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Isolating toxicophoric scaffold on *trans*-dehydrocrotonin

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Abstract

A proposed mechanism for toxicity of *trans*-dehydrocrotonin was performed by means of density functional theory calculations related to exploration of its electronic structure. The preferential electron transfer was located mainly under furan ring as nucleophilic moiety. The HOMO values and the highest spin density contribution at the furan ring can be related with a probable and preferential metabolism by means of oxidation reaction such as epoxidation. Simplified derivatives show great impact on electron donating capacity for each moiety. Furan and cycle-hexenone increase electron donating capacity by synergistic effect. Lactone moiety decreases electron donating capacity. A toxicity mechanism on furan ring as nucleophilic moiety was proposed to give epoxide and aldehyde as reactive intermediate.

Keywords: *trans*-dehydrocrotonin, oxidation, electron transfer, metabolism, toxicity, DFT.

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