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**Selective detection of Cu<sup>2+</sup> and S<sup>2-</sup> by a colorimetric chemosensor: Experimental and theoretical calculations**

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**Abstract**

A multifunctional colorimetric chemosensor **1**, based on 4-(diethylamino)-2-hydroxybenzaldehyde and 2,3-diamino-5-bromopyridine, has been synthesized and characterized. Sensor **1** detected instantly both Cu<sup>2+</sup> and S<sup>2-</sup> by the color change from pale yellow to deep yellow. The binding modes of **1** with Cu<sup>2+</sup> and S<sup>2-</sup> were found to be the 1:1 stoichiometry through Job plot and ESI-mass spectrometry analysis, respectively. In addition, the detection limit of **1** for Cu<sup>2+</sup> was found to be 68.6 nM, which was much lower than WHO guideline (31.5 μM) in drinking water. Importantly, sensor **1** could be used to quantify Cu<sup>2+</sup> in water samples. Moreover, **1** exhibited a high selectivity for S<sup>2-</sup> in the presence of other anions. The sensing mechanisms of Cu<sup>2+</sup> and S<sup>2-</sup> by **1** were explained by theoretical calculations.

**Keywords:** colorimetric chemosensor, naked-eye, copper ion, sulfide, theoretical calculations

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