عنوان مقاله:

Investigation of ADMET properties and interaction of Amygdalus persica compounds with coagulation factor VIIa

محل انتشار:

دومین همایش بین المللی زیست شناسی و علوم آزمایشگاهی (سال: 1402)

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خلاصه مقاله:

A.persica (Rosaceae) is a common folk medicine in China. Some compounds have been found to be effective inthe blood clotting process. However, conducting experimental analysis on the effects of these differentcompounds on the extrinsic pathway and especially factor VII is time-consuming and expensive. Therefore, thisstudy used computational analyses, such as binding, physicochemical, and pharmacokinetic servers, to identifypotential coagulation activity in A.persica compounds. In this research, the ADMET lab web server, DiscoveryStudio, and Autodock were used to assess the proper binding to target proteins and predict theirphysicochemical and ADMET (adsorption, distribution, metabolism, excretion, and toxicity) properties.Coagulation factor (F) VIIa was selected as target protein and docking studies revealed that all compounds wereeffective on this factor, while Hespridin showing better binding results. Moreover, ADMET studies showed thesafety profile of these compounds. In conclusion, carboxylic groups Hespridin, along with alcoholic groups ofKaempferol, Naringenin, Quercetin play a role in interacting with FVIIa. Additionally, based on the ADMETcharacteristics and suitable pharmacokinetic potentials of these compounds, they could be introduced ascandidates for blood coagulants with fewer side effects in bleeding disorders. However, further studies arenecessary to evaluate the precise components of A.persica with the ability to bind coagulation factors

کلمات کلیدی:

Amygdalus persica , molecular docking, coagulation factor VIIa, plant, ADMET