Electronic Supplementary Material (ESI) for Analyst
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Supporting Information for

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**,[1] **2**,[2] and **3**[1] 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_3CN. UV/Vis titration experiments were performed using 5 μM of probe **1** in CH_3CN/HEPES solution (1/99, v/v) with varying concentrations of the metal nitrate salts.

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2. More Spectroscopy Data

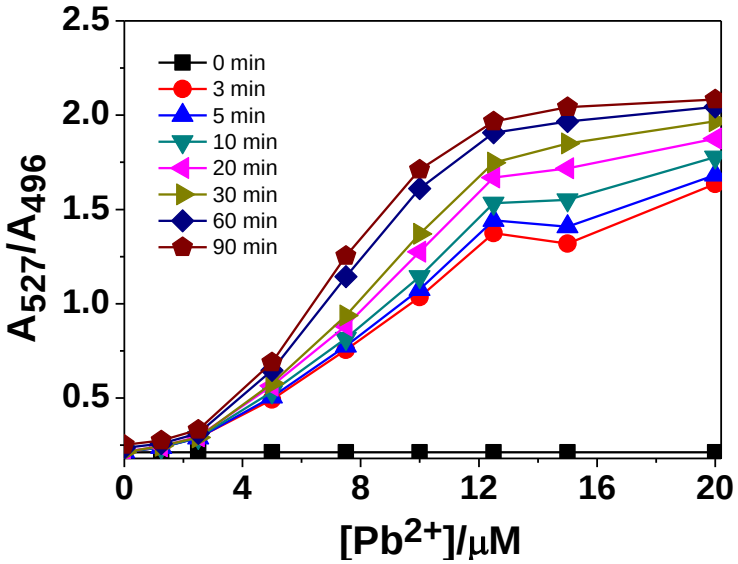

Fig. S1 Absorption ratio (A_{527}/A_{496}) of probe **1** (5 μM) upon addition of varied concentrations of $Pb(NO_3)_2$. Incubation time = from bottom to top: 0, 3, 5, 10, 20, 30, 60, 90 min. All data were obtained in HEPES buffer (10 mM, pH 7.4, 1% CH_3CN) at 25 ^oC.

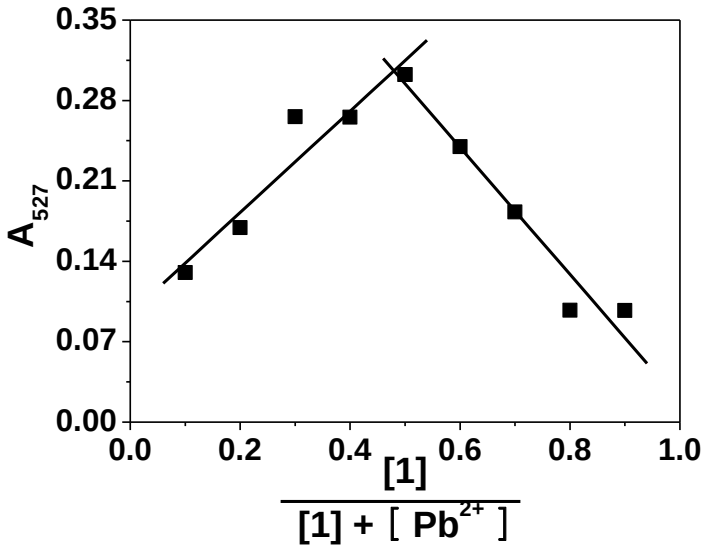

Fig. S2 Job's plot of a 1:1 complex of **1** and Pb^{2+}, where the absorbance at 527 nm is plotted against the mole fraction of **1** at an invariant total concentration of 40 μM in HEPES buffer (10 mM, pH 7.4) containing 1% CH_3CN.

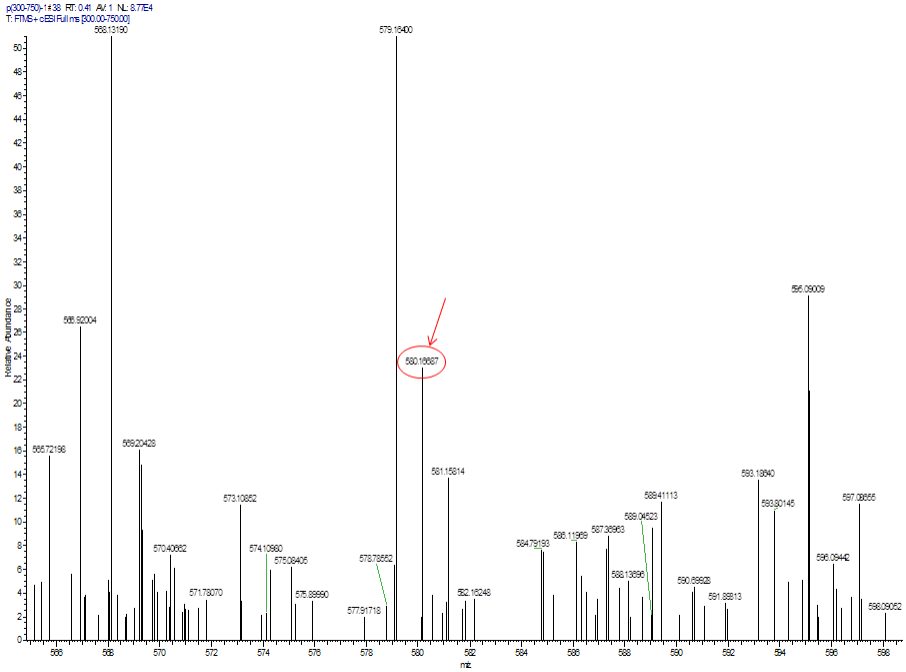

Fig. S3 ESI-MS spectrum of **1**-Pb^{2+} complex.

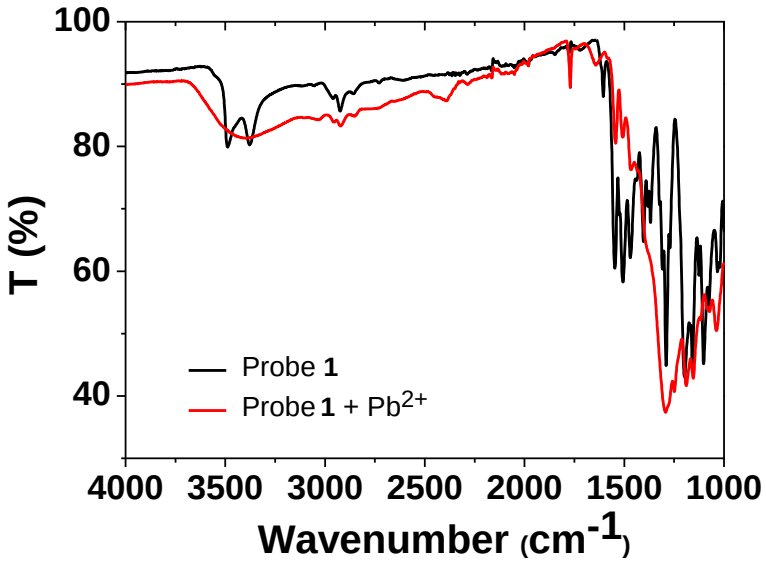

Fig. S4 Infrared spectra of **1** and **1**-Pb(II) adduct.

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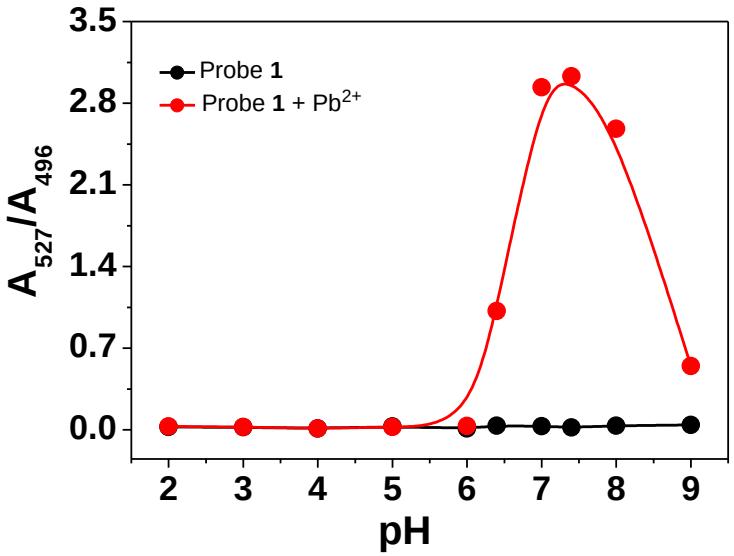

Fig. S5 Absorption ratio (527 over 496 nm) of **1** (5 μM) and **1** treated with Pb(II) ions (4 equiv.) in different pH buffer systems containing 1% CH_3CN as a cosolvent at 25 ^oC. Incubation time is 30 min.

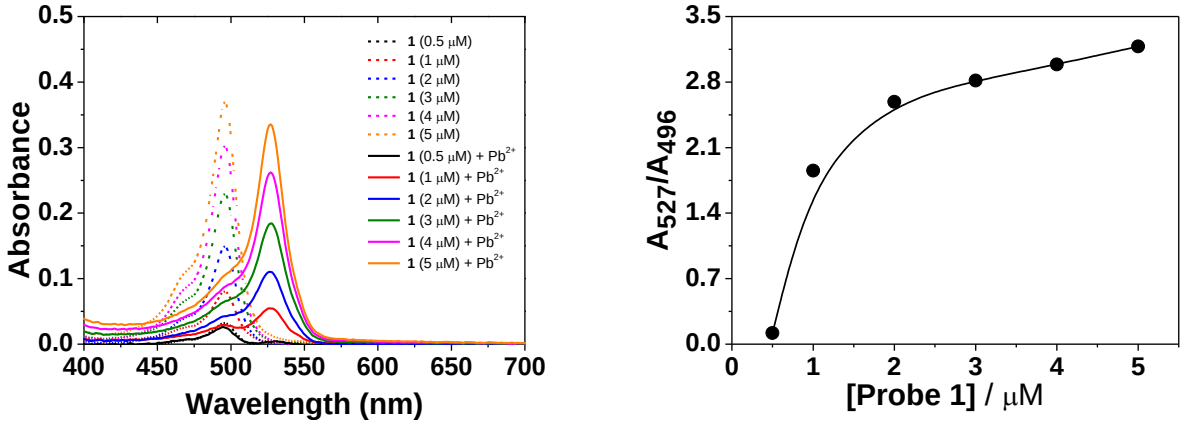

Fig. S6 Absorption spectra of probe **1** (0.5 - 5 μM) upon addition of corresponding 4 equiv. of Pb^{2+} in HEPES buffer (10 mM, pH 7.4, containing 1% acetonitrile) at 25 ^oC.

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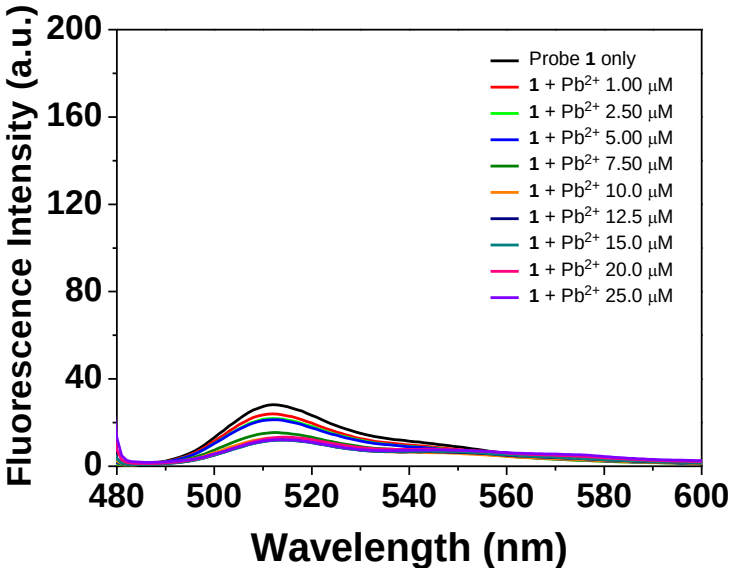

Fig. S7 Fluorescence emission spectra of **1** (5 μM) in the presence of various concentrations of Pb^{2+} (Excited at 460 nm). All spectra were taken at 30 min in HEPES buffer (10 mM, pH 7.4, 1% CH_3CN) at 25 ^{o}C.

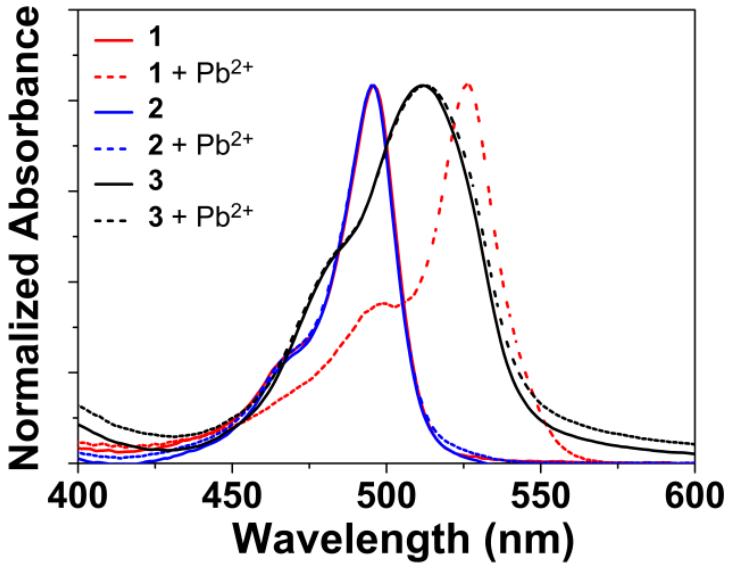

Fig. S8 Normalized UV-visible spectra of compounds **1**–**3** (5 μM) upon addition of 4 equiv. of $Pb(NO_3)_2$. All data were taken at 30 min in HEPES buffer (10 mM, pH 7.4, 1% CH_3CN) at 25 °C.

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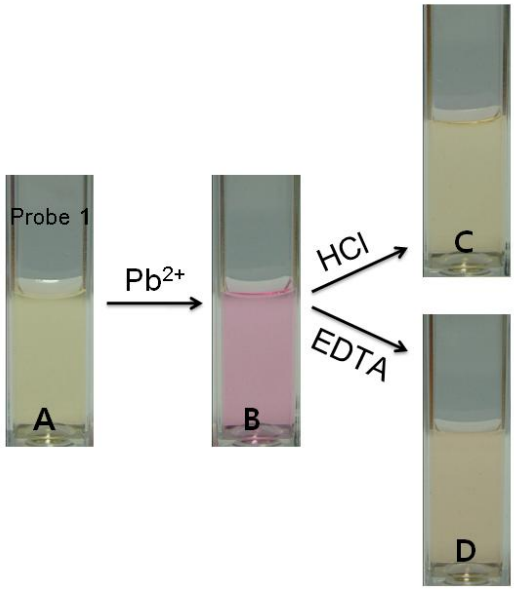

Fig. S9 Color change of probe **1** in the absence (a) and presence (b) of $Pb(NO_3)_2$. Subsequently, either HCl (c) or EDTA (d) was added to the **1**-Pb(II) adduct.

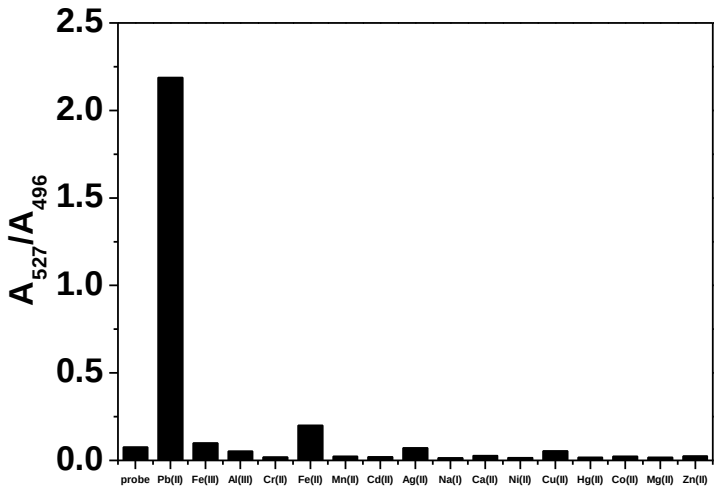

Fig. S10 Absorption ratio (527 over 496 nm) of **1** (5 μM) upon addition of different metal ions (4 equiv.) in HEPES buffer (10 mM, pH 7.4, 1% CH_3CN, 25 °C). All data were measured at 30 min after addition of each metal ion.

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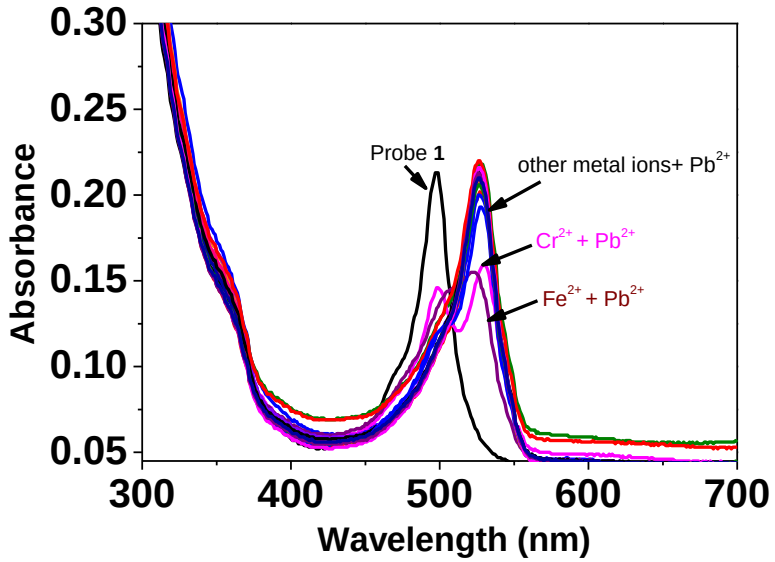

Fig. S11 Absorption spectra of probe **1** upon addition of different metal ions (4 equiv.) and subsequent addition of Pb(II) ions (4 equiv.) to each mixture.

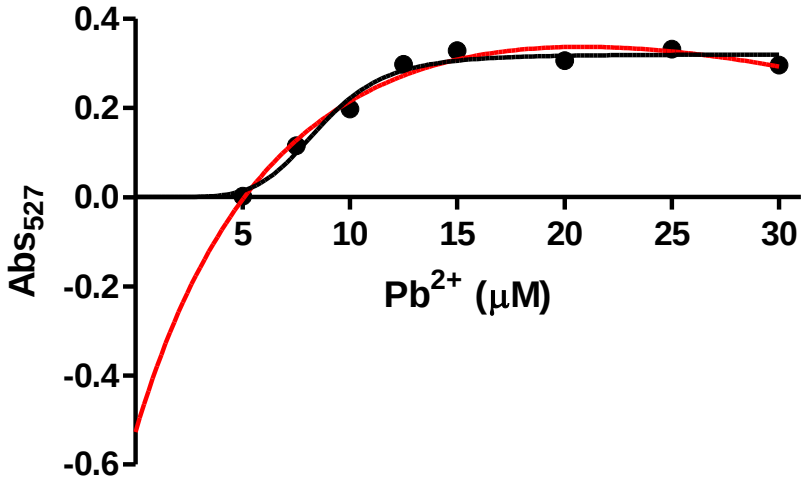

Fig. S12 Absorbance at A_{527} of probe **1** (5 μM) upon addition of varied concentrations of $Pb(NO_3)_2$. Determination of dissociation constant was assessed from titration curve of Pb^{2+} with probe **1** (5 μM) and calculated using one-site binding model on GraphPad Prism version 5.

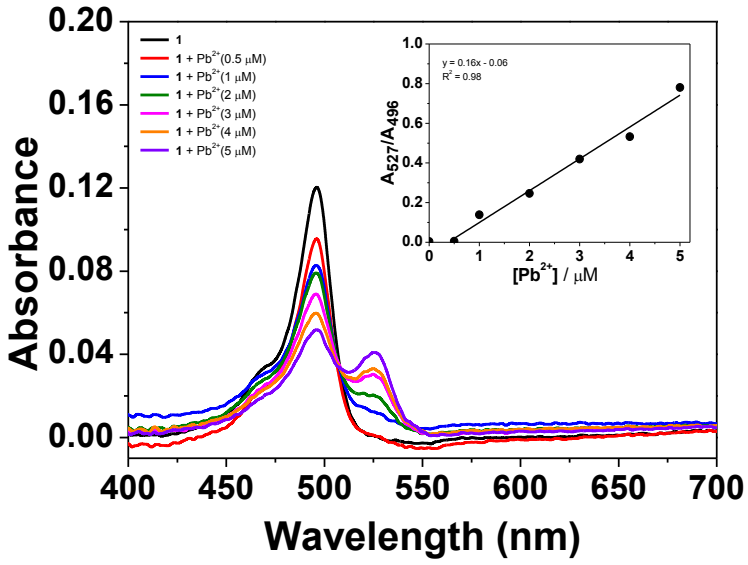

Fig. S13 Absorption spectra of probe **1** (1 μM) upon addition of different concentrations of Pb^{2+} (0.5 – 5 μM) in HEPES buffer (10 mM, pH 7.4, containing 1% acetonitrile) at 25 ^{o}C. Detection limit was determined to be 1 μM.

3. References

1. T.-I. Kim, J. Park, S. Park, Y. Choi and Y. Kim, *Chem. Commun.*, 2011, **47**, 12640.
2. J.-Y. Liu, H.-S. Yeung, W. Xu, X. Li and D. K. P. Ng, *Org. Lett.*, 2008, **10 (23)**, 5421.