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List of Abstracts of Oral Presentation

Biological Sciences

Abstract No: BO-04

Identification of plant based anti-diabetic drug leads: A computer-based drug discovery approach

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Diabetes mellitus is known to be one of the fastest-rising chronic metabolic diseases with multiple etiologies. The disease is characterized by chronic hyperglycemia resulting from defects in insulin secretion, insulin action or both. Available therapeutic agents, come with their fair share of side effects. Plant-derived medications that have been used for centuries in the treatment of diabetes in ayurveda and folk medicine have gained a lot of attention in recent years. Studies have shown that plants consist of many bioactive compounds with anti-diabetic properties. Computer-aided drug discovery is slowly gaining popularity with molecular docking accelerating drug discovery by providing structure-based interactions between ligand and receptor proteins. This study was designed to use computational methods to identify the best anti-diabetic compounds devised from ten selected plants. A total of ten plants and three target receptor proteins were selected for *in silico* screening based on the literature. The selected plants were *Nigella sativa L., Coccinia grandis (L.) Voigt, Cheilocostus speciosus (J.Koenig) C.D.Specht, Momordica charantia L., Strychnos potatorum L.f, Gymnema sylvestre (Retz.) R.Br., Aloe vera (L.) Burm.f., Scoparia dulcis L., Abutilon indicum (L.) Sweet, and Trigonella foenum-graceum L.* A phytochemical compound library with a total of 952 ligands was prepared using IMPPAT database. The main target receptor proteins, include α-glucosidase, α-amylase and dipeptidyl peptidase-IV (DPP-IV), based on their key roles in the maintenance of glucose homeostasis. The 3D protein structures were downloaded from the RCSB Protein Data Bank. Miglitol, sitagliptin and acarbose were selected as reference drugs for each target protein to conduct a comparative study. Biovia Discovery Studio was used to visualize the target protein and prepare the protein for virtual screening. UCSF Chimera and PyRx Autodock were used for the energy minimization of the proteins and the virtual screening respectively. Schrodinger Maestro was used for the dynamic simulation studies with the OPLS-2005 force field and TIP3P Solvent model. The compound library was screened by carrying out flexible docking against each target protein. The search space for virtual screening was defined to include all the critical inhibitor-binding sites based on the literature. All the compounds having binding affinity less than 6 kcal/mol were rejected. Only the compounds with promising binding energy values, depending on each target, were subjected to the target-ligand interaction analysis conducted using Biovia Discovery Studio. The binding affinity and interaction patterns of phytochemical ligands were evaluated against three receptor proteins. The best three molecules for each protein were selected based on the best hydrogen bond interactions since they determine the specific, energetically favorable ligand binding at the target sites. The selected 12 molecules were further analyzed for the best target-ligand binding conformation and subjected to molecular dynamics simulation. Compound 27 and compound 85 in *T. foenum-graceum* with RMSD less than 3Å and hydrogen bond retention above 75% in 100NS simulation were identified as promising therapeutic drug leads for the treatment of diabetes. *In vitro* screening for the antidiabetic activities would be conducted using α-glucosidase, α-amylase and DPP-IV assays to further assess their effectiveness as anti-diabetic drug leads.

Keywords: Anti-diabetic assays, *Cheilocostus speciosus*, *Gymnema sylvestre*, Molecular docking, *Trigonella foenum-graceum*

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