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Cheminformatics-Aninsilico pharmacoinformatics approach in Drug Discovery

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Abstract

Cheminformatics is a novel in silico approach used in drug discovery and designing. Though it is in its budding stage but with the help of cheminformatics identification and analysis of structural and functional behavior of chemical compounds and biological molecules have been made easier. With such progress in the area of biochemistry, bioinformatics make use of such information in computer aided drug designing and development.

Key Words: Drug Discovery; Virtual Chemical Libraries; Open Babel; ChemReader

Introduction

Cheminformatics is a sub discipline of computer molecular science that deals with the information retrieval from chemical databases, three-dimensional molecular and crystal structure modeling, chemical reaction pathway prediction, molecular functional groups and docking sites [1].Cheminformatics originally emerged as a vehicle to help in drug discovery and development process. But now it has numerous application in numerous disciplines such as life sciences, chemistry, biochemistry, structural biology etc [2].This area of research mainly deals with small molecules, whereas bioinformatics covers genes, proteins, and other larger chemical compounds [3]. However both the disciplines are inter-related and quiet novel. Since Cheminformatics is a new field therefore still in its initial stages of development.

Following are some Cheminformatics tools mentioned below that aids in drug delivery and in its related developmental processes [4].

Virtual Chemical Libraries

Chemical databases and libraries contain suppository or imaginary compounds and structures (which do not exist in nature but there is a likelihood that these can be made).These guide the researchers suggesting different desired functionalities that do not exist yet [4]. Virtual libraries can contain information on possible synthesis methods and predicted stability of the different products that come into existence after going through a chemical pathway. It makes use of different chemical and physical principles to identify and choose the best chemical substance for a particular reaction or function, from large libraries of real and virtual molecules. The most suitable candidate can then be confirmed through wet lab experiments [5].

Cheminformatics Tools in Drug Discovery

The most prominent use of Cheminformatics is in drug discovery. The virtual libraries help predict the best substrate for a certain reaction leading to the wet lab experiments of drug discovery process. Before cheminformatics, it took decades for a drug to hit the market. But now with the help of Cheminformatics, this time period has been reduced immensely. Most of the unlikely candidates for a reaction are ruled out in the virtual screening process and then with the help of high throughput screening, a lot of time and manpower is saved [6].

Symyx Draw

It is a free chemical structure drawing program used to draw virtual diagrams of chemical substances. It uses its personal file format as well as the usual chemical file formats like MDL molfile, TGX file etc [7]. One can draw chemical structures and reactions, manually, an also using IUPAC names. It also provides the IUPAC names of the compounds that we have drawn. In addition to this, it allows search and retrieval through chemical databases [8].

ChemDraws

It is a structure drawing tool that allows one to create 3-D chemical structures and reactions with complete chains, rings, functional groups and bonds. It even allows one to find out the structures properties using the tool [9].

ChemReader

It is structure recognition software which retrieves chemical structure diagrams from digital pictures and converts them into computer readable chemical file formats. This information can then be used to search through chemical databases [10].

JME Molecule Editor

It is free java script software that allows users to draw and edit molecular diagrams along with creating substructure queries (queries regarding the molecular structures and its substructures). It can convert structures into numerous file formats [11].

Wendi

Wendi is a web engine for nonobvious drug information. A type of web based integrative data mining tool that is used to find associations between a query compound and scholarly publications, biological properties, genes and diseases that are usually ambiguous using multiple information sources [12].

ChemMine Tool

It is a tool that works online for analysis of small molecule and provides an interface between Cheminformatics and data mining tools for different analytical studies in chemical genomics and drug discovery [13].

CML

CML is chemical markup language, a combination of text and non textual information of chemical structure on the internet [14].

PubChem

It is a database for small molecules and their experimental biological activity. It combines and provides search, retrieval, visualization, analysis access tools [15].

PLSR

PLSR or Partial Least Squares Regression is a chemmetrics tool which relates and works on two matrixes on the basis of some predesigned models, and analyses data in the existence of many nonsensical and even incomplete variables [16].

Open Babel

It is a chemical format converting software that converts structures into different chemical formats [17].

Conclusion

Recognition and assessment of morphological and functional interactions of chemical compounds and biological molecules is one of the most important requirements for medical research which is made easier with the advent of Cheminformatics. A developing field which is progressing rapidly in the biochemical world.

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