REVIEW ARTICLE

Applications of Computer Science in Pharmacy: An Overview

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ABSTRACT

Computer is mandatory in this advanced era and pharmacy and related subjects are not exception to it. This review mainly focuses on the various applications, softwares and use of computers in pharmacy. Computer science and technology is deeply utilized in pharmacy field everywhere like in pharmacy colleges, pharmaceutical industries, research centers, hospital pharmacy and many more. Computer significantly reduces the time, expenditure, and manpower required for any kind of work. Development of various softwares makes it trouble-free to handle huge data. In short, computers are playing critical role in pharmacy field, without computers pharmacy research will be long-lasting and expensive.

KEY WORDS: Computer Science; Softwares; Pharmacy; Research; Computer Applications; Pharmaceutical Industries

Pharmacy field plays a crucial role in patient healthcare. It is a huge field which is present worldwide. To run pharmacy field professionally and efficiently, it requires huge management and manpower. But now a days use of computers in pharmacy field reduced the manpower and time. Computers are almost related to every corner of pharmacy field. These are utilized in the drug design technique, retail pharmacy shop, clinical research centers, crude drug identification, drug storage and business management, hospital and clinical pharmacy, in pharmacy colleges for computer assisted learning.

Internet is huge collection of data. It is available in just one click. Various search engines like Google, Yahoo, Rediff, Bing help in searching online data related to pharmacy field just one have to enter his or her area of interest in search engine.

In Pharmacy field, effective use of computers started from 1980. Since then there is great demand of computers in pharmacy field. Computers are having their own advantages like reduction in time, accuracy, reduction in man power, speed, multitasking, non-fatiguness, high memory, data storage and many more.[1]

USE OF INTERNET IN PHARMACY

Internet is collection of huge data. And this data is available for us in just a one click. Internet is useful tool in literature survey. Books are also available on the internet. Various research journals can be easily accessed via internet.[2] There are number of web-sites which are related to pharmacy field. Some of these web sites are as follows;[3]

1. www.phrma.org
   Organization representing America's pharmaceutical research companies provides details of drug development, industry news, and health guides.
2. www.healthcareforums.com
   Created to facilitate interaction among healthcare professionals on specific topics which includes discussion of cases, research and other relevant issues.
3. www.astra.com
   This is official web-site of ASTRA pharmaceuticals which produces medications for respiratory tract, cardiovascular and gastrointestinal diseases, and for pain relief. Includes press releases.
4. www.biogen.com
   Company principally engaged in developing genetically-engineered human pharmaceuticals. With career advice, and drug information.
5. www.gene.com
   Develops pharmaceuticals mostly for the treatment of genetic disorders. Includes a listing of the major drugs and their uses.
6. www.genzyme.com
   Company that specializes in biotechnology and health care products. With career, product, and services information.
7. www.pfizer.com/main.html
   Find out about research projects and career opportunities at this Pfizer pharmaceuticals. Includes health education and pharmaceutical advice section.
8. www.roche.com
   Roche produces pharmaceuticals and products for treatment of HIV, obesity and cardiac conditions. Offers news and company information.
9. www.pharmweb.net/pwmirror/pwk/pharmwebk.html
   Listing of international pharmaceutical regulatory bodies including the US Food and Drug Administration.
10. http://www.druginfonet.com
    Drug information, disease information, Ask the Expert, Pharmaceutical Manufacturer Information, Healthcare news and information, Medical References / libraries.
11. http://www.fda.gov/default.htm
    Useful for checking adverse reaction reports for dietary supplements and drug interactions. The Orange book approved drug products is also available on-line here, as well as orphan drug products (with links to other web-sites for rare disease/orphan product information). Contains an alphabetical listing of drugs licensed in the US and the corresponding package inserts.

Lists the latest information on drug recalls, drug shortages, and changes in labeling

12. www.ijpc.com
    Alphabetical Index of formulations found in the International Journal of Pharmaceutical Compounding. Specialty articles on compounding
13. http://www.pharmainfo.com
    Pharmaceutical News, Pharmaceutical Articles, and Pharmaceutical blogs
14. www.fda.gov/cvm/
    Searchable listing provides facts and figures on all animal drug products approved by the FDA.
15. www.aaps.org
    Information on officers, activities and membership from the American Association of Pharmaceutical Scientists
16. http://www.sciencedirect.com
    Contains research and review articles related to pharmacy field

USE OF COMPUTERS IN RETAIL PHARMACY SHOP

Computers are used by community pharmacist for various functions. Some accounting functions are like preparation of prescription label, providing a receipt for patient, generation a hard copy record of transactions, calculating total prescription cost, automatically ordering the low quantity products via electronic transitions, preparation of annual withholding payrolls.

Managerial functions include generation of multiple sales analysis for a day, month, weak and to date for number of prescriptions handled and amounts in cash. Estimation of profits and financial ration analysis, calculation of number of prescription handled per unit time, printing of billing and payment details. [4, 5]

Computers can be effectively used for purchasing and inventory control in retail pharmacy shops. Whenever an item is added to the stock or removed from the stock, immediately position of the stock can be updated by computers. For annual auditing, records of numerous items are required; this can be easily handled by using various computer softwares. Billing process can also be computerized. Demands of various products can be easily evaluated by using computers by tracking the movements of stock.
Complete search of the drug information is necessary for the pharmacist to satisfy the queries about pharmacological actions, drug interactions, adverse drug reactions, toxicology. This search job is simplified by use of computers. The computerized information recovery is time saving and satisfying with the extra advantage of more detailed and timely than manual search. For gathering of information international data banks are available such as World standard drug database, Drug bank, MEDLARS (Medical Literature Analysis and Retrieval System) and DIALOG. [6]

Drug Bank database is a unique bioinformatics and cheminformatics resource that combines detailed drug (chemical, pharmacological and pharmaceutical) data with comprehensive drug target (sequence, structure, and pathway) information. The database contains 6826 drug entries including 1431 FDA-approved small molecule drugs, 133 FDA-approved biotech (protein/peptide) drugs, 83 nutraceuticals. Additionally, 4435 non-redundant protein (i.e. drug target/enzyme/transporter/carrier) sequences are linked to these drug entries.[6]

MEDLARS (Medical Literature Analysis and Retrieval System) are a computerized biomedical bibliographic retrieval system. It was launched by the National Library of Medicine in 1964 and was the first large scale, computer based, retrospective search service available to the general public. In 1971 an online version called MEDLINE ("MEDLARS Online") became available. Along with this pharmacist can maintain all the record related to the patient, his/ her history, disease state, interactions shown by medicine which will be useful to the pharmacist while dispensing the medicine to that patient next time.

HOSPITAL AND CLINICAL PHARMACY

Hospital pharmacy is division of hospital which monitors on the receiving and allotment of drugs

and medicines and professional supplies, stores them and dispenses to inpatient, outpatient and may have a manufacturing extension to manufacture pharmaceuticals and parenteral in bulk.

Clinical pharmacy is the branch of Pharmacy where pharmacists and pharmacon omists provide patient care that optimizes the use of medication and promotes health, wellness, and disease prevention.[2]

Patient record maintenance is vital job in hospitals but with the help of computers, data can be maintained easily and also updated time to time. Maintenance of stock means inventory control can be achieved very well by using computers. For this purpose, periodic or perpetual inventory control systems may be adapted. Computers can play role like,[2, 7]

- To detect the items which have reached minimum order level.
- To prepare list of items to be purchased and their quantities.
- To prepare purchase orders for vendors and to avoid duplication.
- To detect the infrequently purchased items for possible return or elimination from pharmacy's drug supply.
- To produce periodic summary and purchasing and inventory control statistics.
- Maintaining patient medical record.
- Drug information services.
- Patient monitoring.

Softwares like Microsoft Excel are useful in maintenance of all type of numerical data.

Clinical pharmacist may use computers for therapeutic drug monitoring; which are very potent and having very narrow therapeutic range like cardiac glycosides, anticonvulsants. Computer program are designed to calculate drug dosage to suit individual patients need.

Apart from this, drug interactions may be screened by using programs like MEDIPHOR (monitoring and Evaluating of Drug interactions by a pharmacy oriented reporting) and PAD (Pharmacy Automated Drug Interaction Screening).[6]

COMPUTERS IN EDUCATION

Computers and information technology have become essential to pharmacy field education and teaching. Various methods getting integrated in teaching process. "Chalk to talk" approach is changing to the "Display and deliver" approach. Use of multimedia packages, hypertext video chats, web based education, multimedia based education, intelligent tutoring system, digital libraries, simulation laboratories, tele-education are finding place in normal teaching process at post graduate as well as undergraduate level and it is increasing day by day. Sensible use of computers in imparting education to pharmacy student has been found attractive and satisfying. "Computer Aided Learning" (CAL) is becoming an important part of education system.[8] CAL system has its own vital merits as follows;

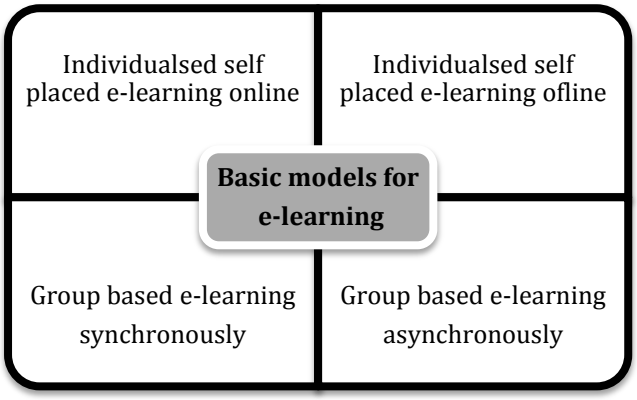
- It is well structured that means information is well organized and readily accessible to user.
- CAL system is individualized which allows user to work privately and without any interference.
- Elegant way to present information through graphics, animation which is attractive.
- Rapid response to user's queries.
- It is enjoyable as it overcomes tradition approach of blackboard and most of times one way communication.
- User satisfaction can be achieved as it can be used multiple times.
- It is convenient as it can be used at home or work place.
- Dynamic means its content can be easily modified and upgraded depending upon current information.
- It is self-evaluating, resource effective, dependable, simulative and numerically judicious.

Along with CAL, distance learning, digital libraries, e-learning are another important applications of computers for education.

E-learning[8]

E-learning is commonly referred to the intentional use of networked information and communications technology in teaching and learning. A number of other terms are also applied to e-learning like online learning, virtual learning, distributed learning, network and web based learning. There are four basic models for e-learning as follows;

Figure 1: Models for e-learning



a. *Individualized self-paced e-learning online* refers to situations where an individual learner is accessing learning resources such as a database or course content online via an Intranet. A typical example of this is a learner studying alone or conducting some research on the Internet or a local network.

b. *Individualized self-paced e-learning offline* refers to situations where an individual learner is using learning resources such as a database or a computer-assisted learning package offline (i.e., while not connected to an Intranet). An example of this is a learner working alone off a hard drive, a CD or DVD.

c. *Group-based e-learning synchronously* refers to situations where groups of learners are working together in real time via an Intranet. It may include text-based conferencing, and one or two-way audio and videoconferencing. Examples of this include learners engaged in a real-time chat or an audio-videoconference.

d. *Group-based e-learning asynchronously* refers to situations where groups of learners are working over an Intranet, where exchanges among participants occur with a time delay (i.e., not in real time). Typical examples of this kind of activity include on-line discussions via electronic mailing lists and text-based conferencing within learning managements systems.

Digital Libraries[9, 10]

Digital libraries are an electronic collection of real or virtual resources which is available anywhere in the world online or offline. Digital Libraries have received large interest in the recent years because they allow access to digital information from anywhere across the world. They have become widely accepted and even preferred information sources in areas of education, science and others. The speedy expansion of Internet and the increasing interest in development of digital library related technologies and collections helped to speed up the digitization of printed documents in the past few years.

There are several advantages of digital libraries as;

1. Minimizing storage space.
2. Cutting down the cost of library maintenance and resource distribution.
3. Information which cannot be provided in printed format can be presented by using digital libraries like audio and videos.
4. Easy for distribution via internet, Compact disk (CD) and Digital Versatile Disk (DVD).
5. Less time required to search specific things i.e. within a matter of seconds.
6. Multiple accesses.

Beside these aspects computers are finding their place in classrooms for the purpose of presenting data in the form of Power-points, which allows easy understanding for the student by using graphics, animation and attractive presentation. Students are also using various computer programs for completing their projects, assignments.

Pharmacology is branch which is mainly concerned with the drug action on organism (Pharmacodynamic) and effect of organism's body on drug (Pharmacokinetic). Various types of experiments are done in study of drug on animal models. In the pharmacy colleges also in routine practicals experiments on animals or animal parts are involved. After doing such experiments there is need to support result with numeric data. For such purpose various tests like ANOVA, Student's 't' tests, Chi square test are need to be carried out. These tests require very lengthy calculation which is time consuming. For performing these tests there are certain softwares in which you have to just feed values and results are generated within seconds. List of such softwares is as follows;

- XLSTAT
- OpenStat
- Prism
- SAS (Statistical analytical softwares)
- Minitab
- Excel
- SYSTAT
- MYSTAT

Computer assisted learning (CAL) in pharmacology is also getting popularity in these days. For doing practical, many of animals are killed every year. Such experiments can be presented to the students using computer assistance which save life of animal as well as time.[11]

Computer assisted learning has found to be having number of advantages as;

1. Learning through animated models, which is very interesting for students.
2. By running program again and again same topic can be revised number of times and when required.
3. For teachers, it also becomes very easy to explain particular topic via animation.

COMPUTERS IN PHARMACEUTICAL ANALYSIS

Computers in pharmaceutical analysis are mainly utilized for data storage, processing of data, searching of various files. Also various instruments like UV Visible spectrophotometer, Infra red instrument, HPLC, Microscopes, Mass spectrometer come along with particular softwares. These softwares do all necessary process required for analysis purpose. Also these programs contain in built libraries which prove useful for searching of data related to different chemical entities. For example if a mass spectrum of any unknown chemical is obtained then instructions can be given to the program to find out similar mass spectrum among the library which is present in it, which will help to find out unknown chemical entity.

For interpretation of IR spectra commercial software packages are available. Sadtler Standard infra-red collection and Sadtler commercial infrared collection contain over 1,20,000 spectra.[6]

COMPUTER ADDED DRUG DESIGN

Drug design, also sometimes referred to as rational drug design, is the inventive process of finding new medications based on the knowledge of the biological target. This type of drug design can be assisted by computer softwares. Software will generate number of lead molecules depending upon the feed data and among these; compound of interest can be developed and tested. If such process is carried out manually then it will be time consuming and tedious. But use of computer reduces time hugely. [12, 13]

Molecular modeling and molecular graphics have shown dramatic growth and are becoming integral part of drug discovery process. Molecular modeling is the generation, manipulation and representation of three dimensional form of molecule. Molecular graphics refers to the use of computer graphics to represent the molecular structure. In the past synthetic chemists have used molecular models, but computer modeling has enhanced the detailed display of molecular structures.[14]

Various types of softwares are available, like[15] AutoDock (The Scripps Research Institute), CombiBUILD (Sandia National Labs), DockVision (University of Alberta), HINT! (Virginia

Commonwealth University), LIGPLOT (University College of London), SITUS (Scripps Research Institute), DOCK (UCSF Molecular Design Institute), Sanjeevani (Indian Institute of Technology, New Delhi), Bio-Suite (Tata Consultancy Services Ltd.), Maestro, Macro Model 5.5, Delphi.

Some popular drugs are discovered by using computer assisted drug design.[1] (Table - 1)

Table 1: Marketed Pharmaceuticals whose discovery was assisted by computers

Generic name	Brand name	Year approved in United States	Discovery assisted by	Activity
Norfloxacin	Noroxin	1983	QSAR	Antibacterial
Losartan	Cozzar	1994	CADD	Anti-hyeprtensive
Dorzolamide	Truspot	1995	CADD/ SBDD	Antiglaucoma
Ritonavir	Norvir	1996	CADD	Antiviral
Indinavir	Crixivan	1996	CADD	Antivairal
Donepezil	Aricept	1997	QSAR	Anti-Alzheimer's
Zolmitriptan	Zomig	1997	CADD	Animigraine
Nelfinavir	Viracept	1997	SBDD	Antiviral
Amprenavir	Agenerase	1999	SBDD	Antiviral
Zanamavir	Relenza	1999	SBDD	Antiviral
Oseltamavir	Tamiflu	1999	SBDD	Antiviral
Lopinavir	Aluviran	2000	SBDD	Antiviral
Imatinib	Gleevec	2001	SBDD	Antineoplastic
Erlotinib	Tarceva	2004	SBDD	Anineoplastic
Ximelagatran	Exanta	2004	SBDD	Anticoagulant

QSAR: *Quantitative structure-activity relationship, CADD: Computer Assisted Drug Design, SBDD: Structure Based Drug Design*

COMPUTERS IN MANAGEMENT OF CLINICAL TRIALS[1]

Clinical trials are the important part of current drug development which provides information about risk and benefits of any medication. Data collection and management are very crucial in clinical trials. The astonishing advancement in computer hardware and software technology has had tremendous impact on clinical trials data collection and management. Before explosion of information technology, clinical trials are relied upon either manual method or somewhat on computers. Softwares can be used for the trial database, data collection/data entry, randomization, registration, study management tools, and statistical analysis.

Communication between volunteer and physician is very important. Various computer assisted methods can be utilized for communication purpose like;

- e-mail
- Web-sites
- Video conferencing

E-clinical softwares

E-clinical softwares consist of integrated suits of application s that support clinical research process, including various ways of data collection, data entry, remote data capture, batch data load. These suites enable to quickly and easily design studies, capture clinical data, some examples of e-clinical softwares are

1. Oracle clinical V4i® from Oracle Corporation.
2. Data LabsXC® from Data labs, Inc.
3. Trial master® from Omnicomm systems.
4. Cliniplus® Data management from DZC software solution, Inc.
5. Openclinica by Akaza research (Cambridge, MA)

Pharmacokinetics is the science which deals with the rate of absorption, metabolism, distribution and elimination of drug and it's metabolites in the body. Pharmacokinetic analysis is basically carried out to get information on renal clearance, volume of distribution, metabolic deposition, absorption and multiple dosing of drug. This type of analysis can be carried out by using different softwares.

Classically, long manual calculations had to be performed and semilogarithmic paper was used for drawing plots. Now the boring computations can be left to the computer, and complicated plots and semilogarithmic plots can be precisely and quickly drawn. There are different approaches to pharmacokinetics using differential equations with the help of softwares.

NONLIN is the software which allows you to o perform statistical regression analyses to estimate the values of parameters for linear, multivariate, polynomial, and general nonlinear functions. The regression analysis determines the values of the parameters which cause the function to best fit the observed data that you provide.

KINPAK is software used to obtain Area under curve (AUC), Peak plasma concentration (C_{max}) and peak plasma time (t_{max})

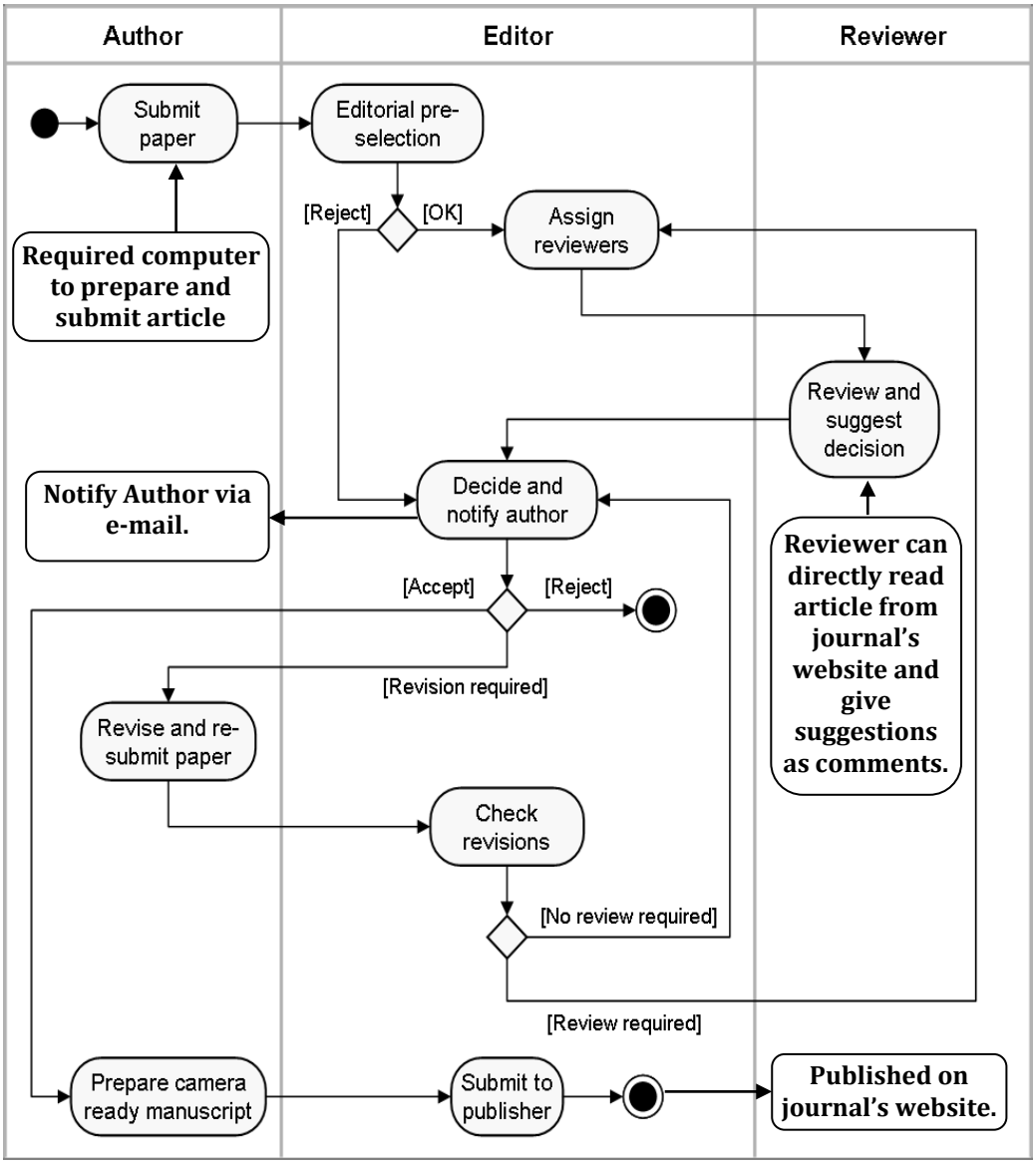
ESTRIP and STRIPACT are programs which are also used for mathematical analysis. These softwares help in therapeutic drug monitoring of patient.

Other softwares like SAS, SAM and BMDP are used for calculation of regression analysis.[6]

COMPUTERS IN PUBLICATION[16, 17]

Publication of research work is an important aspect in any field and pharmacy field is not exception to it. Publishing research is a vital element of researcher's professional life. However, writing is not every researcher's desired activity and the difficulty of getting a paper published can be nerve-wracking. However use of computers in writing and editing makes it very effortless and versatile to prepare and publish article. Computer may be required at the different stages for the author, publisher and reviewer.

Figure 2: Different steps of article preparation where computer applications are necessary



For writing paper, Microsoft word software is most commonly used software which is available on each computer and it is very easy to operate. Other such programs are Notepad, WordPad. Microsoft word provides numerous tools to carry out easy typing and processing options for documents. Microsoft word is provided with options like spell check which automatically checks the spellings and suggests the correct spelling, also corrects the grammatical mistake, provided with option of inserting page numbers, tables of required size, graphics, footnotes and many more.

When it comes to publishing articles, conventional ways are very tedious and time taking. But use of computers and internet makes it very easy. Internet can display the list of different journals by just one click, their guidelines for writing research paper and submission process. Internet provides help to publisher to choose appropriate journal for publishing his or her article. Submitting of the article by use of internet is very easy and one step process as compared to sending article via simple mail which is time taking process. Most journals today offer the opportunity to submit paper via journals web site which is called as "electronic submission" or "e-submission". E-submission is faster mode of submitting paper by just one click. Publishers can also send back articles to the author for corrections, if any, by e-mail. Publishers also publish articles online which is free to review by everyone and depending upon the number of reviews for any article, publishers can also decide rank for the article.

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