

Supplementary Information

Coumarin-Based Fluorescent Probes for Dual Recognition of Copper(II) and Iron(III) Ions and Their Application in Bio-Imaging. *Sensors* 2014, 14, 1385-1371

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Supplementary Information

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Figure S1. Fluorescence spectra of excitation (black color line) and emission (red color line) of **BS1** ($2\ \mu\text{M}$), $\lambda_{\text{Exc}} = 340\ \text{nm}$, $\lambda_{\text{Em}} = 458\ \text{nm}$. Slit 5.0/5.0.

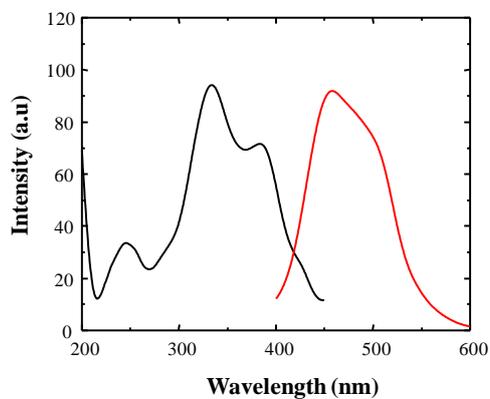


Figure S2. Fluorescence spectra excitation (black color line) and emission (red color line) of **BS2** ($2\ \mu\text{M}$), $\lambda_{\text{Exc}} = 364\ \text{nm}$, $\lambda_{\text{Em}} = 437\ \text{nm}$. Slit 5.0/5.0.

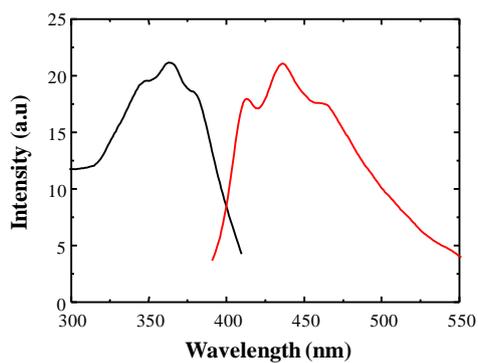


Figure S3. Fluorescence spectra excitation (black color line) and emission (red color line) of **3** ($2\ \mu\text{M}$), $\lambda_{\text{Exc}} = 336\ \text{nm}$, $\lambda_{\text{Em}} = 454\ \text{nm}$. Slit 5.0/5.0.

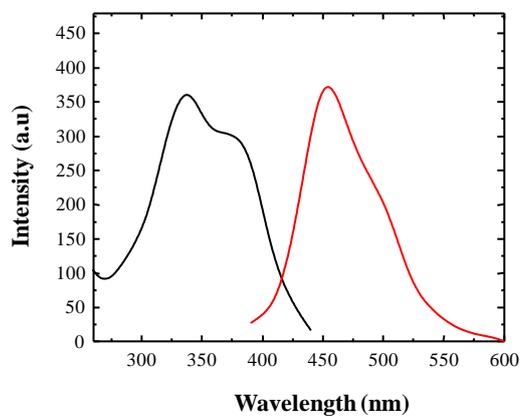


Figure S4. $^1\text{H-NMR}$ spectra of **3** in $\text{DMSO-}(d_6)$ at 300 K. Red color represents $t = 0$ and light blue color represents spectrum after water addition (10 %).

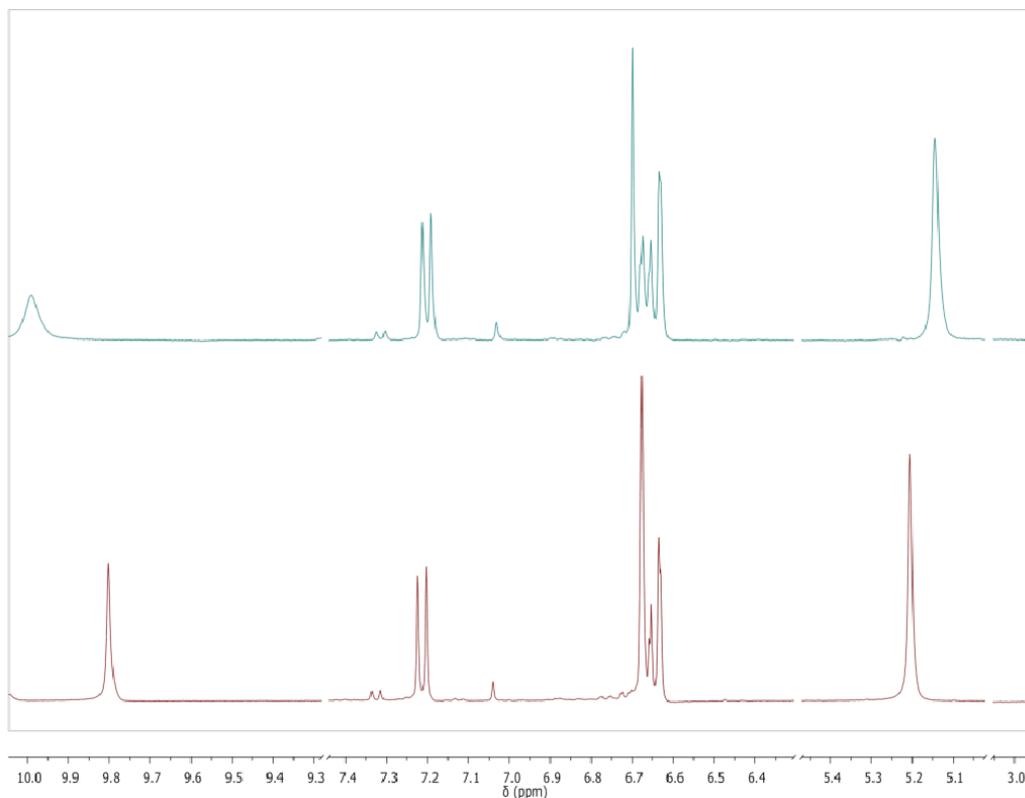


Figure S5. $^1\text{H-NMR}$ spectra of **BS2** at different incubation times. (A) Spectrum of a freshly prepared solution of **BS2**; (B) Spectrum of a solution containing **BS2** after 120 min. of incubation and (C) Spectrum of a solution containing **BS2** plus water.

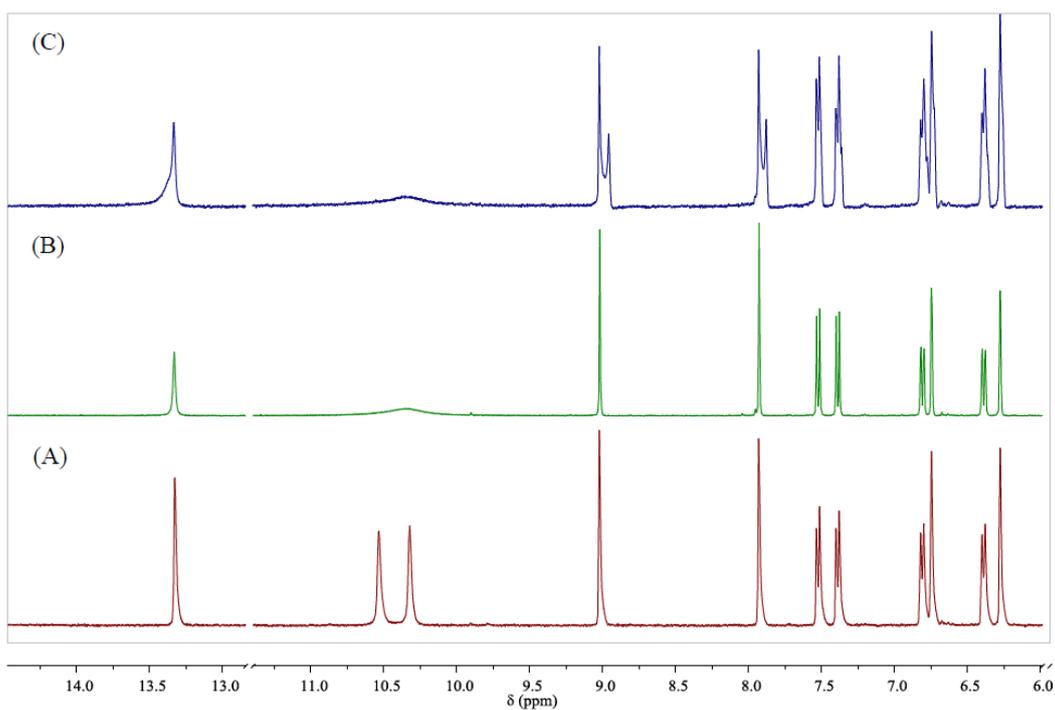


Figure S6. (A) Fluorescence spectra (2 μM) of **BS1** recorded upon the addition of copper ion (0–300 equiv.) in aqueous solution (30 mM HEPES buffer, pH 7.4, 1% DMSO). Excitation at 340 nm (slit = 5.0/5.0); (B) Fluorescence spectra (2 μM) of **BS1** recorded upon the addition of iron ion (0–300 equiv.) in aqueous solution (30 mM HEPES buffer, pH 7.4, 1% DMSO). Excitation at 340 nm (Slit = 5.0/5.0).

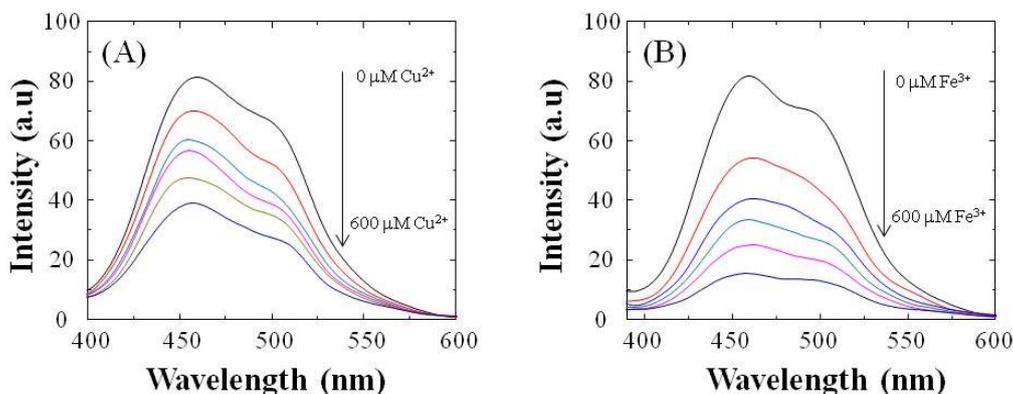


Figure S7. Reaction profile for the *auto-decomposition* reaction of **BS1**.

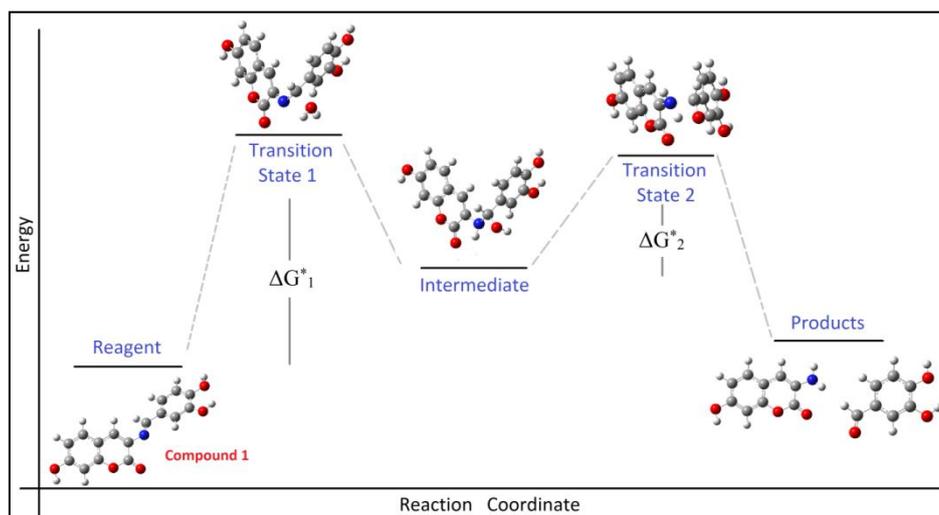


Figure S8. Calculated structure for the binding modes for the complex formed between **BS2** and copper ion.

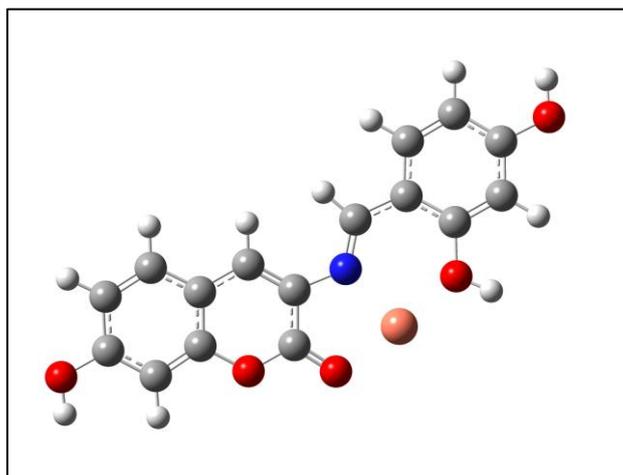


Figure S9. Changes in fluorescence intensity (expressed as Relative Fluorescence Units “RFU”) of solution **3** (2 μM) induced by different metal ions. In graph (A) the black bars represent the fluorescence intensity due to **3** alone, grey bars represent the fluorescence intensity due to **3** plus 300 equiv. of miscellaneous metal ions and the white bars represent the fluorescence intensity of the above solution upon further addition of 10 equiv of Fe^{3+} ($\lambda_{\text{em}} = 454 \text{ nm}$); In graph (B) the black bars represent the fluorescence intensity due to **BS2** alone, grey bars represent the fluorescence intensity due to **BS2** plus 300 equiv. of miscellaneous metal ions and the white bars represent the fluorescence intensity of the above solution upon further addition of 10 equiv of Fe^{3+} ($\lambda_{\text{em}} = 437 \text{ nm}$).

