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A REVIEW: DIFFERENT SOFTWARE USED IN PHARMACY

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Abstract: Software is a computer program and related data that provide the instructions to the computer to perform particular task. 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. 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 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, and identify genome responsible for expression of particular characteristics. Hence, in the present article e, we have enlisted the subject wise different software names, websites and their features used in the milieu of pharmacy.

Keywords: Software, Websites, Pharmaceuticals, Computer Program.

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INTRODUCTION

Softwares are programs that help to process the data as wanted. There are two major kinds of softwares:

1. **System software:** It is software that helps the computer to run its own resources.

2. **Application software:** Application software on the other hand is "end-user" software.

These are programs designed to address general and special purpose applications.

1. 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 [1].

2. 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.

3. Softwares used 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 [2].

4. Softwares used in Pharmaceutics help for predicting the dissolution rate, biopharmaceutical characterization, accurate and precise stability profile, etc. of formulated dosage form [3].

5. Softwares used in Pharmacognosy give information on herb activity, interactions, mechanisms of action and supporting data underlying the use of herb for health [3].

6. Software used 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 [4].

7. Computers have been successfully utilized in pharmaceutical technology to improve productivity and to provide solutions for time-consuming manual task. Various computer applications are classified as - Data and information management systems, Interactive voice response systems, Group collaboration tools, Document management and publishing systems, Internet based applications and tools, Problem solving application,

Communication aids, Laboratory automation, Process control, Computer based training. In data and information management systems the available data management programs are material inventory system, formulation information system, clinical supplies inventory system, clinical supplies labeling, stability information system, analytical information system, and quality assurance information system [5].

8. Computers can also be used for expiry date prediction, laboratory automation, in pharmacokinetics for fitting blood- level data to the appropriate model (single, two or multiple compartments) and calculate model parameters, such as absolute rate constant, elimination rate constant, half-life, volume of distribution to evaluate bioavailability parameters such as peak plasma concentration and area under the concentration time curve obtainable from a blood level curve [6].

9. To calculate dosage regimens in patients with renal failure. Currently the growing trend is to make use of physiologically based pharmacokinetic models to study the behavior of drugs in animals and extrapolate data to humans and predict concentration of drugs in human body fluids [7].

10. To solid dosage form dissolution allows for nearly complete automation. Sampling, analysis, quantization, data handling and reporting are all performed by the computer according to the analysis parameters specified before each run or included in a set up table. Automation has played a key role in the development of dissolution system, which attempts to simulate changes in pH in the gastro intestinal tract or the presence of bile salts [7].

11. Computerized process control systems are used to measure process variables through sensors at predefined intervals, make appropriate decisions and APTI ijper Indian Journal of Pharmaceutical Education & Research. The computer mainly records the measurements, compares with standards and transmits signals to regulating devices to make the necessary changes. This automation is limited by availability of pharmaceutical processing equipment. The practical applications can be seen in automated tableting and automated freeze-drying [7].

12. Pharmacy Software Reviews is a grass roots effort to improve pharmacy software in the market today. As a member of the pharmacy software community you can: review your software to send a message about what needs to be improved to your vendor; review your software to help others starting out or changing software; request features as a community to let your vendor know what features are important. You can also use the features search, reviews and feature requests to find a new pharmacy system. Join us and be part of the voice of the pharmacy software community [8].

Softwares used in different fields of pharmacy:

1. Softwares used in Pharmacology

The softwares used in pharmacology, are mainly related to minimize the efforts needed in determining the pathway of the drug and consequently its adverse reactions. Further the softwares are extensively used in determining the pharmacokinetic principles of the particular drug in a particular individual. The various softwares used are as follows:

a) **Computerized drug-drug interaction (DDI):** screening is widely used to identify potentially harmful drug combinations in the inpatient and outpatient setting. The performance of this software was checked by creating 6 mock patient profiles containing 37 drug pairs, 16 of which are clinically meaningful DDIs that pose a potential risk to the safety of the patient. Each profile was entered into the computer pharmacy system and the system response in terms of the presence or absence of a DDI alert was recorded for each drug pair. The percentage of correct responses and the sensitivity, specificity, positive predictive value and negative predictive value of each system to correctly [9].

b) **The Introductory Pharmacokinetic Workshop package (COACS)**: The objective of this software package is to teach the basic principles of pharmacokinetics through computer simulations. Valuable tool to understand the basic pharmacokinetic principles and to appreciate the interplay of various pharmacokinetic parameters. The program allows the student to evaluate the impact of changing one or more of pharmacokinetic parameters on the concentration time profile of the drug. The program covers intravenous bolus and, oral drug administration, constant rate and intermittent intravenous infusions, single and multiple drug administration, linear and non-linear drug elimination, one and two-compartment pharmacokinetic models. U.S. EPA benchmark dose software and the software by Kalliomaa are used for dichotomous data on dose- response and dose- effect data on the liver, kidneys, CNS and tumors. Dose modeling for various data of doses is done on these software using log logistic model and some flexible models like Hill &Mult model, needed for S-shaped continuous data. But a slight problem with this software is that the models used to describe the data need more software levels. Thus the output depends a lot on the model selection [10].

c) **SPINA, CINA, MINA and PC-SCOPE:** These are complete guiding systems to assist the anesthetist to deliver simultaneously many drugs to a patient. This system is constituted of three

modules. The first module SPINA is used to select the most appropriate IV drug from a database considering patient's age, weight, disease state and surgery. It helps to evaluate its pharmacokinetics. The second module CINA is used to prepare the infusion sheet. The third module, MINA is used for the start up and control of drug delivery and to synchronize the infusion pumps. It is also possible to interact on the preprogrammed infusion sequences. To achieve a closed loop regulation PC-SCOPE was developed. It manages data acquisition [11].

d) **Pk-fit:** This software is used to fit nonlinear models to kinetic and dynamic data. Directly connected to the spreadsheet, a statistical software component manager is available. In the data manager, Pk-fit includes the non compartmental analysis module, the compartmental analysis module, the nonlinear kinetic process module, the drug absorption module, the pharmacodynamic data modeling module, the simultaneous fitting module and user-defined library module. Software similar to Pk-fit is packages like PCNONLIN, MODFIT, MKMODEL, NONMEM, and SIPHAR [12].

e) **Pulse Analysis System (PAS):** The software takes an inspiration from an integral part of Chinese Indian J. Pharm. Educ. Res. 42(4), Oct-Dec, 2008: 404. The software reads pulses of 12 internal organs within minutes. According to acupuncture, every organ has a meridian through which energy and blood flows. There are 12 such pulses and even a slight imbalance in the Yin (structural) and Yang (functional) forces can be detected through PAS. The 6 Yin pulses on the left hand are liver, heart, spleen, lungs, kidney and pericardium. Yang-Gall bladder, small intestine, stomach, large intestine, 3 cavities and urinary bladder. PAS has a pulse wave sensor attached to the computer. As the sensor reads each pulse, the data is analyzed and within seconds detailed health matrix flashes on screen. In PAS, distribution of wood, fire, earth, metal and water, these elements in 12 organs. There should be an overall Yin-Yang balance of 90 for ideal health. PAS is diagnostic. The level of diagnosis is accurate. It can be used for preventive diagnosis e.g. If hypertension/ diabetes runs in family then PAS can tell if one possess the tendency to develop hypertension/ diabetes. Thus preventive measures can be taken [13].

f) **Qik Prop:** It is software designed for pharmacological considerations. It provides rapid ADME characteristic predictions of drug candidates [14].

g) **METEOR:** The software predicts the metabolic fate of a parent compound and it also evaluates the likelihood that each predicted metabolite could be found in vivo. This evaluation considers

physicochemical parameters; such as log P. Metabolites can be restricted to those most likely to be of interest by user-defined controls. The feature included are, selection of confidence levels for metabolite generation, sequence termination at excretable metabolites, the potential to make species specific predictions, restriction to either Phase I / Phase II processes [15].

h) **UNISTAT:** UNISTAT's optional Analysis of Biostatistical Method in Biological Assay and furthermore, it is also a complete implementation of the specification given in European Pharmacopoeia, Statistical Analysis of Results of Biological Assays and Tests. Potency calculations can be performed employing parallel line, slope ratio and quantal response methods, complete with fiducially confidence Other types of bioassays and effective dose (or ED50) applications can be analyzed using UNISTAT's Nonlinear Regression and Logit/ Probit / Weibull procedures [16].

2. Softwares used in Medicinal Chemistry

The major application of softwares in pure chemistry is for QSAR. It is possible to elucidate the influence of various physiological properties on drug potency and to predict activity values for new compounds within certain limits. QSAR technology employs complex computers, molecular graphics and sophisticated software's. They may be of enormous assistance to those trying to generate the large databases result from massive efforts in drug research.

a) **DEREK**: It is run on Windows. It is a rule based expert system that predicts toxicological hazard of chemical based on an analysis of their molecular structure. The software uses structure activity relationship (SAR) and gives some consideration to physicochemical properties to derive its predictions. All outcomes are peer reviewed by expert toxicologists and Indian J.Pharm. Educ. Res. 42(4), Oct-Dec, 2008405 are supported by literature references. Alerts cover a wide range of toxicological end points, including carcinogenicity, mutagenicity and skin sensitization [17].

b) **Auto Nom:** It is a chemical naming software system for windows and Macintosh Operating System. It uses a proprietary algorithm based on IUPAC nomenclature rules to generate IUPAC names automatically from chemical structures. The latest version of this software (4.0 version) includes features as, chiral interpretation (R, S configuration) and double bond topology (E, Z descriptors), support for CAS ring system naming conventions, ability to number atom loc ants within named structure [18].

c) **MDL-ISIS:** Integrated scientific Information system serves as an information management framework

for discovery data. It has extensive chemical representation features or powerful chemical structure, chemical reaction or 3D model searching capabilities. ISIS is also an application development environment that allows extending software beyond chem drawing and data basing to managing chemical inventories, creating electronic lab journals and managing therapeutic level lead candidates [19].

d) **V-life MDS (2.0 Version):** It is a QSAR software. QSAR Plus module for evaluation of several molecular descriptors along with a facility to build the QSAR equation and use it for predicting the activities of the test or new molecules. These features are managed through an MS- Excel type work sheet28. The k- nearest neighbor (kNN) method used for generating relationship of activity with descriptors [20].

e) **GLIDE (4.0 Versions):** This is another type of the QSAR softwares. It is provided by Schrodinger. The software is exclusively used for docking. Docking simulate as it is called in scientific terms is one the important methods for achieving a foray in new compounds. The docking procedure mainly helps in understanding the action of the drug on the molecular level. The process of the action of the drug in our body mainly starts with its binding to specific enzymes, which further helps in catalyzing the drug's action. The drug binds to the active site of the enzyme forming the presence of various amino acid residues. The extent of binding of the drug to the enzyme is generally related with its extent of action. This software gives a score, which determines the extent and efficiency of the binding ability of a drug. Thus the scores of established drugs are fed to the software. When a new analogue of the drug is found, its score is compared with the score of the standard for that particular enzyme. If the score is greater than that of the established drug, then it can be assumed that the new analogue has better action than the established drug, at least at the molecular level [21].

f) **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 [22].

g) **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 [23].

3. Software's used in Pharmaceutics:

The softwares used in pharmaceutics mainly are involved in predicting the

dissolution extents of the formulated dosage form. Dissolution is an important parameter to determine the in vitro–in vivo correlation. Further the softwares are also used to determine the pharmacokinetic profile of the drug. The softwares also help in getting a precise stability profile of the particular drug.

a) **ZOREL**: Software developed for the purpose of studying drug release kinetics from compressed matrices. The program, written in FORTRAN, uses raw dissolution data for input. It initially corrects the dissolution data for drug and/or volume losses occurring at the time of sampling and on the basis of the weight of the dosage form and drug content, estimates the values of amount and percent drug released at various times for each formulation unit. The value of log mean fraction released are computed and regressed against log time to yield the values of kinetic constants K and release exponent (n) and subsequently calculations are made for mean dissolution time (MDT). For swelling matrices the respective contributions of the diffusion and the polymer relaxation along with the constant of k1 and k 2 are also computed. Based on the phenomenological analysis, the software predicts the type of release viz. Fickian, non Fickian (anomalous) or zero order. In addition the values of mean percent release are calculated and observations. The values of rate of drug release and t50%, t60% up to t90% of the drug release are computed using the program [24].

b) **ALOGPS**: Interactively calculates and compares lipophilicity and aqueous solubility of chemical compounds using 6 programs – CLOGP, XLOGP, IA_ logP, IA_logs, LOGKOW and ALOGPS itself [25].

c) **CALACO**: It is a windows data conversion program, which can perform conversions in the following categories – Acceleration, angle, area, energy, length, power, pressure, speed, temperature, time, volume and weight. CALACO provides pop-up definition for each unit. Sometimes a unit maybe used in 2 different measurement systems. The software helps in knowing full definitions of units. It also has features to calculate boiling points at reduced pressures and perform density calculations [26].

d) **pKa:** It is a highly accurate and automated tool for predicting pKa's for a wide range of molecules. The module utilizes quantum chemical methods to reliably predict pKa in combination of correlated quantum chemistry, self – consistent reaction field (SCRF) continuum treatment of solvation and systematic correction to account for approximation in both ab initio and continuum solvation models [27].

e) **WinNonlin**: It is the industry standard for pharmacokinetic, pharmacodynamic, and noncompartmental analysis. In addition to its extensive library of built-in PK, PD and PK/PD models, WinNonlin supports custom, user-defined models to address any kind of data. WinNonlin provides a complete solution with data management, statistical, modeling and visualization tools in one package.Additional tools enable exploration of drug's properties through nonparametric superposition, semi compartmental modeling, deconvolution and nonparametric analysis of crossover studies [28].

f) **PCP-Disso v2.08 software:** It is software for dissolution studies of a chemical moiety. This software can obtain dissolution profiles of various drugs at desired pH. Thus the drug release time can be calculated. The software also helps to find out the order of kinetic degradation of a particular drug [29].

g) **Automated packaging component analyzer**: It is used to automatically verify the incoming printed components against a pre-approved master [30].

h) **Biopharmaceutics**: It designed to introduce the applications of biopharmaceutics to oral drug delivery [31].

i) **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 [32].

4. Softwares used in 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 [33].

a) **Biota:** Biota manages specimen-based spatially and taxonomically referenced data for ecologists, conservation biologists, evolutionary biologists, systematists, museums and herbaria [34].

b) **DfD:** DfD is offering a variety of nearest-neighbor and transect methods commonly used by ecologists to estimate animal and plant densities.

c) **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 [35, 36].

CONCLUSION

Pharmaceutical software's have become the essential tool in the various fields/areas of pharmacy eg. Research, Teaching, Quality control, Quality assurance, Drug

development, Biostatistics, Bioinformatics etc. Pharmaceutical software's decreased the human efforts, error, time utilization in particular task without compromising the quality of work with great accuracy and efficiency. These software's are utilized by the various institutes globally related to science and medicine.

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Fig 1: UNISTAT Software

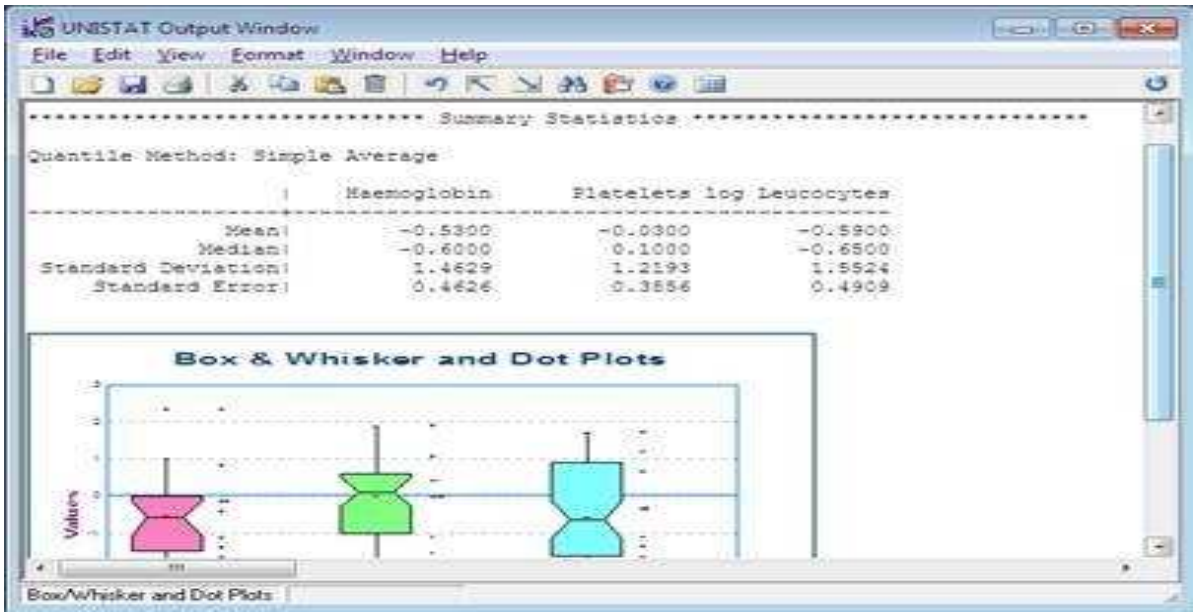


Fig 2: DEREK Software

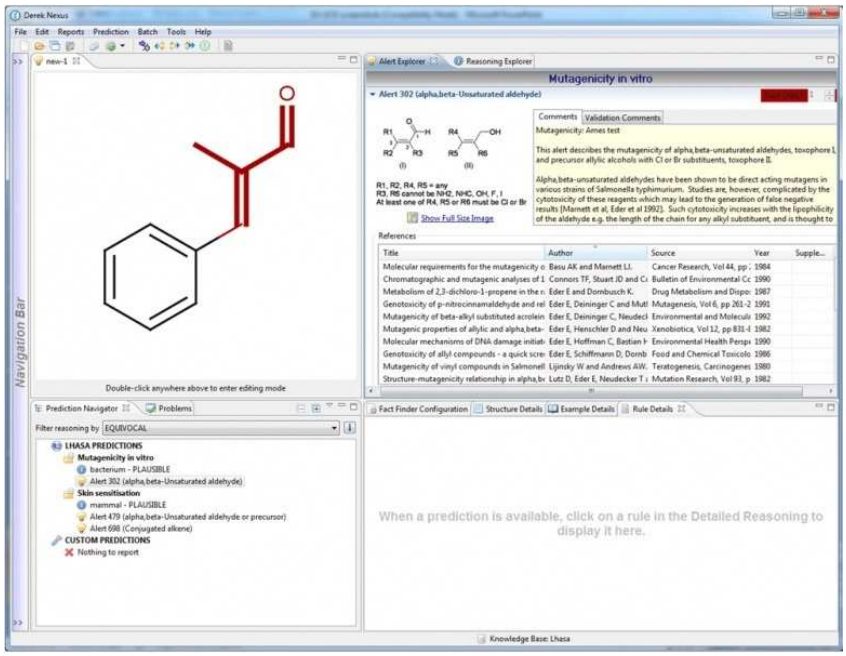


Fig 3: AUTO NOM Software

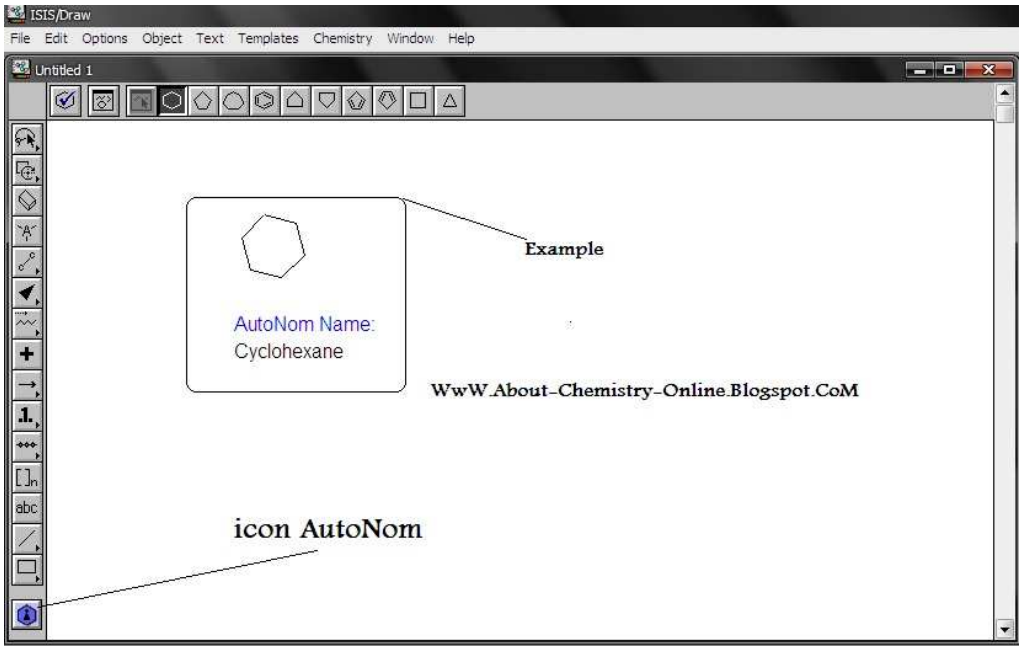


Fig 4: MDL-ISIS Software

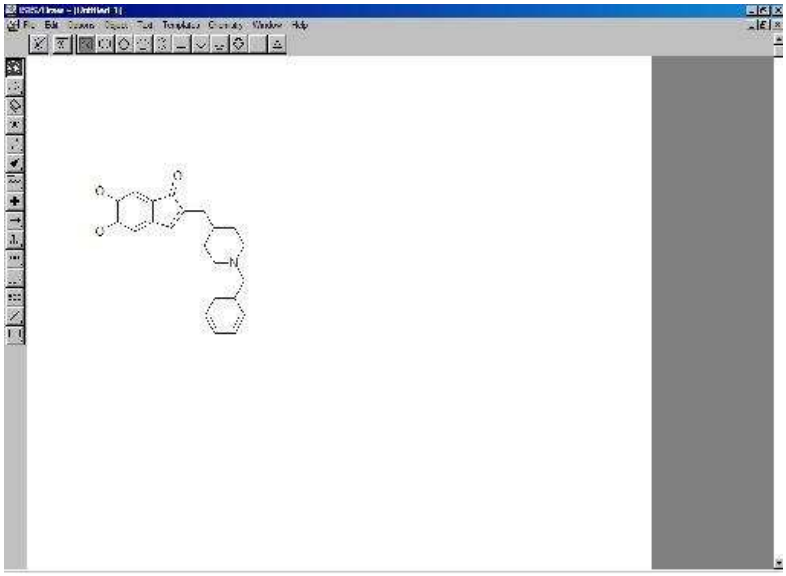


Fig 5: MDS Scripting Console

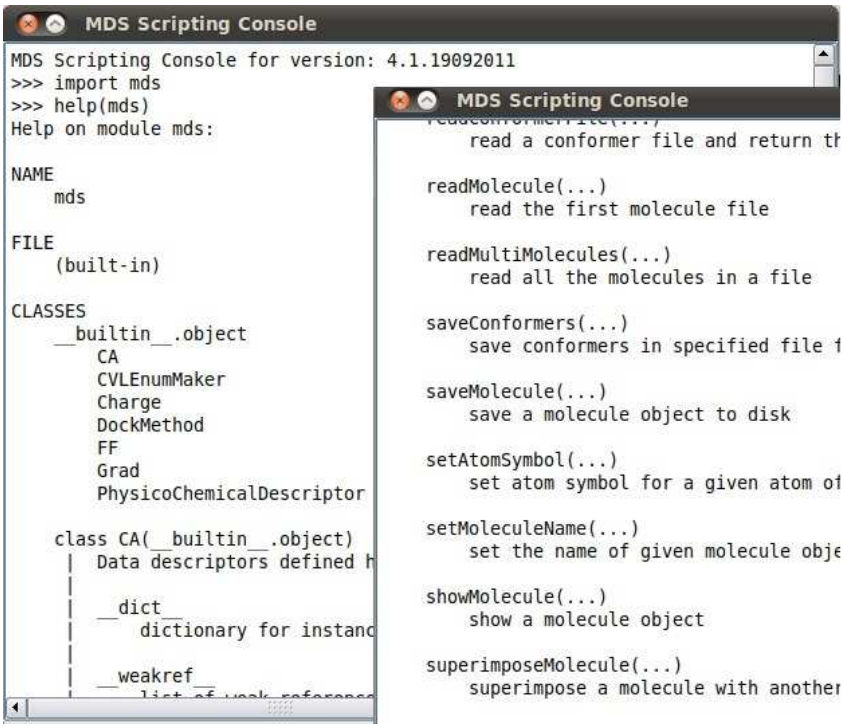


Fig 6: Ciara

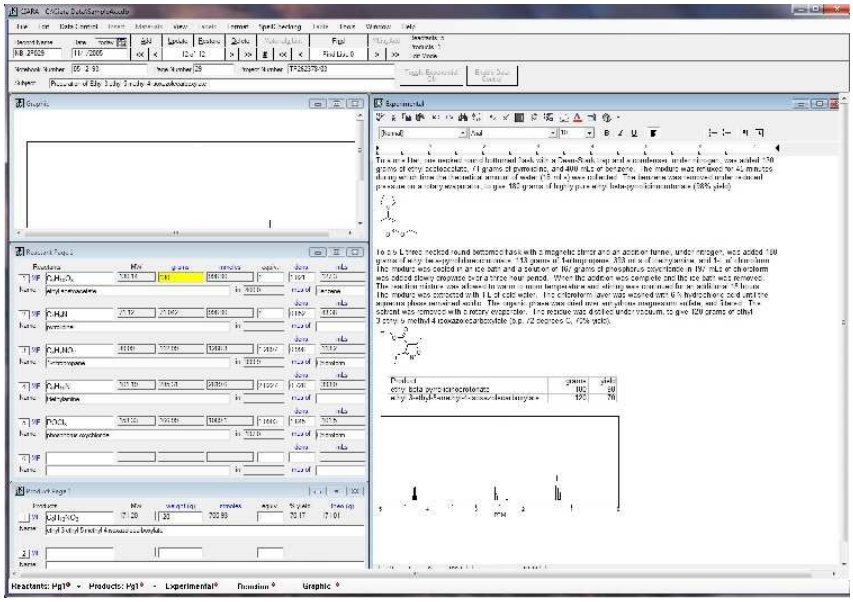


Fig 7: CHARMm-CNX SOFTWARE

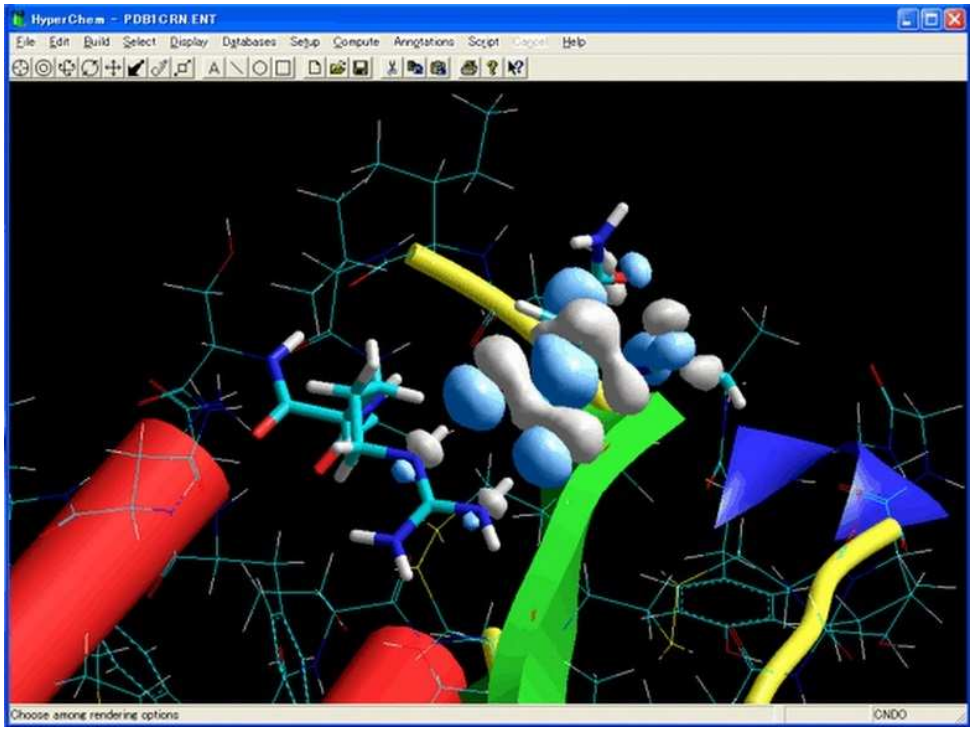


Fig 8: CALACO SOFTWARE

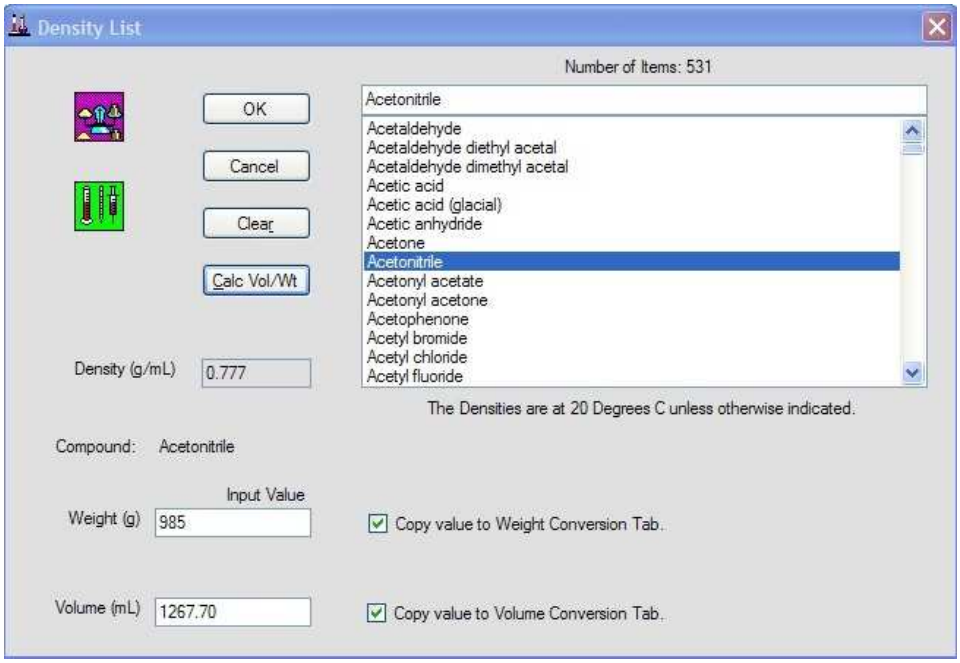


Fig 9: pKa software

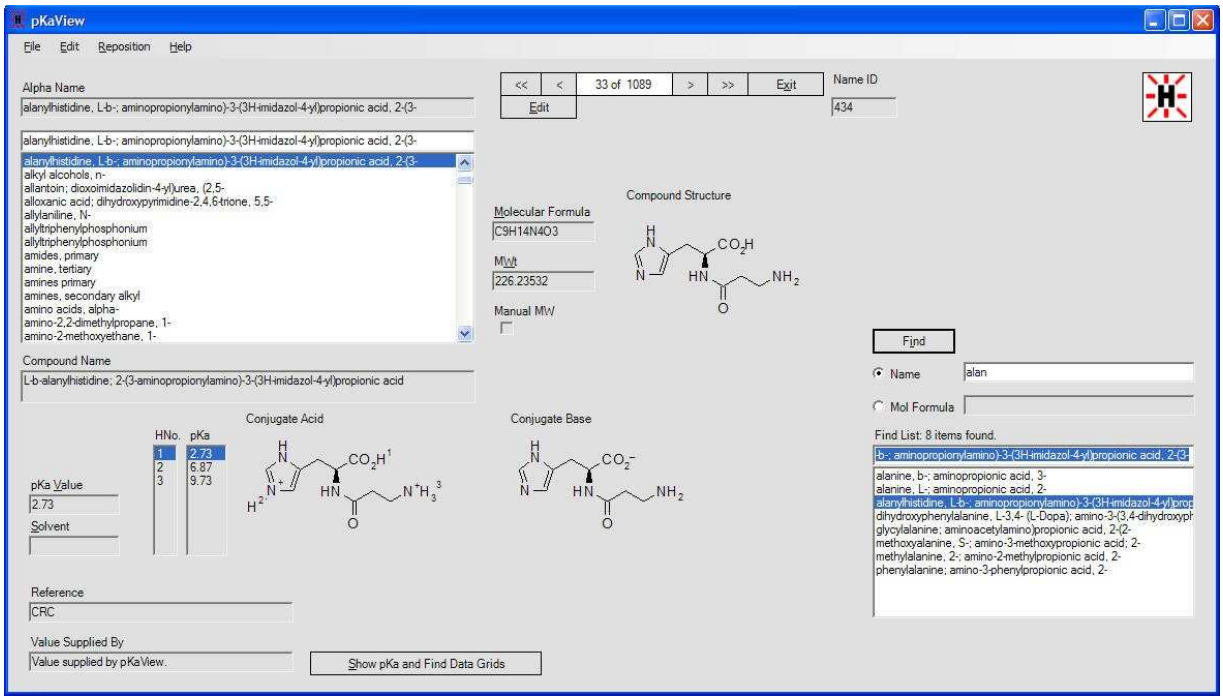


Fig 10: Win NONLIN Software

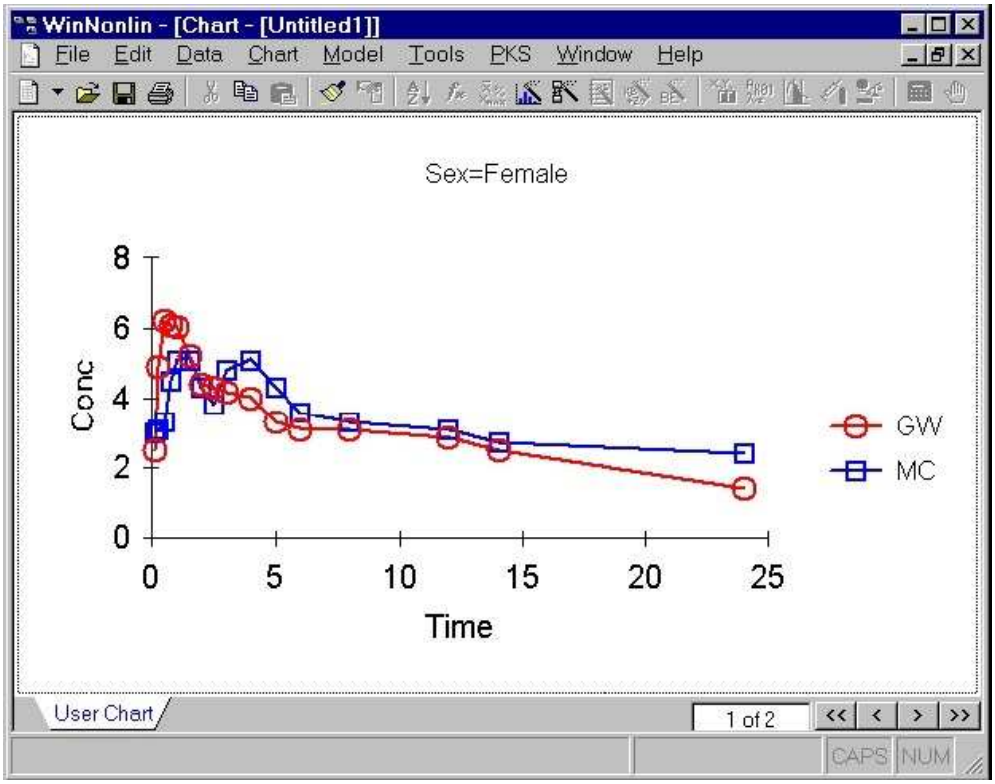


Fig 11: BIO OFFICE Software

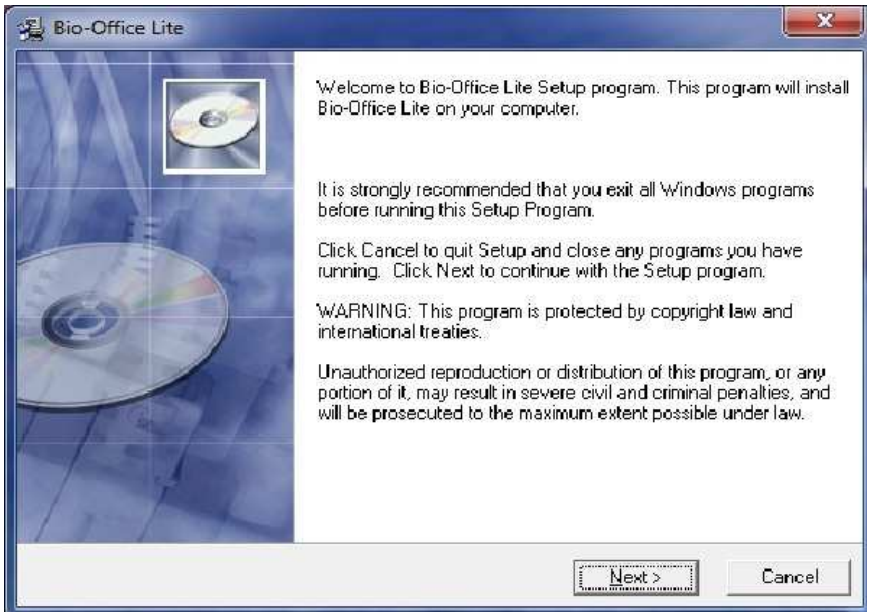


Fig 12: BIOTA- SOFTWARE

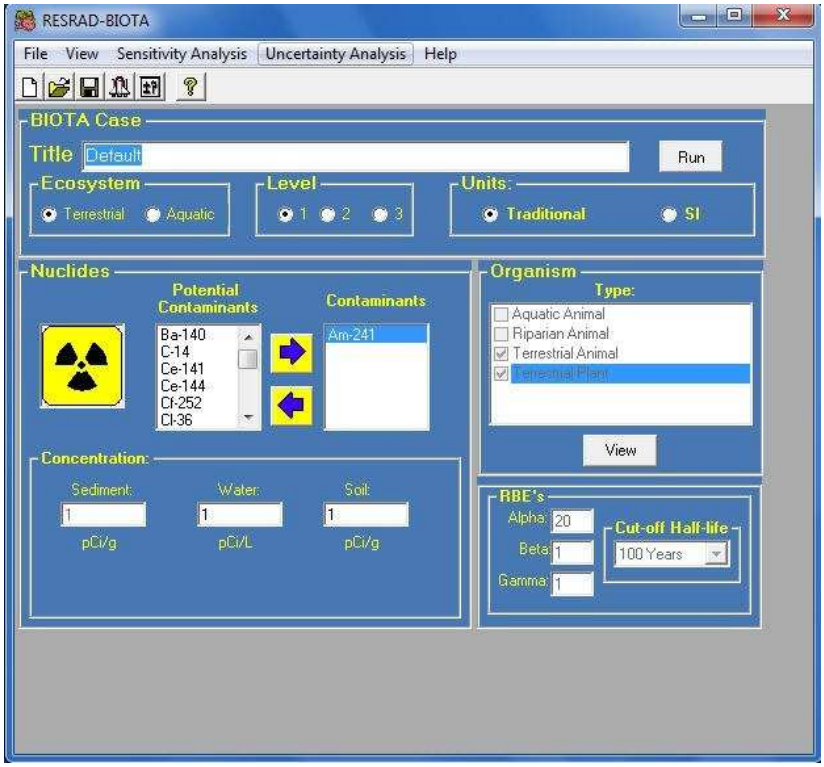
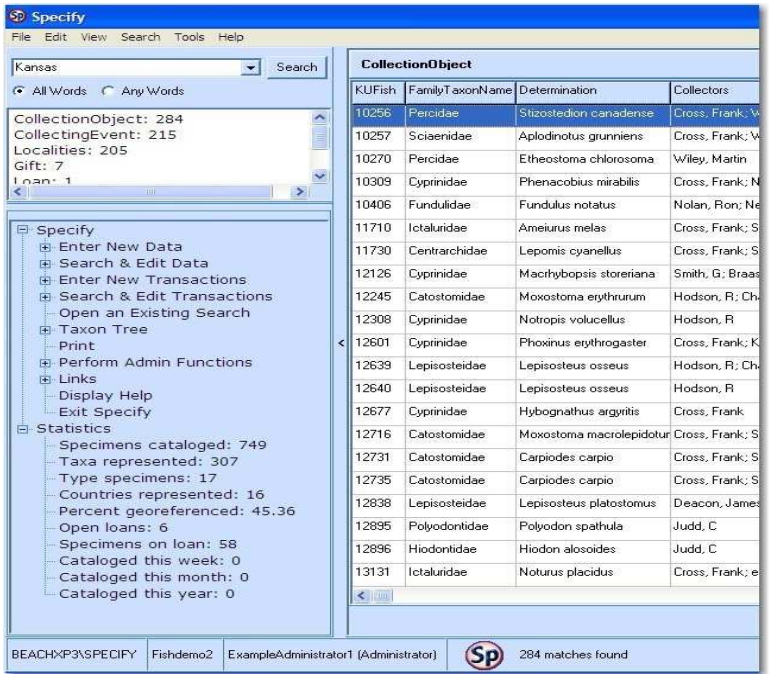


Fig 13: SPECIFY-Software



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