

Short Communication

Chemoinformatics: The stakeholder of Information Solutions for Chemical and Allied Medical Domain

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Abstract: Chemoinformatics or Cheminformatics is an important interdisciplinary field that integrate the domain of chemistry and information science with computer science. In other words, it is the application and integration of Informatics with chemical Science. This concept originated some years back but gained popularity as a knowledge domain in the domain of chemical sciences very recently. It plays a vital role in storing large data sets related to chemical science and converting or transforming it into knowledge to make better and faster decision. Here, the methods or algorithm incorporated into it, assist the professionals to identify the better and appropriate chemical compound to also meet the need of medical and allied domain as they are the ultimate end users of the end product of chemical science. In spite of having several benefits, there are so many misconceptions are still there with Chemoinformatics. This paper explains the general role of Chemoinformatics, its application, brief evaluation and future potentials.

Keywords: Chemoinformatics, Cheminformatics, Chembioinformatics, Chemical Information, Information Science, Information Systems, Informatics, Chemical Computing, Health Science, Pharmaceutical Sciences.

Introduction

Chemoinformatics is a branch of informatics that deals with the use of computer in formulating computational technique in the field of chemistry and chemical science to assist the researchers and learners in making make better decision [08], [15]. This is dedicated to provide solutions in designing, creation, organization, management, retrieval, analysis, dissemination, presentation and use of chemical and allied information. In earlier days, this use to be considered as a technique or method but the advances in informatics, chemical science and interdisciplinary research rejuvenate and coined it as Chemoinformatics and established an interdisciplinary domain or study area around the globe. There are several programs offered by universities around the world related to 'Chemoinformatics' as MS-Chemoinformatics or PhD. The domain 'Chemoinformatics' has been differentiated by academic community in several ways such as; chemical computing, chemical information science, Bioinformatics etc. [09], [10], [13]. As Chemoinformatics deals with storing, manipulating, processing chemical information; thus many experts earlier explained Chemical Information studies as a

method or procedure to find out relationship between structure and properties of a chemical compound.

Objective

The main aim and objective of this study is includes:-

- To understand Chemoinformatics; its nature and characteristics.
- Identify the role and application of Chemoinformatics; in chemistry and chemical sciences.
- To find out the future potential of Chemoinformatics research and innovation.
- To learn the principle and structure of Chemoinformatics.
- To differentiate Chemoinformatics with Bio-Informatics and allied domain.

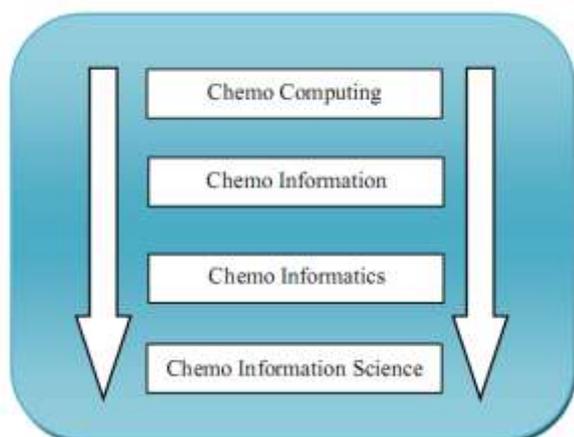


Fig: 1 showing the Chemoinformatics and its smaller to larger gradients at a glance

Chemoinformatics

Chemoinformatics plays an important place in chemistry and chemical research and this was coined and gifted by FK Brown, G Pavis, Hann, R Green, Johann Gosteign, the chemical scientist with computing expertise. Though, Chemoinformatics is primarily responsible for providing information about chemical and its compound but in modern time, it deals with identification and recognition of small molecular structure and properties of the chemical compound. The chemical science produces huge amount of data that are too complex to understand the structure of compound with its biological activity. In order to understand and take better decision, the data require further processing and analysis using various theoretical calculation. In many instances, this process itself become complex due to manual computation and lead to several errors. To avoid such situation and to take better decision, the whole process i.e. from data generation to analysis, require automation and to do so, chemical sciences should interact with the computing environment. This will not only improve the process but also enhance the accuracy and safety of data. The attempt of better information processing and visualization of results build the domain of Chemoinformatics [15].

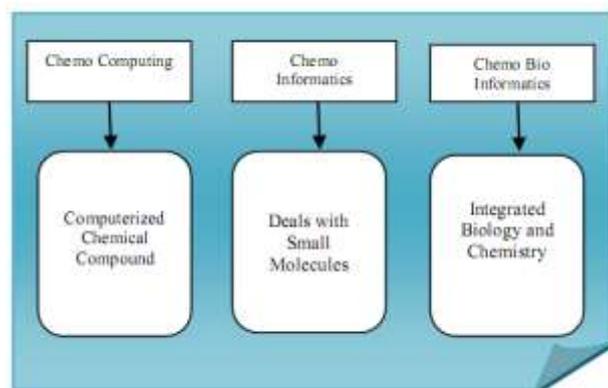


Fig: 2: Depicted role of domain deals with Chemical Information- Partially and Fully

The related nomenclature of Chemoinformatics could be Cheminformatics or Chemical Informatics. Though literature review also indicates its synonyms or closely related nomenclature as Chemobioinformatics, Molecular Informatics etc. Thus, Chemoinformatics is a field or process of integrating Information Technology and management application in drug management, chemical structure visualization, chemical compound relationship etc. Chemoinformatics application, in many ways, closely associated with Bioinformatics and Medical Informatics, as it provide information related to the chemical composition and structure in identifying the abnormalities in humans and choosing the best drug therapy in delivery of quality healthcare [3], [4], [8].

Chemoinformatics: Applications and Utilization

Chemoinformatics is basically a process and method responsible for several activities but fundamentally responsible for data analysis of chemical structure and its compound for choosing the best agent available during the drug discovery process. Chemoinformatics is useful to find out new lead structure and optimize them to drug condition [10], [18-20]. As stated by FK Brown, "The use of Information Technology and Management has become a critical part of drug discovery process. Chemoinformatics is the mixing of these 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". Thus it is an application of Information Science, Management Science and computing to solve chemical problems [8], [14, 13]. Let discuss some of the traditional, emerging application of Informatics in chemistry or chemical sciences:-

- In analytical chemistry, Chemoinformatics is useful in analysis and synthesizing data to make a healthy prediction about quality, origin and age of the investigated objects [9], [15].
- Drug Science and Drug development needs Chemoinformatics application for identification and selection of new lead structure and their optimization, establishment of quantities structure, definition analysis of structural discovery, drug screening, discovery of several compound has been done with Chemoinformatics. In addition to these, comparison of chemical libraries; its planning is also possible with this. The pharmaceutical systems, critical researcher today move a screening based to a knowledge based paradigm [1], [2], [10].
- Virtually, Chemoinformatics is required for the storage and retrieval of chemical structure and associated large data sets with the help of computational tools and technologies, multimedia systems, drawing software etc. The application can also be utilized as an eLearning tool, where the knowledge related to chemical

science can be shared among researcher and learner.

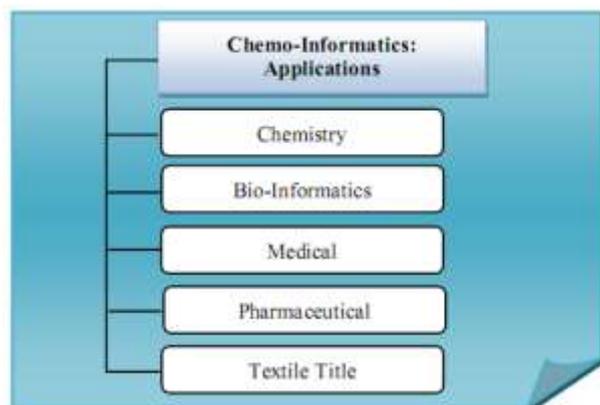


Fig: 3:-Chemical Informatics and its applications in allied domain

Thus, Chemoinformatics is required for the cross linking of data to information for the prediction of physical, chemical and biological properties of the chemical compounds. The decision regarding the absorption, distribution and metabolic properties of drug is possible through such domain and techniques [11-13]. In other words, Chemoinformatics helps the structural analogue, property analogue, and mechanistic analogue of the compound. As Chemoinformatics helps in avoiding the conventional chemical synthesizing and biological testing, thus it helps in saving the cost. In many instances; the availability of low cost medicine in many ways is due to the practice of Chemoinformatics. The Regenerative Medicine is also considered as one of the important beneficiaries of Chemoinformatics, [10], [15].

Chemoinformatics: time need and future potentials

The advance in the field of chemical sciences including organic, inorganic and allied has given rise to the generation of dynamic knowledge which is not only unique but large (more than 50 million chemical compound) and managing these large data sets is possible through Chemoinformatics [1]. The Chemoinformatics has the potentials in analyzing and simplifying the large data sets to such an extent that it add knowledge to the researchers and collaborators in drug discovery, choosing the best agent possible for treating disease and disease conditions. It also promote interdisciplinary research of chemistry, information science, informatics, Biological, Medical Science and so on. Presently, the practice of Chemoinformatics is not only limited data management and mining but also related to molecular modeling, structure presentation, reaction presentation, 2D and 3D modeling etc. The future of Chemoinformatics can be seen an established educational discipline in universities across the globe. As stated earlier, it is an interdisciplinary area and may not require a separate full-fledged department or unit

but can be managed by the professionals available in chemistry, IT and allied domain [10,15].

Findings

The following findings can be seen as an establishment of Chemoinformatics as a broad domain:

- Chemoinformatics has become an essential component in today's chemical, allied and medical science.
- Chemobioinformatics, the integrated form of Chemoinformatics and Bioinformatics has marked as a frontier in designing the best drug therapy in genomics or gene science.
- Chemoinformatics has slowly gained the popularity not as a process, method and mechanism but also as an academic domain.
- Chemoinformatics is widely popular and useful in physical, analytical, organic, inorganic chemistry, drug design, medical science, research and so on.

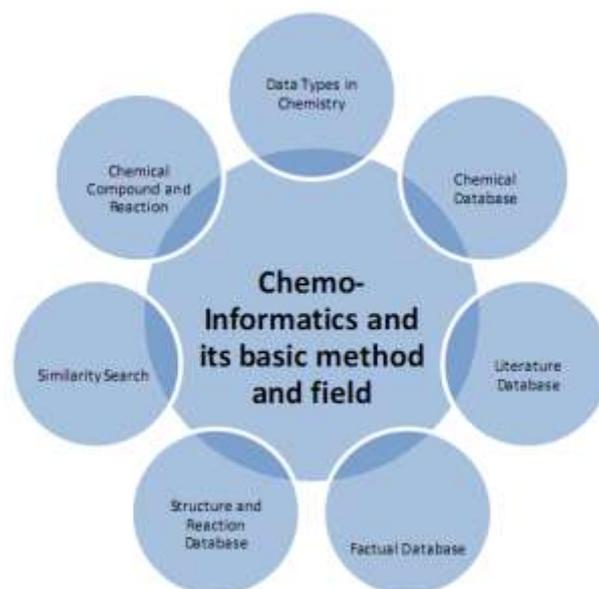


Fig: 4- Depicted some basic method and basic field of Chemo-Informatics

Suggestion

Chemoinformatics can be seen as an established domain in the present era but still, there are lot of things that are required to be done and looked into while dealing with it. Some of those are:

- There is a need to create more awareness among the researcher and learner about Chemoinformatics to distinguish the computational chemistry with Chemoinformatics as they perceive both as one.
- The short-term and long-term educational program can be seen as one of the solution to achieve maximum knowledge and awareness. But this responsibilities lies on the domain expert in the area

of chemical sciences, information science, computer science and engineering.

- The workshops, conferences, seminars can also be seen as a solutions in disseminating the benefits of Chemoinformatics to the large mass. The institution those are pioneered in Chemoinformatics can take these initiative to go further and promote the discipline.

Conclusion

Chemistry plays an important role for science and technological development. There are millions of chemical data that are not only helpful to choose the best drug therapy, but also in many perspectives for the development of a healthy human being. But these data are required to be managed well to aid in better decision making where Chemoinformatics plays a greater role. This has not only streamlined the process of data management and generation of knowledge, but also enhances the knowledge of researchers and learner in the field of chemical, pharmaceutical, biotechnology, allied and medical science. This can be seen as a major stakeholder as an information solution and support in better product designing and development of drug therapy for the betterment of mankind across the globe.

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