Supplementary Information

A highly selective off-on fluorescent chemodosimeter for Hg^{2+} based on a anthracene-bis(phosphinesulfide) conjugate

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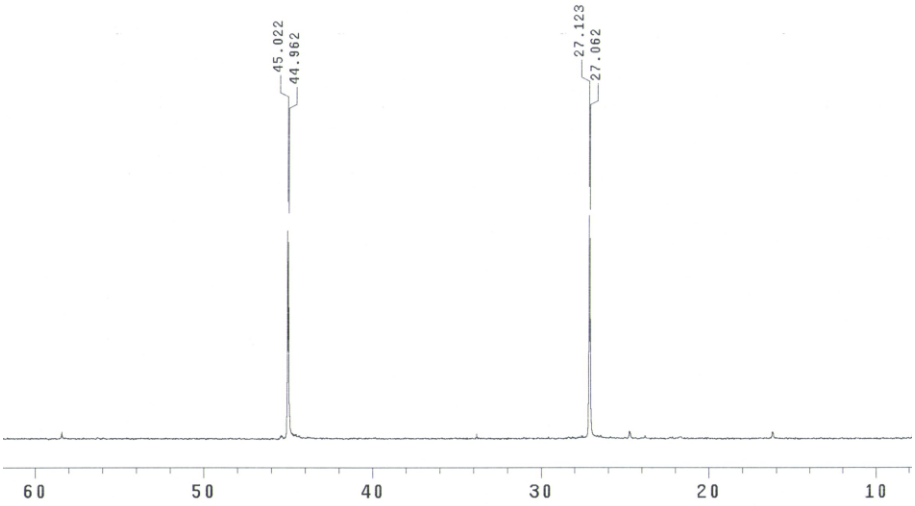

Figure S1. ^{31}P NMR spectrum of **L**^{1} (δ in ppm, $CDCl_3$, 25 °C).

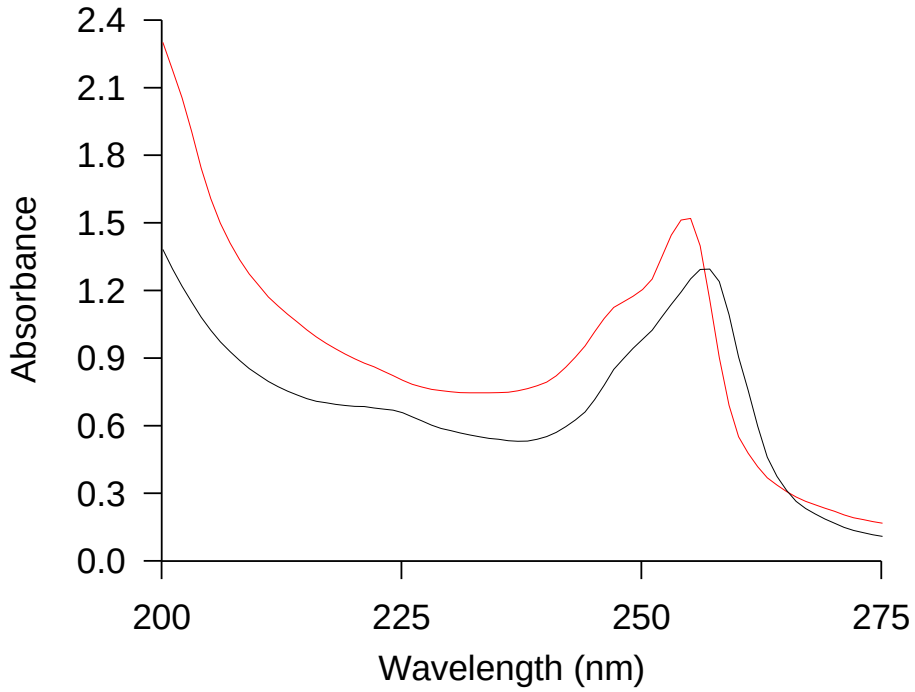

Figure S2. UV-Vis spectra of **L**^{1} (black line) (2.79×10^{-5} M) and of a solution of **L**^{1} (red line) in MeCN/H_2O 4:1 (v/v), 25°C, upon addition of Hg^{2+} ion, recorded after 1 h ([Hg^{2+}]/[**L**^{1}] molar ratio of 0.5).

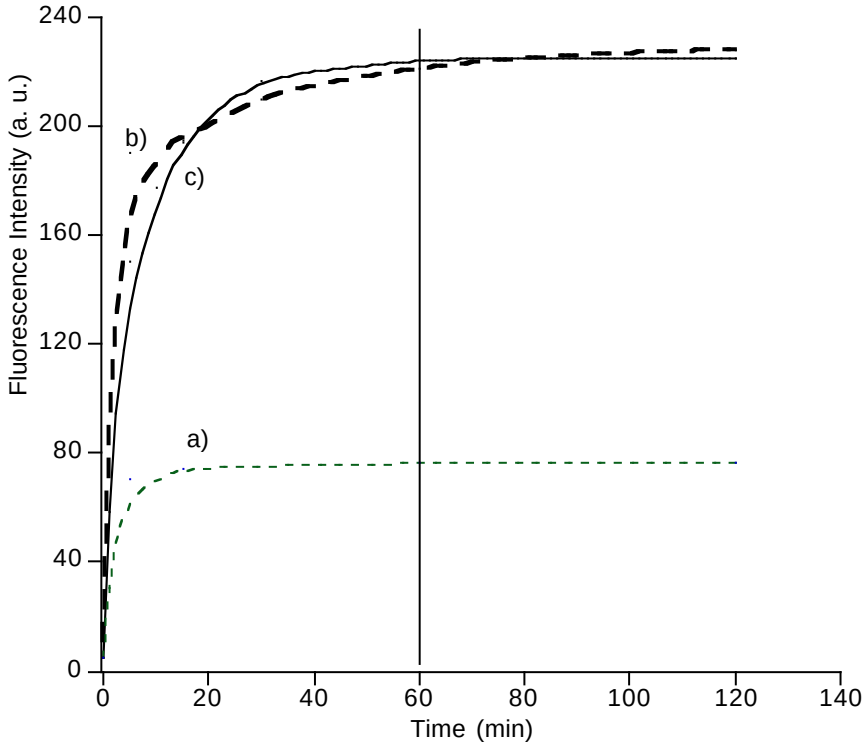

Figure S3. Time trace of the fluorescence intensity at 411 nm of the reaction of $\mathbf{L}^1$ (2.79×10^{-5} M) and Hg^{2+} at the $[Hg^{2+}]/[\mathbf{L}^1]$ molar ratio of a) 0.25; b) 0.5, c) 1. MeCN/H_2O 4:1 (v/v), 25 °C, λ_{ex} = 376 nm.

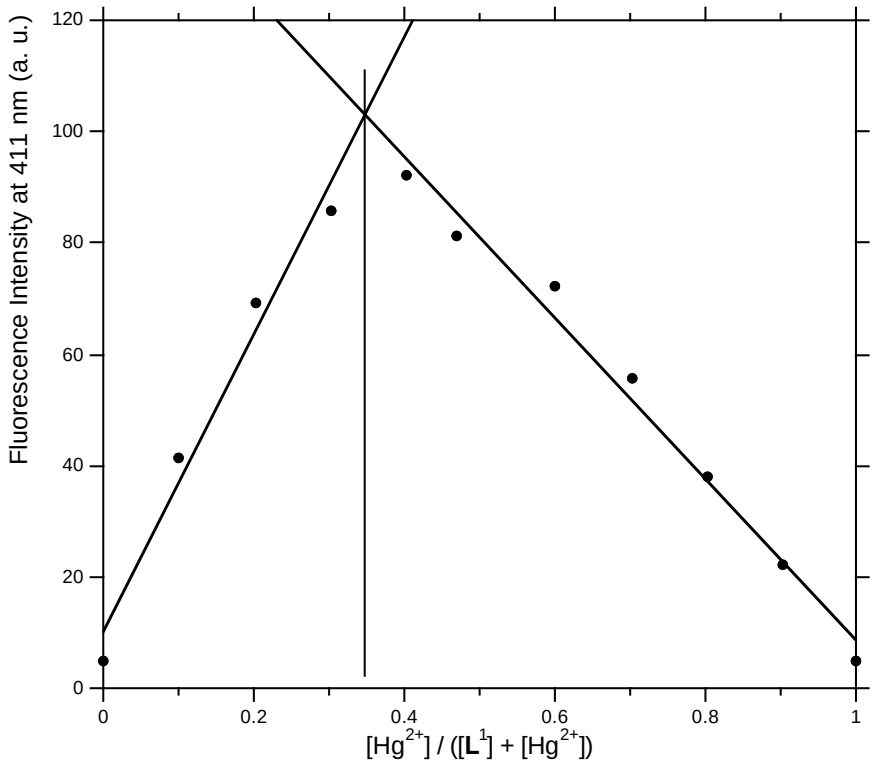

Figure S4. Job's plot data for the system Hg^{2+}- $\mathbf{L}^1$. The total concentration of $\mathbf{L}^1$ and Hg^{2+} was 2.8×10^{-5} M. Spectra were measured at 25 °C after 1 h the preparation of solutions. λ_{ex} = 376 nm.

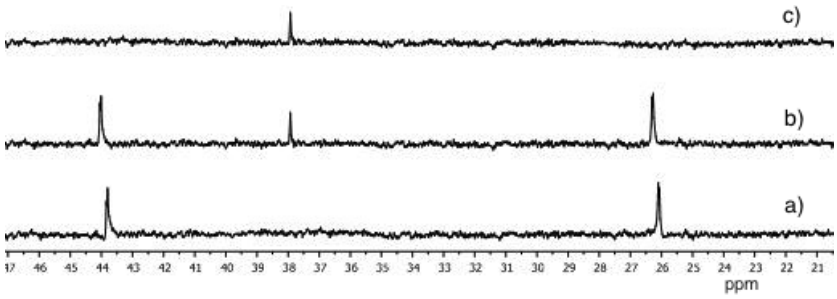

Figure S5. ^{31}P NMR spectra in $CDCl_3$ of (a) $\mathbf{L}^1$ (1.35×10^{-3} M), and (b) after the addition of $Hg(ClO_4)_2$ in CD_3CN ($[Hg^{2+}]/[\mathbf{L}^1]$ molar ratio of 0.5) recorded after 20 min from the mixing, (c) the solution from (b) recorded after 1 h from the mixing; δ in ppm, 25 °C).

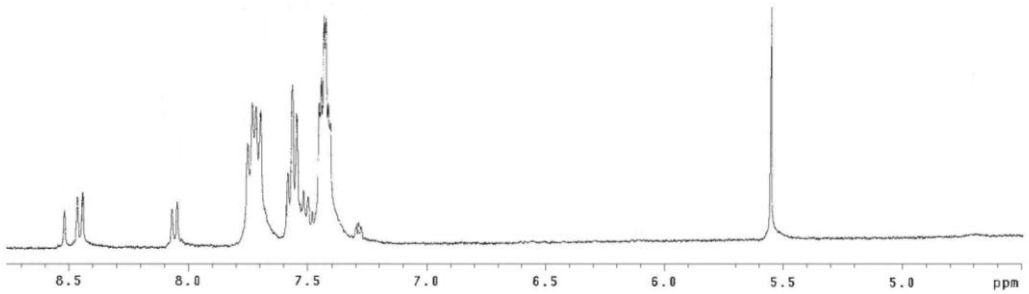

Figure S6. ^{1}H NMR spectrum of the solution obtained from the reaction of $\mathbf{L}^1$ in $CDCl_3$ (1.35×10^{-3} M) with $Hg(ClO_4)_2$ in CD_3CN ($[Hg^{2+}]/[\mathbf{L}^1]$ molar ratio of 0.5.) after the separation of the solid complex $[Hg\mathbf{L}_2]$; δ in ppm, 25 °C).

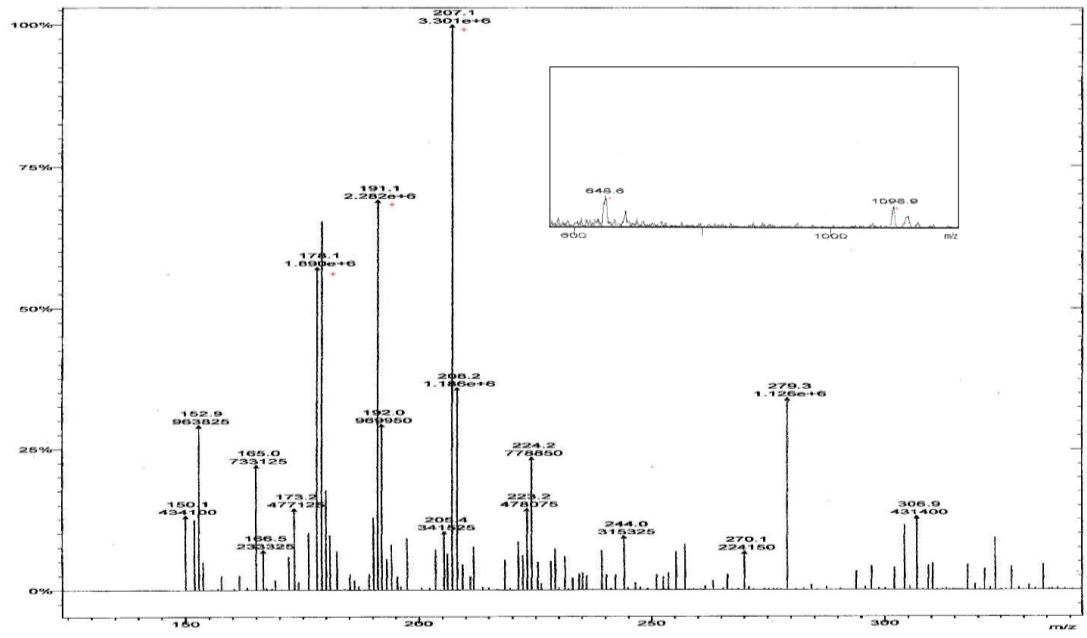

Figure S7. Atmospheric Pressure Chemical Ionisation Mass (APCI) spectrum of $\mathbf{L}^1$ (4.35×10^{-7} M) in MeCN upon addition of Hg^{2+} ion. $[Hg^{2+}]/[\mathbf{L}^1]$ molar ratio of 0.5. Spectrum recorded after 1h from the mixing.