STRUCTURE AND BINDING SITES OF MOST STABLE CHELATES OF NEUTRAL, MONO- AND DI-DEPROTONATED FORMS OF QUERCETIN WITH DIVALENT METAL CATIONS

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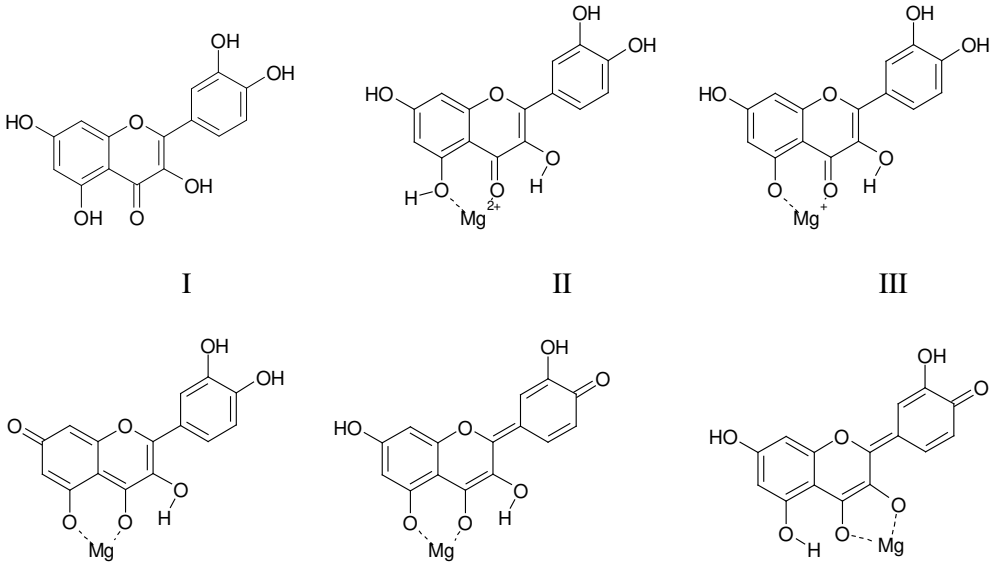
Flavonoids are important group of polyphenolic compounds commonly occurring in fruit and vegetables. They can bind to biological polymers, chelate metal ions, catalyze electron transport, and scavenge free radicals. It is general agreement that flavonoids possess both excellent iron-chelating and radical-scavenging properties. However, is has been much discussion and controversy regarding their relative contribution to antioxidant activity. The ability of flavonoids to chelate redox active metal ions like Fe^{2+} is very important for their antioxidant activity because site-specific scavenging may occur. If Fe^{2+} or Ni^{2+} cation chelated by the flavonoid is still catalytically active then radicals are formed in the vicinity of the flavonoid molecule that can be scavenged immediately. It is expected that in this case the flavonoid would have synergetic action, which would make it a more potent antioxidant.

In this work we present results of our experimental and theoretical studies using quercetin (I) as a flavonoid model compound and several divalent cations: Mg^{2+}, Fe^{2+}, Ni^{2+} and Cu^{2+}. Experimental study is based on UV-VIS absorption spectroscopy and cyclic voltammetry. In our theoretical study we use B3LYP/6-311G**//B3LYP/6-31G* model chemistry to obtain optimum results with respect to accuracy and calculation time. The LANL2DZ basis set developed to handle heavy atoms after the third row of the periodic table seemed to be too slowly convergent in energy minimization, and quadratic convergence method (SCF=QC) occurred to be too much time consuming. Structures II-VI were found theoretically as the most stable. The important result of our work is a finding that a doubly deprotonated quercetin forms species with quinone structure.



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