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

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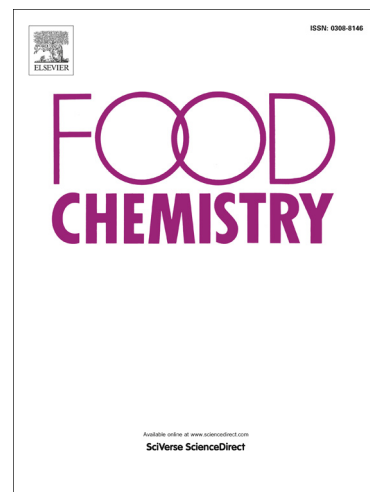
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1 Electronic structure of some thymol derivatives correlated with the
2 radical scavenging activity: Theoretical study

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13 **ABSTRACT**

14

15 Molecules acting as antioxidants capable of scavenging reactive oxygen species
16 (ROS) are of utmost importance in the living cell. Thymol derivatives exhibit
17 various antioxidant activities and potential health benefits. Exploration of
18 structure-radical scavenging activity (SAR) was approached with a wide range
19 of thymol derivatives. To accomplish this task, the DPPH experimental assay
20 along with quantum-chemical calculations were also employed for these
21 compounds. By comparing the structural properties of the derivatives of interest,
22 their antioxidant activity was explained by the formation of an intramolecular
23 hydrogen bond and the presence of unsaturated double bond ($-\text{CH}=\text{CH}$
24 substituent) in their radical species. Moreover, the delocalization of odd electrons
25 in these radicals has been investigated by natural bond orbital analysis and
26 interpretation of spin density maps. Reactivity order of the compound towards
27 the ROS: $\text{HO}\cdot$, $\text{HOO}\cdot$, and $\text{O}_2\cdot^-$ was found to be as $\text{HO}\cdot > \text{HOO}\cdot >> \text{O}_2\cdot^-$.

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

30

31 **Abbreviations**

32 DFT: Density Functional Theory

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

34 BDE: Bond Dissociation Energy

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