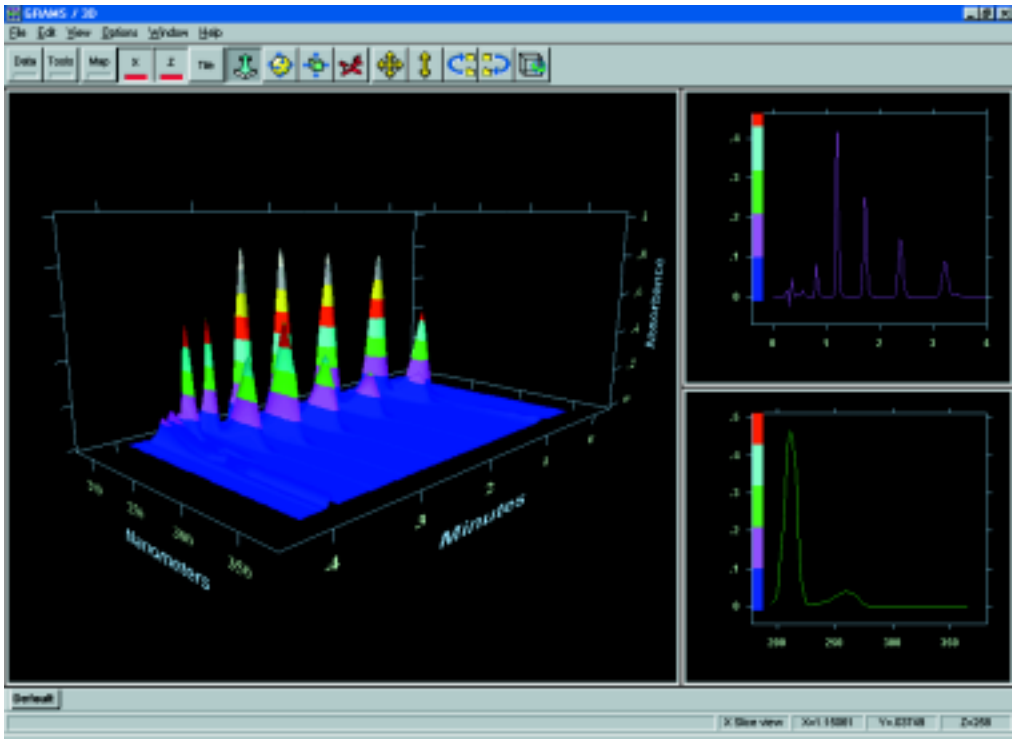
Thermo Galactic Product Catalog

Spectroscopy Software Solutions

GRAMS/3D provides high quality 3D graphics with performance previously only attainable on expensive workstations. GRAMS/3D is a GRAMS/32 add-on that places real-time, interactive 3D graphic visualization on the extensive list of capabilities already included in the Galactic product line. Now you can manipulate large 3D data sets in real-time on your PC and see the unseen information hidden in multidimensional data.

Real-time Data Rotation

Unlike simple 3D plotting and rendering packages, GRAMS/3D is true real-time interactive visualization software. Using a fast and intelligent 3D graphics engine, GRAMS/3D makes it possible to view large three dimensional data sets from any angle in real-time. GRAMS/3D's zoom capabilities allow you to examine even the smallest features of your data. GRAMS/3D updates the display many times per second, even as you zoom and rotate the data.



■ *GRAMS/3D makes it possible for you to see your data in a whole new dimension. Users can "slice" data in different dimensions to extract individual features.*

■ *Zoom capabilities allow you to view data from any angle and examine even the smallest features in real-time.*

True 3D Rendering

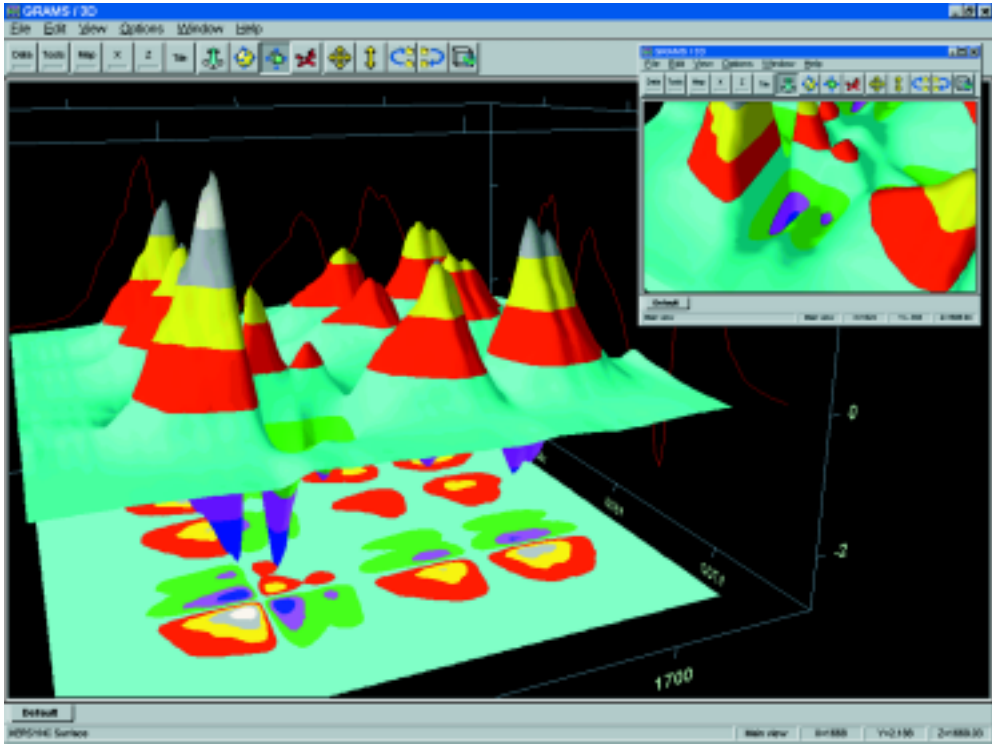
The display speed of GRAMS/3D

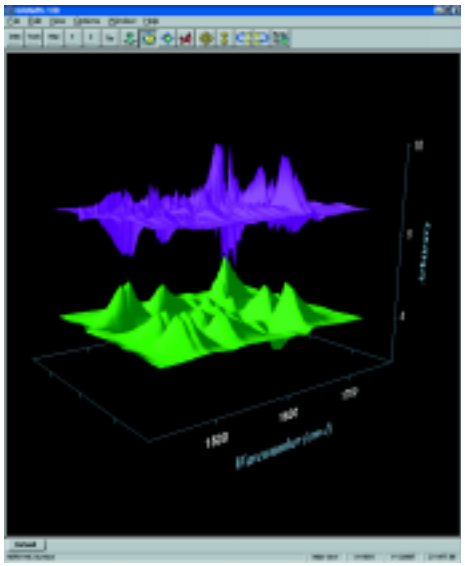
makes it practical to utilize a full range of interactive "camera" movements and perspectives. It provides a camera eye view as you rotate and zoom around your data. GRAMS/3D offers full control over camera angle and position, movement sensitivity, and perspective distance. Intuitive navigation of the camera with a mouse makes this comprehensive visualization package easy to use.

Workstation Power and Speed

GRAMS/3D brings the power of a workstation to the Windows desktop.

It is the only PC-based product that can work with large, irregularly shaped data sets. GRAMS/3D quickly and easily animates data sets with millions of data points in real-time. It is the fastest PC-based 3D data visualization package available.





■ *Simultaneously compare multiple data sets and enhance data features with shading and lighting effects to expose hidden valleys and peaks.*

See Unseen Information

Using a variety of tools and options, GRAMS/3D can help you see the unseen information hidden in multidimensional data. You can display data in several graphical formats such as wire frame, solid, or contour. An assortment of colors as well as banded and gradient color fills allow you to emphasize the subtle differences or similarities in your data. You can enhance data features with shading and lighting effects to provide the best definition of data and to expose hidden valleys and peaks.

GRAMS/3D includes a Gallery of pre-designed popular views, allowing quick selection of the best way to display your data. You can create your own views and add them to the Gallery to use with other data files.

Compare Multiple Data Sets

GRAMS/3D is ideal for examining data from a variety of instrumentation including GC-IR, HPLC-DAS, multidimensional spectroscopy, 2D-NMR, 2D-IR, or spectroscopic mapping experiments. You can compare multifile experiments, such as spectral kinetics, and quickly see the differences or similarities. Multiple data sets can be simultaneously compared.

GRAMS/3D makes it possible for you to see your data in a whole new dimension. Bring the power of a graphics workstation to your laboratory with GRAMS/3D and see the information you've been missing in your data.

Spectral ID®

■ *Spectral ID optionally integrates with CambridgeSoft's powerful structure editing tools.* ■ *Accurately remove a library spectrum from a mixture with the Auto-Subtract feature.* ■ *Spectral ID also incorporates powerful Mass Spec searching features.*

Spectral ID is the most comprehensive spectral search software available. It is easy-to-use, fast, and compatible with most commercial libraries. Spectral ID is capable of creating and searching libraries for many analytical techniques such as MS, IR, Raman, UV-VIS, Fluorescence, NIR, and other data types. Fast and accurate spectral matching is almost effortless with Spectral ID.

Unmatched Compatibility

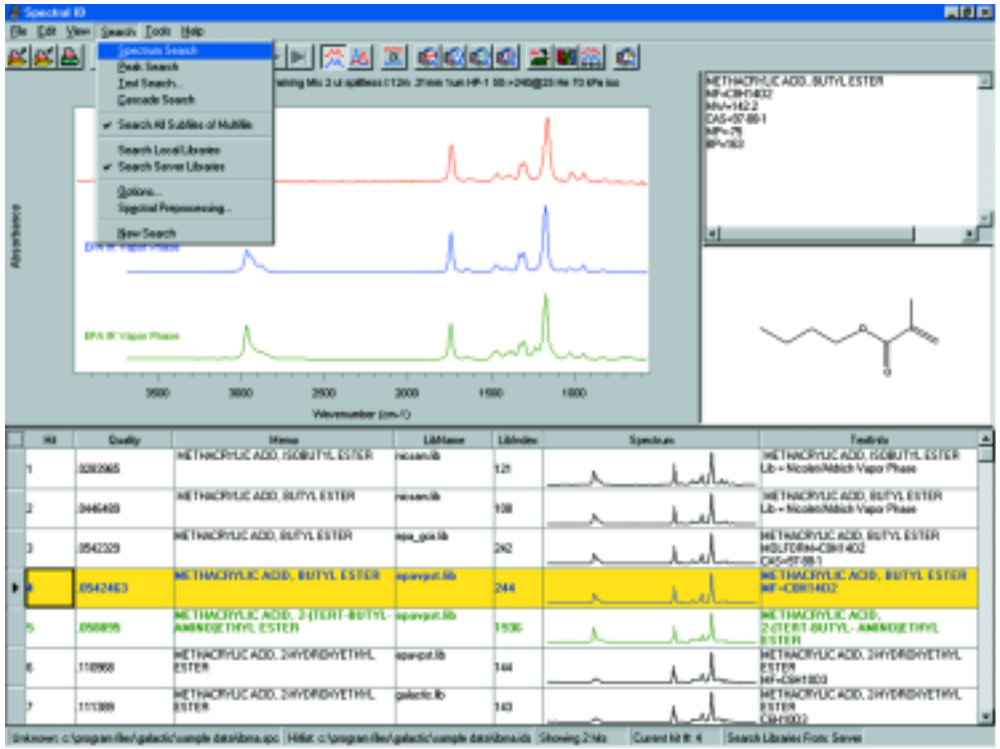
There is no spectral search product on the market that is compatible with more commercial libraries than Spectral ID. Over 750,000 spectra can be searched in the hundreds of commercial collections from Aldrich, Bio-Rad Sadtler, Chemical Concepts, Nicolet-Aldrich, NIST, Wiley, and other vendors. Spectral ID also supports structure display and optional structure editing. A molecule window in the search form allows molecular structures to be displayed for library hits.

Not only is it compatible with more libraries, Spectral ID can also read nearly any instrument data file format. Using Galactic's unique SmartConvert™ technology, Spectral ID can load spectra from hundreds of different file formats. There's no need for clumsy exporting of data files from your instrument software. Simply open the file from the menu, or drag-and-drop it on the Spectral ID window, and it is automatically translated and loaded. Spectral ID also includes automatic links for easy integration with both GRAMS/32 and Agilent/HP Chemstation software.

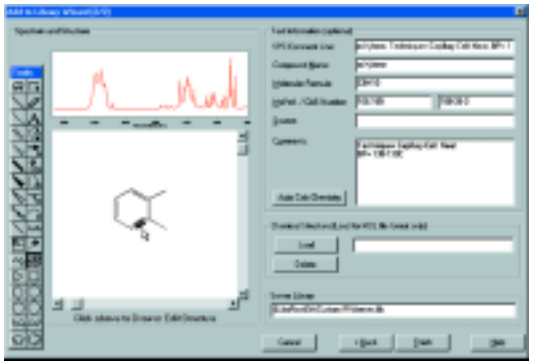
For users who want to create their own libraries, Spectral ID can easily add spectra directly into the library. You can add spectra by selecting individual files, a whole directory, or an entire list of files.

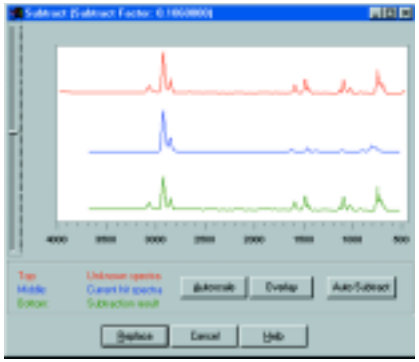
Ease of Use

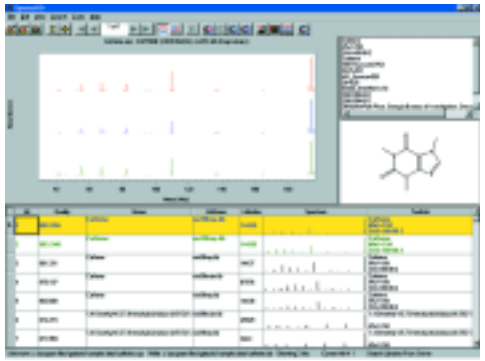
Spectral ID provides 6,000 spectra out of the box. It automatically searches your hard disk for existing libraries and gives you instant access to them. When a new spectrum is opened, Spectral ID selects only the appropriate spectral libraries for searching. Spectral ID's QuickAdd feature lets you add new spectra to your libraries with a single mouse click.



■ *Spectral ID's multi-paned window interface allows simultaneous viewing of unknown and library spectra, search hit quality lists, structures, and chemical and physical property information.*







Network Enabled

While Spectral ID is a powerful desktop spectral searching application, its real power comes from the ability to efficiently share spectral libraries over a network. Installing the optional Spectral ID Server software on a networked computer running Windows NT Workstation or Windows NT Server provides each networked Spectral ID user instant access to all your commercial* and user-created libraries. When your spectral libraries are installed on a Windows NT computer, the tasks of tracking, updating, and configuring your search data are all managed from a single location. Rights and restrictions can be granted for creating, editing, and searching server-based libraries.

Spectral ID Server uses a true Client/Server architecture providing fast searches even over slow networks or dial-up connections. Spectral ID Server performs all the calculations on the Windows NT computer, so only the unknown spectrum and hit list results travel across the network connection. With Spectral ID Server, spectral library searching can become a company-wide activity rather than a specialty.

Versatility

Spectral ID provides a large variety of proven and powerful search algorithms and pre-filter operations for both optical and Mass Spectrometry data. These include both full spectrum and peak matching algorithms for optical spectroscopy, as well as the ability to selectively exclude multiple regions.

Unlike other search packages, region selection and data preprocessing in Spectral ID have no impact on performance; it is always *FAST*. In addition to a variety of other calculation options, an automatic subtraction feature allows you to quickly remove the spectrum of a match from the spectrum of a mixture sample, then optionally search the remainder.

Powerful text searching capabilities allow you to query libraries based on key words, compound names, CAS numbers and other information. Text search operators allow AND/OR operations. Text searching can be performed across all library types (e.g. IR and MS) so you can retrieve all the spectra available for a given compound. Advanced search capabilities even let you combine Text, Peak, and Full Spectrum searches to selectively refine your searches.

Speed

Galactic has developed a reputation for high performance software and it continues with Spectral ID. Spectral ID can search tens of thousands of spectra in just a few seconds, eliminating the need to break searches into smaller sets to gain acceptable performance. Spectral ID Server offers the same performance in a networked environment. By investing in a Windows NT computer to support your spectral libraries, all networked users can take advantage of the speed provided by one fast CPU. For example, a typical server class machine is capable of searching over 80,000 IR spectra in under 4 seconds! Spectral ID and Spectral ID Server offer optimum speed and accurate results. Spectral searching has never been easier!

** Licensing policies for commercial libraries are set by each library vendor. Contact Galactic for specific information.*

PLSplus/IQ™

■ *A spectral region editor provides easy click-and-drag region selection to help remove undesirable variations.* ■ *An interactive 3D scatter plot viewer is useful for examining sample scores.* ■ *Easily customize prediction reports.*

PLSplus/IQ includes powerful multivariate analysis tools for building quantitative calibrations as well as qualitative models for discriminant analysis. This powerful software links qualitative and quantitative methods to provide a complete spectroscopic model of your samples. PLSplus/IQ also includes calibration transfer capabilities that allow calibrations to be moved from instrument to instrument. It is *the* complete solution for analysts looking to apply chemometric calibrations in the laboratory and on the production line.

Creating a Training Set

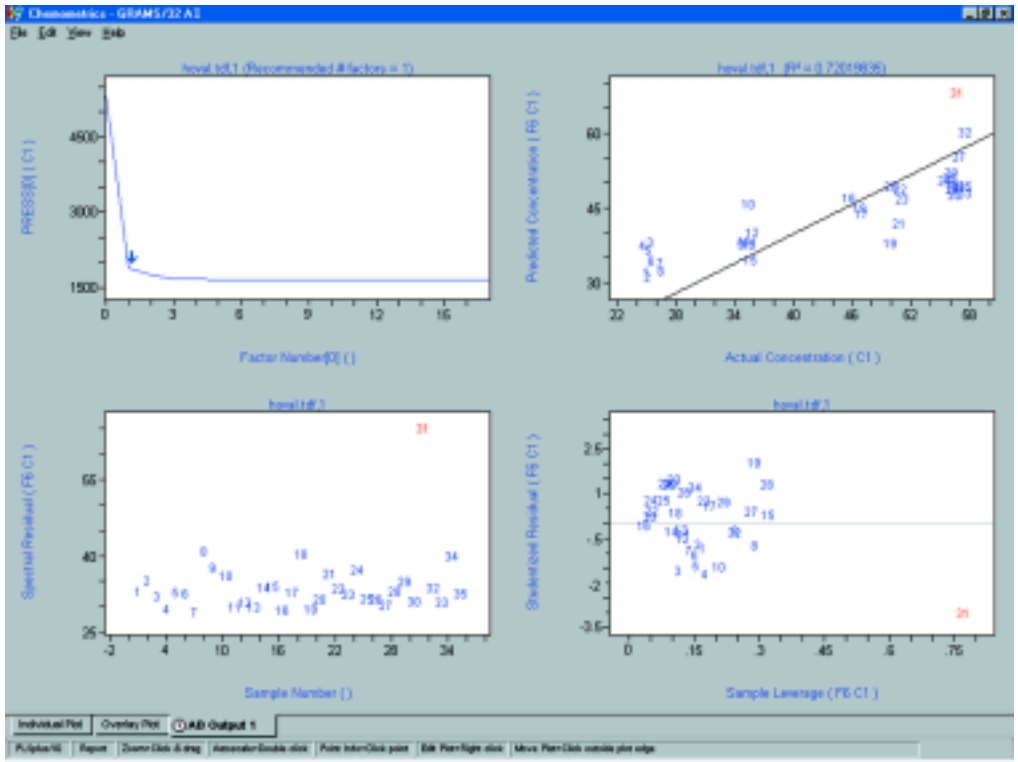
Creating, editing, and storing training set data are all accomplished with the PLSplus/IQ Training Set Editor. This easy-to-use editor works like a spreadsheet and can accept data from typed input as well as the Windows Clipboard. Users can import files from previous versions of PLSplus and Discriminate as well as data sets with constituent information from other vendor formats.

Setting Up Experiments

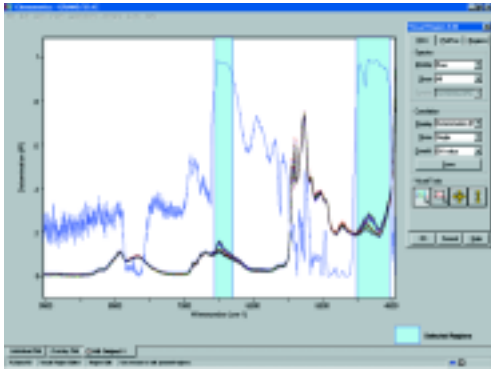
PLSplus/IQ's unique Experiment Manager organizes all your calculated data with a copy of your original raw calibration data (spectra and constituents). The Experiment Manager also keeps a running history of all attempted calibration models and can easily clone your experiments to try multiple variations of similar conditions.

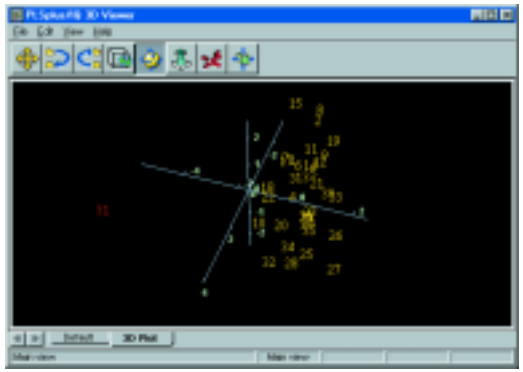
The Experiment Manager includes the most popular multivariate algorithms (PLS-1, PLS-2 and PCR) as well as qualitative methods, including PCA, for performing simple data exploration and visualization. Galactic's PCA/MDR discriminant analysis algorithm is also included for constructing complete models of spectra without any constituent information.

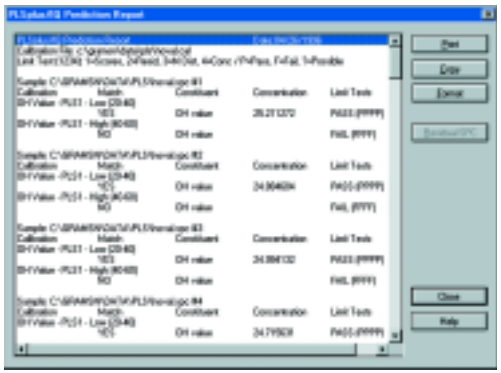
Advanced diagnostics such as Self Prediction, Leverage Validation, and Cross Validation will help you to determine the correct calibration model. Sample rotations can be set for



■ *The Report Viewer displays multiple plots simultaneously from one or more experiments. Users can mark outliers directly on the plots and save a new experiment with the marked outliers removed.*







one or more samples at a time using different ordering options to give the best distribution during cross validation. Individual samples and constituents can be marked as outliers to create better calibrations after pilot experiments have been run and analyzed. In addition, the highly optimized code insures that the calculations are fast.

PLSplus/IQ also includes a variety of popular data preprocessing methods that are automatically applied during both calibration and sample prediction.

Viewing Experiment Results

With the PLSplus/IQ Report Viewer you can view and plot all calculated data and a variety of diagnostic indicators that are stored in PLSplus/IQ training data file experiments. This powerful feature assists in optimizing the calibration model, determining if there are any outliers in the training set, evaluating model performance, and determining the number of factors to use in the final calibration file.

With the custom report generator you can preview and print all calculated data or copy it to the clipboard for use in spreadsheets or word processors. After determining optimum conditions, you can save your final calibrations. Multiple calibrations can be saved in the same file, even from different training sets.

Predicting Samples

The PLSplus/IQ Prediction Setup allows you to specify how a spectrum is analyzed and how to output the results each time you execute a prediction. Users can predict samples against multiple calibrations to compare calibration accuracy and performance.

Qualitative tests can be performed using quantitative models as if the calibrations were designed for that purpose. Using Discriminant Analysis as a prefilter before applying the quantitative calculations allows PLSplus/IQ to select the calibration that best matches the sample spectrum. In addition, outlier samples can be quickly and easily determined during sample prediction, giving you the utmost assurance of the results.

You can customize the prediction report to include constituent quantities, Mahalanobis Distance, Model Limits Tests, and spectral residual. Users can organize the report by constituent, calibration, or sample and print, copy, or save the report to an ASCII file.

Each copy of PLSplus/IQ includes three additional licenses for distribution of your calibration model to other GRAMS/32 computer systems. In addition, many instrument systems can use the calibrations directly.

Transferring Calibrations

PLSplus/IQ includes a tool to allow calibrations to be transferred to other instruments and/or sample devices with minimal re-measurement (typically a single spectrum). PLSplus/IQ includes Galactic's SECT method (*Spectroscopic Effect Correction Transfer*) which adjusts for wavelength or frequency shifting between instruments.

GRAMS/32 AI

GRAMS/32 AI Version 6 is a comprehensive data processing and data management software package. Its advanced processing and ability to handle all types of spectral and chromatographic data from virtually any analytical instrument set the industry standard in scientific software. The AI version introduces many improvements including an enhanced user interface and a collection of updated processing routines based on Microsoft's Active X technology. These ActiveApps™ are more robust and powerful than their predecessors, allowing faster processing and providing more reliable results.

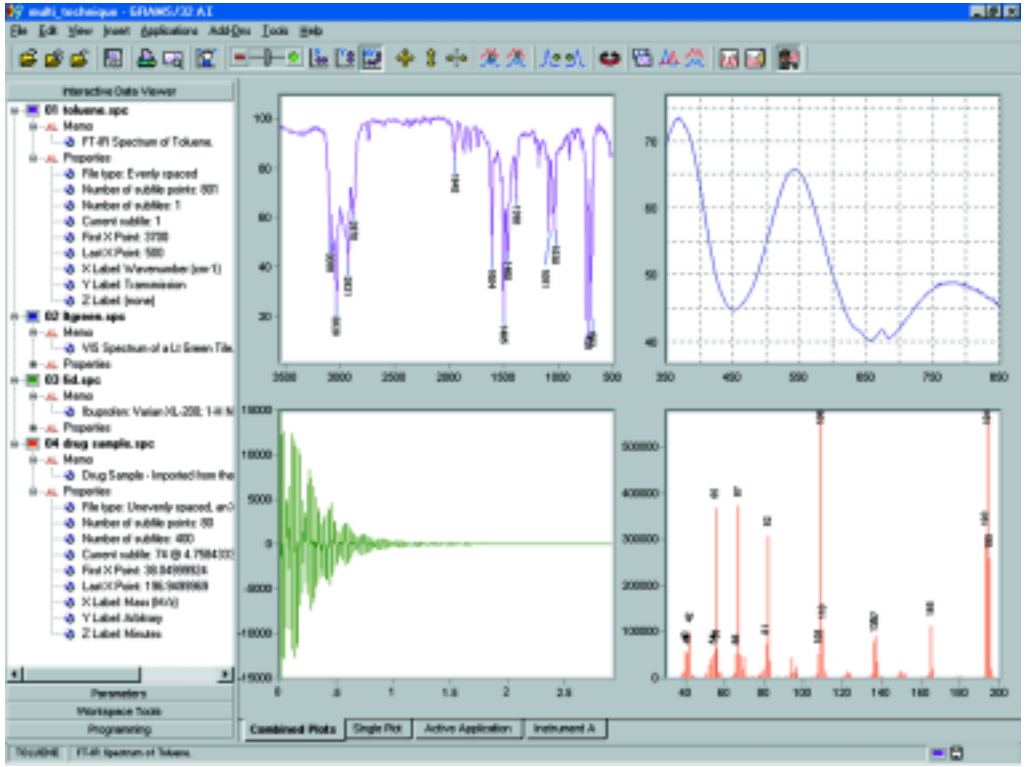
As always, GRAMS/32 utilizes the universal Galactic SPC file format, allowing you to integrate your entire laboratory, easily share data with colleagues, and process analytical data at your desk, freeing up valuable instrument workstations.

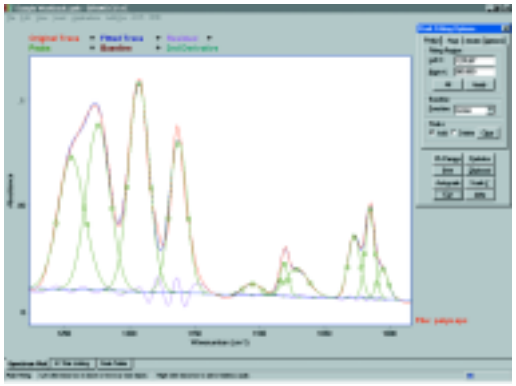
Work with all Data Formats

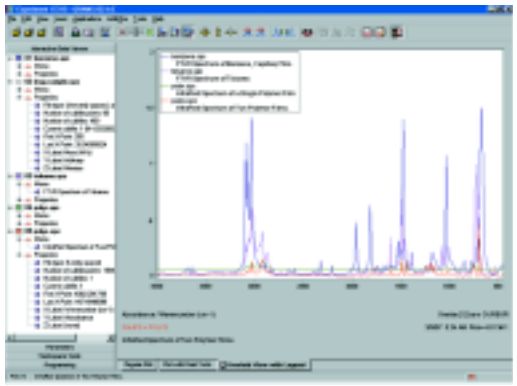
GRAMS/32 is the only software package capable of reading hundreds of analytical instrument and industry standard file formats. With Galactic's SmartConvert™ technology, GRAMS/32 automatically identifies a data file's format, converts it, and opens it for processing or viewing. In addition to supporting data files from most analytical instruments including Agilent/HP, Beckman, Bio-Rad, Bomem, Bruker, Finnigan, Gilson, Hitachi, MicroMass, Nicolet, PerkinElmer, Shimadzu, Varian, Waters, and many others, GRAMS/32 also handles general purpose data formats such as ASCII, JCAMP, and AIA/ANDI. The Galactic *My Instrument*™ standard allows GRAMS/32 to control and collect data from a growing list of analytical instrumentation. For more information see *Data Acquisition: My Instrument*.

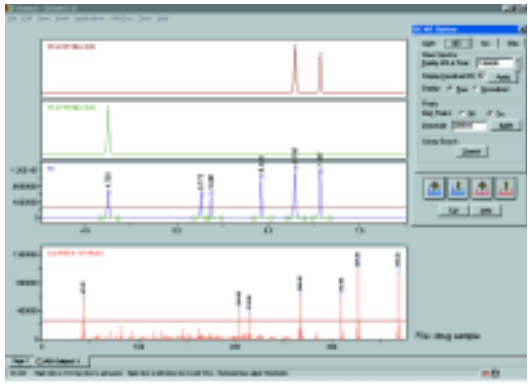
Intuitive, User-Friendly Interface

The GRAMS Assistant offers a user-friendly interface with features that benefit new and experienced users. This easy-to-use interface allows you to quickly navigate through open data files, expose important file information, access parameter settings, and customize your workspace, all with a click of the mouse.









Workspace Customization

With GRAMS/32 you can create a customized environment for reporting, viewing, and processing your data. Multi-page workbooks store your specific data display preferences. Workbook pages or even an entire workbook can be automated to perform specific functions or process data. The Toolbar Builder makes it easy to add buttons for one-click access to frequently used applications or display modes.

Powerful Data Processing

Fast and flexible data processing on both single and multi-dimensional data files puts GRAMS/32 at the forefront of spectroscopy software. An extensive library of applications allows you to perform calculations on virtually any data type. From simple data smoothing and mathematical operations to advanced peak fitting and self-deconvolution, GRAMS/32 helps you to obtain results with confidence.

Technique Specific Processing

In addition to general purpose processing routines, GRAMS/32 provides technique specific applications for a variety of instrumental techniques. Each copy of GRAMS/32 ships with your choice of one of the following Application Packs. Additional applications may be purchased separately.

IR/Raman Application Pack: Contains applications to calculate ATR pathlength correction, interferogram compute, Kramers-Kronig transform, standard Raman shift, and a Diode Array/CCD calibration technique.

UV/VIS/NIR Application Pack: Performs popular colorimetric analyses such as L*A*B and L*U*V using all standard CIE illuminants. It also includes multiplicative scatter correction, standard normal variate, and de-trending transforms.

NMR Application Pack: Allows you to graphically manipulate or automatically process 1D NMR data in both time and frequency domains. A one-step processing routine allows you to FFT, phase, integrate, and pick peaks.

Chromatography Application Pack: Provides a graphical drag-and-drop environment that allows you to easily build analysis methods. Peak picking and identification, model calibration, and quantitation can be done with just a few mouse clicks.

GC-MS Application Pack: Allows you to display and analyze data from GC-MS experiments. A variety of tools for single ion chromatogram calculation, automatic peak identification, visual parameter adjustment, and peak analysis are also provided.

Visual Programming

The GRAMS/32 Macro Wizard allows you to create custom processing routines to accommodate specific experimental needs. With the Macro Wizard you can automate a series of processing routines with no formal programming. Array Basic™, Galactic's powerful programming language, allows advanced users to customize GRAMS/32 to solve virtually any analytical problem.

Links with Other Galactic Products

GRAMS/32 easily integrates with PLSplus/IQ and can share data with other Galactic applications, such as Spectral ID, Spectral DB, and GRAMS/3D.

Spectral DB™

■ *Spectral DB's grid view allows quick browsing through your data.* ■ *Spectral DB can be launched directly from GRAMS/32 where it will automatically populate the database form and archive your spectral or chromatographic data to a sharable database.*

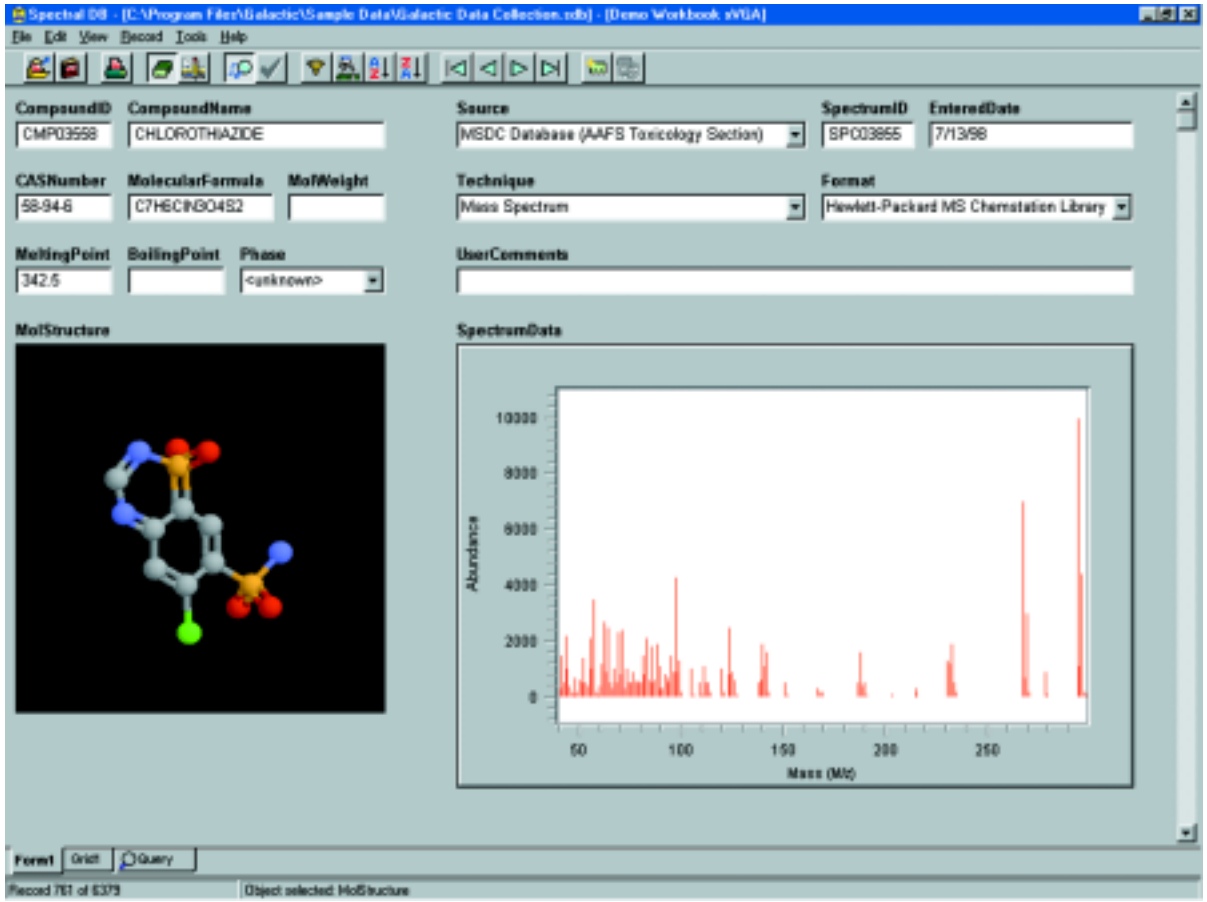
Spectral DB is a unique data management tool for organizing spectra and chromatograms into a database. Today's laboratories are working with increasingly large amounts of analytical data. It can be difficult to effectively manage such large data stores, resulting in lost information and decreased productivity. Spectral DB can help your lab solve this problem. Data stored with Spectral DB can be easily saved, organized, retrieved, viewed, and shared with others in your workgroup. If organizing and managing spectral and chromatography data files have become a problem in your lab, Spectral DB is the solution.

Flexibility and Ease of Use

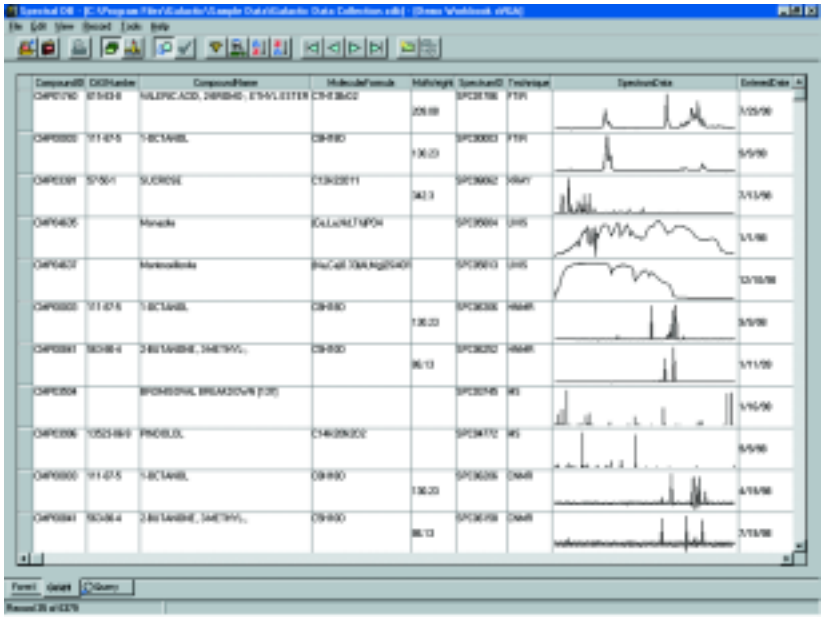
Spectral DB has an intuitive user interface that provides simple form building and layout tools for easy browsing and querying, and a flexible grid display for sorting. With Spectral DB your analytical data is always stored at full resolution. When you retrieve files, you get back the actual spectrum or chromatogram data, not just a picture or image. You can interact with the data on the forms and zoom and scroll for closer inspection. A simple click of the mouse will automatically launch the data into GRAMS/32 for additional data processing.

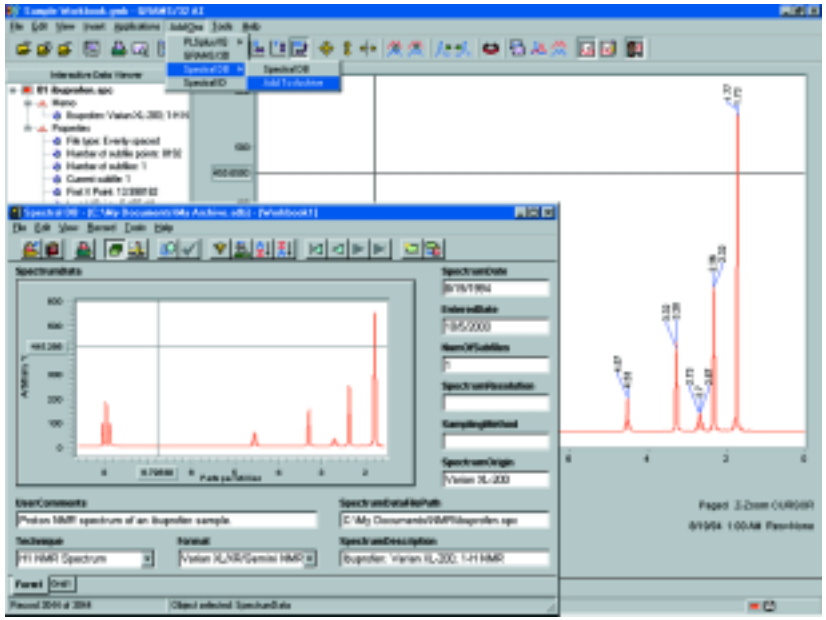
Supported Data Types

Spectral DB includes GRAMS/32's powerful SmartConvert™ technology. SmartConvert gives Spectral DB the ability to read hundreds of analytical instrument and industry standard file formats. This means you can just "drag and drop" your data file into Spectral DB where it will be automatically converted to the industry standard Galactic SPC format for database storage. Your database can contain spectra, chromatograms, chemical structures, and picture images along with text and numeric information.



■ *Spectral DB displays the spectra, structure, and text information in configurable forms.*





Intuitive Form Layout and Design

One of the most powerful features in Spectral DB is its simple form building and layout tools. When creating a new form, Spectral DB automatically arranges the database fields onto the form. You can rearrange the items you want and delete the ones you don't. Data can also be viewed using a tabular grid that displays all the information in the database columns.

Workbooks

It is often convenient to use multiple forms to view and browse the contents of a database. Spectral DB allows you to group multiple forms into a multi-page workbook. You can add tabular grid displays as workbook pages and even create multiple workbooks for a specific database. All workbooks are stored inside the database itself so they will never get lost or be out of order.

Browsing and Querying

Spectral DB makes it easy to find and retrieve data, as well as group data together with similar properties such as a project or notebook number. Querying and browsing are easy too. Fill in the query form and with a click of the mouse find your data files and any information associated with them. You can view query results using any page in your workbook, including different forms and grid displays. The data can be automatically transferred into GRAMS/32 for processing.

Ready-to-Use Database Templates

Spectral DB comes with predefined templates of functional spectral and laboratory archives. They can be used straight out of the box or as a foundation for customized page layouts. These templates allow for easy implementation and quick setup, enabling you to be instantly productive.

Scale-Up to Corporate-Wide Data Management

Spectral DB is ideal for individuals or small workgroups to share and manage their analytical data. It is also the perfect starting point for labs who ultimately need to share their data on a larger scale. Spectral DB databases can be transferred to large scale database systems based on Galactic's Spectral Server™ software. For more information on Spectral Server, please see *Corporate Solutions*.

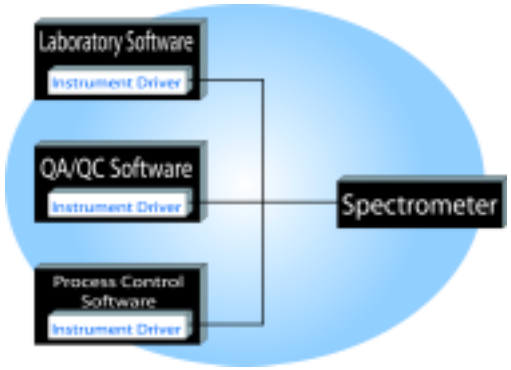
My Instrument Technology

A standard Windows-based programming interface for analytical instrumentation

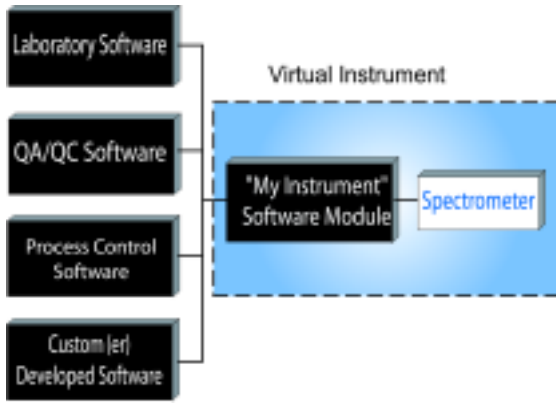
Galactic has been in the instrument control business for over 15 years. Our experienced staff of programmers and engineers has either developed or contributed to the development of control and data acquisition software for over 100 different instrument models from over 20 vendors. These include NMR, Raman, IR, FT-IR, UV-VIS, NIR, GC, HPLC, and a variety of other instrument types. This experience has allowed us to evaluate the analytical instrumentation market from a unique point of view, observing first hand the needs of users, vendors, and developers in our industry. These observations have prompted Galactic to propose an entirely new approach to instrument control and data acquisition called *My Instrument*. This technology is not a product and it is not proprietary. It is a new interface that Galactic supports and has made openly available for the benefit of the entire analytical instrumentation community.

The Problem

Most analytical instruments use a dedicated software package supplied by the manufacturer to control and acquire, view, process, and print data. Most of the time this is the only software that can be used with the instrument. If the manufacturer's software doesn't meet all of your data handling needs, it can be very frustrating. The PC printer market once faced the same problem. Printers were purchased based on the software that could run them, or software was purchased based on which printers were available. Obviously, this was not a logical approach to purchasing hardware or software, and was not acceptable to the PC market as a whole. The problem was solved when popular operating systems introduced standardized interfaces for applications and printers. *My Instrument* brings this type of universal interface to the analytical instrumentation market.



■ *Traditional instrumentation software is dedicated to running one specific instrument.*



The Solution

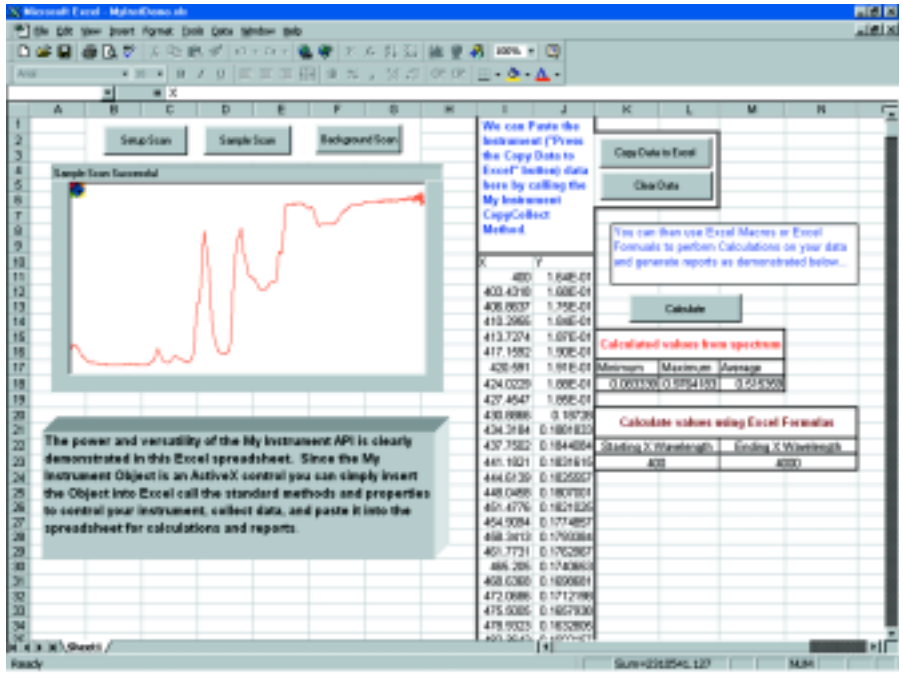
My Instrument technology allows programs to be written that can talk to virtually any instrument that supports the interface. This allows you to choose software most appropriate for your needs. While one software package may be preferred for running an instrument in a research lab, another might be better for running routine or automated analysis. *My Instrument* gives you the freedom to choose the software that will work best for you.

Additional Benefits

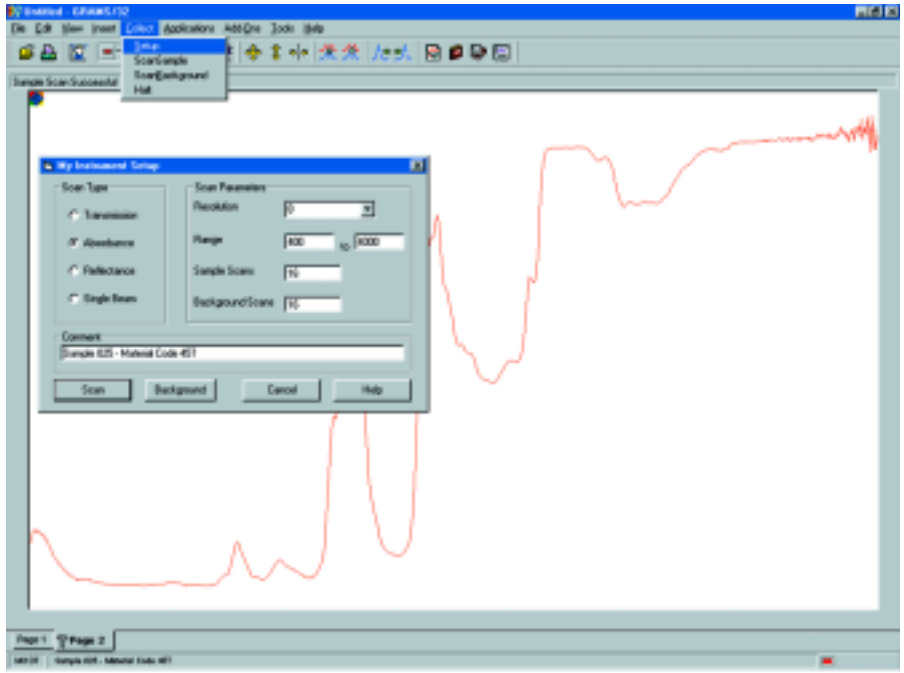
One of the most frustrating tasks in an analytical lab is customizing instrumentation software to perform a task that it doesn't support out of the box. Although most vendors provide some form of macro language to accomplish the task, each implementation is different. Since the *My Instrument* interface is based on Microsoft's Active X technology, it can be automated from almost any standard programming language, such as Visual Basic or C++. It is also compatible with the built-in macros provided by most Office applications such as Excel, Word, Access, or even PowerPoint. The ability to use industry standard tools and applications makes customization quick and efficient.

Who Supports It

As with any standard, if it is not supported it is not very useful. Currently, over 30 instrument manufacturers are developing instrument control software that uses the *My Instrument* standard. Techniques supported include UV/VIS, FT-IR, Fluorescence, NIR, Diode Array, and Raman. Galactic's GRAMS/32 AI is fully compatible with the *My Instrument* standard and automatically recognizes and integrates any installed *My Instrument* software into its menu and workbook pages. For the most up-to-date information on who supports *My Instrument*, visit the website at **www.myinstrument.com**



■ *The versatility of the My Instrument interface is demonstrated by using Excel to directly acquire and analyze data from a NIR instrument.*



■ *GRAMS/32 automatically recognizes My Instrument compatible software and incorporates the instrument control dialog into its menus.*

Corporate Solutions

■ *Administrators can also monitor software access by tracking the usage statistics for each product.* ■ *A quick glance at the Configuration Manager tells the administrator which software products are installed, the version numbers, allowable seating, etc.*

Galactic software is designed to meet your corporate needs. From site licenses to data sharing between corporate facilities located around the globe, Galactic has solutions to make your group, department, or entire company more efficient.

Service Plus Plans

All Galactic Software comes with the option to purchase the Galactic Service Plus Plan (SPP). It is the ultimate insurance policy that combines professional technical assistance with the latest in product functionality. The Galactic SPP provides you with unlimited, priority technical support and automatic product upgrades.

Unlimited Telephone Support

Galactic's Technical Support staff will provide assistance with installing the software, technical guidance, tips and suggestions, or information about available bug fixes and workarounds. There are no limits to the number of callers (site license customers) or the number of calls to the Technical Support Department. Our Technical Support staff is available to take your calls Monday through Friday, 8:30 a.m. to 5:00 p.m. Eastern Standard Time.

Product Upgrades

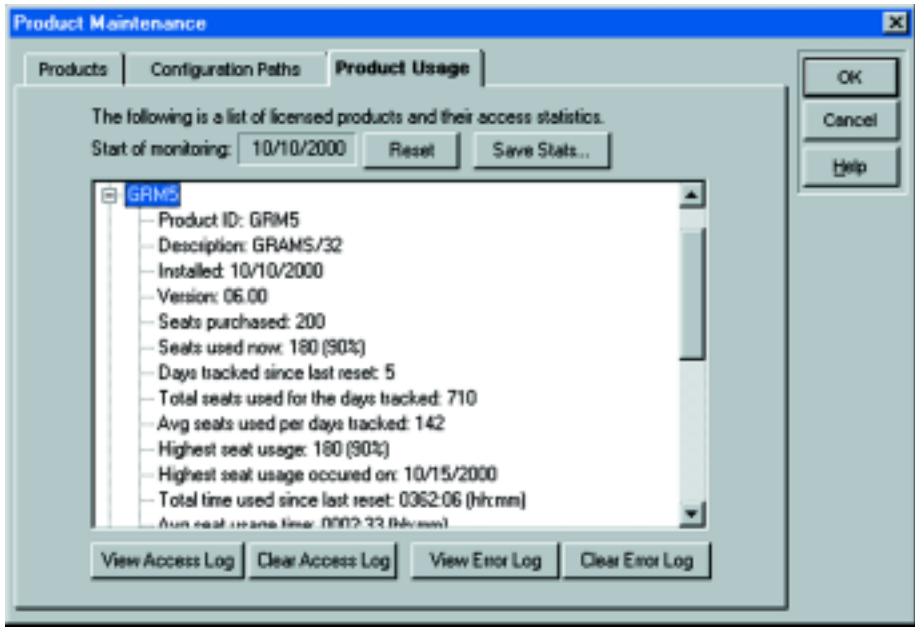
We continually invest in and improve the functionality of our software products and want you to have the benefit of our latest technology at all times. For this reason, all major and minor upgrades are automatically shipped, upon commercial release, to you or your registered System Administrator (site license customers). Patches are available as needed through the technical support department. Some programs are even posted on our web site for downloading.

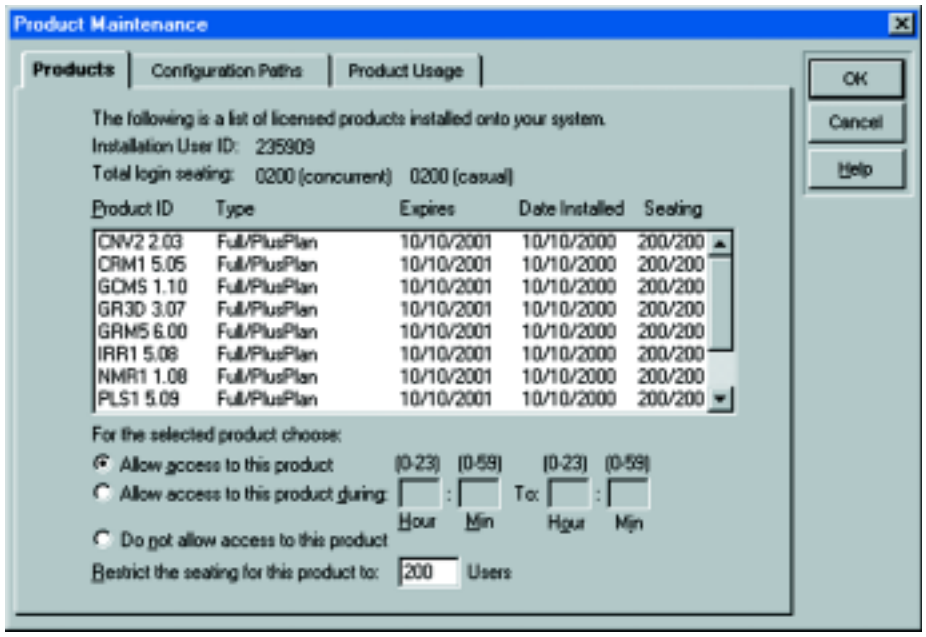
Software Site Licenses

Site licenses are available for Galactic's entire product line. Part-time licenses at discounted prices are provided for casual users, allowing you to support a large amount of users without spending a large amount of money. From five users to hundreds, Galactic has a solution for your corporate computing needs.

All Galactic software products are equipped with features that allow easy roll-out, user management, and automatic updating in a multi-user network environment. Our software supports a multiple client configuration, allowing users to choose either a full or "lite" install depending on storage capabilities of the client computer and network bandwidth. Software updates are simple too. Install an update on your server and all client machines are automatically updated the next time the program is used. A built in messaging system notifies users before an update begins. Additionally, user accesses are automatically logged for review of product usage.

Site license security and user management are controlled by the Galactic Configuration Manager. All users are identified by their network login name, eliminating the need for aliases or new user names. Additionally, all user profiles are stored on the file server so any user can login to any computer where the client software is installed and access his profile. You can set up user groups and permissions, controlling access to software products and features on a user or group basis.





Analytical Information Management Systems

Many modern labs are dealing with increasingly large amounts of data that are stored in many different file formats. Retrieving your archived data or referencing that of a colleague can be almost impossible, resulting in duplicated work and lost productivity. An Analytical Information Management System (AIMS) can solve this problem, making it easy to retrieve and share data files, regardless of their file format.

Spectral Server™ is the first generation of commercially available AIMS software. It implements all of Galactic's trusted technology for data translation, display and processing, archiving, and spectral searching on a centralized network server. It is specifically designed for storing and sharing all types of analytical data using industry standard databases.

Spectral Server is an open-ended laboratory solution. This means your AIMS can be developed around your instruments and data to meet the specific needs, rules, and standard practices of your organization. Spectral Server's modular design allows easy integration with existing data management tools such as chemical structure databases and Laboratory Information Systems (LIMS). Spectral Server can be implemented as custom client/server software or as a web server.

For more information please contact our sales department at 603-898-7600/800-862-6004 or e-mail us at sales@galactic.com