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Pharmacoinformatics in Modern Drug Discovery

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Review Article

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ABSTRACT

Pharmaceutical science having many branches which helps us to develop many novel drug discoveries and development. Pharmacoinformatics is one of the relevant and novel topics which elucidating the drug discovery process by using various tools. Pharmacoinformatics in India can be available in National Institute of Pharmaceutical Education and Research. As we know that it is an emerging filed which combines the bioinformatics and pharm field together to develop novel compounds in current research.

INTRODUCTION

The Pharmacoinformatics is an emerging field in which the drug development and modernization of drug discoveries using various bioinformatics field by using various statistical methods and algorithms like artificial Neural Networks, Capacity Building, Cluster analysis and data mining, Computing paradigms, Education, Information representation, Pharmacoinformatics infrastructure, Pharmacovigilance, Pharmacy management, Reporting systems, etc. Pharmacoinformatics is a newly launched branch in India at National Institute of Pharmaceutical Education and Research in the year of 2003. The drug development using in vitro methods is a time taking and costly process [1-6]. By using Pharmacoinformatics we can develop various types of drug candidates by using different computational tools and it is cheap and less time taking than the in vitro methods [7-13].

The drugs which were developed has been conducted several tests and then they can be developed by using in vitro methods. By using these methods the novel drug discovery in pharmaceutical fields were increased and the candidates who were developed are going through different tests to exceed their biological activities.

PHARMACOINFORMATICS AND THEIR BRANCHES IN DRUG DISCOVERIES

Pharmacoinformatics is also known as the interface of technology with the practice of pharmacy **(Figure 1)** [14-16]. It is an emerging field in which we use several disciplines like Pharmacogenomics, Bioinformatics and Cheminformatics for the invention of drugs for the clinical use of medications in individuals and populations. In pharmacy, this field helps us to develop new drug candidates by using different technologies [17-22].

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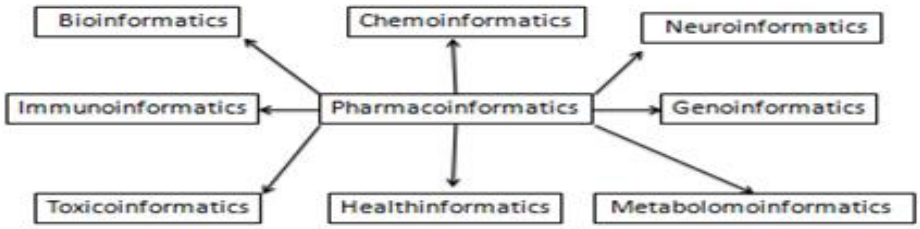
Figure 1: Classification of Pharmacoinformatics.



Pharmacogenomics

Pharmacogenomics was first invented by Pythagoras. When he is performing scientific studies on fava bean injection with haemolytic anemia and oxidative stress accidentally he found about genes were responsible for favism and he recognized it has a genomic studies [23-30]. However, the term pharmacogenomics was first coined by Frienrich Vogel in the year of 1959. Later, in 1960 the twin studies supported us to recognize the genomic involvement in metabolism of drug candidates. The pharmacogenomics is the study of the role of the genome in drug response.

The name itself indicates that the combination of pharmacology and genomics. The studies help us to recognize the drug biological actions (Pharmacodynamics and Pharmacokinetics). The term pharmacogenomics started using from 1990's and the studies on pharmacogenomics helps pharmaceutical development of novel drug candidates for curing effected individuals. By using these studies we can predict the inherited genetic variation on drug response in patients by comparing their correlated gene expression or biological actions like pharmacodynamics actions or pharmacodynamics actions which includes absorption, distribution, metabolism and elimination as well as targeted drug receptor effects [31-35]. Pharmacogenomics enclose a more genome-wide association approach, incorporating genomics and epigenetics for drug response.

The first novel FDA approval of a pharmacogenetic test was performed on alleles in CYP2D6 and CYP2C19 in the year of in 2005.

Bioinformatics

Bioinformatics is a trending field, which combines the biological studies with informatics techniques to develop effective pharmaceutical drug candidates [36-42]. The term bioinformatics came to now in 1990's and it was first invented by Paulien Hogeweg and Ben Hesper in the year of 1970's. It was an emerging field in pharmaceutical science for developing novel drug molecules by performing various in silico methods **(Figure 2).** Various computational tools were used for drug design and development. Current days the term bioinformatics has enlarged and incorporated too many other fields of biological sciences like gene expression, protein-protein interaction studies and microarrays, functional analysis of biomolecules and new drug entities [43-51]. The above mentioned fields will use different kind of databases, algorithms and statistical methods to perform their functions.

Figure 2: Bioinformatics in drug discovery process.

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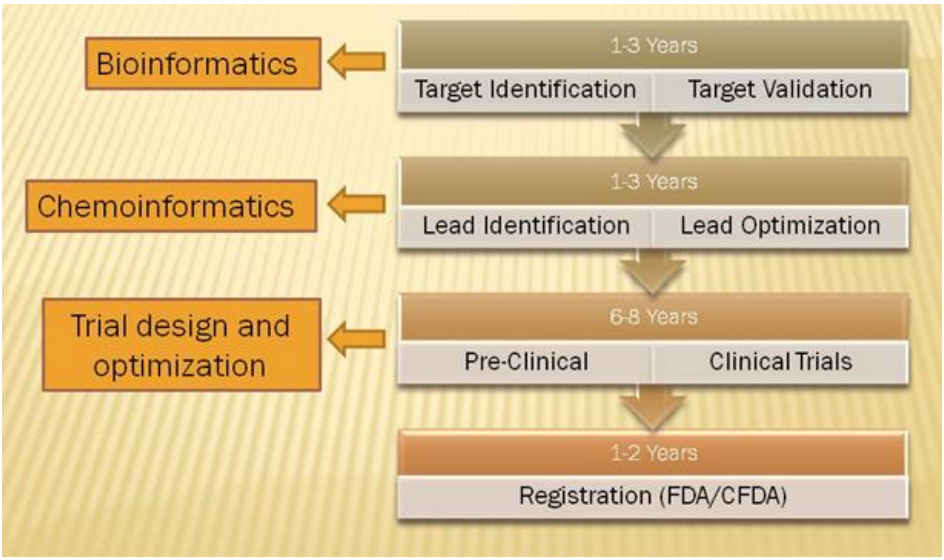


There are three important sub-disciplines in Bioinformatics: the development of new algorithms and novel statistical methods, which helps us to assess relationships among members of large data sets;the analysis and interpretation of many types of data containing nucleotide and amino acid sequences, protein domains, and protein structures;and the evolution and implementation of novel tools that enable efficient access and management of different types of information" [52-58].

Chemo informatics

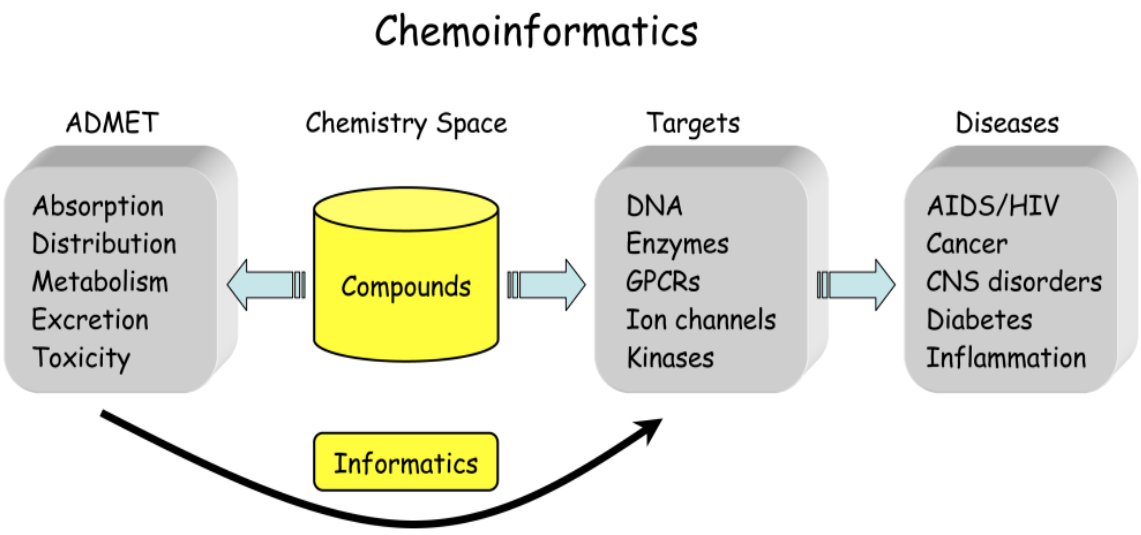
Chemo informatics is the informatics technique to solve chemical problems with the help of informatics tools. It helps in all types of chemistry related fields like chemistry from analytical chemistry to develop novel drug molecules. At present, we are facing several problems and still many chemical challenges waiting for clear solutions by using Cheminformatics **(Figure 3)** [59-65].

The term Cheminformatics first mentioned by Frank Brown in 1998.

Chemical Data →Storage in Databases →Data Information →Data Retrieval →Analysis

Chemo informatics is the arrangement of information resources to transform data into information and information into knowledge for the intended purpose of making better decisions faster in the area of drug lead identification and organization. So chemo informatics is helpful in drug design, Greg Paris came up with a much broader definition [66-72].

Figure 3: Flow char of Cheminformatics in drug discovery.



The current schema of Cheminformatics in drug designing is given below: Analysis of predesigned drug structure structural property prediction (QSAR) property prediction by smiles format perform some modification in

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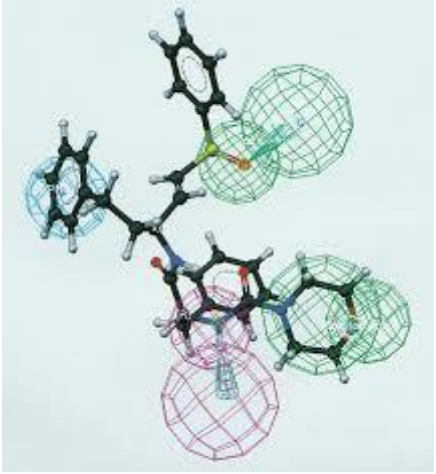
prior drug again predict the drug property if variation occurs in novel structure save that structure and design a fragment library [73-81]. Cheminformatics is a generic term that encompasses the design, creation, organization, management, retrieval, analysis, dissemination, visualization, and use of chemical information.

Quantitative Structure Activity Relationship (QSAR)

Quantitative structure-activity relationships methods are used to show a relationship of structural and/or property descriptors of compounds with their biological activities **(Figure 4)** [82]. These descriptors explaining the properties like steric, topologic, electronic, and hydrophobic of numerous molecules, have been determined through empirical methods, and only more recently by computational methods [83-91].
A QSAR generally takes the form of a linear equation:

{Biological Activity = Const + (C1 P1) + (C2 P2) + (C3 P3) + ...}

Figure 4: Descriptors of compounds with their biological activities.



Discovery Studio is a comprehensive life science modeling and simulation suite of applications focused on optimizing the drug discovery process [92-94]. Capabilities include molecular simulations, quantum mechanics /molecular mechanics, pharmacophore modeling, QSAR, protein-ligand docking, protein homology modeling, sequence analysis, docking studies and antibody modeling, etc.

CONCLUSION

After thoroughly reviewing many topics we have discussed several information technology endeavored to the pharmaceutical industry which helps for novel drug discovery [95-101]. In future, these attempts were expected to grow both in terms of their reliability and scope. Pharmacoinformatics would be an emerging technology field and it becoming an essential component of pharmaceutical sciences and industry for novel discoveries.

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