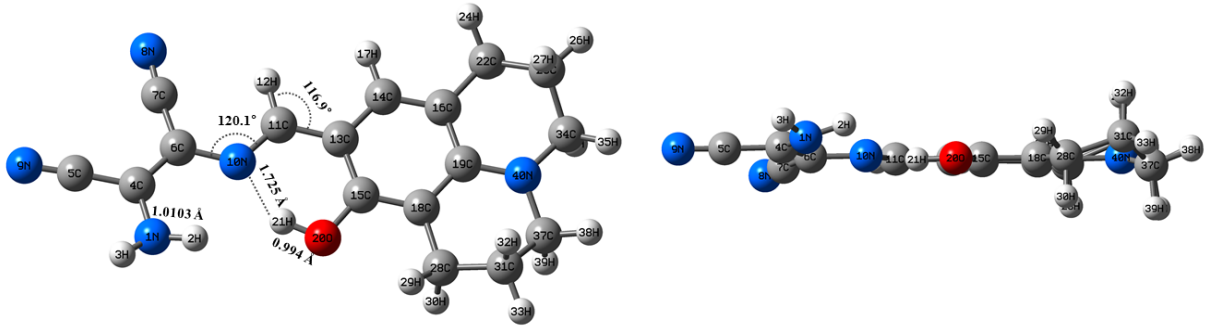
Supporting information

A diaminomaleonitrile based selective colorimetric chemosensor for copper(II) and fluoride ions

Tae Geun Jo, Yu Jeong Na,* Jae Jun Lee, Myoung Mi Lee, Sun Young Lee, Cheal Kim*

[a]Department of Fine Chemistry and Department of Interdisciplinary Bio IT Materials, Seoul National University of Science and Technology, Seoul 139-743, Korea. Fax: +82-2-973-9149; Tel: +82-2-970-6693; E-mail: meureen@hanmail.net and chealkim@seoultech.ac.kr

(a)



(b)

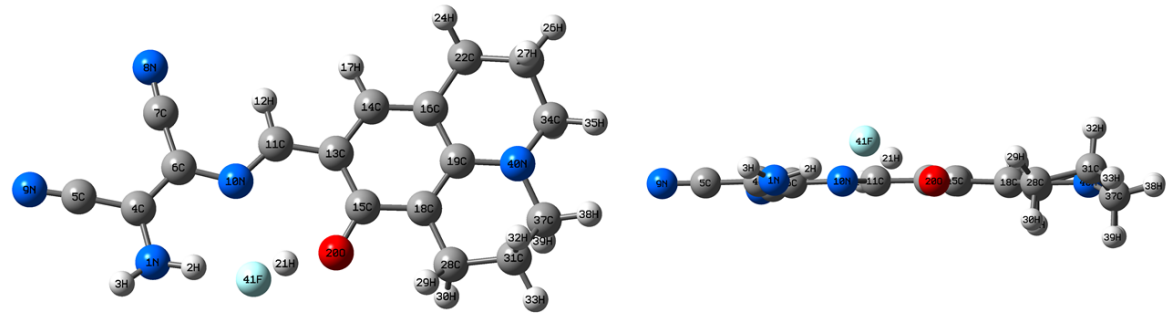


Fig. S1 The optimized structures of **1** (a) and **1**-F^- species (b) from B3LYP level

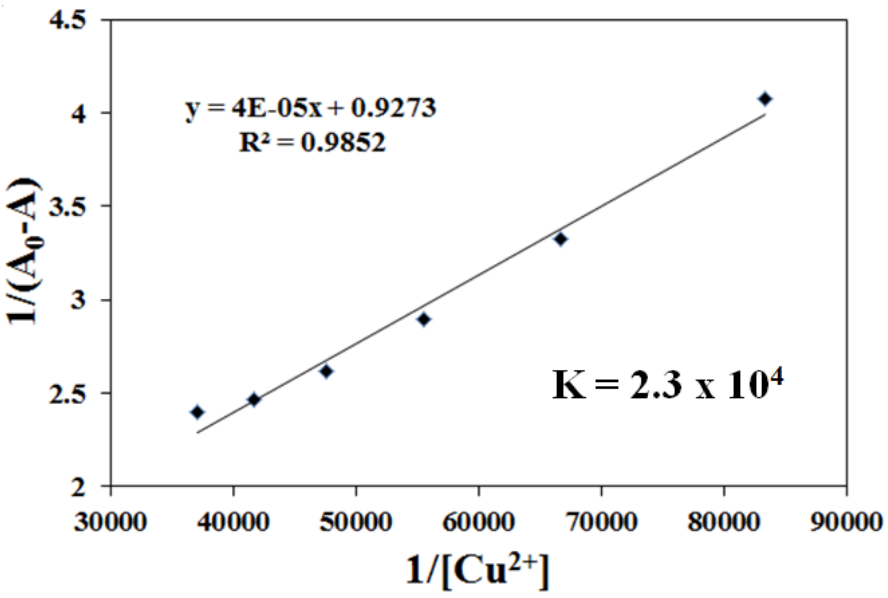


Fig. S2 Benesi-Hildebrand plot (absorbance at 450 nm) of **1**, assuming a 1:1 stoichiometry for association between **1** and Cu^{2+}.

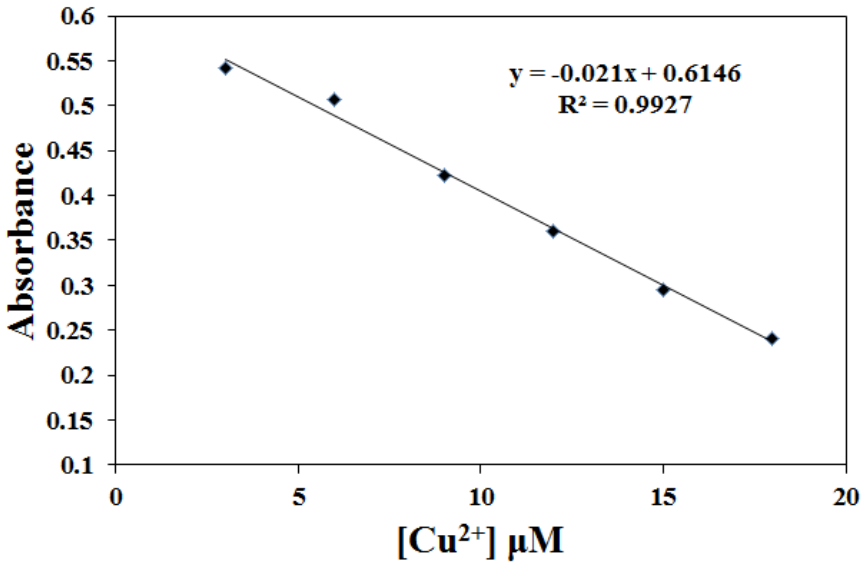


Fig. S3 Determination of the detection limit based on absorbance change (450 nm) of **1** (10 µM) with Cu^{2+}.

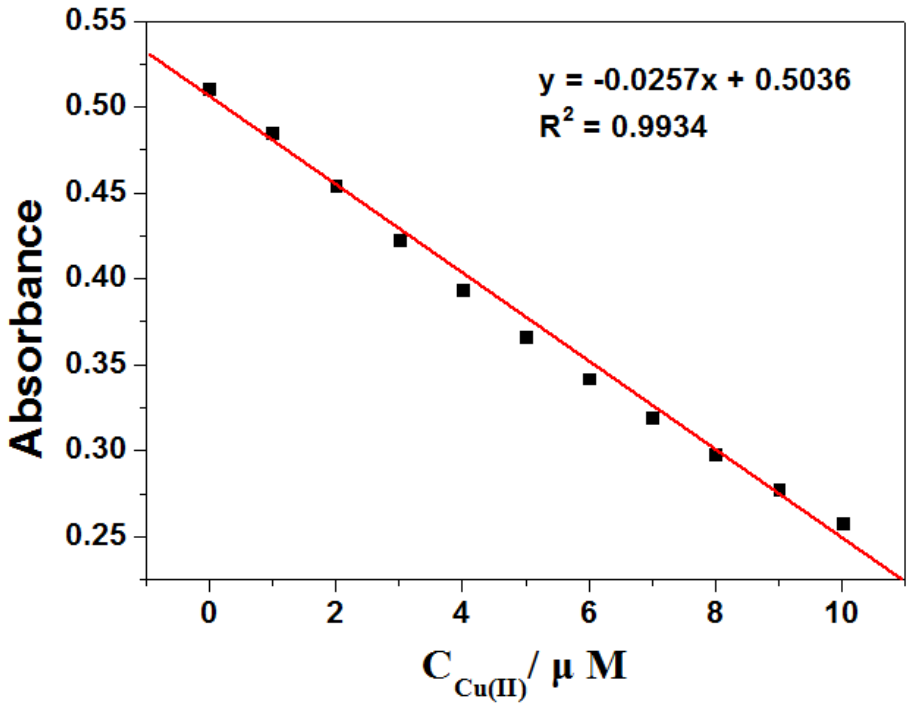


Fig. S4 Absorption (at 460 nm) of **1** as a function of Cu(II) concentration. [**1**] = 10 μmol/L, [Cu(II)] = 0-10.0 μmol/L.

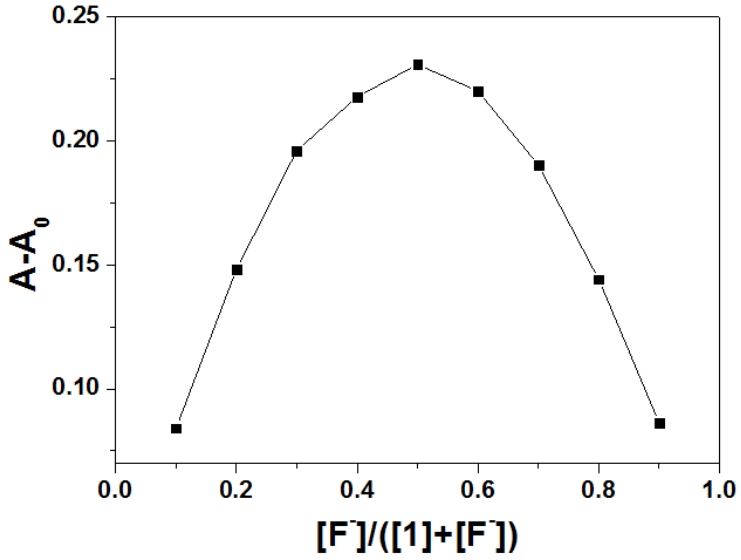


Fig. S5 Job plot of receptor **1** and fluoride. Absorbance at 460 nm was plotted as a function of the molar ratio $[F^-]/([\mathbf{1}] + [F^-])$. The total concentration of fluoride with receptor **1** was 2.0 x 10^{-5} M.

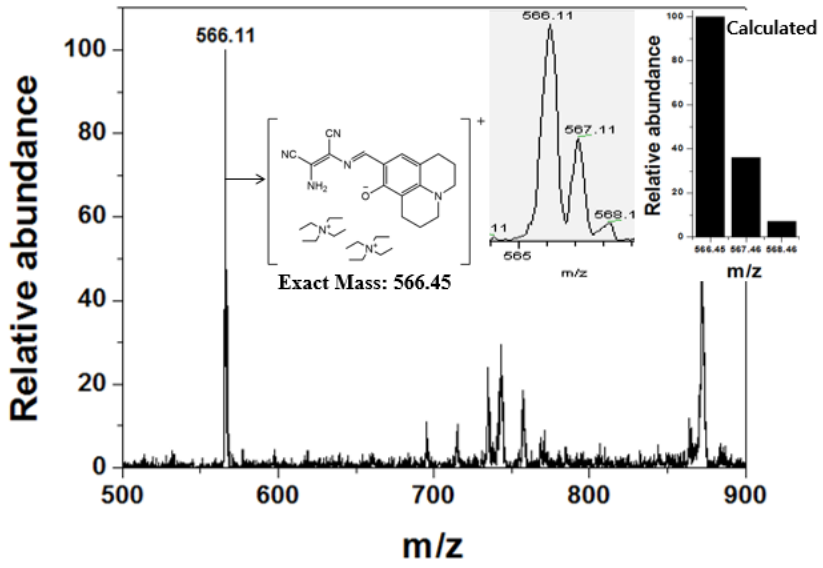


Fig. S6 Positive-ion electrospray ionization mass spectrum of **1** (0.1 mM) upon addition of F^- (0.1 mM).

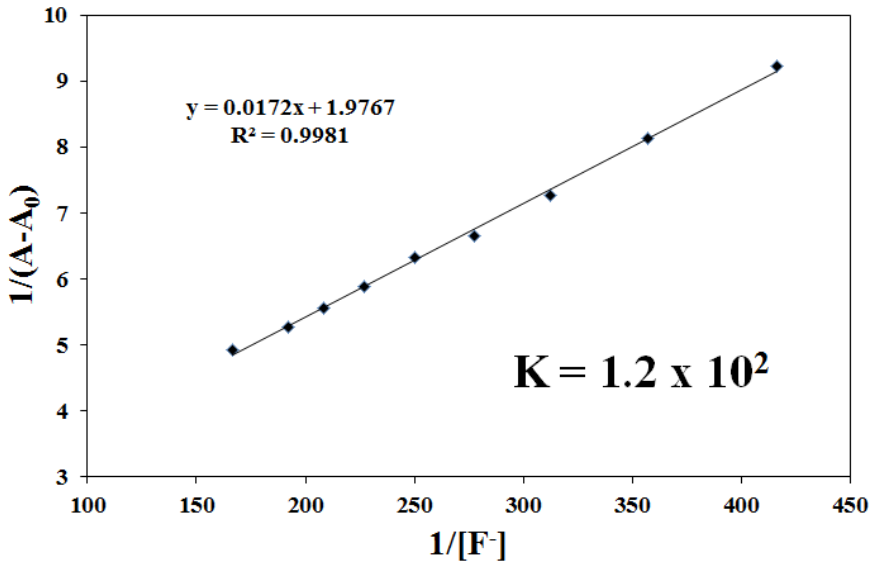


Fig. S7 Benesi-Hildebrand plot (absorbance at 460 nm) of **1**, assuming a 1:1 stoichiometry for interaction between **1** and F^-.

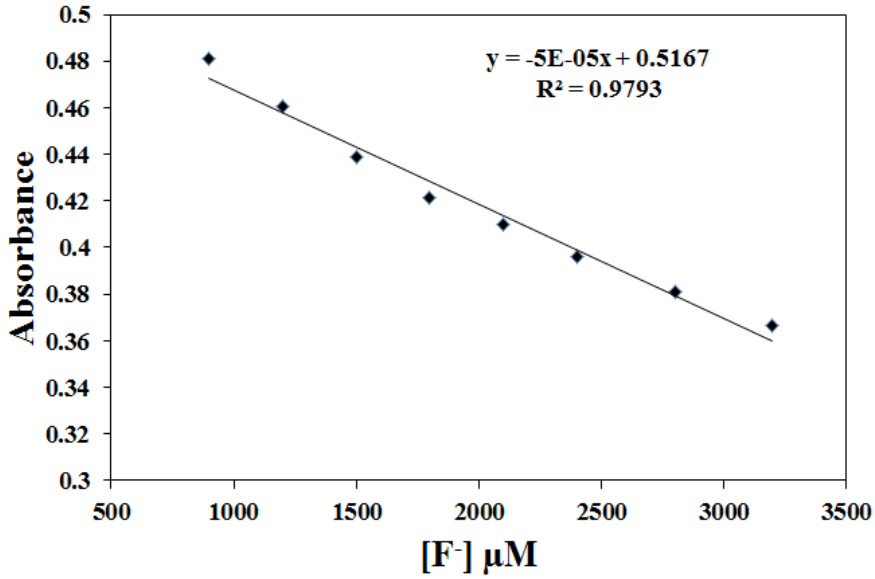


Fig. S8 Determination of the detection limit based on absorbance change (460 nm) of **1** (10 µM) with F^-.

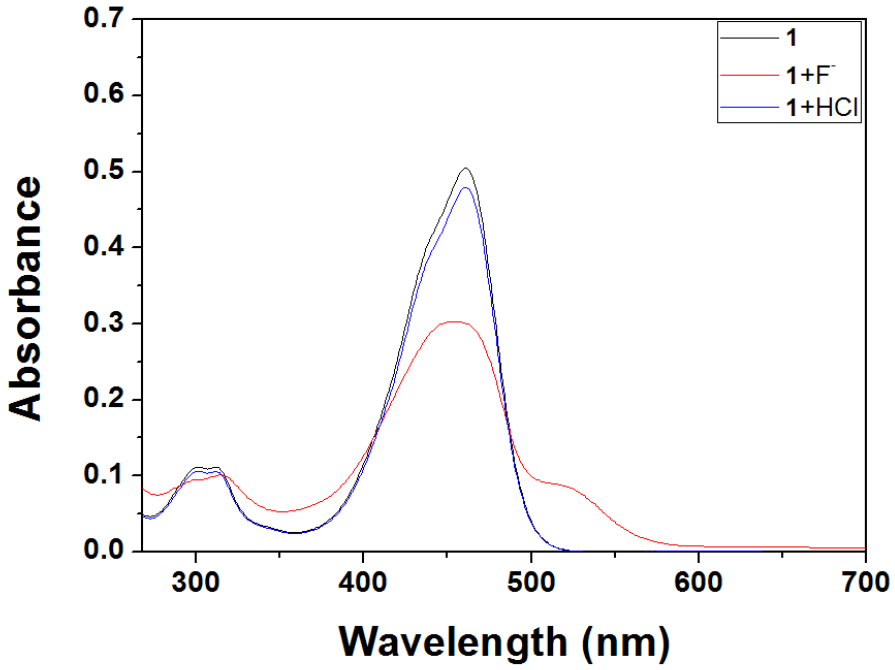


Fig. S9 Reversible changes in absorbance of **1** (20 μM) after the sequential addition of F^- and HCl.

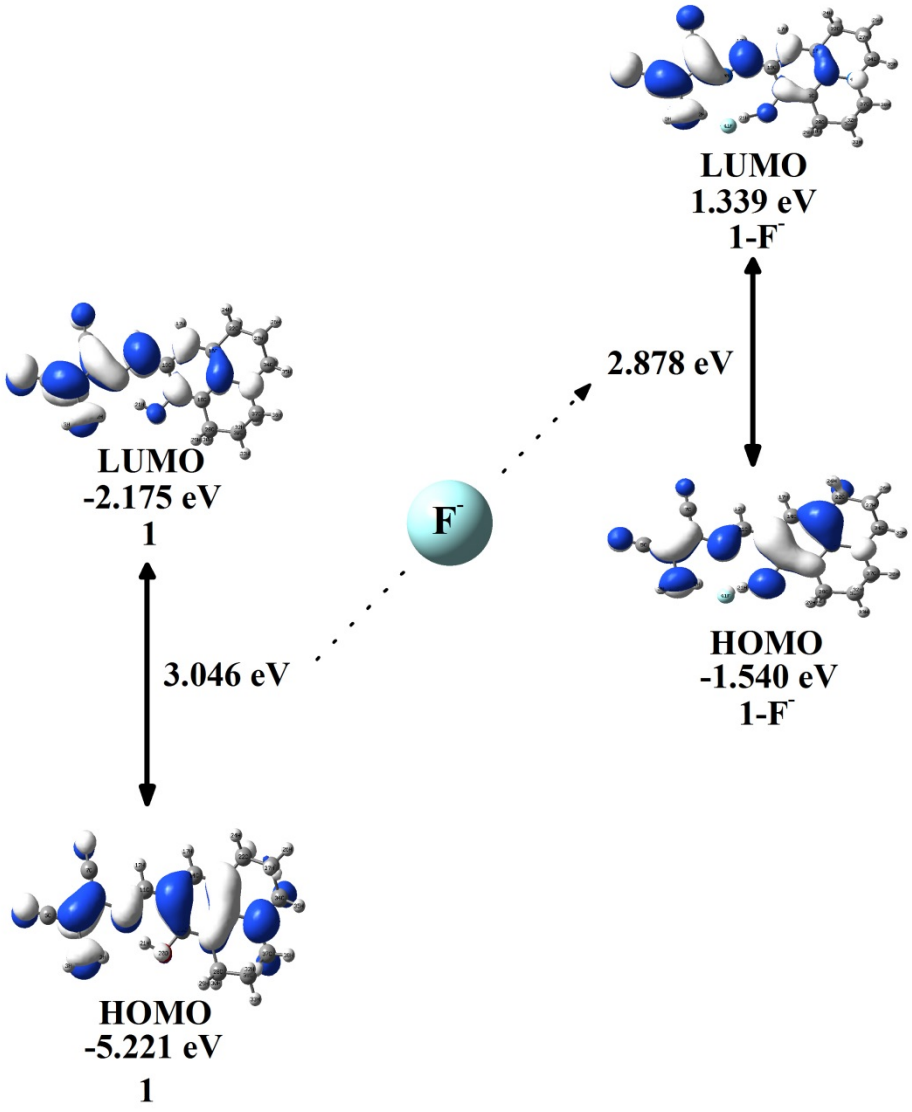


Fig. S10 HOMO-LUMO energy gaps of **1** and **1**-F^- species (isovalue = 0.025).