



611/ E2

Computational design and investigation of antioxidant activity of phenolic compounds and their derivatives

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Among various types of antioxidants, phenolic antioxidants form an important class of compounds, which serves to inhibit the oxidation of materials of both commercial and biological importance.

Density functional theory (DFT) calculations (**BP86** level of theory and **6-311++ G (2df, 2p)** basis set) have been performed on some structurally simple phenolic antioxidants first, and then on novel designed, phenolic derivatives. Moreover, the polarity of the solvent medium has been included in calculating bond dissociation energy (BDE) and ionization potentials (IP). Both H-atom transfer (HAT mechanism) and single electron transfer (SET mechanism) pathways have been investigated by calculating the phenolic O–H bond dissociation energy (BDE) and ionization potentials (IP) in three different phases (gas, aqueous and cyclohexane). How the antioxidant activity of phenolic derivatives is perturbed by electron donor and withdrawing substituents present at ortho, meta, and para positions and the dimerized of phenolic derivatives have also been computationally investigated.

The presence of electron donating substituents on the structure at the ortho and para positions of the phenol increased the antioxidant activity significantly. When secondary and tertiary amine groups were introduced to phenolic antioxidants, the BDE and IP values decreased noticeably (IP from 7.04 to 5.23 and 1.97 eV, BDE from 71.01 to 70.62 and 69.00 kcal/mol). In aqueous phase the designed phenolic antioxidants showed better activity owing to Hydrogen bonding. The effect of solvent on IP values was higher than on BDE, showing that the SET mechanism was highly solvent dependent compared to HAT mechanism. These theoretical computational predictions were superimposable with experimental results reported in literature. When designed novel amino derivatives were dimerized and those monomers were linked through conjugated alkyl chains, they demonstrated much better antioxidant properties (lower BDE) than the monomers themselves (68.05 to 65.04 kcal/mol).

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