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# A VITAL ROLE OF PHARMACOINFORMATICS

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**ABSTRACT:** *The rapid growth of the internet and the World Wide Web has led to the development of pharmacoinformatics technologies to assist oncology healthcare professionals in delivering optimum pharmaceutical care and health related outcomes. There is an increasing recognition that information technology can be effectively used for drug discovery. The work in pharmacoinformatics can be broadly divided into two categories - scientific aspects and service aspects. The scientific component deals with the drug discovery and development activities, whereas the service oriented aspects are more patient centric. Pharmacoinformatics subject feeds on many emerging information technologies like neuroinformatics, immunoinformatics, biosystem informatics, metabolomics, chemical reaction informatics, toxicoinformatics, cancer informatics, genome informatics, proteome informatics, biomedical informatics, The minimizing the time between a drug's discovery and its delivery to the marketplace and maintaining high productivity in the manufacturing processes. During a product's lifecycle many complex decisions must be made to achieve these goals. To better support the development and manufacturing processes at each stage, we have proposed a new epitome to facilitate the management and transfer of data information and knowledge. In future these information technology efforts are expected to grow both in terms of their reliability and scope. Thus, this emerging technology (pharmacoinformatics) is becoming an essential component of pharmaceutical sciences.*

**KEYWORDS:** Pharmacoinformatics, Immunoinformatics, Chemoinformatics, Bioinformatics.

## INTRODUCTION

Informatics and internet technologies are becoming extremely popular in today's health-care system. The emergence of the worldwide web has affected the way in which health-related information is distributed and accessed over cyberspace. The internet is rapidly gaining importance, not just for health-care professionals, but also for patients, by enabling them to search for drug-related and other health-related information [1]. Pharmacoinformatics is the study, invention and effectuation of discipline where technology with any aspect of drug delivery, from the basic sciences to the clinical use of medications in individuals and populations. Informatics is commonly defined as the "use of computers to manage data and information" and represents the nexus of people, information, and technology. Includes pharmacy technologies involved in the preparation, delivery, and management of medication use within health care delivery systems [2, 3]. Many applications of pharmacoinformatics currently exist within the health-care sector. These applications have important roles in helping to reduce DRPs in the oncology setting. Studies on the effectiveness of support systems for clinical decisions, e-prescribing, and drug-order entry have shown benefits in reducing medication errors [4-5], and in the prevention and management of chronic diseases [6].



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## Classification of Pharmacoinformatics

Pharmacoinformatics is new emerging information technologies like neuroinformatics, immunoinformatics, bioinformatics, Metabolomics, chemo-informatics, toxico-informatics, cancer informatics, genome informatics, proteome informatics, biomedical informatics are basic tools provided for the purpose of drug discovery [7]. Shows the current statuses of the activities in pharmacoinformatics are given in (fig. 1).

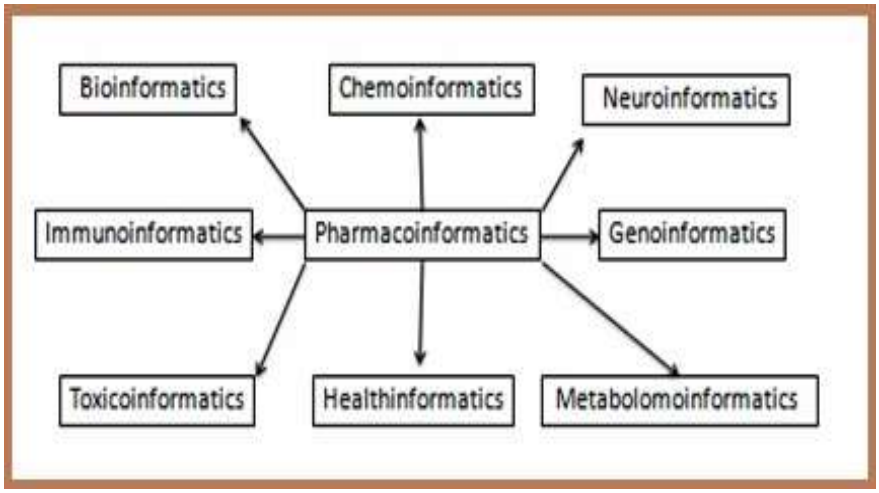


**Figure.1: Classification of Pharmacoinformatics**

### 1. Bioinformatics

Bioinformatics is the combination of biology and information technology. The discipline encompasses any computational tools and methods used to manage, analyze and manipulate large sets of biological data. Essentially, bioinformatics has three components:

- The creation of databases, allowing the storage and management of large biological data sets.
- The development of algorithms and statistics to determine relationships among members of large data sets.
- The use of these tools for the analysis and interpretation of various types of biological data, including DNA, RNA and protein sequences, protein structures, gene expression profiles, and biochemical pathways [8].

The term bioinformatics first came into use in the 1990s and was originally synonymous with the management and analysis of DNA, RNA and protein sequence data. Computational tools for sequence analysis had been available since the 1960s, but this was a minority interest until advances in sequencing technology led to a rapid expansion in the number of stored sequences in databases such as GenBank. Now, the term has expanded to incorporate many other types of biological data, for example protein structures, gene expression profiles and protein interactions. Each of these areas requires its own set of databases, algorithms and statistical methods [9-10].



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**Molecular bio-informatics:** bioinformatics is conceptualizing biology in terms of molecules (in the sense of physical chemistry) and applying "informatics techniques" (derived from disciplines such as applied maths, computer science and statistics) to understand and organize the information associated with these molecules, on a large scale. In short, bioinformatics is a management information system for molecular biology and has many practical applications [11-12]. Bioinformatics and medical informatics (BIOMI) are multidisciplinary fields at the intersection of computing and informatics, mathematics and statistics, biology, chemistry, and engineering [13]. Bioinformatics is the combination of biology and information technology. The discipline encompasses any computational tools and methods used to manage, analyze and manipulate large sets of biological data. The National Center for Biotechnology Information (NCBI 2001) defines Bioinformatics as "Bioinformatics is the field of science in which biology, computer science, and information technologies merge into a single discipline [14-15]. There are three important sub-disciplines within Bioinformatics: the development of new algorithms and statistics with which to assess relationships among members of large data sets; the analysis and interpretation of various types of data including nucleotide and amino acid sequences, protein domains, and protein structures; and the development and implementation of tools that enable efficient access and management of different types of information [16]." Basically, bioinformatics has three components: The creation of databases, allowing the storage and management of large biological data sets. The development of algorithms and statistics to determine relationships among members of large data sets. The use of these tools for the analysis and interpretation of various types of biological data, including DNA, RNA and protein sequences, protein structures, gene expression profiles, and biochemical pathways [11, 15].

**Bioinformatics and internet:** Bioinformatics is largely, although not exclusively, a computer-based discipline. Computers are important in bioinformatics for two reasons: First, many bioinformatics problems require the same task to be repeated millions of times. In such cases, the ability of computers to process information and test alternative solutions rapidly is indispensable [17]. Second, computers are required for their problem-solving power. Typical problems that might be addressed using bioinformatics could include solving the folding pathways of protein given its amino acid sequence, or deducing a biochemical pathway given a collection of RNA expression profiles. Internet plays an important role to retrieve the biological information. Bioinformatics emerging new dimension of biological science includes computer science, mathematics and life science. The Computational part of bioinformatics use to optimize the biological problems like metabolic disorder, genetic disorders [18-19].

The Internet provides various facilities for Bioinformatics such as;

**World Wide Web (WWW) Virtual Library:** This directory, provided by Cato Research Ltd., contains over 1000 URLs specific to biotechnology, pharmaceutical development, and related fields [18].

**Subject Specific Sites:** These sites are more likely to concentrate on a particular area of Bioinformatics. These sites are further divided into the various areas of Bioinformatics e.g. genomic comparisons [19].



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**General Bioinformatics Web Sites:** Many of the sites are offering the same sorts of links and many to other Bioinformatics sites; many have links to a Sequence Retrieval System or other facilities for sequence retrieval. These are categorized as under: Academic Sites and Corporate/Government Sites [18].

**Access to Journals:** Providing access to journals such as; Nature, Science, Molecular biology and Evolution, Nucleic Acids Research, Bioinformatics.

**As a Centre for Biotechnology Information:** One can explore extensive sites of resources and including newsletters, Bioinformatics databases, and links to the major medical bibliographic databases. It not only connects to textual databases but also to Protein Structure Servers. These include 3DB browser, biomolecular modeling and structural classification of proteins etc [19].

**Searching Database**

**Types of Biological Databases Accessible:** There are many different types of database but for routine sequence analysis, the following are initially the most important. Primary Database (Nucleic Acid Protein): EMBL, Genbank, DDBJ, SWISS-PROT. Secondary databases: PROSITE, Pfam. Composite databases: Combine different sources of primary databases. Example: NRDB OWL [18-19].

**Some bioinformatics research and service centers:** National Center for Biotechnology Information (NCBI) in the USA; European Bioinformatics Institute (EBI) in the UK; Swiss Institute of Bioinformatics (SIB); Australian National Genome Information Service (ANGIS); Canadian Bioinformatics Resource (CBR); Peking Center of Bioinformatics (CBI); Singapore Bioinformatics Centre (BIC); South-African National Bioinformatics Institute (SANBI) [18].

**Table: 1. Databases Information Contain Type of databases [7, 18-19]**

| Category | Name | Description | Source |
|---|---|---|---|
| Sequence databases | GenBank | Genetic sequence database | http://www.ncbi.nlm.nih.gov |
| | EMBL | Nucleic acid and protein databases | http://www.ebi.ac.uk/embl/index.html |
| | Uni–Prot | Protein database | http://www.uniprot.org |
| Genome databases | dbEST | Expressed Sequence Tags database | http://www.ncbi.nlm.nih.gov/dbEST/index.html |
| | GDB | Human Genome Database | http://www.gdb.org/ |
| | Ensembl | Genome database | http://www.ensembl.org/index.html |
| Secondary protein databases | Pfam | Protein family database with multiple sequence alignments and hidden Markov models | http://www.sanger.ac.uk/Software/Pfam/ |
| | PROSITE | Protein family and domain database | http://us.expasy.org/prosite/details.html |
| Protein interaction databases | BIND | Bimolecular Interaction Network Database | http://www.bind.ca |



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## 2. Genome Informatics

This is a relatively well-known topic being closely related to bioinformatics through sequence analysis. Genome informatics as a field encompasses the various methods and algorithms for analyzing and extracting biologically relevant information from the rapidly growing biological and essential sequence databases [19]. The Genome Informatics program supports research in computational biology that will enable the development of tools for sequence analysis, gene mapping, complex trait mapping and genetic variation. These tools include mathematical and statistical methods for the identification of functional elements in complex genomes; the identification of patterns in large datasets (for example, microarray data); and the mapping of complex traits and genetic variations (for example, single nucleotide polymorphisms, or SNPs).The program also encourages development and maintenance of databases of genomic and genetic data. This emphasis includes new tools for annotating complex genomes so as to expand their utility. The program also supports the production of robust, exportable software that can be widely shared among different databases in order to facilitate database interoperability. These bioinformatics resources will allow the scientific community efficient access to genomic data, which will enable new types of analyses. The analyses, in turn, will allow for the computer modeling and subsequent experimental validation of the complex pathways and networks that ultimately determine the phenotype of a cell or the causes of many human diseases [20-21]. A number of online resources and servers are available that assist in genome informatics research. Few of them are – Fly Base [22], KEGG (Kyoto Encyclopedia of Genes and Genomes) [23], and Ensemble Compara Database [24], cis RED database, genome SCOUT gene RAGE, CoGenT++. In India, Institute of Genomics and Integrated Biology (IGIB) is one of the leading institutes working in the field of genome informatics. Personalized medicine is the idealized medical practice to give right drugs to right patients at right times. Finding SNPs is considered as a premise for this practice, but it is by no means the sufficient effort. Good practice must be supported by well trained medical professionals who can easily access relevant data and knowledge. Such an informational environment would be called the infrastructure for personalized medicine [25].

## 3. Immunoinformatics

Immunoinformatics is another major area in biomedical research where computational and informational technologies are playing a major role in the development of drugs and vaccines. This field is still in its infancy and it covers both modeling and informatics of the immune system and is the application of informatics technology to the study of immunological macromolecules, addressing important questions in immunobiology and vaccinology. Data sources for immunoinformatics include experimental approaches and theoretical models, both demanding validation at every stage. Major immunological developments include immunological databases, sequence analysis, structure modeling, modeling of the immune system, simulation of laboratory experiments, statistical support for immunological experimentation, and immunogenomics [26-27]. The field of immunoinformatics has direct influence in the following areas: (a) improve transplantation outcomes (b) identify novel genes involved in immunological disorders (c) decipher the relationship between antigen presentation pathways and human disease



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(d) predict allergenicity of molecules including drugs (e) personalized medicine (f) vaccine development.

**Table 2: Some Selected Immunoinformatics Databases and Tools** [18, 28-31]

| Databases and Tools | Brief Description | URL |
|---|---|---|
| IMGT, the international ImMunoGeneTics information system | A sequence, genome, and structure database for immunogenetics data | http://imgt.cines.fr |
| HIV Molecular Immunology Database | A database of HIV – specific B - cell and T - cell responses | http://www.hiv.lanl.gov/content/immunology/index.html |
| MHCPEP | Database of MHC - binding peptides | http://wehih.wehi.edu.au/mhcpep/ |
| FIMM | Database of Functional Immunology | http://research.i2r.astar.edu.sg/fimm/ |
| SYFPEITHI | Database and prediction server of MHC ligands | http://www.syfpeithi.de/ |
| BIMAS | Bioinformatics and Molecular Analysis Section (MHC peptide - binding prediction) | http://bimas.dcrt.nih.gov/molbio/hla_bind/ |

## 4. Neuroinformatics

Neuroinformatics may be defined as the organization and analysis of neuroscientific data using the tools of information technology. The information sources in neuroinformatics include behavioral sciences (psychological description) and medicinal (including drugs and diagnostic images) and biological (membranes, neurons, synapses, genes, etc.) aspects. The aim of neuroinformatics is to unravel the complex structure – function relationship of the brain in an integrative effort. Neuroscientists work at multiple levels and are producing enormous amounts of data. Distributed databases are being prepared and novel analytical tools are being generated with the help of information technology. Producing digital capabilities for web-based information management systems is one of the major objectives of neuroinformatics. Apart from data sharing, computational modeling of ion channels, neurons and neural networks, second messenger pathways, morphological features, and biochemical reaction are also often included in neuroinformatics. The initial ideas on neuroinformatics can be traced to the work of Hodgkin and Huxley, who initiated computational neuronal modeling. Current efforts in the direction include studies related to modeling the neuropsychological tests, neuroimaging, computational neuroscience, brain mapping, molecular neuroimaging, and magnetic resonance imaging [18].



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**Table: 3. Selected List of Important Neuroinformatics Tools and Databases [18, 32-34]**

| Databases | Brief Description | URL |
|---|---|---|
| Brain Architecture Management System (BAMS) | Repository of brain structure information; contains to date around 40,000 connections | http://brancusi.usc.edu/bkms/ |
| Brain Map | For meta - analysis of human functional brain-mapping literature | http://brainmap.org/ |
| Surface Management System (SuMS) | A surface - based database to aid cortical surface reconstruction, visualization and analysis | http://sumsdb.wustl.edu/sums/index.jsp |
| L - Neuron | Computational Neuroanatomy Database | http://www.krasnow.gmu.edu/LNeuron |
| GENESIS | Neural Simulator | http://www.genesissim.org/GENESIS/ |
| NeuroScholar | MySQL Database frontend with management of bibliography, histological and tracing data | http://www.neuroscholar.org |

## 5. Toxic Informatics

Toxicoinformatics involves the use of information technology and computational science for the prediction of toxicity of chemical molecules in the living systems. Early prediction of toxicological parameters of new chemical entities (NCEs) is an important requirement in the drug discovery strategy today. This is being emphasized in the wake of many drug withdrawals in the recent past. Computational methods for predicting toxicophoric features is a cost effective approach toward saving experimental efforts and saving animal life. Current efforts in Toxicoinformatics are mainly based on QSTR (quantitative structure – toxicity relationships) and rule - based mechanistic methods. QSTR is a statistical approach, in which a correlation is developed between structural descriptors of a series of compounds and their toxicological data. In this approach, a model can be trained with the help of a set of known data, validated using many approaches, and then used for the prediction of toxicological parameters. The only limitation of this approach is that the predictive power of these models gets reduced when chemicals' belonging to a class outside the series of molecules is used for the construction of the model. Toxicity prediction tools using this approach include TOPKAT and CASE/M-CASE. TOPKAT mainly employs electrotopological descriptors based on graph theory for the development of QSTR models. TOPKAT uses linear free - energy relationships in statistical regression analysis of a series of compounds. In this software, the continuous/dichotomous toxicity end points are correlated to the structural features like electronic topological descriptors, shape descriptors, and substructure descriptors. CASE (Computer Automated Structure Evaluation) and M - CASE are Toxicoinformatics software packages that have the capability to



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automatically generate predictive models. A hybrid QSTR artificial expert system - based methodology is adopted in CASE - based systems [35-38].

## 6. Metabolome Informatics

Metabolomics is an emerging new ominous science analogous to genomics, transcriptomics, proteomics, etc. Metabolomics is the lesser-known cousin to genomics and proteomics. An understanding of the pharmacokinetics of a drug can play a major role in reducing the probability of bringing a new chemical entity (NCE) with inappropriate ADME/Toxicity profile to the market. Drug metabolism and toxicity in the human body are primarily assessed during clinical trials, and preclinical assessment of the same involves study on *in vivo* and *in vitro* systems. In silico models for predicting pharmacokinetic properties based on the experimental results can greatly reduce the cost and time required for the experiments. These methods range from modeling approaches such as QSARs, to similarity searches as well as informatics methods like ligand-protein docking and pharmacophore modeling. Metabolic biotransformation of any NCE may profoundly affect the bioavailability, activity, distribution, toxicity, and elimination of a compound; the effects of probable metabolism are now considered in the early stages of drug discovery with the help of computer - aided methods. In silico prediction of metabolic biotransformation occurring at the liver cytochrome enzymes (CYP450 enzymes) are being studied [18, 39]. Many databases and software systems are available in this field for the early prediction of substrates of CYP450 enzymes. Some of the databases and predictive systems for metabolic information of drugs are given in Table. The Human Drug Metabolism Database (hDMdb) project is a nonprofit, internet database of xenobiotic metabolic transformations that are observed in humans [40]. The predictive systems available for metabolism are mainly expert systems based on experimental data representing the metabolic effects (database) and/or rules derived from such data (rule - base). The rules may either be induced rules, which are quantitative, derived from a statistical analysis of the metabolic data, or knowledge - based rules derived from expert judgment [41]. Plant breeding and assessment of crop quality, Food assessment and safety, Toxicity assessment, Nutrition assessment, Medical diagnosis and assessment of disease status, Pharmaceutical drug development, Yield improvement in crops and fermentation, Biomarker discovery, Technological advances in analytical chemistry, Genotyping, Environmental adaptations, Gene-function elucidation, Integrated systems biology.



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**Table: 4. Databases and Tools for Metabolism Informatics** [18, 39-41]

| Databases and Tools | Brief Description | URL |
|---|---|---|
| Human Drug Metabolism Database (hDMdb) | IUPAC project for a web-based model database for human drug metabolism information | http://www.iupac.org/projects/2000/2000 -010-1-700.html |
| MDL Metabolite | Comprised of a database, registration system, and browsing interface | http://www.mdl.com/products/predictive/metabolite/index.Jsp |
| Biofrontier/P450 | Human cytochrome P450 information and predictive system | http://www.fqs.pl/ |
| METEOR (LHASA Ltd., Leeds, UK) | Predictions presented as metabolic trees | http://www.lhasalimited.org/ |
| META (Multicase, Inc.) | Uses dictionaries to create metabolic paths of query molecules | http://www.multicase.com/products/prod05.htm |

## 7. Healthcare Informatics

Biomedical Informatics is an emerging discipline that has been defined as the study, invention, and implementation of structures and algorithms to improve communication, understanding and management of medical information." Medical informatics is more concerned with structures and algorithms for the manipulation of medical data, rather than with the data itself. This suggests that one difference between bioinformatics and medical informatics as disciplines lies with their approaches to the data there are bioinformatics interested in the theory behind the manipulation of that data and there are bioinformatics scientists concerned with the data itself and its biological implications. Medical informatics, biomedical informatics, clinical informatics, nursing informatics, etc. come under the service-oriented sectors. Other topics like cancer informatics, diabetes informatics are specific therapeutic area based information technology topics. These topics are also related to pharmacoinformatics as a whole because the information obtained from these subjects leads to decision making in pharmaceutical industry. For example, medical informatics deals with medicines and health care. The databases associated with this filed include the feedback received response to a drug. Thus, future designing of the drugs can be made to suit the needs of the patients. Electronic health record (EHR) systems, Hospital Information Systems (HIS), Decision Support Systems (DSS), etc. are the major components of healthcare informatics [43]. Medical Information Science is the science of using system-analytic tools to develop procedures (algorithms) for management, process control, decision making and scientific analysis of medical knowledge - *Ted Short life.* Medical Informatics comprises the theoretical and practical aspects of information processing and communication, based on knowledge and experience derived from processes in medicine and health care - *Jan van Bemm.* Medical Informatics (MI) is the study of information processing as it is used in healthcare. It might have been called medical computing, but the French-derived term informatics is more commonly used internationally and probably conveys a broader set of concerns, including the uses and flows of information that may have little to do with computers. Like many engineering



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fields, MI has scientific aspects that focus on the description, modeling and interpretation of how information is actually generated, disseminated and used, and underlying constraints or natural laws that govern these activities. MI is also deeply concerned with the design of appropriate medical information processing systems, with tradeoffs in their implementation, and with ways to evaluate their effectiveness [44]. Some have suggested health informatics as a better, broader term, meant to encompass aspects of health care that are not traditionally the focus of medicine, such as preventive care, nutrition, patient education, epidemiology, etc. Related terms include bioinformatics, which is the study of information processing in biological sciences. Opinion currently varies on whether bioinformatics is part of medical informatics, or-if it forms a distinct discipline-how it relates. Most expect that progress in understanding the molecular basis of disease will bring these fields closer together, if not to merger. Telemedicine (or the recent European coinage telematique) focuses on one aspect of MI, access to and use of medical information at a distance. At MIT, in line with our traditions of institutional flexibility, we have no official organization that does medical informatics, but a number of small foci around the research and teaching interests of faculty in different Departments and Laboratories [42-45]. Pharmacoinformatics preventing adverse drug reactions in hospital patients. Health informatics is concerned with the systematic processing of data, information and knowledge in medicine and healthcare, increasingly delivered by a mix of public and private organisations. Health informatics is delivered by operational health practitioners, academic researchers and educators, scientists and technologists in operational, commercial and academic domains. The ultimately focus is to improve patient safety and organisational effectiveness to achieve better outcomes [45].

**Nursing informatics (NI)** is a specialty that integrates nursing science, computer science, and information science to manage and communicate data, information, knowledge, and wisdom in nursing practice. NI supports consumers, patients, nurses, and other providers in their decision making in all roles and settings. This support is accomplished through the use of information structures, information processes, and information technology opportunities in Health broadly cover the following facets, sometimes in combination and with grey boundaries between them [46].

## 8. Chemo informatics

Chemo informatics is the application of informatics methods to solve chemical problems. All areas of chemistry from analytical chemistry to drug design can benefit from chemo informatics methods. And there are still many challenging chemical problems waiting for solutions through the further development of chemo informatics [46]. The term "Chemoinformatics" appeared a few years ago and rapidly gained widespread use. Workshops and symposia are organized that are exclusively devoted to Chemoinformatics, and many job advertisements can be found in journals. The first mention of Chemoinformatics may be attributed to Frank Brown [47]. 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. Chemical Data →Storage in Databases →Data Information →Data Retrieval →Analysis The current schema of chemoinformatics in drug designing is given below: Analysis of predesigned drug structure structural property prediction (QSAR) property prediction by smiles format perform some modification in prior



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drug again predict the drug property if variation occurs in novel structure save that structure and design a fragment library [48].Chemoinformatics is a generic term that encompasses the design, creation, organization, management, retrieval, analysis, dissemination, visualization, and use of chemical information. The needs for chemoinformatics recent chemical developments for drug discovery are generating a lot of chemical data. These developments are combinatorial chemistry and high-throughput screening. Some scientists have described this situation as a chemical information explosion. This has created a demand to effectively collect, organize, and apply the chemical information [49-50]. Chemo informatics which deals with the information of the molecules, chemical reaction informatics also plays an important role in the field of pharmacoinformatics. Chemical reaction informatics enable a chemist to explore synthetic pathways, quickly design and record completely new experiments from scratch or by beginning with reactions found in the reaction databases. Chemical reaction informatics a database consists of the following information -Reactants and products, Atom mapping, which allows you to tell which atom, becomes which product atom through the reaction, Information regarding reacting center(s), The catalyst used, The atmosphere, including pressure and composition, The solvent used, Product yield, Optical purity, References to literature. The chemical reaction informatics would essentially assist the chemist in giving access to reaction information, in deriving knowledge on chemical reactions, in predicting the course and outcome of chemical reactions, and in designing syntheses. Specifically, the following tasks can be accomplished by analysis tools in chemical reaction informatics- Storing information on chemical reactions, Retrieving information on chemical reactions, Comparing and analyzing sets of reactions, Defining the scope and limitations of a reaction type, Developing models of chemical reactivity, Predicting the course of chemical reactions, Analyzing reaction networks, Developing methods for the design of syntheses, etc. Applications of Chemo informatics**:** Chemical Information, All fields of chemistry, Analytical Chemistry, Organic Chemistry, Drug Design and Textile Industry [51].

## CONCLUSION

Drug discovery and development requires the integration of multiple scientific and technological disciplines. These include chemistry, biology, pharmacology, pharmaceutical technology and extensive use of information technology. The latter is increasingly recognised as Pharmacoinformatics. As discussed above, there is several information technology efforts related to the pharmaceutical sciences which are useful for drug discovery. In future, these efforts are expected to grow both in terms of their reliability and scope. Thus, this emerging technology (pharmacoinformatics) is becoming an essential component of pharmaceutical sciences.

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