

عنوان مقاله:

Investigation of plant flavonoids as potential dengue protease inhibitors

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خلاصه مقاله:

Introduction: Dengue infection is one of the worldwide problems with an increasing rate. Dengue virus (DENV) belonging to Flaviviridae family carries a positive single strand RNA, consists of four serotypes, gives rise to dengue shock syndrome, undifferentiated fever (DF), and dengue hemorrhagic fever. Unfortunately, there is no licensed drug available for various serotypes and the vaccine candidates are still under investigation. Flavonoids are a group of important phytochemicals of many plants used against various viruses. Therefore, the present study was designed to screen the subset of plant flavonoids against the DENV NS₂/NS₃ protease of 3L6P and 2VBC of serotype 1 and serotype 4 respectively by in silico docking. Methods: Flavonoids were subjected to docking study using AutoDock Vina. The lead molecule was further investigated for its dengue viral protease inhibition. Further the cytotoxicity of lead molecule was tested by 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) assay. Absorption, distribution, metabolism, excretion and toxicity (ADMET) study was performed using OSIRIS software. Results: The flavonoids amentoflavone, quercetin-3-O-β-D-glucopyranoside, avicularin, reynoutrin, silymarin and scutallarein showed potential interactions in both serotype 1 and serotype 4 and hence these flavonoids can be served as potential lead candidates to stop viral replication. Amentoflavone, the lead molecule, showed potential in-vitro protease inhibition activity and also the concentration was below the minimal effective level for the in-vitro cytotoxicity test conducted. Conclusion: This finding has laid the groundwork for eventual identification of these flavonoids in developing potential inhibitor candidates for further development by in-vitro extraction and chemical modification .methods

کلمات کلیدی:

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