Supporting information

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

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**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$^{2+}$. 

\[
y = 4E-05x + 0.9273 \\
R^2 = 0.9852
\]

\[K = 2.3 \times 10^4\]
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. [I] = 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⁻]/([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⁻.

\[ y = 0.0172x + 1.9767 \]

\[ R^2 = 0.9981 \]

\[ K = 1.2 \times 10^2 \]
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).