

Supporting Information

Facile Synthesis of Rhodamine-Based Highly Sensitive and Fast Responsive Colorimetric and Off-On Fluorescent Reversible Chemosensors for Hg²⁺: Preparation of a Fluorescent Thin Film Sensor

Chatthai Kaewtong,^{*a} Banchob Wannoo,^a Yuwaporn Uppa,^b Nongnit Morakot,^a
Buncha Pulpoka^c and Thawatchai Tuntulani^c

^a*Supramolecular Chemistry Research Unit, Department of Chemistry and Center of Excellence for Innovation in Chemistry, Faculty of Science, Mahasarakham University, Mahasarakham, 44150, Thailand.*

^b*Department of Chemistry, Faculty of Engineering, Rajamangala University of Technology Isan Khon Kaen Campus, Khonkaen 40000, Thailand.*

^c*Supramolecular Chemistry Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand.*

kchatthai@gmail.com

Contents

Figure S1. Fluorescence spectral changes of L1 after the addition of 5 equiv of various cations.	S3
Figure S2. FT-IR spectra of L2 , L2 ⊃ Hg ²⁺ and L2 ⊃ Hg ²⁺ after treatment with dilute NaOH.	S4
Figure S3. The B3LYP/LanL2DZ level-computed molecular orbitals contoured, HOMOs (Down) and LUMOs (Up) at an iso-surface value of 0.05 a.u. for L1 • Hg ²⁺ , L2 • Hg ²⁺ , L3 • Hg ²⁺ and L4 • Hg ²⁺	S4
Figure S4. ¹ H NMR spectrum of <i>N</i> -(rhodamine B)lactam-ethylenediamine (L1).	S5
Figure S5. ¹ H NMR spectrum of <i>N</i> -(rhodamine B)lactam-diethylenetriamine (L2).	S5
Figure S6. ¹ H NMR spectrum of <i>N</i> -(rhodamine B)lactam-triethylenetetramine (L3).	S6
Figure S7. ¹ H NMR spectrum of <i>N</i> -(rhodamine B)lactam-tetraethylenepentamine (L4).	S6

Experimental General methods

NMR spectra were recorded on a Varian 400 MHz spectrometer in deuterated chloroform and DMSO- d_6 . MALDI-TOF mass spectra were recorded on a Biflex Bruker Mass spectrometer using 2-cyano-4-hydroxycinnamic acid (CCA) or 2,5-dihydroxy-benzoic acid (DHB) as the matrix. ESI-Mass spectra were recorded on a Bruker Daltonics microTOF. UV-vis absorption measurements were performed on a Perkin Elmer Lambda 25 UV/VIS spectrometer. Fluorescent spectra were recorded using a Perkin Elmer luminescence spectrometer LS50B. Infrared spectra were obtained on a Nicolet Impact 410 using KBr pellet. Column chromatography was carried out using silica gel (Kieselgel 60, 0.063 – 0.200 mm, Merck). All reagents were standard analytical grade and used without further purification.

Commercial grade solvents, such as acetone, hexane, dichloromethane, methanol and ethyl acetate, were distilled before use. MeCN was dried over CaH_2 and freshly distilled under a nitrogen atmosphere prior to use.

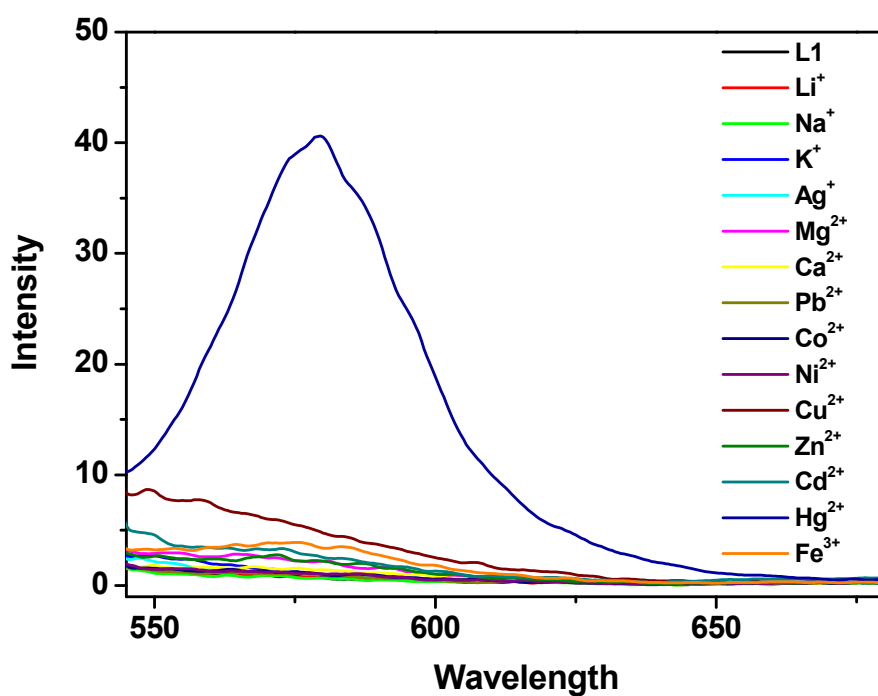


Figure S1. Fluorescence spectral changes of L1 after the addition of 5 equiv of various cations.

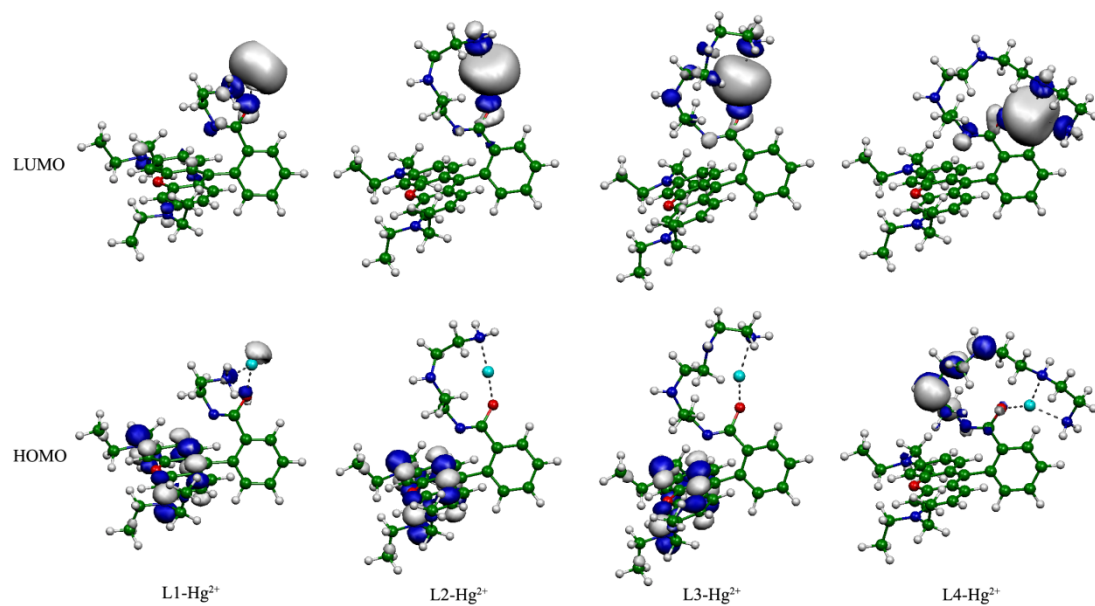


Figure S2. The B3LYP/LanL2DZ level-computed molecular orbitals contoured, HOMOs (Down) and LUMOs (Up) at an iso-surface value of 0.05 a.u. for **L1•Hg²⁺**, **L2•Hg²⁺**, **L3•Hg²⁺** and **L4•Hg²⁺**.

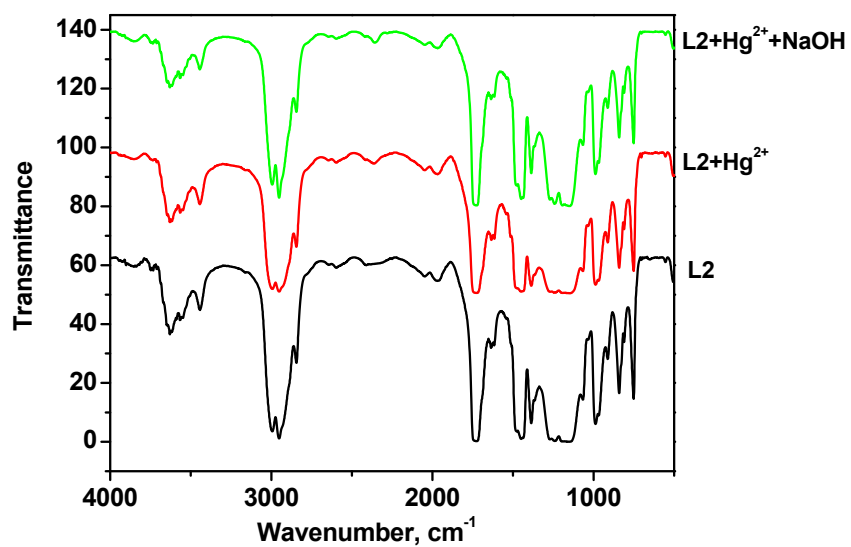


Figure S3 FT-IR spectra of **L2**, **L2•Hg²⁺** and **L2•Hg²⁺** after treatment with dilute NaOH.

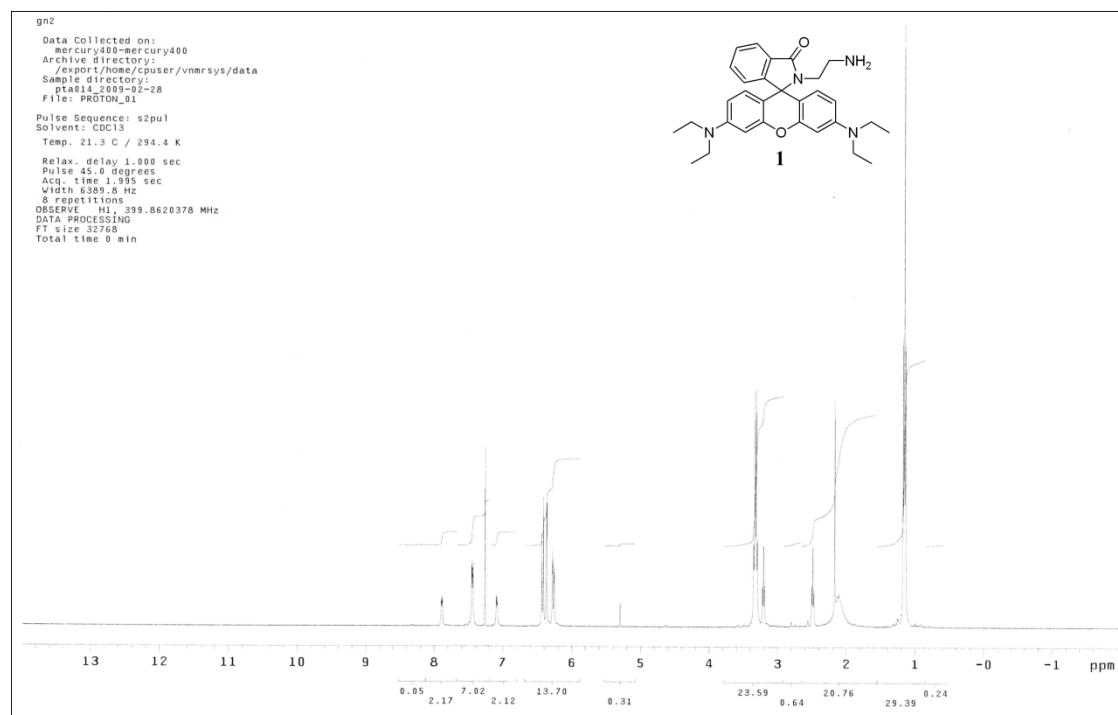


Figure S4. ^1H NMR spectrum of *N*-(rhodamine B)lactam-ethylenediamine (**L1**).

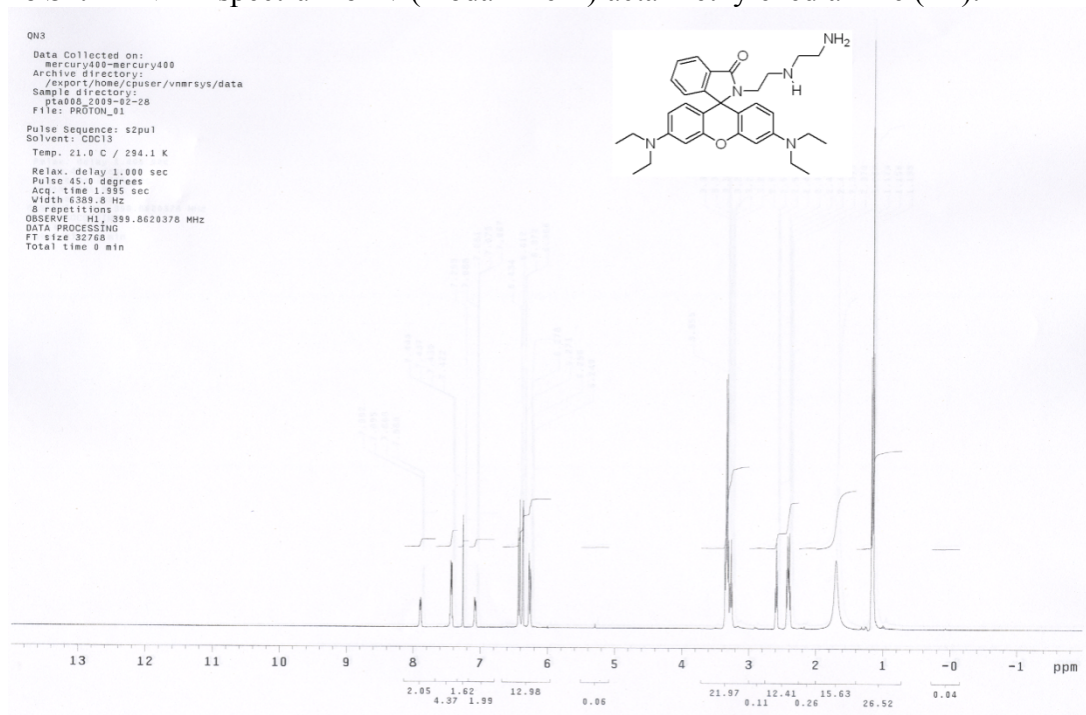


Figure S5. ^1H NMR spectrum of *N*-(rhodamine B)lactam-diethylenetriamine (**L2**).

