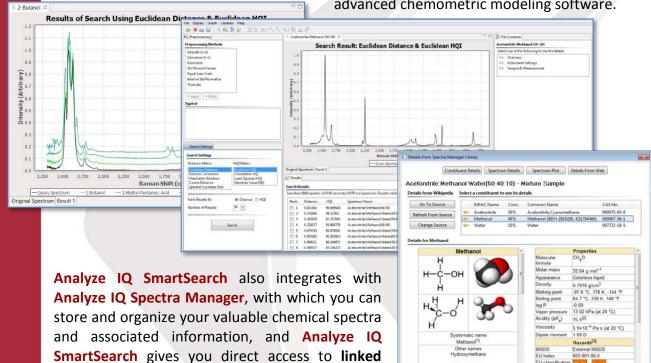# Analyze IQ® SmartSearch
Fast Spectrum Searching and Mixture Analysis

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

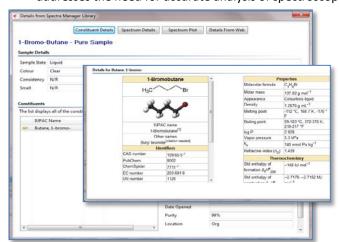## Download a free evaluation of Analyze IQ SmartSearch or find out more at www.AnalyzeIQ.com

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
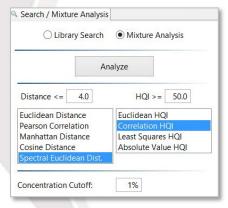✦ Hit Quality Index metrics: Euclidean HQI, Correlation HQI, Least Squares HQI, Absolute Value HQI

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

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