

Supporting Information

A Pyrene based schiff base probe for selective fluorescent turn-on detection of Hg²⁺ ions with live cell application

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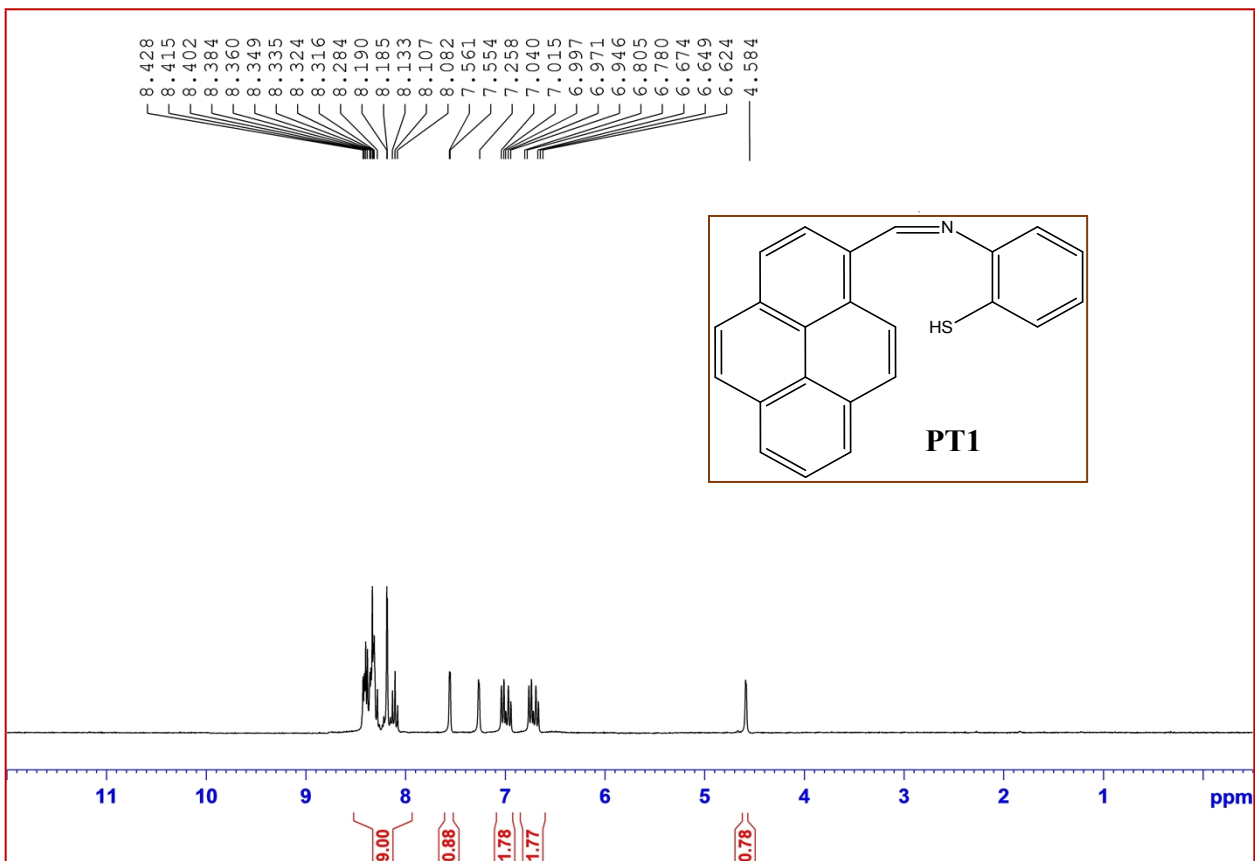


Fig. S1 ^1H NMR spectrum of **PT1** in $d\text{-Cl}_2$.

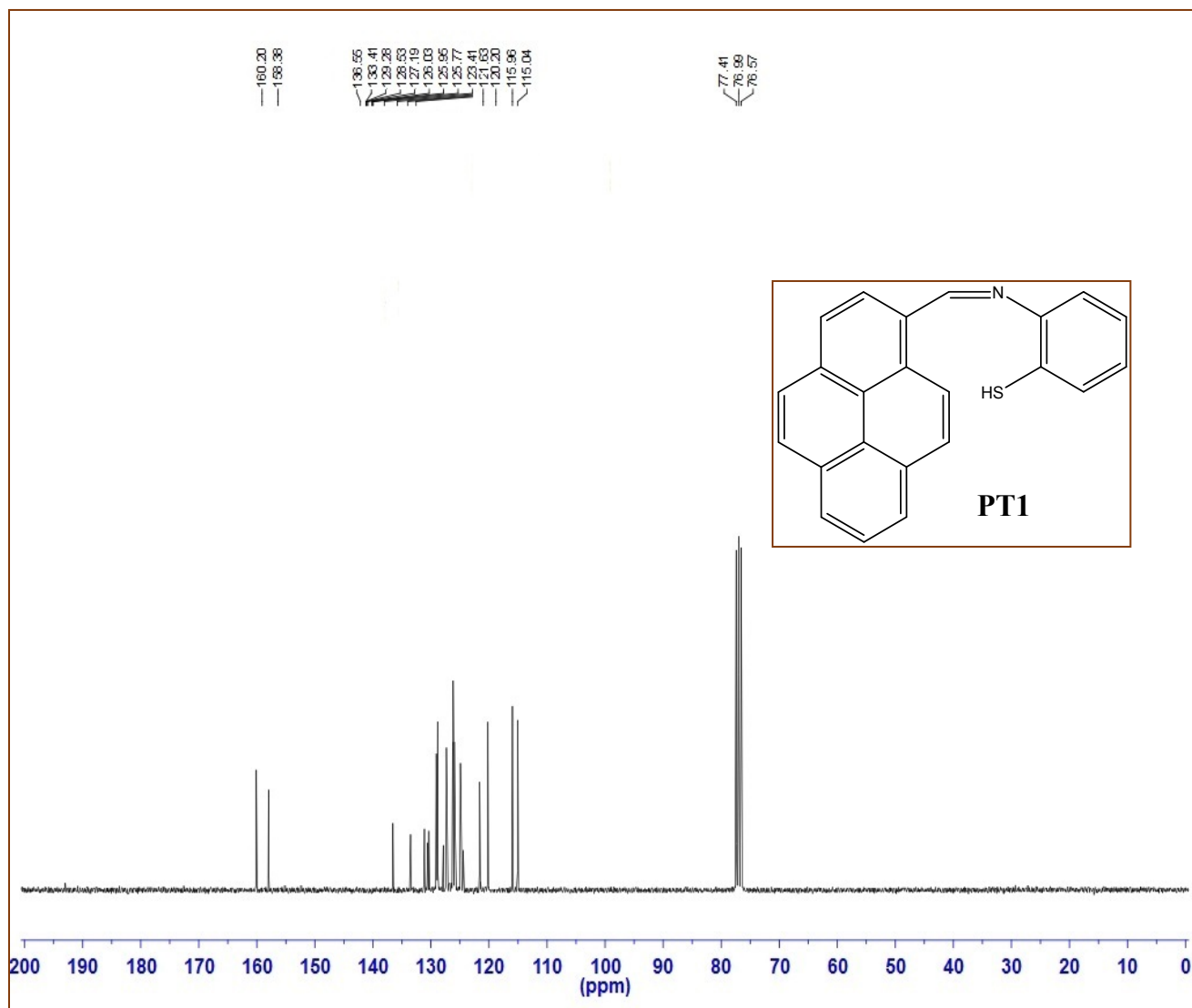


Fig. S2 ^{13}C NMR spectrum of **PT1** in d -Chloroform.

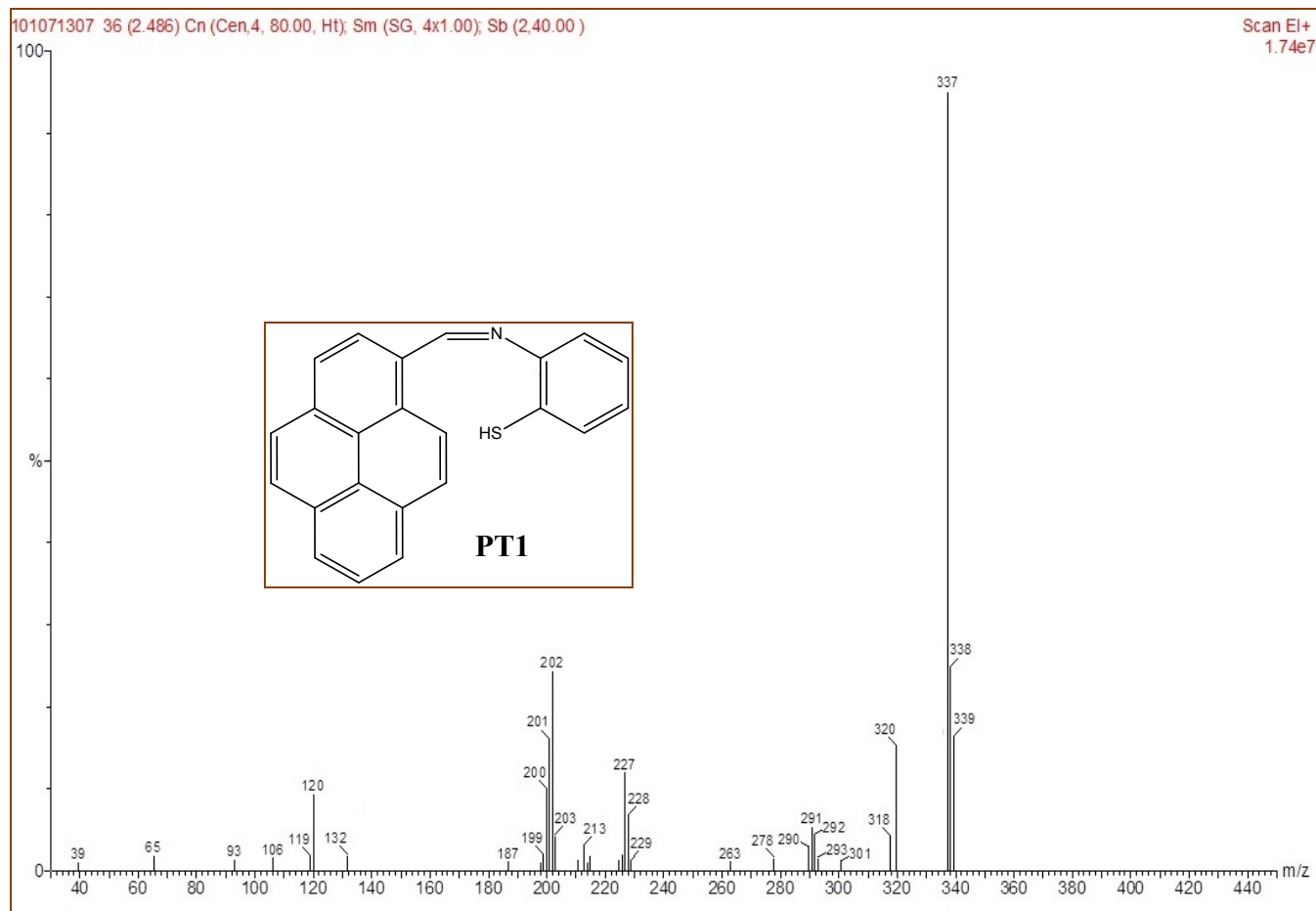


Fig. S3 Mass (FAB) spectrum of **PT1**.

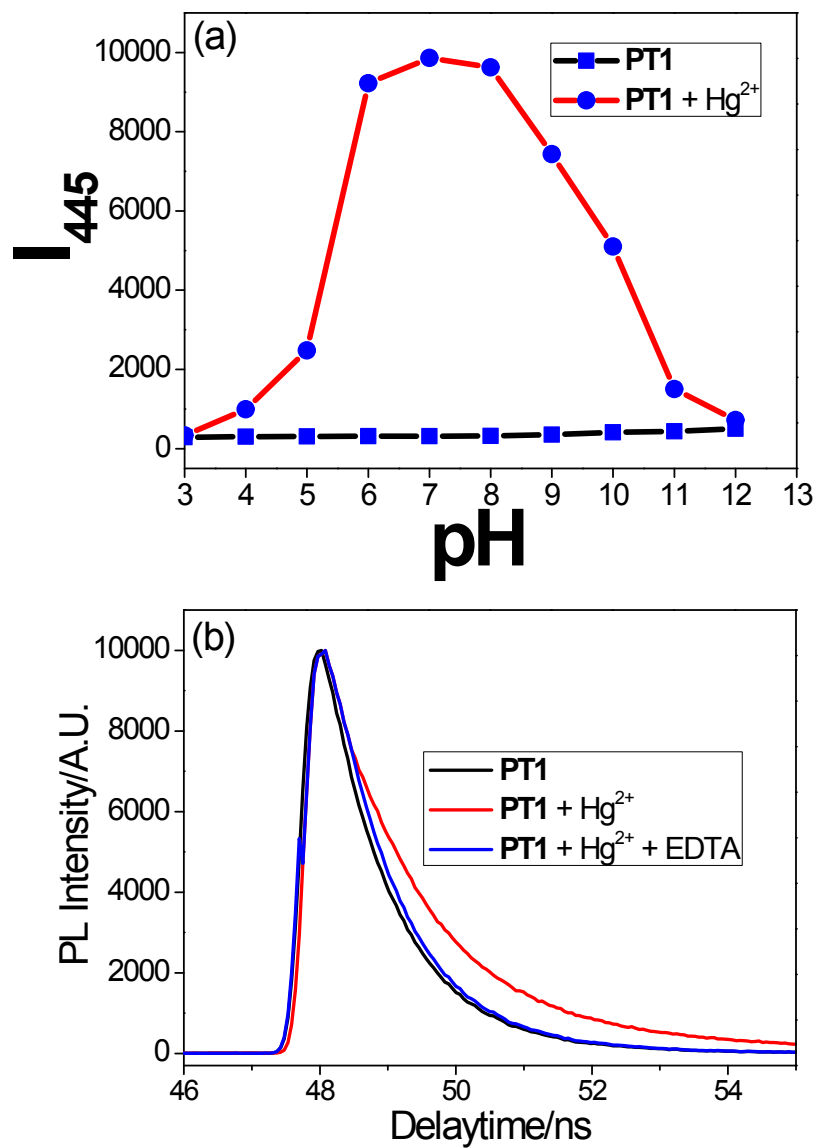
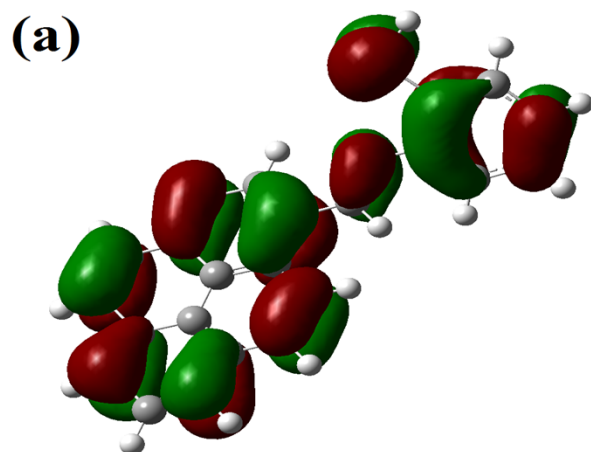
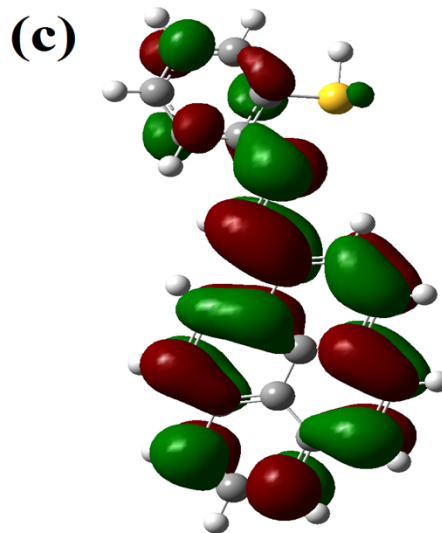


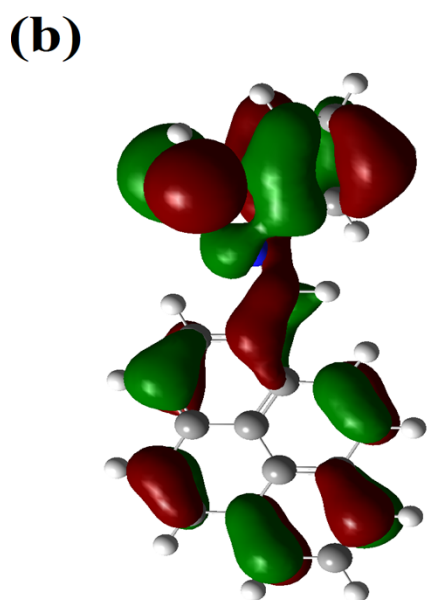
Fig. S4 (a) pH effect on **PT1** and **PT1+Hg²⁺** systems and (b) TRPL spectra of **PT1**, **PT1+Hg²⁺** and **PT1 + Hg²⁺ + EDTA**.



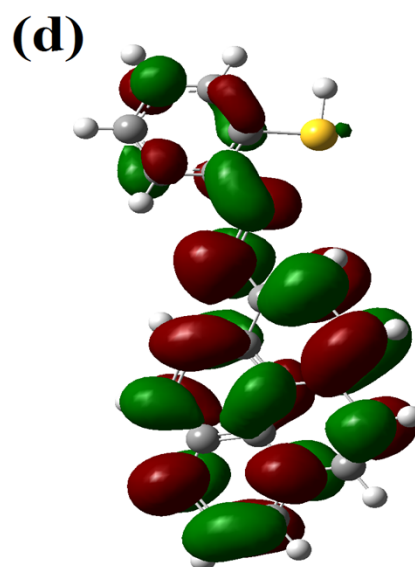
PT1 (HOMO)



PT1 (LUMO)

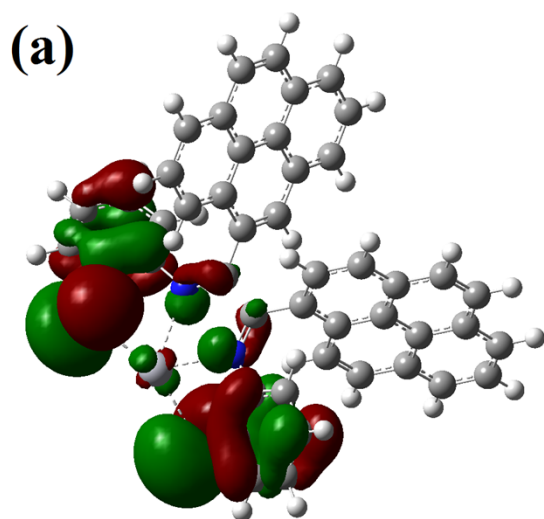


PT1 (HOMO-1)

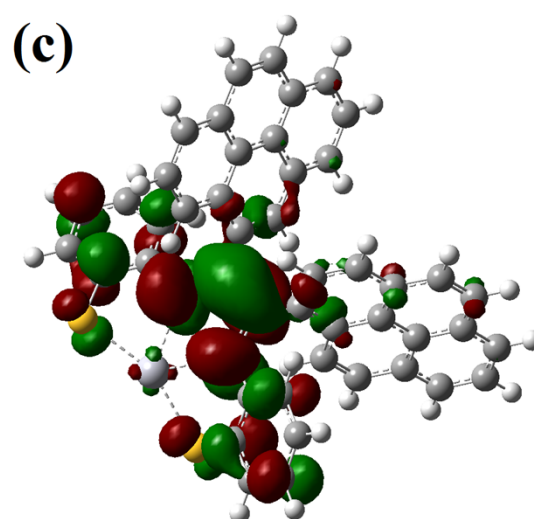


PT1 (LUMO+1)

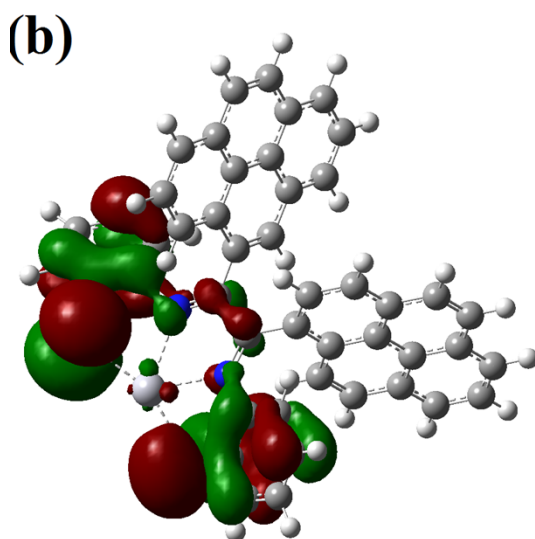
Fig. S5 HOMOs and LUMOs of PT1.



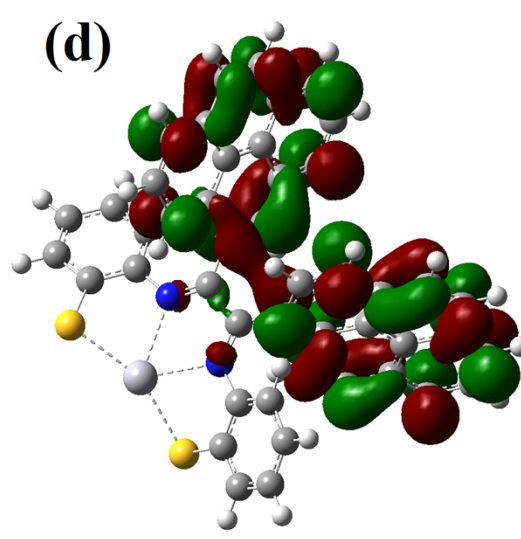
PT1-PT1* (HOMO)



PT1-PT1* (LUMO)



PT1-PT1* (HOMO-1)



PT1-PT1* (LUMO+1)

Fig. S6 HOMOs and LUMOs of **PT1-PT1*** excimer for **PT1-Hg²⁺** complex formation.

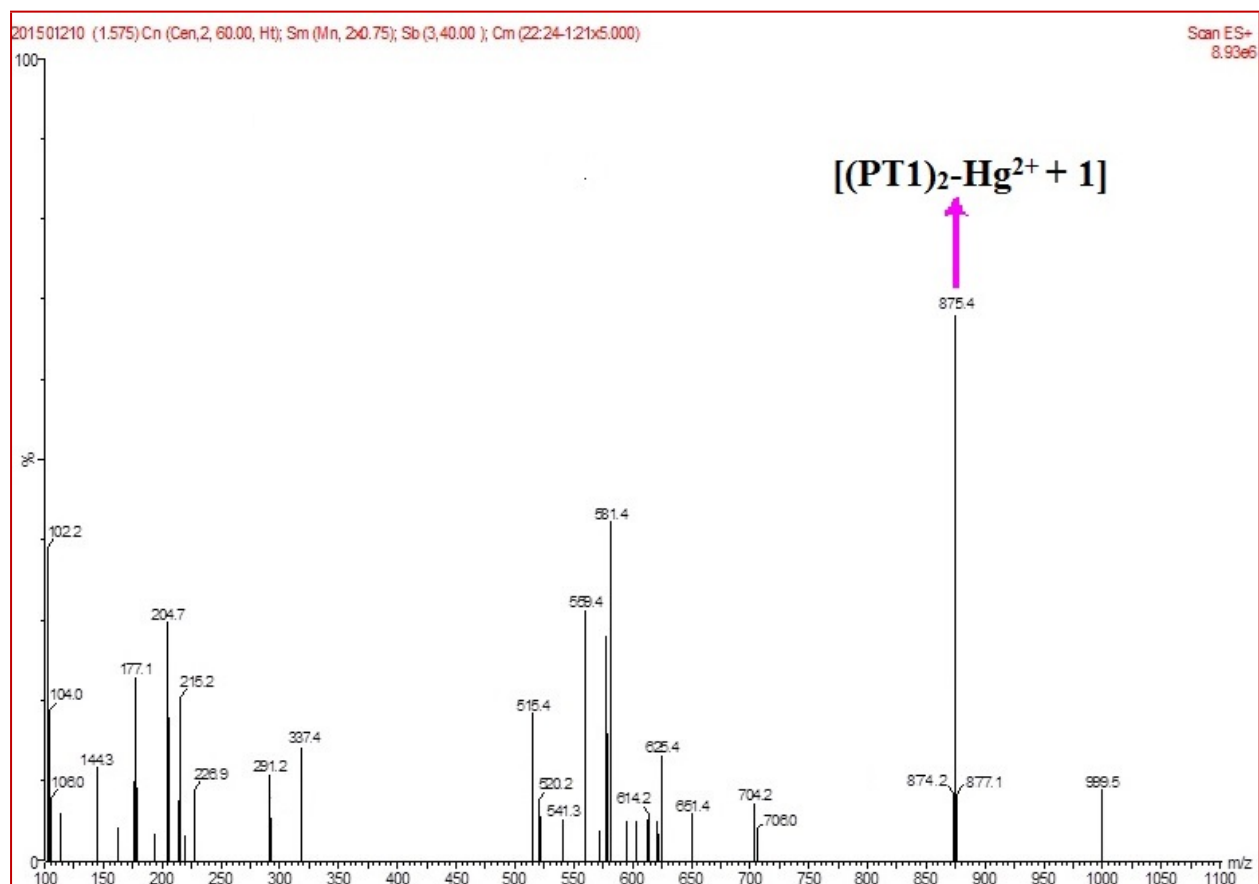


Fig. S7 ESI-Mass spectrum of $(PT1)_2-Hg^{2+}$ complex during $PT1-PT1^*$ excimer formation.

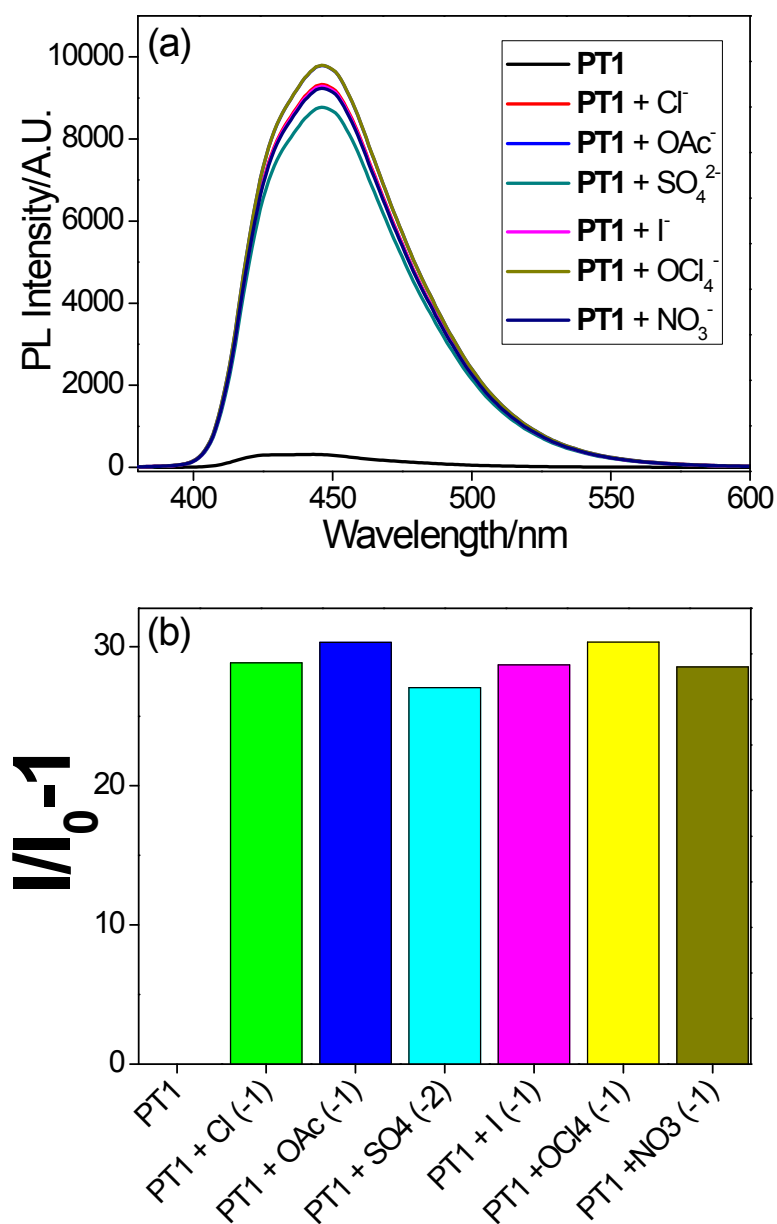


Fig. S8 (a) Sensor responses and (b) folds of enhancement of **PT1** towards Hg^{2+} in presence of different counter ions (CH_3COO^- , NO_3^- , Cl^- , I^- , ClO_4^- and SO_4^{2-} were taken as counter ions)

Table 1 TRPL decay constants (τ) of **PT1** and its sensor complexes.

Compound	τ_1 (ns)	τ_2 (ns)	A_1 (%)	A_2 (%)	τ_{Avg} (ns)
PT1	0.7321	2.2891	35.58	64.42	2.63
PT1 +Hg ²⁺	1.0491	5.9600	96.16	3.84	3.14
PT1 +Hg ²⁺ + EDTA	0.7516	2.2960	35.31	64.69	2.68