

# KnowItAll Software Training

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## Searching

# Searching

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## How to Perform a Basic Spectral Search

### Purpose

These exercises demonstrate how to perform spectral searches using KnowItAll.

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### Objectives

These exercises will teach you:

- How to select databases for searching
  - How to configure and perform various spectral searches
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### Background

Spectral searching against reference databases is frequently used in both the analysis of unknown compounds and in compound verification. KnowItAll SearchIt application facilitates this purpose.

#### Training Files Used in This Lesson

C:\Users\Public\Documents\Wiley\KnowItAll\Samples folder

- Acetic anhydride.dx
- Multi-Technique Sadtler Demo Database - Wiley [DEMO].sdbx

#### KnowItAll Applications Used

- SearchIt
- Minelt

## KnowItAll IR and Raman Search Algorithms

A background in the algorithms used by KnowItAll will be beneficial. For IR and Raman spectral comparison, KnowItAll uses the following algorithms:

### Correlation

This is the default algorithm for searching in KnowItAll and it conforms to the industry standard for correlation algorithms. The Correlation algorithm is similar to the Euclidean Distance algorithm. The difference between the two is in the way the spectra are treated before the comparison. Each spectrum is mean centered prior to performing the dot product normalization. This approach can improve search results for noisy spectra and spectra that have baseline issues, particularly with a baseline offset that is the result of a negative spike or chemical noise. It is slightly more time-consuming than the Euclidean Distance algorithm. The search speed is slower because each spectrum in the database must be mean centered and then normalized prior to the comparison. The search results that are obtained with the Correlation algorithm are spectrally similar to the unknown, even if the unknown compound is not in the database. The Correlation algorithm is heavily weighted by peak areas. Broad features are weighted much more strongly than sharp features. The algorithm is most tolerant to peak shifts and non-linearities in relative band intensities.

### Correlation (Classic)

The Correlation algorithm that was found in all versions of KnowItAll prior to KnowItAll 2020 is similar to the Euclidean Distance algorithm. However, it did not conform to the industry standard for correlation algorithms. Beginning with KnowItAll 2020, the Correlation algorithm does conform to the industry standard and it is the default algorithm used for searching in KnowItAll. To provide backward compatibility for customers who want to reproduce prior search results, the previous correlation algorithm is now provided as Correlation (Classic).

### Euclidean Distance

The Euclidean Distance algorithm measures the point-to-point differences between a pair of spectra. The results that are obtained with the Euclidean Distance algorithm are spectrally similar to the unknown, even if the unknown compound is not in the database. This algorithm, however, can yield degraded search results when the unknown spectrum has a sloping or offset baseline. The Euclidean Distance algorithm is heavily weighted by peak areas. Broad features are weighted much more strongly than sharp features. This algorithm is most tolerant to peak shifts and non-linearities in relative band intensities.

### First Derivative Euclidean Distance

Use this algorithm to reduce the effects of baseline slope or offset in the unknown. Although search speed is slightly slower than with the Euclidean Distance algorithm, the First Derivative Euclidean Distance sometimes gives improved search results, especially when the unknown spectrum is a mixture of two or more compounds. The First Derivative Euclidean Distance algorithm is heavily weighted by changes in slope. Sharp features are weighted much more strongly than broad features. The algorithm is also very sensitive to peak shifts. Small shifts can make the algorithm miss a similar result.

**Second Derivative Euclidean Distance** Use the Second Derivative Euclidean Distance algorithm to compare the second derivative of a reference spectrum to that of the query spectrum.

## Optimized Corrections: A Breakthrough Technology for Spectral Searching

Spectral searching is one of the most important tools researchers use to classify or identify materials, yet it continues to be plagued by errors and imperfections. During a spectral search, a sample spectrum is compared to a database of reference spectra. To ensure that an optimal match is found in the database, spectra can be adjusted to compensate for differences between spectra caused by variability in instruments, accessories, environmental conditions, and other factors.

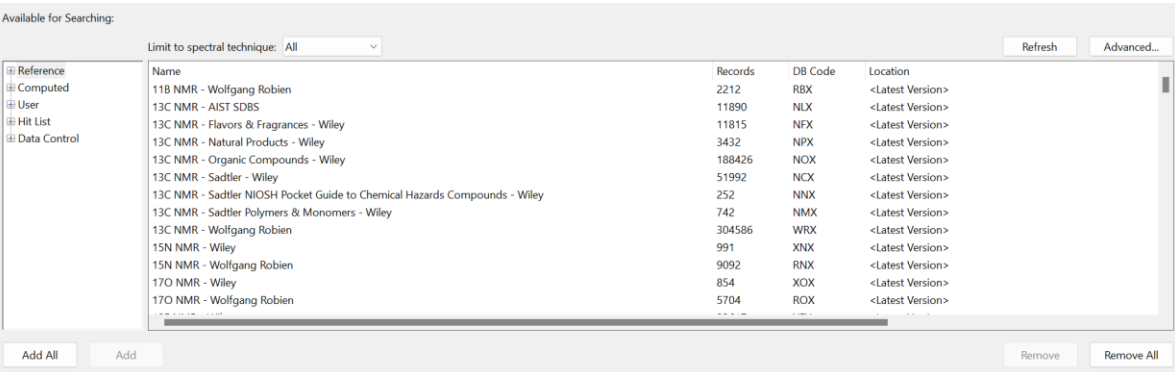
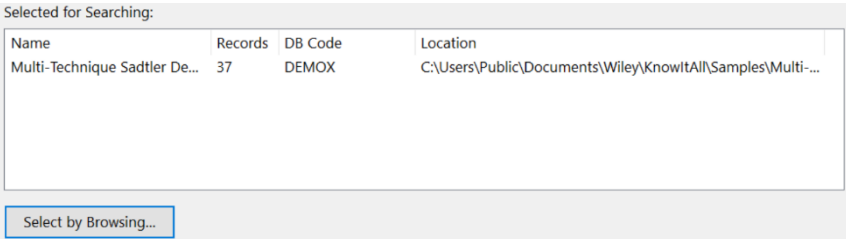
According to ASTM's guide on spectral searching<sup>1</sup>, various algorithms and manual methods exist to adjust spectra to get reasonable match scores when two compared spectra of the same compound differ for various reasons. While these methods may work in selected cases, subtle discrepancies such as a shift of the X-axis are very hard to identify and correct manually. The inflexible mathematical algorithms typically employed do not compensate for these types of errors in spectra that are flawed.


Manual corrections can be made by expert spectroscopists, but those less experienced in spectroscopy are often unaware of how to perform the necessary corrections on their sample spectrum to achieve the best search result. To address this growing concern, Wiley has introduced Optimized Corrections, a breakthrough patented technology that performs a computationally complex set of multiple corrections on query and reference spectra in a search to find the optimal match between the query and each individual reference spectrum. This training guide will demonstrate how the Optimized Corrections technology yields better matches between query and reference spectra than can be attained using rigid search algorithms alone or with manual methods to optimize spectra for searching.

Optimized Corrections consider the full spectrum during a selected range(s) search.

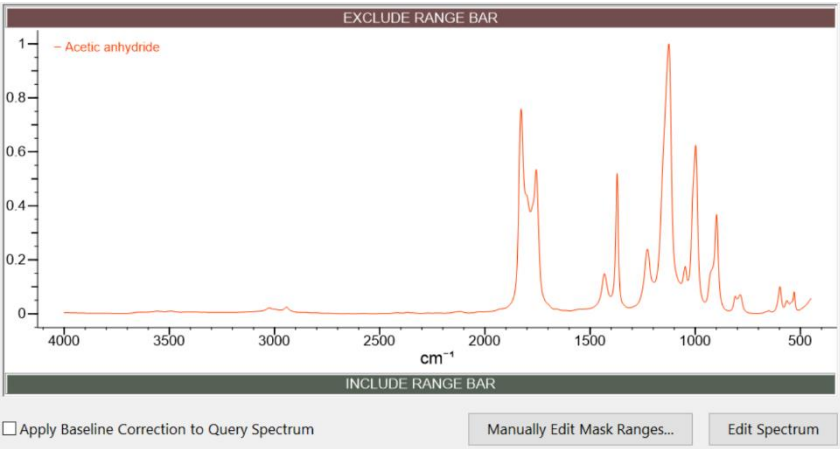
<sup>1</sup> E2310-04 - Standard Guide for Use of Spectral Searching by Curve Matching Algorithms with Data Recorded Using Mid-Infrared Spectroscopy, 2009. ASTM International Web Site. <http://www.astm.org/Standards/E2310.htm> (accessed March 4, 2015).



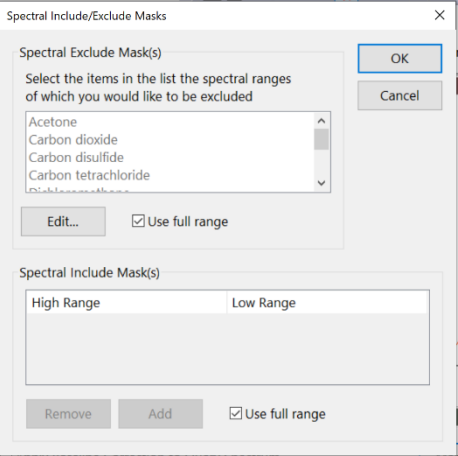
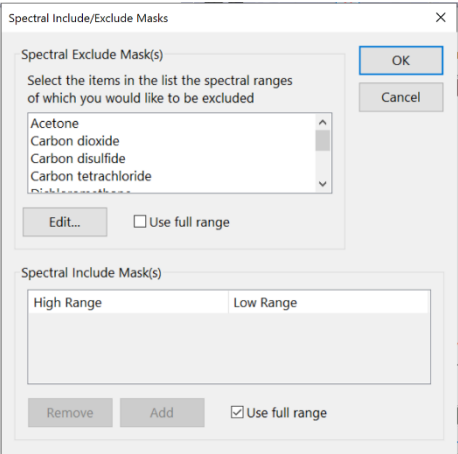
4	<p>To the left of the <b>Available for Searching</b> window, expand each branch in the tree structure to display a particular database category—<b>Reference, User, Hit List</b>— and specify whether network, local, or all databases are displayed. The available databases are displayed at the right of the window.</p>	<p>The <b>Reference</b> category is shown below. The database <b>Name</b>, number of <b>Records</b>, <b>Location</b> and version are displayed for each database.</p>  <p><b>NOTE:</b> Your display may look different depending on whether or not you have access to databases available online.</p> <p>Click <b>Advanced</b> on the top right to open the <b>Advanced Options</b> dialog box, where you can control how you access online databases and add or remove local database locations. Click <b>Refresh</b> to update the display after settings are changed.</p>
5	<p>Click <b>Select by Browsing</b> button located at the lower left.</p>	<p>The <b>Browse for a Database or Hit List</b> dialog box opens.</p>
6	<p>Navigate to “C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples”. Open <b>Multi-Technique Sadtler Demo Database - Wiley (DEMO).sdbx</b>.</p>	<p>The database is displayed in the <b>Selected for Searching</b> list.</p> 

7	<p>If necessary, uncheck the <b>All Hits</b> check box and set <b>Hit List Size Limit</b> to 50.</p> <p><b>NOTE:</b> When performing a spectral or peak search using more than two or three databases, it is better to limit the number of hits. Checking <b>All Hits</b> or using a larger value can drastically reduce the search speed.</p>	<p>The <b>Hit List Size Limit</b> is equal to 50:</p> 
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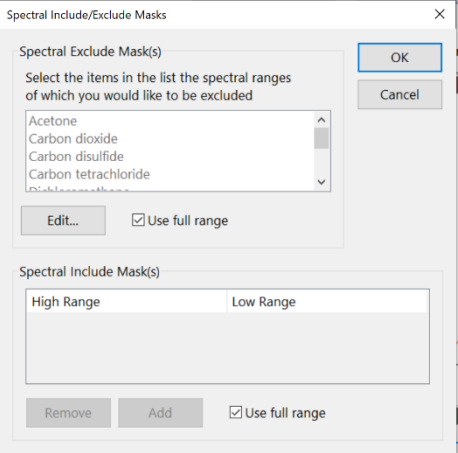
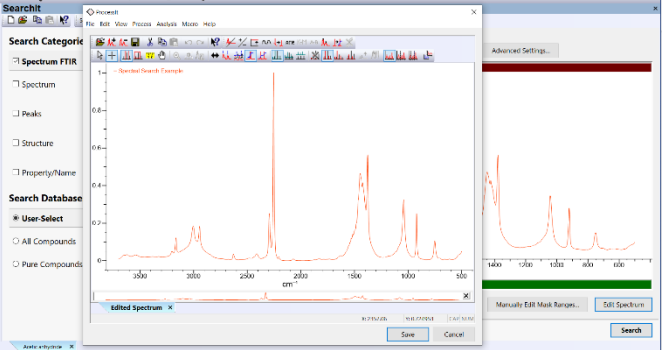
## Open the spectral file

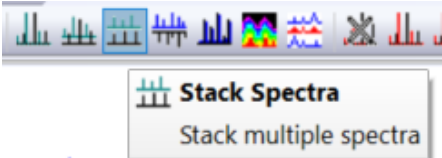
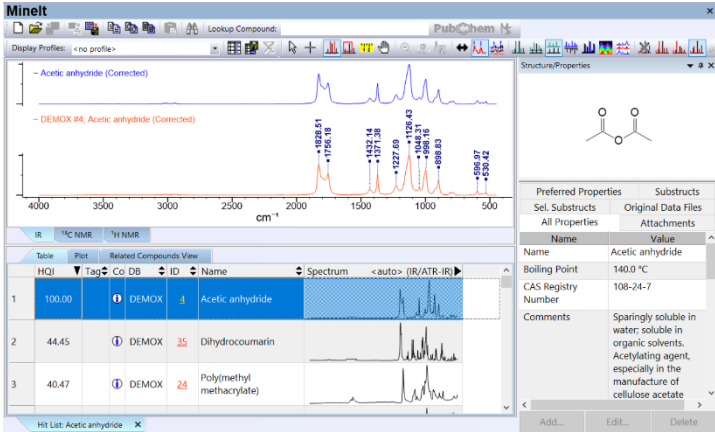
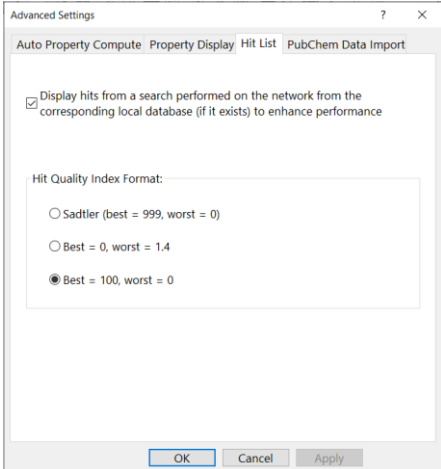
	Action	Result
1	<p>Click the <b>Spectrum</b> button under <b>Search Categories</b>.</p> <p>Navigate to "<b>C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\IR</b>".</p> <p>Select <b>Acetic anhydride.jdx</b>.</p> <p>Click <b>Open</b>.</p> <p><b>Note:</b> You can use the <b>Files of Type</b> filter to limit the display to specific types of files, such as JCAMP (*.dx, *.jdx), or to display all files (*.*)</p>	<p>An <b>Open</b> dialog box appears. The spectrum is recognized as an IR spectrum and displayed in the spectral pane in the <b>Spectrum</b> tab:</p>  <p><b>NOTE:</b> You can use the checkbox at the bottom to "Apply Baseline Correction to Query Spectrum", if desired. However, KnowItAll automatically corrects the baseline.</p>

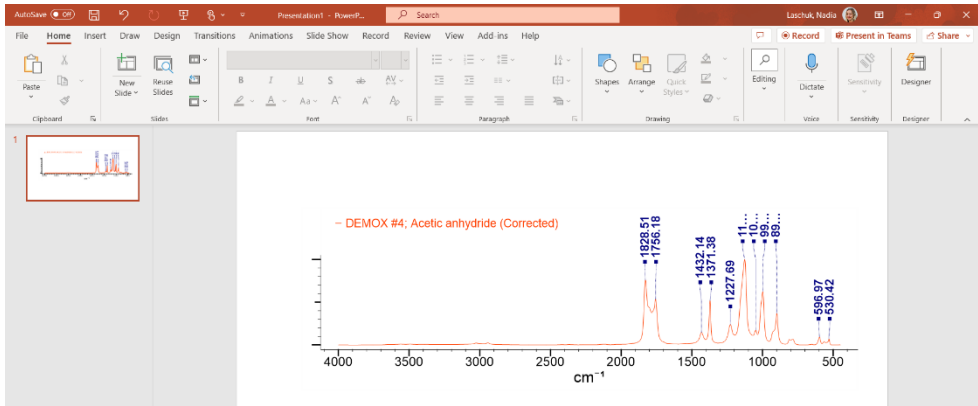
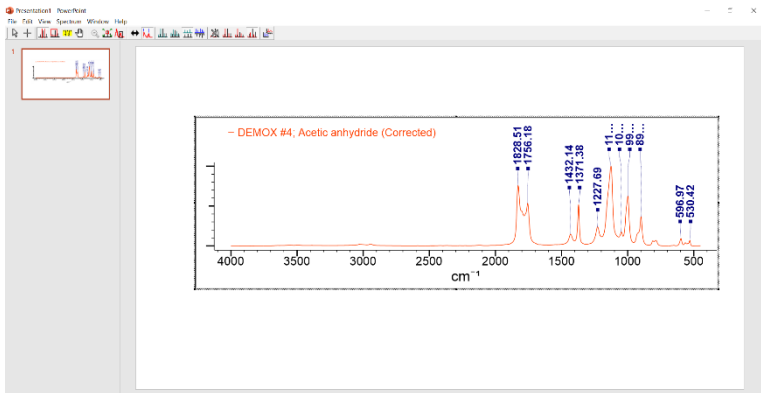
## Fine-tune before searching

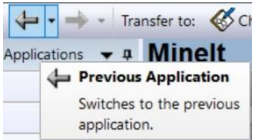
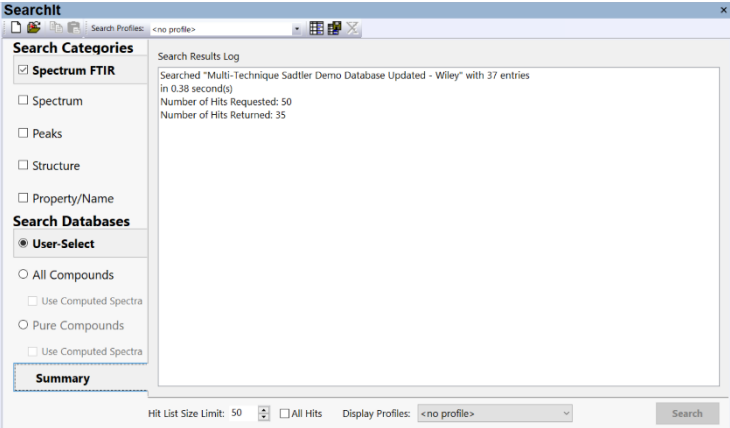
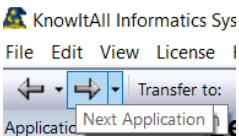
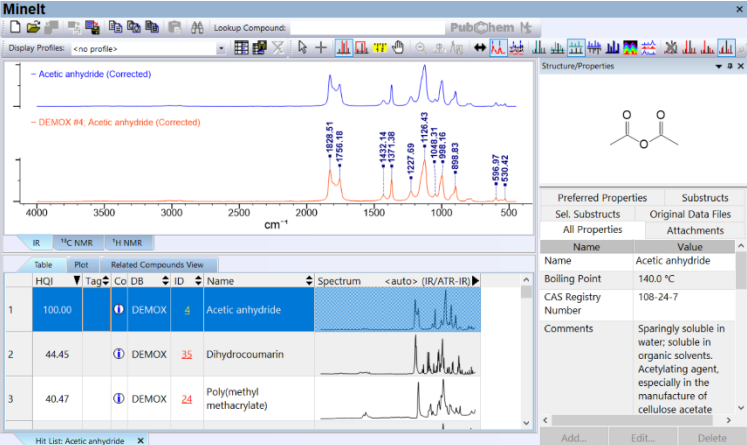
	Action	Result
1	<p>Click <b>Manually Edit Mask Ranges</b>.</p> <p><b>NOTE:</b> You can also click and drag in the <b>Spectral</b> pane's <b>Exclude Range Bar</b> and <b>Include Range Bar</b> after closing the <b>Spectral Include/Exclude Masks</b> window.</p>	<p>The <b>Spectral Include/Exclude Masks</b> dialog box opens:</p> 
2	<p>Deselect the <b>Use full range</b> checkbox under the list of <b>Spectral Exclude Mask(s)</b>. Select some to see how they work.</p> <p><b>Note:</b> The use of these masks will be demonstrated later in this lesson:</p>	<p>The list of pre-defined <b>Exclude Masks</b> becomes available:</p> 



	Action	Result
3	Reselect the <b>Use full range</b> checkbox under the list of <b>Spectral Exclude Mask(s)</b> .	Any selected <b>Spectral Exclude Masks</b> are removed from the spectrum: 
4	Click <b>OK</b> to close the <b>Spectral Include/Exclude Masks</b> dialog box.	The <b>Spectral Include/Exclude Masks</b> dialog box is closed.
5	Click <b>Edit Spectrum</b> at the bottom right of the spectral pane.	The spectrum is transferred to the popped-up <b>ProcessIt</b> application, where you can correct potential searching problems and save the corrected spectrum into the <b>SearchIt</b> spectrum pane. 
6	Click <b>Cancel</b> .	The spectrum is returned to the <b>SearchIt</b> application. Changes made in the <b>ProcessIt</b> application are not saved.

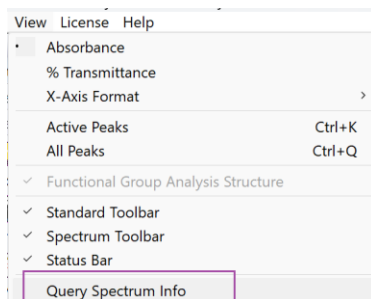
	Action	Result
7	<p>Click <b>Search</b> and <b>Minelt</b> will open In <b>Minelt</b> click to choose <b>Stack Spectra</b></p>  <p>view:</p>	<p>The search results are automatically displayed in the <b>Minelt</b> application as a hit list, sorted by HQI. Both the unknown spectrum and the selected database spectrum are displayed.</p>  <p>The <b>HQI</b> value measures how close the reference spectrum is to that of the query. The default scale of <b>HQI</b> is 0-100.</p>
8	<p><b>Note:</b> The <b>HQI</b> (Hit Quality Index) is displayed for each search result, which has settings under: <b>File &gt; Preferences &gt; Hit List</b>. Click <b>Cancel</b> to close the dialog.</p>	<p>The <b>Advanced Settings</b> dialog is launched:</p> 

	Action	Result
9	<b>TIPS</b>	<ul style="list-style-type: none"> <li>You can tag individual hits in the hit list as either "Accept," "Tentative" or "Reject" using the <b>Hit List &gt; Tag As</b> menu option or by double-clicking in the <b>Tag</b> column. You can then sort the hit list based on your tags.</li> <li>You can edit which columns in the hit list are displayed by right-clicking in the data table at the bottom left, selecting the <b>Edit Columns...</b> option, and selecting which columns you would like to display as well as the order in which they are displayed.</li> </ul>
10	From the <b>Edit</b> menu, select <b>Copy Active Spectrum</b> . Then open an MS Office tool (PowerPoint, for example). Right-click on the screen and select <b>Paste</b> .	<p><b>KnowItAll</b> objects such as the spectral pane can be copied and embedded into MS tools.</p> 
11	Double-click the object in PowerPoint.	<p><b>KnowItAll</b> spectrum manipulation toolbar is shown in PowerPoint. For example, you can turn on peak labeling.</p> 

	Action	Result																																
12	<p>In <b>KnowItAll</b>, click the <b>Back</b> button (located below the <b>File</b> menu).</p> 	<p>You are returned to the <b>SearchIt</b> application, where a <b>Summary</b> tab has been added to the main <b>SearchIt</b> window:</p> 																																
13	<p>Click the KnowItAll <b>Next Application</b> button.</p> 	<p>You are returned to <b>Minelt</b> and the hit list.</p>  <table border="1" data-bbox="751 1117 1270 1295"> <thead> <tr> <th>Hit#</th> <th>HQI</th> <th>Tag</th> <th>Co</th> <th>DB</th> <th>ID</th> <th>Name</th> <th>Spectrum</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>100.00</td> <td></td> <td>DEMOX</td> <td></td> <td></td> <td>Acetic anhydride</td> <td></td> </tr> <tr> <td>2</td> <td>44.45</td> <td></td> <td>DEMOX</td> <td>35</td> <td></td> <td>Dihydrocoumarin</td> <td></td> </tr> <tr> <td>3</td> <td>40.47</td> <td></td> <td>DEMOX</td> <td>24</td> <td></td> <td>Poly(methyl methacrylate)</td> <td></td> </tr> </tbody> </table>	Hit#	HQI	Tag	Co	DB	ID	Name	Spectrum	1	100.00		DEMOX			Acetic anhydride		2	44.45		DEMOX	35		Dihydrocoumarin		3	40.47		DEMOX	24		Poly(methyl methacrylate)	
Hit#	HQI	Tag	Co	DB	ID	Name	Spectrum																											
1	100.00		DEMOX			Acetic anhydride																												
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3	40.47		DEMOX	24		Poly(methyl methacrylate)																												

Note: one can view the metadata of query spectrum by

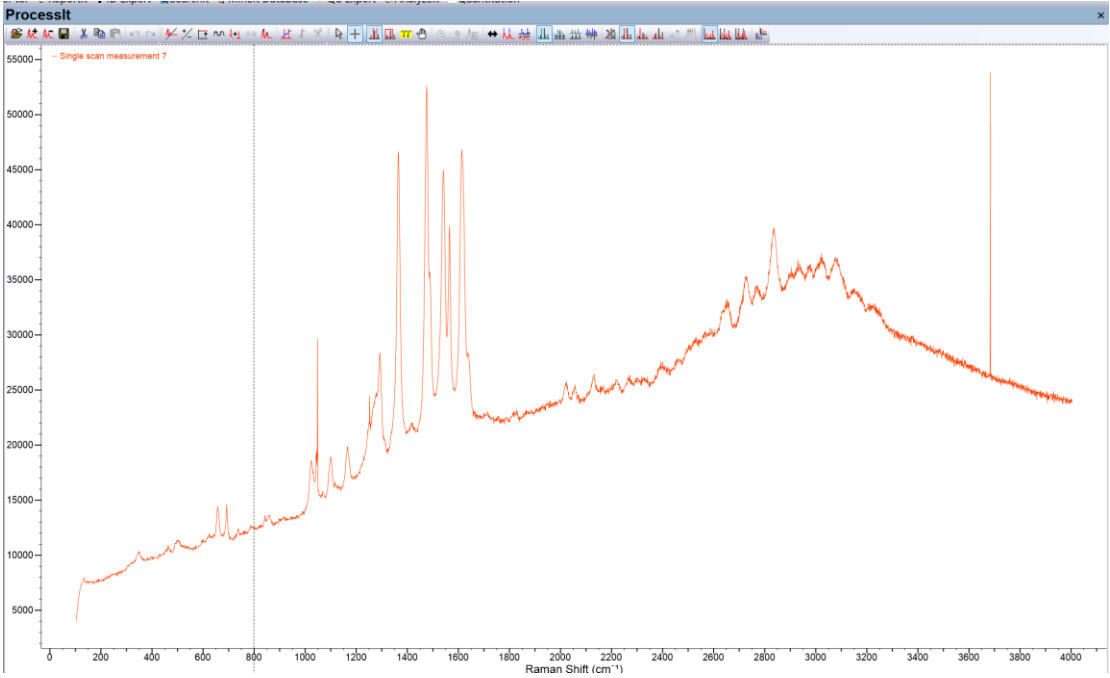
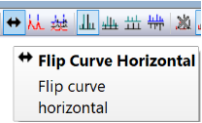
- In **SearchIt**, click **View > Query Spectrum Info**

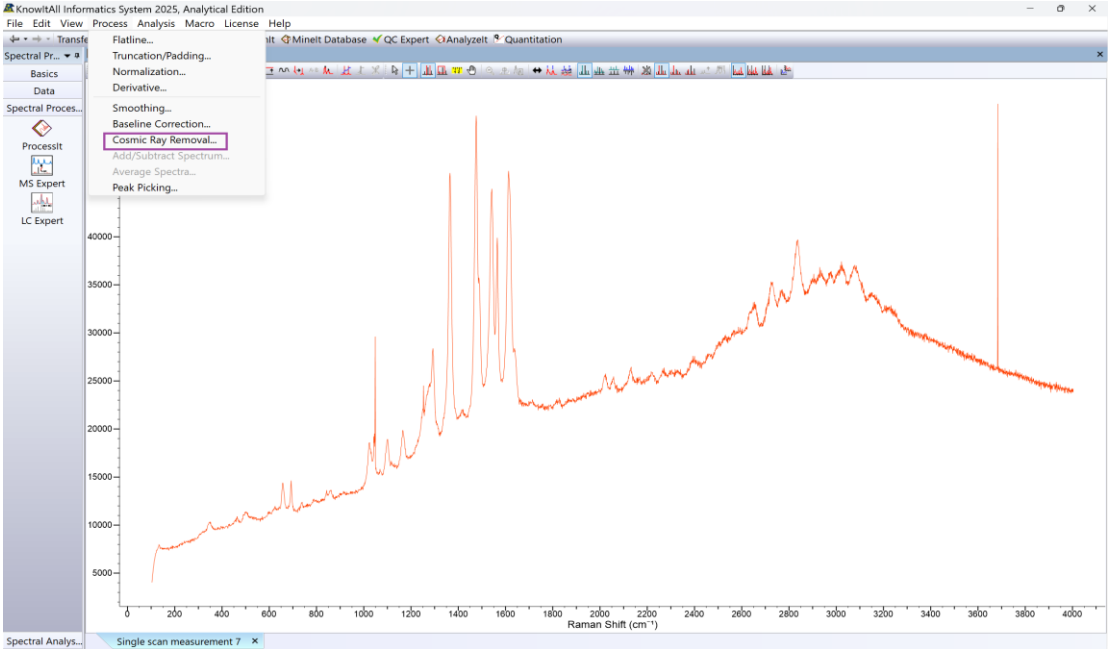
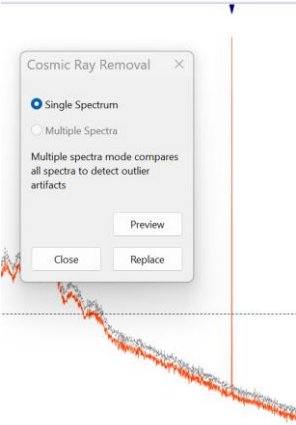


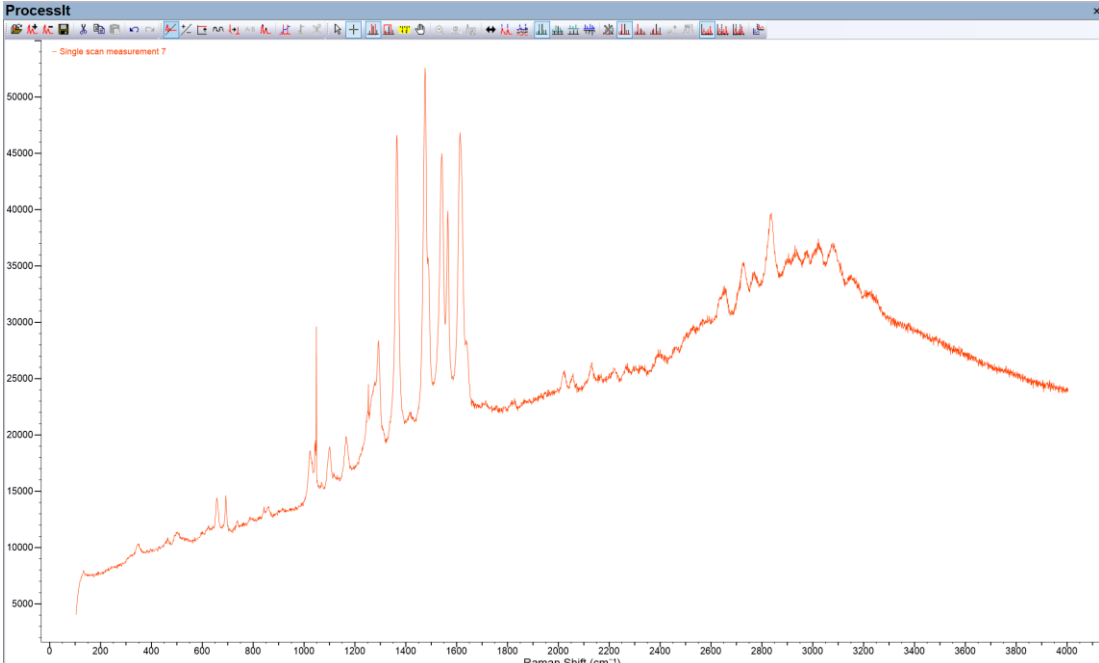
- In a **Minelt** hit list, click **View > Windows/Tables > Query Spectrum Info**.

## Raman-specific fine-tuning before searching

### Example 1 – Cosmic Ray Correction

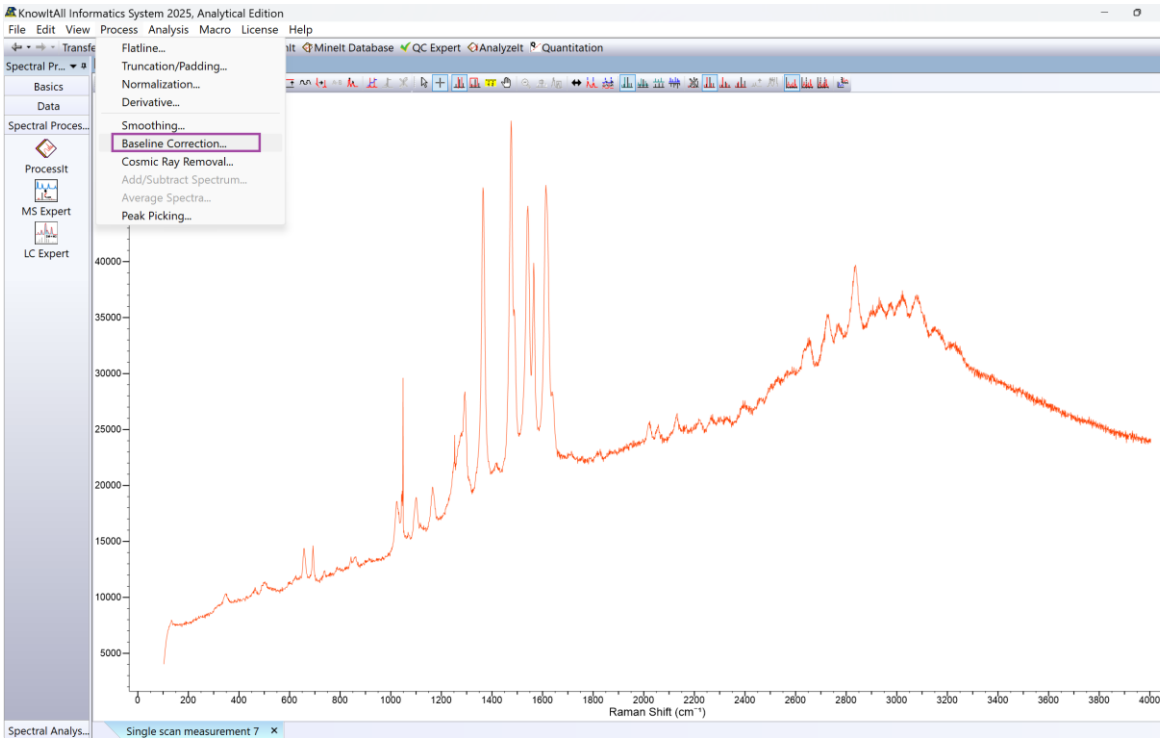
	Action	Result
1	<p>Start <b>ProcessIt</b> application</p> <p>Click <b>Open Spectroscopy Data File</b></p> <p>Navigate to “<b>C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\Raman</b>”.</p> <p>Select <b>Co and Fe complexes on porous substrate.wdf</b>.</p> <p>Click <b>Open</b>.</p>	<p>The spectrum will be displayed and the Baseline Correction popup window will appear with the baseline options.</p>  <p>Note: Depending on user/instrument setup, Raman X-axis could be low (left) to high (right) or vice versa.</p> <p>One can flip by using a button in the toolbar:</p> 

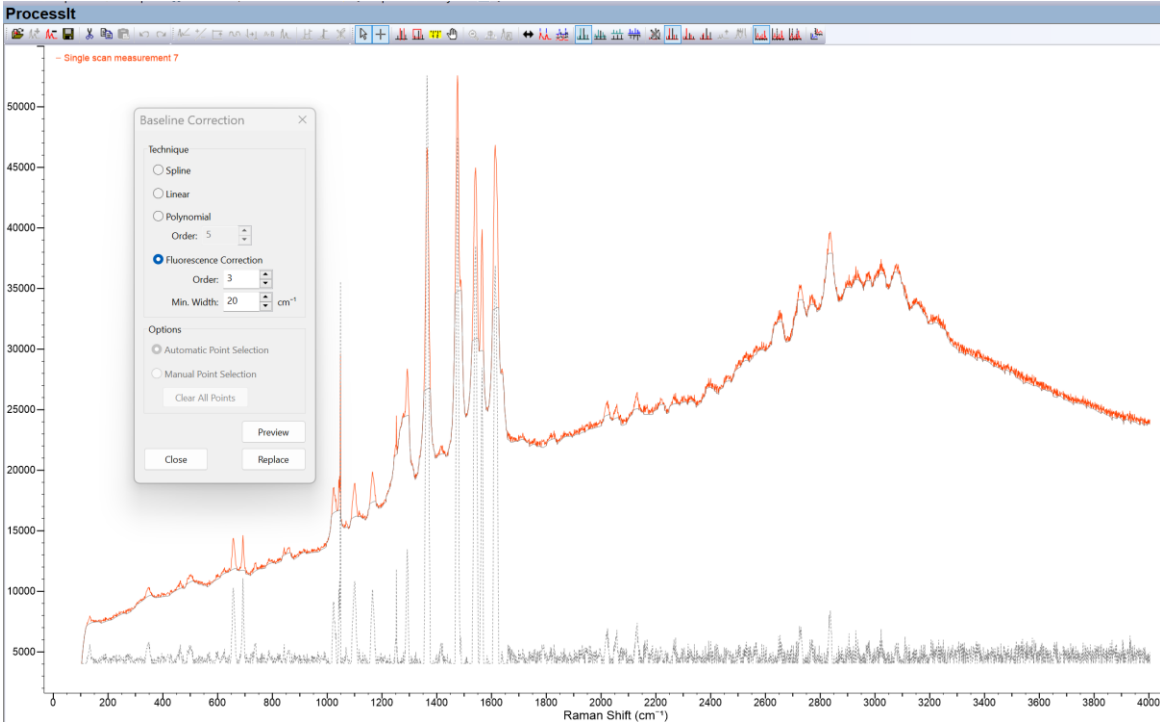
	Action	Result
2	<p>Select <b>Cosmic Ray Removal</b> from the <b>Process</b> menu</p>	
3	<p>Select for <b>Single Spectrum</b></p> <p>Note: One can apply Cosmic Ray correction to multiple Raman spectra opened in <b>ProcessIt</b>.</p>	 <p>The cosmic ray is marked by a down arrow:</p>

	Action	Result
4	Hit the <b>Replace</b> button.	 <p>The screenshot displays a Raman spectrum plot within a software window titled "ProcessIt". The plot shows a single scan measurement with intensity on the y-axis (ranging from 0 to 50,000) and Raman Shift in cm⁻¹ on the x-axis (ranging from 0 to 4000). The spectrum exhibits several sharp peaks in the 1000-1800 cm⁻¹ region and a broad, multi-peaked region between 2000 and 3500 cm⁻¹.</p>



### Example 2 – Fluorescence Correction

Action	Result
<p>1</p> <p>One can just continue with the cosmic ray correction result in the previous sample, or open a sample with strong fluorescence by using Click <b>Open Spectroscopy Data File</b></p> <p>In this case, we will continue from previous example.</p> <p><b>Process &gt; Baseline Correction and Replace</b> button</p>	 <p>The screenshot displays the 'Spectral Process' menu in the KnowItAll Informatics System. The 'Baseline Correction...' option is highlighted with a red box. The background shows a Raman spectrum plot with 'Raman Shift (cm<sup>-1</sup>)' on the x-axis (0 to 4000) and intensity on the y-axis (0 to 40000). The spectrum shows a broad, rising baseline starting around 1000 cm<sup>-1</sup>, characteristic of fluorescence, which is the target for the correction.</p>

	Action	Result
2	<p>Select <b>Cosmic Ray Removal</b> using the <b>Process</b> menu item</p> <p>You may preview the various <b>Baseline Correction</b> techniques. You will find that <b>Fluorescence Correction</b> does the best job.</p> <p>Hit the <b>Replace</b> button.</p>	 <p>Processed spectrum will be ready for downstream searching.</p>

# Searching

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## How to Create Search Profiles and Use the Minelt profile to display results

### Purpose

This exercise demonstrates how to use search profiles and use the Minelt profile to display search results.

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### Objectives

This exercise will teach you:

- How to apply a search profile
  - How to create a search profile
- 

### Background

Search Profiles are pre-defined combinations of search parameters such as Databases and Hit List Size Limit that can be stored for later use. Using search profiles makes searching easier, especially when the same type of search is repeated.



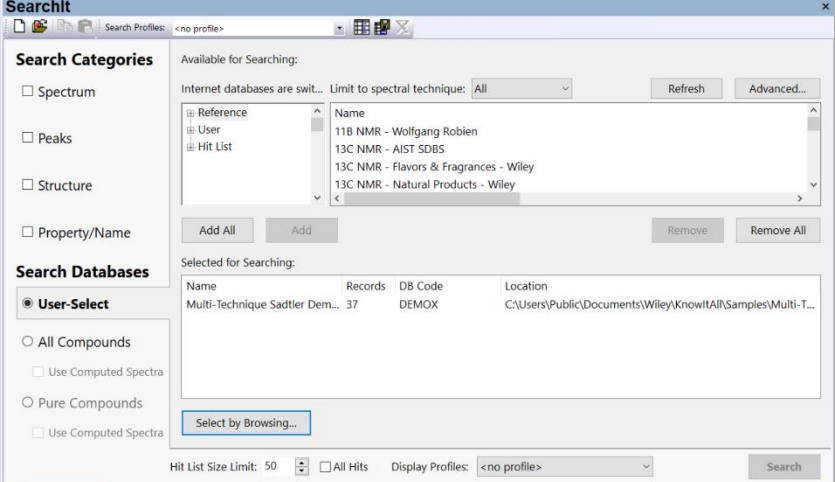
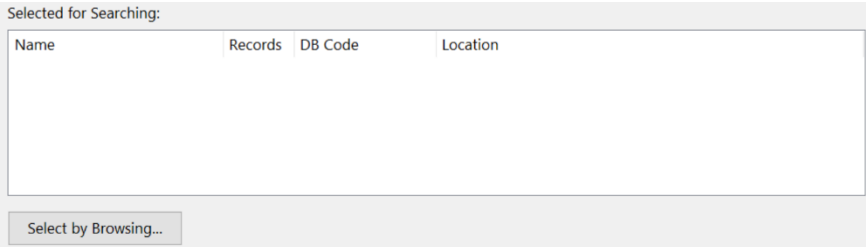
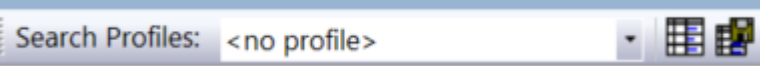
Minelt profiles are preferences of hit list information display, it is defined in Minelt. It can be tied to a search.

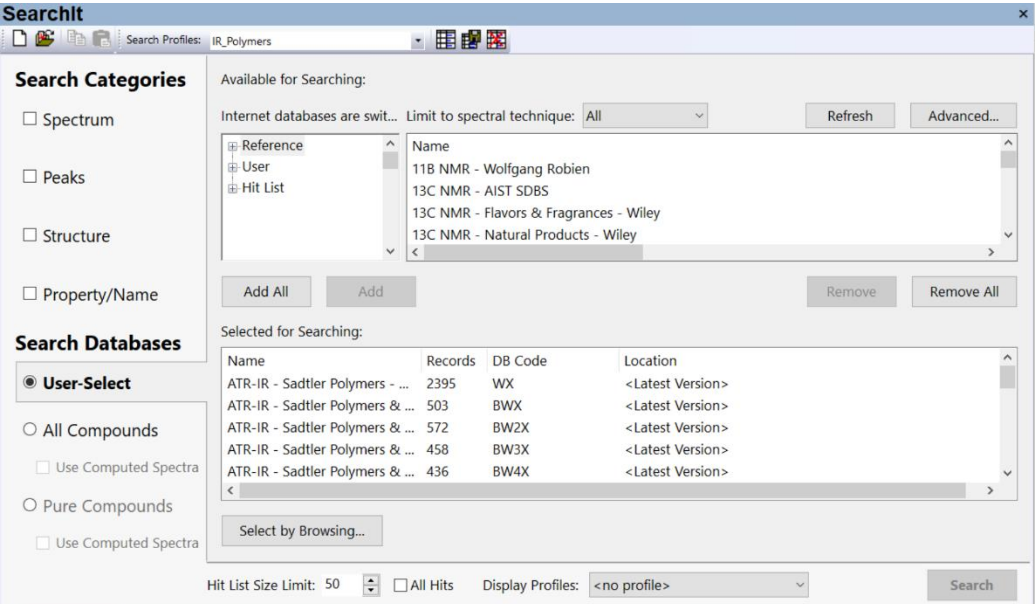
#### Training Files Used in This Lesson

#### KnowItAll Applications Used


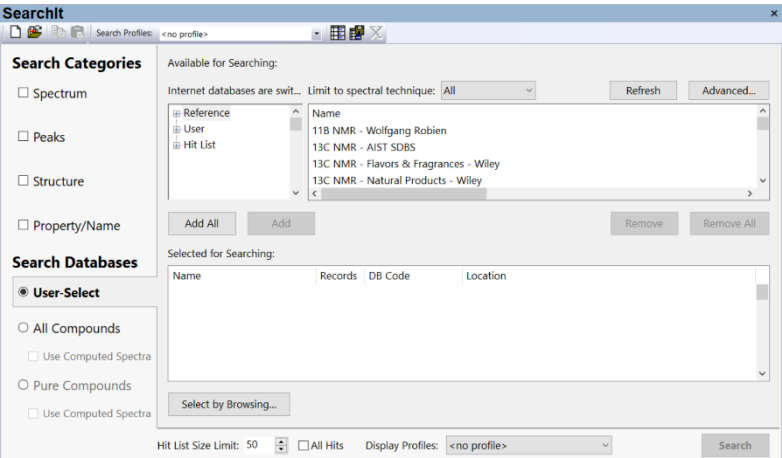

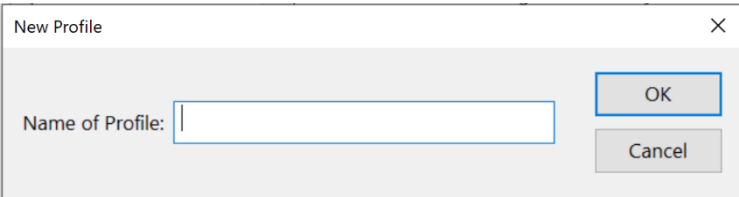
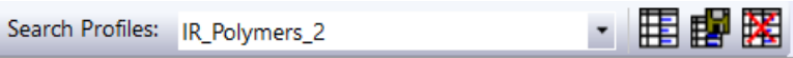
- SearchIt

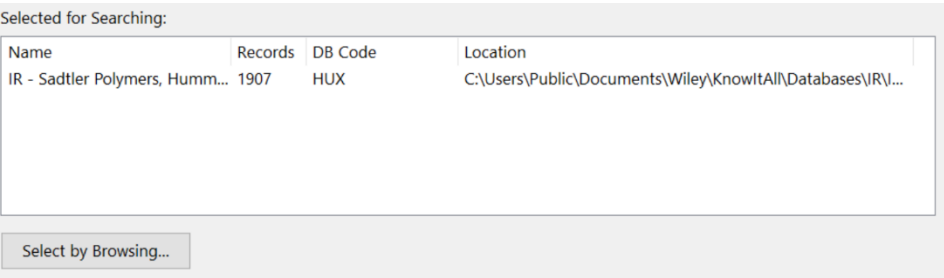
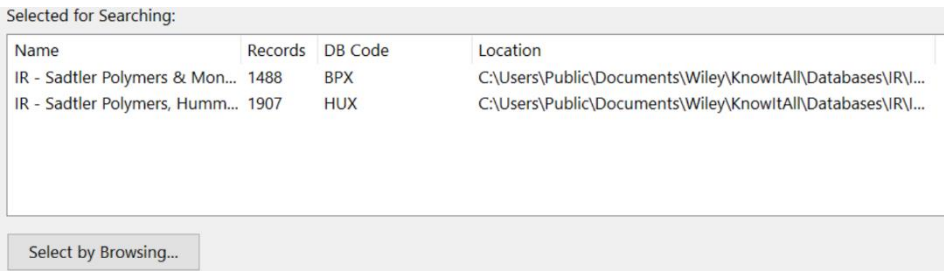
## Apply a pre-defined search profile

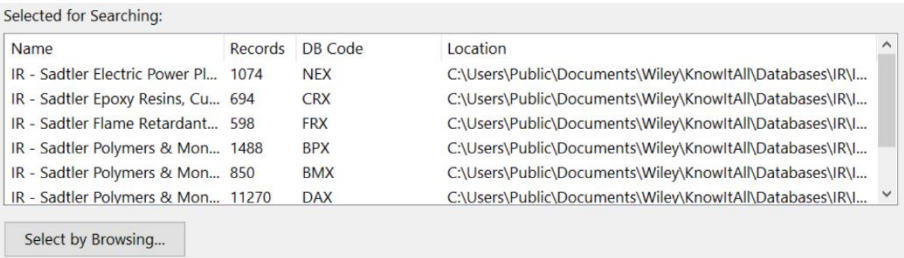

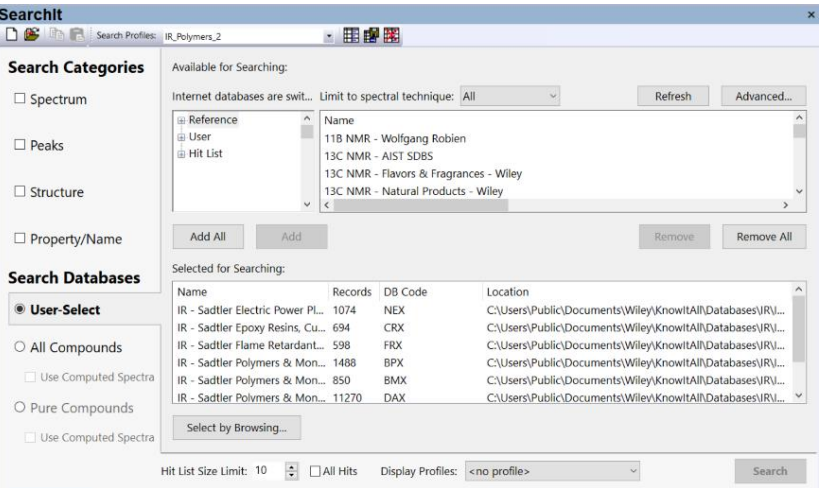
	Action	Result
1	<p>Do one of the following:</p> <ul style="list-style-type: none"> <li>If the <b>SearchIt</b> application is not open, navigate to the <b>Data</b> toolbox and click its icon.</li> </ul>  <ul style="list-style-type: none"> <li>If the <b>SearchIt</b> application is already open, click the SearchIt Close button  to close the current search.</li> </ul>	<p>The <b>SearchIt</b> application's <b>User-Select</b> tab is displayed, and the <b>Selected for Searching</b> list displays the databases last used:</p> 
2	<p>If databases are already selected for searching, click <b>Remove All</b> to clear the selections. You can also double-click individual entries to remove them from the list.</p>	<p>The <b>Selected for Searching</b> databases section is cleared:</p> 
3	<p>If necessary, choose <b>View &gt; Profile Toolbar</b> to display Search Profiles tools.</p>	

Action	Result																								
4 Select the <b>IR_Polymers</b> profile using the <b>Search Profiles</b> dropdown menu.	<p>Polymer databases are displayed in the <b>Selected for Searching</b> list:</p>  <p>The screenshot shows the SearchIt application window with the following components:</p> <ul style="list-style-type: none"><li><b>Search Categories:</b> A list of checkboxes for Spectrum, Peaks, Structure, and Property/Name, all of which are currently unchecked.</li><li><b>Search Databases:</b> A section with a radio button selected for "User-Select". Below it are options for "All Compounds" and "Pure Compounds", each with a "Use Computed Spectra" checkbox.</li><li><b>Available for Searching:</b> A list of internet databases including "11B NMR - Wolfgang Robien", "13C NMR - AIST SDBS", "13C NMR - Flavors &amp; Fragrances - Wiley", and "13C NMR - Natural Products - Wiley".</li><li><b>Selected for Searching:</b> A table listing the databases selected for the search.</li></ul> <table border="1" data-bbox="1003 699 1801 852"><thead><tr><th>Name</th><th>Records</th><th>DB Code</th><th>Location</th></tr></thead><tbody><tr><td>ATR-IR - Sadtler Polymers - ...</td><td>2395</td><td>WX</td><td>&lt;Latest Version&gt;</td></tr><tr><td>ATR-IR - Sadtler Polymers &amp; ...</td><td>503</td><td>BWX</td><td>&lt;Latest Version&gt;</td></tr><tr><td>ATR-IR - Sadtler Polymers &amp; ...</td><td>572</td><td>BW2X</td><td>&lt;Latest Version&gt;</td></tr><tr><td>ATR-IR - Sadtler Polymers &amp; ...</td><td>458</td><td>BW3X</td><td>&lt;Latest Version&gt;</td></tr><tr><td>ATR-IR - Sadtler Polymers &amp; ...</td><td>436</td><td>BW4X</td><td>&lt;Latest Version&gt;</td></tr></tbody></table> <p>At the bottom of the window, there is a "Hit List Size Limit" set to 50, an "All Hits" checkbox, a "Display Profiles" dropdown menu set to "&lt;no profile&gt;", and a "Search" button.</p>	Name	Records	DB Code	Location	ATR-IR - Sadtler Polymers - ...	2395	WX	<Latest Version>	ATR-IR - Sadtler Polymers & ...	503	BWX	<Latest Version>	ATR-IR - Sadtler Polymers & ...	572	BW2X	<Latest Version>	ATR-IR - Sadtler Polymers & ...	458	BW3X	<Latest Version>	ATR-IR - Sadtler Polymers & ...	436	BW4X	<Latest Version>
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## Create a new search profile

	Action	Result
1	Click the SearchIt <b>Close</b> button  , then click <b>Remove All</b> to clear the contents of the <b>Selected for Searching</b> list.	<p>The <b>User-Select</b> tab is displayed. The <b>Selected for Searching</b> list is empty:</p> 
2	Click the <b>Add a New Profile</b> button  on the <b>Profile</b> toolbar.	<p>The <b>New Profile</b> dialog box opens.</p> 
3	Type in the name of the new profile [ <b>IR_Polymers_2</b> ].  Click <b>OK</b> .	<p>The new profile name is displayed in the <b>Search Profiles</b> text box:</p> 
4	Specify <b>IR</b> in the <b>Limit to spectral technique</b> drop-down list.	<p>Only databases with IR spectra are displayed in the <b>Available for Searching</b> list. Note that <b>Multi-Technique Sadtler Demo Database - Wiley</b> is included in the list because it includes IR spectra.</p>

	Action	Result
5	In the <b>Available for Searching</b> list, click to select <b>IR – Sadtler Polymers, Hummel – Wiley</b> (DB Code HUX). Click <b>Add</b> .	The HUX database is added to the <b>Selected for Searching</b> list: 
6	In the <b>Available for Searching</b> list, double-click <b>IR — Sadtler Polymers &amp; Monomers (Basic) 1 — Wiley</b> (DB Code BPX).	The BPX database is added to the <b>Selected for Searching</b> list: 

	Action	Result																																						
7	Continue adding databases BMX, CRX, DAX, FRX and NEX.	<p>The selected databases are added to the <b>Selected for Searching</b> window:</p>  <table border="1" data-bbox="793 386 1692 560"> <thead> <tr> <th>Name</th> <th>Records</th> <th>DB Code</th> <th>Location</th> </tr> </thead> <tbody> <tr> <td>IR - Sadtler Electric Power Pl...</td> <td>1074</td> <td>NEX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...</td> </tr> <tr> <td>IR - Sadtler Epoxy Resins, Cu...</td> <td>694</td> <td>CRX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...</td> </tr> <tr> <td>IR - Sadtler Flame Retardant...</td> <td>598</td> <td>FRX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...</td> </tr> <tr> <td>IR - Sadtler Polymers &amp; Mon...</td> <td>1488</td> <td>BPX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...</td> </tr> <tr> <td>IR - Sadtler Polymers &amp; Mon...</td> <td>850</td> <td>BMX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...</td> </tr> <tr> <td>IR - Sadtler Polymers &amp; Mon...</td> <td>11270</td> <td>DAX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...</td> </tr> </tbody> </table> <p>Select by Browsing...</p>	Name	Records	DB Code	Location	IR - Sadtler Electric Power Pl...	1074	NEX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...	IR - Sadtler Epoxy Resins, Cu...	694	CRX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...	IR - Sadtler Flame Retardant...	598	FRX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...	IR - Sadtler Polymers & Mon...	1488	BPX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...	IR - Sadtler Polymers & Mon...	850	BMX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...	IR - Sadtler Polymers & Mon...	11270	DAX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...										
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8	On the <b>User-Select</b> tab, change the Hit List Size Limit to 10.	<p>Hit List Size Limit: 10 <input type="checkbox"/> All Hits</p>																																						
9	Click the <b>Save Current Profile</b> button  on the Profile toolbar. A message box asks if you wish to overwrite the current profile. Click <b>Yes</b> to save the new profile.																																							
10	Close the current search by clicking <b>X</b> , then select the newly created <b>IR_Polymers_2</b> search profile.	<p>The databases and search settings associated with this profile are displayed:</p>  <p><b>Search Categories</b></p> <ul style="list-style-type: none"> <li><input type="checkbox"/> Spectrum</li> <li><input type="checkbox"/> Peaks</li> <li><input type="checkbox"/> Structure</li> <li><input type="checkbox"/> Property/Name</li> </ul> <p><b>Search Databases</b></p> <ul style="list-style-type: none"> <li><input checked="" type="radio"/> <b>User-Select</b></li> <li><input type="radio"/> All Compounds <ul style="list-style-type: none"> <li><input type="checkbox"/> Use Computed Spectra</li> </ul> </li> <li><input type="radio"/> Pure Compounds <ul style="list-style-type: none"> <li><input type="checkbox"/> Use Computed Spectra</li> </ul> </li> </ul> <p><b>Available for Searching:</b></p> <p>Internet databases are swit... Limit to spectral technique: All <input type="button" value="Refresh"/> <input type="button" value="Advanced..."/></p> <table border="1" data-bbox="961 987 1596 1089"> <thead> <tr> <th>Reference</th> <th>Name</th> </tr> </thead> <tbody> <tr> <td><input type="checkbox"/></td> <td>11B NMR - Wolfgang Robien</td> </tr> <tr> <td><input type="checkbox"/></td> <td>13C NMR - AIST SDB5</td> </tr> <tr> <td><input type="checkbox"/></td> <td>13C NMR - Flavors &amp; Fragrances - Wiley</td> </tr> <tr> <td><input type="checkbox"/></td> <td>13C NMR - Natural Products - Wiley</td> </tr> </tbody> </table> <p><input type="button" value="Add All"/> <input type="button" value="Add"/> <input type="button" value="Remove"/> <input type="button" value="Remove All"/></p> <p><b>Selected for Searching:</b></p> <table border="1" data-bbox="961 1157 1596 1284"> <thead> <tr> <th>Name</th> <th>Records</th> <th>DB Code</th> <th>Location</th> </tr> </thead> <tbody> <tr> <td>IR - Sadtler Electric Power PL...</td> <td>1074</td> <td>NEX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...</td> </tr> <tr> <td>IR - Sadtler Epoxy Resins, Cu...</td> <td>694</td> <td>CRX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...</td> </tr> <tr> <td>IR - Sadtler Flame Retardant...</td> <td>598</td> <td>FRX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...</td> </tr> <tr> <td>IR - Sadtler Polymers &amp; Mon...</td> <td>1488</td> <td>BPX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...</td> </tr> <tr> <td>IR - Sadtler Polymers &amp; Mon...</td> <td>850</td> <td>BMX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...</td> </tr> <tr> <td>IR - Sadtler Polymers &amp; Mon...</td> <td>11270</td> <td>DAX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...</td> </tr> </tbody> </table> <p>Select by Browsing...</p> <p>Hit List Size Limit: 10 <input type="checkbox"/> All Hits Display Profiles: &lt;no profile&gt; <input type="button" value="Search"/></p>	Reference	Name	<input type="checkbox"/>	11B NMR - Wolfgang Robien	<input type="checkbox"/>	13C NMR - AIST SDB5	<input type="checkbox"/>	13C NMR - Flavors & Fragrances - Wiley	<input type="checkbox"/>	13C NMR - Natural Products - Wiley	Name	Records	DB Code	Location	IR - Sadtler Electric Power PL...	1074	NEX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...	IR - Sadtler Epoxy Resins, Cu...	694	CRX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...	IR - Sadtler Flame Retardant...	598	FRX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...	IR - Sadtler Polymers & Mon...	1488	BPX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...	IR - Sadtler Polymers & Mon...	850	BMX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...	IR - Sadtler Polymers & Mon...	11270	DAX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...
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## Use Minelt profile for hit list display

New in the KnowItAll 2024 release, one can specify how a search hit list is to be displayed in SearchIt simply by expanding the highlighted drop list:

The screenshot shows the SearchIt application window with the following components:

- Search Categories:** Spectrum, Peaks, Structure, Property/Name.
- Search Databases:** User-Select (selected), All Compounds, Pure Compounds.
- Available for Searching:** Internet databases are switched. Limit to spectral technique: All. Buttons: Refresh, Advanced...
- Selected for Searching:** A table listing databases with columns: Name, Records, DB Code, Location.
- Hit List Size Limit:** 50.  All Hits.
- Display Profiles:** A dropdown menu currently set to "<no profile>".
- Search:** A button to execute the search.

Name	Records	DB Code	Location
IR - Sadtler Electric Power Pl...	1074	NEX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...
IR - Sadtler Epoxy Resins, Cu...	694	CRX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...
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IR - Sadtler Polymers & Mon...	11270	DAX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...

# Searching

## How to Search a Database of Spectra by Peak

### Purpose

This exercise demonstrates how to perform a peak search.

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### Objectives

This exercise will teach you:

- How to configure a peak search
- 

### Background

The **SearchIt** application provides the capability of using peak information to perform a search of spectral or chromatographic data. This allows users to compare peak tables from databases to a peak table that you enter or extract from a spectrum.

#### Training Files Used in This Lesson



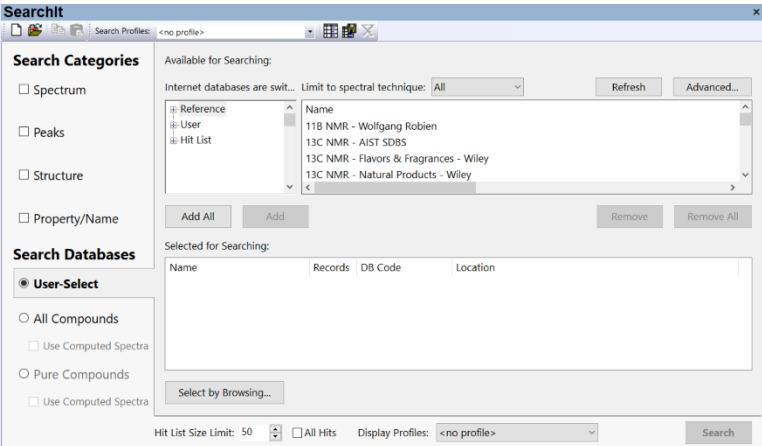
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\IR

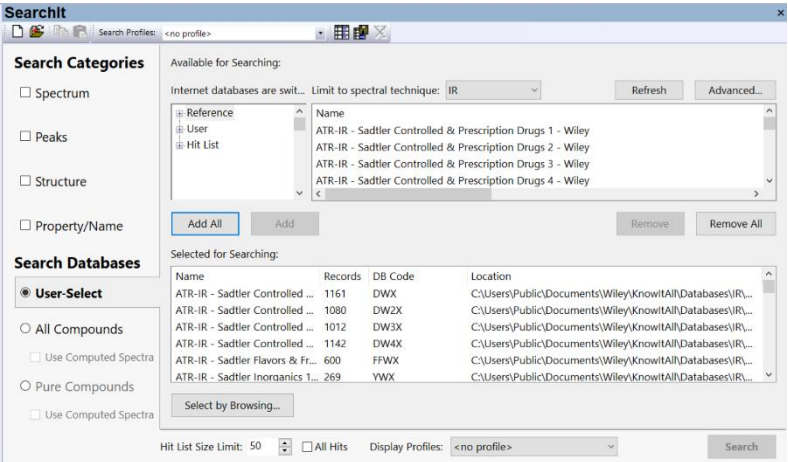
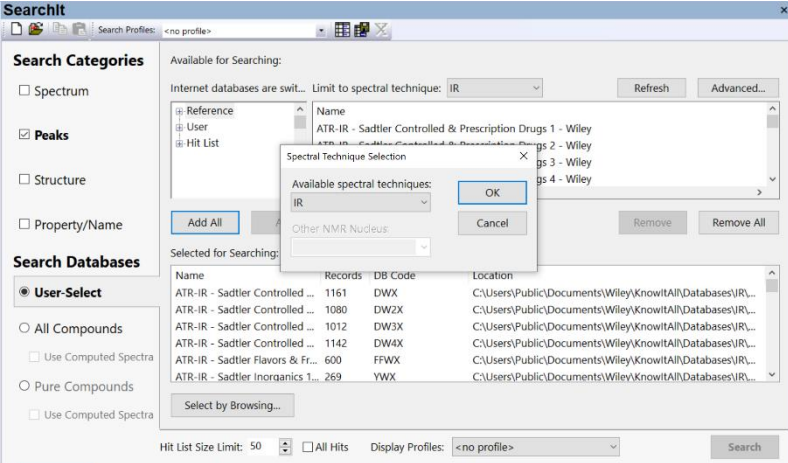
- Ethyl acrylate.dx

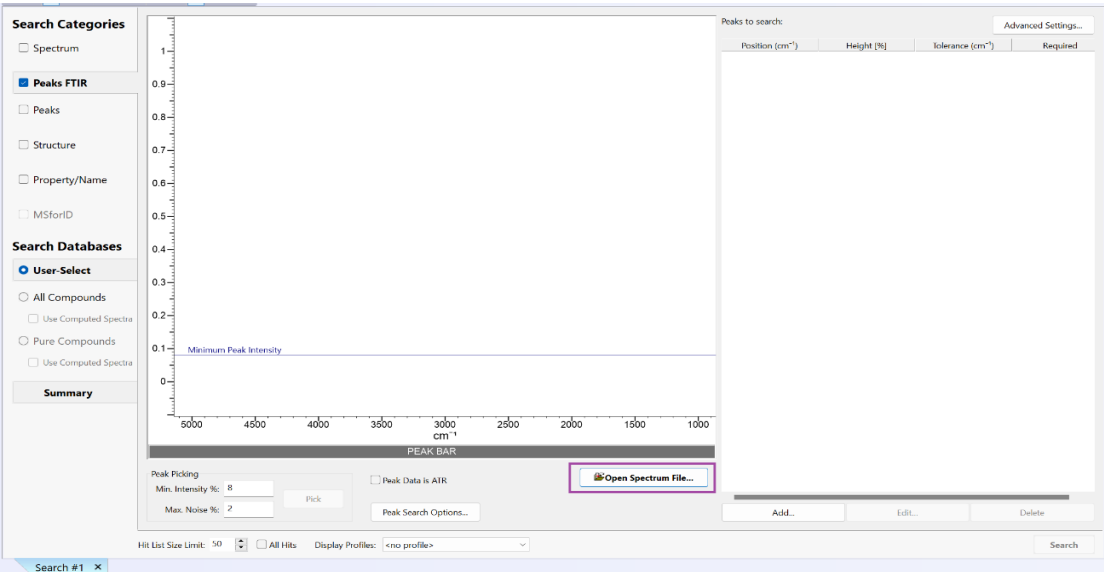
#### KnowItAll Applications Used

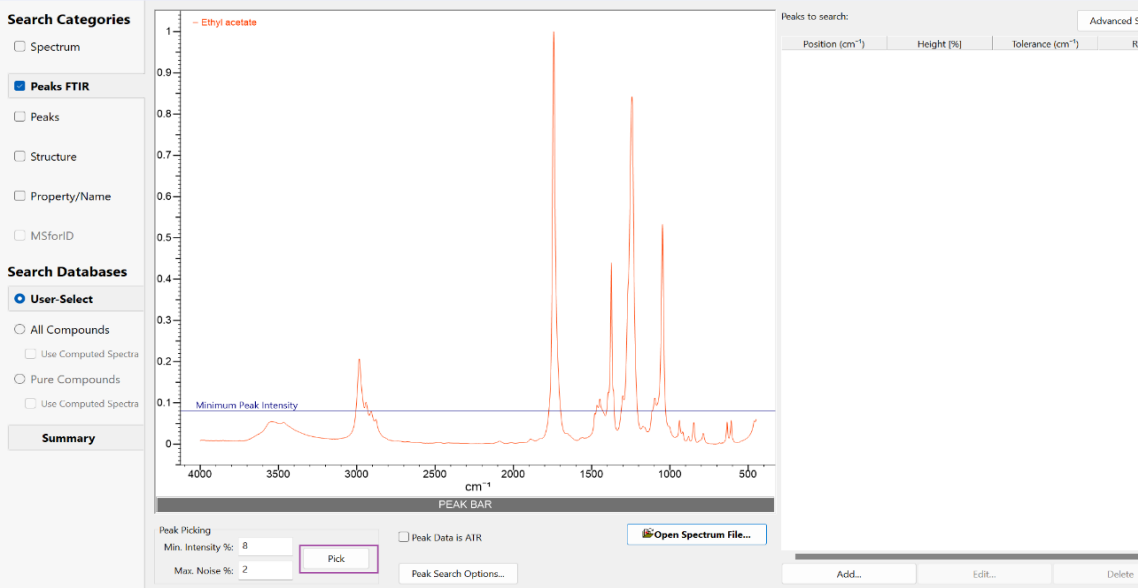
- SearchIt
- Minelt

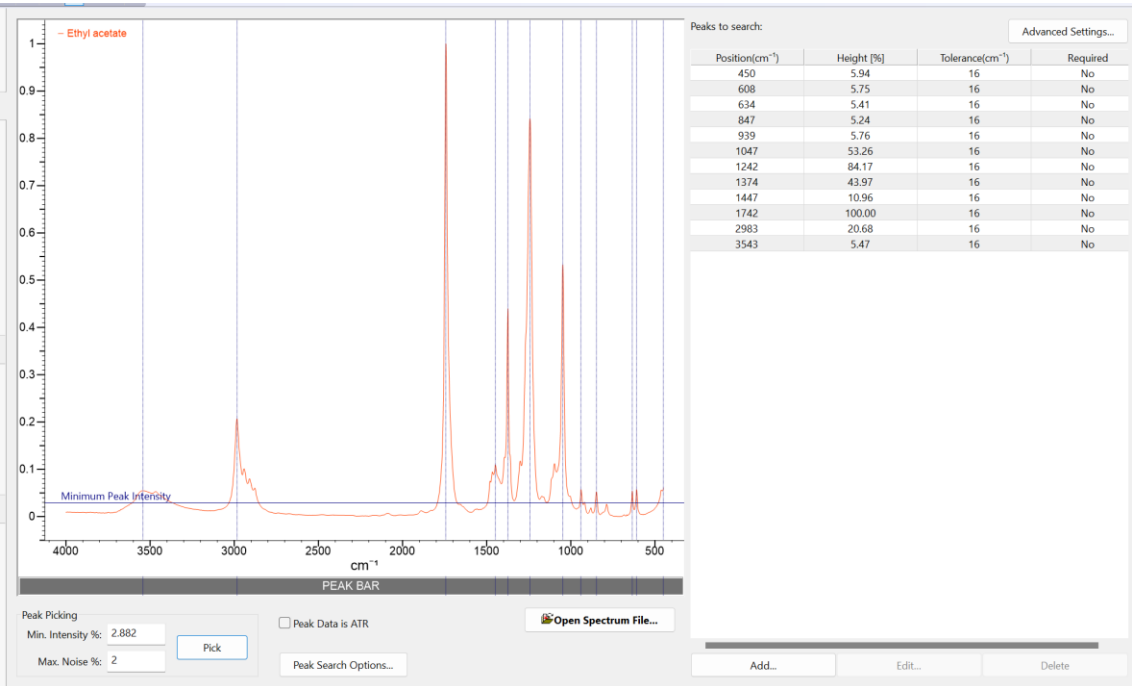
## Configure and perform a peak search

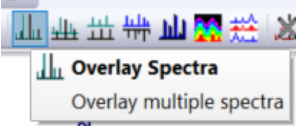
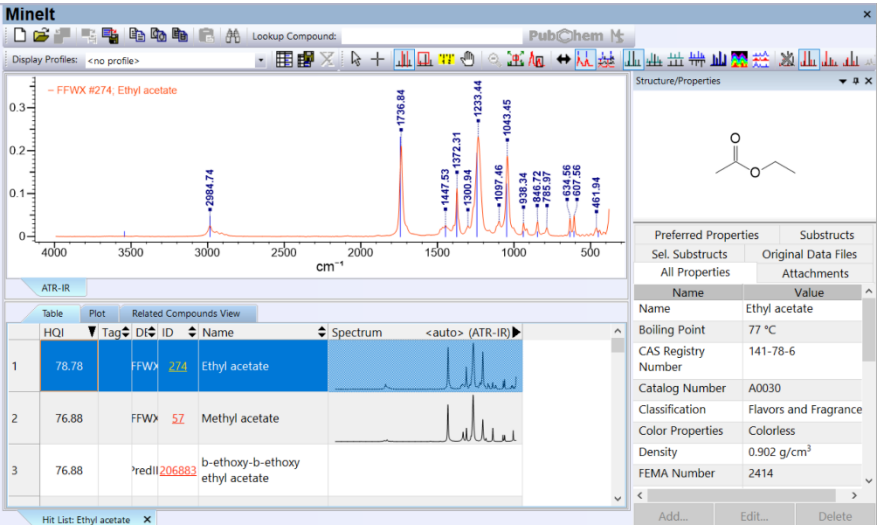
	Action	Result
1	<p>Do one of the following:</p> <ul style="list-style-type: none"><li>If the <b>SearchIt</b> application is not open, navigate to the <b>Data</b> toolbox and click its icon.</li></ul>  <p>If the application is already open, click the <b>Close</b> button  to close the current search.</p>	<p>The <b>SearchIt</b> application's <b>User-Select</b> tab is displayed, and the <b>Selected for Searching</b> list displays the databases last used:</p> 

	Action	Result
2	<p>If databases are already selected for searching, click <b>Remove All</b> to clear the selections. Set <b>Limit to spectral technique to IR</b>. Click <b>Add All</b>.</p>	<p>The Wiley IR database library has been added to the <b>Selected for Searching</b> window:</p> 
3	<p>Under <b>Search Categories</b> click <b>Peaks</b>. Choose <b>IR</b> in the pop-up dialog.</p>	<p>The <b>Spectral Technique Selection</b> dialog appears, and user selects option for <b>IR</b>:</p> 

	Action	Result
4	Click <b>OK</b> .	<p>The <b>Peaks FTIR</b> search dialog is displayed:</p> 

	Action	Result
5	<p>Click <b>Open Spectrum File</b> button located toward the bottom</p> <p>Navigate to <b>“C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\IR”</b>.</p> <p>Open <b>Ethyl acetate.jdx</b>.</p>	<p>The selected spectrum is displayed:</p>  <p>The screenshot displays the following interface elements:</p> <ul style="list-style-type: none"> <li><b>Search Categories:</b> Spectrum (unchecked), <b>Peaks FTIR</b> (checked), Peaks (unchecked), Structure (unchecked), Property/Name (unchecked), MSforID (unchecked).</li> <li><b>Search Databases:</b> <b>User-Select</b> (selected), All Compounds (unchecked), Use Computed Spectra (unchecked), Pure Compounds (unchecked), Use Computed Spectra (unchecked).</li> <li><b>Summary:</b> A button at the bottom of the search panel.</li> <li><b>Peak Picking:</b> Min. Intensity %: 8, Max. Noise %: 2, and a highlighted <b>Pick</b> button.</li> <li><b>Other Controls:</b> "Open Spectrum File..." button, "Peak Data is AIR" checkbox, and "Peak Search Options..." button.</li> <li><b>Table:</b> A table titled "Peaks to search:" with columns for Position (cm<sup>-1</sup>), Height (%), Tolerance (cm<sup>-1</sup>), and a "Required" column.</li> </ul>

	Action	Result																																																				
6	Click <b>Pick</b> .	<p>The <b>peak table</b> is created based on the current settings:</p>  <p>The screenshot displays an IR spectrum for Ethyl acetate. The x-axis represents wavenumber in cm<sup>-1</sup>, ranging from 4000 to 500. The y-axis represents relative intensity from 0 to 1. A horizontal blue line indicates the 'Minimum Peak Intensity' at approximately 0.05. A 'PEAK BAR' is visible at the bottom of the plot area. To the right of the plot is a 'Peaks to search:' table with columns for Position (cm<sup>-1</sup>), Height (%), Tolerance (cm<sup>-1</sup>), and Required. Below the table are 'Add...', 'Edit...', and 'Delete' buttons. At the bottom of the interface, there are 'Peak Picking' controls including 'Min. Intensity %' (set to 2.882), 'Max. Noise %' (set to 2), a 'Pick' button, and a checkbox for 'Peak Data is ATR'. An 'Open Spectrum File...' button is also present.</p> <table border="1" data-bbox="1465 375 1906 602"> <thead> <tr> <th>Position(cm<sup>-1</sup>)</th> <th>Height (%)</th> <th>Tolerance(cm<sup>-1</sup>)</th> <th>Required</th> </tr> </thead> <tbody> <tr><td>450</td><td>5.94</td><td>16</td><td>No</td></tr> <tr><td>608</td><td>5.75</td><td>16</td><td>No</td></tr> <tr><td>634</td><td>5.41</td><td>16</td><td>No</td></tr> <tr><td>847</td><td>5.24</td><td>16</td><td>No</td></tr> <tr><td>939</td><td>5.76</td><td>16</td><td>No</td></tr> <tr><td>1047</td><td>53.26</td><td>16</td><td>No</td></tr> <tr><td>1242</td><td>84.17</td><td>16</td><td>No</td></tr> <tr><td>1374</td><td>43.97</td><td>16</td><td>No</td></tr> <tr><td>1447</td><td>10.96</td><td>16</td><td>No</td></tr> <tr><td>1742</td><td>100.00</td><td>16</td><td>No</td></tr> <tr><td>2983</td><td>20.68</td><td>16</td><td>No</td></tr> <tr><td>3543</td><td>5.47</td><td>16</td><td>No</td></tr> </tbody> </table>	Position(cm <sup>-1</sup> )	Height (%)	Tolerance(cm <sup>-1</sup> )	Required	450	5.94	16	No	608	5.75	16	No	634	5.41	16	No	847	5.24	16	No	939	5.76	16	No	1047	53.26	16	No	1242	84.17	16	No	1374	43.97	16	No	1447	10.96	16	No	1742	100.00	16	No	2983	20.68	16	No	3543	5.47	16	No
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7	<b>TIP</b>	<p>You can remove a peak from the <b>peak table</b> by selecting the peak and clicking the <b>delete</b> button or by double-clicking it in the peak bar. Similarly, you can <b>add</b> or <b>edit</b> peaks using the corresponding buttons at the bottom of the table.</p>																																																				

	Action	Result
8	<p>Click <b>Search</b>. In <b>Minelt</b>, click <b>Overlay Spectra</b> view.</p> 	<p>Search results are automatically displayed in the <b>Minelt</b> application:</p>  <p>For each entry, the <b>Spectral</b> pane displays the hit list spectrum along with the peaks used to perform the search.</p>



# Searching

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## How to Search Spectral Databases Using a Limited Range in a Spectrum

### Purpose

This exercise demonstrates how to search spectral databases using a limited spectral range with the KnowItAll Informatics System's SearchIt application.

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### Objectives

This exercise will teach you:

- How to use the Include Range bar when configuring a spectral search
  - How to use the Search Masks dialog box when configuring a spectral search
- 

### Background

Using a limited range spectral search is slightly faster because fewer points are needed for computation. Using a limited range also focuses a spectral search on feature-rich areas such as the fingerprint region in the IR below 1500 wavenumbers and can be used in place of spectral subtraction by ignoring regions where impurities have peaks.

#### Training Files Used in This Lesson

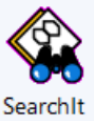

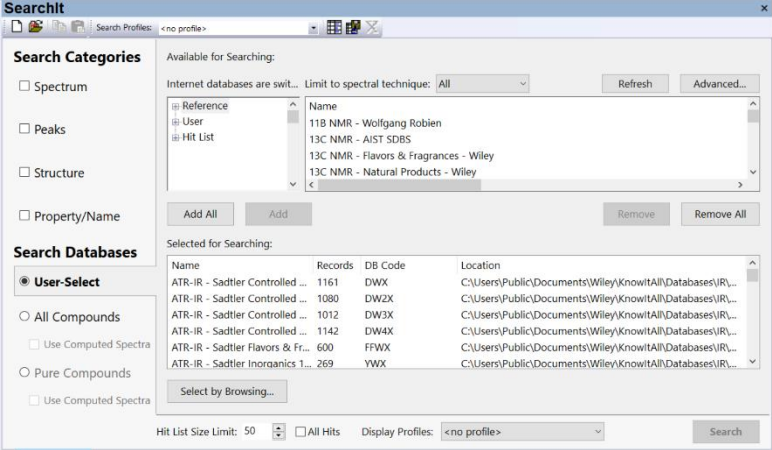
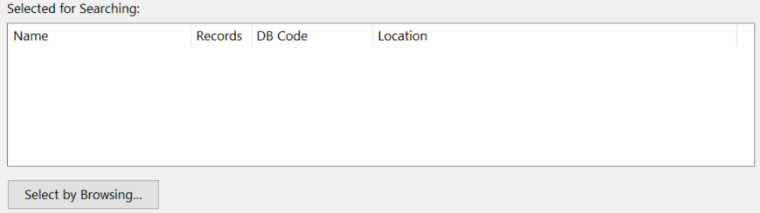
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\IR

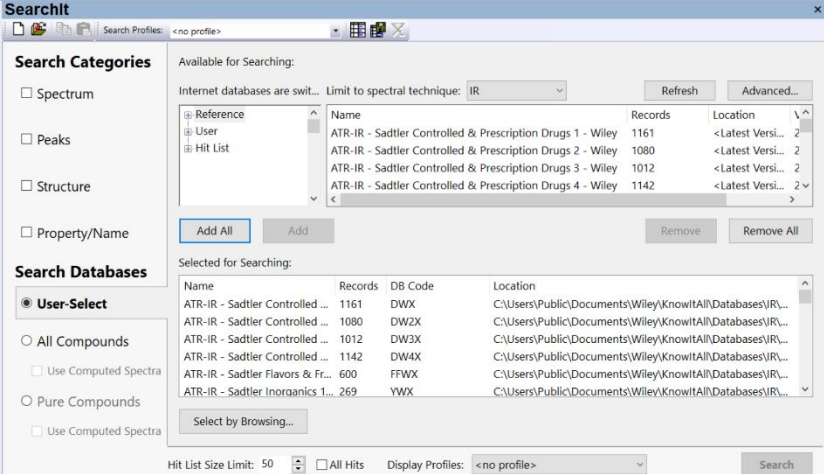
- Acetonitrile.jdx

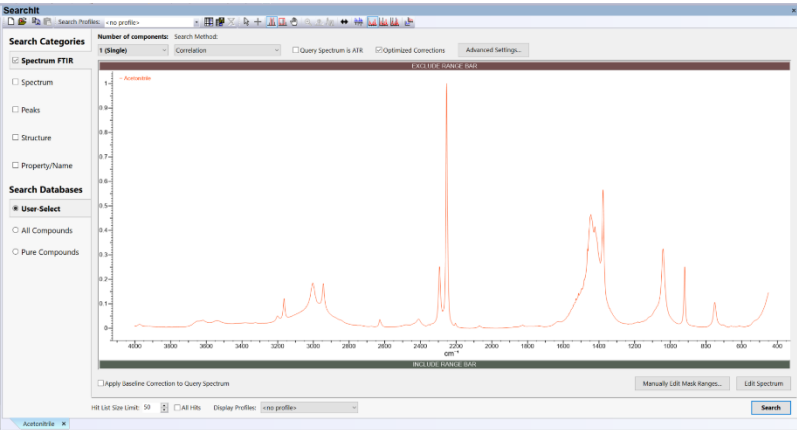
#### KnowItAll Applications Used

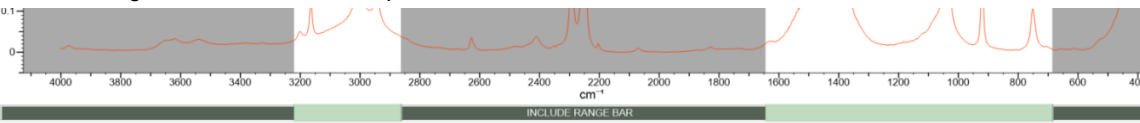

- SearchIt
- Minelt

## Configure a spectral search


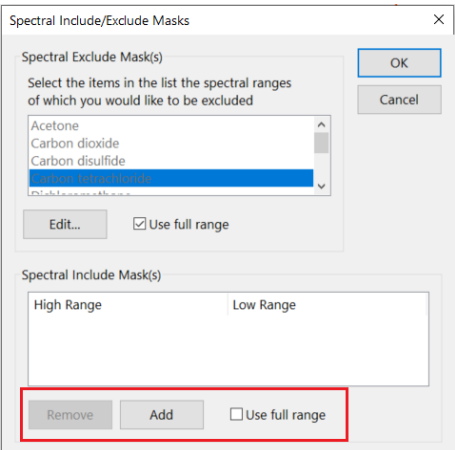
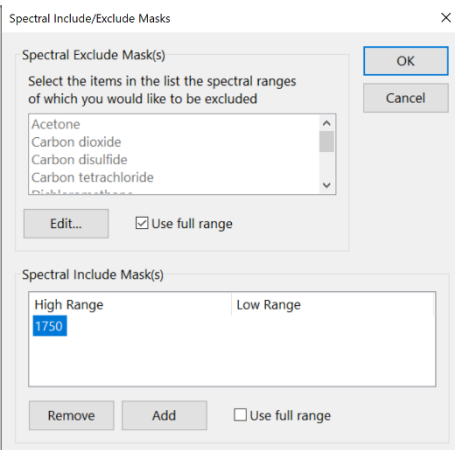
	Action	Result
1	<p>Do one of the following:</p> <ul style="list-style-type: none"> <li>If the <b>SearchIt</b> application is not open, navigate to the <b>Data</b> toolbox and click its icon.</li> </ul>  <ul style="list-style-type: none"> <li>If the <b>SearchIt</b> application is already open, click the <b>SearchIt Close</b> button  to close the current search.</li> </ul>	<p>The <b>SearchIt</b> application's <b>User-Select</b> tab is displayed and the <b>Selected for Searching</b> list displays the databases last used:</p> 
2	<p>If databases are already selected for searching, click <b>Remove All</b> to clear the selections.</p>	<p>The <b>Selected for Searching</b> window is cleared:</p> 

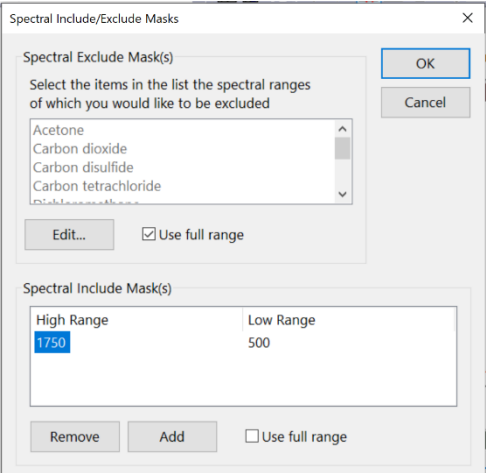
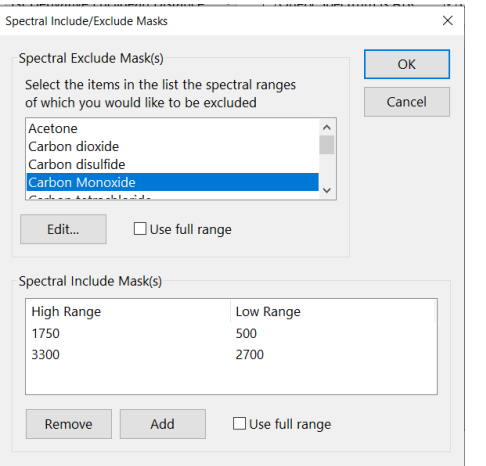
	Action	Result																												
3	In the <b>Available for Searching</b> Dialog, choose <b>IR</b> for <b>Limit Spectral Technique</b> to. Click <b>Add All</b> .	<p>The Wiley IR database collection is displayed in the <b>Selected for Searching</b> list:</p>  <p>The screenshot shows the SearchIt dialog box with the following details:</p> <ul style="list-style-type: none"> <li><b>Search Categories:</b> Spectrum, Peaks, Structure, Property/Name (all unchecked).</li> <li><b>Search Databases:</b> User-Select (selected), All Compounds, Pure Compounds (all unchecked).</li> <li><b>Available for Searching:</b> Internet databases are switched on. Limit to spectral technique: IR. Buttons: Refresh, Advanced...</li> <li><b>Selected for Searching:</b> <table border="1"> <thead> <tr> <th>Name</th> <th>Records</th> <th>DB Code</th> <th>Location</th> </tr> </thead> <tbody> <tr> <td>ATR-IR - Sadtler Controlled &amp; Prescription Drugs 1 - Wiley</td> <td>1161</td> <td>DWX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR...</td> </tr> <tr> <td>ATR-IR - Sadtler Controlled &amp; Prescription Drugs 2 - Wiley</td> <td>1080</td> <td>DW2X</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR...</td> </tr> <tr> <td>ATR-IR - Sadtler Controlled &amp; Prescription Drugs 3 - Wiley</td> <td>1012</td> <td>DW3X</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR...</td> </tr> <tr> <td>ATR-IR - Sadtler Controlled &amp; Prescription Drugs 4 - Wiley</td> <td>1142</td> <td>DW4X</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR...</td> </tr> <tr> <td>ATR-IR - Sadtler Flavors &amp; Fr...</td> <td>600</td> <td>FFWX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR...</td> </tr> <tr> <td>ATR-IR - Sadtler Inorganics 1...</td> <td>269</td> <td>YWX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR...</td> </tr> </tbody> </table> </li> </ul>	Name	Records	DB Code	Location	ATR-IR - Sadtler Controlled & Prescription Drugs 1 - Wiley	1161	DWX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR...	ATR-IR - Sadtler Controlled & Prescription Drugs 2 - Wiley	1080	DW2X	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR...	ATR-IR - Sadtler Controlled & Prescription Drugs 3 - Wiley	1012	DW3X	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR...	ATR-IR - Sadtler Controlled & Prescription Drugs 4 - Wiley	1142	DW4X	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR...	ATR-IR - Sadtler Flavors & Fr...	600	FFWX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR...	ATR-IR - Sadtler Inorganics 1...	269	YWX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR...
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4	Click <b>Spectrum</b> under <b>Search Categories</b> .	An <b>Open</b> dialog box appears.																												

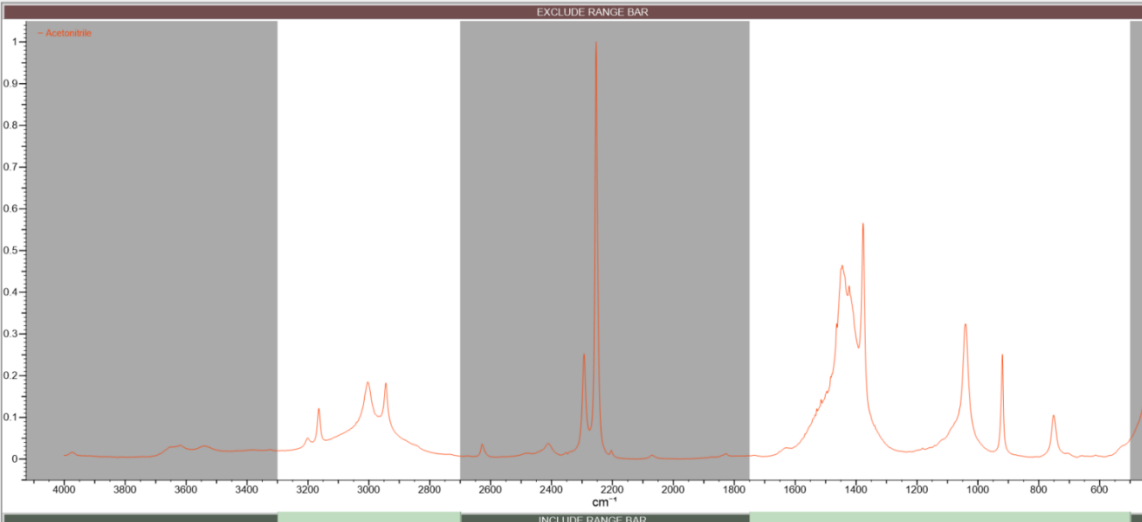
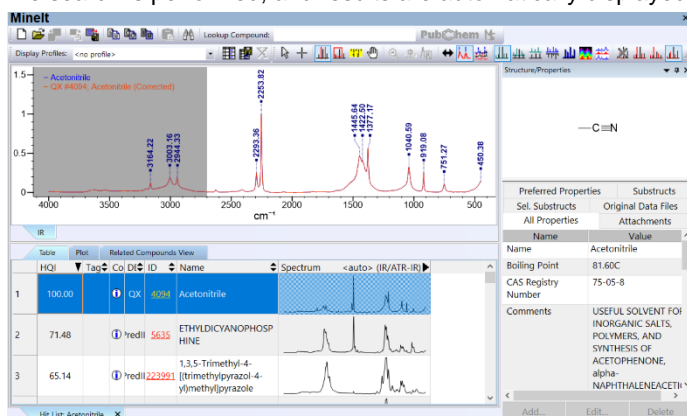

	Action	Result
5	<p>Navigate to “C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\IR”. Open <b>Acetonitrile.jdx</b>.</p> <p><b>Note:</b> You can use the <b>Files of Type</b> filter to display JCAMP files (or all files).</p>	<p>The spectrum is displayed.</p> 
6	<p>Click, drag, and release within the <b>Include Range Bar</b> to define an <b>Include</b> region.</p>	<p>The Include region is green in the <b>Include Range Bar</b>; the included spectral region has a white background. Spectral regions that will not be included in the search have a gray background:</p>  <p>Using the <b>Include Range</b> feature allows you to set one or more ranges to be included in a spectral search. This feature is primarily used on a per search basis. Although the ranges set using this method will be remembered until they are changed, the ranges are not permanently saved.</p>

	Action	Result
7	<p>Click and drag to define a second Include region.</p> <p><b>Note:</b> To move a region horizontally, click within the region on the <b>Include Range Bar</b> and drag to a new location.</p>	<p>A second region is selected on the spectrum:</p>  <p>The image shows an IR spectrum with a wavenumber axis from 4000 to 400 cm<sup>-1</sup>. Two regions are highlighted in grey: one from approximately 3200 to 2800 cm<sup>-1</sup> and another from approximately 1600 to 1000 cm<sup>-1</sup>. Below the spectrum is a black 'INCLUDE RANGE BAR' with two green segments corresponding to the highlighted regions. A white cursor is positioned over the right edge of the second green segment.</p>
8	<p><b>TIPS:</b></p>	<p>To re-size a region, move the cursor into the <b>Include Range Bar</b> and position the cursor over an endpoint, then drag and release. The cursor changes to a cross with a double arrowhead.</p>  <p>The image is a close-up of the 'INCLUDE RANGE BAR' showing a green segment. A white cursor with a black cross and double arrowheads is positioned over the right endpoint of the green segment.</p> <p>To remove a single region, either click within the region on the <b>Include Range Bar</b> and drag to either side away from the spectral pane, or right-click within the region and choose <b>Yes</b> on the message box that opens.</p> <p>To remove all regions, click the trash can icon at the right end of the <b>Include Range Bar</b>.</p>

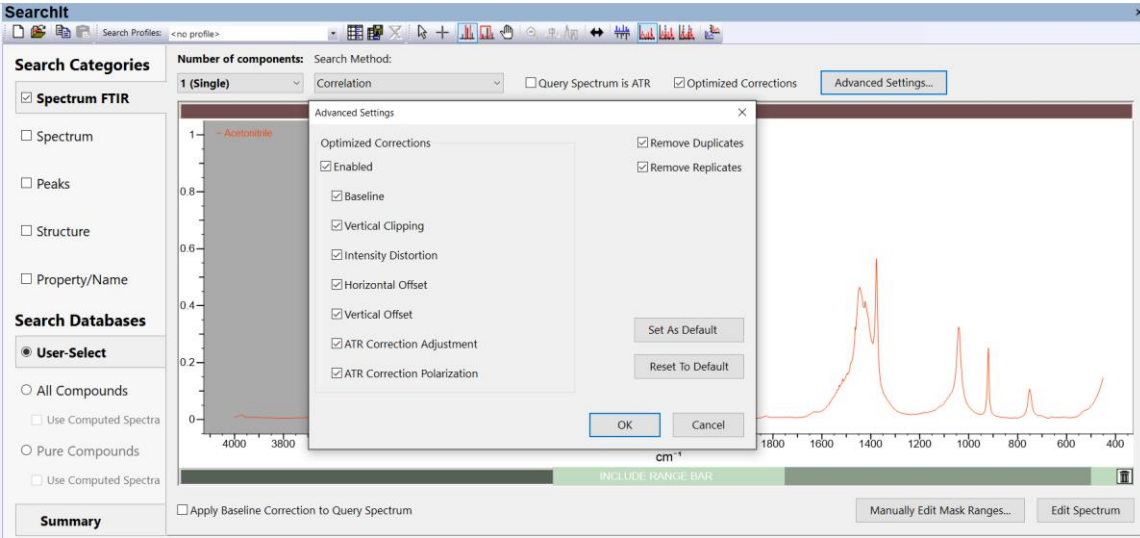
## Use the Search Masks dialog box

	Action	Result
1	<p>Clear the previous search range by clicking the trash can icon on the right side of the <b>INCLUDE RANGE BAR</b></p>  <p>Click <b>Manually Edit Mask Ranges</b>. Unclick <b>Use full range</b> and click <b>Add</b> under <b>Spectral Include Mask(s)</b></p> <p><b>Note:</b> Any <b>Include</b> regions defined using the <b>Include Range Bar</b> are displayed in the list of <b>Spectral Include Mask(s)</b>. However, if <b>Use full range</b> is checked, these regions will not be used.</p>	<p>The <b>Spectral Include/Exclude Masks</b> dialog box opens.</p> 
2	<p>Click to select the <b>High Range</b> value in the remaining Include region and type in '1750.'</p>	<p>1750 is added as a <b>High Range</b> value:</p> 

	Action	Result
3	Click to select the <b>Low Range</b> value in the remaining Include region and type in '500.'	<p>500 is added as a <b>Low Range</b> value:</p> 
4	Click <b>Add</b> to create another Include region. Type '3300 in the new <b>High Range</b> text box, then click in the <b>Low Range</b> column and type '2700.'	<p>The ranges are added to the <b>Spectral Include Masks</b>:</p> 

	Action	Result																																														
5	Click <b>OK</b> .	<p>The dialog box closes, and the search spectrum is displayed with the re-defined <b>Include</b> regions.</p>  <p>The image shows an IR spectrum for Acetonitrile. The x-axis represents wavenumber in cm⁻¹, ranging from 4000 to 400. The y-axis represents transmittance from 0 to 1.0. A red line represents the spectrum. Two grey shaded regions are labeled 'EXCLUDE RANGE BAR' at the top, covering approximately 3500-3000 cm⁻¹ and 2000-1800 cm⁻¹. A green shaded region at the bottom is labeled 'INCLUDE RANGE BAR', covering the entire range from 4000 to 400 cm⁻¹. Several peaks are visible, with a prominent one at approximately 2200 cm⁻¹.</p>																																														
6	Click <b>Search</b> .	<p>The search is performed, and results are automatically displayed in the <b>Minelt</b> application as a hit list.</p>  <p>The image is a screenshot of the Minelt application interface. At the top, it shows 'Minelt' and 'PubChem'. Below that is a search bar with 'Acetonitrile' entered. The main area displays an IR spectrum of Acetonitrile with several peaks labeled with their wavenumbers: 3164.22, 3063.16, 2944.25, 2283.82, 1465.84, 1377.07, 1046.59, 819.28, 751.27, and 469.38. To the right of the spectrum is a 'Structure/Properties' panel showing the chemical structure of Acetonitrile (C≡N) and a table of properties:</p> <table border="1" data-bbox="1281 1104 1470 1339"> <thead> <tr> <th>Name</th> <th>Value</th> </tr> </thead> <tbody> <tr> <td>Name</td> <td>Acetonitrile</td> </tr> <tr> <td>Boiling Point</td> <td>81.60C</td> </tr> <tr> <td>CAS Registry Number</td> <td>75-05-8</td> </tr> <tr> <td>Comments</td> <td>USEFUL SOLVENT FOR INORGANIC SALTS, POLYMERS, AND SYNTHESIS OF ACETOPHENONE, alpha-NAPHTHALENEACETI...</td> </tr> </tbody> </table> <p>Below the spectrum is a 'Hit List' table:</p> <table border="1" data-bbox="787 1185 1260 1339"> <thead> <tr> <th>HIQI</th> <th>Tag</th> <th>CO</th> <th>DI</th> <th>ID</th> <th>Name</th> <th>Spectrum</th> <th>&lt;auto&gt;</th> <th>(IR/ATR-IR)</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>100.00</td> <td></td> <td>CX</td> <td>4099</td> <td>Acetonitrile</td> <td></td> <td></td> <td></td> </tr> <tr> <td>2</td> <td>71.48</td> <td></td> <td>iredi</td> <td>5633</td> <td>ETHYLDICANOPHOSPHINE</td> <td></td> <td></td> <td></td> </tr> <tr> <td>3</td> <td>65.14</td> <td></td> <td>iredi</td> <td>223991</td> <td>1,3,5-Trimethyl-4-(trimethylpyrazol-4-yl)methylpyrazole</td> <td></td> <td></td> <td></td> </tr> </tbody> </table> <p>Clicking on the information icon  in the results table displays <b>Optimized Corrections</b> that have been performed.</p>	Name	Value	Name	Acetonitrile	Boiling Point	81.60C	CAS Registry Number	75-05-8	Comments	USEFUL SOLVENT FOR INORGANIC SALTS, POLYMERS, AND SYNTHESIS OF ACETOPHENONE, alpha-NAPHTHALENEACETI...	HIQI	Tag	CO	DI	ID	Name	Spectrum	<auto>	(IR/ATR-IR)	1	100.00		CX	4099	Acetonitrile				2	71.48		iredi	5633	ETHYLDICANOPHOSPHINE				3	65.14		iredi	223991	1,3,5-Trimethyl-4-(trimethylpyrazol-4-yl)methylpyrazole			
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Action	Result
<p>7 Close the <b>Optimized Corrections</b> window, then use the KnowItAll <b>Back</b> button to return to the <b>SearchIt</b> application.</p> <p>Click <b>Advanced Settings</b> on the <b>Spectrum FTIR</b> tab.</p>	<p>The <b>Advanced Settings</b> dialog box opens:</p>  <p>The screenshot shows the SearchIt application interface. On the left, the 'Search Categories' panel has 'Spectrum FTIR' selected. The 'Advanced Settings' dialog box is open, displaying various optimization options. The 'Optimized Corrections' section is checked and includes: 'Enabled', 'Baseline', 'Vertical Clipping', 'Intensity Distortion', 'Horizontal Offset', 'Vertical Offset', 'ATR Correction Adjustment', and 'ATR Correction Polarization'. The 'Remove Duplicates' and 'Remove Replicates' options are also checked. The background shows an FTIR spectrum plot with a peak labeled 'Acetanilide' at approximately 1650 cm⁻¹. The x-axis is labeled 'cm⁻¹' and ranges from 4000 to 400. The y-axis ranges from 0 to 1.0. At the bottom of the dialog, there are buttons for 'Set As Default', 'Reset To Default', 'OK', and 'Cancel'. Below the dialog, there is a checkbox for 'Apply Baseline Correction to Query Spectrum' and buttons for 'Manually Edit Mask Ranges...' and 'Edit Spectrum'.</p> <p>The <b>Advanced Settings</b> dialog can be used to control the applied <b>Optimized Corrections</b>.</p>

# Searching

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## How to Search Spectral Databases Using a Mask to Exclude Regions in Your Search

### Purpose

This exercise demonstrates how to create masks to exclude regions in a spectral search.

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### Objectives

This exercise will teach you:

- How to create and use Exclude Masks when configuring a spectral search
- 

### Background

Exclude Masks allows you to ignore regions during spectral searching and can be defined for a variety of compounds such as solvents or impurities. Such masking allows for an easy method to remove these regions from consideration during a search.

Unlike Include Regions, which is not permanent, Exclude Masks can be saved and re-used.

#### Training Files Used in This Lesson

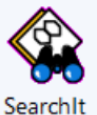

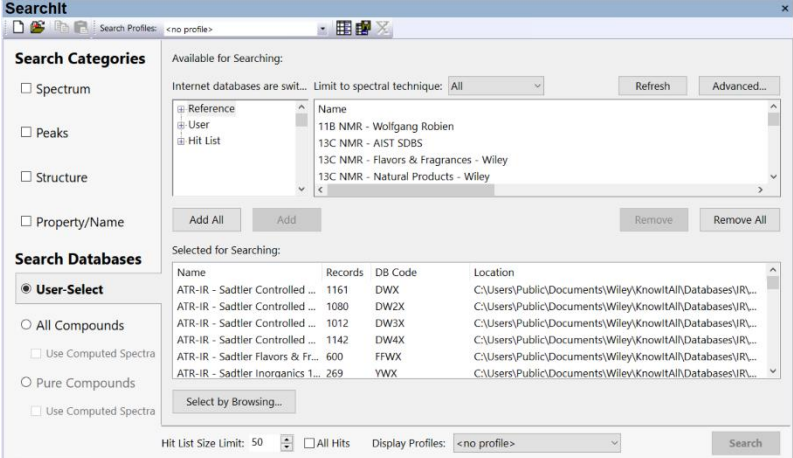
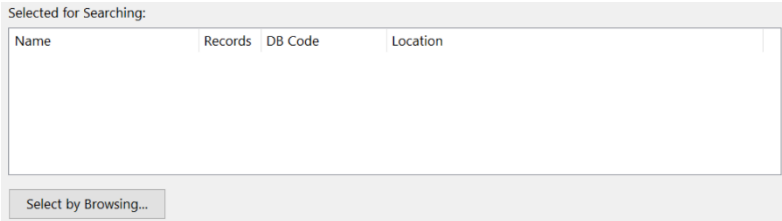
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\IR

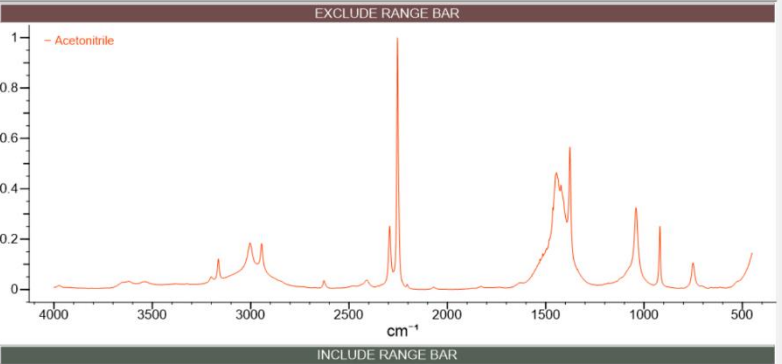
- Acetonitrile.jdx

#### KnowItAll Applications Used

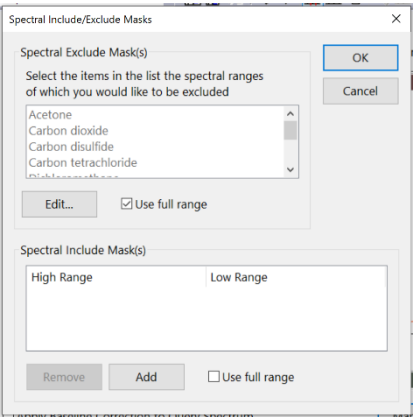
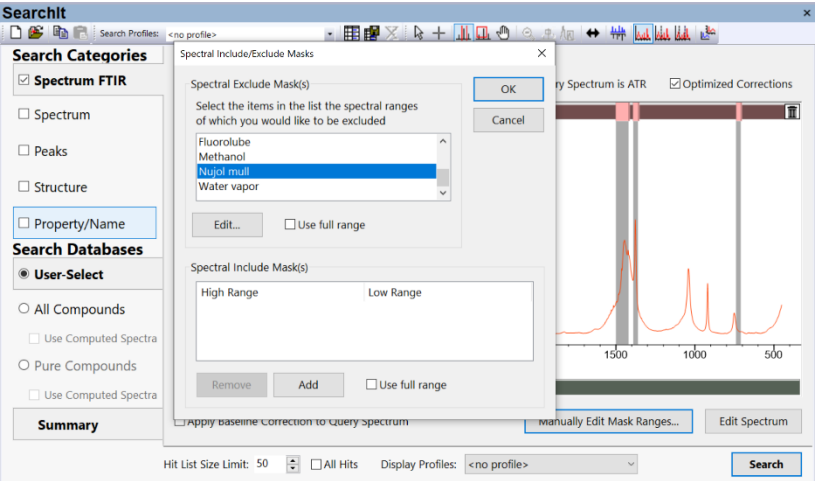
- SearchIt
- Minelt

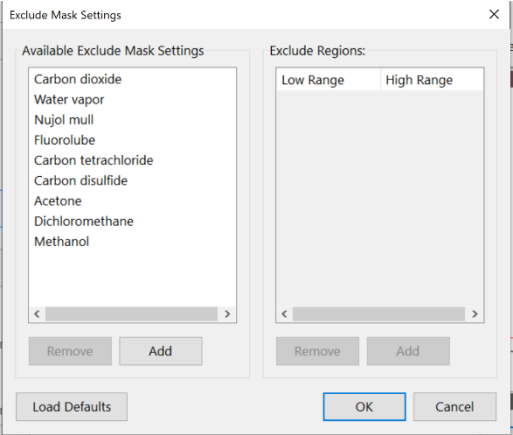
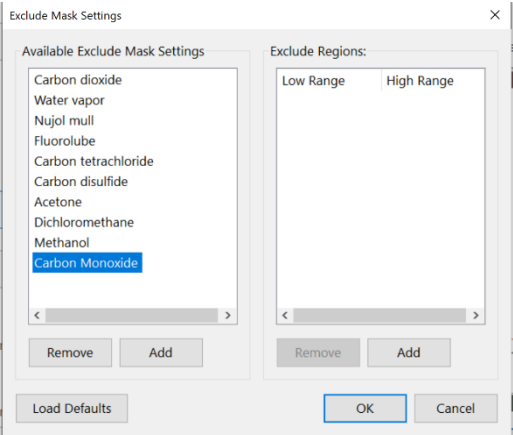
## Configure a spectral search

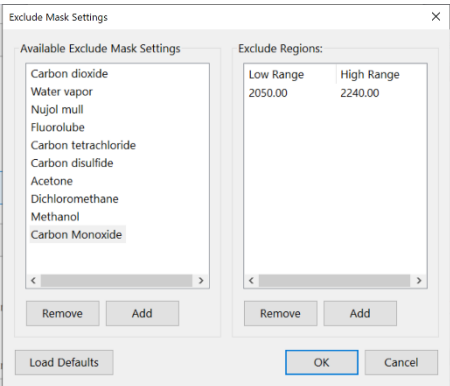
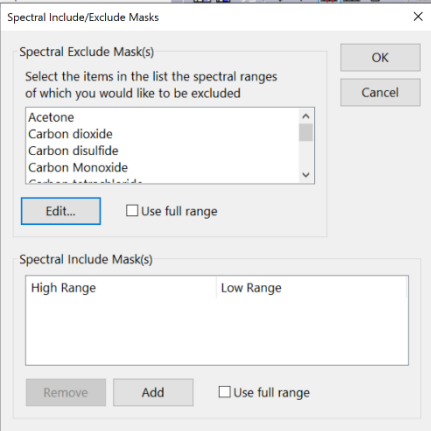
	Action	Result
1	<p>Do one of the following:</p> <ul style="list-style-type: none"> <li>If the <b>SearchIt</b> application is not open, navigate to the <b>Data</b> toolbox and click its icon.</li> </ul>  <ul style="list-style-type: none"> <li>If the <b>SearchIt</b> application is already open, click the <b>SearchIt Close</b> button  to close the current search.</li> </ul>	<p>The <b>SearchIt</b> application's <b>User-Select</b> tab is displayed and the <b>Selected for Searching</b> list displays the databases last used:</p> 
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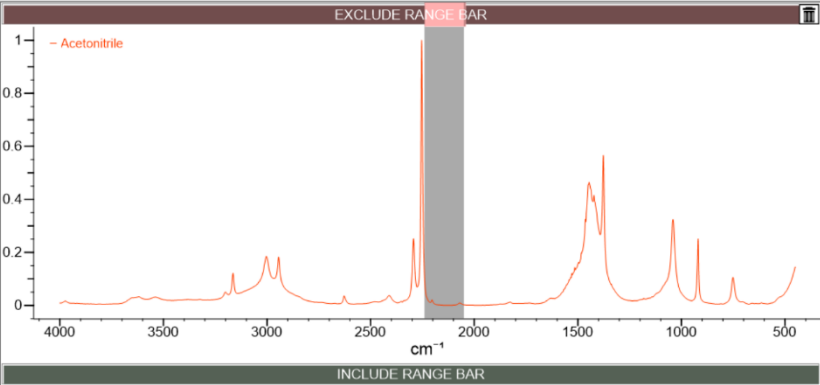
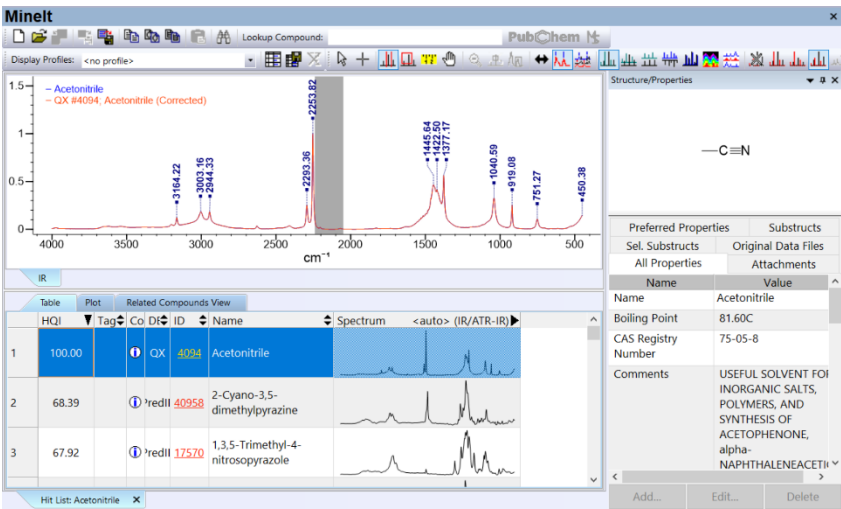
	Action	Result																												
3	Select IR using the <b>Limit to spectral technique</b> control. Click <b>Add All</b> .	The Wiley IR database collection is displayed in the <b>Selected for Searching</b> list: <div data-bbox="793 354 1619 594" style="border: 1px solid gray; padding: 5px; margin: 10px 0;">             Selected for Searching:             <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th>Name</th> <th>Records</th> <th>DB Code</th> <th>Location</th> </tr> </thead> <tbody> <tr> <td>ATR-IR - Sadtler Controlled ...</td> <td>1161</td> <td>DWX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...</td> </tr> <tr> <td>ATR-IR - Sadtler Controlled ...</td> <td>1080</td> <td>DW2X</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...</td> </tr> <tr> <td>ATR-IR - Sadtler Controlled ...</td> <td>1012</td> <td>DW3X</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...</td> </tr> <tr> <td>ATR-IR - Sadtler Controlled ...</td> <td>1142</td> <td>DW4X</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...</td> </tr> <tr> <td>ATR-IR - Sadtler Flavors &amp; Fr...</td> <td>600</td> <td>FFWX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...</td> </tr> <tr> <td>ATR-IR - Sadtler Inorganics 1...</td> <td>269</td> <td>YWX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...</td> </tr> </tbody> </table> <p style="text-align: center; margin-top: 5px;">Select by Browsing...</p> </div> <p><b>Note:</b> Many of the databases have only IR spectra, but others—such as the Multi-Technique Sadtler Demo Database - Wiley—include other types of spectra and structures.</p>	Name	Records	DB Code	Location	ATR-IR - Sadtler Controlled ...	1161	DWX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...	ATR-IR - Sadtler Controlled ...	1080	DW2X	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...	ATR-IR - Sadtler Controlled ...	1012	DW3X	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...	ATR-IR - Sadtler Controlled ...	1142	DW4X	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...	ATR-IR - Sadtler Flavors & Fr...	600	FFWX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...	ATR-IR - Sadtler Inorganics 1...	269	YWX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...
Name	Records	DB Code	Location																											
ATR-IR - Sadtler Controlled ...	1161	DWX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...																											
ATR-IR - Sadtler Controlled ...	1080	DW2X	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...																											
ATR-IR - Sadtler Controlled ...	1012	DW3X	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...																											
ATR-IR - Sadtler Controlled ...	1142	DW4X	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...																											
ATR-IR - Sadtler Flavors & Fr...	600	FFWX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...																											
ATR-IR - Sadtler Inorganics 1...	269	YWX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...																											
4	Click <b>Spectrum</b> under <b>Search Categories</b> .	An <b>Open</b> dialog box appears.																												
5	Navigate to “C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\IR”. Open <b>Acetonitrile.jdx</b> . <p><b>NOTE:</b> You can use the Files of type filter to display JCAMP files (or all files).</p>	The spectrum is displayed in the IR Spectrum tab: <div data-bbox="793 769 1587 1187" style="border: 1px solid gray; padding: 5px; margin: 10px 0;">  <p style="text-align: center; margin-top: 5px;"> <input type="checkbox"/> Apply Baseline Correction to Query Spectrum           <span style="margin-left: 100px;">Manually Edit Mask Ranges...</span> <span style="margin-left: 20px;">Edit Spectrum</span> </p> </div>																												

Use the Search Masks dialog box

	Action	Result
1	Click <b>Manually Edit Mask Ranges</b> .	<p>The <b>Spectral Include/Exclude Masks</b> dialog box opens.</p> 
2	Uncheck <b>Use full range</b> under the list of <b>Spectral Exclude Mask(s)</b> , then click to select the <b>Nujol mull</b> exclude mask.	<p>Excluded regions are highlighted in bright red on the <b>Exclude Range Bar</b>, and in gray in the spectrum. The carbon dioxide exclude mask includes two regions:</p> 

	Action	Result
3	Click <b>Edit</b> on the <b>Spectral Include/Exclude Masks</b> dialog box.	The <b>Exclude Mask Settings</b> dialog opens: 
4	Click <b>Add</b> . Type in "Carbon Monoxide", then click outside the text box.	A text box appears under <b>Available Exclude Mask Settings</b> , which allows for entering "Carbon Monoxide": 

	Action	Result
5	<p>With <b>Carbon Monoxide</b> selected in the list of <b>Available Exclude Mask Settings</b>, click <b>Add</b> under the list of <b>Exclude Regions</b> or click under <b>Low Range</b>. Type in low and high range values (2050 and 2240).</p>	<p>A text box appears under <b>Exclude Regions</b> that allows for entering the <b>Low Range</b> and <b>High Range</b> values:</p> 
6	<p><b>TIPS:</b></p>	<p>Alternatively, you can manually set exclude ranges using the <b>Exclude Range Bar</b> and clicking and dragging to select regions. See the section above on <a href="#">How to Search Spectral Databases Using a Limited Range in a Spectrum</a>. Manually setting the exclude range works in the same way as manually setting the include range.</p>
7	<p>Click <b>OK</b></p>	<p>The <b>Exclude Mask Settings</b> dialog box closes, and the new carbon monoxide mask is added to the list of <b>Exclude Masks</b>.</p> 

	Action	Result																																																								
8	Select the new <b>Carbon Monoxide</b> mask, then click <b>OK</b> to close the <b>Spectral Include/Exclude Masks</b> dialog box.	<p>The dialog box closes, and the search spectrum is displayed with the newly defined exclude region:</p> 																																																								
9	Click <b>Search</b> .	<p>The search results are automatically displayed in the <b>Minelt</b> application as a hit list.</p>  <table border="1" data-bbox="785 1117 1304 1317"> <thead> <tr> <th>HQI</th> <th>Tag</th> <th>Co</th> <th>Di</th> <th>ID</th> <th>Name</th> <th>Spectrum</th> </tr> </thead> <tbody> <tr> <td>100.00</td> <td>QX</td> <td>4094</td> <td></td> <td></td> <td>Acetonitrile</td> <td></td> </tr> <tr> <td>68.39</td> <td>redil</td> <td>40958</td> <td></td> <td></td> <td>2-Cyano-3,5-dimethylpyrazine</td> <td></td> </tr> <tr> <td>67.92</td> <td>redil</td> <td>17570</td> <td></td> <td></td> <td>1,3,5-Trimethyl-4-nitrosopyrazole</td> <td></td> </tr> </tbody> </table> <p>Structure/Properties</p> <p><chem>C#N</chem></p> <table border="1" data-bbox="1388 1045 1621 1317"> <thead> <tr> <th colspan="2">Preferred Properties</th> <th colspan="2">Substructs</th> </tr> <tr> <th colspan="2">All Properties</th> <th colspan="2">Attachments</th> </tr> <tr> <th>Name</th> <th>Value</th> <th></th> <th></th> </tr> </thead> <tbody> <tr> <td>Name</td> <td>Acetonitrile</td> <td></td> <td></td> </tr> <tr> <td>Boiling Point</td> <td>81.60C</td> <td></td> <td></td> </tr> <tr> <td>CAS Registry Number</td> <td>75-05-8</td> <td></td> <td></td> </tr> <tr> <td>Comments</td> <td>USEFUL SOLVENT FOR INORGANIC SALTS, POLYMERS, AND SYNTHESIS OF ACETOPHENONE, alpha-NAPHTHALENEACETI</td> <td></td> <td></td> </tr> </tbody> </table>	HQI	Tag	Co	Di	ID	Name	Spectrum	100.00	QX	4094			Acetonitrile		68.39	redil	40958			2-Cyano-3,5-dimethylpyrazine		67.92	redil	17570			1,3,5-Trimethyl-4-nitrosopyrazole		Preferred Properties		Substructs		All Properties		Attachments		Name	Value			Name	Acetonitrile			Boiling Point	81.60C			CAS Registry Number	75-05-8			Comments	USEFUL SOLVENT FOR INORGANIC SALTS, POLYMERS, AND SYNTHESIS OF ACETOPHENONE, alpha-NAPHTHALENEACETI		
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# Searching

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## How to Subtract One Spectrum from Another

### Purpose

This exercise demonstrates how to use the spectral subtraction feature in the KnowItAll Informatics System.

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### Objectives

This exercise will teach you:

- How to use the spectral subtraction feature in KnowItAll
- 

### Background

You can use the ProcessIt applications to perform a point-by-point subtraction of one spectrum from another. This capability is useful when analyzing mixtures or composite spectra.

#### Training Files Used in This Lesson

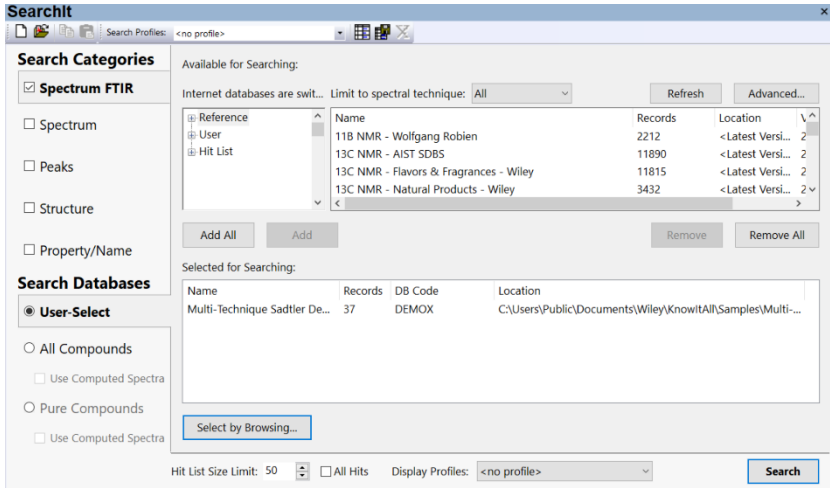
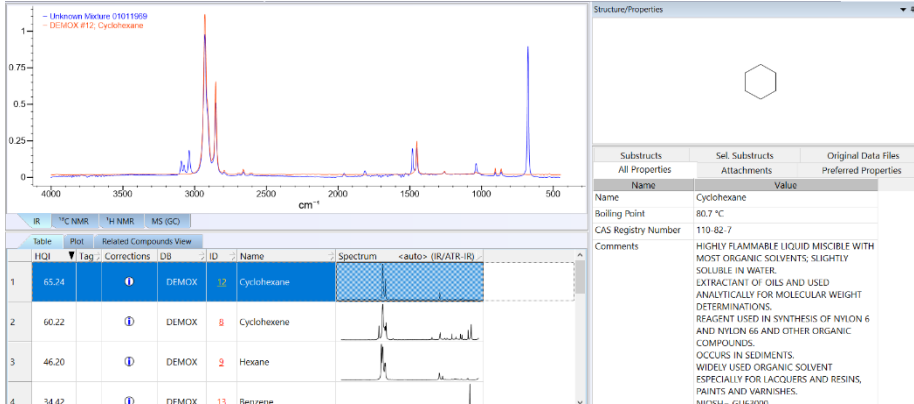
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Mixture Analysis\IR Examples

- Unknown Mixture 01011969.jdx

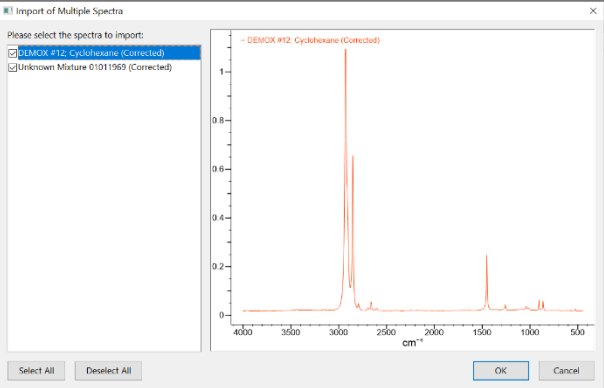
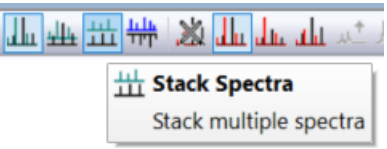
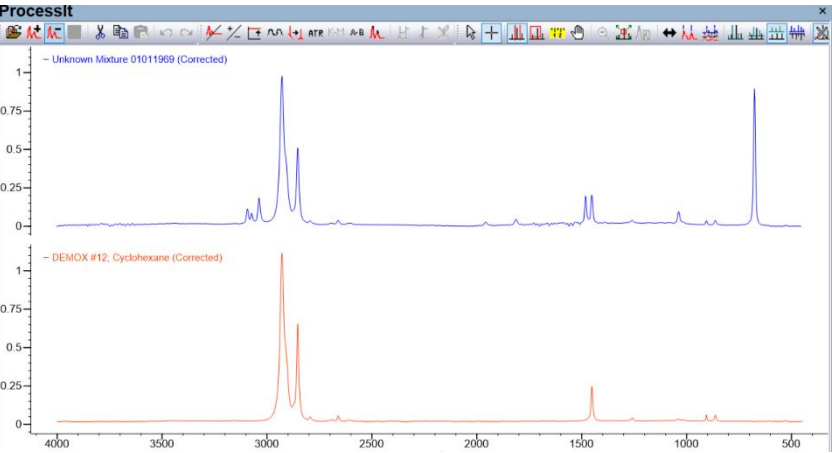
#### KnowItAll Applications Used


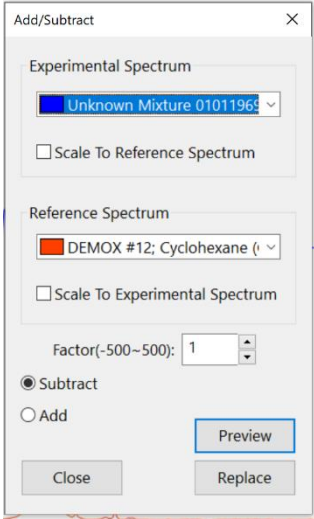
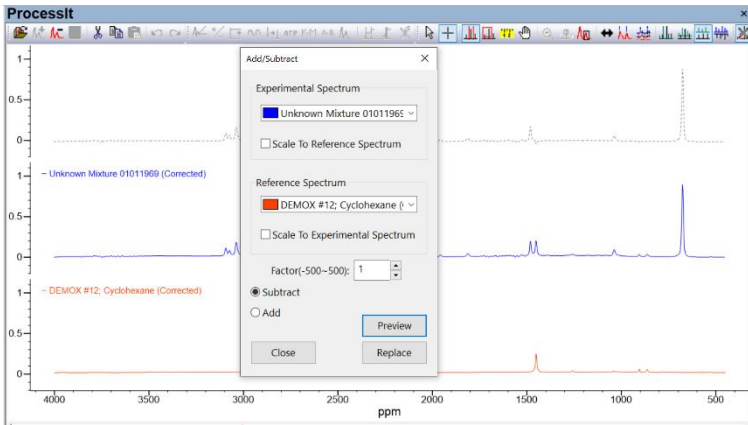
- SearchIt
- Minelt
- ProcessIt

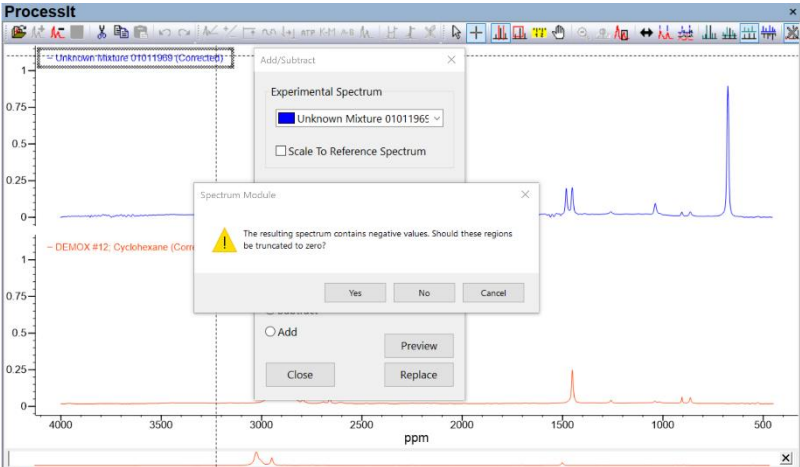
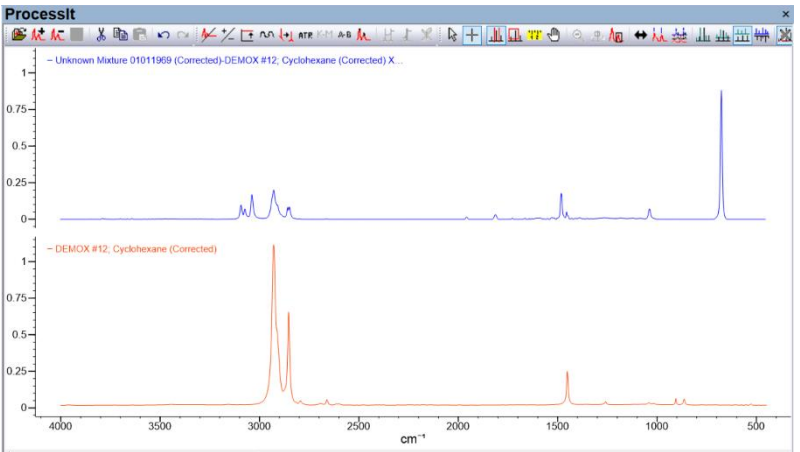
## Set up a spectral search against a mixture

	Action	Result																																			
1	<p>In the <b>SearchIt</b> application, navigate to “C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\Mixture Analysis\IR Examples” and open <b>Unknown Mixture 01011969.jdx</b>.</p> <p>Limit the database search to <b>Multi-Technique Sadtler Demo Database – Wiley</b> from “C:\Users\Public\Public Documents\Wiley\KnowItAll\Sample” folder by using the <b>Open by browsing</b> button.</p>	<p>The FTIR spectrum is opened in <b>SearchIt</b> and the DEMOX database is selected for searching:</p> 																																			
2	Click <b>Search</b> .	<p>Results are displayed in the <b>Minelt</b> application. The first hit is <b>cyclohexane</b>. Both spectra, the query and the first hit are displayed in the spectral pane.</p>  <table border="1" data-bbox="777 1209 1354 1380"> <thead> <tr> <th>Table</th> <th>Plot</th> <th>Related Compounds View</th> <th>ID</th> <th>Name</th> <th>Spectrum</th> <th>&lt;auto&gt; (IR/AIR-IR)</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>65.24</td> <td></td> <td>DEMOX</td> <td>Cyclohexane</td> <td></td> <td></td> </tr> <tr> <td>2</td> <td>60.22</td> <td></td> <td>DEMOX</td> <td>Cyclohexane</td> <td></td> <td></td> </tr> <tr> <td>3</td> <td>46.20</td> <td></td> <td>DEMOX</td> <td>Hexane</td> <td></td> <td></td> </tr> <tr> <td>4</td> <td>34.47</td> <td></td> <td>DEMOX</td> <td>Benzen...</td> <td></td> <td></td> </tr> </tbody> </table>	Table	Plot	Related Compounds View	ID	Name	Spectrum	<auto> (IR/AIR-IR)	1	65.24		DEMOX	Cyclohexane			2	60.22		DEMOX	Cyclohexane			3	46.20		DEMOX	Hexane			4	34.47		DEMOX	Benzen...		
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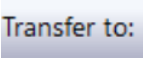
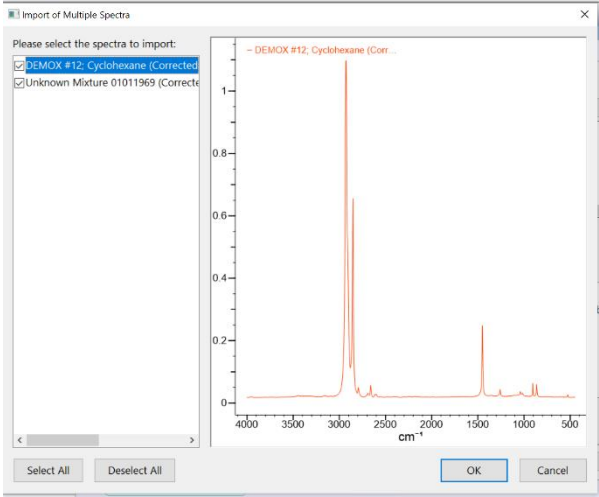
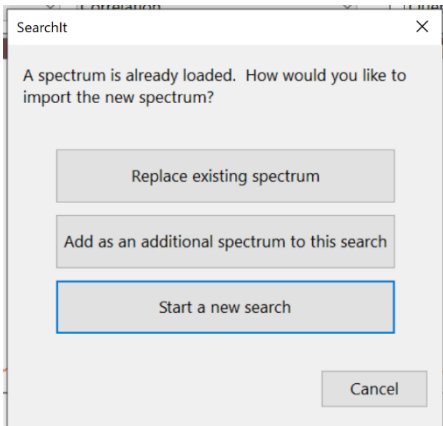
## Create a difference spectrum

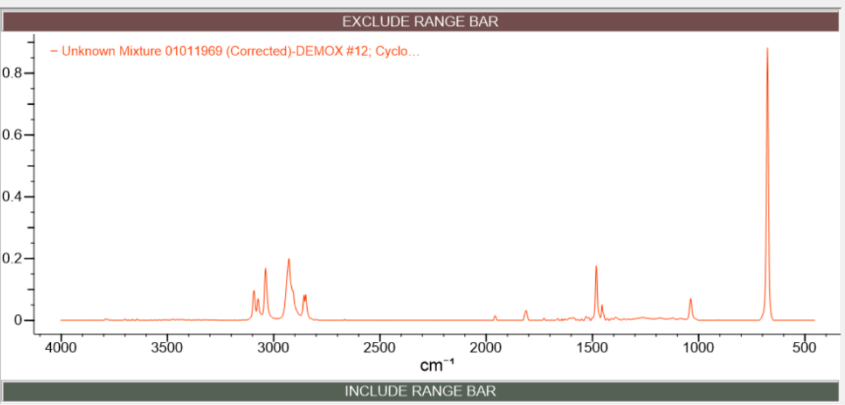
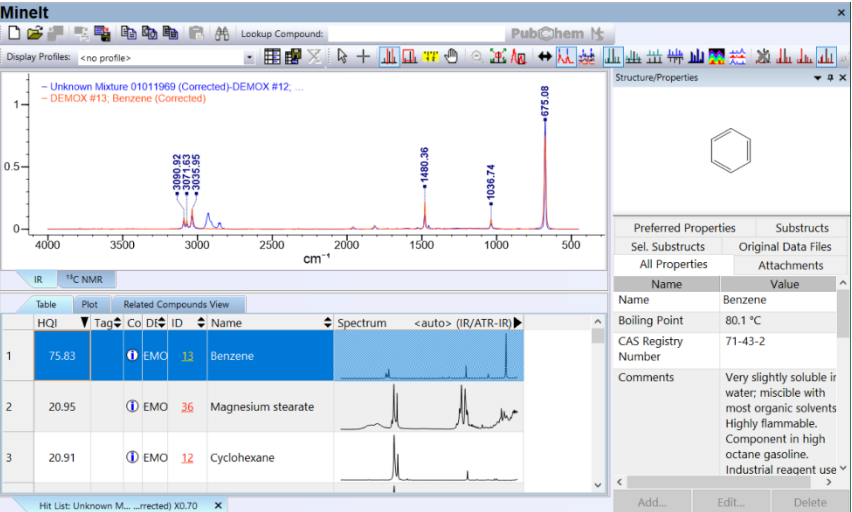
	Action	Result
1	With the hit list displayed in <b>Minelt</b> and the first record selected, click <b>ProcessIt</b> in the <b>Transfer to</b> bar.	<p>The <b>Import of Multiple Spectra</b> dialog box opens.</p>  <p>Both the query spectrum and the first hit are displayed.</p>
2	Click <b>Select All</b> , then click <b>OK</b> on the <b>Import of Multiple Spectra</b> dialog box. Click <b>Stack Spectra</b> view. 	<p>Both spectra—the mixture and the first hit, cyclohexane—are transferred to the <b>ProcessIt</b> IR application:</p>  <p><b>NOTE:</b> Use spectrum toolbar buttons to adjust the display. The Stacked display is preferable to Offset or Overlay for spectral subtraction.</p>

	Action	Result
3	<p>Choose <b>Process &gt; Add/Subtract Spectrum</b>.</p> <p><b>NOTE:</b> You can also use the toolbar button . The command is not available unless two or more spectra are open.</p>	<p>The <b>Add/Subtract</b> dialog box opens. The active spectrum is assumed to be the reference spectrum:</p> 
4	<p>Make sure the mixture spectrum is the <b>Experimental Spectrum</b>, and cyclohexane is the <b>Reference Spectrum</b>. If needed, change these assignments using either of the drop-down lists. Click <b>Preview</b>.</p>	<p>A preview of the difference spectrum is provided:</p> 

	Action	Result
5	On the <b>Add/Subtract</b> dialog box, adjust <b>Factor</b> to ~0.7. Click <b>Replace</b> .	<p>A message box opens and asks whether negative values should be truncated to zero:</p>  <p>The screenshot shows the ProcessIt software interface. The main window displays two IR spectra: a blue one for 'Unknown Mixture 01011969 (Corrected)' and a red one for 'DEMOX #12: Cyclohexane (Corrected)'. The x-axis is labeled 'ppm' and ranges from 4000 to 500. An 'Add/Subtract' dialog box is open, showing 'Unknown Mixture 01011965' selected in the dropdown menu, with a 'Scale To Reference Spectrum' checkbox. A 'Spectrum Module' warning dialog box is also open, displaying a yellow warning icon and the text: 'The resulting spectrum contains negative values. Should these regions be truncated to zero?'. Below the warning dialog, there are radio buttons for 'Add' and 'Replace', and buttons for 'Close', 'Preview', and 'Replace'.</p>
6	Click <b>Yes</b> .	<p>The mixture spectrum is replaced by a difference spectrum:</p>  <p>The screenshot shows the ProcessIt software interface after the 'Yes' button was clicked. The main window now displays a single IR spectrum in blue, representing the difference spectrum. The x-axis is labeled 'cm<sup>-1</sup>' and ranges from 4000 to 500. The spectrum shows a prominent peak at approximately 2900 cm<sup>-1</sup> and a smaller peak at approximately 1500 cm<sup>-1</sup>. The title bar of the window reads: 'Unknown Mixture 01011969 (Corrected)-DEMOX #12: Cyclohexane (Corrected) X...'.</p>

**Repeat the search using the difference spectrum**

	Action	Result
1	Click <b>SearchIt</b> in the <b>Transfer to</b> bar. 	The <b>Import of Multiple Spectra</b> dialog box opens. 
2	De-select <b>DEMOX #12 Cyclohexane</b> so that only the difference spectrum is selected. Click <b>OK</b> .	A message box opens: 

	Action	Result															
3	Click <b>Start a new search.</b>	<p>The difference spectrum is loaded in <b>SearchIt:</b></p> 															
4	<p>Click <b>User-Select</b> tab and make sure the <b>Multi-Technique Sadtler Demo Database - Wiley</b> is selected for searching.</p> <p>Click <b>Search.</b></p>	<p>Results are displayed in the <b>Minelt</b> application. The first hit is benzene, the other component of the mixture.</p>  <table border="1" data-bbox="772 1133 1365 1339"> <thead> <tr> <th>Table</th> <th>Plot</th> <th>Related Compounds View</th> </tr> <tr> <th>HQI</th> <th>Tag</th> <th>Co DI ID Name Spectrum &lt;auto&gt; (IR/ATR-IR)</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>75.83</td> <td>EMO 13 Benzene</td> </tr> <tr> <td>2</td> <td>20.95</td> <td>EMO 36 Magnesium stearate</td> </tr> <tr> <td>3</td> <td>20.91</td> <td>EMO 12 Cyclohexane</td> </tr> </tbody> </table>	Table	Plot	Related Compounds View	HQI	Tag	Co DI ID Name Spectrum <auto> (IR/ATR-IR)	1	75.83	EMO 13 Benzene	2	20.95	EMO 36 Magnesium stearate	3	20.91	EMO 12 Cyclohexane
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# Searching

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## How to Perform a Structure Search

### Purpose

This exercise demonstrates how to perform a structure search using the SearchIt application.

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### Objectives

This exercise will teach you:

- How to perform an exact match structure search
  - How to perform a substructure search
- 

### Background

In the SearchIt application, scientists can use a structure fragment as a search term to locate chemical structures containing that structural skeleton. This capability is useful for retrieving structure fragments because a substructure search always analyzes the entire molecular structure of a compound—not just the largest fragment.

#### Training Files Used in This Lesson

C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Structures



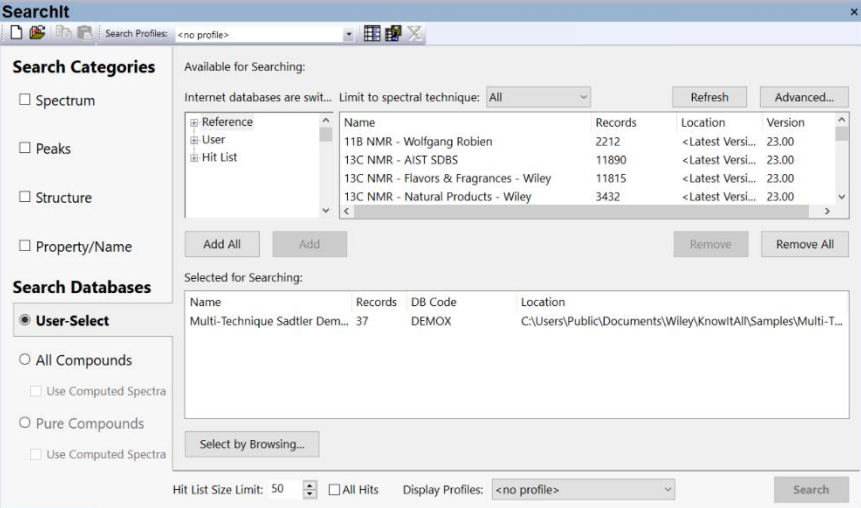
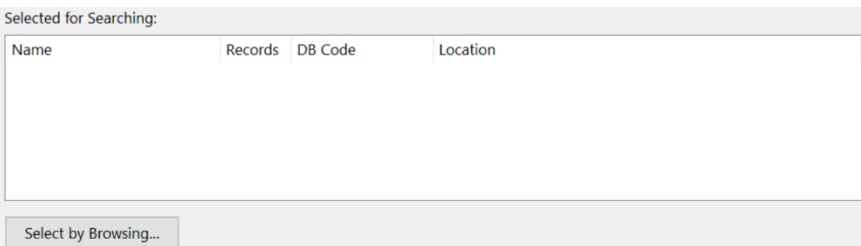
- tryptophan.dsf
- benzenethiol.dsf

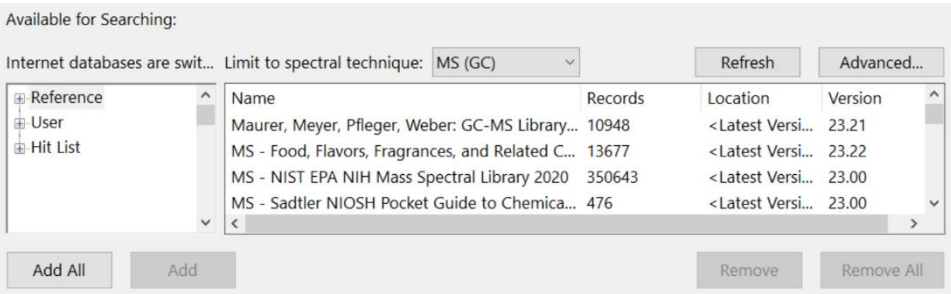

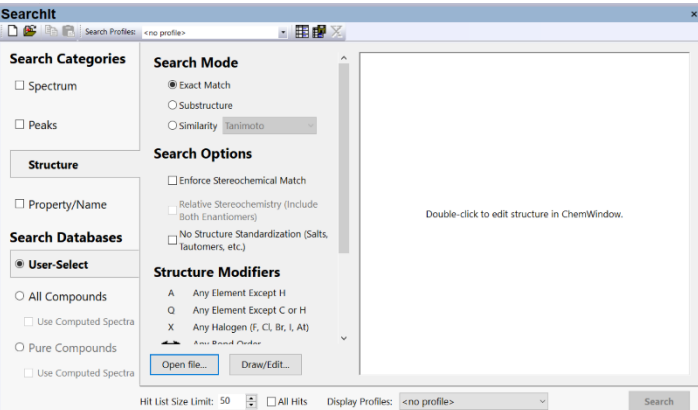
#### KnowItAll Applications Used

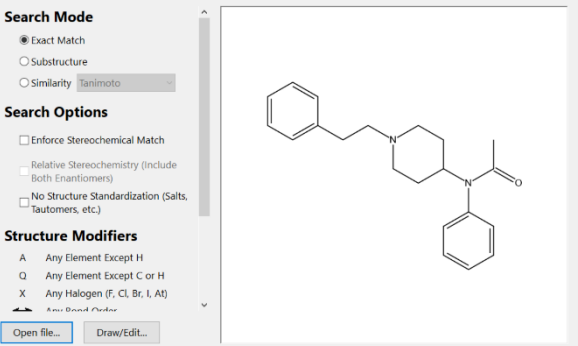
- SearchIt
- Minelt
- ChemWindow®



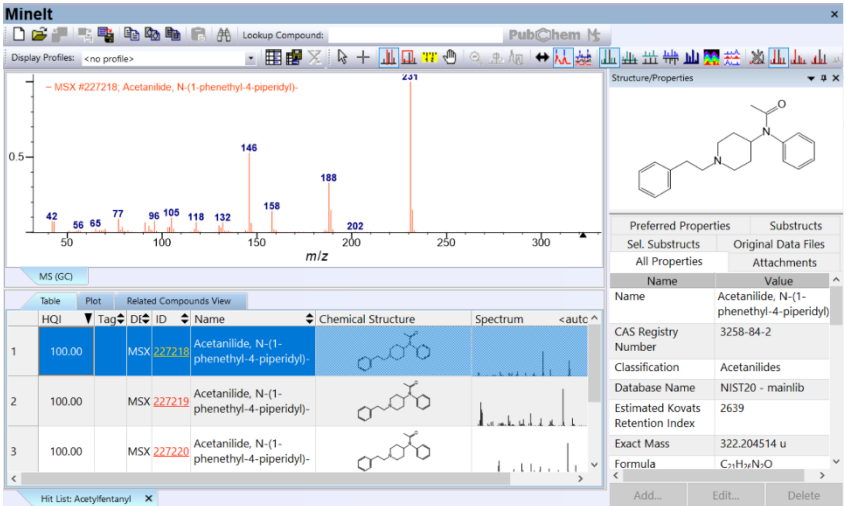
## Configure an exact structure match search

	Action	Result
1	<p>Do one of the following:</p> <ul style="list-style-type: none"> <li>If the <b>SearchIt</b> application is not open, navigate to the <b>Data</b> toolbox and click its icon.</li> </ul>  <p><b>SearchIt</b></p> <ul style="list-style-type: none"> <li>If the <b>SearchIt</b> application is already open, click the <b>SearchIt Close</b> button  to close the current search.</li> </ul>	<p>The <b>SearchIt</b> application's <b>User-Select</b> tab is displayed and the <b>Selected for Searching</b> list displays the databases last used:</p> 
2	<p>If databases are already selected for searching, click <b>Remove All</b> to clear the selections.</p>	<p>If databases are already selected for searching, click <b>Remove All</b> to clear the selections:</p> 

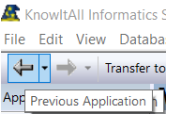
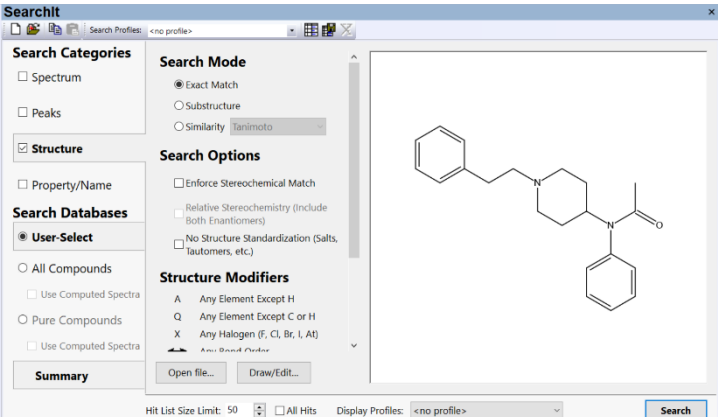
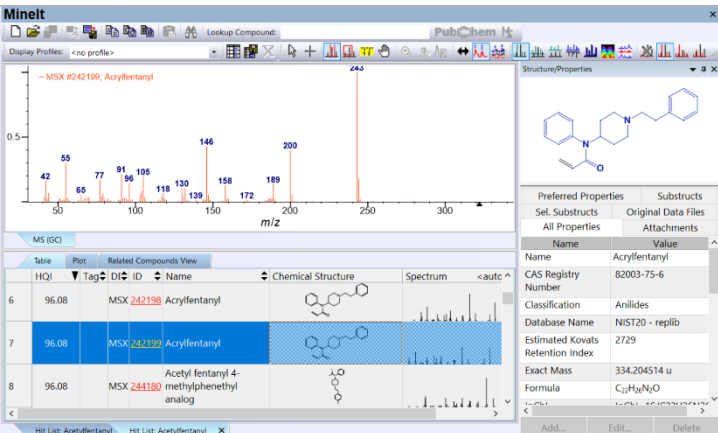
	Action	Result																				
3	Set <b>Limit to Spectral Technique</b> to <b>MS (GC)</b> .	<p>Only databases with MS spectral data are displayed:</p>  <p>Available for Searching:</p> <p>Internet databases are swit... Limit to spectral technique: MS (GC) Refresh Advanced...</p> <table border="1"> <thead> <tr> <th>Name</th> <th>Records</th> <th>Location</th> <th>Version</th> </tr> </thead> <tbody> <tr> <td>Maurer, Meyer, Pflieger, Weber: GC-MS Library...</td> <td>10948</td> <td>&lt; Latest Versi...</td> <td>23.21</td> </tr> <tr> <td>MS - Food, Flavors, Fragrances, and Related C...</td> <td>13677</td> <td>&lt; Latest Versi...</td> <td>23.22</td> </tr> <tr> <td>MS - NIST EPA NIH Mass Spectral Library 2020</td> <td>350643</td> <td>&lt; Latest Versi...</td> <td>23.00</td> </tr> <tr> <td>MS - Sadtler NIOSH Pocket Guide to Chemica...</td> <td>476</td> <td>&lt; Latest Versi...</td> <td>23.00</td> </tr> </tbody> </table> <p>Add All Add Remove Remove All</p>	Name	Records	Location	Version	Maurer, Meyer, Pflieger, Weber: GC-MS Library...	10948	< Latest Versi...	23.21	MS - Food, Flavors, Fragrances, and Related C...	13677	< Latest Versi...	23.22	MS - NIST EPA NIH Mass Spectral Library 2020	350643	< Latest Versi...	23.00	MS - Sadtler NIOSH Pocket Guide to Chemica...	476	< Latest Versi...	23.00
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MS - NIST EPA NIH Mass Spectral Library 2020	350643	< Latest Versi...	23.00																			
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4	<p>Select database <b>MS – NIST EPA NIH Mass Spectral Library xxxx – Main Library</b> for searching.</p> <p>xxxx is the year of the library</p>	<p>The selected database is added to the <b>Selected for Searching</b> window:</p>  <p>Selected for Searching:</p> <table border="1"> <thead> <tr> <th>Name</th> <th>Records</th> <th>DB Code</th> <th>Location</th> </tr> </thead> <tbody> <tr> <td>MS - NIST EPA NIH Mass Spe...</td> <td>350643</td> <td>MSX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\MS\...</td> </tr> </tbody> </table>	Name	Records	DB Code	Location	MS - NIST EPA NIH Mass Spe...	350643	MSX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\MS\...												
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MS - NIST EPA NIH Mass Spe...	350643	MSX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\MS\...																			
5	Click <b>Structure</b> under <b>Search Categories</b> .	<p>The <b>Structure Search</b> dialog is displayed:</p>  <p>SearchIt</p> <p>Search Profiles: &lt;no profile&gt;</p> <p><b>Search Categories</b></p> <p><input type="checkbox"/> Spectrum</p> <p><input type="checkbox"/> Peaks</p> <p><b>Structure</b></p> <p><input type="checkbox"/> Property/Name</p> <p><b>Search Databases</b></p> <p><input checked="" type="radio"/> User-Select</p> <p><input type="checkbox"/> All Compounds</p> <p><input type="checkbox"/> Use Computed Spectra</p> <p><input type="checkbox"/> Pure Compounds</p> <p><input type="checkbox"/> Use Computed Spectra</p> <p><b>Search Mode</b></p> <p><input checked="" type="radio"/> Exact Match</p> <p><input type="radio"/> Substructure</p> <p><input type="radio"/> Similarity Tanimoto</p> <p><b>Search Options</b></p> <p><input type="checkbox"/> Enforce Stereochemical Match</p> <p><input type="checkbox"/> Relative Stereochemistry (Include Both Enantiomers)</p> <p><input type="checkbox"/> No Structure Standardization (Salts, Isomers, etc.)</p> <p><b>Structure Modifiers</b></p> <p><input type="checkbox"/> A Any Element Except H</p> <p><input type="checkbox"/> O Any Element Except C or H</p> <p><input type="checkbox"/> X Any Halogen (F, Cl, Br, I, At)</p> <p>Open file... Draw/Edit...</p> <p>HIT List Size Limit: 50 <input type="checkbox"/> All Hits Display Profiles: &lt;no profile&gt; Search</p>																				

	Action	Result
6	<p>Click <b>Open file...</b> button.</p> <p>Navigate to “C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\Structures” and select <b>Acetylfentanyl.cdx</b>.</p> <p><b>Note:</b> You can also click <b>Draw/Edit</b> to create a structure using the <b>ChemWindow</b> application.</p>	<p>The structure is displayed in the <b>Structure</b> tab:</p>  <p>The screenshot shows a search interface with the following sections:</p> <ul style="list-style-type: none"><li><b>Search Mode:</b> Radio buttons for Exact Match (selected), Substructure, and Similarity. A dropdown menu is set to Tanimoto.</li><li><b>Search Options:</b> Checkboxes for Enforce Stereochemical Match, Relative Stereochemistry (include Both Enantiomers), and No Structure Standardization (Salts, Tautomers, etc.).</li><li><b>Structure Modifiers:</b> A list of modifiers: A (Any Element Except H), Q (Any Element Except C or H), X (Any Halogen (F, Cl, Br, I, At)), and an expandable list for Bond Order.</li><li>Buttons for <b>Open file...</b> and <b>Draw/Edit...</b></li></ul> <p>The chemical structure displayed is Acetylfentanyl, which consists of a piperidine ring substituted with a propylphenyl group and an acetophenone group.</p>

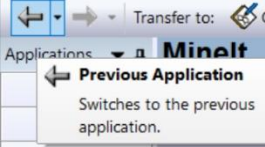
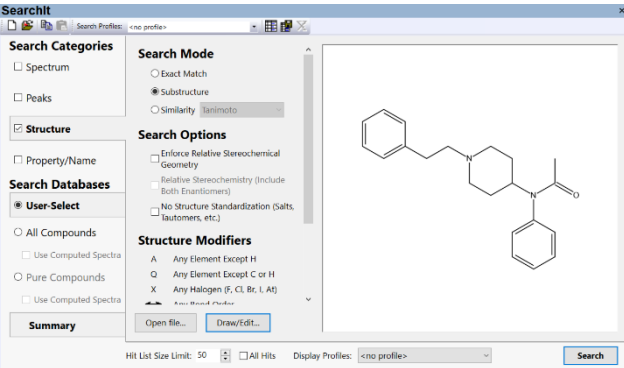

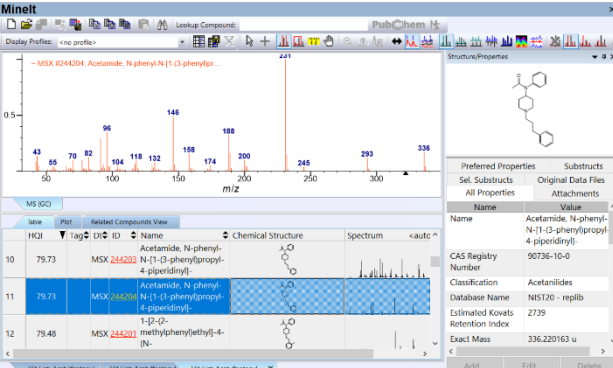
## Perform an exact structure match search

	Action	Result																																								
1	Select <b>Exact Match</b> under <b>Search Mode</b> , then click <b>Search</b> .	<p>Exact matches are displayed in the <b>Minelt</b> application:</p>  <p>The screenshot displays the Minelt application interface. At the top, the title bar reads "Minelt" and "PubChem". Below the title bar, there is a "Lookup Compound:" field. The main area is divided into two panes. The left pane shows a mass spectrum plot with the x-axis labeled "m/z" and the y-axis labeled "0.5". The plot title is "- MSX #227218; Acetanilide, N-(1-phenethyl-4-piperidyl)-". The spectrum shows several peaks, with the most prominent one at m/z 241. Other labeled peaks include 42, 56, 65, 77, 96, 105, 118, 132, 146, 158, 188, and 202. The right pane shows the chemical structure of Acetanilide, N-(1-phenethyl-4-piperidyl) and a table of properties. The table has columns for "Name" and "Value".</p> <table border="1"><thead><tr><th colspan="2">Preferred Properties</th><th colspan="2">Substructs</th></tr><tr><th colspan="2">All Properties</th><th colspan="2">Attachments</th></tr><tr><th>Name</th><th>Value</th><th></th><th></th></tr></thead><tbody><tr><td>Name</td><td>Acetanilide, N-(1-phenethyl-4-piperidyl)</td><td></td><td></td></tr><tr><td>CAS Registry Number</td><td>3258-84-2</td><td></td><td></td></tr><tr><td>Classification</td><td>Acetanilides</td><td></td><td></td></tr><tr><td>Database Name</td><td>NIST20 - mainlib</td><td></td><td></td></tr><tr><td>Estimated Kovats Retention Index</td><td>2639</td><td></td><td></td></tr><tr><td>Exact Mass</td><td>322.204514 u</td><td></td><td></td></tr><tr><td>Formula</td><td>C<sub>17</sub>H<sub>19</sub>N<sub>2</sub>O</td><td></td><td></td></tr></tbody></table> <p>Hit List: Acetylfentanyl X</p>	Preferred Properties		Substructs		All Properties		Attachments		Name	Value			Name	Acetanilide, N-(1-phenethyl-4-piperidyl)			CAS Registry Number	3258-84-2			Classification	Acetanilides			Database Name	NIST20 - mainlib			Estimated Kovats Retention Index	2639			Exact Mass	322.204514 u			Formula	C <sub>17</sub> H <sub>19</sub> N <sub>2</sub> O		
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## Configure and perform a substructure search

	Action	Result
1	<p>Click the KnowItAll <b>Back</b> button to return to <b>SearchIt</b>.</p>  <p>If you are not on the <b>Structure</b> tab, click to resume a structure search.</p>	<p>The <b>Structure</b> search dialog is displayed:</p> 
2	<p>Select <b>Substructure Search</b>, then click <b>Search</b>. Click through the records to search results.</p> <p><b>NOTE:</b> Rather than finding only exact matches for the search structure, the substructure search returns records that contain the query structure as a part of the database structure.</p>	<p>The substructure search produces more hits than the exact match search. The substructure is highlighted in blue and additional fragments are displayed using black coloration:</p>  <p>Note that the original hit list is still available and can be accessed by clicking the appropriate tab (at the lower left corner).</p>

## Configure and perform a similarity search

	Action	Result												
1	Click the KnowItAll <b>Back</b> button to return to <b>SearchIt</b> . 	The <b>SearchIt Structure</b> search dialog is displayed: 												
2	Click the <b>Similarity Search</b> radio button. Use the default scoring method, <b>Tanimoto</b> .	Tanimoto is selected for the <b>Search Mode</b> : 												
3	Click <b>Search</b> .	Structure which are similar to the searched structure are displayed in the <b>Minelt</b> application:  <table border="1" data-bbox="787 1226 1228 1380"> <thead> <tr> <th>Name</th> <th>Chemical Structure</th> <th>Spectrum</th> </tr> </thead> <tbody> <tr> <td>10 79.73 MSX 244203 Acetamide, N-phenyl-N-[1-(3-phenylpropyl)-4-piperidinyl]</td> <td></td> <td></td> </tr> <tr> <td>11 79.71 MSX 244304 Acetamide, N-phenyl-N-[1-(3-phenylpropyl)-4-piperidinyl]</td> <td></td> <td></td> </tr> <tr> <td>12 79.48 MSX 244201 methylphenylethyl-4-[N-]</td> <td></td> <td></td> </tr> </tbody> </table>	Name	Chemical Structure	Spectrum	10 79.73 MSX 244203 Acetamide, N-phenyl-N-[1-(3-phenylpropyl)-4-piperidinyl]			11 79.71 MSX 244304 Acetamide, N-phenyl-N-[1-(3-phenylpropyl)-4-piperidinyl]			12 79.48 MSX 244201 methylphenylethyl-4-[N-]		
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# Searching

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## All Compounds and Pure Compounds Database Selections

### Purpose

This exercise demonstrates how to use the All Compounds and Pure Compounds Database Selections

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### Objectives

This exercise will teach you:

- How to use All Compounds and Pure Compounds Database Selections
  - How to interpret the search result
- 

### Background

All Compounds and Pure Compounds database selections link data by structure, name, InChI, CAS Registry Number or synonym.

#### Training Files Used in This Lesson



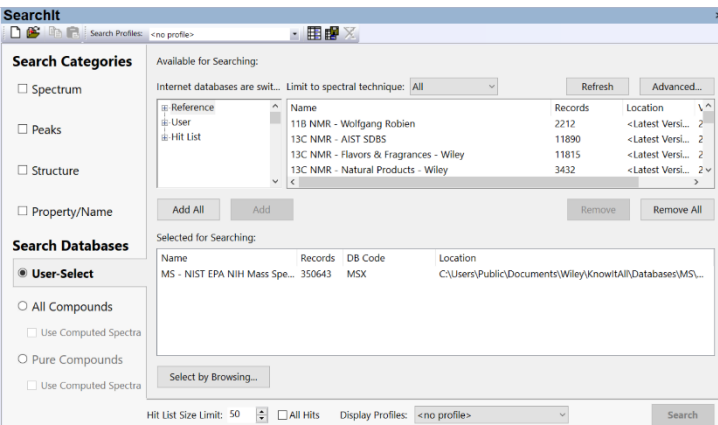
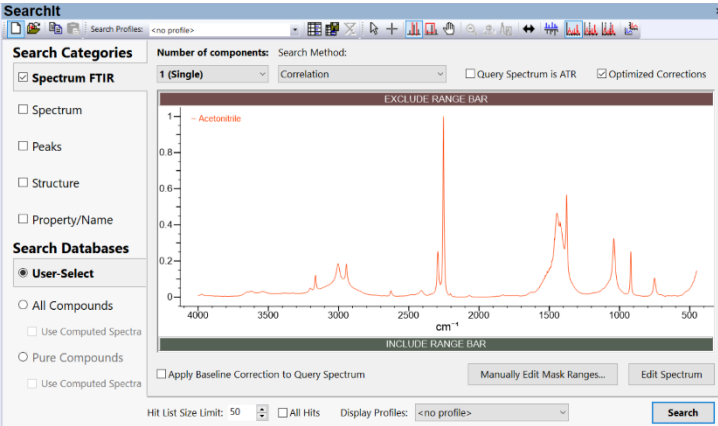
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\IR

- Acetonitrile.jdx

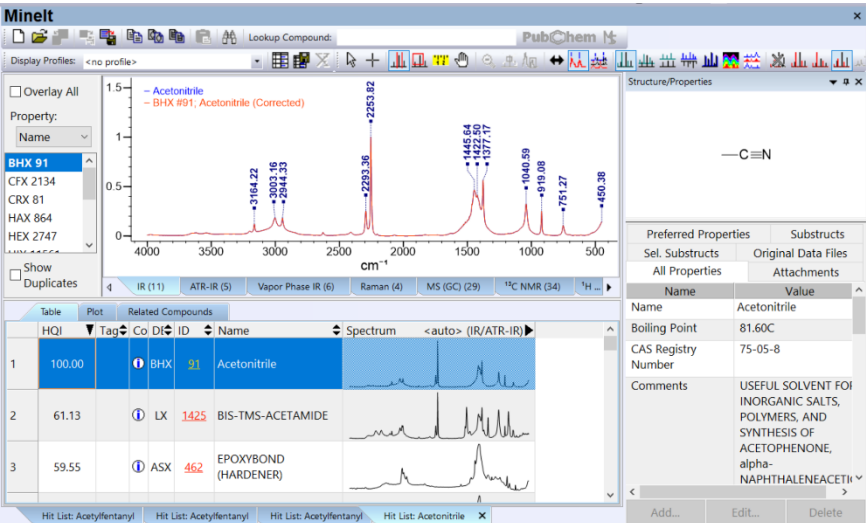
#### KnowItAll Applications Used

- SearchIt
- Minelt

## Configure and perform an All Compounds search

	Action	Result
1	<p>Do one of the following:</p> <ul style="list-style-type: none"> <li>If the <b>SearchIt</b> application is not open, navigate to the <b>Data</b> toolbox and click its icon.</li> </ul>  <p>SearchIt</p> <ul style="list-style-type: none"> <li>If the <b>SearchIt</b> application is already open, click the SearchIt <b>Close</b> button  to close the current search.</li> </ul>	<p>The <b>SearchIt</b> application's <b>User-Select</b> tab is displayed and the <b>Selected for Searching</b> list displays the databases last used:</p> 
2	<p>Click <b>Spectrum</b> under <b>Search Categories</b>. Navigate to C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\IR" and select <b>acetonitrile.jdx</b>.</p>	<p>The spectrum for acetonitrile is displayed:</p> 
3	<p>Select the <b>All Compounds</b> option under <b>Search Databases</b>.</p>	<p>The <b>All Compounds</b> search option is selected.</p>



	Action	Result
4	Click <b>Search</b> .	<p>The search is performed, and results are displayed in the <b>Minelt</b> application:</p>  <p>Compared to the <b>User-Select</b> database search, you will see additional information related to the hit:</p> <ul style="list-style-type: none"> <li>• Replicates are displayed in the upper-left panel. They do not participate in this search and navigating through them does not change the value of HQI (Hit Quality Index). The bold ID signifies the hit spectrum.</li> <li>• Other spectrum information related to the hit compound is displayed in tabs under the spectrum pane.</li> </ul>
5	<b>TIPS:</b>	<ul style="list-style-type: none"> <li>• <b>User-Select</b> – User selects which databases to search. This is where you can include user databases in a search.</li> <li>• <b>All Compounds</b> – All licensed reference databases. Records are linked by structure, name, InChI, CAS Registry Number or synonym.</li> <li>• <b>Pure Compounds</b> – All Compounds with the exclusion of commercial compounds.</li> </ul>

# Searching

## How to Perform a Multi-Technique Spectral Search

### Purpose

This exercise demonstrates how to perform a multi-technique spectral search using the KnowItAll Informatics System.

### Objectives

This exercise will teach you:

- How to configure a multi-technique spectral search
- How to analyze the results of a multi-technique search

### Background

A multi-technique spectral search permits the optimization of chemical similarity based on several analytical techniques to maximize the chemical knowledge obtained on the unknown compound.

#### Training Files Used in This Lesson



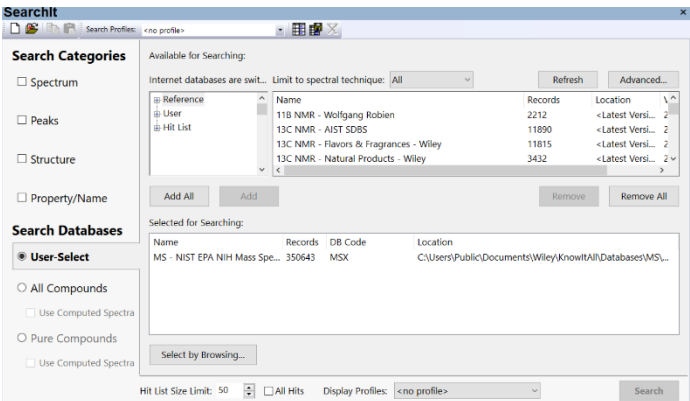
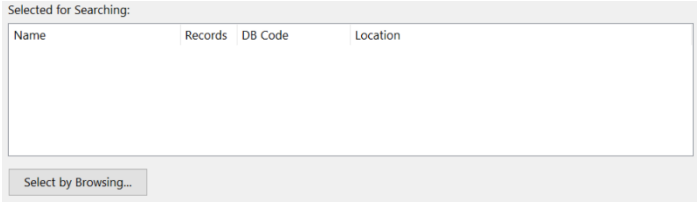
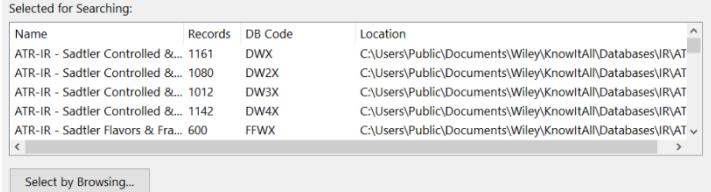
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Si  
multaneous Multi-Technique Searching folder

- Unknown D IR.jdx
- Unknown D Raman.jdx

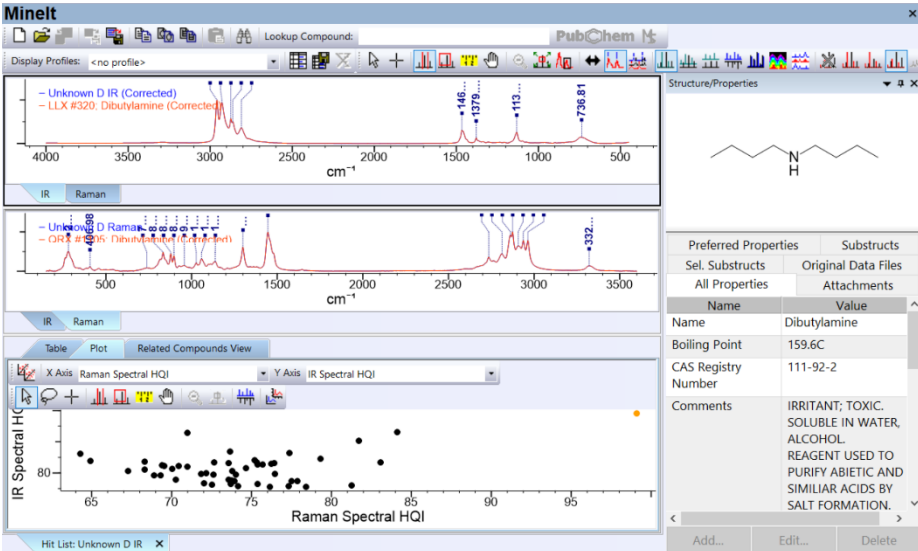
#### KnowItAll Applications Used

- SearchIt
- Minelt



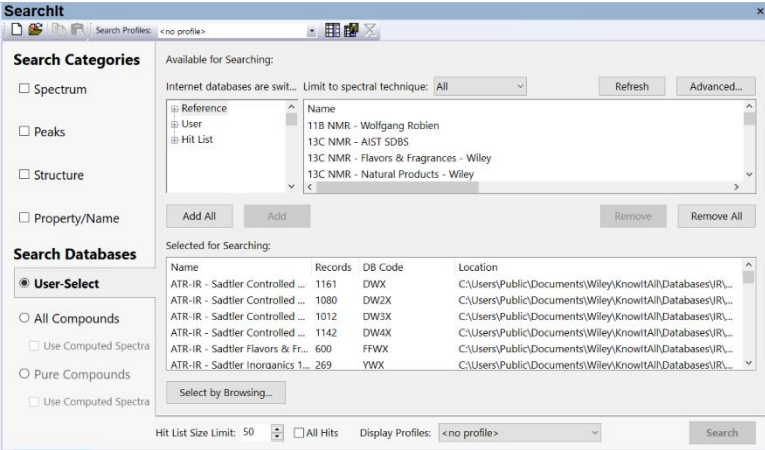
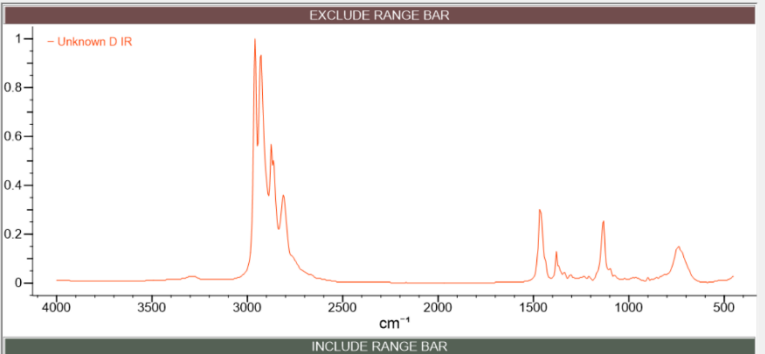
## Configure and perform a multi-technique spectral search with the User-Select Search Databases option

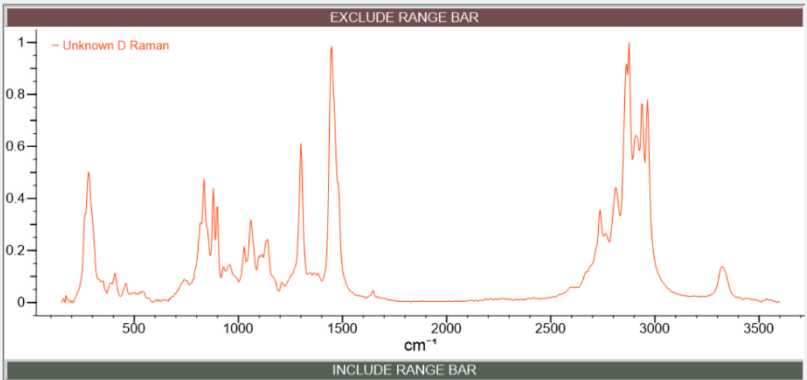
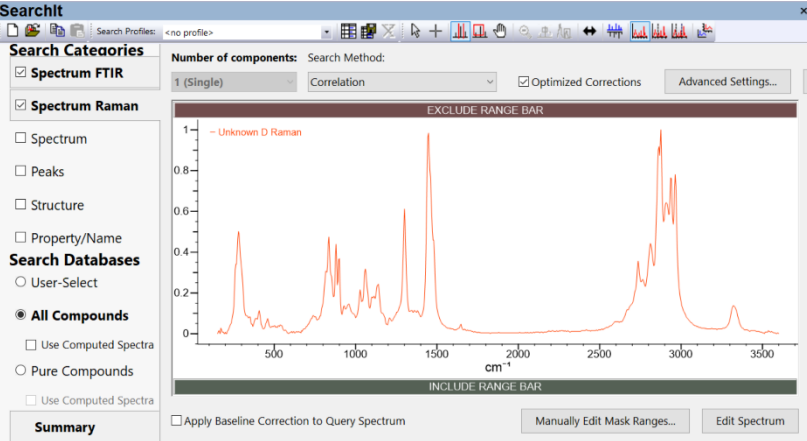
	Action	Result
1	<p>Do one of the following:</p> <ul style="list-style-type: none"> <li>If the <b>SearchIt</b> application is not open, navigate to the <b>Data</b> toolbox and click its icon.</li> </ul>  <p><b>SearchIt</b></p> <ul style="list-style-type: none"> <li>If the <b>SearchIt</b> application is already open, click the <b>SearchIt Close</b> button  to close the current search.</li> </ul>	<p>The <b>SearchIt</b> application's <b>User-Select</b> tab is displayed, and the <b>Selected for Searching</b> list displays the databases last used:</p> 
2	<p>Select <b>User-Select</b> under <b>Search Databases</b> option. If databases are already selected for searching, click <b>Remove All</b> to clear the selections</p>	<p>The <b>Selected for Searching</b> databases section is cleared:</p> 
3	<p>Using the <b>Limit to spectral technique</b> tab, select <b>IR</b> then click <b>Add All</b>. Repeat for <b>Raman</b>.</p>	<p>All of the available IR and Raman databases are added to the <b>Selected for Searching</b> window:</p> 

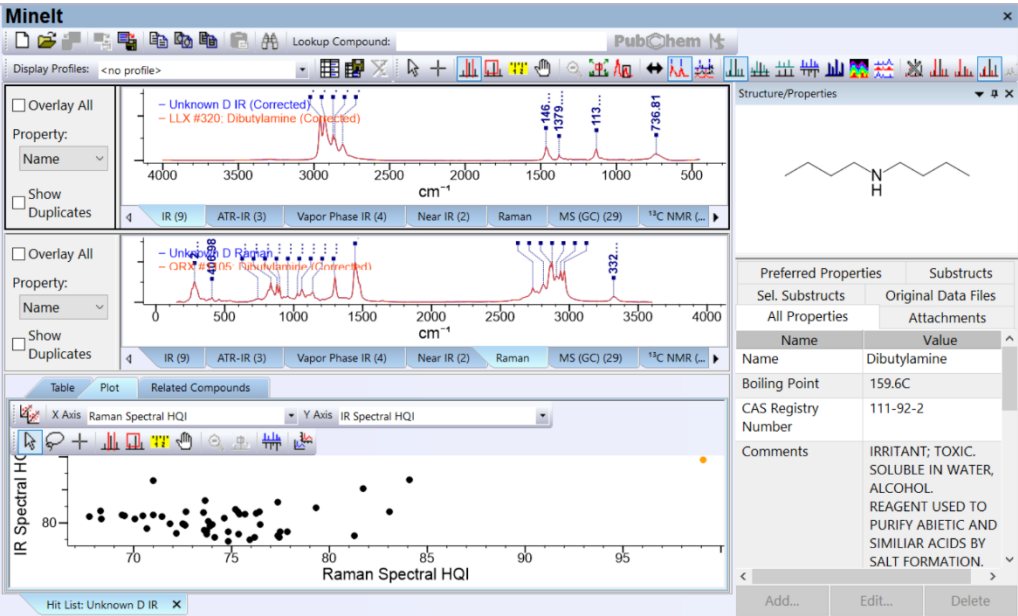
	Action	Result
4	<p>Click <b>Spectrum</b> under <b>Search Categories</b>.</p> <p>Navigate to “C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\Simultaneous Multi-Technique Searching”.</p> <p>Open <b>Unknown D IR.jdx</b>.</p>	<p>An IR spectrum is displayed in the <b>SearchIt spectrum</b> window:</p> 
5	<p>Click <b>Spectrum</b> under <b>Search Categories</b> to add another spectrum.</p> <p>From the folder “C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\Simultaneous Multi-Technique Searching”, choose <b>Unknown D Raman.jdx</b>.</p>	<p>The Raman spectrum is added to the search:</p> 

	Action	Result
6	Click <b>Search</b> .	<p>The search results are displayed in the <b>Minelt</b> application:</p>  <p>Because this was a multi-technique search, the <b>Database</b> pane's <b>Plot</b> tab automatically displays a scatter plot representing HQI values for the two spectral techniques. The point with the highest HQI values is selected at the upper right. You can click on the dots in the plot to view the different search results, or click <b>Table</b> tab to view tabular results.</p>

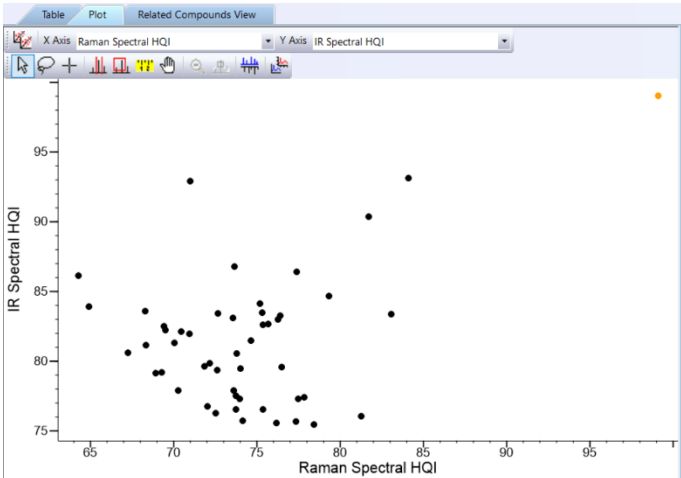
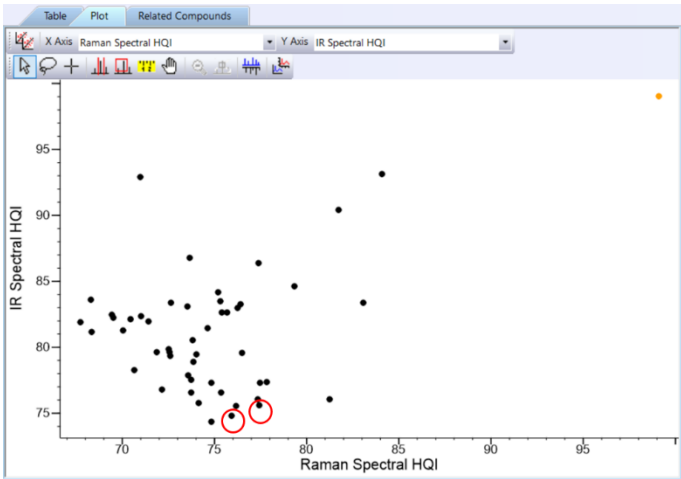
## Configure and perform a multi-technique spectral search with the All Compounds Search Databases option

	Action	Result
1	<p>Do one of the following:</p> <ul style="list-style-type: none"> <li>If the <b>SearchIt</b> application is not open, navigate to the <b>Data</b> toolbox and click its icon.</li> </ul>  <ul style="list-style-type: none"> <li>If the <b>SearchIt</b> application is already open, click the <b>SearchIt Close</b> button  to close the current search.</li> </ul>	<p>The <b>SearchIt</b> application's <b>User-Select</b> tab is displayed, and the <b>Selected for Searching</b> list displays the databases last used:</p> 
2	<p>Click <b>Spectrum</b> under <b>Search Categories</b>. Navigate to C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\Simultaneous Multi-Technique Searching" and select <b>Unknown D IR.jdx</b>.</p>	<p>The spectrum is displayed in the <b>SearchIt</b> application:</p> 

	Action	Result
3	<p>Click <b>Spectrum</b> under <b>Search Categories</b> to add another spectrum.</p> <p>From the folder "C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\Simultaneous Multi-Technique Searching", choose <b>Unknown D Raman.jdx</b>.</p>	<p>The Raman spectrum is added to the search:</p>  <p>The plot shows a Raman spectrum with intensity on the y-axis (0 to 1) and wavenumber on the x-axis (0 to 3500 cm<sup>-1</sup>). The spectrum is labeled "Unknown D Raman" and shows several peaks, with the most prominent ones around 1500 and 3000 cm<sup>-1</sup>. The plot is framed by "EXCLUDE RANGE BAR" at the top and "INCLUDE RANGE BAR" at the bottom.</p>
4	<p>Check <b>All Compounds</b> under <b>Search Databases</b> option.</p>	<p><b>All Compounds</b> search is selected under <b>Search Databases</b>:</p>  <p>The screenshot shows the SearchIt software interface. On the left, under "Search Categories", "Spectrum FTIR" and "Spectrum Raman" are checked. Under "Search Databases", "All Compounds" is selected with a radio button. The main window displays the same Raman spectrum plot as in the previous step, with the "All Compounds" search method selected. The interface includes a toolbar at the top, a "Number of components" dropdown set to "1 (Single)", and a "Search Method" dropdown set to "Correlation". There are also checkboxes for "Optimized Corrections" and "Apply Baseline Correction to Query Spectrum".</p>

	Action	Result																																
5	Click <b>Search</b> .	<p>The search results are displayed in the <b>Minelt</b> application:</p>  <p>Because this was a multi-technique search, the <b>Database</b> pane's <b>Plot</b> tab automatically displays a scatter plot representing HQI values for the two spectral techniques. The point with the highest HQI values is selected at the upper right.</p> <table border="1" data-bbox="1535 613 1818 966"> <thead> <tr> <th colspan="2">Preferred Properties</th> <th colspan="2">Substructs</th> </tr> <tr> <th colspan="2">Sel. Substructs</th> <th colspan="2">Original Data Files</th> </tr> <tr> <th colspan="2">All Properties</th> <th colspan="2">Attachments</th> </tr> <tr> <th>Name</th> <th>Value</th> <th colspan="2"></th> </tr> </thead> <tbody> <tr> <td>Name</td> <td>Dibutylamine</td> <td colspan="2"></td> </tr> <tr> <td>Boiling Point</td> <td>159.6C</td> <td colspan="2"></td> </tr> <tr> <td>CAS Registry Number</td> <td>111-92-2</td> <td colspan="2"></td> </tr> <tr> <td>Comments</td> <td colspan="3">IRRITANT; TOXIC. SOLUBLE IN WATER, ALCOHOL. REAGENT USED TO PURIFY ABIETIC AND SIMILIAR ACIDS BY SALT FORMATION.</td> </tr> </tbody> </table>	Preferred Properties		Substructs		Sel. Substructs		Original Data Files		All Properties		Attachments		Name	Value			Name	Dibutylamine			Boiling Point	159.6C			CAS Registry Number	111-92-2			Comments	IRRITANT; TOXIC. SOLUBLE IN WATER, ALCOHOL. REAGENT USED TO PURIFY ABIETIC AND SIMILIAR ACIDS BY SALT FORMATION.		
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	Action	Result
6	Examine the example shown in the Results. Compare the scatter plot of the <b>User-Select</b> database search and that of <b>All Compounds</b> search.	<p data-bbox="804 321 1157 345"><b>User-Selected</b> database search:</p>  <p data-bbox="804 841 1176 865"><b>All Compounds</b> database search:</p>  <p data-bbox="804 1360 1566 1385">They are more points near the circled region including the circled points.</p>

	Action	Result
7	Using the search results from Step 5, examine the circled points.	<p>These two records are the stereoisomers whose IR and Raman spectral records are linked not by structure, but by other features in the record (name, InChI, CAS Registry Number or synonym).</p> <p><b>(S) Isomer:</b></p>  <p><b>(R) Isomer:</b></p> 