

Theoretical Investigation of Metal Chelating Activity in Phenolic CompoundsAslı ÖZTÜRK KIRAZ¹, İzzet KARA², Yeşim KARA³, Soner ÖZGEN⁴¹*Pamukkale University, Science and Art Faculty, Physics Dep., 20070, Denizli, Turkey*²*Pamukkale University, Education Faculty, Mathematics and Science Educ., 20070, Denizli, Turkey*³*Pamukkale University, Science and Art Faculty, Biology Dep., 20070, Denizli, Turkey*⁴*Firat University, Science and Art Faculty, Physics Dep., Elazığ, Turkey*

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Aim of the study: Flavonoids are generally composed of polyphenol compounds of plant origin with various biological and chemical activities. Since the presence of carbonyl and hydroxyl groups they can coordinate metal ions and form complexes. Flavonoids can chelate metal ions preventing them in the participation to form free radicals, and protect against oxidative stress. Many studies have confirmed that flavonoids can behave as antioxidants because of their chelating properties. In this study, inhibition of free radicals using some flavonoid compounds chelate with the Fe⁺² and Cu⁺² are examined to determine their antioxidant effects.

Material and Methods: We have utilized B3LYP/6-31G+(d,p) method to explore the antioxidant effects and structure–activity relationships of some flavonoid chelate with Fe⁺² and Cu⁺². The electronic properties and various molecular descriptors such as the BDE, HOMO and E_{gap} of the chelate complexes have also been obtained and studied, which are relevant to show evidence of antioxidant activity.

Results: Flavonoids are common to chelate iron and copper, by that removing a random factor for the development of free radicals. So quercetin form complexes with Cu⁺² and Fe⁺² show strong antioxidant activity. It is also important to understand the properties of the flavonoids chelating with metal-ions for developing new molecules.

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Keywords: polyphenol compounds, metal chelating activity, electronic properties, antioxidant activity.