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REVIEW ARTICLE

Use of Computer Software and Databases in Different Fields of Pharmacy: A Meta-Analysis

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ABSTRACT

Objective: To present an overview of different software and databases being used in various fields of pharmacy along with their effect and achievements.

Methodology: We conducted a systematic review of the published literature on the use of different computer software in the field of pharmaceutical sciences using SciFinder and Google Scholar and exploring different database sites for information. The sites were searched for articles published from 2001 up to 2016 demonstrating the use of computer assisted technologies being utilized in various subjects of Pharmacy. A total of 60 studies meeting our criteria were further analyzed to examine relationship between computer applications and pharmacy. Among these 5 belonged to each subject-Pharmaceutics, Pharmacology, Pharmacognosy, Clinical Pharmacy, Industrial Pharmacy, Hospital Pharmacy, and Pharmaceutical Research. Besides few databases that are widely used in pharmaceutical sciences were also discussed.

Conclusion: The frequent use of computers could be visualized in almost every walk of the field that established the role of computer technology with the passage of time in almost every branch of Pharmaceutical Sciences allowing transformation of older methodologies and paving the way for innovation.

INTRODUCTION

The modern era is an era of technology and computer. The rapid use of computer advancement has affected every field of study and Pharmacy is no exception. The technological advancements require computer skills to be utilized in Pharmaceutical Sciences as well for appreciable outcomes. A variety of tasks are performed by pharmacists with the use of computers including critical tasks of patient care. The use of computer applications, either hardware or software is increasing with the passage of time and importance of computer acquiring skills is prominent from the curricular guidelines of the students of pharmacy around the globe. A variety of computer programmes are available for teaching pharmacy subjects to students which not only improve learning but improve overall study outcomes [1].

This study aims to provide an updated meta-analysis for the use of computer software being used in the field of Pharmacy. The time period selected spreads over 15-year period from the 2001 to 2016. The software is being used over a broad range of subjects and seems to improve considerably over the past.

PHARMACEUTICS

Pharmaceutics is commonly defined as the science of new drug design. It is the discipline of

pharmacy that deals with the process of turning a new chemical entity (NCE) or old drugs into a dosage form to be used safely and effectively by patients. The study of Pharmaceutics requires various procedures involved in conversion of chemical substance to a dosage form.

Drug release studies have critical importance in new solid dosage form designing. It is also considered as the most investigated subject in Pharmaceutics. The use of computer software like Modes Lab Dragon and Hyper Chem have helped to provide cross comparision of experimental and calculated values of partition coefficients of ionized form of drug substance. Among these Hyper Chem was found to be most reliable [2].

In this regards the DDSolver software has been used to perform *in vivo* and *in vitro* drug release in Immediate Release and Extended Release dosage forms [3-5].

DDSolver is well known and freely available software being used for the purpose in Pharmaceutics. The software is capable of performing multi task operations including Ratio Test, f1 and f2 factor calculation, Rescigno Indexes, Confidence Interval and various others methods [13] Similarly, comparisons can be made for dissolution profiles of formulations.

A more recent advancement is its use in data profile comparisons and drug release pattern in Microspheres preparation and specific Drug Delivery System [6-9]. The drug release can be easily quantified and dissolution profiles can be easily compared for similarity factor. The method has also been found to be superior to routinely used excel sheets on computer [10].

PHARMACOLOGY

Pharmacology defined as the branch in science concerned with the effects of the drugs on living organisms (pharmacodynamics) and the effects of living organisms with the drugs (pharmacokinetics) or it may be defined as the study of the interaction and effects between chemicals and biological systems and *vice versa*.

The programing software like Property Calculator help student predict likeness of Drug using “Lipinsiki Rule of 5” [11]. These are helpful in providing comprehensive knowledge of drug design. Another software named TDT software application is recently been introduced to develop innovative methodologies to aid discovery of new compound [10,12,13].

Special Computer Software can be used to predict and compare doses of drug substance [13].

HyperChem software is quite helpful in providing understanding of pharmacological and toxicological profiles of drug substances at molecular level [14].

Apart from that, different freely accessible platform is available on web to evaluate Pharmacokinetic and toxicity properties of drug substances such as pk CSM. Software like Win Nonlin are available for determination of pharmacokinetic parameters.

On the other hand, we also have we also have PK/PD computer simulations which can be used as an alternative to pre-built PK/PD complex models [15].

CEqual is software available for SPECT Data analysis (Single photon emission computed tomography images. SPECT is a nuclear medicine tomographic imaging technique using gamma rays [14]. CDS Software is Clinical Decision Support program available for detecting drug Interactions.However studies have demonstrated missing of some clinically significant Interactions [16].

Research studies demonstrate continuous progression in computer assisted learning in Pharmacology [17]. Software named CAL helps to demonstrate action of drugs on living tissues. The software has been used in research study demonstrating to be an effective method of teaching practical aspects of Pharmacology [18].

Similarly, PASS (Prediction of Activity Spectra for Substances) is computer software available for prediction of activities of drug substances. The program is useful for elucidation of unknown therapeutic mechanisms of drug substances [2].

PHARMACOGNOSY

A subject in which involves scientific and systematic study of physical, chemical and biological characters of crude drugs along with their method of cultivation, collection and preparation [19].

The INVDOCK is automated computer software used to identify potential therapeutic and toxicity protein targets of several bioactive compounds isolated from medicinal plants.

Another research study demonstrates use of an inverse docking software named SELNERGY used to identify putative binding biological targets [20].

The extracts obtained from the medicinal plants also require HPLC analysis. At this point also, computer aided optimization of HPLC analysis of different extracted compounds is performed. For this purpose of optimization, a computer-based program is available with the name Dry Lab G which is widely used for optimization of RP-HPLC for separating extracts as required [21].

PHARMACEUTICAL INDUSTRY

The pharmaceutical industry discovers, develops, produces, and markets drugs or pharmaceutical drugs for use as medications. Pharmaceutical companies may deal in generic or brand medications and medical devices.

A variety of computer software are available in Industry for optimization of Industrial process for research and development, procurement of raw material, manufacturing and storage of drugs.

Computer software named ATLAS is available for combining two techniques such as that used in sequential determination of Aspirin and Vitamin C using laser induced phytochemical silver substrate synthesis in a moving flow cell [22].

The recent advancement in the field of pharmaceutical formulation has been marked with the impact of computer aided programs software FCAD (Formulation Computer Aided Design) is used to develop and test *silico* capsule and tablet formulations. Such software including ACD/ Auto Chrom based on QbDprinciles. These programs utilize artificial intelligence for rapid identification of stationary phase and mobile phase which help save effort and time [23].

Dry Lab automated computer program is extensively being utilized to develop HPLC methods. The programming tools of DryLab allow rapid calculations of chromatograms and present peak movements with slight variation in pH of eluent [24].

The advancement also requires fast, accurate and reliable production methods. One such example is that of Fused Deposition Modelling (FDM): a process acquired in Pharmaceutical Manufacturing Process providing 3D printing with a standard manufacturing process [25].

HOSPITAL PHARMACY

In a Hospital setting a critical role is to be played by a Pharmacist. A major work is analysis of Drug Interactions by both retail and hospital pharmacists. Micromedex is recently developed computer software for screening drug Interactions in patients [26].

Medical reference and information system providing access to database through computer-based software are capable of analysing medications prescribed by physicians [27].

Inventory control is an essential task to be performed in a long-term care Pharmacy of hospitals. Six Sigma has shown to be an effective processing program for inventory analysis with a few out of Specifications OOS events [28].

CLINICAL PHARMACY

The pharmacists in the field of Clinical pharmacy are aimed to provide patient care that optimizes use of medications promotes health care, wellness and disease prevention. This is done in collaboration with physicians and other health care professionals [29]. It may involve specialist computer software for use of therapeutic and diagnostic materials, computer databases and statistical analysis programs [30].

A variety of tasks are performed under use of computer software including prescription

monitoring, medical errors, pharmacokinetic and therapeutic drug level monitoring etc. Computer software named Decision Analysis Tree Age is used in a complex procedure of cerebrospinal fluid shunts transfer for treatment methodology for infections [31].

Another more recent development is acoustic analysis using computerized Speech lab and Multi-dimensional voice program software in patients with Parkinson's disorder after treatment with levodopa [32].

MEDICINAL CHEMISTRY

Drug discovery is major part of Medicinal Chemistry. The search for new drug molecule is complex and time consuming. The newer applications of different software have reformed the drug discovery process through their use in detecting drug target interactions and QSAR (Quantitative Structure Activity Relationships) studies, energy minimization and docking studies in drug design. These include software like PBPK/PD modeling software, PKUDDS, APIS JAVA, Perl and Phyton, CADD software libraries [33].

Drug Guru (Drug Generation Using Rules) is a web-based computer program for transformational changes in the chemical structure on the basis of rules of thumb from historical lore of drug discovery programs. The analogs produced could be evaluated for synthesis in future [34].

An innovative processor is KPP Software for computer simulation of chemical kinetic systems. The program allows development of kinetic schemes for chemical moieties and numerical integration methods [35].

Another useful software is the PaDEL Descriptor for the purpose of calculating molecular Descriptors and fingerprints and has been considered as a useful addition to already available molecular descriptor software [36].

The researches promise continuous optimization in the Docking procedure through use of MPI-DOCK for large scale drug like chemicals ultimately strengthening the databases

PHARMACY LABS

PHARMACOLOGY LAB

Researches present keen interest of undergraduate and graduate students in CAL (Computer Assisted Learning) The software utilizes sound, video and animated graphics to replace animal issue-based practical's being performed in routine classical laboratory practical. The simulated experiments have shown to provide better understanding and confidence of the subject among students [37].

PHARMACEUTICAL RESEARCH

An important role is being played by computer software with the development of useful databases. One such effective database is ACD-IDEA providing compiled existing data records of in vivo doses of compounds making it valuable for the purpose of research and education [38].

New Drug Discovery is the major element of Pharmaceutical Research which has been revolutionized with the advent of modern technological advancements in CADD.CADD-Computer Aided Drug Design is of prime importance for analyzing early stage drug discovery making it comparatively much simpler and less time consuming [39].

Furthermore, the genetic research has opened new horizons in the field of research with development of diversity calculators [40].

1. **SciFinder**

   It provides access to a wide-range of reliableresource ofliterature, chemical compounds and reactions inchemistry, biochemistry, chemical engineering, materials science, nanotechnology, physics, environmental science and other science and engineering disciplines. SciFinder consists of six Chemical Abstract Service databases including Chemical Abstracts (CAplus), CAS Registry, CASREACT, CHEMCATS, CHEMLIST, MARPAT plus Medline. It covers around 44 million journal citations,

abstracts and patents etc. from 1907 to present [41].

2. Scopus

It is a bibliographic database that contains abstract and peer-reviewed literature: from scientific journals, books, and conference proceedings and patents from 1995 to present. It covers nearly 22,000 titles from over 5,000 publishers, of which 20,000 are peer-reviewed journals in the science, technology, medicine, social sciences, and arts and humanities. It is driven by Elsevier [42].

3. Web of Science

It gives access to the cross-disciplinary research, which permits comprehensive survey of specialized sub-fields within educational or scientific categories. It links multiple databases, publications and researchers through citations and organized indexing in curated data banks covering all scientific disciplines. It is powered by Clarivate analytics and includes 59 million records and backfiles dating back to 1898 [43].

4. BIOSIS Previews

It's a largest database service containing biological Abstracts in the form of articles reports, reviews, meetings, patents and material from books, from 1926 to present. It contains literature with profound, international, reportage on a wide range of subject areas including life sciences and biomedical sciences . *Biological Abstracts* consists of 350,000 references for almost 5,000 primary journal and monograph titles. *Biological Abstracts/RRM* additionally includes more than 200,000 non-journal citations [44].

5. Springer Materials

Springer Materials provides numerical and graphical data on more than 3000 physical and chemical properties of over 250,000 materials and chemical systems curated data and advanced functionalities to support research in materials science, physics, chemistry, engineering and other related fields [45].

6. Cambridge Structural Database (CSD)

Established in 1965, the CSD is the world's repository for small-molecule organic and metal-organic crystal structures. Containing over 875,000 entries from x-ray and neutron diffraction analyses, this unique database of accurate 3D structures has become an essential resource to scientists around the world [46].

7. NIST Chemistry Web Book

It provides entree to a wide variety of thermochemical, ion energetics, physical, solubility, spectroscopic and chromatographic data for around 40,000 compounds. It is maintained by National Institute of Standards and Technology (NIST), USA [47].

8. Merck Index

Merck index is the oldest known available encyclopedia now available online with over 11,500 monographs for chemicals, drugs, and biologicals. It is driven by the Royal Society of Chemistry (RSC) [48].

9. Reaxys

It gives access to data and citations from the *Beilstein* (organic), *Gmelin* (inorganic and organometallic) databases from 1771 to date. It also includes Patent chemistry databases comprised of organic chemistry (1830- 1980) and life science

patents (1976-present). Provided by Elsevier [49].

10. Google Scholar

It is an easily reachable bibliographic database that almost gave access to around 160 million documents. It represents almost all type of books, conference papers, technical reports, dissertations, preprints, theses, abstracts and other scholarly literature, including court opinions and patents [50].

11. PubChem

Information on the biological activities of small molecules. Provided by the National Center for Biotechnology Information (NBI), USA [51].

12. PubMed

More than 24 million citations for biomedical literature from MEDLINE, life science journals, and online books; citations may include links to full-text content from PubMed Central and publisher web sites. Provided by The National Center for Biotechnology Information (NBI), US National Library of Medicine, and National Institute of Health (NIH), USA [52].

13. Science of Synthesis

It covers major synthetic reactions reported from the early 1800s to date in the fields of organic and organometallic chemistry. It is driven by Thieme [53].

14. Spectra Lab

Spectral data system that uses empirical spectral data (2.2 million MS, NMR, and IR spectra) and advanced software to help chemists, toxicologists, and life scientists identify chemical substances. Provided by Wiley [54].

15. World Wide Protein Data Bank (wwPDB)

This database provides information about the three Dimension structures of proteins, nucleic acids, and complex assemblies. Provided by Worldwide Protein Data Bank Foundation [55].

16. ZINC

This database contains the collection of commercially-available chemical compounds prepared especially for computer-generated screening; contains over 35 million compounds in ready-to-dock 3D formats. Provided by the Irwin and Shoichet Laboratories, USA [56].

17. Spectral Database for Organic Compounds (SDBS)

Integrated spectral database system for organic compounds; includes six different types of spectra (EI-MS, ^{1}H-NMR, ^{13}C-NMR, FT-IR, Raman, ESR) for ca. 34.600 compounds. Provided by National Institute of Advanced Industrial Science and Technology (AIST), Japan [57].

18. ChEMBL

Open data resource provide broad coverage across a diverse set of targets, organisms and bioactivity measurements published in scientific literature, together with a variety of accessible search for more than 1 million compounds and 5200 protein targets. Provided by the European Bioinformatic Institute (EMBL-EBI), UK [58].

19. Chemical Entities of Biological Interest (ChEBI)

Focuses on small chemical compounds. Provided by the European Bioinformatic Institute (EMBL-EBI), UK, as part of the Open Biomedical Ontologies (OBO Foundry) effort [59].

20. Chem Inform Rxn Finder

Search engine for the *Chem Inform Reaction Library* (CIRX), which contains over 2 million reactions and covers data from 1990 to the present from ca. 100 journals; a tool for the synthetic organic chemist. Provided by Wiley [60].

21. TOXNET

Group of databases covering chemicals and drugs, diseases and the environment, environmental health, occupational safety and health, poisoning, risk assessment and regulations, and toxicology. Provided by Toxicology and Environmental Health Information Program (TEHIP), USA [61].

22. Chem Planner

This helps chemists design viable synthetic routes to their target molecules by predicting synthetic strategies and exposing a wide spectrum of relevant synthetic methods and available building blocks. Provided by Wiley [62].

23. Derwent World Patent Index (DWPI^{SM})

The database contains more than 23.1 million records with more than 15.3 million images from 1963 to date [63]. Provided by Thomson Reuters.

24. Drug Bank

Bioinformatics and cheminformatics resource that combines detailed drug data with comprehensive drug target information. Provided by the Canadian Institutes of Health Research, Alberta Innovates – Health Solutions, and by the Metabolomics Innovation Centre (TMIC) [64].

25. Inorganic Crystal Structure Database (ICSD)

Completely identified inorganic crystal structures; contains about 177,000 peer-reviewed data entries. Provided by FIZ Karlsruhe – Leibniz – Institute für Information infrastructure GmbH, Germany [65].

26. International Patent Documentation Center Database (INPADOC)

International patent collection; contains patent families and legal status information; updated weekly. Provided by the European Patent Office (EPO) [66].

27. IUPAC Standards Online

This Database provides information about standards and recommendations as given by International Union of Pure and Applied Chemistry. Provided by Walter de Gruyter GmbH [67].

28. Spectral Database for Organic Compounds (SDBS)

Integrated spectral database system for organic compounds; includes six different types of spectra (EI-MS, ^{1}H-NMR, ^{13}C-NMR, FT-IR, Raman, ESR) for ca. 34.600 compounds. Provided by National Institute of Advanced Industrial Science and Technology (AIST), Japan [68].

29. Open Food Tox

This database provides information about to summaries of toxicological data used by the European Food Safety Authority (EFSA) in its risk assessment; toxicity of chemicals found in the food and feed chain; updated on a yearly basis. Provided by EFSA [69].

30. MMs INC Search

It is useful for exploring commercially available compounds for virtual screening and cheminformatics utilization. Provided by the University of Padova, Italy [70].

CONCLUSION

With advancement of new technologies in searchable organizational database enhancing data visibility (analysis, data capture, monitoring, decision making) and institutional knowledge about respective scientific discipline, which previously have been produced with considerable investments of time, money, and other resources. Use of computer software in virtually all areas of Pharmaceutical Sciences have come out to be an effective tool for pharmaceutical research and development to improve efficiency and productivity in all areas related to drug discovery and development.

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