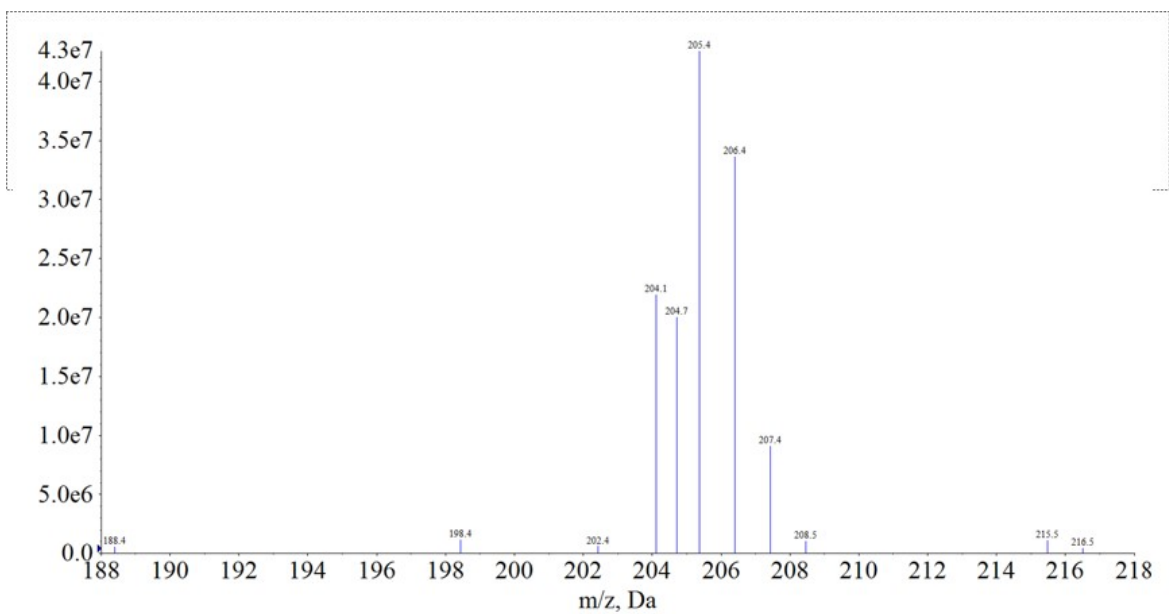


Figure S2. Mass spectra of compound D1

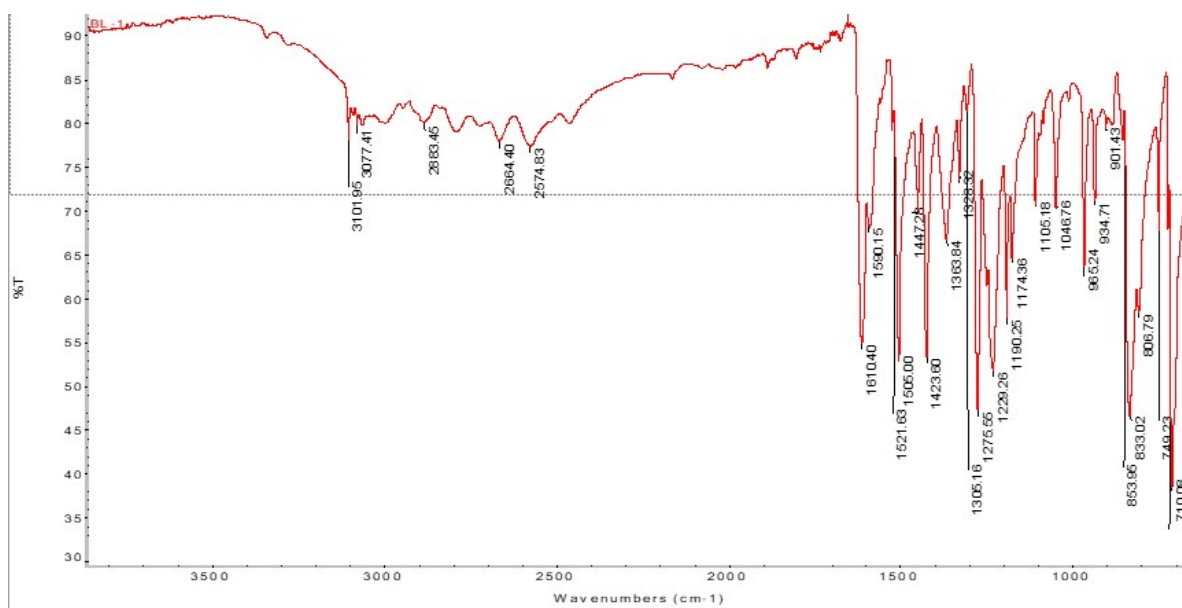


Figure S3. FT-IR spectra of compound D1

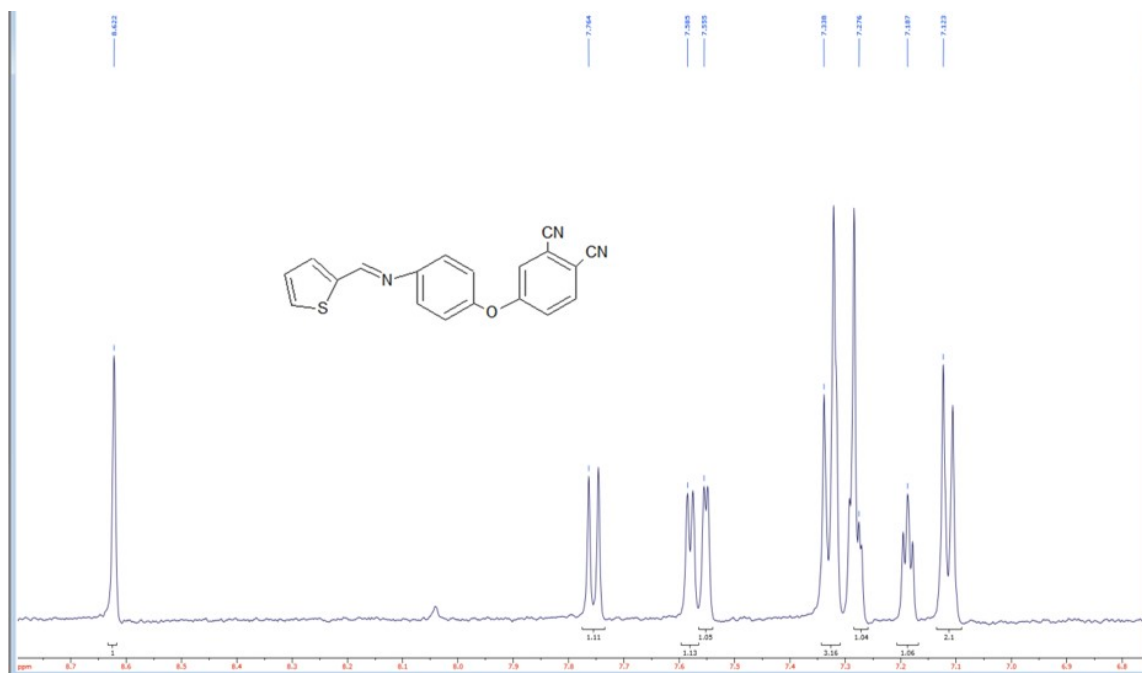


Figure S4. ¹H-NMR spectra of compound D2

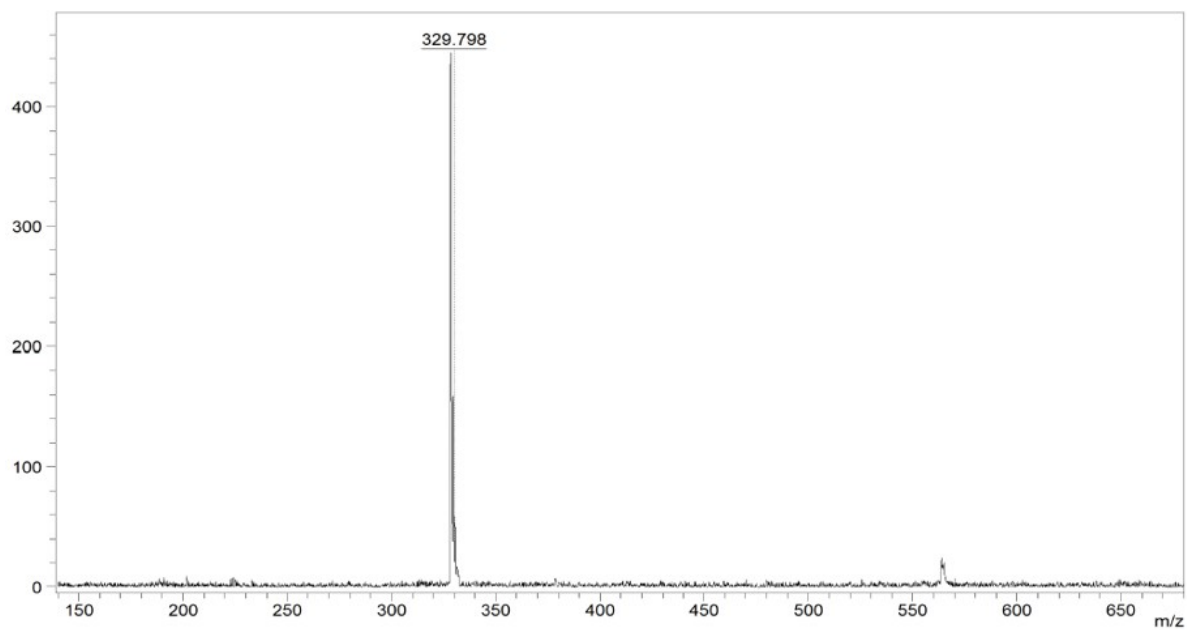


Figure S5. Mass spectra of compound D2

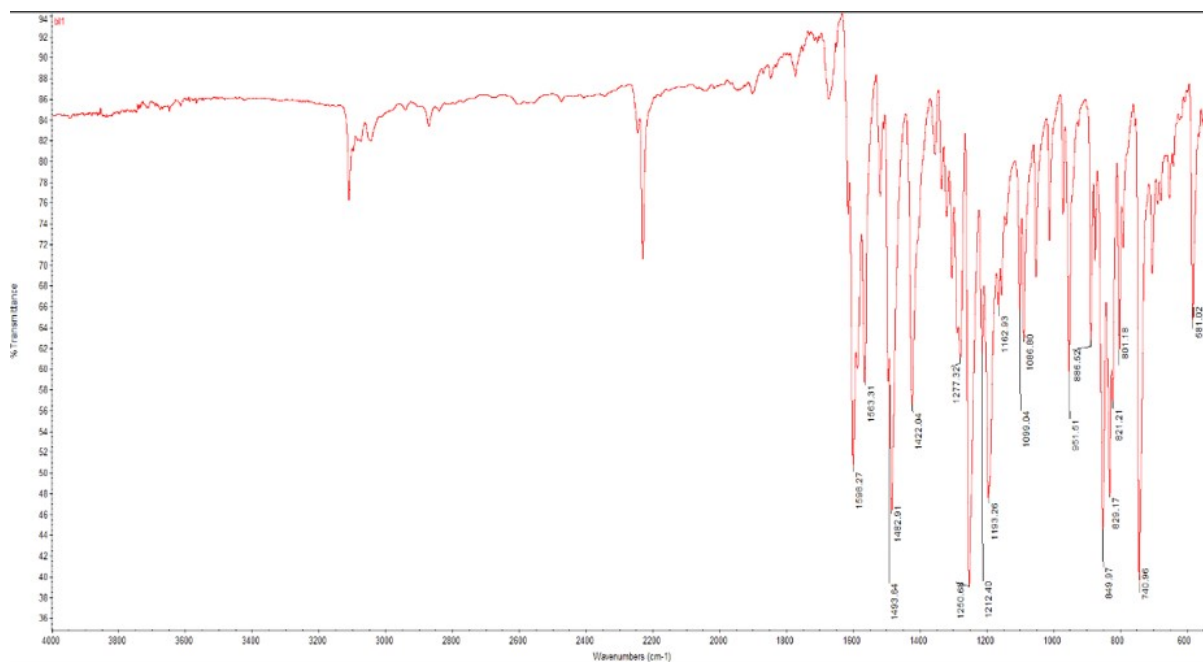


Figure S6. FT-IR spectra of compound D2

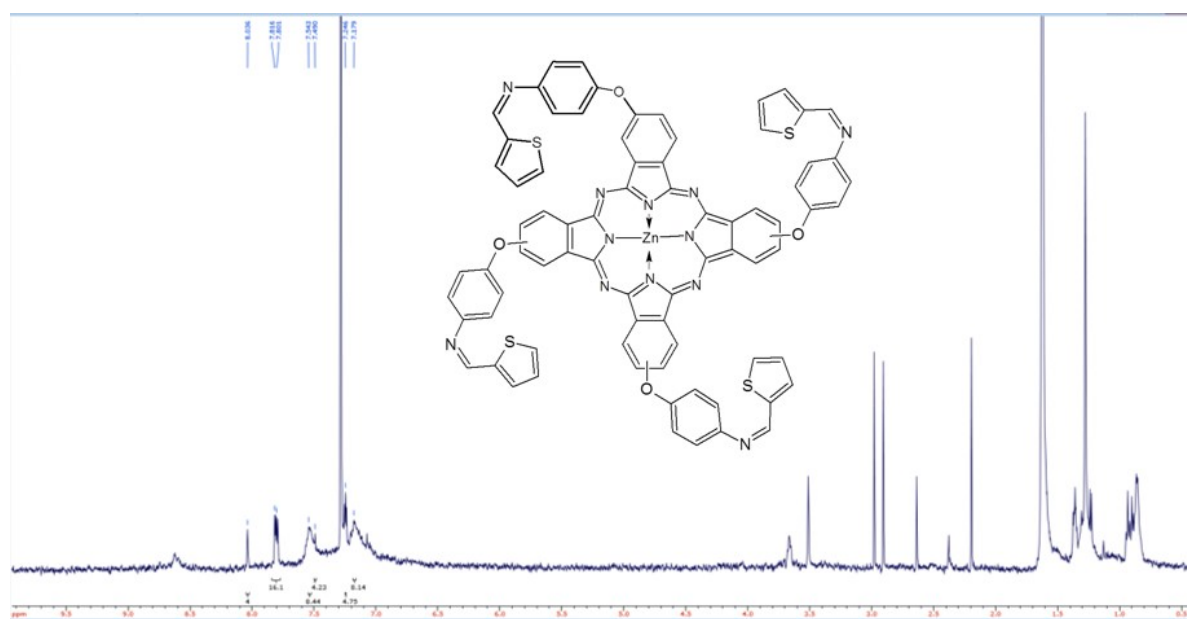


Figure S7. ¹H-NMR spectra of compound D3

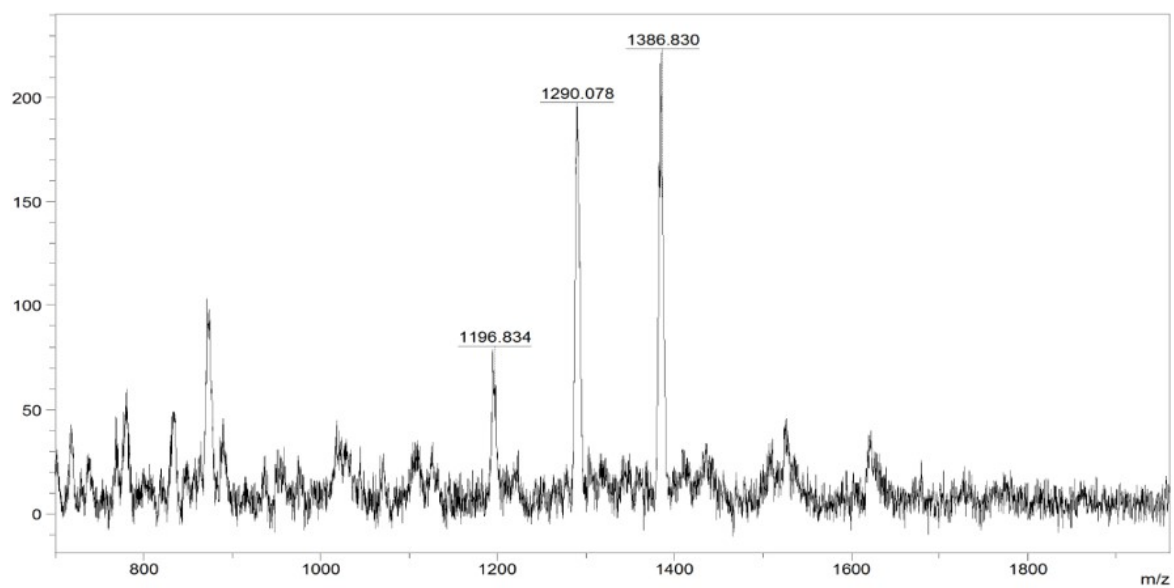


Figure S8. Mass spectra of compound D3

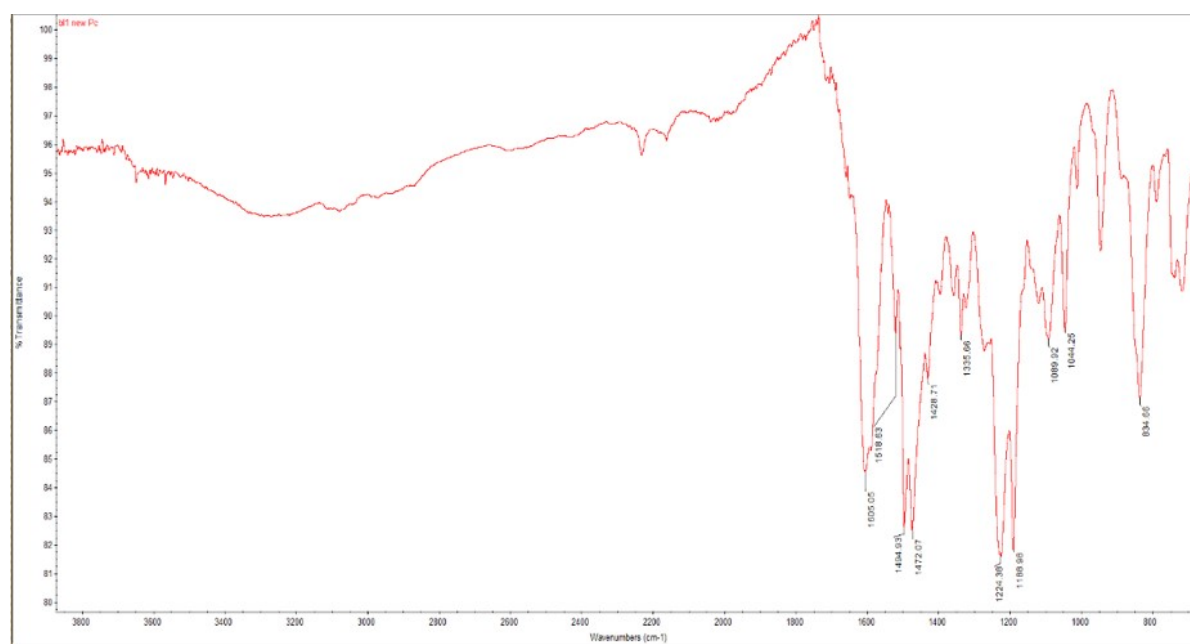


Figure S9. FT-IR spectra of compound D3

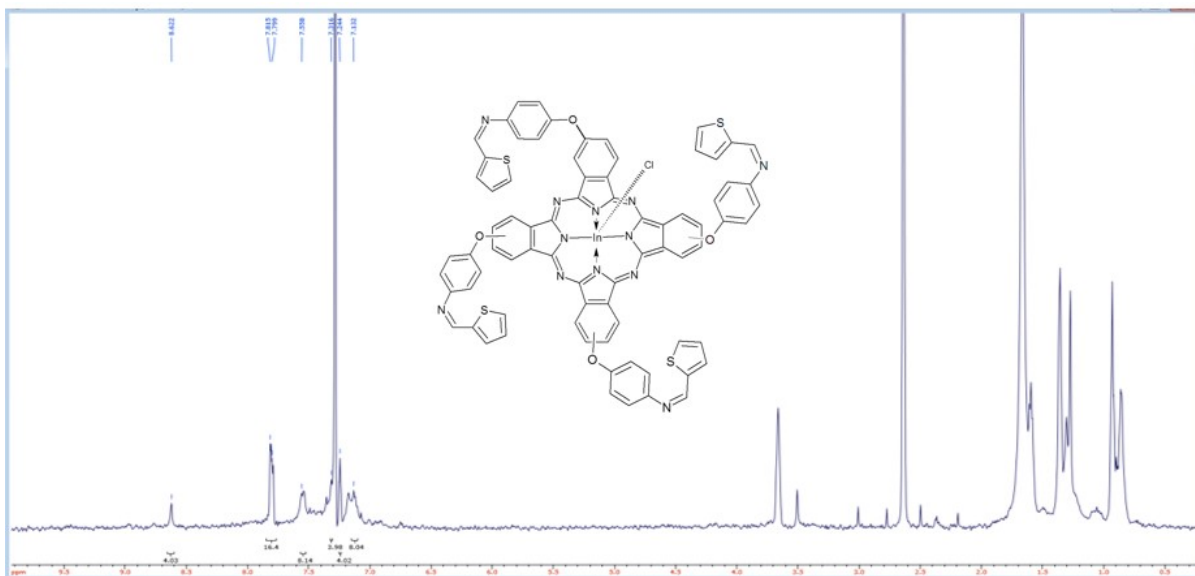


Figure S10. ¹H-NMR spectra of compound **D4**

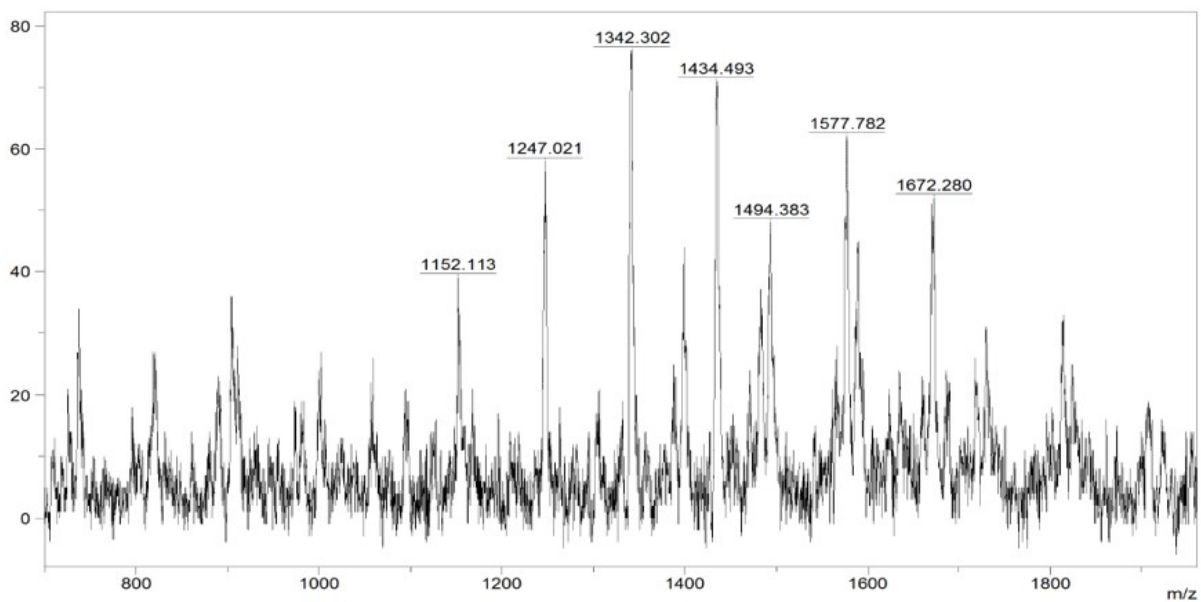


Figure S11. Mass spectra of compound **D4**

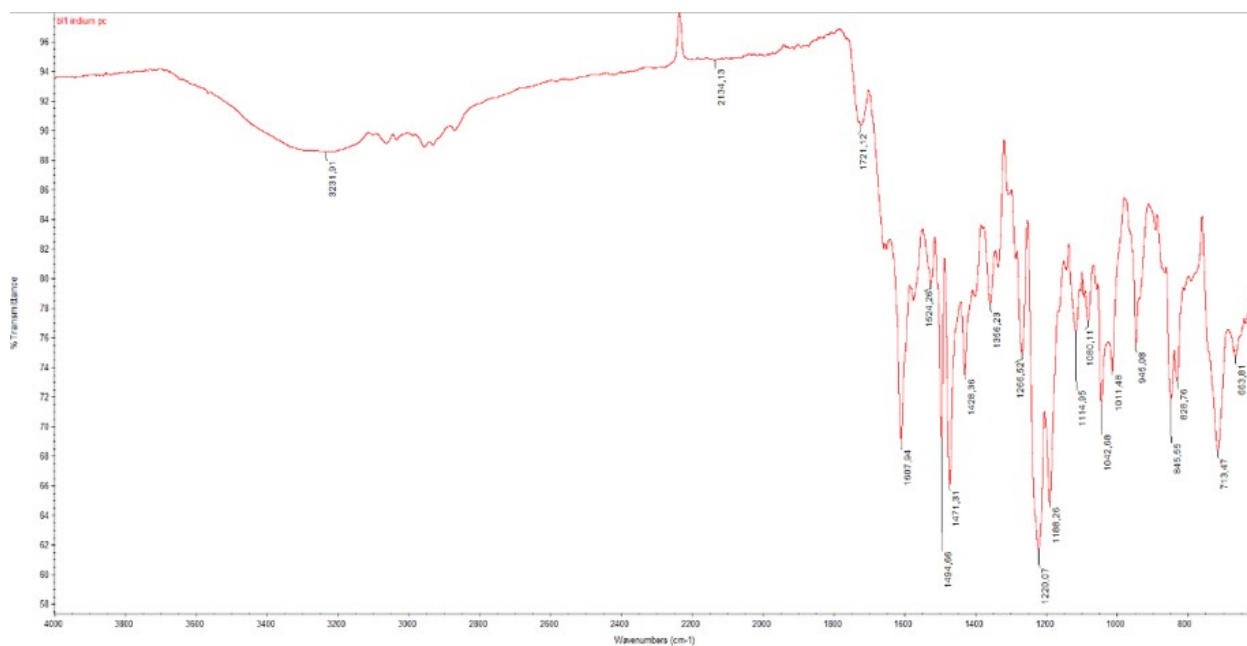


Figure S12. FT-IR spectra of compound D4