



## AN OVERVIEW OF COMPUTERS UTILISATION IN PHARMACY ACADEMIC AND INDUSTRIAL PROSPECTIVE

**Vasundhara Bandlamudi\*<sup>1</sup> and Ramarao Nadendla<sup>1</sup>**

<sup>1</sup>Department of Pharmaceutical Analysis, Chalapathi Institute of Pharmaceutical Sciences, Lam Guntur.

\*Corresponding Author: Vasundhara Bandlamudi

Department of Pharmaceutical Analysis, Chalapathi Institute of Pharmaceutical Sciences, Lam Guntur.

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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 various fields of pharmacy profession in academics and industry as well. Computer technology is deeply utilized in pharmacy field everywhere like in pharmacy colleges, pharmaceutical industries, research centres, 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.

**KEYWORDS:** Computer Science; Softwares; Pharmacy; Research; Computer Applications; Pharmaceutical Industries.

### INTRODUCTION

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-fatigueness, high memory, data storage and many more.<sup>[1]</sup>

### 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.<sup>[2]</sup> There are number of web-sites which are related to pharmacy field. Some of these web sites are as follows;<sup>[3]</sup>

#### 1. [www.phrma.org](http://www.phrma.org)

Organization representing America's pharmaceutical research companies provides details of drug development, industry news and health guides.

#### 2. [www.healthcareforums.com](http://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](http://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](http://www.biogen.com)

Company principally engaged in developing genetically-engineered human pharmaceuticals. With career advice, and drug information.

#### 5. [www.gene.com](http://www.gene.com)

Develops pharmaceuticals mostly for the treatment of genetic disorders. Includes a listing of the major drugs and their uses.

**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 websites 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 labelling.

**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>.

17. <http://onlinelibrary.wiley.com/>.

18. <https://www.ncbi.nlm.nih.gov/pubmed/>.

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 analyses for a day, month and week 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.

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.<sup>[4]</sup>

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.<sup>[4]</sup>

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 pharmaconomists provide patient care that optimizes the use of medication and promotes health, wellness, and disease prevention.<sup>[2]</sup>

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,<sup>[2,5]</sup>

- 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).<sup>[4]</sup>

### 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.<sup>[6]</sup> 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.

### 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 reduce time hugely.<sup>[7-8]</sup>

Molecular modelling and molecular graphics have shown dramatic growth and are becoming integral part of drug discovery process. Molecular modelling 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 modelling has enhanced the detailed display of molecular structures.<sup>[9]</sup>

Various types of softwares are available, like<sup>[10]</sup> Auto Dock (The Scripps Research Institute), Combi BUILD (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.<sup>[1]</sup> (Table - 1).

**Table 1: Marketed Pharmaceuticals whose discovery was assisted by computers**

Generic name	Brand name	Year Approved in united sates	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

### COMPUTERS IN MANAGEMENT OF CLINICAL TRIALS<sup>[1]</sup>

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 applications 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 its 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 semi logarithmic paper was used for drawing plots. Now the boring computations can be left to the computer and complicated plots and semi logarithmic 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 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<sub>max</sub>) and peak plasma time (t<sub>max</sub>) 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.<sup>[6]</sup>

**Softwares for CDM Most of the CDMS used in pharmaceutical companies are commercial.<sup>[11]</sup>**

Softwares	Features
ORACLE CLINICAL	Integrated CDM and remote data capture
CLINTRIAL	Provide real time data access and enhanced data quality
MACRO EDC	for all trials from phase 1-4
RAVE Flexible,	scalable, configurable
E Clinical Suite	Simple, fast and affordable for collection of data
Open Clinica	EDC
Open CDMS	enable researches to manage full cycle of their clinical research
Trial DB	EDC
Phosco	EDC

**Softwares for Pharmacovigilance<sup>[11]</sup>**

Softwares	Features
ARIS g	Leading Pharmacovigilance and clinical safety system Manage adverse event reporting and adverse reaction Applicable for vaccines, biologics, devices Flexible and scalable Can be used by small companies and large organisations
PvNET	Supports to segregate data entry, scientific assessment Extensive data validation and cross validation checks MedRA version management Covers full spectrum of developing good safety report
ARGUS	Manage data from multiple sources Access flexible drug safety databases
Oracle AERS	Reporting and analysis of serious adverse events of all medicinal products
PV Works	Collect and report safety data to meet all common international regulations
Clintrace	Clinical research, post approval marketing, drug surveillance
Pcv manager	Based on E2b and medDRA industry data standards

**REFERENCES**

1. Ekins Sean, "Computer Application in Pharmaceutical Research and Development", Wiley Interscience: A John Wiley and Sons, INC., Publication, 2006; 3: 37.
2. Patil D. J., "Hospital and Clinical Pharmacy", Published by Nirali Prakashan, Second Edition, March 2008; 10.1 – 10.5.
3. "Pharmacy website" submitted by Aadepu on Saturday, 11/29/2008 – 16:51 available at <http://www.pharmainfo.net/og/pharmindia/pharmacy-websites> last cited on 7 September 2011.
4. Shaha Y. I., Paradkar A. R., Dhayagude M. G., "Introduction to Biostatistics and Computer Science-For Pharmacy and Medical Student", published by Nirali Prakashan, Tenth Edition, August 2008; 8.1 – 8.5.
5. Fisher Richard, "Information Technology for Pharmacist" Published by Pharmaceutical Press, 2006; 169-171.
6. Naidu Som, "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, 2nd revised edition, 2006; 1-3.
7. Doucet Jean-Pierre, Weber Jacques, "Computer Aided Molecular Design: Theory and Application", Acedmic Press limited, Second printing, 1997; 1-10.
8. Perun Thomas J., Propst Catherine, "Computer Assisted Drug Design: Methods and Applications", Marcel Dekker INC., 2007; 19-52.
9. Duane D Miller, Structure Activity relationship and drug design, "Remington: The Science and practice of Pharmacy", Lippincott Williams and Wilkins, 20th Indian edition, Volume I, 477.
10. "Structure based drug design and molecular modelling" available at [http://www.imb-jena.de/~rake/Bioinformatics\\_WEB/dd\\_tools.html](http://www.imb-jena.de/~rake/Bioinformatics_WEB/dd_tools.html) last cited on 7 September 2011.
11. <https://www.omicsonline.org/abstract/review-of-the-softwares-used-in-pharmacovigilance-and-clinical-trials>.