Electronic Supplementary Information

Mercaptoimidazo-phenazine based a Blue Fluorescent Sensor for Ultra-sensitive Detection of Mercury (Ⅱ) ions in Aqueous Solution

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Materials and methods

All the cations Fe^{3+}, Hg^{2+}, Ag^{+}, Ca^{2+}, Cu^{2+}, Co^{2+}, Ni^{2+}, Cd^{2+}, Pb^{2+}, Zn^{2+}, Cr^{3+},and Mg^{2+} was added in the form of perchlorate salts, which were purchased from Alfa-Aesar Chemical, and stored in a vacuum desiccator. All other reagents and solvents were commercially available at analytical grade and were used without further purification. ^{1}H NMR spectra were recorded using a Mercury-400BB spectrometer at 400 MHz for ^{1}H NMR and 600 MHz for ^{13}C NMR. The fluorescence spectra were recorded with a Shimadzu RF-5301 spectrofluorimeter. The IR was performed on a Digilab FTS-3000 FT-IR spectrophotometer. Mass spectra were recorded on an esquire 6000 MS instrument equipped with an electrospray (ESI) ion source and version 3.4 of Bruker Daltonics Data Analysis as the data collection system.

Synthesis of compound Z-3

3-aminophenazin-2-ol (0.013mmol, 0.0033g) and potassium hydroxide (0.02 mol, 1.12g) were added to H_2O/EtOH (1:4). The solution was heated until the solid dissolved. Cooling to the room temperature and adding the carbon disulfide (10 ml) to the solution. The solution was stirred and refluxed for 7h, after cooling to room temperature, the precipitate was filtrated, washed with hot absolute ethanol three times, recrystallized with DMF to get yellow-green powdery product.

Z-3: yield: 45%; m.p. > 300℃; ^{1}H NMR (DMSO–d_6, 600MHz) δ 14.41 (s, 1H), 8.17-7.69 (m, 6H). ^{13}C NMR (DMSO-d_6, 150MHz) δ 182.31, 151.10, 141.79, 141.40, 141.16, 140.53, 130.43, 130.12, 128.54, 128.47, 109.27, 105.38, 104.55; IR (KBr cm^{-1}) v: 2675 cm^{-1} (-SH); ESI–MS *m/z* $[M + H]^+$ Calcd for $C_{13}H_7OS$ 253.03; Found 254.08.

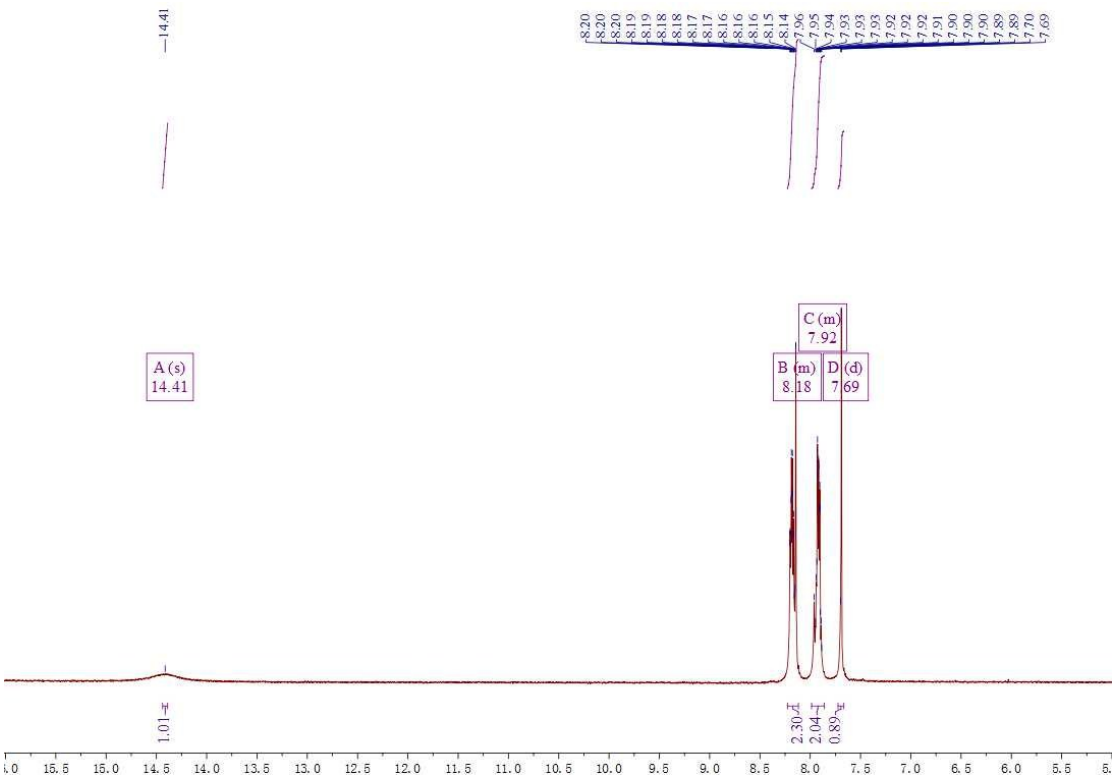


Fig. S1 ^{1}H NMR spectra of compound **Z-3**.

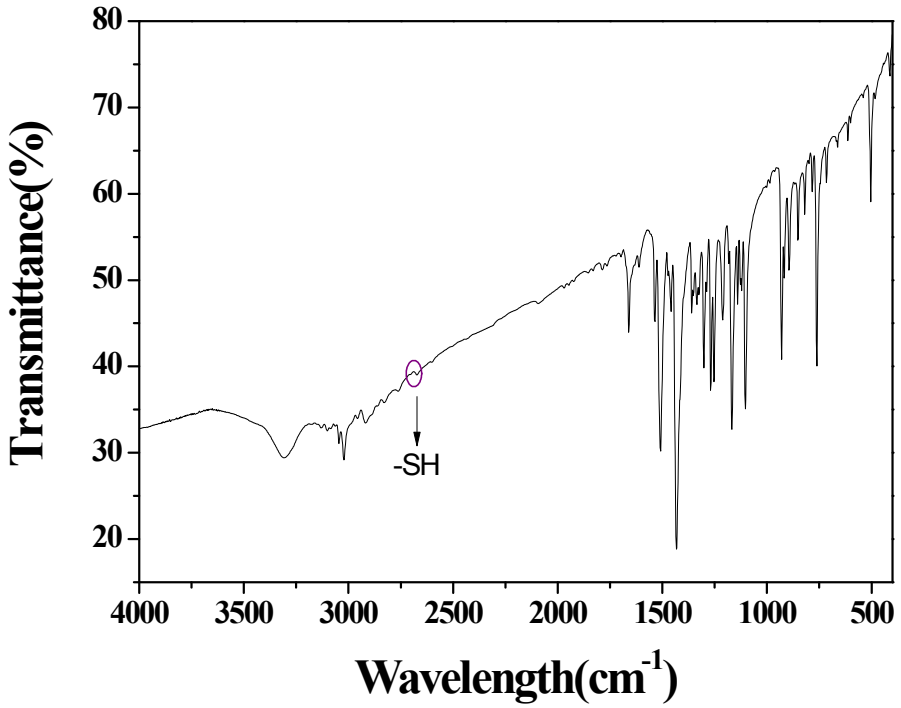


Fig. S2 IR spectrum of **Z-3**.

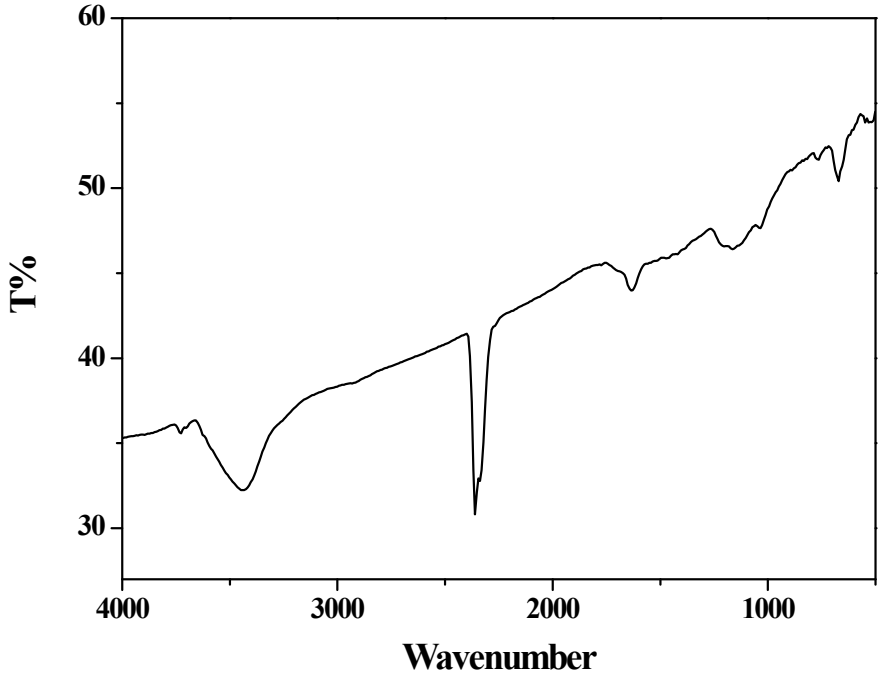


Fig. S3 IR spectrum of **Z-3** + Hg^{2+}.

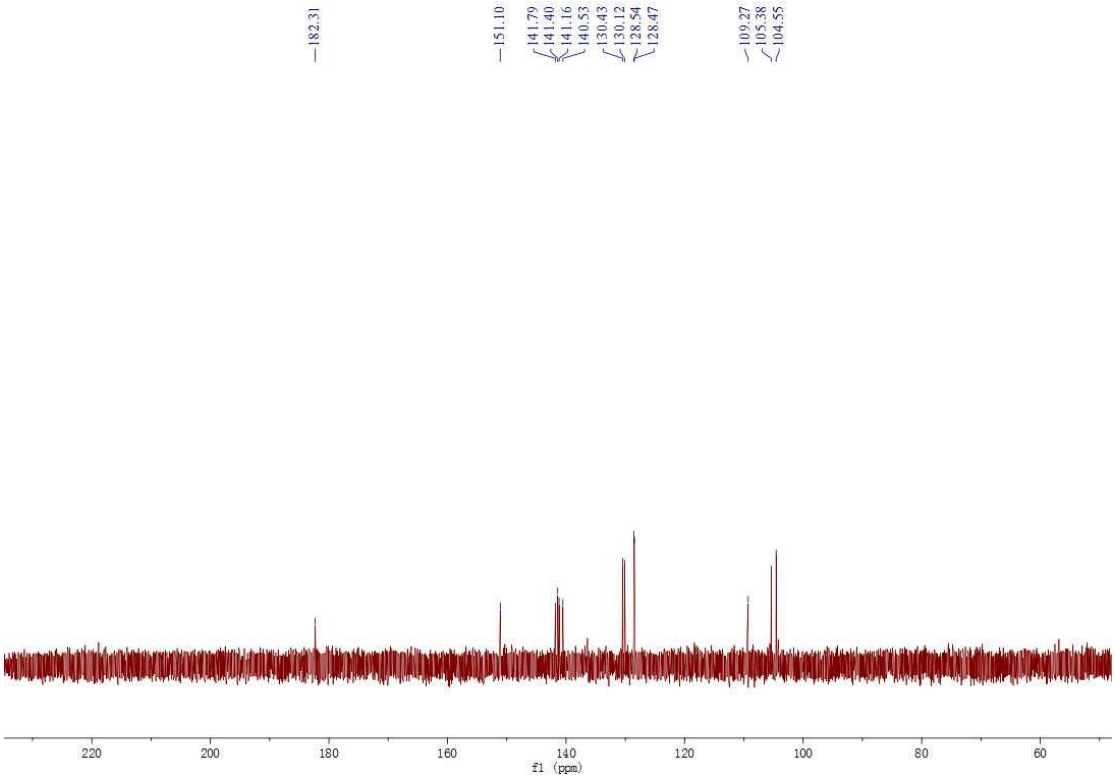
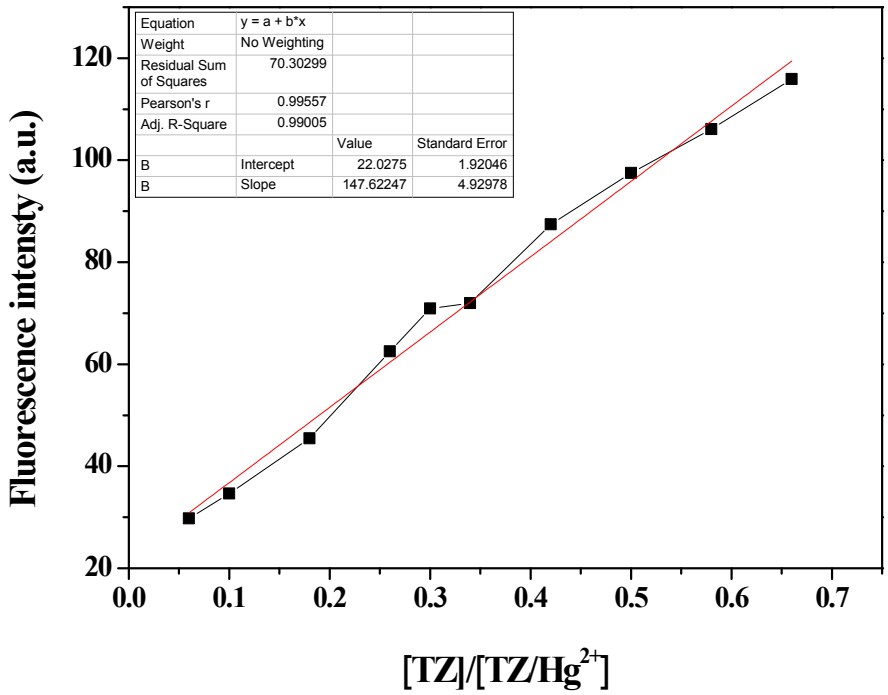


Fig. S4 The ^{13}C NMR spectra of **Z-3**.



Linear Equation: $Y = 147.622 \times X + 22.028$ $R^2 = 0.99005$

$S = 147.622 \times 10^6$ $\delta = 0.1053$ (N = 20) K = 3

$LOD = K \times \delta / S = 2.14 \times 10^{-9}$ M

Fig. S5 The photograph of the fluorescent spectrum linear range.

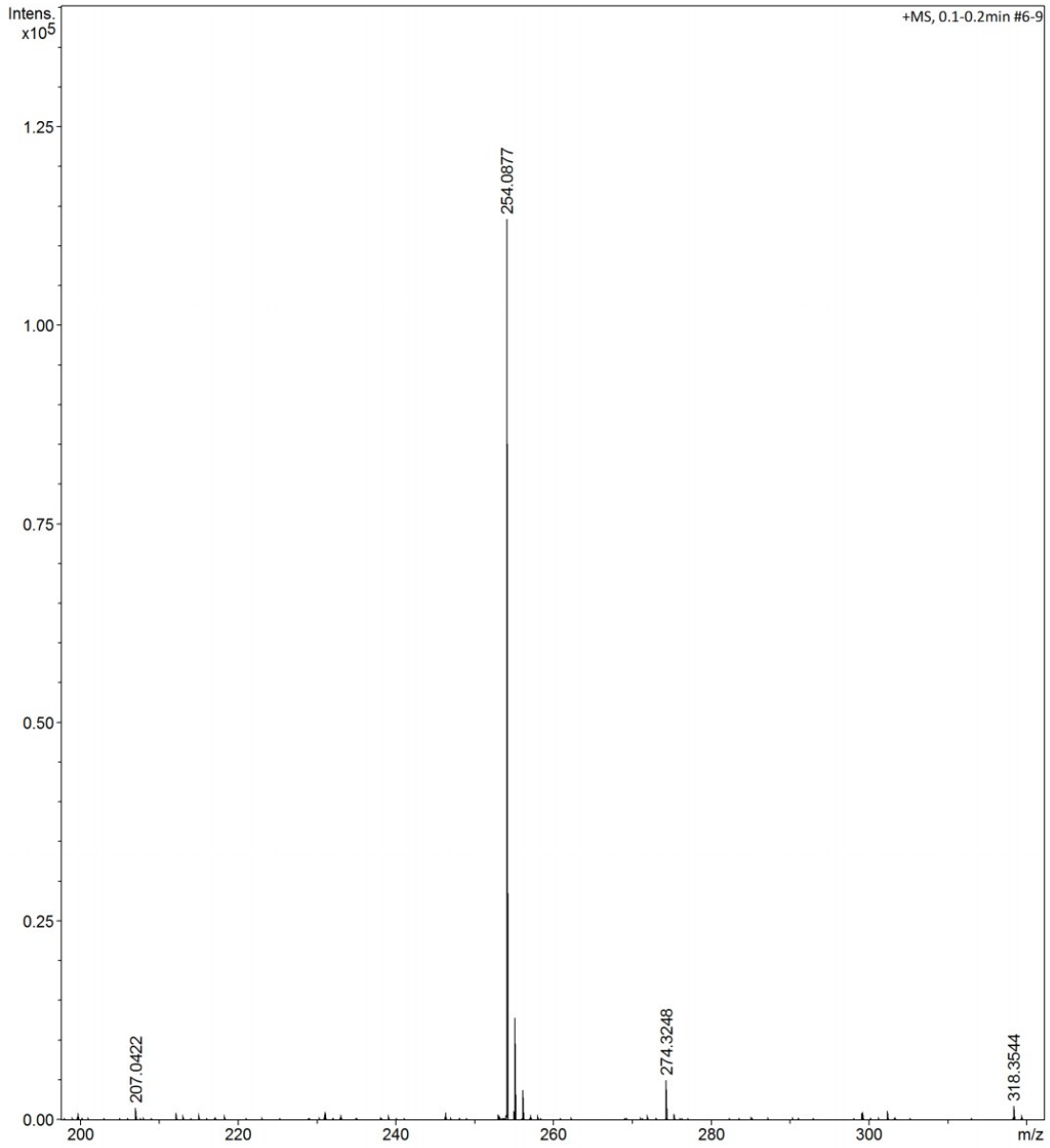


Fig. S6 ESI-MS spectra of **Z-3**.