Structure Activity Relationship of Biologically Active Flavonoids

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Structure Activity Relationships (SAR) is relations between the molecular structure and biological activity of compounds and is used to determine the chemical groups responsible for evoking a target biological effect in the body, predict expected pharmacological activity, discover and develop new compounds. Flavonoids belong to the large group of natural polyphenolic compounds ubiquitously found in plants. Many reports illustrated that these secondary metabolites are responsible for the variety of pharmacological structure dependent activities, including antioxidant, antitumor, anti-inflammatory, antiviral and chemopreventive;it was suggested that the biological effects of flavonoids might depend on their anti-oxidant activity. The chemical nature of flavonoids depends on their structural class, degree of hydroxylation, other substitutions and conjugations. Flavonoids occur both in freestate and as glycosides. The common characteristic of the flavonoids (flavones, flavonols, flavanols, and flavanones) is the basic 15-carbon flavan structure ($C_6C_3C_6$; Fig.1). Classes of flavonoids differ in the level of saturation of the C ring. Individual compounds within a class differ in the substitution pattern of the A and B rings that influence the phenoxyl radical stability and the antioxidant properties of the substances. By several investigators have been demonstrated that the free radical-scavenging potential of natural polyphenolic compounds appears to depend on the number and location of free −OH groups on the flavonoid skeleton; flavonoids with multiple hydroxyl groups are more effective antioxidants than those with only one; the presence of the ortho-3,4-dihydroxy structure increases the antioxidative activityof these compounds;pro-oxidant effect of flavonoids are related to the presence of hydroxyl groups, especially in the B ring. The SAR studiesshowed that hydrophobicity and electronic property are key factors in the antibacterial activity of flavonoids; for example, high positive charges on C3 lead to an increase in antibacterial activity. Data from literature suggest thatoccurrence, position, structure, and total number of sugar moieties in flavonoid (flavonoids glycosides) play an important role in antioxidant activity;aglycones are more potent antioxidants than their corresponding glycosides.In conclusion we can say that SAR is key to many aspects of drug discovery, it can provide useful tools for revealing the nature of flavonoid action and may also help in the design of new and efficient flavonoids, which could be used as potential therapeutic agents.

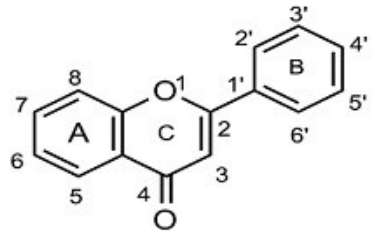

Fig. 1: Basic structure of flavonoid
Methods: Published scientific literature and journals from different sources

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