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DFT study on the synergistic effect of antioxidant and lipid solubility of catechins with structural modification

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With the aid of density functional theory (DFT), the optimized structures of catechins and their derivatives have been obtained. The synergistic effect of antioxidant and lipid solubility has also been explored with the analysis of the thermodynamics enthalpies of the hydrogen abstraction reaction with DPPH and the spin densities of radical products. It is concluded that the structure modifying on the phenolic hydroxyl site of EGCG results in the pronounced electron delocalization and the enhancement of product free radical stability, leading to a significant improvement in antioxidant activity. Furthermore, the structure modification significantly reduces molecular polarity and enhances the lipid solubility of catechins and their derivatives, resulting in a synergistic effect between antioxidant activity and lipid solubility. On this basis, the effects of solvent polarity differences on the antioxidant activity and lipid solubility of catechins and their derivatives have been analyzed. It is suggested that differences in solvent polarity primarily influences the relative strength of antioxidant activity and lipid solubility at different sites, but does not alter the highest activity sites and the positive impact of structural modification on both antioxidant and lipid solubility.

Keywords: Catechins, Antioxidant, Lipid solubility, Solvent polarity, Density functional theory