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Molecular Docking Insights to Anti-Diabetic Drug Discovery Using Bioactive Compounds

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Abstract

Diabetes mellitus is a metabolic disorder that has become a global health problem. About 500 million people where estimated to be living with diabetes in 2018 with about 20 million in Africa and 2 million cases in Nigeria. Bioactive compounds offer an advanced starting point in the search for highly specific and potent modulator of bimolecular function as well as novel drugs, which can be studied with more precision by using computer aided drug design (CADD). Molecular docking employed for predicting the interactions between receptor and ligands is an integral aspect in drug discovery. The main objective is to attain ligand-receptor complex with optimized conformation and with the intention of possessing less binding free energy. Several studies have used this method to explore the potency of bioactive compounds to predict better alternatives in the search for an anti-diabetic drug with very effective therapeutic role and minimal side effects. This has been carried out by using several compounds such as Quercetin and Yohimbine among others, against endogenous targets such as Glycogen phosphorylase, Peroxisome Proliferator-activated Receptor (PPAR)-y, Glucokinase, Protein Tyrosine Phosphatase 1-beta (PTP-1B), GLUT4, etc. In Silico tools such as Protein Database (PDB), GenBank and softwares such as Autodock and modeller are of major importance to these studies.The paper seeks to examine bioactive compounds that have been successfully identified through molecular docking and their molecular targets as well as recent advances in the use of molecular docking in the novel discovery and explanation of mechanisms of actions of some bioactive compounds in anti-diabetic drug discovery.

Biography

Teibo, Oluwafemi John is a biochemist and a researcher currently doing his Postgraduate training at the University of Ibadan, Ibadan, Oyo State, Nigeria. He has interest in Biochemistry and Molecular Biology, Bioinformatics and Computational Biology. He is a student member of Genetics Society of Nigeria and International Society of Computational Biology. He is also the Project Manager and General Secretary of Team Brainiac Organization. He is currently undergoing H3ABionet: Introduction to Bioinformatics course in Africa. He has some publications to his credit.

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