

Abstract Submitted
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Study on the Molecular Characteristics and Pharmacological Activity of Polyphenols as Antioxidants HANSOL KIM, RICHARD KYUNG, CRG-NJ — Polyphenols are the largest group of phytochemicals widely used as biologically active compounds in pharmacology, medicine, and as potential agents for the prevention and treatment of oxidative stress-related diseases. Many of them have been found in plant-based foods and some are structurally and functionally related to flavonoids phenolic compounds. In this project, thermodynamic and stereochemical properties of several types of biochemical molecules that can be used as a biological antioxidant were studied. Computational and biomedical simulations were used, and have been proven useful in assessing the physicochemical stability of molecules. Molecular editing programs were used to model, optimize, and compare the resulting molecular optimization energies of the phenolic compounds. Various polyphenols were tested when OH groups and functional groups were differently attached to the molecules: those with more OH groups and substituents, and those attached farther apart, or were with less functional groups. For all the types of functional groups attached, the optimization energy of the compounds in which the clusters attached were distanced is usually lower than that of the isomer in which the functional groups are close to each other.

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