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Online Server-Based ADME Analysis of Phytomolecules for the Management of Hyperglycaemia

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ABSTRACT

Background: Diabetes mellitus is a metabolic disorder which is characterized by a defect in insulin secretion, insulin action, or both. In the Indian traditional system of medicine, various herbal medicines are used to treat diabetes mellitus. Drug discovery is a time consuming as well as costly process to develop novel molecules or identify from an existing library of compounds, to increase the speed search of novel compounds various computational methods are used using different software's which helps in the prediction of desired activity and ADMET analysis of lead molecule without conducting any *in-vitro* or *in-vivo* test. For the same purpose, we used online server-based ADME screening of natural compounds for the management of diabetes.

Objective: Server-based screening and identification of lead compounds from natural products for the management of diabetes.

Methods: Through a literature survey, we identified around 400 phytomolecules molecules as a candidate molecule for the search of the antidiabetic compound, their canonical smile were obtained from PubChem (<https://pubchem.ncbi.nlm.nih.gov/>). ADME analysis of selected molecules was performed by Swissdock (<http://www.swissadme.ch/index.php>) for the identification of novel compounds we had also performed a similarity search using the same software on zinc database.

Results: ADME analysis of selected 400 molecules from natural products and similarity search shows that only 30 molecules have a drug-likeness property based on the Lipinski rule of five although plant-based molecules work differently as compared to the allopathic system of medicine.

Conclusion: ADME screening plays important role in the development of drug molecules, numbers of chemical compounds failed in the preclinical and clinical stage of drug development because of poor ADME properties, it could be helpful for the development of novel phytomolecules for the management of diabetes.



Aims & Scope

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