Supporting Information

for

Selective Off-On Fluorescent Chemosensor for Detection of Trivalent Iron ions in the Aqueous Media

Liang Huang[a], Fengping Hou[a], Ju Chen[b], Pinxian Xi*[a], Fengjuan Chen[a], Decheng Bai[b] and Zhengzhi Zeng*[a]

Key Laboratory of Nonferrous Metal Chemistry and Resources Utilization of Gansu Province, State Key Laboratory of Applied Organic Chemistry and College of Chemistry and Chemical Engineering, Lanzhou University, Lanzhou 730000, P. R.China.

Email: zengzhzh@yahoo.com.cn, xipx@lzu.edu.cn

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1. Instruments, reagents and experimental procedures

^{1}H and ^{13}C NMR spectra were taken on a Varian mercury-400 spectrometer with TMS as an internal standard and $CDCl_3$ as solvent. Absorption spectra were determined on a Varian UV-Cary100 spectrophotometer. Fluorescence spectra measurements were performed on a Hitachi F-4500 spectrofluorimeter. All pH measurements were made with a pH-10C digital pH meter. HRMS were determined on a Bruker Daltonics APEXII 47e FT-ICR spectrometer.

All the materials for synthesis were purchased from commercial suppliers and used without further purification. Methanol for spectra detection was HPLC reagent without fluorescent impurity.

Procedures of metal ion sensing

Stock solutions of the metal ions (2.5 mM) were prepared in deionized water. A stock solution of **L1**(1 mM) was prepared in DMF: CH_3CN (1:1 v/v). The solution of **L1** was then diluted to 5 μM with EtOH/ H_2O (3:7, v/v) solution. In titration experiments, each time a 2 mL solution of **L1** (5μM) was filled in a quartz optical cell of 1 cm optical path length, and the Fe^{3+} stock solution was added into the quartz optical cell gradually by using a micro-pippet. Spectral data were recorded at 2 min after the addition. In selectivity experiments, the test samples were prepared by placing appropriate amounts of metal ion stock into 2 mL solution of **L1** (5μM). For fluorescence measurements, excitation was provided at 505nm, and emission was collected from 515 to 650 nm.

Cell Culture

The EJ cell line was provided by Institute of Biochemistry and Cell Biology (China). Cells were grown in H-DMEM (Dulbecco's Modified Eagle's Medium, High Glucose) supplemented with 10 % FBS (Fetal Bovine Serum) in an atmosphere of 5 % CO_2, 95 % air at 37°C. Cells (5×10^8/L) were plated on 18 mm glass coverslips and allowed to adhere for 24 hours. Then the cells treated with **L1** (0-10 μM) and incubated for 12 hours for MTT assay. Experiments to asses Fe^{3+} uptake were performed in the same media supplemented with 100 μM $FeCl_3$ for 2h.

Fluorescence Imaging

Fluorescent pictures were taken on Zeiss Leica inverted epifluorescence /reflectance laser scanning confocal microscope. Excitation of 1-loaded cells at 515 nm was carried out with a HeNe laser. Emission was collected using a 560 nm long-pass filter. Emission was collected from 570 to 625 nm. Before the experiments, cells were washed with PBS buffer and then incubated with 20 μM **1** in DMF-PBS (1:49, v/v) for 20 min at 37 ℃. Cell imaging was then carried out after washing cells with PBS.

2. Supplementary spectra data

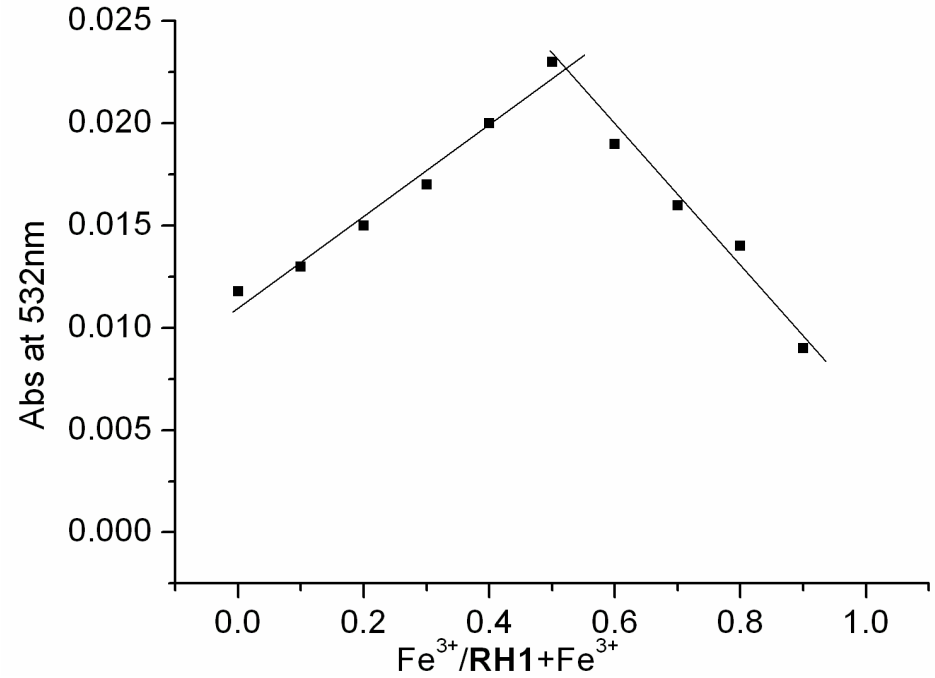

Fig. S1 Job's plots according to the method for continuous variations, indicating the 1:1 stoichiometry for the **L1**-Fe^{3+}.

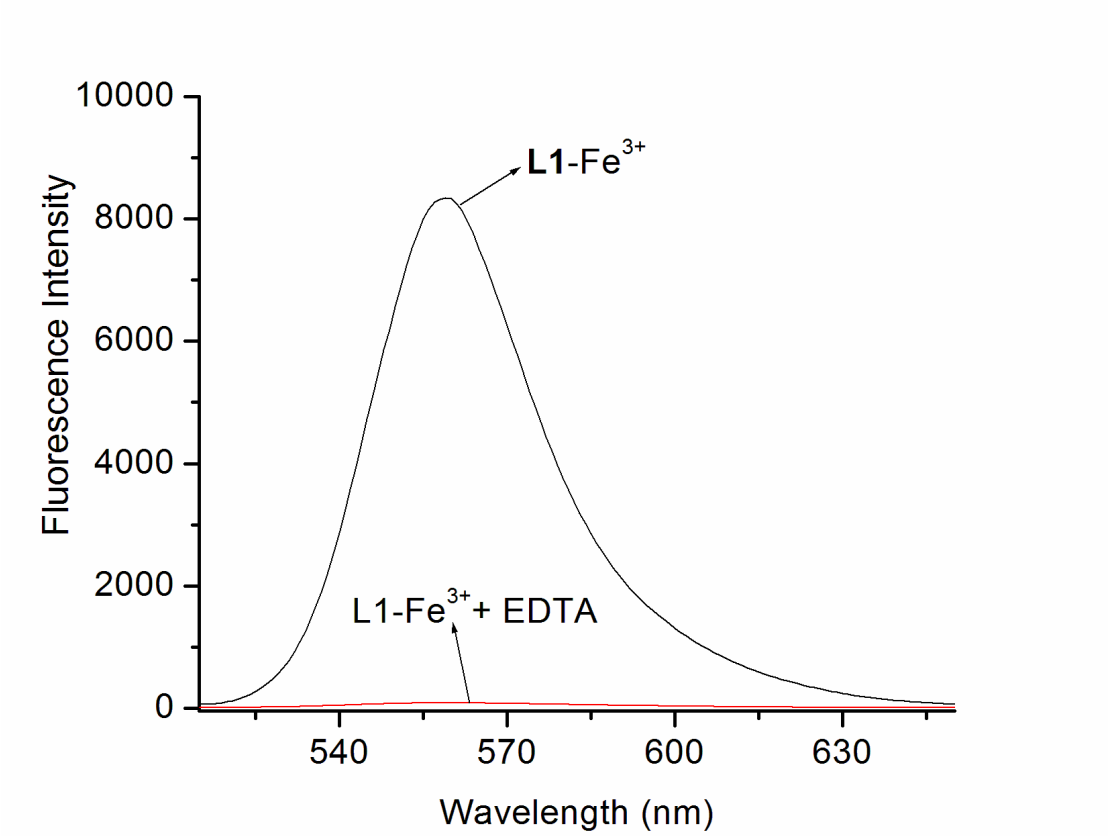

Fig. S2 Fluorescence spectra of **L1** (5 μM) and Fe^{3+} (100 μM) upon the addition of excess EDTA.

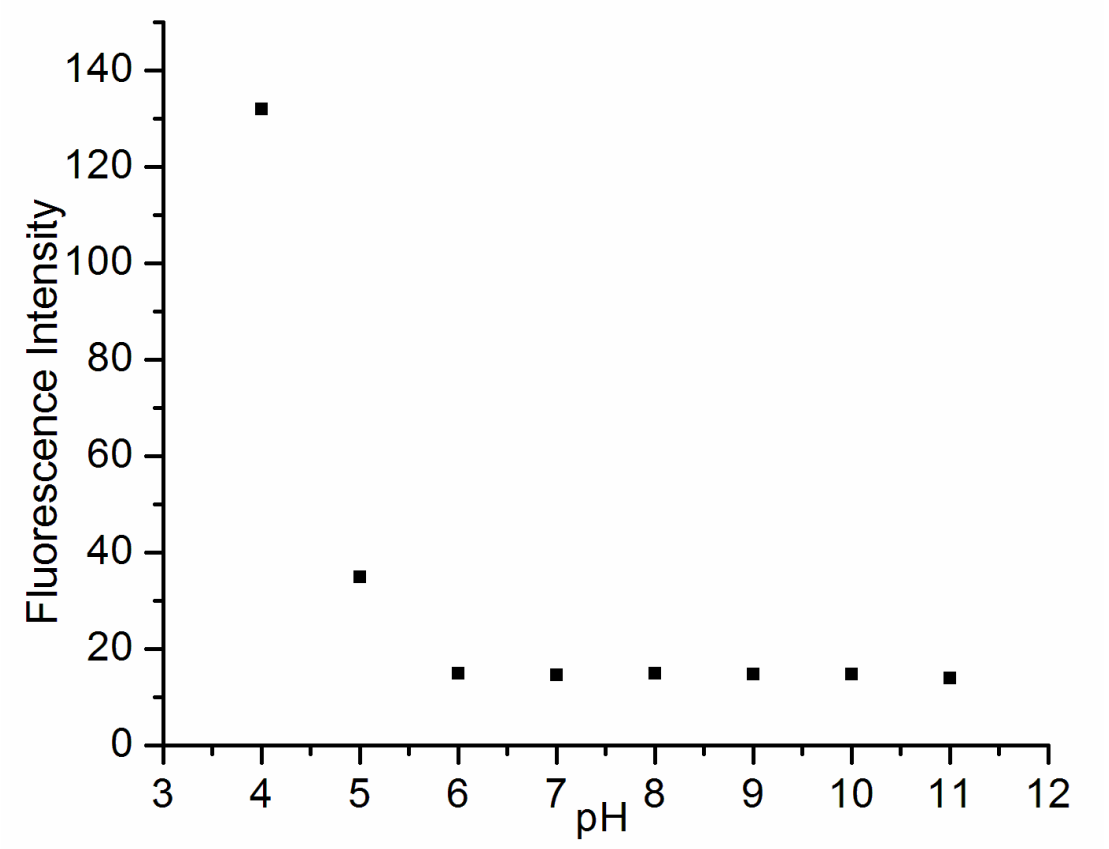

Fig. S3 Fluorescence spectra of **L1** (5 μM) in EtOH/ H_2O (3:7, v/v) solutions at various pH values.

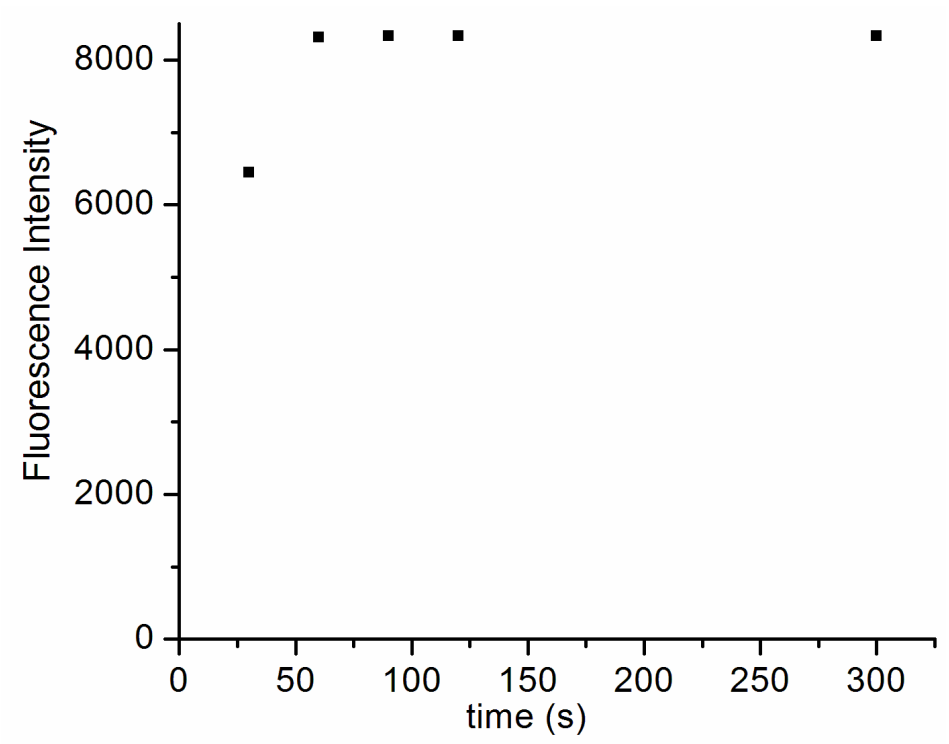

Fig. S4 Time course of the response of **L1** (5 μM) to 20 equiv Fe^{3+} in EtOH/ H_2O (3:7, v/v) solutions.

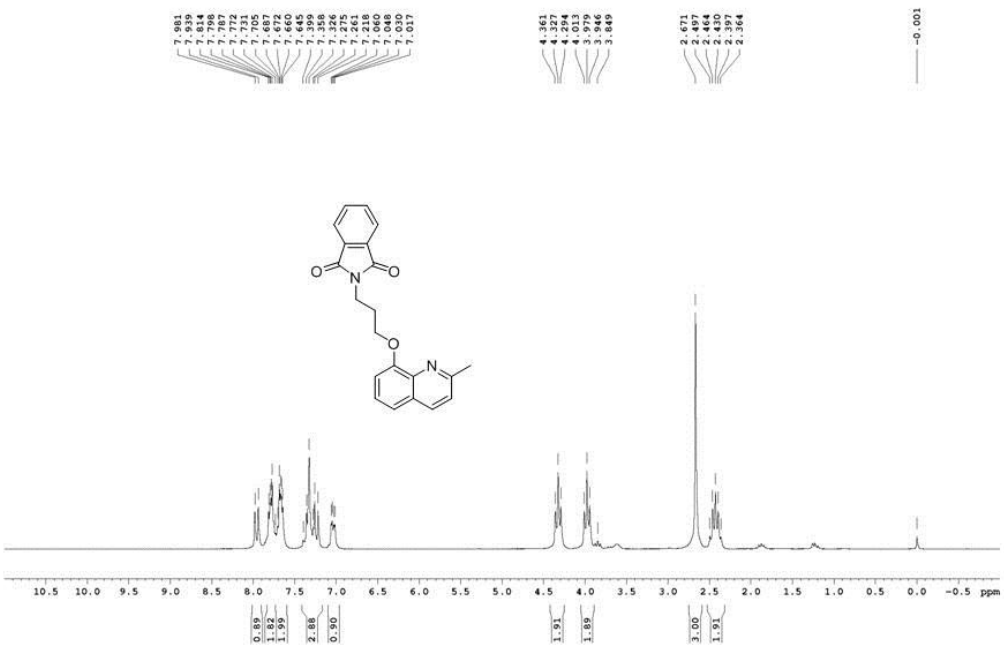

Fig.S5 ^{1}H NMR ($CDCl_3$, 200 MHz) spectrum of **2**.

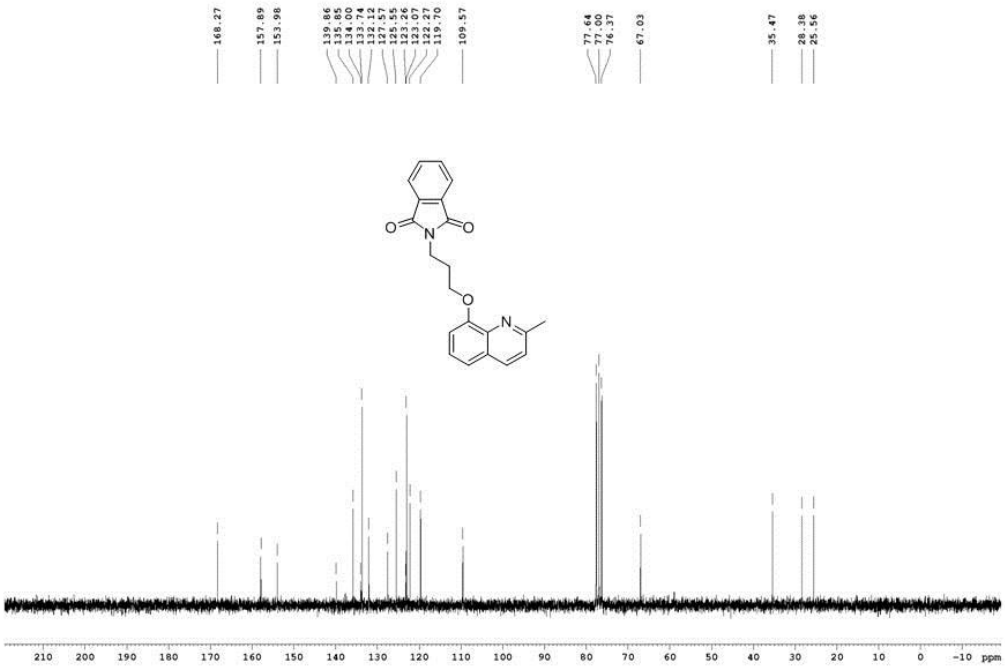

Fig. S6 ^{13}C NMR ($CDCl_3$, 50MHz) spectrum of **2**.

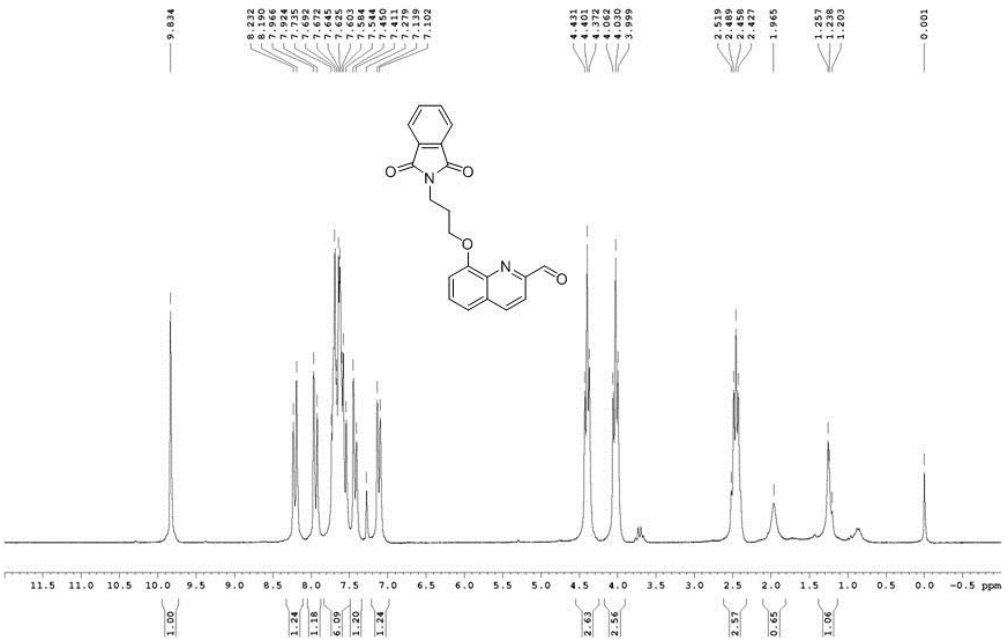

Fig.S7 ^{1}H NMR ($CDCl_3$, 200 MHz) spectrum of **3**.

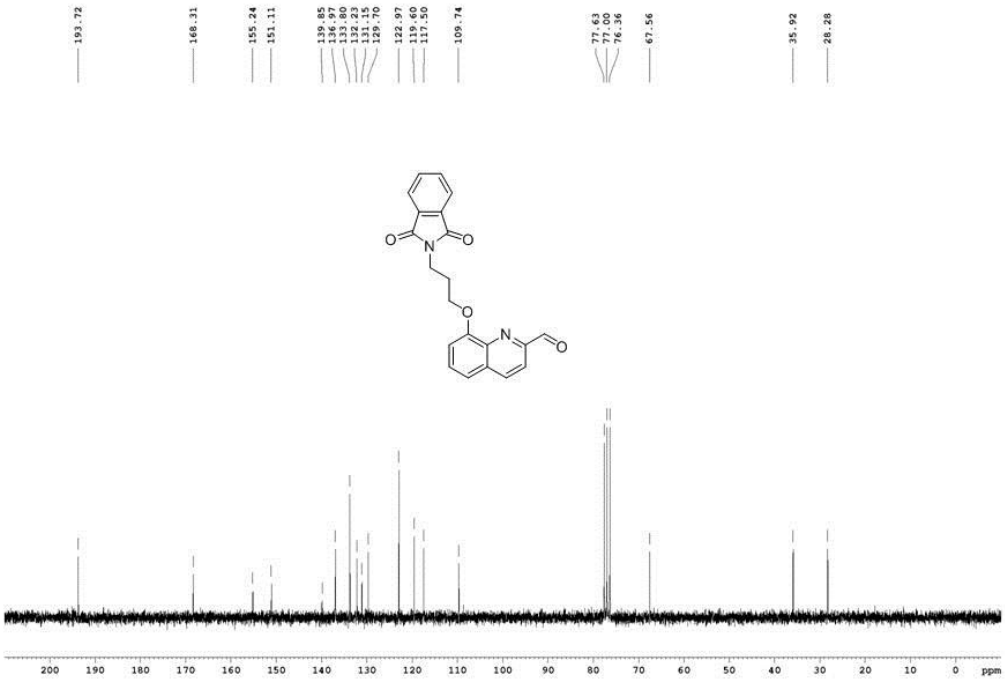

Fig. S8 ^{13}C NMR ($CDCl_3$, 50MHz) spectrum of **3**.

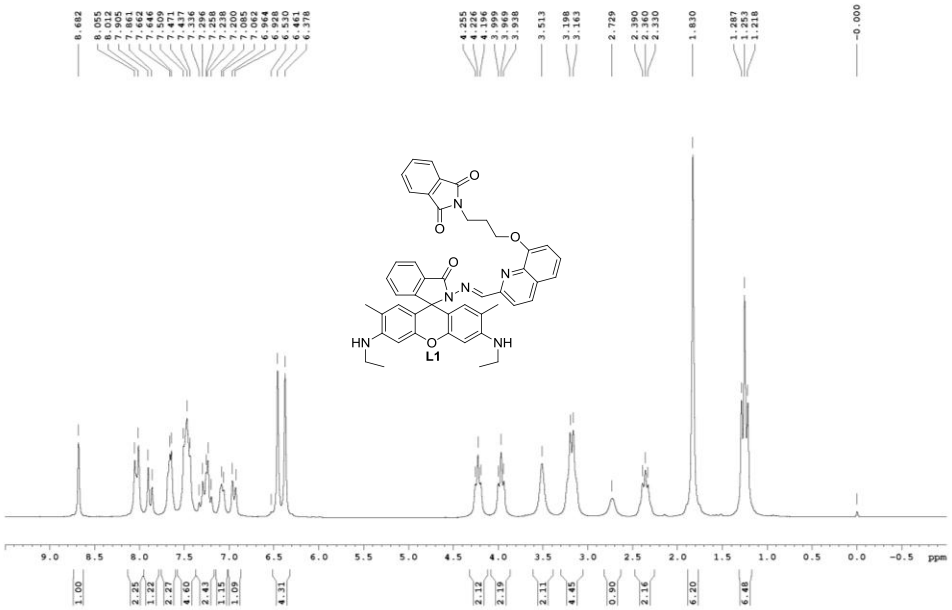

Fig.S9 ^{1}H NMR ($CDCl_3$, 200 MHz) spectrum of **L1**.

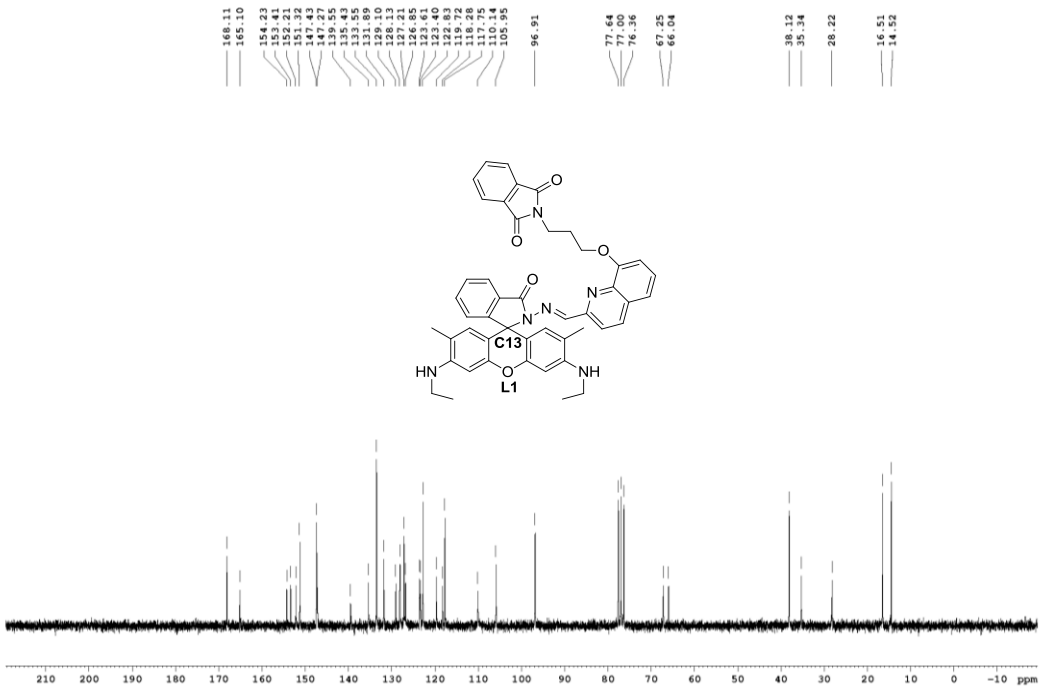

Fig. S10 ^{13}C NMR ($CDCl_3$, 50MHz) spectrum of **L1**.

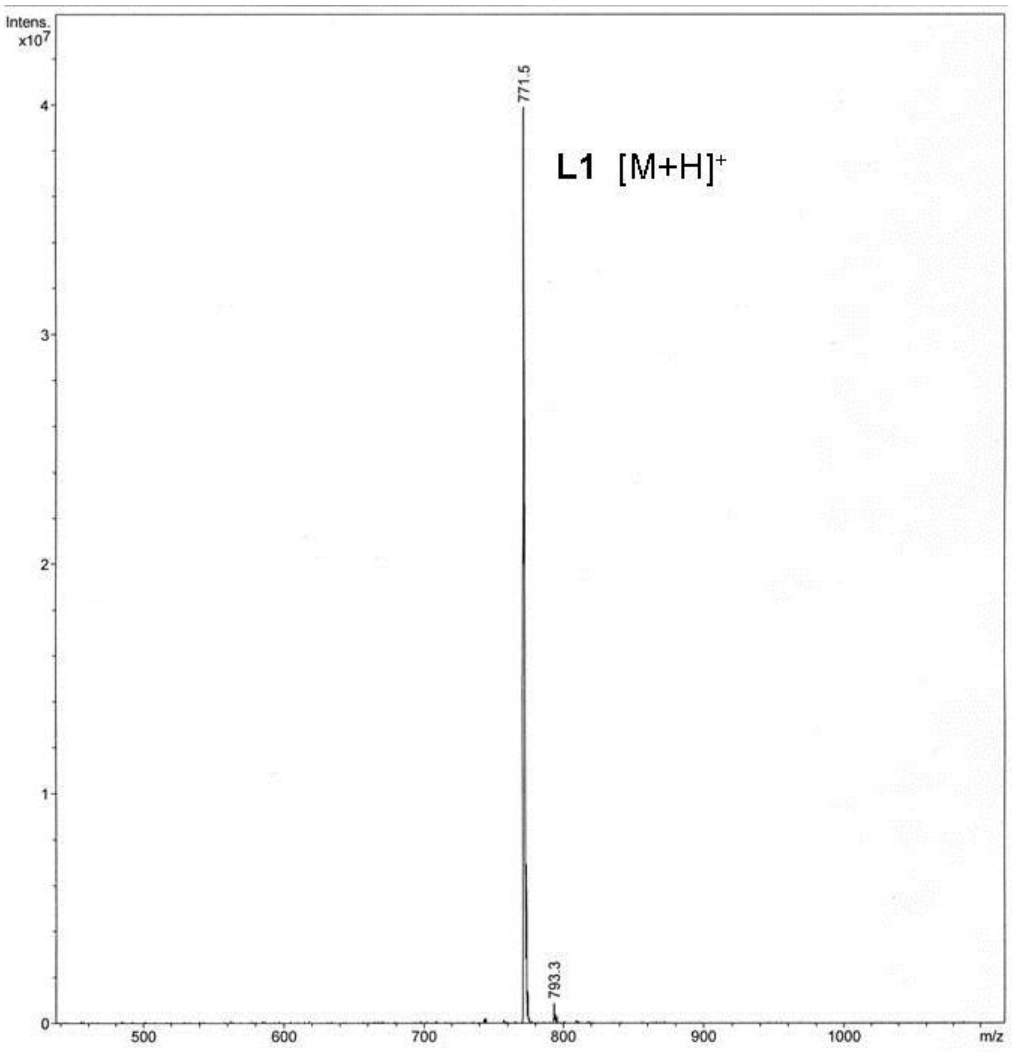

Fig.S11 ESI mass spectrum of **L1.**

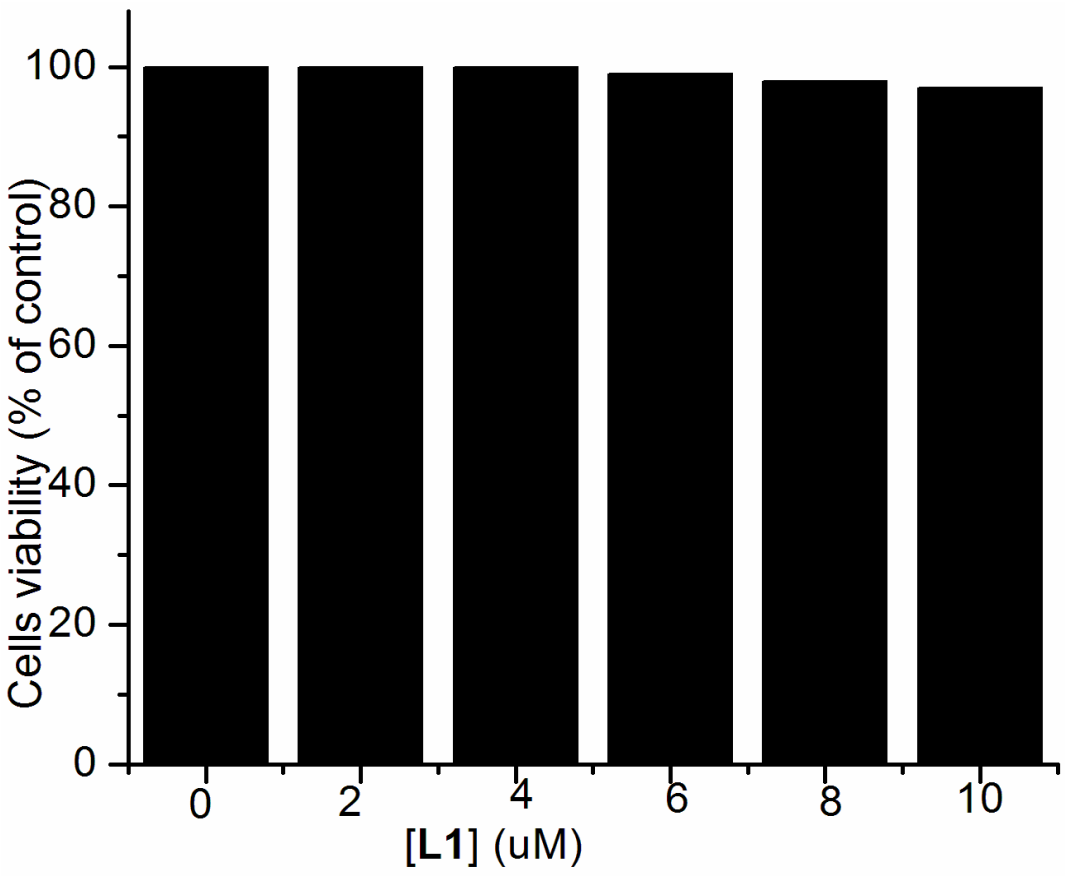

Fig.S12 MTT assay of **L1**