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DIACAN: Integrated Database for Antidiabetic and Anticancer Medicinal Plants

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Abstract:

Medicinal plants and plant derived molecules are widely used in traditional cultures all over the world and they are becoming large popular among biomedical researchers and pharmaceutical companies as a natural alternative to synthetic medicine. Information related to medicinal plants and herbal drugs accumulated over the ages are scattered and unstructured which make it prudent to develop a curated database for medicinal plants. The Antidiabetic and Anticancer Medicinal Plants Database (DIACAN) aims to collect and provide an integrated platform for plants and phytochemiclas having antidiabetic or anticancer activity.

Availability: http://www.kaubic.in/diacan

Background:

Nature has provided an innumerable number of culturally important medicinal plants that have been indispensable for the treatment of various diseases and maintaining health. Plants produce a wide variety and high diversity of secondary metabolites, which are not required for the immediate survival of the plant but which are synthesized in response to stress as a means to protect themselves from organisms, diseases or the environment **[1]**. Plant kingdom is a promising source of chemical constituents that are of high value to human beings because of their profound physiological effect on the mammalian system and can be used as a source for new pharmacologically active compounds.

Cancer is the second leading cause of mortality at present and it strikes more than one-third of the world's population. Influence of natural products in the area of anticancer drug discovery is quite marked, both for use as such and as platforms for developing more effective molecules **[2]**. Phytochemicals ISSN 0973-2063 (online) 0973-8894 (print) Bioinformation 9(18): 941-943 (2013) obtained from medicinal plants seems to be one of the most feasible and promising approaches for chemoprevention [3].

Diabetes has emerged as the leading cause of premature illness and mortality in both developed and developing countries and it is estimated that 25% of the world population is affected by this disease **[4]**. Although numerous synthetic drugs were developed, medicinal plants and their derivatives were widely considered in the treatment of diabetes because they are effective, non-toxic, with less or no side effects and are considered to be excellent candidates for oral therapy **[5]**.

Despite recent improvements made in the treatment of cancer and diabetes, there is a growing interest in herbal drugs due to the undesired side effects associated with chemotherapy and oral hypoglycemic agent **[6, 7].** Currently, a few plant based products are being used to treat cancer and diabetes. However, a myriad of unexplored potentially useful plant products exist that have shown very promising anti-cancer and antidiabetic

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properties **[8].** Antidiabetic and Anticancer Medicinal Plants Database (DIACAN) is unique in providing a comprehensive platform for antidiabetic/anticancer medicinal plants,

taxonomical hierarchy, phytoconstituents isolated from the plants, and medicinal properties obtained through literature mining.

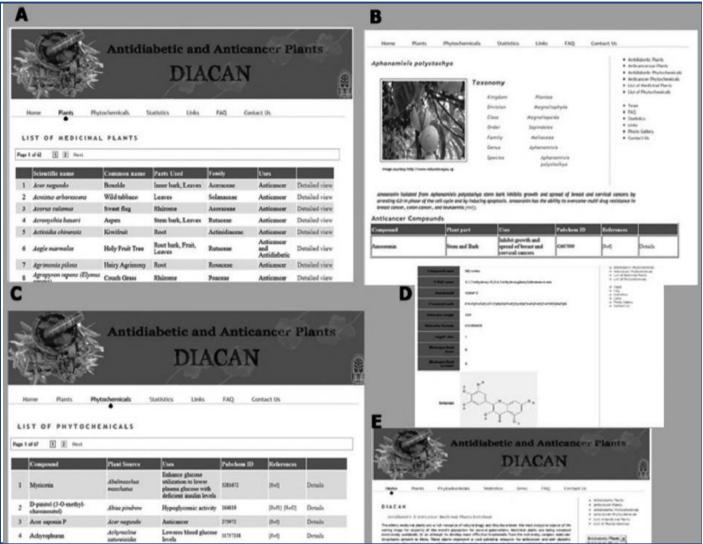


Figure 1: Screenshots of the web-interface of the DIACAN. **A)** Medicinal plants and their bioactivity listed alphabetically; **B)** Detailed description page for individual Medicinal Plant; **C)** Plant derived phytoconstituents and their uses arranged in the order of alphabetical list of Medicinal plants; **D)** Property of Phytoconstituent and 2D structure; **E)** Drop down search box for alphabetical listing.

Methodology:

Database Architecture and Implementation

MySQL 5.0 (http://www.mysql.com/), an object-relational database management system was used (RDBMS) at the backend which stores information as tables and performs SQL (Structured Query Language) queries that provides speed and flexibility in data retrieval. Hypertext Preprocessor (PHP) programming language along with HTML and JavaScript was used as the front end in order to provide dynamism to the Web interface. DIACAN was deployed on Apache HTTP server and runs on a server managed by the Windows operating system.

DataBase Access

The lists of antidiabetic plants, anticancer plants, antidiabetic phytochemicals and anticancer phytochemicals have been ISSN 0973-2063 (online) 0973-8894 (print)

alphabetically indexed based on plant name in the database. The user can click on the medicinal plant detailed view link and a new page will appear that display the details of the plant and its activity towards diabetes or cancer (Figure 1). The corresponding page for each plant is comprised of (i) general information including scientific name of the plant, taxonomic classification, image of the plant, image courtesy, ii) detailed description regarding the bioactivity of the plant and related references with literature citation, iii) phytoconstituents isolated from the plant having antidiabetic or anticancer activity, plant part from which the compound was isolated, description regarding the activity of compound with related reference, iv) PubChem ID, and compound detail view hyperlink. By clicking on detailed view hyperlink user can view the compound chemical properties of like IUPAC name, molecular formula,

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molecular weight, hydrogen bond donor, canonical smiles and 2D structure of the phytochemical. Drop down search box with scientific names in alphabetical order is also provided for easy retrieval of data. A photo gallery of medicinal plants is also provided in the database. DIACAN is also having cross references to databases like PubChem and PubMed.

Utility:

DIACAN will be a specialized, first of its kind value-added database that will enable effortless pursuit of relevant knowledge on anticancer and antidiabetic medicinal herbs and phytoconstituents, thus making it a unique resource in the area of cancer and diabetes. DIACAN will help in the process of Drug Discovery by providing a promising starting point for *in silico* screening of phytochemicals.

Future development:

We are working to elaborate the database by incorporating data on disease targets of phytoconstituents and geographic location of the medicinal plants. Additional search and retrieval features will also be added to enhance the usability of the web interface.

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