Review Article

A Short and Snappy Overview on the Attribution of Computers in Pharmacy

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ABSTRACT

The knowledge, relevance and applications of computer are obligatory in the present era that Pharmacy and its allied branches have incorporated in the study. Computers are the effectual tools for trouble-free and efficient admittance to pertinent information space across exponentially emergent research sources. It has become a vital factor in field of biomedical research. Computers endow with web based knowledge space with diverse searching capabilities. Computing technology has been deeply utilized in colleges, pharmaceutical industries, research centers, hospital pharmacies, publications, drug designing and many more. In the present paper, focuses on the various applications of computers in Pharmacy, softwares used for diverse facilitations. Researcher can visualize various approaches by using computers with prominent functional characteristics of data set, to simplify exploratory methods that steer the investigation which will discover some newer unforeseen information. With further exploration of newer applications in computing technology, eminence in pharmaceutical research can be seen.

Keywords: Computing technology, Softwares, Pharmaceutical Research, Computer Applications, Pharmaceutical Industries, Drug designing.

INTRODUCTION

Computers in pharmacy are used for the drug data information, maintenance of records and files, creation, modification, addition and deletion of data in patient files so as to generate reports (drug management) and business details. The Pharmacy field is awe fully benefitted by utilization of computers for accomplishment and comparison of the information to yield precise results.[1]

New drug discovery, drug design analysis, and manufacturing of drugs employ computing technology. It has become practically feasible only through the advancing of various hardwares and softwares. The computers play a very pertinent role in receiving details, storage, processing and dissemination. This incessant surge of information represents the effective functioning of any system.[1]

Effective use of computers in Pharmacy started from 1980s. Since then there has been immense requirement of computing technology in Pharmacy field. The merits include like time reduction, accuracy, man power reduction, speed, multitasking, elevated memory, efficient data storage etc.[2]

Fundamental uses of Computers in Pharmacy are enlisted as follows:

Computing technology in Retail Pharmacy

Computing technology is responsible for providing a receipt to the patient and for the record money transactions. Also, order of low quantity of products via electronic transitions can be done easily with database system. It is responsible for the multiple analyses in prescription handling. The estimation of profit and other financial analysis can be easily computed. It helps in generation of printed of billing and other expense details. There can be a control on inventories. The stock position gets rationalized right away. It helps in easy maintenance of drug data information. The queries related to toxicology, adverse drug reactions, and drug-drug and drug-food interactions can be easily satisfied.[3, 4]

Computer aided drug designing (CADD)

CADD is a discrete and sophisticated drug designing process. It is a process of assertion of new medications.[5] A well defined feed information along with refined graphics software improves the scope in designing of new molecules, with better efficiency in terms of action.[6,7]

Computing technology in Hospital pharmacy

Computing technology is useful in receiving and allotment of drugs. Database can be maintained about the details of every individual. A record of professional supplies can be maintained. The database keeps a record of dispensed drugs to each inpatient and outpatient along with their information records. Patient monitoring is made easy (record of blood pressure, pulse rate, temperature).[8]

Computing technology in storage and retrieval of data

Computing technology helps in storage of data storage of data and subsequent recovery of (retrieval) due to the alterations coming up. It is commonly practical in the procedure of admittance of patient, nursing and clinical staff, beds in hospital, operation theatres, intensive care unit (ICU), pharmacies, radiological service, etc. Computer accounts and records in sequence the information related

to diagnosis, medication, demography, clinical information etc. about the patient.[9]

Computing technology and Pharmaceutical industry

Information system aggregates information technology with public which is enviable and handy. Pharmaceutical companies implementing their operations by information managing technologies amplify the odds of accomplishment and escalate the competence in their production run.[10, 11]

With the advancements in computing technology, it led to the structured analysis and biological information management which is essential for the study of various biological processes. Bioinformatics helps in data implementation and out benefits the data into reliable therapeutics thus emerging as an important tool for the development of standardized computer organizations.[12] Bioinformatics facilitates the development of novel drug molecules by via receptor based pharmacophore gizmo; generating pharmacophores by optimization of The structural targets are optimized by generation Pharmacophores, at protein level with specific binding site were used for virtual screening so as to obtain the set of ligand that demonstrate significant activities.[13, 14]

Computing technology and Pharmacoinformatics

It is the new computing technology which is inclusive of bioinformatics, genoinformatics, healthinformatics, immunoinformatics, metaboloinformatics and neuroinformatics essential for the drug discovery.[15] The computing technology is required for the transferring of information and data. Medical informatics focuses on use of information processing within the clinical setting for medical billing, patient and resource scheduling, and patient care. Clinical informatics utilizes clinical decision support systems, providing feedback and directives to healthcare service provider for increasing patient compliance.[16-18]

"In silico" research informatics has developed a conduit for medical invention and exploration at every facet of healthcare.[19] With the profound analysis of medical information and advancements creates the prospect for rapid knowledge in health applications and to aid in bio medical research, having the safety as preliminary concern. This will facilitate in building a digital policy for medical study assuring the appropriate valuation of medical statistics and depict consequential conclusions.[19]

Computing technology in Diagnostic laboratories

Manual procedures are tedious and time consuming whereas automated computerized instruments finish number of tasks with precise result in conclusion. Laboratory Information System (LIS) control huge sum of data.[19, 20] Instrument's utility is as pre-processors, converting the raw data in the digital format and finally the numerical values in the reports. The advancement of swaying computing technology offer enhanced and improved view and perception in radiology department. Computerized Tomography (CT) and Magnetic Resonance Imaging (MRI) are inherently digital.[21, 22]

Computer aided learning

Digital libraries play very crucial role in updating the latest advancements in drug discovery and subsequent new therapies associated. Thus, there is ready access to the information in a well-organized manner through computing technology, this aides learning easy and accessible. Simulative techniques help in self-evaluating process which is involved in decision making.[23]

Computing technology in Clinical trial management

In drug development, preclinical and clinical trials are the significant part which evaluates pharmacological profit along with the toxicological hazard coupled with the medication. Computing technology with the use of software helps in ensuring the safe therapeutic window for the drug candidates. Some examples are Cliniplus® Data management from DZC software solution, Inc., Data LabsXC® from Data labs, Inc., Electronic data capture from DSG Inc., Openclinica by Akaza research (Cambridge, MA), Oracle clinical V4i® from Oracle Corporation and Trial master® from Omnicomm systems.[24]

Computing technology in Adverse Drug Events (ADE) control

There has been a competition for exploration of newer approaches for therapeutics for diseases, between various pharmaceutical companies for the development of the new drug molecules. The implementation of food, drug and cosmetics act in 1938 imparted improved drug safety.[25,26] However, there is lack of appropriate access and elucidation of drug safety data challenge and will continue to persevere. With development of computerized depot of post marketing voluntary adverse drug events, it has become easy to analyze various adverse drug events. In this regard, he drug regulatory agencies and pharmaceutical industry have constructed a computerized repository of premarketing as well as post marketing clinical trial data which will ensure the effective data analysis and decision making ultimately leading to the implementation of novel software for evaluating and monitoring the adverse drug events.[27] Reconfiguration of data bases and validation is a vital aspect before analysis of adverse drug events data. There are several database designed with the help of computing technology such as adverse event reporting systems, spontaneous reporting system which is coded with COSTART (coding symbol for thesaurus of adverse reaction terms) dictionary, further upgraded with MedDRA (medical dictionary for regulatory activities) system for coding.[28, 29]

Computing technology in Pharmaceutical formulations

The optimized formulation needs the approval from regulatory bodies before ther introduction of a new drug in the market, after its development in to a quality product. Accurate choice of additives is vital for the

provision like efficacy, safety and stability. With the developing computing technology the data processing can be done in multidimensional way in order to explore relationships, within the data set and optimized formulation so as to predict the outcome.[30] Neural network is an attempt which mimics the processing of human brain.[31] Genetic algorithm mimics the evolutionary process of self organization and adaptation.[32] Fuzzy logic mimics the skill of human brain to draw conclusion and generation of responses on the basis of incomplete or imprecise information.[33] The FDA suggested for the use of design of experiments (DOE) as it ensures a structured and well organized method for determination of the relation between factors affecting a process and the response of that process. It is much easier for non-statisticians to use. DOE software enables a user to easily choose from a range of various experimental designs. It makes easy to define the design space by entering high and low values for components.

The pharmaceutical Quality by Design (QbD) is a methodical approach to progress that begins with predefined aim and lays stress on the product,process understanding and process control., QbD is emerging to augment the safe assurance, of the effective drug supply to the consumer thereby promising for significant improvement in manufacturing quality performance.

It includes;

- Beginning with a target product profile.Defining of a target product quality profile
- Gathering of relevant prior knowledge about the drug substance and potential excipients and process operations.
- Designing of a formulation and identification of the critical material (quality) attributes of the final product.
- Designing of a manufacturing process to produce a final product.
- Identification of the critical process parameters and input (raw) material attributes.
- Establishment of a control strategy for the entire process.

Learning system based on a computational technique which can simulate the neurological processing ability of the human brain. It has been applied to solve various problems related to the QSARs (quantitative structure–activity relationships, QSPRs (quantitative structure–pharmacokinetic relationships), estimation of diffusion coefficient and prediction of the skin permeability and the mechanism of drug action.

Computing technology in Toxicology and risk assessment

- It incepted in 1962, *In silico* toxicity predictions have made great strides Following recommendation have been made to overcome the problems: More toxicity data, for greater consistency.
- Mechanistic appreciation of clear toxicity.

Some softwares used in toxicology were listed below;

- DEREK Nexus: Prediction of toxicological profiles.
- Literature examination for functionality of data.
- Hazard Expert: Identification of noxious molecules. Bioavailability calculations, accumulation and other parameters of consideration.
- VirtualToxLab: Docking and QSAR hybrid approach.
- MetaDrug: Systems pharmacology platform built on data from MetaBase. It is helpful in prediction of prediction of mechanism of action, toxicity, and off-target effects.
- TOPKAT: Prediction of toxicity measures in *in vitro* assays and animal models.
- Percepta Toxicity modules: Prediction of acute toxicity, aquatic toxicity, hERG channel inhibition, endocrine disruption, genotoxicity, and irritation and health effects.
- ADMET Predictor: Prediction of endocrine disruption, phospholipidosis, hERG channel inhibition, skin sensitization, and so on.[34-36]

Computing technology in Drug disposition

Data quantity is the limiting factor in case of ADMET modelling. Some of the recent versions are gastro plus, Lancaster CA, PK-SIM, and ADME/TOX web.[37-41]

Recent developments

Joint analysis of vast data sets in incongruent formats and focus on various biological facts is the key challenge for qualitative, testable and validated frame work. Integration of Pharmacy disciplines can find a solution to this problem.[42]

Computing technology in Research publication

Publication of several investigations, some useful examinations, scrutinies, and other research works are the important countenances. Submission and publication of research works by scholars in the form of manuscript has become convenient with the use of computing technology thereby, improving the quality of publications. The main aim of the researcher is to publish their own research work and computing technology plays vital role in it. The computers help in making suitable corrections, necessary editing which makes the document very facile and multifaceted so as to make it viable for publication. Computers provide different softwares for the accessible typing and processing, correction of spellings, grammatical mistakes and administer other editing points for consideration. Computing technology helps in

facilitation of the information about submission process (E-submission process).[43, 44] After publication, articles are free for anyone to review. Few types of software useful in research publication are given below:

- Ithenticate: Plagiarism detection.
- Graph pad prism: Illustrations of experimental data in to graphical representations and analysis of kinetic data.
- Chem Draw and Corel Draw: These softwares are effectively utilized to draw chemical structures and their view as three dimensional (3D) models.
- IBM SPSS Statistics is an integrated product for addressing from planning to data collection to analysis, reporting and deployment.

Computing technology and Digital library

Digital libraries are the electronic assortment of real or virtual resources which facilitates access of data anywhere**.** This has paced up the digitalisation of written and printed documents in the past few years.[45, 46]

Advantages of Digital Library include;

- Effective utilization without wastage.
- Lowered expenses for maintenance and distribution of resources.
- Storage of information in audio and video formats.
- Multiple users can access the data.
- Compatible searching.
- Easy distribution in various formats.

CONCLUSION

Computers thus offer effectiveness with the computing technology as for easy and efficient access to germane knowledge space across disjoined and exponentially emergent research sources. It is thus a crucial success factor for the field of biomedical research. Computers provide web based knowledge with diverse search options beyond common search engines. One can foresee different approaches by using computing technology to ease the exploratory methods which will guide for the search paths and discovery of unanticipated facts. With further improvement and investigation of applications of computing technology, newer approaches and subsequent credibility can be achieved in pharmaceutical research.

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REFERENCES

1. Sean E, Computer Application in Pharmaceutical Research and Development", Wiley Interscience: A John Wiley and Sons Publication, 2006.
2. Ekins Sean, "Computer Application in Pharmaceutical Research and Development", Wiley Interscience: A John Wiley and Sons, INC., Publication, 3, 2006, 37.
3. Patil DJ Hospital and Clinical Pharmacy Published by Nirali Prakashan, Second Edition, 2008, 10.1-10.5.
4. Yadav S, Yadav M, Computer assisted pharmacy services [CAPS] - A step towards pharmacy automation, Pharma buzz - A national pharma monthly magazine, 4, 2009, 24-29.
5. Jean-Pierre D, Jacques W, Computer Aided Molecular Design: Theory and Application, Acedmic Press limited, 1997, 1-10.
6. Thomas PJ Catherine P, Computer Assisted Drug Design: Methods and Applications Marcel Dekker INC, 2006, 19-52.
7. Miller DD, Remington: The Science and practice of Pharmacy. Lippincott Williams and Wilkins, 20th Indian edition, 1, 2006, 477.
8. Yadhav AV, Yadhav BV, Hospital and clinical pharmacy Second year diploma in pharmacy published by Nirali prakashan fifteenth edition, 2008, 153-154.
9. Richard F, Information Technology for Pharmacist Published by Pharmaceutical Press, 2006, 169-171.
10. Udayakumar M, Hemavathi K, Shanmugapriya P, Seenivasagam R, Receptor-Based Pharmacophore Tool for Design and Development of Next- Generation Drugs International, Int J Bioinform Res Appl, 9, 2013, 487-516.
11. Lexin wang, Computer-simulated pharmacology experiments for undergraduate pharmacy students: experience from an Australian university. Indian journal of pharmacology, 33, 2001, 280-282.
12. Stein L1, Creating a bioinformatics nation. Nature, 417, 2002, 119-120.
13. Goodford PJ, A computational procedure for determining energetically favorable binding sites on biologically important molecules, J Med Chem, 28, 1985, 849-857.
14. Bohm HJ, The computer program LUDI: a new method for the de novo design of enzyme inhibitors, J Comput Aided Mol Des, 6, 1992, 61-78.
15. Seenivasagam R, Hemavathi K, Sivakumar G, Niranjan V, Discovering novel carriers for oral insulin tablets: a pharmacoinformatics approach, Int J Bioinform Res Appl, 9, 2013, 184-206.
16. Szarfman A, Tonning JM, Doraiswamy PM, Pharmacovigilance in the 21st century: new systematic tools for an old problem. Pharmacotherapy, 24, 2004, 1099-1104.
17. Mallick M, Odedra D, Vidyarthi AS, Shankaracharya, Meropenem: a potent drug against superbug as unveiled through bioinformatics approaches, Int J Bioinform Res Appl, 9, 2013, 109-120.

18. Etheredge LM, A rapid-learning health system. Health Aff (Millwood), 26, 2007, w107-118.
19. Gohlke H, Hendlich M, Klebe G, Knowledge-based scoring function to predict protein-ligand interactions. J Mol Biol, 295, 2000, 337-356.
20. Gohlke H, Hendlich M, Klebe G, Predicting binding modes, binding affinities and 'hot spots' for protein-ligand complexes using a knowledge-based scoring function, Perspectives in Drug Discovery and Design, 20, 2000, 115-144.
21. Sotriffer CA, Gohlke H, Klebe G, Docking into knowledge-based potential fields: a comparative evaluation of Drug Score, J Med Chem, 45, 2002, 1967-1970.
22. Hansch C, Maloney PP, Fujita T, Correlation of biological activity of phenoxyacetic acids with Hammett subsistent constants and partition coefficients, Nature, 194, 1962, 178-180.
23. Naidu S, E-learning - A guidebook of Principles, Procedures and Practices, Published on behalf of the commonwealth educational media center for Asia by Dr. Usha V. Reddi, Director, CEMCA, New Delhi, 2006, II revised edition, 1-3.
24. FDA Science Forum: Advancing Public Health through Innovative Science, Washington, DC. April 27, 2005.
25. Shaha YI, Paradkar AR., Dhayagude MG, Introduction to Biostatics and Computer Science- For Pharmacy and Medical Student, Nirali Prakashan, Tenth Edition, 2008, 8.1 -8.5.
26. Barnett ST, James JA, Measuring the clinical development process, Appl Clin Trials, 4, 1995, 44-52.
27. Szarfman A, Tonning JM, Doraiswamy PM, Pharmacovigilance in the 21st century: new systematic tools for an old problem, Pharmacotherapy, 24, 2004, 1099-1104.
28. Reviewer Guidance Conducting a Clinical Safety Review of a New Product Application and Preparing a Report on the Review. U.S. Department of Health 13a and Human Services, Food and Drug Administration, Center for Drug Evaluation and Research (CDER) February 2005.
29. Gould AL, Practical pharmacovigilance analysis strategies, Pharmacoepidemiol Drug Saf, 12, 2003, 559-574.
30. Bourquin J, Schmidli H, van Hoogevest P, Leuenberger H, Comparison of artificial neural networks (ANN) with classical modelling technologies using different experimental designs and data from a galenical study on a solid dosage form, Eur J Pharm Sci, 6, 1998, 287-300.
31. Rowe RC, Colbourn EA, Applications of neural computing in formulation, Pharmaceutical Visions Spring Edition, 2002, 4-7.
32. Colbourn EA, Rowe RC, Modelling and optimization of a tablet formulation using neural networks and genetic algorithms, Pharm Tech Eur, 8, 1996, 46-55.
33. Rowe RC, Woolgar CG, Neuro-fuzzy logic in tablet film coating formulation, Pharm Sci Technolo Today, 2, 1999, 495-497.
34. Barratt MD, Rodford RA, The computational prediction of toxicity, Curr Opin Chem Biol, 5, 2001, 383-388.
35. Norinder U, *In silico* modelling of ADMET- a mini review of work from 2000 to 2004, SAR QSAR Environ Res, 16, 2005, 1-11.
36. Wolber G, Langer T, LigandScout: 3-D pharmacophores derived from protein-bound ligands and their use as virtual screening filters, J Chem Inf Model, 45, 2005, 160-169.
37. Swaan PW, Szoka FC Jr, Oie S, Molecular modeling of the intestinal bile acid carrier: a comparative molecular field analysis study, J Comput Aided Mol Des, 11, 2007, 581-588.
38. Langer T, Eder M, Hoffmann RD, Chiba P, Ecker GF, Lead identification for modulators of multidrug resistance based on *in silico* screening with a pharmacophoric feature model, Arch Pharm (Weinheim), 337, 2004, 317-327.
39. Mao Q, Unadkat JD, Role of the breast cancer resistance protein (ABCG2) in drug transport, AAPS J, 7, 2005, E118-133.
40. Ekins S, Johnston JS, Bahadduri P, D'Souza VM, Ray A, et al., In vitro and pharmacophore-based discovery of novel hPEPT1 inhibitors. Pharm Res, 22, 2005, 512-517.
41. Sheiner LB, Ludden TM, Population pharmacokinetics/dynamics, Annu Rev Pharmacol Toxicol, 32, 1992, 185-209.
42. Sheiner L, Wakefield J, Population modelling in drug development. Stat Methods Med Res, 8, 1999, 183-193.
43. Michael D, Basics of research paper writing and publishing. Int J of Technology Enhanced Learning, 6, 2014, 105-123.
44. Fleming G, Typing your research paper: Tips for working on the computer, 2014.
45. Ambati V, Balkrishnan N, Reddy R, Pratha L, Jawahar CV, The digital library of India project: Process, Policies and Architecture, 2006.
46. Sood A, Chandrasekharan U, Digital libraries in India - A baseline Study, A report commissioned by Educational Development Center (EDC), 2004.

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