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Antioxidant Properties of a Simmondsin: A Theoretical Study

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Aim of the study: Simmondsin is an extract of jojoba seeds and a part of the chemical family of flavonoids. Flavonoids are generally composed of polyphenol compounds of plant origin with various biological and chemical activities. Several experimental studies have been shown that antioxidant activity of simmodsin but there is no theoretical study. Because of hydroxyl (OH) groups in the structure of simmodsin, it can scavenge free radicals produced in vivo.

Material and Methods: In this study, the antioxidant activity of a simmodsin have been calculated using density functional theory (DFT), at B3LYP/ 6-31G+(d,p) level. For the antioxidant activity we must calculate the OH bond dissociation enthalpies (BDE) for hemolytic O-H bond breaking and the ionization potential (IP) in the gas phase at 298.15 K.

Results: The antioxidant estimation of simmodsin has been determined. Our calculations represented that IP and ΔE_{iso} are electronic properties responsible for the excellent antioxidant activity of the simmodsin is a flavonol class, which is one of the most antioxidant natural phenolic compound.

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Keywords: simmodsin,density functional theory (DFT), antioxidant activity.