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Comparative Study of Antioxidant Potential of Selected Dietary Vitamins; Computational Insights

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Received: 29 March 2019; Accepted: 22 April 2019; Published: 26 April 2019

Abstract: 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, single electron transfer–proton transfer, and sequential proton loss–electron transfer were discussed 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.

Keywords: antioxidant; HAT; SET–PT; SPLET; BDE; IP; PDE; PA; ETE

1. Introduction

The origin of the harmful process called oxidative stress lies in the extreme production of free radicals such as reactive oxygen species (ROS),reactive nitrogen species (RNS), and reactive sulfur species (RSS) with half-lives of only a few nanoseconds, whose effects can seriously alter cell structures (e.g., membranes) and damage biomolecules such as lipids, lipoproteins, proteins, and nucleic acids [1–3]. Among various types of antioxidants, natural vitamins represent a wide group of chemically distinct, water-soluble, and biologically active compounds which serve to inhibit or delay the oxidation of important macromolecules of cells by scavenging those free radicals [4,5]. These antioxidants may also have potential to protect against a number of disease conditions such as aging, atherosclerosis, cancer, autoimmune conditions, asthma, and arthritis. Some vitamins (vitamin C and vitamin B6) have been often been reported as antioxidants which have the capability to limit the oxidative damage in humans and lower the risk of certain chronic diseases [6–8].

It is broadly recognized that the most vital structural characteristic which facilitates effective antioxidant activity is the presence of one or more conjugated OH groups or COOH groups, which boosts the ability of such a molecule to quench the free radicals [4,5]. There are three major proposed mechanisms which can be used to clarify how antioxidants release the atomic hydrogen from their OH group or COOH group and scavenge free radicals; (1) the hydrogen atom transfer (HAT) mechanism, (2) the single electron transfer–proton transfer (SET–PT) mechanism, and (3) the sequential proton loss–electron transfer (SPLET) mechanism [6,9].Though bond dissociation energy (BDE) is used as a key factor to determine antioxidant capacity of the HAT mechanism, adiabatic ionization potential (IP) and proton dissociation enthalpy (PDE) are used to determine antioxidant efficiency of the SET–PT