Computational Investigation of Antioxidant Activity of Dietary Vitamins; DFT Study

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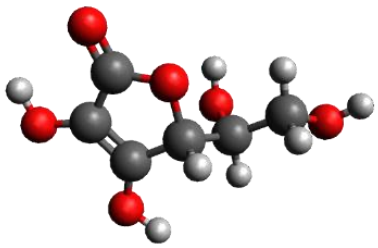
Among numerous types of antioxidant compounds, dietary vitamins form an important class of chain-breaking compounds which have a potential to quench reactive radical intermediates produced during the oxidative processes of both biological and commercial importance materials. According to the recent investigations, the possible role of antioxidants in prevention of human diseases has taken a leading role. Antioxidants are also capable to defend against number of disease conditions such as aging, atherosclerosis, cancer, asthma, arthritis and autoimmune diseases. Antioxidants as external supplements are used to maintain the concentration of free radicals as low as possible and to avoid the oxidative stress. They are heavily used in food industry to maintain the quality of the ready-to-eat foods, and to boost the shelf life.

The computational chemistry has become a versatile tool to investigate wide range of thermodynamic properties which are hardly measurable, as well as to predict the trends between them. The efficiency of an antioxidant can be successfully estimated by analyzing the potential energy surface (PES) of the reaction with a certain radical. This potential energy surface permits calculation of the activation and reaction energies, entailing that both kinetic and thermodynamic approaches to the interested reaction are presented. As well as the computed parameters provide useful information on the radical scavenging power without considering reaction pathway.
Density functional theory (DFT) was used to explore the antioxidant properties of some naturally occurring dietary vitamins, and the reaction enthalpies related to various mechanisms of primary antioxidant action, i.e., hydrogen atom transfer (HAT), single electron transfer–proton transfer (SET–PT), and sequential proton loss–electron transfer (SPLET) have been investigated in detail. B3LYP, M05-2X, and M06-2X functionals were utilized in this work. For aqueous phase studies, the integral equation formalism polarized continuum model (IEF–PCM) was employed.

From the outcomes, hydrogen atom transfer (HAT) was the most probable mechanism for the antioxidant action of this class of compounds. Comparison of found results with experimental data (available in literature), vitamin C possesses the lowest enthalpy values for both proton affinity (PA) and bond dissociation energy (BDE) in the aqueous phase, suggesting it as the most promising candidate as an antioxidant. Accordingly, these computational insights encourage the design of structurally novel, simple vitamins which will be more economical and beneficial in the pharmaceutical industry.



Computationally optimized geometry of vitamin-C

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