HKCP ALUMNI BULLETIN

Issue-XII Feb- 2014

From the Editors Desk:

Dear Alumni,

I am pleased to present the 12th issue of alumni bulletin. A cultural week and Orane 2014 was celebrated from 23rd Jan to 28th Jan. It was full of activities as sports day; many competitions were organized as indoor –outdoor games, mehendi, tattoo making, face painting, rangoli, dumb charades and mono acting. Our students participated in inter college competitions like Rx sports, RX cultural and RX tech-fest. On nation level students has participated in Manthan- 2013.

In Success secret series the present issue carries an article "SOFTWARES IN PHARMACEUTICAL RESEARCH"

As ever we always work towards giving you more and more of news about college, do send us your views and suggestions.

With best wishes

SheelaYadav

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Campus News:

- A PTA meeting was held on 11th Jan 2014.
- A photo session for Impulse was organized on 13th Jan.
- The cultural week was organized under the guidance of principal madam.
- A sport day was organized on 23rd and 24th Jan. Students were participated in various out doors and in doors games.
- On 25th Jan students were participated in nail art, mehandi, face painting, tattoo making, rangoli ect.
- On 26th Jan, The Republic day was celebrated.
- On 28th Jan "Orane" annual day was celebrated. The students were awarded with trophy and certificates for their achievements.
- For Academic Year 2012-2013; Tarjani form 1st year M.Pharm, Gaurave from final year, Mitchell lobo from 3rd year, Anamika Pandey from 2nd yr, Prabhuta Makwana fron 1st yr; got 1st prize.
- Under the guidance of Dr. Anubha Khale and Sunita Ogale madam; in manthan two groups from our college were participated and their ppt selected on 34th and 35th position.
- For RX sports; Maulik and Nihkil from 2nd yr got 2nd prize for Bowling, Vivek from 2nd yr for NFS got 2nd prize, Yasin from 4th yr got 2nd prize for Fifa, for carom doubles (girls) Rohini and Varsha from 3rd yr got 3rd prize ect.
- RX cultural; 1st prize for spelling buzz Rahul from 2nd ye, 2nd prize for personality Zaid from 4th yr, 3rd prize for Hogathon John from 2nd yr, 3rd prize for poetry writing Salma shaikh from 4th yr.
- RX Tech-fest; From 4th yr Zaid and Akshay got 1st prize for poster presentation, 3rd for oral presentation.
- Pharma observer and Impulse-14 was released on 28th Jan.
- Convocation ceremony was held on 18th Feb.

Name: Megha Rajan

: **II-B-10, Lotus CHS, Hanuman Nagar, Katemanivili, Kalyan (East)**
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PREVIOUS EXPERIENCE:

Acharya Chemicals as Trainee Officer QA for 4 months

EDUCATIONAL QUALIFICATIONS

Degree	Institute/ University	Class	Year of passing
M.Pharm (Quality Assurance)	C.U. Shah college of Pharmacy, SNDT University	Distinction Grade A	2013
B. Pharm	L.H Hiranandani College of Pharmacy, Mumbai University	First class	2010

M. PHARM. DISSERTATION WORK (QUALITY ASSURANCE)

Title of Thesis : **Novel extraction techniques for extraction and isolation of Biomarker from *Convolvulus pluricaulis***

Research Mentor : **Dr. (Mrs.) Pratima .A. Tatke**

PRESENTATIONS

1. **Presentation on "Interferons" at L.H. Hiranandani College of Pharmacy**
2. Poster presentation at 64th IPC, Chennai on Compariso of various extraction techniques for isolation of scopoletin from *Convolvulus Pluricaulis*.

Dr. Ritesh A. Fule

Date of Birth: 17.10.1984

Address: 602, A1 Tower, Riddhi Gardens, Malad (E), Mumbai.

Marital status: Married

Language known: English, Marathi, Hindi

Educational Qualifications

Examination	Institution (name, place, state of Institution)	%Marks
Ph.D. Tech (Pharmaceutics)	Institute of Chemical Technology, Mumbai (ELITE status)	
(UGC- SAP Funding) N/A		
M.Pharm (AICTE)	Bombay College of Pharmacy, Kalina, Mumbai, Maharashtra (Govt. Aided)	1st class
B.Pharm	Govt. College of Pharmacy, Amravati University	1st class

Skills and Expertise (4 year of complete research experience in Formulation development)

Scientific reviewer

Working as a Scientific Reviewer for research, review articles for Journal of Pharmacy Research an international peer reviewed journal published by Elsevier publishers.

Ph.D. (Tech.). Research Topic

"Innovative drug delivery systems for Antimalarials in Fixed dose form"

Research Supervisor: Prof. Purnima D. Amin

Place of research work: Institute of Chemical Technology

List of Publications in Peer-Reviewed Journals (published / accepted / under review) -15

Patents

1. Indian Patent with complete specification (1674/MUM/2013) filled entitled "Pharmaceutical Dosage Form Comprising Antimalarial Ingredients In A Solid Dispersion Using Hot Melt Extrusion Technology" (Ritesh A. Fule, Tarique S. Meer, Purnima D. Amin)

2. Indian patent entitled "Preparation and use of oligosaccharide imprinted mesoporous silica" got published with patent application number 2056/MUM/2011 in 19/7/2011; Meer Tariq Ali, Patole Rahul K, Fule Ritesh Amol, Amin Purnima Dhanraj.

3. Indian patent entitled "Once a daily oral sustained release gastroretentive formulation of lafutidine" got published with patent application number 3203/MUM/2011; Khan Furqan, Dhamecha Dinesh, Ghadlinge Shyam, Fule Ritesh Amol.

Presentations (oral / poster) in Conferences / Workshops / Seminars

Posters presented-5

Awards and honors

1. Awarded 1st Prize for poster presentation entitled "Engineering novel pfLDH inhibitors for falciparum species" in Medicinal chemistry at the 61st Indian Pharmaceutical Congress held at Ahmedabad from December 12th to 13th, 2009.

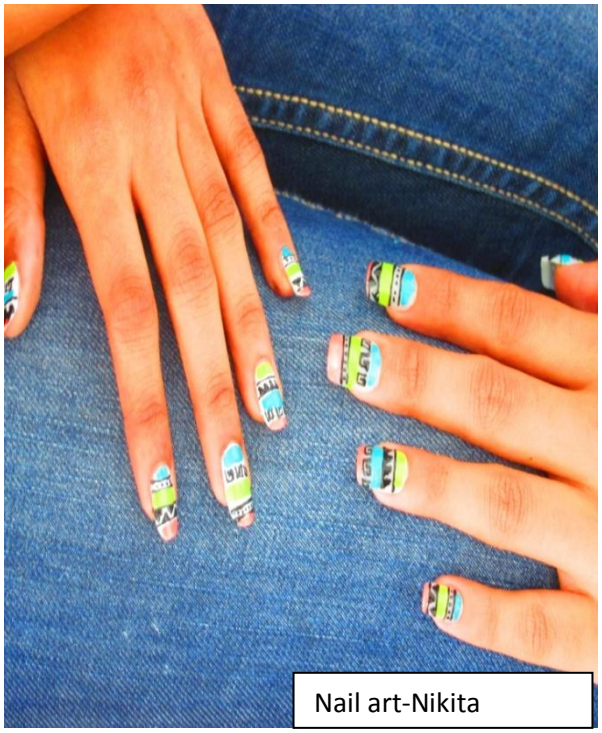
2. Awarded Gold medal for the poster presentation entitled "Design and synthesis of novel inhibitors of pfLDH for plasmodium falciparum" at DIA conference in Mumbai, 2009.

Photo Gallery:

PTA meetting 11-01-14

Sports Day 23-24 Jan

Darshna Kadam-



Nail art-Nikita

Impulse-2014

The Pharma Observer

Annual Day-2013-14

Annual Day-2013-14

Convocation ceremony

Convocation ceremony

Success Secrets Series:

Article by: Mrs. Ojaswi Ghadge

SOFTWARES IN PHARMACEUTICAL RESEARCH

The article is mainly aimed for the readers who have not used computers in their pharmaceutical research and development process and to make them feel inspired by the ideas and to make them to be desired to learn more. The information is easily available on internet, the only thing is researchers should be aware that such aids do exist which will make their research process smoother.

It's a compilation of information on many of the softwares, which are helpful in the wide area of Pharmaceutical research. It is also my hope that the vision of this article will be realized by computers being directly associated with the continued success of the pharmaceutical, biotechnology, and associated industries, to ultimately speed the delivery of therapeutics to the waiting patients.

In less than a generation we have seen the impressive impact of computer science on many fields, which has changed not only the ways in which we communicate in business but also the processes in industry from product manufacturing to sales and marketing. Computing has had a wide influence by implementation of predictions based on statistics, mathematics, and risk assessment algorithms. These predictions or simulations represent a way to rapidly make

decisions, prototype, innovate, and, importantly, learn quickly from failure. The computer is really just a facilitator using software and a user interface to lower the threshold of entry for individuals to benefit from complex fields such as mathematics, statistics, physics, biology, chemistry, and engineering. Without necessarily having to be an expert in these fields the user can take advantage of the software for the desired goal whether in the simulation of a process or for visualization and interpretation of results from analytical hardware.

Within the pharmaceutical industry we have progressed from the point where computers in the laboratory were rarely present or used beyond spread-sheet calculations. Now computers are ubiquitous in pharmaceutical research and development laboratories, and nearly everyone has at least one used in some way to aid in his or her role. It should come as no surprise that the development of hardware and software over the last 30 years has expanded the scope of computer use to virtually all stages of pharmaceutical research and development (data analysis, data capture, monitoring and decision making, Computers as Data Analysis and Data Management Tools in Preclinical Development, Statistical Modeling in Pharmaceutical Research and Development, Chemoinformatics Techniques for Processing ChemicalStructure Databases, Electronic Laboratory Notebooks, Protein Crystallograph, Computer Algorithms for Selecting Molecule Libraries for Synthesis, Computer Methods for Predicting Drug Metabolism orAnalyzing Adverse Drug Events).

There are many excellent books, papers published that are focused on in-depth discussions of computer-aided drug design, bioinformatics, or other related individual topics.

General Programming Tools

Accelrys provides high-quality scientific information products and services to the fine-chemical, pharmaceutical, agrochemical, biotechnology and academic research community.

- Accord for Microsoft Access is a chemical database, relational, multi-user and fast.
- Accord for Microsoft Excel, Synopsys' bestselling chemical spreadsheet, is used by thousands of chemists world-wide to transform raw chemical data into meaningful information.
- With the Accord VBX, developers can rapidly integrate Accord's chemical capabilities into their own Visual Basic applications.
- With the Accord Software Development Kit (SDK), developers can integrate Accords' chemical capabilities into their own applications, such as Notes, Access, Word, Foxpro, Paradox or Omnis 7.
- Accelrys also produces five corporate reaction databases, Solid-Phase Synthesis, Methods in Organic Synthesis, Biocatalysis, Protecting Groups and Bioster.

ChemBuddy (http://www.chembuddy.com) offers a variety of Chemical calculators for labs and education. We offer three chemical calculators, easy to use Windows applications that balance chemical equations, do stoichiometric calculations, convert concentrations and calculate pH.

Calculators help you easily prepare lab reports, solve textbook questions, check results of your homework, prepare solutions, calculate titration results or prepare quizzes and tests for students.

EBAS (Equation Balancing and Stoichiometry calculator) balances reaction equations, calculates stoichiometric masses and number of moles of reagents and finds limiting reagents. All you have to do is to enter substance formulas and their known amounts. Program has a built in concentration and ideal gas calculators to further speed up calculations. EBAS exports balanced reactions as TXT, RTF, HTML, LaTeX and UBBC code making it easy to incorporate equations into papers, on line lectures and lab reports.

CASC (Concentration and Solution Calculator) calculates concentrations and converts between molar, molal, percent w/w and w/v concentrations and molar fractions. These conversions require knowledge of solution density and CASC uses built in database of density tables of over 300 compounds for the highest possible accuracy. You may use it to prepare printable solution recipes and to calculate concentrations of solutions regardless of the way they were prepared by mixing other solutions or by dissolving solids.

BATE (Base Acid Titration and Equilibrium calculator) calculates pH of any solution containing strong or weak acid and/or base with up to four dissociation steps. Built in database contains dissociation constants for many popular acids and bases. Program also calculates acid base titration curves and allows calculation of ionic strength and activity coefficients if necessary. You may compose solutions in several easy ways for example entering concentrations, entering mass of substance and volume of solvent or entering volumes of acid and base solutions mixed.

All programs have easy and intuitive user interface and they were designed for the flexibility and versatility. All possible calculations are done automatically whenever you enter any information which not only speeds up finding answer but also helps twiddling with parameters and solving what-if scenarios. Results of calculations can be always saved and printed for further reference. All built in databases can be modified and extended by user.

IMSL Libraries IMSL supplies two libraries of subroutines for graphics, Mathematics and Statistics. IMSL/IDL is an array oriented interactive command language complete with graphics and a robust set of mathematical, statistical, image processing and signal processing functions which allow visual exploration of numerical data. Exponent Graphics is a library of graphical subroutines that alleviates the task of coding low-level graphics primatives. The IMSL Libraries is an extensive set of 900 Fortran subroutines for applications in general applied mathematics, special functions and for analyzing and presenting statistical data. Libraries are also available for C programming needs. All of the IMSL software runs on a wide variety of platforms.

SolMis (Solubility/Miscibility) is a program available from Tarko Laszlo, Center of Organic Chemistry (CCO) - Bucharest, Romanian Academy. The program solves five solubility/miscibility problems:

- what are the best solvents to dissolve a given compound
- what is miscibility of two given compound
- what are the best solvents to separate two compounds by extraction / precipitation

- what is the best solvent to dissolve a given compound in the presence of a given poor solvent
- what is the solubleness of a given compound within a given good solvent / poor solvent mixture

By an improvement routine the program may "learn" how to solve problems that involve whimsical chemical groups. The SolMis software (a small archive of an installation kit) will be sent only by E-mail.

Spectra Heap is a software product and a spectral lines database for atomic emission analysis created on the basis of the spectral tables issued earlier as separate publications.

Technical Data Analysis and Graphing

Axum Technical data analysis and graphing program for Windows which provides over 80 2D and 3D graphs. Panel plots based on TRELLIS graphics are also supported.

ChemSpread is an SGI-based statistical/spreadsheet program for use in analysing and correlating structural, electronic, and biological data of chemical compounds. Its primary uses are in the fields of drug design and agrochemicals.

CrossGraphs is a new software tool that helps you visualize, understand, and report complex, multidimensional data in analysis databases and data warehouses.

Uniquely architected to present data in arrays of graphs that reveal important trends and relationships, CrossGraphs is the industry's only data visualization product that can automatically divide data into subsets and iteratively create many graphs, one graph per subset, on one or many pages without programming. This unique combination of cross-tabulation and statistical graphics lets you scan graphs along rows, columns, and diagonals to discover relationships in higher-dimensional data and compare patterns across many subsets of the data. CrossGraphs supports over a dozen built-in types of graphs.

CrossGraphs runs on industry-leading platforms including, personal computers with Windows 3.1, Windows for Workgroups 3.11, Windows95, and Windows NT; Sun workstations with SunOS or Solaris; and Hewlett-Packard workstations with HP-UX. The system interfaces to a variety of data sources including dBase, Oracle, text data files, SAS datasets, and ODBC-compliant sources. A Customization Option lets programmers extend CrossGraphs with new graph types and user interfaces designed specifically for their company's unique needs. This option also supports integration with other software, via Windows OLE automation.

Application areas include High Throughput Compound Screening (HTS) and Combinatorial Chemistry.

DataMontage is a Java class library that enables you to display information-dense collections of timelines, time-series graphs, and time-stamped notes within Java applets or applications. You can stack graphs and timelines vertically or arrange them in rows and columns to see patterns

spanning multiple variables. Flexible control over the color, shape, and size of graph and timeline symbols lets you encode multiple attributes and highlight significant data points.

Design-Ease software for design of experiments (DOE) helps experimenters make breakthrough discoveries. Wizards make it easy to set up two-level factorial, general factorial, fractional factorial and Plackett-Burman designs. The program also provides simple one-way designs. A point and shoot interface with progressive toolbar icons leads the user to statistically valid predictive equations. Graphics simplify the analysis at every step.

Design-Expert software for design of experiments (DOE) includes all of the features of Design-Ease plus powerful DOEs for process optimization including three-level factorials, central composite, Box-Behnken and d-optimal designs. The program also offers mixture experiments including simplex, extreme vertices and d-optimal designs; combined mixture/process designs plus screening for up to 24 components. Rotatable 3D response surface maps (RSM) lead experimenters to the peak of performance. Design-Expert then uses sophisticated multiple response optimization routines to find the "sweet spot" that meets all specifications. Design-Expert is one of Stat-Ease's design of experiments (DOE) software packages available.

EasyFit is a distribution fitting software designed to facilitate probability data analysis and best model selection. It allows to easily and quickly selecting the probability distribution which best fits to your data. EasyFit supports over 30 probability distributions, goodness of fit tests, and high-quality graphs. A 30-day free trial is available for download at http://mathwave.com/downloads.html. EasyFit is available from MathWave Technologies.

ECHIP: Software for Design of experiments (DOE). ECHIP software produces 3D diagrams and 2D contour plots. You can view 2D and 3D plots simultaneously. This gives you a more complete understanding of how the plotted control variables affect your response variable. You can rotate a 3D plot to identify any peaks or valleys that might otherwise be obscured. The combination of contour and 3D plots for each response variable which makes it easier to find optimum and robust settings to get the maximum output, And achieve it consistently.

The software handles the analysis, computing all coefficient values, and checking the lack-of-fit statistic to assess how good your model is. This is where lesser DOE packages fall down. They make you do the analysis separately, expecting you to know what analysis is best for your experiment and how to perform it. If the analysis indicates that you need another experiment, ECHIP lets you augment existing designs. The application gives you a new set of experimental runs to perform, combining the data from the original experiment with the results of the new experimental runs for the analysis.

Version 6.4.1 Release - This CD contains multiple versions of ECHIP so that you can install under Windows 95/98/NT and above (Using ECHIP 6.3.2) and Macintosh 7/8 (ECHIP 6.2.1 for Macintosh)

Version 7.2 Pre-Release - This newest version of ECHIP is now shipping. Windows 95/98/NT and above and Macintosh 7/8.

Fortner Visualization Suite is a collection of three tools which can be used to analyze and manipulate sophisticated plots, images, and 3D renderings of data. The components are Plot - a plotting tool that is optimized for huge datasets, Transform - for analysis of matrix and image data, and Slicer - a volumetric visualization tool.

LeoAnalyst is an application for most common statistical analysis of data with intuitive friendly user interface. Distribution, approximation, signal revealing, 3D presentation function of two arguments, near neighbor method. Platform - all windows OC beginning Win95.

LeoCalculator is an application for performing calculation of mathematical expressions that could include not only basic operations but also functions and brackets. http://www.leokrut.com/LeoCalculator.zip
Platform - all windows OC beginning Win95. http://www.leokrut.com

Mathcad is a live worksheet-based program which performs numerical and symbolic calculations, graphs, annotates, etc. The program is available for Windows and MacOS.

Mathematica is a technical computing system that seamlessly integrates a numeric and symbolic computational engine, graphics system, programming language, documentation system, and advanced connectivity to other applications."

MINITAB is a general statistical analysis package for Macintosh, Windows and PC platforms. The program provides:

- basic statistics
- regression analysis
- multivariate analysis
- nonparametrics
- experiment design
- exploratory data analysis
- time series
- statistical process control
- spreadsheet-like data editor
- presentation quality graphics

MultiSimplex is new Windows-based chemometric software for experimental design and optimization. The optimization is based on practical trials that are performed step-by-step. The computation algorithms in the software are the simplex methods and fuzzy set membership functions.

MultiSimplex can simultaneously handle up to 15 control variables and up to 15 response variables with different, and conflicting, optimization objectives. Algorithms, objectives, etc. can be changed "on the fly", On-line help and manual, Extensive database and graphical display of results. It is designed for Microsoft Windows NT and Windows 95. Also it is Microsoft Office

97 Compatible. It requires Microsoft Excel. Supported platforms: 486 or Pentium PC's and Windows 3.1/3.11, Windows 95 or Windows NT 3.51/4.0.

Origin is a technical graphics and data analysis program for Windows 3.1 and Windows 95. Functions available include full analysis (regression, FFT, baseline and peak analysis), nonlinear curve fitting, presentation, etc.

Pestode is comprised of two freeware programs to estimate parameters in ODEs by quasilinearization. A library of ODE models is used in one program. Users can submit their own models to be added. An option to use a "stiff" integration method is available. Eleven examples illustrate use of PESTODE. A second program for estimation of rate constants in networks of first order Rxns with three examples is included.

PractiCalc - A brand new CALCULATOR for your PC. More powerful than your usual calculator - more user-friendly than a spreadsheet. PractiCalc provides both conventional and unique calculator operation and facilities. PractiCalc processes your calculations, equations and expressions giving the result as you type. PractiCalc's extensive built-in functions and user-defined formula combine to allow flexible and extendible mathematical expressions. Practicalc offers a comprehensive range of conversion operators and a special conversion screen. PractiCalc is the prime choice for anyone who uses a computer - from professional scientists, engineers to financial information processors including computer scientists, educators, students and the layperson. PractiCalc runs in all Windows environments, 95 thru XP.

PrestoPlot (Version 1.16) is a freely available, windows-based 2D plotting tool. Among the many improvements and bug fixes are:

- Vector plots.
- Plot arbitrary 1D functions (including cartesian, polar and parametric plots).
- Perform interactive non-linear curve fitting of 1D data sets with an arbitrary number of fit parameters.
- Move and resize graphs using the mouse.
- Zoom and scroll graphs using the wheel mouse and middle mouse button.

PlotData is a software package consisting of a plotter with data analysis capability. Data can be plotted on the screen, viewed, edited, analyzed, differentiated, integrated, calculated and reproduced graphically. Many sets of data can be overlapped to solve systems of equations graphically. The three versions of PlotD11A.ZIP are available.

ProWorks is the provider of top quality data visualization solutions. Since 1986 ProWorks has been the affordable, timesaving graphics choice for developers, financial institutions, business and scientific applications. Our award-winning Flipper series is used by developers and software professionals in major industries throughout the world. Continually expanded and updated, the Flipper components provide a cost-efficient solution for adding virtually any type of scientific or business charts to Windows applications and web pages. Flipper is backed by on-going, high quality technical support. Supported OS include WinNT 3.x, WinNT 4.x, Win XP, Windows 2000.

Qmol is a program for viewing molecular structures and animating molecular trajectories. Originally based on the molview demo program by Mark Kilgard (from his book, Programming OpenGL for the X Window System) and inspired by the Xmol program. Qmol is similar to programs like VMD , MolMol , weblab, Swiss-Pdb Viewer, MolScript, RasMol, gOpenMol and ICM, but opts for a fast, easy to use user interface with a set of features focused on the display of proteins and small molecules. It supports the following (on the Windows platform - features under *uix are unfortunately rather limited):

- Display wire frame, stick figure, ball and stick, point, space-filling, solid and flat ribbon, trace and tube molecular structures from a PDB file.
- Display of multiple molecular models (as used in NMR).
- Animate molecular trajectories stored in a DCD (i.e. CHARMm/Xplor binary trajectory) file in either big- or little-endian formats.
- Kabsch rotate all structures in a trajectory against the initial structure.
- Interactively measure bond lengths, bond angles and torsion angles.
- Dynamically adjust user selected torsion angles.
- Display atom labels.
- Display coordinate axis.
- Dynamic modification of the color scheme (including color-by-element, color-by-atom-number, color-by-residue-number, color-by-temperature and color-by-occupancy).
- Dynamic lighting.
- Adjust atomic radii (including radii-by-temperature and radii-by-occupancy).
- Print to any Windows supported printer and copy images to the Windows clip board.
- Generate AVI movies from a molecular trajectory.
- Assign secondary structure via the STRIDE program.
- Stereo view.
- Directly query the Protein Data Bank and display the resulting structure.
- Detect and display hydrogen bonds (using the energetic criterion of Kabsch and Sander).
- Use the wheel mouse to zoom in and out.
- NEW: User defined clipping plane with rendered sphere/plane intersections.

- NEW: Paste temperature and occupancy PDB fields from the windows clipboard.

SciPredict is a free program with optional models (after a 10 day trial period) that can be purchased at $150 each. The program models are based on the training of a Bayesian Regularized Neural Network. Preditions can be made individually by inputting SMILES strings or by processing files of SMILES strings or SD files. SciMetrics offers chemical prediction models for Vapor Pressure, Henry's Law, LogP, Water Solubility as well as the toxicity of chemicals to Tetrahymena Pyriformis and Fathead Minnow.

The Sigma Suite of programs provide data analysis, equation development and graphing. The programs include:

- **SigmaPlot:** A library of 2D and 3D graph types, mathematical transforms and summary statistics. Automatically fits and plots polynomial regressions up to 10th order and 95% or 99% confidence and prediction levels.
- **SigmaStat, TableCurve, PeakFit:** Advanced data fitting and analysis programs. Can be used to separate and fit up to 100 overlapping, difficult to resolve peaks on spectroscopy, chromatography and electrophoresis data.
- **SigmaScan, SigmaScan Pro and SigmaGel:** Image measurement and analysis software for digital images.

SigmaXL is a leading provider of user-friendly Excel add-in tools for statistical and graphical analysis. Our flagship product, SigmaXL, was designed from the ground up to be cost-effective, powerful, and easy to use. Features include:

- Measurement Systems Analysis with confidence intervals
- Multiple Linear Regression that accepts both continuous and categorical predictors
- Capability Combination Report
- Weibull Analysis
- Control Chart Tools
    - Add Data to existing control chart
    - Split limits by historical group
    - Scroll through chart data
    - Easy to read summary of test violations
- **Stat-Ease:** Design-Expert software is an experimental design program available from http://www.statease.com/
- **STATISTICA:** Complete Windows and Macintosh based data analysis and graphing programs with thousands of on-screen customizable, presentation-quality graphs fully integrated with all procedures.

- **StatView** is a statistical analysis package which runs on both Macintosh and Windows platforms. Statview provides a variety of statistical analyses and the ability to create high quality presentation graphics. Links between data and results are interactive so that changes to the data are immediately reflected in the models.
- **SYSTAT** is a dynamic data explorer for Windows. Features for data management, interactive, exploratory data analysis, comprehensive statistics, and high quality graphics.

SymbMath is a computer algebra system that can perform exact numeric, symbolic and graphic computation.

Visual Math for Java: is a Java applet to serve as graphic calculator, equation solver, plotter of functions, derivatives and integrals.

Spartan: Spartan is a powerful tool for computer aided drug design. The easy-to-use interface delivers a new suite of molecular modelling features as well as quantum calculation tools for chemists working in drug discovery. Pharmaceutical scientists can perform conformational analysis and can quantify 3D molecular similarity based on structure, chemical function, and pharmacophore models. Many of the leading Pharmaceutical companies are already using Wave function software to fast-track development of new drugs.

Key Benefits of Spartan

Ease of Use

Spartan offers construction, manipulation, and analysis (both computational and statistical) from a single, user friendly interface. The end result is that Spartan is easier to master, without compromising the limitations of its functionality. This maximizes the return on investment for pharma research companies.

Seamless Databases Access

Spartan integrates access to the leading molecular and spectroscopy databases seamlessly from within the graphical interface.

Efficient Molecular Modelling

Spartan includes easy to use 3D builders for Organic, Inorganic, Peptides, and Nucleotides --it offers a new substituent builder for generating virtual libraries, and one can use ChemDraw (directly from within Spartan) to build in 2D and seamlessly convert the 2D molecule to 3D within Spartan.

Conformer Library Generation

A new capability has been added to provide generation of libraries of diverse conformers. This is based on a systematic search of conformation space using MMFF molecular mechanics, followed by a procedure to eliminate conformers that occupy "similar space". Conformer libraries are intended for use in similarity analysis. Conformer libraries corresponding to common drugs (5,000 entries) and to the Maybridge compendium, "Compounds for Drug Discovery Chemistry" (70,000 entries) are provided via the Spartan Molecular Database (SMD).

Similarity Analysis

A new capability has been developed for assessing and quantifying the similarity of one or more "templates" (either molecules or pharmacophores), to one or more "libraries" (including libraries of diverse conformers). Similarity between molecules may either be based on structure or on CFD's, whereas similarity between molecules and pharmacophores is based solely on CFD's. A scoring function based on rms deviations between selected atomic centers or between CFDs (automatically adjusted to account for unfavorable intramolecular interactions) has also been provided.

Reference:

1. http://www.computational-chemistry.co.uk/pharmaceutical-research-software.html
2. http://www.pharmaresearch.in/?page=17e62166fc8586dfa4d1bc0e1742c08b
3. Computer applications in Pharmaceutical Research and Development, Sean Ekins, A JOHN WILEY & SONS, INC., PUBLICATION
