

Spectra Lab
Desktop version
Quick-start
Guide

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

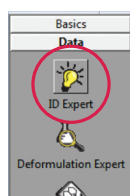
● ID Expert™ (IR/Raman)	3
● Deformulation Expert™ (IR)	5
● QC Expert™ (IR)	6
● SearchIt™ & MineIt™ for GCMS	9
● SearchIt™ & MineIt™ for NMR	13

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.



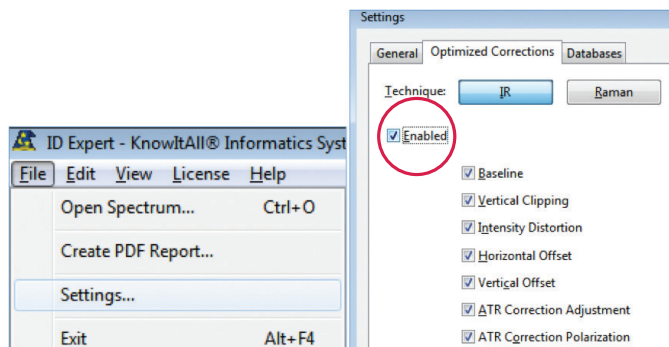
Select the appropriate file and click “open”. ID Expert will recognize if the file is an IR or Raman spectrum and begin to search for a match in the databases. The results will be displayed in the results window. A score of over 90% and ideally over 95% is a good match.

Score	Info Name	Chemical Structure
99.09	2-NAPHTHYL ACRYLATE	
80.45	BISPHENOL A DIACRYLATE	
71.45	METHACRYLIC ACID, 2,3-EPOXYPROPYL ESTER	

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

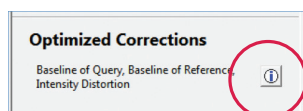


If the search finishes without finding a reasonable 1-component hit, it will then run a 2-component, then 3-component and so on. If no hit is found, make sure “Optimized Corrections” is enabled for the appropriate technique in the “Optimized Corrections” tab under File->Settings.

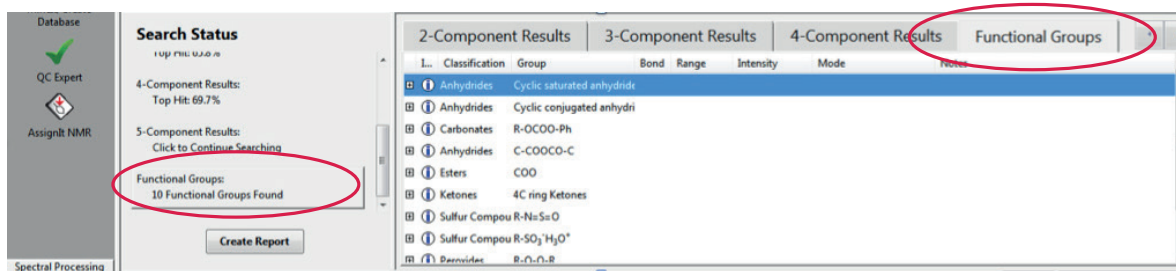


ID Expert™ (IR/Raman)

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.



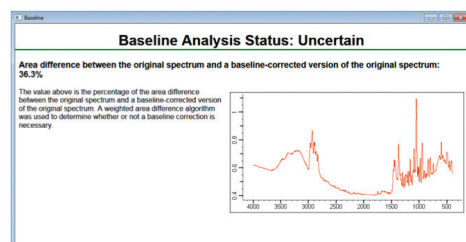
If **no hit is found** in any search, the “Functional Groups” analysis will suggest which functional groups could be present to help with further analysis through other techniques.



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.

Checklist	Status	Fix?
Baseline	?	<input type="checkbox"/>
Noise	✓	<input type="checkbox"/>
Contaminants	✓	<input type="checkbox"/>
Technique	✓	<input type="checkbox"/>

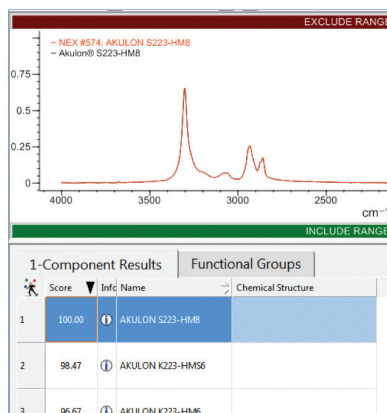
Click the “i” icon to see what the problem is



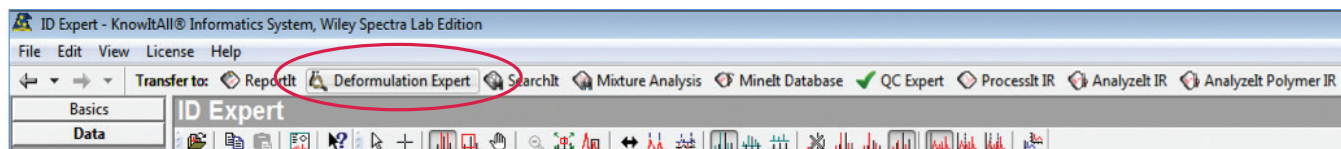
Then check “Fix” to use have Spectra Lab correct the problem. ID Expert then restarts the query with the corrected spectrum.

Deformulation Expert™ (IR)

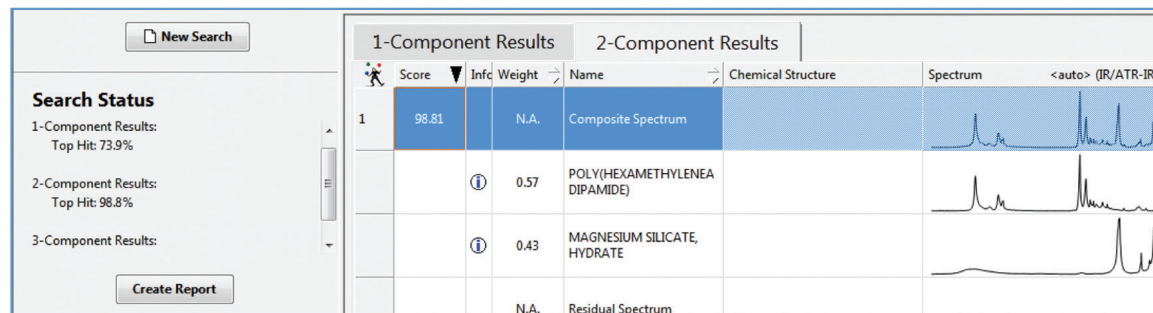
Deformulation Expert is used to examine the components of a formulated product by IR spectroscopy. Open a spectrum in ID Expert and let the spectral search run. This will match the IR spectrum of the complete product.



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.



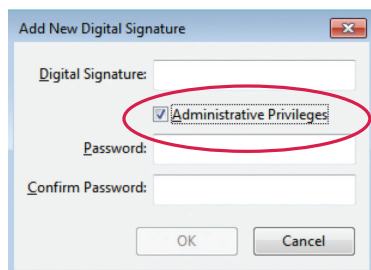
QC Expert™ (IR)

One-Time Configuration

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



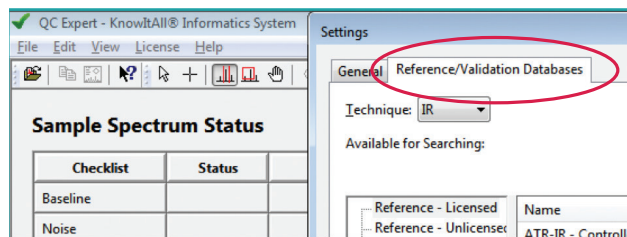
After loading QC Expert for the first time, you will get a “There are no users defined for this application” message. Click “OK”, add your digital signature and password, make sure “Administrative Privileges” is checked then click “OK”.



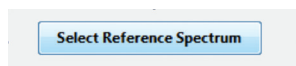
Add the relevant details and verify. Then add any user accounts in the same way but uncheck “Administrative Privileges”.

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”.

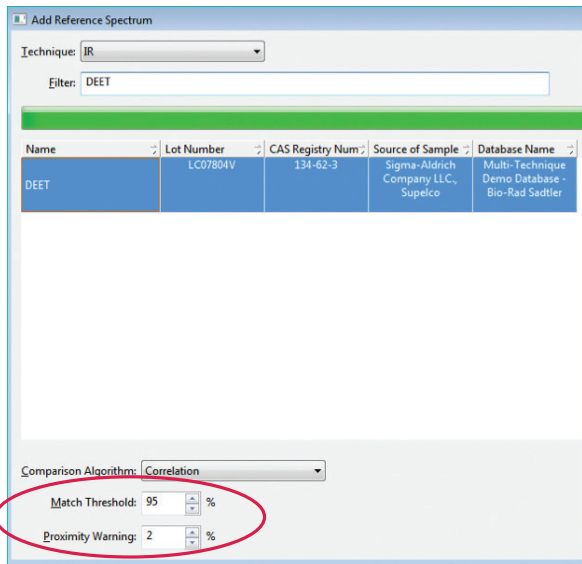


To select a reference spectrum, click “Select Reference Spectrum”.



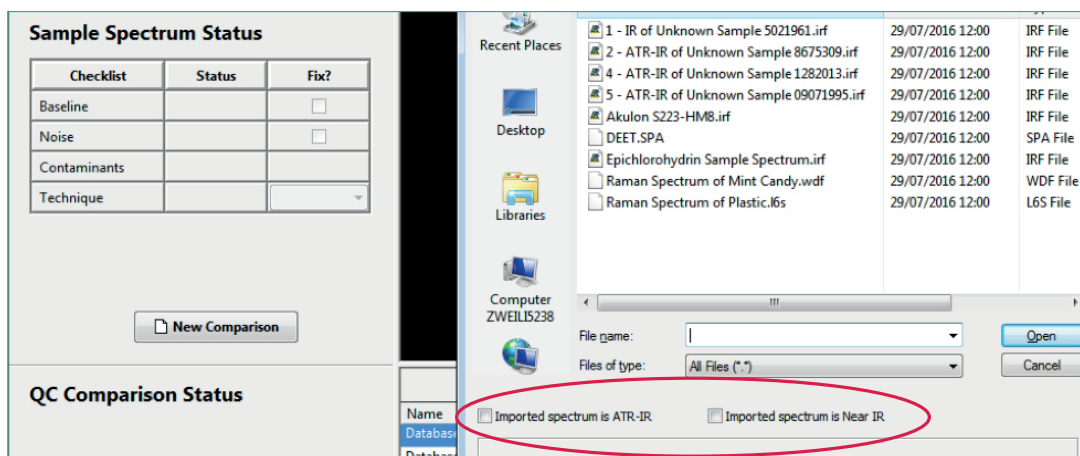
QC Expert™ (IR)

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”.



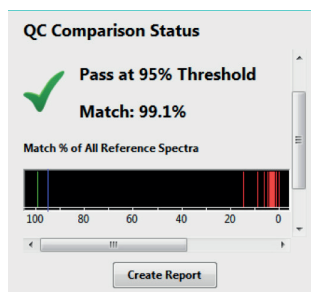
Running a sample

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.

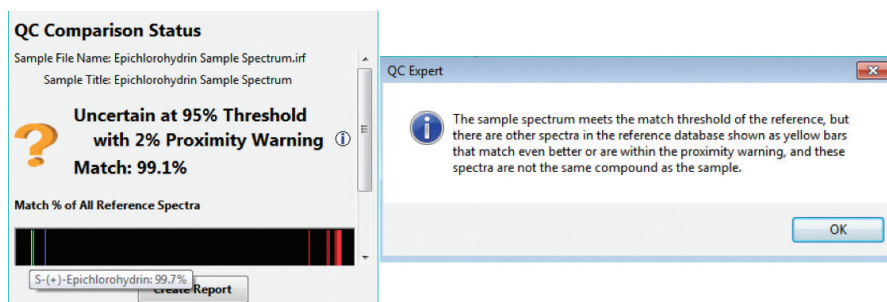


QC Expert™ (IR)

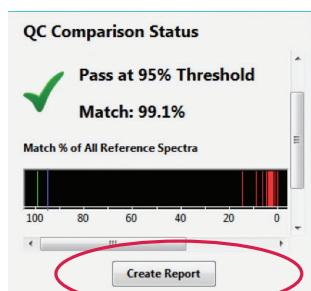
The “QC comparison status” will then show “pass” “fail” if the sample and reference spectra match or don’t match.



“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.

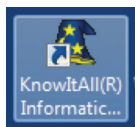


To create a digitally-signed report Click on “create report”, select your name from the “digital signatures” drop-down, enter the password, fill out the sample information, then click “OK”.



SearchIt™ & Minelt™ for GCMS

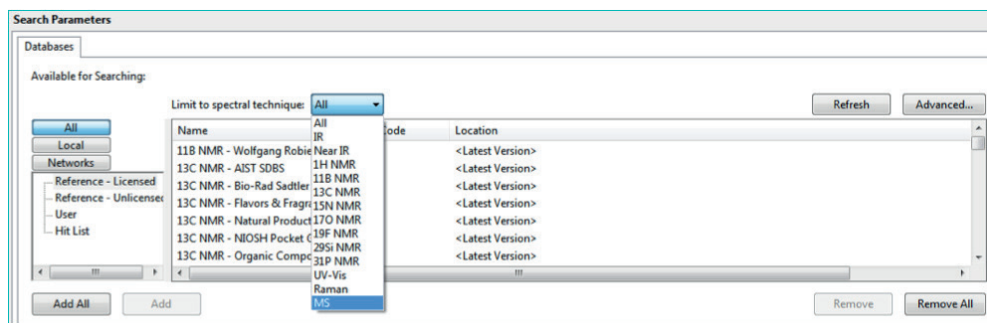
Open Wiley Spectra Lab by double-clicking on the “Know-it-All” icon on your desktop.



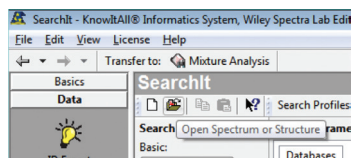
Select SearchIt in the left-hand toolbar.



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



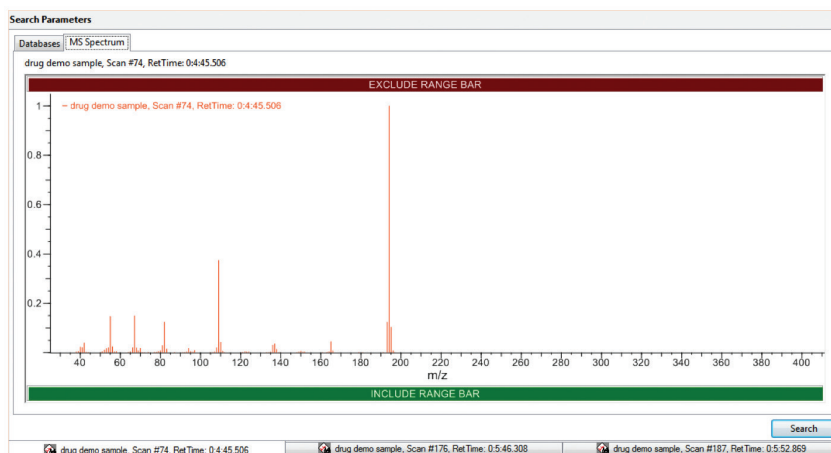
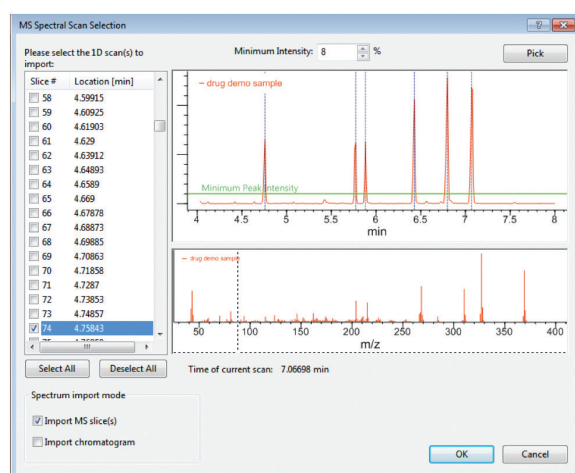
Click the “Open Spectrum or Structure” button on the top SearchIt toolbar to open the spectrum file, select the desired file then click “Open”.



SearchIt™ & Minelt™ for GCMS

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™ & Minelt™ 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.

The screenshot displays the Minelt software interface. The top toolbar includes a "Transfer to:" dropdown menu with "ReportIt" selected. The main window shows a mass spectrum plot with a peak at m/z 194. Below the plot is a table of search results:

Table	Plot	HQI	Tar	DI	ID	Name	Spectrum
1		98.64		MT	20440	1H-PURINE-2,6-DIONE, 3,7-DIHYDRO-1,3,7-TRIMETHYL-	Analytical Techniques
2		98.64		WMS	273687	1H-PURINE-2,6-DIONE, 3,7-DIHYDRO-1,3,7-TRIMETHYL-	Analytical Techniques
3		98.02		MS	228814	Caffeine	Analytical Techniques
4		97.91		AF	675	Caffeine	Analytical Techniques
5		97.91		WMS	295632	1H-PURINE-2,6-DIONE, 3,7-DIHYDRO-1,3,7-	Analytical Techniques

The right panel shows the chemical structure of Caffeine (1,3,7-trimethylxanthine) and its properties:

- Name: 1H-PURINE-2,6-DIONE, 3,7-DIHYDRO-1,3,7-TRIMETHYL-
- CAS Registry Number: 58-08-2
- Formula: C₈H₁₀N₄O₂
- Mol.Weight: 194.190 g/mol
- Nominal Mass: 194 g
- Owner: Database Compilation Copyright (C) 2007 John Wiley & Sons, Inc.; All Rights Reserved
- Source File Reference: Original Number: 8_LMCM-43019-218V; WILEYID: 20440

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.

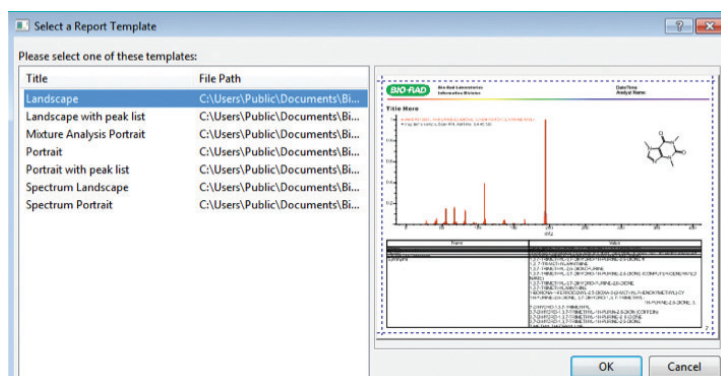


To make a report, click “Transfer to: ReportIt” on the top toolbar.

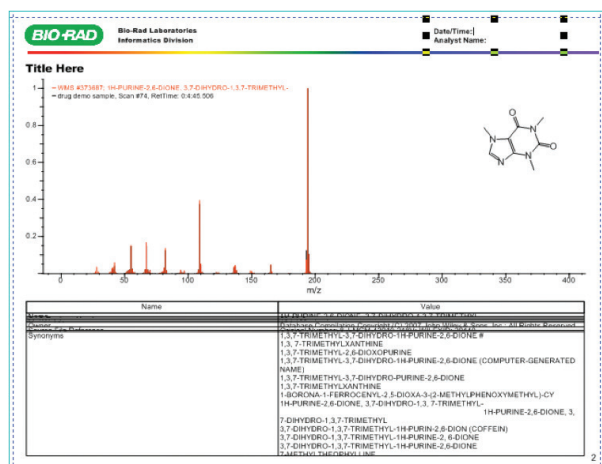
The screenshot shows the Minelt software interface with the "Transfer to:" dropdown menu in the top toolbar. The "ReportIt" option is highlighted, indicating the process of generating a report.

SearchIt™ & Minelt™ for GCMS

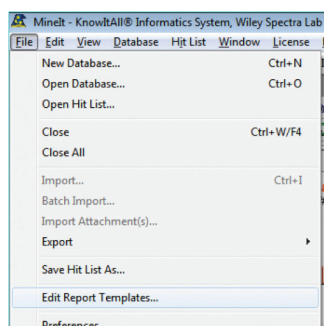
Select the type of report template to use and click “OK”



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.

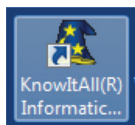


Report templates can be customized, including the layout, by clicking “Edit Report Templates” in the “File” menu in the main “Minelt” window.

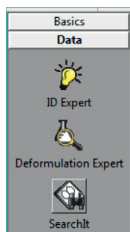


SearchIt™ & Minelt™ for NMR

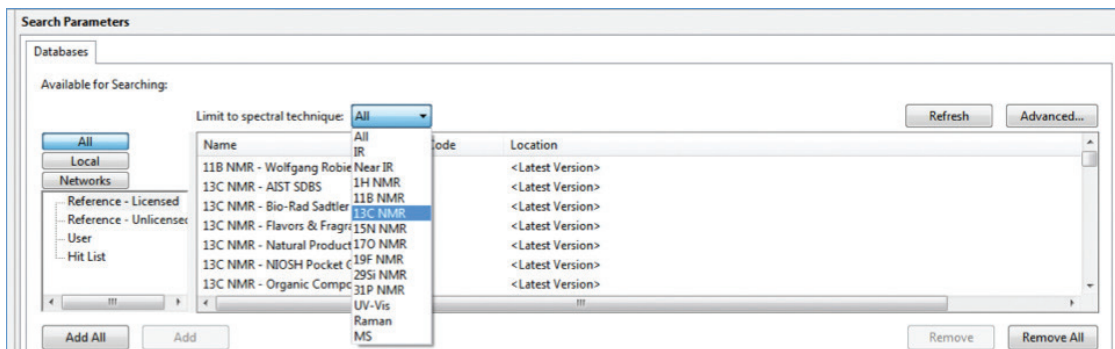
Open Wiley Spectra Lab by double-clicking on the “Know-it-All” icon on your desktop



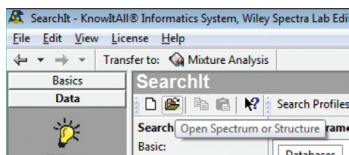
Select SearchIt in the left-hand toolbar.



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.

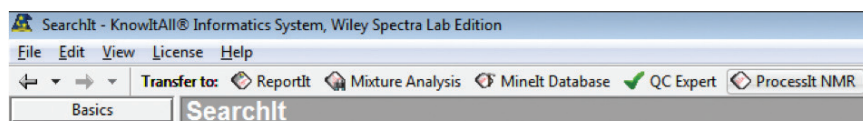


Click the “Open Spectrum or Structure” button on the top SearchIt toolbar to open the spectrum file, select the desired file then click “Open”.

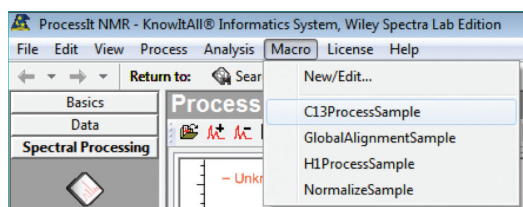


SearchIt™ & Minelt™ for NMR

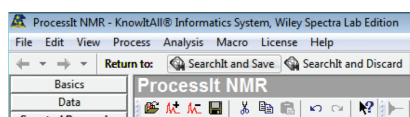
To process the spectrum, click “Transfer to ProcessIt NMR”



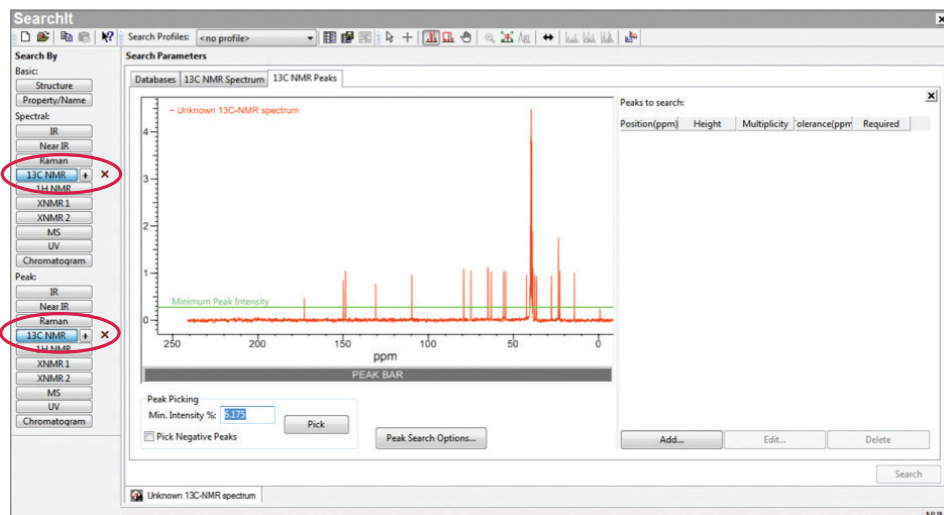
To apply processing macros, click “Macro” and either create or edit a macro or apply an existing one. For 13C NMR, the in-built “C13ProcessSample” can be used for minor spectral corrections.



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

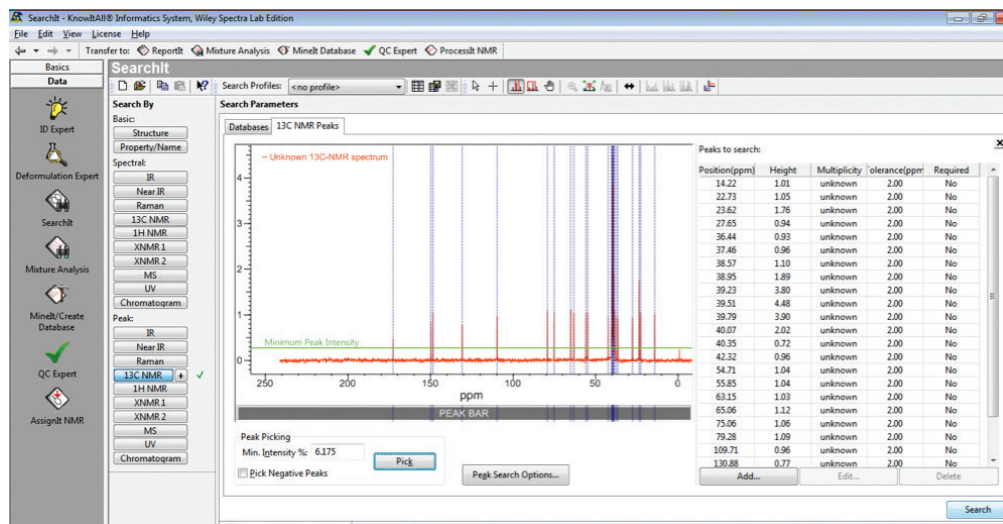


On the “SearchIt” screen, click the corresponding technique under “Peak” on the left-hand side, then click the corresponding technique under “Spectral” in the menu above to deselect it. Set the minimum peak intensity by either typing the value into the “Min. Intensity” box or by dragging the green line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



SearchIt™ & Minelt™ for NMR

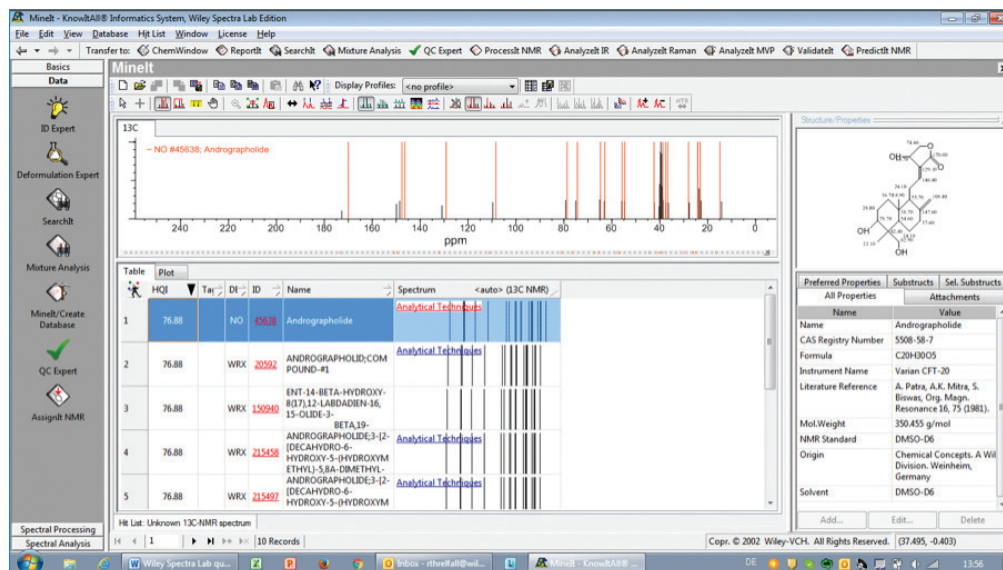
A peak list will appear on the right and to start the search click “Search” under the peak list.



The screenshot displays the SearchIt software interface. On the left, a sidebar contains various analysis tools. The main window shows a 13C NMR spectrum with a peak list table on the right. The table lists peak positions, heights, multiplicities, and tolerances.

Position(ppm)	Height	Multiplicity	tolerance(ppm)	Required
14.22	1.01	unknown	2.00	No
22.73	1.05	unknown	2.00	No
23.62	1.76	unknown	2.00	No
27.65	0.94	unknown	2.00	No
36.44	0.93	unknown	2.00	No
37.46	0.96	unknown	2.00	No
38.57	1.10	unknown	2.00	No
38.95	1.89	unknown	2.00	No
39.23	3.80	unknown	2.00	No
39.51	4.48	unknown	2.00	No
39.79	3.90	unknown	2.00	No
40.07	2.02	unknown	2.00	No
40.35	0.72	unknown	2.00	No
42.32	0.96	unknown	2.00	No
54.71	1.04	unknown	2.00	No
55.85	1.04	unknown	2.00	No
63.15	1.03	unknown	2.00	No
65.96	1.12	unknown	2.00	No
75.06	1.06	unknown	2.00	No
79.28	1.09	unknown	2.00	No
109.71	0.96	unknown	2.00	No
130.88	0.77	unknown	2.00	No

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



The screenshot displays the Minelt software interface. The main window shows a list of search hits with columns for HQI, Name, and Spectrum. The top hit is selected, and its details are shown in a table on the right.

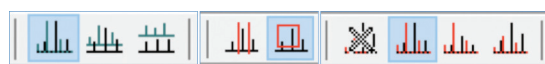
HQI	Name	Spectrum
76.88	NO #45638; Andrographolide	Analytical Techniques
76.88	WRX 20294 ANDROGRAPHOLIDE;COM POUND-#1	Analytical Techniques
76.88	WRX 150940 ENT-14-BETA-HYDROXY-107,112-LABDADIN-16, 15-OLIDE-3-	Analytical Techniques
76.88	WRX 215458 BETA,19- ANDROGRAPHOLIDE;3-[2- DECAHYDRO-6- HYDROXY-5-HYDROXYM ETHYL]-3,8A-DIMETHYL- ANDROGRAPHOLIDE;3-[2- DECAHYDRO-6- HYDROXY-5-HYDROXYM	Analytical Techniques
76.88	WRX 215492	Analytical Techniques

Structure Properties table:

Name	Value
Name	Andrographolide
CAS Registry Number	5508-58-7
Formula	C20H30O5
Instrument Name	Varian CFT-20
Literature Reference	A. Patra, A.K. Mitra, S. Biswas, Org. Magn. Resonance 16, 73 (1981).
Mol.Weight	350.455 g/mol
NMR Standard	DMSO-D6
Origin	Chemical Concepts, A Weil Division, Weinheim, Germany
Solvent	DMSO-D6

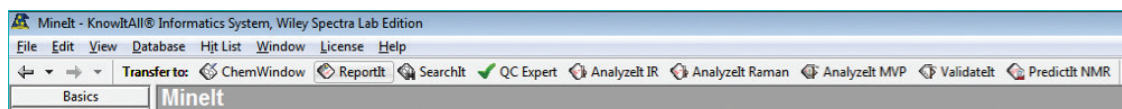
A hit quality index of >50 indicates a relatively good hit. Where some peaks don't overlap well between reference and sample spectra, additional analysis with other techniques is recommended.

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

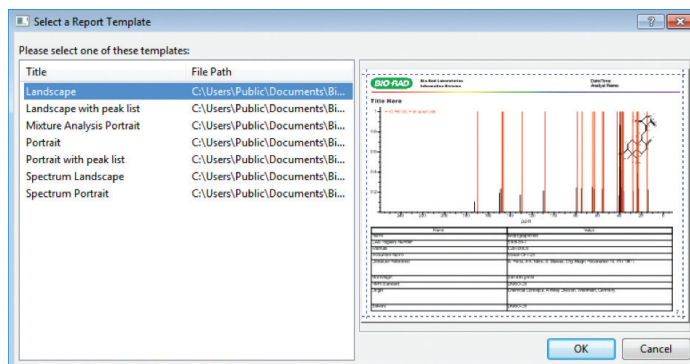


SearchIt™ & Minelt™ for NMR

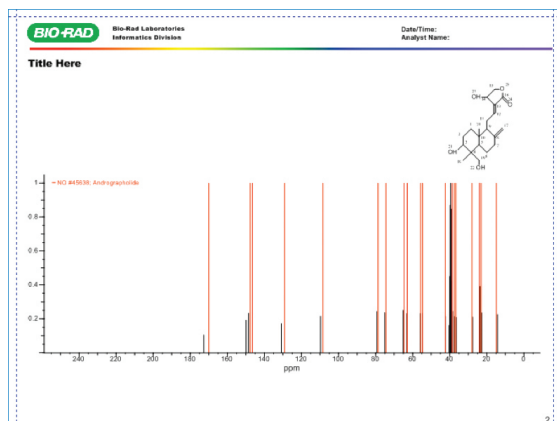
To make a report, click “Transfer to: ReportIt” on the top toolbar.



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



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 “Minelt” window.

