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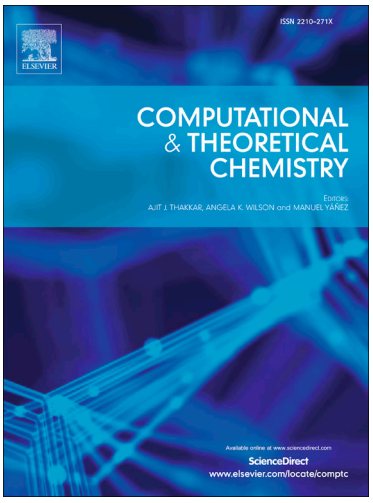

Computational Study of the Chemical Reactivity of the Blue-M1 Intermediate Melanoidin

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Computational Study of the Chemical Reactivity of the Blue-M1 Intermediate Melanoidin

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Abstract

This study assessed eight density functionals that include CAM-B3LYP, LC-ωPBE, M11, MN12SX, N12SX, ωB97, ωB97X, and ωB97XD related to the Def2TZVP basis sets together with the SMD solvation model. These are assessed in calculating the molecular properties and structure of the Blue-M1 intermediate melanoidin pigment. Notably, the chemical reactivity descriptors for the system are calculated via the Conceptual Density Functional Theory. The choice of active sites applicable to nucleophilic, electrophilic as well as radical attacks is made by linking them with Fukui functions indices, electrophilic Parr functions, and condensed dual descriptor $\Delta f(\mathbf{r})$. The predicted maximum absorption wavelength tends to be considerably accurate relative to the experimental value. The study found the MN12SX and N12SX density functionals to be the most appropriate in predicting the chemical reactivity of the molecule under study.

Keywords: Melanoidins; Blue-M1; Conceptual DFT; Chemical Reactivity; Dual Descriptor; Parr Function; Maximum Absorption Wavelength

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