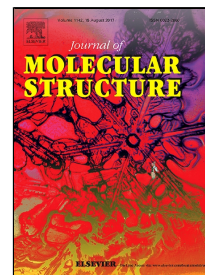


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Synthesis, Crystal Structure Analysis, Molecular Docking Studies and Density Functional Theory Predictions of the Local Reactive Properties and Degradation Properties of a novel halochalcone



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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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