GRAMS Suite

For over 20 years, Thermo Scientific GRAMS spectroscopy software suite has been the premier solution for visualizing, processing and managing spectroscopy data. Due to its broad compatibility with many different instrument data types, researchers in the pharmaceutical, chemical, petroleum, consumer products, and food industries as well as academia, use the GRAMS Suite to solve some of their most difficult data analysis problems. With a powerful collection of processing routines and a simple-to-operate user interface, the GRAMS Suite has made thousands of researchers more productive by eliminating reliance on multiple instrument software packages, reducing overall software training costs and improving data access and collaboration.

Thermo Scientific GRAMS Suite – A Solution for Visualizing, Processing, and Managing Spectroscopy Data

Complete Software Suite

The GRAMS Suite provides a broad collection of tools to meet the needs of scientists engaged in a wide variety of spectroscopic experiments and disciplines. The GRAMS Suite is comprised of a collection of complementary and fully integrated applications and modules centered on the core GRAMS/AI™ spectroscopy data processing and reporting software.

The GRAMS Suite includes several productivity applications that can be used alone, or in conjunction with GRAMS/AI:
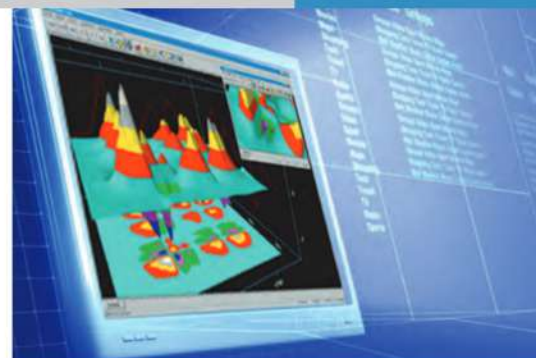
- GRAMS/3D for visualizing multi-dimensional data sets;
- Spectral DB for creating shared workgroup databases for managing spectral data;
- Spectral ID for performing qualitative spectral identifications;
- GRAMS IQ™ for creating qualitative and quantitative chemometric calibration models;
- IQ Predict for deploying GRAMS IQ calibrations;
- QuickQuant for creating simple quantitative calibration models;
- ExcelExchange for data interchange with Microsoft Excel; and
- Active Multifile Tool for creating and manipulation of three-dimensional data sets.

In addition, several third-party vendors offer GRAMS-compatible applications including modules for reaction monitoring and chiral protein analysis.

Broad Data File Compatibility

Using its unique SmartConvert™ technology, the GRAMS Suite is compatible with data files from hundreds of different instrument control applications including Agilent/HP, Beckman, Bio-Rad, Bruker, Gilson, Hitachi, PerkinElmer, Shimadzu, Varian and Waters/Micromass. The GRAMS Suite also supports a number of general-purpose data formats such as SPC, ASCII, JCAMP, and AnDI/NetCDF. For storing data, all GRAMS Suite applications utilize the universal SPC file format enabling scientists to share data with colleagues easily and analyze it at their desks rather than occupying valuable instrument workstations. In addition, GRAMS/AI includes the GRAMS Convert application, which can be used to quickly and easily find, identify, and convert all supported foreign data files to the SPC file format at once.
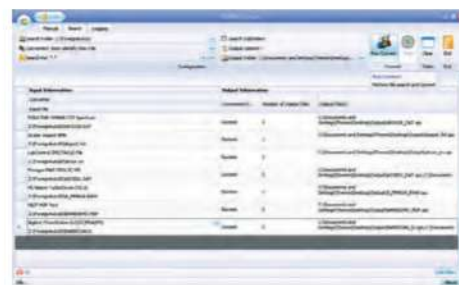
GRAMS Convert – can intelligently scan multiple directories converting known file formats into the industry standard GRAMS .SPC format.

Thermo
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Thermo Scientific GRAMS/AI™ – Comprehensive spectral data visualization and processing

Ready for the Enterprise

While the GRAMS Suite is an excellent tool for the individual scientist, it also enables large research organizations to realize increased productivity from using common data processing software and sharing their data. The software can be deployed to stand-alone PCs for individual users, or to a file server for organization-wide access. The GRAMS Suite offers IT Administrators tools for centralized license and installation management, 21 CFR Part 11 access control and security configurations, and data and spectral library sharing tools to simplify software deployment and long-term maintenance.

The Industry Standard Application for Data Processing and Visualization

GRAMS/AI is a comprehensive data processing, visualization and reporting package which forms the core of the GRAMS Suite. Its advanced processing routines, data comparison and visualization features and its ability to handle data from virtually any analytical instrument have set the industry standard in scientific software.

One Tool for Multiple Instruments

GRAMS/AI can work with data from nearly any kind of analytical instrument including optical spectroscopy (FTIR, Raman, NIR, UV-Vis, Fluorescence), NMR, and hyphenated techniques (LC/GC-MS, LC-PDA). Data can be directly read from its original format using the GRAMS Suite SmartConvert™ technology, which automatically recognizes hundreds of different file formats.

GRAMS/AI can also directly acquire data from a number of instruments via its unique My Instrument plug-in interface. GRAMS/AI includes capabilities for interchanging data with Microsoft Excel, real time visualization of large data sets with GRAMS/3D, and can access data from other GRAMS Suite applications such as Spectral DB workgroup databases and Spectral ID search libraries.

Customizable Workspace

GRAMS/AI offers a simple, intuitive user interface with features that benefit both new and experienced users. The software enables users to quickly navigate through open data files, expose important file information, access parameter settings, and customize the workspace, all with a click of the mouse.
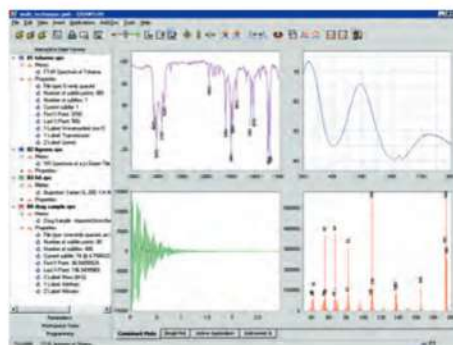
GRAMS/AI can read files from multiple types of instrumentation software and provides a single, integrated environment for working with the data. GRAMS/AI Workbook templates simplify creating custom workbooks for viewing and processing data.

With GRAMS/AI users can create customized environments for viewing, reporting, and processing their data. Multi-page workbooks store specific data display preferences; customized workbook pages, or even automated automation to perform specific functions or process data. Workbooks allow insertion of drawing objects including annotations, lines, and arrows. Use the included Design Science Equation Editor to add mathematical formulas. Even add buttons directly on the workspace and link them to macros or other common functions to create a custom data work-up environment. An integrated Toolbar Builder makes it easy to add buttons for one-click access to frequently used applications or display modes. All user configurations can be stored in a Workbook file which can be used over and over again with different data sets.

Powerful Data Processing

Fast and flexible data processing puts GRAMS/AI at the forefront of spectroscopy software. An extensive library of built-in data processing routines provides users with tools to analyze virtually any type of instrument data. From simple data smoothing to advanced peak fitting to tools for specific instrument types, GRAMS/AI tracks all file changes in the file's Audit Log section, providing results with confidence.

Standard Data Processing Library: Baseline correction (multi-point, polynomial fit), Peak fitting (Gaussian, Lorentzian, Voigt, and other functions), Smoothing, Derivatives, Automatic spectral subtraction, Spectral unit conversion, and more.

IR/Raman Application Pack: ATR pathlength correction, Interferogram compute, Kramers-Kronig transform, Raman shift correction, and a CCD spectrometer calibration routine.

UV/VIS/NIR Application Pack: Performs popular colormetric analyses such as L*A*B and L*U*V using all standard CIE illuminants.
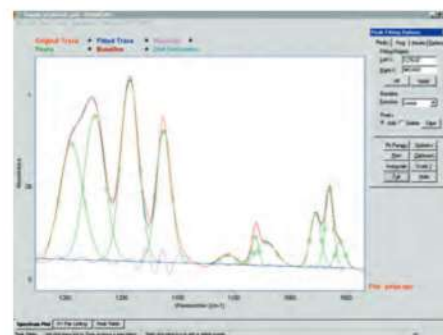
The Peak Fitting routine can automatically identify and optimize a set of known peak and baseline functions to any data set.

NMR Application Pack: 1D NMR data processing; includes a unique one-step routine that can perform a complete data work-up on FID signals including FFT, phase, integrate, and peak identification.

Chromatography Application Pack: Easily build chromatographic analysis methods; peak picking and identification, model calibration, and quantitation.

GC-MS Application Pack: Analyze data from GC-MS experiments; calculate and compare single and total ion chromatograms, automatic peak identification, and spectral library searching (using the Spectral ID GRAMS Suite application).

Customization and Programming

With GRAMS/AI, users can create their own custom data processing applications. The integrated Macro Wizard allows linking of existing routines together with no formal programming to accommodate repetitive experimental needs. Advanced users can take advantage of the embedded Array Basic™ programming language to develop customized routines to solve virtually any analytical problem.

Instrument Control

GRAMS/AI can interface directly to instruments for full control and data acquisition via the embedded My Instrument interface. Any spectrometer that has a My Instrument driver available can be directly connected to GRAMS/AI. Instrument integration with GRAMS/AI is simple; the software recog-

nizes all My Instrument drivers installed on the same PC and automatically updates the GRAMS/AI menus and toolbars to access them. Data is displayed in GRAMS/AI in a special workbook page in real time as it is collected and is automatically transferred into the current workbook for processing once the run is complete.

A number of spectrometer vendors now offer My Instrument drivers for their instrumentation. To get more information on this unique technology see www.thermoscientific.com/grams under the 'Resources' section, users can also contact their instrument vendor to check availability of a driver. Instrument vendors should contact sales.informatics@thermofisher.com for more information on how to develop My Instrument drivers.

GRAMS IQ™ & IQ Predict™ – Chemometric analysis tools

Comprehensive Chemometric Data Modeling for Spectroscopists

Multivariate data analysis methods have become common tools in applying modern spectroscopic instruments to solve qualitative and quantitative analysis problems. Chemometric techniques such as PLS, PCR, PCA, and discriminant analysis have become standard approaches to quickly analyzing complex samples from their spectral signatures.

The GRAMS IQ application extends the capabilities of the GRAMS Suite with an intuitive graphical user interface for creating robust chemometric calibration models for the laboratory and the production line. The separate IQ Predict module can also be used to deploy GRAMS IQ calibrations to multiple GRAMS/AI users.

GRAMS IQ - Powerful Tools for Easy Model-Building

Creating robust chemometric models generally requires trying out many different approaches to working up the data. GRAMS IQ is designed to make this process as simple as possible for both qualitative and quantitative models. GRAMS IQ provides the user with the tools to create, maintain, and extend chemometric data sets. Spectral files can be quickly added - including foreign formats using SmartConvert. GRAMS IQ records the training sample information as well as allowing the user to enter custom information about each sample, if desired. Unique tools allow the user to create multiple combinations of modeling conditions to investigate as a series of separate "experiments". Relationships between these experiments are recorded and displayed for the
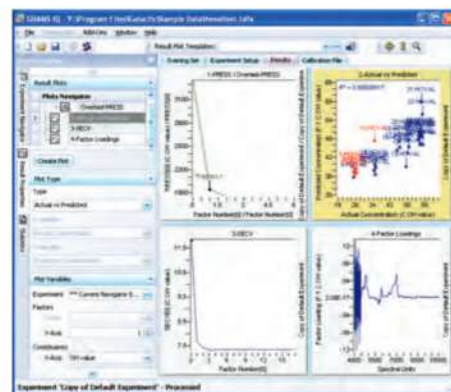
user. Each experiment consists of a collection of settings that completely define the model to be calculated. This includes the model type (including PLS-1, PLS-2, PCR, and a PCA-based discriminant analysis), data preprocessing options (such as scatter and pathlength correction, variance scaling, derivatives), and the spectral regions. Advanced diagnostics such as Self Prediction, Leverage Validation, and Cross Validation help the user to determine the correct model parameters. The parameters and results of each experiment are stored and organized hierarchically using the Experiment Navigator.

GRAMS IQ can display multiple plots of results from different experiments to help determine the best possible combination of calibration parameters.

Spectral files can be quickly added – including foreign formats using SmartConvert.

The Experiment Setup tab region selector offers correlation tools to guide selection of the best spectral regions for calibration.

Once experimental calculations have been performed, users can view and plot all calculated data and a variety of diagnostic indicators that are stored in calculated ex-

periments. Users can compare results of various calibration approaches using the wide variety of built-in plots, or create their own data analysis plots. This assists in optimizing the calibration model, determining if there are any outliers in the training set, evaluating model performance, and determining the number of principal components to use in the final calibration file.

All calculated data and graphs can be exported to a rich text document for reporting purposes. Finally, once the optimum conditions are determined, users can save one or more calibrations to a file for use in prediction. The calibration is linked to the training set data for audit purposes.
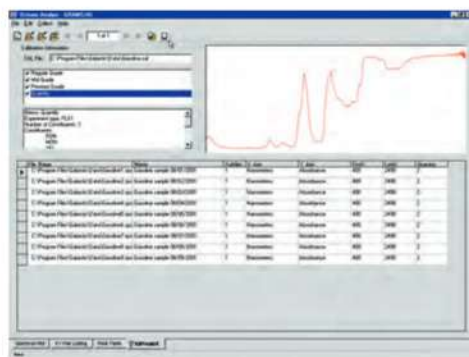
Deploy Calibrations with IQ Predict

Prediction of unknown samples is handled by IQ Predict. Able to run independently of GRAMS/AI and GRAMS IQ, IQ Predict allows users to load one or more spectra and predict them against any GRAMS IQ calibration model.

With GRAMS IQ™, multiple calibrations can be combined in a single file to create a complete collection of all analyses to be

performed on each sample spectrum. This allows creating optimal calibrations separately for different components, comparing performance of different calibrations, or even using qualitative selection criteria that allows IQ Predict to choose the best calibration for the sample being analyzed.

Users can define the output report format and criteria to treat and identify "mismatched" samples.

The IQ Predict ActiveApp module can be used to apply GRAMS IQ calibrations to spectral data from within GRAMS/AI or as a separate stand-alone application. Prediction reports can be formatted for easy output to printers, files or for input into other applications.

Automate Prediction

The IQ Predict module is also ideal for deploying calibrations to multiple systems where the operators are not chemometrics experts and do not need the power of the full GRAMS IQ package. IQ Predict can automatically detect and interface with any My Instrument module installed on the same PC, allowing users to directly apply calibrations and get results immediately as spectra are collected for new samples.

IQ Predict can be configured to operate in "auto-predict" mode which provides a simplified interface which is ideal for routine analyses, repetitive measurements, quality control, and fieldwork. It can also operate in a fully interactive mode which provides a full-featured user interface with complete manual control for loading, collecting, and predicting spectra. It even includes an automation interface which allows it to be incorporated into custom programs to run with no user interaction.

In addition, GRAMS IQ calibration files are compatible with a number of commercial spectrometer applications.
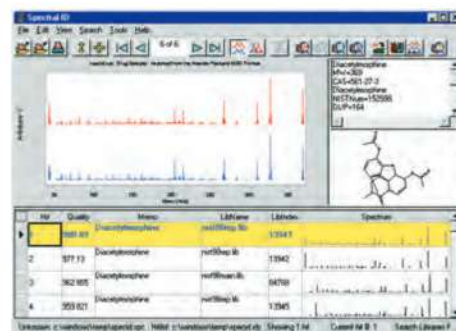
Spectral ID – Spectral library searching®

Qualitative Material Identification using Spectral Library Searching

Spectral pattern matching or "library searching" is one of the most efficient and effective methods for qualitative identification of compounds, and Spectral ID is the most comprehensive searching software available. Fast and easy to use, it is compatible with Mass Spectrometry, IR, Raman, UV-Vis, Fluorescence and NIR data.

Data Compatibility

Spectral ID is compatible with more data than any other spectral search product on the market. Users can easily create their own custom library collections and add spectra easily using the QuickAdd feature, or by importing entire directories or lists of raw data files. Commercial spectral library collections from Aldrich, Chemical Concepts, Thermo Scientific Omnic, NIST, Wiley, and other vendors can be combined with custom-built collections to give users broad coverage of compounds in a single search.

Spectral ID can also read nearly any instrument data file for searching. Using Thermo Scientific GRAMS Suite SmartConvert™ technology, the software automatically recognizes hundreds of different file formats. Spectral ID can automatically link and share data with both GRAMS/AI and Agilent/HP Chemstation software.

Quickly browse and compare search results with the original spectrum. The Library Wizard makes it easy to create custom search library collections from spectral data files.

Versatile Search Options

Spectral ID combines proven and powerful search algorithms with a number of pre-filter options to give quick and accurate qualitative identifications. Users can combine Text, Peak, and Full Spectrum searches, select specific spectral regions or whole spectra and even automatically remove the spectrum of a match from the spectrum of a mixture sample, then search the remainder spectrum again.

Spectral ID's highly optimized library engine is designed to give results fast; there is little degradation in performance no matter how many pre-filters or options are combined in a search.

Network Enabled

With the optional Spectral ID Server software, organizations that routinely and widely use spectral searching can share and centrally manage spectral libraries. The Spectral ID user software can perform searches on the central server collections, or use libraries on the local PC. For more information, see the Enterprise Solutions section of this brochure.

Thermo Scientific Spectral DB™ – Spectral data management

Organize and Share Instrument Data

As scientists work with increasingly large amounts of instrument data, keeping track of their samples and experiments is becoming more and more difficult. Often, researchers find themselves dealing with more information than they can effectively manage. Spectral DB provides individuals and small workgroups an effective data management tool for organizing spectra and chromatograms into a simple, searchable database.

Databases of Instrument Data

The Spectral DB application is a simple tool to organize and index large numbers of instrument data files. Its meta-data entry and indexing system makes it easy to find and retrieve data, as well as group data with similar properties together, such as a project, compound ID, or notebook number. Querying and browsing are easy; simply fill the search criteria directly into the data viewing form and click the mouse. Data can be viewed using the supplied workbook forms, in a grid view, or users can create their own forms and workbooks. Once the desired data set is located, it can be automatically transferred into GRAMS/AI for processing.

Building databases in Spectral DB is simple as well. Files from instrument control applications can be loaded right into the database using the GRAMS Suite SmartConvert™ technology. Databases can also be setup to allow insertion of picture images, MOLfile chemical structures, and alphanumeric text. Databases can optionally be password protected to prevent undesired modification, and can be shared using simple network file sharing protocols with no additional database license or software necessary. In addition, Spectral DB supports Oracle and Microsoft SQL Server for true client-server performance or simple network file-sharing for workgroup use.

Workbook and Form Interface

Spectral DB uses a familiar workbook user interface which can contain one or more forms for viewing and searching the database. When creating a new form, Spectral DB automatically arranges all the database fields onto the page; users can rearrange the fields and remove ones that are not necessary. To make new users more productive, databases can be created using one of the supplied templates and the embedded forms

can be quickly modified to match the user's needs. Workbook forms can be set up to include data viewer windows, text fields, chemical structure and image viewers, and tabular grid displays. Spectral DB stores workbooks directly inside the database itself so they will never get lost or be out of order and can be used by other scientists that have access to the database.
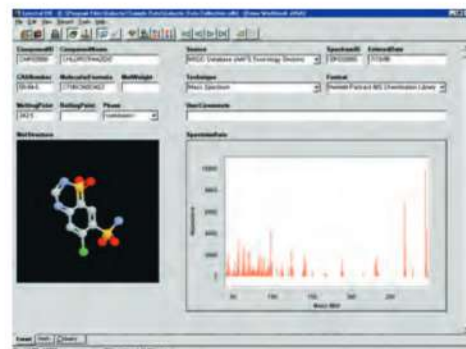
Create customized workbook forms for viewing and searching database collections. Collate data from multiple instrument types and applications into a single, searchable database.

Thermo Scientific GRAMS/3D – Multidimensional data visualization

Real Time Data Visualization for Multi-dimensional Experiments

Unlike static 3D plotting and rendering packages, GRAMS/3D is a true real-time visualization software application that offers scientists an interactive tool to view all the information in multidimensional data sets such as GC-IR, LC-PDA, multidimensional spectroscopy, 2D-NMR, 2D-IR, or spectroscopic mapping experiments.

True 3D Visualization

Multidimensional data from analytical instrumentation is often complex, irregularly shaped, and hard to analyze using simple two dimensional plots. GRAMS/3D is designed specifically to provide real-time 3D

visualization of large multidimensional data sets containing millions of data points. The unique data extraction and rendering algorithms in GRAMS/3D makes it practical to view and analyze these data sets as a whole rather than in pieces. The application uses an interactive "camera" approach to look at data surfaces from multiple angles and perspectives. Users have full control over the camera angle, position, zooming, movement sensitivity, lighting effects, and perspective distance, which can all be changed in real time while viewing the data. Camera navigation is simple and intuitive, connecting common movements of the mouse with camera position, angle and distance.

See the Hidden Information in Any Data Set

GRAMS/3D offers a collection of visualization tools that enable researchers to see subtle and minute variations hidden in multidimensional data sets that are just not possible to observe with less powerful plotting applications. Data can be viewed in one of several different graphical formats including wire frame, shaded solid, gradient solid, or contour plots. Users can control contour level and surface colors to provide the best data definition and expose hidden valleys and peaks, as well as display or hide axes and labels. Views can include extracted two dimensional "slices" and multiple data sets can be displayed simultaneously in stacked

or overlaid modes to compare data from multiple 3D experiments. Users can save all their view settings to a file and reuse their views with other data sets. GRAMS/3D includes a Gallery of pre-designed popular views, allowing quick selection of the best way to display a data set. User-created custom views can also be added to the Gallery.

As with all the GRAMS Suite applications, nearly any data file can be loaded into
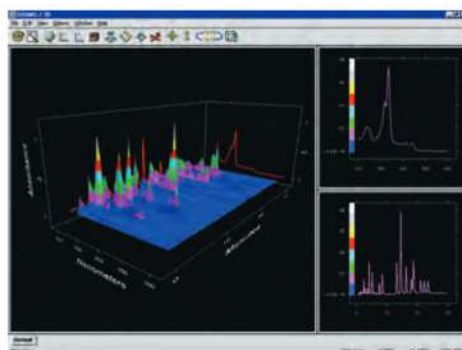
GRAMS/3D using the SmartConvert™ technology. GRAMS/3D can also receive data directly from the GRAMS/AI application.

Data "slice" extraction and perspective tools add an extra dimension to exploring 3D data sets. Real time zooming, coloring and shading features help visualize the small and subtle variations in large multidimensional data sets.

# ExcelExchange™ and QuickQuant™ – ActiveApps expand GRAMS/AI capabilities

ExcelExchange for Data Transfer Between GRAMS and Excel

ExcelExchange allows transferring of data between GRAMS/AI spectral data files (in SPC format) and Microsoft Excel worksheets. Data can be transferred in both directions: from an SPC file into a worksheet or from a worksheet into an SPC file. A simple-to-use wizard guides the whole process. ExcelExchange can import and export SPC files that contain single spectra. It also works with SPC multifiles where the sub-spectra share a common set of x-axis values.

ExcelExchange is an effective way to import ASCII data sets with a large number of data points into GRAMS/AI and to export multidimensional spectral data sets into Excel for special calculations.

QuickQuant for Univariate Quantitation

In situations with simple sample types, multivariate calibration methods like PLS are often too complex and unnecessary.
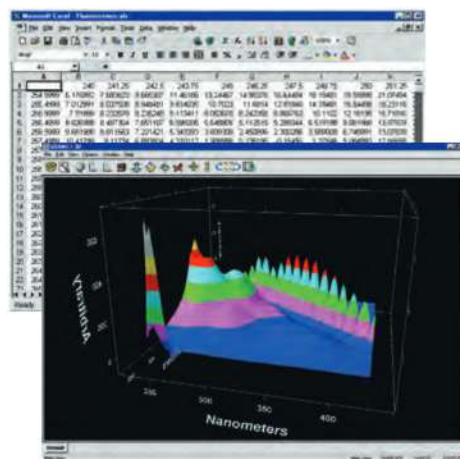
Use ExcelExchange to easily share data between GRAMS Suite applications and Microsoft Excel.

Therefore, the GRAMS Suite offers the QuickQuant module for performing least squares regression calibration analysis of spectral data.

QuickQuant features a wizard-based calibration builder which guides the user through the process of creating or editing a calibration. Multiple component bands and baselines can be graphically defined and adjusted. Users can apply linear, quadratic, or cubic equations to compute the final calibration.

Sample prediction reports are easy to create, simple to interpret, and can be output to the display, printer, clipboard, text file, or any combination thereof. QuickQuant is also fully compatible with My Instrument™ modules for applying calibrations directly to sample spectra collected from a compliant instrument.

Envision – Complex data visualization

Multi-format Instrument Data Viewer

Envision is a multi-format instrument data viewer with the capacity to host plug-in processing and reporting modules.

Envision enhances GRAMS SmartConvert technology to support the GAML open standard XML instrument data format. This allows capture of comprehensive meta-data and simplifies communication with an increasing number of 3rd party products.

Envision can transfer data quickly and easily to other products within the GRAMS Suite. The integral web browser allows seamless connectivity with enterprise data management portals and web based search tools.

With the Inform report design tool, which allows creation of custom templates, Envision allows users to apply standardized reports to data originating from multiple instrument vendors.
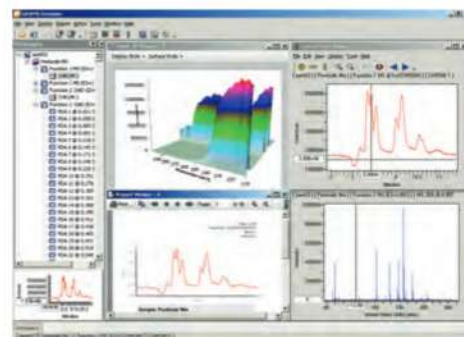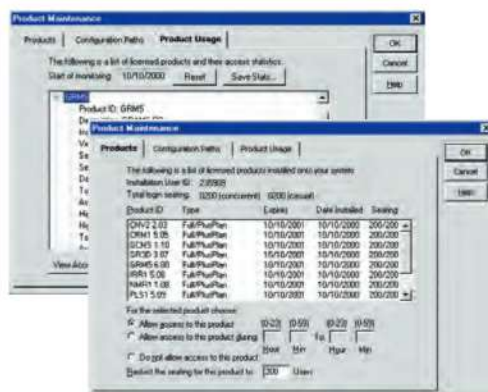

GRAMS Suite Enterprise Solutions

Network Software Deployment and Management

For organizations with large numbers of users, managing software distribution, license usage, and user configurations can consume a significant amount of a company's IT resources. The GRAMS Suite offers a number of powerful tools to minimize the management burden of deploying software applications in the corporate enterprise.

Distributed License Management and User Configuration

The GRAMS Suite Configuration Manager allows system administrators to easily manage site license installations, deploy new software and updates, and define user and group profiles all from a single console. All GRAMS Suite applications and modules can be deployed to users from a central file server; when a user runs an application, the software checks the server and installs updates automatically. Software can be configured to install all components on the user's PC, or run in a "minimal footprint" configuration directly from the server for systems where workstation revalidation is an issue. Administrators can define user profiles and groups, control what GRAMS Suite applications a user or group can access

(and when), and what permissions they have within the applications. All user profiles are managed from the server so a user's settings and permissions are the same regardless of which PC they use to access the GRAMS Suite. The Configuration Manager also maintains and tracks license usage, allowing organizations to manage their GRAMS Suite licenses most effectively.

The GRAMS Suite can be deployed in the enterprise with controlled access for specific users and applications.

Configurable Data Security

The GRAMS Suite includes tools to configure applications to restrict each user's ability to make changes to data. By default, any

modifications made to a data set are always tracked in the file's audit logs. However, the Configuration Manager offers administrators additional settings to ensure data authenticity and integrity. For example, data file overwrite warnings and file integrity checking features can be enabled to prevent and discover data set tampering. Data copying and pasting can be disabled and the optional eSignature tool allows applying and validating electronic signatures in data sets processed by the GRAMS/AI application.

Networked Spectral Library Sharing

When using the Spectral ID application, networked organizations can take advantage of the Spectral ID Server option to share and centrally manage their custom-built and purchased spectral library collections. In addition to allowing companies to more efficiently share their valuable libraries, this option also provides administrators with tools to restrict access and assign permissions to specific users to update the databases. Shared access server-based searching is the fastest and most efficient method for deploying spectral search libraries in distributed organizations which perform moderate to high numbers of spectral searches.

GRAMS Suite Supported Data File Formats

All Thermo Scientific GRAMS Suite applications share the unique SmartConvert™ technology, which allows the software to automatically recognize and load data files from hundreds of different instrument control applications. The following is a partial list of the data formats supported.

ABB Bomem DA3/DA8 FT-IR
ABB Bomem ExaminIR/ NetworkIR/WorkIR
ABB Bomem GRAMS
Acorn NMR NUTS
Acton Research SpectraSense
Agilent ChemStation LC/GC/PDA/MS
Agilent HP LAS GC/LC Chromatography
Agilent/HP 1040 Diode Array (PAWS)
Agilent/HP 1090 Diode Array (PAWS)
Agilent/HP 8452/8453 UV-Vis
Agilent/HP ChemStation GC/LC/ MS/PDA
Agilent/HP IRD ChemStation GC-IR (DOS)
Alton Instruments LS2000
Amersham Biosciences Unicorn Chromatography
Analect Instruments FT-IR
Analytical Spectral Devices FieldSpec
Analytical Spectral Devices LabSpec
Analytical Spectral Devices PSII UV-Vis
AnDI/netCDF Chromatography
AnDI/netCDF FT-IR
AnDI/netCDF Mass Spectrometry
Ando Instruments AQ 6312B
Applied Automation Optichrom Advance
Applied Biosystems/MDS Sciex Analyst
ASCII XY - Constant X Spacing
ASCII XY - High Precision X
ASCII XY - Variable X Spacing
ASCII Y-only (Single column)
ASI ReactIR
AVIV UV-Vis/CD

Beckman - All UV-Vis/Fluorescence
Beckman 32 Karat Chromatography
Beckman DU60 UV-Vis (ASCII)
Beckman FT1000/2000 FT-IR
Beckman Gold Chromatography
Bio-Rad BioDimensions PDA
Bio-Rad Digilab 3200 FT-IR
Bio-Rad Digilab IMX FT-IR
Bio-Rad Sadtler
Bio-Tek Instruments Kroma System 3000
Brimrose NIR
Bruins Instruments Omega Series UV-Vis/NIR
Bruker AMX/X32 Series NMR
Bruker Aspect NMR
Bruker ATS FT-IR
Bruker AXS DIFFRAC/plus XRD/XRF
Bruker ESP300 ESR
Bruker OPUS FT-IR
Bruker PC WIN-NMR
Bruker XWIN-NMR
Buck GRAMS-IR
Buck GRAMS-UV

Chemagnetics CMX NMR
Creon-LabControl SPECTACLE

Digilab/Bio-Rad Win-IR
Dilor Microdil 28 Raman (V2)
Dilor Microdil 28/Z24 Raman (V1)
Dionex-Lee Scientific 600 Chromatography

EG&G PAR CCD
EG&G PAR OMA88
EG&G PAR ProcessVision
EG&G Spectrum Master MAESTRO II

Finnigan ITDS GC-MS
Finnigan Xcalibur GC/LC/MS/PDA
Foss NIRSystems NSAS NIR
Foss NIRSystems Vision NIR

GBC Spectral UV-Vis
GE Nicolet NMR
GE OMEGA NMR
Gilson Unipoint Chromatography
Groton Technology PF1 PDA
Groton Technology SoloNET PDA
Guided Wave NIR

Hamilton Sundstrand AnaGRAMS
Hamilton Sundstrand Analect FT-IR
Hamilton Sundstrand PIONIR
Hitachi D7000 HSM Chromatography
Hitachi R-1200/1100 NMR
Hitachi R-1500 NMR
Hitachi-GRAMS 3400 UV-Vis
Horiba FT-IR

IBM 9420 UV-Vis
IBM IR30 FT-IR
Interspectrum/Spectrolab PFS2000

Jasco J-600 CD
Jasco J-700 CD
Jasco Spectrum Manager IR/UV/FL/Raman/CD
J-CAMP DX (V4.24)
JEOL Delta NMR (Generic format)
JEOL GX/EX NMR
JEOL WinSpec FT-IR
JMBS Diamir
JY Horiba DataMax
JY Horiba ISA PRISM Raman
JY Horiba ISA SpectraMax Raman (DOS)
JY Horiba SpectraMax (Windows)
JY Horiba Spex Raman

Kontron DS450 Chromatogram
Kratos MACH3 GC-MS

LDC SM5000 Diode Array
Lecroy 8818A Digital Oscilloscope
Lecroy 9400 Series Digital Oscilloscopes
Lecroy LC7200 Digital Oscilloscope
Linear Instruments DOS-based PDAs
LTI PowerScan NIR
LTI SpectraMetrix NIR

Micromass MassLynx LC/GC-MS
Micromass MassLynx LC/MS/PDA
NIST MSP Mass Spectrometry

Ocean Optics Ocean32 UV-Vis
Ocean Optics OOBase32 UV-Vis
Optical Solutions PS-1/PS-E Spectrometer
Otsuka UV-Vis DAD

PE Sciex Analyst
PerkinElmer Access Chrom
PerkinElmer TurboChrom
PerkinElmer 7000 Series FT-IR
PerkinElmer FL DataManager
PerkinElmer FL Winlab
PerkinElmer IR AutoIMAGE
PerkinElmer IR DataManager FT-IR
PerkinElmer Nelson 2600 Chromatography
PerkinElmer Nelson Access Chromatography
PerkinElmer PC137 SAM
PerkinElmer PEGRAMS 1000/1600/2000
PerkinElmer PIONIR NIR
PerkinElmer Spectrum IR
PerkinElmer TravelIR FTIR
PerkinElmer Turbochrom (up to V3.3)
PerkinElmer TurboMass GC/LC/MS
PerkinElmer UV DataManager
PerkinElmer UV Winlab
Perseptive Biosystems Voyager TOF-MS
Perten GRAMS
Perten PerCon NIR
Pharmacia LKB GelscanXL
Phillips IR/40 FT-IR
Polymer Laboratories Cirrus GPC
Polymer Labs Cirrus GPC/SEC
Prolab Resources/Teknivent GC-MS V1

Radiomatic FLO-1
Renishaw WiRE Raman
Roper Scientific Princeton Instruments CCD

Scientific Software, Inc. EZ Chrom Elite™ Chromatography
SensIR - All FT-IRs
Shimadzu Class-VP
Shimadzu Hyper-IR
Shimadzu Hyper-UV
Shimadzu QP5000 GC-MS
Shimadzu UV160/265
Siemens DIFFRAC/DIFFRA Cplus XRD/XRF
Spectra Physics 4200 Integrator
Spectra Physics ChromStation
Stanford Research SR265

TA Instruments Universal Analysis DSC/TGA
Techmag MacNMR
Telos Labs Spectrogram FT-IR
Temet Instruments FT-IR
Thermo Scientific Elemental VG PlasmaQuad ICP-MS
Thermo Scientific Xcalibur GC/LC/MS/PDA
Thermo Scientific Atlas Chromatography
Thermo Scientific Finnigan ChromQuest
Thermo Scientific Finnigan Masslab
Thermo Scientific Finnigan Xcalibur Chromatography System
Thermo Scientific Multichrom
Thermo Scientific Nicolet Omnic IRDATA & GROUP Files
Thermo Scientific Nicolet Omnic Series Files
Thermo Scientific Solaar
Thermo Scientific Spectronic Helios UV-Vis
Thermo Scientific Thru-Put Target Chromatography
Thermo Scientific SPC (GRAMS)
Thermo Scientific ICON FT-IR
Thermo Scientific WinFIRST FT-IR
Thermo Scientific OMNIC Atlas FT-IR
Thermo Scientific OMNIC FT-IR
Thermo Scientific OMNIC Series FT-IR
Thermo Scientific PC-IR FT-IR
Thermo Scientific RESULT FT-IR
Thermo Scientific SX/DX FT-IR
Thermo Scientific InstaSpec
Thermo Scientific RUNNES II
Thermo Scientific Aminco-Bowman 2
Thermo Scientific SLM 3000 UV-Vis
Thermo Scientific SLM Universal UV & FL
Tracor Northern TN-6500
Tracor Northern TN-6600

Varian Cary UV-Vis (OS/2)
Varian Cary WinUV
Varian Cary-GRAMS UV-Vis
Varian Galaxie
Varian Saturn 3 GC-MS
Varian Saturn 5 GC-MS
Varian Star GC Chromatography
Varian VNMR
Varian XL/XR/Gemini NMR
Varian/Chemagnetics SpinSight NMR

Waters 990/991 Diode Array
Waters Maxima 820 Chromatography

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