Supporting Information

Title: A Reversible E_m-FRET Rhodamine-Based Chemosensor for Carboxylate Anions Using a Ditopic Receptor Strategy

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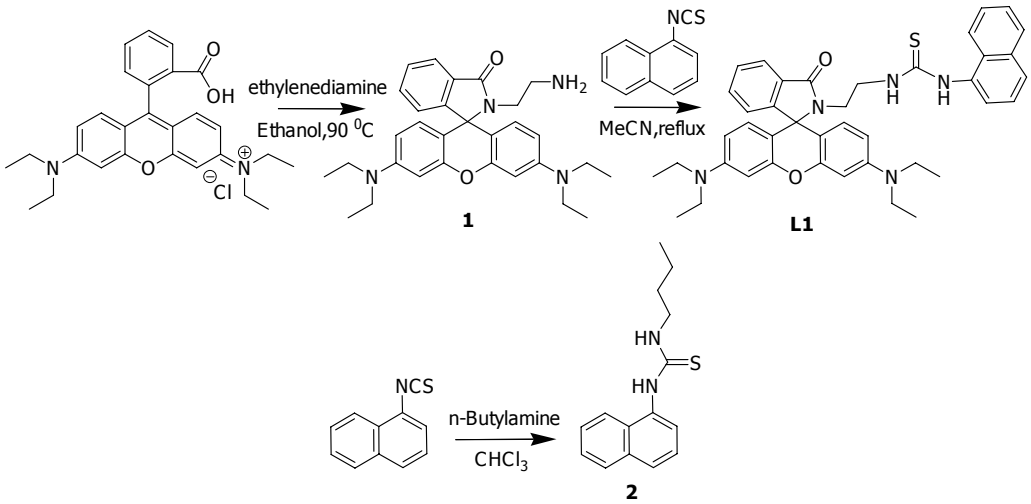


Scheme S1. Synthetic pathways of **L1** and **2**

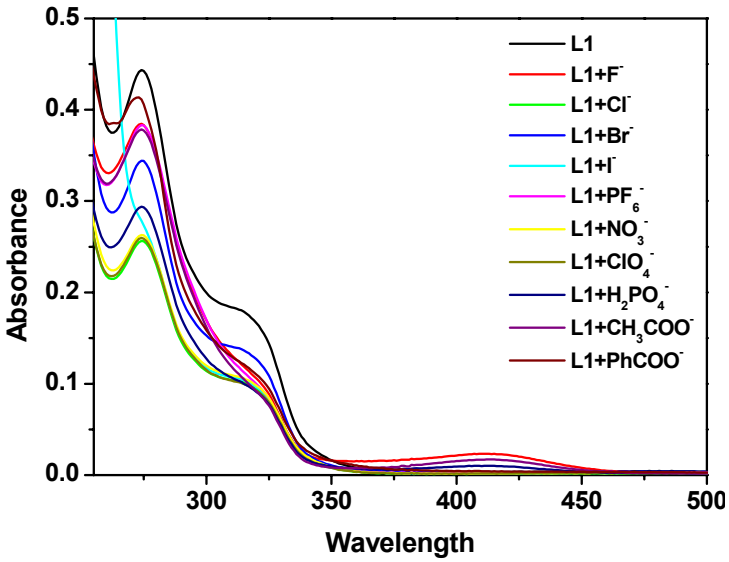


Fig. S1 UV-vis spectra of **L1** upon addition of various anions. Conditions: **L1** (10 μM) in MeCN, TBAX (30 equiv) in MeCN.

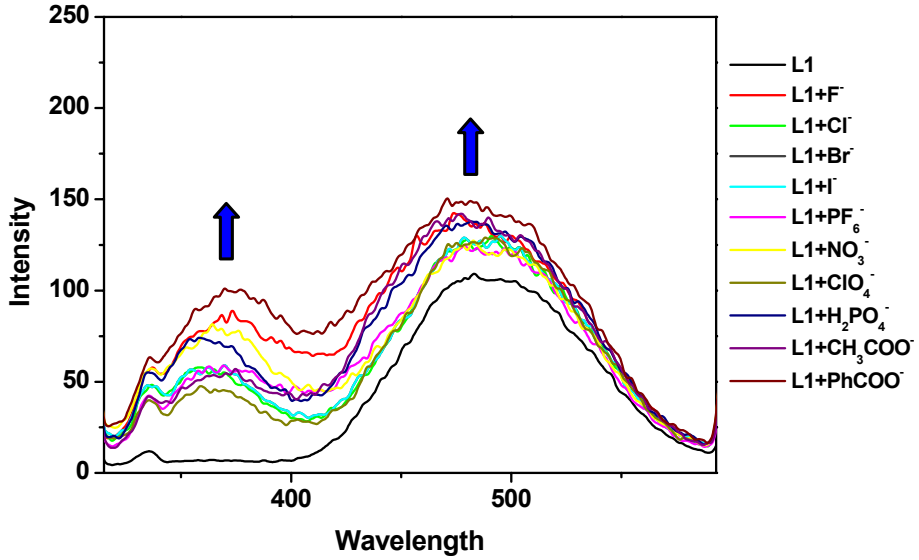
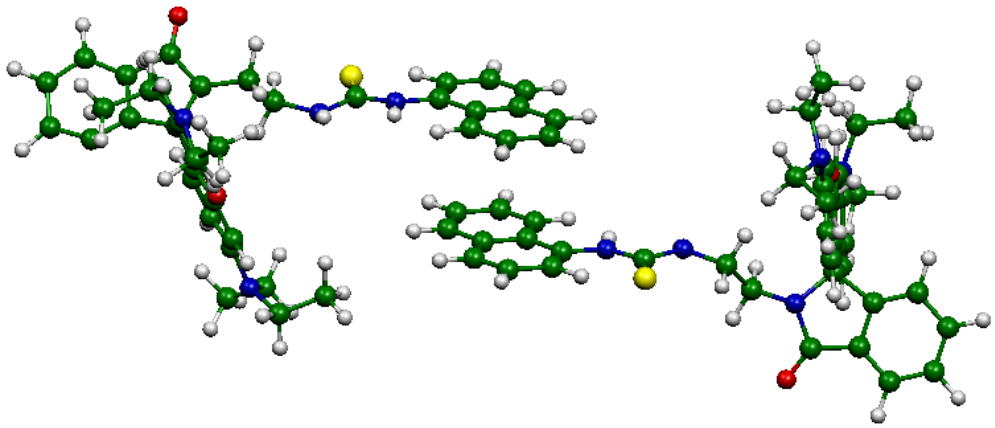


Fig. S2 Fluorescence emission spectra of **L1** upon addition of various anions. Conditions: **L1** (10 μM) in MeCN, excitation at 300 nm, TBAX (30 equiv) in MeCN.



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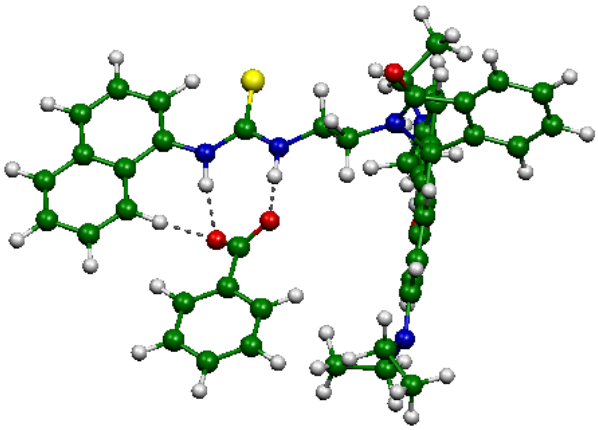
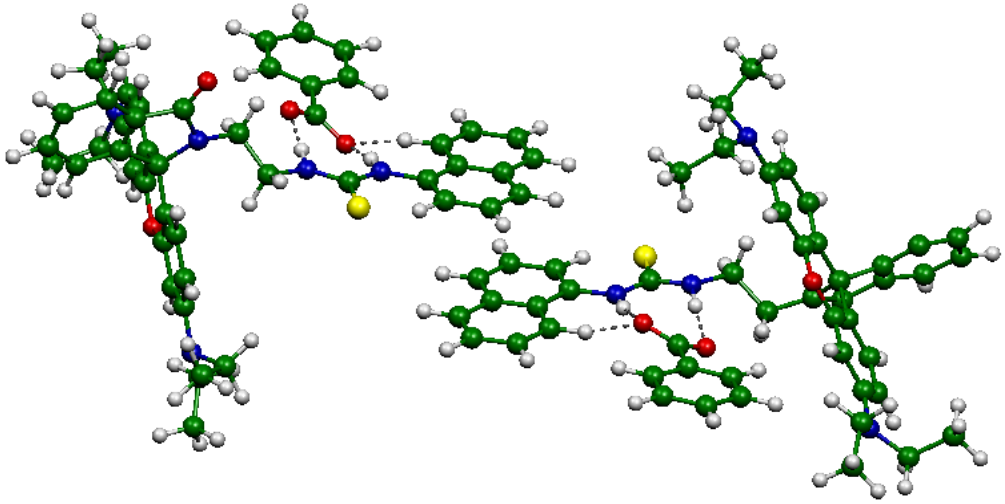


b)



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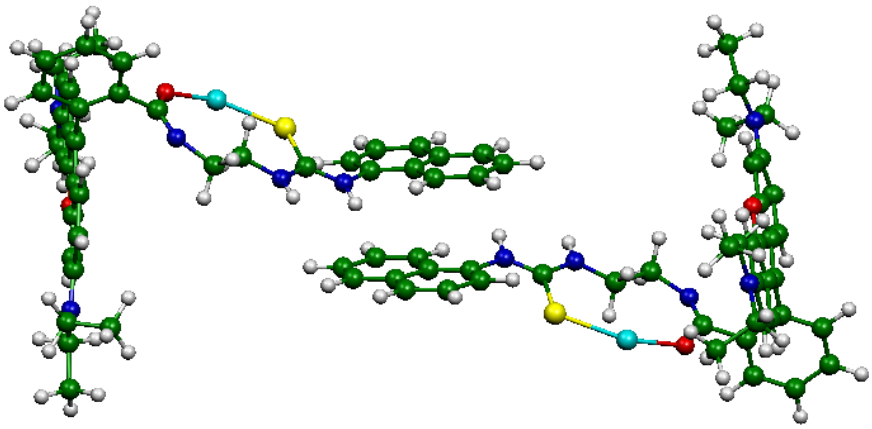

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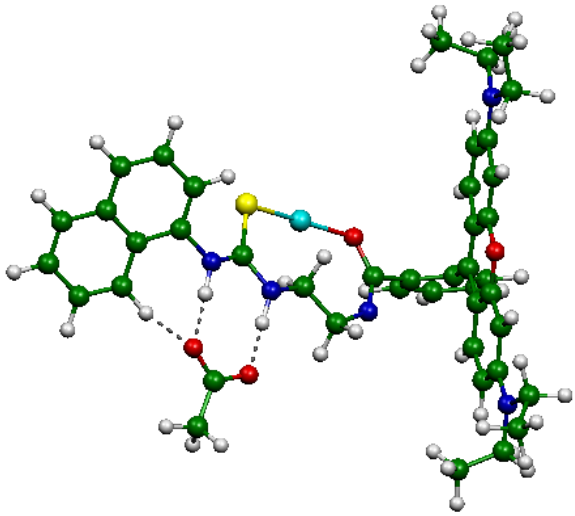

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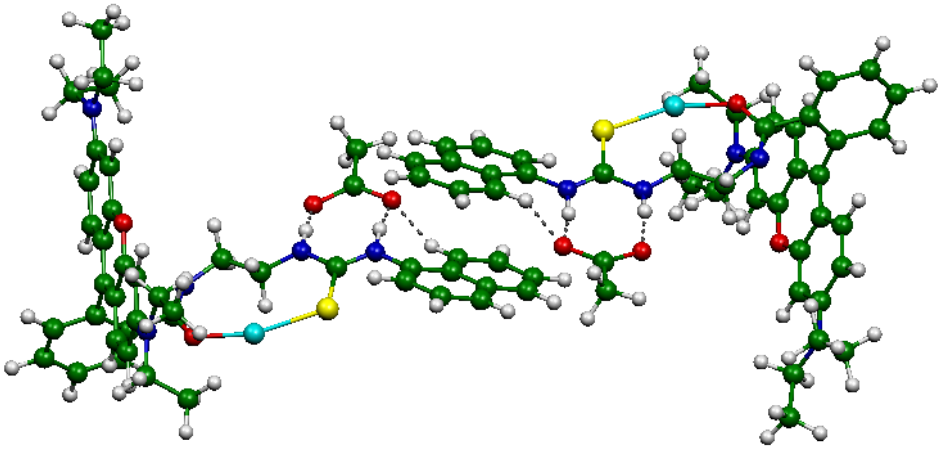

f)

Fig. S3 Proposed binding modes of (a) **L1**, (b) **L1**+$PhCOO^-$ (1:1), (c) **L1**+$PhCOO^-$ (2:2), (d) **L1**+Cu^{2+}, (e) **L1**·Cu^{2+}+CH_3COO^- (1:1), (f) **L1**·Cu^{2+}+CH_3COO^- (2:2) were generated with the MOLEKEL 4.3 program.[S1]

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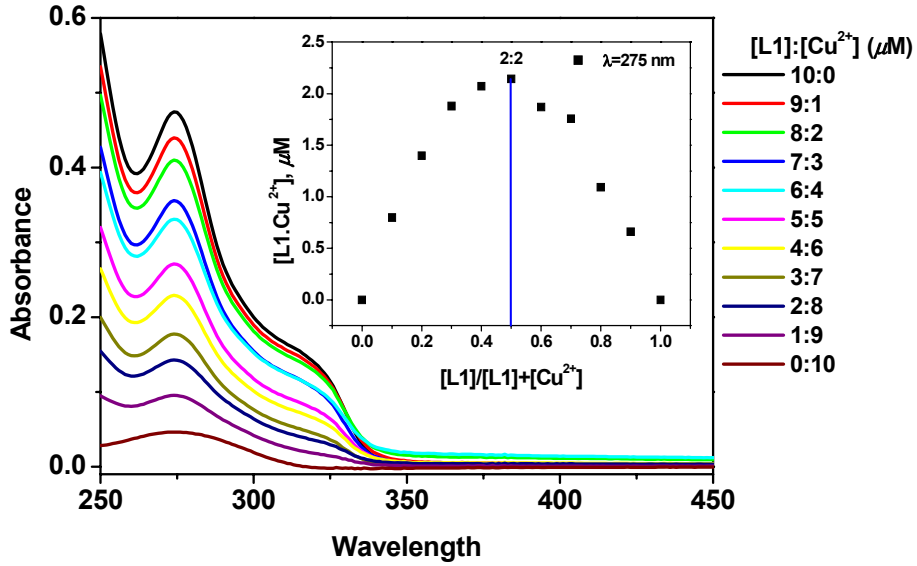

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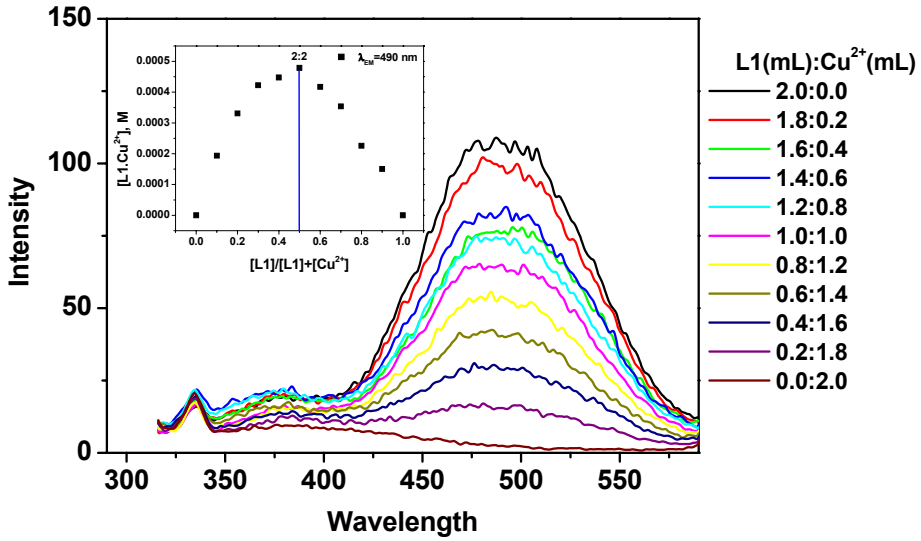
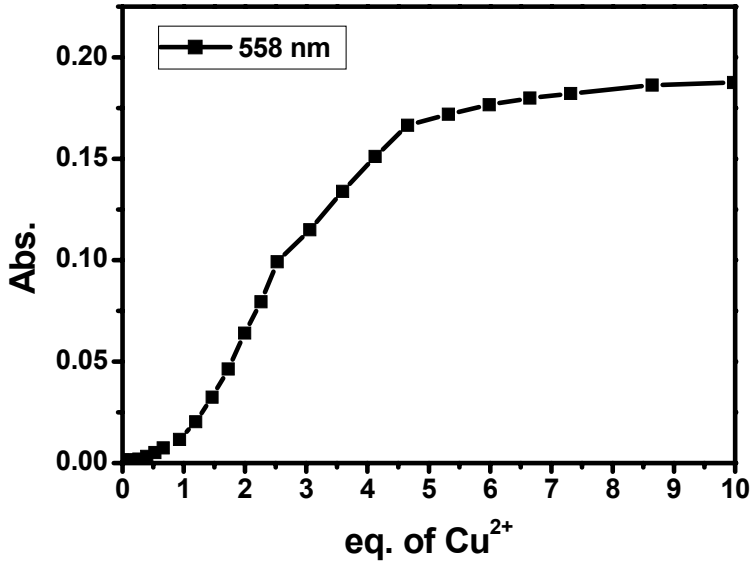


b)

Fig. S4 Job plot[S2] between receptor **L1** and various Cu^{2+} concentrations. The total concentration of **L1** + Cu^{2+} was kept constant at 10 μM. The complex concentration, [HG] was calculated by the equation; [HG] = $\Delta A/A_0$*[H]. (a) UV-vis spectra at 275 nm, (b) fluorescent spectra at 490 nm (λ_{ex} 300 nm).



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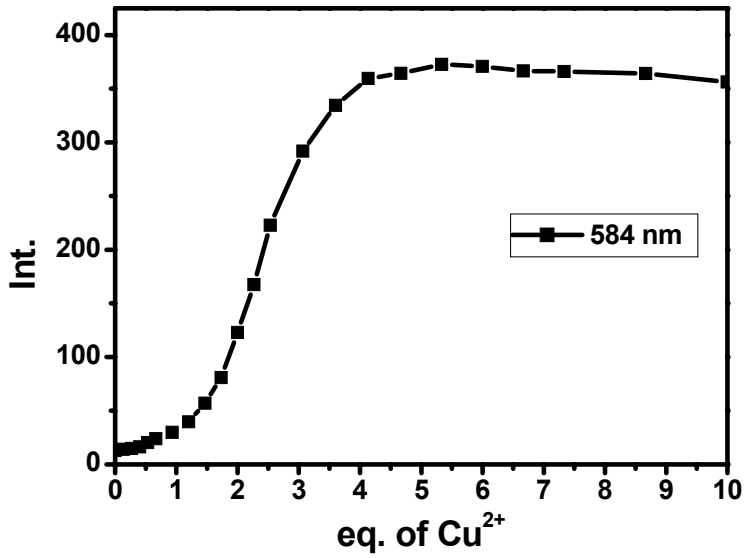
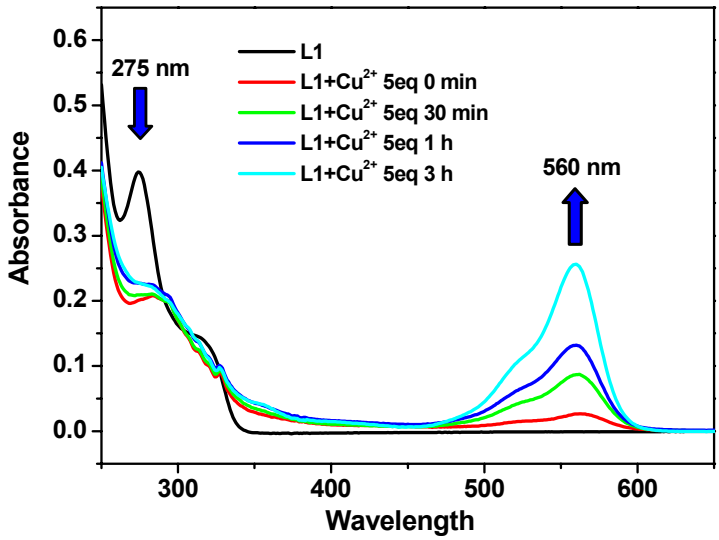


b)

Fig. S5 Mole ratio plots[S3] between receptor **L1** and various Cu^{2+} concentrations (equiv). (a) UV-vis spectra at 558 nm, (b) fluorescent spectra at 584 nm (λ_{ex} 300 nm).



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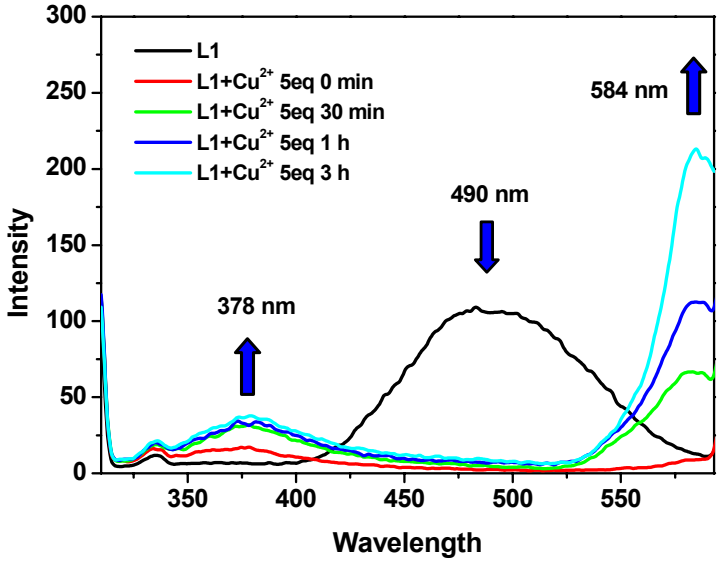

b)

Fig. S6 Time evolution of sensor **L1** (10 μM) in MeCN in the presence of 5.0 equiv. of Cu^{2+} ion. Spectra changes of UV-vis intensity at 275, 560 nm (a) and fluorescence intensity at 490 and 584 nm, λ_{ex} = 300 nm (b) as a function of time (0.0 to 3.0 h).

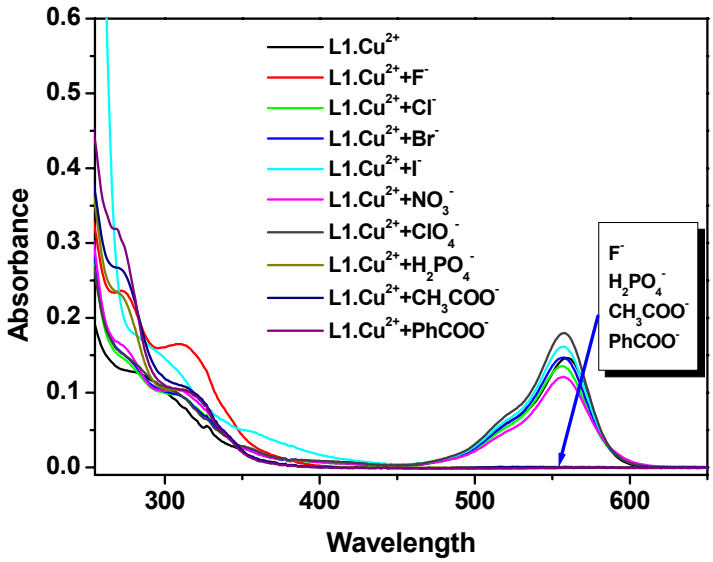

Fig. S7 UV-vis spectra excess of **L1•Cu**$^{2+}$ upon addition of various anions. Conditions: **L1•Cu**$^{2+}$ (10 μM) in MeCN, TBAX (30 equiv.) in MeCN.

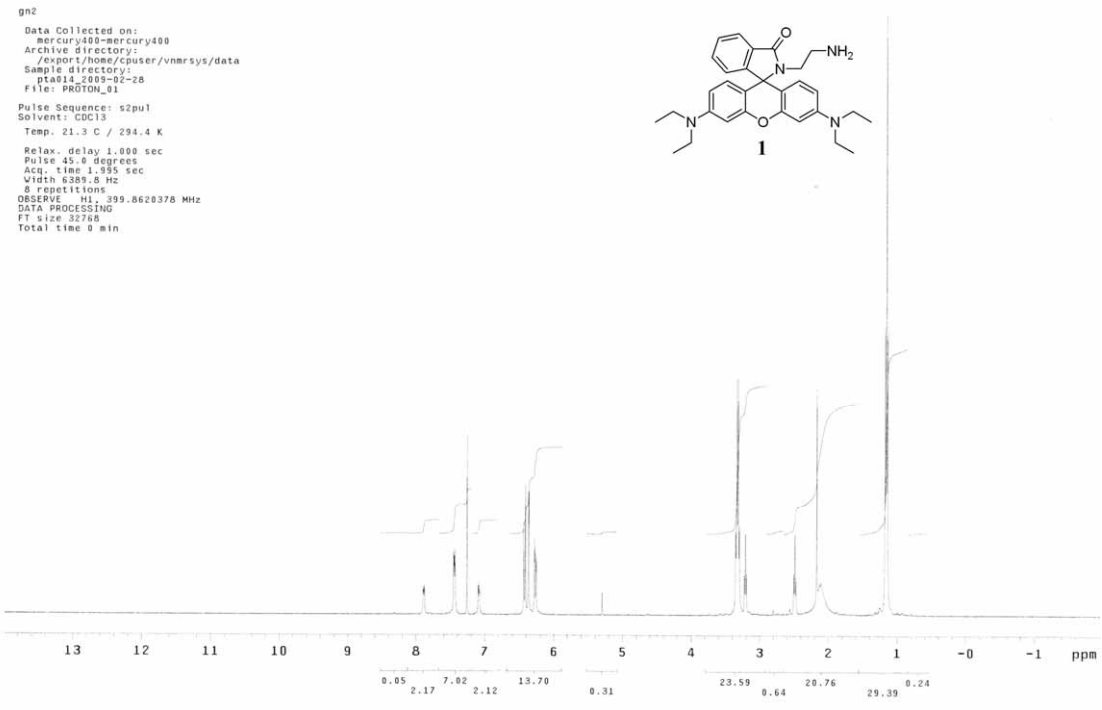

Fig. S8 ^{1}H NMR spectrum of *N*-(rhodamine B)lactam-ethylenediamine (**1**).

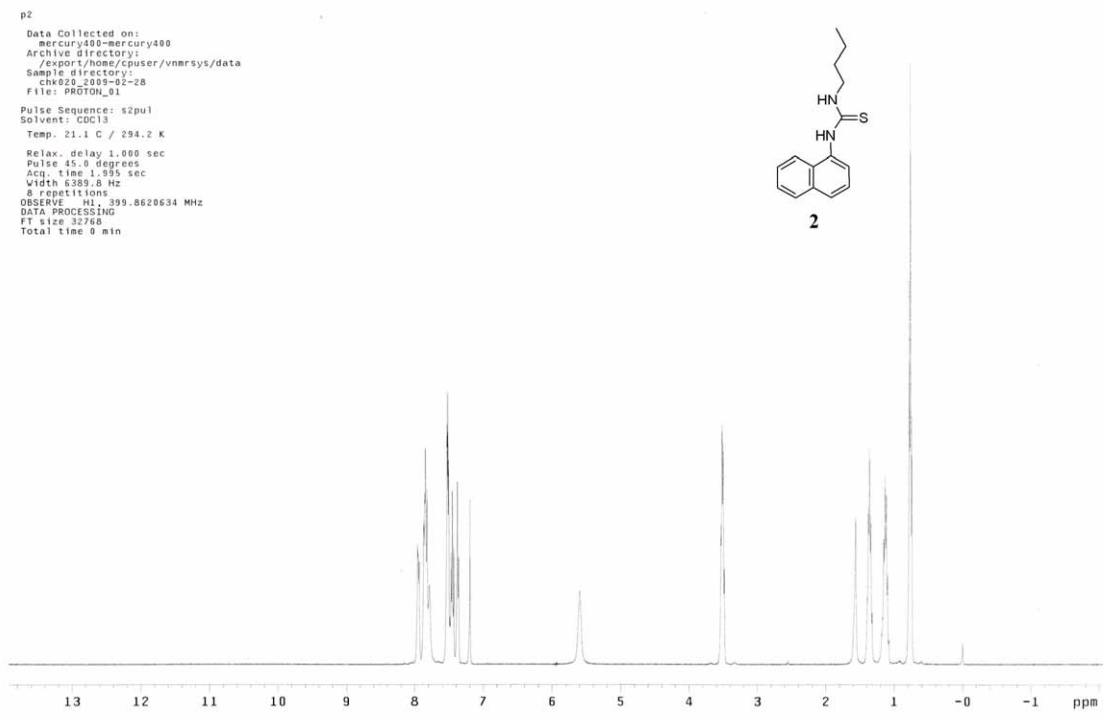

Fig. S9 ^{1}H NMR spectrum of 1-butyl-3-(naphthalen-1-yl)thiourea (**2**).

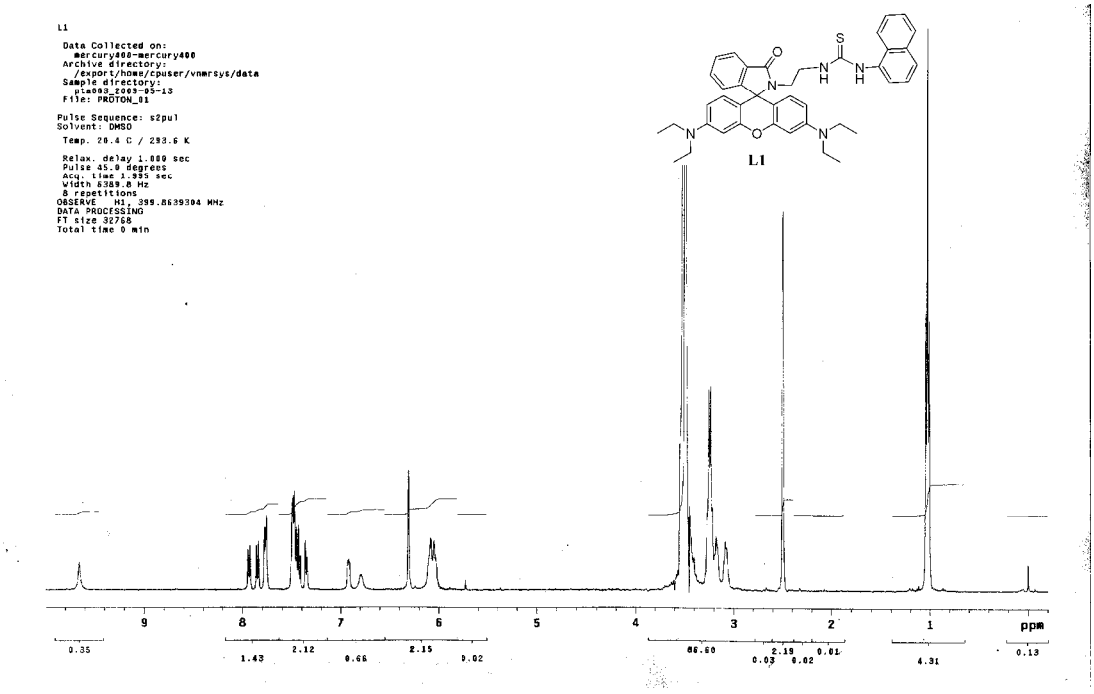

Fig. S10 ^{1}H NMR spectrum of *N*-(Rhodamine B)lactam-*N´*-naphthylthiourea-ethylenediamine (**L1**).

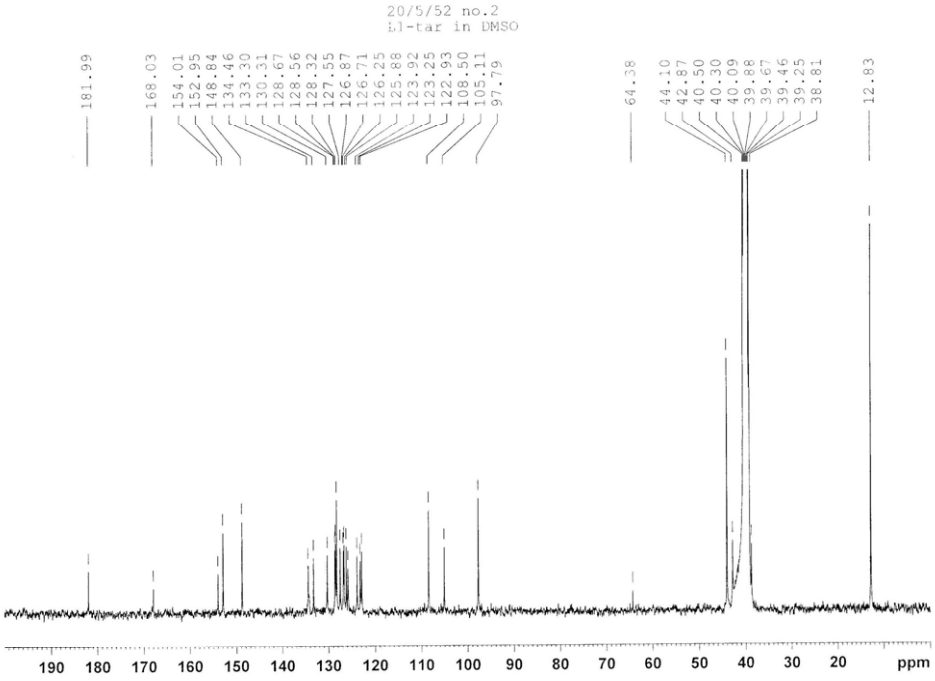

Fig. S11 ^{13}C NMR spectrum of *N*-(Rhodamine B)lactam-*N*′-naphthylthiourea-ethylenediamine (**L1**).

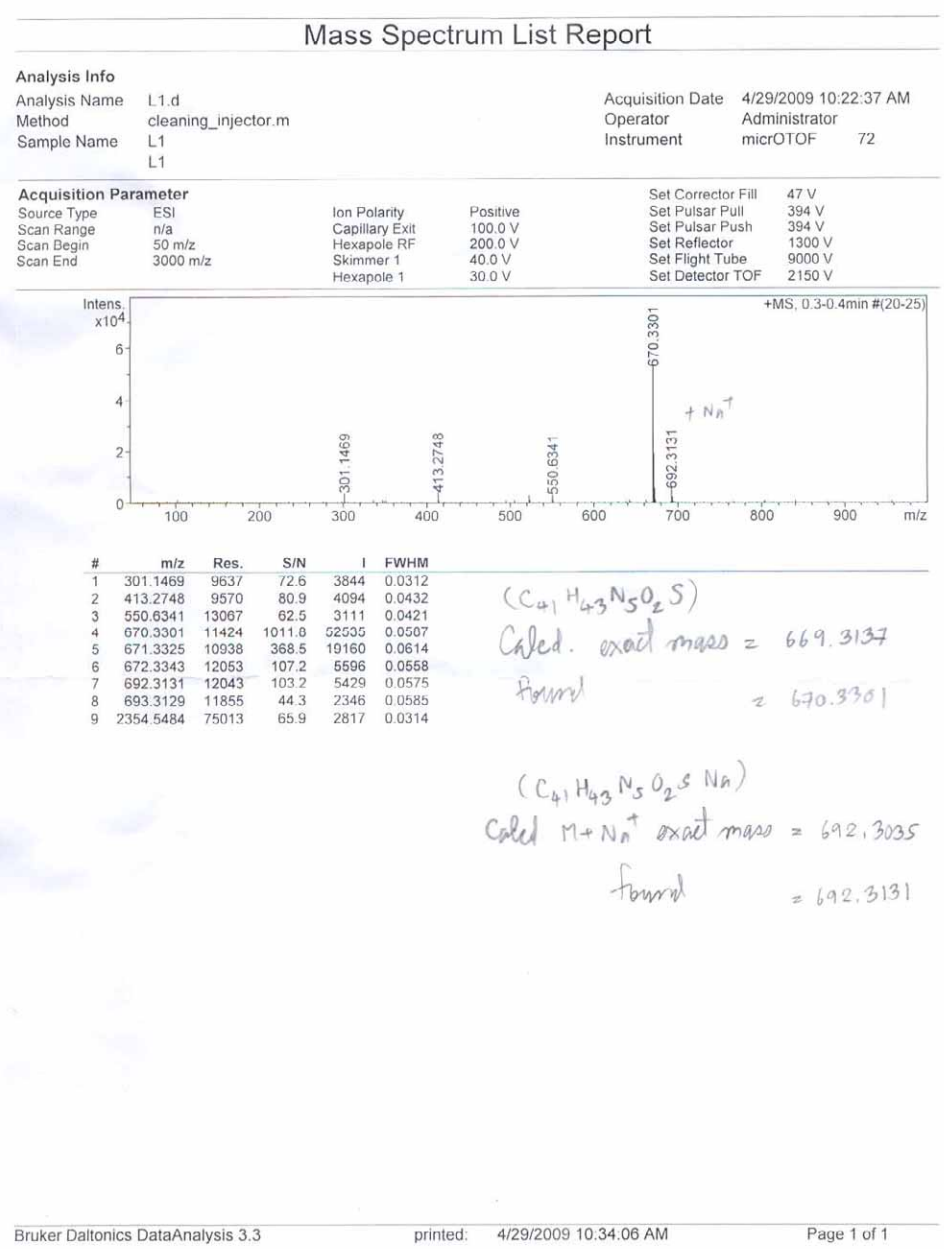

Fig. S12 ESI-Mass spectrum of *N*-(Rhodamine B)lactam-*N*′-naphthylthiourea-ethylenediamine (**L1**).

S1 P. P. Flükiger, H.P. Lüthi, S. Portmann, J. Weber, Swiss Center for Scientific Computing, Manno (Switzerland), 2000–2002, MOLEKEL 4.3

S2 P. Job, Ann. Chim., 1928, 9, 113.

S3 J. H. Yoe and A. E. Harvey, J. Am. Chem. Soc., 1948, 70, 648.