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InfoMetrix

The Premier Chemometrics Company

Multivariate Data Analysis and Automation

For the Lab…

…for the Process

The Premier Chemometrics Company

Infometrix is a leading developer of software products in the field of Chemometrics, employing pattern recognition and modeling techniques for the analysis of multivariate data sets in chemistry and biotechnology. Our research and development efforts are directed toward software that will be completely integrated with instrumentation to provide better solutions to complex problems in chemistry, engineering and other sciences.

Since 1978, Infometrix has been developing chemometrics tools and has produced a series of chemometrics software packages, as well as a variety of chemometrics solutions specially bundled for analytical instrument companies. The Infometrix mission is to provide high quality, easy-to-use software for the handling of multivariate data. Please visit our web site at http://www.infometrix.com to view product details, pricing and application notes.

Life Sciences
Clinical, Bacterial Identification,
Pharmaceutical, PAT
Food and Beverage, Agriculture,
Adulteration
Physiology, Metabolomics and
Proteomics
Olfactory – E Nose, Flavors and
Fragrance, E Tongue
Environmental
Air quality
Toxic waste disposal
Industrial spills and apportioning
Forensics
Archaeology
Physical Sciences
Criminal forensics
Counterfeiting
Arson
Elemental Analysis

Industrial/Manufacturing
Chemical
Petroleum and Gas
Fuels and energy
Exploration
Production and manufacturing
Automated analysis
Quality screening, MSPC, SCADA
Minerals and Mining
Analytical Instrumentation
Chromatography, GC, LC, Data alignment
Spectroscopy, NMR, Optical, MS
Algorithms and Math
QSAR and QPSR
Calibration Regression
Classification
Data exploration and mining
Data alignment
Manufacturing Quality Control
Database

We are collecting an ever increasing amount of data. In a day an analytical instrument can generate data on many samples, each with hundreds of variables. Chemometrics software is designed to extract meaningful information efficiently from such large data sets. Today's technology demands this approach: one that acknowledges not only the nonspecific and multivariate nature of most instrumented data but also common bottlenecks in the data analysis process

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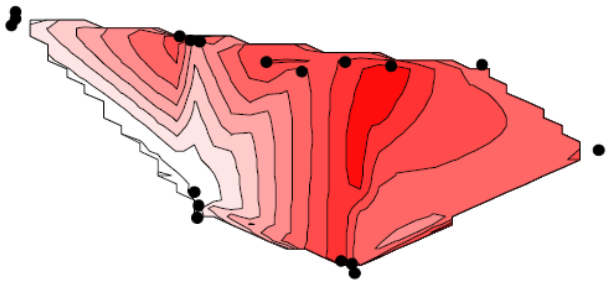
Pirouette®

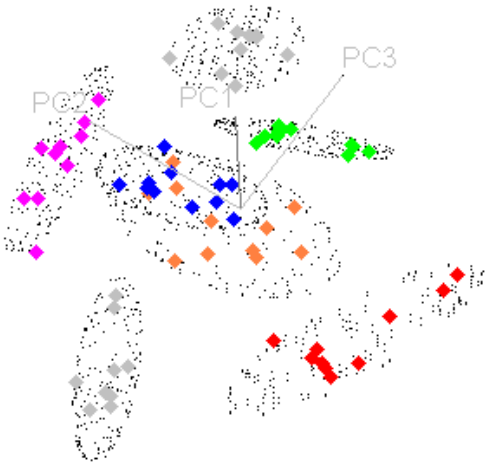
Comprehensive Chemometrics
Modeling Software

Pirouette 4.5, our most comprehensive chemometrics package, is designed specifically for Windows Vista, 7, 8, 10. Modeling and prediction tools for data exploration, pattern recognition, property correlation, and mixture analysis methods are implemented in a single program. Infometrix designed and developed the Pirouette software over 25 years ago to address the need for a tool to organize and understand complex data. We focused primarily on analytical instruments, but soon found uses in areas as diverse as clinical applications, environmental monitoring, refinery quality control and database management. The software balances the necessary algorithmic requirements with a simple user interface and is used for:

- Data mining, visualization and organization;
- Classification analysis to identify the origin of a sample;
- Quantitative analysis to estimate a concentration or other property that is hard to measure more directly; and
- Unmixing signals to identify and apportion the component parts of a mixture.

Mapping the impact of a pollution source on soils in the area





Pirouette is the ideal means for organizing complex data, whether it is a survey of polluted sites where you want to apportion the root causes to building a quality control system for an on-line analyzer. Pirouette is the tool that enables the construction of both quantitative and qualitative models, and makes them easy to integrate into the laboratory or the process environment.

A qualitative model showing groupings and probability envelopes

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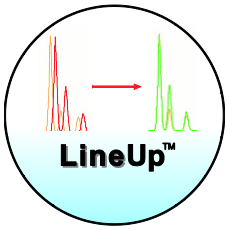
A simple to use yet very powerful interface facilitates interacting with raw and processed data. Support for many common instrument and data exchange file formats make importing data painless. Thousands of subsets can be created from a single data file, allowing the user to exercise many different what-if scenarios without having to collect additional data. All calculated products are saved in a single file and can be retrieved and manipulated via the Object Manager, a unique data handling system. Transfer of calibration options allow spectra to be adjusted appropriately for prediction with a model from another source. You can even run multiple instances of Pirouette to maximize efficiency.

Even the Pirouette demo has substantial capability. Load any supported file type, including Pirouette native format files, with results present. Use the visualization tools to evaluate your data or data sent to you from a Pirouette user. When you are ready to jump into multivariate analysis, purchase a license to unlock Pirouette's algorithms.

InStep™

Automated Chemometrics
Prediction Software

InStep 3.5 is a Visual Basic client that is a compliment to Pirouette for automating predictions. InStep 3.5 provides the ability to take a Pirouette model, integrate it into a method or a procedure, and put it to use right away. The software is designed to be integrated into a method or a process by either using a watched folder or being explicitly called on a command line. Methods and Reports are developed through an intuitive form-based interface. Hierarchical prediction strategies are possible, and functioning example methods included with the package demonstrate method concepts. Reports can be configured to include only the predicted values or a suite of prediction diagnostics and can be written to individual files or accumulated in one master file. We also open up all of our computational capabilities through the Infometrix Product Access Kit (IPAK) so that integrators and software developers can access all of the chemometrics functions in their own software. Examples of these integrations abound spanning product offerings from Agilent, Bio-Rad, ChromPerfect, GeoMark, Northwest Analytics, PerkinElmer, Siemens and many others.



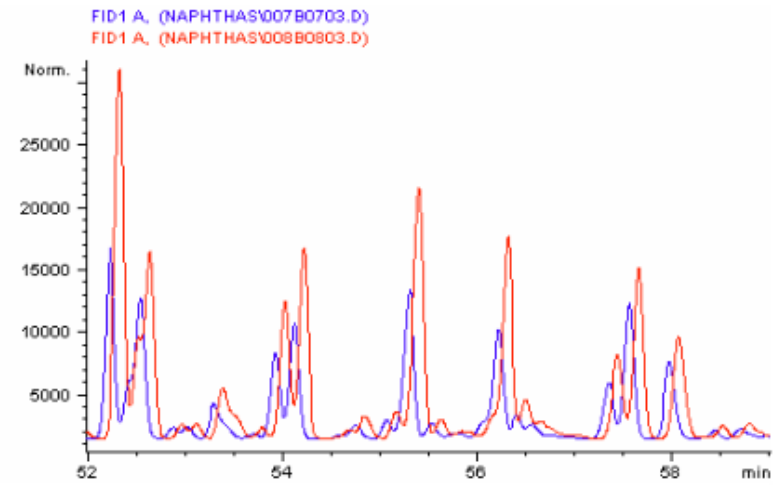
LineUp™

Software for Alignment
of Chemical Analysis Profiles

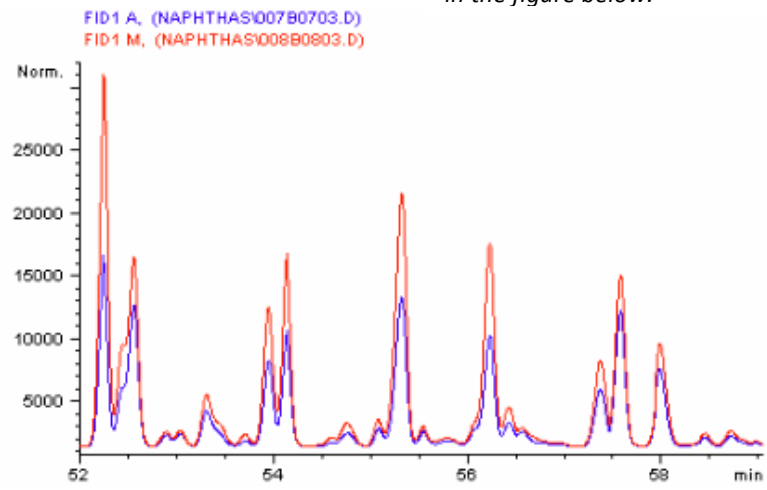
LineUp™ 3.5 is an alignment utility for chromatographic and spectroscopic data. LineUp will process files in several data formats, including Agilent ChemStation chromatography systems

(*.CH files) and many other instrument systems (PerkinElmer TotalChrom, ThermoFisher Atlas, Waters Empower, Dionex Chromeleon, etc.) through the AIA data interchange format for chromatography (*.CDF files). We also support ThermoGalactic's GRAMS spectroscopy software (*.SPC files), a very common data interchange format and files in the Infometrix ASCII format (*.DAT) can also be aligned. In addition, accessory files are included for automating the alignment process with ChemStation and with the EZChrom Elite system. With the advent of LineUp 3.0, the executable became a COM client of IPAK. New to version 3.5 is a graphical user interface that allows you to manage LineUp parameters and view chromatograms, raw and aligned, from a single window.
Using a multivariate correlation method, LineUp will adjust a chromatogram's retention axis to more closely resemble that of a target. In doing so, LineUp can adjust for variations in column loading, column aging and changes in flow. The same approach can be applied to spectroscopic data, especially useful for corrections to Raman spectra.

By largely eliminating retention time variation, LineUp becomes an excellent partner with Infometrix' Pirouette pattern recognition methods and data visualization tools. Together, LineUp and Pirouette can automate the interpretation of chromatographic data. Please see the product specifications for more details.



An example of a sample requiring alignment is drawn from the petroleum industry in which complex mixtures are frequently encountered. The figure to the left shows two chromatograms of similar material where many peaks have shifted significantly in the second sample with respect to those in the first. After aligning the sample to the target (respectively, the red and blue trace), the misalignment has been almost completely eliminated, as seen in the figure below.



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