Molecular modeling of flavonoids that inhibits xanthine oxidase

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摘要.

Abstract

The inhibition of xanthine oxidase activity by various flavonoids was assessed. All of the tested flavonoids were competitive inhibitors, and from the kinetic analysis suggested that flavonoids bind to the reactive site. To further understand the stereochemistry between these flavonoids and xanthine oxidase, structure-based molecular modeling was performed. Apigenin was the most potent inhibitor which showed the most favorable interaction in the reactive site. The bicyclic benzopyranone ring ofapigenin stacked with phenyl of Phe 914, and the phenolic group stretched to the space surrounding with several hydrophobic residues. Quercetin and myricetin composed a 3-hydroxyl group on benzopyranone which resulting in reduction of binding affinity. The phenolic group of genistein positioned in opposite orientation comparison with apigenin, and resulted in a weaker interaction with xanthine oxidase. Isovitexin showed the weakest inhibitory effect among the compounds tested. The bulky group ofsugar in isovitexin may hamper its interaction with xanthine oxidase. (c) 2002 Elsevier Science (USA).