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Chemosensor development of Cu2+ recognition using 1,5-diphenylthiocarbazone: Optimization, COSMO-RS and DFT studies

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Abstract
The sensitive and selective chemosensor for copper(II) ions (Cu2+) was successfully optimized using the 1,5-diphenylthiocarbazone (DPT) compound. The result showed that dimethyl sulfoxide (DMSO) in a 9:1 (DMSO:water) ratio at a pH of 3 was the optimum medium for DPT to act as chemosensor of Cu2+ recognition. The DPT chemosensor did not encounter any interference from other metal ions, including Fe3+, Ag+, Cr3+, Pb2+, Mg2+, Cd2+, Zn2+, K+, Ni2+ and Co2+. The presence of Cu2+ led to an absorption peak at 658 nm, where the color changed from cantaloupe to gray-green color indicating the interaction by the formation of the DPT-Cu complex in 2:1 stoichiometry. The theoretical σ-profile calculation using conductor-like screening model for real solvents (COSMORS) showed the compatibility of DPT with the DMSO solvent through hydrogen bonding. In the density functional theory (DFT) calculations, the formation energy of DPT and DPT-Cu were -1113.79645660 and -2435.71832681 a.u., respectively. Under optimal conditions, a detection limit of 6.08 μM for the DPT chemosensor for Cu2+ recognition can compete with the flame atomic absorption spectroscopy (FAAS) value of 6.21 μM. Finally, DPT was able to provide less expensive, more portable and convenient chemosensor for Cu2+ recognition in environmental water samples. © 2019 Sociedade Brasileira de Química.

Author Keywords
Chemosensor; Colorimetric; COSMO-RS; DFT; Test strip

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