

# Going software in the neural network

Feeling fuzzy about the logic being use on your data? This selection of software offers packages for database development, data acquisition coupled with statistical analysis and systems for scientific imaging.

## ACSL BioMed 3.1

From MGA Software

*Simulate clinical trials with computer-assisted trial design software*

Working closely with several pharmaceutical companies, MGA has incorporated new functionality into its software for simulating clinical drug trials. Pharmacologists can now simulate proposed clinical trials on specific patient populations, such as pediatrics, smokers and the elderly, and gain insight into these designs before initiating the trials. According to MGA, the program can now predict how variations in trial populations, such as having a significant number of elderly persons, will influence the proposed study. Complex populations can be described and incorporated into any number of trial designs using an intuitive, point-and-click user interface. Once a complex population is defined for one trial, it can be used again or modified for future trial designs.

**Reader Enquiry No. 100**

## Topkat 5.0

From Oxford Molecular Group

*Computational toxicology software developed by Health Designs*

This Windows-based program assesses various toxicity metrics based solely on their molecular structures. Because the program can evaluate the specific contribution to a toxicity metric of any user-defined substructural moiety, it can guide a scientist in designing chemical structures having minimal toxicity. By identifying toxic compounds, this technology can also aid in reducing the number of animals used in the toxicity testing of new chemical entities. It features a technology called optimum prediction space (OPS) and integrates a host of algorithms to generate and test the acceptability of predictions and to identify particular molecular substructures for hypothesizing possible molecular sites of toxicity. Topkat is now operating in Windows 3.1 and Windows95 and incorporates an easily-learned interface, extensive on-line help and modules for assessing rodent carcinogenicity, Ames mutagenicity, developmental toxicity potential, rat oral LD<sub>50</sub>, rat oral chronic LOAEL, skin sensitization (GPMT), fathead minnow LC<sub>50</sub>, *daphnia magna* EC<sub>50</sub> and LogP. Additional modules are to be released soon for eye and skin irritancy (rabbit), mouse inhalation LC<sub>50</sub>, rat maximum tolerated dose and aerobic biodegradability.

**Reader Enquiry No. 101**



C<sup>2</sup>Diversity samples potential drug compounds.

## C<sup>2</sup>Diversity

From Molecular Simulations

*A program that analyses chemical diversity, or similarity, for use in the design and evaluation of compound libraries and reagent sets for combinatorial chemistry*

Users can intelligently sample potential drug candidates so that a reduced set can be synthesized and screened. C2 Diversity helps to design libraries for synthesis, both at the start of a combinatorial chemistry experiment, and throughout the various iterations of obtaining and using structure activity relationship data to design new libraries. This program helps to reduce the final number of compounds that need to be synthesized, and allows more rational judgement into the combinatorial chemistry process.

**Reader Enquiry No. 102**

## Imaging

### Scope-Pro

From Media Cybernetics

*Software that automates the movement of microscopes, stages and accessories*

This is the latest module for the ImagePro Plus scientific image analysis program. The module is designed to control complex equipment in a simple, repeatable manner. It reduces the need to look through the ocular during image acquisition and to adjust microscope controls manually. The software also automatically controls magnification, focus, motorized filter wheels, shutters, filter sliders and lamps settings, automating repetitive routines for increased efficiency. It supports brands of microscopes and stages that include Zeiss AxioPlan, Olympus Provis, Ludl MAC 2000, Prior H128 series, Sutter Lambda 10-2 filter wheels and shutters and Vincent Associates' shutters. Repetitive functions can be programmed using the Auto-Pro macro or Visual Basic program. By integrating control of the stage into a macro program, users can incorporate any of Image-

Pro's 200 some analysis and processing routines into a fully automated image capture, analysis and data collection process.

**Reader Enquiry No. 103**

## Snapper development kit

From Active Imaging

*A software development kit for this range of modular image acquisition boards, which is now available for Macintosh system 7.0*

Snapper can acquire images in excess of 25 frames per second, supporting standard or non-standard analog video formats, composite-colour, s-video, RGB and 16-bit digital image acquisition. Triggered acquisition and support for asynchronous reset cameras, such as Pulnix TM-6AS, Hitachi IM-C1, JAI 1550 Progressive Scan, three-chip colour and more, make Snapper well suited for a variety of both industrial and scientific applications. In addition, the digital acquisition module offers specific camera support for an increasing range of cameras, including Pulnix TM9701, Dalsa CL-CX line-scan, Kodak Megaplex 1.4 and Photometrics SenSys. The Mac SDK includes example applications, as well as a Quicktime VDIG, supporting all of the acquisition modules. This allows it to be used immediately with any application supporting Quicktime VDIGs, such as AVID Photoshop, Fusion video recorder, IP Lab Spectrum, and others.

**Reader Enquiry No. 104**

## Image

From Zeiss

*A series of image analysis packages that includes a package written specifically for use with Power Macintosh computers*

This is a full range of counting, measurement, image, image enhancement and image archiving applications. Users can employ grey-scale or colour acquisition, processing and analysis. This package is said to work seamlessly with other Macintosh-based applications, such as Microsoft Excel and Word, and should be well suited for biological and industrial research applications.

**Reader Enquiry No. 105**

## BioBench

From National Instruments

*This is the Virtual Instrumentation Company's software for physiological data acquisition and analysis*

This program is offered as a low-cost turnkey package for Windows95/NT and requires no programming to get users up

and running. It can automatically configure and acquire data from many physiological instruments from a variety of manufacturers, as well as acquire data directly from sensors, via the company's plug-in data acquisition hardware. This system interfaces to instruments through a generic BNC connector. Analysis functions include histogram, fast Fourier transform and peak detection. Users can set alarms to trigger when data reaches certain levels. For example, an application monitoring a laboratory subject can trigger an alarm once blood pressure, temperature or respiration reaches a predetermined point.

**Reader Enquiry No. 106**

### Proc-StatXact

From Cytel

*A new version of StatXact software that comes as a seamless extension of SAS software*

This SAS add-on product allows users of SAS releases 6.11 and 6.12 to perform exact tests on small, sparse or unbalanced data sets with no interruption to processing within the SAS environment. This new capability is said to save time and to ensure greater objectivity and better documentation of analyses. Even more important, the ability to use exact tests automatically rather than chi-square approximations on small or unbalanced safety, efficacy and carcinogenicity tables, should greatly reduce the chance of expensive delays in the review process due to the potential inaccuracy of applying large sample methods to these data sets. Before the release of this package, SAS users who needed to apply the StatXact procedure for computing exact P-values on selected data sets had to delay a SAS production run while they ran the tests using a standalone version. This procedure required users to identify manually suspicious tables from SAS output, enter them into StatXact, run the exact tests and finally insert the results back into their SAS report. This program eliminates these delays and allows users to apply StatXact's high-speed exact and Monte Carlo algorithms to every single table in a large batch run. The Automatic Pilot feature is designed to overcome the risk of hanging up the computer by applying an exact test to a data set that is too large for such processing. It detects data sets that are too large for exact-test processing and automatically switches to Monte Carlo inference.

**Reader Enquiry No. 107**

### Windmill data acquisition

From Windmill

*Three new or improved applications that increase the versatility of this data acquisition and control software suite*

Applications in this suite include Replay, Alarm Logger and Test-Seq. Replay plays

backlogged data files graphically, allowing the user to scroll through data files looking for significant events. Users can fast forward through uneventful stretches and pause for a more detailed look when something catches their eye. Alarm Logger has been improved with user-specified help messages that can now be shown when an alarm occurs and give instructions on the corrective action to take. Auto-dialing alerts engineers to alarms by telephone, and users can insist on a delay before being alerted to an alarm. This can be useful when monitoring temperatures in a refrigerator where briefly opening and closing a door should not trigger an alarm. There is also password protection to prevent unauthorized users from acknowledging alarms. Test-Seq is a program that interprets an ASCII file of commands and controls measurement and control equipment appropriately. It allows a digital pulse to be output for a specified time period. Other commands let users ramp the values sent to an output channel, monitor and act on alarms, implement control loops, send sequences of keystrokes to other applications, and so on.

**Reader Enquiry No. 108**

### Life Science Workbench

From MDL

*This package that comprises Screen and Isis for Excel, providing comprehensive informatics solutions for high-throughput discovery and other aspects of research*

Workbench contains flexible and efficient tools for developing, registering and searching methodology information and for capturing, analysing and registering results. The Screen component is designed to accommodate the variety of sample sources available to high-throughput screening laboratories. It manages plate inventory in a hierarchy of storage plates, master plates, daughter plates and assay plates. Users may select any plate format, map samples from each type of plate to the next and transfer the sample to plates with different formats, maintaining a complete audit trail. There is also the ability to track the age and volume of samples in plates, print reports and the uploading of compound, sample or plate information using Screen's flexible file import system.

**Reader Enquiry No. 109**

### Statistica Connectivity kit

From StatSoft

*A program that links data acquisition and analysis in a Windows environment*

This system is designed to bring statistics and analytical graphics together with external sources of data, such as real-time data acquisition and monitoring systems, measurement devices, data collectors or laboratory equipment. The kit can read data via serial ports or from PC-bus-compatible interface cards,

such as the universal, high-performance Rockwell/Datamyte InterGage card. The kit also includes options to facilitate connecting Statistica to specialized databases that store the relevant information. This integrated system should find use in a variety of environments from simple workstations or small production facilities to large enterprise-wide computing environments. Simple set-up dialogues help with configuration, beginning with how to specify the hardware settings for the source of data and the variables to be used to receive the stream of raw data. Data files that have been configured to receive data from a database or measurement device and can be updated with a single click or keystroke (when data are not imported but received in run time, options are provided to update data continuously or only when requested, to append data or replace them). These updated data files can then be analysed interactively using any part of Statistica or previously created custom scripts.

**Reader Enquiry No. 110** □

*These notes are compiled by Brendan Horton from information provided by the manufacturers. For more details, fill in the reader service card bound inside the journal.*

#### ADVERTISEMENTS

#### Coming Soon!

SeqWeb™, the new web interface to the popular Wisconsin Package for sequence analysis, is coming in April 1998.

<http://www.gcg.com/seqweb.html>



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