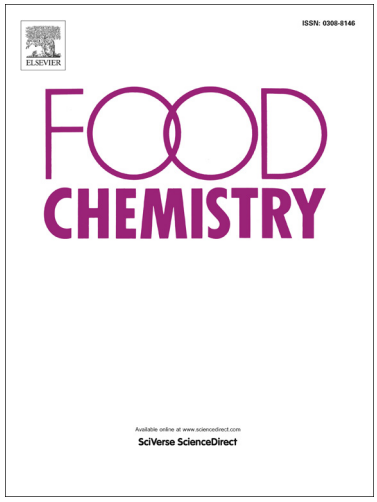

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Electronic structure of some thymol derivatives correlated with the radical scavenging activity: Theoretical study

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ABSTRACT

Molecules acting as antioxidants capable of scavenging reactive oxygen species (ROS) are of upmost importance in the living cell. Thymol derivatives exhibit various antioxidant activities and potential health benefits. Exploration of structure-radical scavenging activity (SAR) was approached with a wide range of thymol derivatives. To accomplish this task, the DPPH experimental assay along with quantum-chemical calculations were also employed for these compounds. By comparing the structural properties of the derivatives of interest, their antioxidant activity was explained by the formation of an intramolecular hydrogen bond and the presence of unsaturated double bond (–CH=CH substituent) in their radical spices. Moreover, the delocalization of odd electrons in these radicals has been investigated by natural bond orbital analysis and interpretation of spin density maps. Reactivity order of the compound towards the ROS: HO•, HOO•, and O_2•$^-$ was found to be as HO•> HOO•>> O_2•$^-$.

Keywords: Thymol radical scavenging activity, Reactive oxygen species, Bond dissociation energy, DPPH assay, DFT study, Ionization potential.

Abbreviations

DFT: Density Functional Theory

B3LYP: Becke, three-parameter, Lee-Yang-Parr

BDE: Bond Dissociation Energy