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The substitution group and solvent effect on the chemical behavior of chlorine-functionalized Ferulic acid

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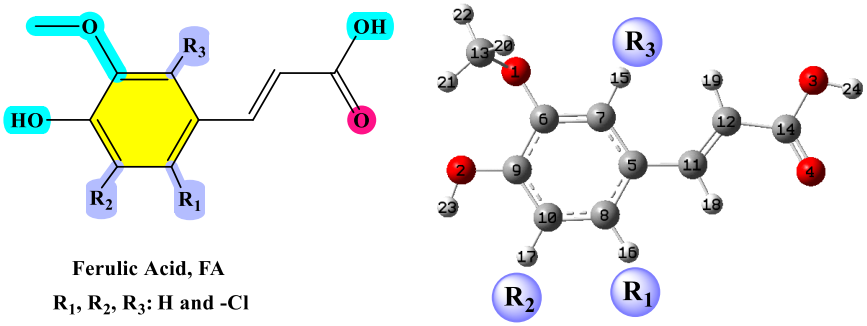
Ferulic acid (FA) as a member of the phenolic compounds have occurred in the plants commonly, especially in popocorns, bamboo shoots, rice, and wheat [1]. Also, it is the main metabolite of the chlorogenic acids in humans together with caffeic and isoferulic acid. G16W package [2] is used to perform the quantum mechanical simulations. Herein, the DFT/B3LYP/6-311++G** [3,4] level computations are conducted to structural optimization and confirmation of the FA and its chlorinated derivatives depicted in Figure 1. Then, the FMO and MEP computations are performed to elucidate the reactivity direction [5] and site of the compounds. Also, the TD-DFT computations have been conducted to evaluate the UV-Vis characterization. The pharmacokinetics, bioavailability, and drug-likeness features of the compounds are also evaluated [6].



Key Words: *Ferulic acid, UV-Vis, FMO, NBO, MEP*

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