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COSMO-RS and DFT studies on development and optimization of quercetin as a chemosensor for Fe $^{3+}$ recognition in aqueous medium (Article)

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Abstract

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Quercetin is known as a bioflavonoid compound that has been successfully optimized to be a chemosensor probe for Fe $^{3+}$ recognition. The sensitivity of quercetin towards Fe $^{3+}$ increased in DMSO:deionized water with a 9:1 ratio at pH 4. There was also no significant interference from other metal ions, such as K $^{+}$, Cr $^{3+}$, Ag $^{+}$, Cd $^{2+}$, Mg $^{2+}$, Pb $^{2+}$, Co $^{2+}$, Ni $^{2+}$, Zn $^{2+}$ and Cu $^{2+}$ in the selectivity optimization. The detection limit of the probe was 20.5 μM. The stoichiometry of 1:1 quercetin:Fe $^{3+}$ was calculated using the Job plot method. The sigma profile was calculated using COSMO-RS, which showed that quercetin formed stronger hydrogen bonds with the DMSO solvent. Density functional theory (DFT) calculations, such as molecular electrostatic potential (MEP) and the Fukui function, were performed to visualize and clarify the region of interaction between quercetin and Fe $^{3+}$. The TD-DFT method was successfully used to investigate the electronic properties of quercetin and quercetin–Fe $^{3+}$ and it showed good agreement between experimental and theoretical results.

Author keywords

Chemosensor | Colorimetric | COSMO-RS | DFT | Quercetin | Test strip

Indexed keywords

Engineering controlled terms: Deionized water | Density functional theory | Design for testability | Electronic properties | Hydrogen bonds | Metal ions | Metals | Phenols | Physiology | Probes

Engineering uncontrolled terms: Chemosensor | Colorimetric | COSMO-RS | Quercetin | Test strips

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