### Title: Quantum mechanical study of antioxidative ability and antioxidative mechanism of chrysin in solution

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**Abstract:**

Introduction: Chrysin is a biologically active natural molecule that present in many plants and belongs to flavonoids family. Flavonoids are the most important class of polyphenolic compounds, which in addition to their important biological roles in plant pigmentation, nitrogen fixation, and chemical defense possess anti-cancer, anti-inflammatory, antibacterial, antiviral, and anti-allergic properties that are a consequence of their antioxidant properties. Antioxidants are compounds that can prevent biological and chemical substances from oxidative damage by reactive oxygen species such as the hydroxyl radical, the superoxide radical, singlet oxygen and lipid peroxyl radicals. The objectives of this study are to investigate the antioxidant of chrysin including hydroxyl radical scavenging activity.

Method: Quantum mechanical calculation were carried out using the Gaussian program series 2003 with DFT method at the B3LYP/6-311++G** level in gas and solvent phase by using PCM method.

Results: The interaction between chrysin and hydroxyl radical has been simulated by using quantum mechanical calculations and B3LYP/ 6-311++G** method. The results of our calculations indicate that the oxidation of chrysin by hydroxyl radical is an exothermic reaction about 27 kcal /mol. Our calculation has been done in the gas and in solution phase.

Conclusions: According to our calculated results, chrysin has tendency to donate an electron to active radicals, converting them to more stable non reactive species and terminating the free-radical chain reaction. The molecular properties that we used to investigate a possible antioxidant mechanism of chrysin were the spin density distribution of the radical formed after the abstraction of the hydrogen atom.

**Chrysin, Antioxidant, QM calculation, Exothermic**

**Presentation:** Poster