

Assessment of Pharmaceutical Software in Various Field

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Abstract—With the recent development of software, becoming a key for progress in each and every field of pharmacy. Drug designing software has potential role to design drug in pharmaceutical field. The drug designing software are used to analyze molecular modeling, gene sequence, molecular docking and behavioral study. Auto Docking used for molecular docking. CADD is very potential feature of software for drug display analyze. In a pharmaceutical industry their comes complexity in data and product, so now days various advanced software is used to handle these parameters. Electronic Data Capture [EDC] software is a tool used for the collection, management, and analysis of clinical trial data in the health care and pharmaceutical industries. It simplifies and automates the process of capturing and storing data electronically, replacing traditional paper- based methods. In the realm of clinical trials, pharmaceutical software simplifies the complex process of trial design, participant recruitment, data collection, and analysis. It offers functionalities for protocol management, electronic data capture, adverse event reporting, and statistical analyses. Clinical Trial Management System [CTMS] software assists in the overall planning, coordination, and management of clinical trials. Pharmaceutical software is also designed to support pharmacists in hospitals by providing tools for medication management, drug interaction checks, dosage calculations, and patient information systems. These software solutions improve medication safety, enable accurate prescription verification, facilitate patient-specific dosing, and enhance clinical decision-making. Pharmaceutical software serves as a critical asset in drug design and development, pharmaceutical industry management, clinical trial operations, and hospital pharmacist workflows. Its diverse functionalities optimize processes, improve productivity.

Keywords— Drug discovery, Drug Design Software, Pharma industry software, Electronic data capture.

I. INTRODUCTION

Software is a set of programs that tells a computer what task it should perform. It consists of a series of code written by a programming language, which is then interpreted by a computer. As a result, it facilitates our work by keeping all the records, carrying out the required calculations, and much more.

Exploration of software have become a key component of the drug discovery and development in pharmaceutical industry, playing a crucial role in expanding new bio - active drugs across a range of therapeutic areas. Proper used of software and computer based modern methods has reduced several hindrances in the process of drug discovery and new drug development. The handling, storage and distribution of pharmaceuticals is a complex task. So, we used a various advanced software to handle all parameters [1].

In the field of pharmaceutical industry software are used to collect and maintained all document. Drug design is a process which involves the identification of a compound that displays a biological action and end when the biological action and chemical synthesis of new compound or drug are optimized. The process of drug discovery and development is very convenient with the invention of various computational software and tools. Drug design and discovery mostly done with the help of software like structure-ligand based design and lead optimization. The invention of computational tools used for Novel Doses Drug design and discovery is one of the fast - developing recent achievements for Molecular Docking. Molecular docking is such a structure - based drug design methods in which molecules interact to each other and also

predict the binding mode and affinity between receptors and ligands. The technology has been widely used now which not only record data but also greatly improves the efficiency and reduce the research cost and in case of industry reduced labor cost

The modern era is an era of technology and computer. The rapid use of computer has affected every field of study and pharmacy is no exception. A variety of task are performed by pharmacists with the use of software and some particular apps. With the recent advancements in pharmaceutical industry the complexes are handle by digital or data - based computer work. We hope to illustrate the significance of pharmaceutical software in numerous fields with this review [2].

II. SOFTWARE USED IN DRUG DESIGNING AND DEVELOPMENT

Drug designing is a process which involve the identification of a compound that displays a biological profile and end when the biological profile and chemical synthesis of the new chemical entity are optimized. Drug designing and development of new pharmaceutical product is generally known as complex process which takes a lot of time and resources for developing. It is also known as rational drug design and it is method of finding new medication based on the biological receptors and target molecules. Drug designing and development involve the designing of small molecules which is complementary to the biological receptors to which they bind and interact to cause pharmacological action. The drug molecule are the primary components in the drug formulations, which combined with the numbers of compound [3].

Selection of drug molecules for the designing and development

For the initial stage of drug designing and development using software, the choice of drug is a crucial component. When choosing drug compounds, the following considerations must be made-

- A polar drug that is soluble in water is required.
- Both hydrophilic and lipophilic properties must be present in a drug's structure.
- Drugs need to pass through cell membranes.[4]

Types of drugs- designing and development

There are mainly four types of drugs- designing and discoveries which are given below-

- Ligand based drug design [LBDD]
- Structure based drug design [SBDD]
- Rational drug design
- Computer- Aided drug design [5]

Ligand-Based Drug-Design [LBDD]

In LBDD, the target protein's 3D structure is unknown, but it is known which ligands bind to the intended target location. These ligands are applicable to create a model or molecule for a pharmacophore that possesses all required structural characteristics to adhere to active target site [6]. Pharmacophore-based approaches and quantitative-structure activity relationships (QSARs) are two common ligand-based methodologies. It is presumed in LBDD that molecules with comparable structures also share the same biological properties and interact with the target protein [7].

Structure based drug design

Structure based drug design is one of the earliest methods in drug design, that helped in search of new drug. It makes calculation while design provides structural as well as structural information, ligand dynamic and electronic characteristics. Structure based drug design development is

based on understanding of the biological target 3D structure. [8]

Rational drug design

The creation of medications based on an analysis of the structure and function of specific molecules is known as rational drug design. The goal of rational design is the creation of medications that work. The three major steps involved in rational drug design are:

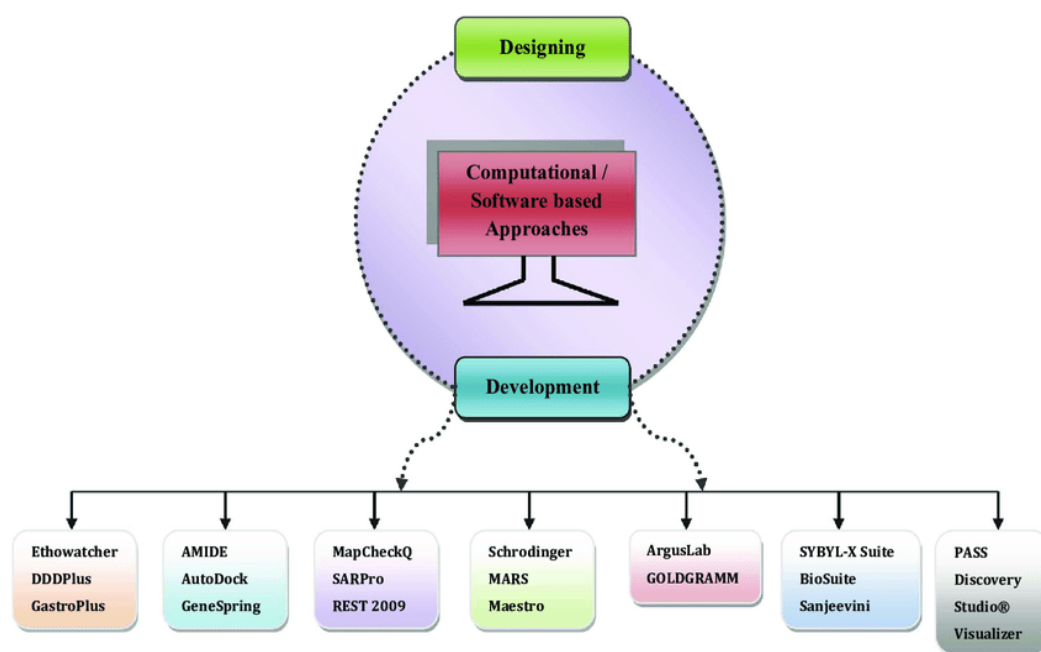
- Step 1: Identification of receptor or enzyme.
- Step 2: Characterize the structure and function of identified receptors or enzyme.
- Step 3: design a drug-molecules that interact with the receptor or enzyme in therapeutically beneficial way.[9]

Computer-Aided drug design

Chemical biology and computational drug design techniques are used in drug discovery to effectively identify and optimize lead molecules. The primary goals of chemical biology are to clarify a target's biological role and a chemical modulator's mode of action. However, to help identify promising candidate medications, computer-aided drug design leverages structural knowledge of either the target (structure-based) or known ligands with bioactivity (ligand-based) knowledge. Pharmaceutical corporations and academic research groups are now using a variety of virtual screening techniques to shorten the time and expense involved in finding a powerful medication. Even though these techniques are developing quickly, further advancements are necessary for next-generation drug discovery instruments. The benefits of structure-based and ligand-based drug design imply that their complementary applications and incorporation into experimental protocols have a significant influence on logical drug design [10].

Drug Designing software

A computer needs a software for its function such as program. This software makes our work simple and easy.



Software Based Programs Used During New Drug Discovery and Development

1. Pharmacokinetic parameters

1. DDD Plus: Study of disintegration and dissolution
2. Gastro Plus: IVIVC for various formulations
3. Map Check: Compare dose and fluency measurement

2. Ligand interaction and molecular dynamics

1. Auto Dock: Ligand – protein interaction evaluation
2. Schrodinger: Ligand – receptor docking
3. GOLD: Protein – ligand docking
4. Bio Suite – Sequence and genome analyzing

3. Image analysis and visualizers

1. AMIDE: Medical image analysis in molecular imaging
2. Imaging Software Scge-Pro: cytogenetic and DNA based analysis
3. Xenone Living Image Software: In vivo imaging display and analysis

4. Molecular modeling and structure activity relationship

1. Maesrto: Molecular modeling analysis
2. Argus Lab: Molecular docking calculation molecular modeling package
3. GRAMM: Protein-protein docking
4. PASS: SAR models creation and analysis

5. Behavioral study

1. Ethowatcher: Behavioral analysis
2. MARS [Multi modal Animal Rotation System]: Animal activity tracking

6. Data Analysis

1. REST 2009 Software: Gene expression data analysis
2. QSAR Pro: Study of protein – protein interaction
3. Gene Spring: For correction method in samples

1. DDD Plus

DDD Plus [Dose Dissolution and Disintegration Plus] is used to study disintegration and dissolution pattern of doses performed and active- ingredients. It used to perform *in-vitro* disintegration and dissolution. It is an advanced computer program employed by formulation of new API, a single calibration experiment is generally required, after which DDD Plus predicts how change in formulation or experimental parameters will affect the dissolution rate. This software provides precise information of dissolution and disintegration rate [11]. DDD Plus allow to choose from one of the following mathematical drug models and to demonstrate the dissolution of a single ingredients using. It is mathematical model which is used for the *in vitro* dissolution to determine physiochemical parameters like- pKa, solubility, diffusion coefficients and density [12].

Application

1. Automatically calculates fluid velocity based on type of apparatus used.
2. It is an optimizing module which uses a single experimented data set to calibrate drugs dissolution rate [13].

2. Auto Dock

Auto Dock is a powerful software tool used in the field of computational biology and drug discovery for performing molecular docking simulations. Molecular docking is a crucial step in the early stages of drug development, where the

interaction between a small molecule (ligand) and a target protein is investigated to predict their binding affinity and geometry. Auto Dock utilizes an algorithmic approach called Lamarckian Genetic Algorithm (LGA) that combines elements of genetic algorithms and local search methods to efficiently explore the conformational space of the ligand and receptor [14]. This allows for the identification of energetically favorable binding poses and the prediction of binding affinities. The software incorporates sophisticated scoring functions that evaluate the complementarity between the ligand and protein, considering factors such as shape, electrostatics, and hydrophobicity. This enables researchers to assess the strength of the interaction and prioritize potential drug candidates based on their predicted binding affinity [15]. Auto Dock has been widely used in clinical trials and drug discovery research due to its versatility, accuracy, and high-throughput capabilities. It has aided in the identification of novel drug candidates, optimization of existing compounds, and understanding the molecular mechanisms underlying drug-protein interactions. Through its user-friendly interface and extensive documentation, Auto Dock allows researchers to prepare and analyze complex molecular systems, visualize docking results, and generate insightful reports. It has proven to be an invaluable tool in the quest for new therapeutic interventions by facilitating virtual screening and lead optimization, ultimately contributing to the acceleration of drug discovery processes in the clinical trials [16].

3. AMIDE

AMIDE (Amide's a Medical Imaging Data Examiner) is a widely used software tool in the field of medical imaging analysis. It is specifically designed for the visualization, analysis, and manipulation of various types of medical imaging data, including positron emission tomography (PET) and single photon emission computed tomography (SPECT) images. AMIDE offers a range of features that enable researchers and clinicians to explore and extract valuable information from medical images. It supports the loading and display of DICOM (Digital Imaging and Communications in Medicine) files, which are the standard format for medical imaging data. The software provides an intuitive user interface that allows users to view multiple image slices simultaneously, adjust the window and level settings, and perform various image manipulations like zooming, panning, and rotating. One of the key functionalities of AMIDE is its ability to perform semi-quantitative analysis of PET and SPECT images [17]. It offers tools for region-of-interest (ROI) delineation, allowing users to define specific areas within the image and extract quantitative data such as standardized uptake values (SUV) for PET studies. This quantitative analysis aids in the assessment of disease progression, response to treatment, and overall evaluation of medical imaging data. AMIDE also provides tools for image registration, which is the process of aligning multiple images to facilitate comparison and fusion of information from different modalities or time points. This feature is particularly useful in longitudinal studies or when combining data from different imaging modalities for comprehensive analysis. Furthermore, AMIDE supports the

overlay of anatomical information onto functional images, allowing users to fuse PET/SPECT data with anatomical reference templates or individual structural images from other modalities like magnetic resonance imaging (MRI). This visual integration enhances the interpretation of functional data within the anatomical context. In summary, AMIDE is a versatile software tool that plays a vital role in the analysis and interpretation of medical imaging data. Its capabilities in image visualization, quantitative analysis, ROI delineation, image registration, and integration of functional and anatomical information make it an essential tool in clinical research, diagnosis, and treatment planning [18].

4. Argus Lab

Argus Lab is a powerful and comprehensive software utilized in the field of drug design and discovery. It is specifically designed to aid researchers, chemists, and pharmaceutical companies in various stages of the drug development process. With its numerous functionalities and advanced tools, Argus Lab enables users to streamline their workflow and make informed decisions. One of the key features of Argus Lab is molecular modeling, which allows scientists to create and manipulate three-dimensional molecular structures. This functionality aids in the visualization and analysis of complex molecular systems, providing insights into their behavior and interactions. It also includes tools for performing molecular docking studies, which assist in predicting the binding affinity and interactions between small drug-like molecules and target proteins.

In addition to molecular modeling, Argus Lab offers various computational chemistry techniques for drug design. These techniques include molecular dynamics simulations, quantum mechanics calculations, and structure-activity relationship (SAR) analysis. These calculations help in assessing the stability, energetics, and activity of potential drug candidates, allowing researchers to prioritize and optimize their designs. Argus Lab also provides a wide range of virtual screening capabilities, which involve screening large chemical libraries or databases to identify potential lead compounds with desired properties. This feature integrates various algorithms and scoring functions to prioritize molecules based on their likelihood of binding to a specific target or exhibiting other favorable characteristics [19].

Furthermore, Argus Lab facilitates the analysis of molecular properties such as molecular descriptors, physicochemical properties, and toxicity predictions. These analyses aid in understanding the drug-likeness, ADME (absorption, distribution, metabolism, and excretion) properties, and potential safety profiles of candidate molecules. Overall, Argus Lab plays a crucial role in drug design by providing an extensive suite of tools for molecular modeling, computational chemistry, virtual screening, and property analysis. Its user-friendly interface and comprehensive feature set make it a valuable software for researchers and pharmaceutical companies involved in the development of new drugs [20].

5. MARS [Multi Model Animal Rotation System] Software

The multi-model animal rotational system software refers to a computer program that aids in the design and management

of rotational grazing systems for livestock. Rotational grazing involves systematically moving animals between different grazing areas to optimize forage utilization, improve soil health, and enhance animal performance. This specialized software is designed to help farmers and land managers plan and implement efficient rotational grazing systems for multiple species of animals, such as cattle, sheep, or goats. It takes into account various factors, including the size and terrain of the grazing area, the number of animals, the desired grazing intensity, and the available forage resources. The software provides a user-friendly interface where users can input information about their specific farming operation, such as the number and types of animals, desired rotation schedule, and available pasture areas. Based on this input, the software generates a rotational grazing plan that optimizes grazing efficiency and animal performance while considering factors like forage regrowth time, animal nutritional requirements, and pasture rest periods. Furthermore, the software can assist in monitoring and tracking key performance indicators of the rotational grazing system, such as forage utilization rates, animal weight gains, and pasture productivity. It may also provide recommendations for adjusting the rotation schedule or making improvements to the grazing infrastructure based on real-time data inputs.

The benefits of using multi-model animal rotational system software include improved pasture management, enhanced animal nutrition, increased forage production, and potential cost savings. By optimizing grazing patterns and ensuring appropriate rest and recovery periods for the pasture, this software can contribute to sustainable and efficient livestock production. It is important to note that while there are several software tools available for rotational grazing management, their features and capabilities may vary. Farmers and land managers should research and select a software program that aligns with their specific needs and goals in managing multi-species rotational grazing systems [21].

6. Gene Spring

Gene spring is a powerful software tool used in the field of genomics and bioinformatics. It is specifically designed for the analysis and interpretation of gene expression data. Gene expression refers to the process by which information encoded in genes is converted into functional products, such as proteins, that determine the characteristics and behavior of cells and organisms. Gene spring provides researchers with a user-friendly interface and a wide range of analytical capabilities to explore gene expression data and extract meaningful insights. It supports various types of micro assay and next-generation sequencing data, allowing users to preprocess, normalize, and filter the data for further analysis. The software offers numerous statistical methods and algorithms for identifying differentially expressed genes, performing clustering and classification analyses, and visualizing results through interactive graphs and heatmaps.

In addition to its data analysis features, Gene springs also facilitates the functional interpretation of gene expression results. It integrates with various databases and resources, such as gene ontology (GO) annotations, pathway databases, and biological literature, to help researchers uncover the

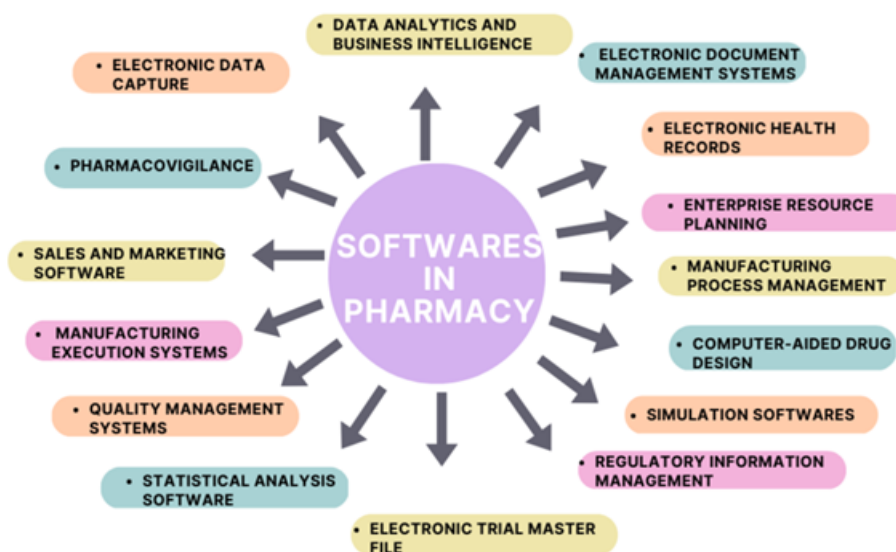
biological significance and potential functions of the identified genes. Overall, Gene spring serves as a valuable tool in genomics research, enabling scientists to explore gene expression patterns, discover potential biomarkers, investigate biological pathways, and gain insights into the underlying molecular mechanisms of various biological processes and diseases [22].

III. THE IMPORTANCE OF PHARMACEUTICAL SOFTWARE IN INDUSTRY

Pharmaceutical software has revolutionized the industry by streamlining various processes and significantly improving efficiency. This software encompasses a wide range of tools and applications designed specifically for the pharmaceutical sector. Let's dive into an introduction to pharmaceutical software in the industry. Pharmaceutical software serves multiple purposes, including research and development, clinical trials, regulatory compliance, manufacturing, supply chain management, quality control, and sales and marketing. These software solutions are tailored to meet the unique needs and challenges of the pharmaceutical industry, transforming the way companies operate and enhancing overall productivity [23]. In the realm of research and development, pharmaceutical software plays a crucial role in accelerating the drug discovery process. It allows scientists to manage and analyze vast amounts of data, aiding in the identification of potential drug targets, the design of experiments, and the optimization of formulation parameters. By utilizing advanced algorithms and predictive models, scientists can expedite the identification of new drug candidates, saving both time and resources. During the clinical trial phase, pharmaceutical software provides comprehensive tools to manage patient data, track study progress, and facilitate collaboration among researchers. These systems enable efficient data collection,

analysis, and reporting, ensuring adherence to strict regulatory requirements and standards. By digitizing and automating manual processes, such software helps reduce errors, improve data integrity, and enhance overall trial efficiency. Moreover, pharmaceutical software addresses quality control and regulatory compliance by implementing robust systems for tracking and managing the manufacturing and distribution of pharmaceuticals. It ensures adherence to stringent quality standards, regulatory guidelines, and safety protocols. This software facilitates the tracking of raw materials, batch records, and manufacturing processes, enabling companies to maintain a high level of product quality and safety. Supply chain management is another critical aspect where pharmaceutical software makes a significant impact. It optimizes inventory control, tracks shipments, and provides real-time visibility into the entire supply chain. By enhancing logistics operations, companies can minimize costs, reduce stockouts, and accurately forecast demand. This, in turn, leads to improved customer satisfaction and the ability to respond swiftly to market demands. Pharmaceutical software also plays a pivotal role in sales and marketing activities. It assists in managing customer relationships, analyzing market trends, and tracking sales performance. These systems enable effective communication with healthcare professionals, facilitate product promotion, and aid in complying with regulatory requirements related to marketing activities. In summary, pharmaceutical software serves as a game-changer in the industry by addressing key challenges and optimizing various processes. From drug discovery to regulatory compliance, manufacturing to supply chain management, and sales to marketing, this software empowers pharmaceutical companies to operate more efficiently, make informed decisions, and ultimately enhance patient care and safety [24].

Types of Pharmaceutical Software used in Industry



Electronic Data Capture

Electronic Data Capture (EDC) software is a tool used for the collection, management, and analysis of clinical trial data

in the healthcare and pharmaceutical industries. It simplifies and automates the process of capturing and storing data electronically, replacing traditional paper-based methods.

EDC software provides a secure and efficient means of data collection by allowing researchers and clinical trial professionals to design electronic case report forms (eCRFs) [25]. These eCRFs consist of specific data fields tailored to capture the necessary information for the study. EDC systems also offer features for data validation and verification, ensuring the accuracy, completeness, and consistency of the collected data. This includes built-in checks for missing data, range validations, and logical checks. By reducing human errors and transcription mistakes commonly associated with paper-based data entry, EDC software improves data quality and integrity. Additionally, EDC software streamlines the data management process by facilitating data cleaning, query management, and tracking. Instead of manually reviewing and resolving discrepancies, the software allows for automated data validation checks and generates queries for clarification when necessary. This accelerates the resolution process, making data cleaning more time-efficient. Moreover, EDC software centralizes data storage, making it easily accessible and searchable for authorized users [26]. It enables collaborative data entry and facilitates remote data entry from multiple sites or locations, enhancing the efficiency and scalability of clinical trials. This centralized storage also improves data security and compliance with privacy regulations, as access to sensitive information can be controlled and monitored. Furthermore, EDC software often integrates with other systems like electronic medical record (EMR) systems or laboratory information management systems (LIMS), enabling seamless data exchange and interoperability. This integration enhances data accuracy, eliminates redundant data entry, and increases data visibility and tracking across different research phases. In summary, electronic data capture software revolutionizes data collection and management in clinical trials by providing a secure, efficient, and automated platform for capturing, maintaining, and analyzing data. It improves data quality, accelerates data cleaning and query resolution processes, facilitates collaboration, and enhances interoperability with other systems [27].

Data Analytics and Business Intelligence

Data analytics and business intelligence are closely related disciplines that involve using advanced techniques to analyze and interpret large sets of data in order to gain valuable insights and make informed business decisions [28]. Data analytics refers to the process of examining raw data to uncover patterns, identify trends, and extract meaningful information. It involves various methods such as data mining, statistical analysis, machine learning, and predictive modeling. By leveraging data analytics, businesses can derive actionable insights from their data, leading to better decision-making, improved operational efficiency, and enhanced business performance [29]. On the other hand, business intelligence (BI) focuses on gathering, analyzing, and presenting data in a way that enables business leaders, managers, and other stakeholders to make data-driven decisions. BI involves using specialized tools and technologies to collect and consolidate data from various sources, transforming it into meaningful and

comprehensible formats such as reports, dashboards, and visualizations. These tools also facilitate data exploration, ad-hoc querying, and the creation of interactive reports, allowing users to gain valuable insights and answer business-related questions efficiently. Overall, the combination of data analytics and business intelligence provides organizations with the means to transform raw data into actionable knowledge. By harnessing these capabilities, businesses can achieve a competitive edge, optimize their operations, identify market trends, understand customer behavior, and ultimately drive growth and innovation [30].

Electronic Health Records

Electronic Health Records (EHR) software refers to a digital system designed to store, manage, and provide access to patient health information in a secure and organized manner. It replaces traditional paper-based medical records with electronic versions, offering numerous benefits to healthcare providers, patients, and the overall healthcare ecosystem. EHR software serves as a comprehensive repository, encompassing a wide range of patient data such as medical history, laboratory results, diagnoses, medications, allergies, immunization records, and more. It allows healthcare professionals to access and update patient information in real-time, ensuring accuracy, continuity of care, and efficient decision-making [31].

Key features of EHR software include:

1. **Patient Data Management:** EHR software allows healthcare providers to enter, store, and retrieve patient information easily. This includes demographics, medical history, chief complaints, vitals, and progress notes.
2. **Interoperability:** EHR systems facilitate seamless communication and data exchange between different healthcare providers and organizations, promoting collaboration, continuity, and coordinated care.
3. **Clinical Decision Support:** EHR software often incorporates clinical decision support tools, such as alerts, reminders, and guidelines, to assist healthcare professionals in making evidence-based decisions, reducing medical errors, and improving patient safety.
4. **Medication Management:** EHRs maintain accurate and up-to-date medication lists, check for possible drug interactions and allergies, and facilitate e-prescribing, enhancing medication safety and prescription accuracy.
5. **Workflow Optimization:** EHR software streamlines various healthcare processes, including appointment scheduling, billing, coding, and documentation, improving overall efficiency and reducing administrative burdens.
6. **Analytics and Reporting:** EHR systems offer analytical capabilities to generate reports, track key performance indicators, and analyze population health data, enabling healthcare organizations to monitor outcomes, identify trends, and facilitate data-driven decision-making. Additionally, EHR software often adheres to strict security and privacy standards, ensuring the confidentiality and integrity of patient data. It provides role-based access controls, audit trails, and encryption mechanisms to protect sensitive information from

unauthorized access or breaches. The widespread adoption of EHR software has transformed healthcare delivery by digitizing and centralizing patient records, enhancing accessibility, interoperability, and care coordination. It promotes efficiency, accuracy, and patient engagement while supporting evidence-based medicine and improving overall healthcare quality [32].

Quality Management Systems

A quality management system (QMS) software is a critical tool used in various industries to ensure that products and services consistently meet the desired quality standards. It helps organizations establish and maintain efficient processes, improve customer satisfaction, and achieve continual improvement [33].

Here are some key aspects and explanations of QMS software in industries:

1. **Centralized Documentation:** QMS software provides a centralized platform for storing and managing quality-related documents such as policies, procedures, work instructions, and forms. This ensures easy access, version control, and compliance with relevant standards or regulations.
2. **Process Automation:** QMS software automates and streamlines various quality processes, such as document control, corrective and preventive actions (CAPA), internal audits, non-conformance management, and change management. It eliminates manual errors, ensures consistency, and saves time.
3. **Risk Management:** An effective QMS software includes risk management features that enable identification, assessment, and mitigation of potential risks in the product or service lifecycle. It helps prioritize actions, minimize adverse effects, and enhance decision-making.
4. **Supplier Management:** Managing suppliers and ensuring their compliance with quality requirements is crucial. QMS software facilitates supplier evaluation, performance monitoring, and supplier corrective actions, ensuring that only approved and reliable vendors are used.
5. **Training and Competence Management:** Training employees on quality procedures, standards, and best practices is essential. QMS software allows organizations to plan, deliver, and track training activities. It also helps assess employee competence and maintain records for compliance purposes [34].
6. **Performance Metrics and Reporting:** QMS software generates real-time reports and performance metrics, providing valuable insights into the effectiveness of quality processes, identifying trends, and areas for improvement. This data-driven approach assists in making informed decisions to enhance overall quality management.
7. **Regulatory Compliance:** Industries often operate under specific regulations or standards (e.g., ISO 9001). QMS software helps organizations comply with these requirements by providing tools for documentation, audits, corrective actions, and ensuring continuous adherence to standards.
8. **Continuous Improvement:** QMS software supports the concept of continuous improvement by allowing organizations to capture and analyze quality-related data, identify root

causes of issues, implement corrective actions, and monitor their effectiveness over time. In conclusion, quality management system software in industries is a comprehensive solution that streamlines quality-related processes, improves compliance, enhances efficiency, and drives continuous improvement. It ensures that products and services meet customer expectations while adhering to relevant standards and regulations [35].

Computer-Aided Drug Design

A computer-aided drug design (CADD) software is a crucial tool in the pharmaceutical industry for developing new drugs. It employs various computational techniques to expedite the process of drug discovery and optimization. Firstly, CADD software aids in the identification and selection of potential drug targets. By analyzing biological structures, such as proteins or enzymes, the software can pinpoint specific sites that could be targeted by a drug molecule. This assists researchers in identifying potential therapeutic targets more effectively, saving time and resources. Once a target has been identified, CADD software facilitates the exploration of chemical compounds that could bind to the target and exhibit desired medicinal properties. This is achieved through virtual screening, where the software screens vast databases of chemical structures and predicts their likelihood of binding to the target and exerting a desired effect. The software also enables the optimization of lead compounds. By utilizing molecular modeling techniques, it can analyze the interactions between the drug molecule and its target, providing valuable insights into how the compound can be fine-tuned to enhance its potency, selectivity, and safety profile. This process, known as lead optimization, aids in the development of more effective and safer drug candidates. Furthermore, CADD software assists in the prediction of pharmacokinetic properties of drug candidates, such as absorption, distribution, metabolism, and excretion (ADME) [36]. These predictions help researchers assess the drug's behavior within the human body, informing decisions about dosage, formulation, and potential interactions with other medications. Additionally, CADD software plays a vital role in predicting the toxicity and safety profile of drug candidates. By analyzing chemical structures and simulating their interaction with biological systems, it can help identify potential risks and guide the selection of compounds with better safety profiles, reducing the chances of adverse effects during clinical trials and post-marketing. Overall, computer-aided drug design software in the pharmaceutical industry accelerates the drug discovery process, streamlines experimentation, reduces costs, and helps researchers make data-driven decisions regarding the selection, design, and optimization of potential drug candidates [37].

Manufacturing Execution Systems

Manufacturing Execution Systems (MES) software is widely used in various industries to optimize and control manufacturing operations. MES software helps improve efficiency, visibility, and traceability of production processes. It can be found in industries such as:

1. Automotive Manufacturing: MES software is used to monitor and control assembly lines, track parts and components, and manage quality control.
2. Aerospace and Defense: Aerospace manufacturers use MES to ensure compliance with strict quality and traceability requirements.
3. Electronics Manufacturing: For companies that produce electronic components and devices, MES software helps manage complex production processes and quality control [38].
4. Pharmaceutical and Life Sciences: In this highly regulated industry, MES ensures compliance with regulatory standards, batch tracking, and quality control.
5. Food and Beverage: MES is used to monitor production, manage recipes, track ingredients, and ensure food safety and compliance.
6. Chemical Manufacturing: It helps manage complex chemical processes, track batch production, and ensure safety and environmental compliance.
7. Medical Device Manufacturing: MES software helps with product traceability, quality assurance, and regulatory compliance in this sector.
8. Oil and Gas: For upstream and downstream operations, MES software helps manage production, track equipment, and ensure safety and regulatory compliance.
9. Textile and Apparel: It aids in managing complex supply chains, tracking raw materials, and ensuring quality in textile and garment manufacturing.
10. Metal and Mining: MES is used to monitor and optimize mining and metal production processes, as well as track resources and quality control.
11. Plastics and Rubber Manufacturing: MES software is used to manage the production of plastic and rubber products, track materials, and maintain quality standards.
12. Packaging Industry: It helps manage the packaging process, track materials, and ensure the quality and safety of packaged products.
13. Paper and Pulp: MES software aids in optimizing paper and pulp production processes, tracking resources, and managing quality [39].
14. Energy and Utilities: In power generation and utility companies, MES can be used for asset management, maintenance, and process optimization.
15. Consumer Goods Manufacturing: For a wide range of consumer products, MES software ensures efficient production and quality control. MES software typically offers features such as real-time monitoring, scheduling, inventory management, quality control, and reporting. It connects with various manufacturing equipment and systems to provide a holistic view of the production process. The choice of MES software and its specific features can vary based on the industry and the needs of the manufacturing organization [40].

IV. SOFTWARE'S IN THE FIELD OF CLINICAL TRIALS

The management and analysis of research data, it serves as a powerful tool to aid researchers, clinicians, and regulatory agencies. Software's used in clinical trials plays a vital role in facilitating tracking and evaluating the safety, efficacy, and

side effects of investigational drugs or medical devices [41]. One of the primary functions of clinical trial software is the electronic data capture (EDC) system. EDC allows for the collection, storage, and management of valuable patient data in a secure and standardized manner. By digitizing the data collection process, researchers can reduce the chance of human error, streamline data entry, and enhance the overall efficiency of the trial. Furthermore, clinical trial software provides features for randomization and stratification of participants, ensuring unbiased allocation to treatment groups. This helps to minimize selection bias and strengthen the validity of the trial's results. Additionally, the software assists in tracking participants' adherence to the study protocol and monitors their progress through automated reminders and notifications. Data management is another critical aspect of clinical trial software. It includes functionalities for data cleaning, validation, and integration to ensure the accuracy and reliability of the collected information. The software can also generate various reports and analytics, allowing researchers to monitor the trial's progress, identify trends, and assess the effectiveness of the interventions being tested. Furthermore, some clinical trial software incorporates advanced statistical analysis tools, enabling researchers to perform complex calculations and generate meaningful insights from the accumulated data. These tools help determine whether the treatment under investigation shows statistically significant differences compared to control groups, aiding in decision-making regarding the potential approval or further development of the intervention. Lastly, compliance and regulatory requirements are crucial in clinical trials. The software assists in maintaining compliance by ensuring data security, privacy, and adherence to relevant regulations such as Good Clinical Practice (GCP) guidelines. It helps with the creation of audit trails, managing user access rights, and tracking any changes made to the data. In summary, the software used in clinical trials provides essential support throughout the entire research process. From data collection and management to analysis and compliance, it enhances efficiency, accuracy, and regulatory compliance, thus contributing to the successful conduct of clinical trials [42].

Application of Software in the Fields of Clinical trials-

In modern clinical trials, there is a myriad of software used to facilitate various aspects of the trial process. These software solutions aim to streamline and enhance data management, analysis, communication, and regulatory compliance. Here are some of the key software applications commonly used in clinical trials:

1. Electronic Data Capture (EDC) Systems: EDC systems are used to collect and manage patient data electronically [43]. They allow for secure and efficient data entry, validation, and tracking during the course of a clinical trial [44].
2. Clinical Trial Management System (CTMS): CTMS software assists in the overall planning, coordination, and management of clinical trials. It helps researchers track study progress, monitor participant enrollment, manage regulatory

compliance, and facilitate collaboration between various stakeholders.

3. Randomization and Trial Supply Management (RTSM) Systems: RTSM systems, also known as Interactive Response Technology (IRT) systems, are used to randomize participants into different study groups and manage the supply of investigational products. These systems help ensure unbiased allocation and efficient inventory management.

4. Electronic Trial Master File (eTMF) Systems: eTMF solutions are employed to digitally organize and store essential trial documents, such as study protocols, informed consent forms, regulatory submissions, and monitoring reports. They facilitate efficient document management, version control, and regulatory compliance.

5. Clinical Data Management Systems (CDMS): CDMS software allows for effective data cleaning, coding, and analysis in clinical trials. These systems help ensure data accuracy, integrity, and adherence to specific data standards [45].

6. Safety Management Systems: Safety management software is critical for adverse event reporting, safety monitoring, and pharmacovigilance. These systems enable the capturing, tracking, and analysis of safety-related data for early detection of adverse events or trends.

7. Statistical Analysis Software: Statistical analysis software, such as SAS or R, is employed to conduct data analysis and generate meaningful insights from clinical trial data. These tools help researchers analyze efficacy, safety, and other relevant outcomes.

8. Electronic Patient-Reported Outcome (ePRO) Systems: ePRO systems collect patient-reported data, such as quality of life measurements or symptom assessments, directly from study participants through electronic devices. These systems improve data accuracy, reduce recall bias, and enhance patient compliance [46].

9. Regulatory Compliance Software: Regulatory compliance software assists in ensuring adherence to applicable regulations and guidelines during clinical trials. These tools can help with tracking and managing regulatory requirements, facilitating inspections, and maintaining compliance documentation. It's important to note that the specific software used can vary depending on the trial's nature, complexity, and requirements. Clinical trial sponsors, contract research organizations (CROs), and research institutions often select software solutions tailored to their specific needs, ensuring efficient and compliant trial management [47].

V. PHARMACEUTICAL SOFTWARE USED BY PHARMACISTS

Pharmacists in hospitals used a variety of software to manage patient medication and perform their duties efficiently. The role of software in hospitals used by pharmacists is to help them perform various tasks related to medication management, patient care, and communication. Some of the functions that software can provide for hospital pharmacists are:

Dispensing and labelling: Software can help pharmacists enter, verify, and print prescriptions and medication orders for patients. Software can also generate barcodes and labels for

medications to ensure accurate identification and administration.

Compounding and manufacturing: Software can help pharmacists prepare and produce sterile and non-sterile products, such as injections, infusions, mixtures, creams, and ointments. Software can also monitor the quality and safety of the products, such as temperature, pH, sterility, and stability.

Inventory and supply chain: Software can help pharmacists manage the stock levels, ordering, receiving, and distribution of medications and supplies. Software can also track the expiry dates, batch numbers, and locations of medications to prevent wastage and ensure availability [48].

Clinical decision support: Software can help pharmacists access patient records, drug information, guidelines, and protocols to support their clinical decisions. Software can also alert pharmacists to potential drug interactions, allergies, adverse effects, dosing errors, and therapeutic duplications.

Patient care services: Software can help pharmacists provide patient-centered services, such as medication reconciliation, medication review, medication education, discharge counselling, and follow-up. Software can also document the outcomes and interventions of these services and generate reports for quality improvement.

Communication and collaboration: Software can help pharmacists communicate and collaborate with other health professionals, such as prescribers, nurses, technicians, and administrators. Software can also facilitate the electronic transmission of prescriptions, orders, results, and feedback between different departments and settings.

Software plays an important role in hospital pharmacy by enhancing the efficiency, accuracy, safety, and quality of the services that pharmacists provide. However, software is not a substitute for the professional judgement and skills of pharmacists. Pharmacists should always use software with caution and verify the information and results that software provides [49].

Types of Software

There are several types of software that pharmacists use in hospitals to manage patient care and medication. Some of the most popular ones are:

1. **Electronic Health Records (EHR):** EHR systems store patients' data, including medical and family history, laboratory and other test results, prescribed medications history, and more. The ability for authorized physicians to create and maintain patient health information and then share it with other providers across multiple healthcare organizations is the most significant aspect of an EHR. This does not only automate and streamline the providers' workflow, but also visibly improves the patient's care. EHRs reduce errors, improve patient safety, and support better patient outcomes [50].

2. **Hospital Management Systems (HMS):** HMS software is used to manage hospital operations such as patient registration, appointment scheduling, billing, inventory management, and more. It helps to streamline hospital workflows and improve efficiency.

3. Pharmacy Information Systems (PIS): PIS software is used to manage medication orders, dispensing, inventory management, and more. It helps pharmacists to ensure that patients receive the right medication at the right time.

4. Clinical Decision Support Systems (CDSS): CDSS software provides pharmacists with real-time clinical decision-making support based on patient data such as medical history, lab results, allergies, etc. It helps pharmacists to make informed decisions about medication orders [51].

5. Telepharmacy Software: Tele pharmacy software enables pharmacists to provide remote pharmacy services such as medication therapy management (MTM), medication reconciliation, and more. It helps to improve access to pharmacy services in remote areas.

6. E-prescribing Software: E-prescribing software allows physicians to electronically send prescriptions to pharmacies. It helps to reduce errors associated with handwritten prescriptions [52].

7. Medication Administration Record (MAR) Software: MAR software is used to document medication administration in hospitals. It helps nurses to ensure that patients receive the right medication at the right time.

8. Medication Reconciliation Software: Medication reconciliation software is used to compare a patient's current medication regimen against their previous medication history. It helps pharmacists to identify discrepancies and ensure that patients receive the right medication.

9. Medication Dispensing Software: Medication dispensing software is used to automate the process of dispensing medications in hospitals. It helps pharmacists to ensure that patients receive the right medication at the right time.

10. Pharmacy Analytics Software: Pharmacy analytics software is used to analyze pharmacy data such as prescription volume, revenue, inventory levels, etc., and generate insights that can help pharmacists make informed decisions about their operations [53].

VI. CONCLUSION

Pharmaceutical software plays a crucial role in various aspects of the pharmaceutical industry, including drug design and development, clinical trials, and hospital operations. In drug design and development, pharmaceutical software assists researchers in analyzing and manipulating molecular structures, predicting the efficacy of drug candidates, and modeling their interactions within the human body. This enables scientists to optimize the design of potential drugs and enhance their safety and effectiveness before proceeding to costly and time-consuming clinical trials. During clinical trials, pharmaceutical software helps manage and analyze large amounts of data collected from patients, allowing researchers to closely monitor the safety and efficacy of experimental drugs. This software provides tools for data organization, statistical analysis, and visualization, supporting the efficient identification of any adverse effects or therapeutic benefits. Within the pharmaceutical industry, software solutions facilitate various operations, including inventory management, quality control, regulatory compliance, and documentation. These tools improve efficiency, accuracy, and

traceability throughout the manufacturing and distribution processes, ensuring that pharmaceutical products meet stringent regulatory requirements. Pharmaceutical software also plays a significant role in hospitals, where pharmacists rely on electronic health records (EHR) systems to manage patient medication profiles, drug interactions, and medication dispensation. These systems integrate with clinical decision support tools, providing alerts and recommendations to help pharmacists make informed decisions about drug dosages, potential interactions, and patient-specific considerations. Overall, these software solutions enhance efficiency, safety, and effectiveness in all stages of the pharmaceutical product life cycle, ultimately benefiting both healthcare professionals and patients.

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