KnowItAll Software Training

Searching

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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

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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.

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Optimized Corrections: A Breakthrough Technology for Spectral Searching

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

According to ASTM's guide on spectral searching[1], 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).

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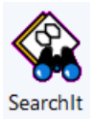
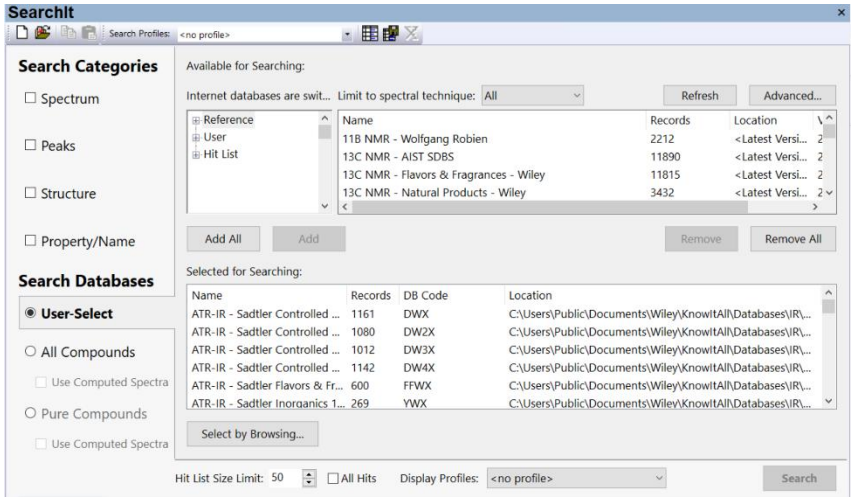
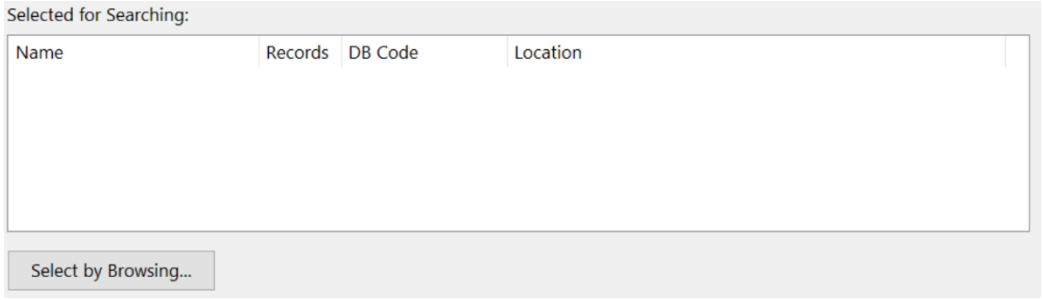
Create a new search and select reference databases

	Action	Result
1	Do one of the following: • If the **SearchIt** application is not open, navigate to the **Data** toolbox and click its icon.  If the **SearchIt** application is already open, click the **Close** button (located in the upper right corner) to close the current search.	The **SearchIt** application is displayed, with the last used databases in the **Selected for Searching** window: 
2	Click on **User-Select** under **Search Databases**.	This option allows users to select the databases they want to search. Users can also include user-created databases in a search.
3	If a list of databases already appears in the **Selected for Searching** pane at the bottom, click **Remove All** to clear this list.	The **User** category is shown below: 

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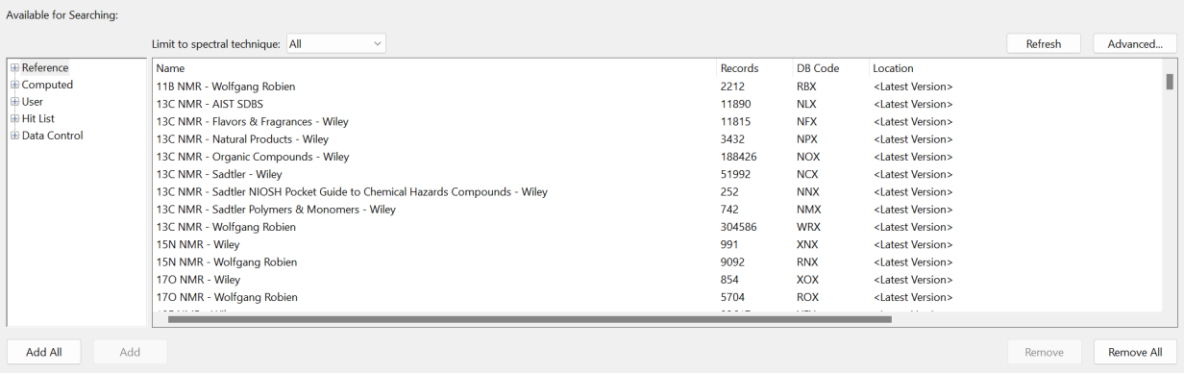
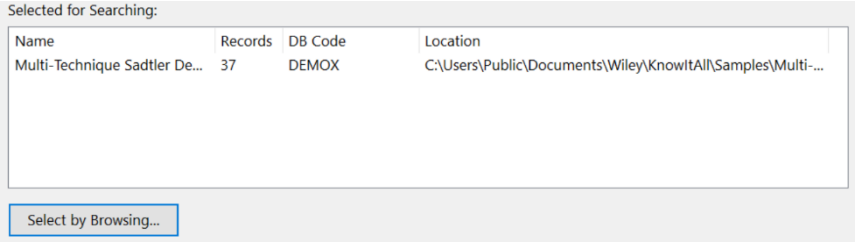
4	To the left of the **Available for Searching** window, expand each branch in the tree structure to display a particular database category—**Reference**, **User**, **Hit List**— and specify whether network, local, or all databases are displayed. The available databases are displayed at the right of the window.	The **Reference** category is shown below. The database **Name**, number of **Records**, **Location** and version are displayed for each database.  **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.
5	Click **Select by Browsing** button located at the lower left.	The **Browse for a Database or Hit List** dialog box opens.
6	Navigate to “C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples”. Open **Multi-Technique Sadtler Demo Database - Wiley (DEMO).sdbx**.	The database is displayed in the **Selected for Searching** list. 

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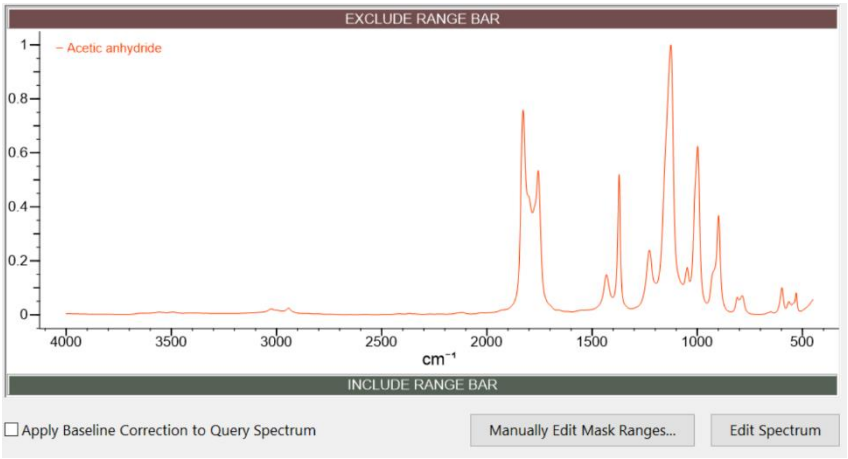
7	If necessary, uncheck the **All Hits** check box and set **Hit List Size Limit** to 50. **NOTE**: When performing a spectral or peak search using more than two or three databases, it is better to limit the number of hits. Checking **All Hits** or using a larger value can drastically reduce the search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

Open the spectral file

	Action	Result
1	Click the **Spectrum** button under **Search Categories**. Navigate to "**C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\IR**". Select **Acetic anhydride.jdx**. Click **Open**. **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 (*.*).	An **Open** dialog box appears. The spectrum is recognized as an IR spectrum and displayed in the spectral pane in the **Spectrum** tab:  **NOTE:** You can use the checkbox at the bottom to "Apply Baseline Correction to Query Spectrum", if desired. However, KnowItAll automatically corrects the baseline.

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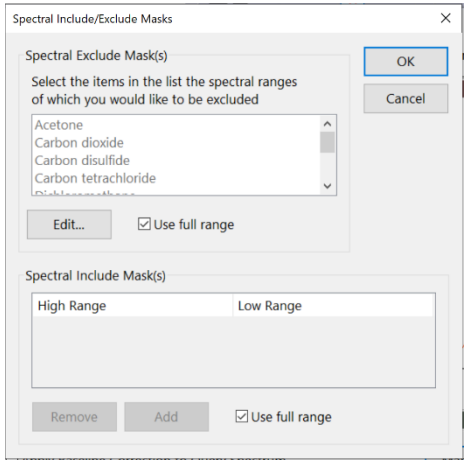
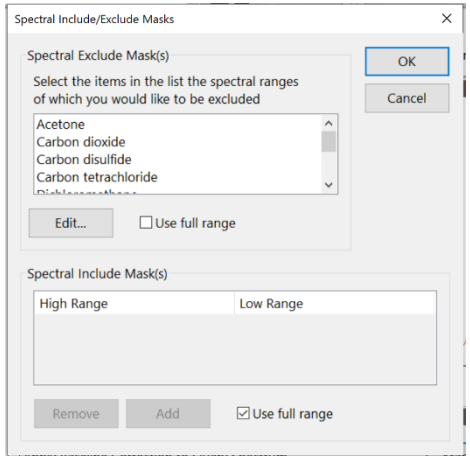
Fine-tune before searching

	Action	Result
1	Click **Manually Edit Mask Ranges**. **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.	The **Spectral Include/Exclude Masks** dialog box opens: 
2	Deselect the **Use full range** checkbox under the list of **Spectral Exclude Mask(s)**. Select some to see how they work. **Note:** The use of these masks will be demonstrated later in this lesson:	The list of pre-defined **Exclude Masks** becomes available: 

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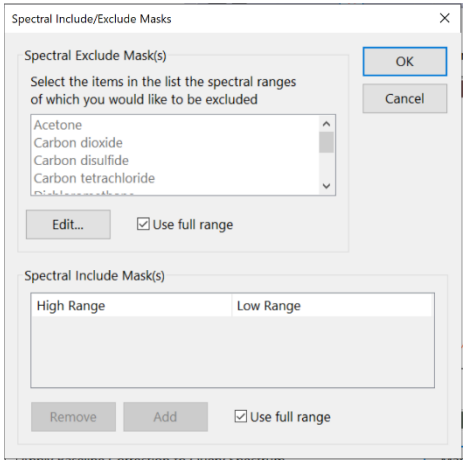
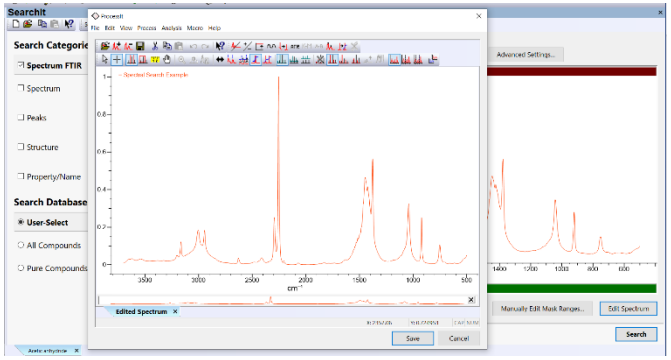
	Action	Result
3	Reselect the **Use full range** checkbox under the list of **Spectral Exclude Mask(s)**.	Any selected **Spectral Exclude Masks** are removed from the spectrum: 
4	Click **OK** to close the **Spectral Include/Exclude Masks** dialog box.	The **Spectral Include/Exclude Masks** dialog box 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** application are not saved.

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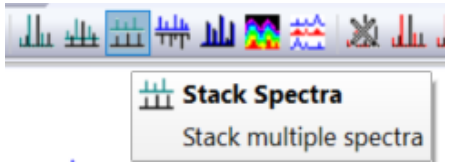
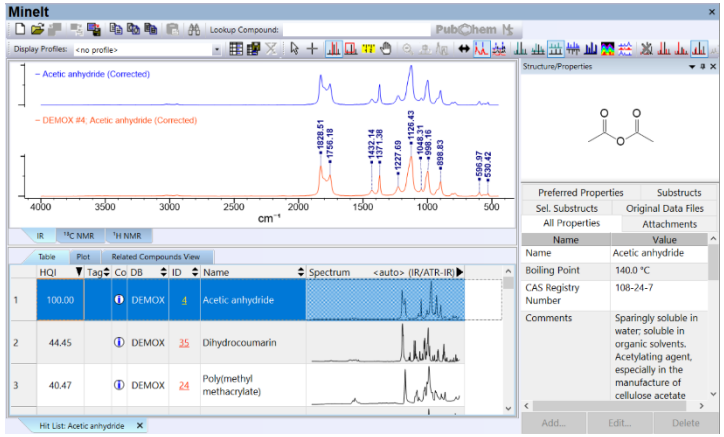
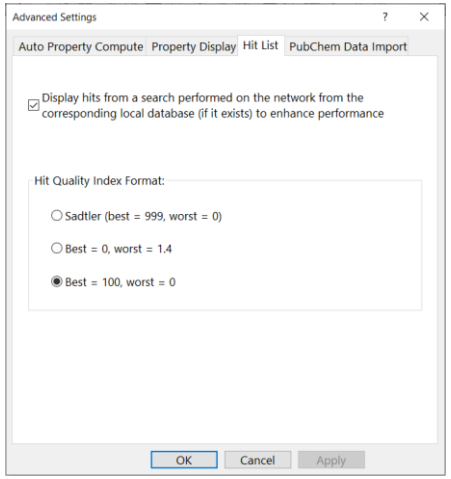
	Action	Result
7	Click **Search** and **MineIt** will open In **MineIt** click to choose **Stack Spectra**  view:	The search results are automatically displayed in the **MineIt** application as a hit list, sorted by HQI. Both the unknown spectrum and the selected database spectrum are displayed.  The **HQI** value measures how close the reference spectrum is to that of the query. The default scale of **HQI** is 0-100.
8	**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.	The **Advanced Settings** dialog is launched: 

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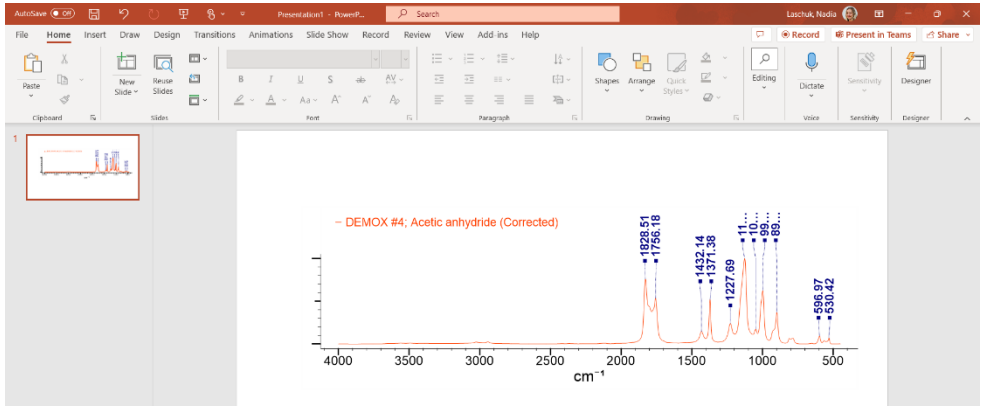
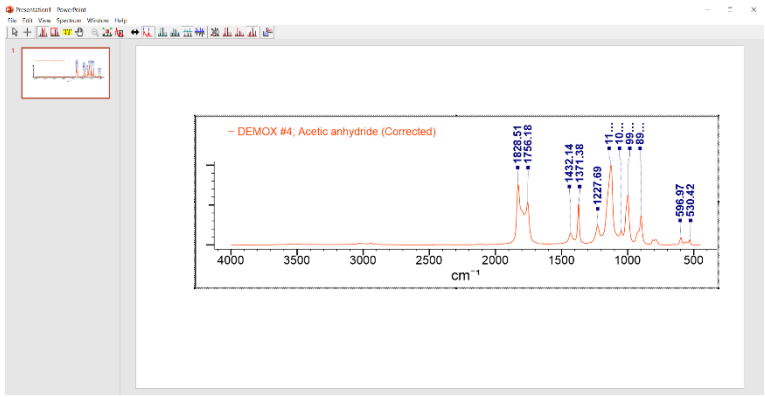
	Action	Result
9	**TIPS**	• You can tag individual hits in the hit list as either "Accept," "Tentative" or "Reject" using the **Hit List > Tag As** menu option or by double-clicking in the **Tag** column. You can then sort the hit list based on your tags. • You can edit which columns in the hit list are 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**.	**KnowItAll** objects such as the spectral pane can be copied and embedded into MS tools. 
11	Double-click the object in PowerPoint.	**KnowItAll spectrum manipulation toolbar** is shown in PowerPoint. For example, you can turn on peak labeling. 

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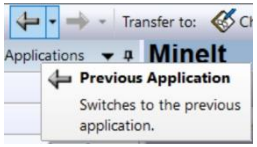
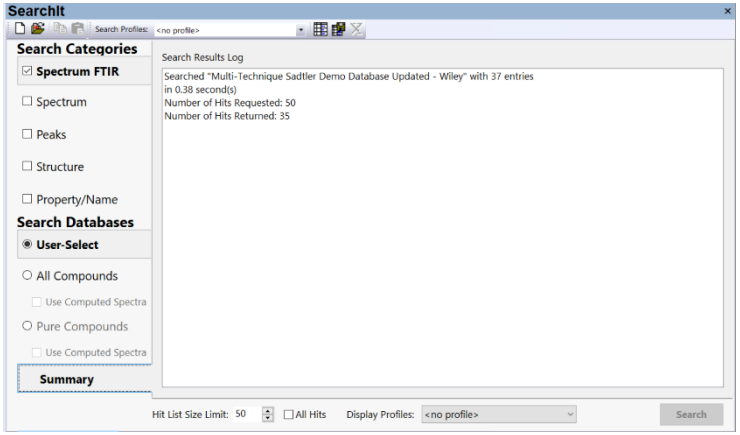
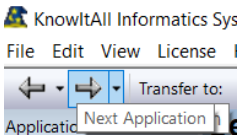
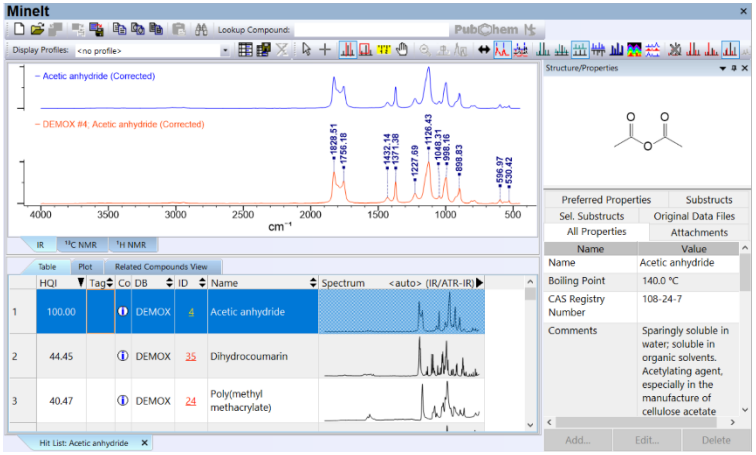
	Action	Result
12	In **KnowItAll**, click the **Back** button (located below the **File** menu). 	You are returned to the **SearchIt** application, where a **Summary** tab has been added to the main **SearchIt** window: 
13	Click the KnowItAll **Next Application** button. 	You are returned to **MineIt** and the hit list. 

Note: one can view the metadata of query spectrum by

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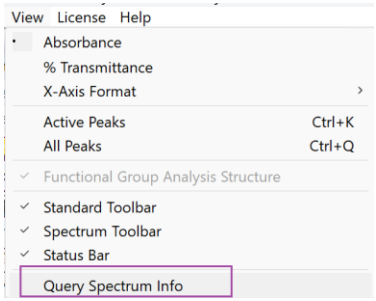
- In **SearchIt**, click **View > Query Spectrum** Info



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

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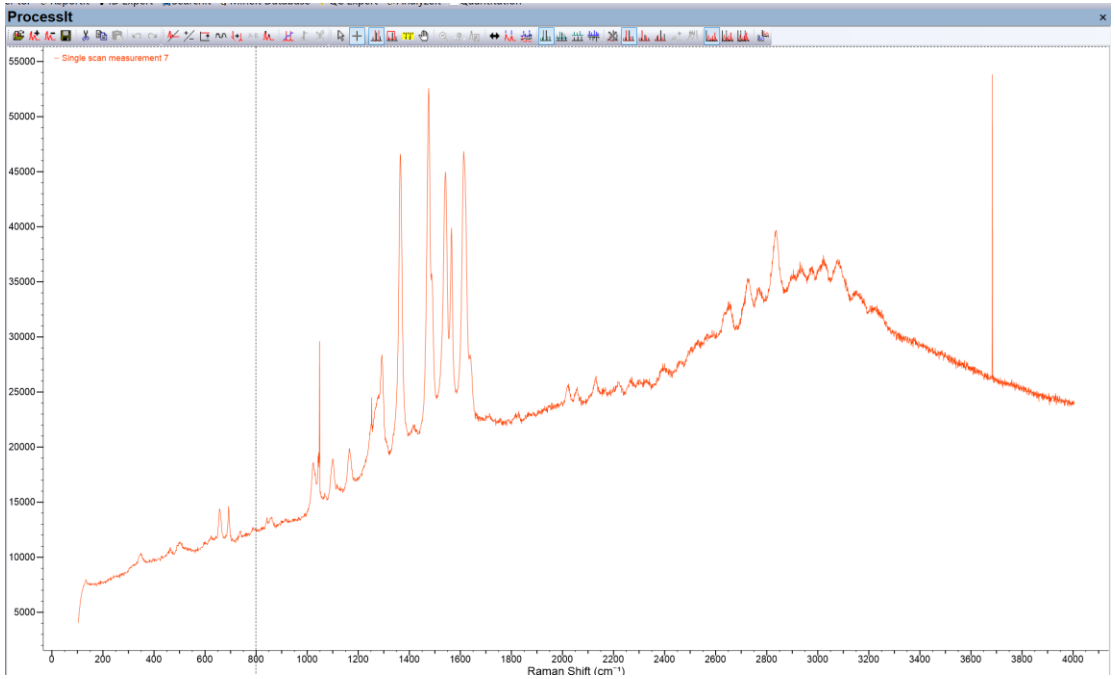
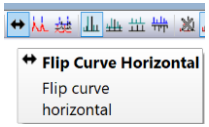
Raman-specific fine-tuning before searching

Example 1 – Cosmic Ray Correction

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

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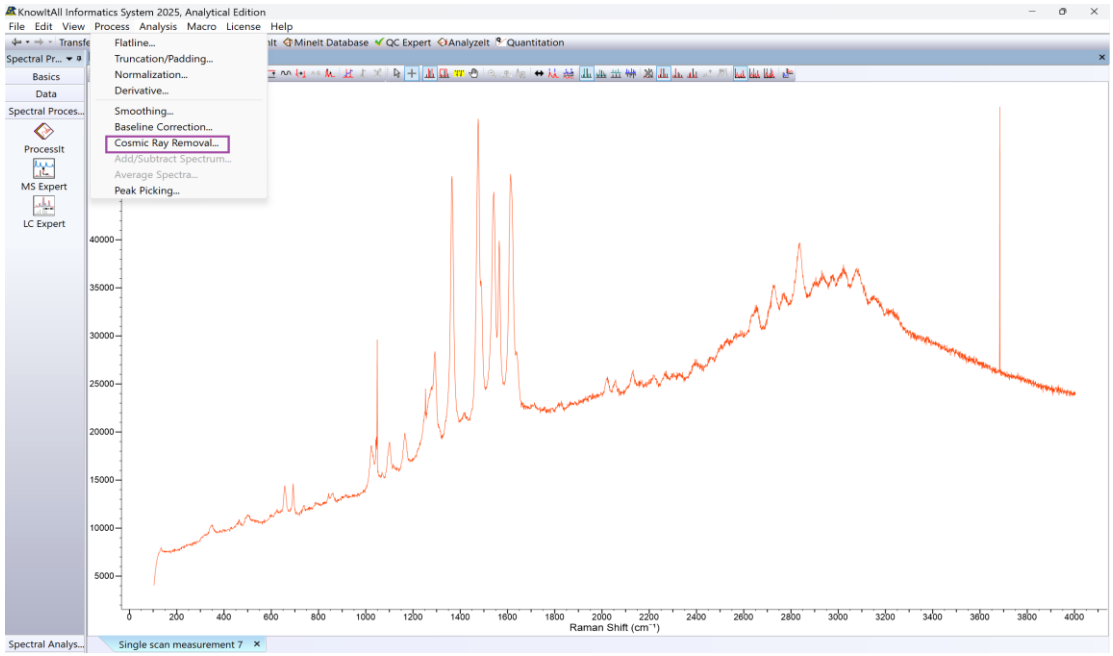
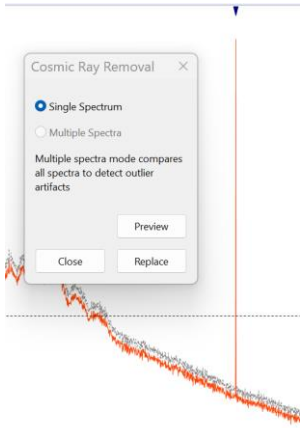
	Action	Result
2	Select **Cosmic Ray Removal** from the **Process** menu	
3	Select for **Single Spectrum** Note: One can apply Cosmic Ray correction to multiple Raman spectra opened in **ProcessIt**.	 The cosmic ray is marked by a down arrow:

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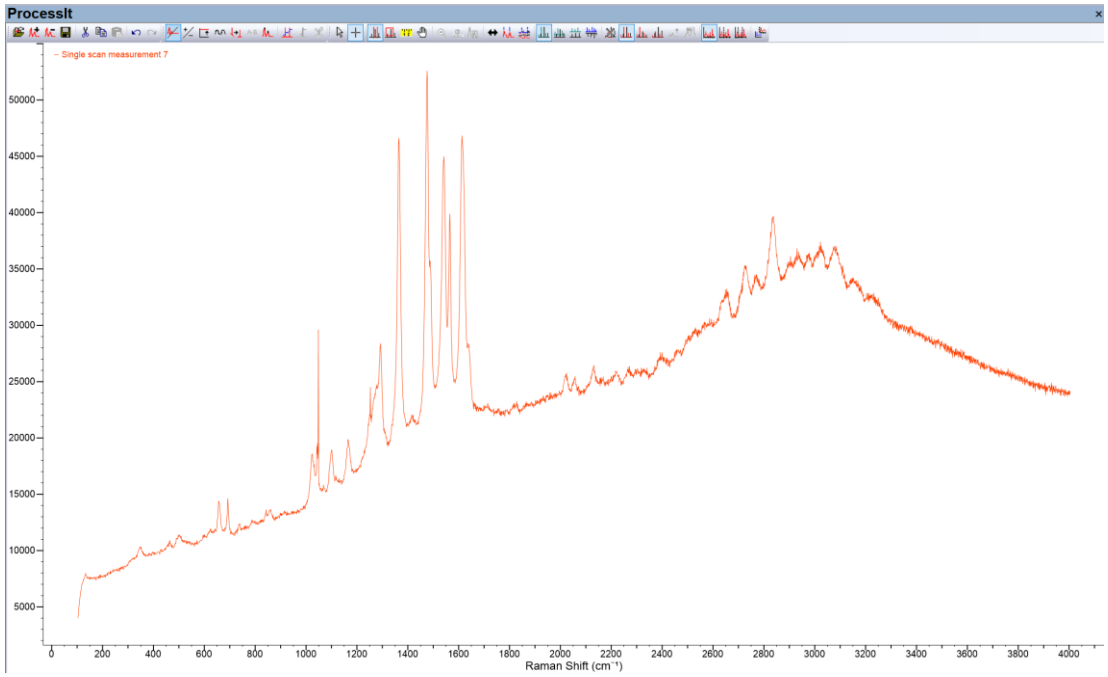
	Action	Result
4	Hit the **Replace** button.	

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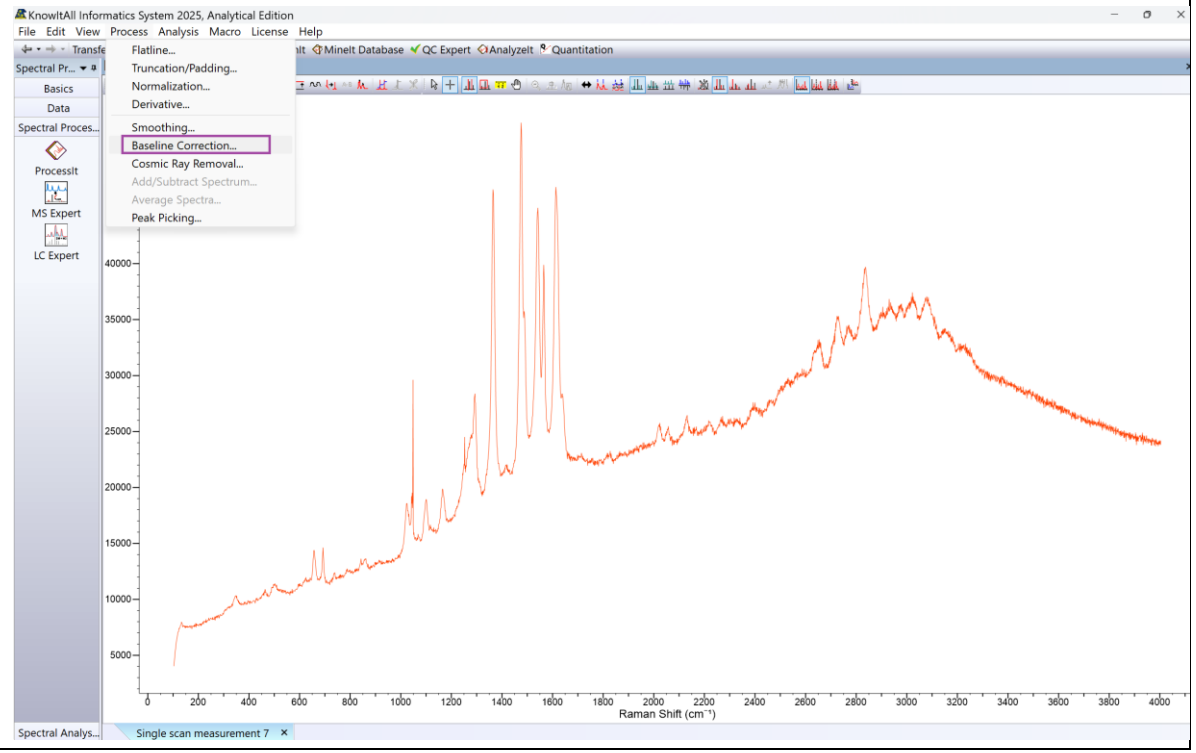
Example 2 – Fluorescence Correction

	Action	Result
1	One can just continue with the cosmic ray correction result in the previous sample, or open a sample with strong fluorescence by using Click **Open Spectroscopy Data File** In this case, we will continue from previous example. **Process > Baseline Correction** and **Replace** button	

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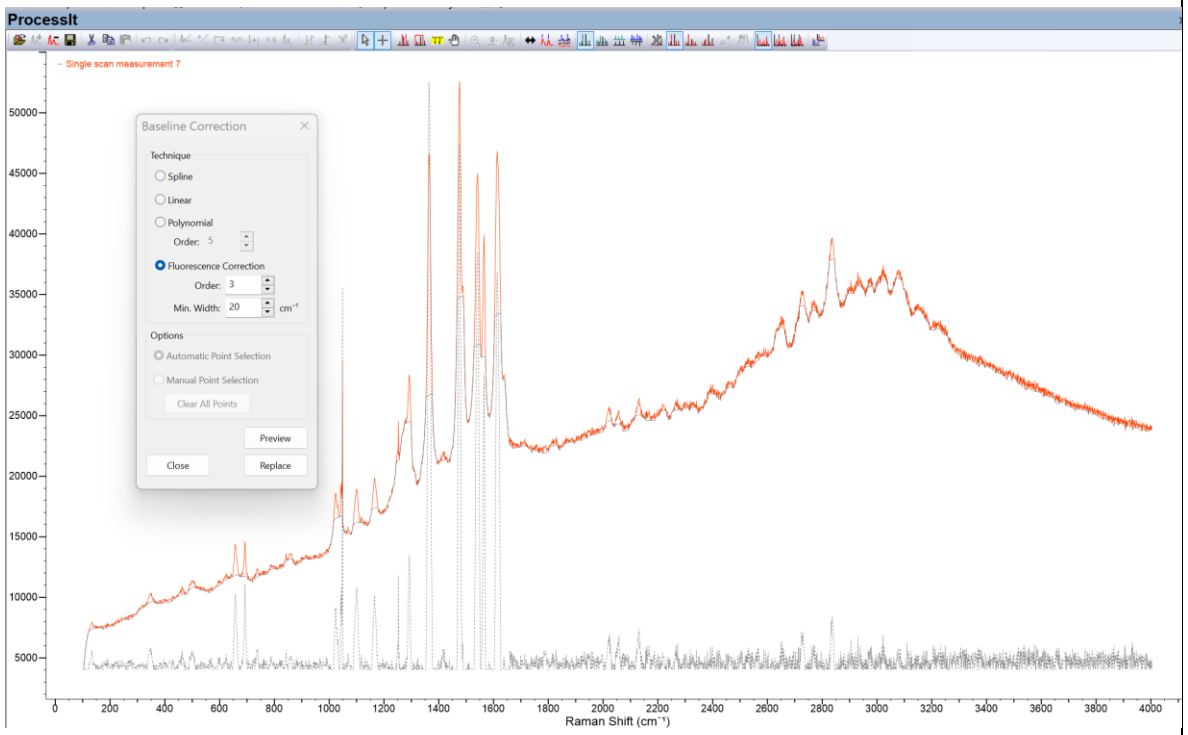
	Action	Result
2	Select **Cosmic Ray Removal** using the **Process** menu item You may preview the various **Baseline Correction** techniques. You will find that **Fluorescence Correction** does the best job. Hit the **Replace** button.	 Processed spectrum will be ready for downstream searching.

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Searching

How to Create Search Profiles and Use the MineIt profile to display results

Purpose

This exercise demonstrates how to use search profiles and use the MineIt 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.

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

Training Files Used in This Lesson

KnowItAll Applications Used

- SearchIt

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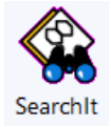
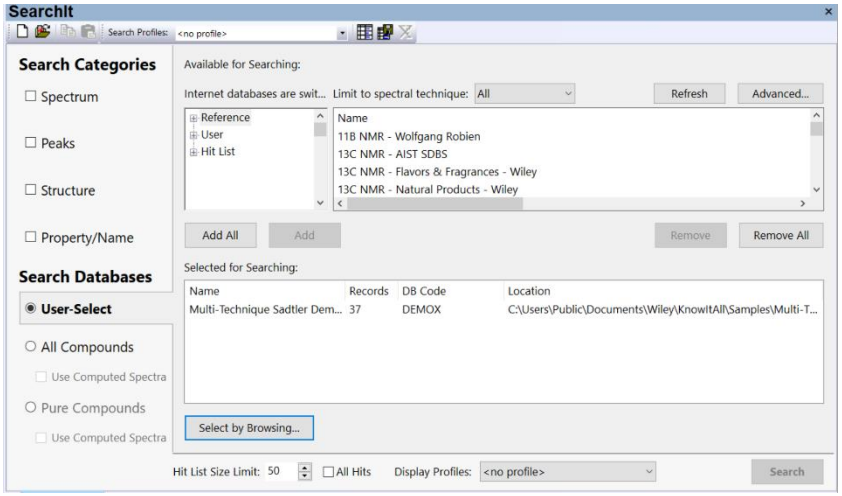
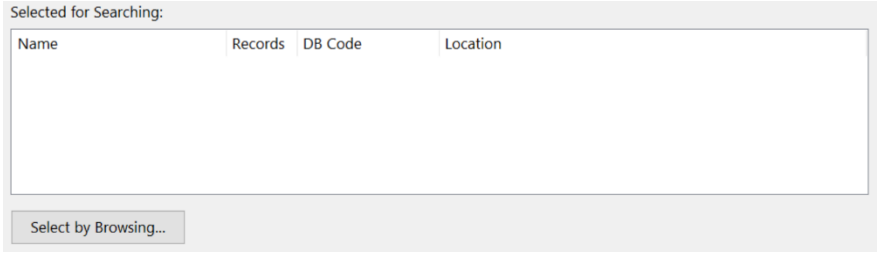
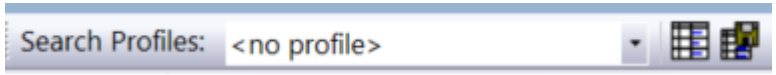
Apply a pre-defined search profile

	Action	Result
1	Do one of the following: • If the **SearchIt** application is not open, navigate to the **Data** toolbox and click its icon.  • If the **SearchIt** application is already open, click the SearchIt Close button to close the current search.	The **SearchIt** application's **User-Select** tab is displayed, and the **Selected for Searching** list displays the databases last used: 
2	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.	The **Selected for Searching** databases section is cleared: 
3	If necessary, choose **View > Profile Toolbar** to display Search Profiles tools.	

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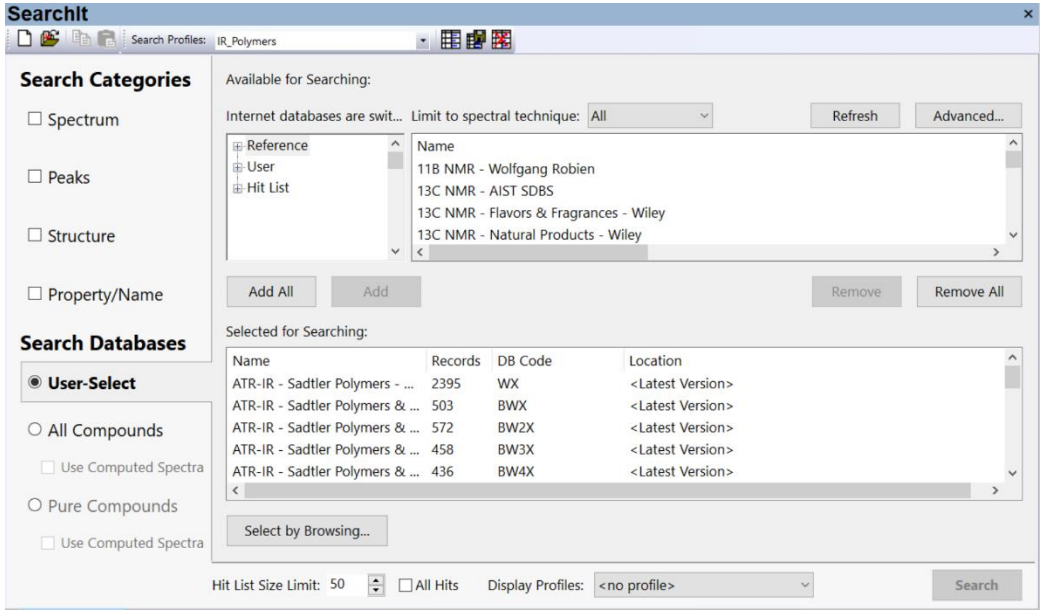
	Action	Result
4	Select the **IR_Polymers** profile using the **Search Profiles** dropdown menu.	Polymer databases are displayed in the **Selected for Searching** list: 

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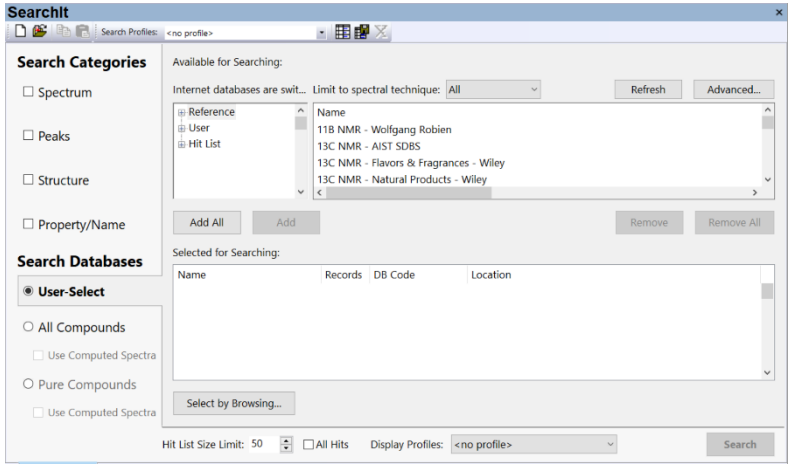
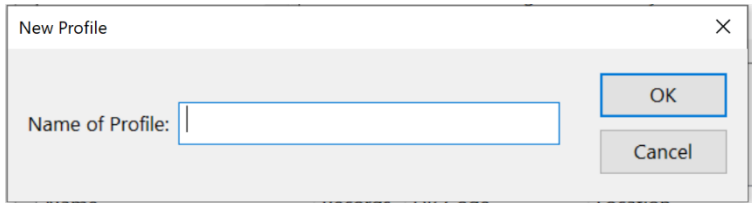
Create a new search profile

	Action	Result
1	Click the SearchIt **Close** button, then click **Remove All** to clear the contents of the **Selected for Searching** list.	The **User-Select** tab is displayed. The **Selected for Searching** list is empty: 
2	Click the **Add a New Profile** button on the **Profile** toolbar.	The **New Profile** dialog box opens. 
3	Type in the name of the new profile [**IR_Polymers_2**]. Click **OK**.	The new profile name is displayed in the **Search Profiles** text box: 
4	Specify **IR** in the **Limit to spectral technique** drop-down list.	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.

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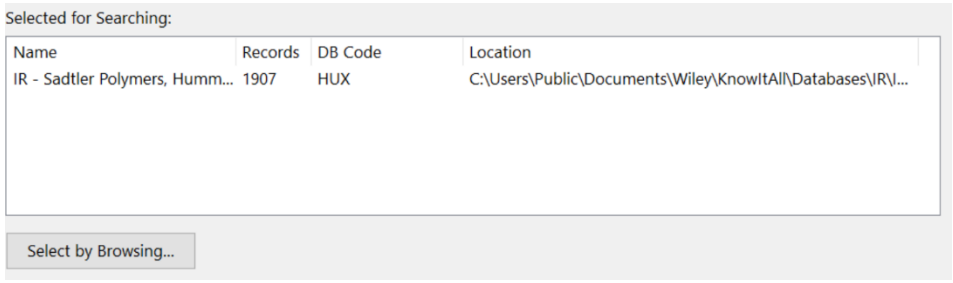
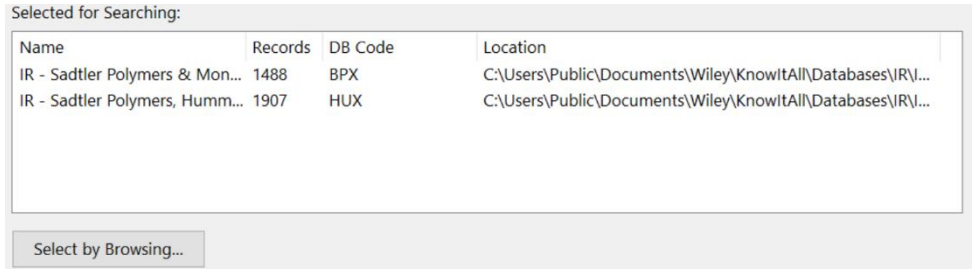
	Action	Result
5	In the **Available for Searching** list, click to select **IR – Sadtler Polymers, Hummel – Wiley** (DB Code HUX). Click **Add**.	The HUX database is added to the **Selected for Searching** list: 
6	In the **Available for Searching** list, double-click **IR — Sadtler Polymers & Monomers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

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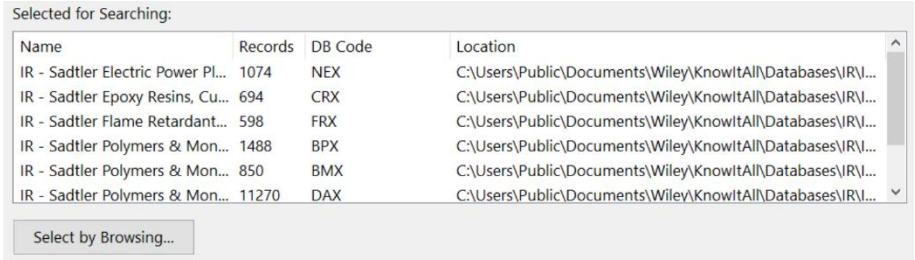
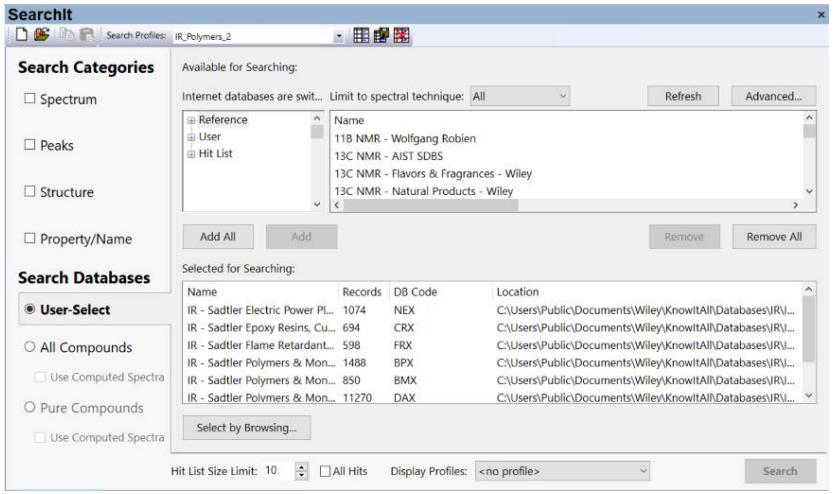
	Action	Result
7	Continue adding databases BMX, CRX, DAX, FRX and NEX.	The selected databases are added to the **Selected for Searching** window: 
8	On the **User-Select** tab, change the Hit List Size Limit to 10.	
9	Click the **Save Current Profile** button  on the Profile toolbar. A message box asks 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.	The databases and search settings associated with this profile are displayed: 

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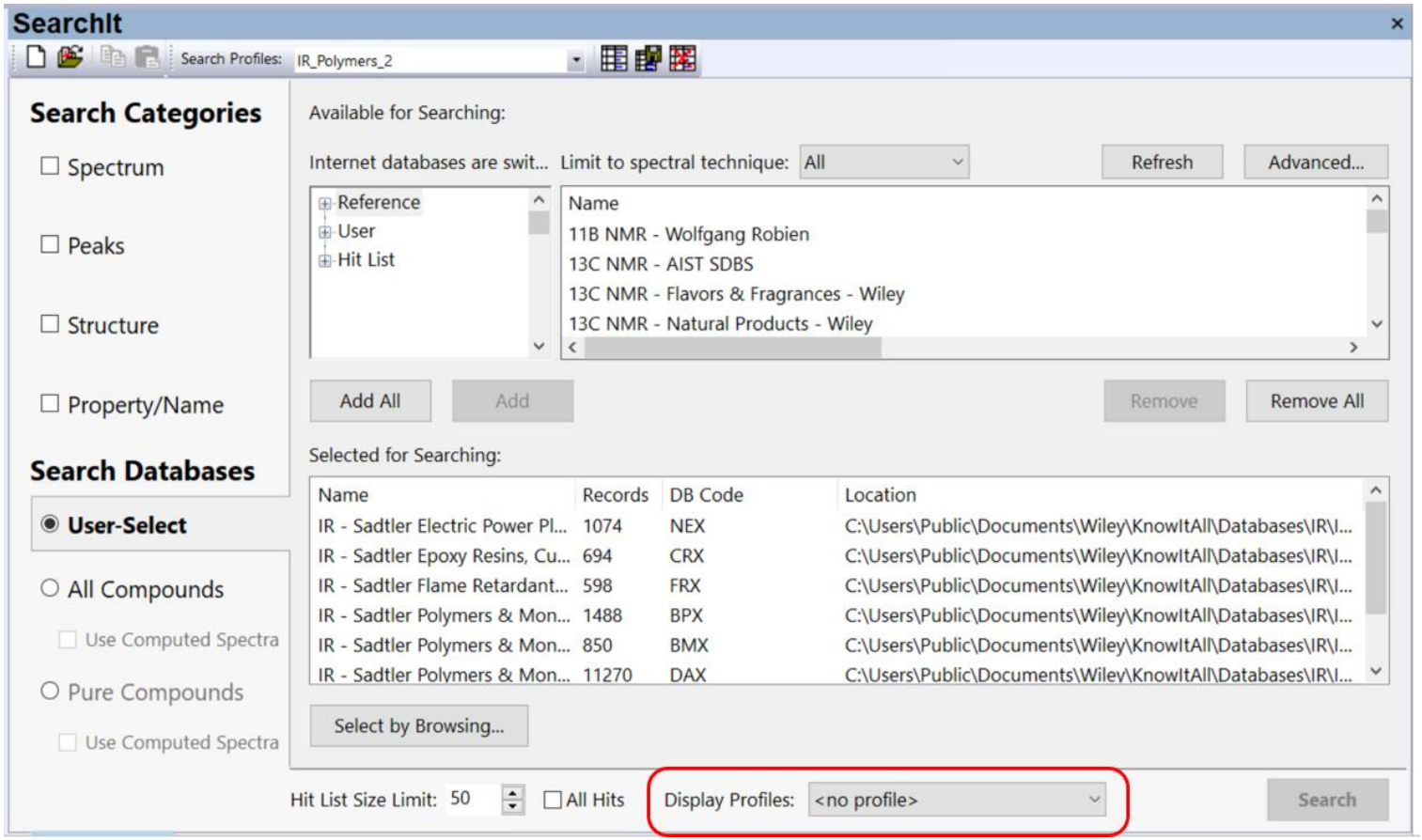
Use MineIt profile for hit list display

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



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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

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

- Ethyl acrylate.dx

KnowItAll Applications Used

- SearchIt
- MineIt

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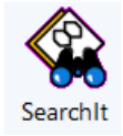
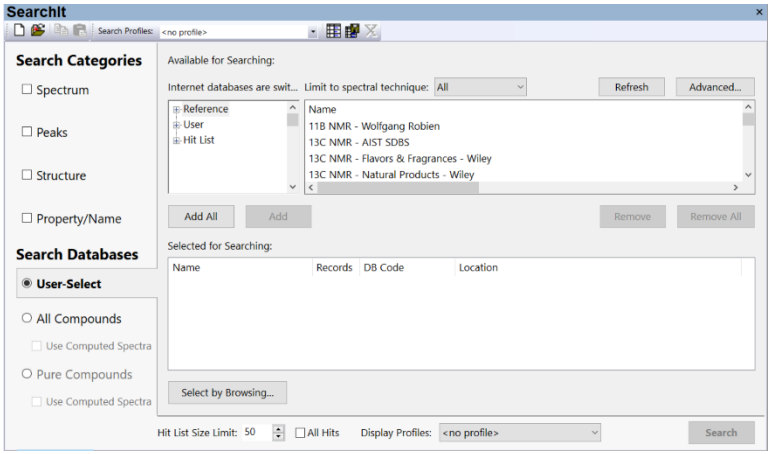
Configure and perform a peak search

	Action	Result
1	Do one of the following: • If the **SearchIt** application is not open, navigate to the **Data** toolbox and click its icon.  If the application is already open, click the **Close** button to close the current search.	The **SearchIt** application's **User-Select** tab is displayed, and the **Selected for Searching** list displays the databases last used: 

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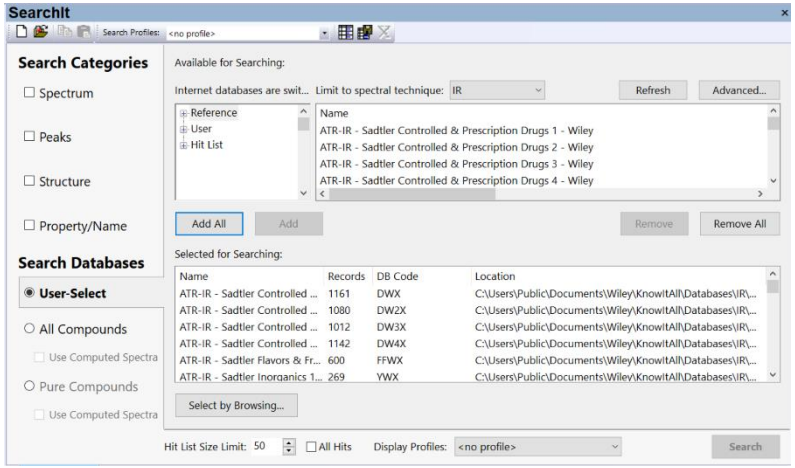
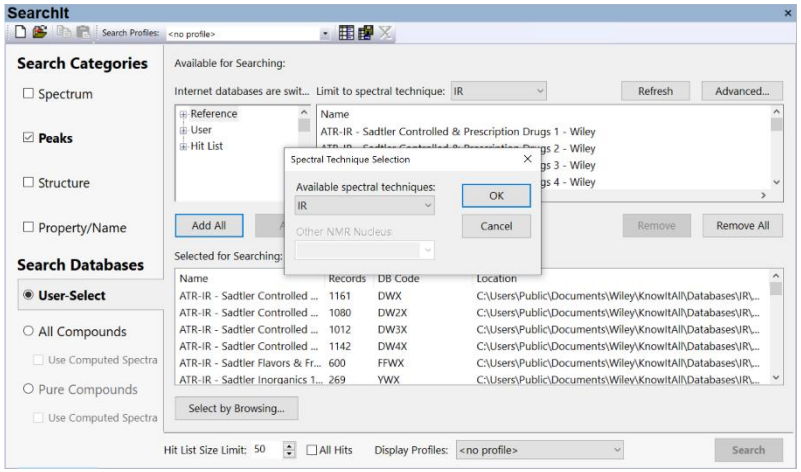
	Action	Result
2	If databases are already selected for searching, click **Remove All** to clear the selections. Set **Limit to spectral technique** to **IR**. Click **Add All**.	The Wiley IR database library has been added to the **Selected for Searching** window: 
3	Under **Search Categories** click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

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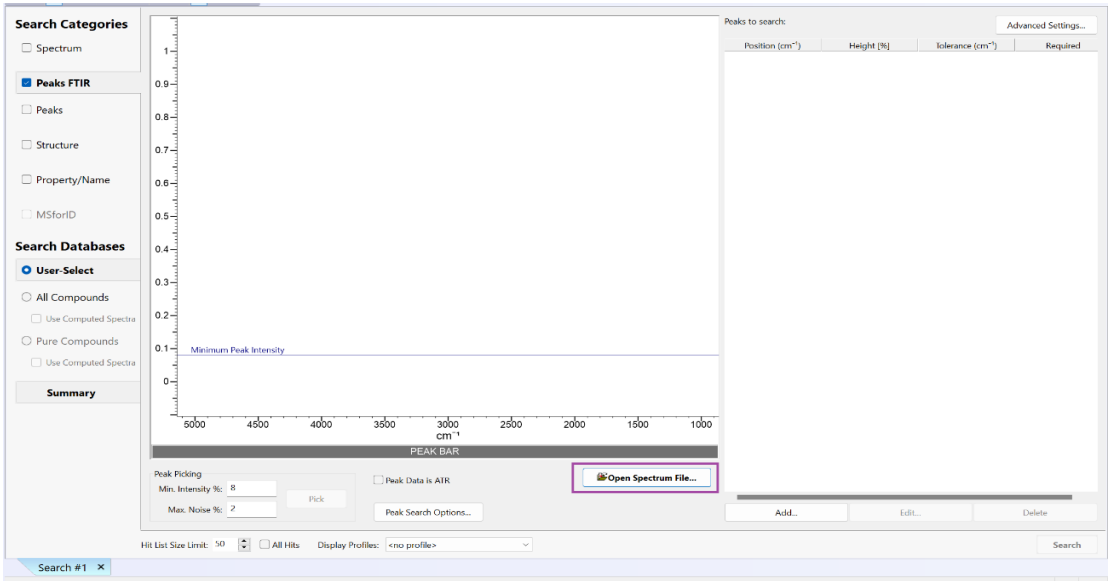
	Action	Result
4	Click **OK**.	The **Peaks FTIR** search dialog is displayed: 

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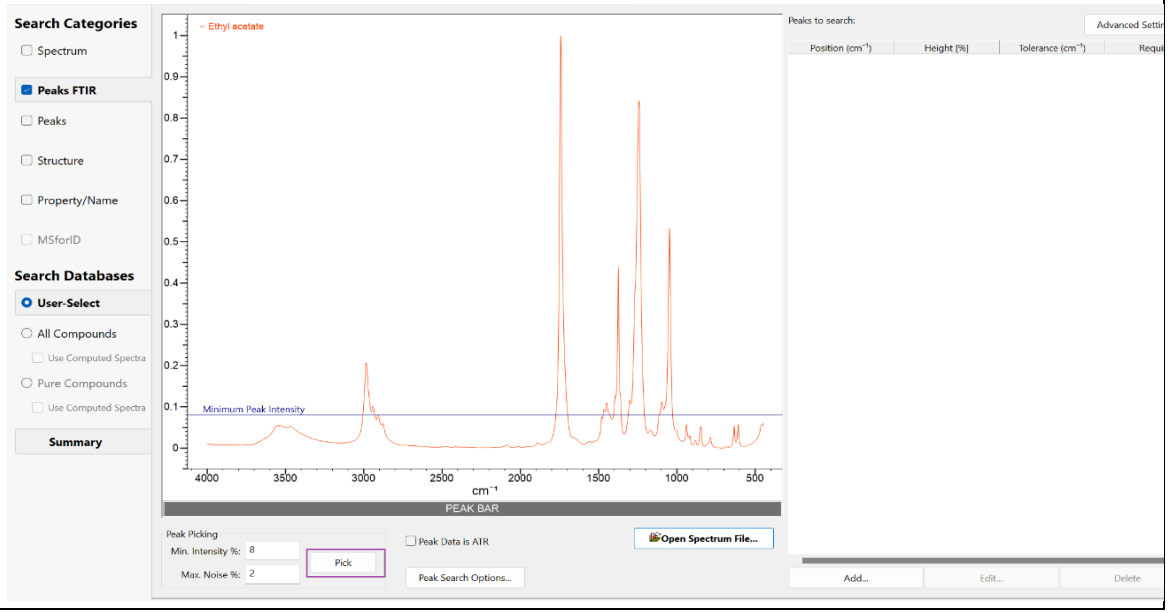
	Action	Result
5	Click **Open Spectrum File** button located toward the bottom Navigate to "**C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\IR**". Open **Ethyl acetate.jdx**.	The selected spectrum is displayed: 

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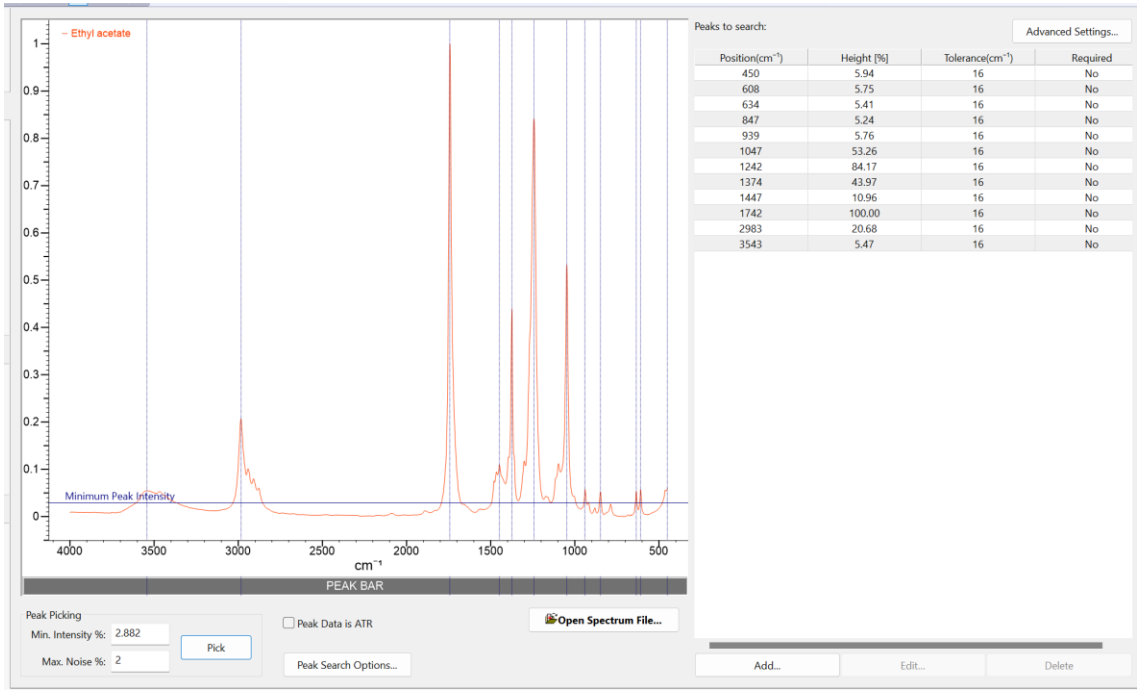
	Action	Result
6	Click **Pick**.	The **peak table** is created based on the current settings: 
7	**TIP**	You can remove a peak from the **peak table** by selecting the peak and clicking the **delete** button or by double-clicking it in the peak bar. Similarly, you can **add** or **edit** peaks using the corresponding buttons at the bottom of the table.

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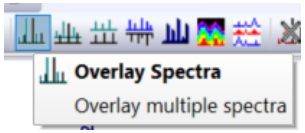
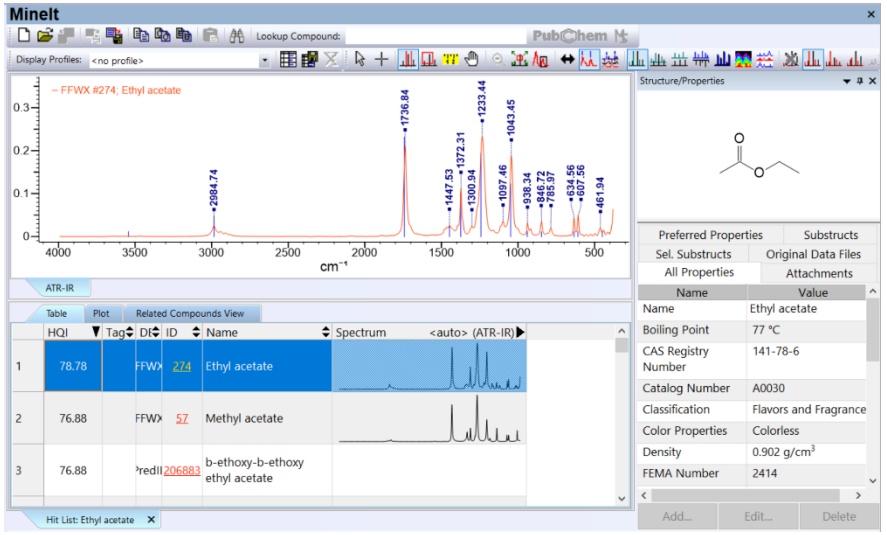
	Action	Result
8	Click **Search**. In **MineIt**, click **Overlay Spectra** view. 	Search results are automatically displayed in the **MineIt** application:  For each entry, the **Spectral** pane displays the hit list spectrum along with the peaks used to perform the search.

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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

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

- Acetonitrile.jdx

KnowItAll Applications Used

- SearchIt
- MineIt

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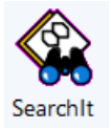
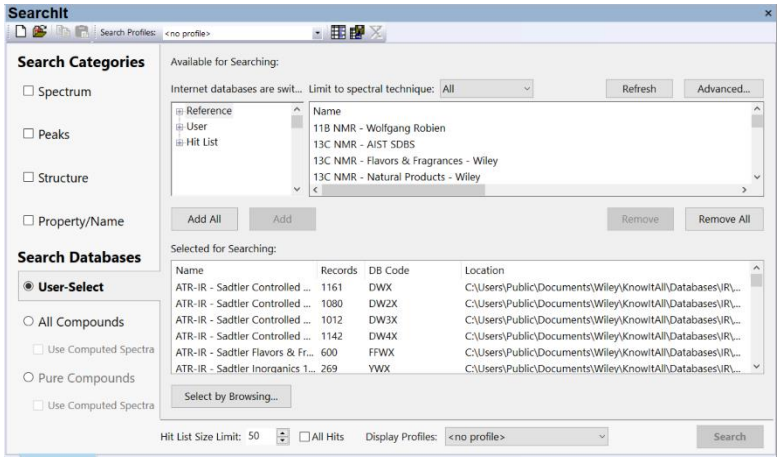
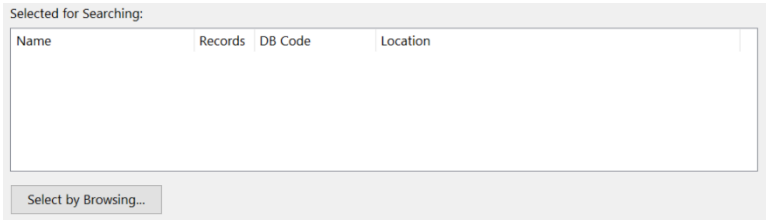
Configure a spectral search

	Action	Result
1	Do one of the following: • If the **SearchIt** application is not open, navigate to the **Data** toolbox and click its icon.  • If the **SearchIt** application is already open, click the SearchIt **Close** button ☒ to close the current search.	The **SearchIt** application's **User-Select** tab is displayed and the **Selected for Searching** list displays the databases last used: 
2	If databases are already selected for searching, click **Remove All** to clear the selections.	The **Selected for Searching** window is cleared: 

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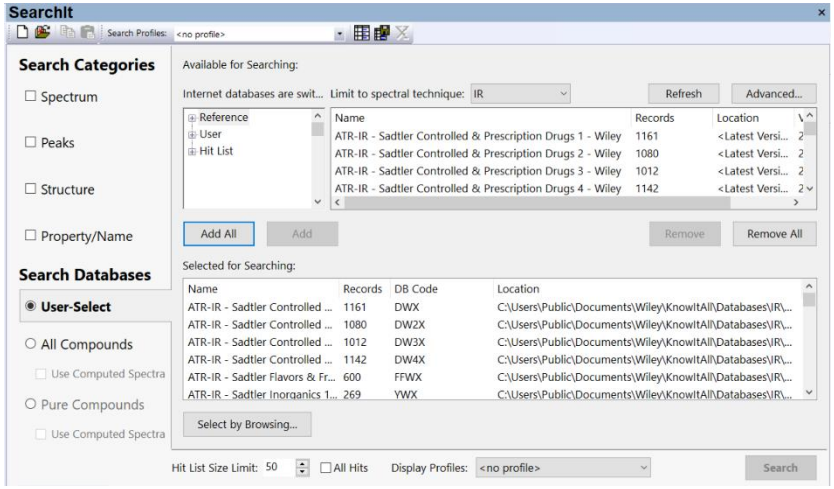
	Action	Result
3	In the **Available for Searching** Dialog, choose **IR** for **Limit Spectral Technique to.** Click **Add All**.	The Wiley IR database collection is displayed in the **Selected for Searching** list: 
4	Click **Spectrum** under **Search Categories**.	An **Open** dialog box appears.

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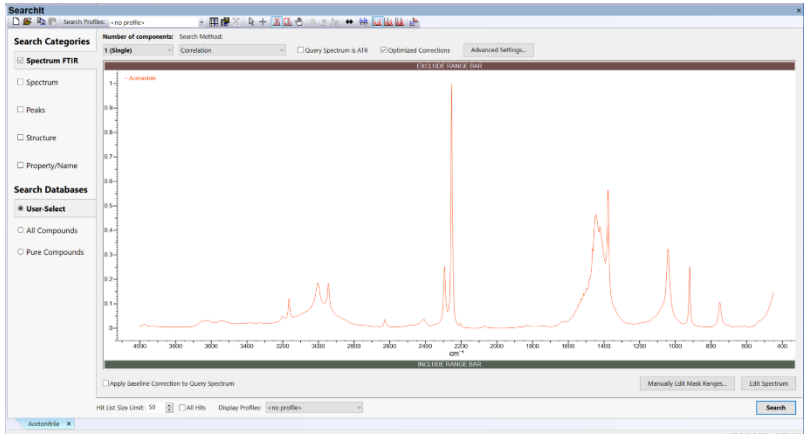
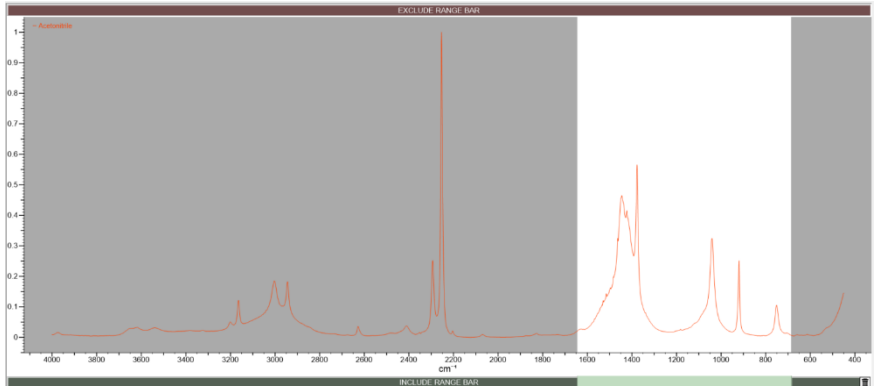
	Action	Result
5	Navigate to “C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\IR”. Open **Acetonitrile.jdx**. **Note**: You can use the **Files of Type** filter to display JCAMP files (or all files).	The spectrum is displayed. 
6	Click, drag, and release within the **Include Range Bar** to define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

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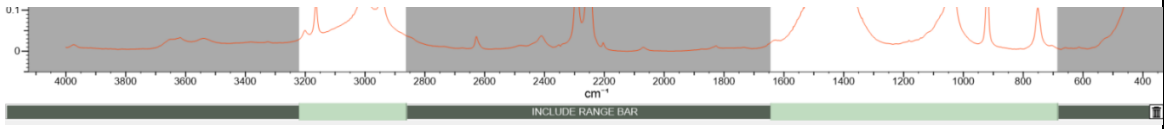
	Action	Result
7	Click and drag to define a second Include region. **Note:** To move a region horizontally, click within the region on the **Include Range Bar** and drag to a new location.	A second region is selected on the spectrum: 
8	**TIPS:**	To re-size a region, move the cursor into the **Include Range Bar** and position the cursor over an endpoint, then drag and release. The cursor changes to a cross with a double arrowhead.  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. To remove all regions, click the trash can icon at the right end of the **Include Range Bar**.

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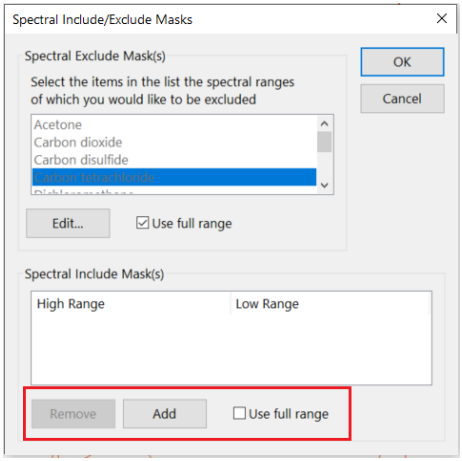
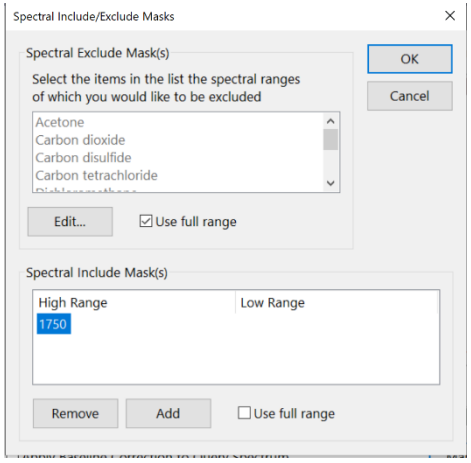
Use the Search Masks dialog box

	Action	Result
1	Clear the previous search range by clicking the trash can icon on the right side of the **INCLUDE RANGE BAR**  Click **Manually Edit Mask Ranges**. Unclick **Use full range** and click **Add** under **Spectral Include Mask(s)** **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.	The **Spectral Include/Exclude Masks** dialog box opens. 
2	Click to select the **High Range** value in the remaining Include region and type in '1750.'	1750 is added as a **High Range** value: 

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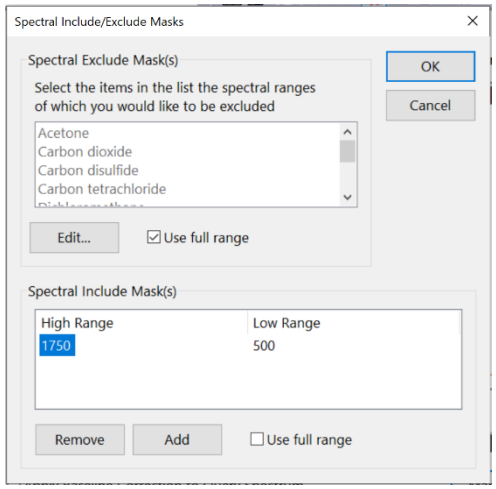
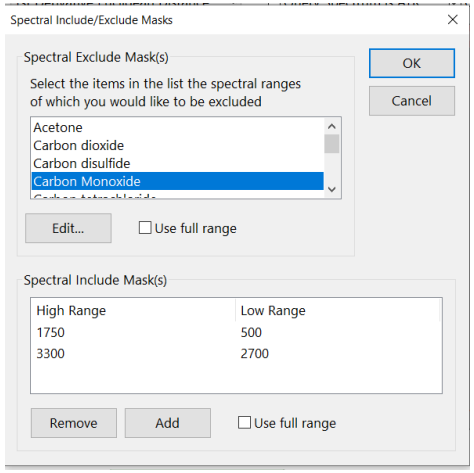
	Action	Result
3	Click to select the **Low Range** value in the remaining Include region and type in '500.'	500 is added as a **Low Range** value: 
4	Click **Add** to create another Include region. Type '3300 in the new **High Range** text box, then click in the **Low Range** column and type '2700.'	The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

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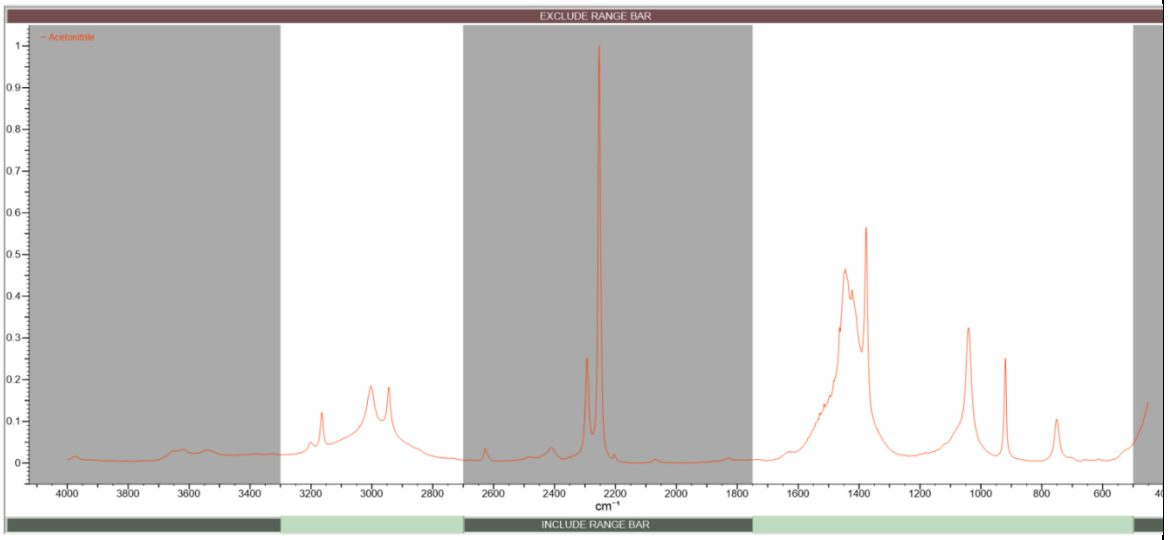
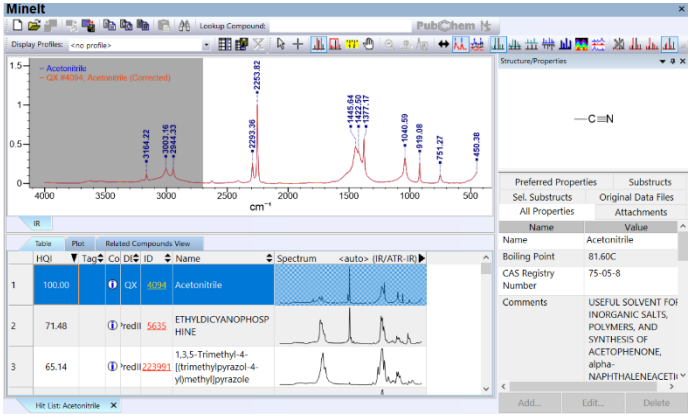
	Action	Result
5	Click **OK**.	The dialog box closes, and the search spectrum is displayed with the re-defined **Include** regions. 
6	Click **Search**.	The search is performed, and results are automatically displayed in the **MineIt** application as a hit list.  Clicking on the information icon ⓘ in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

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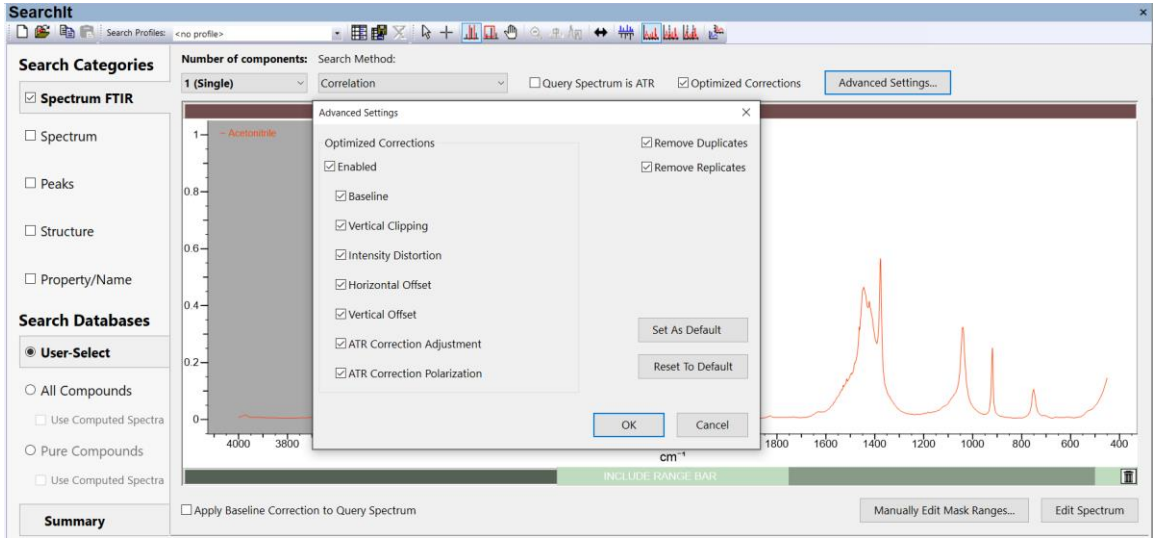
	Action	Result
7	Close the **Optimized Corrections** window, then use the KnowItAll **Back** button to return to the **SearchIt** application. Click **Advanced Settings** on the **Spectrum FTIR** tab.	The **Advanced Settings** dialog box opens:  The **Advanced Settings** dialog can be used to control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

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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

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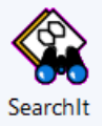
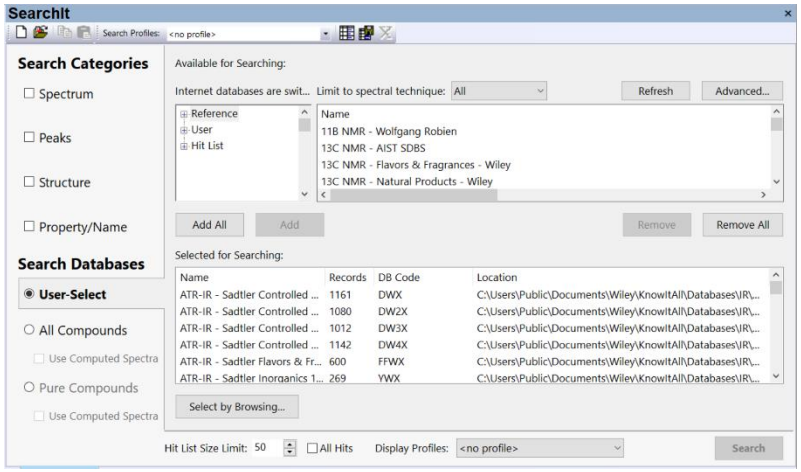
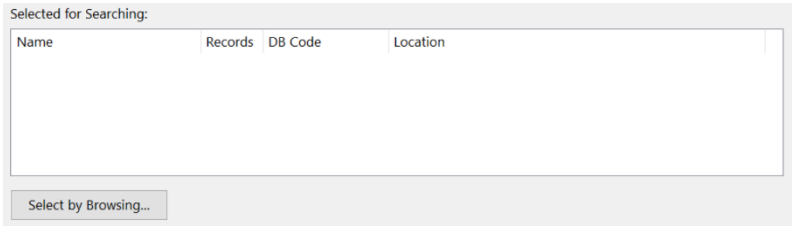
Configure a spectral search

	Action	Result
1	Do one of the following: • If the **SearchIt** application is not open, navigate to the **Data** toolbox and click its icon.  • If the **SearchIt** application is already open, click the SearchIt **Close** button ☒ to close the current search.	The **SearchIt** application's **User-Select** tab is displayed and the **Selected for Searching** list displays the databases last used: 
2	If databases are already selected for searching, click **Remove All** to clear the selections.	The **Selected for Searching** window is cleared: 

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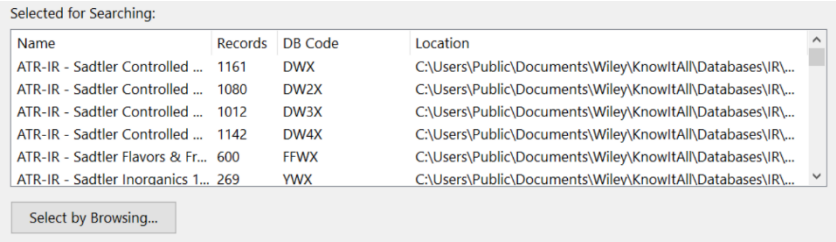
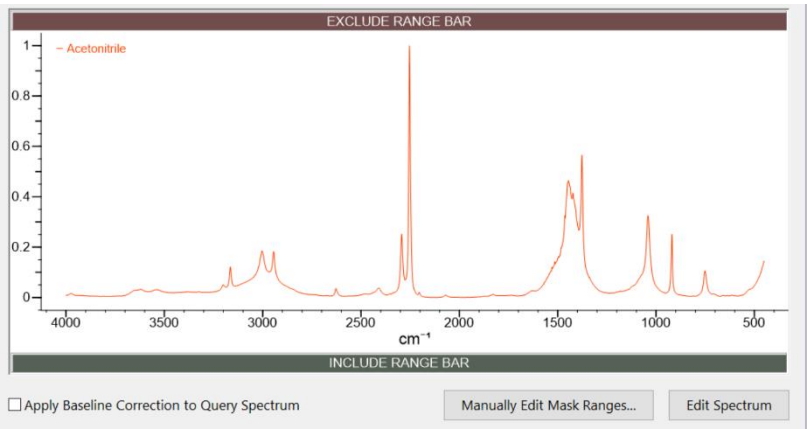
	Action	Result
3	Select **IR** using the **Limit to spectral technique** control. Click **Add All**.	The Wiley IR database collection is displayed in the **Selected for Searching** list:  **Note**: Many of the databases have only IR spectra, but others–such as the Multi-Technique Sadtler Demo Database - Wiley–include other types of spectra and structures.
4	Click **Spectrum** under **Search Categories**.	An **Open** dialog box appears.
5	Navigate to "C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples\IR". Open **Acetonitrile.jdx**. **NOTE**: You can use the Files of type filter to display JCAMP files (or all files).	The spectrum is displayed in the IR Spectrum tab: 

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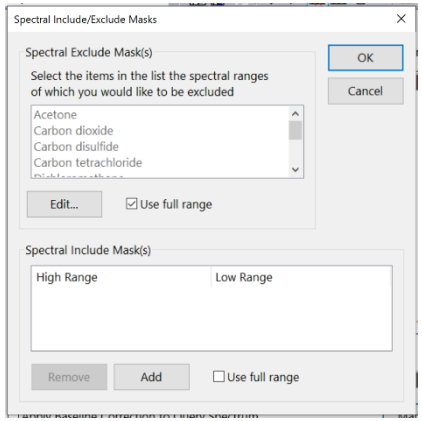
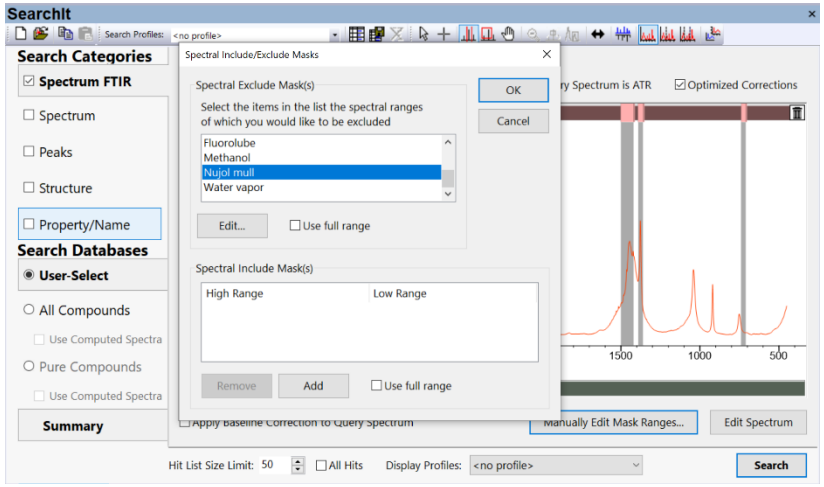
Use the Search Masks dialog box

	Action	Result
1	Click **Manually Edit Mask Ranges**.	The **Spectral Include/Exclude Masks** dialog box opens. 
2	Uncheck **Use full range** under the list of **Spectral Exclude Mask(s)**, then click to select the **Nujol mull** exclude mask.	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: 

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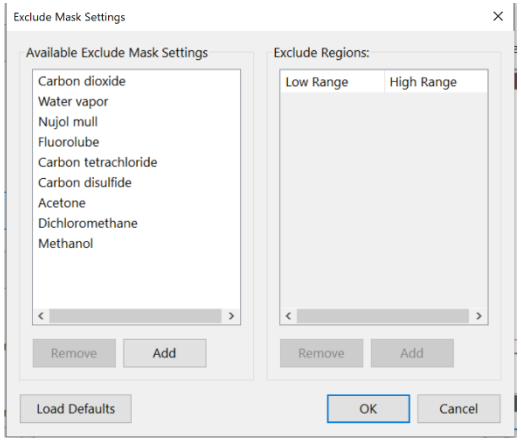
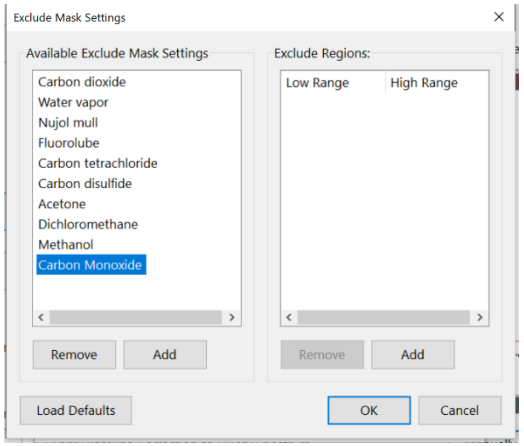
	Action	Result
3	Click **Edit** on the **Spectral Include/Exclude Masks** dialog box.	The **Exclude Mask Settings** dialog opens: 
4	Click **Add**. Type in “Carbon Monoxide**”**, then click outside the text box.	A text box appears under **Available Exclude Mask Settings**, which allows for entering “Carbon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

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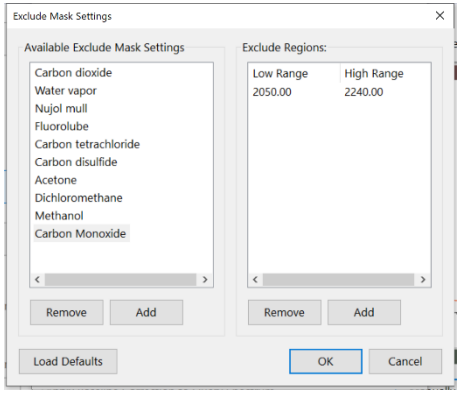
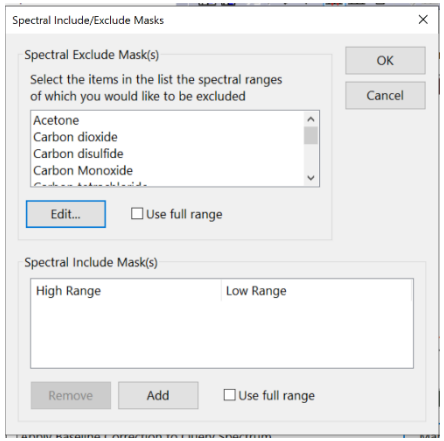
	Action	Result
5	With **Carbon Monoxide** selected in the list of **Available Exclude Mask Settings**, click **Add** under the list of **Exclude Regions** or click under **Low Range**. Type in low and high range values (2050 and 2240).	A text box appears under **Exclude Regions** that allows for entering the **Low Range** and **High Range** values: 
6	**TIPS:**	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.
7	Click **OK**	The **Exclude Mask Settings** dialog box closes, and the new carbon monoxide mask is added to the list of Exclude Masks. 

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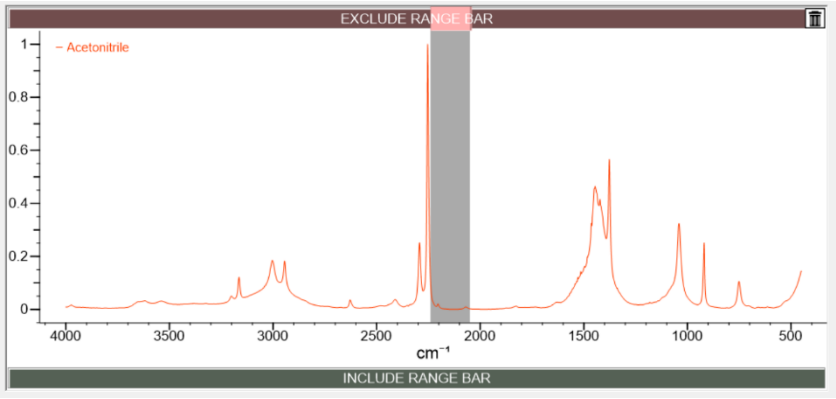
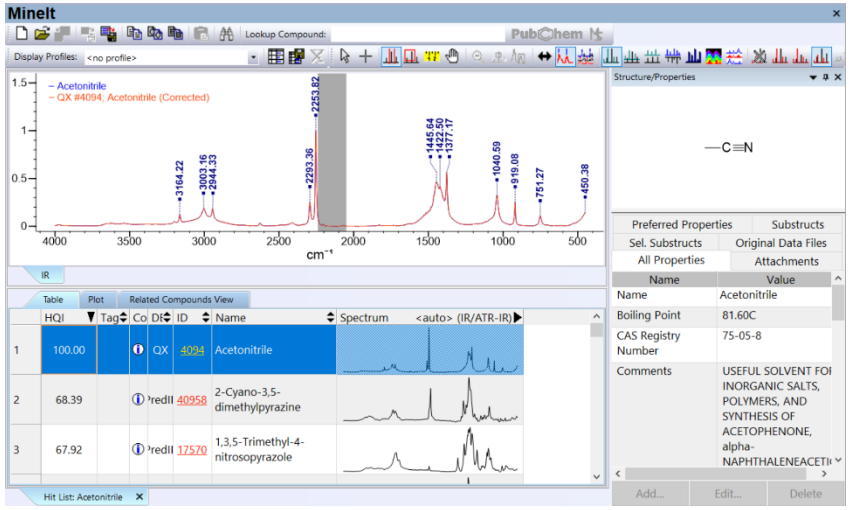
	Action	Result
8	Select the new **Carbon Monoxide** mask, then click **OK** to close the **Spectral Include/Exclude Masks** dialog box.	The dialog box closes, and the search spectrum is displayed with the newly defined exclude region: 
9	Click **Search**.	The search results are automatically displayed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

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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
- MineIt
- ProcessIt

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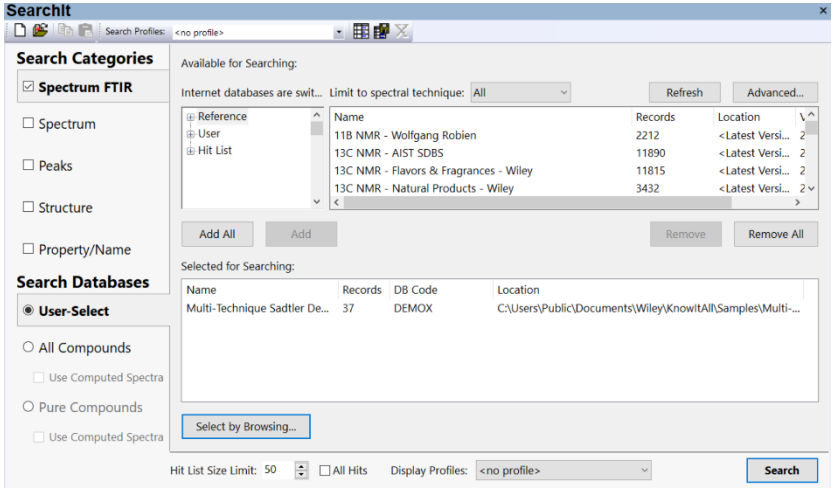
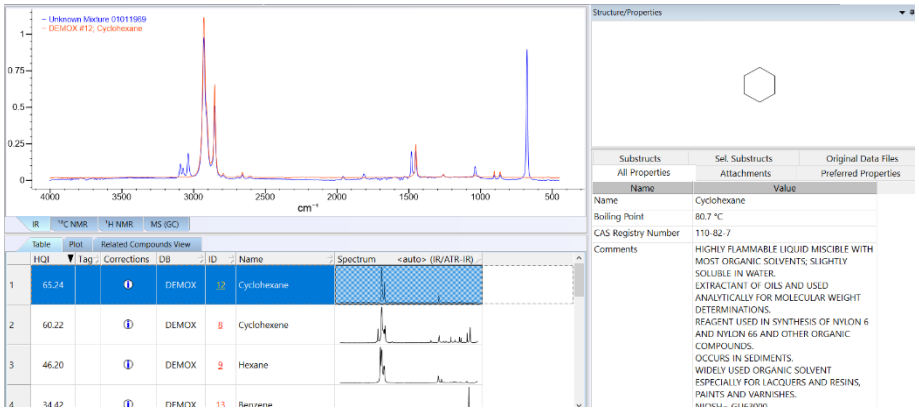
Set up a spectral search against a mixture

	Action	Result
1	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.	The FTIR spectrum is opened in **SearchIt** and the DEMOX database is selected for searching: 
2	Click **Search.**	Results are displayed in the **MineIt** application. The first hit is **cyclohexane**. Both spectra, the query and the first hit are displayed in the spectral pane. 

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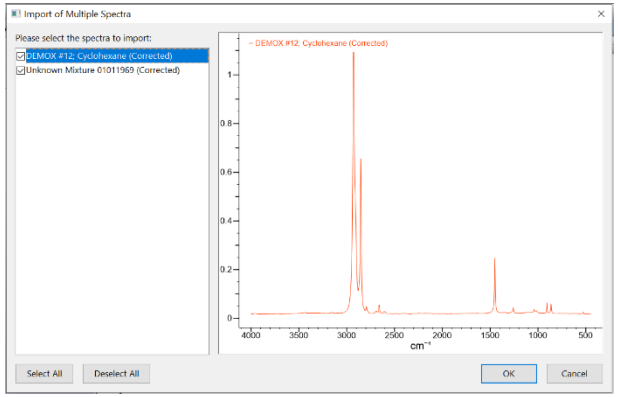
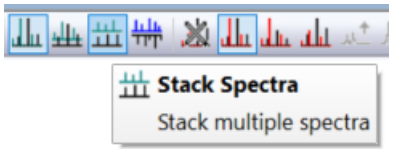
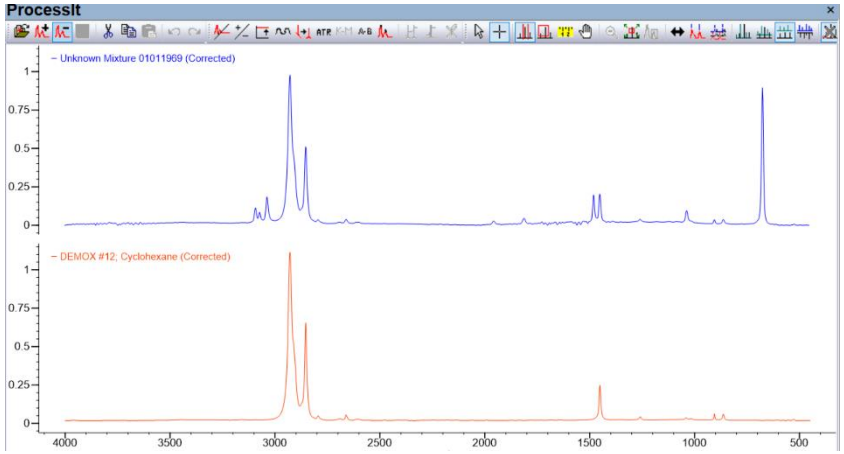
Create a difference spectrum

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

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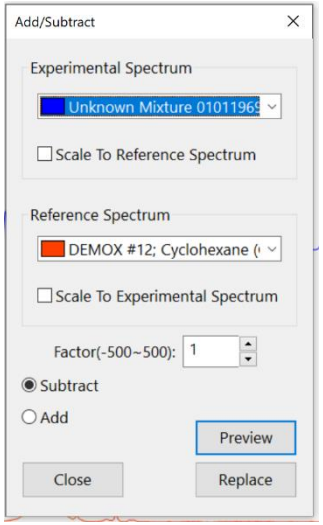
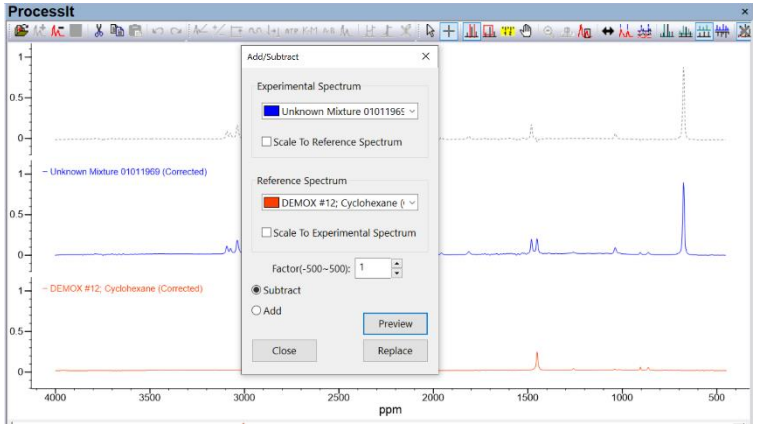
	Action	Result
3	Choose **Process > Add/Subtract Spectrum**. **NOTE**: You can also use the toolbar button  . The command is not available unless two or more spectra are open.	The **Add/Subtract** dialog box opens. The active spectrum is assumed to be the reference spectrum: 
4	Make sure the mixture spectrum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

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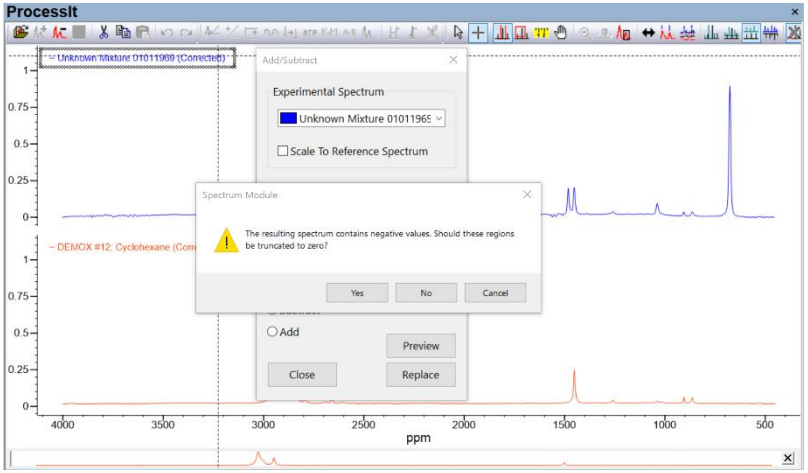
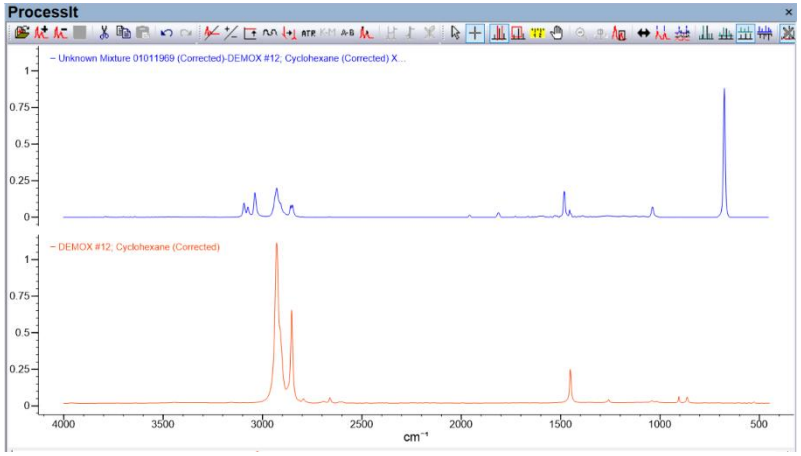
	Action	Result
5	On the **Add/Subtract** dialog box, adjust **Factor** to ~0.7. Click **Replace**.	A message box opens and asks whether negative values should be truncated to zero: 
6	Click **Yes**.	The mixture spectrum is replaced by a difference spectrum: 

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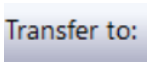
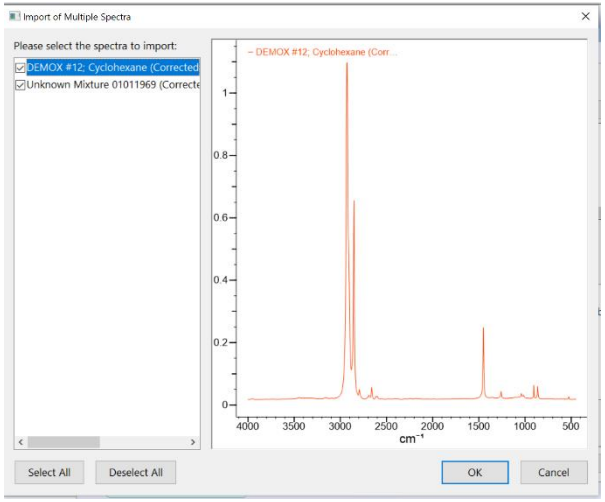
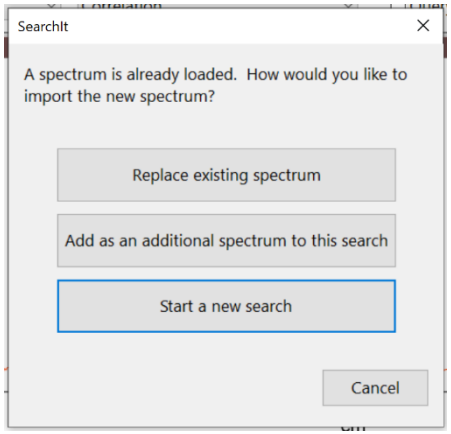
Repeat the search using the difference spectrum

	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: 

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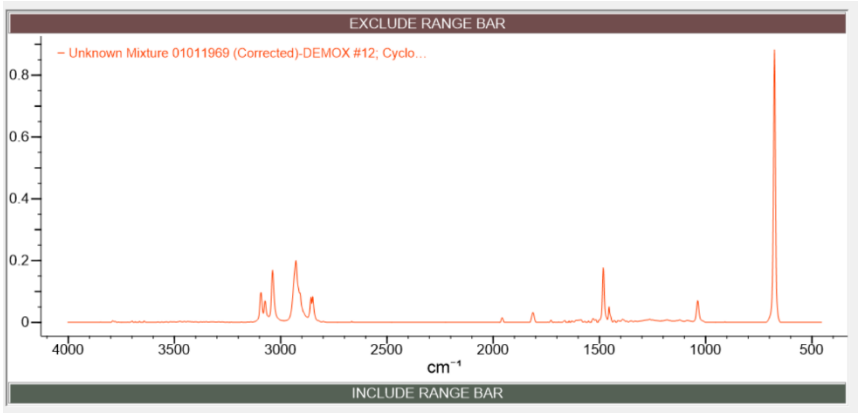
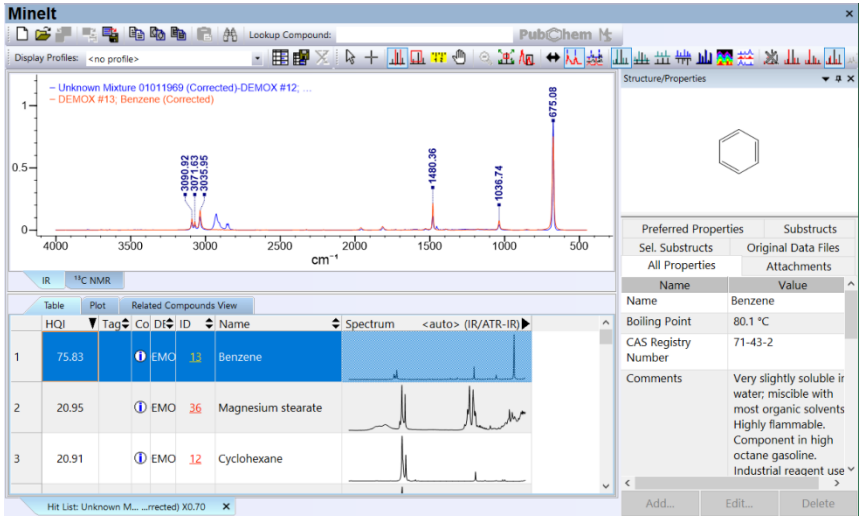
	Action	Result
3	Click **Start a new search**.	The difference spectrum is loaded in **SearchIt**: 
4	Click **User-Select** tab and make sure the **Multi-Technique Sadtler Demo Database - Wiley** is selected for searching. Click **Search**.	Results are displayed in the **MineIt** application. The first hit is benzene, the other component of the mixture. 

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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

- tryptophan.dsf
- benzenethiol.dsf

KnowItAll Applications Used

- SearchIt
- MineIt
- ChemWindow®

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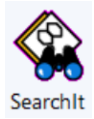
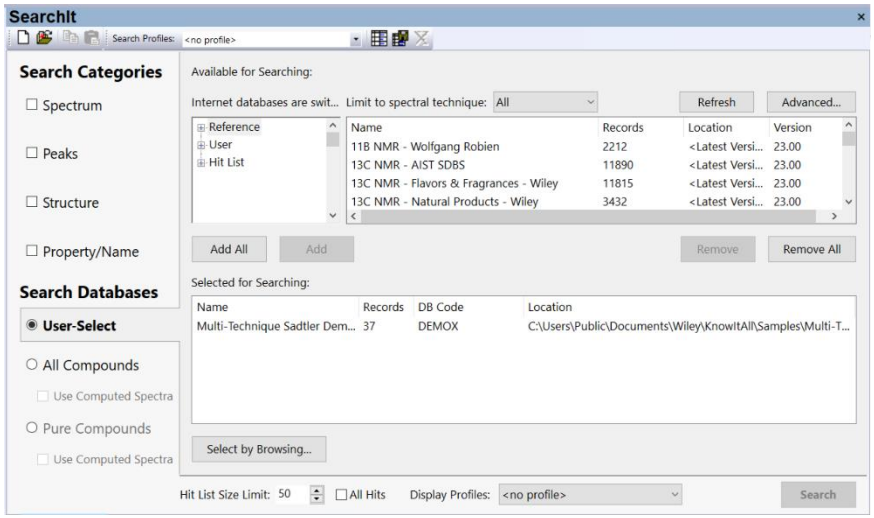
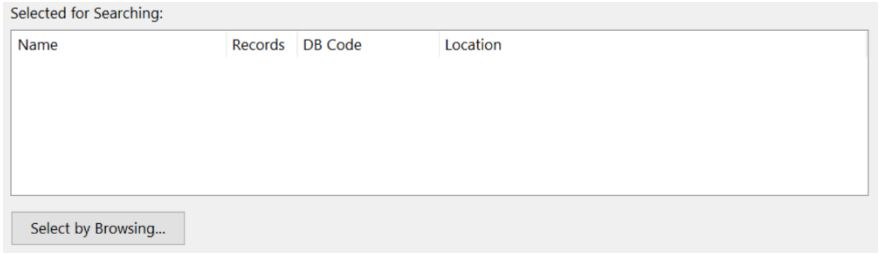
Configure an exact structure match search

	Action	Result
1	Do one of the following: • If the **SearchIt** application is not open, navigate to the **Data** toolbox and click its icon.  • If the **SearchIt** application is already open, click the SearchIt **Close** button ☒ to close the current search.	The **SearchIt** application's **User-Select** tab is displayed and the **Selected for Searching** list displays the databases last used: 
2	If databases are already selected for searching, click **Remove All** to clear the selections.	If databases are already selected for searching, click **Remove All** to clear the selections: 

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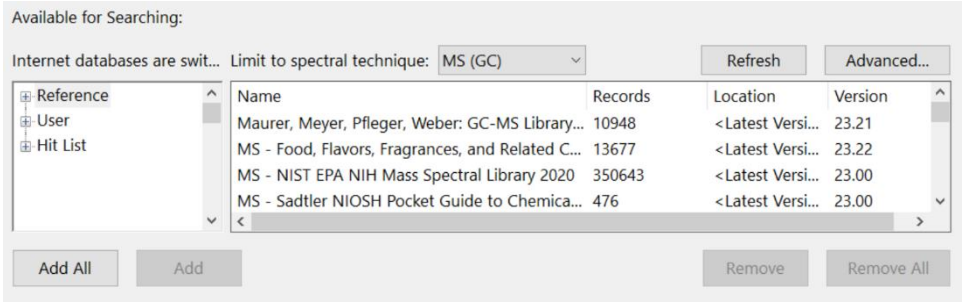
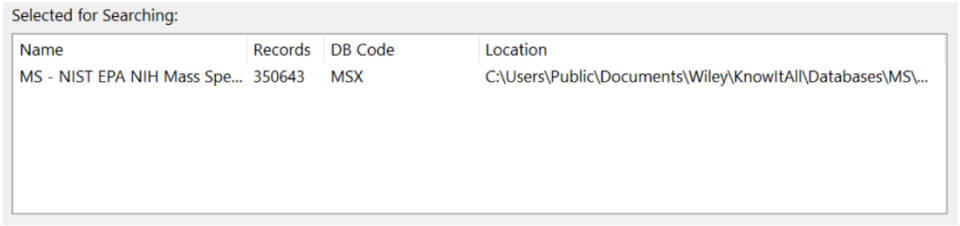
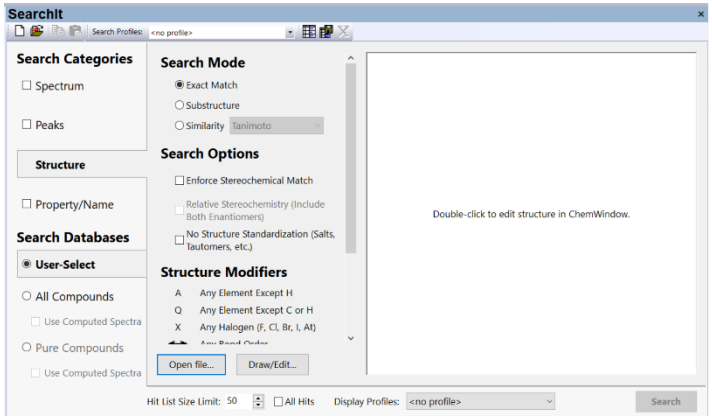
	Action	Result
3	Set **Limit to Spectral Technique** to **MS (GC)**.	Only databases with MS spectral data are displayed: 
4	Select database **MS – NIST EPA NIH Mass Spectral Library xxxx – Main Library** for searching. xxxx is the year of the library	The selected database is added to the **Selected for Searching** window: 
5	Click **Structure** under **Search Categories**.	The **Structure Search** dialog is displayed: 

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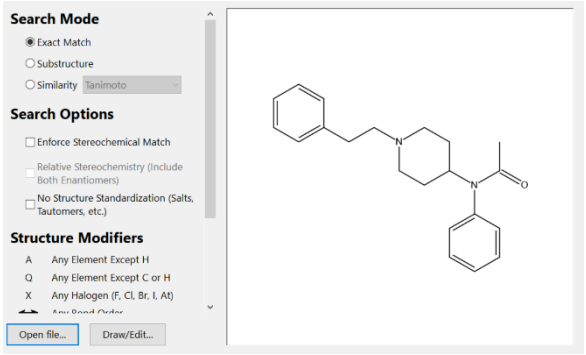
	Action	Result
6	Click **Open file…** button. Navigate to "C:\Users\Public\Public Documents\Wiley\KnowItAll\ Samples\Structures" and select **Acetylfentanyl.cdx**. **Note**: You can also click **Draw/Edit** to create a structure using the **ChemWindow** application.	The structure is displayed in the **Structure** tab: 

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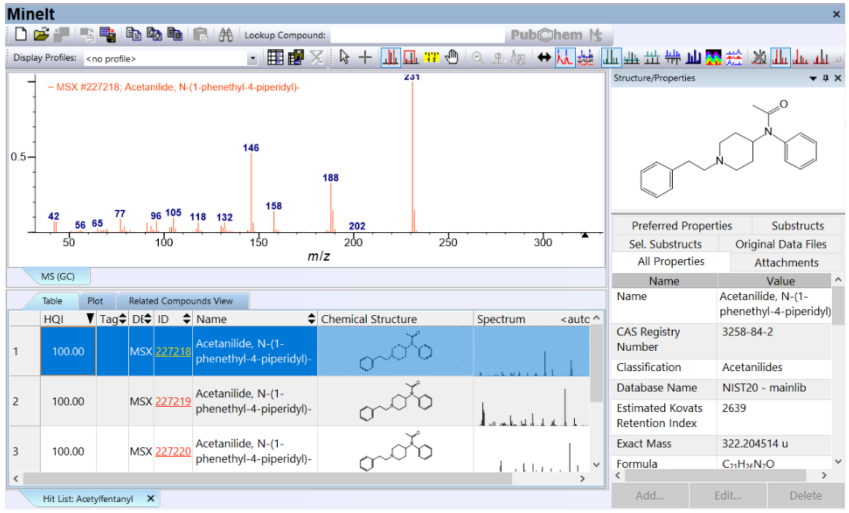
Perform an exact structure match search

	Action	Result
1	Select **Exact Match** under **Search Mode**, then click **Search**.	Exact matches are displayed in the **MineIt** application: 

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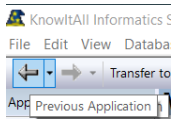
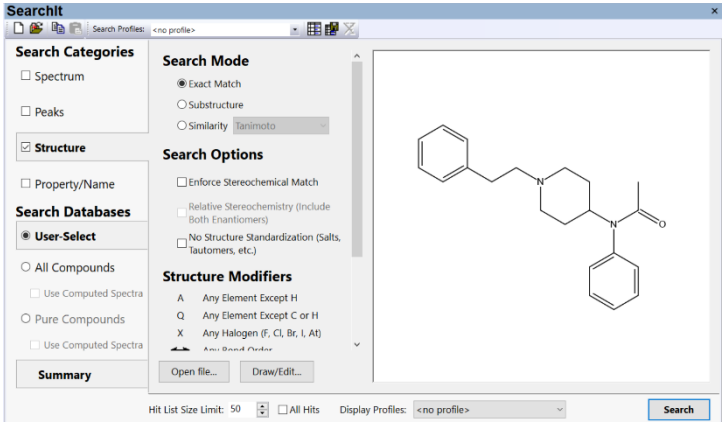
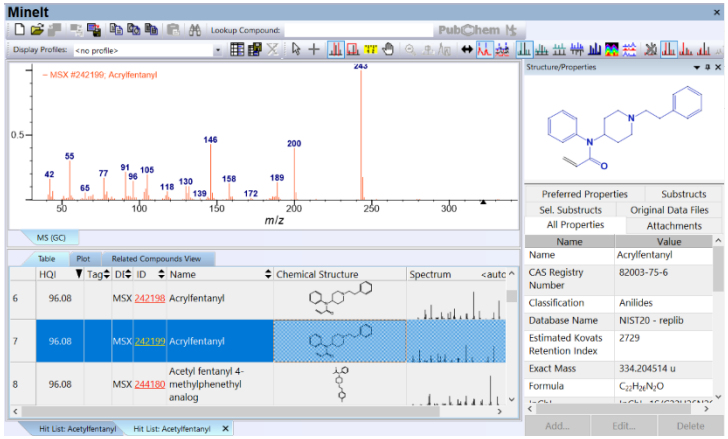
Configure and perform a substructure search

	Action	Result
1	Click the KnowItAll **Back** button to return to **SearchIt**.  If you are not on the **Structure** tab, click to resume a structure search.	The **Structure** search dialog is displayed: 
2	Select **Substructure Search**, then click **Search**. Click through the records to search results. **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.	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:  Note that the original hit list is still available and can be accessed by clicking the appropriate tab (at the lower left corner).

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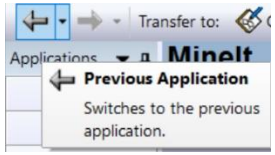
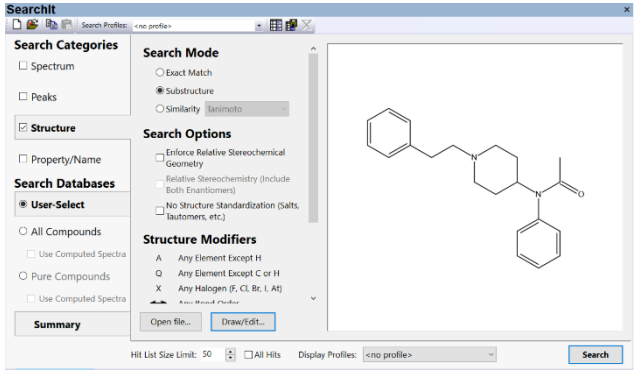
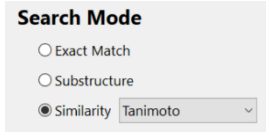
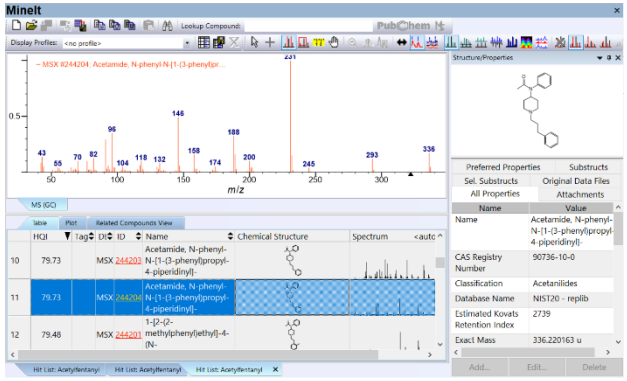
Configure and perform a similarity search

	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 **MineIt** application: 

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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

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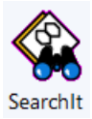
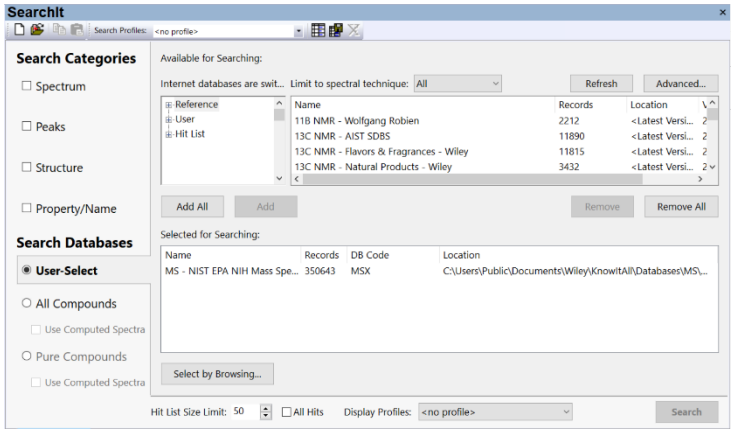
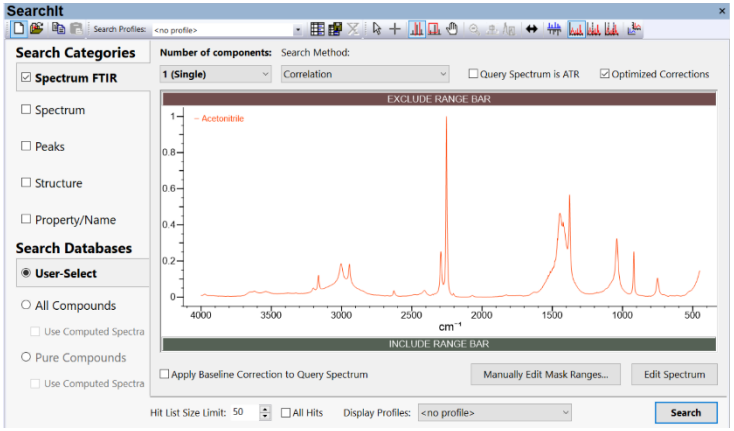
Configure and perform an All Compounds search

	Action	Result
1	Do one of the following: • If the **SearchIt** application is not open, navigate to the **Data** toolbox and click its icon.  • If the **SearchIt** application is already open, click the SearchIt **Close** button ☒ to close the current search.	The **SearchIt** application's **User-Select** tab is displayed and the **Selected for Searching** list displays the databases last used: 
2	Click **Spectrum** under **Search Categories**. Navigate to C:\Users\Public\Public Documents\Wiley\KnowItAll\ Samples\IR" and select **acetonitrile.jdx**.	The spectrum for acetonitrile is displayed: 
3	Select the **All Compounds** option under **Search Databases**.	The **All Compounds** search option is selected.

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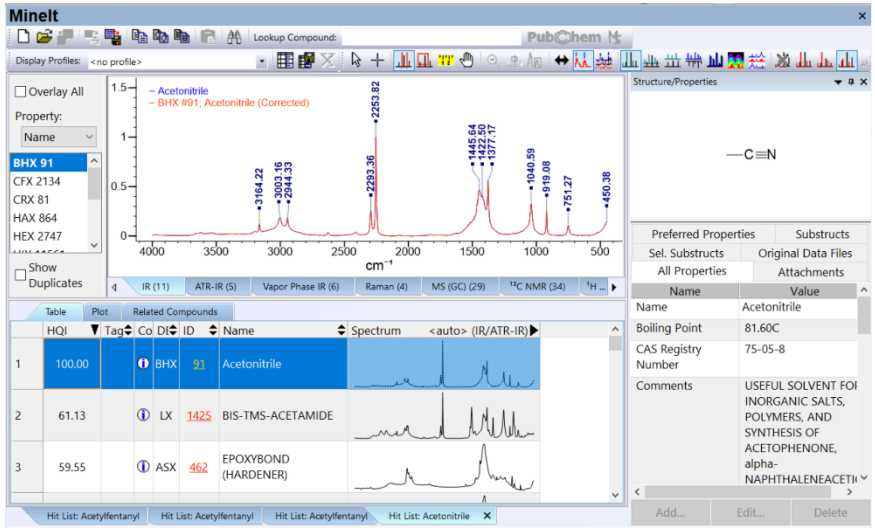
	Action	Result
4	Click **Search**.	The search is performed, and results are displayed in the **MineIt** application:  Compared to the **User-Select** database search, you will see additional information related to the hit: • Replicates are displayed in the upper-left panel. They do not participate in 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:**	• **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.

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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\Simultaneous Multi-Technique Searching folder

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

KnowItAll Applications Used

- SearchIt
- MineIt

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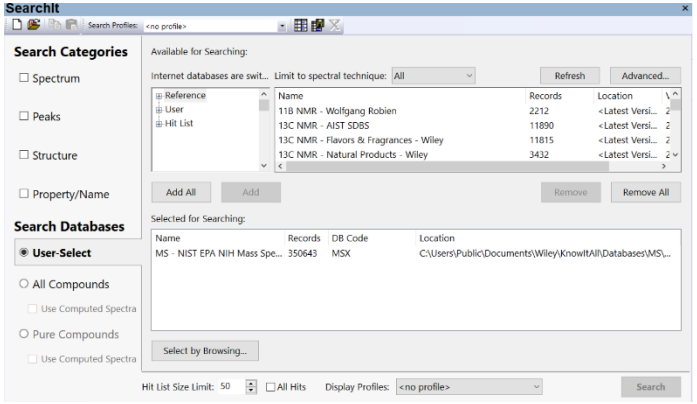
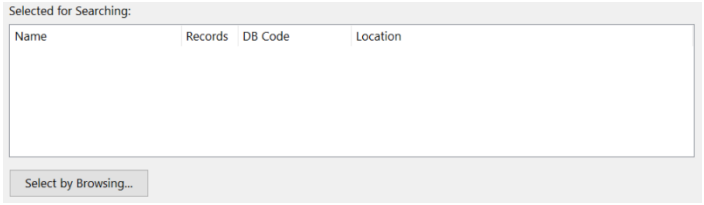
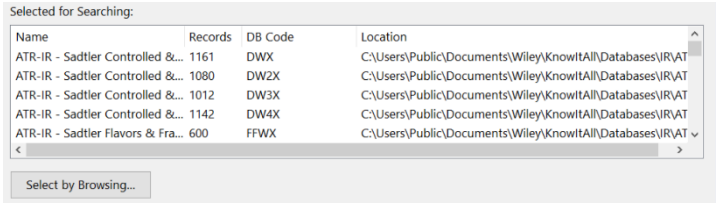
Configure and perform a multi-technique spectral search with the User-Select Search Databases option

	Action	Result
1	Do one of the following: • If the **SearchIt** application is not open, navigate to the **Data** toolbox and click its icon.  • If the **SearchIt** application is already open, click the SearchIt **Close** button ✕ to close the current search.	The **SearchIt** application's **User-Select** tab is displayed, and the **Selected for Searching** list displays the databases last used: 
2	Select **User-Select** under **Search Databases** option. If databases are already selected for searching, click **Remove All** to clear the selections	The **Selected for Searching** databases section is cleared: 
3	Using the **Limit to spectral technique** tab, select **IR** then click **Add All.** Repeat for **Raman**.	All of the available IR and Raman databases are added to the **Selected for Searching** window: 

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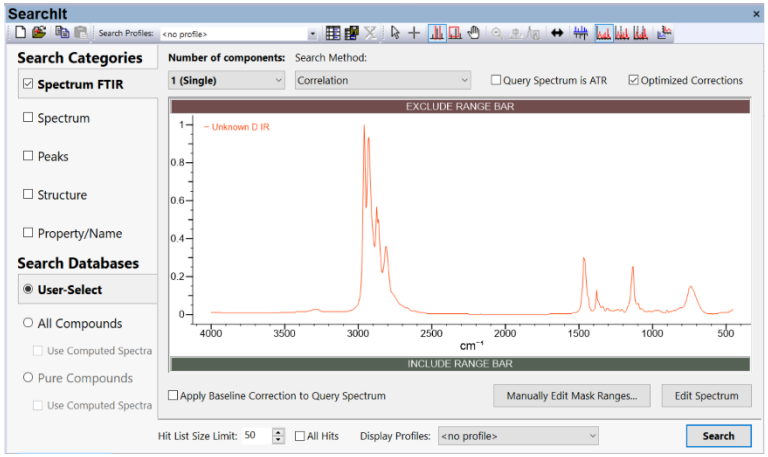
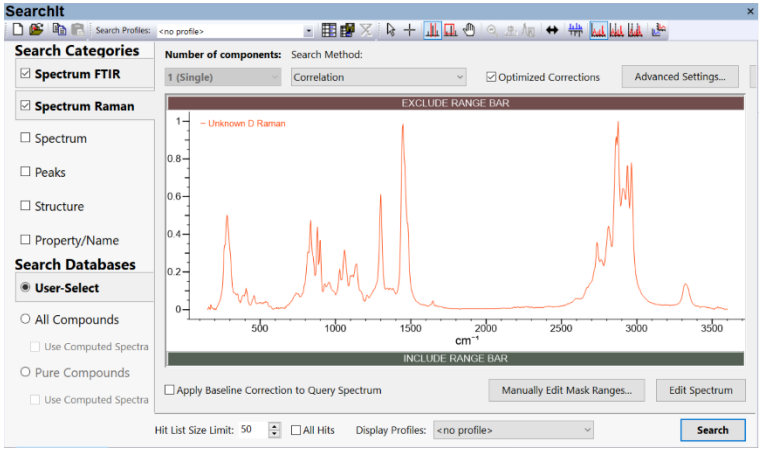
	Action	Result
4	Click **Spectrum** under **Search Categories**. Navigate to “C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples \Simultaneous Multi-Technique Searching”. Open **Unknown D IR.jdx**.	An IR spectrum is displayed in the **SearchIt spectrum** window: 
5	Click **Spectrum** under **Search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

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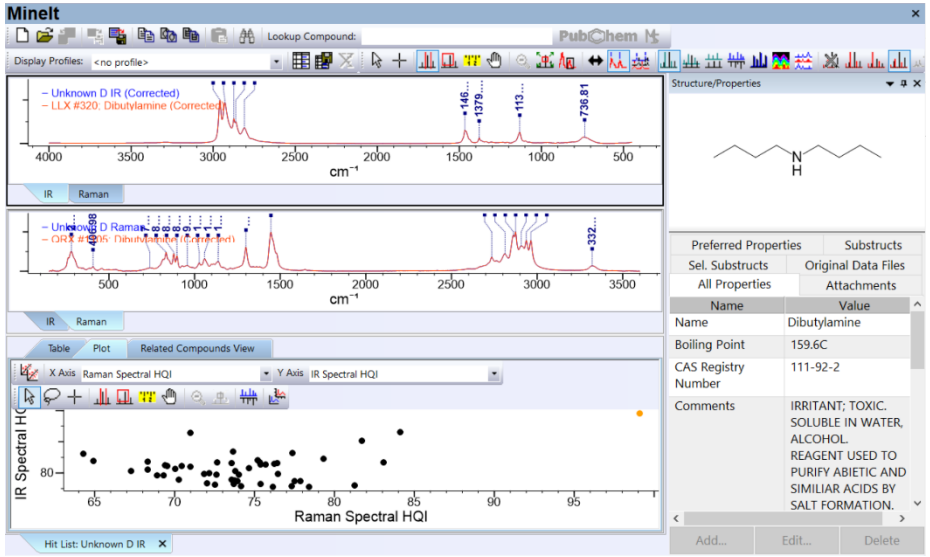
	Action	Result
6	Click **Search**.	The search results are displayed in the **MineIt** application:  Because this was a multi-technique search, the **Database** pane's **Plot** tab automatically displays a scatter plot representing HQI values for the two spectral techniques. The point with the highest 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.

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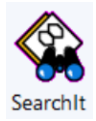
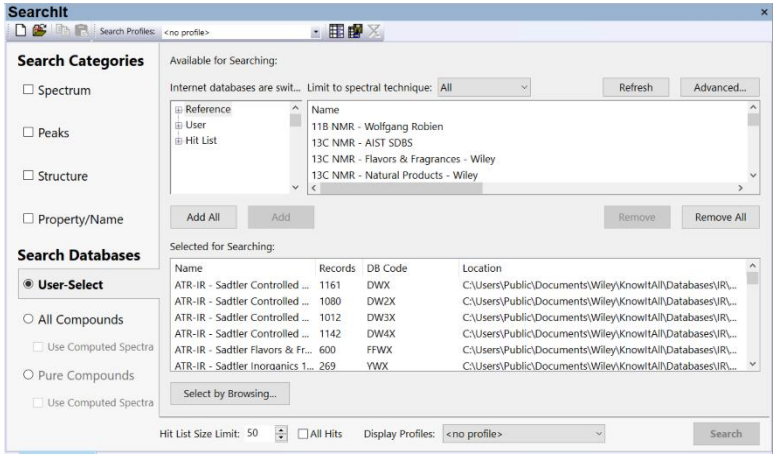
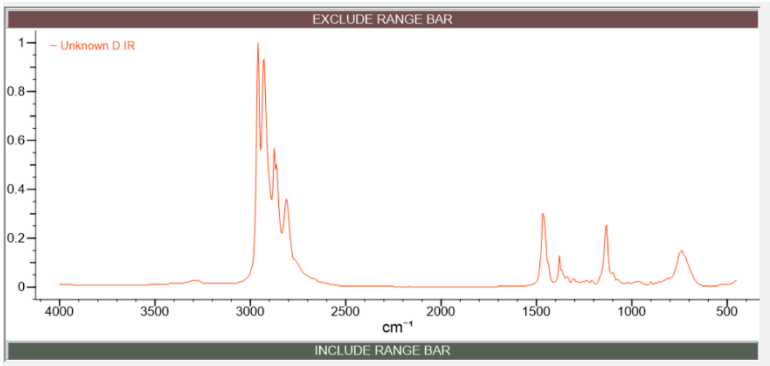
Configure and perform a multi-technique spectral search with the All Compounds Search Databases option

	Action	Result
1	Do one of the following: • If the **SearchIt** application is not open, navigate to the **Data** toolbox and click its icon.  • If the **SearchIt** application is already open, click the SearchIt **Close** button ☒ to close the current search.	The **SearchIt** application's **User-Select** tab is displayed, and the **Selected for Searching** list displays the databases last used: 
2	Click **Spectrum** under **Search Categories**. Navigate to C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples \Simultaneous Multi-Technique Searching" and select **Unknown D IR.jdx**.	The spectrum is displayed in the **SearchIt** application: 

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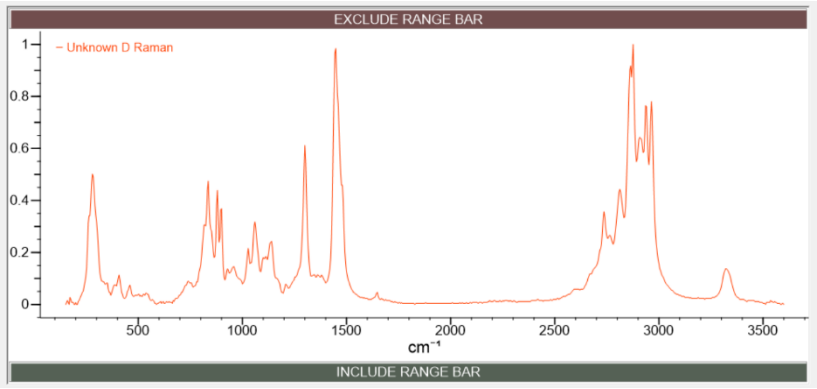
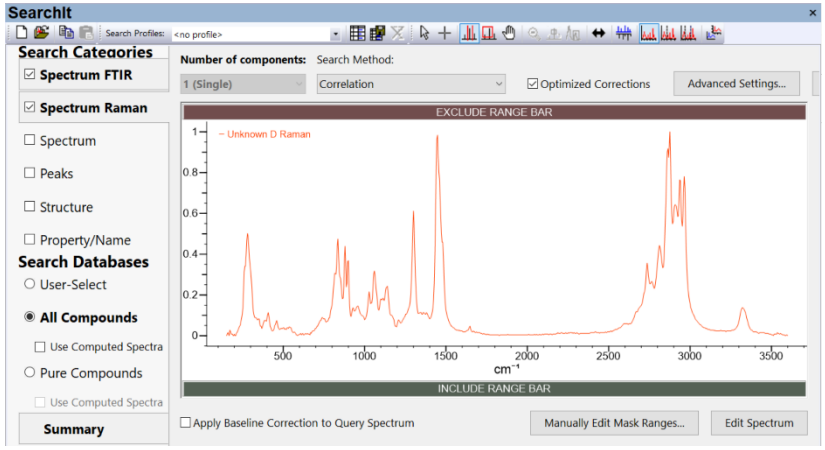
	Action	Result
3	Click **Spectrum** under **Search Categories** to add another spectrum. From the folder "C:\Users\Public\Public Documents\Wiley\KnowItAll\Samples \Simultaneous Multi-Technique Searching", choose **Unknown D Raman.jdx**.	The Raman spectrum is added to the search: 
4	Check **All Compounds**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

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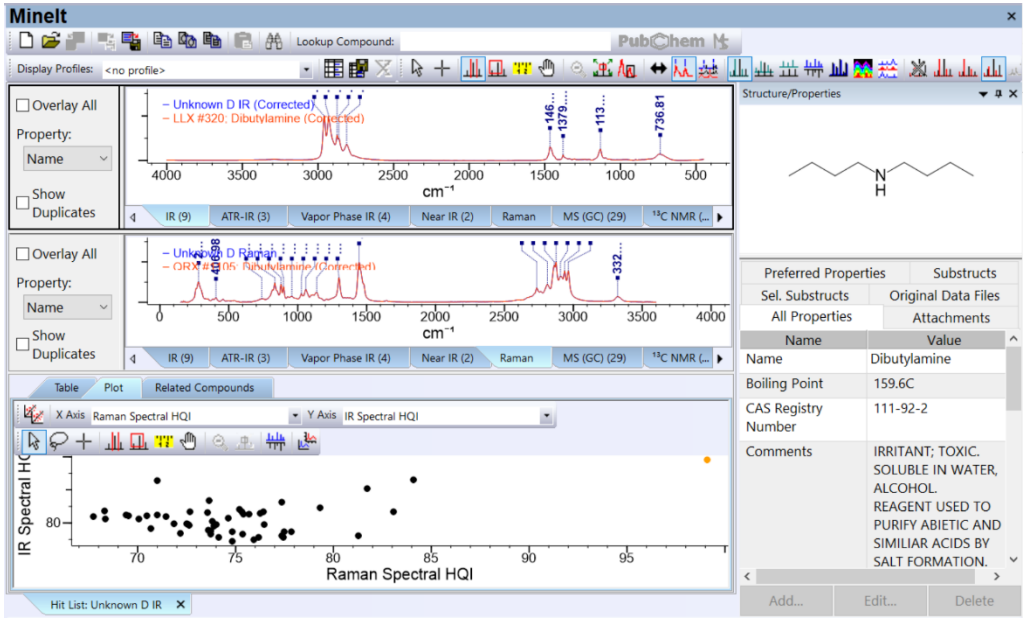
	Action	Result
5	Click **Search**.	The search results are displayed in the **MineIt** application:  Because this was a multi-technique search, the **Database** pane's **Plot** tab automatically displays a scatter plot representing HQI values for the two spectral techniques. The point with the highest HQI values is selected at the upper right.

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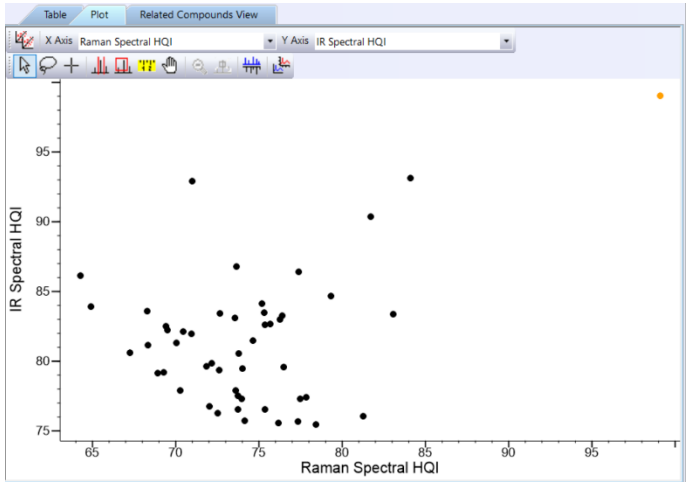
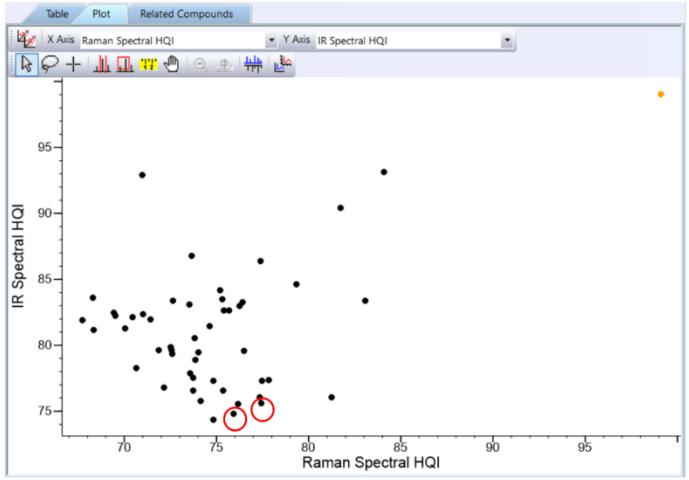
	Action	Result
6	Examine the example shown in the Results. Compare the scatter plot of the **User-Select** database search and that of **All Compounds** search.	**User-Selected** database search:  **All Compounds** database search:  They are more ppints near the circled region including the circled points.

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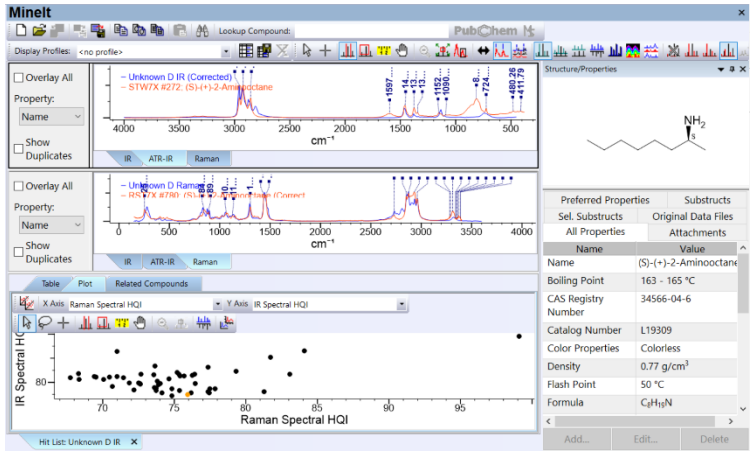
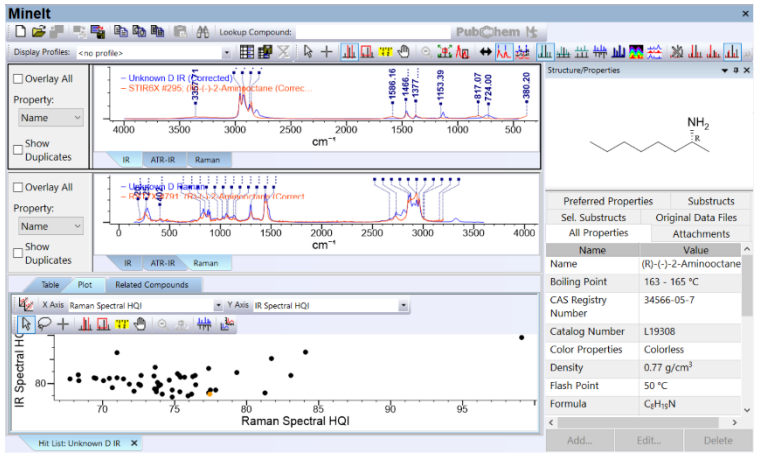
	Action	Result
7	Using the search results from Step 5, examine the circled points.	These two records are the stereoisomers whose IR and Raman spectral records are linked not by structure, but by other features in the record (name, InChI, CAS Registry Number or synonym). **(S) Isomer:**  **(R) Isomer:** 

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