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(In the field of Organic Chemistry)

Virtual screening of new ursolic acid derivatives against HIV-1 protease activity Molecular docking and structure activity relationship studies

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Abstract

Ursolic acids are lipophilic pentacyclic triterpenoid which are found in a wide range of herbs and fruits. In recent years due to the pharmacological effects of ursolic acid along with its low toxicity much attention has been drawn to this compound. Ursolic acid has pharmacological activity such as antimicrobial, antioxidant, antitumor, antiwound and anti-inflammatory. Moreover, it can be used as an alternative medicine for the treatment and prevention of cancer, obesity/diabetes, cardiovascular disease, brain disease, liver disease, and muscle wasting (sarcopenia). In this research, the structure of some ursolic derivatives were optimized using quantum calculations. Then molecular docking of these derivatives with HIV-1 protease enzyme with 3 codes 1HIV, 4MC9, 1HXW was done by MOE software. And the results of molecular docking were analyzed. As we expected, van der Waals interactions of these derivatives with HIV-1 protease enzyme played an important role in the inhibiting of this enzyme. In addition, some derivatives formed hydrogen bond, halogen bond and C-H-π interaction with this enzyme.

Keywords: Ursolic acid, Molecular Docking, HIV-1 protease enzyme, Inhibitor