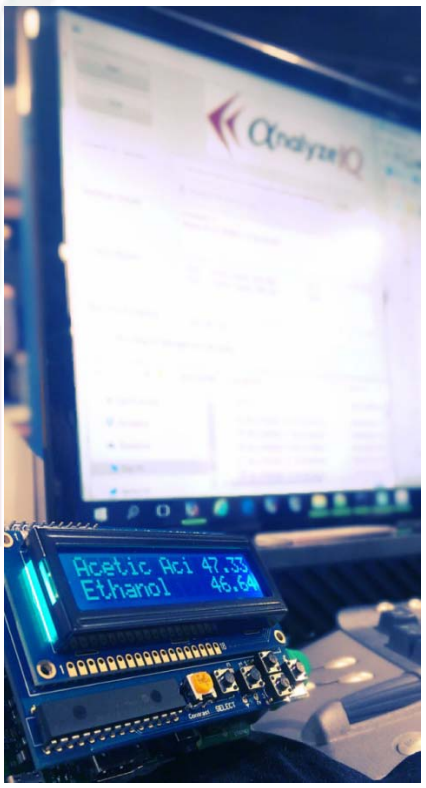
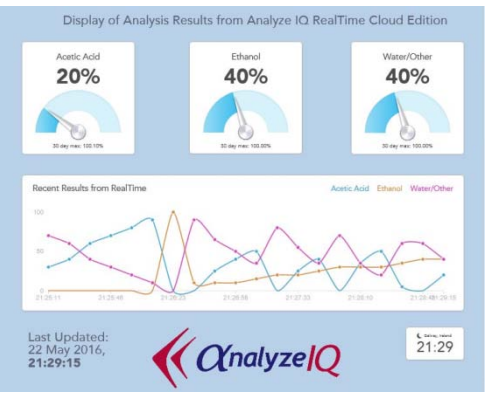
accuracy | insight | speed | confidence

AnalyzeIQ®

INTELLIGENT ANALYTICAL CHEMISTRY SOFTWARE





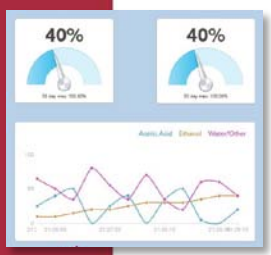
www.AnalyzeIQ.com

Analyze IQ's Vision:

Powerful Intelligent Analytics Everywhere

With rapid advances in miniaturized spectroscopy and the growth of the Internet of Things leading to the new paradigm of Fog Computing, it is becoming possible to have large distributed arrays of spectrometers and other chemical sensors, for applications such as process monitoring, environmental monitoring, and manufacturing control.

For such applications, you need:



- Advanced analytics software to turn your complex data into decisions
- Library search and **library-based mixture analysis** as well as advanced chemometrics, so you can answer broad questions ("what is this?") and specific questions ("is this target present, and in what quantity?")
- The ability to **package and deploy expert knowledge** in fielded applications where it can be applied automatically, or used by personnel without chemometric training
- Analysis of sensor data at the device (**edge computing**), centrally (**cloud computing**), or across combinations of both (**fog computing**), with securely encrypted data transmission when needed
- **Web-based dashboards** so that management personnel can see key details at a glance, on dedicated computers, tablets or phones
- Instrument interfaces, device drivers and user interfaces for **real-time process monitoring**
- Support for multiple operating systems (Windows, Linux, Mac OS and even solutions for Android and iOS) on multiple processor platforms (ARM and Intel, 32bit and 64bit)
- Well engineered software, developed without outsourcing, from an agile independent company that can to develop new software and perform **chemometric modelling**, to provide you with complete solutions.

Analyze IQ® is the only company in this industry that provides all of these capabilities.

Our software framework allows our customers to develop analytical models with **Analyze IQ Lab** and deploy them on the desktop, embedded devices, and the cloud with **Analyze IQ RealTime.** Our software paradigm is carefully architected to enable analytics where they best suit the business need, whether on portable devices, on desktop PCs, or on servers and cloud systems.

We have unlocked the potential of **statistical machine learning**, which normally requires high-powered computers, so that we can support the **multi-scale computing** paradigm, with a single codebase that enables our analytics to be deployed on entirely on miniature devices, or on the desktop, or on the cloud, or distributed from the edge to the cloud in many configurations using **Analyze IQ RealTime**.

AnalyzeIQ®

INTELLIGENT ANALYTICAL CHEMISTRY SOFTWARE

Products

Analyze IQ Lab: Provides rapid & accurate chemometric analysis methods to **turn complex spectral data into decisions**. Its model building wizard allows you to build, evaluate and refine sophisticated models, quickly and reliably.

Analyze IQ SmartSearch allows you to quickly and accurately **search a library** of spectra, to identify the best matches for a spectrum that you wish to identify, and to perform **mixture analyses**, enabling you to answer "what is this?" questions easily and reliably.

Analyze IQ Spectra Manager: Makes it easy for you to **store** and **organize** your valuable spectra and related meta-data, and work with third-party libraries. An ideal alternative to the high cost & effort of implementing a LIMS.

Analyze IQ RealTime: Enables you to **package** chemometric models that have been constructed and validated by expert analysts and **deploy** them in fielded applications, where they can be applied automatically for real time predictions. Available in **Portable**, **Desktop**, or **Cloud** Editions.

Analyze IQ Spectra Library: A carefully-curated collection of 1868 Raman spectra of common organic materials, including laboratory chemicals, hazardous materials, research chemicals, and solvent mixtures.

We also support third-party spectra libraries.

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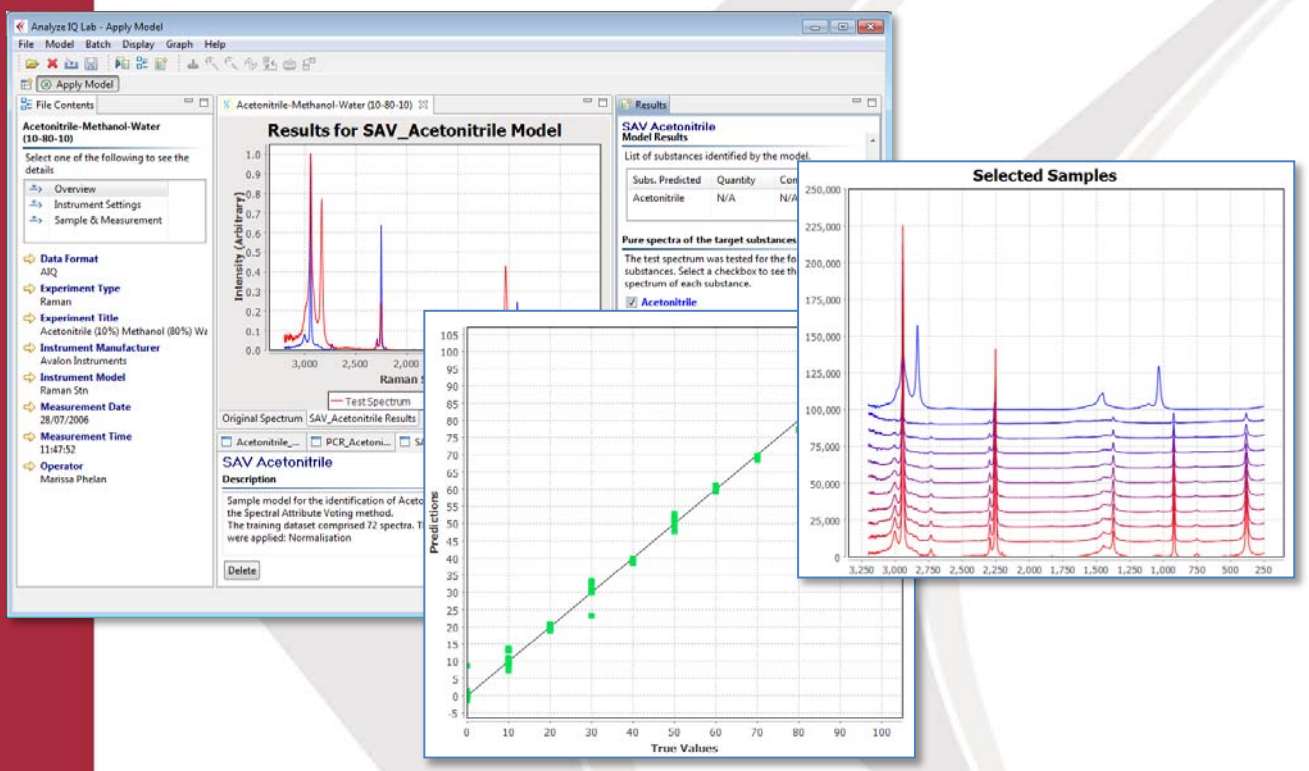
Analyze IQ® Lab:

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.



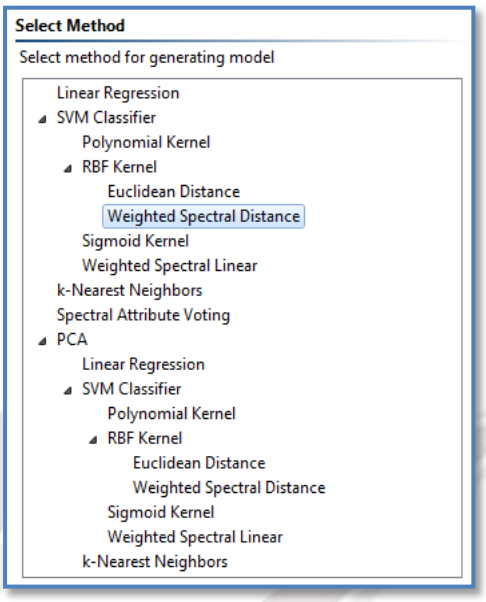
Key features of
Analyze IQ Lab include:

- 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 www.AnalyzeIQ.com

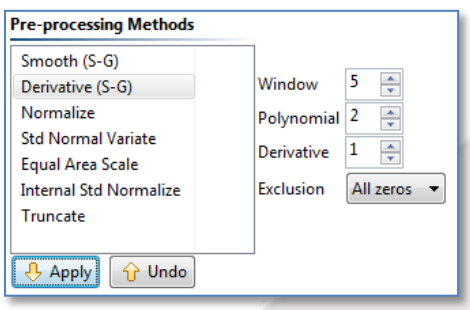
Analyze IQ Lab is the world's most advanced chemometric analysis software package. It is part of the Analyze IQ software suite, which has been developed to address the need for accurate analysis of spectroscopy data.

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-by-step 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.

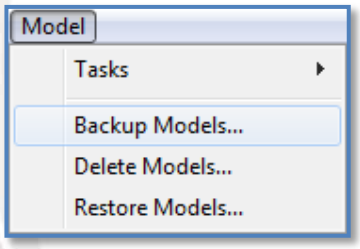


Pre-Processing Methods Include:

- 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.

Analyze IQ Lab

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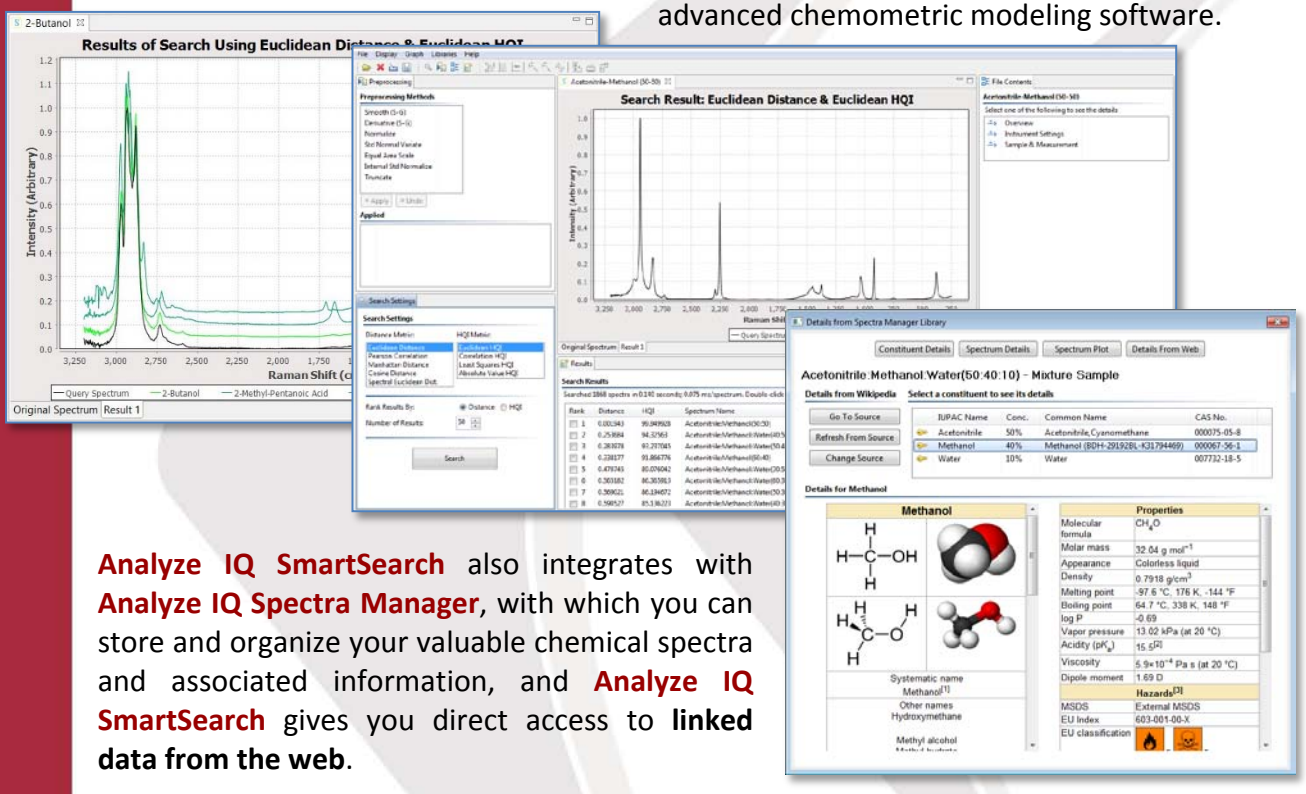
Analyze IQ® SmartSearch

Fast Spectrum Searching and Mixture Analysis

Analyze IQ SmartSearch allows you to search spectrum libraries **rapidly and accurately**, to identify best matches for unknown spectra and key **components of mixtures**. It enables you to answer "what is this?" questions easily and reliably, and provides useful supplementary data.

Analyze IQ SmartSearch provides accurate spectrum matching algorithms to allow you to identify a ranked set of spectra that are the closest matches for a spectrum of interest. It also provides techniques to identify the main components in mixtures. It includes a wide range of well-known comparison metrics, and the innovative new *Spectral Euclidean Distance* algorithm that has been developed for this product.

Analyze IQ SmartSearch is the ideal complement for **Analyze IQ Lab**, the world's most advanced chemometric modeling software.



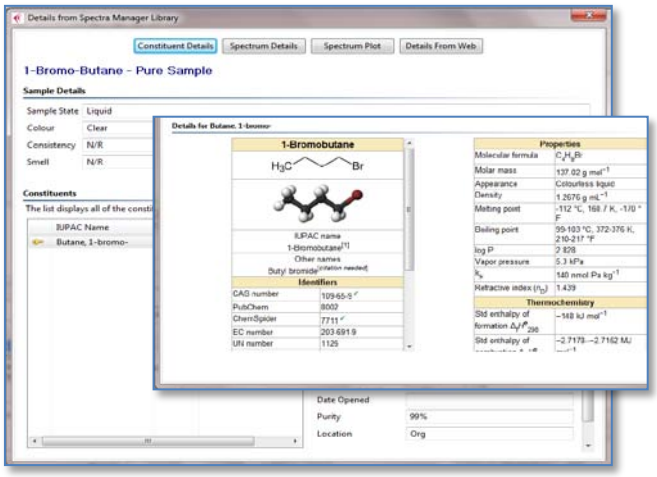
Analyze IQ SmartSearch also integrates with **Analyze IQ Spectra Manager**, with which you can store and organize your valuable chemical spectra and associated information, and **Analyze IQ SmartSearch** gives you direct access to **linked data from the web**.

Key features of **Analyze IQ SmartSearch**:

- High-speed searches with its efficient software design
- High quality mixture analysis to identify key components
- Wide range of spectrum comparison methods & pre-processing methods
- High-performing new *Spectral Euclidean Distance* comparison method
- Modern, clean, graphical user interface: easier to use than competing products
- Works with user-made libraries and third-party libraries in Spectra Manager format
- View relevant chemical information data from linked data sources on the web

Download a free evaluation of Analyze IQ SmartSearch or find out more at www.AnalyzeIQ.com

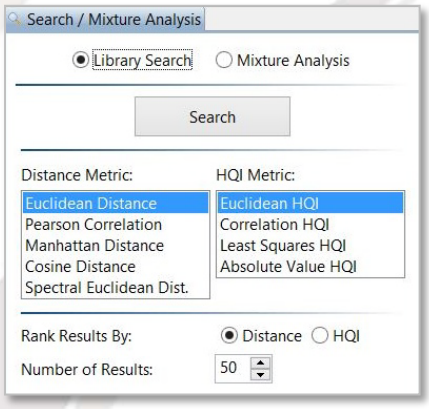
Analyze IQ SmartSearch enables you to search quickly and accurately through a library of spectra, to identify the best matches, and to identify the key components of mixtures. It is part of the Analyze IQ software suite, which addresses the need for accurate analysis of spectroscopy data.



Analyze IQ SmartSearch provides rapid and accurate spectrum matching algorithms to allow you to identify a ranked set of spectra that are the closest matches for a spectrum of an unknown substance of interest.

Analyze IQ SmartSearch also provides techniques for mixture analysis: it rapidly identifies the key components in the query spectrum that match spectra in the library, estimates the contributions of the components to the mixture, and shows residuals.

It includes a wide range of standard comparison metrics and the innovative new *Spectral Euclidean Distance* algorithm, developed for this product, that has been shown to out-perform previous methods (Khan & Madden 2012).



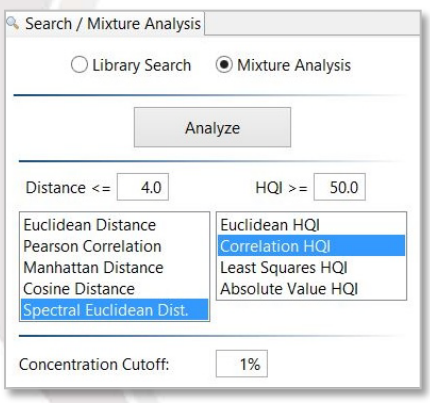
Another **unique feature** is that **SmartSearch** can retrieve and display **linked data from Wikipedia** associated with your results. It can also display information from **Analyze IQ Spectra Manager** about the results.

Useful Set of Spectrum Comparison Metrics:

- Pearson Correlation & Cosine Similarity
- Euclidean Distance & Manhattan (Citiblock) Distance
- Unique *Spectral Euclidean Distance* Measure
- Hit Quality Index metrics: Euclidean HQI, Correlation HQI, Least Squares HQI, Absolute Value HQI

Fast and Effective Analysis of Mixtures:

- Search your library to identify all main components of a query spectrum
- Estimates the contribution of each component identified
- Computes & displays the reconstructed spectrum with its HQI & distance
- Computes and displays the residual
- Batch analyses: select a folder of spectra and get a report with results



Works With Analyze IQ Spectra Manager:

- **Analyze IQ SmartSearch** performs searches against the contents of your **Spectra Manager** libraries
- With **Analyze IQ Spectra Manager** you can sort the contents of your library, insert and remove spectra, and select any entry to view its spectrum and edit associated data

Works With Analyze IQ Raman Spectra Library:

- Raman Spectroscopy users of **Analyze IQ SmartSearch** and **Spectra Manager** can purchase a carefully-curated library of 1868 Raman spectra (1103 pure materials and 765 mixtures), including the exact composition of each material and all associated data
- It contains spectra of a wide range of common organic materials, including laboratory chemicals, hazardous materials, research chemicals, and solvent mixtures

Works With Third Party Spectrum Libraries:

- Third party libraries are supported and we can assist you in importing your own spectra.

Analyze IQ SmartSearch

Reference: S.S. Khan & M.G. Madden*: "New Similarity Metrics for Raman Spectroscopy"*. Chemometrics and Intelligent Laboratory Systems, Volume 114, May 2012.

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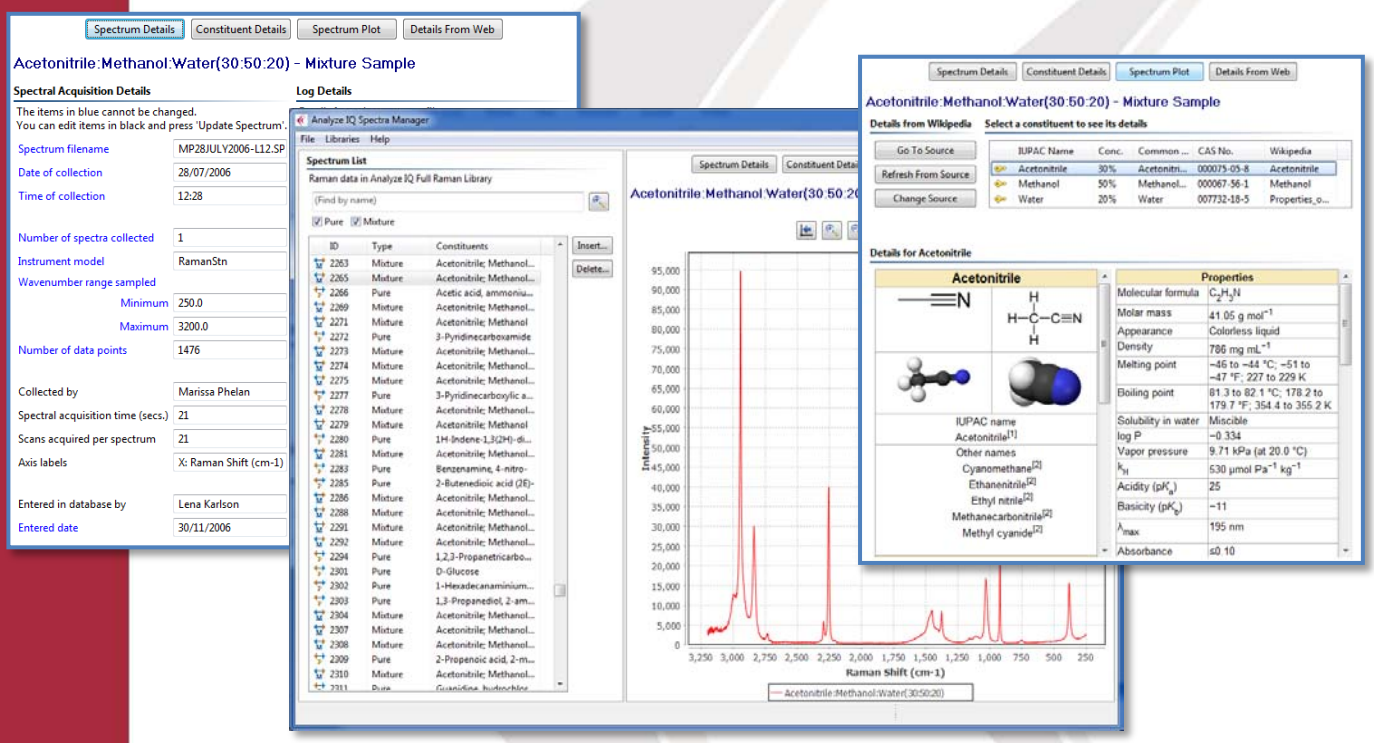
Analyze IQ® Spectra Manager:

Store, Organize, and Link Your Spectral Data

Analyze IQ Spectra Manager allows you to store and organize valuable chemical spectra and associated information, and has a modern, easy-to-use interface.

Your spectra are valuable assets: **Spectra Manager** makes it easy for you to store and organize the spectra and related meta-data. You can build up an in-house library of spectra or use it with third-party libraries. It even gives you direct access to **linked data from the web**.

Spectra Manager is the ideal alternative to the high cost and effort if implementing a LIMS, or the all-too-common approach of keeping spectra in spreadsheets or folders, where associated information and context would be lost.

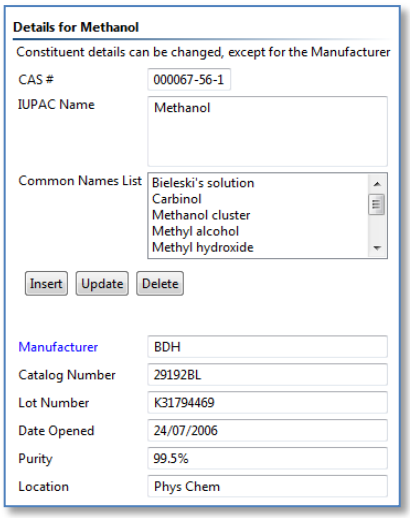


Spectra Manager integrates with **Analyze IQ Lab**, so that you can easily select appropriate spectra from which to build Analyze IQ models.

Spectra Manager also integrates with **Analyze IQ SmartSearch**, so that you can identify best matches for unknown spectra, quickly and reliably.

Download a free evaluation of Spectra Manager
at www.AnalyzeIQ.com

Analyze IQ Spectra Manager is part of the Analyze IQ product suite, which is the world's most advanced chemometrics and spectroscopy analysis software.



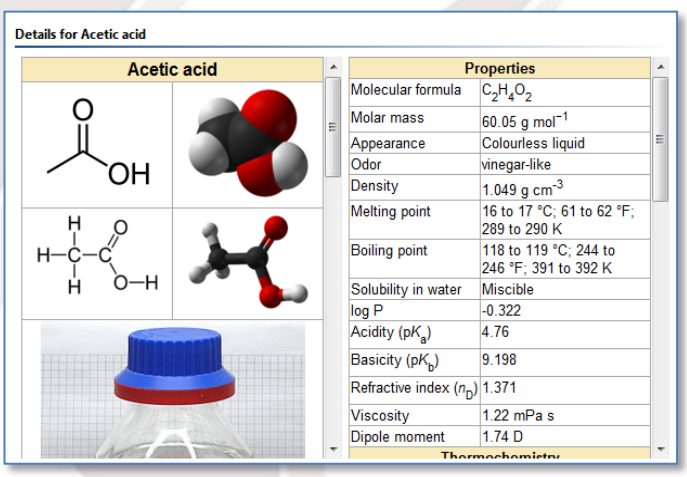
Spectra Manager is the spectral library and data management package that allows you to store and organize spectra and their related meta-data, easily and efficiently.

Its features include:

- Browse spectra and switch between spectrum details, constituent details, plots of spectra, and data from the web
- Store CAS registry numbers and QA details
- For each sample, record important details such as the manufacturer, catalog number, lot number, date opened, and purity
- Full-text search and listing of spectra by IUPAC and common names.
- For mixtures, all the relevant data can be included, so that you can track mixtures that use the same materials by lot numbers.

With **Spectra Manager** you can insert spectra into libraries and remove them, and select any entry to view its spectrum and edit associated data, such as lot number, manufacturer, appearance, IUPAC name, common name, and so on.

Spectra Manager links seamlessly with **Analyze IQ Lab**, allowing users to select data from their database for the development of Analyze IQ models. Functionality is provided to **auto-select** the training set, by scanning the databases for all samples that include the target material and other relevant samples, such as those that contain materials that occur in mixtures with the target material.

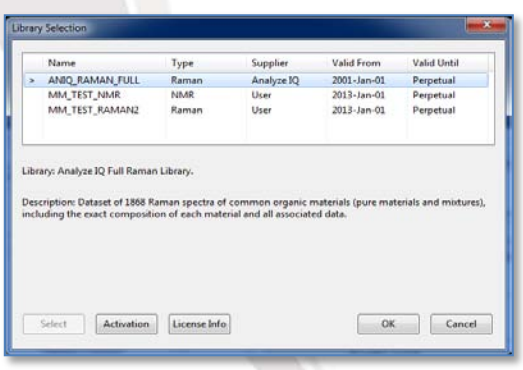


It also links seamlessly with **Analyze IQ SmartSearch**, with which you can search quickly and accurately through your library of spectra, to identify the best matches for a query spectrum.

A **unique feature** of **Analyze IQ Spectra Manager and SmartSearch** is that they can display **linked data from Wikipedia** associated with your data.

Works with Multiple Libraries:

- Analyze IQ Raman Spectra Library
- Third-party commercial libraries
- Build up your own libraries in-house
- Keep libraries on one machine or share them in your department
- We can assist you in importing your spectra or legacy data.



Popular file formats are supported:

- SPC: Thermo-Fisher's GRAMS SPC format
- SpectroML: NIST's XML-based format
- AIQ: format used in the Analyze IQ software suite
- JCAMP-DX: IUPAC's popular JCAMP-DX file format
- XY Text Files and CSV Files

Spectra Manager

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Analyze IQ® RealTime:

Real-Time Process Monitoring & Embedded Chemometric Analyses

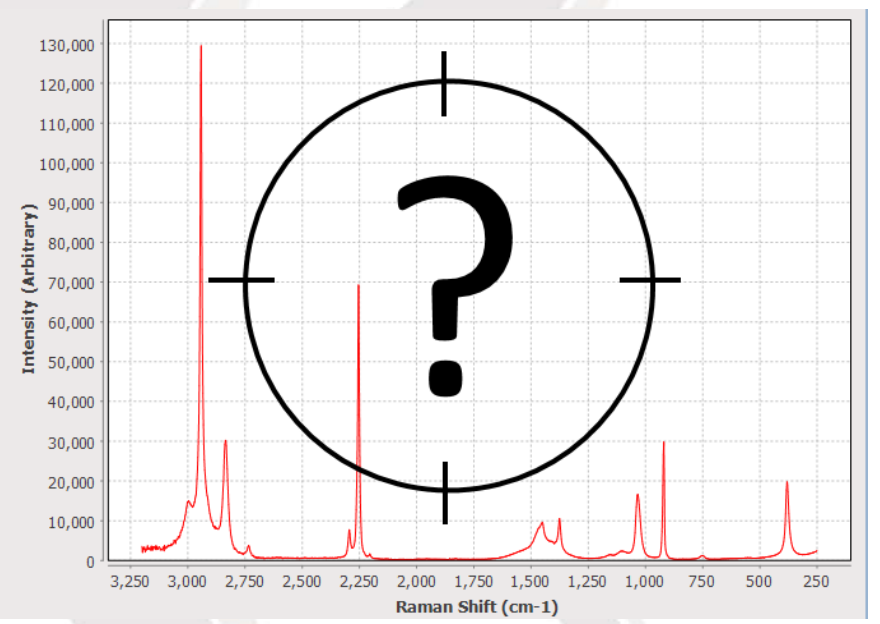
By packaging and deploying analysis models developed by expert chemometricians, **Analyze IQ RealTime** allows analyses to be performed **fully automatically**, thereby enabling operators who are not analysts to make **red-light/green-light decisions** on spectroscopic data in real time.

Analyze IQ RealTime lets you **package and deploy** expert knowledge: chemometric models from **Analyze IQ Lab** that have been constructed and validated by expert analysts can be deployed rapidly in fielded applications, where they can be applied automatically, or by users without chemometric training, for real time predictions.

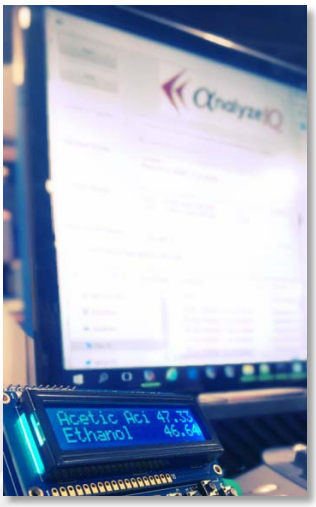
Analyze IQ RealTime is available in **Portable**, **Desktop**, or **Cloud** Editions.

Analyze IQ RealTime is ideal for:

- Real-time process monitoring
- Portable & in-field instrumentation
- Specialist applications
- Materials validation & anti-counterfeiting
- Routine work by non-chemometricians
- Applications in healthcare, pharmaceuticals, law enforcement, and petroleum industries



Contact us now to discuss your application or arrange a demo



Analyze IQ RealTime enables chemometric models from **Analyze IQ Lab** to be integrated in third party products, for fully **automatic, fast, and accurate** quantitative and qualitative chemometric predictive modeling.

It works with models built using **Analyze IQ Lab**, 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.

It is ideal for: real-time process monitoring; portable & in-field instrumentation; specialist applications; materials validation & anti-counterfeiting; and routine work by non-chemometricians.

It is used in applications such as healthcare, pharmaceuticals, law enforcement, and petroleum industries.

Package & Deploy Expert Knowledge

Analyze IQ RealTime's unique advantage is that it allows you to **package and deploy expert knowledge**, since chemometric models that have been expertly constructed and validated by analysts can be deployed in fielded applications, where they can be applied automatically or by end-users without chemometric training.

Because it is based on **Analyze IQ Lab's** industry-leading chemometrics, **Analyze IQ RealTime** provides rapid and accurate chemometric analyses, and it scales well to handle complex combinations of materials and tests. It enables third-party solutions to perform fully automatic analyses, **without any intervention by the end user**: no review of results, no spectral subtraction, just a rapid response.

Error-Free Transfer of Models

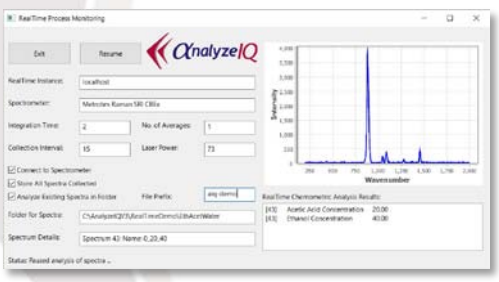
Analyze IQ RealTime uses models that are built with **Analyze IQ Lab**, in the form of binary software code; this **eliminates risk of errors** in transfer or transcription of model information. The models embed preprocessing details within them, so spectra to be analyzed are automatically preprocessed correctly.

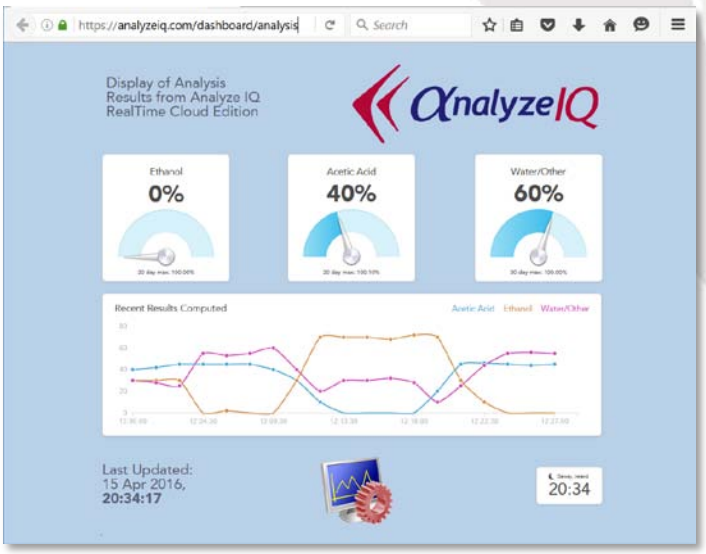
Analyze IQ RealTime has the same Model Manager feature as **Analyze IQ Lab**, allowing you to backup, restore and deploy models conveniently and without any risk of errors.

Scalable from Embedded Devices to the Cloud

Analyze IQ RealTime is a scalable solution:

- **Portable Edition**: runs on embedded computers
- **Desktop Edition**: runs on the same computer as client software, to inter-operate with desktop or handheld devices.
- **Cloud Edition**: responds to analysis requests from multiple client computers, and can be distributed across multiple computers to cope with intensive analysis demands.

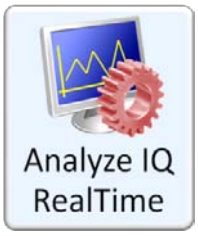




Analyze IQ RealTime is configured to run as a separate process from the client's software, and the two software programs interact using standard inter-process communications and XML-formatted messages. This design allows **Analyze IQ RealTime** to interact with client software developed using virtually any PC-supported software development framework and language. It can also be configured to run as a service on a desktop PC, or on a cloud server.

Customizable

We can customize **Analyze IQ RealTime** for your requirements, support you in integrating it, and develop chemometric models for you. Contact us to discuss this, or for a demonstration.



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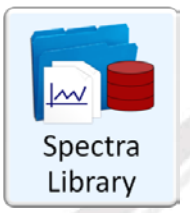
Spectra Libaries

Available for the Analyze IQ® Software Suite

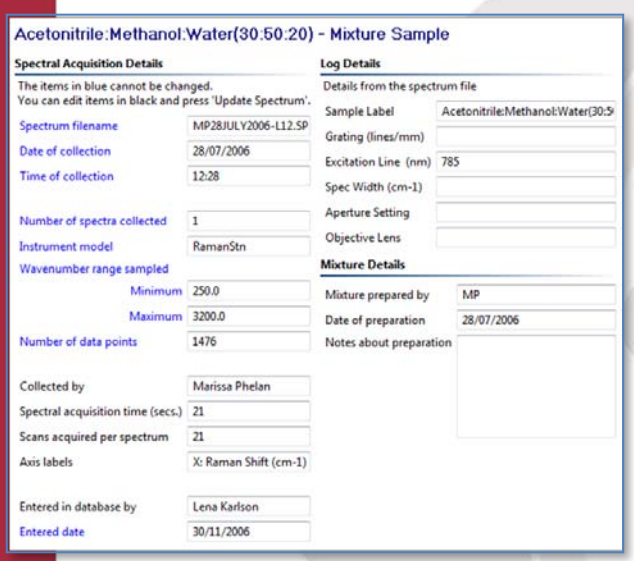
The Analyze IQ Raman Spectra Library is a useful addition to the Analyze IQ software suite for Raman spectroscopy users. It is a carefully-curated library of 1868 Raman spectra (1103 pure materials and 765 mixtures), including the exact composition of each material and all associated data.

The Analyze IQ Raman Spectra Library contains spectra of a wide range of common organic materials, including laboratory chemicals, hazardous materials, research chemicals, and solvent mixtures.



For each spectrum, it stores the exact composition as well as useful meta-data such as the manufacturer, lot number, appearance, purity, IUPAC name, common name, and other details, and also links to Wikipedia details where available.

The library is divided into two subsets, available separately or together:


Acetonitrile:Methanol:Water(30:50:20) - Mixture Sample

Spectral Acquisition Details

The items in blue cannot be changed.
You can edit items in black and press 'Update Spectrum'.

Spectrum filename	MP28JULY2006-L12.SP
Date of collection	28/07/2006
Time of collection	12:28
Number of spectra collected	1
Instrument model	RamanStn
Wavenumber range sampled	
Minimum	250.0
Maximum	3200.0
Number of data points	1476
Collected by	Marissa Phelan
Spectral acquisition time (secs.)	21
Scans acquired per spectrum	21
Axis labels	X: Raman Shift (cm-1)
Entered in database by	Lena Karlson
Entered date	30/11/2006

Log Details

Details from the spectrum file

Sample Label	Acetonitrile:Methanol:Water(30:5
Grating (lines/mm)	
Excitation Line (nm)	785
Spec Width (cm-1)	
Aperture Setting	
Objective Lens	

Mixture Details

Mixture prepared by	MP
Date of preparation	28/07/2006
Notes about preparation	

- **Raman Spectra of Laboratory Materials:** This comprises 1103 spectra covering 899 materials, each of which has a single identified primary constituent
- **Raman Spectra of Mixtures:** This comprises 765 spectra of laboratory-made mixtures of 2 to 4 components.
- **Full Raman Spectra Library:** this includes all 1868 spectra.

The **Raman Spectra Library** is sold as an add-on for other **Analyze IQ SmartSearch** and **Analyze IQ Spectra Manager.**

Third Party Libraries: **Analyze IQ Limited** are resellers of a wide range of libraries and library bundles including: Polymers & Additives, Solvents, Pharmaceuticals, Forensics, Minerals & Inorganics, and many other industry-specific categories.

Download the list of contents of the Raman Spectra Library and contact us for information about third-party libraries at www.AnalyzeIQ.com

Analyze IQ® Lab Application Notes

1: Identifying Acetonitrile in Mixtures

Comparing **SIMCA** (implemented in Unscrambler V8.0) with two **Analyze IQ Lab** techniques. Using 74 samples: 53 with Acetonitrile and 21 without Acetonitrile. Computing average error from 5 runs of 10-fold cross-validation.

Acetonitrile Classification	% Error
Unscrambler: SIMCA	8.65±2.23
Analyze IQ: Weighted Spectral Linear Kernel	2.16±1.54
Analyze IQ: Spectral Attribute Voting	1.08±1.13

2: Chlorinated Solvents; Acetaminophen with Excipients

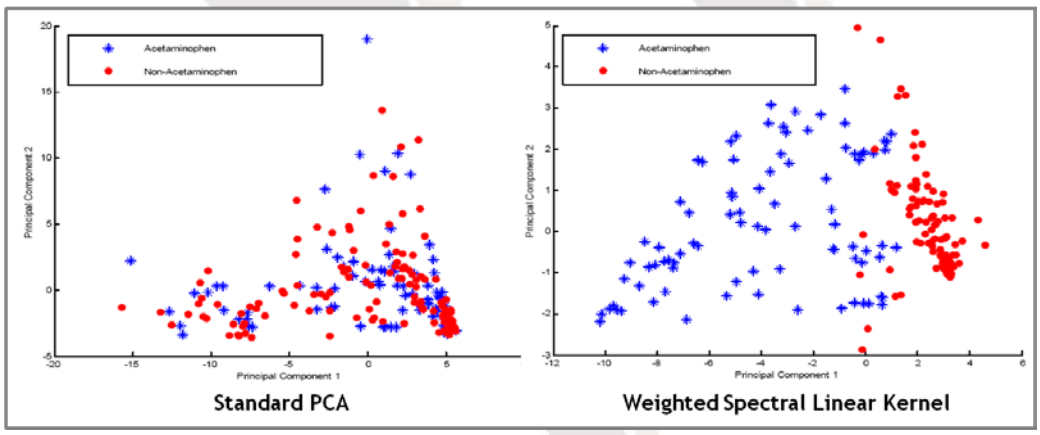
Comparing the standard technique of **Principal Component Regression** with **Analyze IQ Lab**'s kernel-based techniques for classification of a target in a mixture.

Dataset 1: Acetaminophen in various concentrations, mixed with common narcotic excipients; 217 samples in total. **Dataset 2:** Mixtures of chlorinated and non-chlorinated solvents; 230 samples in total. Results from 10 x 10-fold cross-validation.

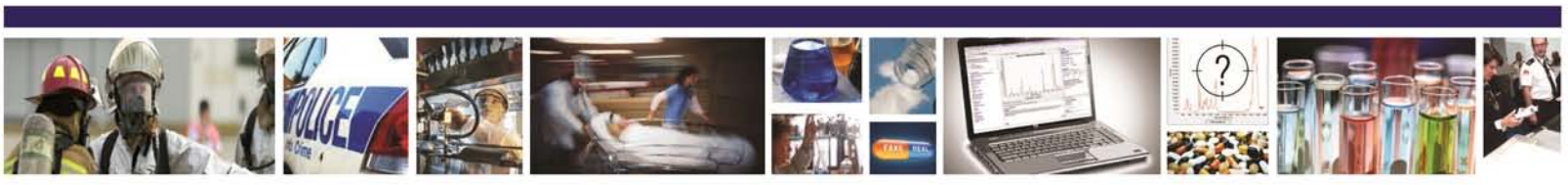
Dataset 1: Acetaminophen + Excipients	PCR Classification	Analyze IQ WS Lin Kernel	Analyze IQ WS RBF Kernel
% Error in Identifying Acetaminophen	4.47 %	1.93 %	0.41 %
Dataset 2: Chlorinated Solvents			
% Error in Identifying 1-1-1 Trichloroethane	18.73 %	2.43 %	2.39 %
% Error in Identifying Dichloromethane	7.87 %	0.96 %	0.87 %
% Error in Identifying Chloroform	13.49 %	0.91 %	0.87 %

3: Visualization of Clusters

Comparing the Principal Components found using standard **Principal Component Analysis** and using Analyze IQ's Weighted Spectral Linear Kernel. Analysis based on a dataset of mixtures with Acetaminophen (blue) and without Acetaminophen (red).



In both cases, we plot PC1 vs PC2. The PCs computed with Analyze IQ's Weighted Spectral Linear Kernel clearly separate the samples, whereas standard PCA does not.



Case Studies

1: Identification and Quantification of Cocaine using ATR-FTIR Spectrometry and Chemometics

Source: Study by National Institute for Criminalistics and Criminology, Drugs and Toxicology Dept., Brussels, Belgium and the University of Antwerp, Chemistry Dept.

Objective: To develop a technique to identify and quantify cocaine in seized drug powders using Attenuated Total Reflectance Fourier Transform Infrared (ATR-FTIR) spectrometry and multivariate analysis methods. ATR-FTIR spectrometry combined with chemometrics is a low-cost and less time-consuming technique in comparison with chromatographic techniques.

Cocaine is the second most commonly seized drugs of abuse entering Belgium, for local consumption and for distribution around Europe. **A challenging issue** when analysing cocaine samples **is the presence of many different adulterants and/or cutting agents** to increase drug volumes and dealer profits. Analyses of cocaine are routinely performed with conventional techniques: colour testing and/or infrared spectrometry for screening and chromatographic techniques for identification and quantification.

Solution: Circa two hundred cocaine powders were an analyzed using a mobile ATR-FTIR spectrometer, gas chromatography-mass spectrometer and gas chromatography-flame ionization detector. The percentage of cocaine in the samples ranged from 12% to 99%. Levarmisole, phenacetin, diltiarzerm, caffeine, hydroxyzine, boric acid, benzocaine and lidocaine were found as by-products. Chemometric analysis was performed on the collected spectral data using the **Analyze IQ® Limited software package, Analyze IQ Lab (Version 3)**. Several pre-processing techniques were tested followed by different chemometric methods to identify and quantify the target cocaine. The most promising models for identification were the Support Vector Machine with Weighted Spectral Linear Kernel (SVMW) and the Spectral Attribute Voting technique, both with an **average error of 0.5%**. For quantification, Principal Component Regression and SVMW were superior with an error prediction of respectively 11.2% and 8.9%.

Result: Based on the results it can be concluded that these models can be used to identify and quantify a wide variety of cocaine mixtures in routine laboratory analyses but also during on-site analysis by law enforcement, Moreover, the use of these models allows **high throughput, low-cost and quick identification and quantification** comparison to the conventional chromatographic techniques.

Reference: *Eliaerts, J. Van Durme, F. Meert, N. Samyn, N. Janssens, K. De Wael, K.: "Identification and Quantification of Cocaine using ATR-FTIR Spectrometry and Chemometrics" , 7th European Academy of Forensic Science Conference (EAFS2015), Prague, Czech Republic.* [Text reproduced with permission.]

Case Studies

2: Rapid Identification of Bacteria from Mass Spectra

Source: Study performed by Dr Pierre Alusta during his PhD research at the University of Arkansas Little Rock, using a commercial Analyze IQ® Lab license.

Objective: To identify unknown bacillus samples rapidly and reliably, including potentially harmful bacteria in a complex matrix such as airborne dust. The client developed a novel technique, Direct Impact Ionization, to ionize bacteria and obtain mass spectra.

Chemometrics was required to positively identify bacteria from their mass spectra.

Solution: Alusta (2012) evaluated and compared several different chemometric software packages for the task of identifying unknown bacilli from their mass spectra, including:

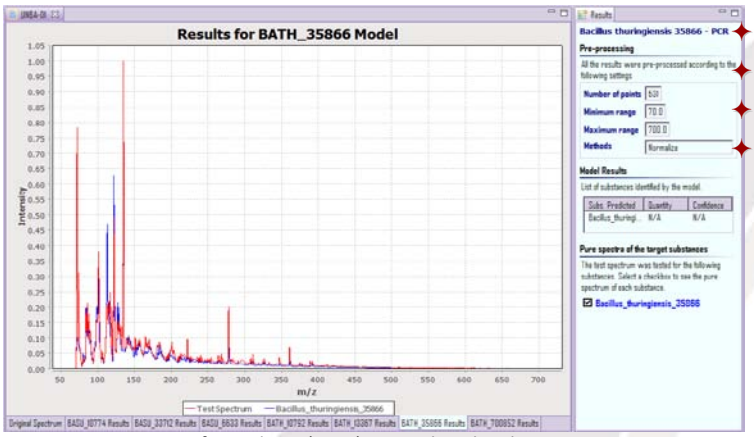


Figure 52 from Alusta (2012). Reproduced with permission.

- **OMNIPrint** V2.0
- **ArrayTrack**
- **Eigenvector SOLO** V6.5.1
- **Analyze IQ Lab** V2.0

In **Analyze IQ Lab**, one model was built and tested for each of the bacilli, using Principal Component Analysis with Linear Regression. The unknown was not included in the training set. A total of 19 models were applied to identifying the unknown bacillus sample.

Results: Unknown samples' spectra were analyzed and correctly identified rapidly with **Analyze IQ Lab**. To confirm the results, traditional determination methods were used in a microbiology lab, re-growing the unknown bacilli and the match found by **Analyze IQ Lab** on agar plates for two days and comparing the cultures (Alusta 2012).

The new methodology using **Analyze IQ Lab** was also evaluated for the task of detecting and identifying potentially harmful bacteria in a complex matrix such as airborne lab dust (Alusta 2012). Again, results were positive.

"The user-friendly Analyze IQ Lab yields robust results and has become an integral tool in our research lab."

- Dr Pierre Alusta, Little Rock, AR, USA

Comparison: **Analyze IQ Lab's performance surpassed that of the other packages**:

- Robust Results: *"Analyze IQ Lab™ v.2.0 software yielded robust results"*, whereas attempts with one alternative package "*looked promising at best"*, and another *"failed to provide numerical output describing close relatedness of data sets"* (Alusta, 2012).
- Ease of Use: *Analyze IQ Lab's user interface "is straightforward and allows the investigator to oversee the entire analysis".* Conversely, a popular competitor is described as having a "*highly-confusingly organized workflow"*, requiring *"a steep learning curve"* and *"help support is meager, if at all present."* (Alusta, 2012).

***Reference**: Alusta, P.: "Rapid Identification of Bacteria Using Mass Spectrometry and Spectral Pattern Recognition", PhD Dissertation, University of Arkansas at Little Rock, 2012.*

Information in this case study is reproduced with permission.

3: Analysis of Fuel Additive

Client: A company producing an innovative fuel additive.

Objective: Determine the concentration (0-300 ppb) of a fuel additive accurately and reliably, using SERS analysis. Comparing peak ratios, they had errors of **50 ppb** on average, and **150 ppb** worst-case.

Our Solution: Using **Analyze IQ® Lab** on a set of reference SERS spectra from the client, we experimented with multiple pre-processing and analysis methods. Best results were obtained using First Order Derivative preprocessing and a Support Vector Machine with Linear Kernel. We also identified that two spectra were mislabeled.

Result: We delivered Analyze IQ chemometric models that:

- Enabled the client to determine the concentration to within **7 ppb**
- Were a **7-fold improvement** on the client's own method
- Made the overall analysis of fuels feasible.

4: Custom Software for Anti-Counterfeiting

Client: A company producing a new anti-counterfeit system.

Objective: The client uses mixtures of up to 12 taggants to create a large number of different combinations of different markers for an anti-counterfeiting system, characterized using NIR and Mid-IR spectroscopy. Using peak-matching software, they were unable to identify the presence/absence of each of their taggants with high reliability in these extremely complex mixtures.

Our Solution: Using **Analyze IQ Lab**, the client was able to build qualitative chemometric models for each taggant and deploy these models on a server using **Analyze IQ RealTime.**

Result:

- The client was able to reliably identify the taggants in complex mixtures
- The solution is highly scalable: adding a new taggant doubles the number of mixtures they can make, but requires just one more taggant model to be added
- They built an instrument using **Analyze IQ RealTime** Cloud Edition, for use across a large area by operatives with minimal training to test for counterfeits.

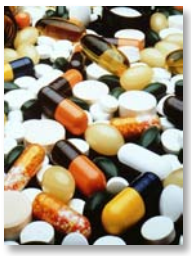
5: Verification of Prescription Drug Cocktails

Client: A company developing a product to verify liquid-based prescription drug cocktails.

Objective: For medical treatments such as chemotherapy, a custom cocktail of drugs is prepared for each patient. Because of the toxicity of such drugs and the potential risk of prescription errors, final verification is important. The client had developed a Raman-based system for characterizing the drug cocktail, but needed analytical software to verify that all components were correct.

Our Solution: Working with the client, we assisted with:

- Integrating **Analyze IQ RealTime** Desktop Edition into each pharmacy-based device
- Building a range of **Analyze IQ Lab** qualitative and quantitative models

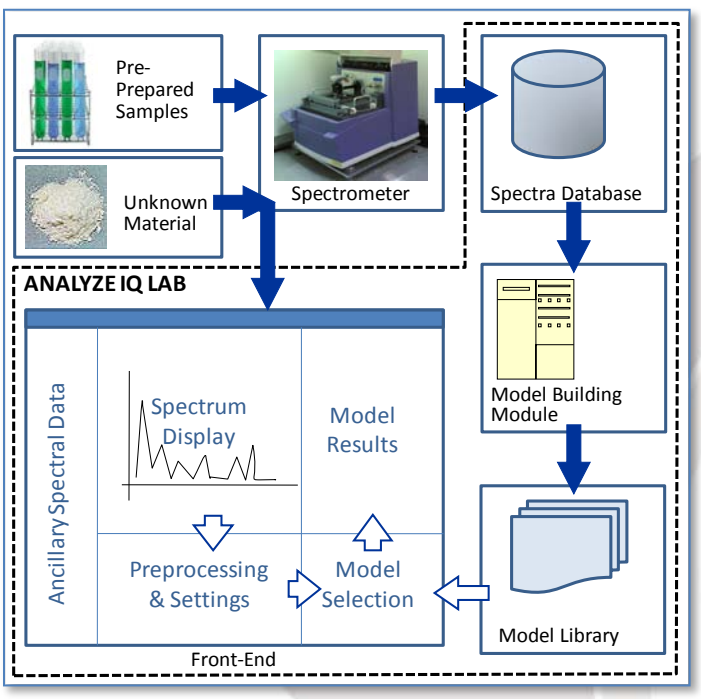


Result: The client was able to speed up bringing their product to market by using Analyze IQ models to perform analyses completely automatically in real-time, to:

- Verify that each expected component of the drug cocktail was present, and no others were
- Verify that each component had the expected concentration.

Technology Overview

We provide the world's most advanced software and services that enable commercial labs, academic researchers, and integrated service providers to rapidly and accurately analyze chemicals. Our products and services are used in Pharmaceutical, Healthcare, Petrochemical, Law Enforcement, Academic and other organizations.



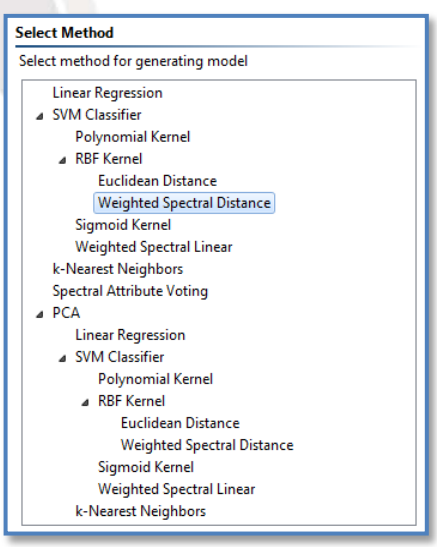
Our technology is used to analyze **all forms of spectral data** used to characterize materials, such as:

- Infra-Red (IR) & Near IR (NIR)
- Fourier transform IR (FT-IR)
- Raman
- X-Ray Fluorescence (XRF)
- Mass Spectrometry
- LIBS
- Surface Enhanced Raman(SERS)

In practical applications, mixtures of materials result in peaks in spectra that may mask or overlap each other, and there may be non-linear relationships between spectrum responses and questions of interest.

Analyze IQ® has a new **model-centred paradigm** for spectral data analysis:

- Prepare and store a range of materials of known composition
- Select from a wide range of chemometric analysis methods, to construct analytical models that compactly summarize all of the spectral data
- Unknown materials can be analyzed instantaneously and accurately using these analytical models that have been tuned to answer specific questions.



Benefits of our unique model-centered paradigm:

- It separates model-building from model usage
- You can 'package and deploy' expert chemometric knowledge encapsulated in models

Analyze IQ models encode all preprocessing and analysis information in them, which eliminates risk in performing analyses with them or in transferring models from the lab to production use.

WWW.ANALYZEIQ.COM

Analytical and Software Services

In addition to developing the world's most advanced chemical analysis software, we provide a range of complementary services that are built on our core expertise. Our services are used in Pharmaceutical, Healthcare, Petrochemical, Law Enforcement, Academic and other organizations.

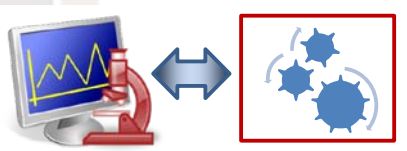
Our services include:

- Custom software development for special-purpose applications
- Custom analysis solutions based on **Analyze IQ® RealTime**
- Bespoke model development and validation
- Software training
- OEM licensing of the Analyze IQ software suite
- Custom versions of the Analyze IQ software product suite, such as with additional features requested by a client or support for extra file formats

Custom Software Development and Analysis Solutions

The **Analyze IQ** technology is an ideal fit for applications requiring fast and high-accuracy testing of complex analytes, such as anti-counterfeiting taggants, biomedical diagnostic markers, and process analytical technologies. It is used with all forms of spectral data, including data from spectroscopic techniques such as infra-red (IR), near infra-red (NIR), Fourier transform IR (FT-IR), Raman, x-ray fluorescence (XRF), Mass Spectrometry, LIBS, SERS, and others.

We have extensive experience of high-quality software development, and evidenced by our software product range. We can provide you with that experience in:



- Integrating **Analyze IQ RealTime** into your software or process: operating on embedded devices, desktop systems, or in a cloud server environment
- Developing custom software solutions for your application
- Development of custom interfaces for instrumentation

Custom Training Courses

Analyze IQ Limited provides on-demand customized software training for clients, at our offices in Ireland or at clients' premises anywhere in the world. A typical one-day or two-day training course will cover:

- Basic concepts of chemometric modeling
- Details of the chemometric analysis methods provided in the Analyze IQ software, including key features and practical advice
- How to use Analyze IQ software to build, evaluate, and work with chemometric models
- Understanding & improving model performance
- Hands-on practice with the Analyze IQ software suite, optionally using data provided by the client.

Training courses are developed and delivered by our senior staff, including our CEO who has held a held a tenured academic position in the National University of Ireland, and has over a decade of experience in university teaching and research.

An example is our Pittcon 1-day course, "Modern Methods for Chemometric Analysis", which has run every year at Pittcon for the past several years and is always popular and highly rated by participants.

Bespoke Model Development and Validation

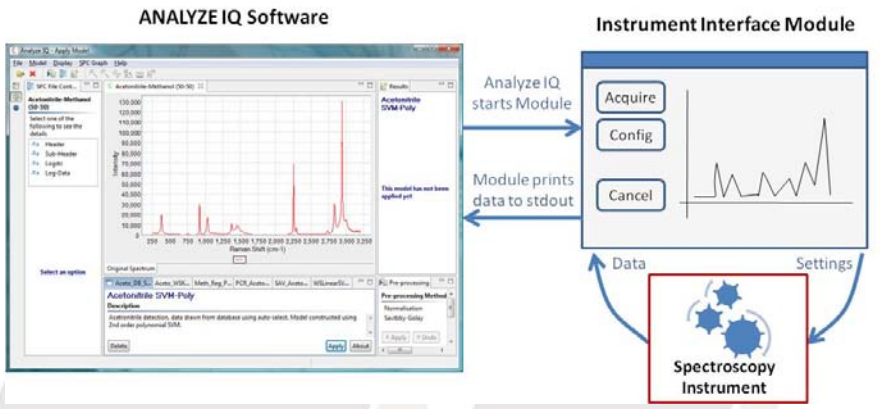
As well as being expert software developers, we are expert chemometricians. We can help you with:

- Validation and analysis of your spectroscopy data
- Bespoke chemometric modeling using Analyze IQ® Lab

Instrument Interfaces

The **Analyze IQ software suite** supports direct interaction with spectroscopy systems via **Analyze IQ Instrument Interface Modules.** These may be developed by the instrumentation manufacturer or by **Analyze IQ Limited**. Key features include:

- Modules may be implemented rapidly and easily by the manufacturer/vendor by re-engineering existing software – in our experience, this is often done in less than a day!
- Modules may be developed in any programming language, as long as they can be deployed on the Operating Systems on which Analyze IQ software runs
- Data is exchanged in a simple text/XML format via the command line
- No need for COM, OLE or other such technologies; this simplifies both testing development greatly
- All Instrument Interface Modules are tested and certified by Analyze IQ Limited prior to deployment.



Partnership Opportunities

We are always interested in developing new partnerships with innovative and forward-looking companies:

- Spectroscopy instrumentation manufacturers
- Vendors and system integrators
- Solution providers in all application domains.

Contact Us to Discuss Our Services & Partnership Opportunities

To **download** our software products, software updates, user manuals, white papers and publications, go to the **User Area** http://www.AnalyzeIQ.com.

To get a fully-functional short-term **evaluation license** for any of the products in the Analyze IQ software suite, please register on our website.

For information on **extending** an evaluation license or **purchasing** a full license, please contact our Sales Department by phone or send email to sales@AnalyzeIQ.com.

For help and **technical support** queries, phone us or send email to support@AnalyzeIQ.com.

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