Electronic Supplementary Information

Highly selective fluorescent probe for detection and visualization of palladium ions in mixed aqueous media

Manoj Kumar,* Naresh Kumar and Vandana Bhalla

Department of Chemistry, UGC Sponsored Centre for Advanced Studies-1, Guru Nanak Dev University, Amritsar-143005, Punjab, India. Email: <u>mksharmaa@yahoo.co.in</u>

- **S2** UV-vis spectra of **1** in the presence of different metal ions.
- **S3** Fluorescence spectra of **1** in the presence of different metal ions.
- S4 Competitive fluorescence response of 1 with Pd²⁺ ions in the presence of Cys and Hcy.
- **S5** Calculations for the detection limit.
- **S6** ¹H NMR spectrum of compound **1**(Full Scale).
- **S7** ¹H NMR spectrum of compound **1**(Expanded).
- **S8** ¹³C NMR spectrum of compound **1**.
- **S9** Mass spectrum of receptor **1**.



Figure S1 UV-vis spectra of **1** (5 μ M) in H₂O:CH₃CN (1:1, v/v) buffered with HEPES, pH = 7.2; in the presence of various metal ions (50 equiv each).



Figure S2 Fluorescence response of **1** (5 μ M) in H₂O:CH₃CN (1:1, v/v) buffered with HEPES, pH = 7.2; at 25 °C; $\lambda_{ex} = 310$ nm in the presence different of metal ions (50 equiv each). Data were given after 3 hour with the appropriate metal ions at 25 °C.



Figure S3 Fluorescence response of **1** (5 μ M) in H₂O:CH₃CN (1:1, v/v) buffered with HEPES, pH = 7.2; at 25 °C; $\lambda_{ex} = 310$ nm with Pd²⁺ ions (50 equiv) in the presence of Cys and Hcy (50 equiv each). Data were given after 3 hour with the appropriate analyte.



Calculations for detection limit:

Figure S5 Figure showing the fluorescence intensity at 372 nm as a function of Pd^{2+} ions concentration.

To determine the detection limit,¹ fluorescence titration of compound **1** with palladium ions was carried out by adding aliquots of palladium solution of minimum concentration and the fluorescence intensity as a function of Pd^{2+} ions added was then plotted.

Equation used for calculating detection limit (DL):

$$DL = C_L \times E_T$$

 C_L = Conc. of Ligand; E_T = Equiv. of Titrant at which change observed.

Thus;

DL = $5 \times 10^{-6} \times 0.008 = 0.04 \times 10^{-6} = 4 \times 10^{-8}$ or

 $= 40 \times 10^{-9} = 40$ nanomolar

¹ G. L. Long and J. D. Winefordner, Anal. Chem., 1983, 55, 712A.

¹H NMR (CDCl₃, 300 MHz, ppm) spectrum of **1** (Full Scale)



¹H NMR (CDCl₃, 300 MHz, ppm) spectrum of **1** (Expanded)



¹³C NMR (CDCl₃, 300 MHz, ppm) spectrum of **1**



Mass spectrum of 1

