QSAR Analysis of the Lipid Peroxidation Inhibitory Activity with Structure and Energetics of 36 Flavonoids Derivatives

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Abstract

The biological activity relationship of 36 flavonoid compounds was investigated using theoretical methods including quantitative structure activity relationships (QSAR) and quantum chemistry calculation. The results suggested that the 5 and/or 8 positions of the substituents of the hydroxyl group in the A ring and the 3' and 4' positions of substituents of the hydroxyl group in the Bring play an important role in flavonoid biological activity. This is probably due to the formation of an intra-molecular hydrogen bond. In addition, the electronic energy, electrostatic energy and bond energy may have an effect on the biological activity of flavonoids. Also, our analysis has shown that the presence of the 1,4 and 1,2-hydroquinone in the A ring and/or the B ring of flavonoids and the contribution of electronic energy, electrostatic energy and bond energy required consideration in the generation of the QSAR model and that the potential compounds will be predicted out of 36 flavonoids.