Analyze IQ[®] Lab: Advanced Chemometric Modeling Made Intuitive

Analyze IQ Lab enables the fast and accurate interrogation of all types of spectroscopic data, with an intuitive & easy-to-use interface that increases productivity and reduces risk of errors.

Analyze IQ Lab provides rapid and accurate analysis methods to turn your complex spectroscopy data into decisions, using both well-established chemometric modeling methods and innovative new techniques based on data mining methods.

Its model building wizard allows you to build, evaluate and refine sophisticated models, quickly and reliably.



Key features of Analyze IQ Lab include:

- Innovative model-based approach yielding fast and accurate results
- + Intuitive user interface, with step-by-step wizard
- Useful range of pre-processing options
- Comprehensive graphics for visualizing effects of pre-processing and performance of models
- Analyze IQ Lab models can be deployed to Analyze IQ RealTime, enabling operators who are not analysts to make red-light/green-light decisions in real time.

Download a free evaluation of Analyze IQ Lab or find out more at <u>www.AnalyzeIQ.com</u>



Analyze IQ Lab is the world's most advanced chemometric analysis software package. It is part of the Analyze IQ software suite, which has been developed to address the need for accurate analysis of spectroscopy data.

Analyze IQ Lab provides rapid and accurate analysis of complex spectra, using both well-established chemometric modeling methods and innovative patent-protected new techniques based on data mining methods. Testing has shown that these proprietary methods are more accurate than standard techniques, particularly when analyzing complex spectra. See our Application Notes for further details.

With Analyze IQ Lab's new model-driven paradigm, you can:

- Analyze data using pre-built models
- Easily build new models customized for your data, using a step-bystep wizard
- Choose from quantitative and qualitative analysis methods, depending on what kinds of question you wish to answer
- Evaluate, refine and improve your models before final deployment
- + Plot your input data and visualize and export your results.

Pre-processing Methods	
Smooth (S-G)	
Derivative (S-G)	Window 5 🚖
Normalize	Polynomial 2 🚔
Std Normal Variate	Derivative 1
Equal Area Scale	
Internal Std Normalize	Exclusion All zeros 🔻
Truncate	
🕂 Apply 🔓 Undo	

Pre-Processing Methods Include:

- Data smoothing
 - Derivatives using Savitzky-Golay method
- Normalization
- Standard Normal Variate Transformation
- Equal Area Scaling
- Truncation with Crop and Notch Options
- Multi-Level Undo

Wide Range of Quantitative and Qualitative Modeling Methods:

- Principal Component Analysis in combination with Linear Regression or any method
- k-Nearest Neighbor Classification & Regression
- + Support Vector Machines with standard kernels: Euclidian, RBF, and Sigmoid
- Support Vector Machines with our proprietary Spectral Kernels
- Our unique Spectral Attribute Voting

And Many Other Unique and Distinctive Features:

- A model-driven paradigm that separates model-building from model usage, so that you can package and deploy expert chemometric knowledge
- + Build models with data from Spectra Manager, from a spreadsheet or from a folder of spectra
- Combines power with ease of use, with features such as its model-building wizard
- Model Backup and Restore: ideal for archiving models and transferring models between computers without any risk of error
- + Batch Analyze Feature: choose M models and N spectra to analyze all MxN combinations
- Support for a wide range of file formats, including: JCAMP-DX; NIST's SpectroML; simple XY text files; Thermo SPC; AIQ text-based XML format; CSV file data from Excel
- Instrument Interface mechanism, to allow for direct acquisition of spectra
- Comprehensive documentation: manuals, worked examples, and sample data.

Select Method Select method for generating model Linear Regression SVM Classifier Polynomial Kernel ⊿ RBF Kernel Euclidean Distance Weighted Spectral Distance Sigmoid Kernel Weighted Spectral Linear k-Nearest Neighbors Spectral Attribute Voting ⊿ PCA Linear Regression SVM Classifier Polynomial Kernel RBF Kernel **Euclidean Distance** Weighted Spectral Distance Sigmoid Kernel Weighted Spectral Linear k-Nearest Neighbors





