A Colorimetric Probe for the Selective Naked-Eye Detection of Pb(II) Ions in Aqueous Media

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1. Materials and Methods

Compounds 1, 2, and 3 were obtained according to the literature procedure. Electrospray ionization mass (ESI-MS) spectra were obtained at national center for inter-university research facilities. Infrared spectra were obtained using PerkinElmer Spectrum 100FT-IR Spectrometers. All absorption spectra were recorded with a Shimadzu UV-2501 spectrophotometer. Fluorescence measurements were recorded on a Hitachi F-7000 fluorescence spectrophotometer at 25 °C using 10 mm quartz cuvettes with a path length of 1 cm. Stock solution of metal nitrate salts (2.04 mM) were prepared in water. Stock solution of probes (0.51 mM) was prepared in CH$_3$CN. UV/Vis titration experiments were performed using 5 μM of probe 1 in CH$_3$CN/HEPES solution (1/99, v/v) with varying concentrations of the metal nitrate salts.
2. More Spectroscopy Data

**Fig. S1** Absorption ratio ($A_{527}/A_{496}$) of probe 1 (5 µM) upon addition of varied concentrations of Pb(NO$_3$)$_2$. Incubation time = from bottom to top: 0, 3, 5, 10, 20, 30, 60, 90 min. All data were obtained in HEPES buffer (10 mM, pH 7.4, 1% CH$_3$CN) at 25 ºC.

**Fig. S2** Job’s plot of a 1:1 complex of 1 and Pb$^{2+}$, where the absorbance at 527 nm is plotted against the mole fraction of 1 at an invariant total concentration of 40 µM in HEPES buffer (10 mM, pH 7.4) containing 1% CH$_3$CN.
**Fig. S3** ESI-MS spectrum of 1-Pb$^{2+}$ complex.

**Fig. S4** Infrared spectra of 1 and 1-Pb(II) adduct.
**Fig. S5** Absorption ratio (527 over 496 nm) of 1 (5 µM) and 1 treated with Pb(II) ions (4 equiv.) in different pH buffer systems containing 1% CH₃CN as a cosolvent at 25 °C. Incubation time is 30 min.

**Fig. S6** Absorption spectra of probe 1 (0.5 - 5 µM) upon addition of corresponding 4 equiv. of Pb²⁺ in HEPES buffer (10 mM, pH 7.4, containing 1% acetonitrile) at 25 °C.
Fig. S7 Fluorescence emission spectra of 1 (5 µM) in the presence of various concentrations of Pb$^{2+}$ (Excited at 460 nm). All spectra were taken at 30 min in HEPES buffer (10 mM, pH 7.4, 1% CH$_3$CN) at 25 °C.

Fig. S8 Normalized UV-visible spectra of compounds 1–3 (5 µM) upon addition of 4 equiv. of Pb(NO$_3$)$_2$. All data were taken at 30 min in HEPES buffer (10 mM, pH 7.4, 1% CH$_3$CN) at 25 °C.
**Fig. S9** Color change of probe 1 in the absence (a) and presence (b) of Pb(NO₃)₂. Subsequently, either HCl (c) or EDTA (d) was added to the 1-Pb(II) adduct.

**Fig. S10** Absorption ratio (527 over 496 nm) of 1 (5 µM) upon addition of different metal ions (4 equiv.) in HEPES buffer (10 mM, pH 7.4, 1% CH₃CN, 25 °C). All data were measured at 30 min after addition of each metal ion.
**Fig. S11** Absorption spectra of probe 1 upon addition of different metal ions (4 equiv.) and subsequent addition of Pb(II) ions (4 equiv.) to each mixture.

**Fig. S12** Absorbance at $A_{527}$ of probe 1 (5 µM) upon addition of varied concentrations of Pb(NO$_3$)$_2$. Determination of dissociation constant was assessed from titration curve of Pb$^{2+}$ with probe 1 (5 µM) and calculated using one-site binding model on GraphPad Prism version 5.
Fig. S13 Absorption spectra of probe 1 (1 µM) upon addition of different concentrations of Pb$^{2+}$ (0.5 – 5 µM) in HEPES buffer (10 mM, pH 7.4, containing 1% acetonitrile) at 25 °C. Detection limit was determined to be 1 µM.

3. References