

Abstract Submitted
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Thermodynamic and Electrostatic Analysis of Flavonol and Tocopherol Analogues in Anti-Aging Products YOOJIN CHO, RICHARD KYUNG, Choice Research Group — This research examined various physical electrostatic interactions and chemical conformations of the anti-aging products due to their ability to deactivate Reactive Oxidation Species (ROS) in the cells. ROS is highly reactive, causing cell's structural and genetic configurations which lead to cell aging or disease. By using the agents that can reduce ROS, cell aging can be delayed significantly. Examining stereo-chemistry and performing computational analysis of thermodynamic stability help determine which of the components in anti-aging antioxidants are most effective. In this research, the enthalpy and chemical safety of anti-aging antioxidants, such as flavonol, flavonoid, and other vitamin E derivatives were studied by calculating and analyzing the molecules thermodynamic stability. The thermodynamic stability was determined by using stereochemical analysis and calculating optimized enthalpy of the molecules. In addition, VES and -TEA were investigated as vitamin E component together with enthalpies of tocopherols and tocotrienols. In this paper, Density Functional Theory (DFT) was used to assess the molecules electron properties.

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