Supporting Information

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1. General Information

1.1 Materials

Fetal bovine serum was obtained from Biological Industries Co., Ltd. Dulbecco's Modified Eagle Medium (DMEM) were purchased from Beijing Solarbio Science & Technoiogy Co., Ltd. Mito-Tracker Deep Red FM was gained by Shanghai Beyotime Co., Ltd. (Shanghai, China). All chemicals were purchased from commercial suppliers and used without further purification. All solvents were purified prior to use. Distilled water was used after passing through a water ultra-purification system. PBS buffer solution was obtained by mixing of 0.05mol/L Na_2HPO_4 water solution and 0.05mol/L KH_2PO4 water solution with the volume ratio 4:1. All chemicals and solvents used were of analytical grade. All solution samples were made by dissolving each solid in water or DMSO.

1.2 Instruments

TLC analysis was performed using precoated silica plates. Using a pH meter (METTLER TOLEDO, Switzerland) to measure pH. Ultraviolet–visible (UV–vis) spectra were recorded on U-3900 UV-Visible spectrophotometer. Hitachi F-7000 fluorescence spectrophotometer was employed to measure fluorescence spectra. Shanghai Huamei Experiment Instrument Plants, China provided a PO-120 quartz cuvette (10 mm). ^1H NMR and ^{13}C NMR experiments were performed with a BRUKER AVANCE III HD 600 MHz and 151 MHz NMR spectrometer, respectively (Bruker, Billerica, MA). Coupling constants (J values) are reported in hertz. ESI-MS was measured with an Thermo Scientific Q Exactive. The cytotoxicity assay was measured by a BioTek ELX808 fully automated microplate reader. And the cells imaging experiments were measured the Zeiss LSM810 Airyscan confocal laser scanning microscope.

1.3 Cell Viability

Cytotoxicity was assessed by performing MTT assay with the HeLa cells. HeLa cells were seeded into 96-well plate at 2×10^3/well and were cultured at 37 °C and 5% CO_2 for 24 h. Different concentrations of **ID-MpH** (0, 5, 10, 15 and 20 μM) were then added to the wells. After incubation for 6 or 12 h, MTT (0.5 mg/mL) was added to each well, and the plate was incubated for another 4 h. The optical densities at 490 nm were measured. The cell viability (%) = $(OD_{sample}-OD_{blank}) / (OD_{control}-OD_{blank}) \times 100$ %. OD_{sample} denotes cells treated with various concentrations of **ID-MpH**; OD_{blank} denotes the plates with DMEM; $OD_{control}$ denotes cells without treated with **ID-MpH**. Each concentration was conducted with three parallel samples, and the results were expressed as mean ± standard deviation (SD).

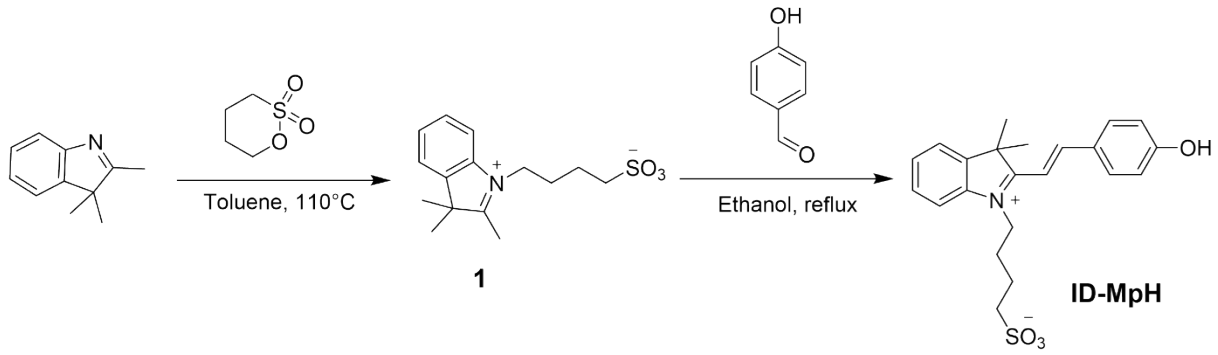
1.4 Cell Culture

Transplanted HeLa and HepG2 cells into Dulbecco's Modified Eagle Medium which contained 10% Fetal Bovine Serum, respectively. The cells were incubated in the constant temperature incubator for approximately 24 hours. Using Trypsin-EDTA solution (0.25%) digested the cells before transferring them to different laser confocal petri dish.

2. Experimental Section

2.1 Synthetic route

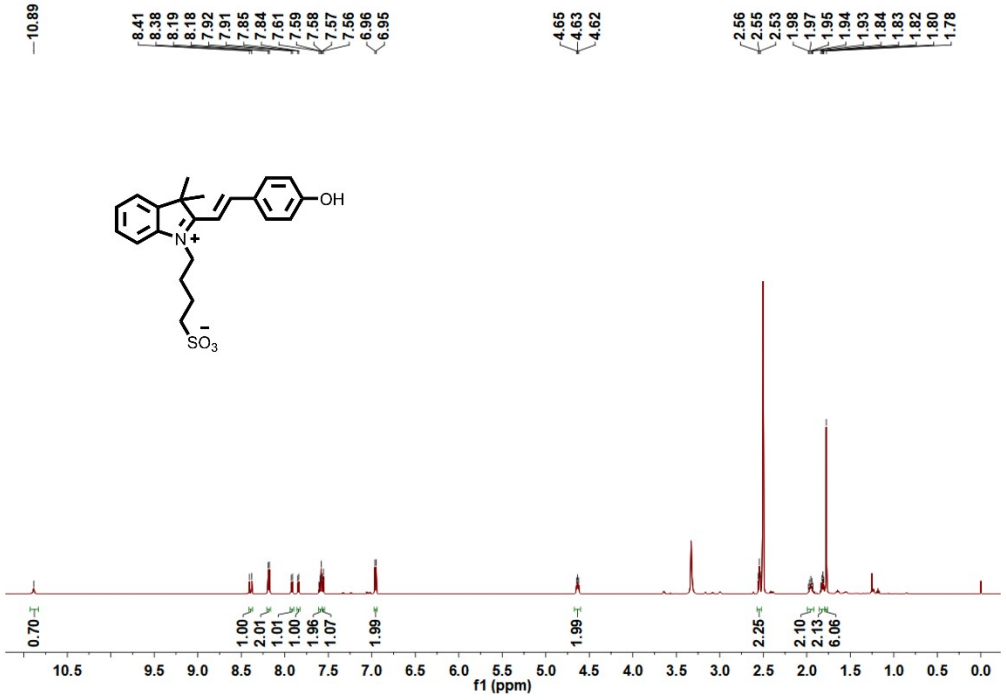
Figure S1: The synthetic route of **ID-MpH.**



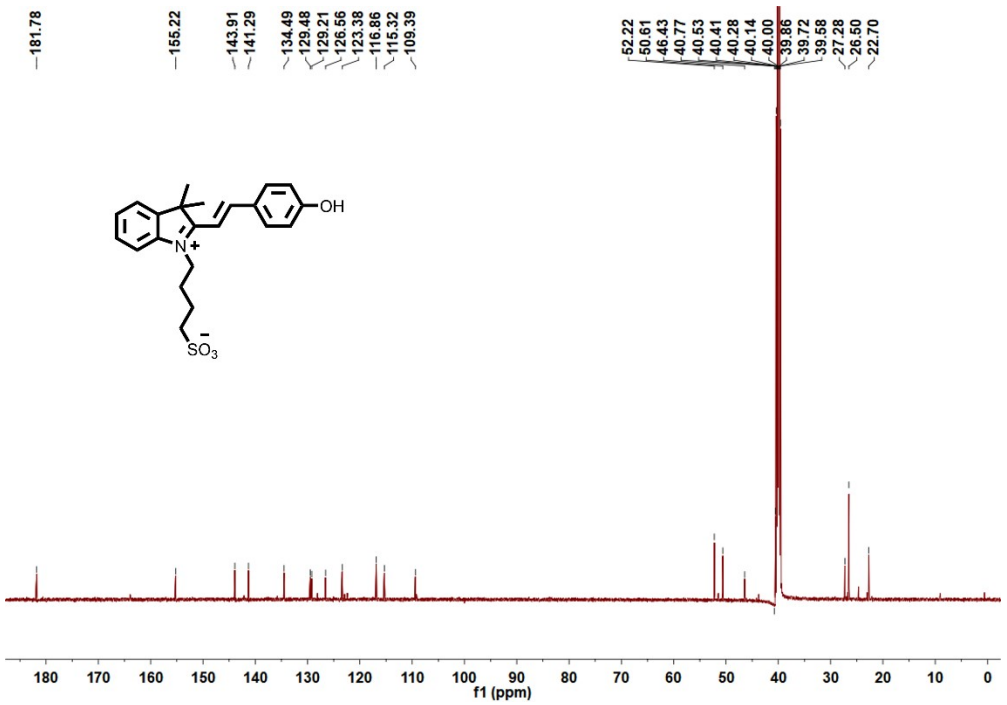
The synthetic route of **ID-MpH**.

2.2 Characterization data for synthesis.

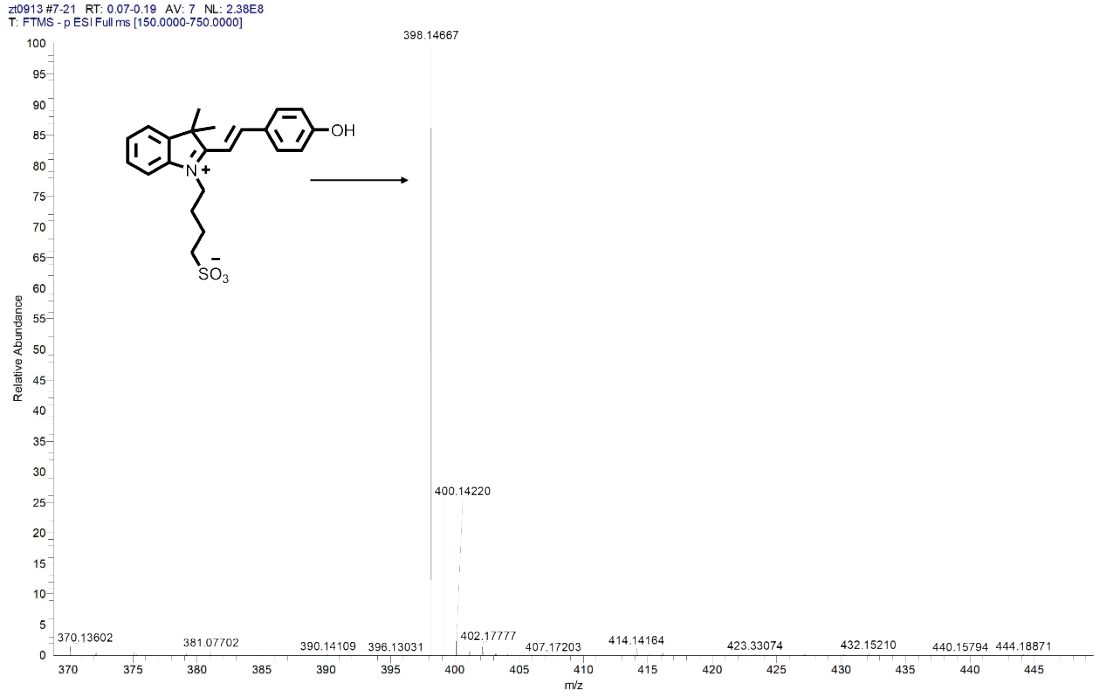
Figure S2: The characterization data of **ID-MpH**.



The ^{1}H MNR (600 MHz) spectra of **ID-MpH** in DMSO-d_6.

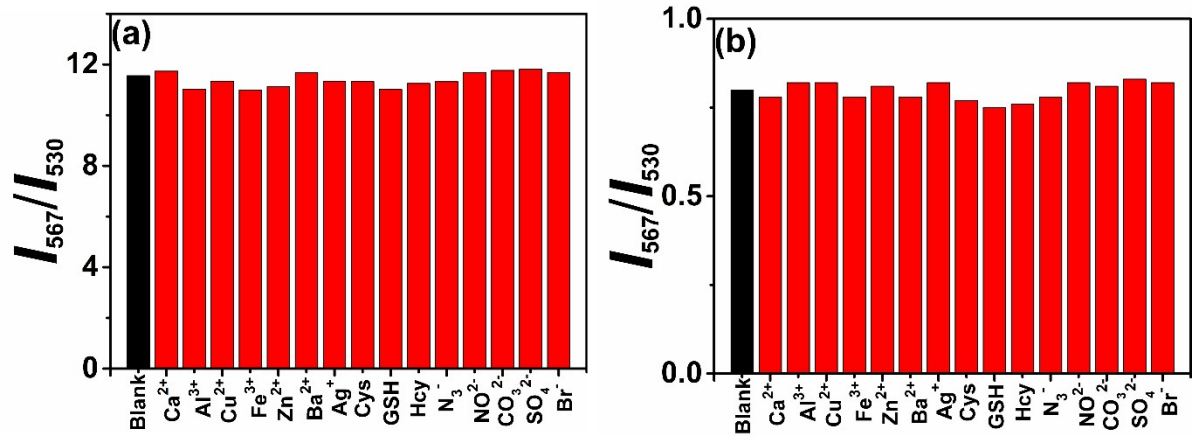


The ^{13}C NMR (151 MHz) spectra of **ID-MpH** in DMSO-d_6.



The ESI-MS of **ID-MpH** : *m*/*z*: [**ID-MpH** - H]$^-$ Calcd. For $C_{22}H_{24}NO_4S^-$ 398.1432, Found 398.1467.

Figure S3: The relative emission intensity at I_{567}/I_{530} of **ID-MpH** to various analytes in phosphate buffer at pH 3 and 9， respectively.



Relative emission intensity at I_{530}/I_{567} of **ID-MpH** (10 μM) in response to other biologically relevant species (100 μM) in phosphate buffer at pH 9 (a) and 3 (b). The first bar represents the relative emission intensity of the free probe, and the remaining bars correspond sequentially to Ca^{2+}, Al^{3+}, Cu^{2+}, Fe^{3+}, Zn^{2+}, Ba^{2+}, Ag^{+}, Cys, GSH (1 mM), Hcy, N_3^-, NO^{2-}, CO_3^{2-}, SO_4^{2-} and Br^-.

Figure S4: The cytotoxicity test.