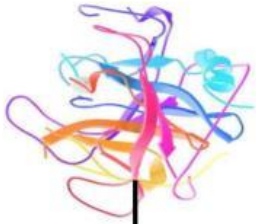
Computational approach on Cheminformatics and Bio-informatics

Dr. Bharati Choudhari

Bioinformatics and Chemoinformatics
The Questions

Bioinformatics: Function

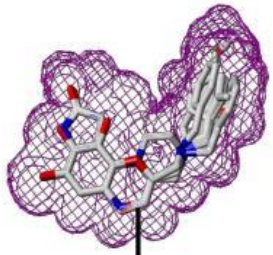


Comparative Genomics

↓

Function

Chemoinformatics QSAR

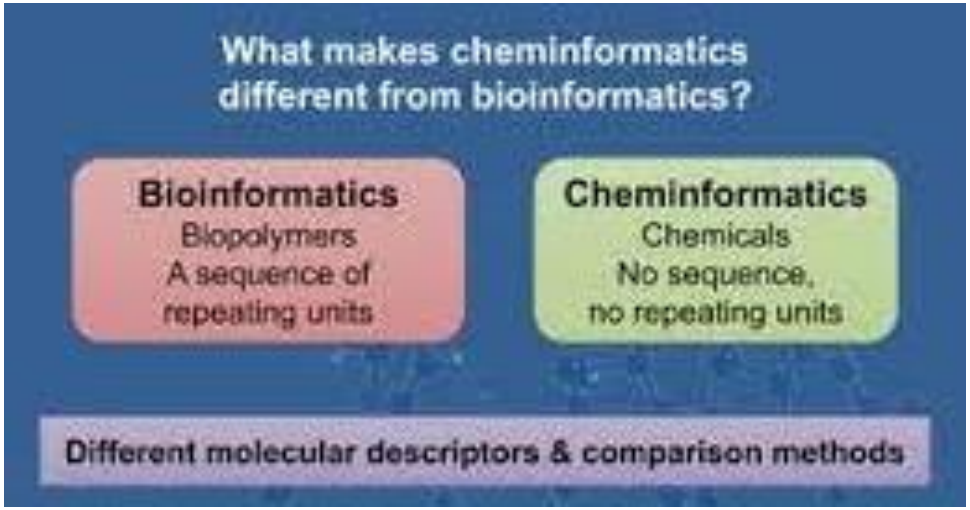


Quantitative Structure-Activity Relationship

↓

Activity/Toxicity

Cédric Notredame (01/11/2014)



Difference between Molecular modeling, Chemoinformatic and Bioinformatics

Molecular modeling	Chemoinformatics	Bioinformatics
Model or mimic the behavior of molecules and molecular systems considering three-dimensional structures	Design, creation, analysis, management, recovery, organization, distribution, visualization and use chemical information	Informational techniques applied to solve biological problems usually at the molecular level
Molecular mechanics	Storage and retreival	Biological databases
Molecular dynamics	Database mining	Sequence alignment
Docking	Molecular descriptors	Gene prediction
Pharmacophore model	Similarity methods	Molecular phylogenetics
Ab initio	Diversity analysis	Structural bioinformatics
DFT	Library design	Genomics and proteomics
Semiempirical	Virtual screening	

Cheminformatics

- Chemoinformatics is the mixing of those information resources to transform data into information and information into knowledge for the intended purpose of making better decisions faster in the area of lead identification and organist ion " **F.K Brown (1998)**

Basic of cheminformatics

What is cheminformatics?

The most accepted definitions of Cheminformatics are…

- 1. "Cheminformatics is the combinationation of chemical synthesis , biological screening and
- data mining approaches used to guide drug discovery and development."

- "C I is the use of computer software to assist in the acquisition , analysis and management of data and information relating to chemical compounds and their properties."

- CI applies IT to chemical data and includes topics such as chemical databases, combinatorial library design, structure-activity relationships and structure based drug design .

- The CI offer programs and databases(mainly for organic and sometimes for inorganic applications) related to small molecules, complementing the activities of the bioinformatics group who concentrate on biological macromolecules

Recent developments such as

- Computational chemistry
- Modern combinatorial chemistry
- Drug design and discovery
- Data sequence, mining and visualisation
- Chemical database design and their management
- Chemical information sources
- Medicinal chemistry etc.,has resulted in the emergence of the discipline of CI, which involves the creation, retrieval, organization, dissemination and processing of chemical information .

Scpoe in Cheminformatics

- CI is the latest area is now becoming a reality in India too
- Till data advance countries like US, UK, Japan and few European countries were working on this .
- In India CI is making inroad in Indian software, Department of Bio-Tech Govt of India , R& D organizations pharmaceuticals and other industries too.
- With thousands of jobs and crores of grants by Govt of India, CI professionals are growing day by day not only in India but also in abroad .
- CI companies are in great need of people with knowledge of chemistry and computer skills to handle the data generated by chemical researchers.

Chemical Information System(CIS)

- The main purpose of this is to identify a chemical substance, find compounds similar to the target compounds and demine the location of the compound, and it is an inventory system.
- **Chemical similarity** searching databases by chemical similarities is among the oldest and most useful techniques in molecular modeling as practiced by the pharmaceutical industry. It works because it is generally true that molecules with similar structure have similar biological activities

Chemical Information System(CIS)…

The chemical information systems and services have been established for many years

(i) Justus Liebig in **1832** founded **Annalender pharmacie**

(ii) Chemical abstarct was started in **1907**

(iii) First compuetr-based system was established over **40 years ago**

- The first journal for the subject , **Journal of chemical documentation** started in **1961.**
- The name changed to **Journal of chemical information and computer science** in **1975.**
- The first book computer handling of chemical structure information appeared on this subject in **1971**
- The first international conference on this subject was held in **1973** at **Noordwijkerhout** and every three years since **1987.**

Milestones in Cheminformatics

(i) Identification of a user-defined structural pattern in a database structure.

(ii) Use of graph -searching Algorithm.

(iii)For the storage and retrieval of **2D chemical structure** .(later, **3D** also)

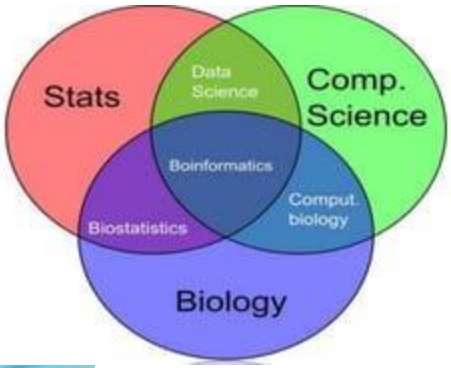
The various companies engaged in making use of CI are …

- **Pharmacopeia** is a software company which includes a BI arm, Genetics computer group as well as molecular simulations, Synopsys scientific systems and oxford molecular group . The last two business form the CI part of pharmacopeia.

- **Chem Navigator** has developed an application that allows researchers to submit a precise structure for comparison with more than one million compounds in its library.
- At chem navigator website, commercially available compounds can be identified , purchased and delivered to the researcher promptly and efficiently.

and many more…….

Bioinformatics



Bioinformatics is the unified discipline formed from the combination of biology, computer science, and information technology.

"The mathematical, statistical and computing methods that aim to solve biological problems using DNA and amino acid sequences and related information." –Frank Tekaia

Why Bioinformatics is necessary?

- The need for bioinformatics has arisen from the recent explosion of publicly available genomic information, such as resulting from the Human Genome Project.
- Gain a better understanding of gene analysis, taxonomy, & evolution.
- To work efficiently on the rational drug designs and reduce the time taken for the development of drug manually

GOALS:

- **Better understand the living cell**
- **How it functions at the molecular level**
- **Solving functional problems using sequence and sometimes structural approaches has proved to be a fruitful endeavor.**

SCOPE:

- Bioinformatics consists of two subfields:
- The development of computational tools and databases.
- The application of these tools and databases in generating biological knowledge to beter understand living systems.

LIMITATIONS

- Bioinformatics has a number of inherent limitations.
- Bioinformatics is by no means a mature field.
- Most algorithms lack the capability and sophistication to truley reflect the reality.
- Errors in sequence alignment, an affect the outcome of structural or phyligenetic analysis.
- Many accurate but exhausitive algorithms cannot be used because of the slow rate computation. Instead, less accurate but faster algorithms have to be used.
- IT IS A GOOD PRACTICE TO USE MULTIPLE PROGRAMS, IF THEY ARE AVAILABLE, AND PERFORM MULTIPLE EVALUATIONS.
- A MORE ACCURATE PREDICTION CAN OFTEN BE OBTAINED IF ONE DRAWS A CONSENSUS BY COMPARING RESULTS FROM DIFFERENT ALGORITHMS.

Bioinformatics is being used in following fields:

- Microbial genome applications
- Molecular medicine
- Personalized medicine
- Preventative medicine
- Gene therapy
- Drug development
- Antibiotic resistance
- Evolutionary studies
- Waste cleanup
- Biotechnology
- Climate change Studies
- Alternative energy sources
- Crop improvement
- Forensic analysis
- Bio-weapon creation
- Insect resistance
- Improve nutritional quality
- Devp. of Drought resistant varieties
- Vetinary Science

Bioinformatics Web Resources

- **NCBI –** The National Center for Biotechnology Information
- **PubMed**
- **EMBL -** European Molecular Biology Laboratory
- **OMIM –** Online Mendelian Inheritance in Man

Applications of Bioinformatics

Bioinformatics joins mathematics, statistics, computer science & information technology to solve complex biological problems.

Applications of Bioinformatics includes:

- Sequence Analysis
- Prediction of Protein Structure
- Genome Annotation
- Comparative Genomics
- Health and Drug discovery