Product note: WiRE software
PN229(EN)-01-A November 2019

RENISHAW
apply innovation™

WiRE™ Software - Spectrum Search

Identification of pure compounds and mixtures

The identification of unknown materials is one of the key uses of Raman spectroscopy. This is normally done with the aid of libraries of spectra. Renishaw's WiRE software, with Spectrum Search, offers access to application-specific spectral libraries and supports a wide range of commercially available ones, enabling you to:

- Identify pure materials
- Identify an unlimited number of components within a mixture using a fully automated process
- Identify mixtures from residual spectra after the subtraction of 'major' components
- Manually mask spectral regions to target identification towards unknown Raman bands
- Build your own custom library, specific to your application

Identify the composition of a mixture

Performing a conventional library search on a spectrum from a mixture often gives unreliable results, as no single spectrum within the library matches well. Manual re-searching of the residual spectrum, after the first hit has been subtracted, is one method to analyse mixtures. While this can be an effective approach, it requires significant user input and can be subjective. With WiRE software you have the option to automate this process by simply defining the maximum number of components that may be in the mixture. The software provides you with the possible compositions of a sample and identification can be performed using multiple libraries at the same time, meaning you only need to analyse once.

Example: analysis of a pharmaceutical tablet

We analysed a pharmaceutical tablet with an inVia™ confocal Raman microscope, using 785 nm excitation and, to achieve a mixed spectrum of multiple components, a low magnification objective lens.

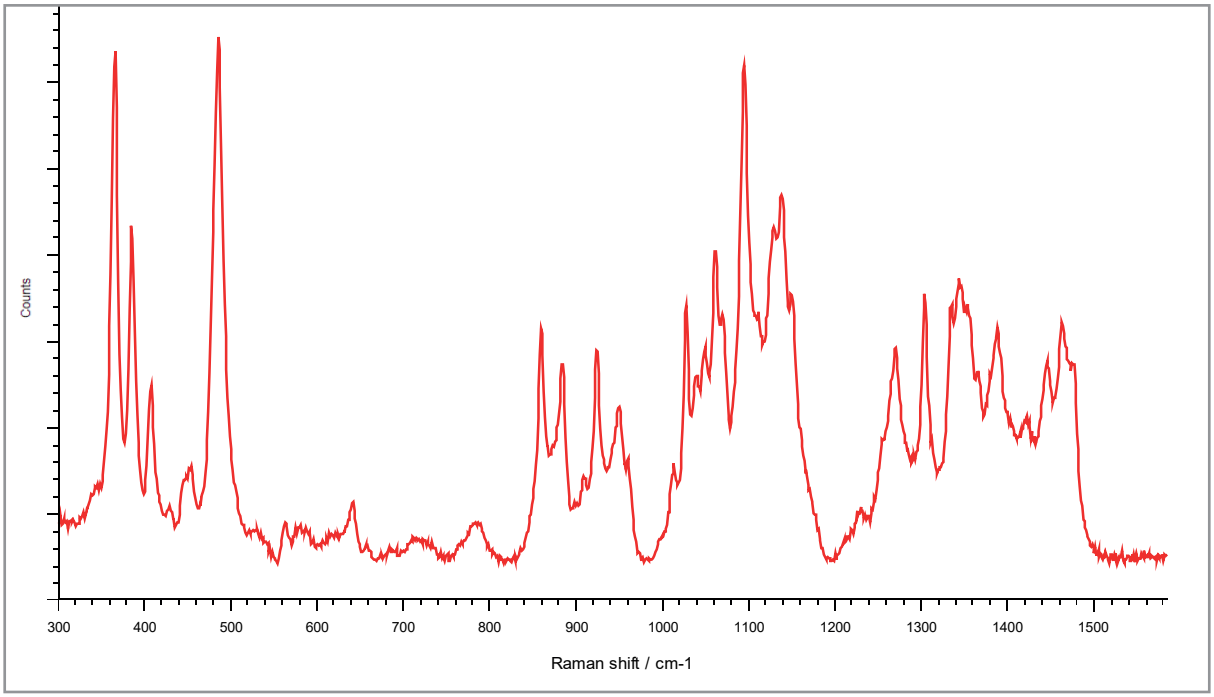
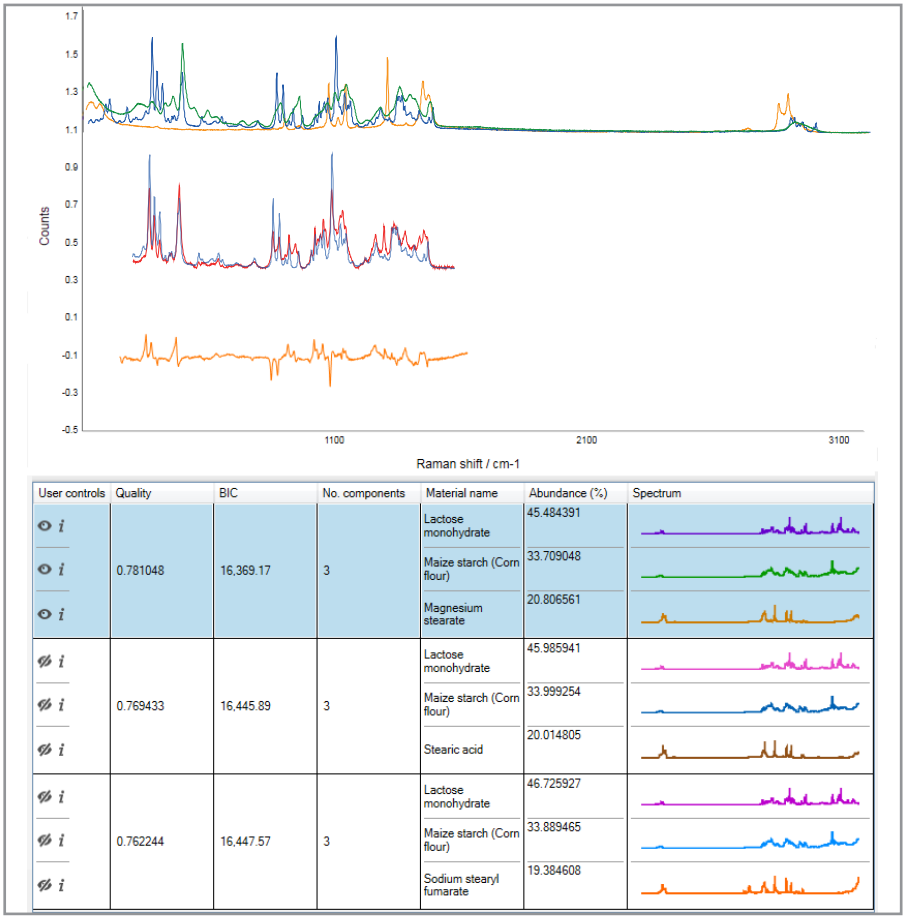


Figure 1. A mixed spectrum of unknown materials from a low spatial resolution tablet analysis

We analysed the spectrum using the 'Automatic' method, requesting a maximum of three components.

The best match was for lactose monohydrate, maize starch and magnesium stearate (Figure 2). The other matches were also for the combination of lactose monohydrate and maize starch, but with either stearic acid or sodium stearyl fumarate. We can therefore be confident that lactose monohydrate and maize starch are present, along with a stearate-related component (most likely magnesium stearate, based on the automatic results).

Figure 2 also shows the spectrum broken down into the components of the best match.



User controls	Quality	BIC	No. components	Material name	Abundance (%)	Spectrum
	0.781048	16,369.17	3	Lactose monohydrate	45.484391	
				Maize starch (Corn flour)	33.709048	
				Magnesium stearate	20.806561	
	0.769433	16,445.89	3	Lactose monohydrate	45.985941	
				Maize starch (Corn flour)	33.999254	
				Stearic acid	20.014805	
	0.762244	16,447.57	3	Lactose monohydrate	46.725927	
				Maize starch (Corn flour)	33.889465	
				Sodium stearyl fumarate	19.384608	

Selected result component overlay (at abundance ratios)

Unknown spectrum overlaid with fit result

Residual

Top result (Highest quality and low BIC)

2nd result

3rd result

Figure 2. Analysis of the pharmaceutical spectrum

- 'Quality' measures the agreement between the fit result and the unknown spectrum
- The Bayesian information criterion (BIC) is a goodness-of-fit measure that is lower for results that describe the compositions in a simpler way
- Abundance gives the fraction of the unknown spectrum that each library spectrum comprises

A combination of the 'Quality' increasing and BIC decreasing (top group hit result in Figure 2) indicates the highest confidence result.

One advantage of this approach is that it doesn't limit how many components can be found. Also, the metrics give a clear comparison between the possible results, helping you to determine which is the optimal set of materials.

Renishaw plc

Spectroscopy Products Division
New Mills, Wotton-under-Edge,
Gloucestershire GL12 8JR
United Kingdom

T +44 (0) 1453 524524
F +44 (0) 1453 524901
E raman@renishaw.com

www.renishaw.com

RENISHAW
apply innovation™

Use library searching with Renishaw's complementary tools

Build your own library with ease.

Library search results are only as good as the contents of the libraries. Renishaw provides an extensive range of high-quality general and application-specific libraries. However, you sometimes need to build your own library of materials of interest to you.

Renishaw's Library Manager makes building libraries easy. Generate a new empty library, name it, and directly add spectra into it, either individually or as a group. Once you have created the library, you can add more spectra with a single mouse-click, without needing to configure any settings. Combining your own libraries with commercially available ones often provides the most comprehensive solution to material identification.

Optimise your data with Intelligent Fitting baseline removal

Library search algorithms have a range of methods for coping with variations in the baseline of your spectra. However, removing the baseline by pre-processing often gives better results.

Renishaw's Intelligent Fitting method automatically targets the broad backgrounds that can be produced by sample fluorescence. Raman bands—both sharp and broad—are left untouched, resulting in great quality spectra that are ideal for library searching.

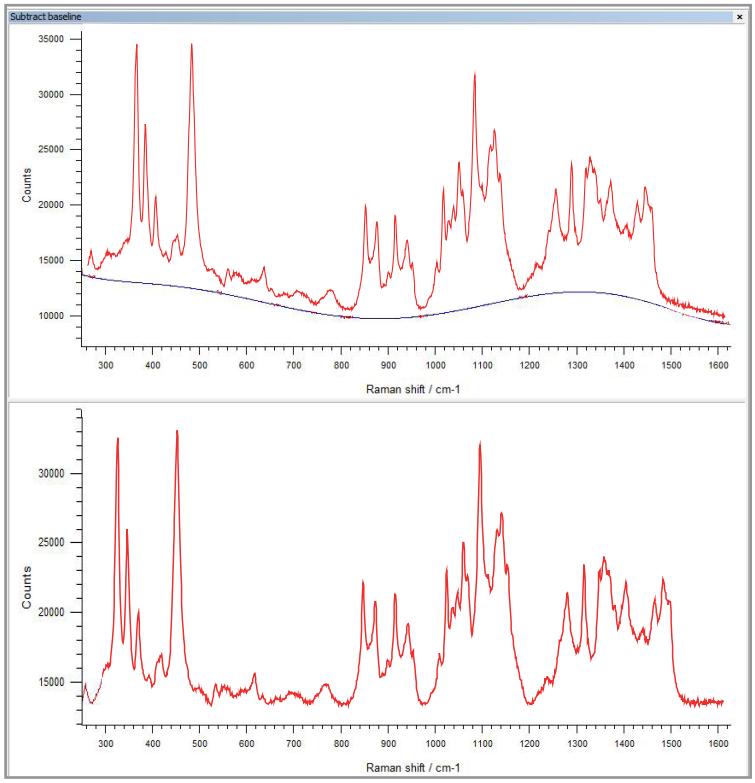


Figure 3. Single click Intelligent Fitting baseline removal example (top - original spectrum with intelligent baseline shown in blue, bottom - baseline removed result)

Intelligent Fitting is just one of many processing tools in Renishaw's WiRE software that ensure you can get the best quality data.

Note: Spectrum Search is an option in the WiRE software, with mixture analysis available in WiRE 5.3 and above.

Renishaw. The Raman innovators

Renishaw manufactures a wide range of high performance optical spectroscopy products, including confocal Raman microscopes with high speed chemical imaging technology, dedicated Raman analysers, interfaces for scanning electron and atomic force microscopes, solid state lasers for spectroscopy and state-of-the-art cooled CCD detectors.

Offering the highest levels of performance, sensitivity and reliability across a diverse range of fields and applications, the instruments are designed to meet your needs, so you can tackle even the most challenging analytical problems with confidence.

A worldwide network of subsidiary companies and distributors provides exceptional service and support for its customers.

Please visit www.renishaw.com/raman for more information.