EP 040

Molecular Docking Study Of Phytocompounds Isolated From The Leaves Of Epiphyllum Oxypetalum Targeting Liver Cirrhosis

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Background : The Epiphyllum oxypetalum (E. oxypetalum) is a family of cactaceae and traditionally, this plant was reported a valuable medicinal property including diseases such as sexually transmitted diseases, liver infection, and antiviral disease. The objective of this study was to investigate the insilico therapeutic role of few compounds extracted from the plants against protein responsible for liver cirrhosis.

Methods : The three-dimensional structure of pyruvate dehydrogenase kinase 2 (PDHK2) used for the present docking study was taken from Protein Data Bank (PDB ID: 3CRK). The ligands used in the study were 4-Hydroxy-2-methylacetophenone, Cyclohexylmethyl hexyl ester, Megastigmatrienone C, Stigmasterol and 3D structure of were retrieved from PubChem database. The ligands were docked to PDHK2 protein using "Autodock 4.2." Essential hydrogen atoms, Kollman united atom type charges, and solvation parameters were included with the aid of AutoDock tools. The final figures were created with the help of Discovery Studio Visualizer (Accelrys San Diego, CA, USA).

Results : Our result shows that the better binding interactions of stigmasterol with PDHK2 compared to the other active compounds. Moreover, we measured various parameters such as minimum inhibition constant, Ki and highest negative free energy. We reported that the binding energy was highest in stigmasterol (-7.77 kcal/mol). The free binding energies were (-6.53 kcal/mol), (-4.68 kcal/mol) and (-4.51kcal/mol) using megastigmatrienone C, 4-hydroxy-2-methylacetophenone and cyclohexylmethyl hexyl ester respectively.

Conclusions : This study may provide the clue that stigmasterol extracted from E. oxypetalum leave shows better potential of inhibition against virulent enzyme involved in cirrhosis and can be used to treat liver cirrhosis.

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