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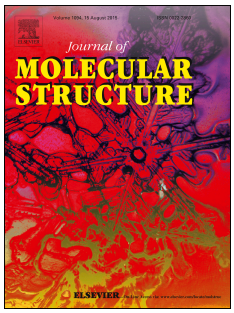

Synthesis, XRD crystal structure, spectroscopic characterization, local reactive properties using DFT and molecular dynamics simulations and molecular docking study of *(E)-1-(4-bromophenyl)-3-(4-(trifluoromethoxy)phenyl)prop-2-en-1-one*

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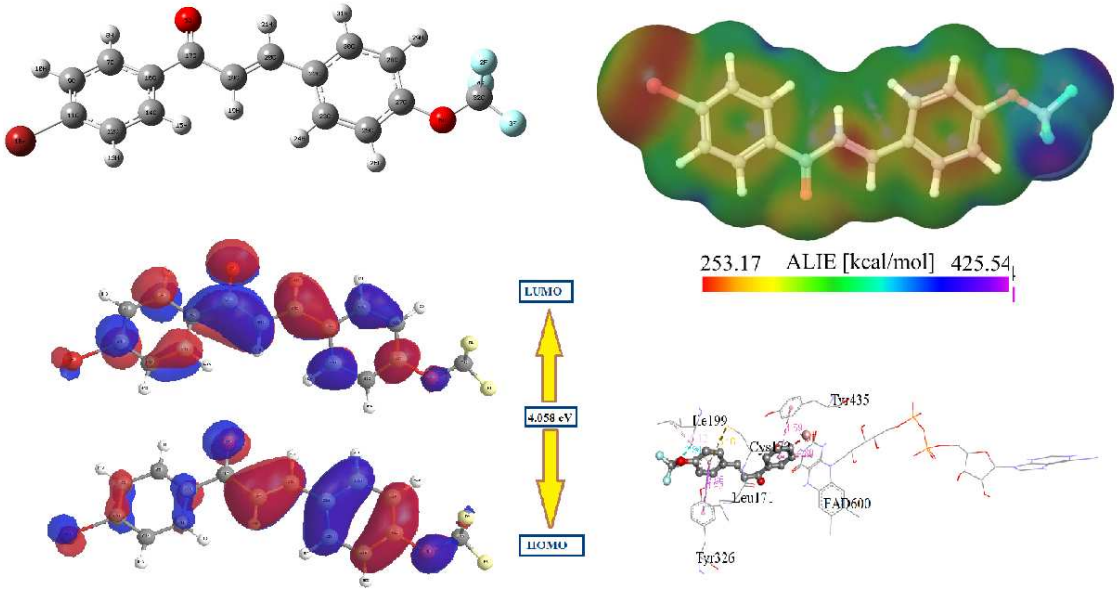
Graphical abstract:

Title of the paper: Synthesis, XRD Crystal Structure, Spectroscopic Characterization, Local Reactive Properties using DFT and Molecular Dynamics Simulations and Molecular Docking Study of *(E)-1-(4-bromophenyl)-3-(4-(trifluoromethoxy)phenyl)prop-2-en-1-one*.



In this work, a new chalcone derivative, *(E)-1-(4-bromophenyl)-3-(4-(trifluoromethoxy)phenyl)prop-2-en-1-one* is synthesized and structurally characterized by single crystal XRD, FT-IR, ^{1}H and ^{13}C NMR. The IR spectrum was recorded and interpreted in details with the aid of Density Functional Theory (DFT) calculations and Potential Energy Distribution (PED) analysis. In order to investigate local reactivity properties of the title molecule, we have conducted DFT calculations of average local ionization energy surface and Fukui functions which were mapped to the electron density surface. In order to predict the open air stability and possible degradation properties, within DFT approach, we have also calculated bond dissociation energies. To determine which atoms of title molecule have pronounced interactions with water molecules, we have calculated radial distribution functions obtained after molecular dynamics simulations. In order to understand how the title molecule inhibits and hence increases the catalytic efficiency of MOA-B enzyme, molecular docking study was performed to fit the title compound into the binding site of MOA-B enzyme.