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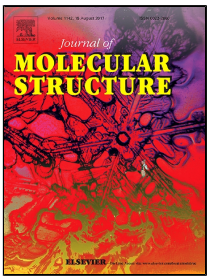

Synthesis, Crystal Structure Analysis, Molecular Docking Studies and Density Functional Theory Predictions of the Local Reactive Properties and Degradation Properties of a novel halochalcone

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Highlights

* Single crystals of a novel chalcone derivative are synthesized and characterized using single crystal X-ray diffraction method.
* Local reactivity properties are investigated by ALIE surfaces and Fukui functions.
* Bond dissociation energies are calculated in order to predict the open air stability and possible degradation properties.
* In order to understand the influence of solvent (water), we have calculated radial distribution functions (RDF) obtained after MD simulations
* Molecular docking study revealed that the title compound might exhibit inhibitory activity against Dihydrofolate reductase (DHFR) enzyme.

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