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NMD SERVER: NATURAL MEDICINES DATABASE FOR DRUG DISCOVERY

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Abstract

Cancer is the most frequently diagnosed disease globally and the second leading cause of the death. Natural Medicines are the alternative form of treatment that includes use of various plants. It is one of the safe treatment option to treat cancer and safer than allopathic medicines in order to reduce side effects. NMD Server: Natural Medicines Database for Drug Discovery is a unique and significant database of its kind, giving researchers, medical practitioners, pharmaceutical industries and students of Life Sciences an instant access to over 354 records of Natural Medicines which may be developed and used for treatment of Cancer. This database constitutes the specific information related to Natural Medicines and their respective target sites. NMD Server: Natural Medicines Database for Drug Discovery provides all the information (database fields) regarding the physiological parameters of database and is considered to be the linked table with pre-determined values and names that are included to aid in populating the fields of the linked tables. There have been many different types of fields with its respective data types that have been designated on the basis of data provided. NMDdock

Tools have been integrated in this database for convenience for users like docking analysis of target and natural medicine, Sensitivity & Specificity analysis of natural medicine, Linear Correlation and Regression tool, Sequence Manipulation of target, Statistical Analysis. For the precise information about any particular drug, connectivity has been made with other databases and applications based highly bioinformatics tools have been embedded for convenience of users.

Keywords

Natural Drug, Target, NLP, Integration, Wrapper, Target Site, NMDdock

1. Introduction

Cancer characterized by uncontrolled growth and abnormal cells, is still the second most typical leading cause of the death within the U.S. According to ACS (American Cancer Society), ~571,950 Americans are expected to die in 2011 due to cancer disease, that means over one, 500 deaths per day. Current diagnosed for various cancers surgery, radiation, hormone care, and chemotherapy (Bernstein, et al 1977). These standard therapies have extended the patients survival, with many limitations. For example, cancer treatment has the cancer therapeutic agents allocating non-specifically in the organic structure, thus these medication have an effect on each cancerous and normal cells (Xu and Wang, 2006) where non-specific distribution of medication limits the therapeutic dose among cancerous cells whereas providing excessive toxicities to normal cells, tissues, as well as organs; and thereby causing many adverse aspect effects together with hairloss, weakness, and organ dysfunction, leading to an occasional superiority of life for cancer patients (Kaushik and Sharma, 2013; Bohari, et al 2011). Over the past several decades, amazing breakthroughs have been created in progressing our understanding of however cancer originates and develops, which has in flip crystal rectifier to higher strategies for each identification and treatment (Chin, et al 2009; Agrawal, et al 1993). Over the past several decades, outstanding breakthroughs have been created in advancing our understanding of but cancer originates and develops, which has in flip crystal rectifier to higher ways for every investigation and dealing (Ahmed, et al 2011). Cancer is the current leading reason for death worldwide, responsible for more or less one quarter of all deaths. Natural Medicine offer tremendous opportunities for multimodal, site-specific drug delivery to these disease sites and natural drug any supply a particularly distinctive set of physical and chemical properties (Wolf, et al 2002; Ye, et al 2011). The NMD Server: Natural Medicines Database for Drug Discovery will attribute hugely towards the treatment of cancer. It makes

itself unique from the other databases by amalgamating various extra ordinary features like the drug information along with the target sites, links to journals, facts about the bioinformatics tools as well as it connects with other databases which is adorning the database.

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2. Approach and Techniques

Database architecture, web user interface and approaches:

2.1 Wrapper- the best feature of this database is usage of wrappers; the wrapper strategy explicitly optimizes the performance criterion. We verified this by comparing the results with those provided by the filter approach FCBF method, where if the data about the drug is not available in this database then it will search the data in drug bank database and it will search out complete query unless and until the user is not being satisfied (Wang, et al 2010; Dunkel, et al 2006).

2.2 Data integrity- has been incorporated to make the database more accurate and consistent, though data warehousing require this accuracy to stand against the errors occurring either by the human error, software or the hardware. Federator data warehouse approach has been highly envisaged in inters operating ability of the medical care and its research (Dobson, et al 2009; Peironcely, et al 2011).

2.3 Data mining and data warehousing- Data and information to be mined is first extracted from an enterprise data warehouse into a data mining database or data mart (Ertl, et al 2008; Hodge, et al 2007). There is some genuine benefit if data is already part of a data warehouse, if the data has already been cleansed for a data warehouse (Newman and Cragg, 2010). Furthermore, many of the problems of data consolidation will be addressed and put in place in maintenance procedures. The data mining database is

logical rather than a physical subset of data warehouse for nmd server: natural medicines database for drug discovery.

2.4 Normalization- Normalization is the process of assembling data in a database (Fiszman, et al 2000; Koehn and Carter, 2005; Mishra and Tiwari, 2011; Csizmadia, 2000). Tables were created for NMD server: a natural medicine database for drug discovery (NMD & account) and establishes relationships between both tables according to rules designed so as to protect the data and to make the database more reliable by eliminating redundancy and inconsistent dependency.

3. Materials and Methodology

Data has been collected and gathered from the reliable database drugbank. Normalization has been done so as to protect the data and to make the database more reliable by eliminating redundancy and inconsistent dependency.

First normal form- eliminate redundant data in individual tables, create a separate table for each set of related data, and identify each set of related data with a primary key.

Second normal form- creates separate tables for sets of values that apply to multiple records, relate these tables with a foreign key.

Third normal form- eliminates fields that do not depend on the key.

- Selection and sampling of the related drug data from drugbank.
- Pre-processing and cleaning of undesirable and redundant data.
- Data mining of the data with its nmd id, compounds name, similar compounds, class, lipinski's rule, pubchem, drugbank, kegg, pdb, cancer type (cell lines), targets with reference, target sequence, target properties over it as well as many other links of related to liver cancers may also be extracted and further searched.

- "NMD server: natural medicines database for drug discovery" database is created with the help of mysql as well as connectivity in the front and back end has been done by php.
- Data security has been done with dcl (data control language) and cookies.
- Transformation and reduction along with wrapping of data with the help of wrappers.
- Evaluation and visualization of the queried data from the database and giving all the respective details about that particular data.
- Link has been added: collection of databases, which resemble to database of databases, this info, has been taken from pubchem.
- Data encryption has been applied as the user can encrypt the utilization of tools and other facilities.
- Link outs for bioinformatics tools from various sources has made it more multi-purpose

Data update has been carried out as well as the valuable comments from the will be considered through the mail which has been provided separately from the developer.

4. Results and discussions

Natural medicines database for drug discovery, where search box is shown in the left, and all the images in the top move to and fro which inbuilt the looks of the web page is denoted in figure 1. Search box displays if the drug name is found. If the drug name is not found then data integrity will be applied and the data source will be caught from drug bank using wrapper and nlp approach. Useful links to other biological databases and bioinformatics on-line tools and off line tools have been given. The user can register and log in through username and password; privileged users are allowed to get the encrypted data. Comment page is placed to get the valuable suggestion of the users. Some tools are

also available for members only like coefficients correlation which is used for find out the sensitivity and specificity of natural drug as denoted in figure 2. Linear correlation and regression is used for find out the correlation between normal gene and cancer gene, sequence manipulation is used for primary level manipulation in genes.

Figure 1: *NMD Server: Natural Medicines Database for Drug Discovery front view page*

Figure 2: *NMD Server: Natural Medicines Database for Drug Discovery; tools for finding Specificity and sensitivity of drug*

3. Significance of Work

It is very difficult to learn and carry out research analysis for the various drugs and its other pharmaco-chemical properties, therefore with the invent of more drugs and its successfully completed clinical trials have made the IT sector to be indulged in the field of drugs and its derivates, With the availability of more and more drugs it is impossible task for the human cranial capacity to retrieve out all the information. Therefore, focusing on all these problems; NMD Server: Natural Medicines Database for Drug Discovery is developed to gather all the information about the drug along with its pharmacological properties enhancing the inclination of medical parameters for the treatment of Liver Cancer. This database is not restricted to the database about Natural Medicines only but also provides links to collection of databases as well as software tools, links and updating column being provided for the users.

4. Conclusion

This is a complete health care database of Natural Medicines for liver cancer. NMD Server: Natural Medicines Database for Drug Discovery provides free access to original peer-reviewed biomedical research regarding Liver Cancer publications including journal articles, current reports, and conference abstracts. Information about current controlled trials, as well as topics related to Liver Cancer and Natural Medicines are also included. Bioinformatics Online Tools (BOI) is a research methods tool. BOI links over with advanced search, user can explore methods concepts and conduct their research, and write up for findings.

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