

Insilico studies on the inhibitory effect of flavonoids on angiotensin converting enzyme activity.

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ABSTRACT

Angiotensin converting enzyme is an exopeptidase that participates in the body's renin-angiotensin system. By catalyzing the conversion of angiotensin I to angiotensin II and degradation of bradykinin, it results in vasoconstriction and hypertension. It is one of the key enzymes involved in cardiovascular, renal and diabetic disorders and thus can act as a potential drug target. Ligands that can block its activity can be applied for designing novel drugs. Flavonoids are polyphenolic secondary metabolites produced by plants. They are naturally available in vegetables and fruits. This study involves insilico interaction analysis of the drug target with flavonoid ligands obtained from vegetables. Computational Biology tools are harnessed for the structural analysis of the target, docking studies and toxicity prediction of the ligands. The results indicate that flavonoids seem to be natural, safe and potent inhibitors of Angiotensin converting enzyme and further facilitate the understanding of their probable mechanism and application in inhibitor based therapy.