Electronic Supplementary Material (ESI) for RSC Advances. This journal is © The Royal Society of Chemistry 2017

Supporting information for

A rhodamine-based chemosensor with diphenylselenium for highly selective fluorescent turn-on detection of Hg^{2+} *in vitro* and *in vivo*

Parthiban Venkatesan, Natesan Thirumalivasan and Shu-Pao Wu*

Department of Applied Chemistry, National Chiao Tung University, Hsinchu 300, Taiwan

*Corresponding author. Tel.: +886-3-5712121-ext56506; Fax: +886-3-5723764 E-mail: <u>spwu@mail.nctu.edu.tw</u>

Contents

- 1. Figure S1. ¹H NMR (300 MHz, DMSO) spectrum of RhoSe
- 2. Figure S2. ¹³C NMR (300 MHz, DMSO) spectrum of RhoSe
- 3. Figure S3. LR ESI⁺ Mass spectrum of RhoSe
- 4. Figure S4. HR ESI⁺ Mass spectrum of **RhoSe**
- **5.** Figure S5. Detection limit for titration of Hg^{2+} (0~3 equiv. respectively) against ratio of fluorescence response for **RhoSe** (10µM) in CH₃OH/H₂O (v/v = 9:1) solution. The excitation wavelength was 510 nm.
- 6. Figure S6. Binding constant for titration of Hg^{2+} (0 to 3.0 eq) against ratio of fluorescence response for (a) RhoSe (10 μ M) in CH₃OH/H₂O (v/v = 9:1) solution. The excitation wavelength was 510 nm.
- 7. Figure S7. Mass Spectrum of RhoSe-Hg²⁺ Complex
- 8. Figure S8. Job plot of the RhoSe-Hg²⁺ complex in CH₃OH/H₂O (v/v = 9:1) solution. The total concentration of RhoSe and Hg²⁺ was 50 μ M. The excitation wavelength was 510 nm.
- 9. Figure S9. HOMO and LUMO levels of RhoSe and RhoSe-Hg²⁺.
- **10. Figure S10.** Strip methods of (a) Color change and (b) fluorescence changes of **RhoSe** (1mM) after addition of various metal ions.
- 11. Figure S11. Cell viability values (%) estimated by an MTT assay versus incubation concentrations of **RhoSe**. HeLa cells were cultured in the presence of **RhoSe** (0–25 μ M) at 37 °C for 24 h.



Figure S1. ¹H NMR (300 MHz, DMSO) spectrum of RhoSe



Figure S2. ¹³C NMR (300 MHz, DMSO) spectrum of RhoSe



Figure S3. LR ESI⁺ Mass spectrum of RhoSe



Figure S4. HR ESI⁺ Mass spectrum of RhoSe



Figure S5. Detection limit for titration of Hg^{2+} (0~1 equiv. respectively) against ratio of fluorescence response for **RhoSe** (10µM) in CH₃OH/H₂O (v/v = 9:1) solution. The excitation wavelength was 510 nm.



Figure S6. Job plot of the **RhoSe-Hg²⁺** complex in CH₃OH/H₂O (v/v = 9:1) solution. The total concentration of **RhoSe** and Hg²⁺ was 50 μ M. The excitation wavelength was 510 nm.



Figure S7. Mass spectrum of RhoSe-Hg²⁺ complex



Figure S8. Binding constant for titration of Hg^{2+} (0 to 3.0 eq) against ratio of fluorescence response for **RhoSe** (10 μ M) in CH₃OH/H₂O (v/v = 9:1) solution. The excitation wavelength was 510 nm.



Figure S9. HOMO and LUMO levels of RhoSe and RhoSe-Hg²⁺.

Rho Se	Ag+	Al ³⁺ C	'd ²⁺	Co ²⁺ Ct	1 ²⁺ C	r 3+	Fe ²⁺ F	e ³⁺	Hg²+	Mg ²⁺	Mn ²⁺	Ni ²⁺	Pb ²⁺	Zn ²⁺
Rho Se	Ag+	Al ³⁺	Cd ²⁺	C0 ²⁺	Cu ²⁺	Cr ³⁺	Fe ²⁺	Fe ³⁺	Hg ²⁺	Mg ²⁺	Mn ²⁺	Ni ²⁺	Pb ²⁺	Zn ²⁺

Figure S10. Strip methods of (a) color change and (b) fluorescence changes of **RhoSe** (1mM) after addition of various metal ions



Figure S11. Cell viability values (%) estimated by an MTT assay versus incubation concentrations of **RhoSe**. HeLa cells were cultured in the presence of **RhoSe** (0–25 μ M) at 37 ^oC for 24 h.