Review Article

A review on worldwide essential software resources in pharmacy

Abstract

Softwares are the collection of computer programs and related data that provide the instructions telling a computer what to do and thereby help to process the data as wanted. These programs are designed to address general and special purpose applications. Softwares used in pharmaceutical sciences cover wide subject areas such as pharmacology, pharmaceutical chemistry, pharmaceutics, pharmacognosy, pharmaceutical biotechnology, etc. Softwares used in pharmacology are mainly related to minimize the efforts needed in determining pharmacokinetic principles of particular drug in individuals, pathways of drug, and consequently, its adverse reactions. Applications of softwares in pharmaceutical chemistry are to elucidate various physiological properties of drugs and to predict activity values for new compounds within certain limits. They may be enormous assistance to those trying to generate the large databases from massive efforts in drug research. However, softwares used in pharmaceutics help for predicting the dissolution rate, biopharmaceutical characterization, accurate and precise stability profile, etc. of formulated dosage form. Softwares used in pharmacognosy give information on herb activity, interactions, mechanisms of action and supporting data underlying the use of herb for health. Wide applications of software in pharmaceutical biotechnology help to increase the predictability of results, identify genes, elucidate protein structure, identify genome responsible for expression of particular characteristics, etc. Hence, in the present article, we have enlisted the subject wise different software names, websites and their features used in the milieu of pharmacy.

Key words:
Resources and pharmacy, softwares, worldwide

Introduction

Now-a-days, it is feasible to understand the complex processes and manage materials, money and manpower effectively and efficiently only due to computer softwares in the field of pharmaceutical sciences. The computer softwares could help to relieve the physicians from routine documentation and other clerical functions, reducing errors and increasing accuracy in transmission and storage of data, and to reduce the usage of animals and chemicals, improve productivity and provide solutions for time consuming manual task, establish consistent standards and continuous monitoring or transactions, and easy and direct access to various information through remotely located terminals.

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It is practically impossible for everyone to find out relevant piece of information without facilitators or knowing a specific universal resource locator (URL), which could be a search engine and facilitates the ever changing global array of information not only in the milieu of pharmaceutical sciences but also in all the related subjects.[1-3] In the present article, we have enlisted the subject wise different software names, websites and their features used in the milieu of pharmacy. They are as follows.

Pharmaceutics

ALOGPS

It interactively calculates and compares lipophilicity

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and aqueous solubility of chemical compounds using six programs, i.e. CLOGP, XLOGP, IA_logP, IA_logs, LOGKOW and ALOGPS.
http://www.vcclab.org

Automated packaging component analyzer
It is used to automatically verify the incoming printed components against a pre-approved master.
http://www.novatech.co.uk/products

Biopharmaceutics
It designed to introduce the applications of biopharmaceutics to oral drug delivery.
http://www.coacs.com/software/published_titles/products/pccal/biopharm.htm

CALACO
It performs conversion in acceleration, angle, area, energy, length, power, pressure, speed, temperature, time, volume and weight.
http://www.vogelscientific.com

Environmental monitoring programme
It is capable of capturing all environmental data in a 21 CFR 11 compliant, fully validated system. It is envisioned for sterile and non-sterile health care industries based on the latest guidelines from FDA, EU, ISO 14644-1 and PDA Technical Report-13.
http://www.novatech.co.uk/products

Finished product and raw material analyzer
It is used for capturing the test data from finished product testing. The application consists of product registration, monograph, certificate of analysis, etc.
http://www.novatech.co.uk/products

Good manufacturing practice
It is intended to give an introduction to Good manufacturing practice (GMP) for medicinal products with respect to pharmaceutical industry.
http://www.coacs.com/software/published_titles/products/pccal/GMP.htm

Introductory pharmacokinetics workshop
It introduces methods and principles involved in calculation of pharmacokinetic parameters such as clearance, half-life, elimination rate constant, volume of distribution and area under the curve.
http://www.coacs.com/software/published_titles/products/pccal/IPW.htm

Laboratory safety
It covers basic laboratory safety, without examining specific hazards. It includes safety signs, basic first aid in the laboratory and the handling of equipment.
http://www.coacs.com/software/published_titles/products/pccal/safety.htm

Methods of filling hard gelatin capsules
It covers all the operations performed by different types of filling machine in the delivery of variety of fill materials to hard gelatin capsules along with some general information applicable to the filling operation.
http://www.coacs.com/software/published_titles/products/pccal/filling.htm

Pharmacokinetics simulations
It simulates the plasma concentration–time profile tool to understand the basic pharmokinetic principles.
http://www.coacs.com/software/published_titles/products/pccal/pksims.htm

pKa
It is a highly accurate and automated tool for predicting pKas for a wide range of molecules.
http://www.pharsight.com/products/prod.home.php

SPSS
SPSS places constraints on internal file structure, data types, data processing and matching files which considerably simplify programming.
http://www.spss.com/spss

Stability program application software
It manages day-to-day activities of stability department within the quality control and/or R & D divisions. According to latest guidelines from the FDA, TPP, ICH and EU among others pertaining to pharmaceutical, chemical, biological and biotechnological fields.
http://www.coacs.com

WinNonlin
It provides a complete solution with data management, statistical modeling and visualization tools in one package.
http://www.pharsight.com/products/prod.home.php

Pharmaceutical Chemistry

Auto nom
It is used to generate IUPAC names automatically from chemical structures.
http://www.mdl.com/products/knowledge/crossfire_beilstein/

CIARA
It stores chemical information and assists in planning chemical reactions. It eliminates tedious and time consuming work of calculating data such as molecular weights, moles, reactant amounts, percent yields, etc.
http://www.vogelscientific.com

CLiDE
CLiDE is a document image processing software, which extracts content (i.e. structures, reactions and text) of chemistry documents.
http://www.chemstore.cambridgesoft.com/software/product.cfm?pid=269

CHARMm CNX
It provides a vast range of functionality for molecular mechanics and dynamics simulation. It can also applied to diverse areas of research including protein modeling, nanotechnology and X-ray and NMR structure determination.
http://www.netsci.org/Resources/Software/index.html

Chem draw PRO/Std
It is designed for chemists to draw chemical notations automatically.
http://www.cambridgesoft.com/products

ChemExper
It is free search tool for physical/chemical characteristics of some 60000 chemicals.
http://www.chemexper.com/

ChemKey
It is devoted to synthetic methodology, asymmetric synthesis, heterocyclic chemistry, organometallic chemistry, stereochemistry, etc.
http://www.euch6f.chem.emory.edu/

ChemSite
It is 3-D molecular modeling program for drawing, displaying and simulating the dynamic behavior of organic and biological molecules.
http://www.chemsw.com/10190.htm

ChemSymphony
ChemSymphony is a platform independent set of interactive JAVA applets that allow 3-D molecular structures to be easily incorporated into HTML documents.
http://www.chemsymphony.com

ChemTK
It is designed to visualize, organize and analyze chemical screening data.
http://www.chemtk.com

ChromView
It imports GC and GC-MS data into other Windows applications such as MS Word, Excel or PowerPoint as high-resolution images.
http://www.chemsw.com/12148.htm

ChemWeb
ChemWeb is a free chemistry drawing program for creation and transfer of 2-D chemical structures across the globe.
http://www.chemwindow.com

DEREK
It predicts the toxicological hazard of chemicals by analysis of their molecular structure.
http://www.netsci.org/Resources/Software/index.html

DIVA
It analyzes chemical and biological data on the desktop.
http://www.netsci.org/Resources/Software/index.html

DMax Chemistry assistant
It automatically finds, formulates, validates and shows scientific hypotheses that best match small molecule screening data.
http://www.pharmadm.com/DMaxChemistryAssistant.asp

DTREG
It generates SVM decision tree and logistic regression models.
http://www.dtreg.com

ECHIP
It produces 3-D diagrams and 2-D contour plots.
http://www.echip.com

Equbits insight
It is an SVM based predictive modeling software application designed for HTS and ADME chemists.
http://www.equbits.com

EROS
Elaboration of Reactions for Organic Synthesis (EROS) is a computer-assisted synthesis program developed by Gasteiger *et al*., which uses a set of rules to propose synthetic routes.
http://www.chemie.uni-erlangen.de/

Felix
It is used for NMR data processing, visualization and analysis.
http://www.netsci.org/Resources/Software/index.html

GC and GCMS file translator
It reads files from a variety of popular GCMS programs, which include Hewlett Packard Chemstation GC, Agilent (Hewlett Packard) Chemstation MS, Finnigan ITDS, etc.
http://www.chemsw.com/12149.htm

GLIDE
It is used for docking. Docking procedure mainly helps in understanding the action of drug at the molecular level.
http://www.schrodinger.com

hmo10
hmo10 is a Huckel molecular orbital calculator.
http://www.simtel.net/pub/pd/42108.html

Insight II
It provides a powerful graphical interface to best of breed algorithms for molecular dynamics and homology modeling.
http://www.netsci.org/Resources/Software/index.html

IMCS Live
It is a robust laboratory equipment calibration tracking and management software program that allows labs to automatically schedule periodic maintenance and inspection events using an extensive array of customizable reports.
http://www.chemsw.com/imcslive.htm

Introduction to mass spectrometry
It covers the fragmentation patterns and interpretation of mass spectra.
http://www.coacs.com/software/published_titles/products/pccal/massspec.htm

Introduction to NMR
It covers description on how NMR works, how NMR spectra interprets, use of delta values and how they are derived, etc.
http://www.coacs.com/software/published_titles/products/pccal/NMR.htm

Introduction to pharmaceutical stereochemistry
It covers basic stereochemistry using examples relevant to pharmacy.
http://www.coacs.com/software/published_titles/products/pccal/stereochemistry.htm

JChem
JChem is a package that contains Java applications and software development tools for chemistry.
http://www.jchem.com/examples.html

Logic and heuristics applied to synthetic analysis
It is a sophisticated retrosynthetic analysis program which can be used to suggest novel synthetic routes.
http://www.lhasalimited.org

Mathematics for pharmacists
It covers several basic mathematical concepts essential to complete calculations for pharmaceutical and life sciences.
http://www.coacs.com/software/published_titles/products/pccal/mathsforPharmacists.htm

MDL-ISIS
It is an integrated scientific information system that serves powerful chemical structures, chemical reactions or 3-D model searching capabilities.
http://www.mdli.com

MultiSimplex
It is new chemometric software for experimental design and optimization.
http://www.multisimplex.com

Nomenclature of organic compounds
It provides an alternative source of information to standard texts.
http://www.coacs.com/software/published_titles/products/pccal/nomenclature.htm

Pharmaceutical analysis – titrimetry
It provides typical calculations of titrimetric assays found in British Pharmacopoeia.
http://www.coacs.com/software/published_titles/products/pccal/titrimetry.htm

ProChemist
It is a 3-D molecular modeling program which includes pKa and solubility calculations, QSAR and chemometrics capabilities.
http://www.pro.chemist.online.fr

Q-Chem
It allows researchers to quickly and accurately analyze molecules of several hundred atoms.
http://www.q-chem.com/

Qmol
Qmol is used for viewing molecular structures and animating molecular trajectories.
http://www.dnastar.com/qmol/

QuantiScan
QuantiScan has functionality similar to that of sophisticated densitometers but at a fraction of the cost. It is able to analyze a wide variety of materials including polyacrylamide and agarose gels, autoradiograms, TLC plates, etc.
http://www.biosoft.com/w/quantiscan.htm

Radiochemistry and radiopharmacy
It provides all the necessary knowledge required for UG and PG students to be able to handle radioisotopes both for laboratory work and in the hospital dispensary.
http://www.coacs.com/software/published_titles/products/pccal/radiochem.htm

Shapes and mechanisms
It intends many animations to emphasize the significance of shape and reactivity within chemical systems.
http://www.coacs.com/software/published_titles/products/pccal/shapesandmechanisms.htm

Simple halogen compounds
It covers halide structure, nomenclature, properties, uses

and types of reaction that halides undergo. These reactions are illustrated using animations.
http://www.coacs.com/software/published_titles/products/pccal/halogencomps.htm

SMOG
Structural Molecular Generation program exhaustively and non-redundantly generates chemical structures for a given molecular formula.
http://www.ccl.osc.edu/pub/chemistry/software/MS-DOS/SMOG

Stat-200
Stat-200 incorporates all the descriptive statistics, parametric and non-parametric statistical tests, graphics and data transforms as per the need for processing, analyzing and presenting data.
http://www.biosoft.com/w/stat200.htm

SYSTAT
It is designed for data management, exploratory data analysis, comprehensive statistics and high-quality graphics.
http://www.spss.com

TOPKAT
It employs robust and cross-validated Quantitative Structural Toxicity Relationship (QTSR) models for assessing various measures of toxicity.
http://www.netsci.org/Resources/Software/index.html

Tsar
Tsar is fully integrated 2-D QSAR package used for library design and lead optimization.
http://www.netsci.org/Resources/Software/index.html

Using chromatographic data to calculate drug content in formulations
It focuses on calculations of the content of active ingredients in formulations using chromatographic data.
http://www.coacs.com/software/published_titles/products/pccal/chromatography.htm

Vcharge
It calculates accurate, conformation-independent, partial atomic charges for an SD file of drug-like compounds in ~0.1 per compound. It is useful for a wide range of modeling and QSAR applications.
http://www.verachem.com/Vcharge

Water!Pro
Water!Pro is a water quality modeling program designed to evaluate most chemical treatments that are applied to drinking water.[4-5]
http://www.chemsw.com/11068.htm

Pharmacology

Alternative therapies
It provides details on alternative therapies, e.g. Acupuncture, Aromatherapy, Osteopathy, Homeopathy and Hypnotherapy.
http://www.coacs.com/software/published_titles/products/pharmacalogy/alternative_therapies.htm

Assay zap
It is a universal assay calculator for RIA, ELISA, IRMA or any other type of assay.
http://www.biosoft.com/w/assayzap.htm

Basic histology of tissues
It is designed to introduce the histology of connective, nervous, muscle and epithelium tissues using text, line drawings (30+) and full-screen histology slides (40+).
http://www.coacs.com/software/published_titles/products/pccal/basichistology.htm

Basic psycho-pharmacology
It introduces the clinical applications of psycho-pharmacology, e.g. the use of anxiolytics.
http://www.coacs.com/software/published_titles/products/pccal/psychopharm.htm

Biological molecules
It provides the structures and properties of molecules which are common to all biological systems.
http://www.coacs.com/software/published_titles/products/pccal/biologicalMolecules.htm

CalcuSyn
It is a definitive analyzer of combined drug effects, which is able to automatically quantify phenomena such as synergism and inhibition.
http://www.biosoft.com/w/calcusyn.htm

CardioLab
It simulates chart recorder outputs of experiments on anesthetized and pithed animals. It can also mimic stimulation of vagal and sympathetic cardiac nerves.
http://www.biosoft.com/w/cardiolab.htm

Clinical trials and drug development
It encompasses the principles of new drug development, human experimentation, clinical trials of therapy.
http://www.coacs.com/software/published_titles/products/pharmacalogy/clinicalTrials.htm

COACS
It evaluates the impact of changing one or more pharmacokinetic parameters on the concentration–time profile of the drug. http://www.coacs.com

Dietary factors in drug metabolism
It is designed to show how dietary factors may affect the metabolism of drugs in the body.
http://www.coacs.com/software/published_titles/products/pharmacalogy/dietary_factors.htm

Drug targets
It focuses on various signal transduction mechanisms associated with drug targets.
http://www.coacs.com/software/published_titles/products/pharmacalogy/Drug_Targets.htm

EP-DOG
EP-DOG simulates the effects of various drugs on dog blood pressure and heart rate.
http://www.indphar.org/sware.htm

EP-Heart for Windows 95/98/2000
EP-Heart simulates the effects of drugs like epinephrine, nor-epinephrine, etc. on frog's heart with feature of examination mode.
http://www.indphar.org/sware.htm

ExPharm for Windows 95/98/2000
ExPharm is an educational software package which simulates the various animal experiments in pharmacology.
http://www.indphar.org/sware.htm

Eye disorders
It is designed to study a variety of eye complaints, which includes stye, allergic and infective conjunctivitis.
http://www.coacs.com/software/published_titles/products/pccal/eyedisorders.htm

Graph pad prism
It helps to organize, analyze and pick appropriate statistical tests and interpret results.
http://www.graphpad.com

Hypertension
It deals with the pathogenesis of hypertension and its management with special consideration of hypertension in pregnancy.
http://www.coacs.com/software/published_titles/products/pccal/hypertension.htm

Ileum
It simulates the effects of drugs on guinea pig ileum *in vitro*.
http://www.biosoft.com/w/ileum.htm

IPA-Tox
It is a data analysis capability within IPA that delivers a focused toxicity and safety assessment of candidate compounds that are being examined using toxicogenomics approaches.
http://www.ingenuity.com/products/ipa-tox.html

Ligand binding
It covers ligand binding and its applications in pharmacology at elementary and advanced levels.
http://www.coacs.com/software/published_titles/products/pharmacalogy/ligandbinding.htm

Local anaesthetics
It provides an overview of local anesthetic drugs and their clinical use.
http://www.coacs.com/software/published_titles/products/pharmacalogy/local_ana.htm

MacDope
MacDope is a pharmacokinetic simulation of drug.
http://www.chime.ucl.ac.uk/resources/Models/

MacMan
MacMan is a simulation program of heart, peripheral circulation and arterial baroreceptors.
http://www.chime.ucl.ac.uk/resources/Models/

MacPee
MacPee is a simulation of heart, kidneys, body fluids, electrolytes and hormones.
http://www.chime.ucl.ac.uk/resources/Models/

MacPuf
MacPuf is a simulation of human respiration, gas exchange and control.
http://www.chime.ucl.ac.uk/resources/Models/

METEOR
It predicts metabolic fate of parent compounds.
http://www.chem.leeds.ac.uk

MLAB
MLAB is an ideal tool for solving simulation and modeling problems such as chemical kinetics, pharmacological compartmental models, multiple site ligand binding, neurophysiological modeling, etc.
http://www.civilized.com/

Movement disorders
It sets Parkinson's disease within the spectrum of movement disorders and uses high-quality graphics, text and animations.
http://www.coacs.com/software/published_titles/products/pharmacalogy/movementdisorders.htm

NeuroSim
NeuroSim is intended for use in teaching neurophysiology at UG and PG level.
http://www.biosoft.com/w/neurosim.htm

PakMed PakNeurol 01
It is the most widely used scoring system in quantifying level of consciousness following traumatic brain injury.
http://www.pakmed.net/access/index.html

PakMed PakPsych 72
It is a set of three self-report scales designed to measure negative emotional states of depression, anxiety and stress.
http://www.pakmed.net/access/index.html

Peripheral blood flow
It helps to learn how to measure peripheral blood flow using this simple non-invasive technique.
http://www.coacs.com/software/published_titles/products/lsc/peripheralblood.htm

PHARM/PCS
It evaluates drug action and safety in experiments on animals and humans.
http://www.pharmpcs.com/

PharmaCalc
PharmaCalc is a pharmacokinetic simulation based on a one-compartment model with linear kinetics.
http://www.pharma.ethz.ch/biopharmacy/research/Simulation/calcloadwin.html

Pharmacology of asthma
It is used to assess respiratory function and peak flow. It is also used to study pathophysiological changes that lead to dyspnea and bronchial hyperresponsiveness.
http://www.coacs.com/software/published_titles/products/pharmacalogy/asthma.htm

PharmaSim
PharmaSim is more complex pharmacokinetic simulation of drug plasma levels based on one or two compartmental models and assume first-order kinetics.
http://www.pharma.ethz.ch/biopharmacy/research/Simulation/pharmasim.html

PharmTools Pro
It is based on drug synergism and dose–effect data analysis.
http://www.pharmsoft.net/

PharmaTutor
PharmaTutor is a simulation program having different program modules such as pharmacokinetics, blood pressure and catecholamine, dose–response curve and neuromuscular signal transmission.
http://www.pharma.ethz.ch/biopharmacy/research/Simulation/pharmatutor.html

Qik Prop
Qik Prop has been designed for pharmacological considerations. It provides rapid ADME characteristic predictions of drug candidates.
http://www.netsci.org/Resources/Software/index.html

Rat blood pressure
It simulates to demonstrate the effects of a variety of pharmacological agents/procedures on blood pressure and heart rate in anesthetized rat (*in vivo*).
http://www.coacs.com/software/published_titles/products/bioscience/ratbp.htm

Series of simulations in human physiology
It is useful for better understanding of theoretical concepts of respiratory system physiology, acid–base balance, etc. in humans.
http://www.physiologyeducation.org/materials/simres.html

Simulated water maze
It explains memory defects with detailed description on nature and use of a water maze.
http://www.coacs.com/software/published_titles/products/pharmacalogy/watermaze.htm

Six second ECG and dynamic cardiac rhythm simulator
It is a human ECG learning software which simulates ECG of human in normal condition and with various cardiac arrhythmias.
http://www.skillstat.com/ECG_Sim_demo.html

Synaptic transmission in the CNS
It aims to teach basic principles of chemical transmission at synapses in the CNS.
http://www.coacs.com/software/published_titles/products/pharmacalogy/CNSTransmission.htm

The circulation
It is a highly interactive program designed to teach the basic physiology of circulation.
http://www.coacs.com/software/published_titles/products/bioscience/circulation.htm

Thyroid hormones
It is designed to teach the basic physiology of the thyroid hormones, which includes location and structure of thyroid glands, synthesis, release, transport, mechanism of action and function of thyroid hormones.
http://www.coacs.com/software/published_titles/products/bioscience/thyroid.htm

Virtual neuromuscular junction
It records the electrical potential associated with neuromuscular transmission at the skeletal neuromuscular junction either by nerve stimulation or by direct current stimulation of the muscle fibers.

http://www.spider.science.strath.ac.uk/PhysPharm/showPage.php?pageName=software_sims

Virtual twich (rat nerve muscle preparation)
This program simulates muscle contractions by two different stimulations such as nerve and by direct electrical to muscle.
http://www.spider.science.strath.ac.uk/PhysPharm/showPage.php?pageName=software_sims

Ulnar nerve conduction
It is designed to measure conduction velocity in motor fibers of peripheral nerves.
http://www.coacs.com/software/published_titles/products/lsc/ulnarnerve.htm

UNISTAT
Various types of bioassays and effective dose (ED_{50}) applications can be analyzed using UNISTAT.[4-8]
http://www.unistat.com/

Pharmacognosy

BioOffice
It includes taxonomists, collection managers, conservation biologists, ecologists and private collectors of biological data or objects and institutions such as universities, museums, national parks, governmental agencies.
http://www.biooffice.at/

Biota
Biota manages specimen-based spatially and taxonomically referenced data for ecologists, conservation biologists, evolutionary biologists, systematists, museums and herbaria.
http://www.viceroy.eeb.uconn.edu/biota

DfD
DfD is offering a variety of nearest-neighbor and transect methods commonly used by ecologists to estimate animal and plant densities.
http://www.pisces-conservation.com/

SPECIFY
It specifies museum and herbarium research data processing. It is used for tracking specimens, tissue management transactions and for mobilizing species occurrence data on to the internet.
http://www.specifysoftware.org

TreeMap
TreeMap is an experimental program for comparing host and parasite trees.[9-13]
http://www.taxonomy.zoology.gla.ac.uk/rod/treemap.html

Life Sciences

Abalone
Abalone is a program for molecular mechanics. It is designed for proteins and nucleic acid simulations.
http://www.agilemolecule.com/Abalone/index.html

AMBER
It is designed to carry out molecular dynamics simulations on biomolecules.
http://www.ambermd.org

AminoXpress
It is multi-functional biochemistry package integrated with modules such as amino acid analysis, mass fragmentation, HPLC retention pattern, etc.
http://www.aminoXpress.com

Basic calculations in pharmacy
It covers basic calculations intended in pharmaceutical sciences.
http://www.coacs.com/software/published_titles/products/pccal/basicCalculations.htm

Biomer
It is an online molecular modeling program used as biopolymer model builders (nucleic acids, proteins, and polysaccharides).
http://www.scripps.edu/~nwhite/Biomer/index.htmlf

BioNumerics
It offers integrated analysis of all major applications in Bioinformatics. It combines information from various genomic and phenotypic sources into one global database and conducts conclusive analysis.
http://www.applied-maths.com/bionumerics/bionumerics.htm

BOSS (molecular mechanics)
It is a general purpose molecular modeling program that performs molecular mechanics calculations.
http://www.en.wikipedia.org/wiki/BOSS_%28molecular_mechanics%29

DDI module
It predicts drug–drug interactions (DDIs) among drugs and metabolites.
http://www.simulations-plus.com/Products.aspx?pID=11andmID=21

EnzFitter
It is designed for analysis of enzyme kinetics experiments.
http://www.biosoft.com/w/enzfitter.htm

FigSys
It is designed for processing, analyzing and presenting data

and creating science documents of all kinds.
http://www.biosoft.com/w/figsys.htm

FlexS
FlexS predicts conformation and orientation of two ligands as assumed when they bind to a protein.
http://www.biosolveit.de/FlexS/

FlexX
It is an extremely fast and highly configurable program used for predicting protein–ligand interactions.
http://www.biosolveit.de/FlexX/

Fundamentals of data collection
It introduces the design of research and methods of data collection in social research. It includes survey design, questionnaires, data sampling, handling techniques, etc.
http://www.coacs.com/software/published_titles/products/derby/fundamentalsofdatacollection.htm

GelCompar II
It offers an impressive list of unique advanced features of phylogenetic and dimensioning algorithms, group verification methods, database quality control techniques, GLP and database protection tools, history recording, etc.
http://www.applied-maths.com/gelcompar/gelcompar.htm

Genchek
It is an integral database system that can used to access, store, organize and retrieve DNA, protein and vector sequences.
http://www.ocimumbio.com/web/bioinformatics/prod_details.asp?prod_id=27

Genup
It is designed for quantitative genetics.
http://www.personal.une.edu.au/~bkinghor/genup.htm

GenVision
It is a genomic visualization package designed to support easy generation of publication quality graphics and maps.
http:/www./biommed.lsu.edu/staticpages/index.php?page=GenVision

Genowiz
It is a powerful gene expression analysis program that has been designed to store, process and visualize gene expression data efficiently.
http://www.ocimumbio.com/web/bioinformatics/prod_details.asp?prod_id=20

HyperTox
It is designed to assist in emergency management of acute clinical toxicology (poisoning) experiments.
http://www.hypertox.com/

Metabolism and transporter module
It is an optional module that extends the capabilities of GastroPlus to include saturable metabolism (gut, liver, and/or any PBPK tissue), saturable carrier-mediated transport by both influx- and efflux-proteins and metabolite tracking.
http://www.simulations-plus.com/Products.aspx?pID=11andmID=9

MPSA
MPSA is a software intended to protein sequence analysis.
http://www.hpc.unm.edu/~aroberts/main/mac_software.htm

MolSuite
It gives molecular modeling with great graphics, physical property calculations, database development and management, all in one complete package
http://www.chemsw.com/12258.htm

Molecular modeling pro
It display molecules as wire frame, ball and stick, spheres and dot surface models.
http://www.chemsw.com/13052.htm

Molecular visualization freeware
It is a software for looking at macromolecular structure and its relation to function.
http://www.umass.edu/microbio/rasmol/

PakMed PakNutri 12
It is a nutritional database presenting nutritional composition of more than 6000 food items for 44 nutrients/food components.
http://www.pakmed.net/access/index.html

PBPKPlus module
It simulates the plasma and tissue concentration–time profiles.
http://www.simulations-plus.com/Products.aspx?pID=11andmID=7

Pharmaceutical microbiology assessment
It consists of series of self-assessment questions on various aspects of pharmaceutical microbiology.
http://www.coacs.com/software/published_titles/products/pccal/microbiology.htm

ProFIT
Protein Fold Identification Tool conducts threading based on an empirical energy function.
http://www.came.sbg.ac.at/software/Profit/profit.html

SigmaPlot
It produces high-quality graphs of research data without spending hours in front of the computer.

http://www.biommed.lsu.edu/staticpages/index.php?page=SigmaPlot

TINKER

It is molecular mechanics and molecular dynamics simulation with complete special features of biopolymers. [4,5,14-16]

http://www.en.wikipedia.org/wiki/TINKER

Conclusion

Therefore, utilization of computer softwares in pharmaceutical sciences is huge across the globe. These internet web resources will also helpful to various organizations, industries, laboratories, researchers, teachers, students, doctors, pharmacists, layman, lawyers and higher authorities, etc. and for all those who are directly or indirectly working in the field of pharmacy, medical, paramedical, engineering, life and other allied subjects, for reshaping and remolding their needs.

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