COSMO-RS and DFT studies on development and optimization of quercetin as a chemosensor for Fe3+ recognition in aqueous medium

By: Normaya, E (Normaya, Erna)[1]; Fazli, M (Fazli, Muhammad)[1]; Ahmad, MN (Ahmad, Mohammad Norazmi)[1]; Bulat, KHK (Bulat, Ku Halim Ku)[2]

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Abstract

Quercetin is known as a bioflavonoid compound that has been successfully optimized to be a chemosensor probe for Fe3+ recognition. The sensitivity of quercetin towards Fe3+ 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+, Cr3+, Ag+, Cd2+, Mg2+, Pb2+, Co2+, Ni2+, Zn2+ and Cu2+ in the selectivity optimization. The detection limit of the probe was 20.5 mu M. The stoichiometry of 1:1 quercetin: Fe3+ 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 Fe3+. The TD-DFT method was successfully used to investigate the electronic properties of quercetin and quercetin-Fe3+ and it showed good agreement between experimental and theoretical results. (C) 2019 Elsevier B.V. All rights reserved.

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Author Information

Reprint Address: Normaya, E (reprint author)

+ Int Islamic Univ Malaysia, Expt & Theoret Res Lab, Dept Chem, Kulliyyah Sci, Kuantan 25200, Pahang, Malaysia.

Addresses:

+ [1] Int Islamic Univ Malaysia, Expt & Theoret Res Lab, Dept Chem, Kulliyyah Sci, Kuantan 25200, Pahang, Malaysia
+ [2] Univ Malaysia Terengganu, Dept Chem, Fac Sci, Mengabang Telipot, Kuala Terengganu 21030, Terengganu Daru, Malaysia

E-mail Addresses: ernanormaya@gmail.com

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