ISSN: 2581-5989
PubMed - National Library of Medicine - ID: 101738774

International Journal of Dental Science and Innovative Research (IJDSIR)
IJDSIR : Dental Publication Service
Available Online at: www.ijdsir.com
Volume – 6, Issue – 2, April - 2023, Page No. : 283 – 292

Chemoinformatics: A powerful tool for dental diagnosis and treatment

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Citation of this Article: A. Alice Nobelika, Dewfrin Fredrick, Arani Nandakumar, Devaki Vijayalakshmi, "Chemoinformatics: A powerful tool for dental diagnosis and treatment", IJDSIR- April - 2023, Volume – 6, Issue - 2, P. No. 283 – 292.

Type of Publication: Original Research Article

Conflicts of Interest: Nil

Abstract

Chemoinformatics is an interdisciplinary approach that employs computational techniques to solve chemistry-related problems. It has found increasing use in dentistry, particularly in the creation of novel pharmaceuticals and dental materials. Recent developments in chemoinformatics in dentistry include molecular docking and virtual screening to identify potential inhibitors of enzymes involved in the pathogenesis of dental caries, machine learning techniques such as random forest and support vector machines to predict the antibacterial activity of natural compounds against oral pathogens, and molecular dynamics simulations to study the mechanical properties of dental composites and to optimise their composition. In addition, machine learning techniques have been applied to predict the adhesive strength of dental adhesives based on their chemical composition. These studies demonstrate the field's potential for devising and optimising dental materials. In dentistry, chemoinformatics has been utilised to examine the interactions between dental materials and buccal tissues. The biocompatibility of dental materials based on their chemical composition has been predicted using molecular docking, molecular dynamics simulations, and machine learning methods. In addition, data mining can

be utilised to extract valuable insights from massive data sets. Understanding the bacterial communities prevalent in the buccal cavity, microbiome analysis can aid in improving oral health.

Keywords: dental application, drug discovery, machine learning, biocompatibility, big data.

Introduction

Chemoinformatics is an interdisciplinary approach that employs computational methods to solve chemistry-related problems. Utilising machine learning, data mining, and molecular modelling techniques, it examines the properties and behaviour of chemical compounds. Chemoinformatics has found increasing use in dentistry in recent years, particularly in developing novel drugs and materials for dental applications. This article summarises recent developments in chemoinformatics in dentistry and provides a thorough overview.

One of the most important applications of chemoinformatics in dentistry is the creation of new pharmaceuticals to treat various dental diseases. For instance, researchers have utilised molecular docking and virtual screening to identify potential enzyme inhibitors involved in the pathogenesis of dental caries (1). Similarly, the antibacterial activity of natural compounds against oral microorganisms has been predicted using machine learning techniques such as random forest and support vector machines (2). These studies illustrate the capacity of chemoinformatics to identify new drug candidates for treating dental diseases.

In addition to medication discovery, chemoinformatics has been applied to develop new dental materials. For instance, molecular dynamics simulations have been used to investigate the mechanical properties of dental composites and optimise their composition (3, 4). Likewise, machine learning techniques have been applied to predict the bonding strength of dental adhesives based on their chemical composition (5, 6). It demonstrate the applicability of chemoinformatics to the design and optimisation of dental materials.

Chemoinformatics in dentistry is also applied to studying the interactions between dental materials and buccal tissues. Molecular docking and molecular dynamics simulations have been used to examine the interactions between dental implants and bone tissue (7). Similarly, machine learning methods have been utilised to predict the biocompatibility of dental materials based on their chemical composition (8). It illustrate the potential of chemoinformatics for comprehending and enhancing the biocompatibility of dental materials.

Drug discovery

The computer-aided approach is utilised to identify potential drug candidates for treating various diseases, including dental diseases. Drug discovery is the process of identifying new medications that can be used to treat, cure, or prevent diseases. Target identification, compound screening, lead optimisation, and preclinical testing are some steps involved. The ultimate goal of drug discovery is to identify safe and effective treatments for diseases that can improve the health and well-being of patients. The conventional method of drug discovery can be time-consuming, costly, and unsuccessful. Chemoinformatics is a promising technique that can accelerate drug discovery by analysing large chemical databases and predicting the biological activity of chemical compounds using computational methods. It employs numerous tools and techniques, such as molecular descriptors, machine learning algorithms, docking and scoring techniques. Molecular descriptors are mathematical representations of molecular properties such as molecular weight, polarity, and solubility. Based on their molecular

descriptors, machine learning algorithms are used to predict the biological activity of chemical compounds. Docking and scoring techniques are utilised to simulate the interaction of chemical compounds with target proteins and to estimate their binding affinity (Figure 1) (9).

In drug discovery and design, one of the benefits of chemoinformatics is that it can identify potential drug candidates with high accuracy and reduce the time and cost associated with conventional drug discovery techniques. It can also enhance the effectiveness of the drug discovery procedure by predicting the biological activity of chemical compounds and reducing the number of compounds that must be tested in the laboratory (10). Despite the benefits of chemoinformatics, there are challenges and constraints associated with this methodology. The importance of data quality to the accuracy of predictions is highlighted by the complexity of chemical interactions and the difficulty of predicting the behaviour of compounds I*n Vivo*.

Material Design

Material design is developing materials with specific properties to satisfy certain requirements. In dental research, material design is essential in developing new dental materials with desirable properties, such as biocompatibility, mechanical strength, and antimicrobial activity. Chemoinformatics enables researchers to predict novel materials' properties and optimise existing ones' performance based on their chemical structure. For instance, it can be used to predict the properties of dental materials such as adhesives, cement, and composites based on their molecular structure, enabling researchers to devise materials with particular properties. High-throughput screening (HTS) is a technique that permits researchers to rapidly screen large libraries of compounds in order to identify those with the desired properties. In conjunction with chemoinformatics, HTS can be used to design and optimise dental materials with specified properties (11). Using chemoinformatics, researchers have developed innovative dental adhesives and composites with better bond strength, durability, mechanical qualities, and antibacterial activity. Material design ideas were used to create novel chemical compounds, which were tested and optimised. These results may impact dentistry and lead to safer and more effective clinical dental materials (Figure 2) (12).

Biocompatibility

Biocompatibility is the capacity of a material to interact with living tissues without producing damage or negative reactions. Biocompatibility is essential for ensuring patient safety and minimising the risk of post-treatment complications. *In Silico* methods such as Molecular docking and molecular dynamics simulations are used to evaluate dental materials' biocompatibility, and these methods anticipate how dental materials interact with biological molecules such as proteins, enzymes, and cell membranes. Molecular coupling can predict the interaction between dental materials and human serum albumin, a blood protein. It can also describe how molecular dynamics simulations can be used to examine the behaviour of dental materials in contact with buccal fluids and tissues. These procedures are less expensive and require less time than conventional in vitro and in vivo tests. In silico methods also enable researchers to examine the interaction of dental materials with biological molecules at the atomic and molecular level, providing valuable insights into the biocompatibility mechanisms (13).

Structure-activity relationship (SAR) analysis

The SAR analysis is a potent instrument for use in the research and development of new drugs. This process

involves the investigation of the connection that exists between the chemical structure of a compound and the biological activity it possesses. Applications of chemoinformatics in drug design and discovery range from predicting biological activity to optimising leads to repurposing existing drugs. Based on their chemical structure, SAR analysis can be used to predict the biological activity of chemical compounds. By analysing the SAR, researchers can identify the structural features essential for biological activity and then design new compounds with enhanced activity.

Utilising SAR analysis for lead optimisation entails modifying existing compounds to enhance their pharmacological properties. By examining the SAR of a lead compound, researchers can identify the structural features responsible for its activity and modify these features to enhance the compound's potency, selectivity, and safety. Identifying new uses for existing drugs is another application of chemoinformatics in drug discovery. Even if they were originally developed for a different indication, SAR analysis could be used to identify structurally similar compounds with potentially similar biological activity (14).

Toxicity prediction

Molecular descriptors are numerical or categorical quantities that describe a molecule's chemical and physical properties and are used to predict its toxicity. These descriptors can be incorporated into models that predict the toxicity of chemical compounds. Prediction of toxicity is a crucial aspect of drug discovery and chemical safety evaluation, as it can help identify potential hazards and guide the selection of safe compounds for further development. Topological, geometrical, electrostatic, and quantum chemical descriptors are the different categories of molecular descriptors. The development of quantitative structure-activity relationship (QSAR) models involves using molecular descriptors and statistical techniques to predict chemical compounds' biological activity or toxicity. The validation and interpretation of QSAR models involve evaluating their predictive ability, robustness, and applicability domain because neglecting model validation and the need to avoid overfitting can lead to spurious correlations and unreliable predictions (15).

Pharmacokinetic studies

The field of pharmacokinetics involves investigating how medications are absorbed, transported throughout the body, metabolized, and excreted. In contrast, pharmacodynamics studies the relationship between drug concentration and its effects on the body. Pharmacokinetics and pharmacodynamics play a vital role in drug discovery and development, as they provide crucial information regarding the safety, efficacy, and appropriate dosage of medications. Pharmacokinetic studies can assist in identifying potential drug candidates with favourable ADME properties, such as high bioavailability and low toxicity, whereas pharmacodynamic studies can assist in determining the optimal dose and administration schedule for a given drug. Drug development relies heavily on several pharmacokinetic and pharmacodynamic parameters, including maximum concentration (Cmax), time to maximum concentration (Tmax), half-life (t1/2), clearance (Cl), and volume of distribution (Vd). These parameters will provide crucial information about drug efficacy, safety, dosing, and potential interactions with other drugs. In order to optimise medication development, in addition to modelling and simulation, pharmacokinetic and pharmacodynamic studies *In Vitro* and *In Vivo* are necessary. (16, 17),

Personalised medicine

Personalised medicine is an approach to healthcare that considers individual differences in genes, environment, and lifestyle when devising treatments. By tailoring treatments to the specific characteristics of each patient, this strategy hopes to improve treatment outcomes and decrease adverse effects. Personalised medicine could have a significant impact on the prevention and treatment of periodontal disease, the diagnosis and treatment of oral cancer, and the management of temporomandibular disorders. Individuals at a higher risk for developing oral diseases could be identified through personalised medicine, allowing for earlier intervention and more targeted treatment. The potential of genomic medicine in dentistry entails using genetic information to guide decisions regarding diagnosis and treatment. Genetic testing could identify individuals at increased risk for developing oral diseases, such as periodontal disease or oral cancer, and guide treatment decisions. The importance of interdisciplinary collaboration in implementing personalised medicine in dentistry cannot be overstated, as it requires input from numerous healthcare professionals, including dentists, geneticists, and pharmacists (18).

Biomaterials design

Teeth and biomaterials are subjected to various mechanical stressors in the oral environment, including compressive, tensile, and shear forces. Therefore, understanding the mechanical properties of teeth and biomimetic materials is essential for developing dental materials with superior mechanical performance and increased durability. The mechanical properties of teeth and biomimetic materials are determined using nanoindentation and tribology techniques. Nanoindentation is a technique involving the application of a small, controlled load to a material's surface and measuring the resulting deformation. Alternatively, tribology studies the interaction between two surfaces in relative motion. Using these techniques, researchers can determine the elastic modulus, hardness, and wear resistance of teeth and biomimetic materials. The evolution of biomimetic materials replicating natural dentition's mechanical properties is accelerating. These materials are designed to possess mechanical properties comparable to natural teeth, such as high wear resistance, tensile strength, and flexibility. Such biomimetic materials have the potential to enhance the durability and performance of dental restorations (19, 20).

Nanotechnology

The application of nanotechnology in dentistry has created new opportunities for developing novel materials and devices for diagnosing and treating various oral diseases. Various dental materials contain nanoparticles, such as restorative materials, dental implants, and drug delivery systems. Nanoparticles are suitable for these applications due to their unique characteristics, including their small size, high ratio of surface area to volume, and surface reactivity. The development of nanosensors and imaging techniques has made possible the use of nanotechnology in the diagnosis of oral diseases such as dental caries and periodontal disease. The use of nanotechnology in the fabrication of scaffolds for oral tissue regeneration has been investigated. However, additional research is required to comprehend the potential dangers and toxicity of incorporating nanoparticles into dental materials and devices. This research is crucial for confronting nanotechnology's difficulties and potential benefits in dentistry (21, 22).

Microbiome analysis

The human buccal cavity is a complex and diverse environment that harbours numerous microorganisms,

including bacteria, fungi, and viruses, as determined by microbiome analysis. The oral microbiome is important in maintaining oral health and is associated with various oral diseases, including dental caries, periodontitis, and oral cancer. The buccal microbiome has garnered interest in recent years because to advances in next-generation sequencing and bioinformatics. Current knowledge of the oral microbiome and its association with several oral diseases necessitates additional research into the potential applications of microbiome analysis in personalised dental medicine. The significance of developing personalised treatments that target the unique microbial community associated with a person's oral disease has also been the subject of research. The microbiome analysis could identify the specific microorganisms responsible for a person's oral disease and design therapies to eliminate them. The high degree of inter-individual variability and the need for large-scale studies to establish a comprehensive understanding of the oral microbiome are obstacles associated with the analysis of the oral microbiome (23, 24).

Data mining

Data mining is extracting hidden and relevant information or patterns from massive datasets. It is a potent instrument that can extract useful information from large and complex datasets to facilitate decision-making processes. In recent years, the healthcare industry has witnessed a substantial increase in the volume and complexity of generated data, creating an opportunity to implement data mining techniques to enhance healthcare outcomes. Data mining is a multi-step procedure that includes data collection, data preparation, data analysis, and knowledge presentation. Identifying the data sources and obtaining the pertinent data is the first step. The second stage involves cleansing, transforming, and organising the data to ensure its high quality and analysability. The third phase is using data mining techniques to identify patterns, relationships, and insights within the data. The results of the data analysis are then presented to the end users in a meaningful and comprehensible manner. The potential of big data analytics in healthcare is highlighted by the ability to identify patient-specific risk factors, predict disease progression, and enhance clinical decision-making. However, data privacy and security, data quality, and the need for a competent workforce to analyse and interpret the data are obstacles that must be overcome (Figure 3) (25, 26).

Conclusion

In dental research, chemoinformatics may be utilised to enhance the design of dental materials, predict the toxicity of chemicals, devise personalised therapies, and get a deeper understanding of the oral microbiota. Microbiome research is an expanding field of study, and nanotechnology provides some encouraging possibilities for creating novel materials and technologies with better features. In drug discovery and development, pharmacokinetic and pharmacodynamic studies are essential for determining a drug's efficacy, safety, and optimal dosage. Data mining is a technique that may be used to get useful insights from massive volumes of data.

Author contribution: All authors listed have equally contributed to the development and writing of this article.

Acknowledgement: The corresponding author would like to acknowledge Kevin Kumar Vijayakumar for proofreading.

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Legend Figures

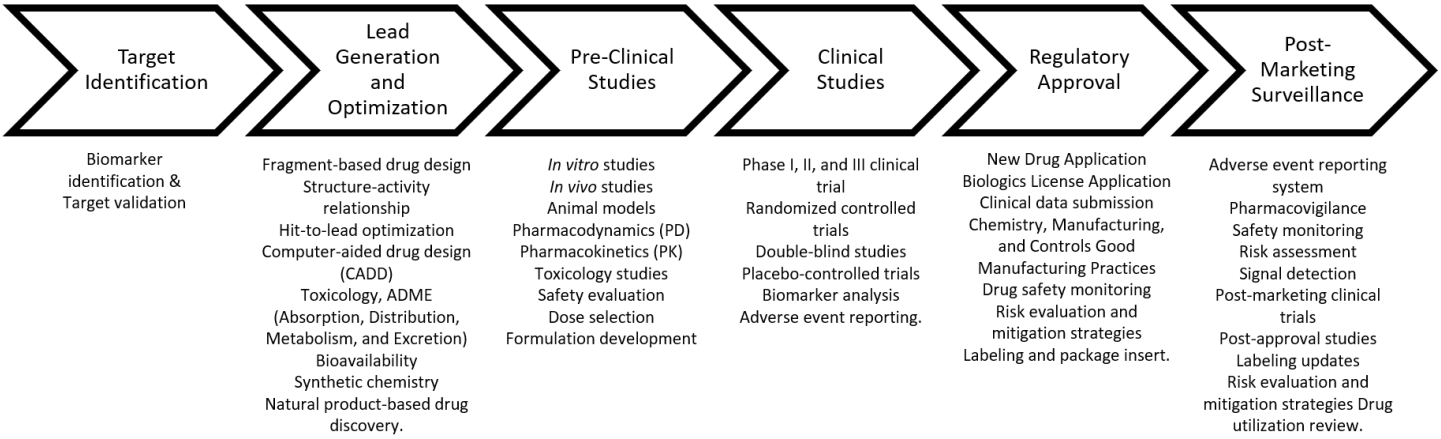

Figure 1: The flowchart illustrates the steps and challenges involved in drug discovery.

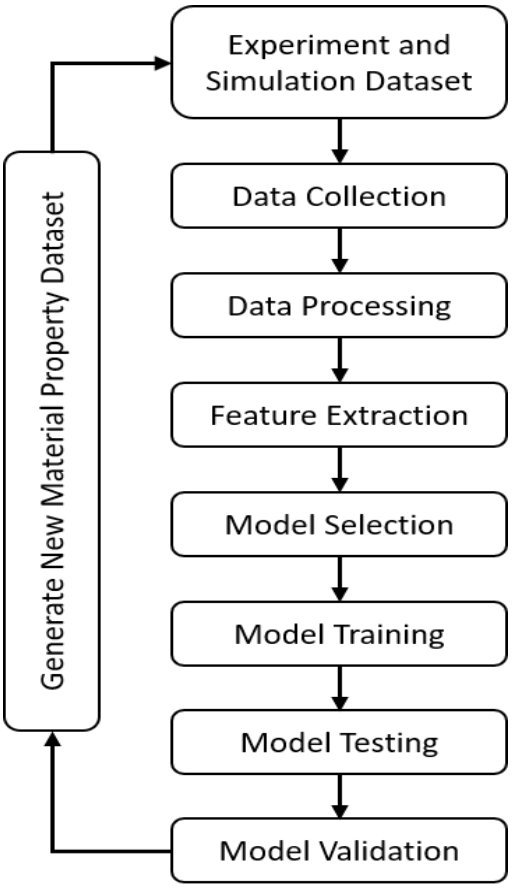

Figure 2: The Flowchart illustrates various steps involves in Material designing using Machine Learning.

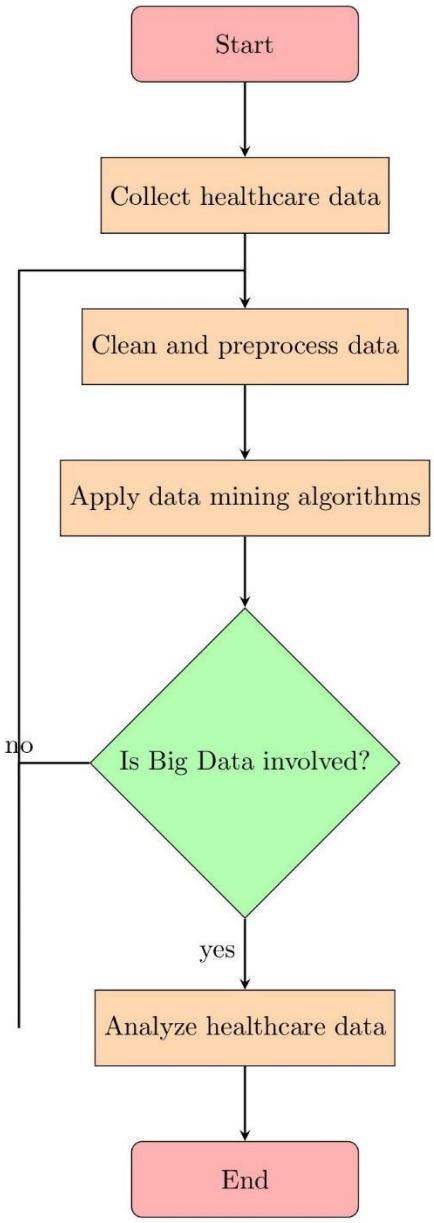

Figure 3: The flowchart illustrates the steps of Data mining and Big Data analysis in in healthcare. The flowchart depicts the progression of a process using distinct shapes for each stage and arcs connecting the shapes.