KnowItAll®
Informatics System

AnalyzeIt™ MVP Multivariate Processing Made Simple

The elegance and power of Infometrix' Pirouette® chemometrics software are a perfect complement to the cheminformatics and comparitive visualization tools in the KnowItAll® system. The result is an advanced tool for multivariate processing to analyze spectroscopic, chromatographic, or numeric data with efficiency and ease. This application offers expert and non-expert users alike a powerful yet intuitive interface for multivariate processing that enables them to:

- Gain insight into hidden patterns and relationships in users' data
- Explore data correlations to answer critical research, development, or production questions
- Facilitate the storage of analysis results for subsequent reference, reporting, or investigation

What is Multivariate Analysis?

Multivariate analysis (including principal component analysis, PCA) refers to the statistical analysis techniques where multiple variables are analyzed to determine the contribution made by each variable to an observed result. It can examine quantitative data in more depth than can usually be obtained from a basic cross-analysis of the data. This permits patterns to emerge from within the data.

Integrated Data Importing, Management, and Data Pre-processing

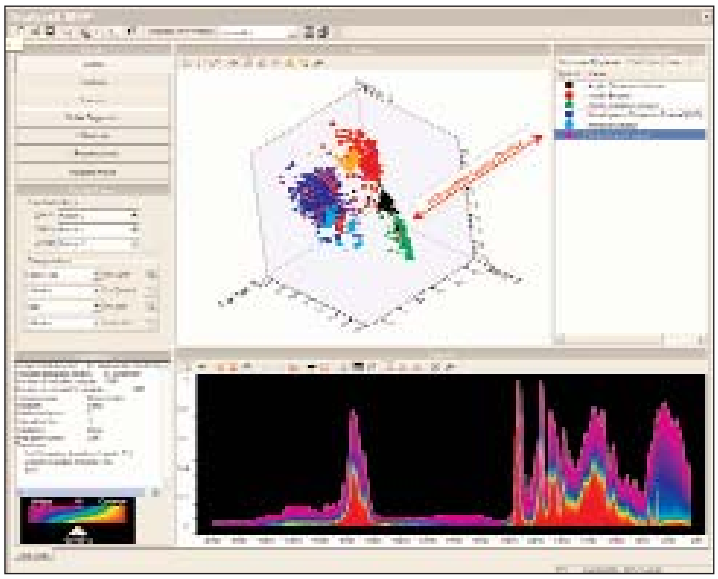
As part of the KnowItAll Informatics System, the AnalyzeIt MVP application seamlessly takes advantage of all of the additional applications in the KnowItAll environment, including data importing and processing of NMR, MS, and other kinds of spectral and chromatographic data via batch mode; database creation, visualization, and searching; and report generation. In addition, the complete list of data pre-processing options familiar to Infometrix' Pirouette customers is incorporated into the AnalyzeIt MVP application, allowing complete flexibility in the multivariate analyses performed. The pre-processing options for PCA include:

- **Pre-processing** (Autoscale, Mean-Center, Pareto, Range Scale, or Variance Scale)
- **Y-Transforms** (1st Derivative, 2nd Derivative, $\log_{10}$, Multiply, Subtract, MSC, SNV, Smooth, Normalize, and Baseline Correction).
- **Binning/Bucketing** (Fixed Width, IntelliBucket™ or User-Defined Range)

AnalyzeIt MVP: IR Example

In this example, a PCA was done on an IR database of automobile paint chips.

Integrated Query Device - The legend at the right is also an integrated Query Device, allowing the user to select one or more paint classes by clicking on the appropriate row or rows in the legend—clicking on the "Water Based Enamel" row in the "Paint Type" legend highlights all points in the scatter plot and displays all spectra that correspond to the paint type selected in the legend.



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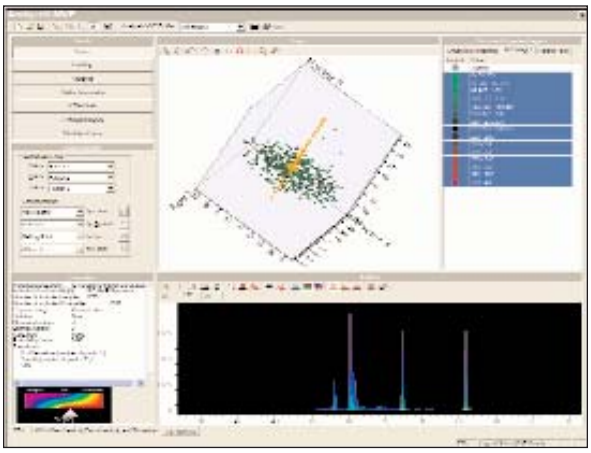

AnalyzeIt MVP: NMR Example

In this example, a PCA was done on an NMR database of organic compounds with a diverse range of functional groups. Note that structures can be made visible via the "Structures/Properties" pane, which allows immediate visualization of the structures associated with selected data points.

Also, the Overlap Density Heatmap slider bar has been moved toward the "common" side to show only those spectral areas with higher levels of similarity.

Plots, Spectra, Structures, and Legends as Integrated Query Devices

The elegance and ease-of-use in the AnalyzeIt MVP application is highlighted by the way in which the plot legends double as simple but powerful query devices, turning the application into an unsurpassed data mining tool. The legends, plots, spectra, and structures are fully interactive and interlinked:

- Select Points ➡ Highlight Legends; Display Spectra and Structures
  If the user selects points in the scatter plot, not only will all corresponding spectra and structures be displayed, but also all rows in all legends corresponding to the selected points will be highlighted.
- Select Legend Row ➡ Highlight Legends; Display Spectra and Structures
  If the user selects a row in any legend, all points corresponding to that legend item will be highlighted in the graph, all corresponding spectra and structures in the data set will be displayed, and most importantly, all corresponding rows in other legends will also be highlighted.

Spectral displays can then be viewed with Bio-Rad's patent pending Overlap Density Heatmap (ODH) technology for powerful comparative visualization. (See *datasheet on Overlap Density Heatmaps for more details*.)

Powerful Plot Display Options for Clear and Compelling Graphics

Several options for data point display are available, with intuitive default values that still give the user complete control to customize all plot display features, including categorization by:

- ***Color*** - Change colors in continuous or categorical coloring schemes
- ***Symbol*** - Plot different categories of data using different symbols
- ***Size*** - Plot different categories or ranges of data with different size symbols
- ***Label*** - Display a data label, including selectively labeled points according to user-specified data ranges

AnalyzeIt MVP also allows one to draw the time-trajectory course of data over time.

Powerful Post-PCA Interpretation Tools

Combined with the MineIt™ and SearchIt™ applications, the resulting loadings plots and the OD consensus spectra of different classes or their difference spectra can be used as a query to search against spectral databases. For example, in the KnowItAll Metabolomics Edition, a database of ^{1}H and ^{13}C spectra and peaks of over 225 common metabolites are provided for identifying biomarkers in NMR-based metabolomics.

The Value of AnalyzeIt MVP

The capabilities of the AnalyzeIt MVP application provide users with a tremendous amount of value, including:

- Giving expert users and non-experts alike an elegant, intuitive, powerful, and easy-to-use informatics environment for performing PCA
- Providing insight into hidden patterns and relationships in large quantities of datasets
- Enabling users to exploit these correlations to answer critical research, development, or production questions
- Facilitating the storage of analysis results for subsequent reference, reporting, or investigation

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