

# 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.

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.<sup>[1-3]</sup> 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](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](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](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/](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](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 pharmacokinetic principles.

[http://www.coacs.com/software/published\\_titles/products/pccal/pksims.htm](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/](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 be 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 a 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 a 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](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](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](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/mathforPharmacists.htm](http://www.coacs.com/software/published_titles/products/pccal/mathforPharmacists.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](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](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](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](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](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](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.<sup>[4-5]</sup>

<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/pharmacology/alternative\\_therapies.htm](http://www.coacs.com/software/published_titles/products/pharmacology/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](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](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](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/calculusyn.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/pharmacology/clinicalTrials.htm](http://www.coacs.com/software/published_titles/products/pharmacology/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/pharmacology/dietary\\_factors.htm](http://www.coacs.com/software/published_titles/products/pharmacology/dietary_factors.htm)

### **Drug targets**

It focuses on various signal transduction mechanisms associated with drug targets.

[http://www.coacs.com/software/published\\_titles/products/pharmacology/Drug\\_Targets.htm](http://www.coacs.com/software/published_titles/products/pharmacology/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](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](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/pharmacology/ligandbinding.htm](http://www.coacs.com/software/published_titles/products/pharmacology/ligandbinding.htm)

### **Local anaesthetics**

It provides an overview of local anesthetic drugs and their clinical use.

[http://www.coacs.com/software/published\\_titles/products/pharmacology/local\\_ana.htm](http://www.coacs.com/software/published_titles/products/pharmacology/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/pharmacology/movementdisorders.htm](http://www.coacs.com/software/published_titles/products/pharmacology/movementdisorders.htm)

### **NeuroSim**

NeuroSim is intended for use in teaching neurophysiology at UG and PG level.

<http://www.biosoft.com/w/neurosim.htm>

### **PakMed PakNeuro1 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](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/calclowwin.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/pharmacology/asthma.htm](http://www.coacs.com/software/published_titles/products/pharmacology/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](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/pharmacology/watermaze.htm](http://www.coacs.com/software/published_titles/products/pharmacology/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](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/pharmacology/CNSTransmission.htm](http://www.coacs.com/software/published_titles/products/pharmacology/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](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](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](http://www.spider.science.strath.ac.uk/PhysPharm/showPage.php?pageName=software_sims)

### **Virtual twitch (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](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](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.<sup>[4-8]</sup>

<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.<sup>[9-13]</sup>

<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](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.html>

### **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](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](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 be used to access, store, organize and retrieve DNA, protein and vector sequences.

[http://www.ocimumbio.com/web/bioinformatics/prod\\_details.asp?prod\\_id=27](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](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 for protein sequence analysis.

[http://www.hpc.unm.edu/~aroberts/main/mac\\_software.htm](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 displays 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 a series of self-assessment questions on various aspects of pharmaceutical microbiology.

[http://www.coacs.com/software/published\\_titles/products/pccal/microbiology.htm](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 remodeling their needs.

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