Electronic Supplementary Information for

Visible Chemosensor Based on Carbohydrazide for Fe(II), Co(II) and Cu(II)
in Aqueous Solution

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Figure S1. UV-vis spectrum of sensor (30 μM).
Figure S2. Job plot for the binding of 1 with Fe$^{2+}$. Absorbance at 642 nm was plotted as a function of the molar ratio $[1]/([1] + [Fe^{2+}])$. The total concentration of ferrous ion with sensor 1 was 3.0 $\times$ 10$^{-5}$ M.

Figure S3. Mass spectroscopy data for Fe(II) plus sensor.
Figure S4. Uv-vis absorption of sensor (1) in the presence of Fe(II) and other metal ions. Conditions: aqueous solution of 30 μM sensor and 1.0 equivalent of Fe(II) and 1.0 equivalent of other metal ion in bis-tris buffer (10 mM) at pH 7.0.

Figure S5. Absorption spectral changes of 1 (30 μM) after addition of increasing amounts of Cu^{2+} in buffer (bis-tris 10 mM, pH 7.0). Inset: Absorption at 370 nm versus the number of equiv of Cu^{2+} added.
Figure S6. Job plots for the binding of 1 with Co$^{2+}$ and Cu$^{2+}$. Absorbance at 370 nm was plotted as a function of the molar ratio $[1]/([1] + [M^{2+}])$. The total concentration of cobalt or copper ion with sensor 1 was $3.0 \times 10^{-5}$ M.

Figure S7. Mass spectrum for Co(II) plus sensor.
Figure S8. Mass spectrum for Cu(II) plus sensor.

Figure S9. Absorption spectral changes of 1 and Cu$^{2+}$ (30 μM) in the absence and presence of 0.5 equiv of different metal ions in buffer (bis-tris 10 mM, pH 7.0).
Figure S10. Reusability of sensor with Fe(II) (a) and Co(II) (b). Conditions: Addition 1 is an aqueous solution of 30 μM sensor. Addition 2 has 20 mM Fe$^{2+}$ or Co$^{2+}$ solution added to the original solution. Addition 3 has had 2.3 μL of 20 mM EDTA added to it. Addition 4 has more Fe$^{2+}$ or Co$^{2+}$, addition 5 has more EDTA, and addition 6 has more Fe$^{2+}$ or Cu$^{2+}$ again.

<table>
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<th>Excited state 1</th>
<th>Wavelength (nm)</th>
<th>Percent (%)</th>
<th>Main Character</th>
<th>Oscillator strength</th>
</tr>
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<tr>
<td>H→L</td>
<td>318.98</td>
<td>93</td>
<td>$\pi \rightarrow \pi^*$</td>
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Figure S11. (a) The theoretical excitation energies and the experimental UV-vis spectrum of sensor. (b) The major electronic transition energies and molecular orbital contributions of sensor (H = HOMO and L = LUMO)

(a)

![Excitation Energies and Experimental UV-vis Spectrum](image1)

(b)

<table>
<thead>
<tr>
<th>Excited state</th>
<th>Wavelength (nm)</th>
<th>Percent (%)</th>
<th>Main Character</th>
<th>Oscillator strength</th>
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<td>H→L+1 (α)</td>
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Figure S12. (a) The theoretical excitation energies and the experimental UV-vis spectrum of Cu(II)-sensor complex. (b) The major electronic transition energies and molecular orbital contributions of Cu(II)-sensor complex (H = HOMO and L = LUMO).
Figure S13. Molecular orbital diagrams of sensor and Cu(II)-sensor complex using TD-DFT.