

KnowItAll Software Training

Searching

Searching

How to Perform a Basic Spectral Search

Purpose

These exercises demonstrate how to perform spectral searches using KnowItAll.

Objectives

These exercises will teach you:

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

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™
- MineIt™

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.



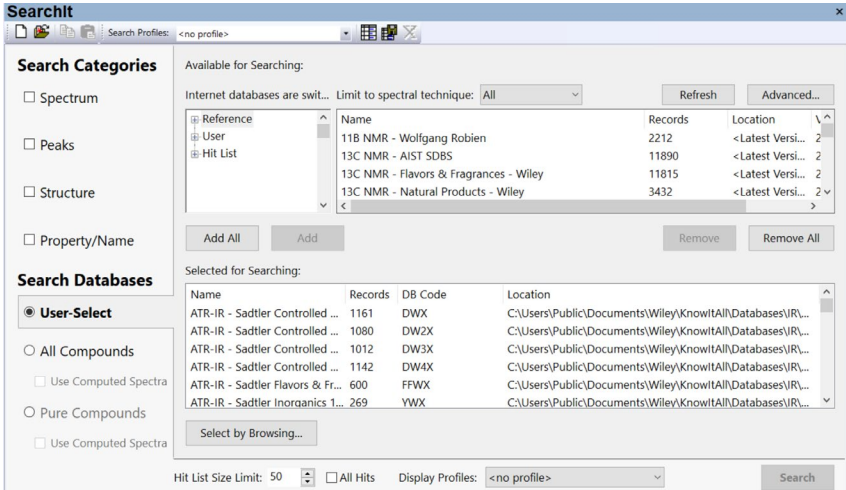
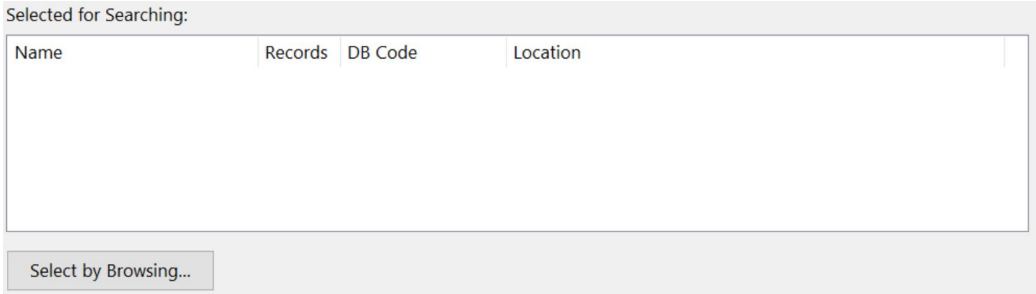
According to ASTM's guide on spectral searching¹, various algorithms and manual methods exist to adjust spectra to get reasonable match scores when two compared spectra of the same compound differ for various reasons. While these methods may work in selected cases, subtle discrepancies such as a shift 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.

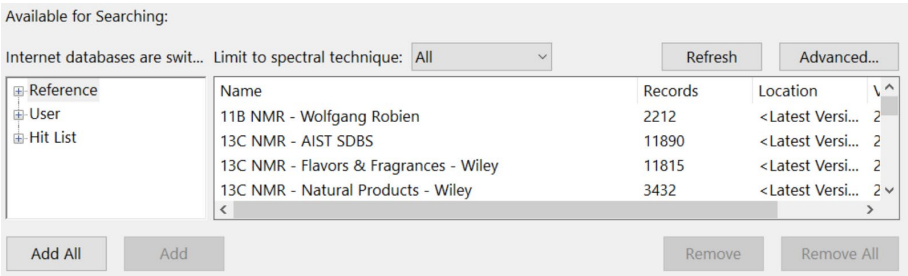
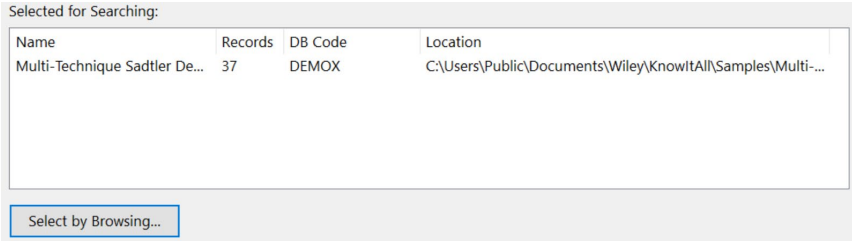

Manual corrections can be made by expert spectroscopists, but those less experienced in spectroscopy are often unaware of how to perform the necessary corrections on their sample spectrum to achieve the best search result. To address this growing concern, Wiley has introduced Optimized Corrections, a 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.

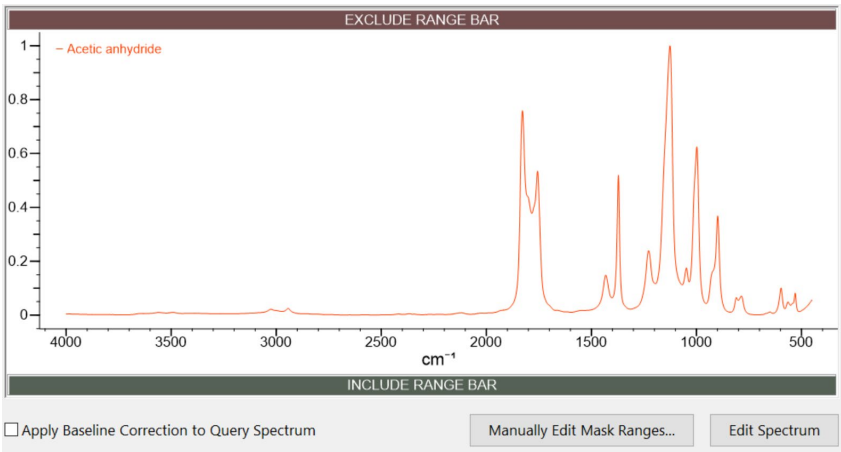
¹ E2310-04 - Standard Guide for Use of Spectral Searching by Curve Matching Algorithms with Data Recorded Using Mid-Infrared Spectroscopy, 2009. ASTM International Web Site. <http://www.astm.org/Standards/E2310.htm> (accessed March 4, 2015).

Create a new search and select reference databases

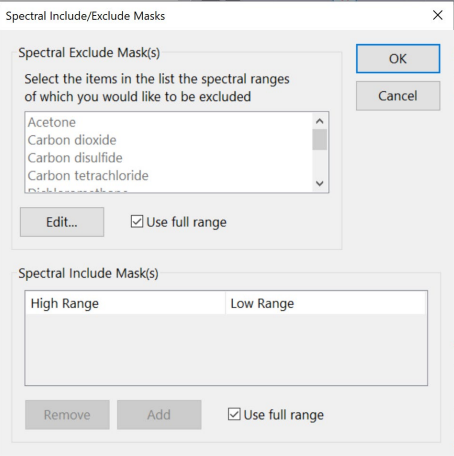
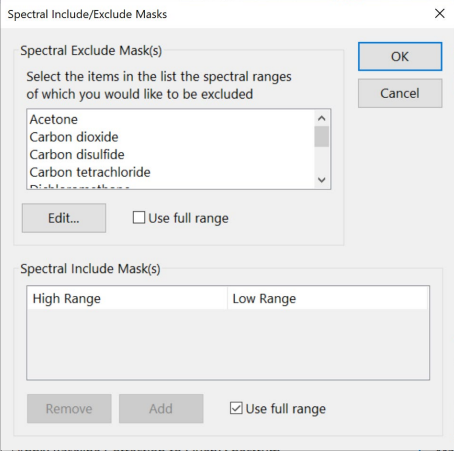
	Action	Result
1	<p>Do one of the following:</p> <ul style="list-style-type: none"> If the SearchIt application is not open, navigate to the Data toolbox and click its icon.  <p>If the SearchIt application is already open, click the Close button  (located in the upper right corner) to close the current search.</p>	<p>The SearchIt application is displayed, with the last used databases in the Selected for Searching window:</p> 
2	<p>Click on User-Select under Search Databases.</p>	<p>This option allows users to select the databases they want to search. Users can also include user-created databases in a search.</p>
3	<p>If a list of databases already appears in the Selected for Searching pane at the bottom, click Remove All to clear this list.</p>	<p>The User category is shown below:</p> 

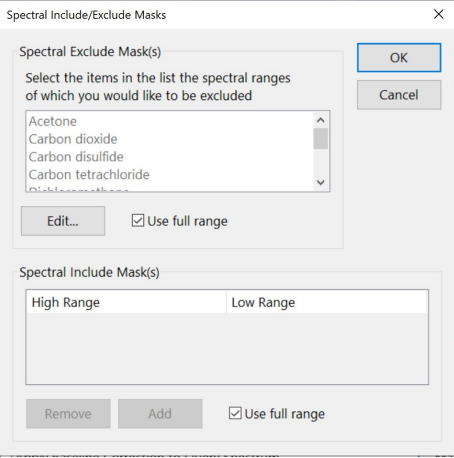
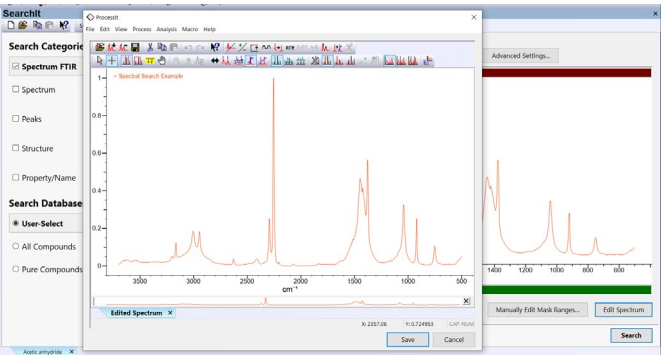
4	<p>To the left of the Available for Searching window, expand each branch in the tree structure to display a particular database category—Reference, User, Hit List— and specify whether network, local, or all databases are displayed. The available databases are displayed at the right of the window.</p>	<p>The Reference category is shown below. The database Name, number of Records, Location and version are displayed for each database.</p>  <p>NOTE: Your display may look different depending on whether or not you have access to databases available online. Click Advanced on the top right to open the Advanced Options dialog box, where you can control how you access online databases and add or remove local database locations. Click Refresh to update the display after settings are changed.</p>
5	<p>Click Select by Browsing button located at the lower left.</p>	<p>The Browse for a Database or Hit List dialog box opens.</p>
6	<p>Navigate to “C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples”. Open Multi-Technique Sadtler Demo Database - Wiley (DEMO).sdbx.</p>	<p>The database is displayed in the Selected for Searching list.</p> 
7	<p>If necessary, uncheck the All Hits check box and set Hit List Size Limit to 50.</p> <p>NOTE: When performing a spectral or peak search using more than two or three databases, it is better to limit the number of hits. Checking All Hits or using a larger value can drastically reduce the search speed.</p>	<p>The Hit List Size Limit is equal to 50:</p> 

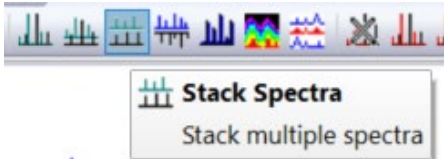
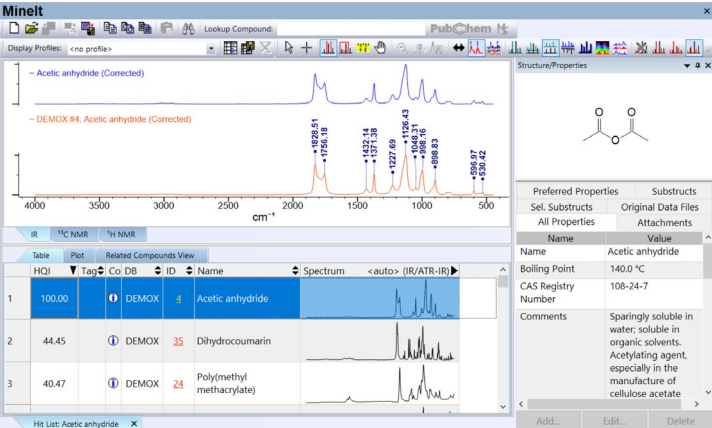
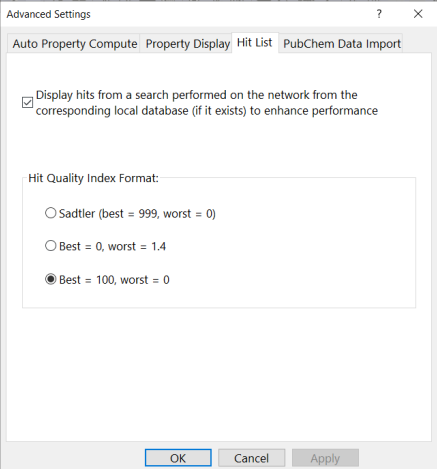
Open the spectral file

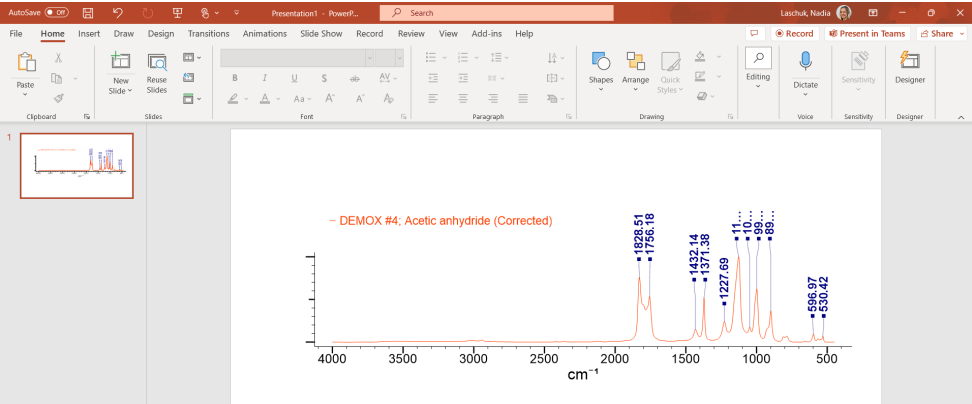
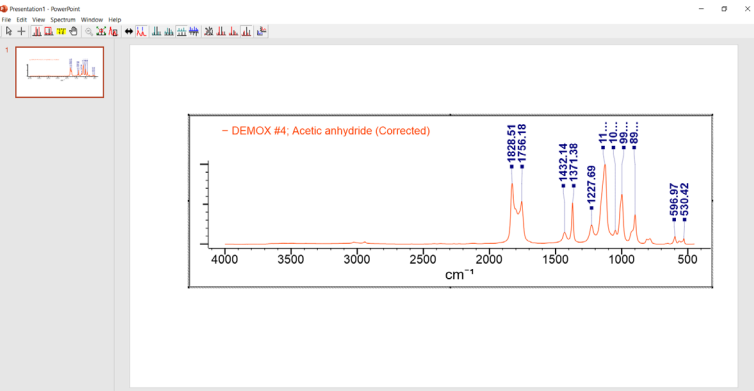
	Action	Result
1	<p>Click the Spectrum button under Search Categories.</p> <p>Navigate to "C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\IR".</p> <p>Select Acetic anhydride.jdx.</p> <p>Click Open.</p> <p>Note: You can use the Files of Type filter to limit the display to specific types of files,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

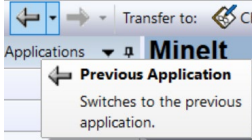
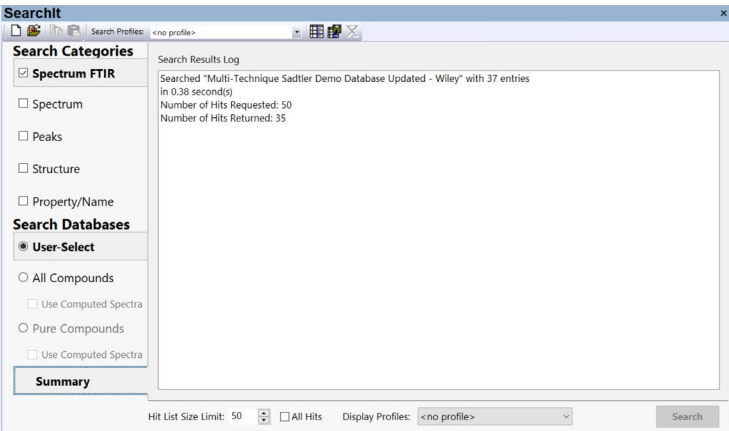
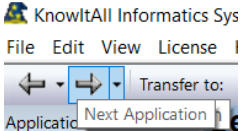
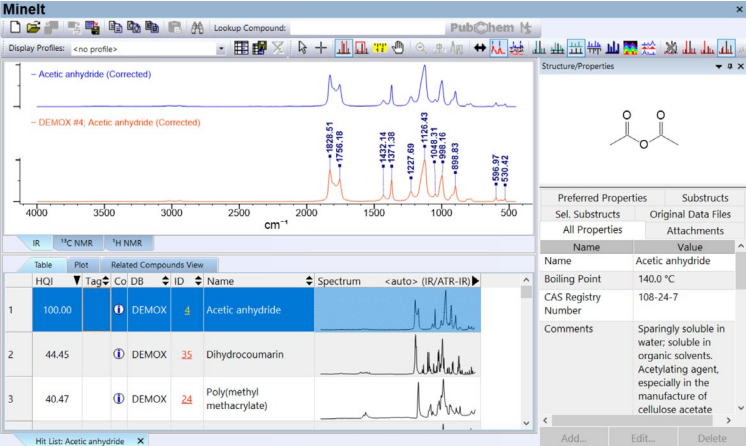
Fine-tune before searching

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

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

	Action	Result																								
7	<p>Click Search. In Minelt, Click to choose Stack Spectra view:</p> 	<p>The search results are automatically displayed in the Minelt application as a hit list, sorted by HQI. Both the unknown spectrum and the selected database spectrum are displayed.</p>  <table border="1" data-bbox="716 641 1213 792"> <thead> <tr> <th>HQI</th> <th>Tag</th> <th>Co</th> <th>ID</th> <th>Name</th> <th>Spectrum</th> </tr> </thead> <tbody> <tr> <td>100.00</td> <td>DEMOX</td> <td>4</td> <td></td> <td>Acetic anhydride</td> <td></td> </tr> <tr> <td>44.45</td> <td>DEMOX</td> <td>35</td> <td></td> <td>Dihydrocoumarin</td> <td></td> </tr> <tr> <td>40.47</td> <td>DEMOX</td> <td>24</td> <td></td> <td>Poly(methyl methacrylate)</td> <td></td> </tr> </tbody> </table> <p>The HQI value measures how close the reference spectrum is to that of the query. The default scale of HQI is 0-100.</p>	HQI	Tag	Co	ID	Name	Spectrum	100.00	DEMOX	4		Acetic anhydride		44.45	DEMOX	35		Dihydrocoumarin		40.47	DEMOX	24		Poly(methyl methacrylate)	
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40.47	DEMOX	24		Poly(methyl methacrylate)																						
8	<p>Note: The HQI (Hit Quality Index) is displayed for each search result, which has settings under: File > Preferences > Hit List. Click Cancel to close the dialog.</p>	<p>The Advanced Settings dialog is launched:</p> 																								

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

	Action	Result															
12	<p>In KnowItAll, click the Back button (located below the File menu).</p> 	<p>You are returned to the SearchIt application, where a Summary tab has been added to the main SearchIt window:</p> 															
13	<p>Click the KnowItAll Next Application button.</p> 	<p>You are returned to Minelt and the hit list.</p>  <table border="1" data-bbox="716 1117 1239 1295"> <thead> <tr> <th>Table</th> <th>Plot</th> <th>Related Compounds View</th> </tr> <tr> <th>HQI</th> <th>Tag</th> <th>Co DB ID Name Spectrum <auto> (IR/ATR-IR)</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>100.00</td> <td>DEMOX 4 Acetic anhydride</td> </tr> <tr> <td>2</td> <td>44.45</td> <td>DEMOX 35 Dihydrocoumarin</td> </tr> <tr> <td>3</td> <td>40.47</td> <td>DEMOX 24 Poly(methyl methacrylate)</td> </tr> </tbody> </table>	Table	Plot	Related Compounds View	HQI	Tag	Co DB ID Name Spectrum <auto> (IR/ATR-IR)	1	100.00	DEMOX 4 Acetic anhydride	2	44.45	DEMOX 35 Dihydrocoumarin	3	40.47	DEMOX 24 Poly(methyl methacrylate)
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Searching

How to Create Search Profiles and Use the Minelt profile for result display

Purpose

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

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.



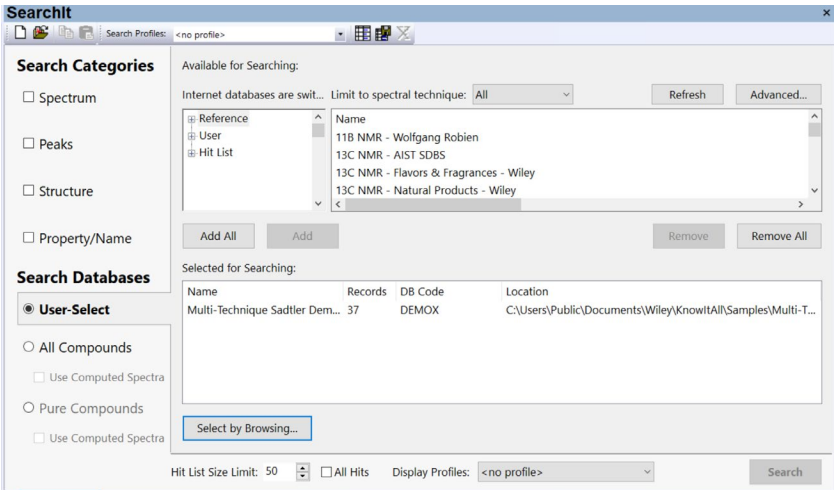
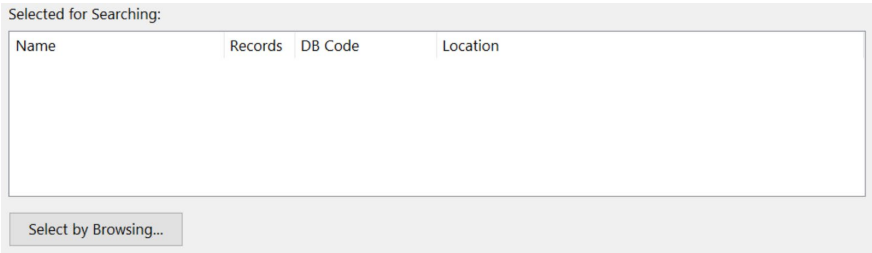
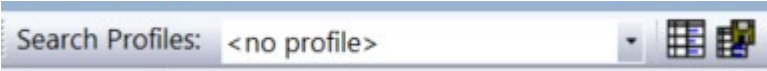
Minelt profiles are preferences of hit list information display, it is defined in Minelt. It can use tied to a search.

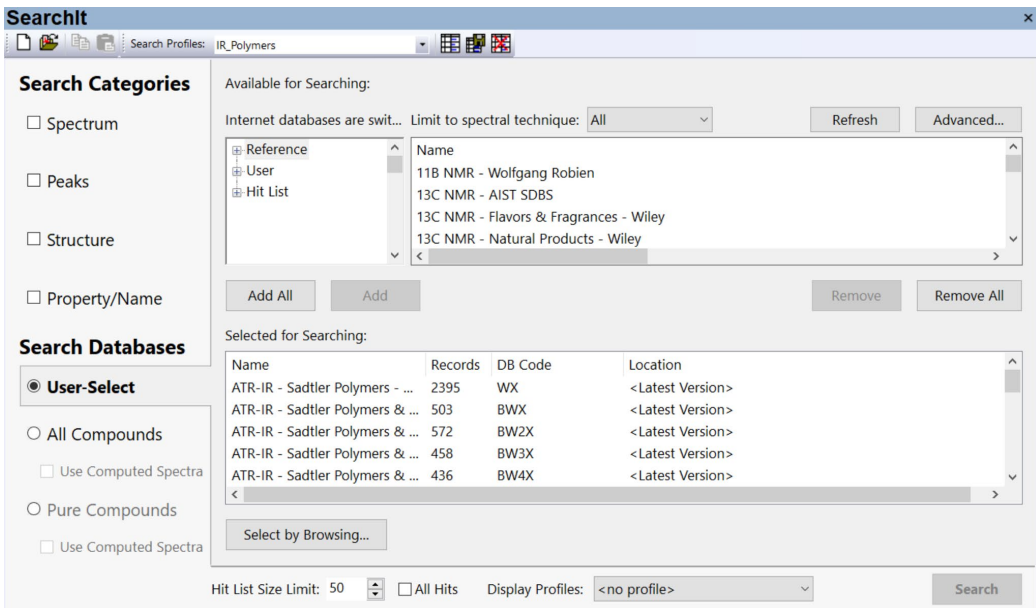
Training Files Used in This Lesson

KnowItAll Applications Used


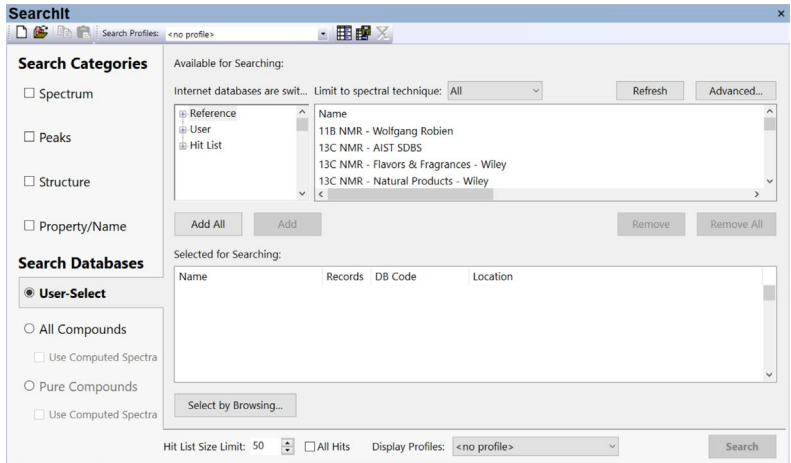

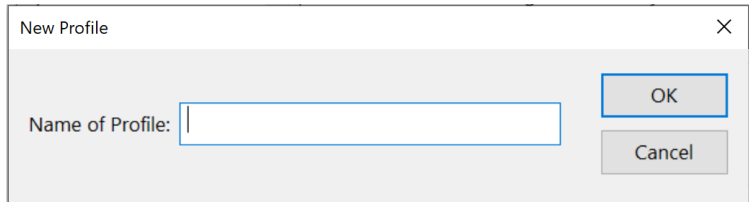

- SearchIt™

Apply a pre-defined search profile

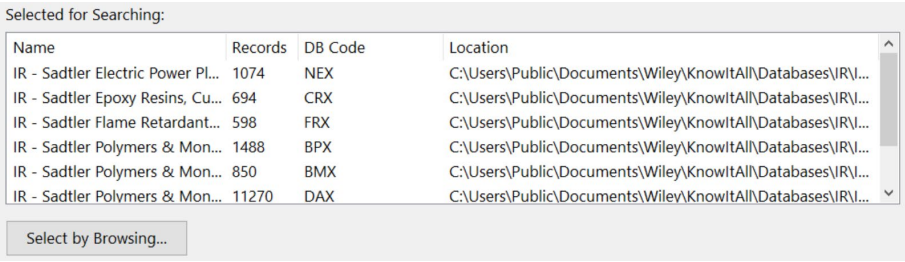
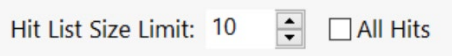

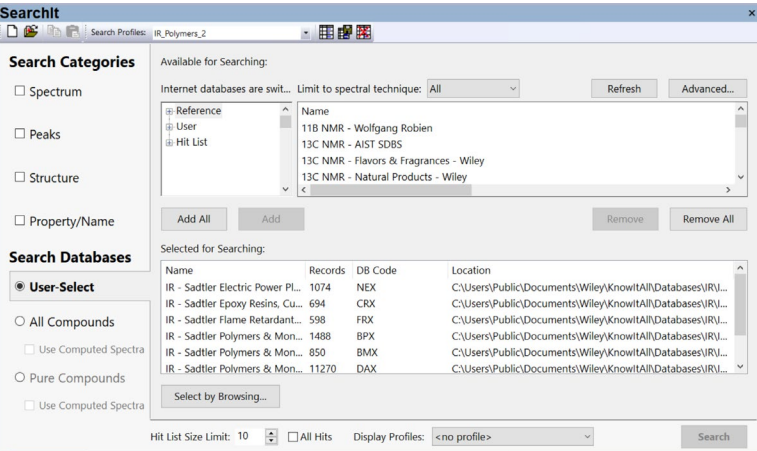
	Action	Result
1	<p>Do one of the following:</p> <ul style="list-style-type: none"> If the SearchIt application is not open, navigate to the Data toolbox and click its icon.  <ul style="list-style-type: none"> If the SearchIt application is already open, click the SearchIt Close button  to close the current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

	Action	Result																								
4	Select the IR_Polymers profile using the Search Profiles dropdown menu.	<p>Polymer databases are displayed in the Selected for Searching list:</p>  <p>The screenshot shows the SearchIt application window with the following details:</p> <ul style="list-style-type: none"> Search Profiles: IR_Polymers Search Categories: <ul style="list-style-type: none"> <input type="checkbox"/> Spectrum <input type="checkbox"/> Peaks <input type="checkbox"/> Structure <input type="checkbox"/> Property/Name Search Databases: <ul style="list-style-type: none"> <input checked="" type="radio"/> User-Select <input type="radio"/> All Compounds <ul style="list-style-type: none"> <input type="checkbox"/> Use Computed Spectra <input type="radio"/> Pure Compounds <ul style="list-style-type: none"> <input type="checkbox"/> Use Computed Spectra Available for Searching: <ul style="list-style-type: none"> Internet databases are swit... Limit to spectral technique: All Reference: 11B NMR - Wolfgang Robien, 13C NMR - AIST SDBS, 13C NMR - Flavors & Fragrances - Wiley, 13C NMR - Natural Products - Wiley Selected for Searching: <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 Polymers - ...</td> <td>2395</td> <td>WX</td> <td><Latest Version></td> </tr> <tr> <td>ATR-IR - Sadtler Polymers & ...</td> <td>503</td> <td>BWX</td> <td><Latest Version></td> </tr> <tr> <td>ATR-IR - Sadtler Polymers & ...</td> <td>572</td> <td>BW2X</td> <td><Latest Version></td> </tr> <tr> <td>ATR-IR - Sadtler Polymers & ...</td> <td>458</td> <td>BW3X</td> <td><Latest Version></td> </tr> <tr> <td>ATR-IR - Sadtler Polymers & ...</td> <td>436</td> <td>BW4X</td> <td><Latest Version></td> </tr> </tbody> </table> Hit List Size Limit: 50 <input type="checkbox"/> All Hits Display Profiles: <no profile> Search button 	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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ATR-IR - Sadtler Polymers & ...	436	BW4X	<Latest Version>																							

Create a new search profile

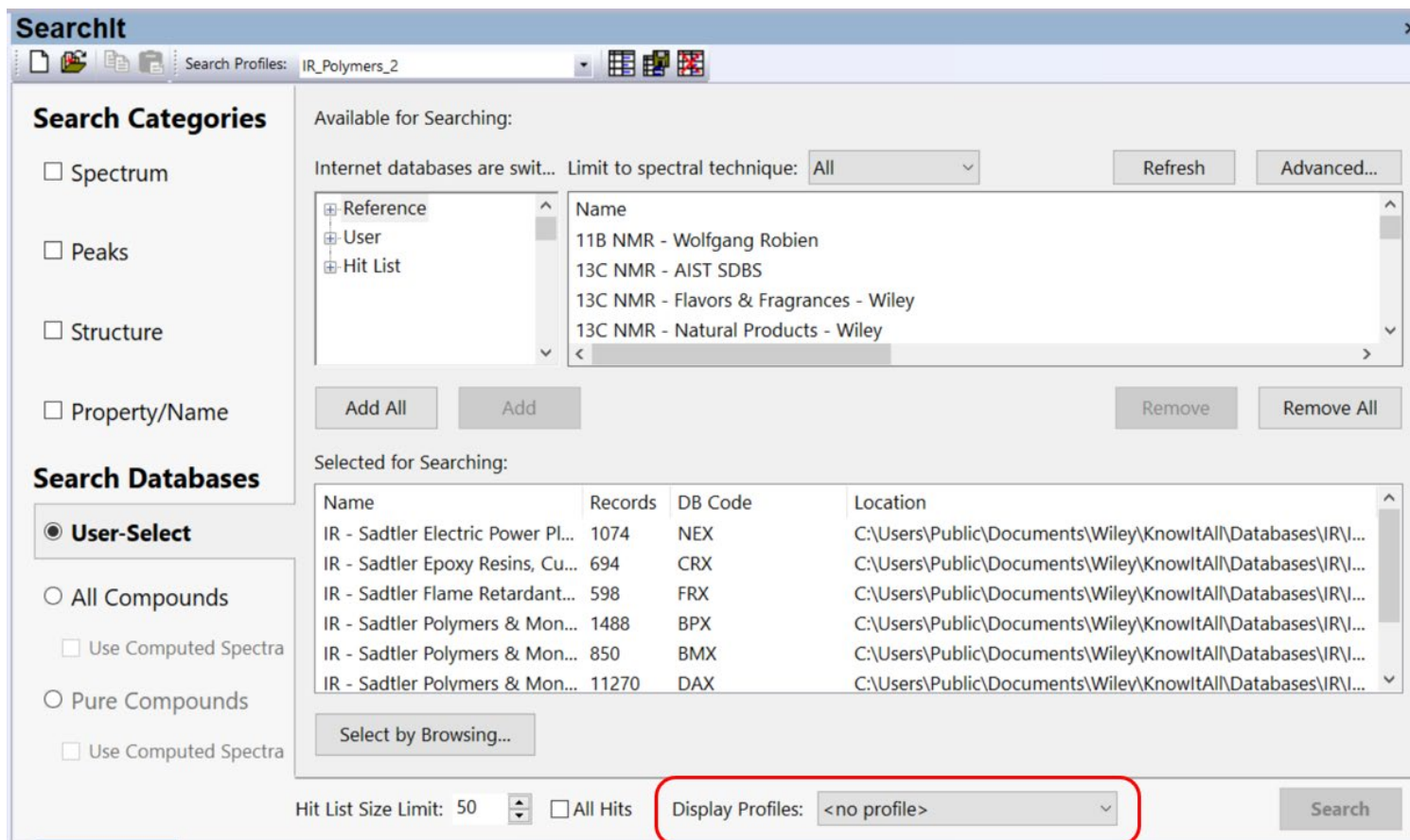
	Action	Result
1	Click the SearchIt Close button  , then click Remove All to clear the contents of the Selected for Searching list.	<p>The User-Select tab is displayed. The Selected for Searching list is empty:</p> 
2	Click the Add a New Profile button  on the Profile toolbar.	<p>The New Profile dialog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

	Action	Result												
5	In the Available for Searching list, click to select IR – Sadtler Polymers, Hummel – Wiley (DB Code HUX). Click Add .	<p>The HUX database is added to the Selected for Searching list:</p> <p>Selected for Searching:</p> <table border="1" data-bbox="701 386 1629 565"> <thead> <tr> <th>Name</th> <th>Records</th> <th>DB Code</th> <th>Location</th> </tr> </thead> <tbody> <tr> <td>IR - Sadtler Polymers, Humm...</td> <td>1907</td> <td>HUX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\I...</td> </tr> </tbody> </table> <p>Select by Browsing...</p>	Name	Records	DB Code	Location	IR - Sadtler Polymers, Humm...	1907	HUX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\I...				
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IR - Sadtler Polymers, Humm...	1907	HUX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\I...											
6	In the Available for Searching list, double-click IR — Sadtler Polymers & Monomers (Basic) 1 — Wiley (DB Code BPX).	<p>The BPX database is added to the Selected for Searching list:</p> <p>Selected for Searching:</p> <table border="1" data-bbox="701 711 1650 889"> <thead> <tr> <th>Name</th> <th>Records</th> <th>DB Code</th> <th>Location</th> </tr> </thead> <tbody> <tr> <td>IR - Sadtler Polymers & Mon...</td> <td>1488</td> <td>BPX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\I...</td> </tr> <tr> <td>IR - Sadtler Polymers, Humm...</td> <td>1907</td> <td>HUX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\I...</td> </tr> </tbody> </table> <p>Select by Browsing...</p>	Name	Records	DB Code	Location	IR - Sadtler Polymers & Mon...	1488	BPX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\I...	IR - Sadtler Polymers, Humm...	1907	HUX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\I...
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	Action	Result																																	
7	Continue adding databases BMX, CRX, DAX, FRX and NEX.	<p>The selected databases are added to the Selected for Searching window:</p>  <table border="1" data-bbox="701 428 1600 600"> <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\I...</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\I...</td> </tr> <tr> <td>IR - Sadtler Flame Retardant...</td> <td>598</td> <td>FRX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\I...</td> </tr> <tr> <td>IR - Sadtler Polymers & Mon...</td> <td>1488</td> <td>BPX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\I...</td> </tr> <tr> <td>IR - Sadtler Polymers & Mon...</td> <td>850</td> <td>BMX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\I...</td> </tr> <tr> <td>IR - Sadtler Polymers & Mon...</td> <td>11270</td> <td>DAX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\I...</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\I...	IR - Sadtler Epoxy Resins, Cu...	694	CRX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\I...	IR - Sadtler Flame Retardant...	598	FRX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\I...	IR - Sadtler Polymers & Mon...	1488	BPX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\I...	IR - Sadtler Polymers & Mon...	850	BMX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\I...	IR - Sadtler Polymers & Mon...	11270	DAX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\I...					
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8	On the User-Select tab, change the Hit List Size Limit to 10.	 <p>Hit List Size Limit: 10 <input type="checkbox"/> All Hits</p>																																	
9	Click the Save Current Profile button  on the Profile toolbar. A message box asks if you wish to overwrite the current profile. Click Yes to save the new profile.																																		
10	Close the current search by clicking X , then select the newly created IR_Polymers_2 search profile.	<p>The databases and search settings associated with this profile are displayed:</p>  <p>Search Categories:</p> <ul style="list-style-type: none"> <input type="checkbox"/> Spectrum <input type="checkbox"/> Peaks <input type="checkbox"/> Structure <input type="checkbox"/> Property/Name <p>Search Databases:</p> <ul style="list-style-type: none"> <input checked="" type="radio"/> User-Select <input type="radio"/> All Compounds <ul style="list-style-type: none"> <input type="checkbox"/> Use Computed Spectra <input type="radio"/> Pure Compounds <ul style="list-style-type: none"> <input type="checkbox"/> Use Computed Spectra <p>Available for Searching:</p> <p>Internet databases are swit... Limit to spectral technique: All Refresh Advanced...</p> <table border="1" data-bbox="861 1045 1453 1143"> <thead> <tr> <th>Name</th> </tr> </thead> <tbody> <tr> <td>11B NMR - Wolfgang Robien</td> </tr> <tr> <td>13C NMR - AIST SDBS</td> </tr> <tr> <td>13C NMR - Flavors & Fragrances - Wiley</td> </tr> <tr> <td>13C NMR - Natural Products - Wiley</td> </tr> </tbody> </table> <p>Add All Add Remove Remove All</p> <p>Selected for Searching:</p> <table border="1" data-bbox="861 1208 1453 1321"> <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\I...</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\I...</td> </tr> <tr> <td>IR - Sadtler Flame Retardant...</td> <td>598</td> <td>FRX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\I...</td> </tr> <tr> <td>IR - Sadtler Polymers & Mon...</td> <td>1488</td> <td>BPX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\I...</td> </tr> <tr> <td>IR - Sadtler Polymers & Mon...</td> <td>850</td> <td>BMX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\I...</td> </tr> <tr> <td>IR - Sadtler Polymers & Mon...</td> <td>11270</td> <td>DAX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\I...</td> </tr> </tbody> </table> <p>Select by Browsing...</p> <p>Hit List Size Limit: 10 <input type="checkbox"/> All Hits Display Profiles: <no profile> Search</p>	Name	11B NMR - Wolfgang Robien	13C NMR - AIST SDBS	13C NMR - Flavors & Fragrances - Wiley	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\I...	IR - Sadtler Epoxy Resins, Cu...	694	CRX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\I...	IR - Sadtler Flame Retardant...	598	FRX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\I...	IR - Sadtler Polymers & Mon...	1488	BPX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\I...	IR - Sadtler Polymers & Mon...	850	BMX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\I...	IR - Sadtler Polymers & Mon...	11270	DAX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\I...
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Use Minelt profile for hit list display

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



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

- Search Profiles:** IR_Polymers_2
- Search Categories:** Spectrum, Peaks, Structure, Property/Name (all unchecked).
- Search Databases:** User-Select (selected), All Compounds, Pure Compounds (all unchecked). "Use Computed Spectra" is also unchecked.
- Available for Searching:** Internet databases are switched on. Limit to spectral technique: All. Buttons: Refresh, Advanced...
- Reference List:**

Name
11B NMR - Wolfgang Robien
13C NMR - AIST SDBS
13C NMR - Flavors & Fragrances - Wiley
13C NMR - Natural Products - Wiley
- Selected for Searching:**

Name	Records	DB Code	Location
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- Bottom Controls:** Hit List Size Limit: 50, All Hits (unchecked), Display Profiles: <no profile> (highlighted with a red box), Search button.

Searching

How to Search a Database of Spectra by Peak

Purpose

This exercise demonstrates how to perform a peak search.

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

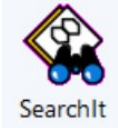

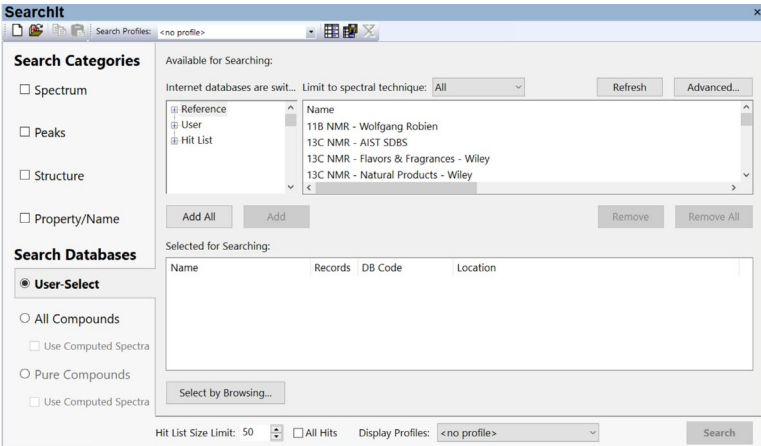
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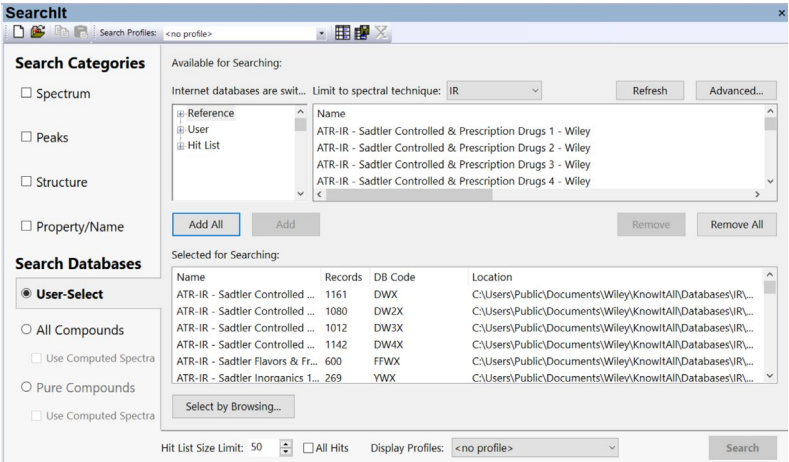
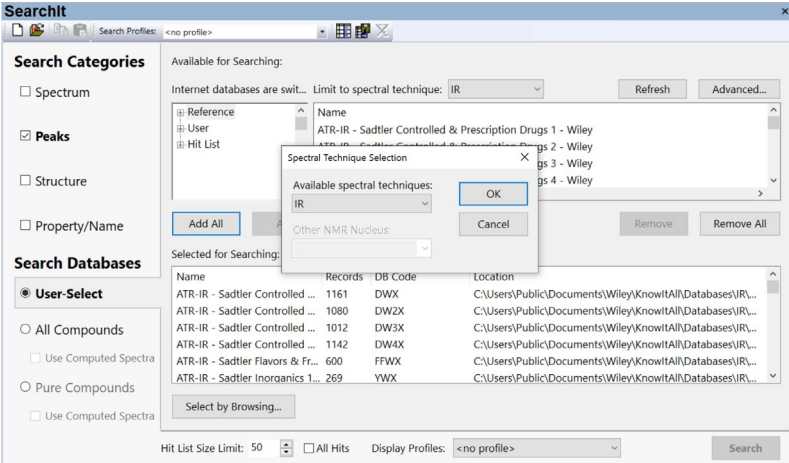
- Ethyl acrylate.dx

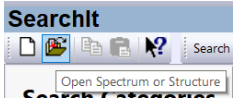
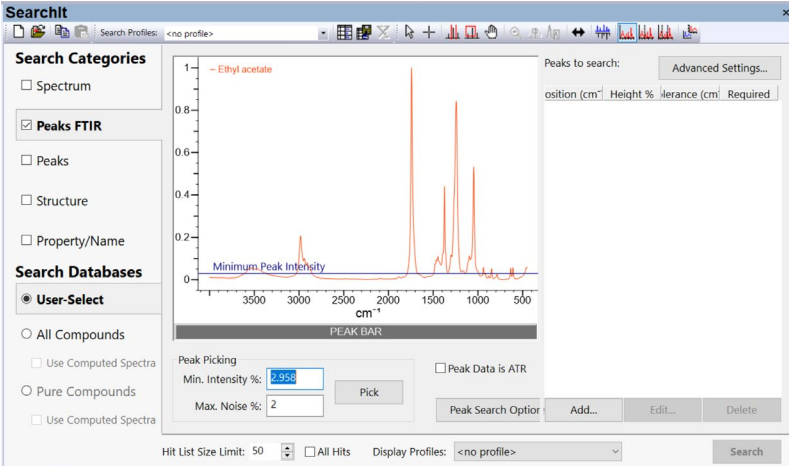
KnowItAll Applications Used

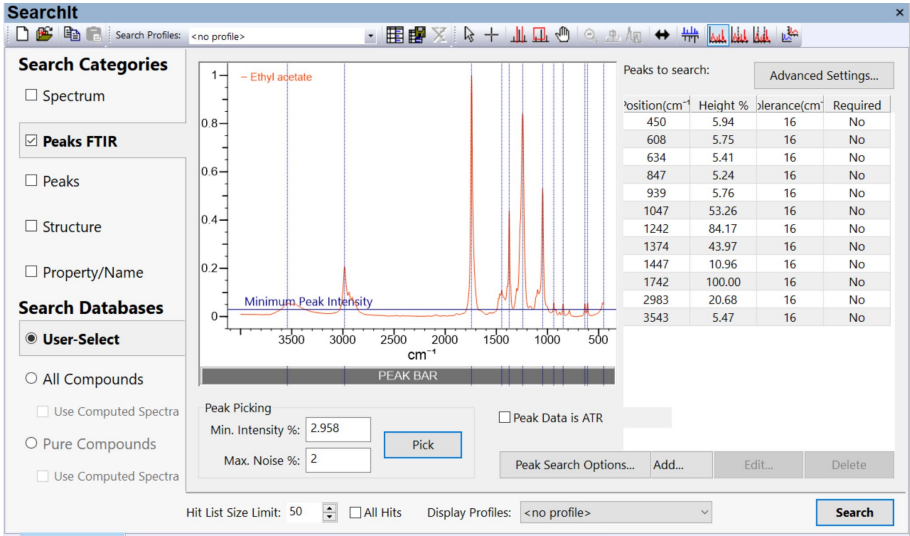
- SearchIt™
- MineIt™

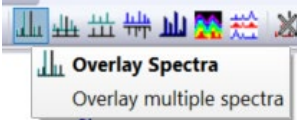
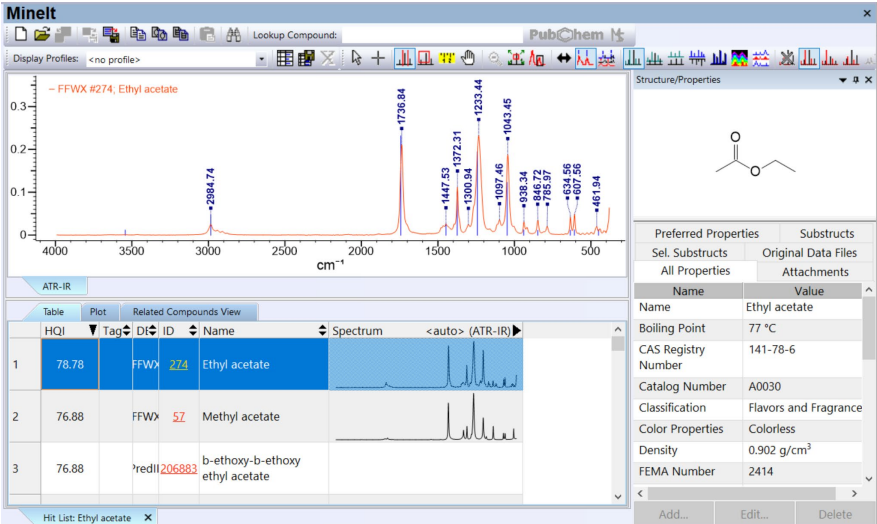
Configure and perform a peak search

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

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

	Action	Result
4	<p>Click OK.</p>	<p>The Peaks FTIR search dialog is displayed:</p> 
5	<p>Click Open Spectrum or Structure.</p>  <p>Navigate to “C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\IR”.</p> <p>Open Ethyl acetate.jdx.</p>	<p>The selected spectrum is displayed:</p> 

	Action	Result																																																				
6	Click Pick .	<p>The peak table is created based on the current settings:</p>  <p>The screenshot shows the SearchIt interface with the following peak table:</p> <table border="1"> <thead> <tr> <th>Position(cm⁻¹)</th> <th>Height %</th> <th>Tolerance(cm⁻¹)</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 ⁻¹)	Height %	Tolerance(cm ⁻¹)	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	TIP	<p>You can remove a peak from the peak table by selecting the peak and clicking the delete button or by double-clicking it in the peak bar. Similarly, you can add or edit peaks using the corresponding buttons at the bottom of the table.</p>																																																				

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

Searching

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.

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

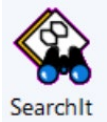

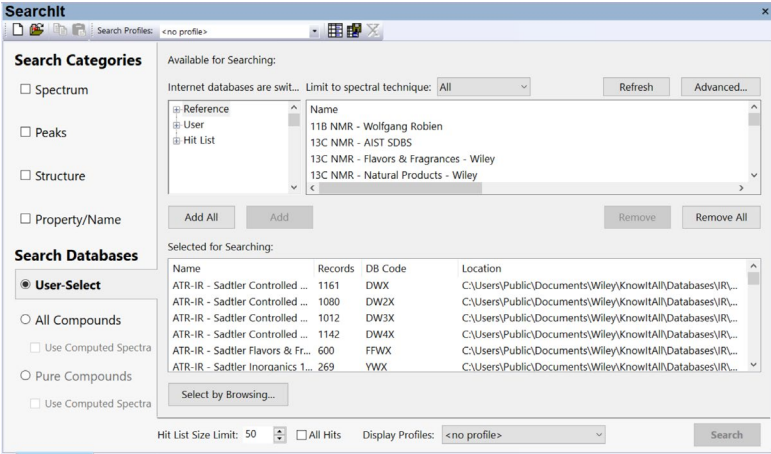
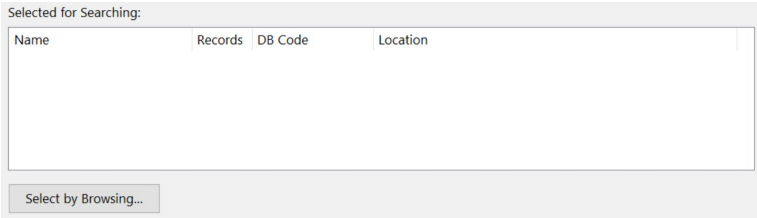
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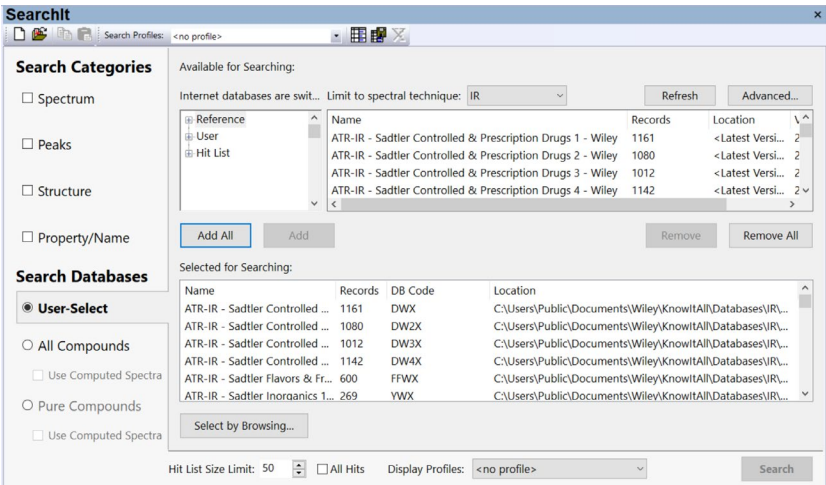
- Acetonitrile.jdx

KnowItAll Applications Used

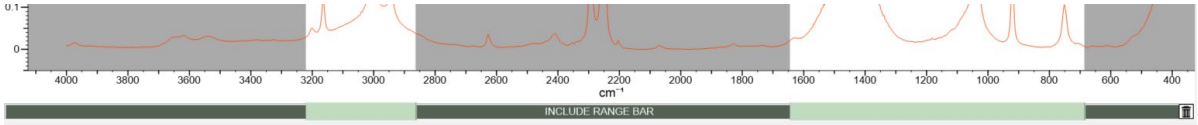

- SearchIt™
- MineIt™

Configure a spectral search


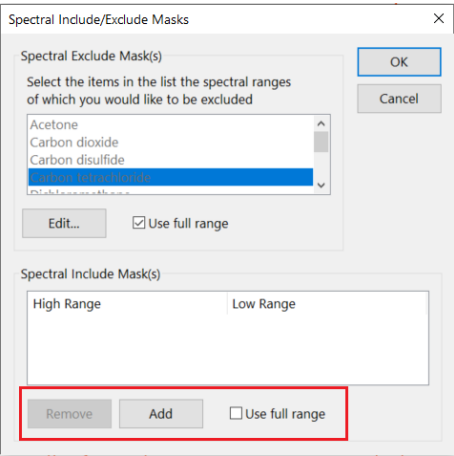
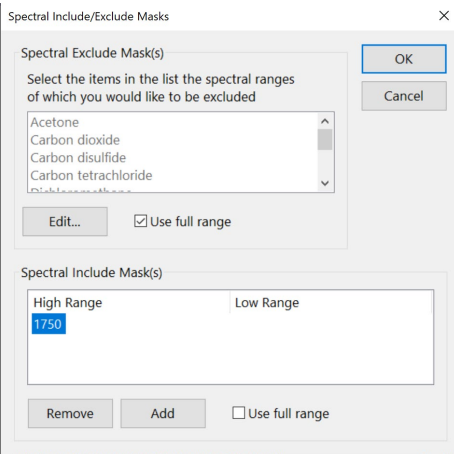
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1	<p>Do one of the following:</p> <ul style="list-style-type: none"> If the SearchIt application is not open, navigate to the Data toolbox and click its icon.  <ul style="list-style-type: none"> If the SearchIt application is already open, click the SearchIt Close button  to close the current search. 	<p>The SearchIt application's User-Select tab is displayed and the Selected for Searching list displays the databases last used:</p>  <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 ...</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 & 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>	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...
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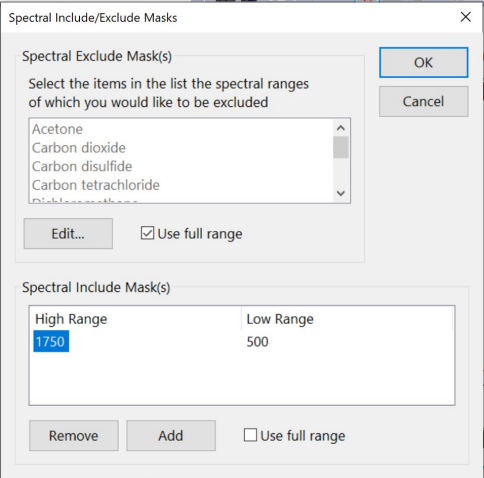
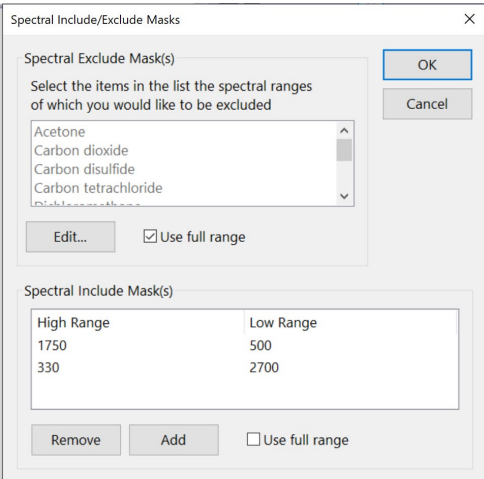
	Action	Result																																																
3	In the Available for Searching Dialog, choose IR for Limit Spectral Technique to. Click Add All .	<p>The Wiley IR database collection is displayed in the Selected for Searching list:</p>  <p>The screenshot shows the SearchIt application window. On the left, under 'Search Categories', 'Spectrum' is selected. In the 'Available for Searching' section, 'Limit to spectral technique' is set to 'IR'. Below this, a table lists available databases. In the 'Selected for Searching' section, a table lists the selected databases. At the bottom, there are controls for 'Hit List Size Limit' (set to 50), 'All Hits', 'Display Profiles' (set to '<no profile>'), and a 'Search' button.</p> <table border="1" data-bbox="877 477 1507 597"> <thead> <tr> <th>Reference</th> <th>Name</th> <th>Records</th> <th>Location</th> </tr> </thead> <tbody> <tr> <td>User</td> <td>ATR-IR - Sadtler Controlled & Prescription Drugs 1 - Wiley</td> <td>1161</td> <td><Latest Versi... 2</td> </tr> <tr> <td>Hit List</td> <td>ATR-IR - Sadtler Controlled & Prescription Drugs 2 - Wiley</td> <td>1080</td> <td><Latest Versi... 2</td> </tr> <tr> <td></td> <td>ATR-IR - Sadtler Controlled & Prescription Drugs 3 - Wiley</td> <td>1012</td> <td><Latest Versi... 2</td> </tr> <tr> <td></td> <td>ATR-IR - Sadtler Controlled & Prescription Drugs 4 - Wiley</td> <td>1142</td> <td><Latest Versi... 2</td> </tr> </tbody> </table> <table border="1" data-bbox="877 656 1507 792"> <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 & Fr...</td> <td>600</td> <td>FFWX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...</td> </tr> <tr> <td>ATR-IR - Sadtler Inoroanics 1...</td> <td>269</td> <td>YWX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...</td> </tr> </tbody> </table>	Reference	Name	Records	Location	User	ATR-IR - Sadtler Controlled & Prescription Drugs 1 - Wiley	1161	<Latest Versi... 2	Hit List	ATR-IR - Sadtler Controlled & Prescription Drugs 2 - Wiley	1080	<Latest Versi... 2		ATR-IR - Sadtler Controlled & Prescription Drugs 3 - Wiley	1012	<Latest Versi... 2		ATR-IR - Sadtler Controlled & Prescription Drugs 4 - Wiley	1142	<Latest Versi... 2	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 Inoroanics 1...	269	YWX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\...
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4	Click Spectrum under Search Categories .	An Open dialog box appears.																																																

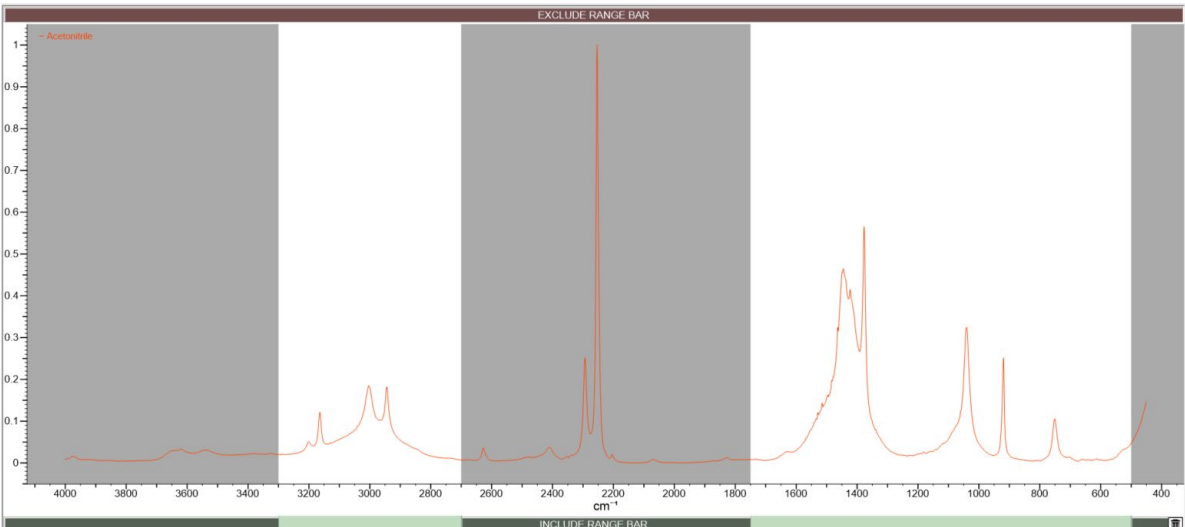
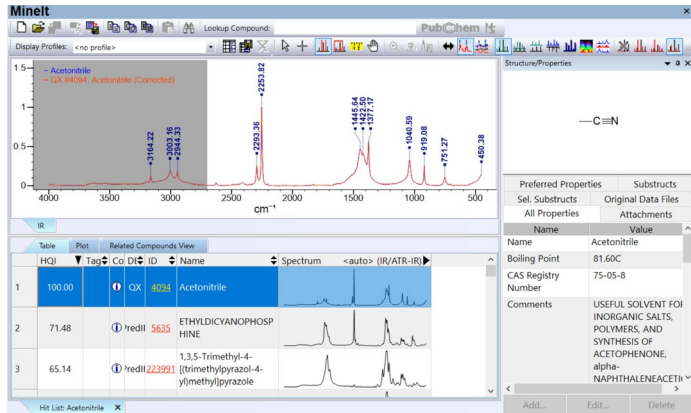

	Action	Result
5	<p>Navigate to “C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\R”. Open Acetonitrile.jdx.</p> <p>Note: You can use the Files of Type filter to display JCAMP files (or all files).</p>	<p>The spectrum is displayed.</p> 
6	<p>Click, drag, and release within the Include Range Bar to define an Include region.</p>	<p>The Include region is green in the Include Range Bar; 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 Include Range 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>

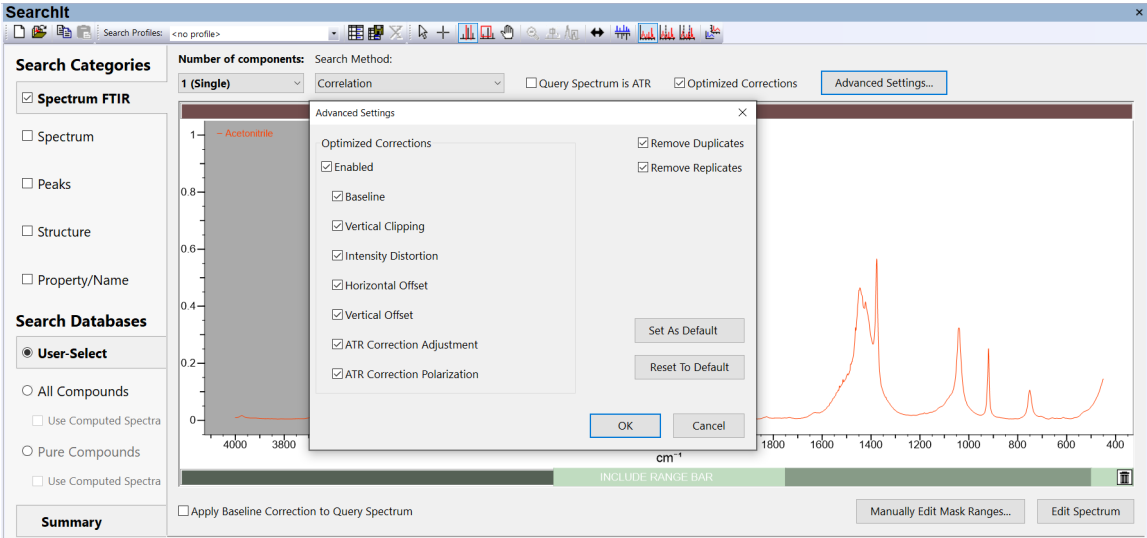
	Action	Result
7	<p>Click and drag to define a second Include region.</p> <p>Note: To move a region horizontally, click within the region on the Include Range Bar and drag to a new location.</p>	<p>A second region is selected on the spectrum:</p> 
8	<p>TIPS:</p>	<p>To re-size a region, move the cursor into the Include Range Bar and position the cursor over an endpoint, then drag and release. The cursor changes to a cross with a double arrowhead.</p>  <p>To remove a single region, either click within the region on the Include Range Bar and drag to either side away from the spectral pane, or right-click within the region and choose Yes on the message box that opens.</p> <p>To remove all regions, click the garbage can icon at the right end of the Include Range Bar.</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 INCLUDE RANGE BAR</p>  <p>Click Manually Edit Mask Ranges. Unclick Use full range and click Add under Spectral Include Mask(s)</p> <p>Note: Any Include regions defined using the Include Range Bar are displayed in the list of Spectral Include Mask(s). However, if Use full range is checked, these regions will not be used.</p>	<p>The Spectral Include/Exclude Masks dialog box opens.</p> 
2	<p>Click to select the High Range value in the remaining Include region and type in '1750.'</p>	<p>1750 is added as a High Range value:</p> 

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

	Action	Result
5	Click OK .	<p>The dialog box closes, and the search spectrum is displayed with the re-defined Include regions.</p> 
6	Click Search .	<p>The search is performed, and results are automatically displayed in the Minelt application as a hit list.</p>  <p>Clicking on the information icon  in the results table displays Optimized Corrections that have been performed.</p>

Action	Result
<p>7 Close the Optimized Corrections window, then use the KnowItAll Back button to return to the SearchIt application.</p> <p>Click Advanced Settings on the Spectrum FTIR tab.</p>	<p>The Advanced Settings dialog box opens:</p>  <p>The Advanced Settings dialog can be used to control the applied Optimized Corrections.</p>

Searching

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.

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

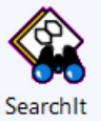

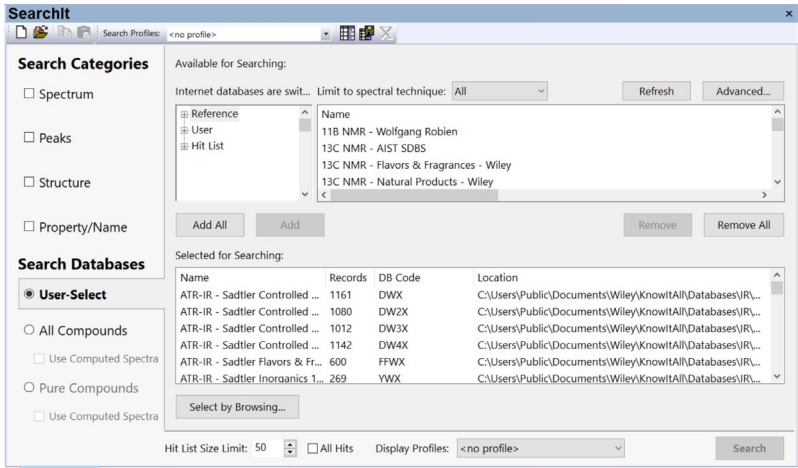
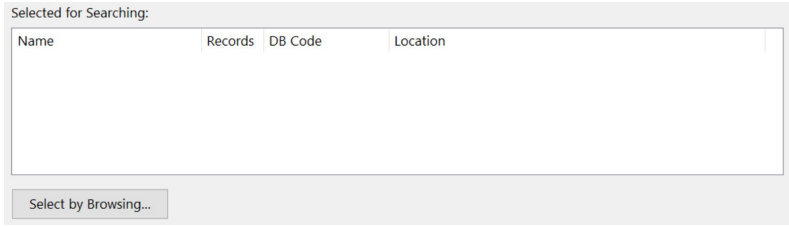
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\IR

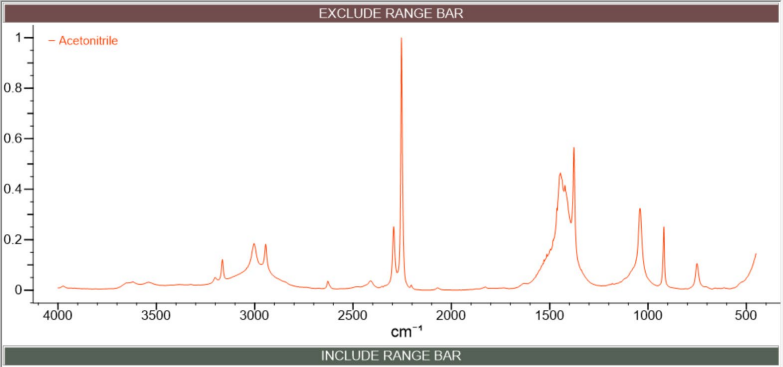
- Acetonitrile.jdx

KnowItAll Applications Used

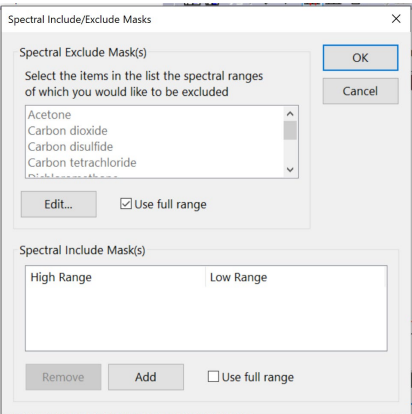
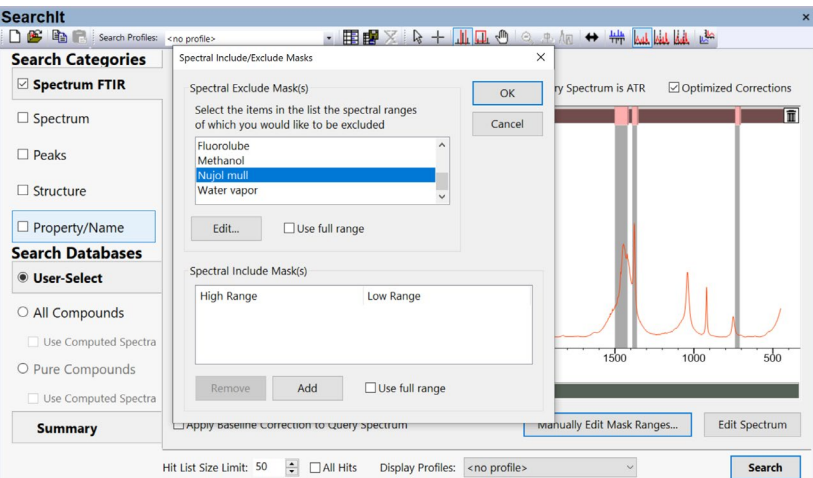
- SearchIt™
- MineIt™

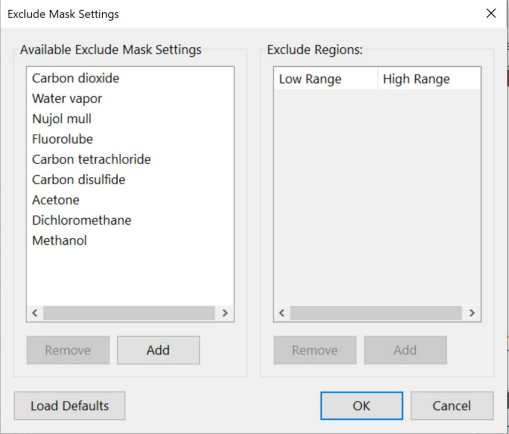
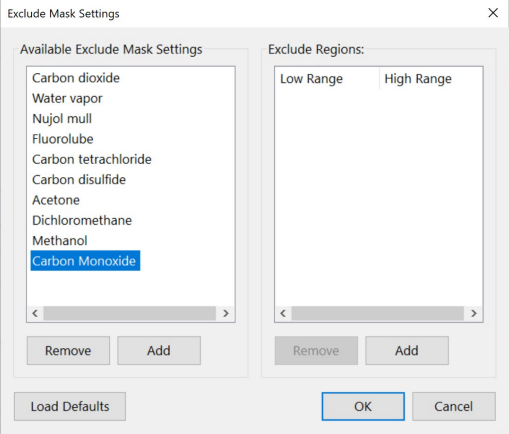
Configure a spectral search

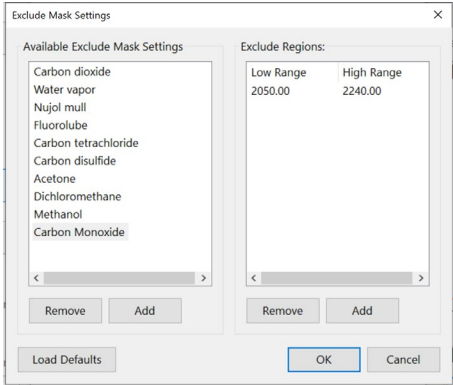
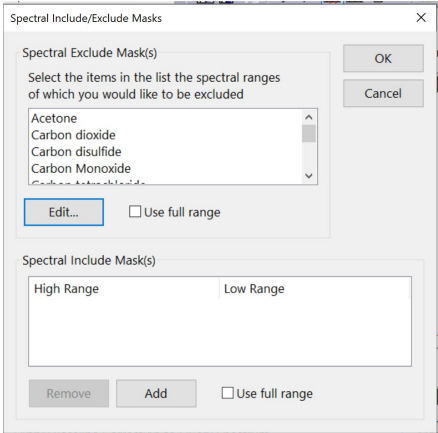
	Action	Result																												
1	<p>Do one of the following:</p> <ul style="list-style-type: none"> If the SearchIt application is not open, navigate to the Data toolbox and click its icon.  <ul style="list-style-type: none"> If the SearchIt application is already open, click the SearchIt Close button  to close the current search. 	<p>The SearchIt application's User-Select tab is displayed and the Selected for Searching list displays the databases last used:</p>  <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 ...</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>DWZX</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 & 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>	Name	Records	DB Code	Location	ATR-IR - Sadtler Controlled ...	1161	DWX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR...	ATR-IR - Sadtler Controlled ...	1080	DWZX	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...
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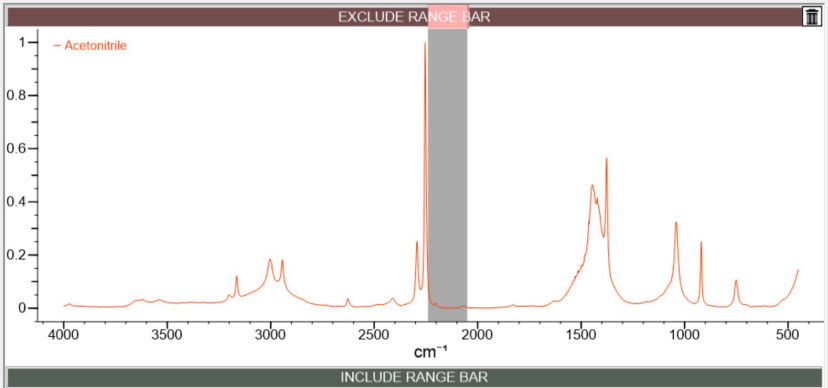
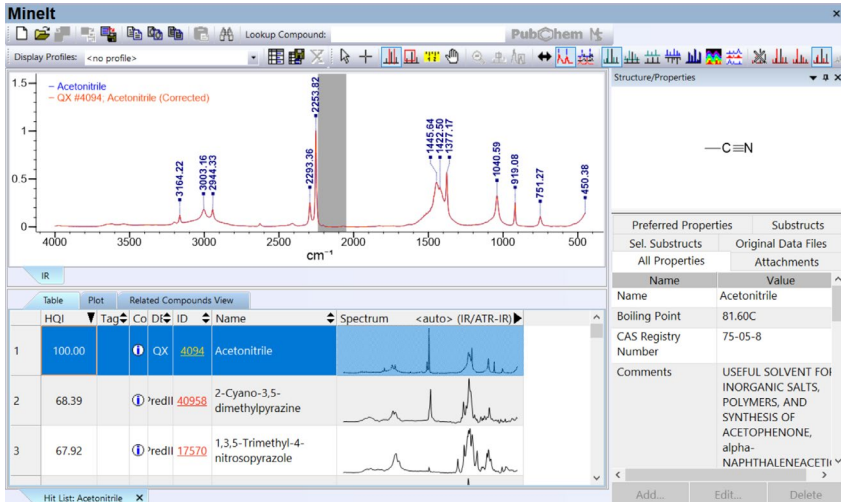
	Action	Result																												
3	Select IR using the Limit to spectral technique control. Click Add All .	The Wiley IR database collection is displayed in the Selected for Searching list: <div data-bbox="709 386 1535 625" style="border: 1px solid gray; padding: 5px; margin: 10px 0;"> Selected 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 & 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="margin-top: 5px;">Select by Browsing...</p> </div> <p>Note: 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\...
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5	Navigate to "C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\IR". Open Acetonitrile.jdx . <p>NOTE: 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="709 829 1507 1247" style="border: 1px solid gray; padding: 5px; margin: 10px 0;">  <p style="margin-top: 5px;"> <input type="checkbox"/> Apply Baseline Correction to Query Spectrum Manually Edit Mask Ranges... Edit Spectrum </p> </div>																												

Use the Search Masks dialog box

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

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

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

	Action	Result
8	Select the new Carbon monoxide mask, then click OK to close the Spectral Include/Exclude Masks dialog box.	The dialog box closes, and the search spectrum is displayed with the newly defined exclude region: 
9	Click Search .	The search results are automatically displayed in the Minelt application as a hit list. 

Searching

How to Subtract One Spectrum from Another

Purpose

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

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

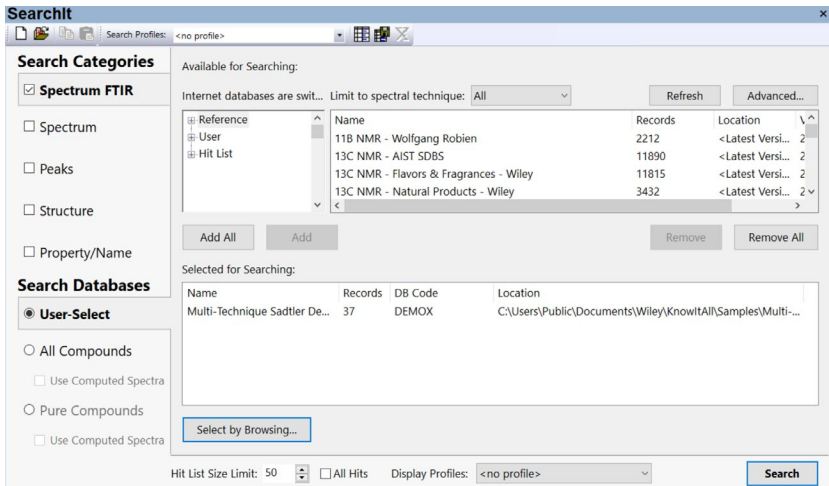
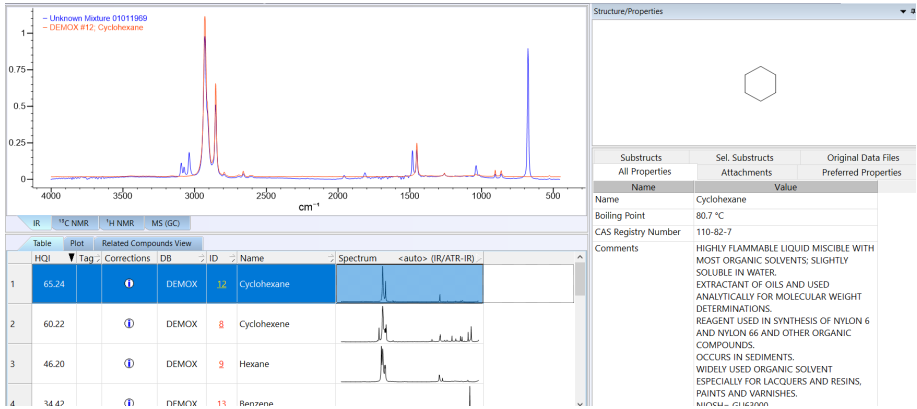
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Mixture Analysis\IR Examples

- Unknown Mixture 01011969.jdx

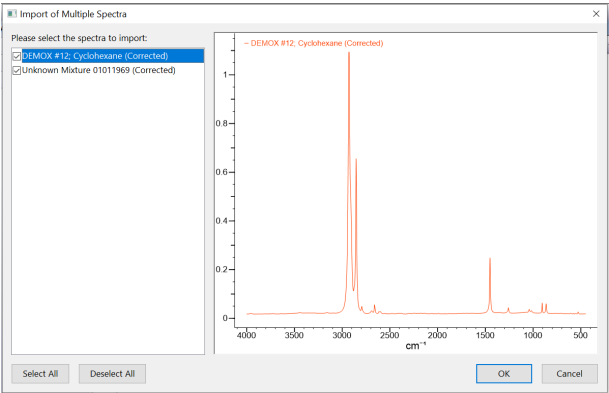
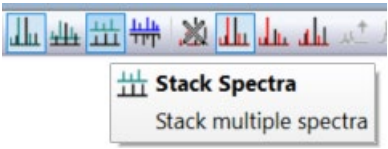
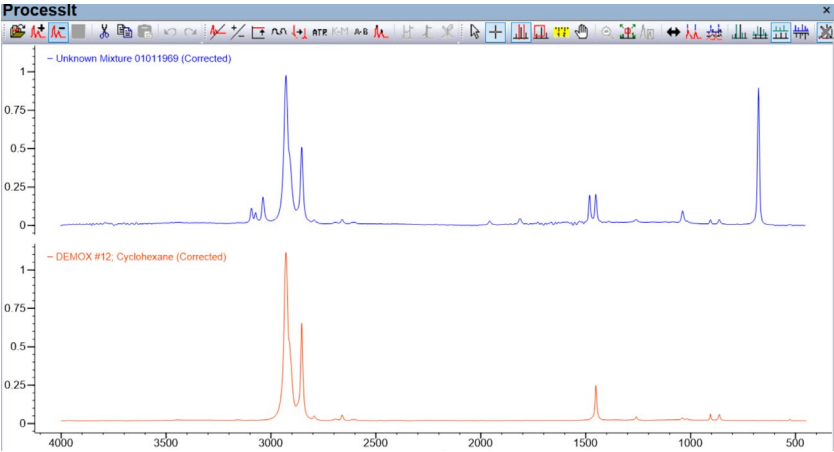
KnowItAll Applications Used


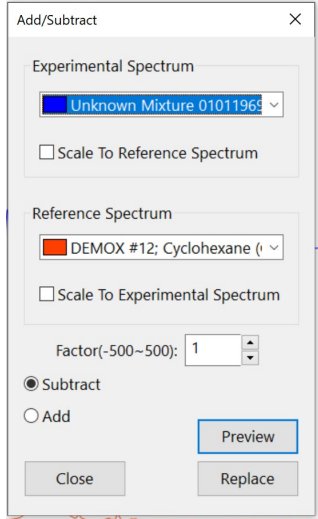
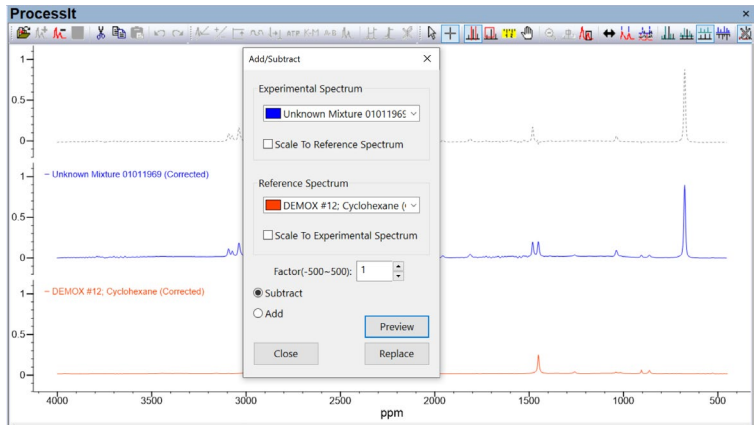
- SearchIt™
- Minelt™
- ProcessIt™ IR

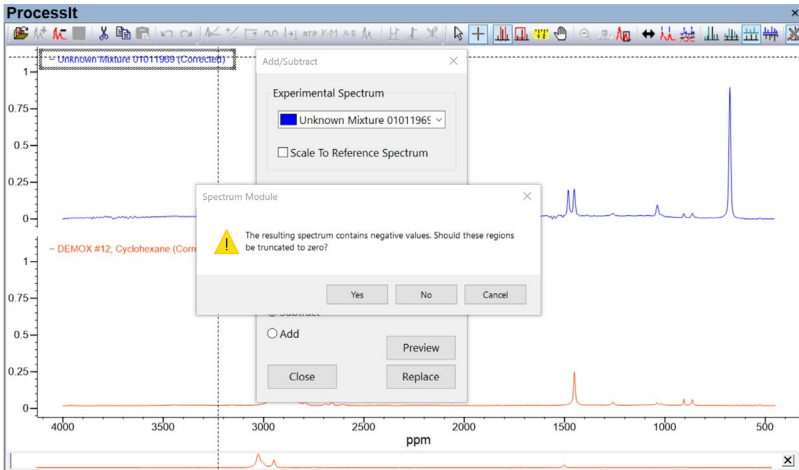
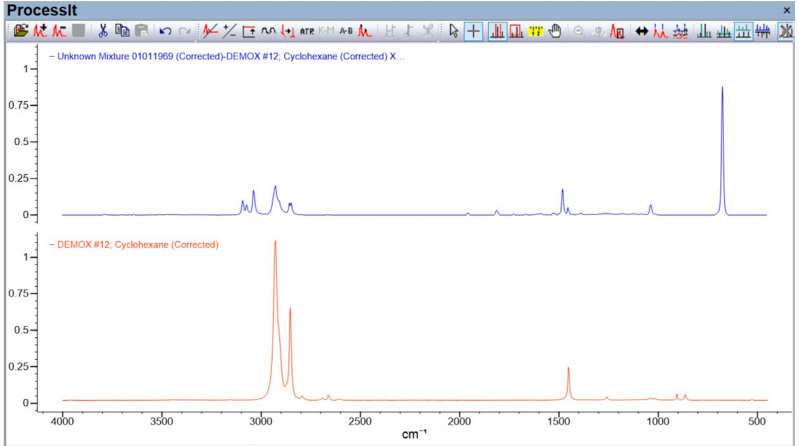
Set up a spectral search against a mixture

	Action	Result																																			
1	<p>In the SearchIt application, navigate to “C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\Mixture Analysis\IR Examples” and open Unknown Mixture 01011969.jdx. Limit the database search to Multi-Technique Sadtler Demo Database – Wiley from “C:\Users\Public\Public Documents\Wiley\KnowItAll\Sample” folder by using the Open by browsing button.</p>	<p>The FTIR spectrum is opened in SearchIt and the DEMOX database is selected for searching:</p> 																																			
2	<p>Click Search.</p>	<p>Results are displayed in the Minelt application. The first hit is cyclohexane. Both spectra, the query and the first hit are displayed in the spectral pane.</p>  <table border="1" data-bbox="821 1219 1396 1382"> <thead> <tr> <th>HQI</th> <th>Tag</th> <th>Corrections</th> <th>DB</th> <th>ID</th> <th>Name</th> <th>Spectrum</th> </tr> </thead> <tbody> <tr> <td>65.24</td> <td></td> <td></td> <td>DEMOK</td> <td>12</td> <td>Cyclohexane</td> <td></td> </tr> <tr> <td>60.22</td> <td></td> <td></td> <td>DEMOK</td> <td>8</td> <td>Cyclohexane</td> <td></td> </tr> <tr> <td>46.20</td> <td></td> <td></td> <td>DEMOK</td> <td>9</td> <td>Hexane</td> <td></td> </tr> <tr> <td>34.42</td> <td></td> <td></td> <td>DEMOK</td> <td>13</td> <td>Benzene</td> <td></td> </tr> </tbody> </table>	HQI	Tag	Corrections	DB	ID	Name	Spectrum	65.24			DEMOK	12	Cyclohexane		60.22			DEMOK	8	Cyclohexane		46.20			DEMOK	9	Hexane		34.42			DEMOK	13	Benzene	
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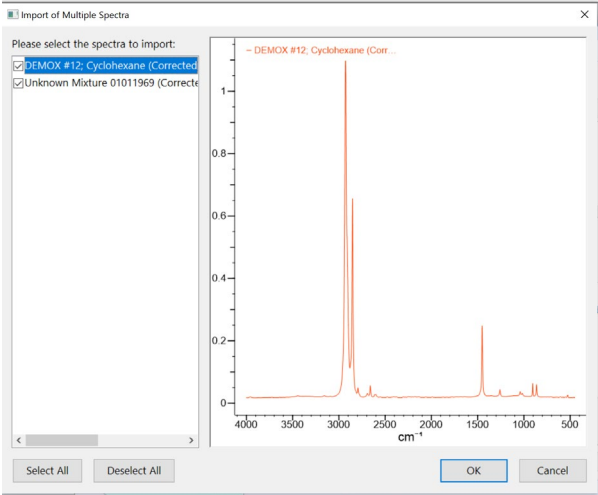
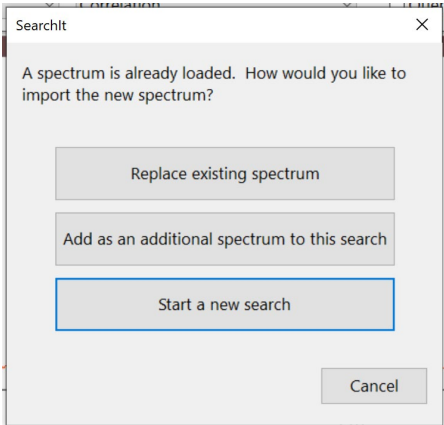
Create a difference spectrum

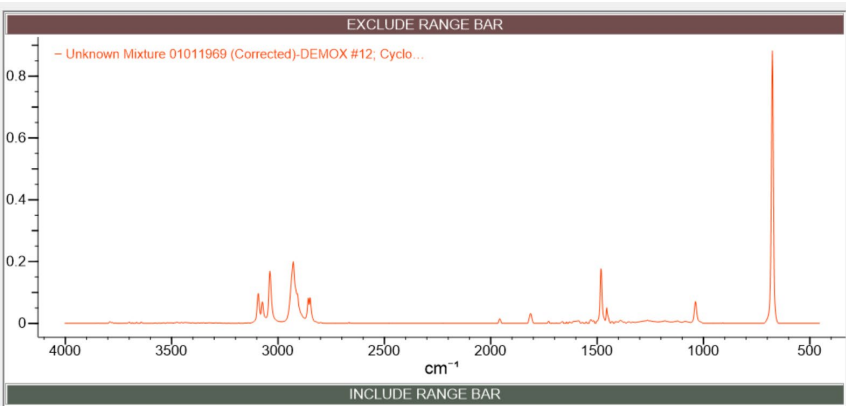
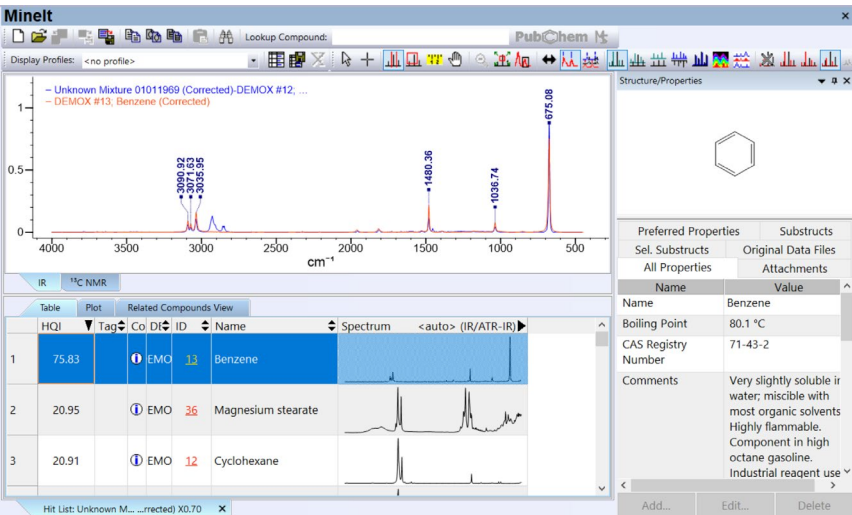
	Action	Result
1	With the hit list displayed in Minelt and the first record selected, click ProcessIt in the Transfer to bar.	<p>The Import of Multiple Spectra dialog box opens.</p>  <p>Both the query spectrum and the first hit are displayed.</p>
2	Click Select All , then click OK on the Import of Multiple Spectra dialog box. In Minelt , click Stack Spectra view. 	<p>Both spectra—the mixture and the first hit, cyclohexane—are transferred to the ProcessIt IR application:</p>  <p>NOTE: 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 Process > Add/Subtract Spectrum.</p> <p>NOTE: You can also use the toolbar button . The command is not available unless two or more spectra are open.</p>	<p>The Add/Subtract dialog box opens. The active spectrum is assumed to be the reference spectrum:</p> 
4	<p>Make sure the mixture spectrum is the Experimental Spectrum, and cyclohexane is the Reference Spectrum. If needed, change these assignments using either of the drop-down lists. Click Preview.</p>	<p>A preview of the difference spectrum is provided:</p> 

	Action	Result
5	On the Add/Subtract dialog box, adjust Factor to ~0.7. Click Replace .	<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 01011965 (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, with 'Unknown Mixture 01011965' selected in the 'Experimental Spectrum' dropdown. The 'Scale To Reference Spectrum' checkbox is unchecked. 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?'. It has 'Yes', 'No', and 'Cancel' buttons. Below the warning, there are radio buttons for 'Add' and 'Replace', along with 'Preview' and 'Close' buttons.</p>
6	Click Yes .	<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 blue IR spectrum representing the difference spectrum, titled 'Unknown Mixture 01011965 (Corrected)-DEMOX #12, Cyclohexane (Corrected) X...'. The x-axis is labeled 'cm⁻¹' and ranges from 4000 to 500. The red reference spectrum for 'DEMOX #12, Cyclohexane (Corrected)' is still visible at the bottom of the plot area.</p>

Repeat the search using the difference spectrum

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

	Action	Result																						
3	Click Start a new search .	<p>The difference spectrum is loaded in SearchIt:</p> 																						
4	<p>Click User-Select tab and make sure the Multi-Technique Sadtler Demo Database - Wiley is selected for searching.</p> <p>Click Search.</p>	<p>Results are displayed in the Minelt application. The first hit is benzene, the other component of the mixture.</p>  <table border="1" data-bbox="653 1138 1178 1341"> <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</th> <th>Spectrum</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>75.83</td> <td>EMO 13</td> <td>Benzene</td> <td></td> </tr> <tr> <td>2</td> <td>20.95</td> <td>EMO 36</td> <td>Magnesium stearate</td> <td></td> </tr> <tr> <td>3</td> <td>20.91</td> <td>EMO 12</td> <td>Cyclohexane</td> <td></td> </tr> </tbody> </table>	Table	Plot	Related Compounds View	HQI	Tag	Co DI ID Name	Spectrum	1	75.83	EMO 13	Benzene		2	20.95	EMO 36	Magnesium stearate		3	20.91	EMO 12	Cyclohexane	
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Searching

How to Perform a Structure Search

Purpose

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

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



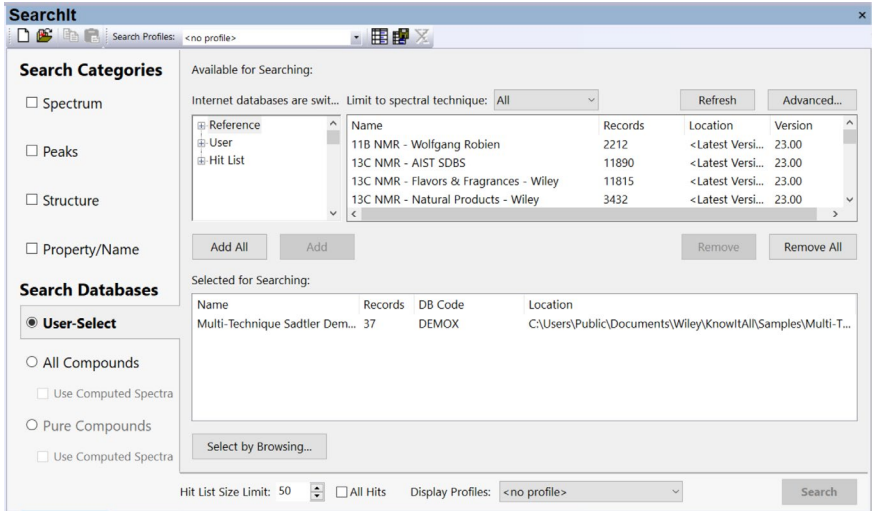
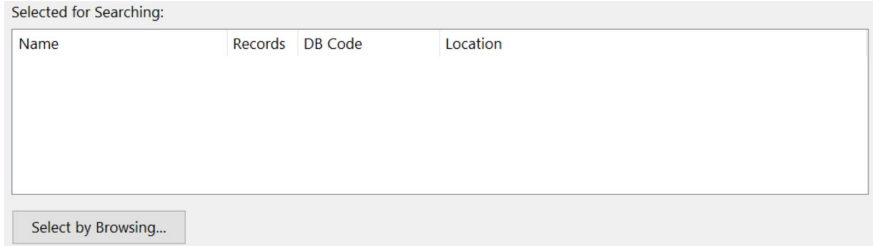
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Structures

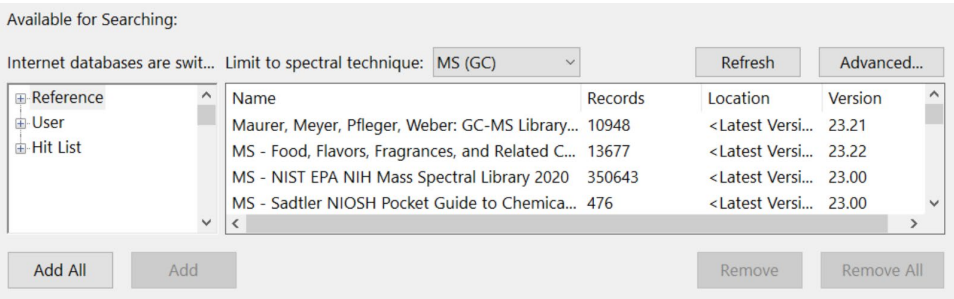
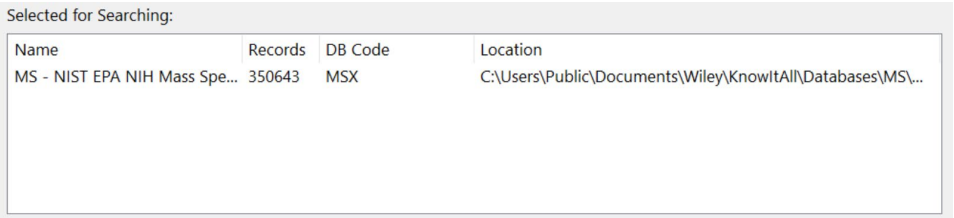
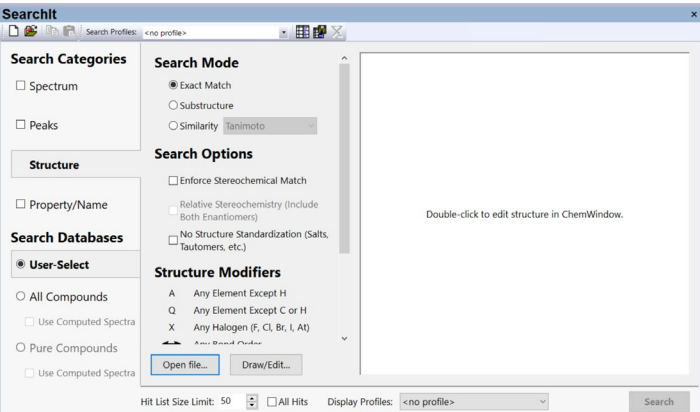
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- benzenethiol.dsf

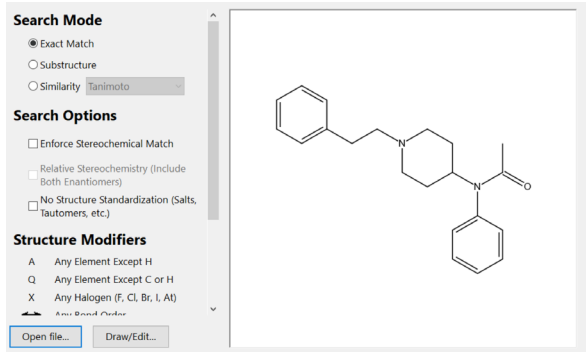
KnowItAll Applications Used

- SearchIt™
- Minelt™
- ChemWindow®

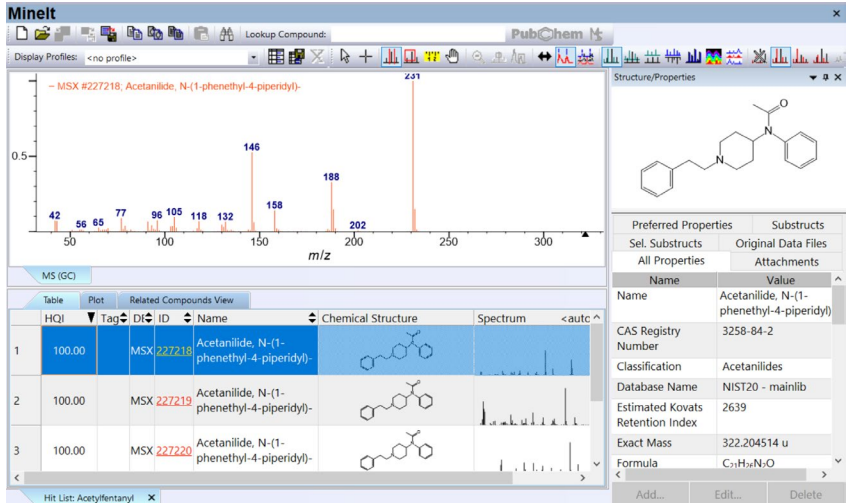
Configure an exact structure match search

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

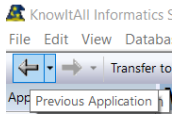
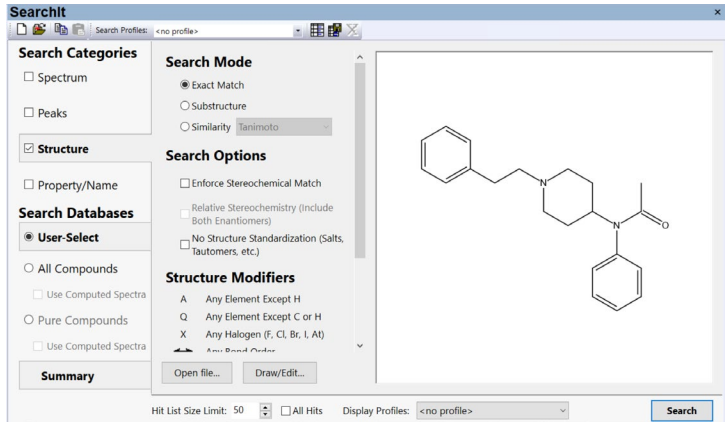
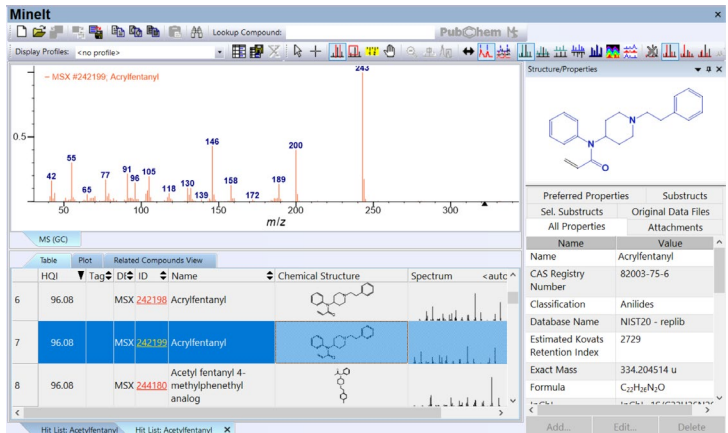
	Action	Result																									
3	Set Limit to Spectral Technique to MS (GC) .	<p>Only databases with MS spectral data are displayed:</p>  <p>Available for Searching:</p> <p>Internet databases are swit... Limit to spectral technique: MS (GC) Refresh Advanced...</p> <table border="1"> <thead> <tr> <th>Reference</th> <th>Name</th> <th>Records</th> <th>Location</th> <th>Version</th> </tr> </thead> <tbody> <tr> <td>User</td> <td>Maurer, Meyer, Pflieger, Weber: GC-MS Library...</td> <td>10948</td> <td><Latest Versi...</td> <td>23.21</td> </tr> <tr> <td>Hit List</td> <td>MS - Food, Flavors, Fragrances, and Related C...</td> <td>13677</td> <td><Latest Versi...</td> <td>23.22</td> </tr> <tr> <td></td> <td>MS - NIST EPA NIH Mass Spectral Library 2020</td> <td>350643</td> <td><Latest Versi...</td> <td>23.00</td> </tr> <tr> <td></td> <td>MS - Sadtler NIOSH Pocket Guide to Chemica...</td> <td>476</td> <td><Latest Versi...</td> <td>23.00</td> </tr> </tbody> </table> <p>Add All Add Remove Remove All</p>	Reference	Name	Records	Location	Version	User	Maurer, Meyer, Pflieger, Weber: GC-MS Library...	10948	<Latest Versi...	23.21	Hit List	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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4	Select database MS – NIST EPA NIH Mass Spectral Library for searching.	<p>The selected database is added to the Selected for Searching 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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5	Click Structure under Search Categories .	<p>The Structure Search dialog is displayed:</p>  <p>SearchIt</p> <p>Search Profiles: <no profile></p> <p>Search Categories</p> <ul style="list-style-type: none"> <input type="checkbox"/> Spectrum <input type="checkbox"/> Peaks Structure <input type="checkbox"/> Property/Name <p>Search Databases</p> <ul style="list-style-type: none"> User-Select <input type="radio"/> All Compounds <input type="checkbox"/> Use Computed Spectra <input type="radio"/> Pure Compounds <input type="checkbox"/> Use Computed Spectra <p>Search Mode</p> <ul style="list-style-type: none"> <input checked="" type="radio"/> Exact Match <input type="radio"/> Substructure <input type="radio"/> Similarity (Tanimoto) <p>Search Options</p> <ul style="list-style-type: none"> <input type="checkbox"/> Enforce Stereochemical Match <input type="checkbox"/> Relative Stereochemistry (include Both Enantiomers) <input type="checkbox"/> No Structure Standardization (Salts, tautomers, etc.) <p>Structure Modifiers</p> <ul style="list-style-type: none"> <input type="checkbox"/> Any Element Except H <input type="checkbox"/> Any Element Except C or H <input type="checkbox"/> Any Halogen (F, Cl, Br, I, At) <p>Open file... Draw/Edit...</p> <p>HR List Size Limit: 50 All Hits Display Profiles: <no profile> Search</p>																									

	Action	Result
6	<p>Click Open file... button.</p> <p>Navigate to “C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\Structures” and select Acetylfentanyl.cdx.</p> <p>Note: You can also click Draw/Edit to create a structure using the ChemWindow application.</p>	<p>The structure is displayed in the Structure tab:</p>  <p>The screenshot shows a search interface with the following sections:</p> <ul style="list-style-type: none">Search Mode: Radio buttons for Exact Match (selected), Substructure, and Similarity (Tanimoto).Search Options: Checkboxes for Enforce Stereochemical Match, Relative Stereochemistry (Include Both Enantiomers), and No Structure Standardization (Salts, tautomers, etc.).Structure Modifiers: 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 a button for Any Bond Order.Buttons for Open file... and Draw/Edit....A central window displaying the chemical structure of Acetylfentanyl: <chem>CC(=O)N(c1ccccc1)C2CCN(CCc3ccccc3)CC2</chem>.

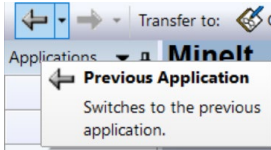
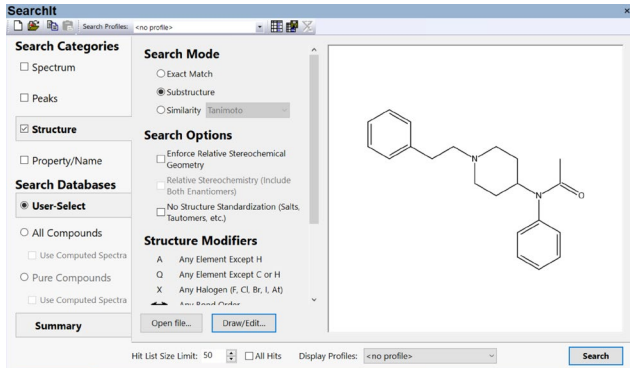
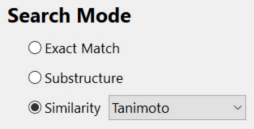
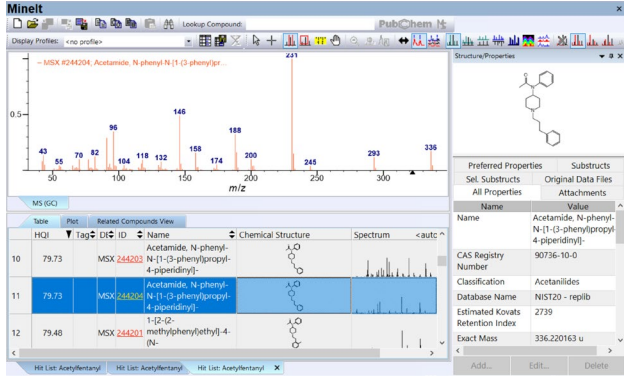
Perform an exact structure match search

	Action	Result																																																		
1	Select Exact Match under Search Mode , then click Search .	<p>Exact matches are displayed in the Minelt application:</p>  <p>The screenshot shows the Minelt application interface. At the top, there is a search bar and a 'Lookup Compound' field. Below this is a mass spectrum plot for MSX #227218, Acetanilide, N-(1-phenethyl-4-piperidyl). The x-axis is labeled 'm/z' and ranges from 50 to 300. The y-axis is labeled '0.5'. The base peak is at m/z 441. Other significant peaks are at m/z 146, 188, 158, 202, 132, 118, 105, 96, 77, 65, 56, and 42.</p> <p>Below the plot is a table of results:</p> <table border="1"> <thead> <tr> <th>Table</th> <th>Plot</th> <th>Related Compounds View</th> <th>HQI</th> <th>Tag</th> <th>DI</th> <th>ID</th> <th>Name</th> <th>Chemical Structure</th> <th>Spectrum</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>100.00</td> <td>MSX 227218</td> <td>Acetanilide, N-(1-phenethyl-4-piperidyl)-</td> <td></td> <td></td> </tr> <tr> <td>2</td> <td>100.00</td> <td>MSX 227219</td> <td>Acetanilide, N-(1-phenethyl-4-piperidyl)-</td> <td></td> <td></td> </tr> <tr> <td>3</td> <td>100.00</td> <td>MSX 227220</td> <td>Acetanilide, N-(1-phenethyl-4-piperidyl)-</td> <td></td> <td></td> </tr> </tbody> </table> <p>At the bottom of the table, there is a 'Hit List: Acetylentanyl' button.</p> <p>On the right side of the application, there is a 'Structure/Properties' panel. It shows the chemical structure of Acetanilide, N-(1-phenethyl-4-piperidyl) and a table of properties:</p> <table border="1"> <thead> <tr> <th>Preferred Properties</th> <th>Substructs</th> </tr> </thead> <tbody> <tr> <td>Sel. Substructs</td> <td>Original Data Files</td> </tr> <tr> <td>All Properties</td> <td>Attachments</td> </tr> <tr> <th>Name</th> <th>Value</th> </tr> <tr> <td>Name</td> <td>Acetanilide, N-(1-phenethyl-4-piperidyl)</td> </tr> <tr> <td>CAS Registry Number</td> <td>3258-84-2</td> </tr> <tr> <td>Classification</td> <td>Acetanilides</td> </tr> <tr> <td>Database Name</td> <td>NIST20 - mainlib</td> </tr> <tr> <td>Estimated Kovats Retention Index</td> <td>2639</td> </tr> <tr> <td>Exact Mass</td> <td>322.204514 u</td> </tr> <tr> <td>Formula</td> <td>C₁₇H₁₇N₂O</td> </tr> </tbody> </table> <p>At the bottom of the properties panel, there are buttons for 'Add...', 'Edit...', and 'Delete'.</p>	Table	Plot	Related Compounds View	HQI	Tag	DI	ID	Name	Chemical Structure	Spectrum	1	100.00	MSX 227218	Acetanilide, N-(1-phenethyl-4-piperidyl)-			2	100.00	MSX 227219	Acetanilide, N-(1-phenethyl-4-piperidyl)-			3	100.00	MSX 227220	Acetanilide, N-(1-phenethyl-4-piperidyl)-			Preferred Properties	Substructs	Sel. Substructs	Original Data Files	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 ₁₇ H ₁₇ N ₂ O
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Configure and perform a substructure search

	Action	Result
1	<p>Click the KnowItAll Back button to return to SearchIt.</p>  <p>If you are not on the Structure tab, click to resume a structure search.</p>	<p>The Structure search dialog is displayed:</p> 
2	<p>Select Substructure Search, then click Search. Click through the records to search results.</p> <p>NOTE: 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 Back button to return to SearchIt . 	The SearchIt Structure search dialog is displayed: 
2	Click the Similarity Search radio button. Use the default scoring method, Tanimoto .	Tanimoto is selected for the Search Mode : 
3	Click Search .	Structure which are similar to the searched structure are displayed in the Minelt application: 

Searching

All Compounds and Pure Compounds Database Selections

Purpose

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

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



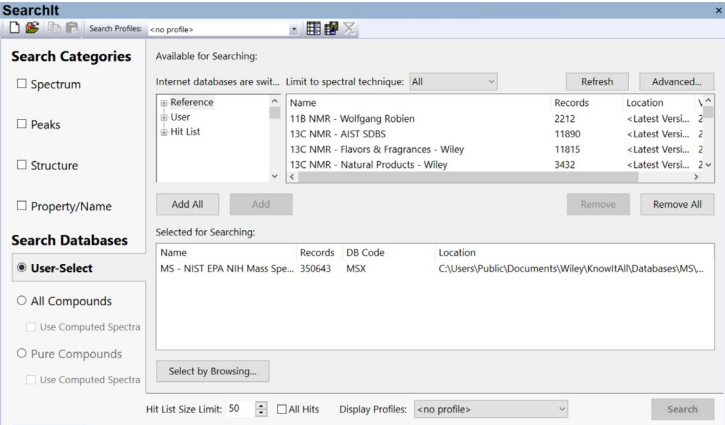
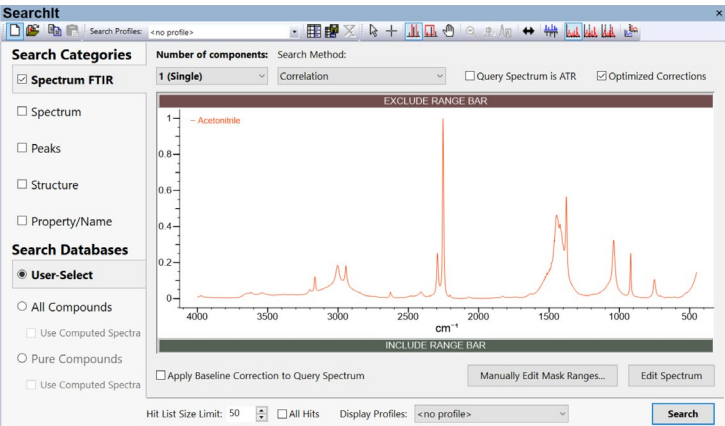
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\IR

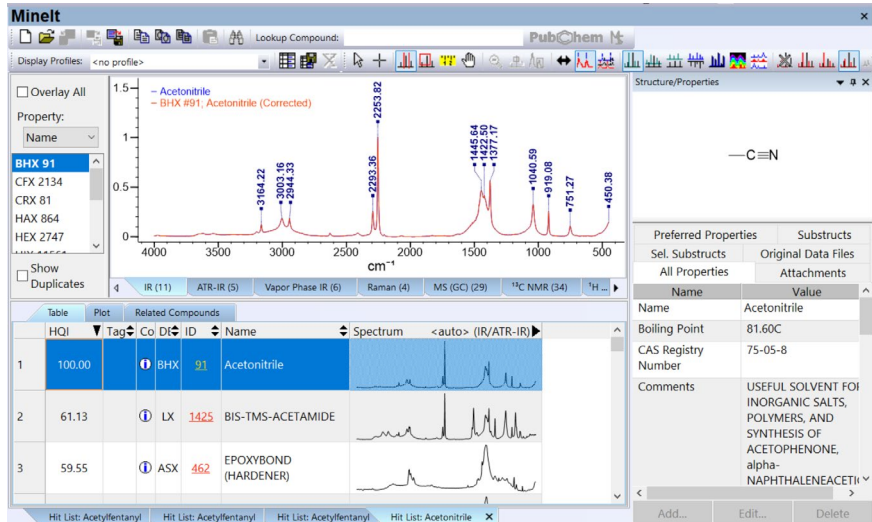
- Acetonitrile.jdx

KnowItAll Applications Used

- SearchIt™
- MineIt™

Configure and perform an All Compounds search

	Action	Result								
1	<p>Do one of the following:</p> <ul style="list-style-type: none"> If the SearchIt application is not open, navigate to the Data toolbox and click its icon.  <p>SearchIt</p> <ul style="list-style-type: none"> If the SearchIt application is already open, click the SearchIt Close button  to close the current search. 	<p>The SearchIt application's User-Select tab is displayed and the Selected for Searching list displays the databases last used:</p>  <p>The screenshot shows the SearchIt application window with the 'User-Select' tab active. Under 'Search Categories', 'Spectrum' is selected. Under 'Search Databases', 'User-Select' is selected. The 'Selected for Searching' table lists several databases:</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\...
Name	Records	DB Code	Location							
MS - NIST EPA NIH Mass Spe...	350643	MSX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\MS\...							
2	<p>Click Spectrum under Search Categories. Navigate to C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\IR and select acetonitrile.jdx.</p>	<p>The spectrum for acetonitrile is displayed:</p>  <p>The screenshot shows the SearchIt application window with the IR spectrum for acetonitrile displayed. The x-axis is labeled 'cm⁻¹' and ranges from 4000 to 500. The y-axis represents intensity from 0 to 1. The spectrum shows several characteristic peaks, with the most prominent one around 2100 cm⁻¹. The interface includes search options like 'Number of components: 1 (Single)' and 'Search Method: Correlation'.</p>								
3	<p>Select the All Compounds option under Search Databases.</p>	<p>The All Compounds search option is selected.</p>								

	Action	Result
4	Click Search .	<p>The search is performed, and results are displayed in the Minelt application:</p>  <p>Compared to the User-Select database search, you will see additional information related to the hit:</p> <ul style="list-style-type: none"> • 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. • Other spectrum information related to the hit compound is displayed in tabs under the spectrum pane.
5	TIPS:	<ul style="list-style-type: none"> • User-Select – User selects which databases to search. This is where you can include user databases in a search. • All Compounds – All licensed reference databases. Records are linked by structure, name, InChI, CAS Registry Number or synonym. • Pure Compounds – All Compounds with the exclusion of commercial compounds.

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



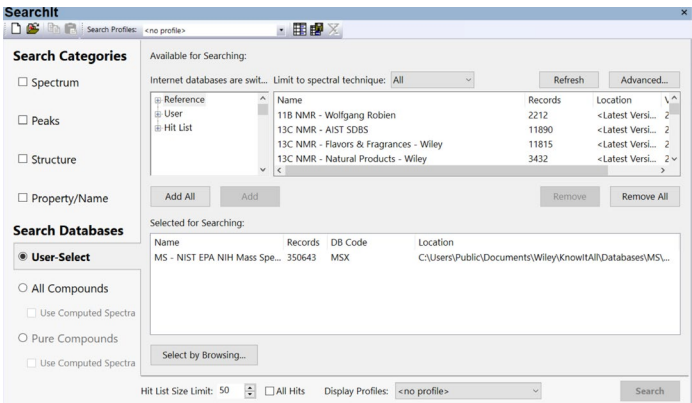
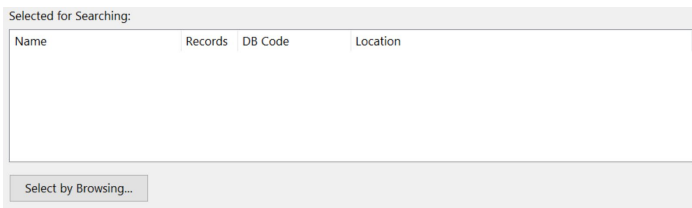
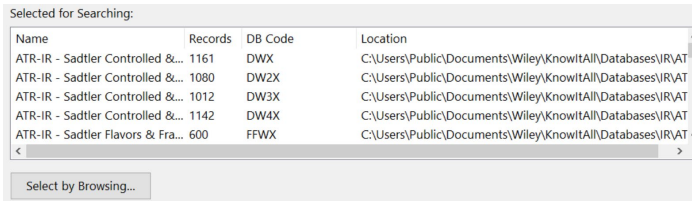
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Si
multaneous Multi-Technique Searching folder

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

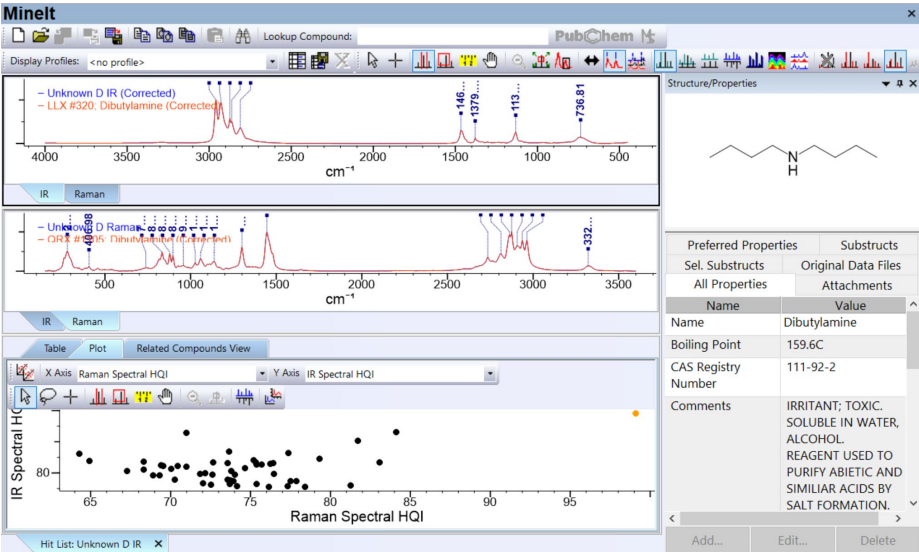
KnowItAll Applications Used

- SearchIt™
- MineIt™



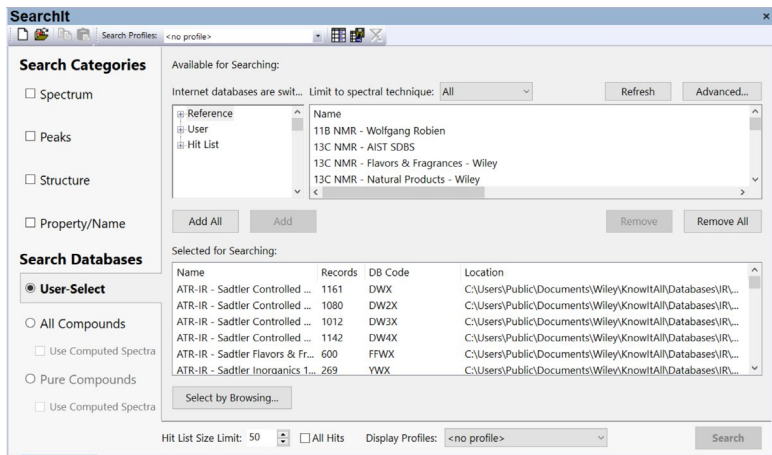
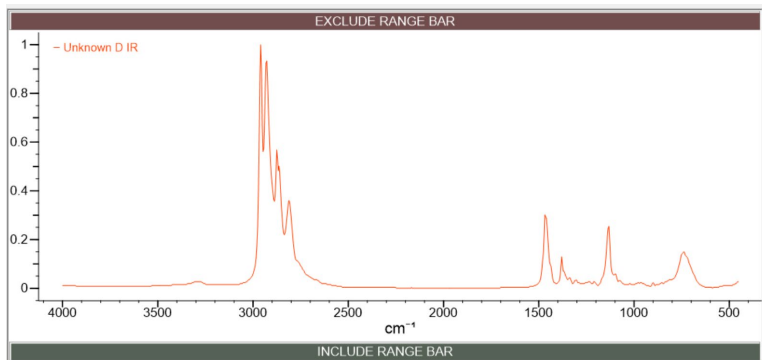
Configure and perform a multi-technique spectral search with the User-Select Search Databases option

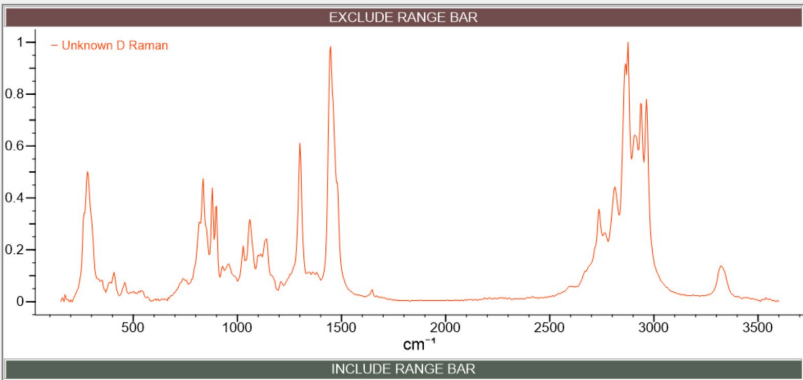
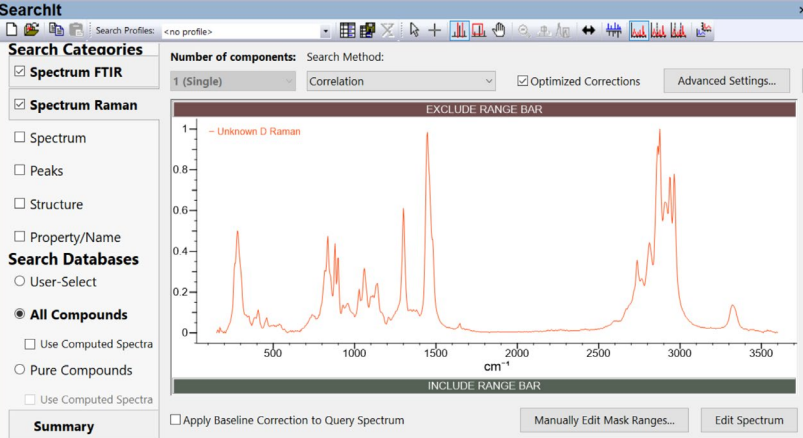
	Action	Result																								
1	<p>Do one of the following:</p> <ul style="list-style-type: none"> If the SearchIt application is not open, navigate to the Data toolbox and click its icon.  <ul style="list-style-type: none"> If the SearchIt application is already open, click the SearchIt Close button  to close the current search. 	<p>The SearchIt application's User-Select tab is displayed, and the Selected for Searching list displays the databases last used:</p>  <p>The screenshot shows the SearchIt application window with the 'User-Select' tab active. The 'Selected for Searching' section contains a table with the following data:</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...																
Name	Records	DB Code	Location																							
MS - NIST EPA NIH Mass Spe...	350643	MSX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\MS...																							
2	<p>Select User-Select under Search Databases option. If databases are already selected for searching, click Remove All to clear the selections</p>	<p>The Selected for Searching databases section is cleared:</p>  <p>The screenshot shows the 'Selected for Searching' section of the SearchIt application, which is currently empty. The table headers are visible, but no data is present.</p>																								
3	<p>Using the Limit to spectral technique tab, select IR then click Add All. Repeat for Raman.</p>	<p>All of the available IR and Raman databases are added to the Selected for Searching window:</p>  <p>The screenshot shows the 'Selected for Searching' section of the SearchIt application, now populated with several IR and Raman databases. The table contains the following data:</p> <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 &...</td> <td>1161</td> <td>DWX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\AT</td> </tr> <tr> <td>ATR-IR - Sadtler Controlled &...</td> <td>1080</td> <td>DW2X</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\AT</td> </tr> <tr> <td>ATR-IR - Sadtler Controlled &...</td> <td>1012</td> <td>DW3X</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\AT</td> </tr> <tr> <td>ATR-IR - Sadtler Controlled &...</td> <td>1142</td> <td>DW4X</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\AT</td> </tr> <tr> <td>ATR-IR - Sadtler Flavors & Fra...</td> <td>600</td> <td>FFWX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\AT</td> </tr> </tbody> </table>	Name	Records	DB Code	Location	ATR-IR - Sadtler Controlled &...	1161	DWX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\AT	ATR-IR - Sadtler Controlled &...	1080	DW2X	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\AT	ATR-IR - Sadtler Controlled &...	1012	DW3X	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\AT	ATR-IR - Sadtler Controlled &...	1142	DW4X	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\AT	ATR-IR - Sadtler Flavors & Fra...	600	FFWX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\AT
Name	Records	DB Code	Location																							
ATR-IR - Sadtler Controlled &...	1161	DWX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\AT																							
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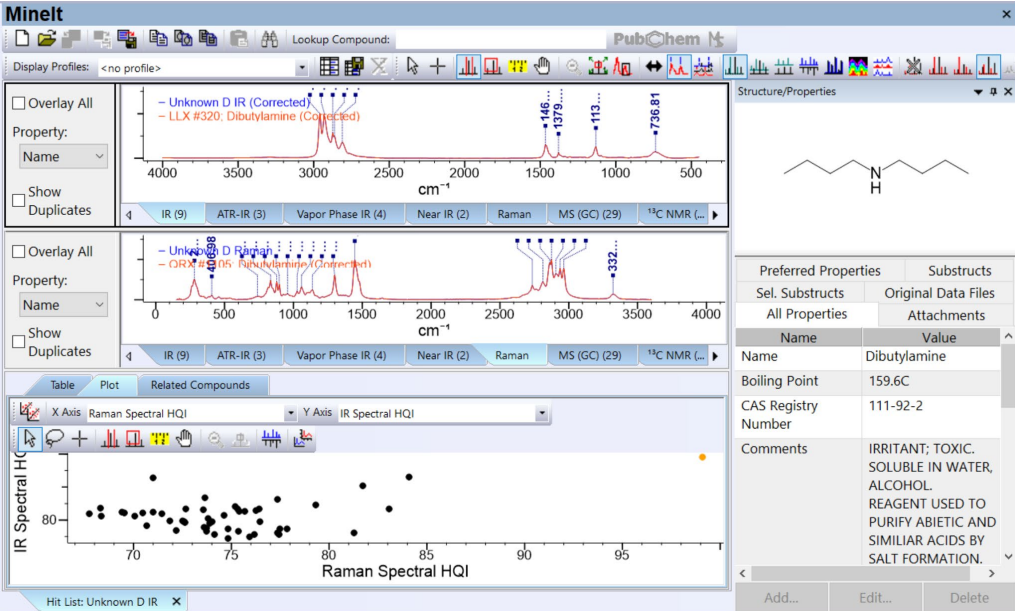
	Action	Result
4	<p>Click Spectrum under Search Categories.</p> <p>Navigate to “C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\Simultaneous Multi-Technique Searching”.</p> <p>Open Unknown D IR.jdx.</p>	<p>An IR spectrum is displayed in the SearchIt spectrum window:</p> 
5	<p>Click Spectrum under Search Categories to add another spectrum.</p> <p>From the folder “C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\Simultaneous Multi-Technique Searching”, choose Unknown D Raman.jdx.</p>	<p>The Raman spectrum is added to the search:</p> 

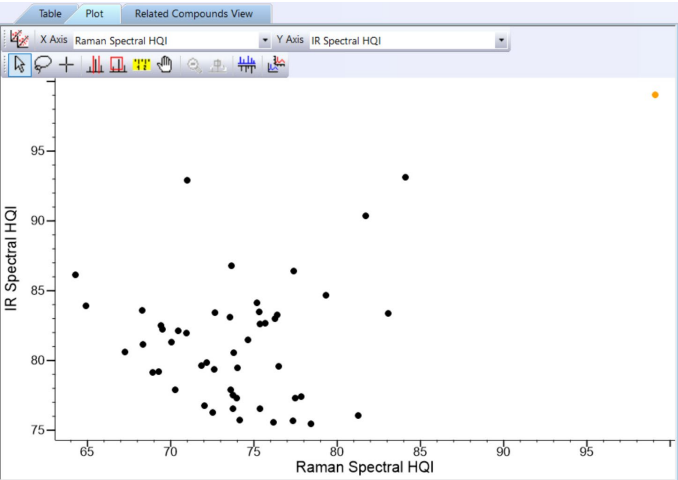
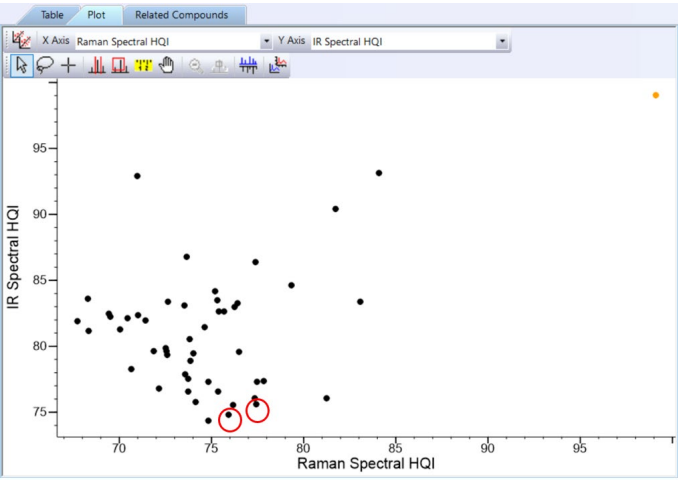
	Action	Result																								
6	Click Search .	<p>The search results are displayed in the Minelt application:</p>  <p>The screenshot displays the Minelt application interface. At the top, the title bar reads 'Minelt' and 'PubChem'. Below the title bar, there are two spectral plots. The top plot is an IR spectrum with the x-axis labeled 'cm⁻¹' ranging from 4000 to 500. It shows two traces: 'Unknown D IR (Corrected)' in blue and 'LLX #320: Dibutylamine (Corrected)' in red. The bottom plot is a Raman spectrum with the x-axis labeled 'cm⁻¹' ranging from 500 to 3500. It also shows two traces: 'Unknown D Raman (Corrected)' in blue and 'ORX #320: Dibutylamine (Corrected)' in red. To the right of the spectra is a chemical structure of dibutylamine, <chem>CCCCNCCCC</chem>. Below the spectra is a scatter plot titled 'IR Spectral HQI' vs 'Raman Spectral HQI'. The x-axis ranges from 65 to 95, and the y-axis ranges from 80 to 100. A single point is highlighted in orange at the top right of the plot. To the right of the plots is a 'Structure/Properties' panel with a table of properties for dibutylamine.</p> <table border="1" data-bbox="1360 630 1612 943"> <thead> <tr> <th colspan="2">Preferred Properties</th> <th>Substructs</th> </tr> </thead> <tbody> <tr> <td>Sel. Substructs</td> <td></td> <td>Original Data Files</td> </tr> <tr> <td>All Properties</td> <td></td> <td>Attachments</td> </tr> <tr> <th>Name</th> <th>Value</th> <td></td> </tr> <tr> <td>Name</td> <td>Dibutylamine</td> <td></td> </tr> <tr> <td>Boiling Point</td> <td>159.6C</td> <td></td> </tr> <tr> <td>CAS Registry Number</td> <td>111-92-2</td> <td></td> </tr> <tr> <td>Comments</td> <td colspan="2">IRRITANT; TOXIC. SOLUBLE IN WATER, ALCOHOL. REAGENT USED TO PURIFY ABIETIC AND SIMILAR ACIDS BY SALT FORMATION.</td> </tr> </tbody> </table> <p>Because this was a multi-technique search, the Database pane's Plot 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 Table tab to view tabular results.</p>	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 SIMILAR ACIDS BY SALT FORMATION.	
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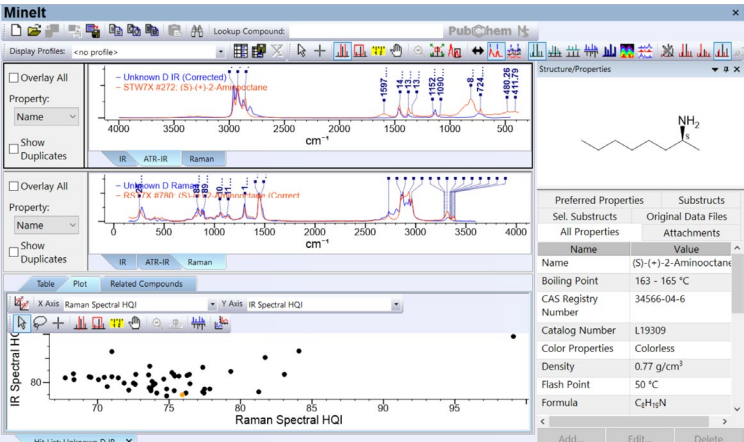
Configure and perform a multi-technique spectral search with the All Compounds Search Databases option

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

	Action	Result
3	<p>Click Spectrum under Search Categories to add another spectrum.</p> <p>From the folder “C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\Simultaneous Multi-Technique Searching”, choose Unknown D Raman.jdx.</p>	<p>The Raman spectrum is added to the search:</p> 
4	<p>Check All Compounds under Search Databases option.</p>	<p>All Compounds search is selected under Search Databases:</p> 

	Action	Result
5	Click Search .	<p>The search results are displayed in the Minelt application:</p>  <p>The screenshot displays the Minelt application interface. At the top, the 'Lookup Compound' field contains 'PubChem'. Below this, there are two IR spectra plots. The top plot shows 'Unknown D IR (Corrected)' and '- LLX #320: Dibutylamine (Corrected)' with peaks at 146, 1379, 1113, and 736.81 cm⁻¹. The bottom plot shows 'Unknown D IR (Corrected)' and '- ORX #05: Dibutylamine (Corrected)' with peaks at 146, 1379, 1113, and 332 cm⁻¹. Below the spectra is a scatter plot titled 'IR Spectral HQI' vs 'Raman Spectral HQI'. The X-axis ranges from 70 to 95, and the Y-axis ranges from 80 to 95. A single point is highlighted in orange at approximately (95, 95). To the right of the plots is a 'Structure/Properties' panel showing the chemical structure of Dibutylamine (SMILES: <chem>CCCCNCCCC</chem>) and its properties: Name: Dibutylamine, Boiling Point: 159.6C, CAS Registry Number: 111-92-2, and Comments: IRRITANT; TOXIC. SOLUBLE IN WATER, ALCOHOL. REAGENT USED TO PURIFY ABIETIC AND SIMILIAR ACIDS BY SALT FORMATION.</p> <p>Because this was a multi-technique search, the Database pane's Plot 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>

	Action	Result
6	<p>Examine the example shown in the Results. Compare the scatter plot of the User-Select database search and that of All Compounds search.</p>	<p>User-Selected database search:</p>  <p>All Compounds database search:</p>  <p>They are more ppints 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>(S) Isomer:</p>  <p>(R) Isomer:</p> 