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Phyto diab care: Phytoremedial database for antidiabetics

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Abstract:

Diabetes, a chronic disease debilitating to normal healthy lifestyle, onsets due to insufficient amount of insulin production or ineffective utilization of the amount produced. Although, pharmaceutical research has brought up remedial drugs and numerous candidates in various phases of clinical trials, off-target effects and unwanted physiological actions are a constant source of concern and contra indicatory in case of diabetic patients. Here we present a phytoremedial database, Phyto Diab Care, broadly applicable to any known anti-diabetic medicinal plant and phytochemicals sourced from them. Utilization of the traditional medicine knowledge for combating diabetes without creating unwanted physiological actions is our major emphasis. Data collected from peer-reviewed publications and phytochemicals were added to the customizable database by means of an extended relational design. The strength of this resource is in providing rapid retrieval of data from large volumes of text at a high degree of accuracy. Enhanced web interface allows multi-criteria based information filtering. Furthermore, the availability of 2D and 3D structures from molecular docking studies with any efficacy on the insulin signaling pathway makes the resource searchable and comparable in an intuitive manner. Phyto Diab Care compendium is publicly available and can be found in online.

Availabilty: http://www.gbpuat-cbsh.ac.in/departments/bi/database/phytodiabcare/HOME%20PAGE/Home%20page.html

Key Words: Diabetes, Phytochemicals, Insulin signaling pathway, Phyto Diab Care.

Background:

Since ancient times, plants have an exemplary source of herbal medicines. Indian literature mention the use of plants in treatment of various human diseases. Research conducted in last few decades on plants mentioned in ancient literature or used traditionally for diabetes have shown anti-diabetic property [1]. Diabetes is considered as the fourth leading cause of deaths by diseases in world. According to International Diabetes federation, the total number of diabetic subjects in India is 41 million in 2006 and that this would rise to 70 million by the year 2025 [2]. Diabetes represents a spectrum of metabolic disorders, which has become a major health challenge worldwide. The treatment of diabetes with synthetic drugs is

generally not preferred because of its high cost and the range of side effects caused [3]. Hence there has been a growing interest in herbal remedies that can be introduced into the general population with the least side effects and the maximal preventive outcome.

Many traditional plants medicines are used throughout the world to treat the Diabetic diseases [4, 5]. Many herbs have been used to cure diabetes since ancient times in countries like India, Egypt, China and some Arabian Peninsula countries. In this database we collected the data of antidiabetic medicinal plants and phytochemicals responsible for their antidiabetic activity and we emphasized the role of information derived

BIOINFORMATION

from various systems of traditional medicine (*Ethno medicine*) and its utility for drug discovery purposes. Keeping in mind the importance of Anti diabetic plants and their phytochemicals, this customizable database provides detailed information on properties, taxonomic information of plants and structure of phytochemicals, which can be used for molecular docking studies on the components of insulin signaling pathway in order to determine the insulinomimetic or insulomimitic properties.

Methodology:

Construction of Phyto Diab Care

PhytoDiabCare is constructed using hypertext mark-up language (html) and can be accessed at http://www.gbpuat-

cbsh.ac.in/departments/bi/database/phytodiabcare/HOME% 20PAGE/Home%20page.html. Data were collected from various literature sources from the web. Phyto Diab Care containing data of about 230 plants and 155 phytochemicals which are obtainted from different plants and possess medicinal properties against diabetes. The PDB structures of 155 phytochemicals were generated through ligbuilder utility of Molecular Operating Environment (MOE) v 2008-10 [6] using the SMILES notation obtained from the PuBChem [7] and convert into 2D and 3D structure and also save them into images. The database can be accessed alphabetically using plant and phytochemical name for information on specific plants.



Figure 1: A screen shot of the PhytoDiabCare database.

Features of PhytoDiabCare

PhytoDiabCare is provided information about the diabetes, insulin receptor, insulin signaling pathway along with its components, 230 anti diabetic plants and 155 phytochemicals, The Anti Diabetic Plant and phytochemicals link display an alphabetically list of medicinal plants and list of phytochemicals respectively. The Anti Diabetic Plants provides Texan information, morphololigal characteristic, anti diabetic properties and economic & other medicinal importance uses of each plant. Besides the information of about phytochemical, the page of each phytochemical provides 2D and 3D structure of

them. **Figure 1** is showing a screen shot of the different pages of PhytoDiabCare database.

Utility to the biological community

Phyto Diab Care emphasizes the information of anti diabetic plants and phytochemicals. The database finds utility to the scientific community for a quick review on the number of plants and phytochemicals for diabetes medicinal plant research and provides enormous scope for development of drugs.

Future development

Continuous updates shall be released to include other plants of anti-diabetic properties periodically and also docking studies of phytochemicals with insulin receptor. The present access method shall be upgraded for faster access to accommodate the growing number of data to browse records on the studied plants and phytochemicals. We plan to develop provisions to search the database to identify plants of interest using keywords.

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