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Indole–Bipyridyl Fluorophores as Dual-Functional Probes for Endoplasmic Reticulum Imaging and Zn^{2+} Sensing in Live Cells

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Absorption and Emission Spectra

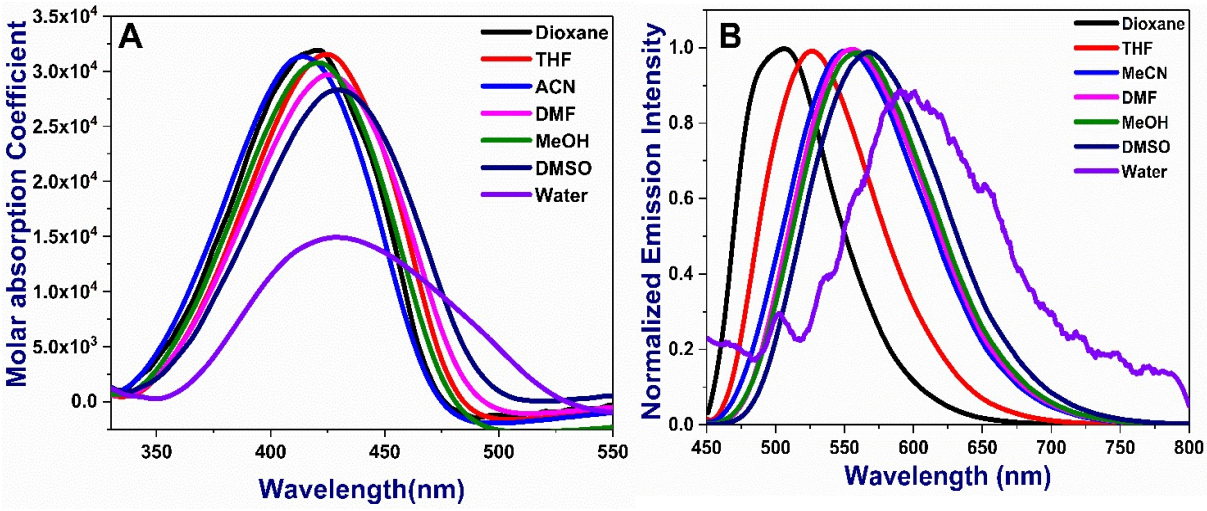


Fig S1 Absorption and Emission spectra of **IBP-1** in various solvents

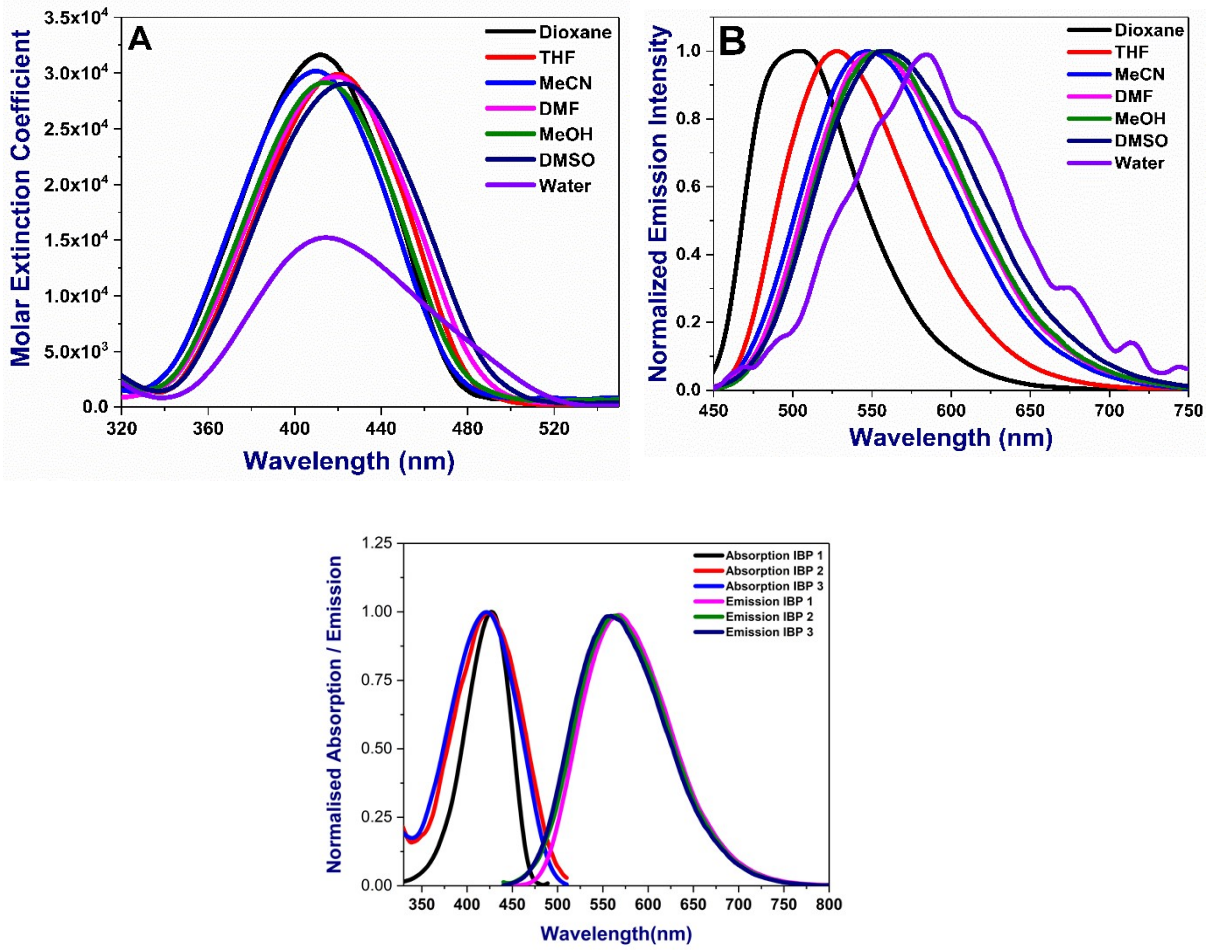
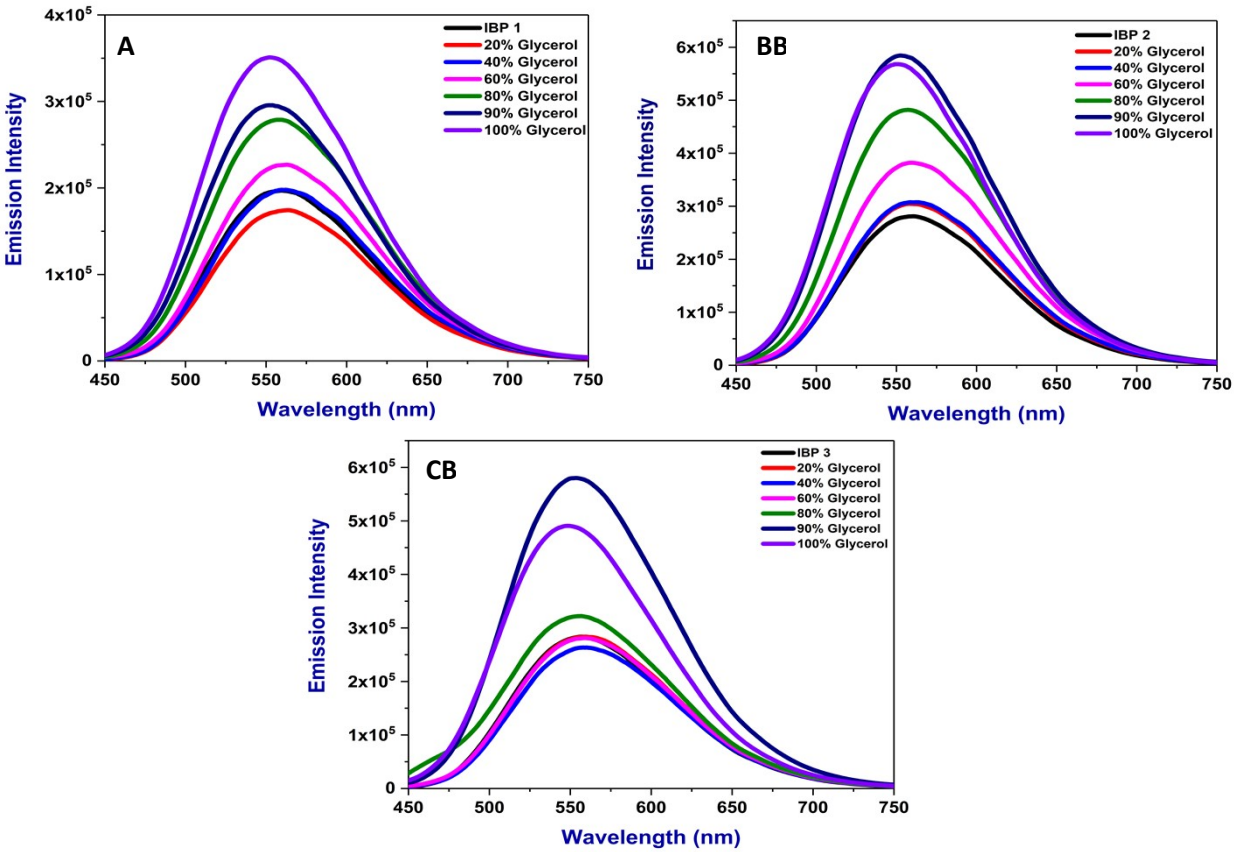


Fig S2: Absorption and Emission spectrum of **IBP-3** in various solvents. The bottom figure is the combined absorption and emission spectra of all three molecules in DMSO revealing a distinct Stokes shift.



Viscosity study

Fig S3 Emission spectrum of (A)**IBP-1,** (B)**IBP-2** and (C)**IBP-3** in glycerol-methanol solution (Concentration: 10 μM).

Zn^{2+}-induced spectral response of IBP-1, IBP-2 and IBP-3

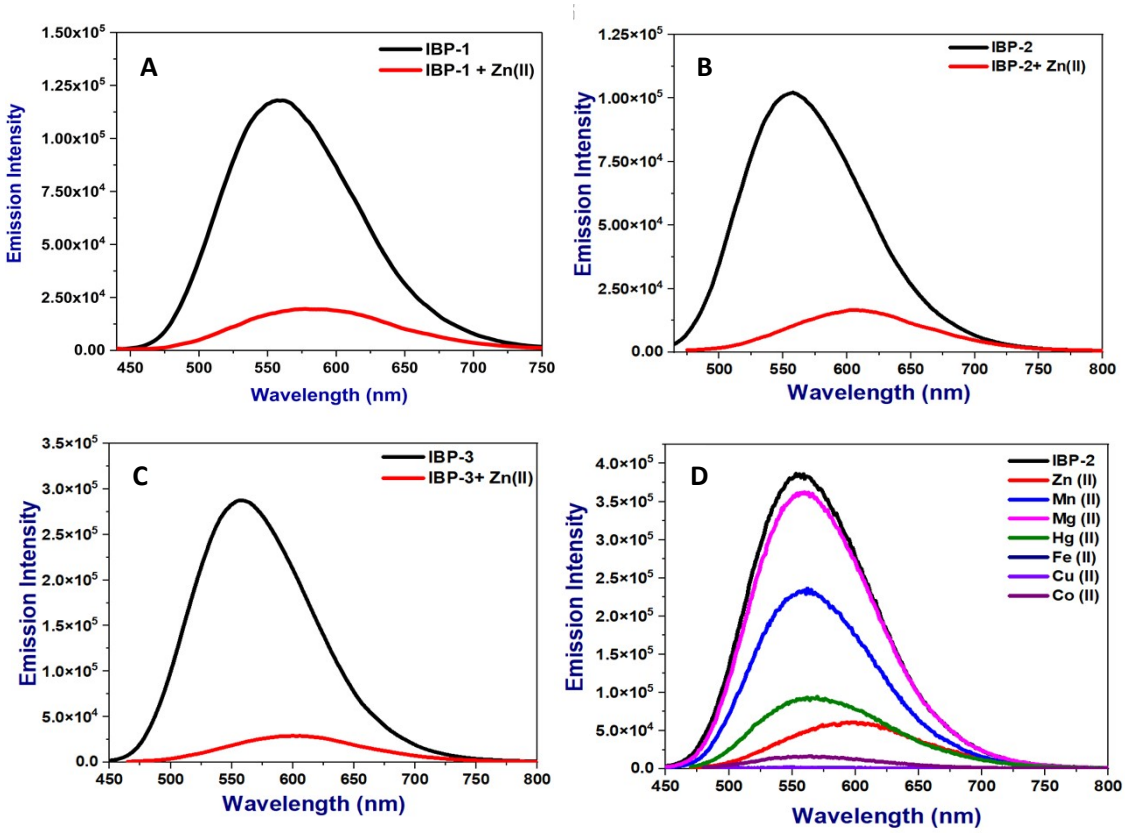


Fig S4: Emission spectra of (A) **IBP-1**, (B) **IBP-2** & (C) **IBP-3** with the addition of Zinc (II) and the selectivity of (D) **IBP-2** with the addition of different metal ions. Only **Zn^{2+}** addition yields a bathochromic shift

Ion, RSS and ROS selectivity test

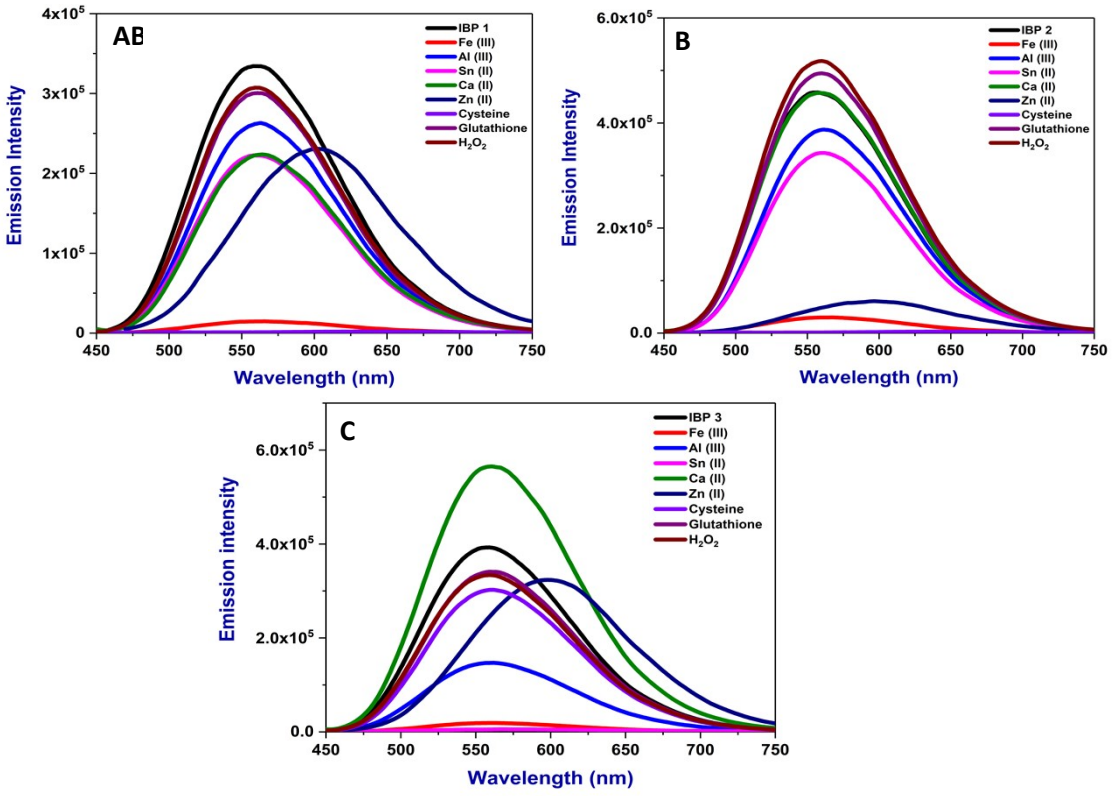


Fig S5. Emission spectra of **IBP-1, IBP-2** and **IBP-3** with the addition of Fe^{3+}, Al^{3+}, Sn^{2+}, Ca^{2+} cysteine, glutathione, H_2O_2 and Zn^{2+} ions

Dye (mL)	Zn^{2+} (mL)	Total (mL)	Mole fraction of Probe (X_{Dye})	Mole fraction of Zn (X_{Zn})	F	F_0	ΔF
0.0	2.0	2.0	0.0	1.0	3225	700000	-696775
0.2	1.8	2.0	0.1	0.9	237860	700000	-462140
0.6	1.4	2.0	0.3	0.7	719694	700000	19694
1.0	1.0	2.0	0.5	0.5	926146	700000	226146
1.4	0.6	2.0	0.7	0.3	908828	700000	208828
1.8	0.2	2.0	0.9	0.1	775042	700000	75042
2.0	0.0	2.0	1.0	0.0	700000	700000	0

Job's Plot Table (IBP2–Zn^{2+} System)

X-axis: Mole fraction of probe (X_{Dye})

Y-axis: = X_{Dye} * ΔF

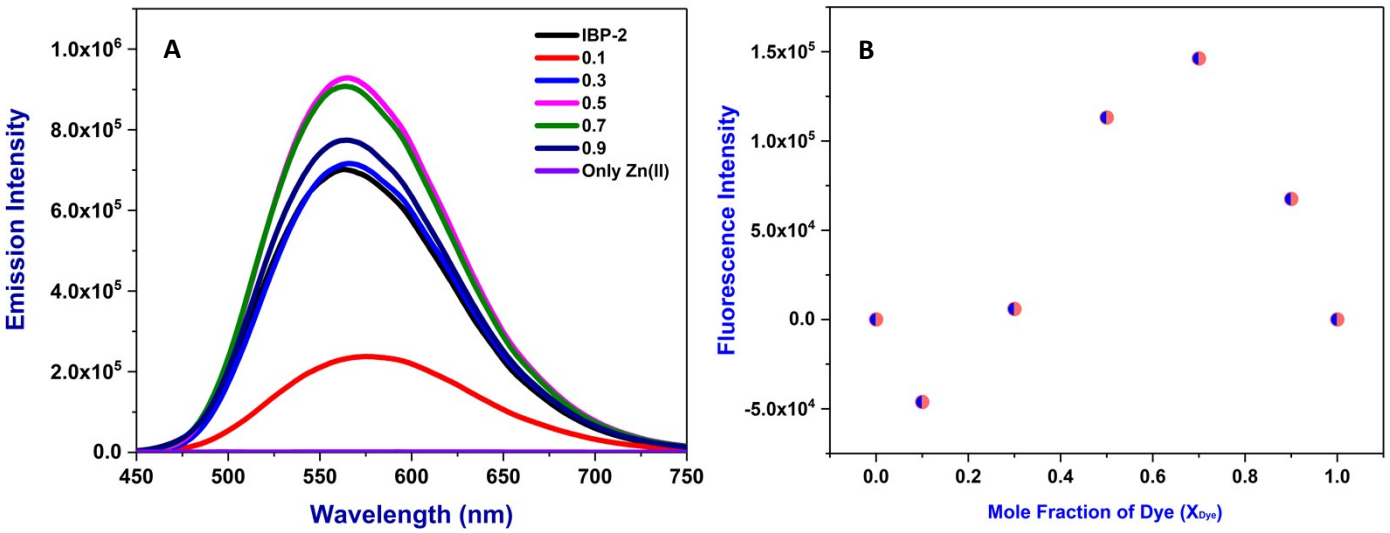


Fig S6. Fluorescence intensity profile of **IBP-2** at different Mole fractions (A)with Zn^{2+} from which Jobs plot is derived. Job's plot (B) of **IBP-Zn^{2+}** complex at 430 nm.

pH response toward IBP-1 probe

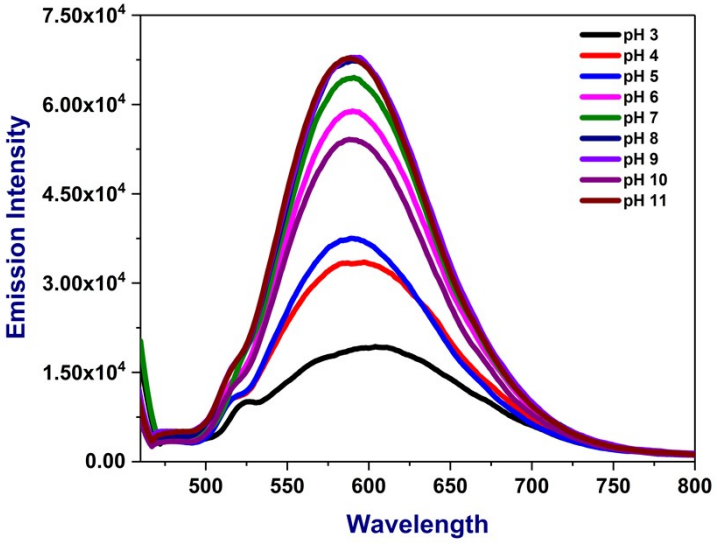


Fig S7. Emission spectra of **IBP-1** at different pH

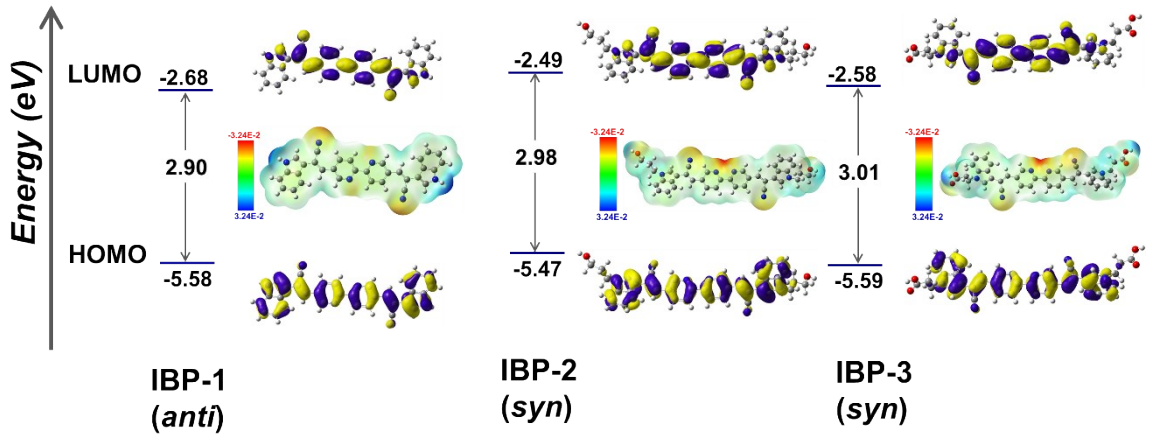


Fig S8. Optimized geometries of **IBP-2** and **IBP-3** in their *syn*-conformations and IBP-1 with *anti*-conformation, highlighting the HOMO–LUMO gap, together with isodensity surface plots of the HOMO and LUMO and the corresponding molecular electrostatic potential (ESP) surfaces.

Live cell imaging

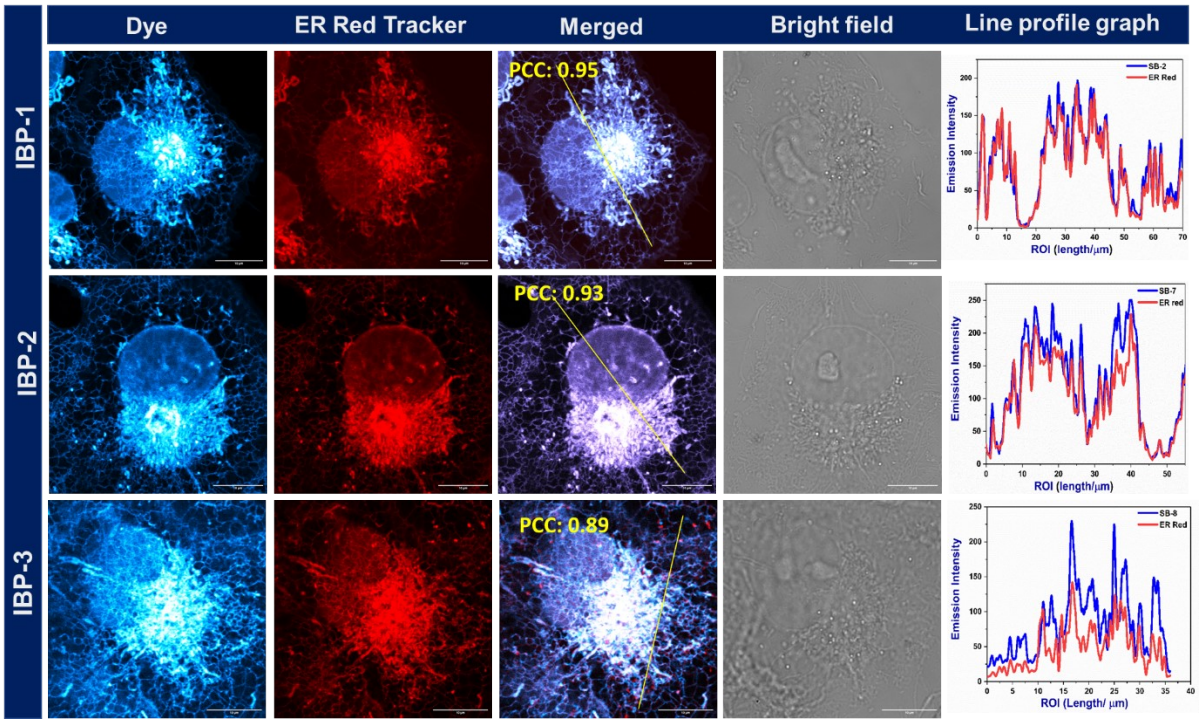


Fig S9. Cellular imaging and colocalization in live **COS-7** cells. Cells are stained with the synthesized molecules (1.5 μM, λ_{ex} :405 nm, λ_{em} : 480-548 nm) for 10 min at 37 °C; **ER tracker Red (**50 nM**,** λ_{ex} :561 nm, λ_{em} :600-645 nm) for 45 min at 37 °C; merged image ; Bright-field image; line profile graph of respective dye; n =15 cells, Scale bar =10 μm.

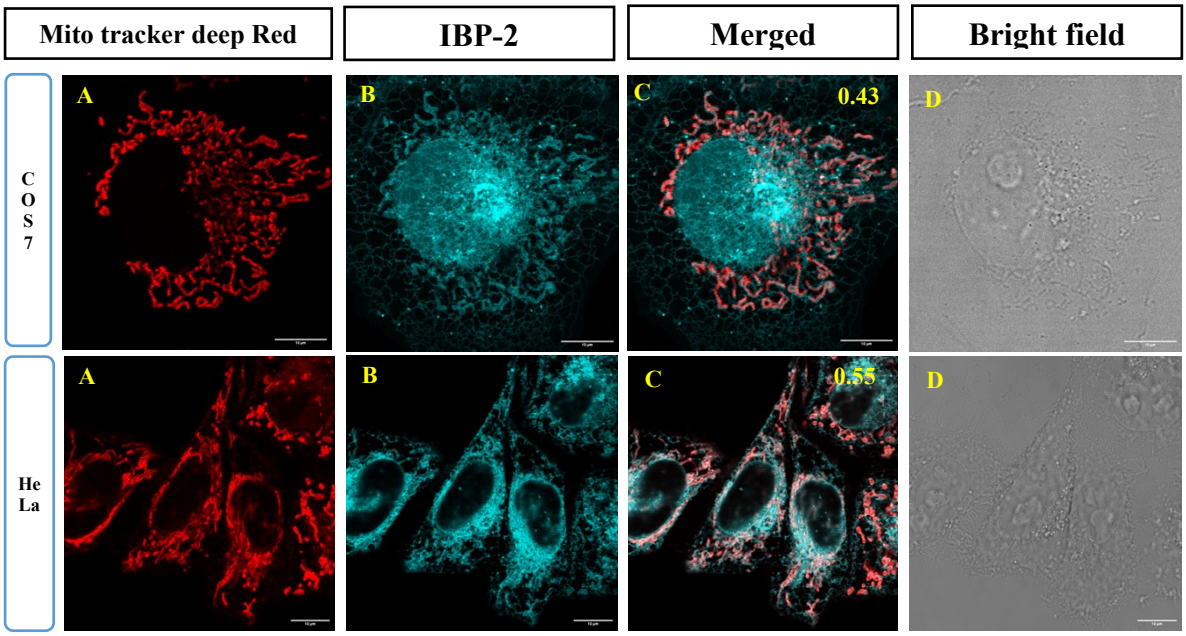


Fig S10. Cellular colocalization of IBP-2 with subcellular organelle tracker in COS-7 and HeLa with CLSM image of MitoTrackerDeep Red (A) IBP-2(B) Merged image (C) Brightfield (D). IBP-2: 1.5 μM, λex :405 nm, λem: 480-548 nm. Mitrotracker Deep Red λex: 633 nm, λem: 645–750 nm. Quantification was performed on n = 15 cells.

Tunicamycin-induced ER-phagy study with IBP 2 dye

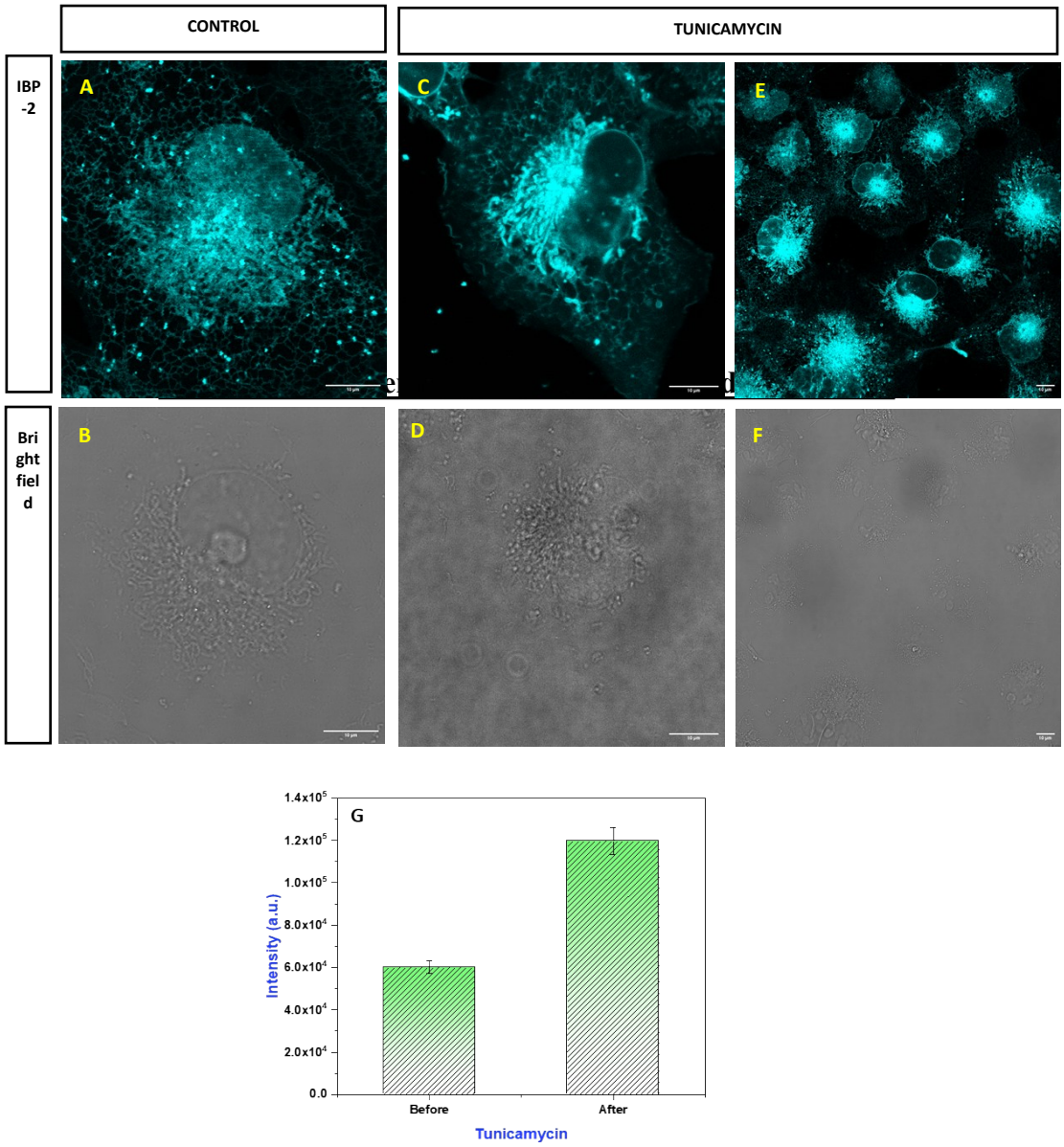
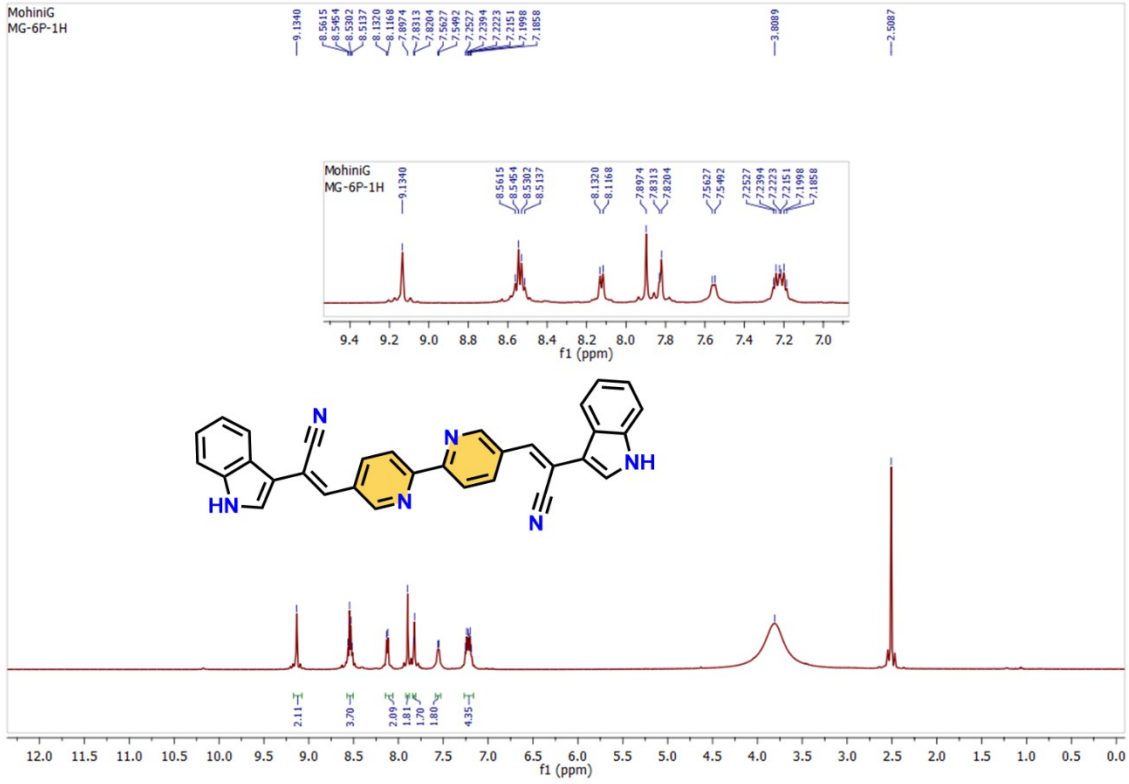
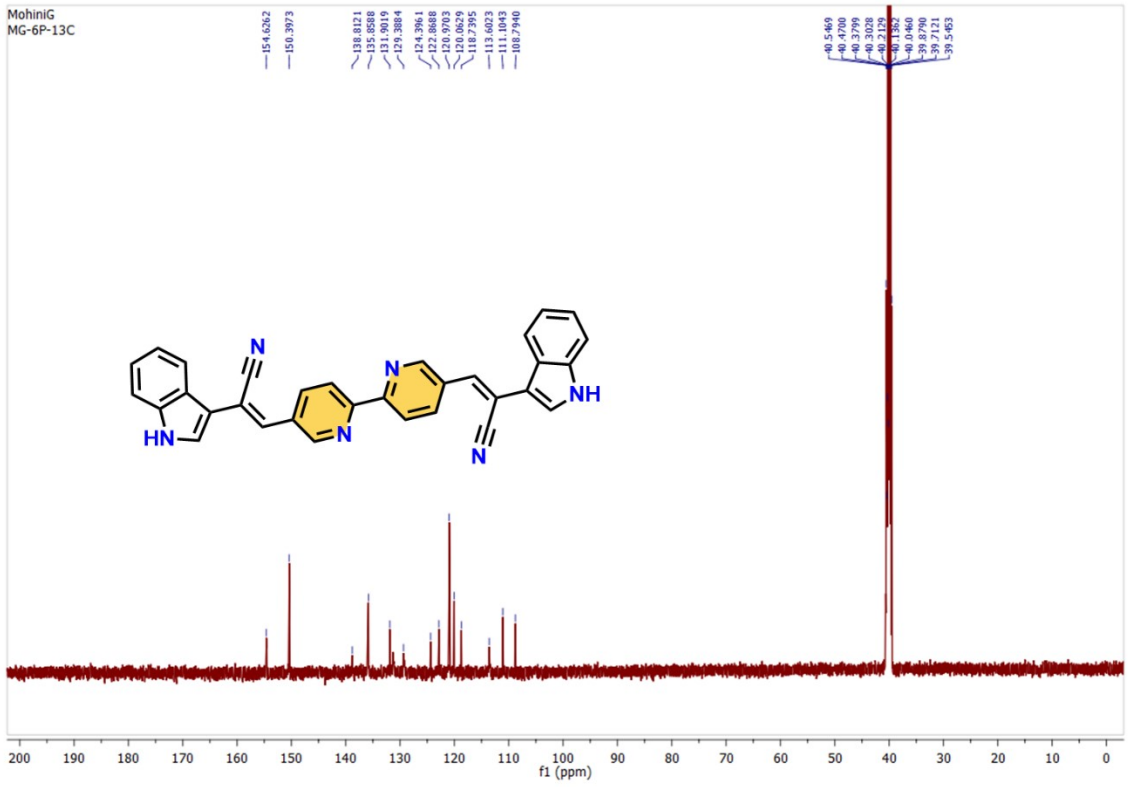


Fig S11 CLSM images of **IBP-2** without (A) and with (C, E) Tunicamycin treatment. The lower panel (B, D, and F) displays the corresponding merged bright-field images. (1.5 µM, λ_{ex} :405 nm, λ_{em} : 480-548 nm) Scale bar: 10 µm, . Quantification was performed on n = 13 cells. The intensity changes are shown in Figure (G).

Fig S12 : ^{1}H and ^{13}C NMR & Mass of IBP-1





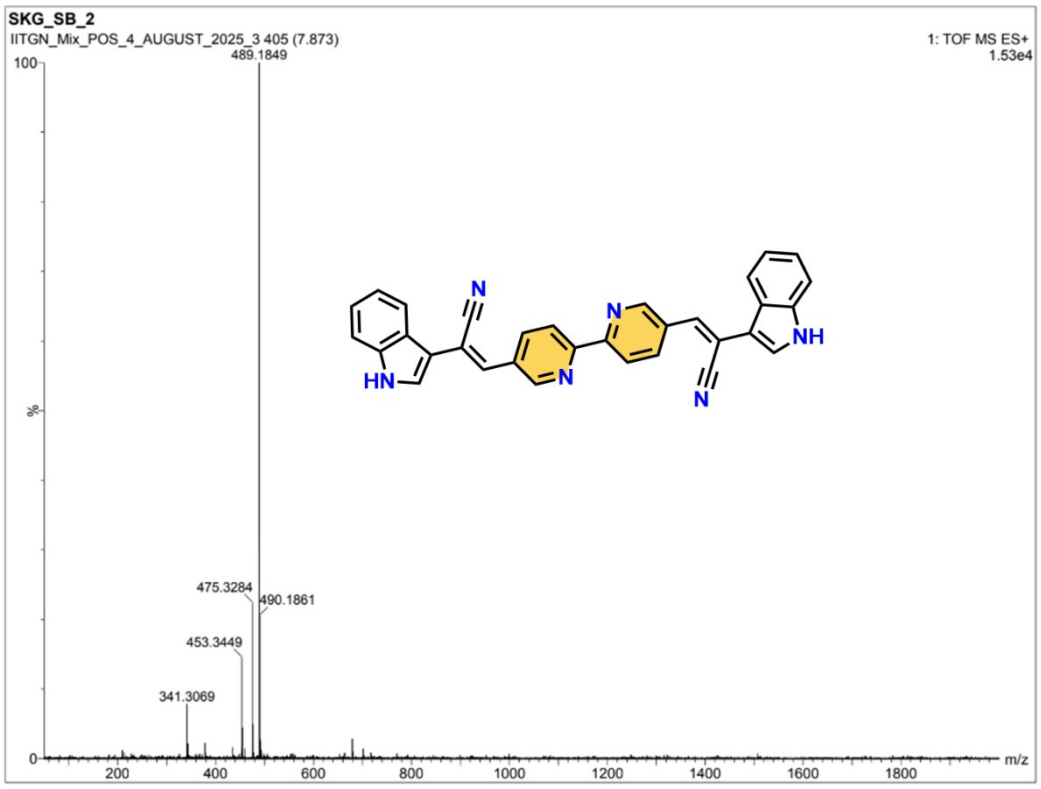
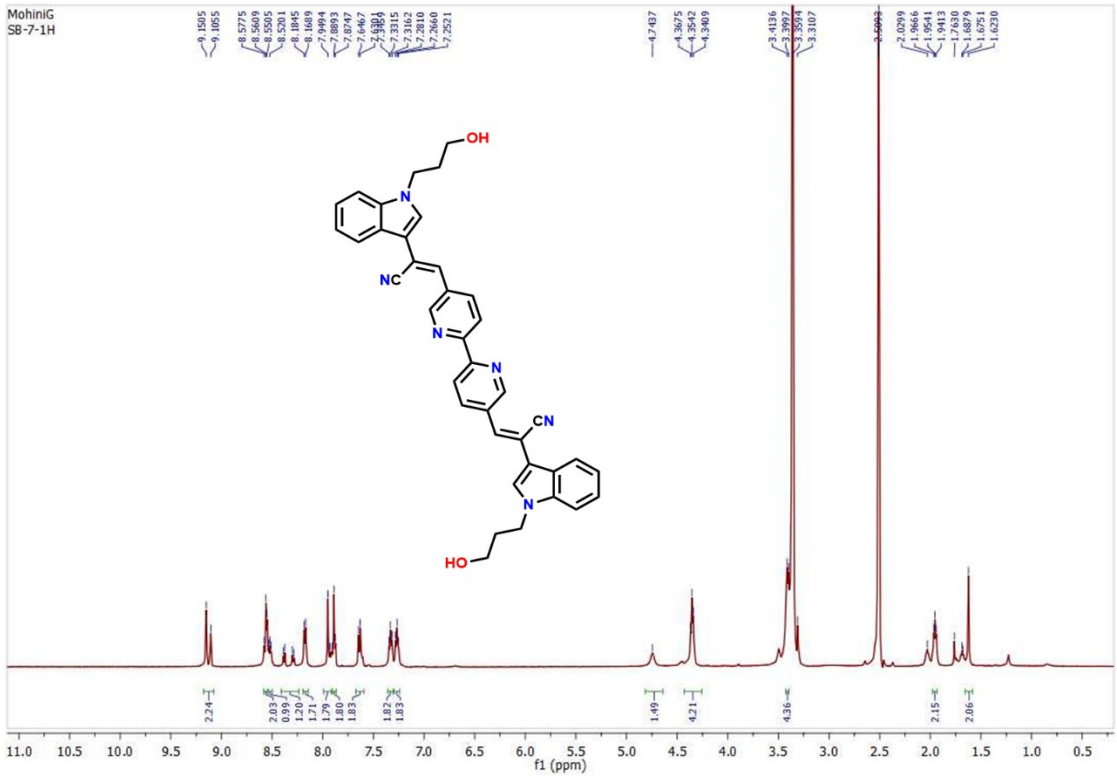
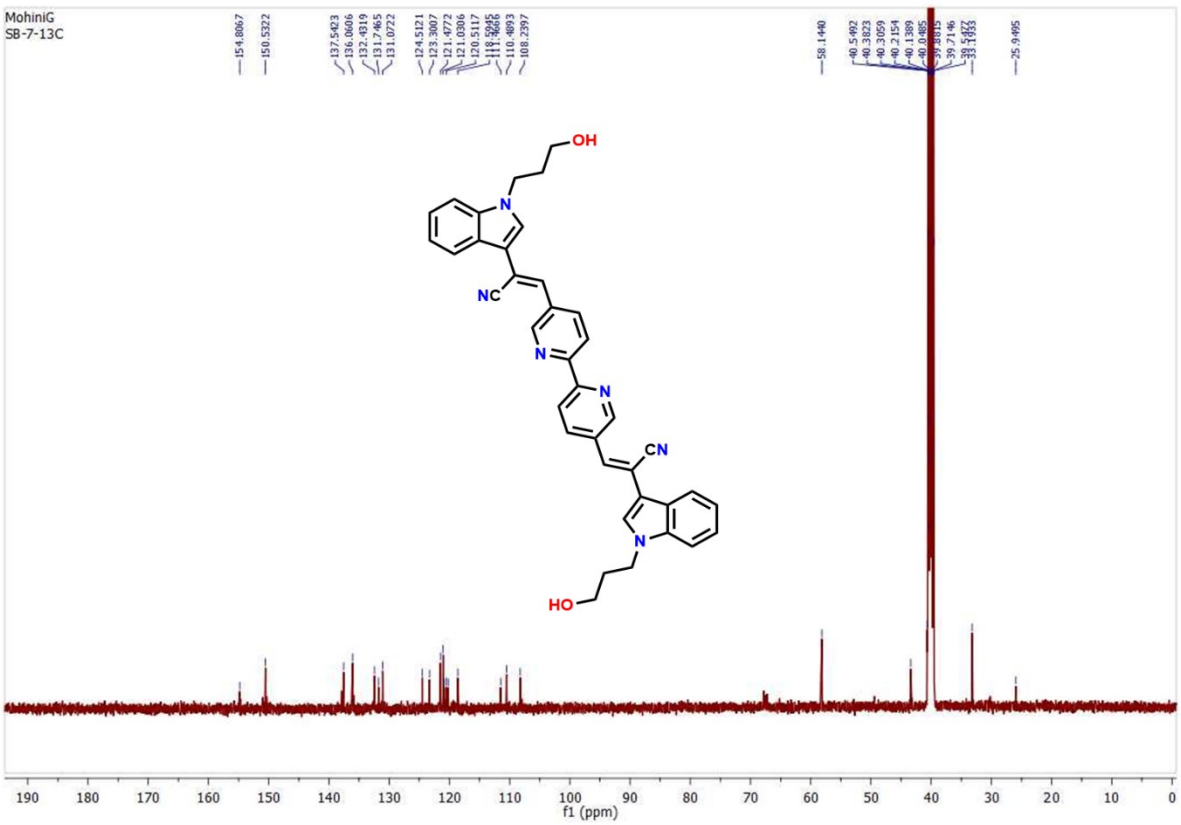


Fig S13: ^{1}H and ^{13}C NMR & Mass of IBP-2

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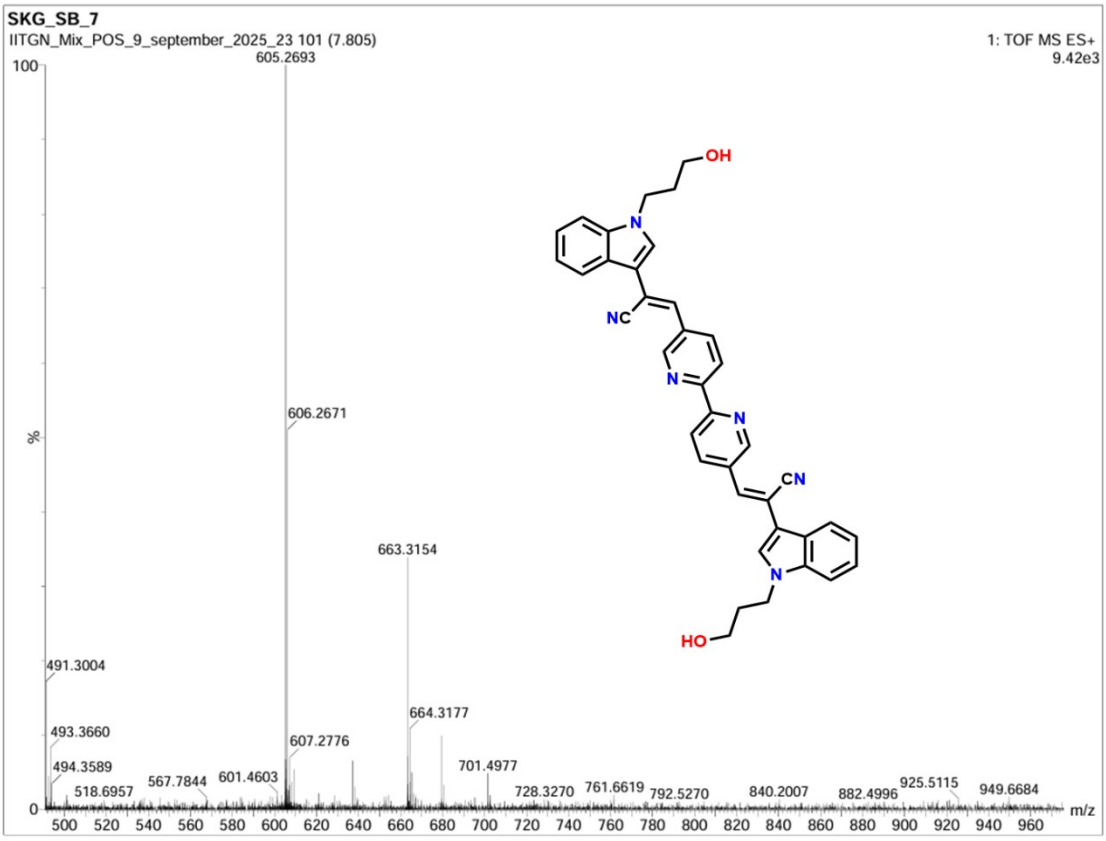
f1 (ppm)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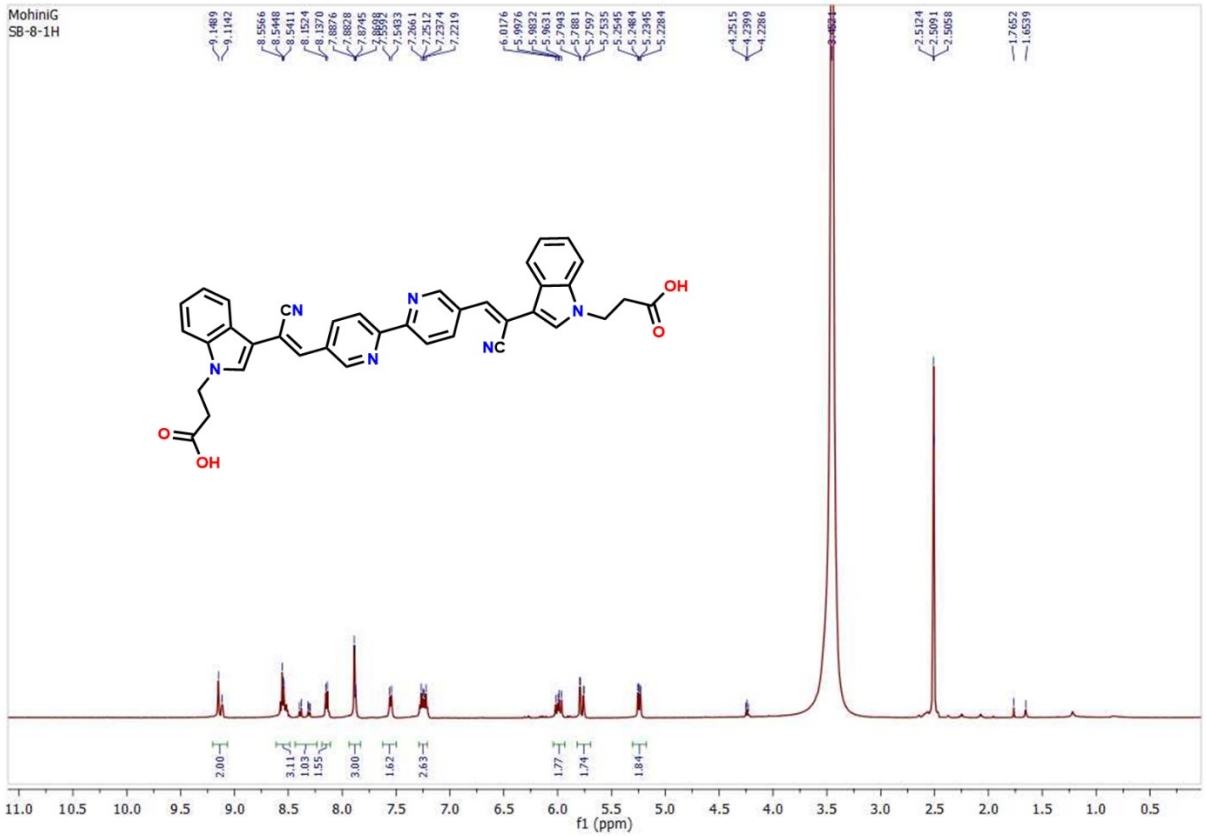
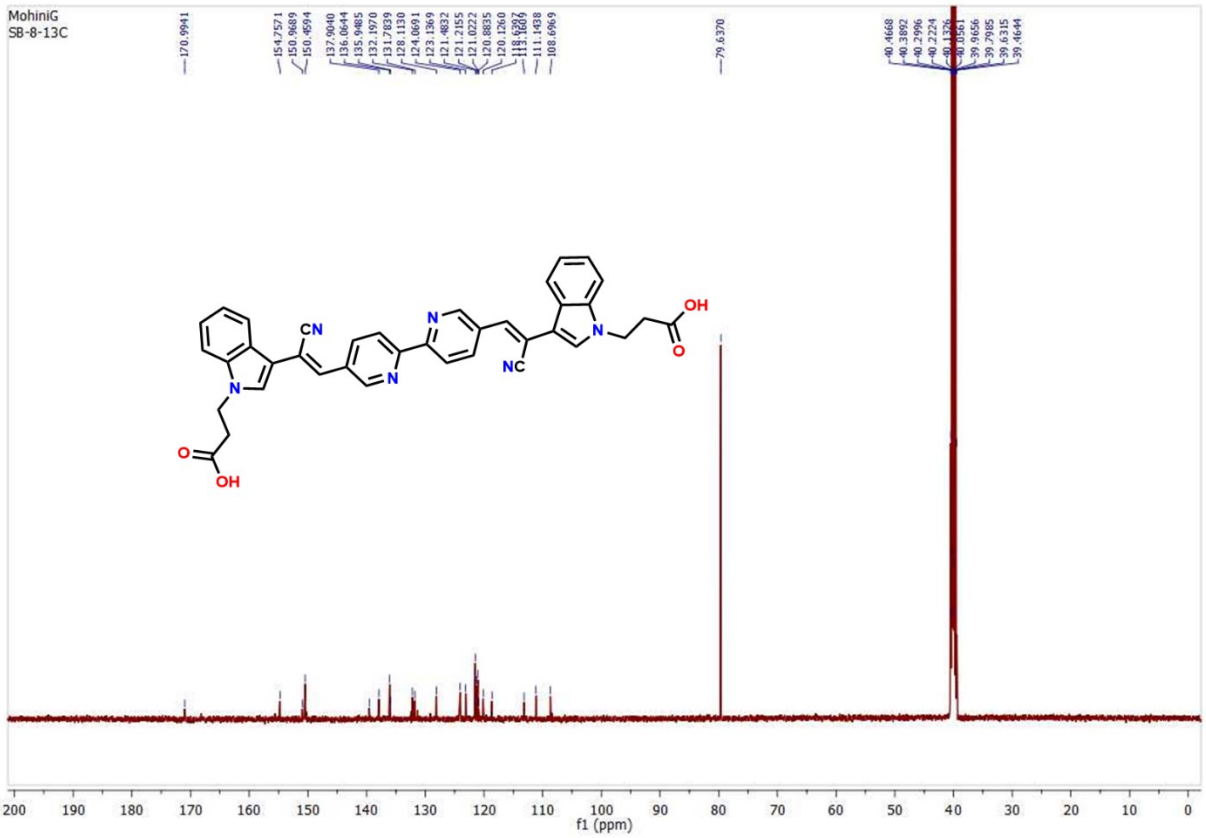
HO

Fig.S14: ^{1}H and ^{13}C NMR & Mass of IBP-3

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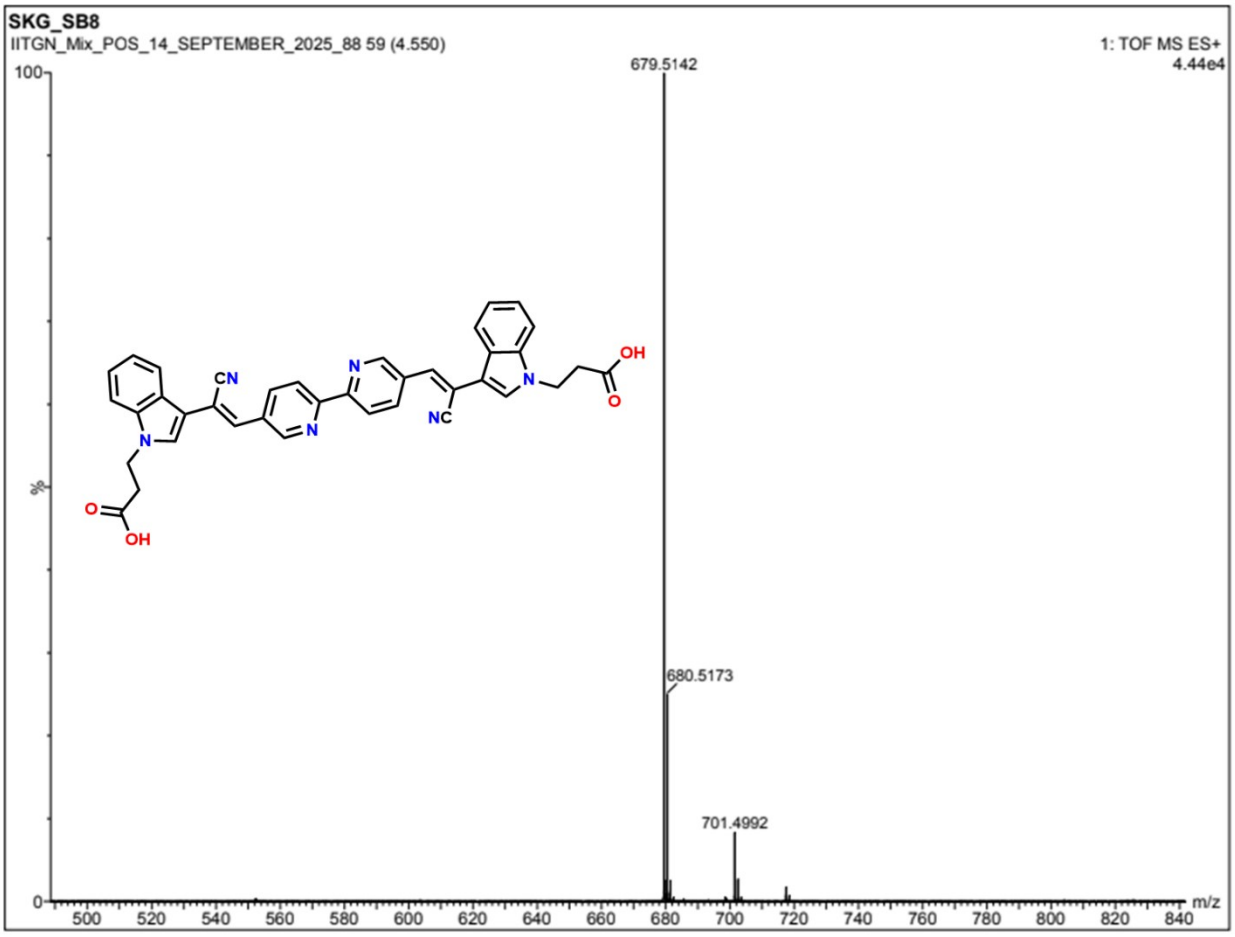
f1 (ppm)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%
0
m/z
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NC
N
OH
O