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(E)-3-(4-Hydroxyphenyl)-1-(4-methoxyphenyl)prop-2-en-1-one: DFT/TD-DFT-based investigations with distinct solvents and *in silico* ADME profiling

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The chalcone scaffold has become one of the privileged structures frequently encountered in medicinal chemistry for the discovery of new and effective drug candidates. In recent years, chalcone derivatives have attracted intense attention from both experimental and theoretical researchers due to their ease of synthesis and wide range of biological activities. Herein, quantum chemical-based calculations have been performed on chalcone derivative (E)-3-(4-hydroxyphenyl)-1-(4-methoxyphenyl)prop-2-en-1-one. Density functional theory (DFT) method has been applied with the B3LYP hybrid functional and 6-311++G (d, p) basis set. The structural, electronic, energetic and reactivity properties of the mentioned chalcone derivative have been examined. Bond parameters and vibrational analysis results are compatible with experimental data. The energy gap (ΔE) values corresponding to acetonitrile, DMSO and water phases have been calculated as 3.753, 3.750 and 3.747 eV, respectively. Also, the reactive regions of the molecule have been visualized with molecular electrostatic potential (MEP) maps. The excited state characteristics of the title compound in water, acetonitrile and DMSO environments have been calculated by the TD-DFT method. All absorption wavelengths could be qualified as $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ transition type. A bioavailability radar has been created by calculating some physicochemical parameters such as lipophilicity, TPSA, and water solubility. ADME properties have been predicted from pharmacokinetics and drug likeness data.

Keywords: Chalcone, DFT, Solvent effect, NBO, ADME profiling