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Study on the Reactive Oxygen Species Scavenging Effects of Natural Polyphenol Molecules Using Biophysical and Computational Analysis SEUNG WOO CHA, RICHARD KYUNG, CRG-NJ — Although there are many types of free radicals, the most prominent and concerning radicals in biological systems are derived from oxygen often called reactive oxygen species. Due to certain conditions, oxygens can accept electrons from the outer environment creating three reactive oxygen species: Superoxide anion, peroxide, and hydroxyl radical. The correlation between natural Polyphenol molecules and the effectiveness in dental disease treatment was studied in this research. For the extract molecules to have better effect, molecules with higher thermodynamic stability and activity are needed for their anti-inflammatory effects and effective activity in radical scavenging. The purpose of this research was to determine the safety of the components used in the Polyphenols for periodontal disease treatment by checking whether there was any noticeable difference in molecular energies of the different molecules or structural isomers. Quantum chemical calculations were helpful in determining whether the compound modeled is stable enough to exist naturally as a compound. Models presenting extremely high optimization energies and/or extremely long optimization times were eliminated from the initial list of possible compounds.

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