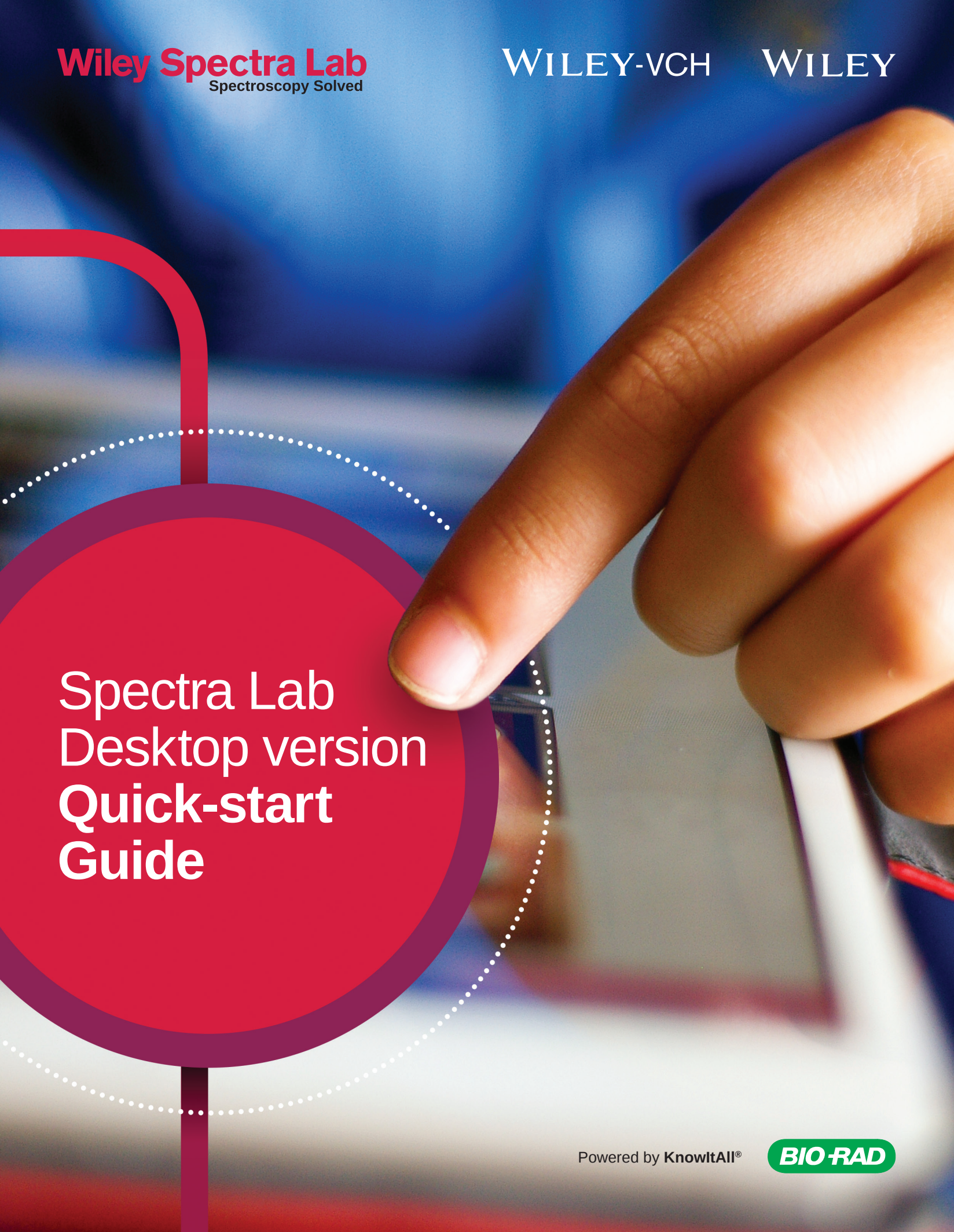
Wiley Spectra Lab
Spectroscopy Solved

WILEY-VCH WILEY



Spectra Lab Desktop version **Quick-start Guide**

Powered by **KnowItAll®**

BIO-RAD

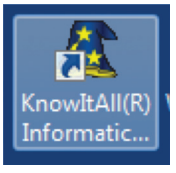
Desktop version Quick-start Guide

Welcome. This guide is to get you started with Wiley Spectra Lab. With millions of spectra and advanced spectroscopy software, Wiley Spectra Lab gives you the best chance of identifying unknown compounds with high confidence in the results. If you should require further assistance or would like a full demonstration of the capabilities of Wiley Spectra Lab, please email us and we will be happy to assist you.

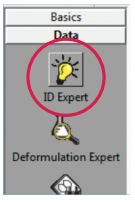
Contents

ID Expert™ (IR/Raman)

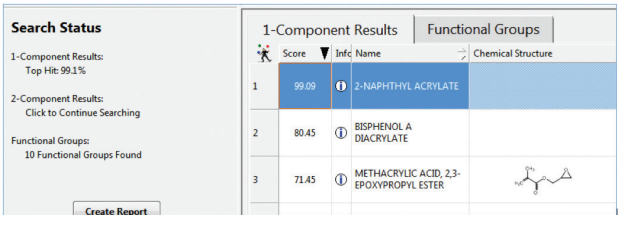
Open Wiley Spectra Lab by double-clicking on the “Know-it-All” icon on your desktop.



Select ID Expert in the left-hand toolbar and you’ll immediately be asked for a data file.

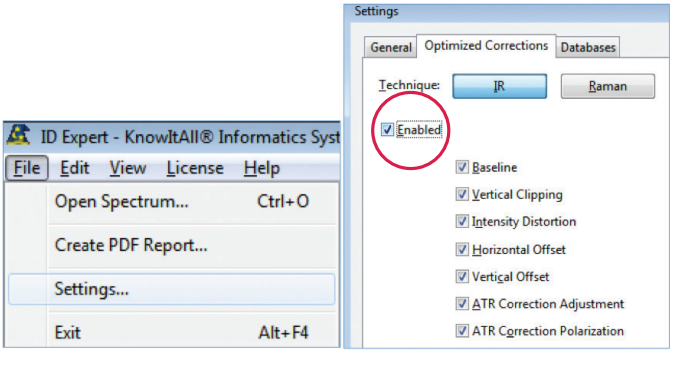


Select the appropriate file and click “open”. ID Expert will recognize if the file is an IR or Raman spectrum and begin to search for a match in the databases. The results will be displayed in the results window. A score of over 90% and ideally over 95% is a good match.



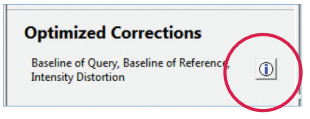
On the top toolbar, you can change the view to Offset/Overlay/Stacked View, box zoom, and scale.

If the search finishes without finding a reasonable 1-component hit, it will then run a 2-component, then 3-component and so on. If no hit is found, make sure “Optimized Corrections” is enabled for the appropriate technique in the “Optimized Corrections” tab under File->Settings.

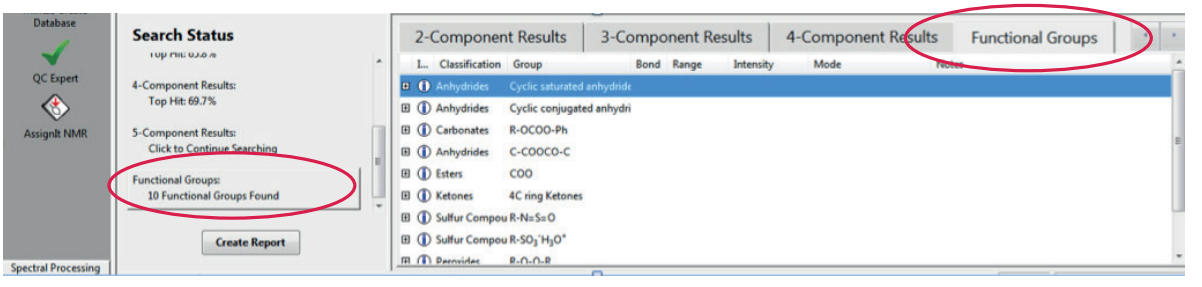


ID Expert™ (IR/Raman)

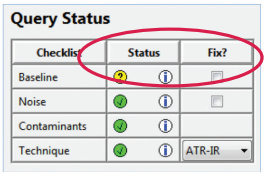
Optimized corrections is a feature unique to Spectra Lab that automatically and instantly performs multiple data and spectral corrections, which would otherwise require lengthy, manual data processing by an expert in each technique. To see which corrections are performed on any spectrum, click the “i” button.



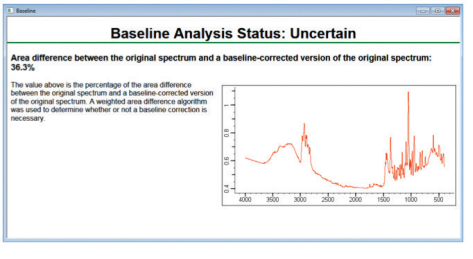
If no hit is found in any search, the “Functional Groups” analysis will suggest which functional groups could be present to help with further analysis through other techniques.



If a yellow question mark appears in the “Query Status” area, Spectra Lab is telling us there is a problem with one or more components of the spectrum.



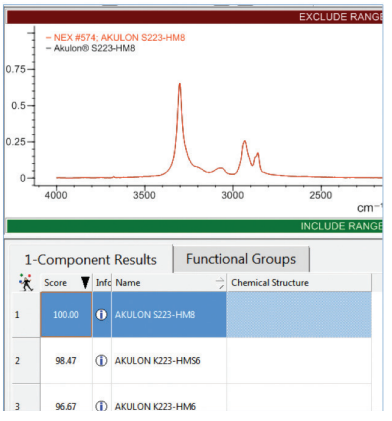
Click the “i” icon to see what the problem is



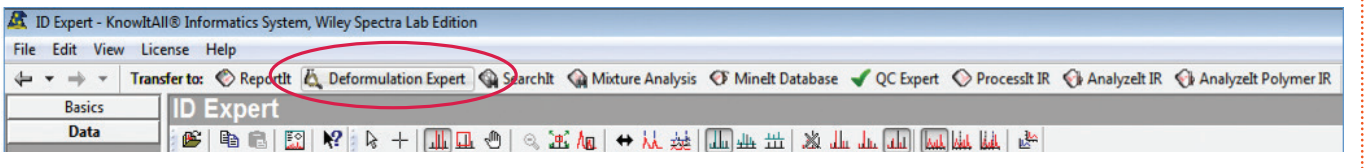
Then check “Fix” to use have Spectra Lab correct the problem. ID Expert then restarts the query with the corrected spectrum.

Deformulation Expert™ (IR)

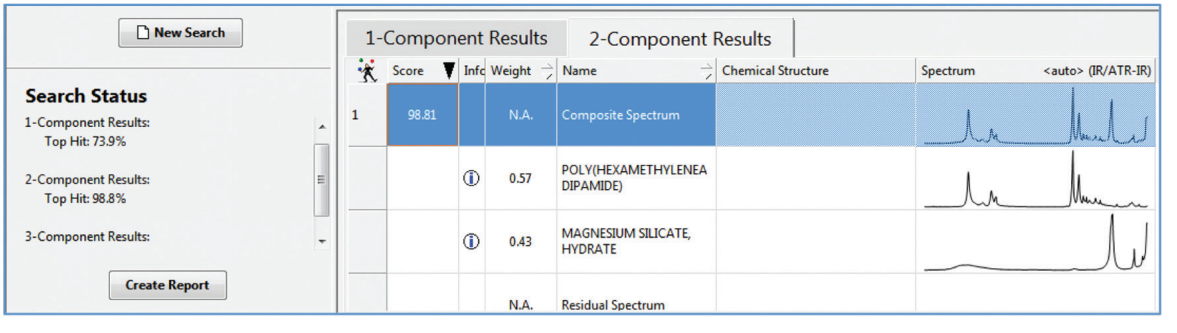
Deformulation Expert is used to examine the components of a formulated product by IR spectroscopy. Open a spectrum in ID Expert and let the spectral search run. This will match the IR spectrum of the complete product.



Transfer the query to Deformulation Expert by clicking “Transfer to: Deformulation Expert”



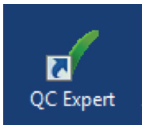
The deformulation analysis will then show the breakdown of the components of the sample.



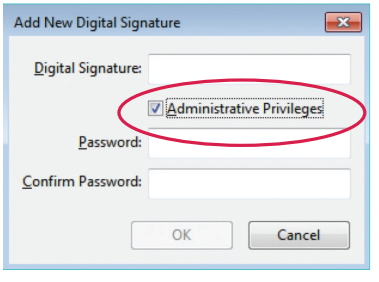
QC Expert™ (IR)

One-Time Configuration

Your copy of Wiley Spectra Lab needs to have an Administrator account configured. Perform these steps before running any samples.



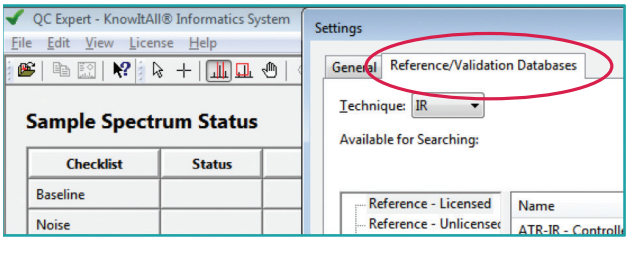
After loading QC Expert for the first time, you will get a “There are no users defined for this application” message. Click “OK”, add your digital signature and password, make sure “Administrative Privileges” is checked then click “OK”.



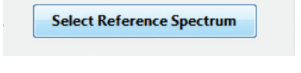
Add the relevant details and verify. Then add any user accounts in the same way but uncheck “Administrative Privileges”.

Setting a Reference Spectrum

To select the reference database, click File->Settings and select the one you want to use on the “Reference/Validation Databases” tab, then click “OK”.

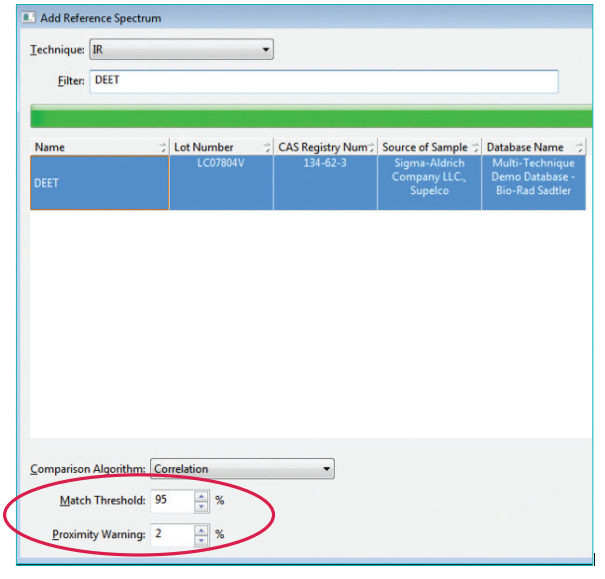


To select a reference spectrum, click “Select Reference Spectrum”.



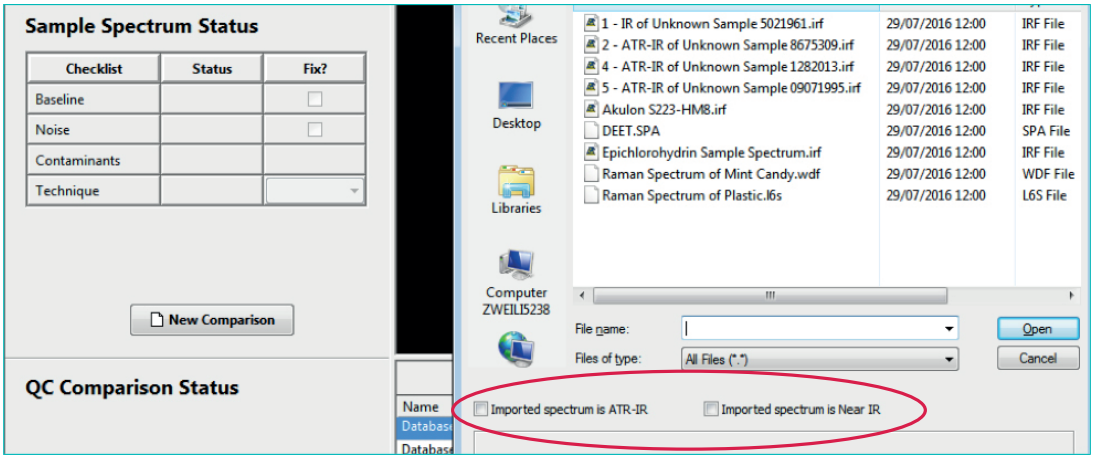
QC Expert™ (IR)

Login as administrator then search for the desired spectrum in the reference database. Set the algorithm, match threshold, and proximity warning parameters in the lower left, then click “OK”.



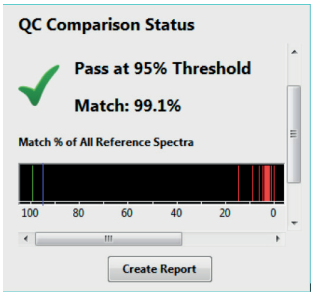
Running a sample

To run a sample, click on “New Comparison” and if the sample is ATR-IR or NIR, this can be indicated. Click “OK” and the analysis will run.

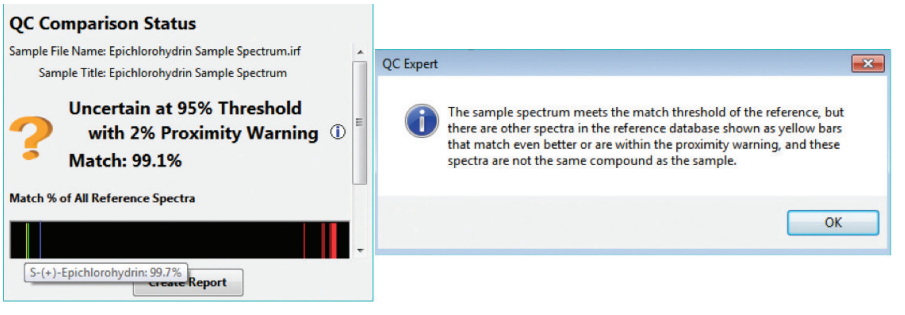


QC Expert™ (IR)

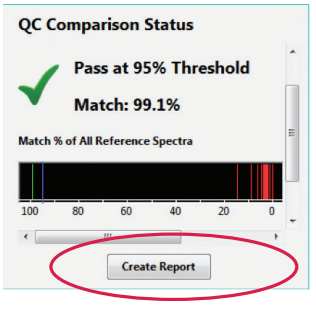
The "QC comparison status" will then show "pass" "fail" if the sample and reference spectra match or don't match.



"Proximity warning" is displayed if the sample and reference spectra match but the sample spectrum also matches another spectrum that isn't the chosen reference spectrum. Click "i" for more information. Hovering over the colored bars will display the names of the spectra that are within the proximity warning parameter.



To create a digitally-signed report Click on "create report", select your name from the "digital signatures" drop-down, enter the password, fill out the sample information, then click "OK".

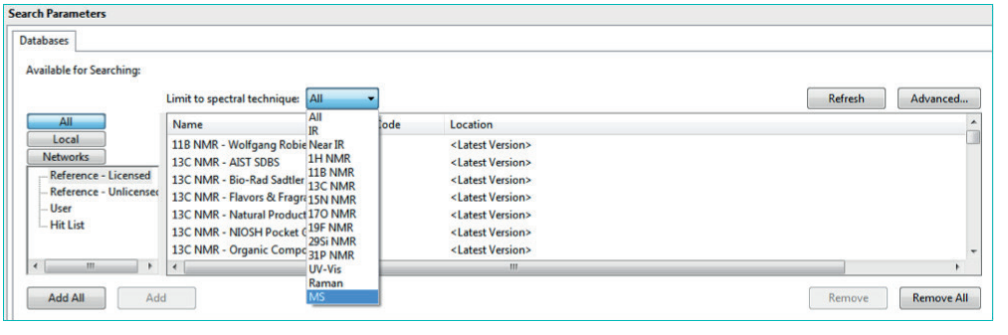


SearchIt™ & MineIt™ for GCMS

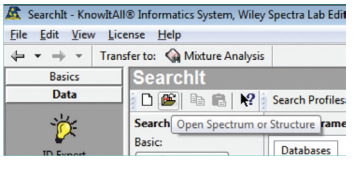
Open Wiley Spectra Lab by double-clicking on the “Know-it-All” icon on your desktop.

Select SearchIt in the left-hand toolbar.

Set “Limit Spectral Technique” to MS then click “Remove All” then “Add All”. This activates only the MS databases for the search.

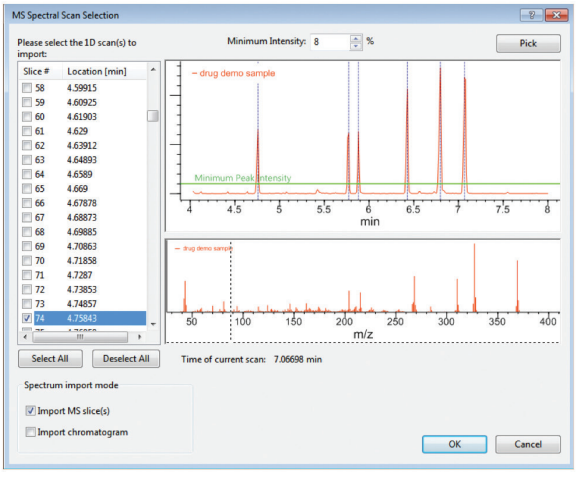


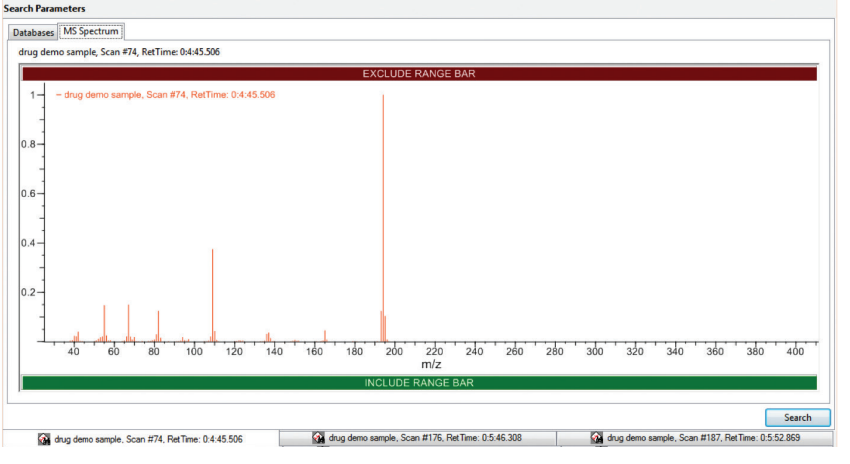
Click the “Open Spectrum or Structure” button on the top SearchIt toolbar to open the spectrum file, select the desired file then click “Open”.



The GCMS chromatogram or total ion chromatogram (TIC) is shown. Set the minimum peak intensity by dragging the green bar up or down to include or exclude peaks.

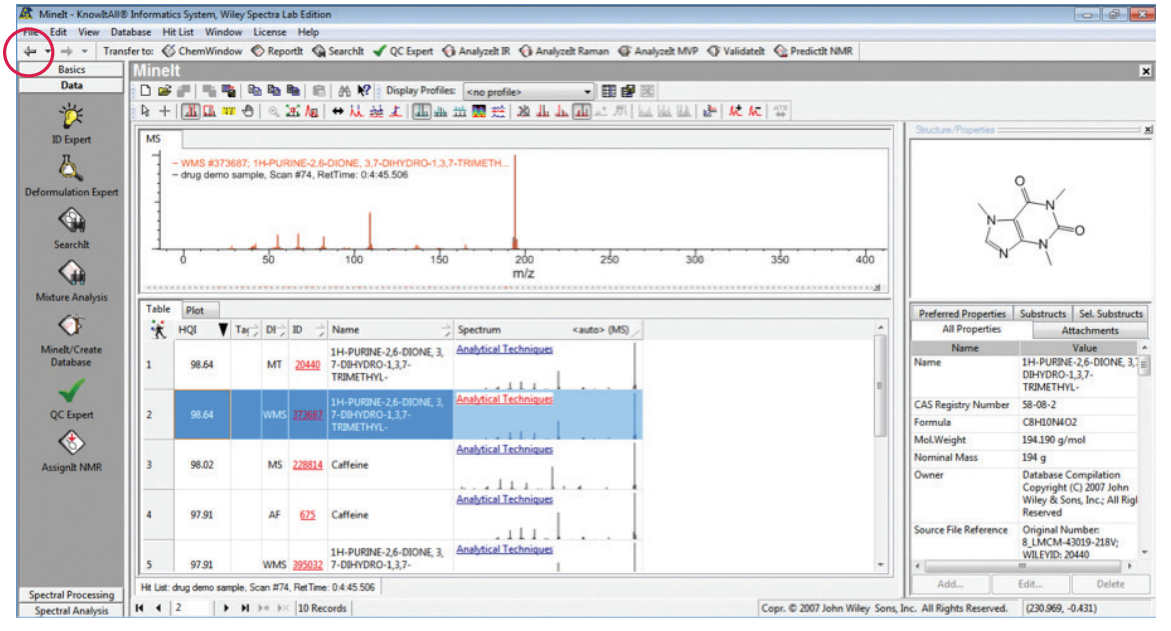
Click “OK” to import all the MS slices. Select the MS slice that you want to identify and click “Search” to start the search.





SearchIt™ & MineIt™ for GCMS

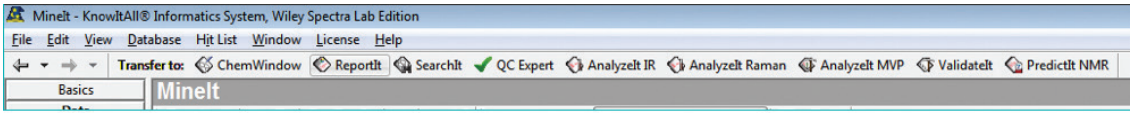
Hits are ranked according to hit quality index (HQI) and spectrum information including synonyms for the selected matching spectrum is displayed on the right.



To identify the next MS slice, click the “back” button on the top left, select the spectrum and click “Search” to start the search.

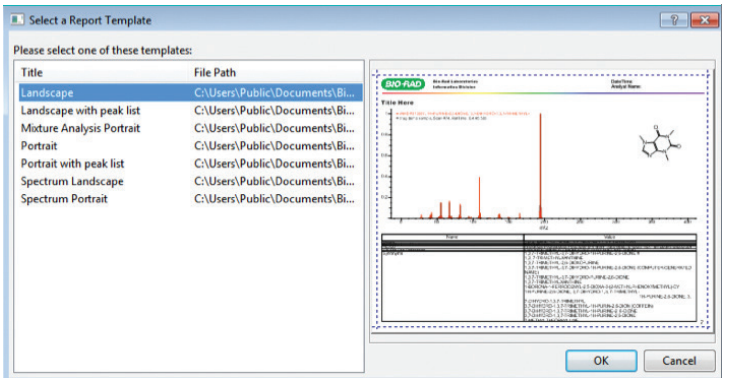
On the top toolbar, you can change the view to Offset/Overlay/Stacked View, box zoom, and scale.

To make a report, click “Transfer to: ReportIt” on the top toolbar.

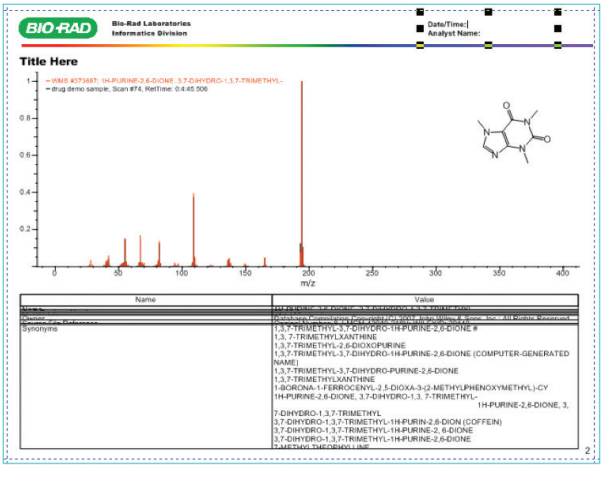


SearchIt™ & MineIt™ for GCMS

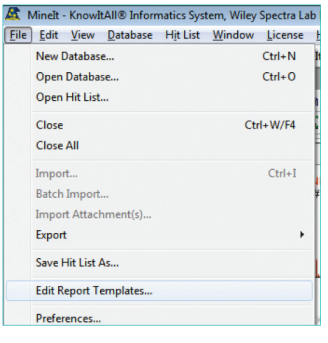
Select the type of report template to use and click “OK”



Double-click on “Title here” on the top left to enter a title and double click on “Date/Time” or “Analyst Name” on the top right to enter the corresponding details.

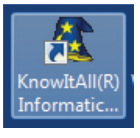


Report templates can be customized, including the layout, by clicking “Edit Report Templates” in the “File” menu in the main “MineIt” window.



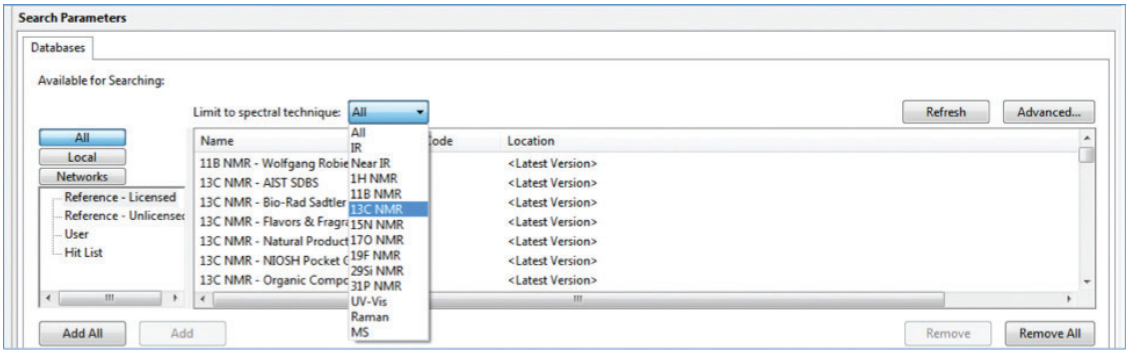
SearchIt™ & MineIt™ for NMR

Open Wiley Spectra Lab by double-clicking on the “Know-it-All” icon on your desktop

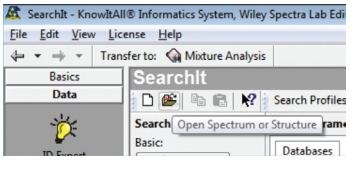


Select SearchIt in the left-hand toolbar.

Set “Limit Spectral Technique” to the appropriate NMR technique then click “Remove All” then “Add All”. This activates only the NMR databases for the search.

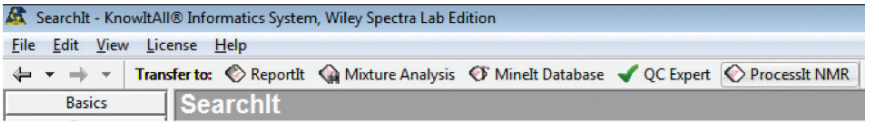


Click the “Open Spectrum or Structure” button on the top SearchIt toolbar to open the spectrum file, select the desired file then click “Open”.

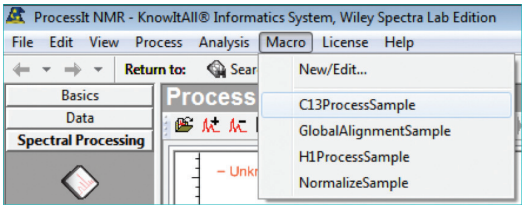


SearchIt™ & MineIt™ for NMR

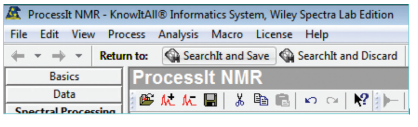
To process the spectrum, click “Transfer to ProcessIt NMR”



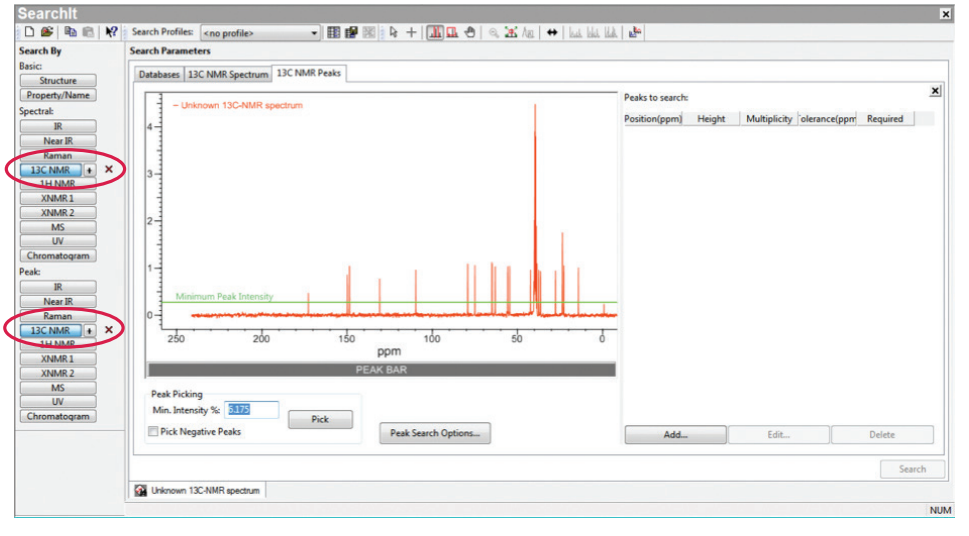
To apply processing macros, click “Macro” and either create or edit a macro or apply an existing one. For 13C NMR, the in-built “C13ProcessSample” can be used for minor spectral corrections.



When processing is complete, click “SearchIt and Save” on the top toolbar.

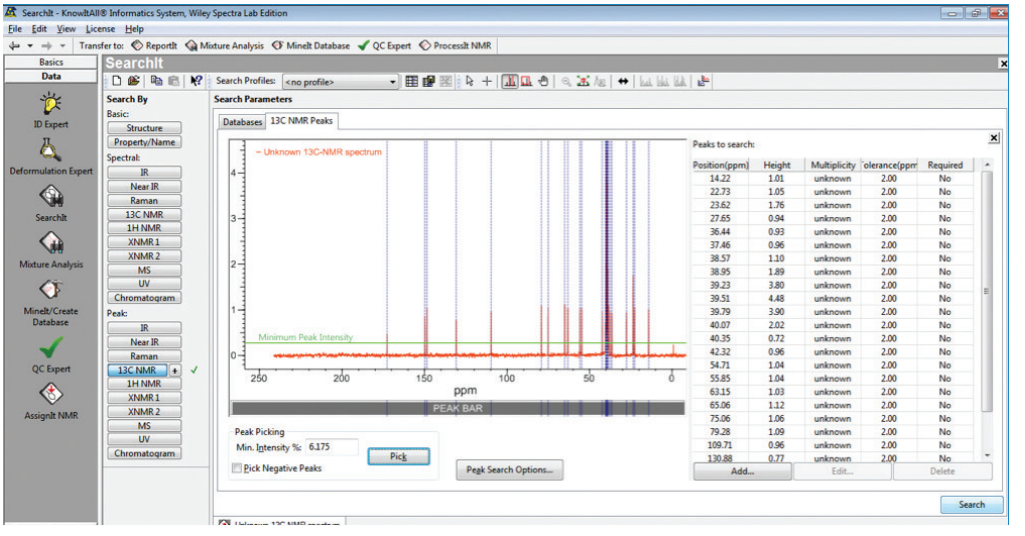


On the “SearchIt” screen, click the corresponding technique under “Peak” on the left-hand side, then click the corresponding technique under “Spectral” in the menu above to deselect it. Set the minimum peak intensity by either typing the value into the “Min. Intensity” box or by dragging the green line to the desired position, then click “Pick” to pick the peaks.



SearchIt™ & MineIt™ for NMR

A peak list will appear on the right and to start the search click “Search” under the peak list.



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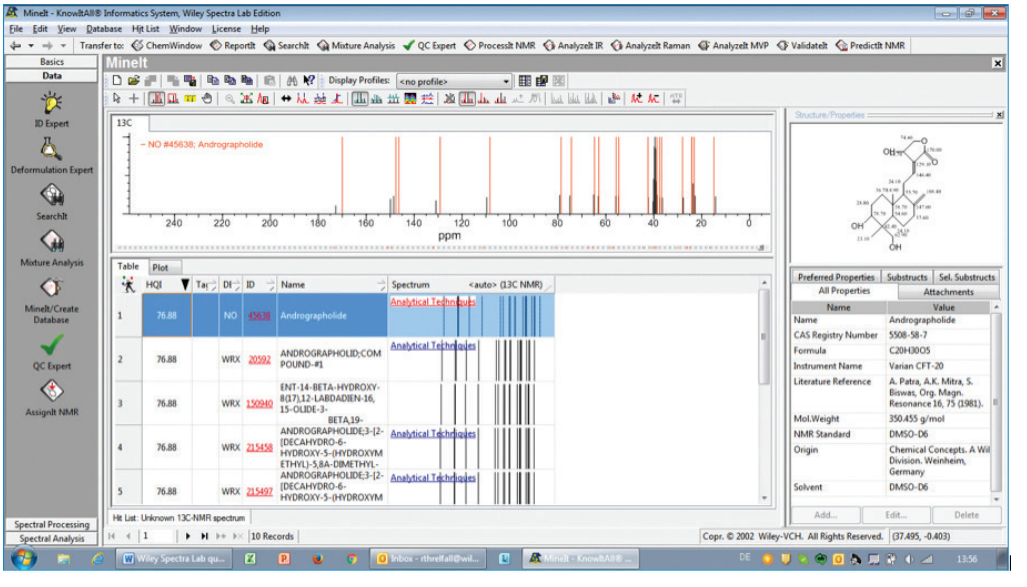

A hit quality index of >50 indicates a relatively good hit. Where some peaks don’t overlap well between reference and sample spectra, additional analysis with other techniques is recommended.

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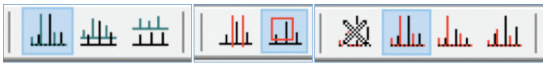
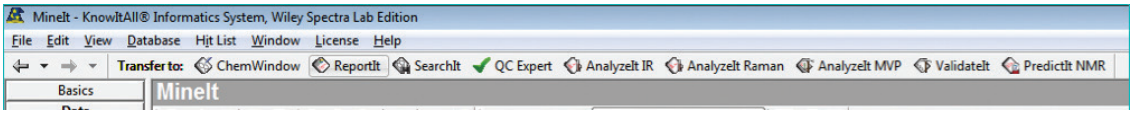
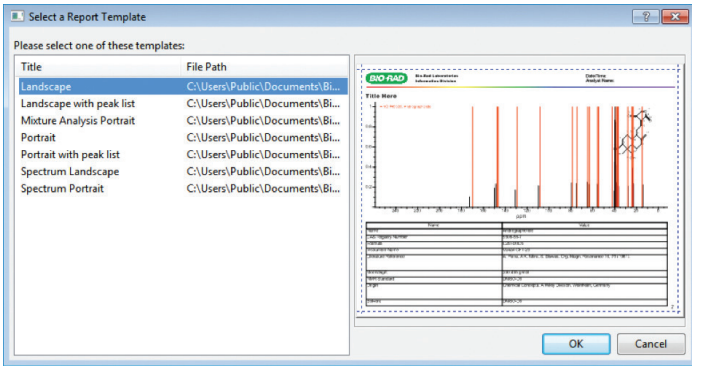


SearchIt™ & MineIt™ for NMR

To make a report, click “Transfer to: ReportIt” on the top toolbar.



Select the type of report template to use and click “OK”



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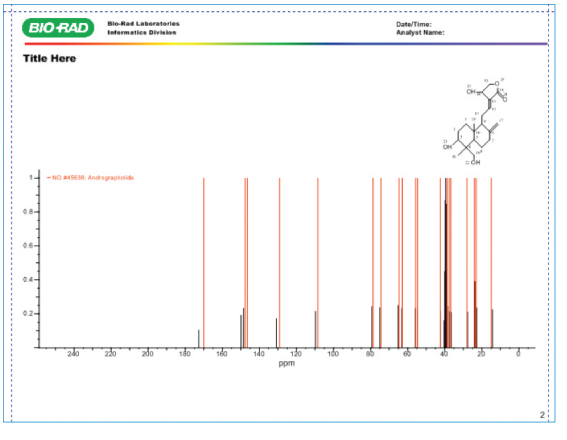

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