KnowItAll Software

Training Guide

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About this Training Guide

This training guide lead you through a series of exercises in the manner of a training course. Each lesson has a folder of example training files associated with it that can be downloaded here: www.knowitall.com/training_files

Lesson	Description	Application Featured
General Features	• Explore the interface • Learn to transfer data from one application to another	KnowItAll "Interface"
1 - Simple Spectral Search / Identification	• Perform a "first pass" analysis of your spectrum against reference spectra • Use patented optimized corrections technology to optimize search results	KnowItAll ID Expert
2 - Searching	• Perform a basic, peak, structure, and multi-technique searches • Create a search profile • Limit search range / exclude search regions • Perform a spectral subtraction • "All" vs. "Pure Compound" search	SearchIt
3 - Mixture Analysis	• Perform mixture analysis • Interpret search results	SearchIt
4 - Create Databases	• Create a database with spectra, structures, properties • Batch import spectra, structures, properties, PubChem properties • Create display profiles	MineIt/Create Databases
5 - Functional Group Analysis	• Browse the knowledgebase of functional groups • Correlate peaks from a structure • Perform spectral analysis by functional group – IR, Raman. IR Polymers • Create User Knowledgebases	AnalyzeIt (IR, IR Polymer, Raman)
6 - Drawing Structures & Reactions	• Use basic ChemWindow tools to create and edit a structure • Create chemical reactions	ChemWindow, ReportIt
7 - Creating Reports	• Use pre-defined report template • Create customized templates	ReportIt
8 - Data Mining & Analysis	• Use patented Overlap Density Heatmaps for visual data mining • Create an overlap consensus spectrum	MineIt
9 - Quality Control Analysis	• Set up administrator account • Select a standard and compare sample	QC Expert

KnowItAll Software Training

General Features

General Features

Introduction to the Basic Applications in the KnowItAll Informatics System

Purpose

This exercise demonstrates the features of the KnowItAll environment.

Objectives

This exercise will teach you:

- How to open individual KnowItAll applications;
- How to access on-line help;
- How to transfer information from one application to another.

Background

All KnowItAll solutions are designed using a unique architecture that allows the seamless transfer of information from one software tool to another without having to leave the main interface.

Training Files Used in This Lesson

- Cholesterol.dsf

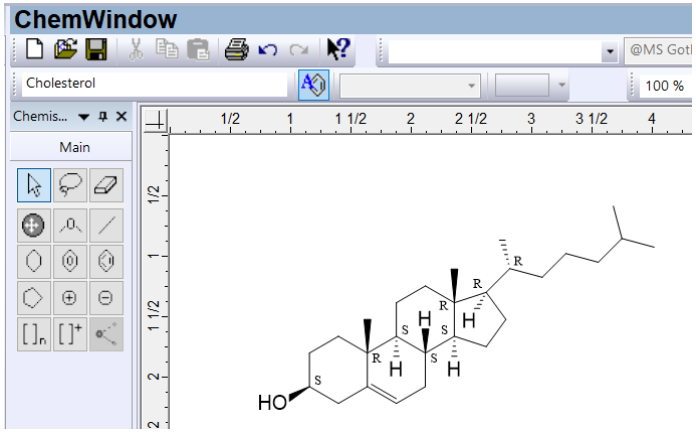
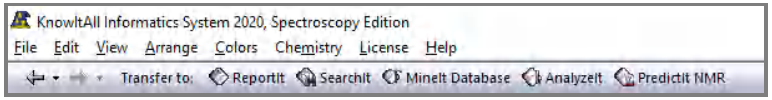
KnowItAll Applications Used

- BrowseIt™
- ChemWindow®
- SearchIt™
- ReportIt™

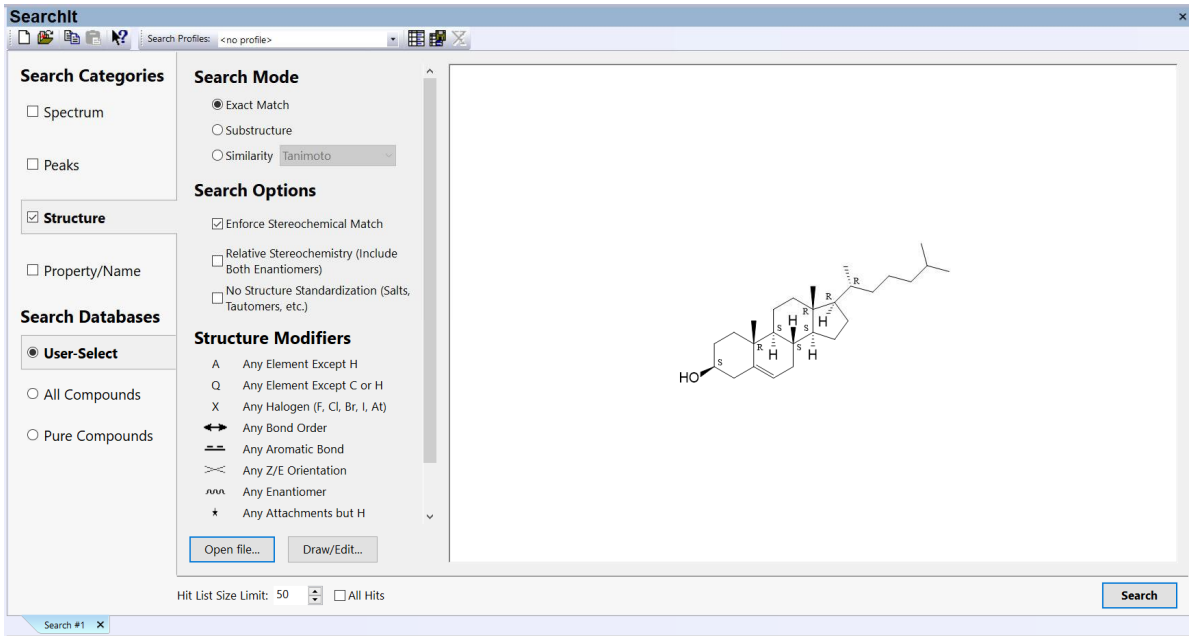
The KnowItAll environment

	Action	Result
1	Open the **KnowItAll Informatics System** by double-clicking its icon on the desktop.	The KnowItAll Informatics System automatically opens to the **BrowseIt** application. This application offers access to a web community designed especially for KnowItAll users and access to training movies and other information. Notice the KnowItAll interface integrates a series of software applications within logically grouped toolboxes, so the user can move from one task to the next and transfer information from one application to another. As you move throughout the KnowItAll Informatics System, notice that certain screen elements are shared by all applications (e.g., Title and Menu bars; Back / Forward buttons; Transfer/Return to bar; and Application Toolboxes.)
2	Explore the online **Help**.	Open the **Help** menu and choose **KnowItAll Help and Training**. This leads user to the online **Help** site.
3	Examine the contents of the **File**, **License**, and **Help** menus.	All KnowItAll Informatics System applications share the same Menu bar, located beneath the Title bar at the top of the application's window. The contents of the Menu bar change to reflect the current application as you move throughout the KnowItAll Informatics System. All applications include File, License, and Help menus. Other menus become available depending on the capabilities of each application.

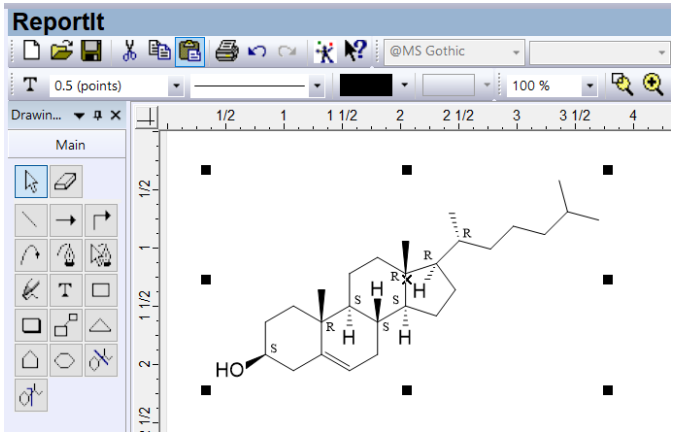
The KnowItAll environment (continued)

	6	Result
4	Click each toolbox title in the Application Toolbox area on the left edge of the application window.	Depending on the edition(s) you have, this area can have **Basics**, **Data**, **Spectral Processing** and **Spectral Analysis**. Click a toolbox title to open it. Click icons within the toolboxes to open and explore different KnowItAll applications.
5	Navigate to the **Basics** toolbox, then open the **ChemWindow** application by clicking its icon.	The application opens to a blank drawing pane.
6	• Choose **File > Open** • Navigate to **KnowItAll > Training Files > General Training > Files > General Features** • Open **Cholesterol.dsf**. **Note**: The **Files of type** filter on the **Open** dialog box allows you to specify which file types are displayed.	The structure opens in the drawing area:  A tab with the structure's name is added. Multiple tabs can be open at the same time.
7	Observe that the **Transfer to** bar (below the menu bar) now shows icons of the applications you can now transfer the structure to.	 You can use the **Transfer to** bar to transfer information or objects from one application to another in KnowItAll. The bar displays all the applications that can accept selected information or objects from the application that is currently in use.

The KnowItAll environment (continued)

	Action	Result
8	Click **SearchIt** in the **Transfer to** bar.	The structure is transferred to the **SearchIt** application: 

The KnowItAll environment (continued)

	Action	Result
9	Click the KnowItAll **Back** button (located below the **File** menu).	You are returned to the **ChemWindow** application. As you use different KnowItAll Informatics System applications, the KnowItAll **Back** and **Forward** buttons and corresponding drop-down lists become available. • Use the KnowItAll **Back** button to return to the most recently used application. • Use the KnowItAll **Back** button drop-down list to go back several steps. Once the KnowItAll **Back** button has been used, the KnowItAll **Forward** button and its drop-down list become available and can be used to move through KnowItAll applications in the opposite direction.
10	Click **ReportIt** in the **Transfer to** bar.	The structure opens in the **ReportIt** application, where you can create a standard report that includes this structure. 

KnowItAll Software Training

Simple Spectral Search / Identification with KnowItAll ID Expert

WILEY

Simple Spectral Search/Identification

How to Use KnowItAll® ID Expert™ to Perform a Simple Spectral Search/Identification

Purpose

These exercises demonstrate how to use KnowItAll® ID Expert™ to Identify IR, Raman and other spectra.

Objectives

These exercises will teach you:

- Perform single component searches, multiple component searches, designer drug classification & functional group analyses simultaneously and view results on a single screen for complete view of all possibilities for the unknown spectrum
- De-convolute industrial material to organic and inorganic chemicals
- How KnowItAll ID Expert's patented optimized corrections technology can help you to find the optimal search results
- Generate PDF report with a single click

Background

Training Files Used in This Lesson

- 2 - ATR-IR of Unknown Sample 8675309.irf
- 4 - ATR-IR of Unknown Sample 1282013.irf
- Deformulation Example.irf
- Mint Candy.wdf

KnowItAll Applications Used

- KnowItAll ID Expert

The KnowItAll ID Expert spectral identification software combined with the KnowItAll Spectral Libraries provides fast answers to scientists identifying unknown spectra.

It's easy to use. Simply open an unknown spectrum and KnowItAll ID Expert automatically performs single component searches, multiple component searches, possible designer drug classification and functional group analyses simultaneously and summarizes the results on a single screen to give a complete view of all possibilities for the unknown. It also can perform analysis using only pure organic and inorganic compound spectra, thus, breaks done industrial material into basic building blocks. If there are problems with the query spectrum, ID Expert has the spectral intelligence to identify issues and fix them using patented Optimized Corrections. Once the user has identified the unknown spectrum, a PDF report can be generated with a single click.

Optimized Corrections: A Breakthrough Technology for Spectral Searching

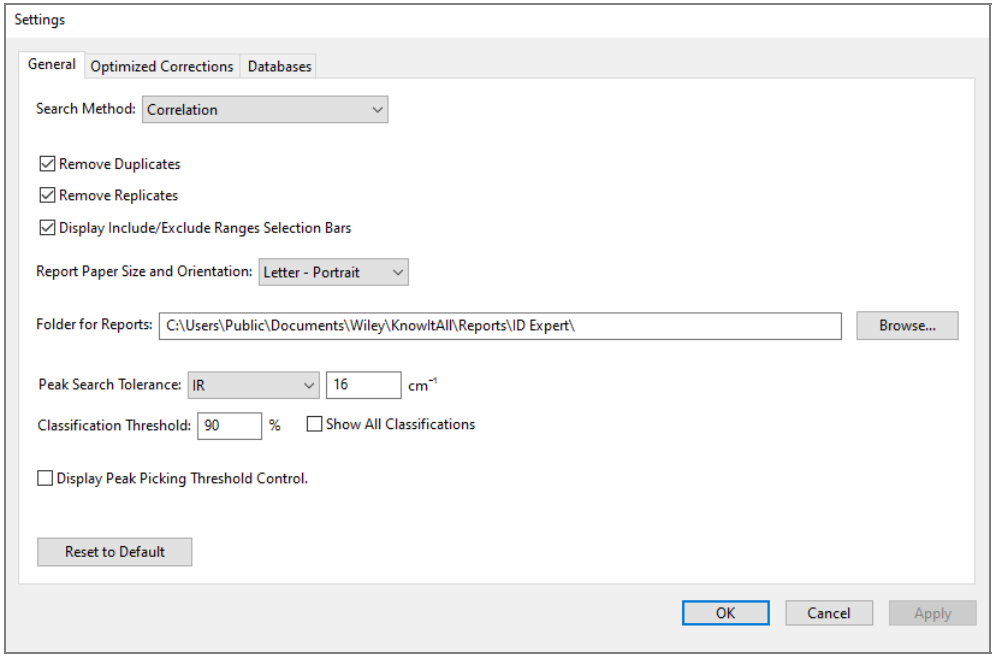
Spectral searching is one of the most important tools researchers use to classify or identify materials, yet it continues to be plagued by errors and imperfections. During a spectral search, a sample spectrum is compared to a database of reference spectra. To ensure that an optimal match is found in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

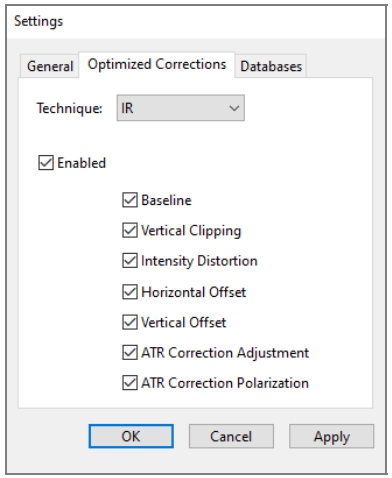
According to ASTM's guide on spectral searching[1], various algorithms and manual methods exist to adjust spectra to get reasonable match scores when two compared spectra of the same compound differ for various reasons. While these methods may work in select cases, subtle discrepancies such as a shift 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.

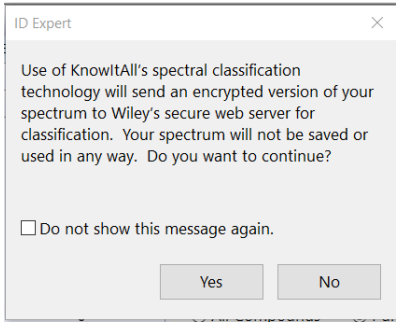
Manual corrections can be made by expert spectroscopists, but those less experienced in spectroscopy are often unaware of how to perform the necessary corrections on their sample spectrum to achieve the best search result. To address this growing concern, Wiley has introduced Optimized Corrections, a breakthrough patented technology that performs a computationally complex set of multiple corrections on all query and reference spectra in a search to find the optimal match between the query and each individual reference spectrum. We 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.

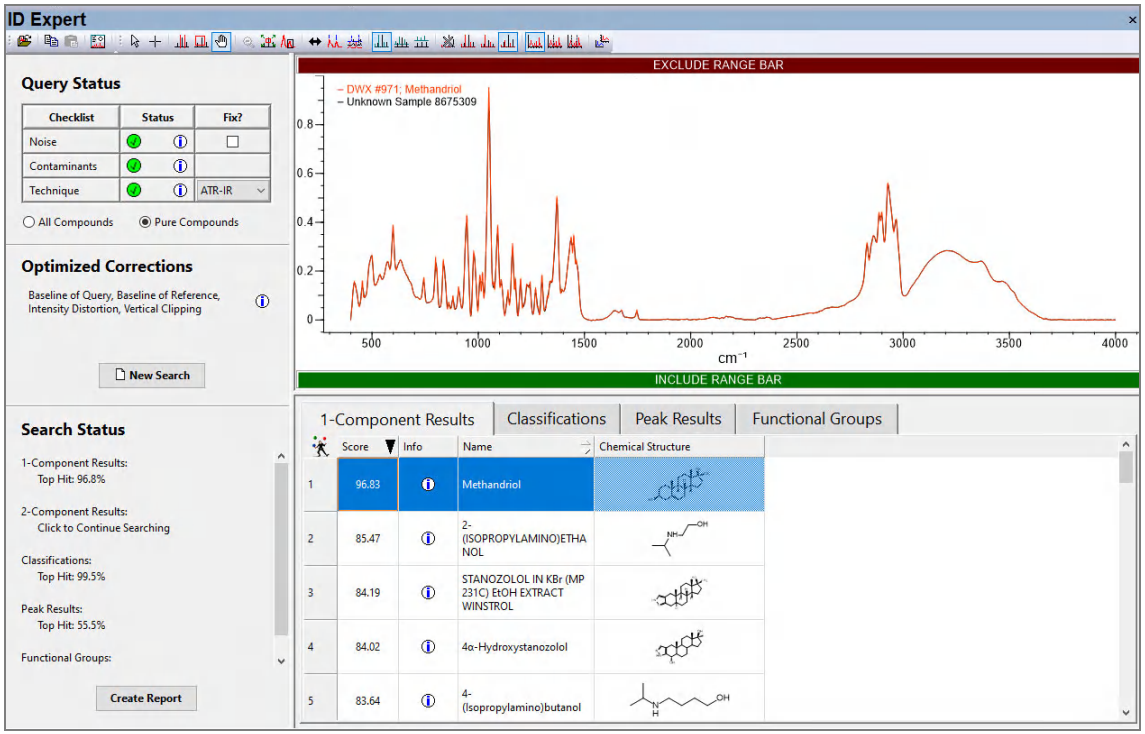
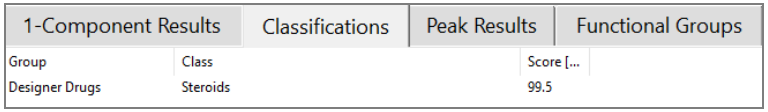
[1] E2310-04 - Standard Guide for Use of Spectral Searching by Curve Matching Algorithms with Data Recorded Using Mid-Infrared Spectroscopy, 2009. ASTM International Web Site. http://www.astm.org/Standards/E2310.htm (accessed March 4, 2015).

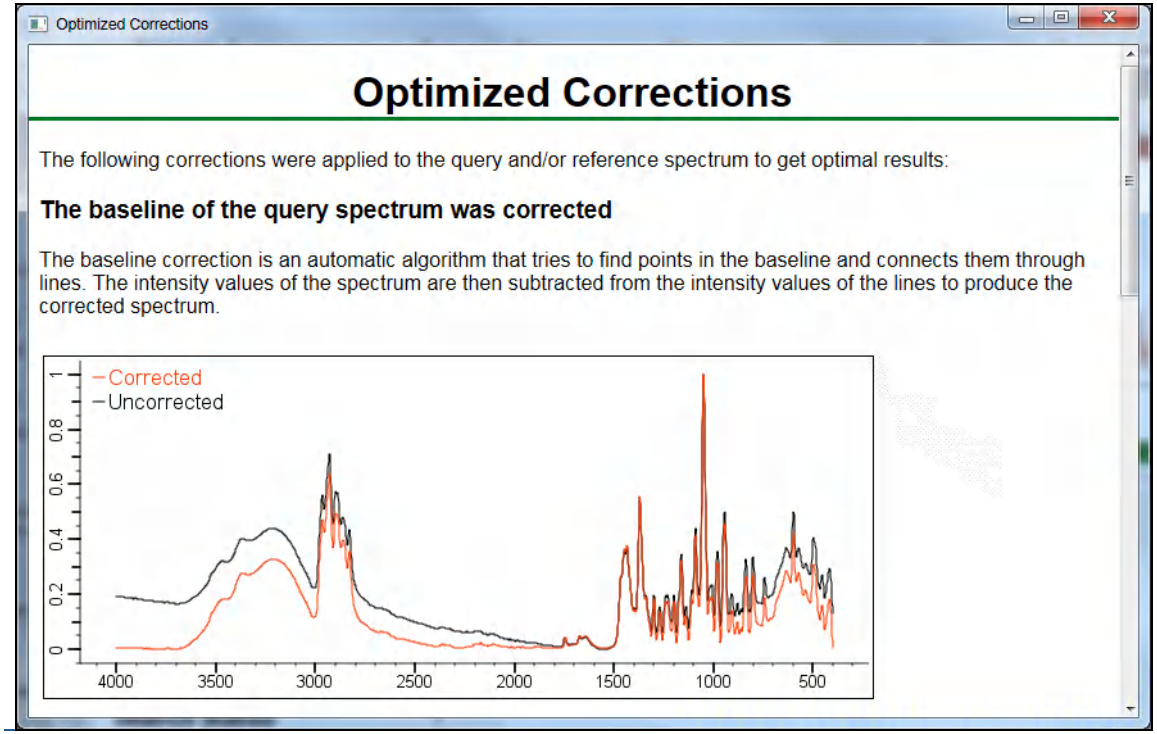
Example 1: 2-ATR-IR of Unknown Sample 8675309.irf

	Action	Result
1	Open the KnowItAll **ID Expert** application, either by double-clicking its icon on the desktop (standalone) mode or by clicking its icon in the KnowItAll application.	The application opens and a Windows **Open** dialog box pops-up.
2	Close the **Open** dialog box, then choose **File > Settings**.	The **Settings** form opens. 

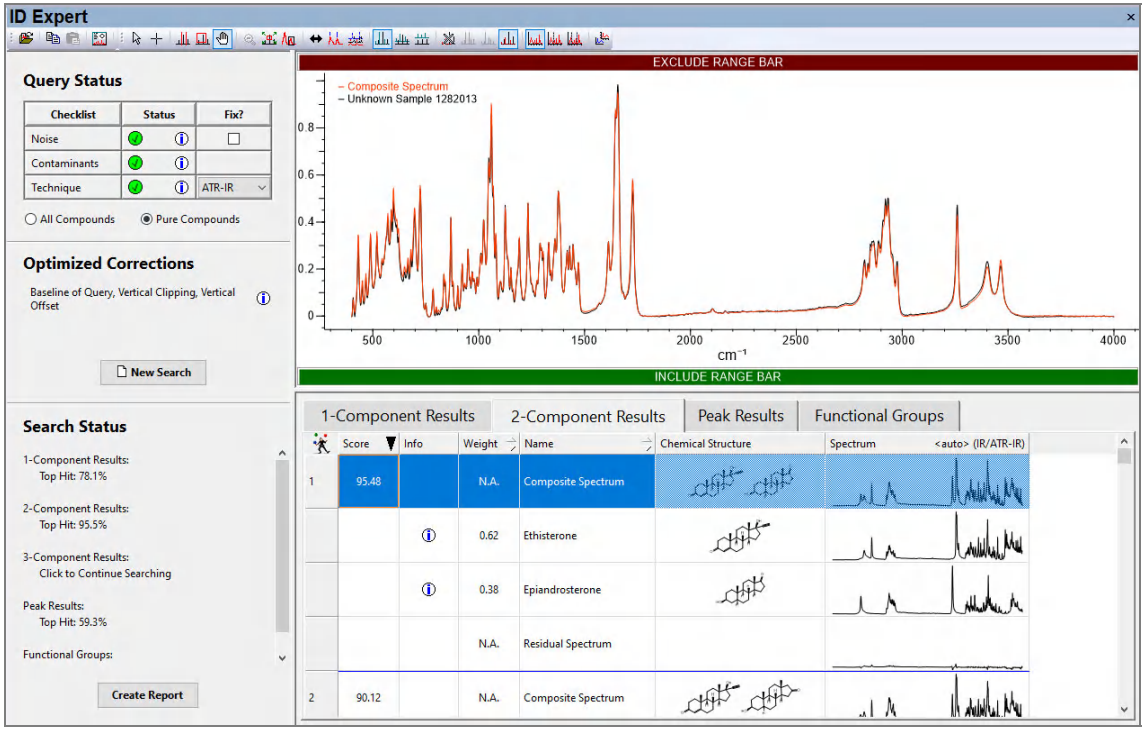
	Action	Result
3	Select the **Optimized Corrections** tab.	 By default, **Optimized Corrections** is enabled for IR, Near IR, Raman, and NMR spectra. With the **Optimized Corrections** checkbox enabled, you can specify which corrections you wish to apply for each spectral technique.
4	Check to see if **Optimized Corrections** for IR is enabled. Click **OK**.	The **Settings** form closes. The word “None” shows under **Optimized Corrections** on the main KnowItAll ID Expert window.

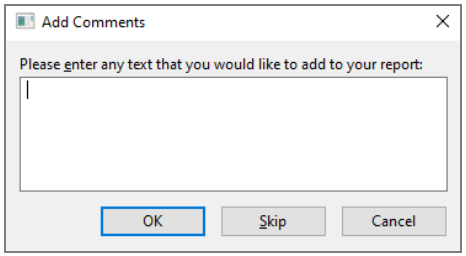
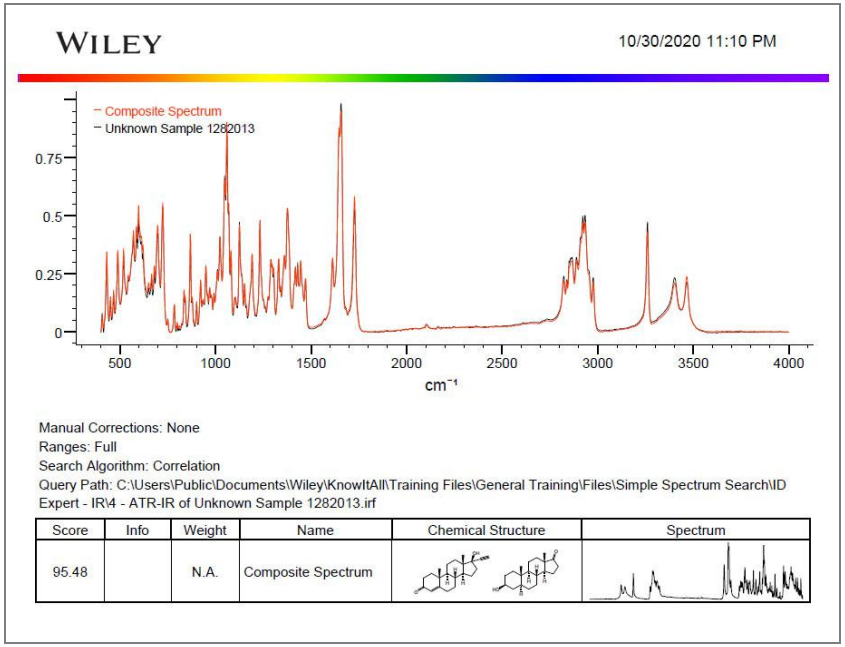
	Action	Result
5	• Click **New Search** in the middle left of the window • Navigate to KnowItAll > Training Files > General Training > Files > Simple Spectrum Search > ID Expert – IR • Select **2 - ATR-IR of Unknown Sample 8675309.irf**. • Check **Imported spectrum** is **ATR-IR** • Click **Open**.	User is prompted for a decision to send the spectrum to the secure Wiley web service for designer drug classification. 

	Action	Result
6	Click either **Yes** or **No**	The search proceeds automatically.  If user selected “Yes” in step 5, and the designer drug classification service return match score above **Classification Threshold** in step 2, then the **Classification** tab is displayed in result table, otherwise, you would not see it. The **Score** is the Hit Quality Index (**HQI**) in 100% unit – a comparison of reference spectrum to query spectrum.
7	Click the **Classification** tab.	 This spectrum is classified as a “Steroids” spectrum. This **score** measures probability for the classification.

	Action	Result
8	Click the information icon ⓘ in the main window's **Optimized Corrections** section.	The **Optimized Corrections** window opens.  Scroll down to view information about all of the optimized corrections that were applied.

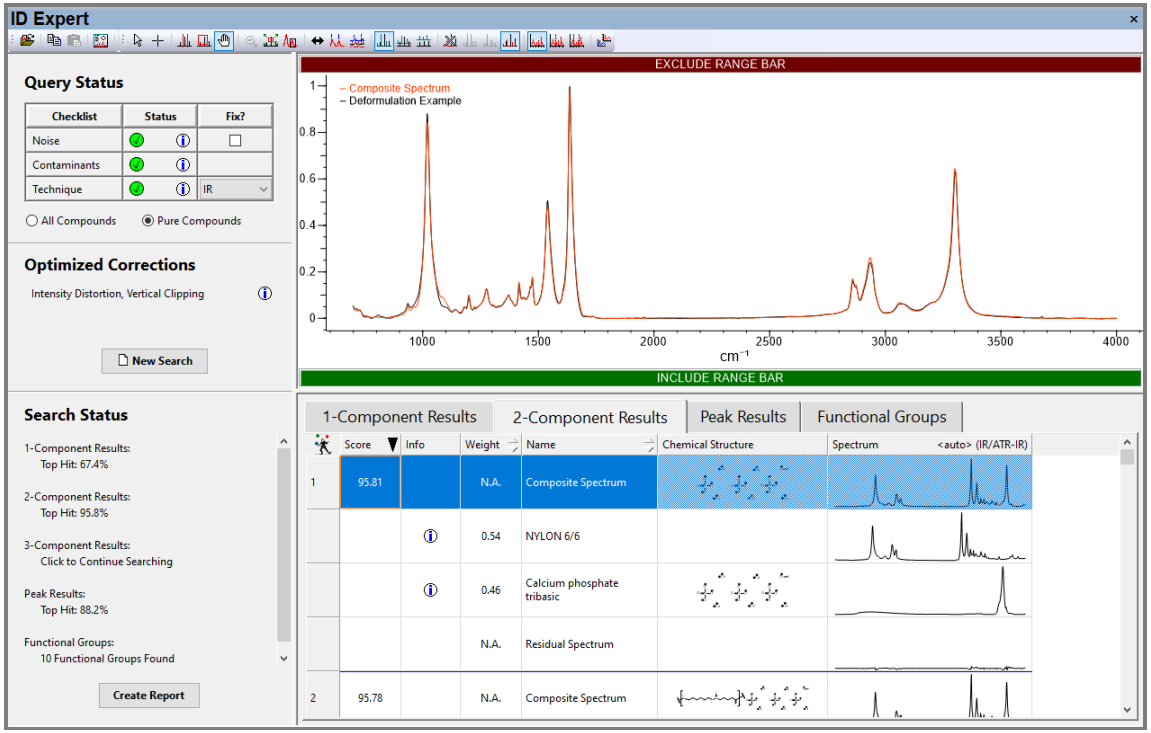
Example 2: 4-ATR-IR of Unknown Sample 1282013.irf

	Action	Result
1	Click **New Search**.	A Windows **Open** dialog box displays.
2	Open the spectral file **4-ATR-IR of Unknown Sample 1282013.irf**. Click **No** at the prompt for submitting the spectrum to Wiley's secure classification server.	The search proceeds automatically: There is no excellent 1-Component match, and KnowItAll ID Expert automatically examines multiple component matches.
3	Allow the search to complete.	The **2-Component Results** tab under **Search Status** flashes, indicating that a good match has been found.
4	Click the **2-Component Results** tab.	The Composite Spectrum, individual component spectra, and Residual Spectrum are displayed: 

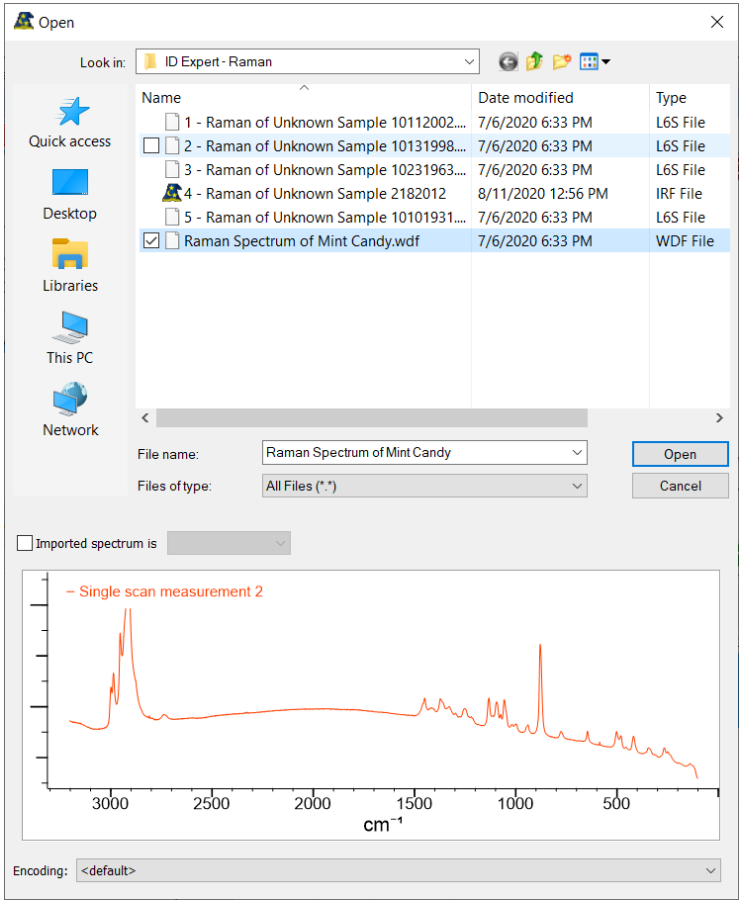
	Action	Result
5	Click **Create Report** below the **Search Status** section.	The **Add Comments** dialog box opens. 
6	Click **OK**.	The report is created, and automatically opens in the Adobe Acrobat Reader: 

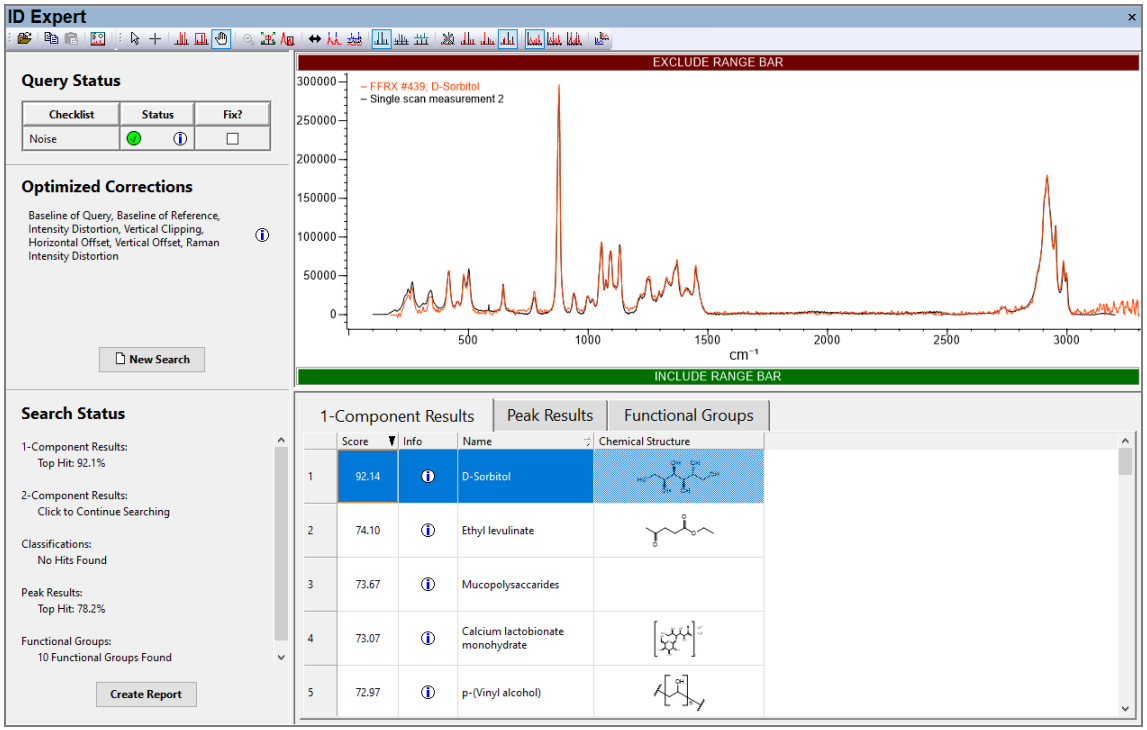
Example 3: Deformulation Example.irf

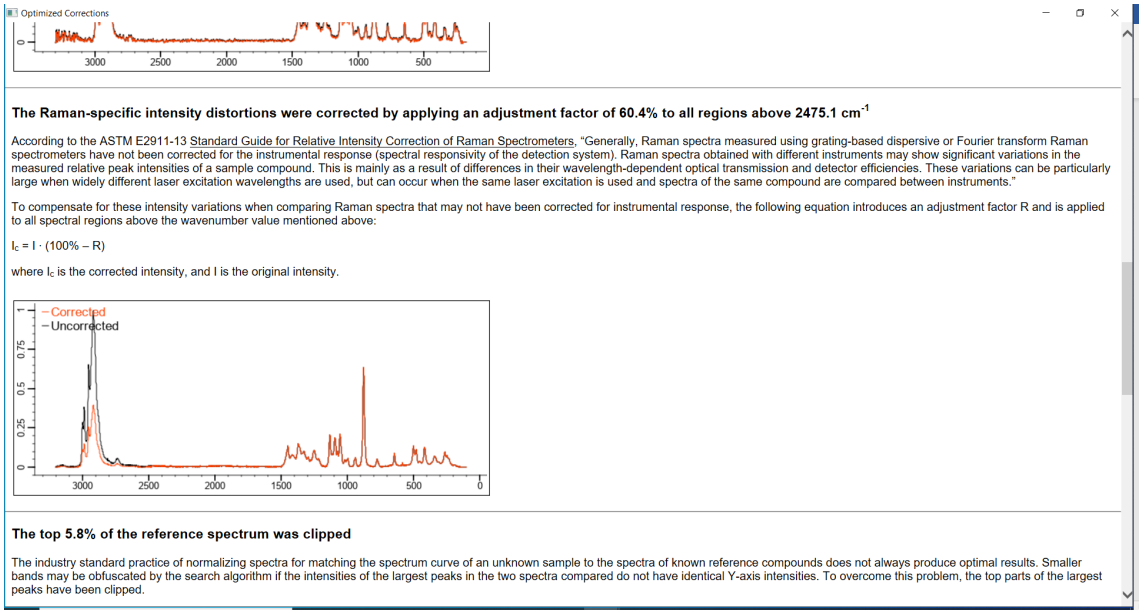
	Action	Result
1	Click **New Search**.	A Windows **Open** dialog box displays.
2	• Navigate to KnowItAll > Training Files > General Training > Files > Simple Spectrum Search > Deformulation • Select **Deformulation Example.irf** • Click **Open** • Click **No** at the prompt for submitting the spectrum to Wiley's secure classification server.	The search proceeds automatically: A perfect match is found – AKOLOUN S223-HM8. However, it is unclear what this material is made of.
3	Click the radio button **Pure Compounds**	ID Expert performs another search, but only on pure organic and inorganic chemical spectra.

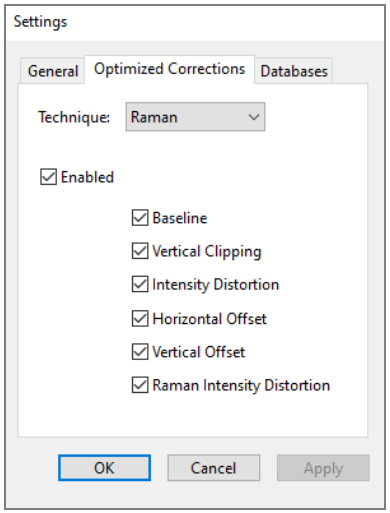
	Action	Result
4	Click the **2-Component Results** tab.	The Composite Spectrum, individual chemical component spectra, and Residual Spectrum are displayed. The sample is possibly made up of NYLON and Calcium salt: 

Example 4: 5 - Raman of Mint Candy.wdf

	Action	Result
1	Click **New Search**.	A Windows **Open** dialog box displays.
2	• Navigate to KnowItAll > Training Files > General Training > Files > Simple Spectrum Search > ID Expert – Raman • Select the spectral file **Raman Spectrum of Mint Candy.wdf** • Click **Open**	From the preview, this is not a “good” spectrum. 

	Action	Result
4	Allow the search to complete, then scroll through the **Search Status** area.	We have a very good match: 

	Action	Result
6	Click the ⓘ for **Optimized Corrections**	 We see that all kinds of spectrum correction have been done for the first hit. One unique to KnowItAll is the "Raman-specific intensity distortion.

	Action	Result
7	Go to **File > Settings**, **Optimize Correction** tab	These are the corrections done for Raman sample and reference spectra: 
8	As an exercise, one can check off **Enabled** and repeat the search to see a very different result.	

KnowItAll Software Training

Searching

Searching

How to Perform a Basic Spectral Search

Purpose

This exercise demonstrates how to perform a spectral search. In this exercise, we will perform a single spectral search, where we compare the IR spectrum of an unknown compound to IR spectra in a single database.

Objectives

This exercise will teach you:

- How to select databases for searching;
- How to use search masks;
- How to configure and perform an IR spectral search.

Background

Spectral searching against reference databases is frequently used in both the analysis of unknown compounds and compound verification.

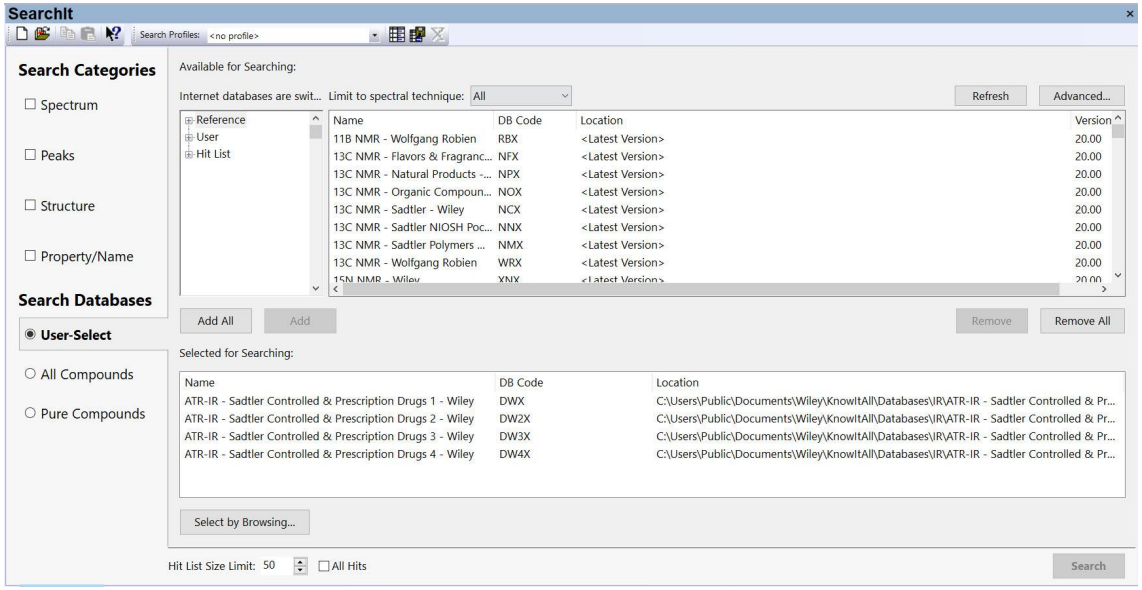
Training Files Used In This Lesson

- Acetic anhydride.dx
- Spectral Search Example.jdx.
- Multi-Technique Sadtler Demo Database – Wiley [DEMO].sdbx

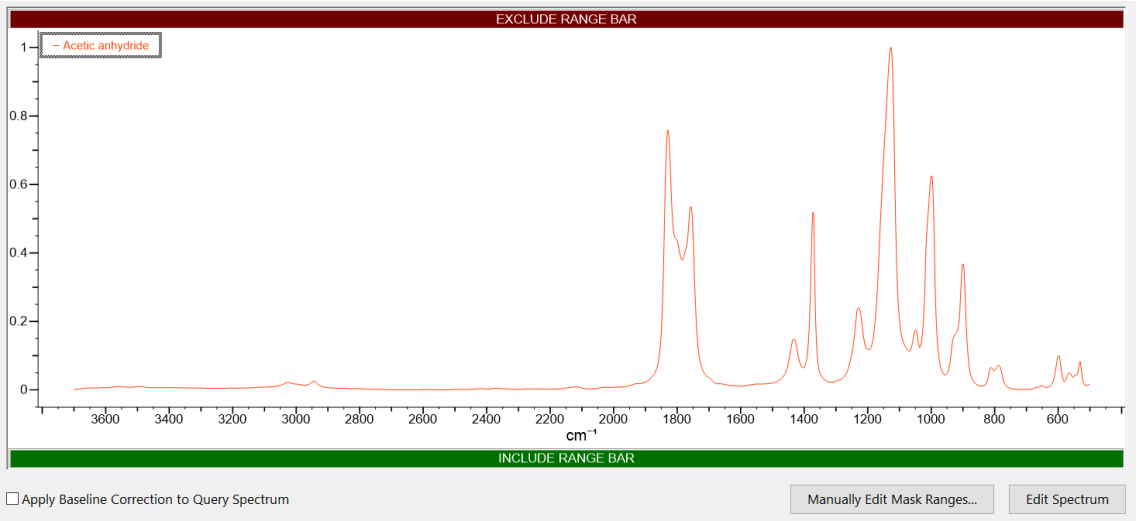
KnowItAll Applications Used

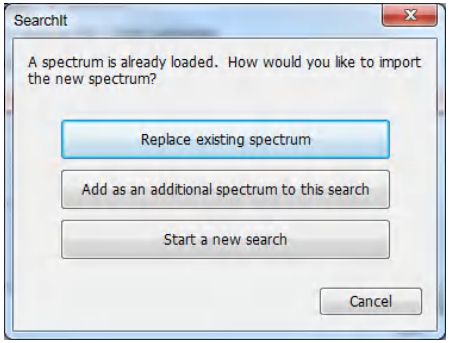
- SearchIt™
- MineIt™
- [optional] ProcessIt™

Create a new search

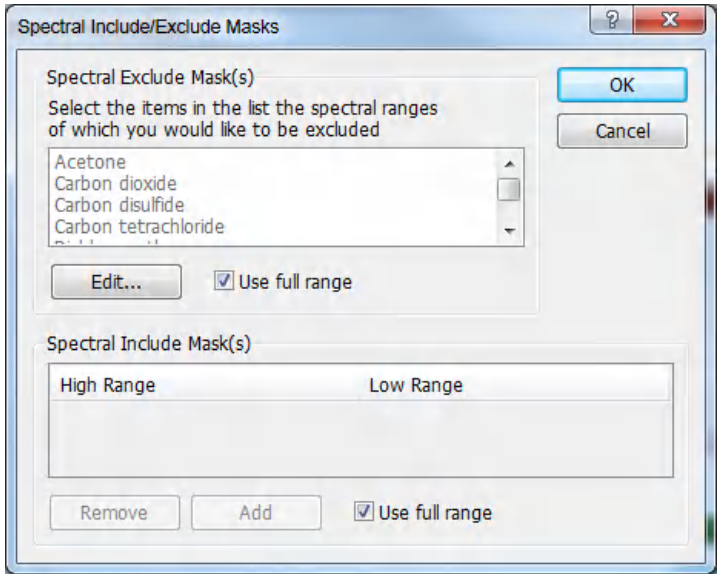
	Action	Result
1	Do one of the following: • If the **SearchIt** application is not open, navigate to the **Data** toolbox and click its icon. • If the **SearchIt** application is already open, click the **Close** button ☒ (located in the upper right corner) to close the current search.	If **SearchIt** application's **User-Select** (under **Search Databases**) tab is selected, the **Selected for Searching** list displays the databases last used. 

Open the spectral file

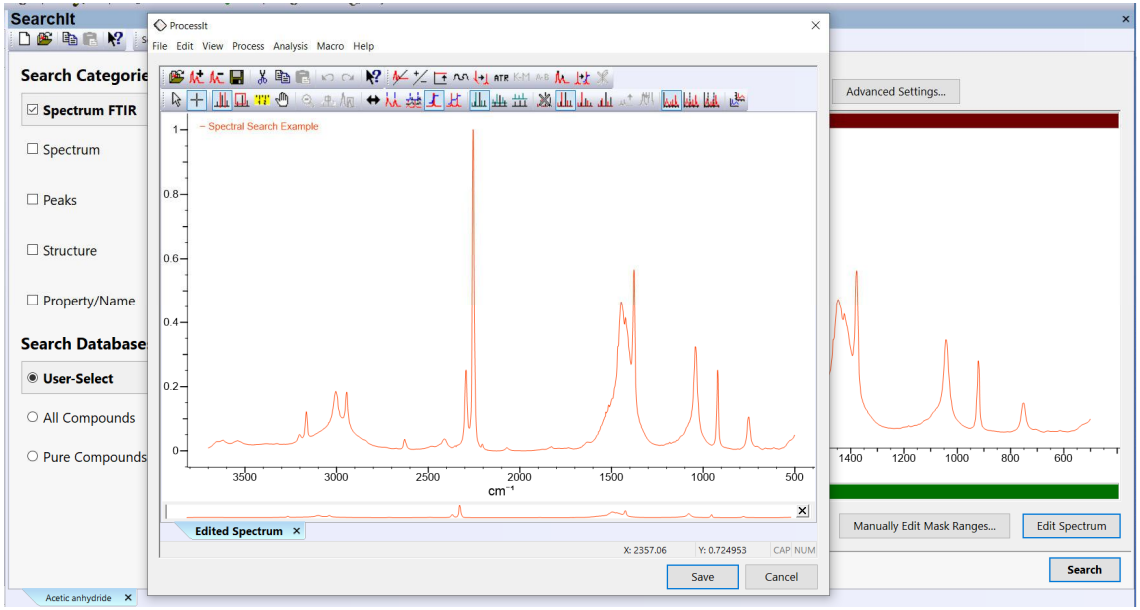
	Action	Result
1	Click the **Spectrum** button under **Search Categories**	An **Open** dialog box appears.
2	• Navigate to **KnowItAll > Training Files > General Training > Files > Searching** • Select **Acetic anhydride.dx**. The lower part of the dialog box displays a preview of the selected spectrum. 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 (*.*). • Click **Open**.	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 the query spectrum, if desired. However, KnowItAll automatically corrects baseline.***
3	To select a different spectral file, press Ctrl+O.	An **Open** dialog box appears.

	Action	Result
4	Select **Spectral Search Example.jdx** from the training files' **Searching** folder. Click **Open**.	A message box appears and offers three choices 
5	Click **Replace existing spectrum** to close the message box and replace the previously displayed spectrum.	The new spectrum is displayed in the spectral pane. **Note**: You can also replace a search spectrum by clicking the SearchIt **Close** button, then clicking the **Spectrum** button in the **Spectral** section of the **Search By** pane.

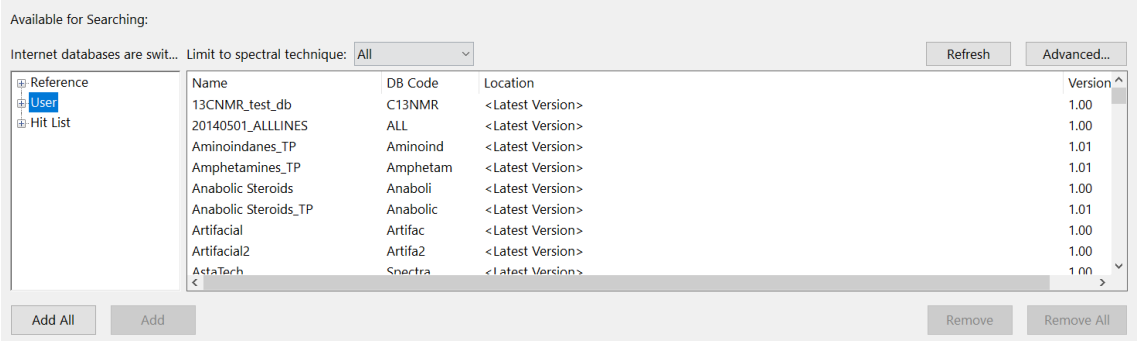
Fine-tune before searching

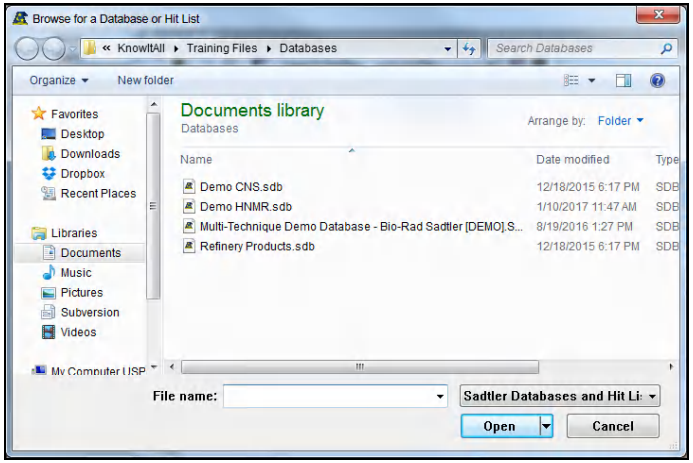
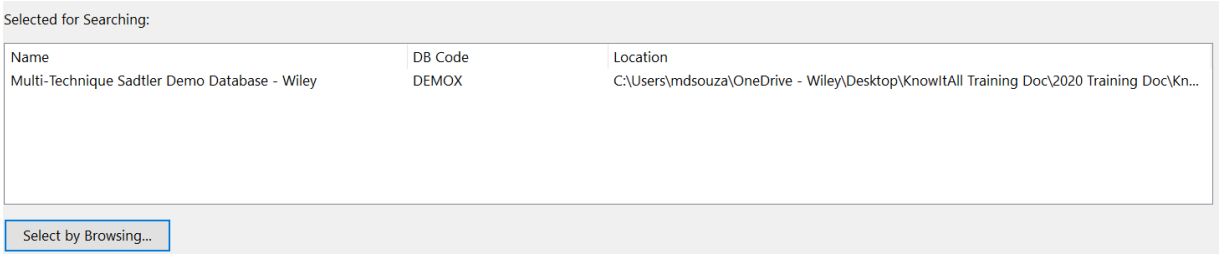
	Action	Result
1	Click **Manually Edit Mask Ranges**.	The **Spectral Include/Exclude Masks** dialog box opens:  **Note**: You can also click and drag in the **Spectral** pane's **Exclude Range Bar** and **Include Range Bar** after closing the **Spectral Include/Exclude Masks** window.
2	Deselect the **Use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

Fine-tune before searching (continued)

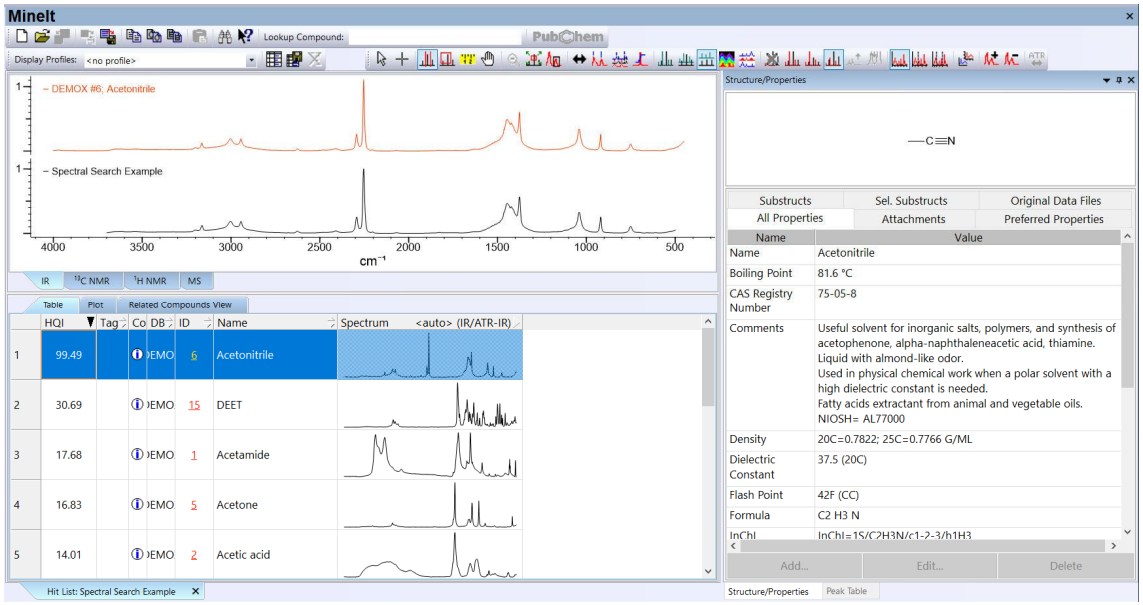
	Action	Result
3	Reselect the **Use full range** checkbox under the list of **Spectral Exclude Mask(s)**.	All Spectral Exclude Masks are removed from the spectrum.
4	Click **OK** to close the **Spectral Include/Exclude Masks** dialog box.	
5	Click **Edit Spectrum** at the bottom right of the spectral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

Open the search database

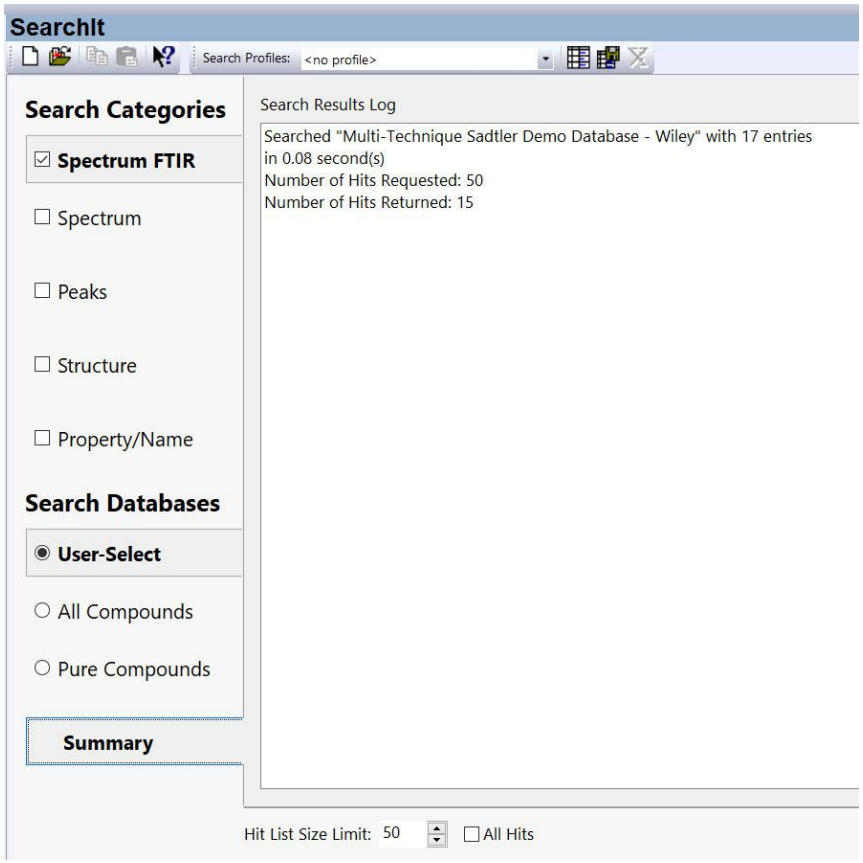
	Action	Result
1	Click on **User-Select** under **Search Databases**	This option allows users to select the databases they want to search. Users can also include user-created databases in a search.
2	If a list of databases already appears in the **Selected for Searching** pane at the bottom, click **Remove All** to clear this list.	
3	Expand each branch in the tree structure on the left of the window 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 **User** category is shown below:  **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.

	Action	Result
4	Click **Select by Browsing** button located at the lower left.	The **Browse for a Database or Hit List** dialog box opens. 
5	Navigate to KnowItAll > Training Files > General Training > Databases and open **Multi-Technique Sadtler Demo Database – Wiley (DEMO)**.	The database is displayed in the **Selected for Searching** list. 
6	If necessary, clear 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 search speed.	

Perform the search

	Action	Result
1	Click **Search**.	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** (Hit Quality Index) value measures how close the reference spectrum is to that of query.
	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.

Perform the search (continued)

	Action	Result
2	Click the KnowItAll **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. 
3	Click the KnowItAll **Forward** button .	You are returned to **MineIt** and the hit list.

Searching

How to Create Search Profiles

Purpose

This exercise demonstrates how to use search profiles.

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.

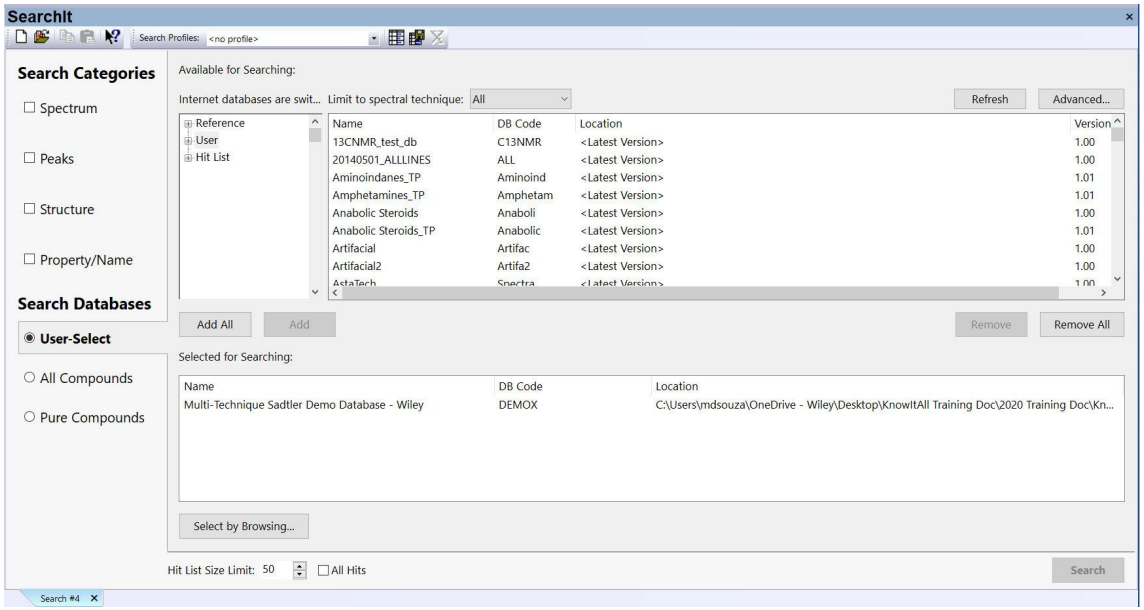
Training Files Used In This Lesson

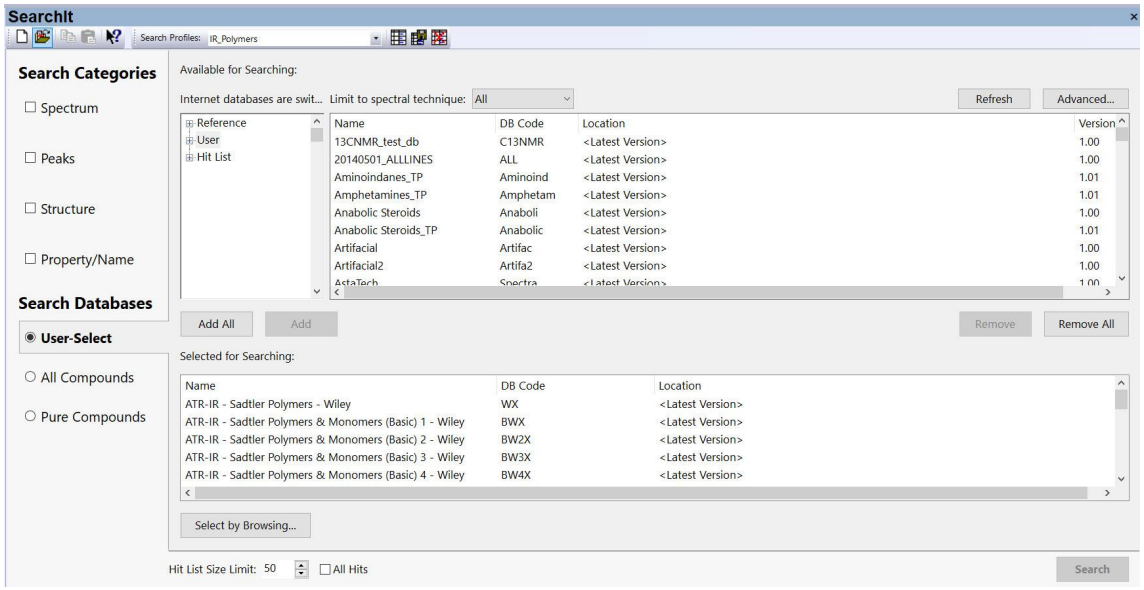
- none

KnowItAll Applications Used

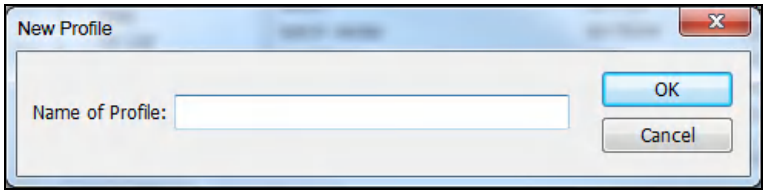
- SearchIt™

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 **Databases** 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.	
3	If necessary, choose **View > Profile Toolbar** to display Search Profiles tools.	

	Action	Result
4	Select the **IR_Polymers** profile.	Polymer databases are displayed in the **Selected for Searching** list. 

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

	Action	Result
7	Continue adding databases BMX, CRX, DAX, FRX, and NEX.	
8	On the **Databases** 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, then select the newly-created **IR_Polymers_2** search profile.	The databases and search settings associated with this profile are displayed.

Searching

How to Search a Database of Spectra or Chromatograms 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.

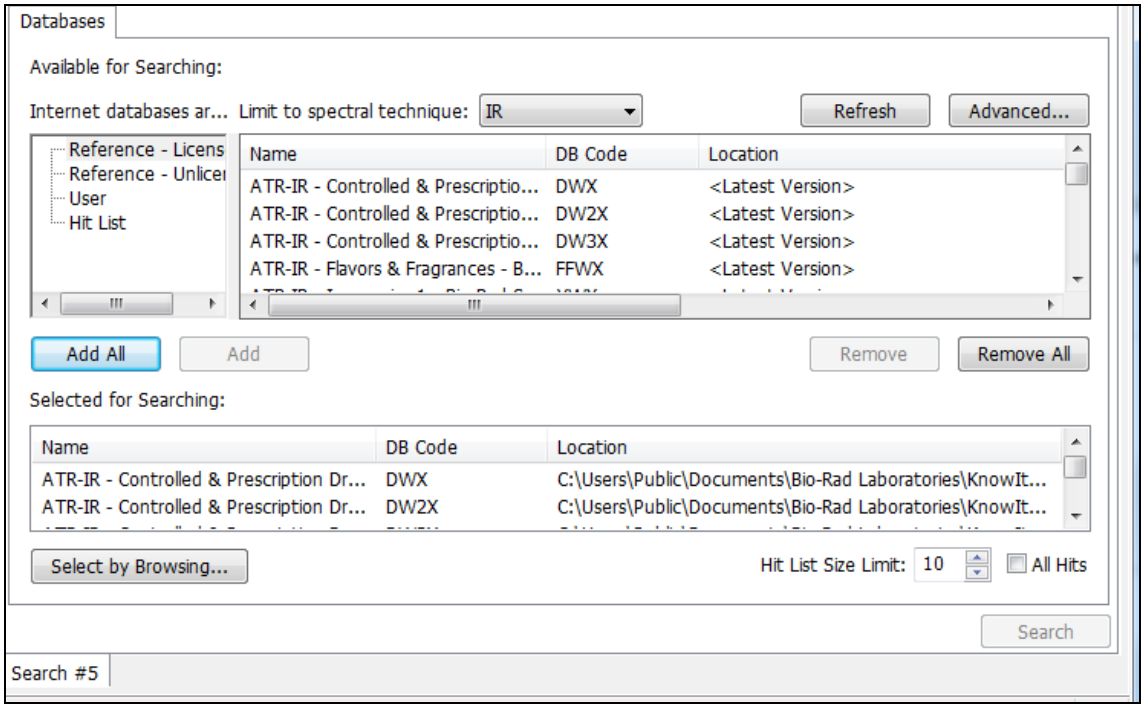
Training Files Used in This Lesson

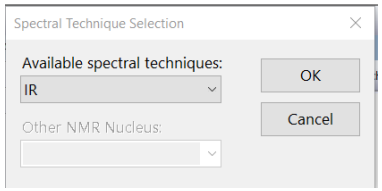
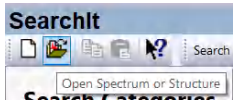
- Ethyl acrylate.dx

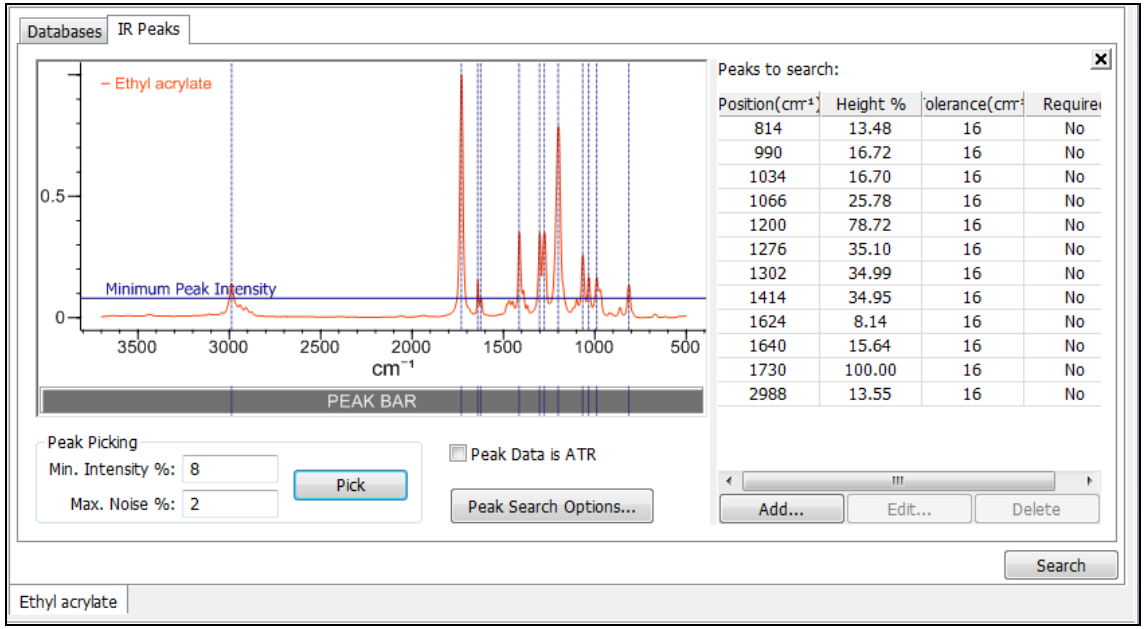
KnowItAll Applications Used

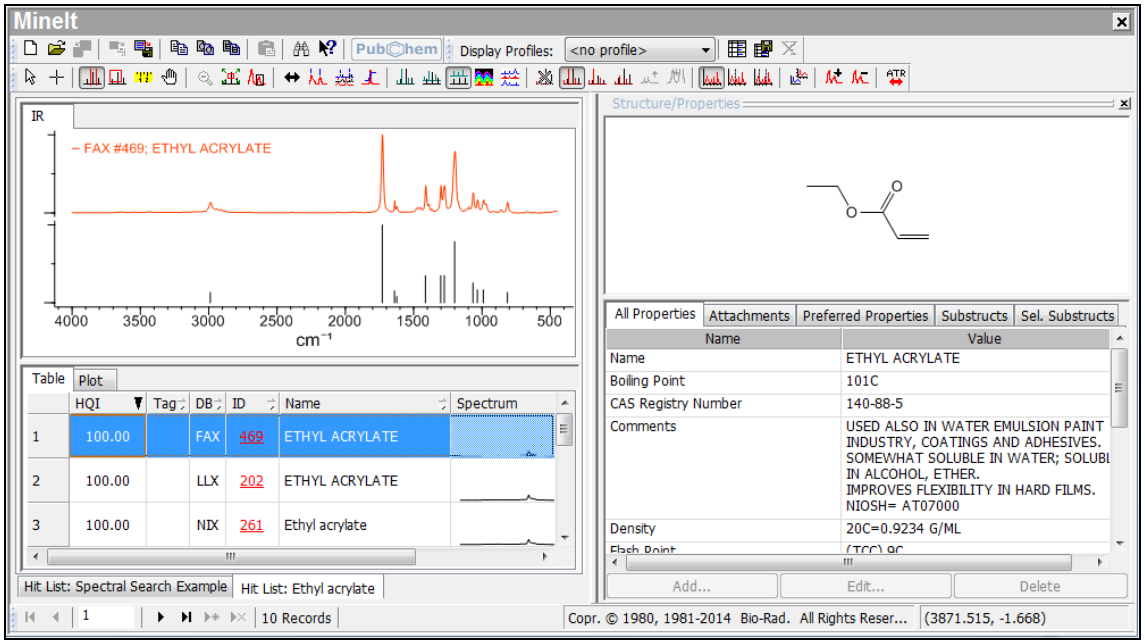
- SearchIt™
- MineIt™

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 **Databases** 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. • Set **Limit to spectral technique** to IR. • Click **Add All**.	

	Action	Result
3	• Under **Search Categories** click **Peaks.** • Choose **IR** in the pop-up dialog. • Click **OK.**	
4	Click **Open Spectrum or Structure**	
5	• Navigate to **KnowItAll > Training Files > General Training > Databases** • Open **Ethyl acrylate.dx**.	The spectrum is displayed.

	Action	Result
6	Click **Pick**.	The peak table is created based on the current settings. 
	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 also add or edit peaks using the corresponding buttons at the bottom of the table..

	Action	Result
7	Click **Search**.	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.

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

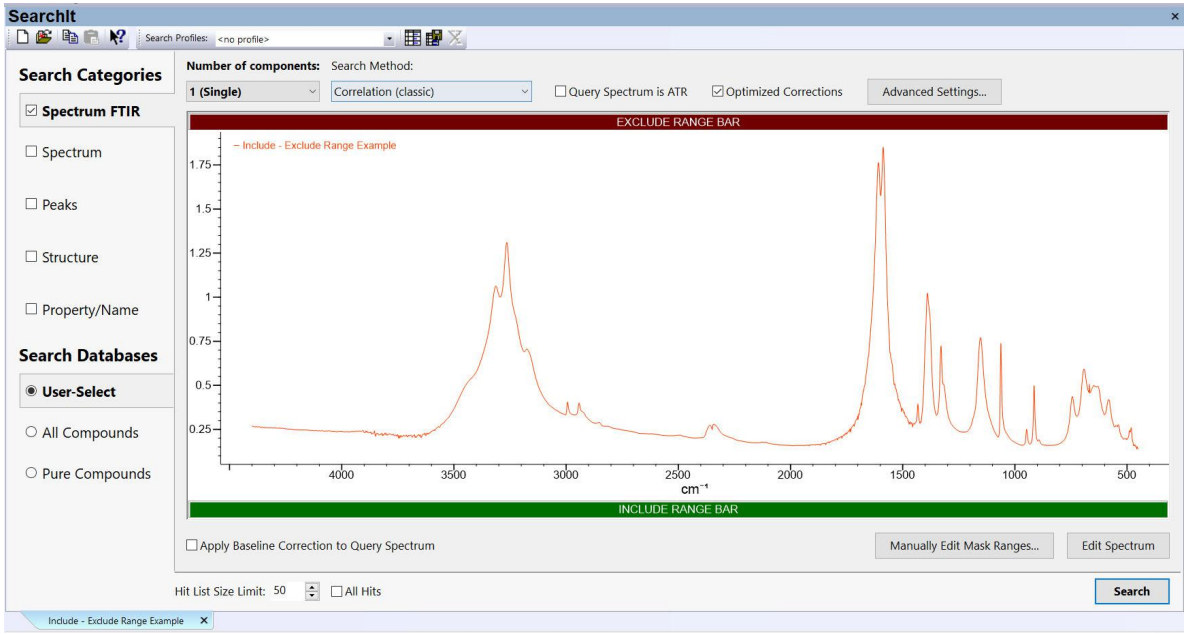
- Include – Exclude Range Example.jdx

KnowItAll Applications Used

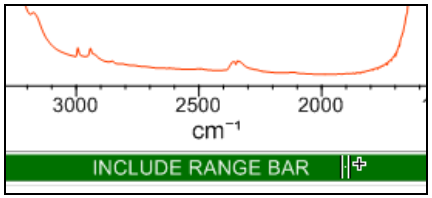
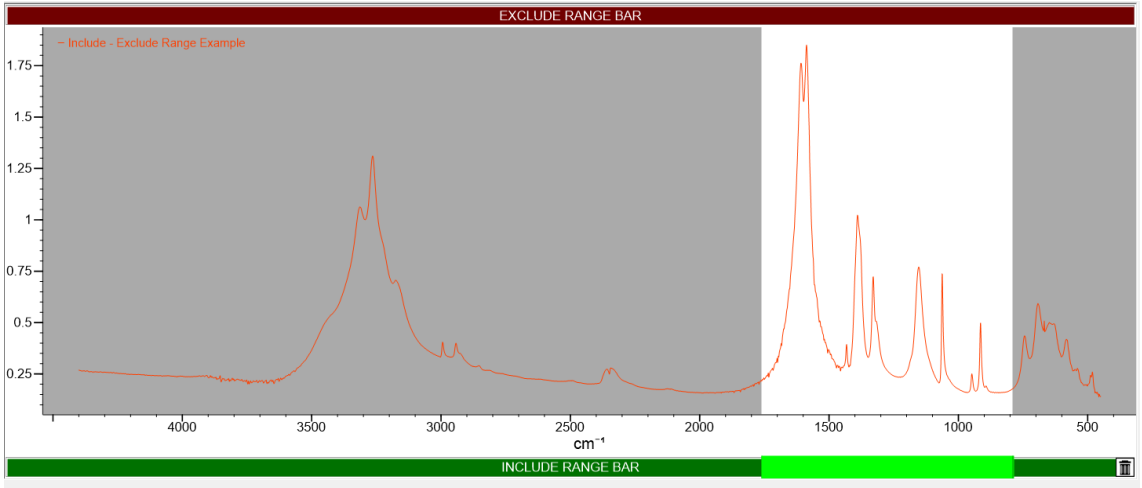
- SearchIt™
- MineIt™

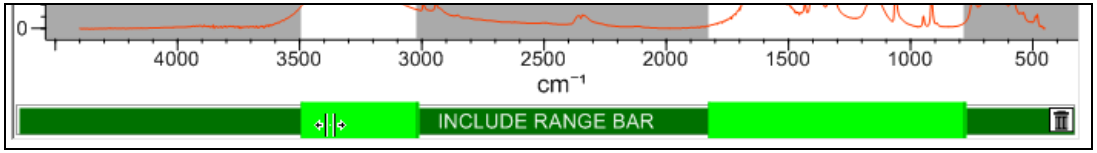
Configure a spectral search

	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 **Databases** 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.	
3	Click **Reference – Licensed** in the tree control.	**Name**, **DB Code**, and **Location** are displayed for the available databases. **Note**: Click **Advanced** to specify **Server Settings**, define local database paths, and find local databases. Expand the tree to view and select network and local database locations. You can also select user databases and hit lists for searching. Finally, you can locate a specific database by clicking **Select by Browsing**.
4	Click **Add All**.	Titles and locations are displayed in the **Selected for Searching** list**.**
5	Click **Spectrum** under **Search Categories**	An **Open** dialog box appears.

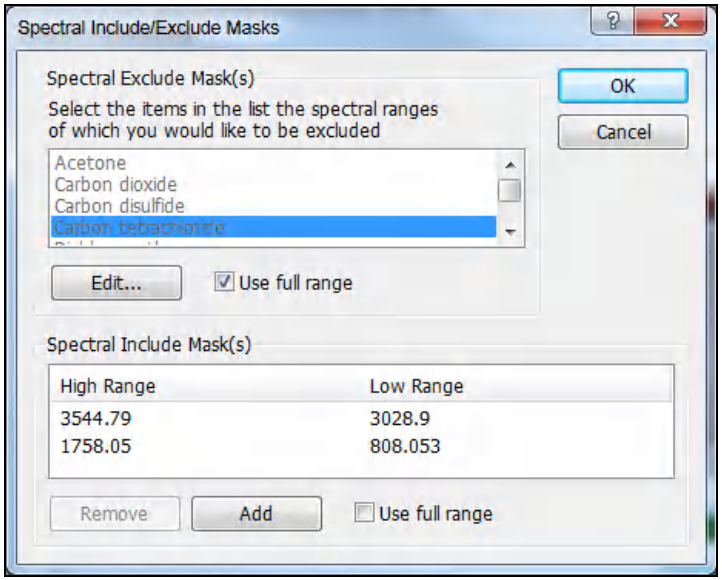
	Action	Result
	• Navigate to **KnowItAll > Training Files > General Training > Files > Searching** • Open **Include -Exclude Range Example.jdx**. **Note**: You can use the **Files of Type** filter to display JCAMP files (or all files).	The spectrum is displayed 

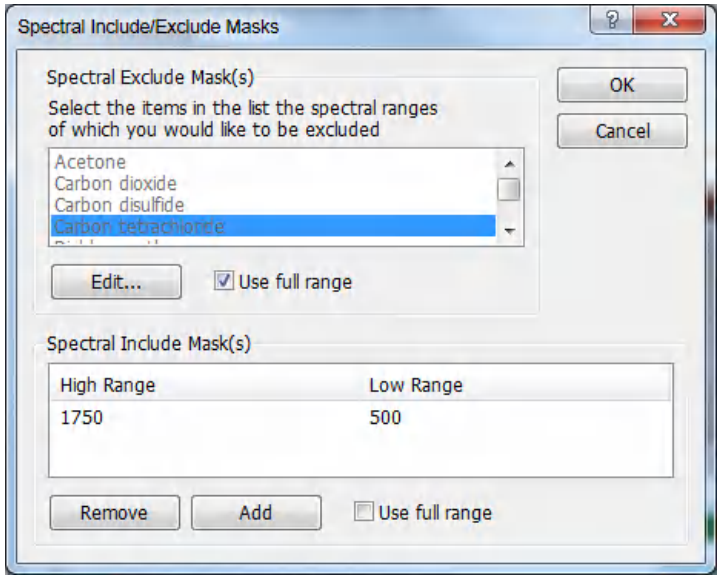
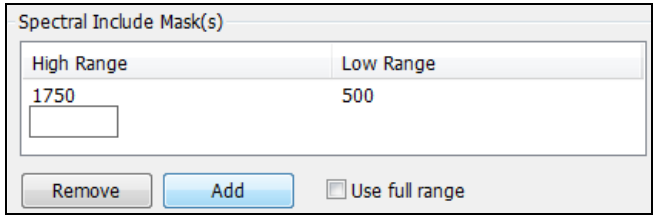
Use the Include Range bar

	Action	Result
1	Move the cursor over the **Include Range Bar** beneath the spectrum.	The cursor changes to a double pipe with a plus sign next to it: 
2	Click, drag, and release within the **Include Range Bar** to define an **Include** region.	The Include region is bright 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.

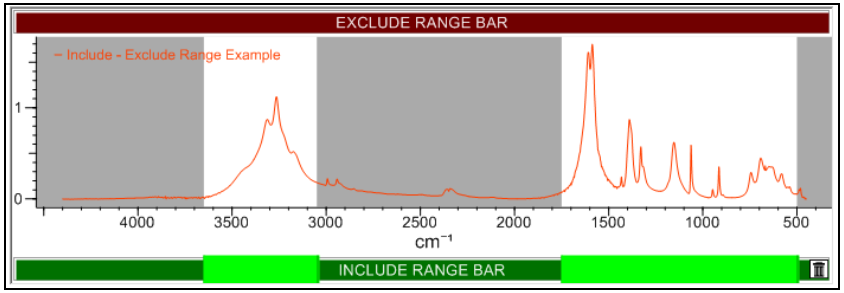
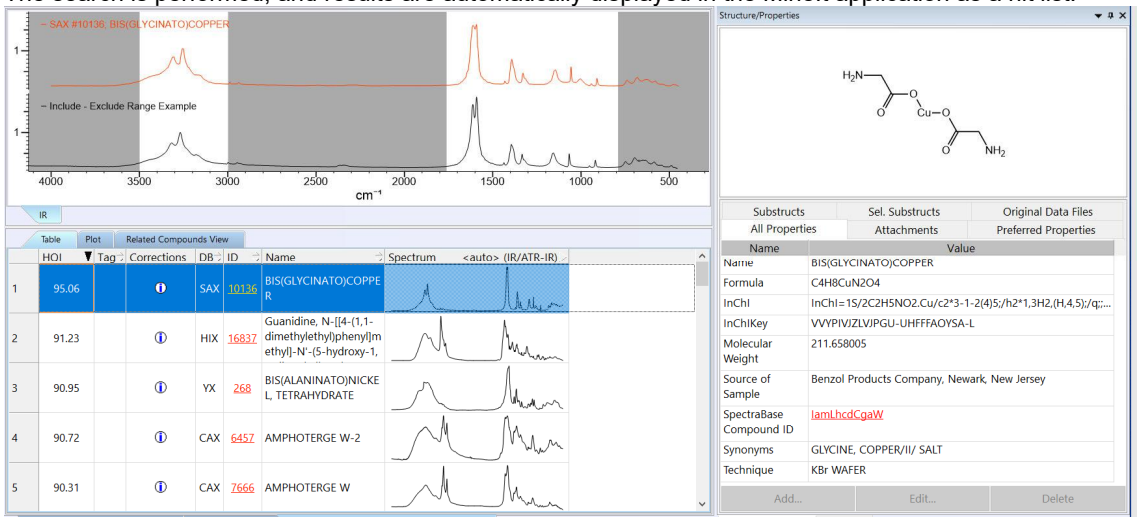
	Action	Result
3	Click and drag to define a second Include region.	
4	To move a region, click within the region on the **Include Range Bar** and drag to a new location.	
	TIP	To remove a single region, either click within the region on the **Include Range Bar** and drag to either side away from the spectral pane, or right-click within the region and choose **Yes** on the message box that opens. To remove all regions, click the garbage can icon at the right end of the **Include Range Bar**.
5	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: 

Use the Search Masks dialog box

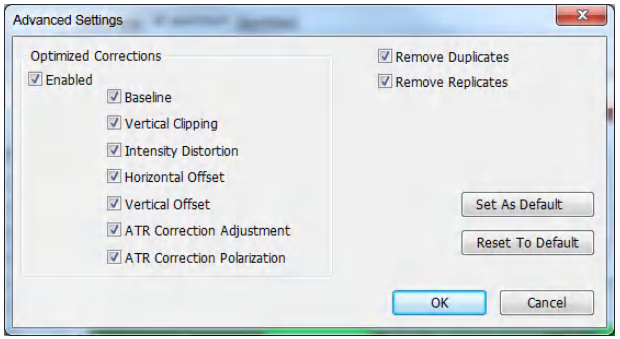
	Action	Result
1	Click **Manually Edit Mask Ranges**.	The **Spectral Include/Exclude Masks** dialog box opens:  Note that any **Include** regions defined using the **Include Range Bar** are displayed in the list of **Spectral Include Mask(s)**. However, if **Use full range** is checked, these regions will not be used.
2	Click to select one of the include regions, then click **Remove**. **Note**: You can select either the high or low value to remove an Include region.	The region is removed from the list.
3	Click to select the **High Range** value in the remaining Include region and type in '1750.'	

	Action	Result
4	Click to select the **Low Range** value in the remaining Include region and type in '500.'	
5	Click **Add** to create another Include region.	A text box with cursor appears in the **High Range** column: 
6	Type '3650' in the new **High Range** text box, then click in the **Low Range** column and type '3050.'	

Use the Search Masks dialog box (continued)

	Action	Result
7	Click **OK**.	The dialog box closes, and the search spectrum is displayed with the re-defined **Include** regions: 
8	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.

Use the Search Masks dialog box (continued)

	Action	Result
9	Close the **Optimized Corrections** window, then use the KnowItAll **Back** button to return to the SearchIt application. Click **Advanced Settings** on the IR Spectrum tab.	The **Advanced Settings** dialog box opens.  Use this dialog box to enable and customize **Optimized Corrections**.

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 allow 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 are not permanent, exclude masks can be saved and re-used.

Training Files Used In This Lesson

- Include-Exclude Range Example.jdx

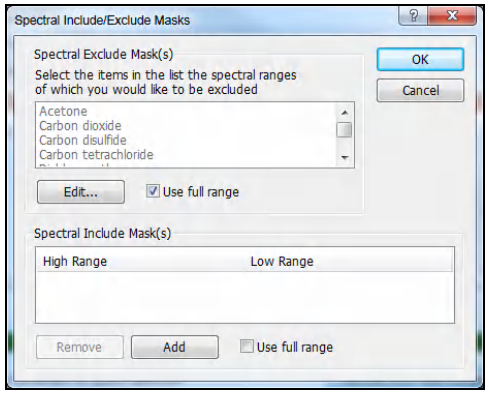
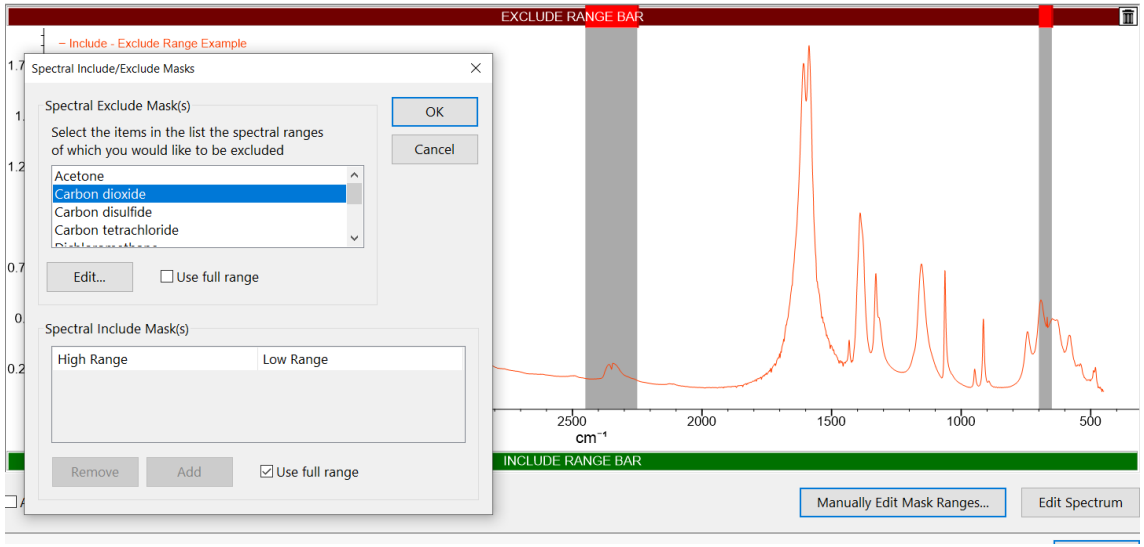
KnowItAll Applications Used

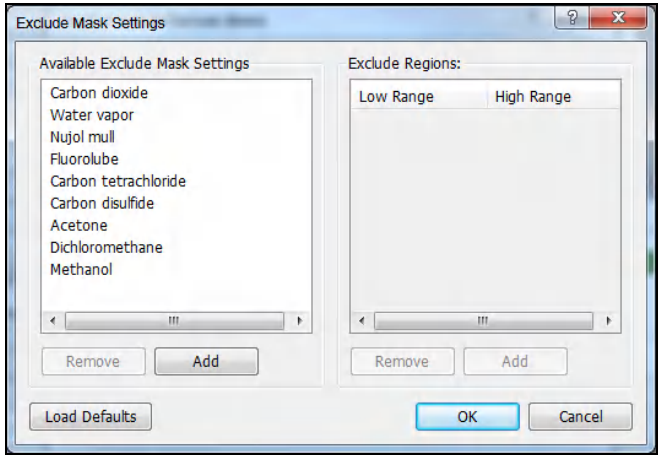
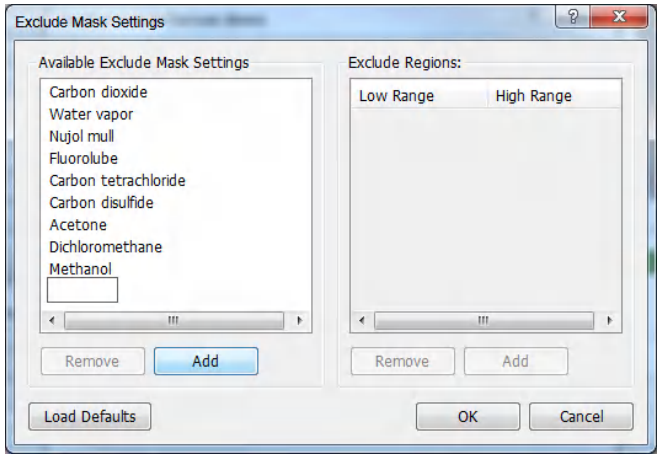
- SearchIt™
- MineIt™

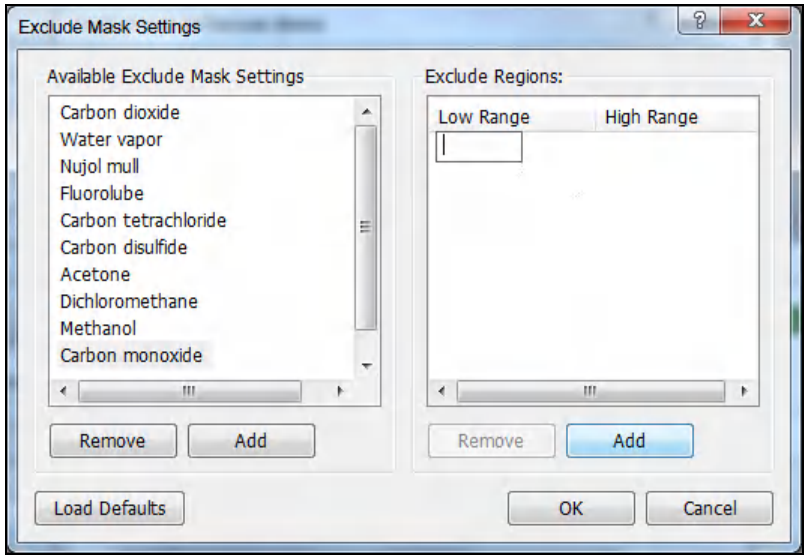
Configure a spectral search

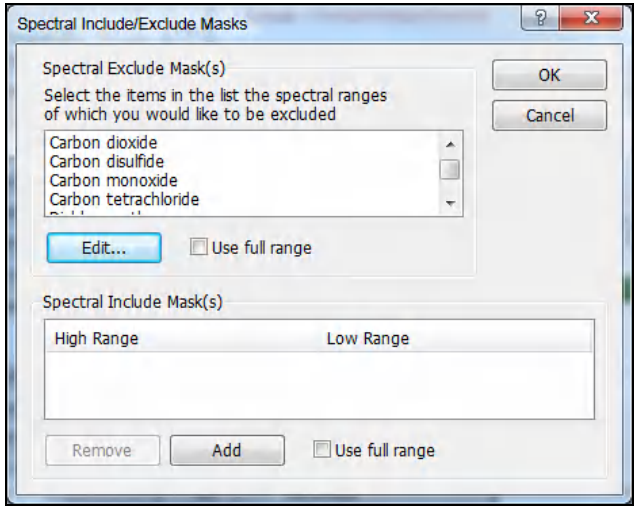
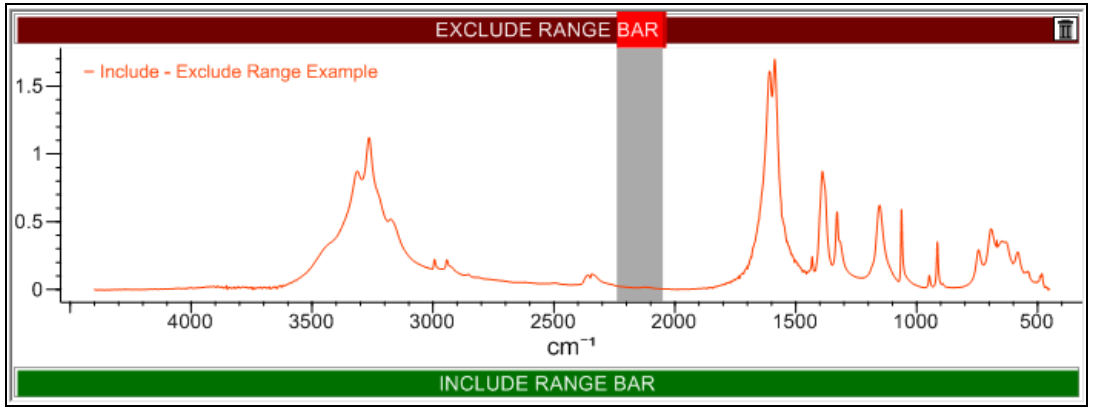
	Action	Result
1	Do one of the following: • If the **SearchIt** application is not open, navigate to the **Data** toolbox and click its icon. • If the **SearchIt** application is already open, click the SearchIt Close button to close the current search	The SearchIt application's **Databases** tab is displayed, 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.	
3	Click **Reference – Licensed** in the tree control.	**Name**, **DB Code**, and **Location** are displayed for the available databases. **Note**: Click **Advanced** to specify Server Settings, define local database paths, and find local databases. Expand the tree to view and select network and local database locations. You can also use user databases and hit lists for searching. Finally, you can locate a specific database by clicking **Select by Browsing**.
4	Select IR using the **Limit to spectral technique** control.	Only databases having IR spectra are displayed. **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.
5	Click **Add All**.	Titles and locations are displayed in the **Selected for Searching** list.
6	Click **Spectrum** under **Search Categories**	An **Open** dialog box appears
7	• Navigate to **KnowItAll > Training Files > General Training > Files > Searching.** • Open **Include-Exclude Range Example.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.

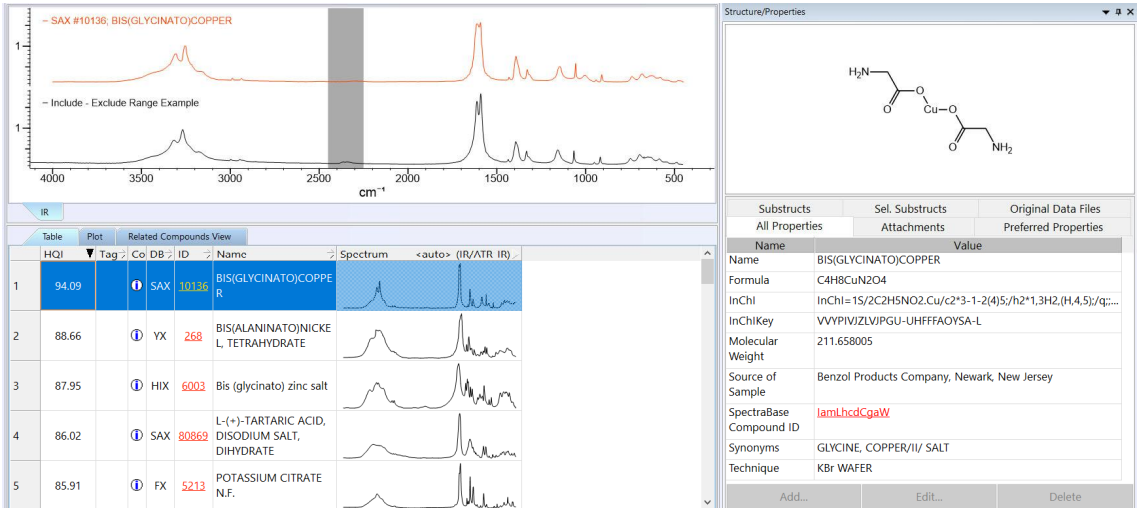
Use the Search Masks dialog box

	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 **Carbon dioxide** 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. 

	Action	Result
3	Click **Edit** on the **Spectral Include/Exclude Masks** dialog box.	The **Exclude Mask Settings** dialog opens: 
4	Click **Add**.	A text box appears under **Available Exclude Mask Settings**. 

	Action	Result
5	Type in **Carbon monoxide**, then click outside the text box.	
6	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**.	A text box appears under **Exclude Regions**. 
	TIP	Alternatively, you can also 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 exactly the same way as manually setting the include range.

	Action	Result
7	Type in low and high range values (2050 and 2240), then click **OK**.	The **Exclude Mask Settings** dialog box closes, and the new carbon monoxide mask is added to the list of exclude masks: 
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: 

	Action	Result
9	Click **Search**.	The search results are automatically displayed in the **MineIt** 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.

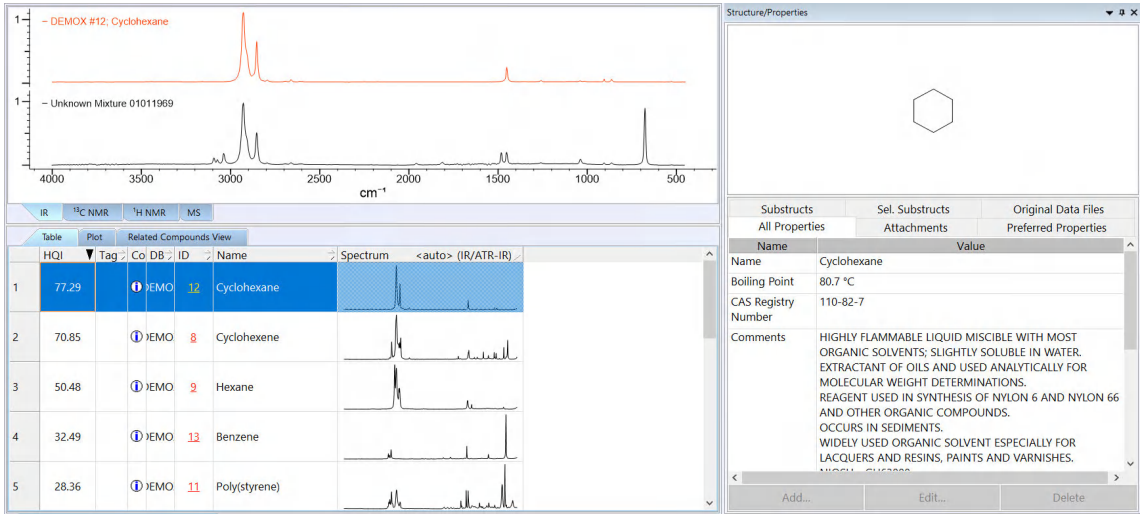
Training Files Used In This Lesson

- Unknown Mixture 01011969.jdx

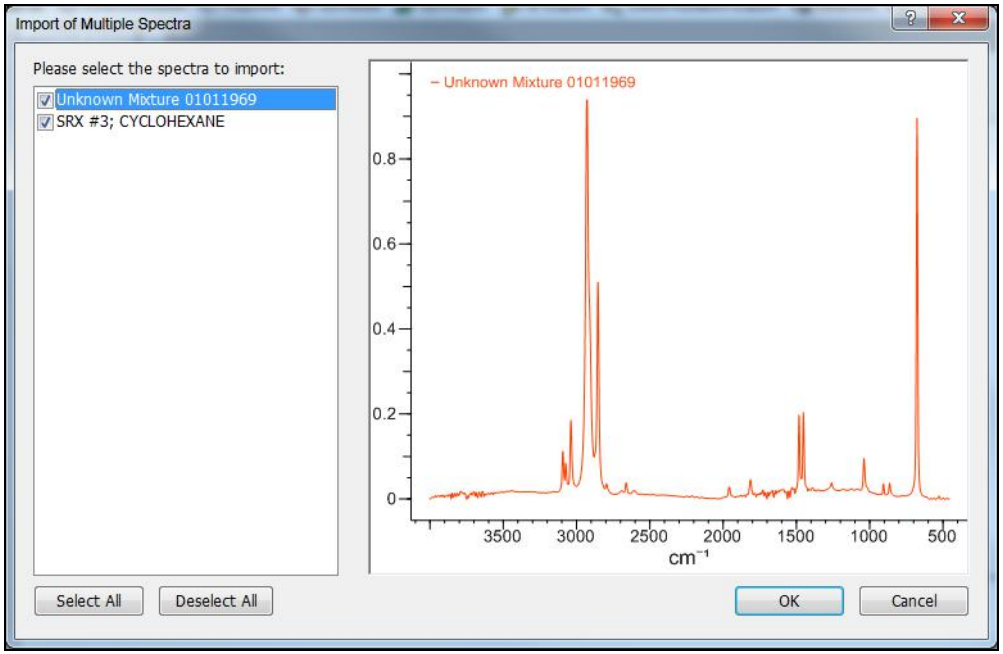
KnowItAll Applications Used

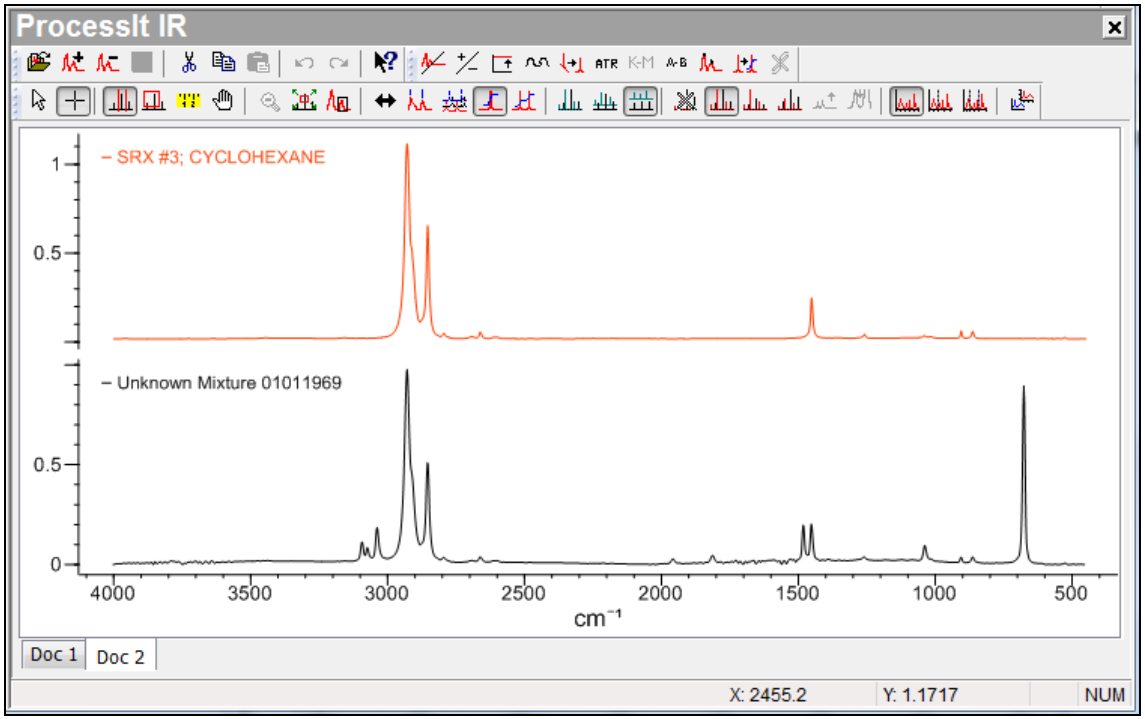
- SearchIt™
- MineIt™
- ProcessIt™ IR

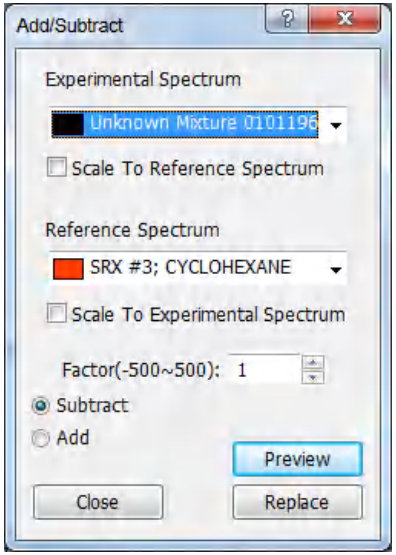
Set up a spectral search against a mixture

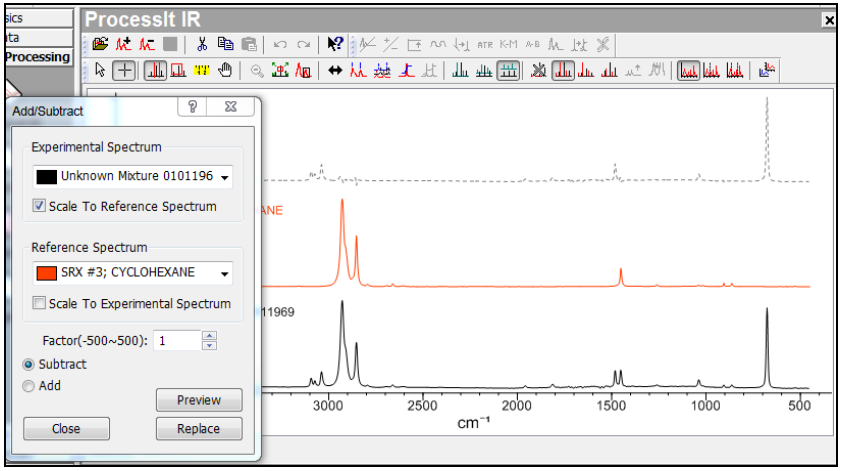
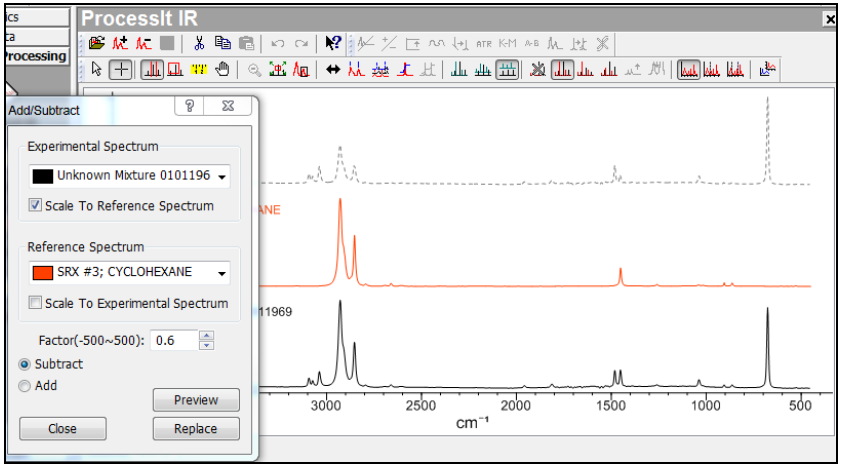
	Action	Result
1	In the **SearchIt** application, set up and perform an IR spectral search using **Unknown Mixture 01011969.jdx** located **in KnowItAll > Training Files > General Training > Files > Searching** folder, and the **Multi-Technique Sadtler Demo Database – Wiley**. ***TIP*** In the **SearchIt** application, click on the **DB Code** column to sort databases alphabetically by code in ascending or descending order.	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. 

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.

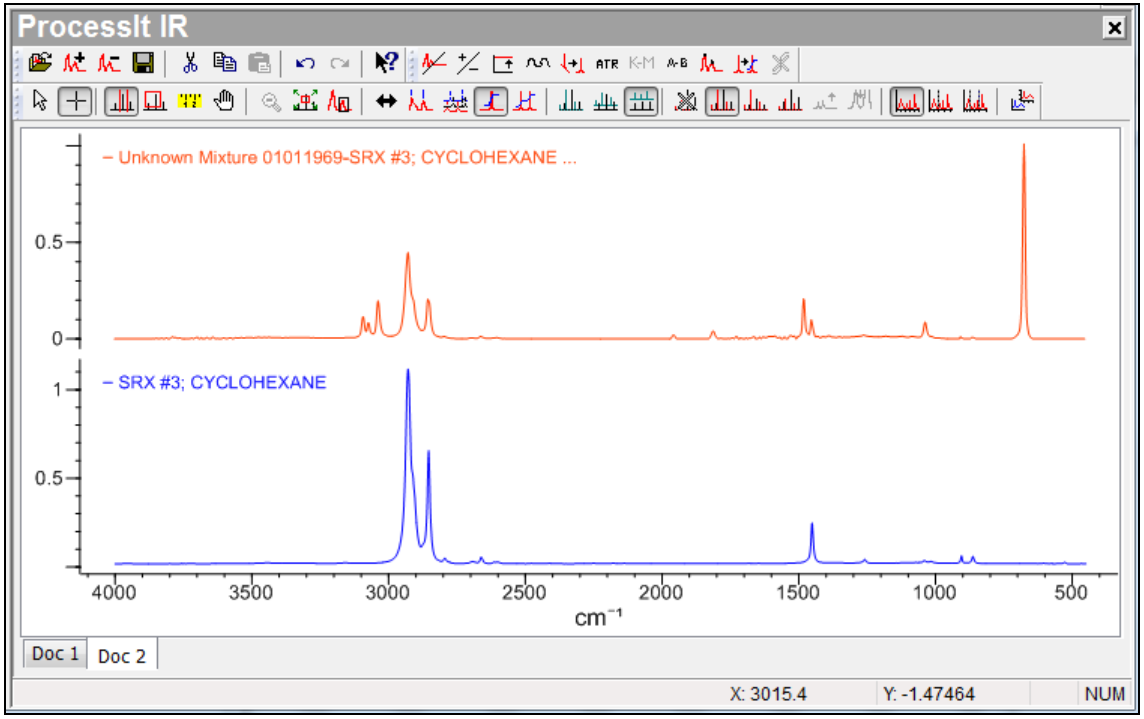
	Action	Result
2	Click **Select All**, then click **OK** on the **Import of Multiple Spectra** dialog box.	Both spectra – the mixture and the first hit, cyclohexane - are transferred to the **ProcessIt** IR application.  **Note**: Use spectrum toolbar buttons to adjust the display. The Stacked display is preferable to Offset or Overlay for spectral subtraction.

	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.	
5	Check **Scale to Reference Spectrum**, set **Factor** to 1, and make sure the **Subtract** radio button is selected.	

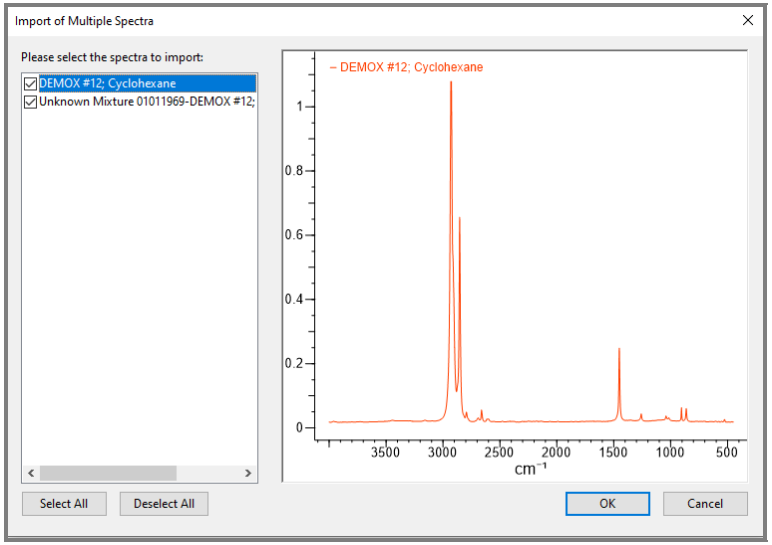
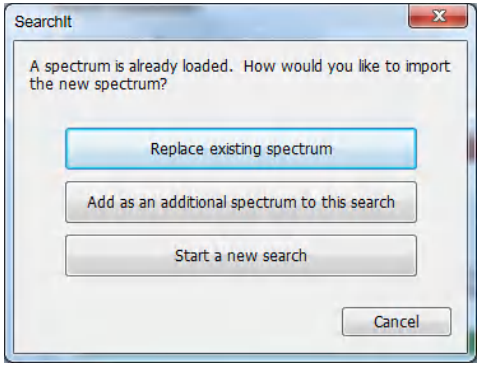
	Action	Result
6	Click **Preview**.	The subtracted spectrum is displayed above the other two. Note the presence of negative peaks in the difference spectrum. 
7	On the **Add/Subtract** dialog box, adjust **Factor** to 0.6.	Negative peaks in the difference spectrum disappear. 

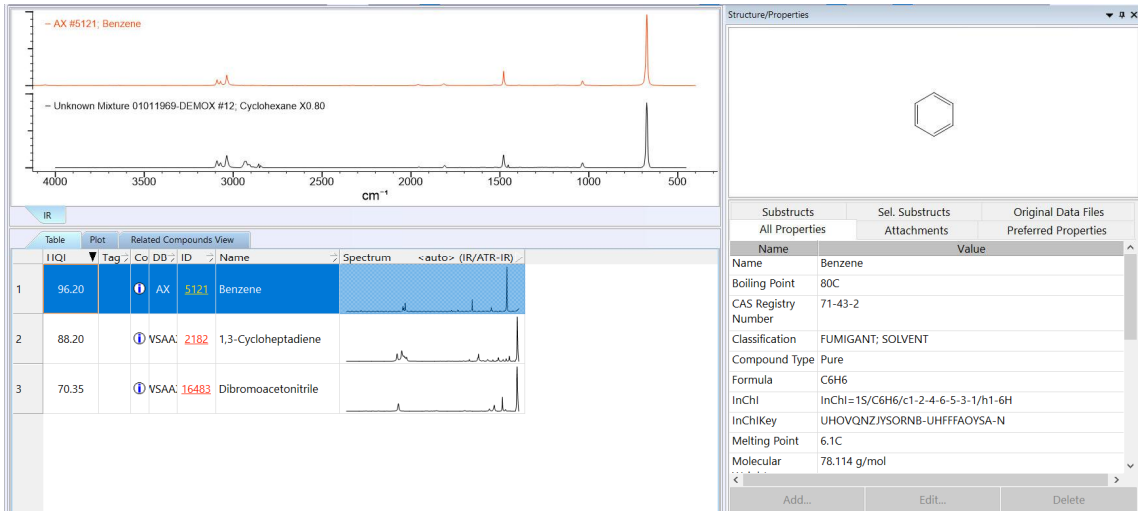
Create a difference spectrum (continued)

	Action	Result
8	Click **Replace**.	A message box opens, and asks whether negative values should be truncated to zero.
9	Click **Yes**.	The mixture spectrum is replaced by a difference spectrum, Unknown Mixture 01011969 - SRX #3, Cyclohexane.



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: 
3	Click **Start a new search**.	The difference spectrum is loaded in **SearchIt**.

	Action	Result
4	Click the **Databases** 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: 

WILEY

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

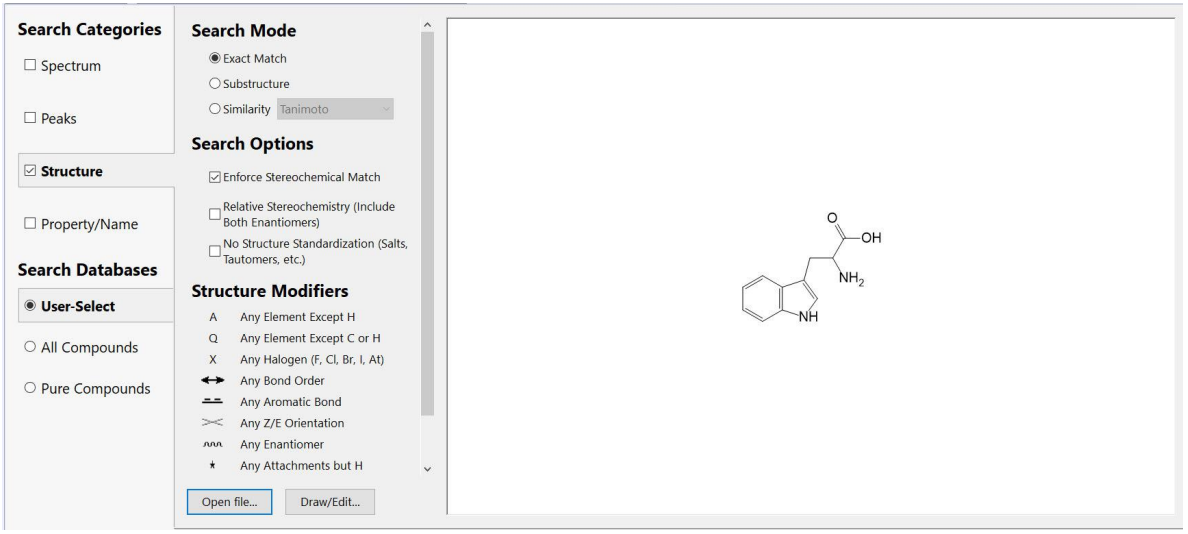
- tryptophan.dsf
- benzenethiol.dsf

KnowItAll Applications Used

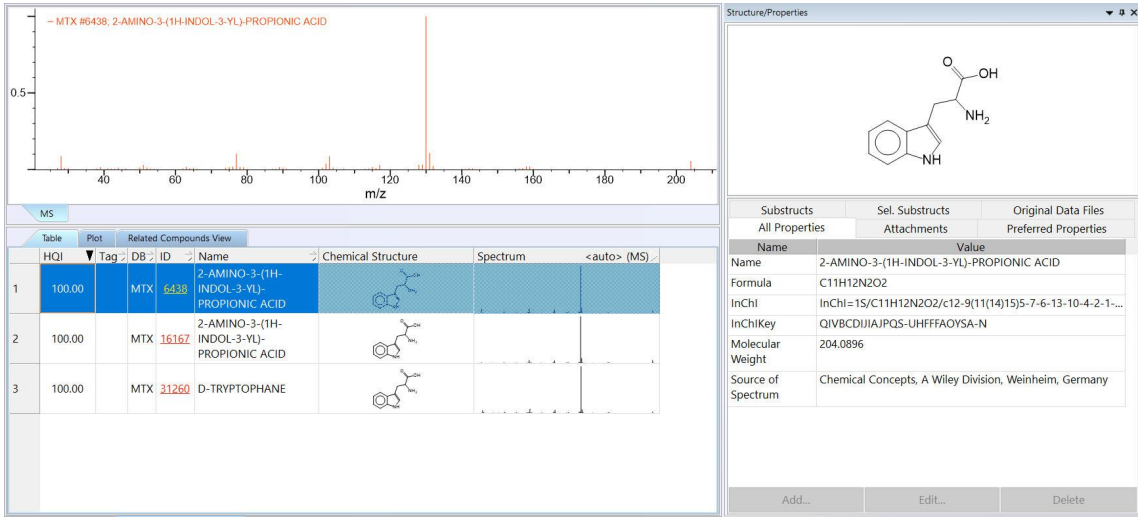
- SearchIt™
- MineIt™
- ChemWindow®

Configure an exact structure match search

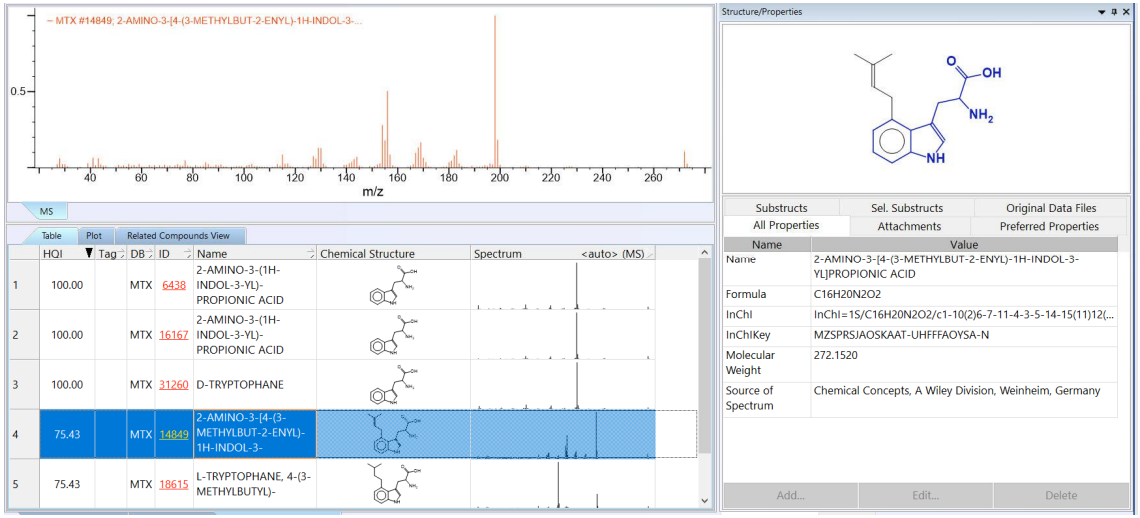
	Action	Result
1	Do one of the following: • If the **SearchIt** application is not open, navigate to the **Data** toolbox and click its icon. • If the **SearchIt** application is already open, click the SearchIt **Close** button to close the current search	The SearchIt application's **Databases** tab 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.	
3	Set **Limit to Spectral Technique** to **MS**.	Only databases with MS spectral data are displayed.
4	Select database **MTX** for searching.	
5	Click **Structure** under **Search Categories**.	

	Action	Result
6	• Click **Open file** on the **Structure** tab. • Navigate to **KnowItAll > Training Files > General Training > Files > Searching**. • Open **Tryptophan.dsf**.	The structure is displayed in the **Structure** tab.  **Note**: You can also click **Draw/Edit** to create a structure using the **ChemWindow** application.

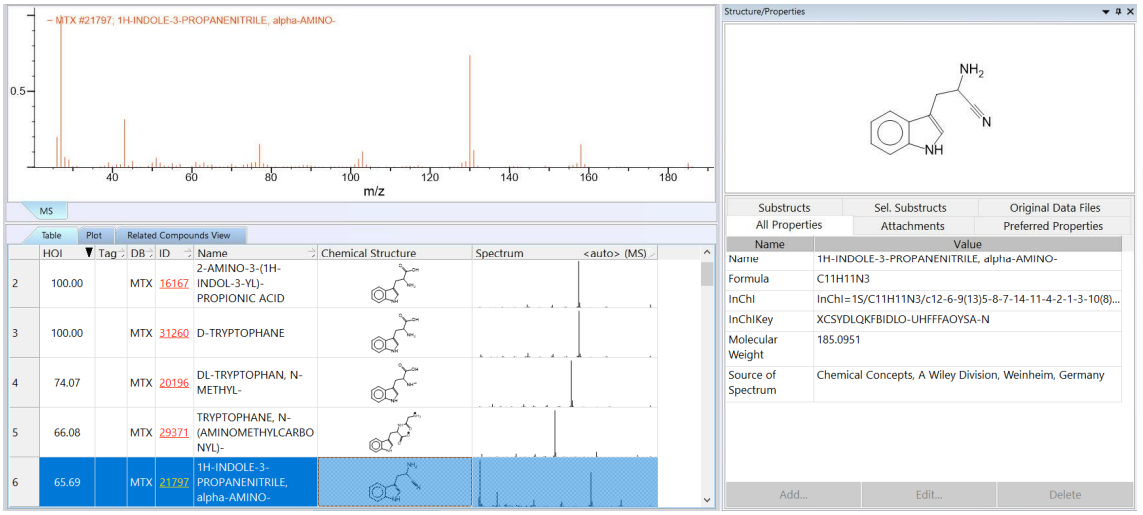
Perform an exact structure match search

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

Configure and perform a substructure search

	Action	Result
1	Click the KnowItAll **Back** button to return to **SearchIt**, then click to select the **Structure** tab.	
2	Select **Substructure Search**, then click **Search**. **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. Note that the original hit list is still available, and can be accessed by clicking the appropriate tab (at the lower left corner). 

Configure and perform a similarity search

	Action	Result
1	Click the KnowItAll **Back** button to return to **SearchIt**	
2	Click the **Similarity Search** radio button. Accept the default scoring method, **Tanimoto**.	
3	Click **Search.**	The results are displayed in the **MineIt** application:  The first hit is the exact structure. The second hit, toluene, is a similar structure.

Searching

All Compounds and Pure Compounds Database Selections

Purpose

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

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Objectives

This exercise will teach you:

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

Background

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

Training Files Used in This Lesson

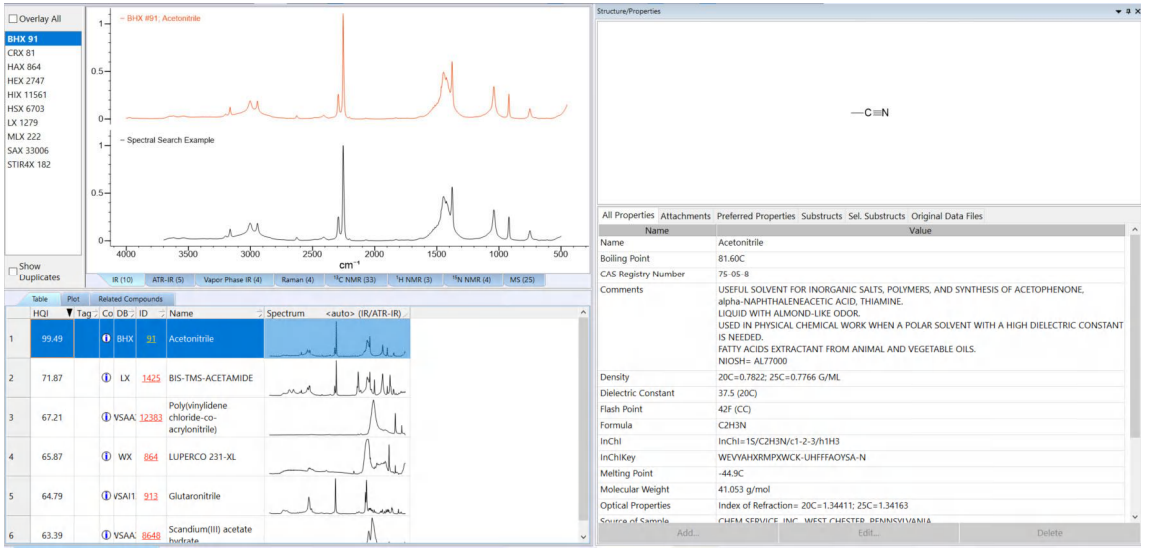
- Spectral Search Example

KnowItAll Applications Used

- SearchIt™
- MineIt™

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 **Databases** tab is displayed, and the **Selected for Searching** list displays the databases last used.
2	Select the **All Compounds** option under **Search Databases**	
3	• Click **Spectrum** under **Search Categories**. • Open **Spectral Search Example.jdx**	

	Action	Result
7	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.

- **User-Select** - User selects which databases to search. This is where one 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

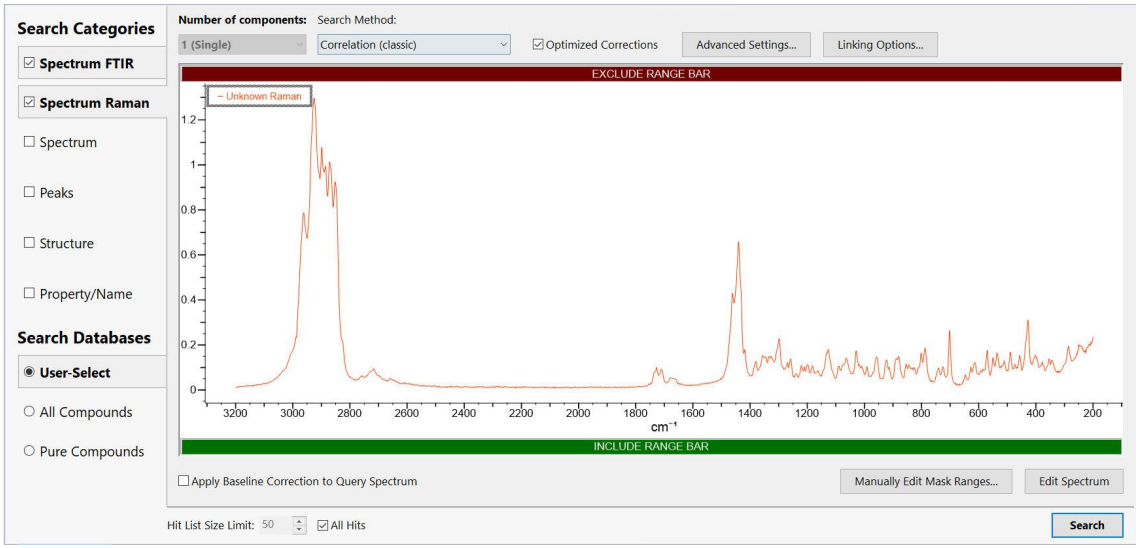
- Unknown IR.jdx
- Unknown Raman.jdx

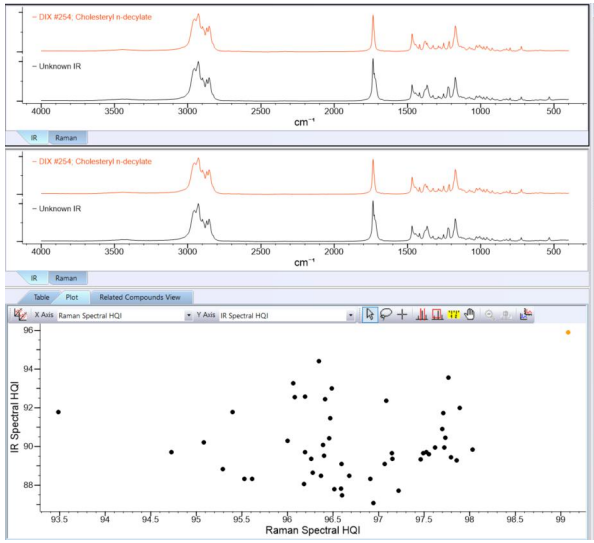
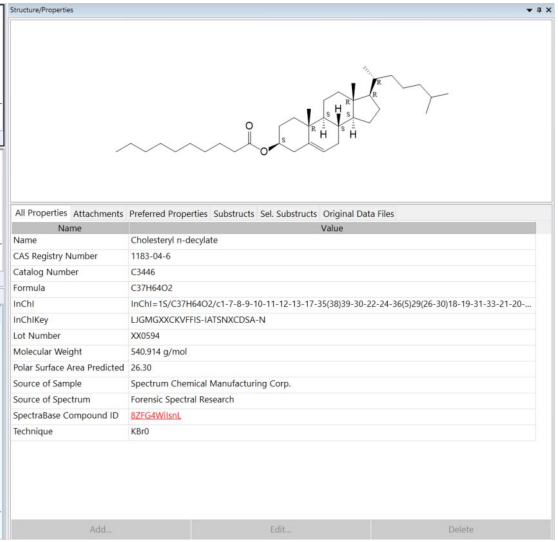
KnowItAll Applications Used

- SearchIt™
- MineIt™

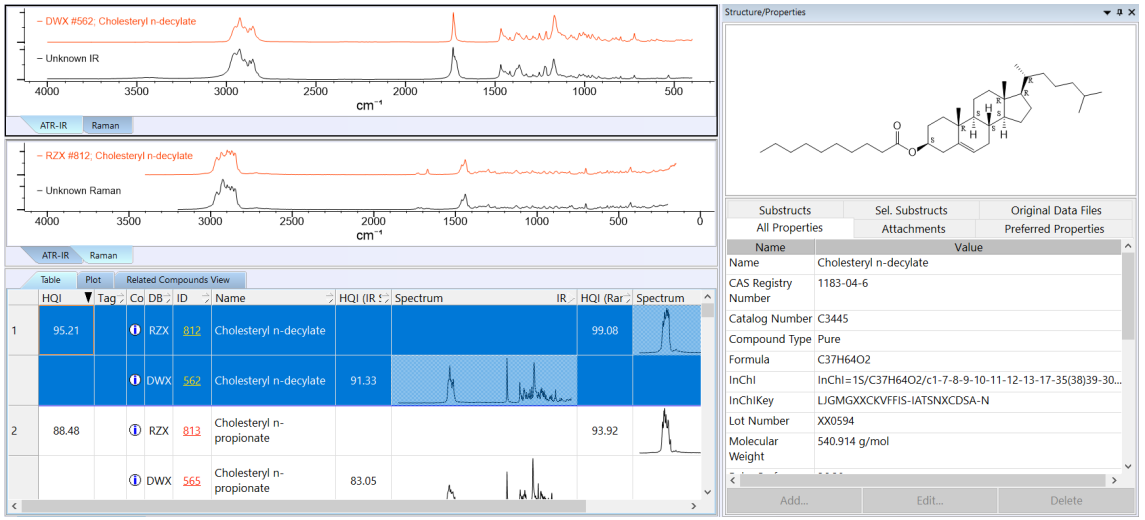
Configure and perform a multi-technique spectral search use User-Select Search Databases option

	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 **Databases** tab is displayed, and the **Selected for Searching** list displays the databases last used.
2	Select **User-Select** under **Search Databases** option	
3	• If databases are already selected for searching, click **Remove All** to clear the selections. • Add all **IR** and **Raman** databases to **Selected for Searching**.	
4	• Click **Spectrum** under **Search Categories**. • Navigate to **KnowItAll > Training Files > General Training > Files > Searching**. • Open **Unknown IR.jdx**	

	Action	Result
5	• Click the new **Spectrum** under **Search Categories**. • Open **Unknown Raman.jdx**.	

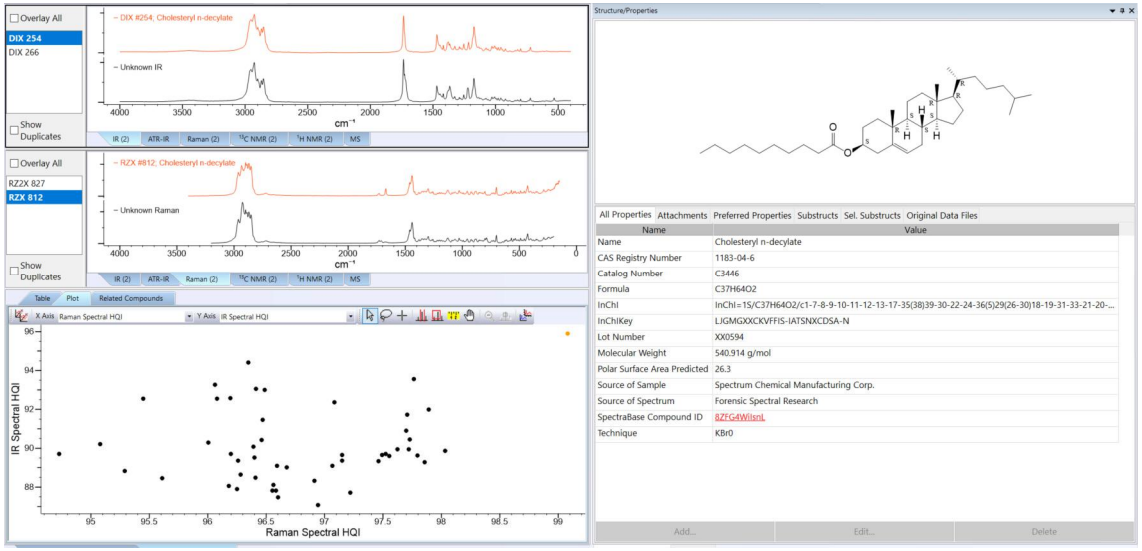
	Action	Result
6	Click **Search**.	The search results are displayed in the **MineIt** application.   Because this was a multi-technique search, the **Database** pane's **Plot** tab automatically displays a scatter plot representing HQI values for the two spectral techniques. The point with the highest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

Examine the search results

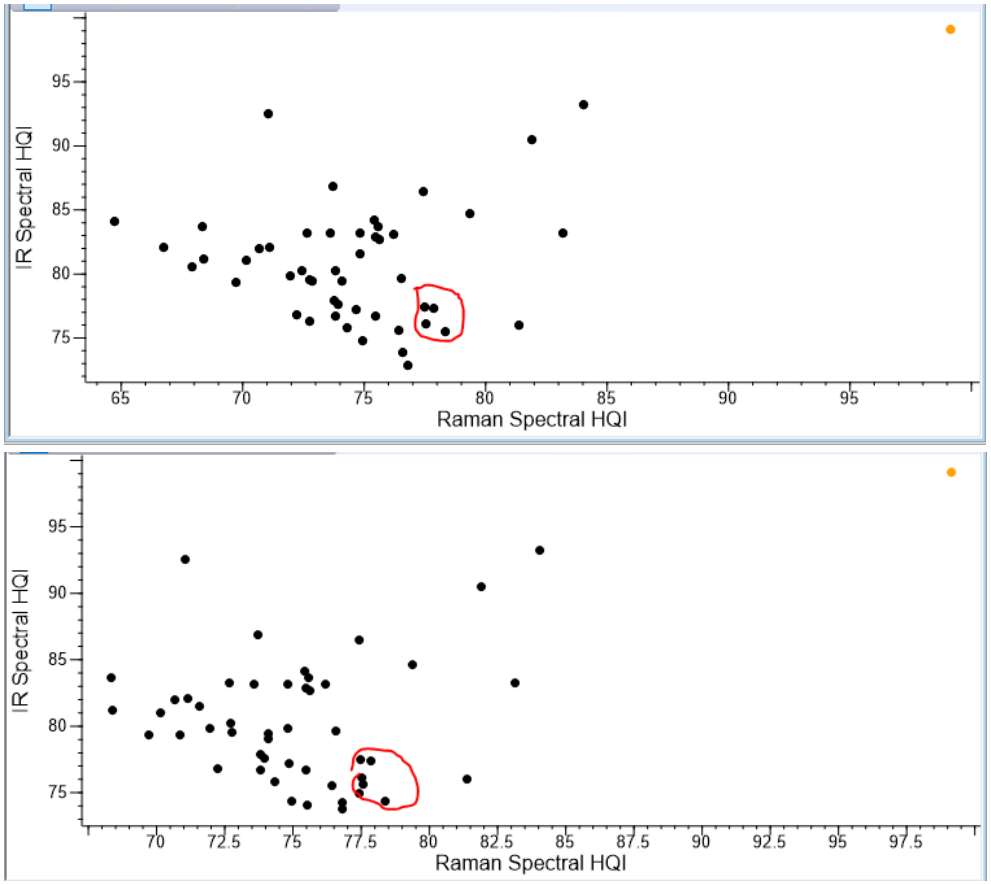
	Action	Result
1	Click the **Table** tab in the **Database** pane.	The corresponding database entries are displayed: 

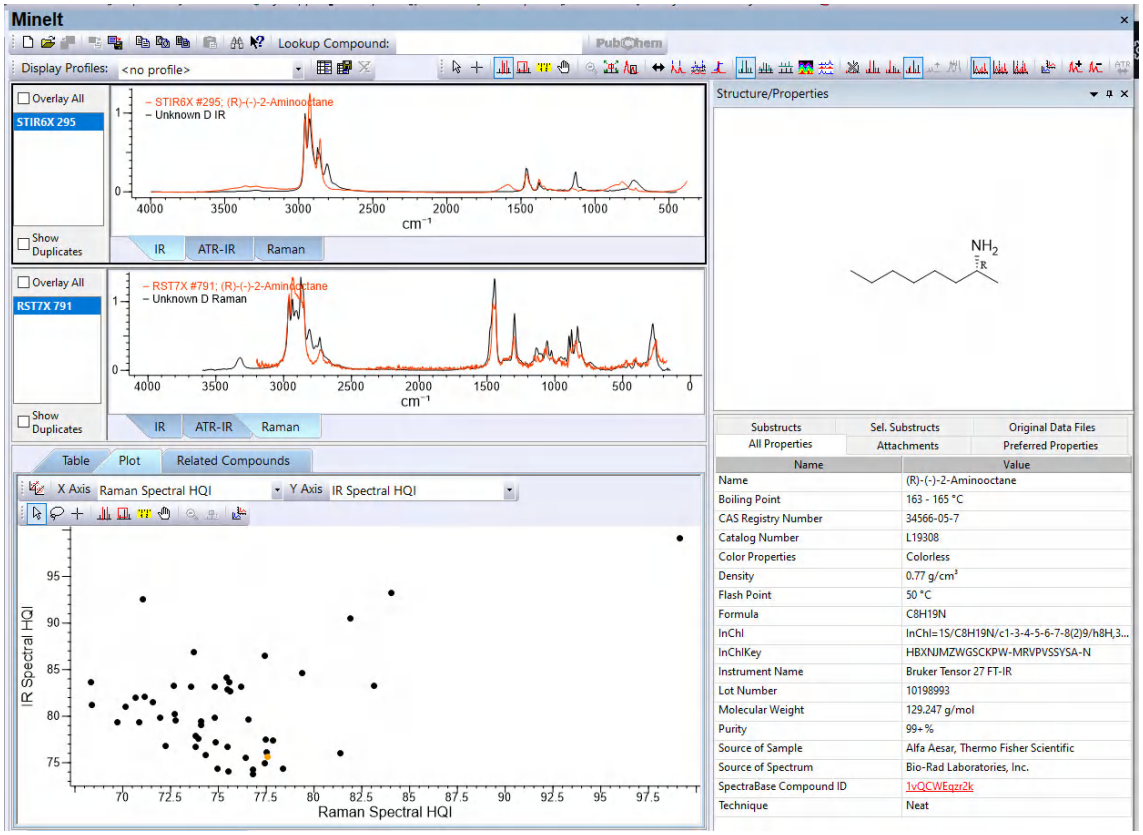
Configure and perform a multi-technique spectral search with All Compounds Search Databases option

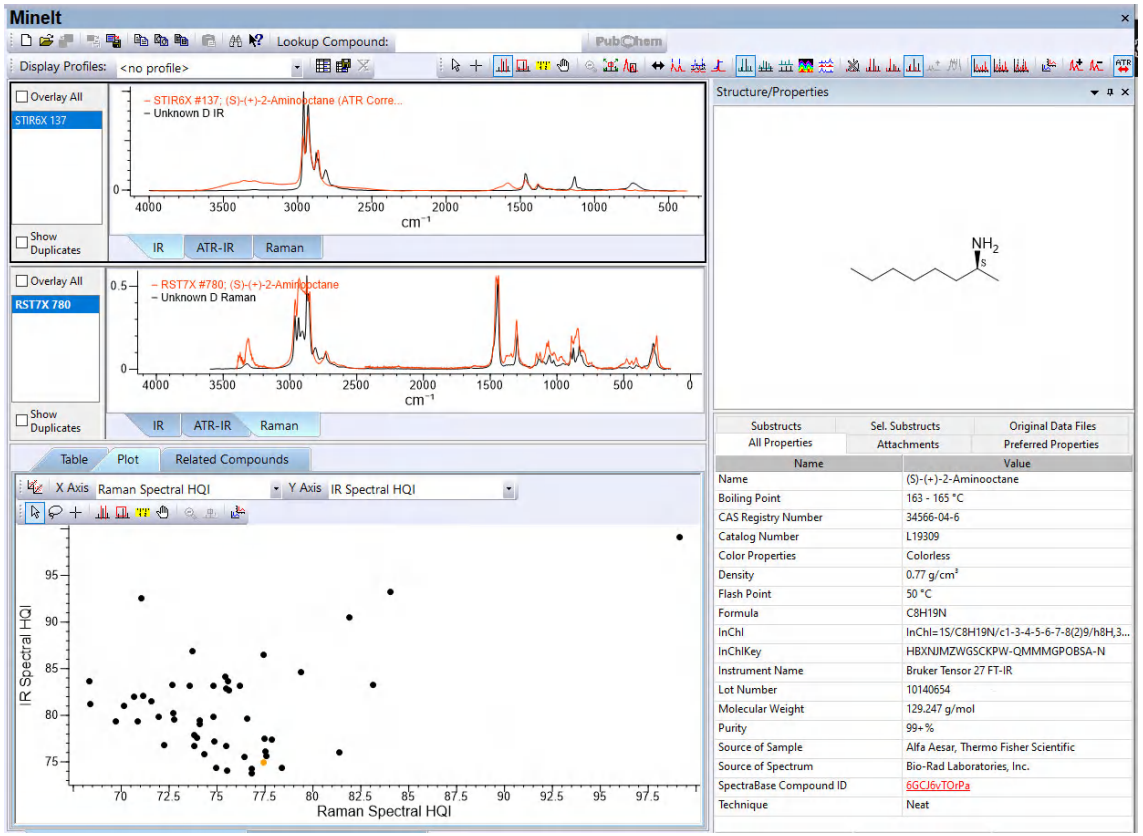
	Action	Result
1	Do one of the following: • If the **SearchIt** application is not open, navigate to the **Data** toolbox and click its icon. • If the **SearchIt** application is already open, click the SearchIt **Close** button to close the current search.	The SearchIt application's **Databases** tab is displayed, and the **Selected for Searching** list displays the databases last used.
2	Check **All Compounds** under **Search Databases** option	
3	• Click **Spectrum** under **Search Categories**. • Open **Unknown IR.jdx**.	

	Action	Result
4	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.

Compare the search result with that from User-Select search

	Action	Result
1		Compare the scatter plot of the **User-Select** database search (top) and that of **All Compound** search (bottom)  We can see that more spots are in this region.

	Action	Result
	Examine the extra spots	 We can see that they 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).

	Action	Result
		 The above is another stereo-isomer.

KnowItAll Software Training

Mixture Analysis

WILEY

Mixture Analysis

How to Analyze Mixture Spectra

Purpose

This exercise demonstrates how to perform a mixture analysis using the KnowItAll Informatics System's SearchIt application.

Objectives

This exercise will teach you:

- How to configure a mixture analysis;
- How to interpret the results of a mixture analysis.

Background

The spectral analysis of mixtures in experimental data is a challenging task. Manual separation of spectral components, even when they are known in advance, is a tedious job. Attempting to do this analysis in an automated fashion creates a whole new level of challenges.

This chapter introduces how to use SearchIt application to perform Mixture Analysis.

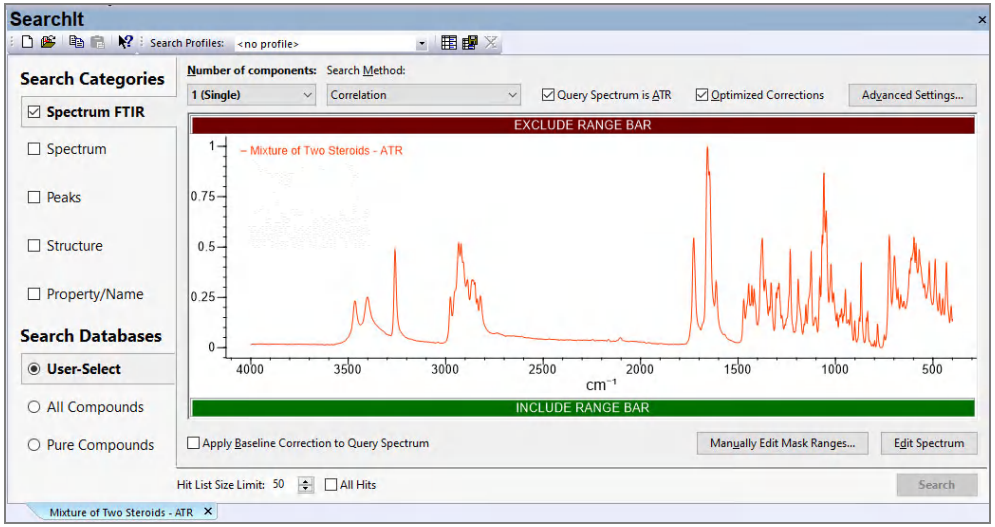
Training Files Used In This Lesson

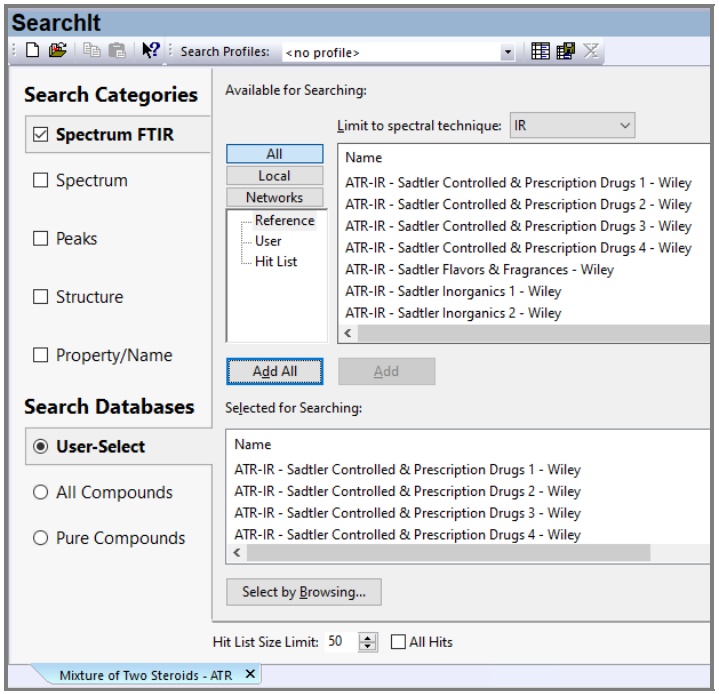
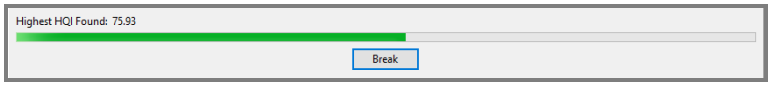
- Mixture of Two Steroids – ATR-IR.irf

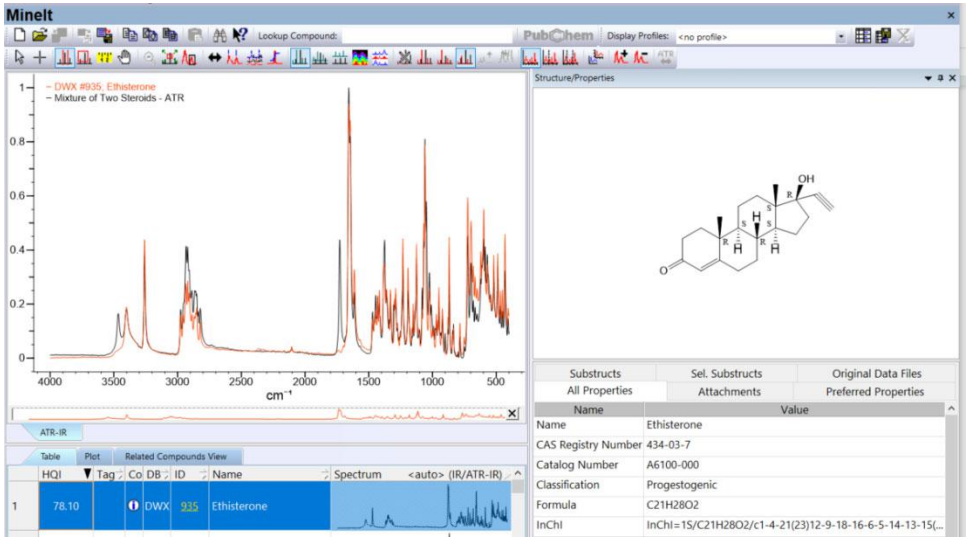
KnowItAll Applications Used

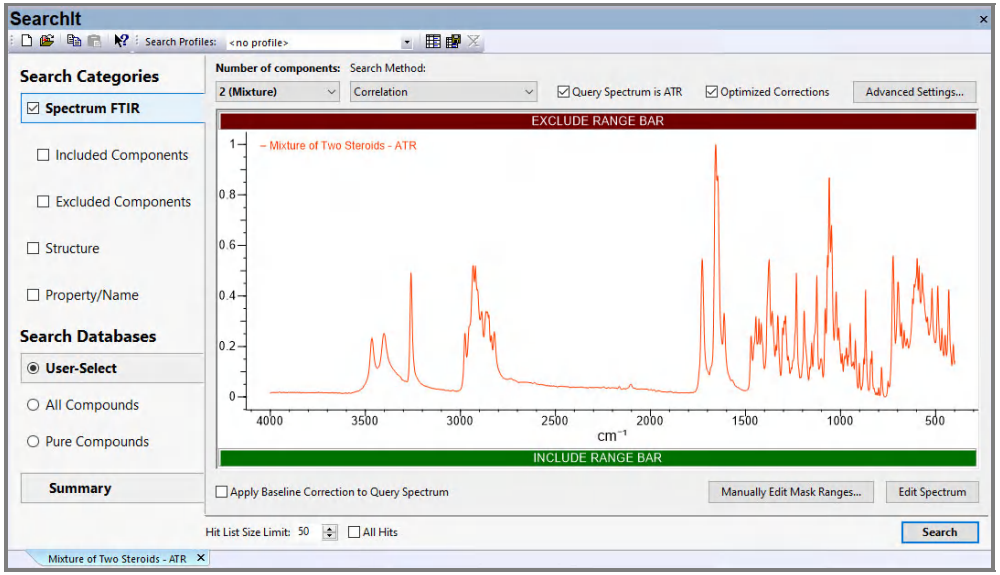
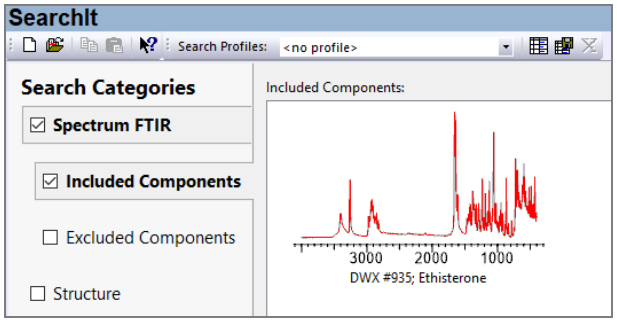
- SearchIt™
- MineIt™

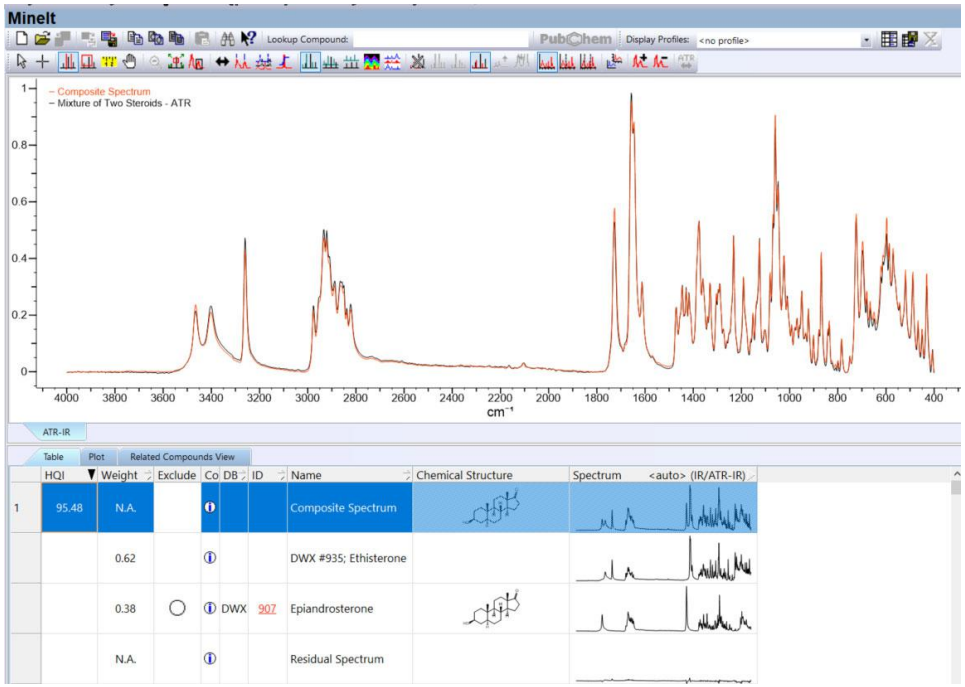
A typical mixture analysis work flow

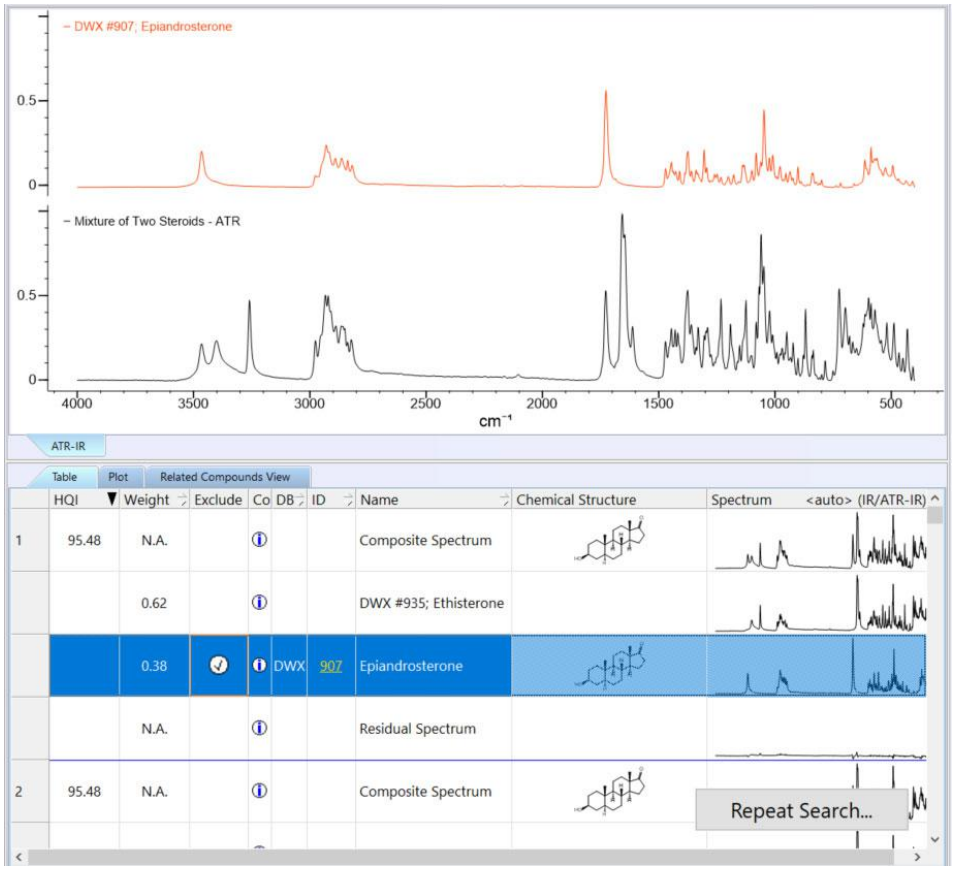
	Action	Result
1	Navigate to the **Data** toolbox and open the **SearchIt** application Check **Spectrum**, and in the resulting **Open** dialog box navigate to KnowItAll > Training Files > General Training > Files > Mixture Analysis and open **Mixture of Two Steroids - ATR-IR**. • Set **Search Method** to **Correlation** • Click on **User-Select** under **Search Databases** • Set **Limit to spectral technique** to **IR** • Click **Add All** at the bottom of **Available for searching** menu	

	Action	Result
1	Do the following: • Set **Search Method** to **Correlation** • Click on **User-Select** under **Search Databases** • Set **Limit to spectral technique** to **IR** • Click **Add All** at the bottom of **Available for searching** menu	
2	Click **Search.**	Wait for the search to complete. 

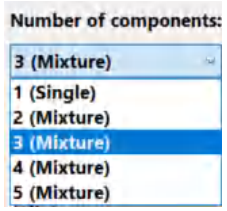
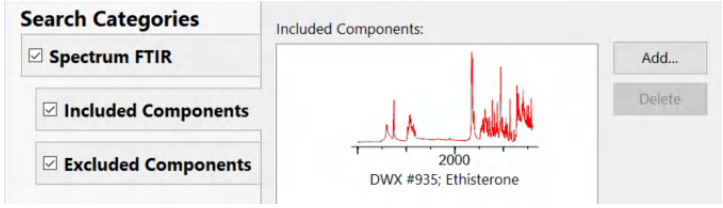
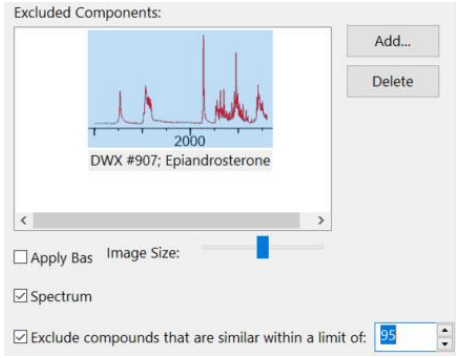
	Action	Result
		One component search result returns to **MineIt** application.  Obviously, the sample is a mixture.
3	Highlight the 1st hit. **Edit** > **Copy Active Spectrum**	

	Action	Result
4	Go back to **SearchIt**, Click the **Spectrum FTIR** button to bring up the query spectrum. Update the **Number of components** to **2 (Mixture)**.	 The **Included Components** and **Excluded Components** checkboxes show up now.
5	Check the **Included Components** Paste the copied spectrum.	

	Action	Result
6	Click the **Spectrum FTIR** button to bring up the query spectrum**.** Click **Search**.	 Now we have a good two-component match. **Note**: Each composite spectrum (row 1) is accompanied by the individual component spectra (middle rows) that comprise the composite, as well as the residual spectrum (last row) – the difference between the query spectrum and the composite. The composite spectra are ranked by how closely they resemble the query spectrum. A relatively flat residual spectrum indicates that the software has correctly identified the individual components of the mixture. The **Weight** value for each component spectrum indicates how much it contributes to the composite spectrum.

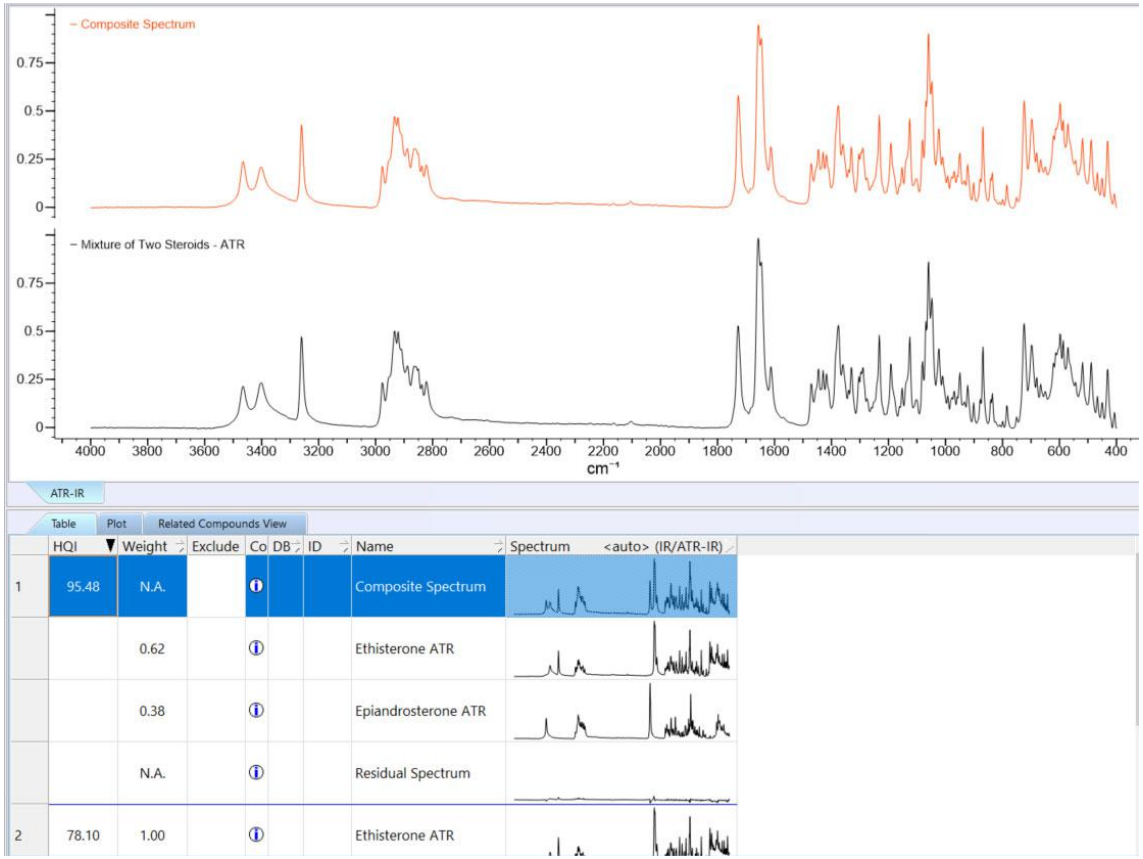
	Action	Result
7	The circle in **Exclude** column can be checked to exclude a component from consideration. Check to exclude **DWX 907**. **Repeat Search** button shows up for user to repeat Mixture Analysis without considering DWX 907	

	Action	Result
8	Click **Repeat Search.**	The new result does not contain excluded DWX 907: 

Notes:	
• You do not have to specify **Included** or **Excluded** components to perform a mixture analysis. You can simply open a spectrum in **SearchIt** and specify **Number of components** to a value larger than 1.	
• You can add **Included** or **Excluded** components from files by clicking the **Add** button.	
• You can exclude spectrally similar records.	

Add all components together

	Action	Result
1	• In the **Data** toolbox, open the **SearchIt** application • Check **Spectrum** • In the resulting **Open** dialog box, navigate to **KnowItAll > Samples > Mixture Analysis > IR Examples** • Open **Mixture of Two Steroids - ATR-IR**. • Set **Search Method** to **Correlation**. • Set **Number of components** to **2 (Mixture)**:	
2	Check **Included Components** **Add** following files from **KnowItAll > Training Files > General Training > Files > Mixture Analysis > Components folder**: • **Epiandrosterone ATR-IR** • **Ethisterone ATR-IR** **Note**: use ctrl key to select multiple files in the **Open** dialog box.	

	Action	Result
3	Click **Search**. **Note**: toggle between different spectra display modes by selecting available options from **View** > **Display Mode**.	 In this case, KnowItAll simply returns possible combinations of two provided components, without going through a database search.

KnowItAll Software Training

Create Databases

Create Databases

How to Build Your Own User Databases of Multiple Analytical Techniques

Purpose

This exercise demonstrates how to use KnowItAll's MineIt™ Database Building feature to create searchable user databases that include multiple analytical techniques. You can also customize properties displayed, create user properties and display profiles.

Objectives

This exercise will teach you:

- How to create a user database;
- How to add spectra to a user database;
- How to add structures to a user database;
- How to add user properties;
- How to perform above tasks in batch; and
- How to create and use a MineIt display profile.

Background

Generating user databases protects intellectual property and promotes sharing of information within an organization. Ultimately, researchers can improve their analyses.

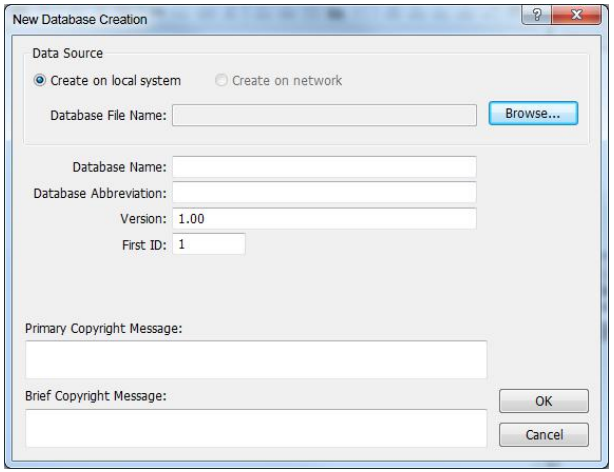
Training Files Used in This Lesson

- IR/Ethyl acetate.dx
- Raman/Ethyl acetate.irf
- BatchImportProperties.csv
- Spectral files from the Batch Import Spectra folder
- MSDS Web Link.txt
- Ethyl acetate MSDS.pdf
- Spectral files from the PubChem/Raman folder

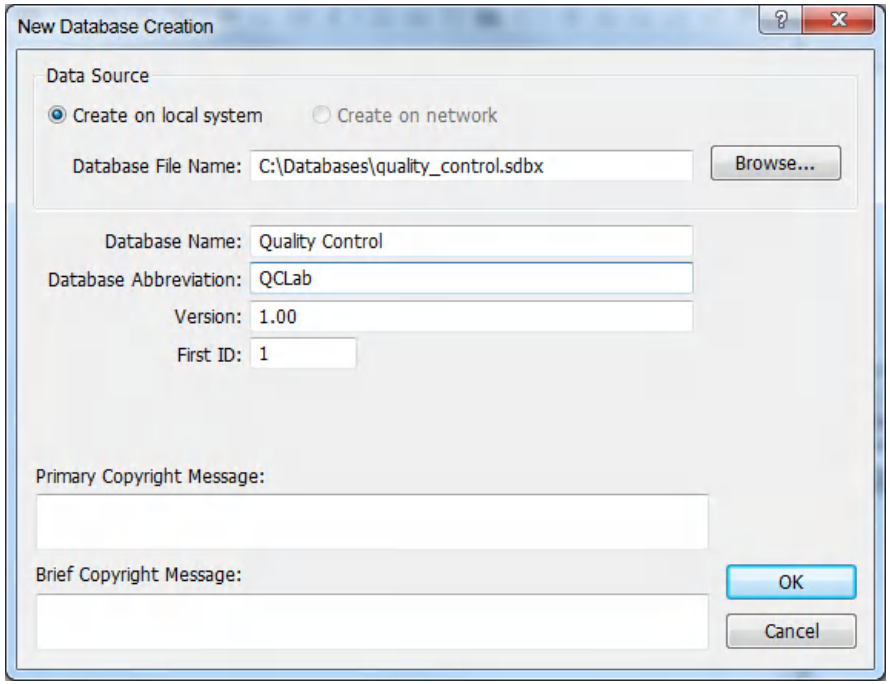
KnowItAll Applications Used

- MineIt™
- ChemWindow®
- BrowseIt™

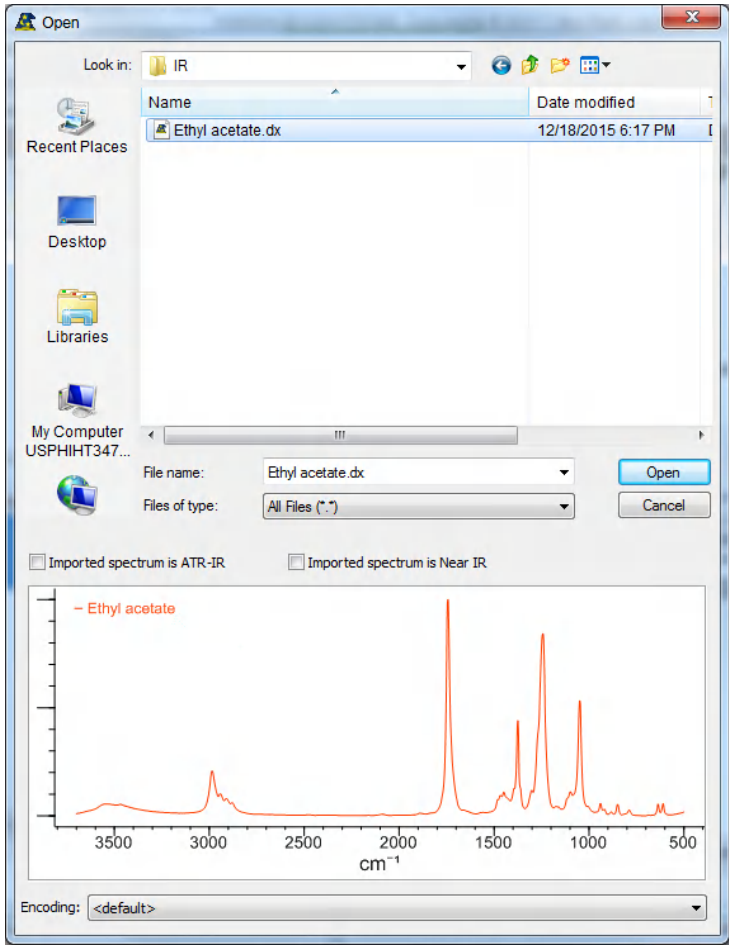
Create a user database

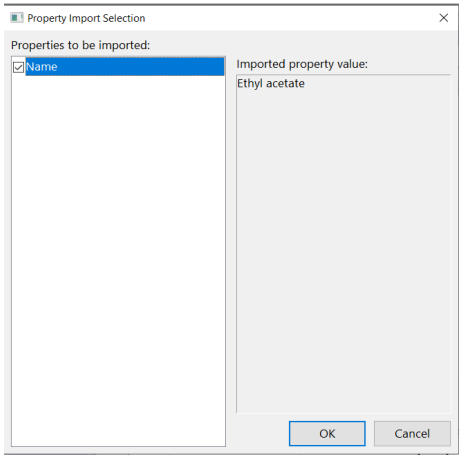
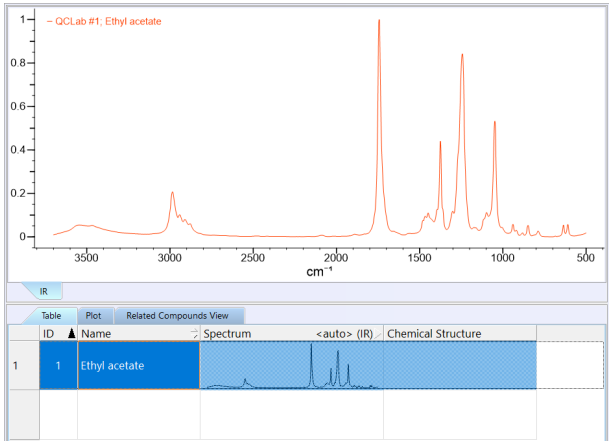
	Action	Result
1	Navigate to the **Data** toolbox and open the MineIt application by clicking the **MineIt/Create Database** icon.	The MineIt application opens.
2	Choose **Database > New**.	The **New Database Creation** dialog box opens. 
3	Select **Create on local system**.	The new database is saved locally.
4	• Click **Browse**. • Create a folder named **Databases** on a local drive • Open the folder, then type in the file name **quality_control** • Click **Save**.	The *.sdbx extension is added automatically. **Note**: The SDBX database format allows spectra to be stored without conforming to a fixed range and resolution. This allows reference spectra to be offered at higher resolution, and allows users to store original spectra as produced.
5	Type **Quality Control** in the **Database Name** text box. **Note**: The file name is used if no other name is specified.	

Create a user database (continued)

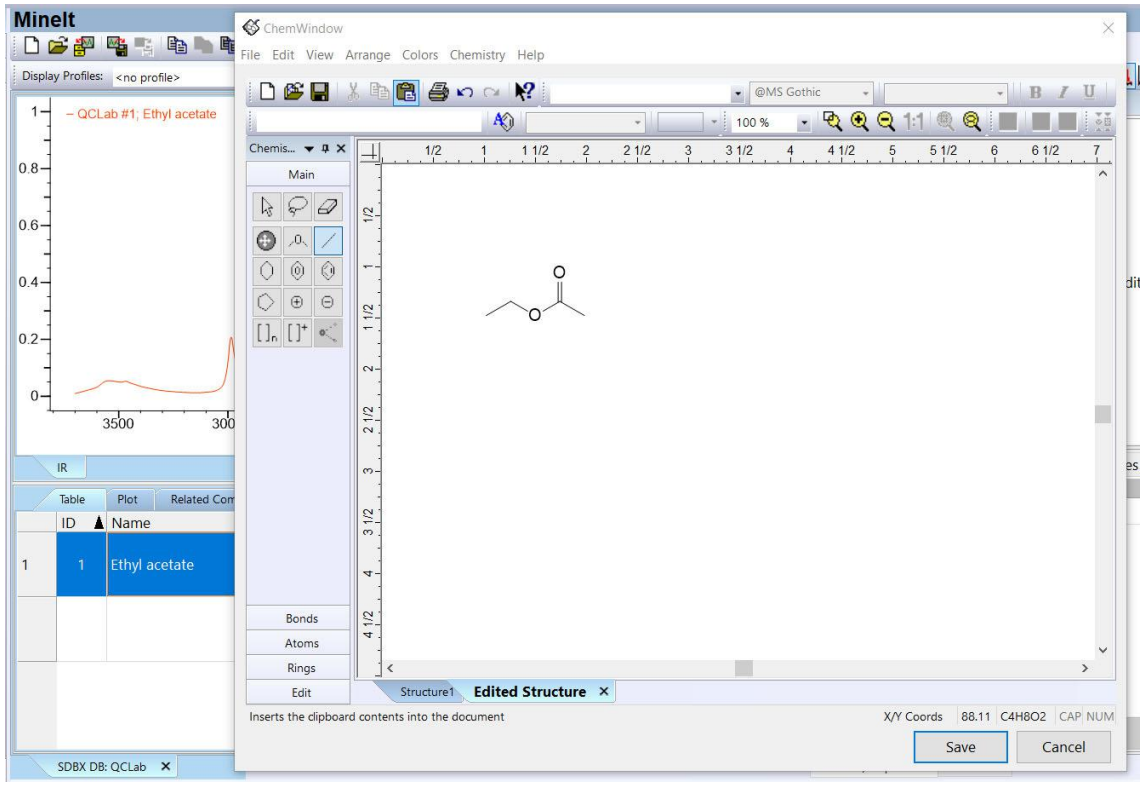
	Action	Result
6	Type **QCLab** in the **Database Abbreviation** text box. **Note**: The abbreviation must be 3-7 characters long.	
7	Enter **Version** number and the **First (starting) ID**, and type in copyright messages. **Note**: You can use the Windows Character Map (Programs > Accessories > System Tools in Windows 7) to copy and paste in the copyright symbol.	
8	Click **OK**.	The new database has been created to receive your data. The Database Abbreviation 'QCLab' appears on the database tab below the database pane (lower left), and copyright information appears in the status area (lower edge of the main window).

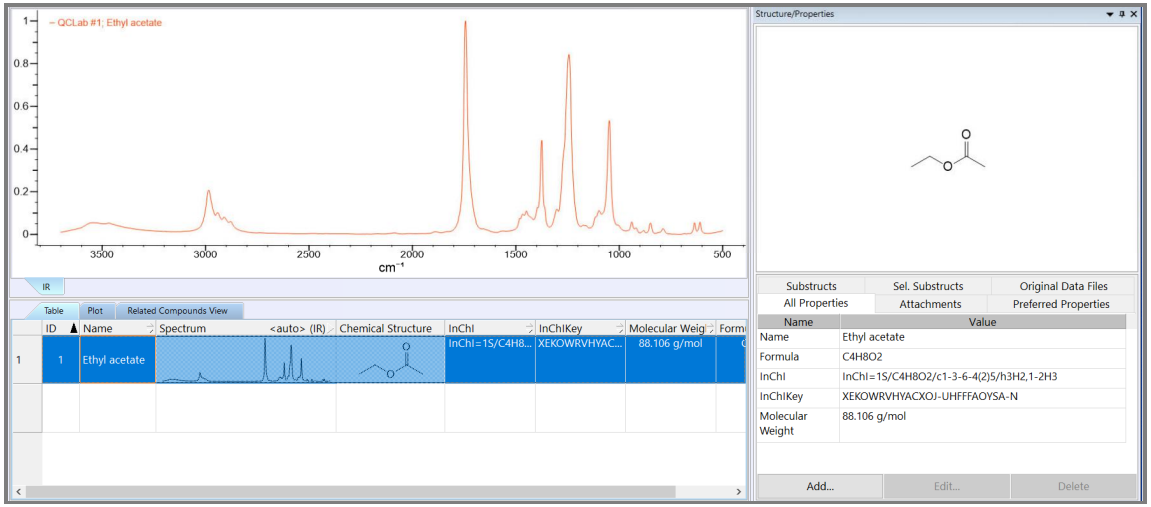
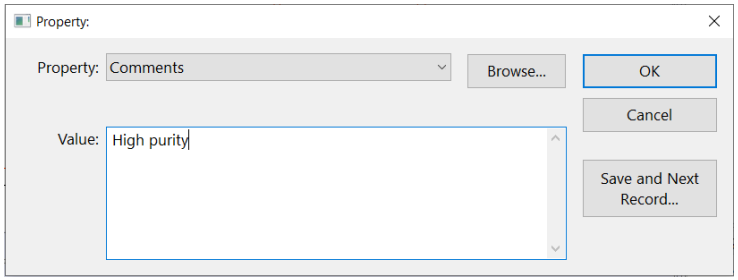
Add the first record to the user database

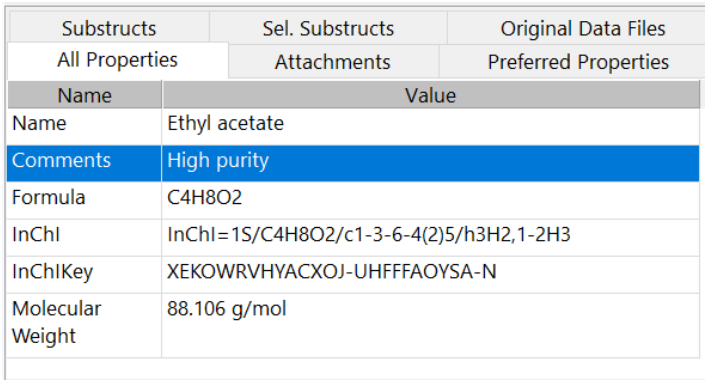
	Action	Result
1	Create the first database record by importing a spectrum: • Choose **File > Import** or press Ctrl+I. • Navigate to **KnowItAll > Training Files > General Training > Files > Creating Databases > IR** • Open **Ethyl acetate.dx** **Note**: Use the **Files of type** filter to locate IRF, JCAMP, and many other specific spectral files.	A Windows **Open** dialog box appears. 

	Action	Result
2	Click **Open**.	The **Property Import Selection** dialog box opens:  This dialog box appears when you transfer information into a user database. All available properties are shown. Select each property in turn; then use the checkboxes to define the action for each property.
3	Click **OK**.	The dialog box closes. The spectrum has been added to the user database as the first record: 

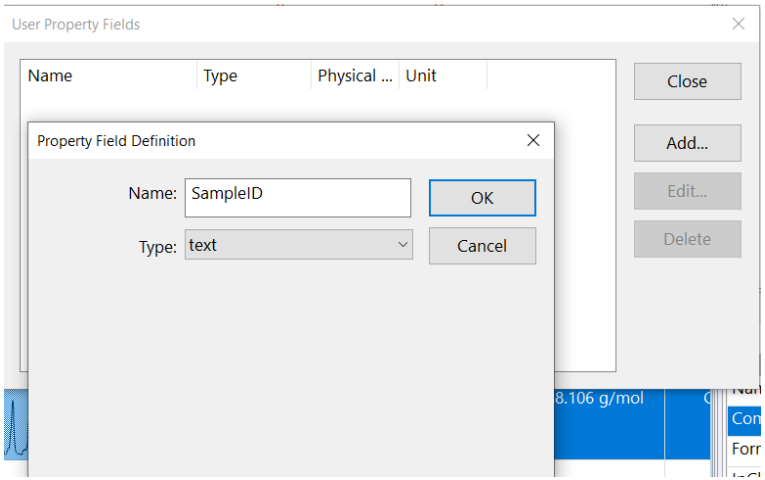
Add a chemical structure and properties to the first database record

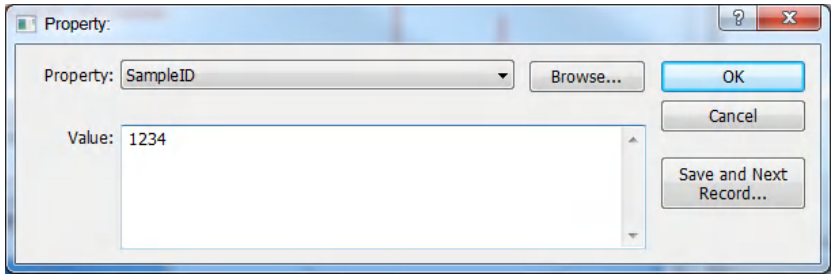
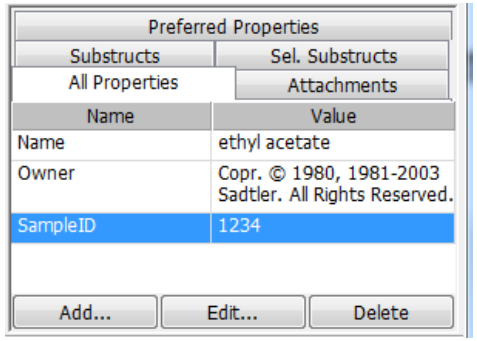
	Action	Result
1	With the first record selected, double-click the Structure/Properties pane at the top right of the window (**Double-click to edit structure in ChemWindow**).	The ChemWindow application pops up. Alternatively, one can use **Transfer to:** to go to the ChemWindow application. 
2	Use the drawing tools to create this structure	

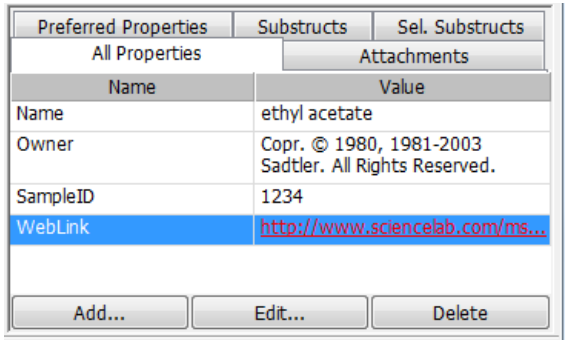
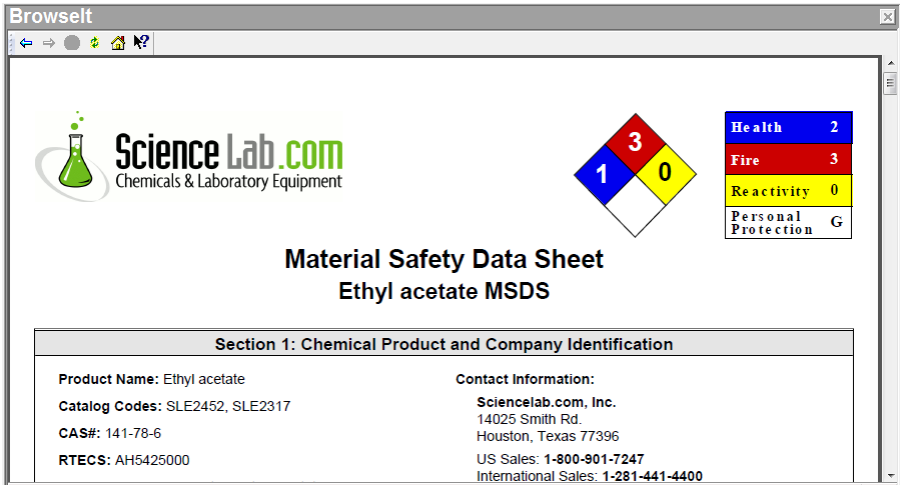
	Action	Result
3	Click **Save**.	The structure is added to the first record, and is displayed both in the **Chemical Structure** column in the **Database** pane and the **Structure/Properties** pane.  NOTE: Some chemical properties such as InChI, InChIKey, Molecular Weight, etc., can be set to be automatically calculated when a structure is saved in a record.
4	Click **Add** at the bottom of the Structure/Properties pane.	The **Property** dialog box appears.
5	Use the drop-down list to select the property you wish to add – **Comments**.	

	Action	Result
6	Click **OK**.	The **Property** dialog box closes, and the name and value of the added property appear in the **Structure/Properties** pane. 
	TIP	You can select multiple database records and use the **Add** or **Edit** button at the bottom of the **Structure/Properties** pane to input the same value for a field.

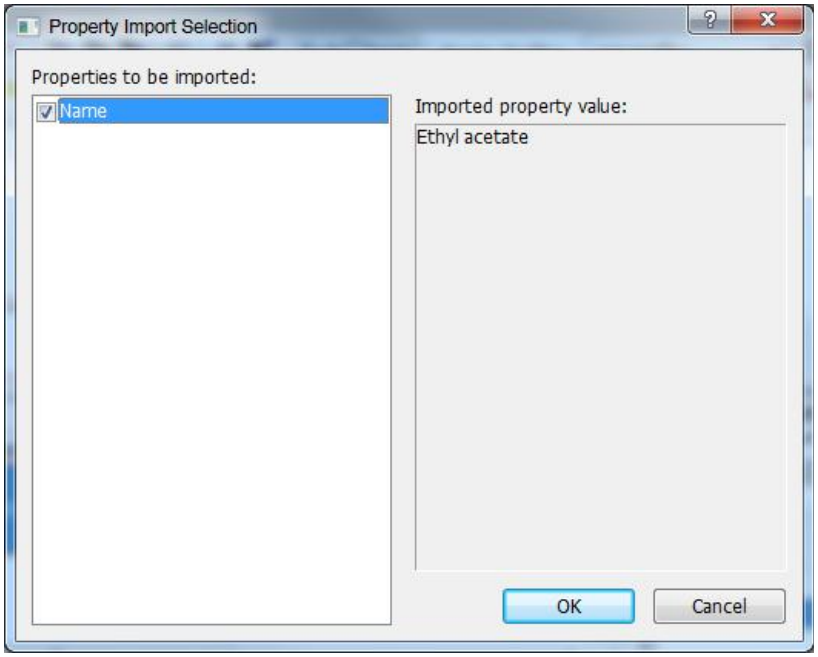
Add user properties

	Action	Result
1	Choose **Database > Define User Property Fields**	The **User Property Fields** dialog box opens.
2	Click **Add**. Use the drop-down list to set **Type** to text.	The **Property Field Definition** dialog box opens.  **Note**: Which controls are available depends on which type of field is specified: numeric, text, or enumeration.
3	Click **OK**, then **Close**	
4	Click **Add** in the **Structure/ Properties** pane.	The **Property** dialog box opens. Note: **Choose View > Windows/Tables > Structure/Properties Table** or press Alt+3 if the pane is not visible.
5	Click the down arrow to display all available properties.	Both pre-defined and user-defined properties are displayed. User-defined properties are at the beginning of the list.
6	Select **SampleID**.	The Value text box is added to the dialog. Note: Which text boxes are added depends on whether the property is numeric, text, or enumeration.

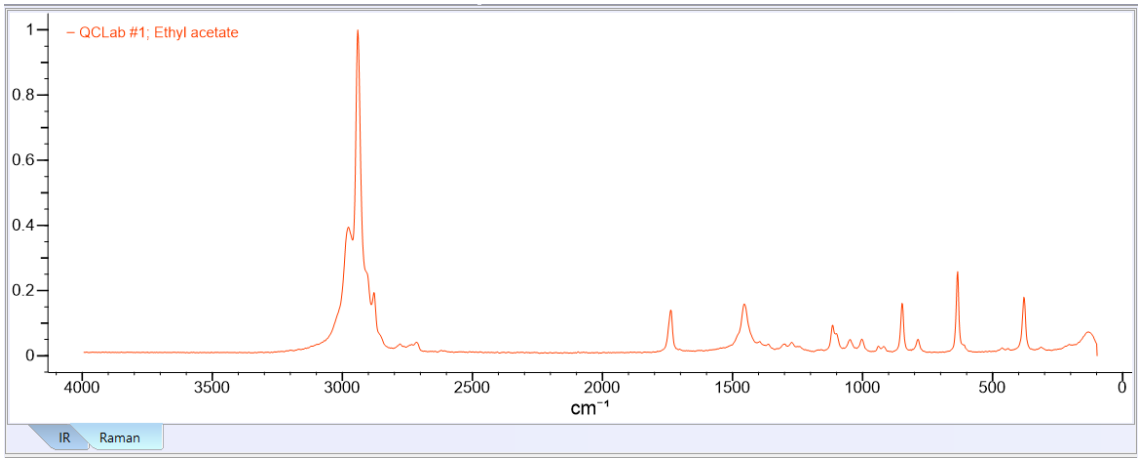
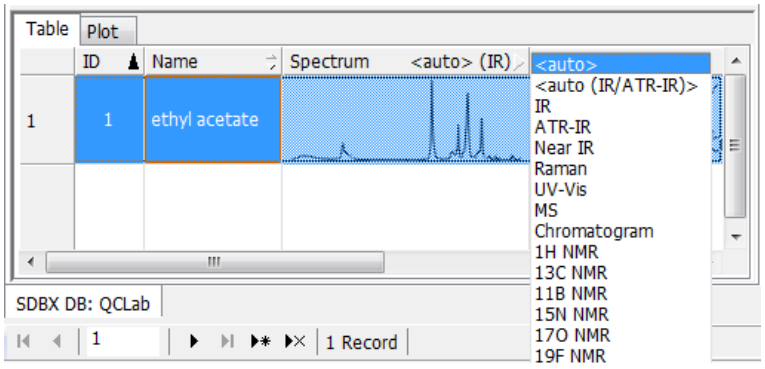
7	Type ‘1234’ in the **Value** text box.	
8	Click **OK**.	The dialog box closes. The property **SampleID** with value 1234 is added to the **Structure/Properties** pane for the first record. 

	Action	Result
9	Repeat steps 1-10 to create the user property WebLink and display it in the **Structure/Properties** pane. Type 'https://pubchem.ncbi.nlm.nih.gov/compound/ethyl-acetate' in the **Property** dialog box's **Value** field. **Note**: You can copy the text string from MSDS Web link.txt in the KnowItAll Training files.	The property **WebLink** with a web address is added to the **Structure/Properties** pane for the first record. 
10	Click the web address in the **Structure/Properties** pane.	The web page opens in the **BrowseIt** application. 
11	Click the KnowItAll **Back** button to return to the **MineIt** application.	

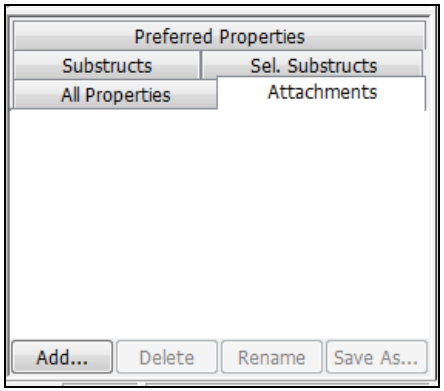
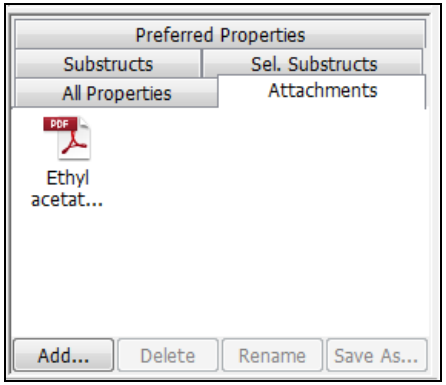
Add another spectrum (Raman) to the first database record

	Action	Result
1	Make sure the first database record is selected, then choose **File > Import.**	The **Open** dialog box with preview pane appears.
2	Navigate to **KnowItAll > Training Files > General Training > Files > Creating Databases > Raman** Open **Ethyl acetate.irf**.	The **Property Import Selection** dialog box opens.  This dialog box appears when you transfer information into a user database. All available properties are shown.

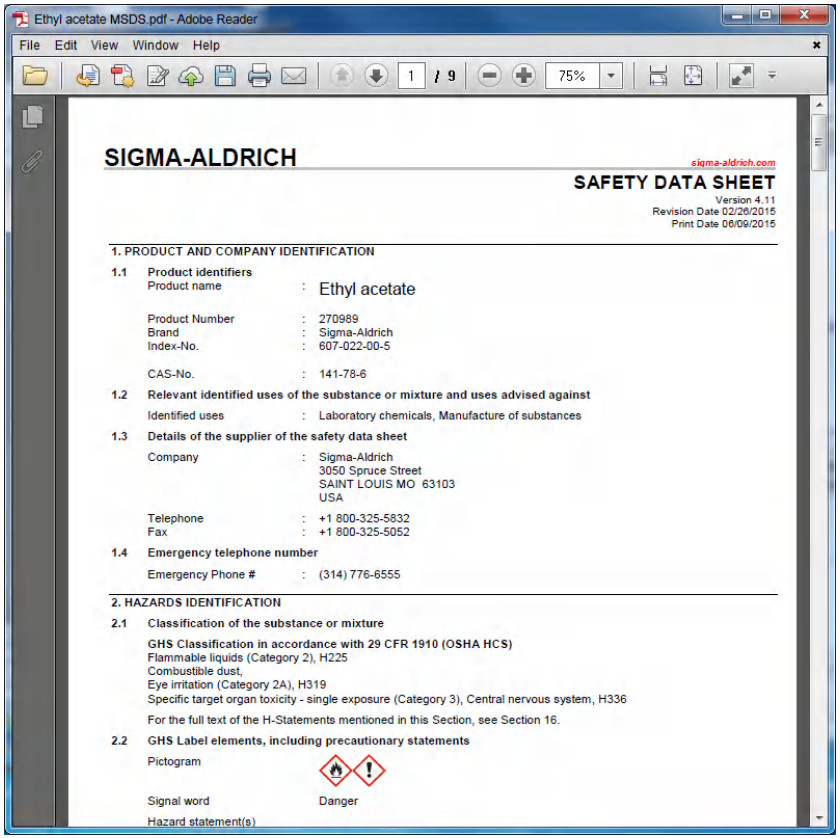
Add another spectrum (Raman) to the first database record (continued)

	Action	Result
3	Click **OK**.	A new **Raman** tab is added to the **Spectral** pane for the display of the Raman spectrum. 
4	Switch between spectra by using the tabs at the bottom left of the spectral pane.	
5	You can also switch between spectra by clicking the arrow in the **Database** pane's **Spectrum** column.	

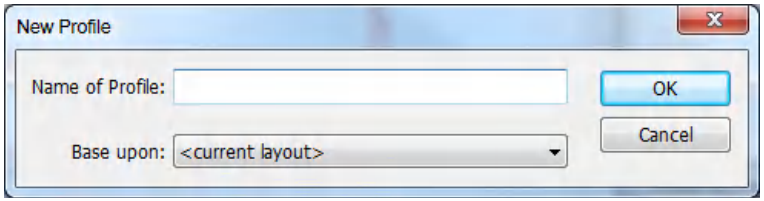
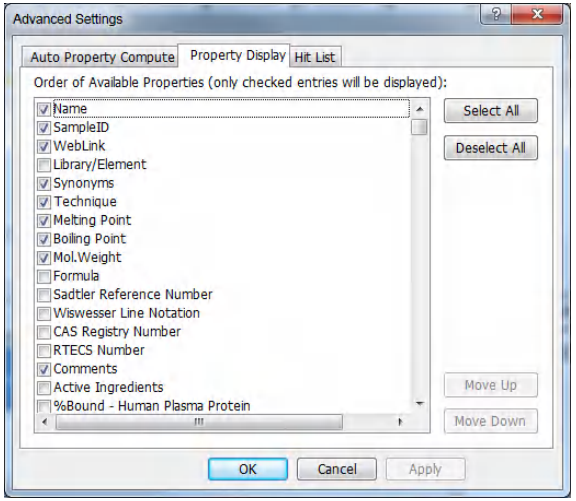
Add an attachment to the first database record

	Action	Result
1	With the first database record selected, click the **Attachments** tab in the **Structure/Properties** pane.	The **Attachments** tab is empty: 
2	Choose **File > Import Attachment(s)…**	A Windows **Open** dialog box is displayed.
3	Navigate to KnowItAll > Training Files > General Training > Files > Creating Databases and select Ethyl acetate MSDS.pdf, then click **Open**.	An icon is added to the **Attachments** tab: 

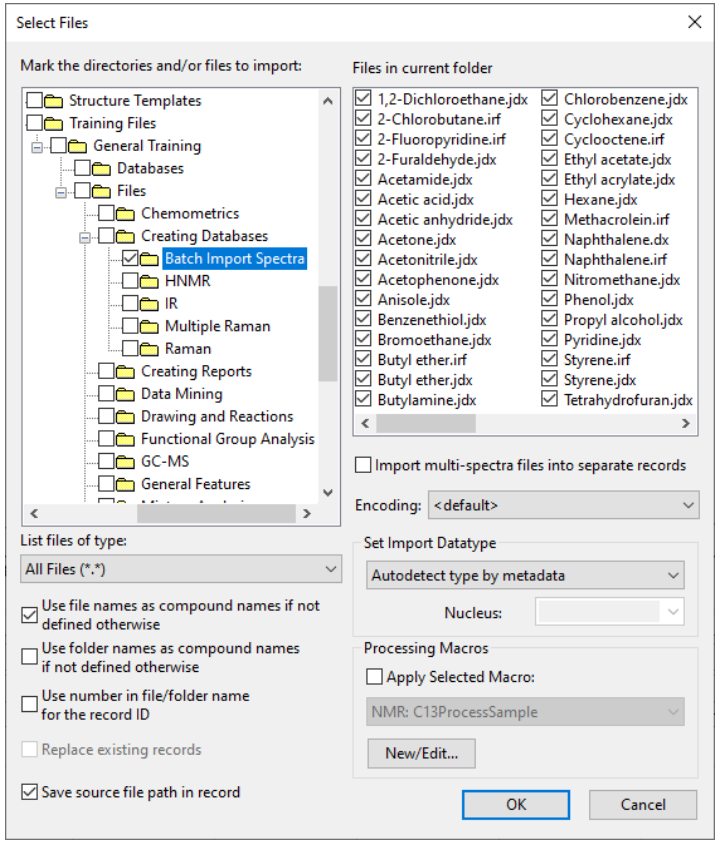
Add an attachment to the first database record (continued)

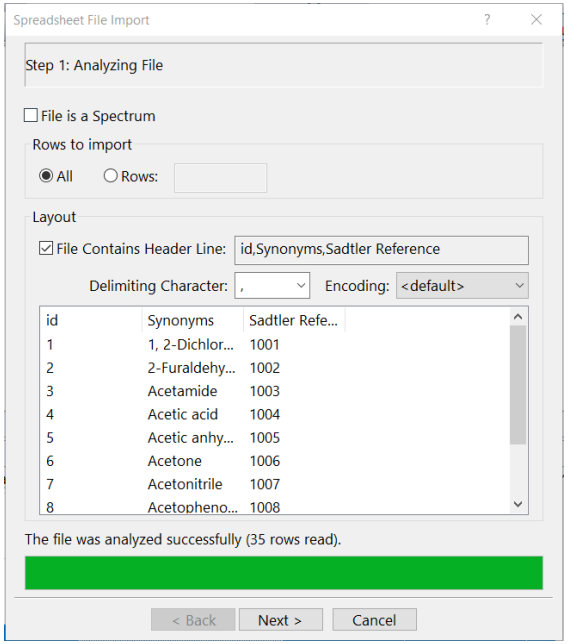
	Action	Result
4	Double click the icon in the **Attachments** tab.	The document opens in its native application – in this case, Adobe Acrobat.  **Note**: Any type of file can be added to a record in a user database using the **Attachments** tab. In addition, you can export an attached file by choosing **File > Export > Attachments**.

Create a new MineIt display profile

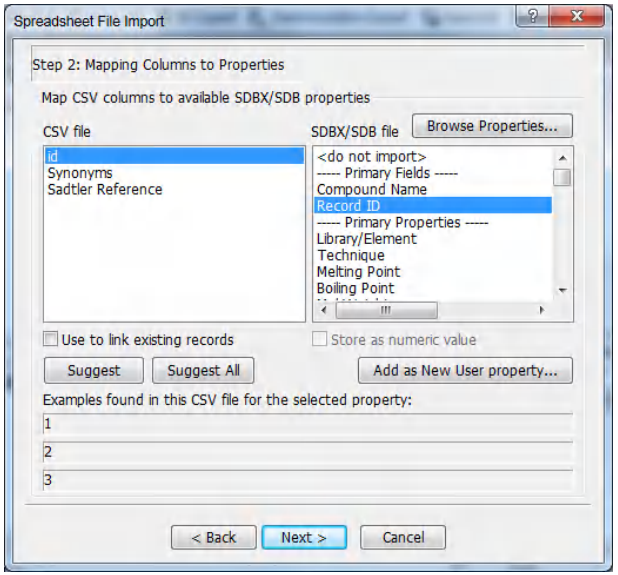
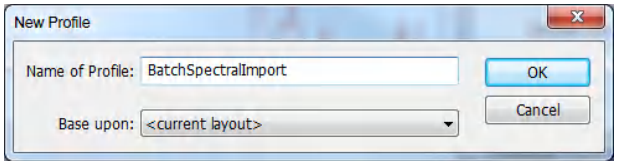
	Action	Result
1	Click the **Add a New Profile** button in the **Profile** toolbar.	The **New Profile** dialog box opens: 
2	Type in the profile name **QC Lab** and click **OK**.	This layout is now available to apply to any database or hit list display in the **MineIt** application.
	TIP	When creating a database and to ensure individual users in your laboratory consistently enter all pertinent information into databases, you should set up preferred properties. To do so, go to File > Preferences. In the Preferences dialog, select the **Property Display** tab. Click on **Deselect All** to clear the properties; then select the properties that you want entered and the order of those properties.  Then the user will enter the information required for that profile. If there is no information for a particular property, it will not appear under All Properties.

Batch Import: many spectra, many records, import properties from a spreadsheet

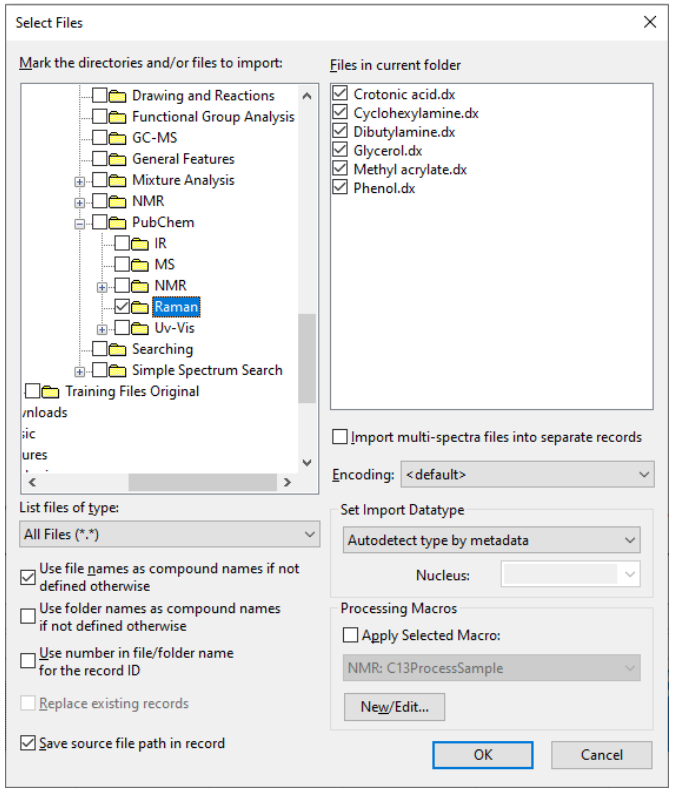
	Action	Result
1	Create a new empty database as in the above example.	
2	Choose **File > Batch Import**, to open the **Select Files** dialog box. Navigate to KnowItAll > Training Files > General Training > Files > Creating Databases > Batch Import Spectra, select all spectral files in the folder and click **OK**. **Note**: Check the box next to a folder name to select all files in the folder.	 A record is created in the new database for each spectral file.

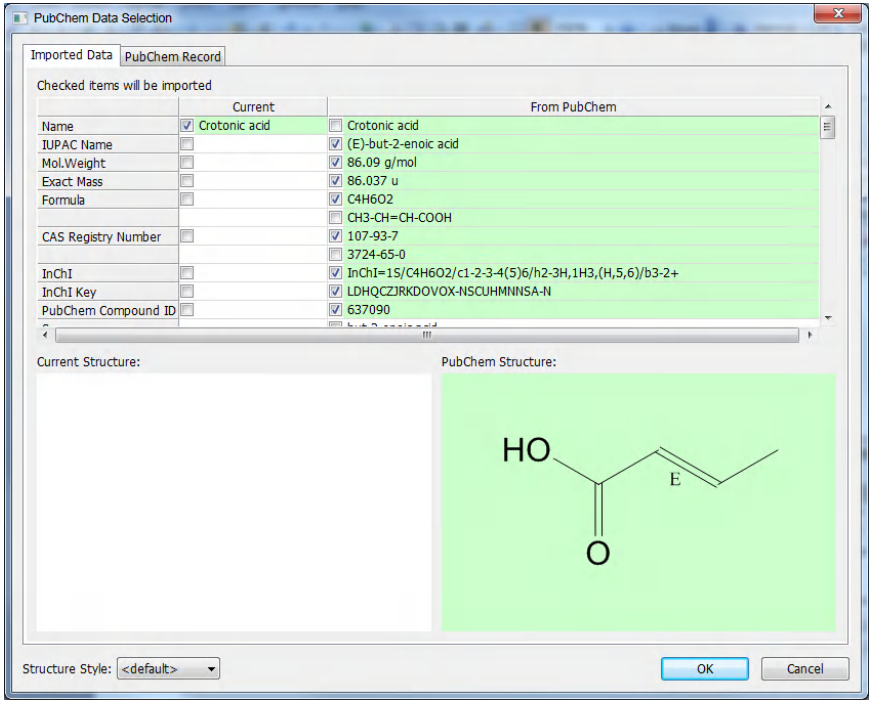
3	• Choose **File > Import** • Navigate to **KnowItAll > Training Files > General Training > Files > Creating Databases** • Select **BatchImportProperties.csv** to map properties to the spectrum files using a spreadsheet • Make sure to check **File Contains Header Line** • Click **Next**	The **Spreadsheet File Import** wizard opens: 

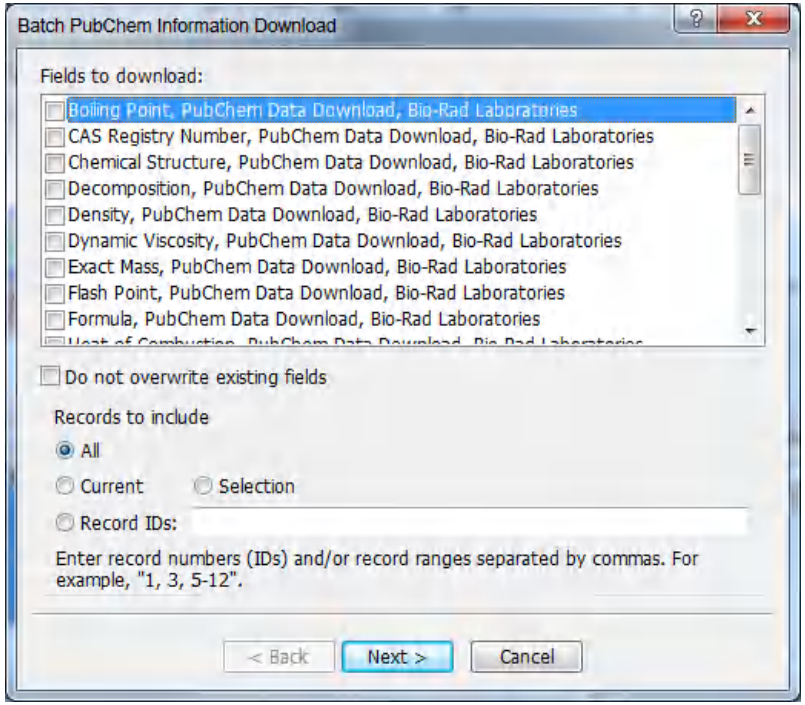
Batch Import: many spectra, many records, import properties from a spreadsheet (continued)

	Action	Result
4	Match • **CSV file** 'id' to **SDBX/SDB file** 'Record ID'; • **CSV file** 'Synonyms' to **SDBX/SDB file** "Synonyms"; • **CSV file** 'Sadtler Reference' to **SDBX/SDB file** 'Sadtler Reference Number'. Alternatively, you can click **Suggest All**, then review the automatic field matches. Click **Next**.	
5	Click **Finish**. You do not have to **Compact database now** at the prompt.	The database now has fields **Synonyms** and **Sadtler Reference** populated by the CSV file.
	TIP	You can rearrange the spreadsheet portion of this database (for example, to get rid of empty structure columns, right-click and choose **Delete Columns**). When edits are completed, you can save this column arrangement as a MineIt profile. Click **Save Current Profile** on the **Profile** toolbar, then type in a name for the new profile:  This profile will be linked with this database. It can also be selected for use with other databases.

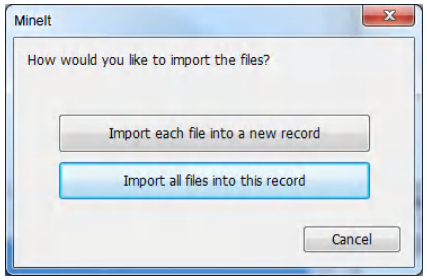
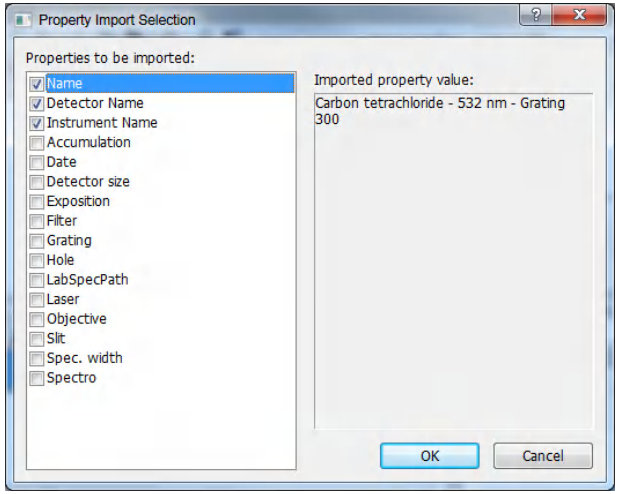
Batch Import: many spectra, many records, import properties from PubChem

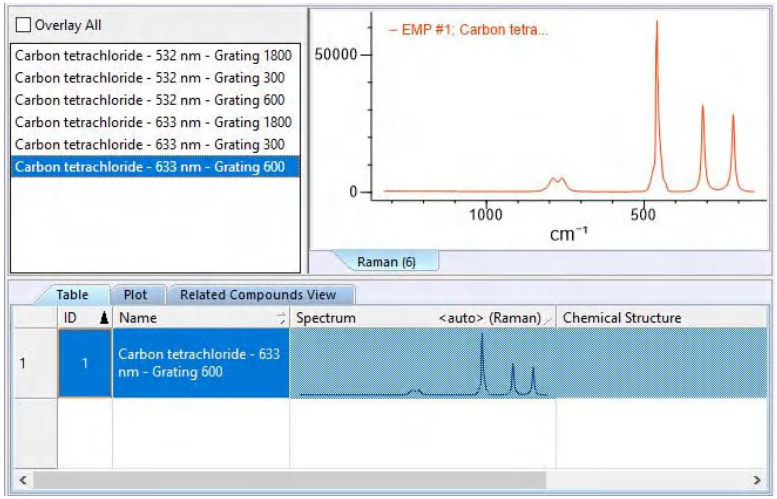
	Action	Result
1	Create a new empty database as in the above example.	
2	• Choose **File > Batch Import** • Navigate to **KnowItAll > Training Files > General Training > Files > PubChem > Raman** • Select all spectral files in the folder • Click **OK**.	 A record is created in the new database for each spectral file.

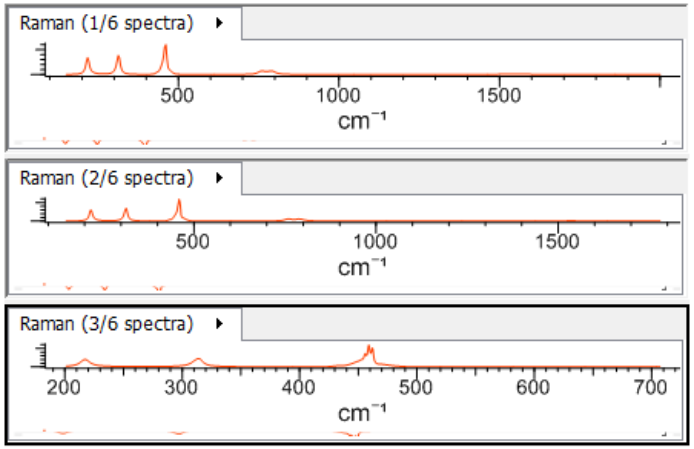
3	Select the first record, then click the **PubChem** toolbar button. 	**PubChem** records are searched. If information is located, the **PubChem Data Selection** dialog box opens: 

	Action	Result
4	Click **OK**.	New properties from **PubChem** are added to the first database record.
5	Select the remaining database records by holding the Shift key, then choose **Database > Batch PubChem Information Download**.	The **Batch PubChem Information Download** dialog box opens: 
6	Check the property fields you wish to add to the database records, then click **Next**.	New properties from PubChem are added to the remaining database records.

Batch Import: many spectra, one record

	Action	Result
1	Create a new empty database as in the above example.	
2	• Choose **File > Import** • Navigate to **KnowItAll > Training Files > General Training > Files > Creating Databases > Multiple Raman** • Select all files in the folder • Click **Open**	A dialog box opens and asks how you want to import the files: 
3	Click **Import all files into this record**.	The **Property Import Selection** dialog opens:  Check the properties you wish to import.

	Action	Result
4	Click **OK** each time the dialog appears.	The dialog box appears once for each spectrum in the record.
5	With the first record selected, observe the **Spectrum** pane.	The tab shows that there are 6 Raman spectra associated with the first record: 
6	Click the name of a spectrum in the left pane to display it.	

	Action	Result
7	Choose **Window > Split Threefold**.	The **Spectral** pane is split into 3 panes, displaying 3 of the 6 spectra: 

Creating Databases (optional section)

How to Create a Database with Structures

Purpose

This exercise demonstrates how to use the KnowItAll's MineIt™ Database Building feature to create searchable user databases that include structures.

Objectives

This exercise will teach you:

- How to create a user database;
- How to add structures to a user database;
- How to display stereochemical properties; and
- How to add user properties.

Background

Generating user databases protects intellectual property and promotes sharing of information within an organization. Ultimately, researchers can improve their analyses.

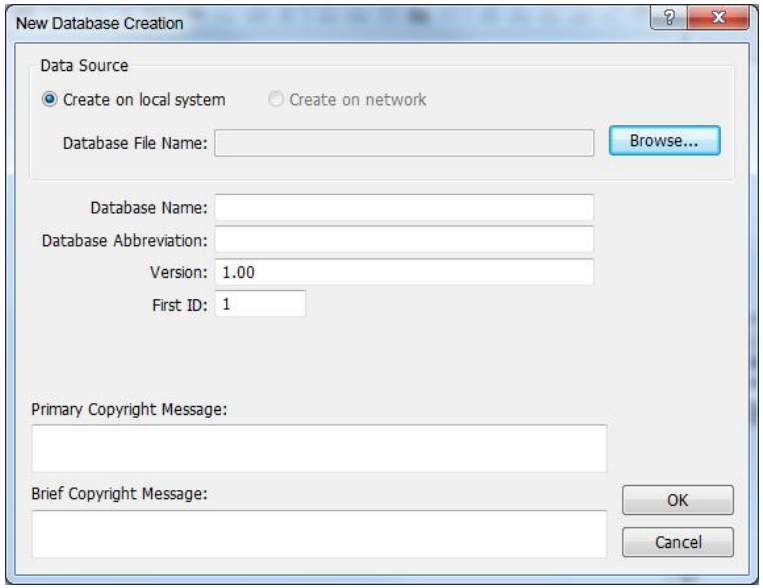
Training Files Used In This Lesson

- benzylpenicillin.dsf

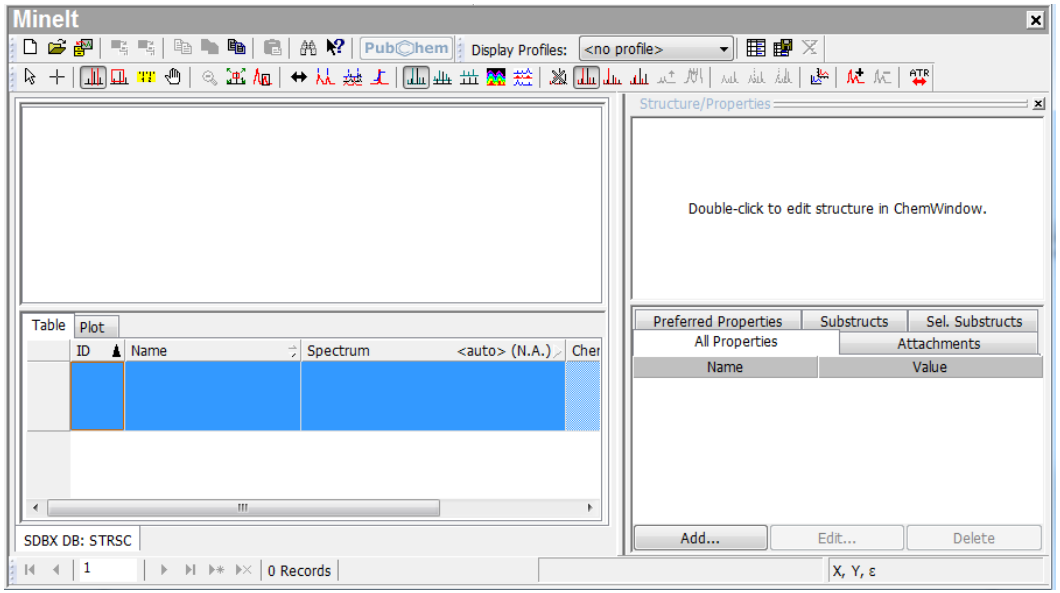
KnowItAll Applications Used

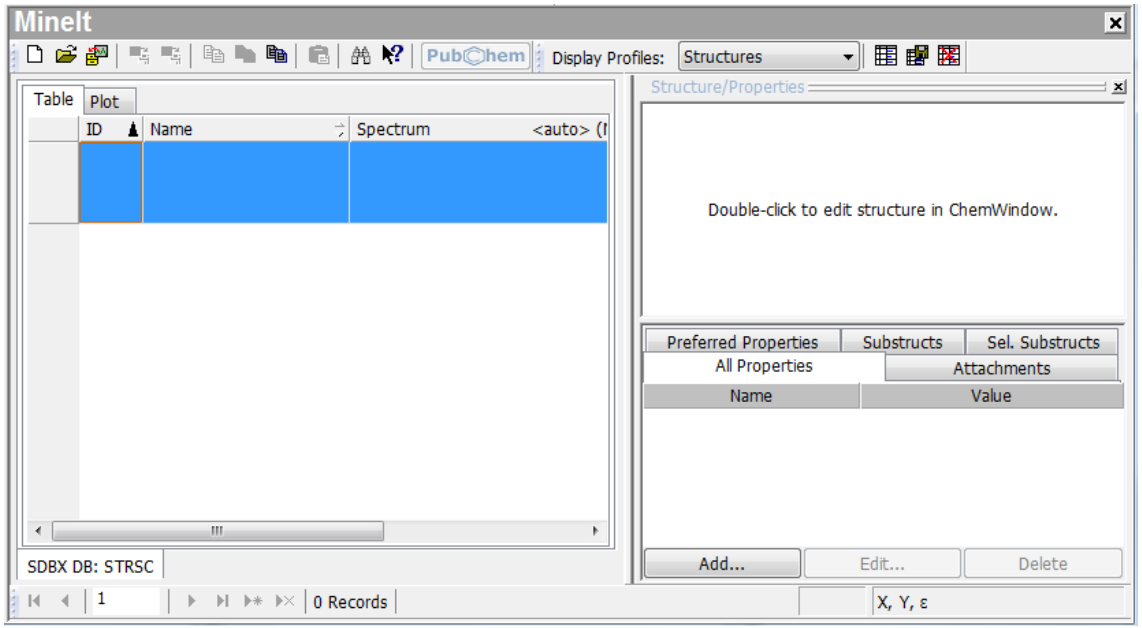
- MineIt™
- ChemWindow®

Create a user database

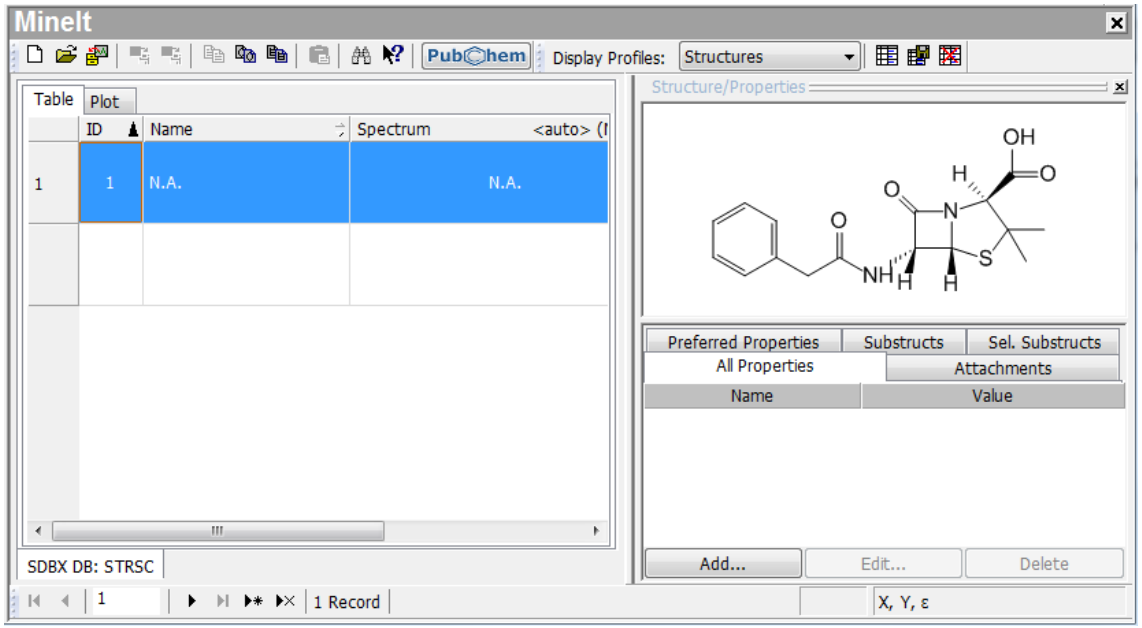
	Action	Result
1	In the MineIt application, choose **Database > New**.	The **New Database Creation** dialog box opens. 
3	Select **Create on local system**.	The new database is saved locally.
4	• Click **Browse** • Navigate to the **Databases** folder you created earlier, • Type **structures-sc** in the **Database File Name** • Click **Save**.	The *.sdbx extension is added automatically. **Note**: The SDBX database format allows spectra to be stored without conforming to a fixed range and resolution. This allows reference spectra to be offered at higher resolution, and allows users to store original spectra as produced.
5	Type **Structures** in the **Database Name** text box. **Note**: The file name is used if no other name is specified.	

Create a user database (continued)

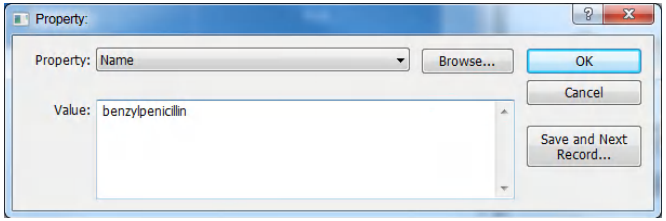
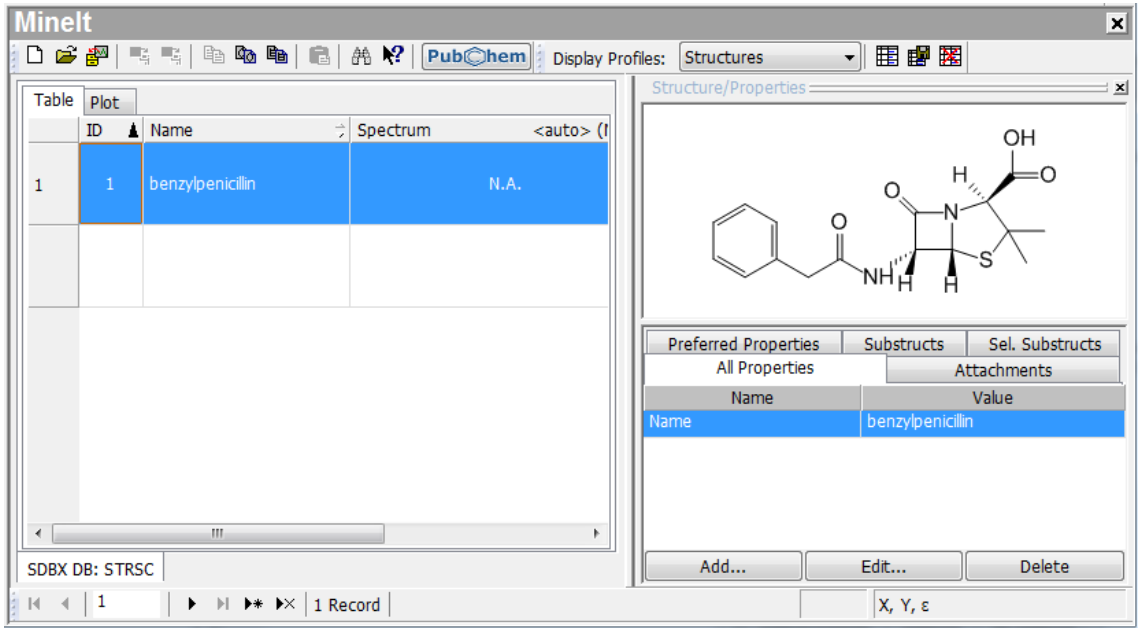
	Action	Result
6	Type 'STRSC' in the **Database Abbreviation** text box. **Note**: The abbreviation must be 3-7 characters long.	
7	Click **OK**.	The new database has been created to receive your data. The Database Abbreviation appears on the database tab. 
8	Choose **View > Windows/Tables > Spectrum Pane** to remove the spectral display from the layout. **Note**: This command (and others like it) toggle the display of different panes in the main window.	

	Action	Result
9	Click the **Add a New Profile** toolbar button  , type the name 'Structures' in the **New Profile** dialog box, then click **OK**.	

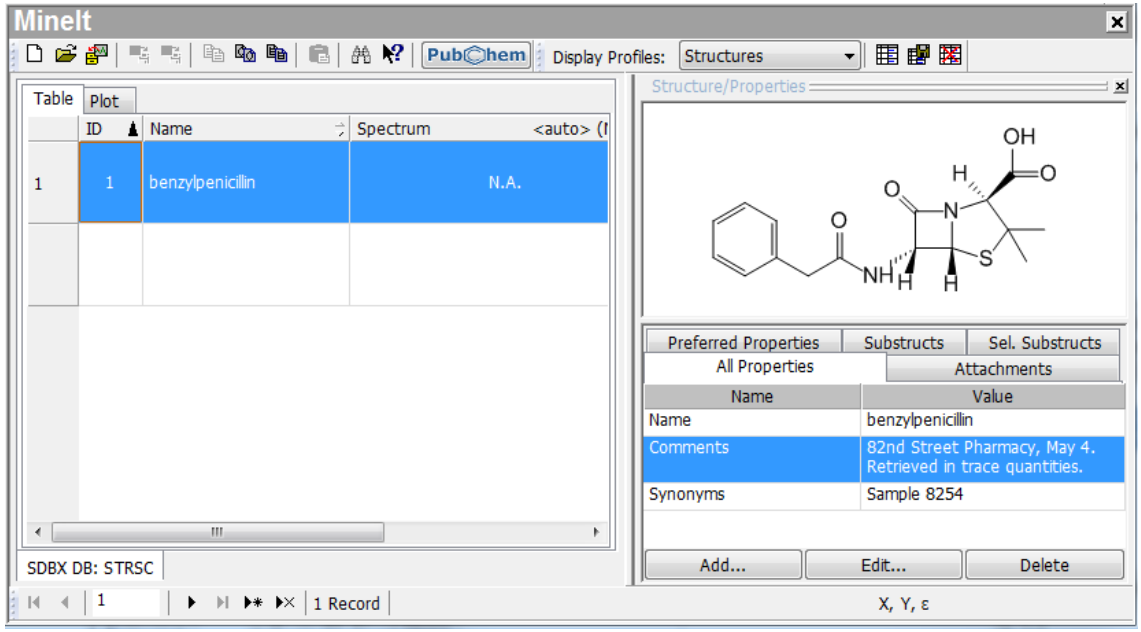
Add a structure to the first database record

	Action	Result
1	• Choose **File > Import** • Navigate **to KnowItAll > Training Files > General Training > Files > Creating Databases** • Open the structure file **Benzylpenicillin.dsf**.	The structure is displayed in the **Structure/Properties** pane: 
2	Open the **View** menu and check **Stereochemistry** if it is not already checked.	Stereochemical descriptors are shown on the structure when **Stereochemistry** is enabled on the **View** menu.

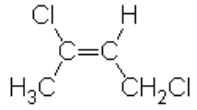
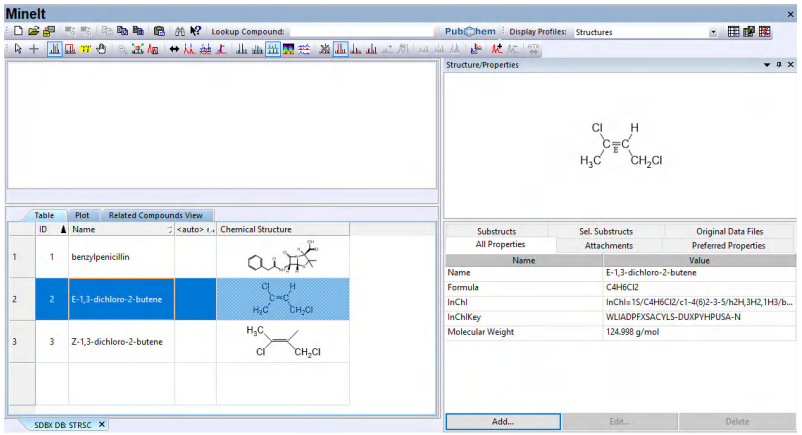
Add properties to the first database record

	Action	Result
1	Click **Add** in the **Structure/Properties** pane.	The **Property** dialog box opens.
2	Select the property **Name**, then type 'benzylpenicillin' in the **Value** text box.	
3	Click **OK**.	The **Property** dialog box closes, and the added property **Name** appears in the **Structure/Properties** pane. 

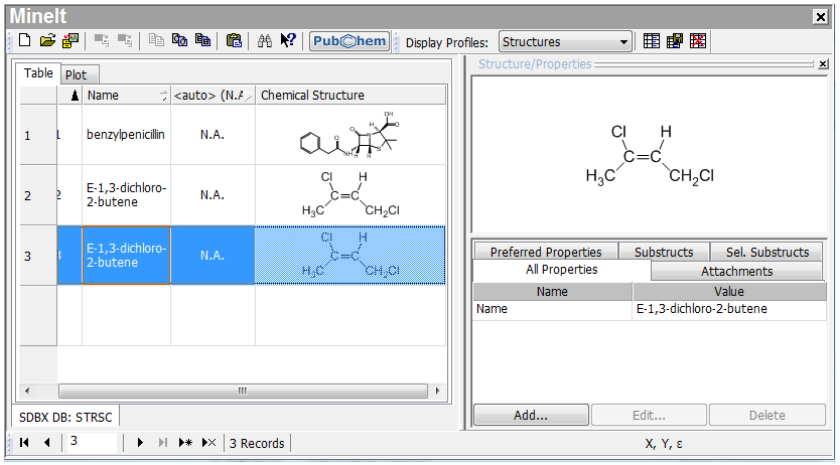
Add properties to the first database record (continued)

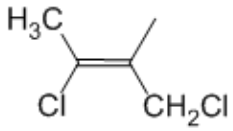
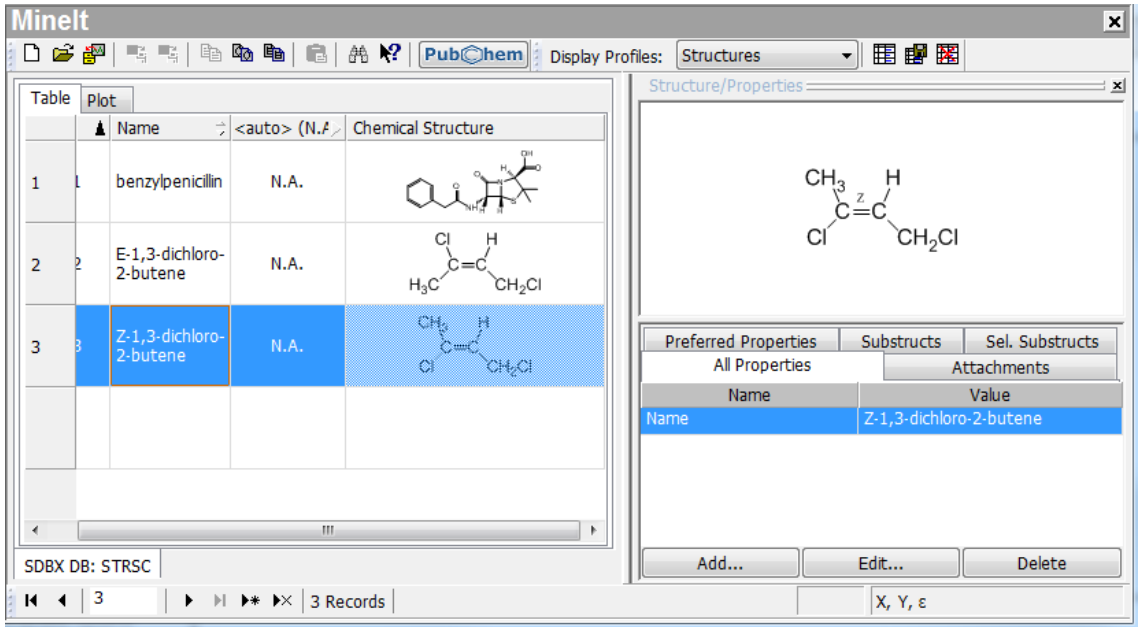
	Action	Result
4	Repeat to add the property **Synonyms** with the value 'Sample 8254.'	
5	Repeat to add the property **Comments** with the value '82nd Street Pharmacy, May 4. Retrieved in trace quantities.'	

Add a second database record

	Action	Result
1	Navigate to the **Basics** toolbox, then open the ChemWindow application by clicking its icon. **Note**: Do not use the **Transfer to** bar in this case.	
2	Draw this structure: 	
3	Use the **Selection** tool to select the structure, then choose **Edit > Copy**.	
4	Use the KnowItAll **Back** button to return to the MineIt application.	
5	With the second database entry selected, choose **Edit > Paste**. A message box asks “Would you like to append the new data as a new record?” Click **OK**.	The structure is added to the second record: 
6	Add the property **Name** with the value ‘E-1,3-dichloro-2-butene.’	

Add a third database record

	Action	Result
1	With the second database record still selected, choose **Edit > Copy Structure**.	
2	Select the third database record and choose **Edit > Paste**. A message box asks “Would you like to append the new data as a new record?” Click **OK**.	The structure and properties are added to the third database record. 
3	With the third database record selected, double click in the **Structure/Properties** pane to open the structure in **ChemWindow**.	

	Action	Result
4	Edit the structure as shown, then click **Return to MineIt Database and Save**. 	The structure is added to the third database record.
5	Edit the property **Name** to 'Z-1,3-dichloro-2-butene.'	

KnowItAll Software Training

Functional Group Analysis

Functional Group Analysis

How to Use the Knowledgebases to Identify or Differentiate Classes of Compounds by Structure or Functional Group

Purpose

This exercise demonstrates how to use the AnalyzeIt™ IR, AnalyzeIt Raman, and AnalyzeIt Polymer IR Knowledgebases to identify or differentiate chemical compounds, and to correlate peaks by structure.

Objectives

This exercise will teach you:

- How to specify the Knowledgebase;
- How to browse by functional group; and
- How to correlate a structure.

Background

The IR and Raman Knowledgebases include group frequencies with over 600 band assignments, corresponding to over 200 functional groups, subdivided into general chemical classes.

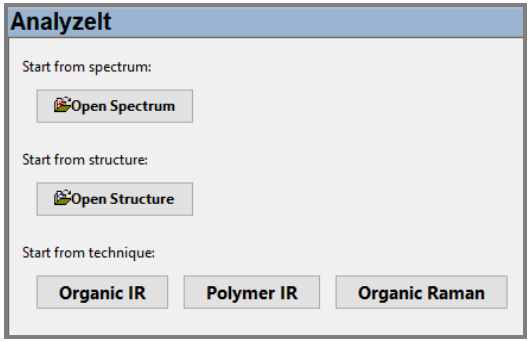
Training Files Used in This Lesson

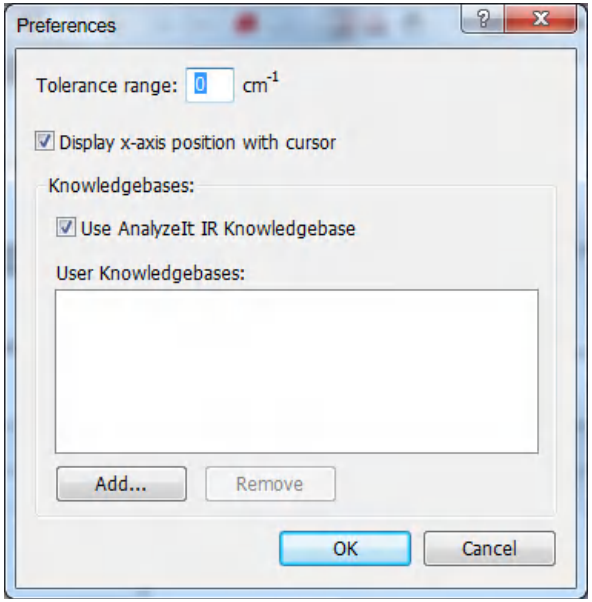
- Test Structure.dsf

KnowItAll Applications Used

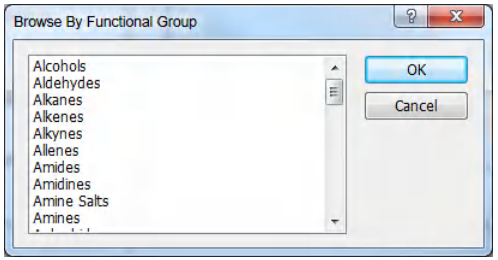
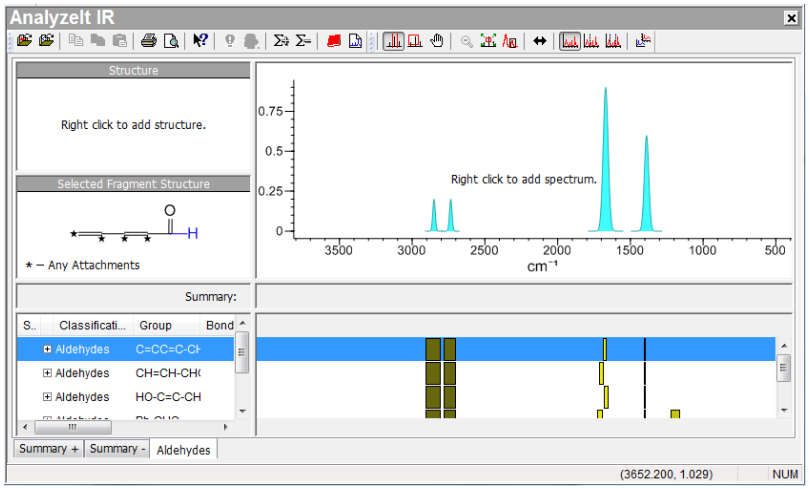
- AnalyzeIt™

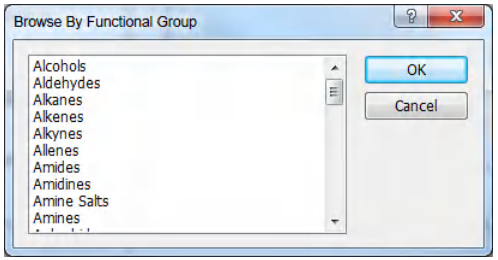
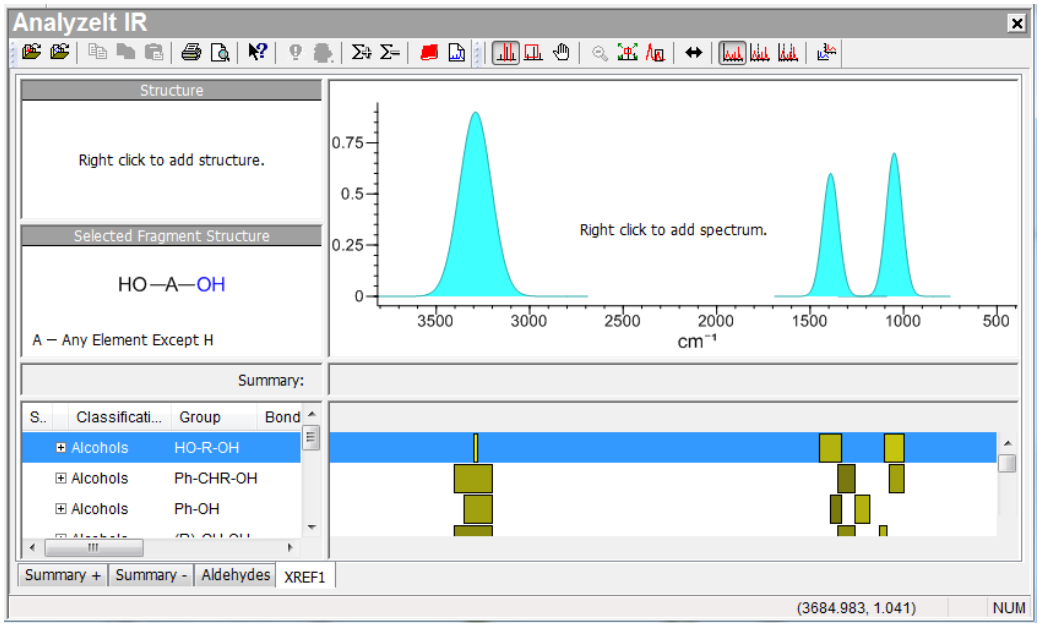
Specify the Knowledgebase

	Action	Result
1	Navigate to the **Spectral Analysis** toolbox	
	Click **AnalyzeIt**	 **Open Spectrum** - starts with any spectrum file. Upon selecting an IR spectrum, **KnowItAll** asks user if it should be put into **Organic IR** or **Polymer IR** application. **Open Structure** - starts with any structure file. Upon selecting a structure file, **KnowItAll** asks user if it should be put into **Organic IR** or **Organic Raman** application. By the same token, • **IR Organic** - starts a blank **AnalyzeIt IR** application • **Polymer IR**- starts a blank **AnalyzeIt Polymer IR** application • **Raman Organic** - starts a blank **AnalyzeIt Raman** application

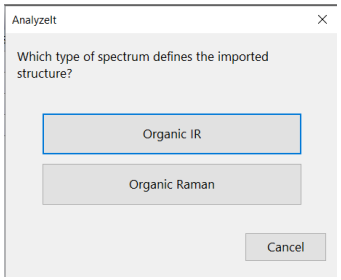
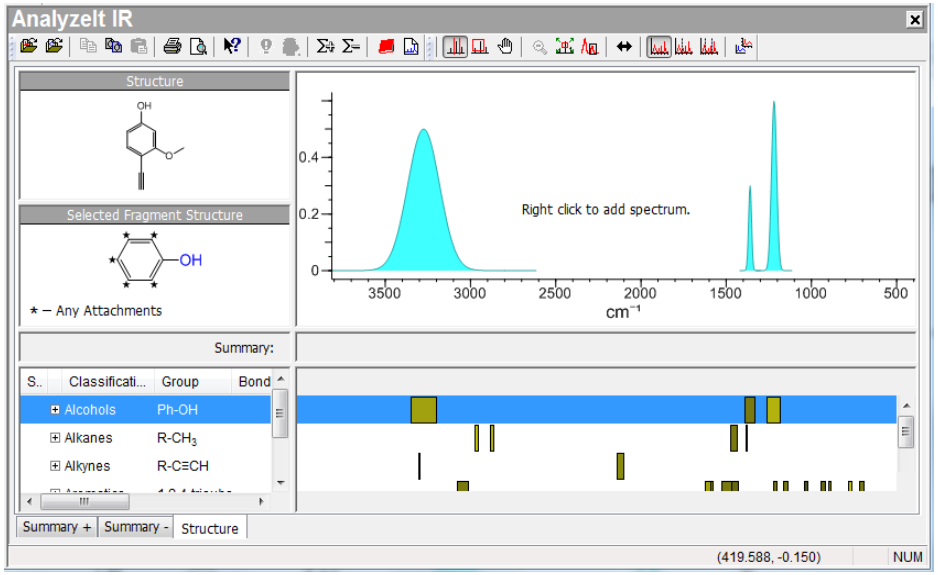
2	Let's start from technique: **Organic IR** Click **Organic IR** and then choose **File > Preferences**.	The **Preferences** dialog box opens:  Setting the **Tolerance range** allows you to determine how precise the matches are between your spectrum peak and the database. You can also choose to display a wavenumber (x-axis position) marker with the cursor as it moves around the **Spectrum** pane. Finally, use the check boxes to select the knowledgebase you wish to use.
3	Make sure **AnalyzeIt IR Knowledgebase** is selected Click **OK**	

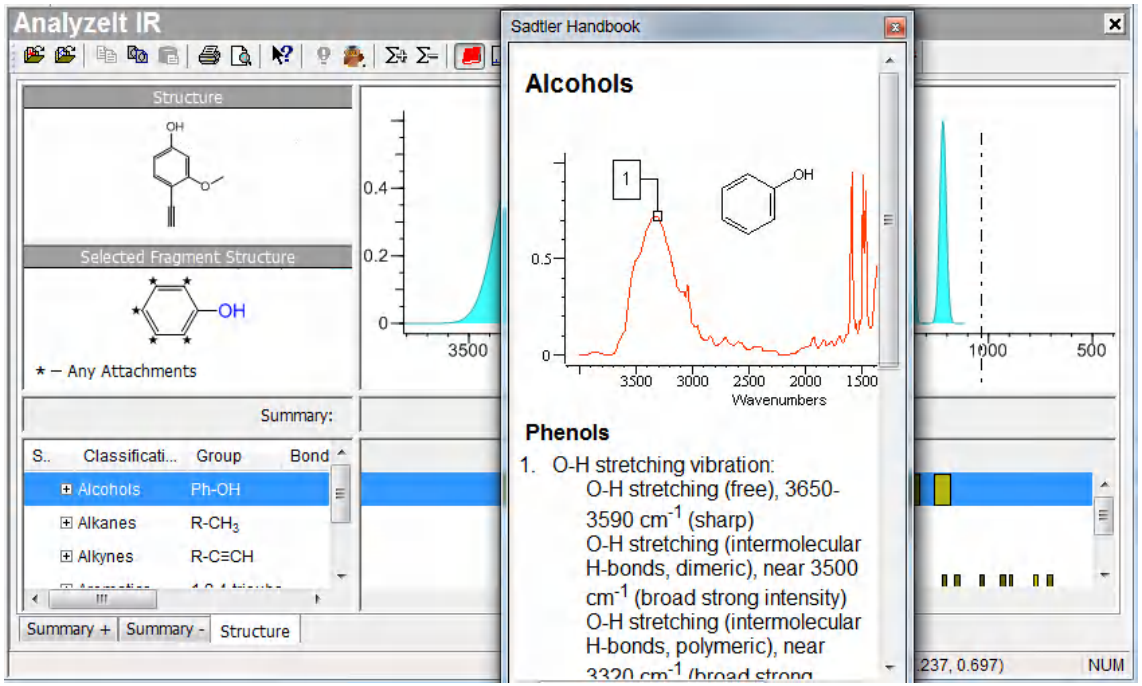
Browse by functional group

	Action	Result
1	Choose **Analyze > Browse a Functional Group**.	The **Browse By Functional Group** dialog box opens: 
2	Select **Aldehydes** and click **OK**.	The **Aldehydes** tab is added to the AnalyzeIt IR display:  Each functional group in the aldehydes group is listed separately in the **Functional Group Data** pane at the lower left, and each entry includes classification, group, bond, range, intensity, mode, and notes. Colored bars in the **Bar Chart** pane at the lower right represent the peaks associated with each functional group class selected in the **Functional Group Data** pane. The bars are intensity coded; lighter color means greater intensity. Corresponding peaks appear in the **Spectrum** pane.

	Action	Result
3	Choose **Analyze > Browse a Functional Group** again.	The **Browse By Functional Group** dialog box opens: 
4	Select both **Alcohols** and **Anhydrides**, then click **OK**. **Note**: Select the first class, then hold down the ctrl key and click to select a second class.	The XREF1 tab is added to the AnalyzeIt IR display:  The tab is labeled XREF1 because it is the first tab containing a combination of classes.

Correlate peaks from a structure

	Action	Result
1	• Choose **File > Close** to clear the previous example display • Click **Open Structure** button • Navigate to **KnowItAll > Training Files > General Training > Files > Functional Group Analysis** • Open **Test Structure.dsf**	A dialog box prompts user to choose between IR or Raman 
2	Click **Organic IR**	After the knowledge base is analyzed, the results are displayed in a **Structure** tab. The **Functional Group Data** pane includes an entry for each group found in the structure. 

	Action	Result
3	Choose **View > Sadtler Handbook** to display the handbook information related to a particular functional group.	The **Sadtler Handbook** pane displays information from the Sadtler Handbook of Reference Spectra - IR for the specific functional group selected in the **Functional Group Data Pane**.  Double clicking the **Sadtler Handbook** pane's title bar allows you to dock and un-dock the pane with reference to the main display.
4	Choose **File > Close**.	The display is cleared.

Functional Group Analysis

How to Perform a Basic Spectral Analysis Using Software-Assisted Functional Group Analysis

Purpose

This exercise demonstrates how to use the AnalyzeIt™ application to perform a basic spectral analysis.

Objectives

This exercise will teach you:

- How to select peaks for correlation; and
- How to use the Summary+ and Summary- tabs.

Background

The AnalyzeIt application can be used to help interpret spectra through the use of its knowledge bases of over 200 functional groups. They can be used to obtain functional group information from a spectrum or a structure, or by browsing the chemical classes included in the knowledge bases.

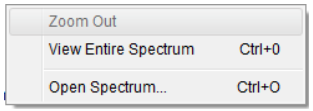
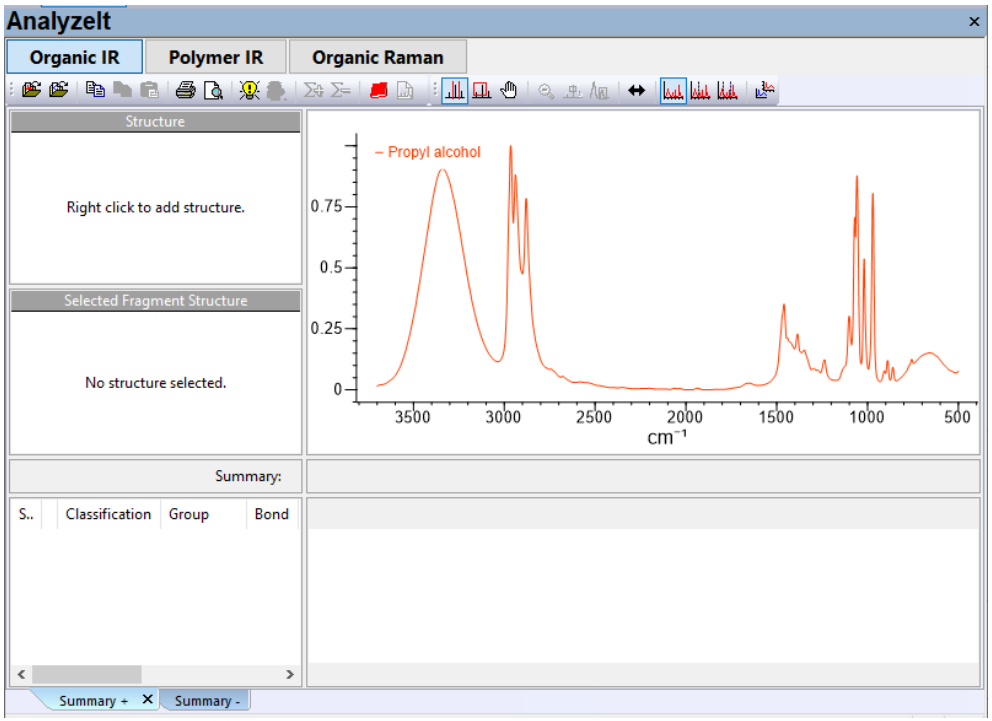
Training Files Used in This Lesson

- Peak Interpretation Example.dx (IR)

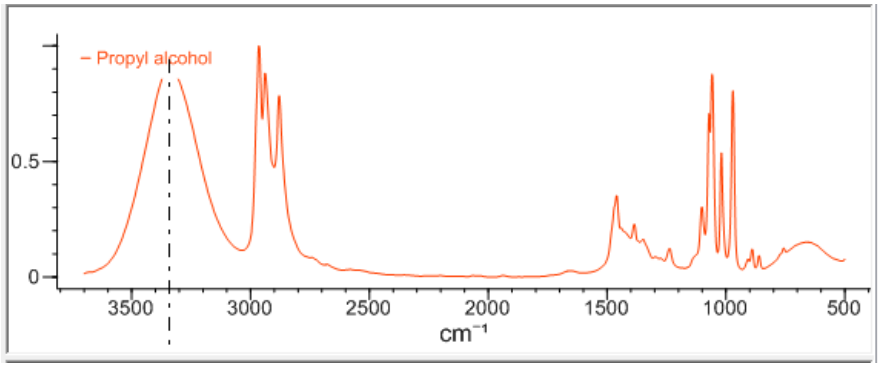
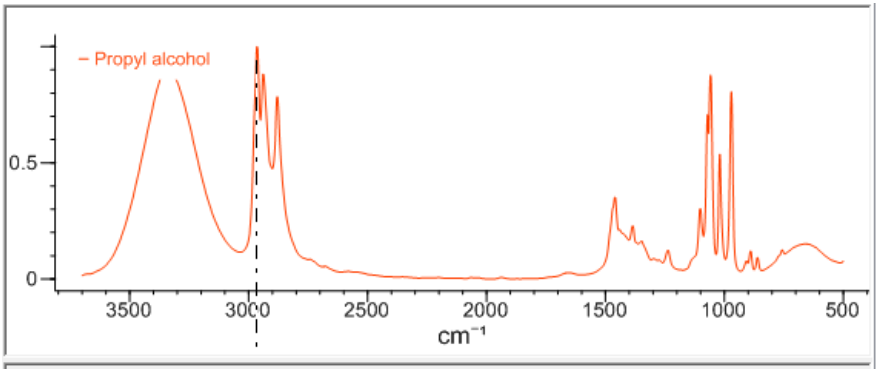
KnowItAll Applications Used

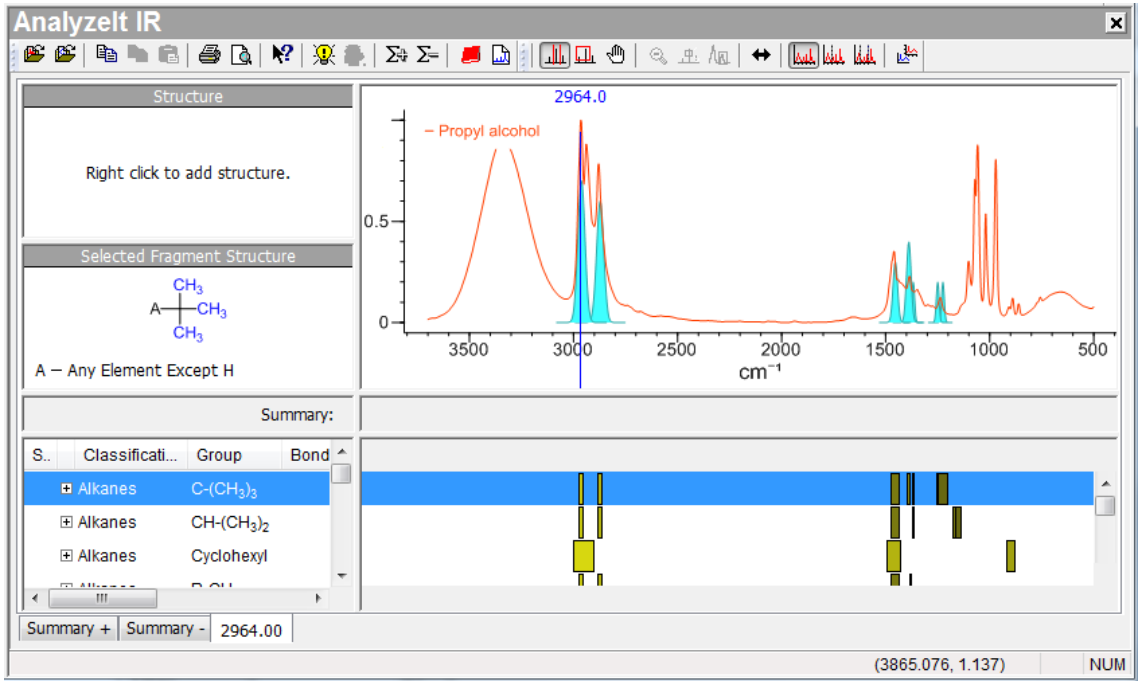
- AnalyzeIt™

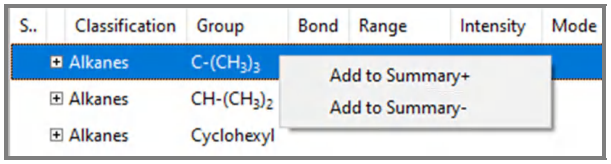
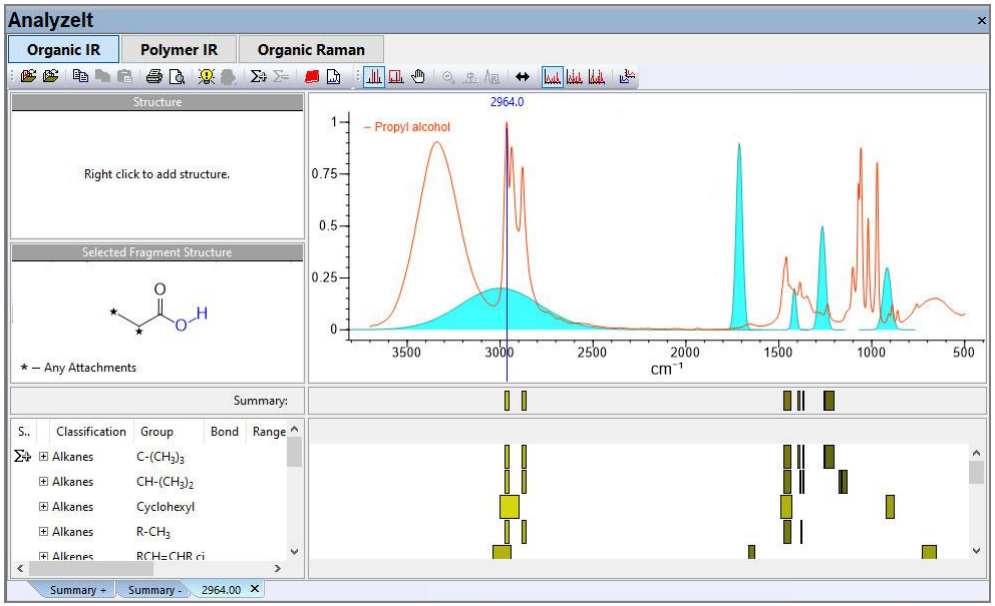
Open a spectrum

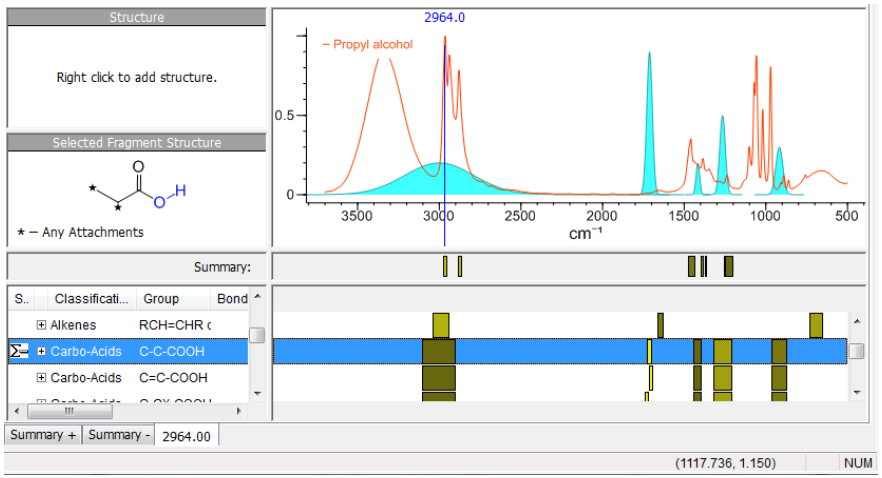
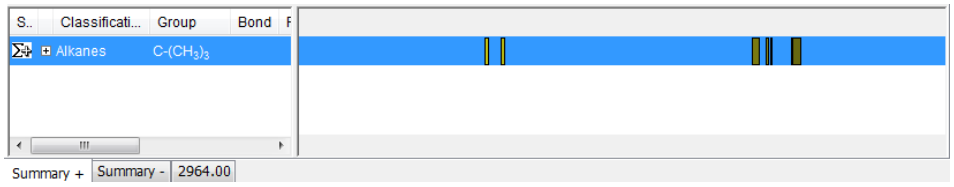
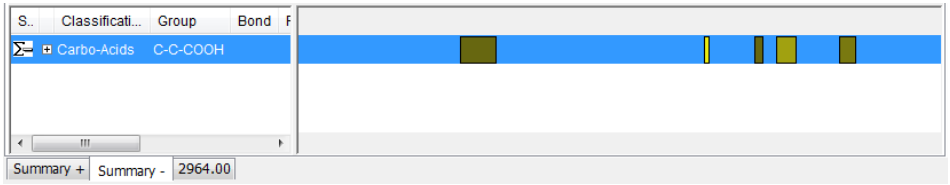
	Action	Result
1	Navigate to the **Spectral Analysis** toolbox, and click **AnalyzeIt** followed by **Organic IR**.	
2	Right-click in the **Spectral Pane**.	A pop-up menu opens: 
3	• Click **Open Spectrum** • Navigate to **KnowItAll > Training Files > General Training > Files > Functional Group Analysis** • Open **Peak Interpretation Example.dx**. • Since this particular spectrum does not have the X-axis unit defined, KnowItAll warns the user with a pop-up saying **The information stored as "Propyl alcohol" does not have X axis unit defined for the spectral trace. KnowItAll will attempt to read the data as cm^{-1}**. • Click **OK**.	The spectrum is displayed: 

Analyze the spectrum

	Action	Result
1	Click the **Suggest** toolbar button  .	The application selects a peak to analyze:  In general, it is best to begin a correlation with a peak above 1500 wavenumbers that is unique and strong. The **AnalyzeIt** application uses a set of rules to select a good starting point.
2	Click the **Suggest** toolbar button again. **Note**: You can also select peaks by clicking in the spectral pane.	Another peak is suggested:  As you click the **Suggest a Peak** toolbar button repeatedly, the application cycles through the suggested starting points.

	Action	Result
3	Click **Suggest** until the second peak (at 2964) is selected and then click the **Correlate** button  .	After the knowledge base is analyzed, the results are displayed in a tab labeled with the wavenumber. 

	Action	Result
4	• Select the alkanes entry C-$(CH_3)_3$ in the **Functional Group Data** pane • Right-click to open the **Summary** pop-up menu. **Note**: The **Summary+** and **Summary–** tabs are created automatically, and are provided to allow you to keep track of functional groups that are consistent with or inconsistent with the measured spectrum.	
5	Because the methyl group correlates well with the spectrum, click **Add to Summary+**.	The peaks are added to the **Summary+** tab and the **Summary Bar Chart** pane (between the spectral display and the **Bar Chart** pane), and a summary plus symbol appears in the **Functional Group Data** pane next to this group. 

	Action	Result
6	Select the first carboxylic acid entry (C-C-COOH) in the **Functional Group Data Pane**, then right-click to open the **Summary** pop-up menu.	
7	Because the results indicate that there should also be a strong band near the 1740 region, move this group to the **Summary–** tab.	
8	Click the **Summary+** tab to display any groups added to this tab.	
9	Click the **Summary-** tab to display any groups added to this tab.	
10	Choose **File > Close**.	The display is cleared.

Functional Group Analysis

How to Perform a Basic Spectral Analysis Using AnalyzeIt™ for Polymer

Purpose

This exercise demonstrates how to use the AnalyzeIt application to perform a basic spectral analysis of polymer

Objectives

This exercise will teach you:

- How to analyze spectra from polymer samples.

Background

The AnalyzeIt Polymer IR Knowledge Base can provide clear and rapid verification and identification of functional groups in the mid-infrared. It features over 100 functional groups and hundreds of interpretation frequencies.

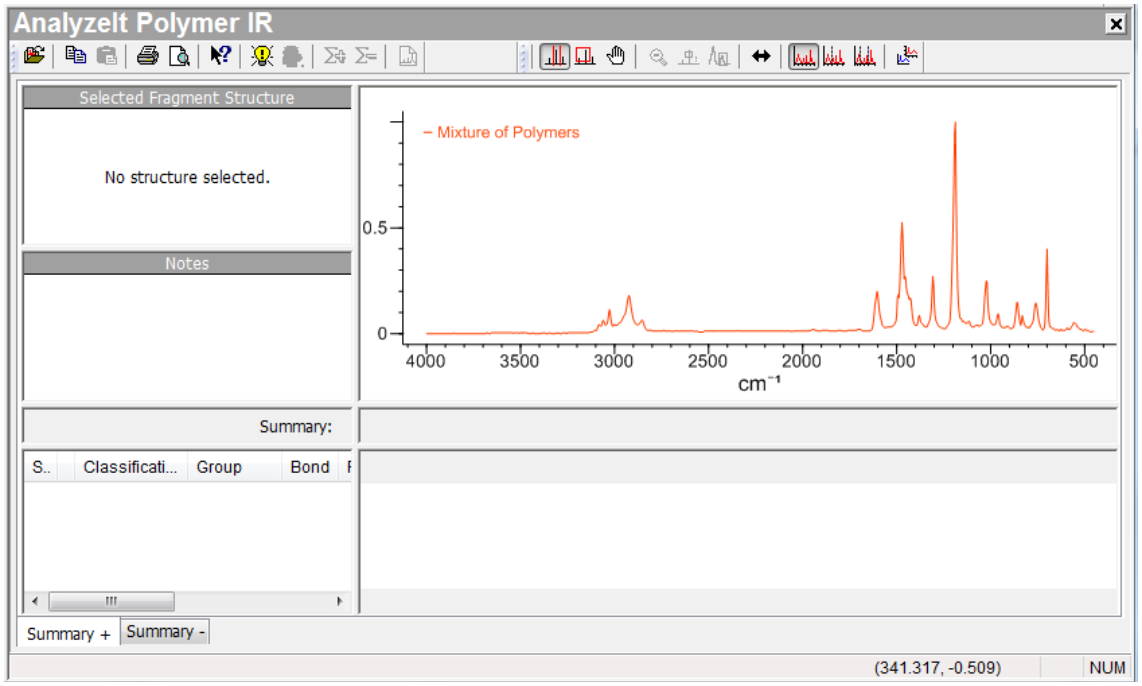
Training Files Used in This Lesson

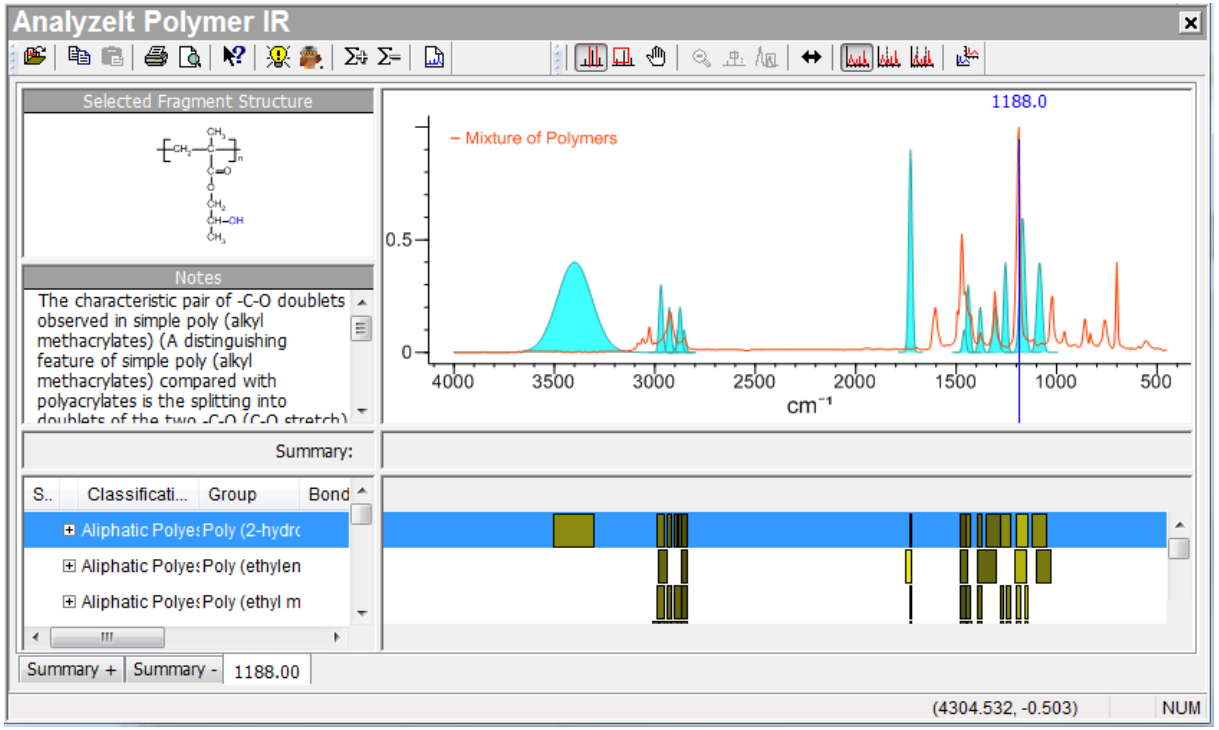
- Mixture of Polymers.irf
- Polystyrene.irf

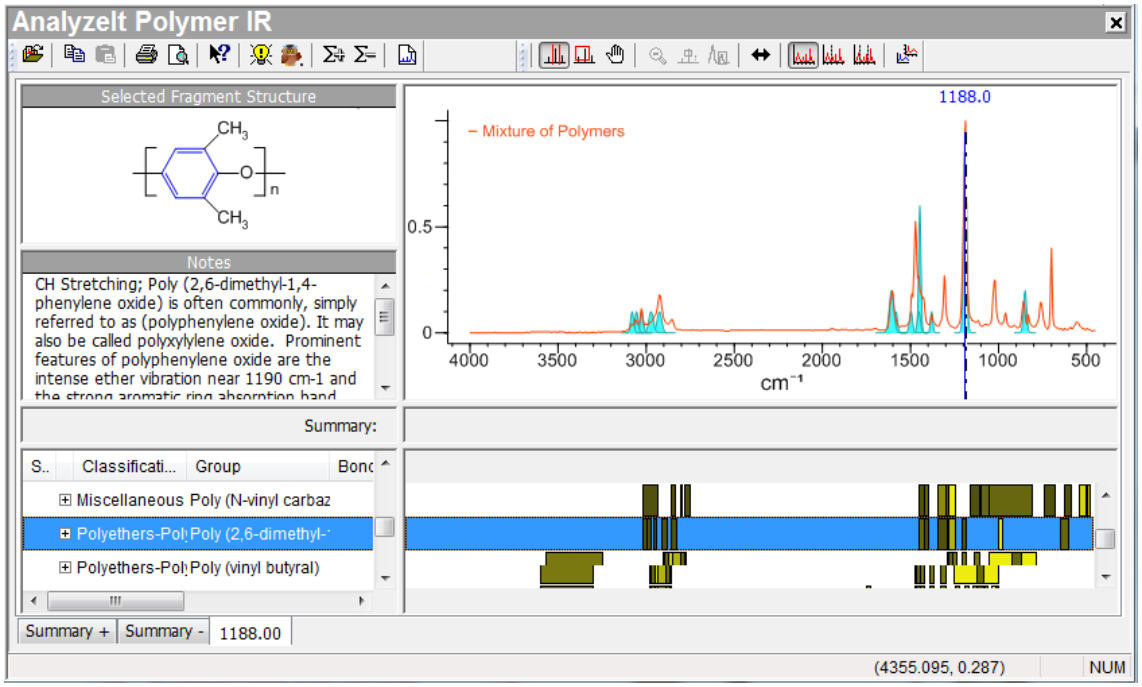
KnowItAll Applications Used

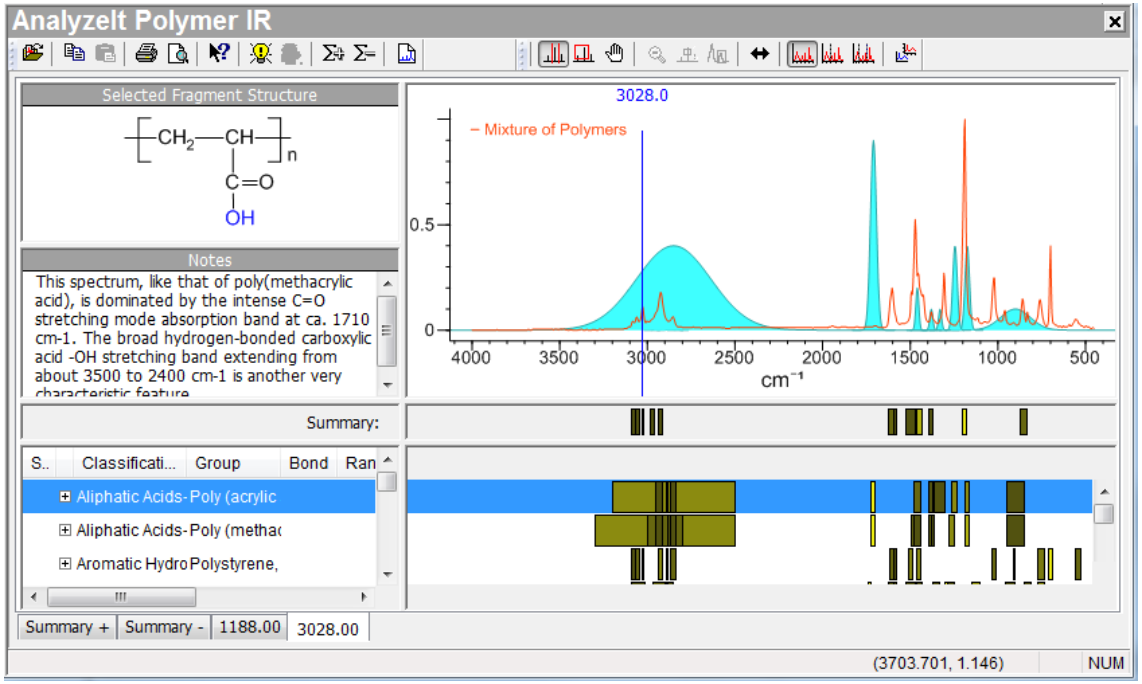
- AnalyzeIt™

Open and analyze a mixture spectrum

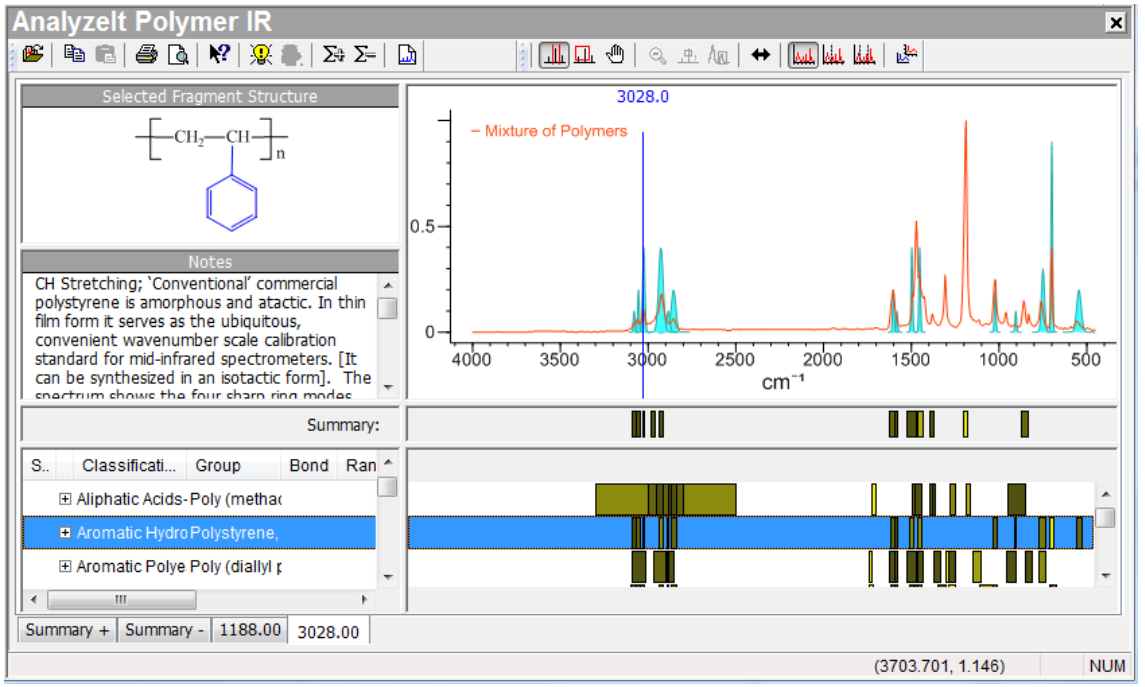
	Action	Result
1	Navigate to the **Spectral Analysis** toolbox, click on **Open Spectrum**	
2	• Navigate to **KnowItAll > Training Files > General Training > Files > Functional Group Analysis** • Open **Mixture of Polymers.irf**. • Click on **Polymer IR** button in the pop-up dialog. **Note**: Use the **Files of type** filter to locate IRF, JCAMP, and many other specific spectral files. You can also select **All files (*.*)**.	The spectrum opens: 

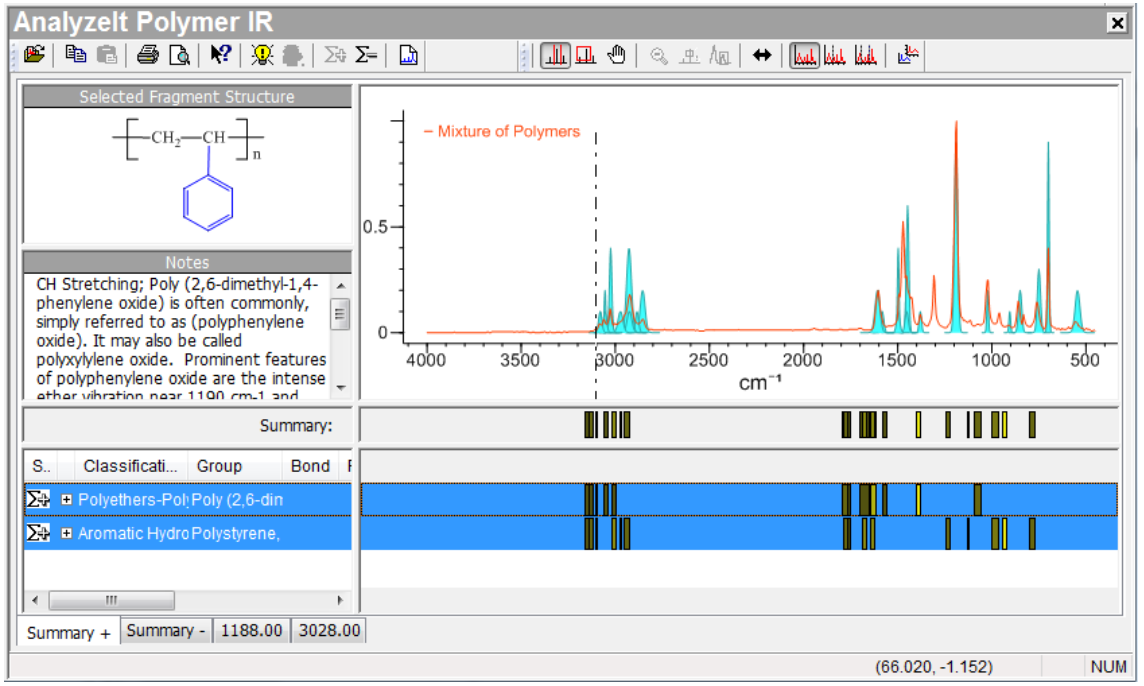
	Action	Result
3	Use the **Suggest** button to select the tallest peak (at 1188), then click the **Correlate** button  . Alternatively, you can double-click a peak to both select it and initiate searching the knowledgebase(s) for functional group matches.	After the knowledgebase is analyzed, the results are displayed in a tab labeled with the wavenumber (1188). 

	Action	Result
4	Select each entry in the **Functional Group Data** pane in turn. Note that the first Polyether-Polymer IR entry (Poly (2,6-dimethyl-1,4-phenylene oxide)) is a good match.	
5	Right-click the entry, then select **Add to Summary+**.	The entry is added to the **Summary+** tab.

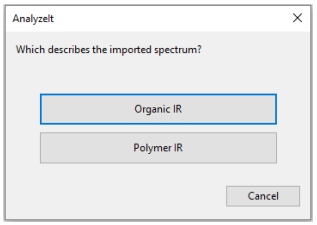
	Action	Result
6	Click the **Suggest** button to select the peak at 3028, then click the **Correlate** button  .	After the knowledge base is analyzed, the results are displayed in a tab labeled with the wavenumber.  Note the detailed notes available with many **Functional Group** entries.

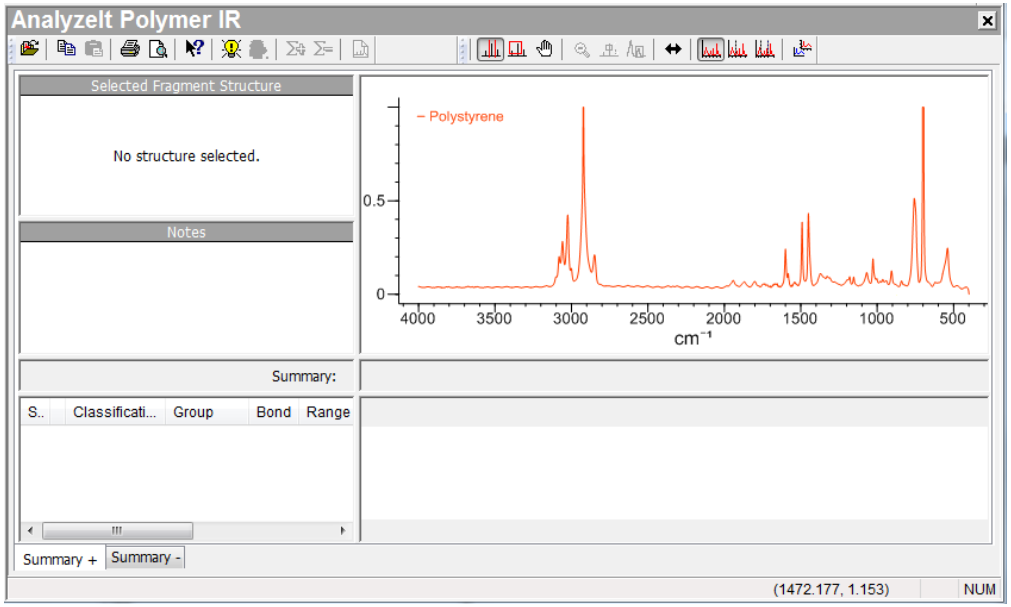
Open and analyze a mixture spectrum (continued)

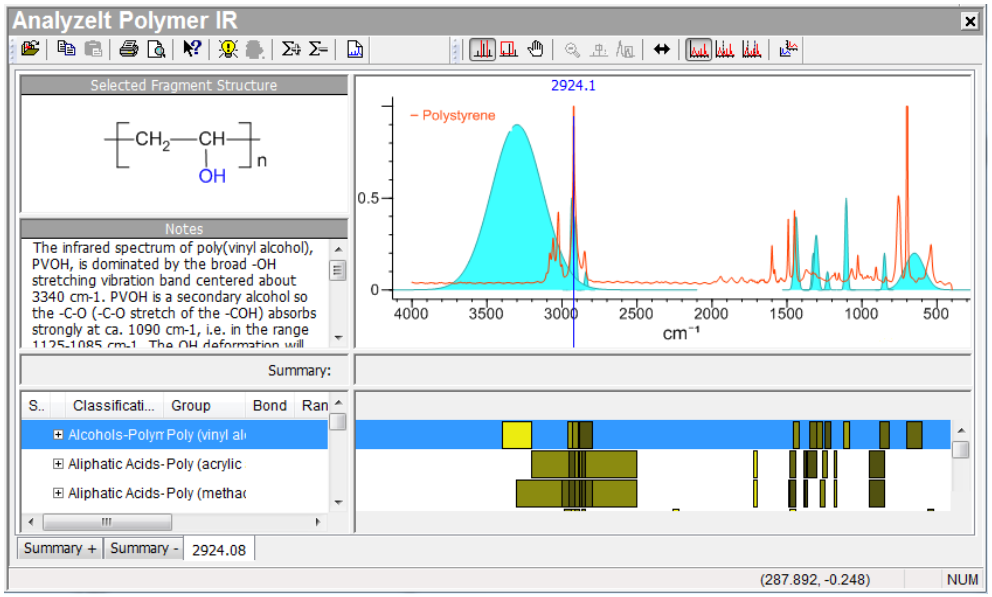
	Action	Result
7	Select each entry in the **Functional Group Data** pane in turn. Note that the Aromatic Hydrocarbon (Polystyrene) entry is a good match.	
8	With the Aromatic Hydrocarbon (Polystyrene) entry selected, right-click then select **Add to Summary+**.	The entry is added to the **Summary+** tab.

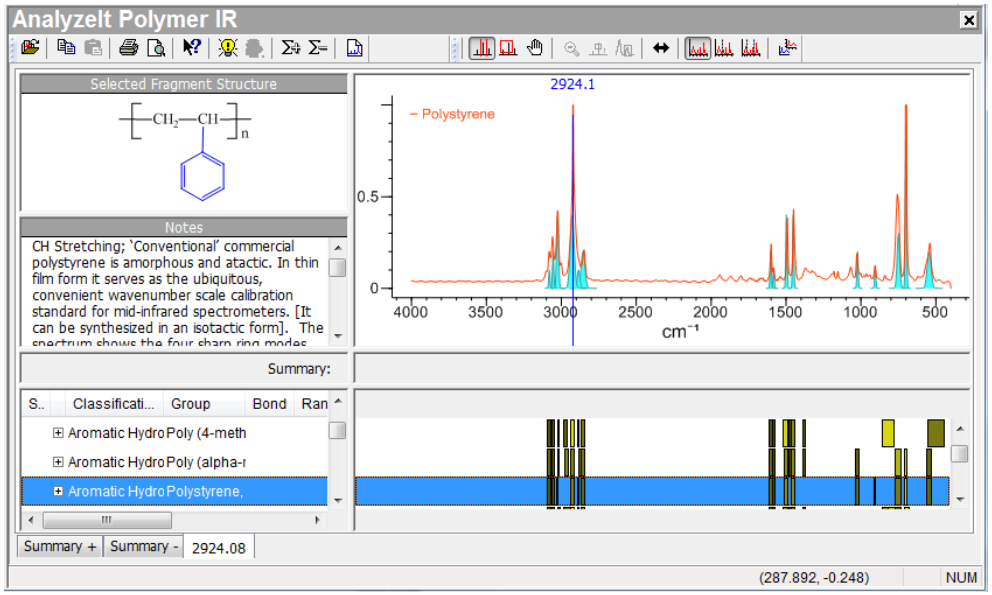
	Action	Result
9	Open the **Summary+** tab and select both entries. **Note**: Select the first entry, then hold down the ctrl key and click to select the second entry.	We see that these functional groups account for most of the peaks in the mixture spectrum. 

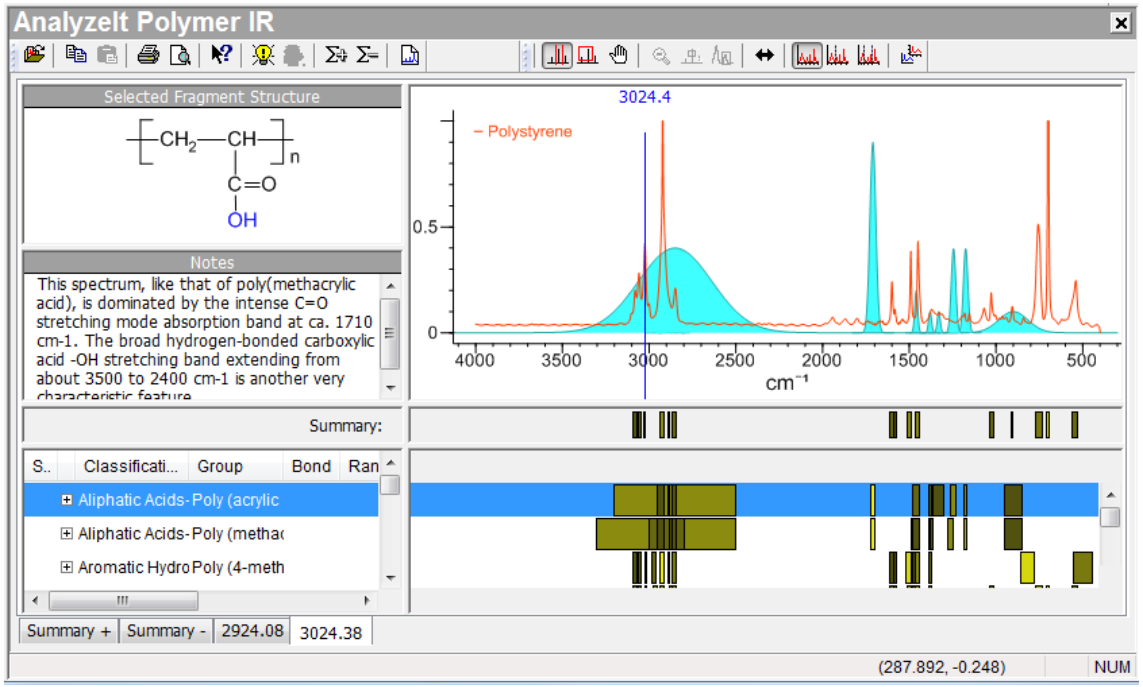
Open and analyze a single component spectrum

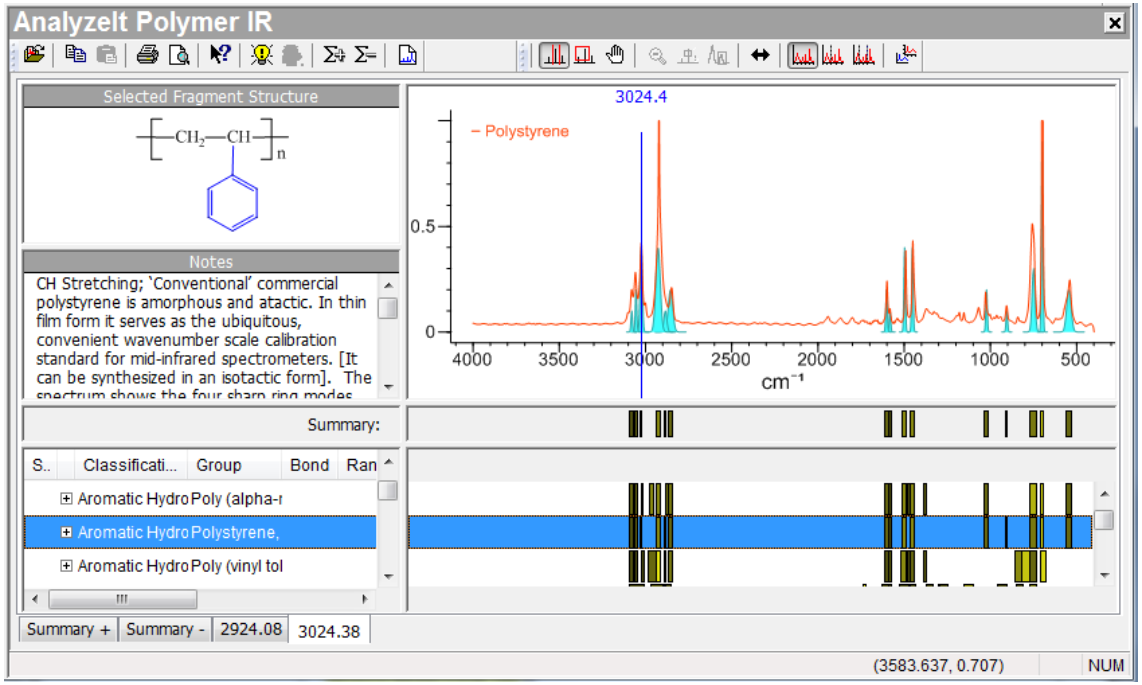
	Action	Result
1	Close the previous analysis by clicking the close button in the upper right-hand corner.	
2	• Choose **File > Open Spectrum**, • Navigate to **KnowItAll > Training Files > General Training > Files > Functional Group Analysis** • Open **Polystyrene.irf**. **Note**: Use the **Files of type** filter to locate IRF, JCAMP, and many other specific spectral files. You can also select **All files (*.*).**	A pop-up dialog displays two options; 

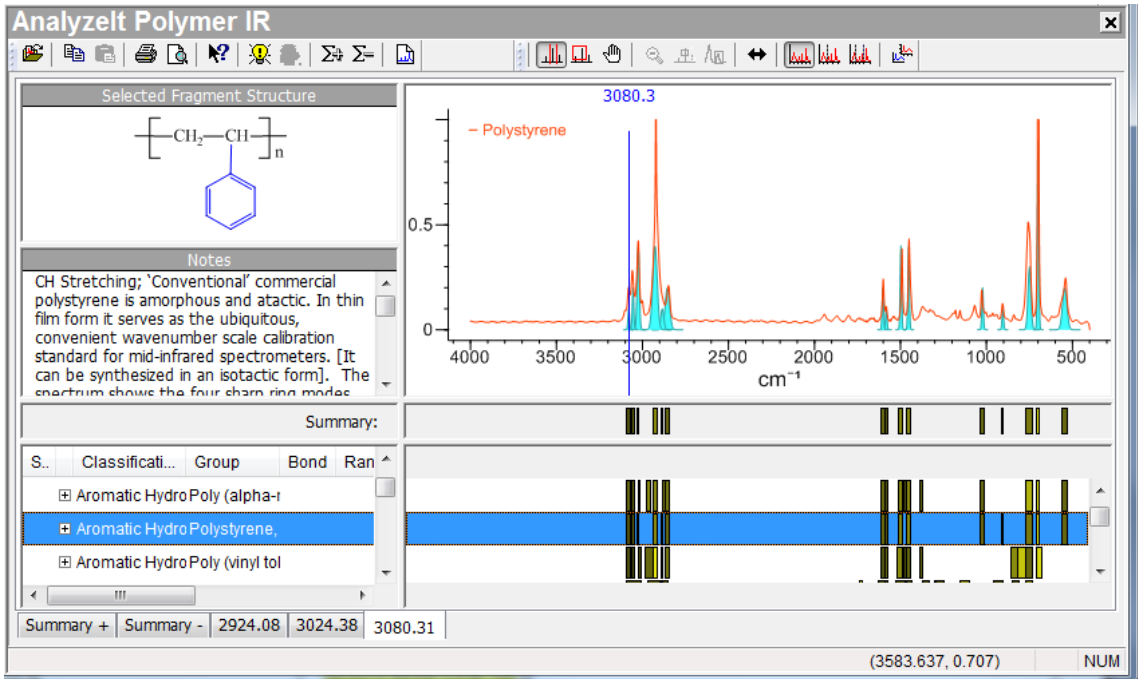
3	Click on **Polymer IR**.	The spectrum opens: 

	Action	Result
3	Click the **Suggest** button to select the peak at 2924.1, then click the **Correlate** button.	After the knowledge base is analyzed, the results are displayed in a tab labeled with the wavenumber (2924.08). 

	Action	Result
4	Select each entry in the **Functional Group Data** pane in turn.	Note that Aromatic Hydrocarbon (Polystyrene) is a good fit: 
5	With the Aromatic Hydrocarbon (Polystyrene) entry selected, right-click, then select **Add to Summary+**.	The functional group is added to the **Summary+** tab.

	Action	Result
6	Click the **Suggest a Peak** toolbar button again, then click the **Correlate** toolbar button.	After the knowledge base is analyzed, the results are displayed in a tab labeled with the wavenumber (3024.38). 

	Action	Result
7	Select each entry in the **Functional Group Data** pane in turn.	Note that the Aromatic Hydrocarbon (Polystyrene) is, once again, a good fit: 

	Action	Result
8	Repeat the process to analyze the third suggested peak (3080.3), then select each entry in the **Functional Group Data** pane in turn.	Aromatic Hydrocarbon (Polystyrene) is a good fit: 

Functional Group Analysis

How to Create a User Knowledgebase

Purpose

This exercise demonstrates how to create and use user Knowledgebases in the AnalyzeIt™ applications.

Objectives

This exercise will teach you:

- How to create a user Knowledgebase;
- How to browse by functional group; and
- How to correlate a structure.

Background

Users can build their own knowledgebases with functional groups and bands from their own data. The knowledgebases can be used in conjunction with KnowItAll's knowledgebases to determine the functional groups in a spectrum.

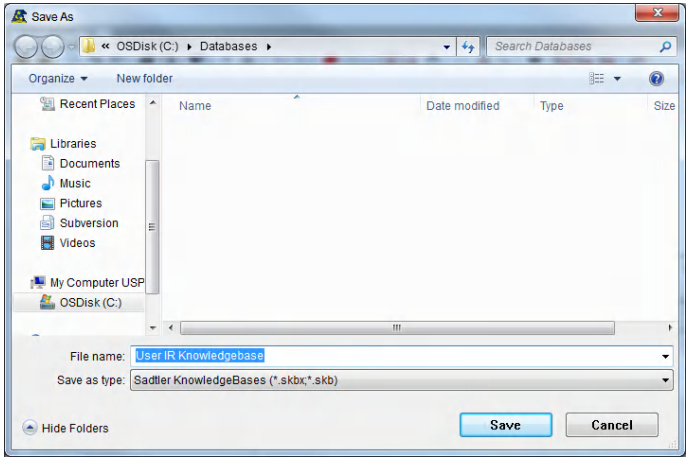
Training Files Used in This Lesson

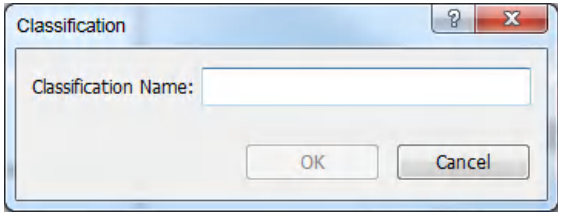
- Test Structure.dsf
- Butylamine.jdx

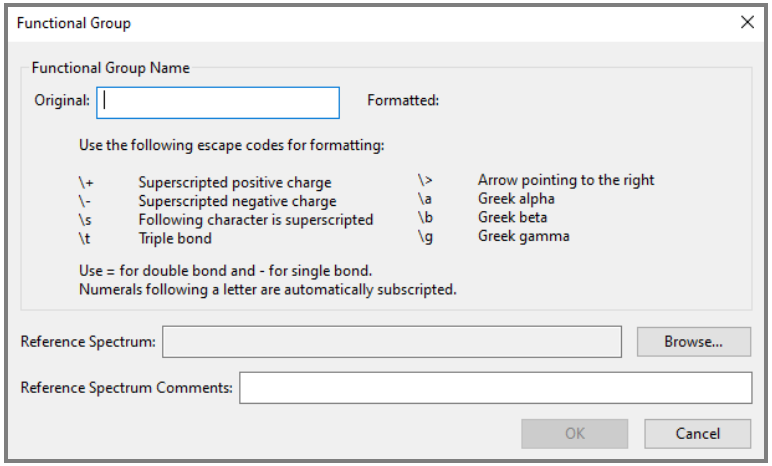
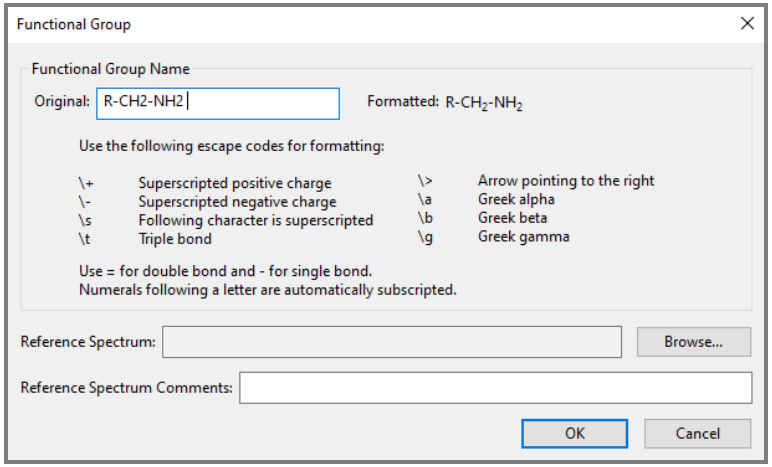
KnowItAll Applications Used

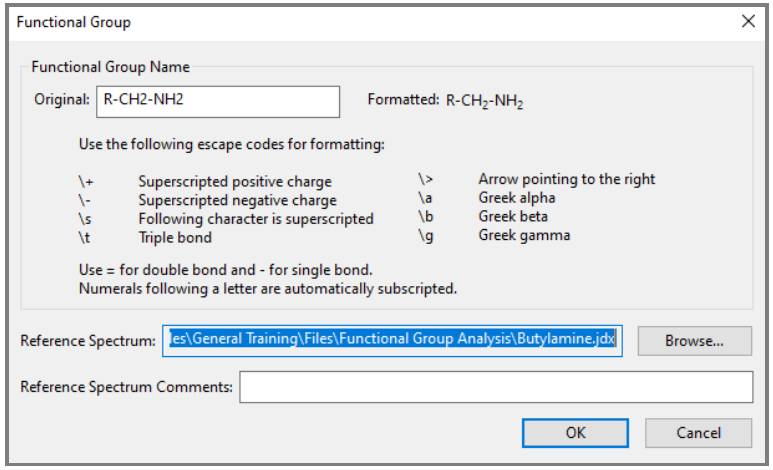
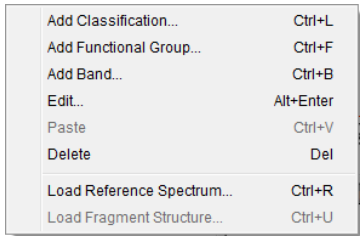
- AnalyzeIt™

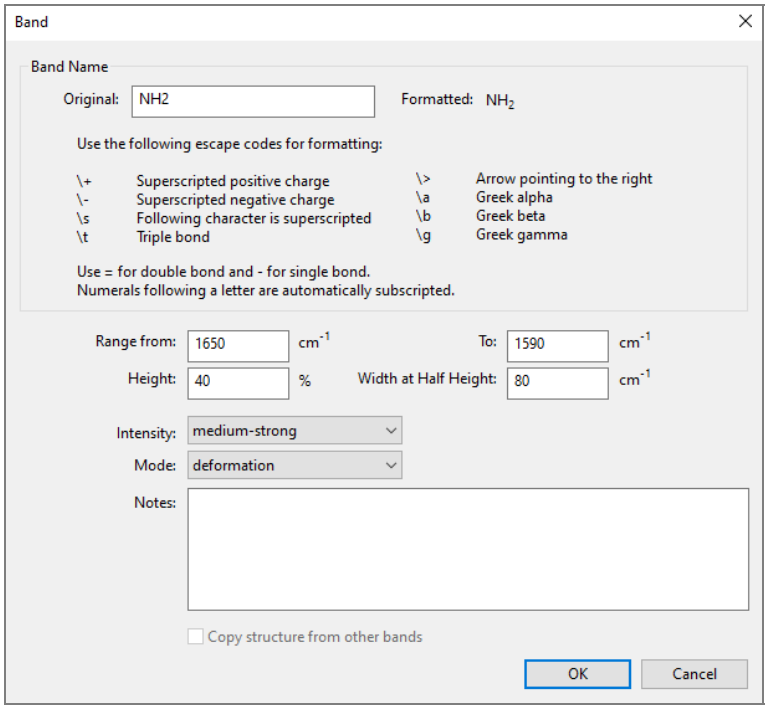
Create a user knowledgebase

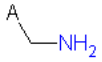
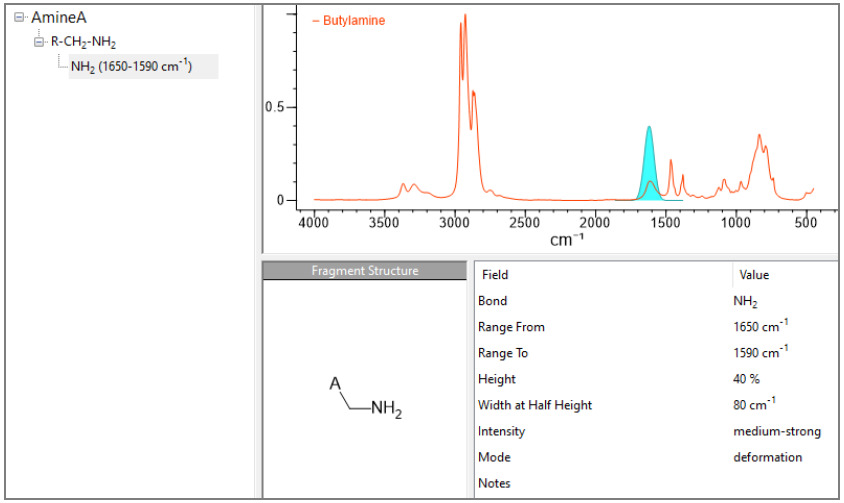
	Action	Result
1	Navigate to the **Spectral Analysis** toolbox and open the **AnalyzeIt** application by clicking its icon. Click **Organic IR** button.	
2	Choose **Knowledgebase > New**.	A **Save As** dialog box opens.
3	Type in a name for the user knowledgebase (such as **User IR Knowledgebase**) and save it to a location on your hard drive.	 The file type - Sadtler Knowledgebase, *.skbx or *.sbk – cannot be changed.

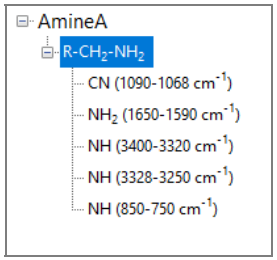
4	Right-click in the **Functional Group Tree** pane (on the left), then select **Add Classification**.	The **Classification** dialog box opens:  Type in AmineA and click **OK**. **Note**: Use a descriptive identifier to make sure the classification appears in the correct order when browsing for a functional group. Add a unique identifier to the end of the classification name to identify the knowledgebase where the entry appears. Changes can be made easily if necessary.

	Action	Result
5	Right-click on the new classification name AmineA, then select **Add Functional Group**.	The **Functional Group** dialog box opens: 
6	Type R-CH2-NH2 in the upper text box.	The text is automatically formatted: 

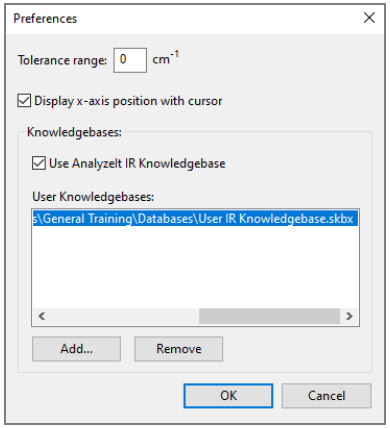
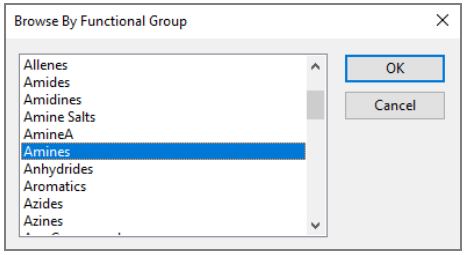
	Action	Result
7	• Click **Browse** • Navigate to **KnowItAll > Training Files > General Training > Files > Functional Group Analysis** • Select **Butylamine.jdx** • The path and file name is displayed in the **Reference Spectrum** text box.	
8	Click **OK** to close the dialog box. Right-click on R-CH_2-NH_2 in the **Functional Group Tree**.	A pop-up menu opens: 

	Action	Result
9	• Click **Add Band**. • Type in NH2, then add other information as follows: • **Range from** 1650 **to** 1590 **Height**: 40 **Width at Half Height**: 80 **Intensity**: medium-strong **Mode**: deformation • Click **OK**.	The **Band** dialog box opens: 
10		

	Action	Result
11	Double-click in the **Fragment Structure** pane to open **ChemWindow**, then draw this structure: 	
12	Click **Save**.	The structure is added to the display: 

<table>
<tr><th></th><th>Action</th><th>Result</th></tr>
<tr><td>13</td><td>Continue the process to add additional bands:
<table>
<tr><th>Band</th><th>Position</th><th>Height</th><th>Width at Half Height</th><th>Intensity</th><th>Mode</th></tr>
<tr><td>NH</td><td>3400-3320</td><td>30</td><td>65</td><td>medium</td><td>anti-symmetric stretching</td></tr>
<tr><td>NH</td><td>3328-3250</td><td>30</td><td>65</td><td>medium</td><td>symmetric stretching</td></tr>
<tr><td>CN</td><td>1090-1068</td><td>40</td><td>40</td><td>medium-weak</td><td>stretching</td></tr>
<tr><td>NH</td><td>850-750</td><td>50</td><td>49</td><td>strong</td><td>wagging</td></tr>
</table></td><td>Knowledgebase information is saved automatically.
 
</td></tr>
<tr><td>14</td><td>Click × in the upper right corner to close the knowledgebase.</td><td></td></tr>
</table>

Specify the user knowledgebase

	Action	Result
1	Navigate to the **Spectral Analysis** toolbox and open the **AnalyzeIt IR** application by clicking its icon.	
2	Choose **File > Preferences**.	The **Preferences** dialog box opens.
3	Click **Add**, then browse to and select the newly created user knowledgebase.	The user knowledgebase is displayed in the **Preferences** dialog box: 
4	Click **OK** to close the **Preferences** dialog box.	
5	Choose **Analyze** > **Browse a Functional Group**.	The contents of the user knowledgebase have been added to the list of functional groups: 

KnowItAll Software Training

Drawing and Reactions

Optional: Drawing and Reactions

How to Draw Chemical Structures

Purpose

The ChemWindow® application is a full-featured 2-dimensional structure drawing program. You can use the ChemWindow application to create chemical structures that can be used throughout the KnowItAll Informatics System for searching, prediction, and reporting chemical composition.

Objectives

This exercise will teach you:

- How to use basic ChemWindow tools to create and edit a structure drawing;
- How to save a structure for further use.

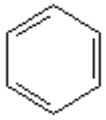
Background

Chemical structures can be used throughout the KnowItAll Informatics System for searching, prediction, and reporting chemical composition.

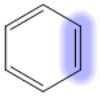
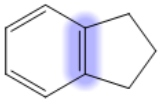
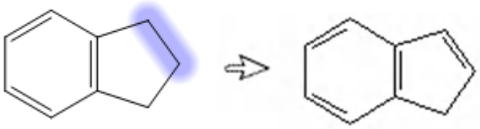
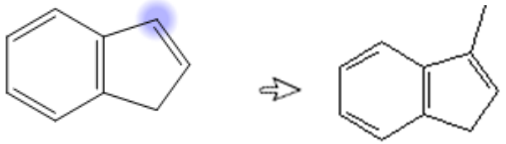
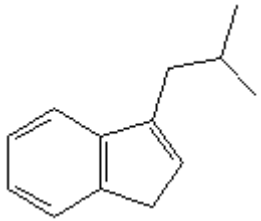
KnowItAll Applications Used

- ChemWindow®

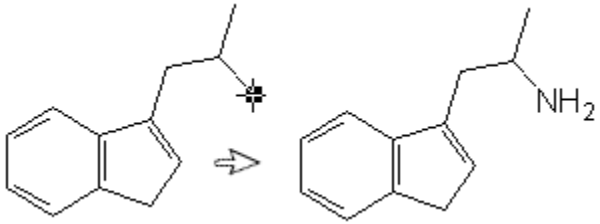
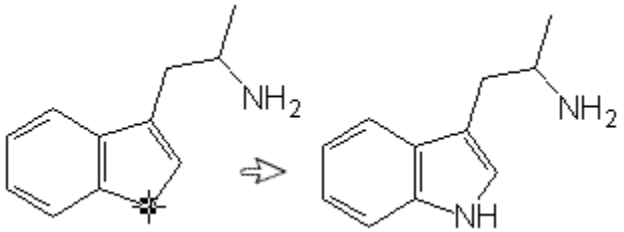
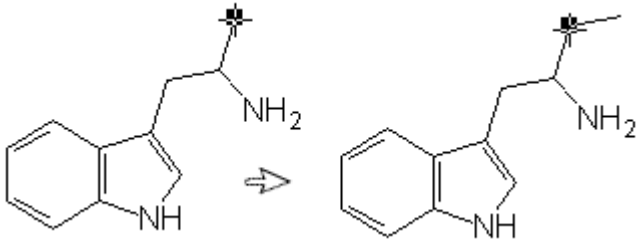
Begin a new structure drawing

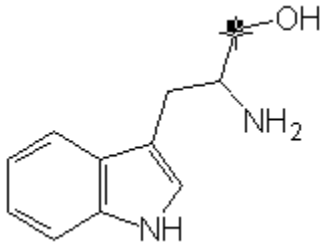
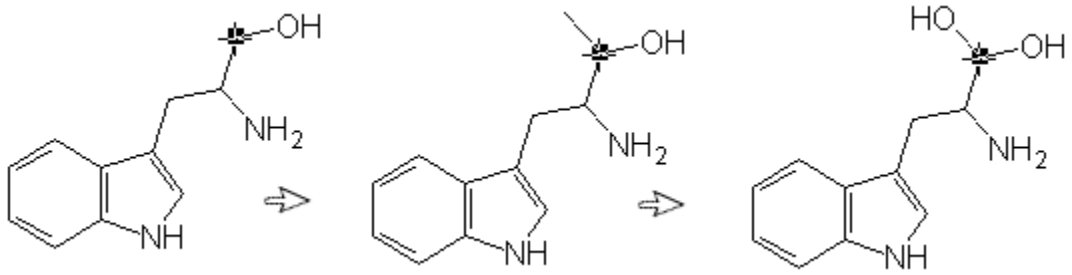
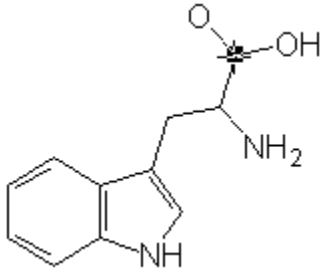
	Action	Result
1	Click the **ChemWindow** icon in the **Basics** toolbox.	The **ChemWindow** application opens to a blank drawing pane.
2	Select the **Benzene Ring** tool  in the **Main** section of the **Chemistry Toolbar**.	
3	Move the cursor into the drawing area, then click to draw a benzene ring.	The benzene ring structure is placed in the drawing area: 
4	If desired, use tools on the zoom toolbar to change the magnification. **Note**: Choose **View > Zoom Toolbar** to toggle the toolbar display.  The **ctrl** + **scroll** function can also be used to zoom in and out quickly.	
5	Use the **Selection** tool  to select the structure and move it within the workspace.	Graphic handles appear when the structure is selected: 

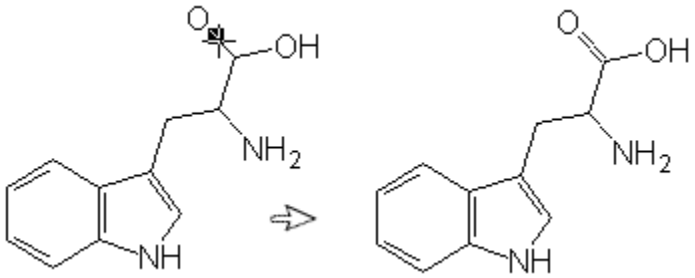
Add features to the structure

	Action	Result
1	Select the **Cyclopentane** tool  , then move the cursor to the highlighted bond on the benzene ring.	
2	Click to join a cyclopentane ring to the benzene ring.	
3	Open the **Bonds** group in the **Drawing Toolbar**, select the **Inside Double Bond** tool  , then use it to add a double bond to the structure.	
4	Select the **Single Bond** tool  , then move the cursor over the atom's hit box as shown. Click to create a single bond.	 **Note**: If you don't release the cursor, you can control the bond direction by dragging.
5	Continue adding single bonds by clicking on hit boxes on atoms.	

Use hot keys to add nitrogen and oxygen atoms

	Action	Result
1	Move the cursor over the terminal carbon, then press n on your keyboard.	**NH_2** appears at the end of the bond:  **Note**: Numbers are automatically displayed as subscripts when using hot keys, which are shortcut keys you can use to quickly label atoms. You can also use the atom label tool to add atoms to a drawing. However, unlike atoms added while using a bond tool, atoms in atom labels are not actually part of the structure, and will not be included when calculating the mass or chemical formula.
2	Repeat to replace a carbon atom with **NH**.	
3	With the single bond tool still selected, place your cursor over the terminal carbon atom and click to add another single bond.	

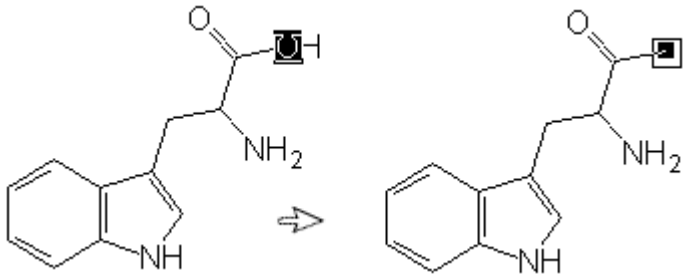
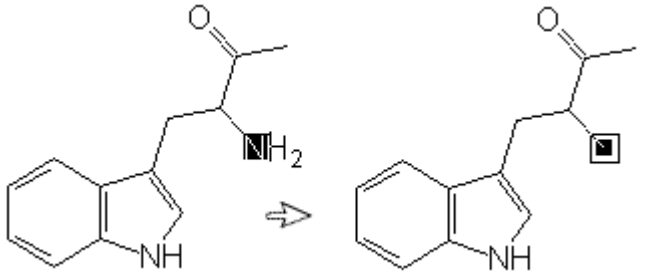
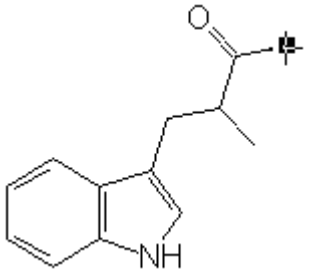
	Action	Result
4	Without moving the cursor, press o on your keyboard.	
5	Click to sprout another single bond, then press o on the keyboard to add a hydroxyl group.	
6	Press o again to remove the hydrogen. **Note**: When using a hot key, you can change the number of hydrogens attached to the atom by pressing the hot key repeatedly.	

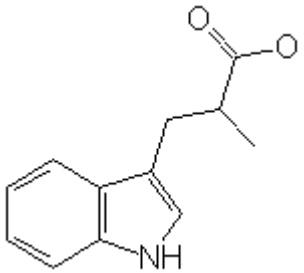
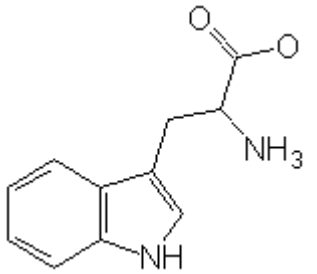
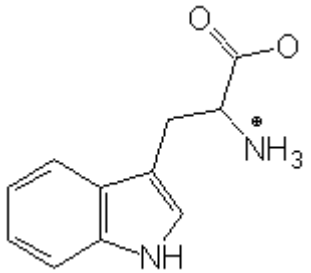
	Action	Result
7	Move the cursor to the hit box on the bond, then click to create a double bond.	

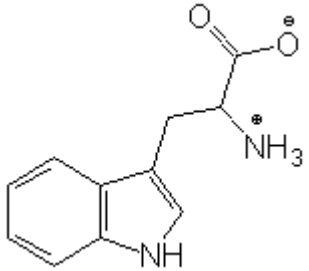
Save the structure

	Action	Result
1	Choose **File > Save**. **Note**: You can also click the **Save** button on the toolbar, or press Ctrl+S.	The **Save As** dialog box opens. The default file type (ChemWindow structure file, *.dsf) is already selected, and will be used for this structure. Other file types include ChemWindow Structure Template & Style (*.dst) and MDL Mol file (*.mol).
2	Navigate to the folder where you wish to save the structure file, then type in the file name “tryptophan.”	
3	Click **Save**.	The structure is saved, and the file name is displayed on the drawing tab.

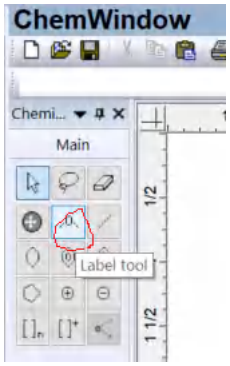
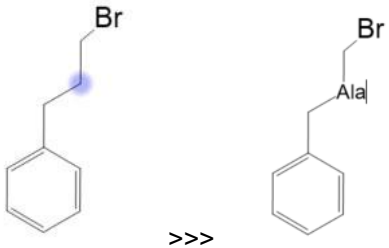
Edit the structure and use atom labels and atom tags

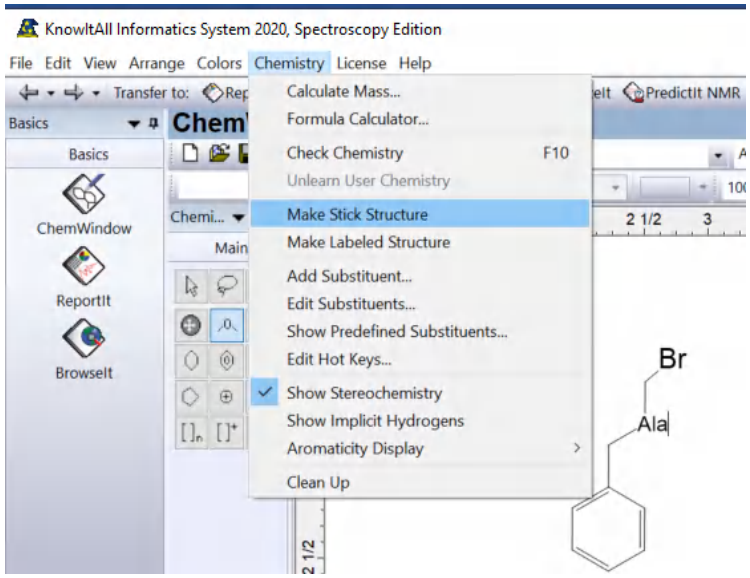
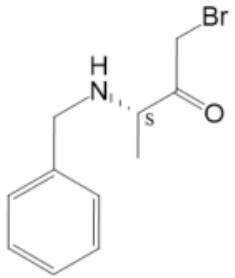
	Action	Result
1	Select the **Eraser** tool  , then click to remove the hydroxyl…	
2	…and amino groups.	
3	Open the **Main** group on the **Drawing Toolbar**, select the **Atom Label** tool  , then click where the hydroxyl group was located.	

	Action	Result
4	Type uppercase O. **Note**: Atom labels are case-sensitive.	
5	Move to the other atom and type uppercase NH3. **Note**: Numbers are automatically displayed as subscripts if the **Text Style** toolbar's **Formula** tool  is selected.	
6	Select the **Positive Charge Atom Tag** tool  to add a positive charge to the atom.	
	TIP	Clicking and dragging a charge allows you more control over the placement of the charge. You can also use the **Lasso** tool to move the charge.

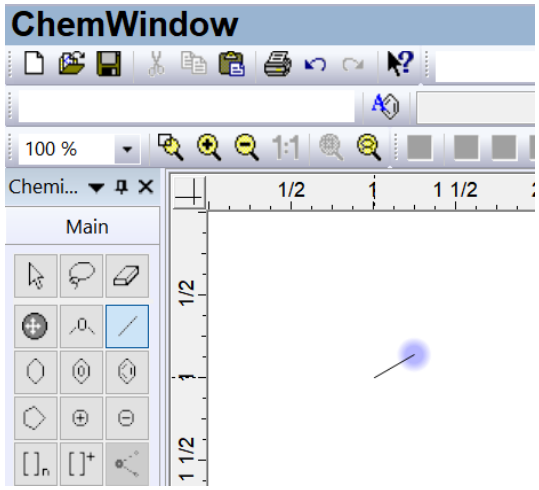
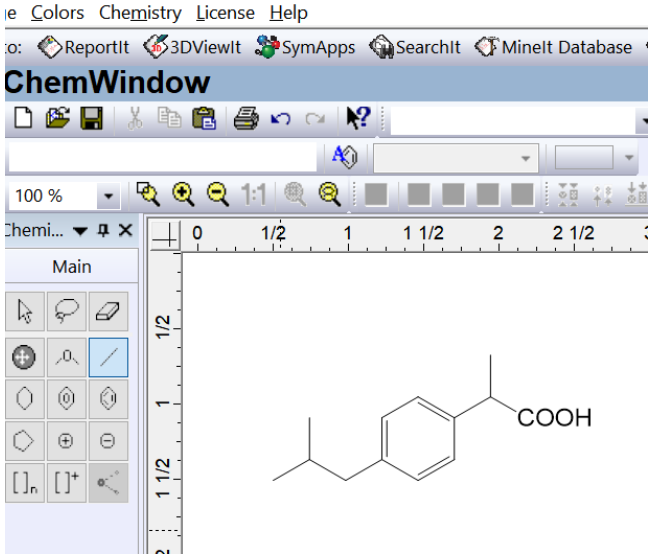
	Action	Result
7	Repeat with the **Negative Charge Atom Tag** tool ⊖ to add a negative charge to the oxygen atom.	
8	Choose **File > Save As** to save the structure with file name **tryptophan2.dsf**.	

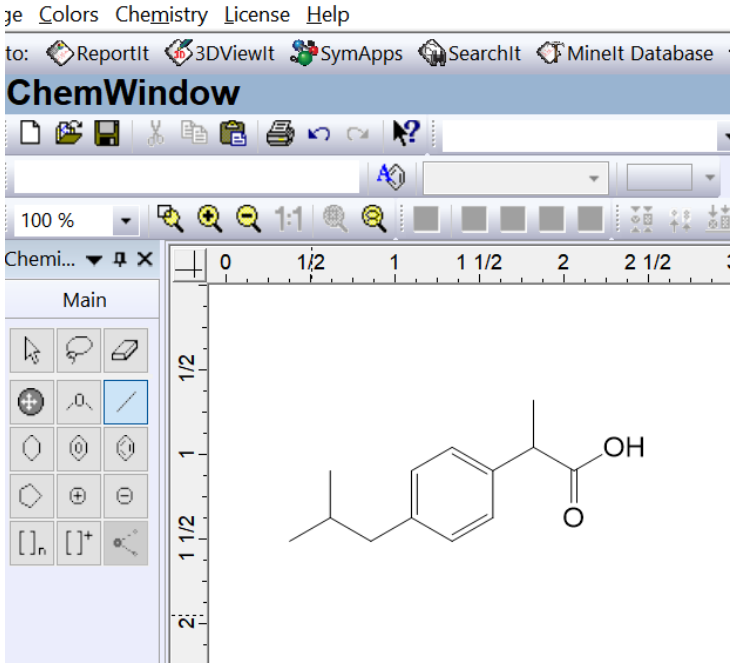
Use pre-defined substituents

	Action	Result
1	Click on the **Label** tool	
2	Select an atom and click to type **Ala** (a pre-defined substituent)	

	Action	Result
3	Click **Chemistry** > **Make Stick Structure**	
4		 The above is the expanded structure

Use Hotkeys

	Action	Result
1	• In the Main toolbox, select the **Standard bond** tool. • Click the structure pane to insert the single bond. The end of the bond will be highlighted automatically.	
2	Type the following characters on your keyboard: `9, 1, 3, 9, O (Capital O)`	

	Action	Result
3	Click **Chemistry** > **Make Stick Structure**	 The above is the expanded structure

Drawing and Reactions

How to Draw Chemical Reactions

Purpose

The ReportIt™ application is a full-featured chemical publishing program. Use the ReportIt application to import objects such as structures and spectra, arrange them on the page, and add text, annotations, reaction arrows, polygons, or orbitals.

The ease with which information can be passed from one KnowItAll Informatics System application to another is especially evident in the way the ReportIt and ChemWindow® applications work together. Use ChemWindow to create structures and transfer them to ReportIt for incorporation in a report. Transfer structures from ReportIt to ChemWindow for editing.

Objectives

This exercise will teach you:

- How to transfer objects between the ChemWindow and ReportIt applications;
- How to use ReportIt tools to create a report that includes chemical reactions.

Background

Scientists can use the KnowItAll ChemWindow and ReportIt applications to add reaction schemes to reports. This capability is useful to anyone communicating the results of laboratory procedures.

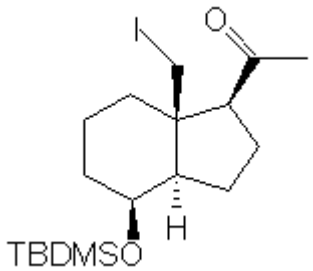
Training Files Used in This Lesson

- Structure 1.dsf
- Structure 2.dsf

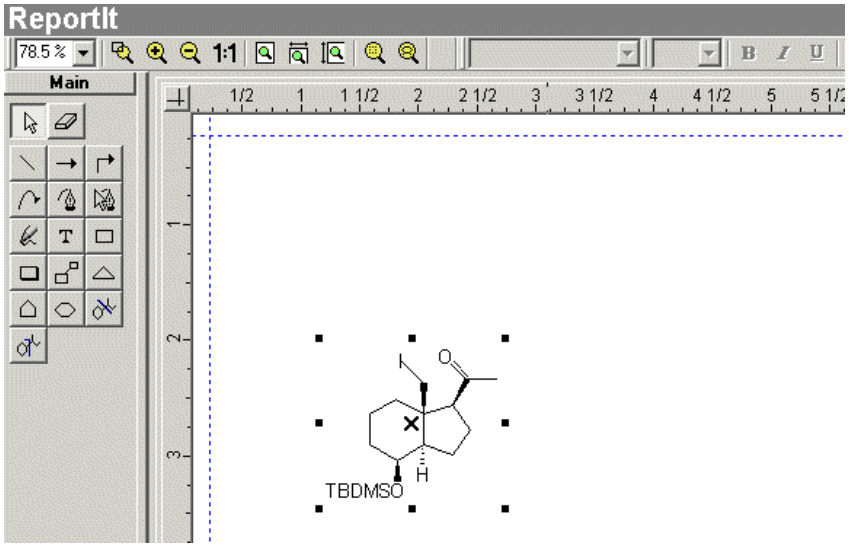
KnowItAll Applications Used

- ChemWindow®
- ReportIt™

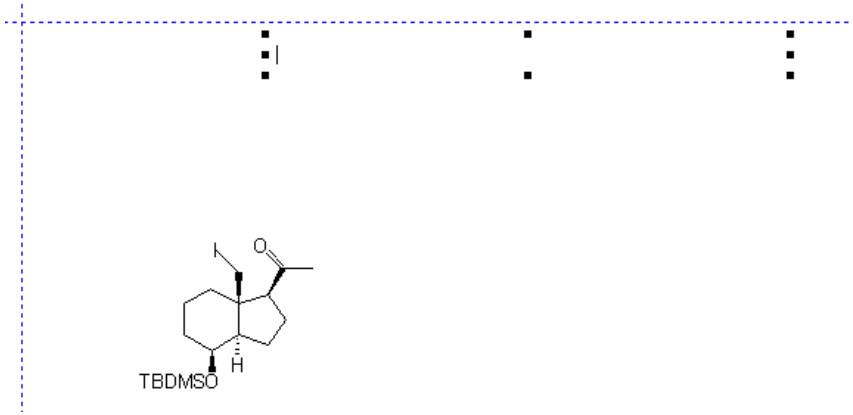
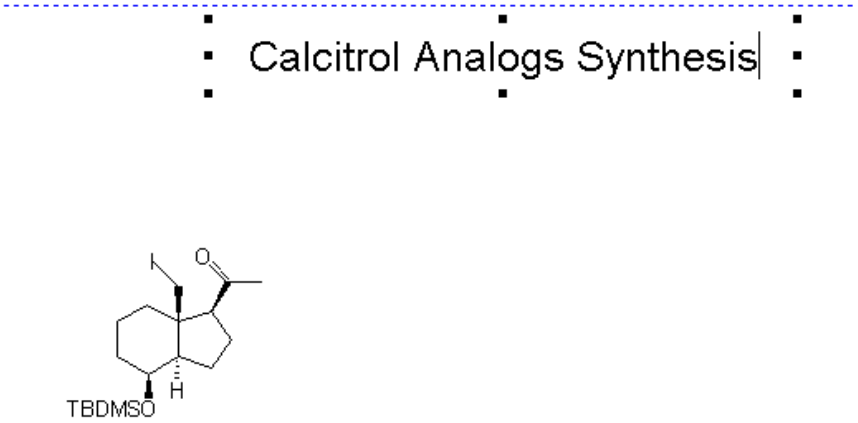
Open a structure in the ChemWindow application

	Action	Result
1	Click the **ChemWindow** icon in the **Basics** toolbox.	The **ChemWindow** application opens to a blank drawing.
2	• Navigate to **File > Open,** then navigate to KnowItAll > Training Files > General Training > Files > Drawing and Reactions • Select **Structure 1.dsf**. • Click **Open**	The file opens in the workspace: 
3	Click **ReportIt** in the **Transfer to** bar.	The structure opens in the **ReportIt** application. It is already selected and can be moved, re-sized, etc.

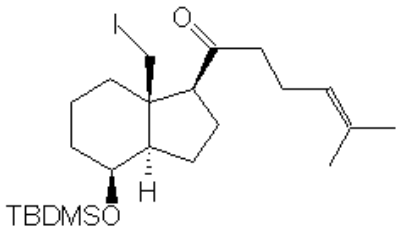
Set up the report

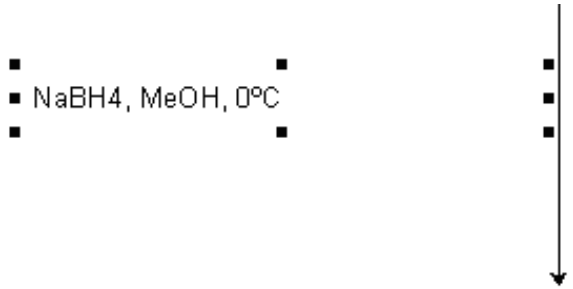
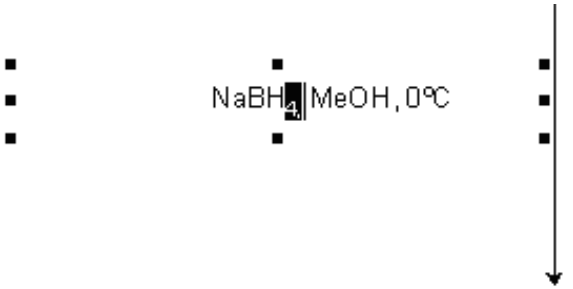
	Action	Result
1	Click the **Fit to Page Width** tool on the **Zoom** toolbar.	The display adjusts so the entire page width is visible.
2	Move the image so it is about 1” in from the left edge, and about 2” below the top of the page. **Note**: Choose **View > Rulers** to display rulers in the drawing area. Choose **File > Preferences** and select the **Templates/Units** tab to specify default measurement units on the drawing area rulers.	

Use Text tools

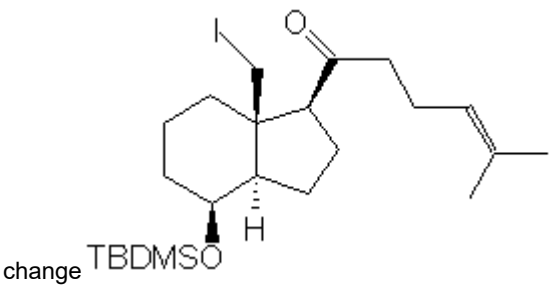
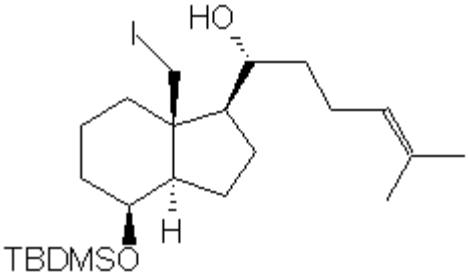
	Action	Result
1	Select the **Text** tool on the **Drawing** toolbar's **Main** group, then click and drag at the top of the page to create a text box.	When you release the mouse button, the text box is bounded by hit boxes and the cursor is inside, ready for typing. Text tools become available. 
2	If necessary, display the **Text Style** toolbar (**View** menu), then adjust the font size to 24.	
3	Type **Calcitrol Analogs Synthesis** then click the **Center Alignment** tool to center the text in the text box.	

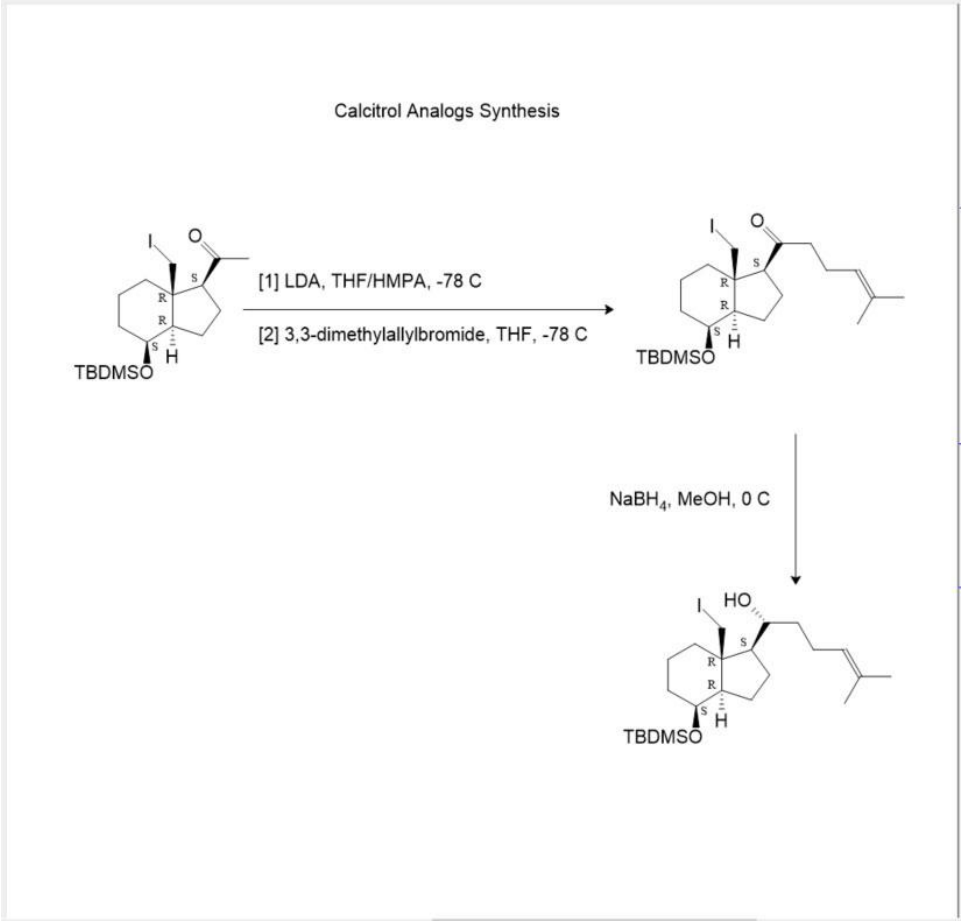
Create reaction arrows, and add a second structure

	Action	Result
1	Select the **Reaction Arrow** tool → in the **Drawing** toolbar's **Main** group, then click and drag to draw an arrow to the right of the structure.	When you release the mouse button, the arrow is selected and ready to be moved or re-sized:  Once the arrow has been drawn, you can resize it, reposition it, and change the direction and style of the arrowhead, if desired. Refer to **ChemWindow** online help or the KnowItAll User Guide for more information.
2	Draw a text box above the arrow and type in the text shown at right. Repeat below the arrow. **Note**: You can type in the degree symbol by opening the **Windows Character map** (Start Menu > Programs > Accessories > System Tools in Windows 10), selecting and copying the symbol, then pasting it in the text box.	[1] LDA, THF/HMPA, -78ºC [2] 3,3-dimethylallylbromide, THF, -78ºC
3	• Use the KnowItAll **Back** button to return to the **ChemWindow** application • Navigate to **File > Open, then navigate to KnowItAll > Training Files > General Training > Files > Drawing and Reactions** • Open **Structure 2.dsf**.	
4	Click **ReportIt** in the **Transfer to** bar.	The drawing is copied into the ReportIt document.
5	Use the **Selection** tool to move the newly-copied structure to the right of the reaction arrow.	
6	Draw another reaction arrow pointing downwards from the newly-copied structure.	

	Action	Result
7	Add a text box to the left of the arrow and type in the text shown at right.	
8	Click the **Right Align** tool ….	
9	…then select '4' in NaBH4 and click the **Subscript** tool .	

Use ReportIt tools to create a third structure

	Action	Result
1	Click the **Selection** tool, then select the second structure, copy it, and paste the copy below the reaction arrow. **Note**: There are many ways to access the copy and paste commands. Right-clicking is one of the easiest.	
2	Double click the newly-pasted structure.	The **Structure** toolbar appears at the right edge of the drawing area.  The **Structure** toolbar can be moved anywhere on the desktop, but remains only as long as the structure is selected.
3	Use the **Structure** toolbar's drawing tools to edit the structure. **Note**: Use the **Atom Label** and **Hashed Wedge Bond** tools to make the changes.	change  to 

	Action	Result
4	Click outside the structure to close the **Structure** toolbar, then click the **Fit to Page** button to view the entire page.	
5	Choose **File > Save**.	

KnowItAll Software Training

Create Reports

Create Reports

How to Create Customized Report Templates

Purpose

KnowItAll users can use report templates to easily generate high-quality documents including structures, spectra, tables, clip art, and more. Reports can be exported using a variety of formats, making it easier to share results with others.

Objectives

This exercise will teach you:

- How to open and use pre-defined KnowItAll report templates;
- How to create and use customized report templates.

Background

In addition to serving as the basis for reports, templates are used when objects and information are transferred to the ReportIt application from other KnowItAll applications. A template must be selected before any transfer can occur. A default template can be selected for each application, or a template can be chosen every time information is transferred to the ReportIt application.

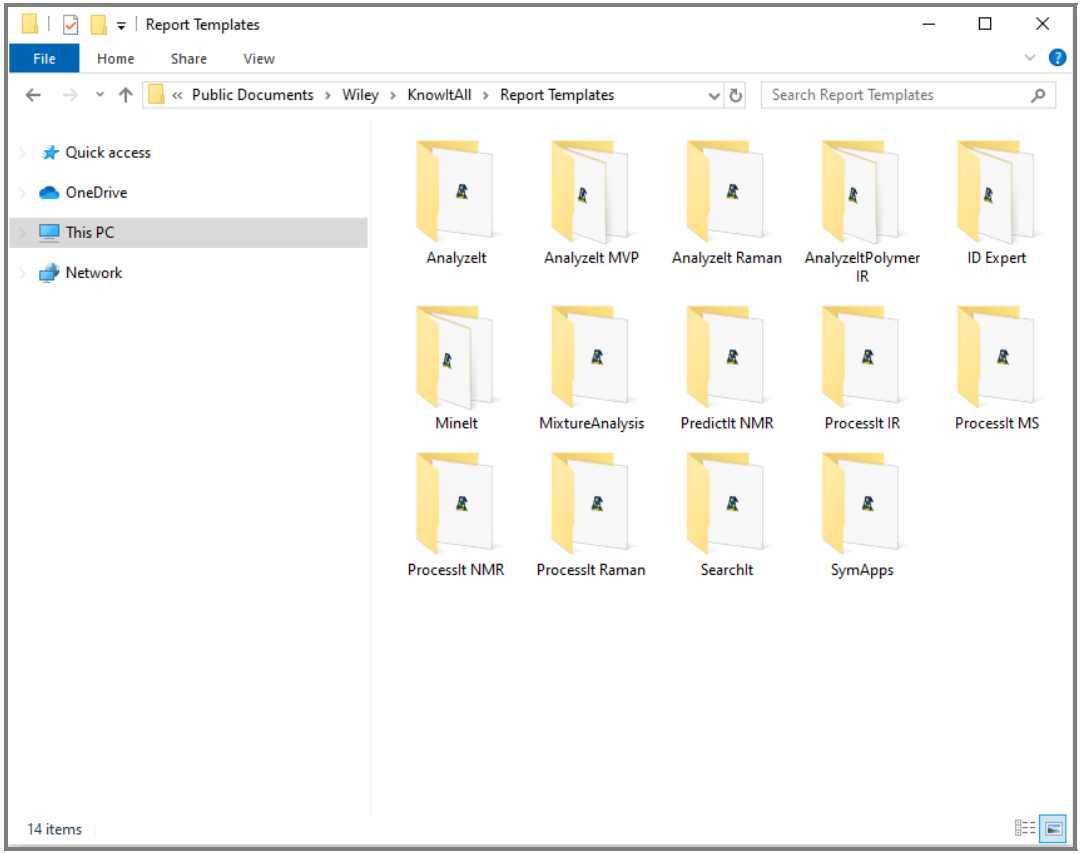
Training Files Used in This Lesson

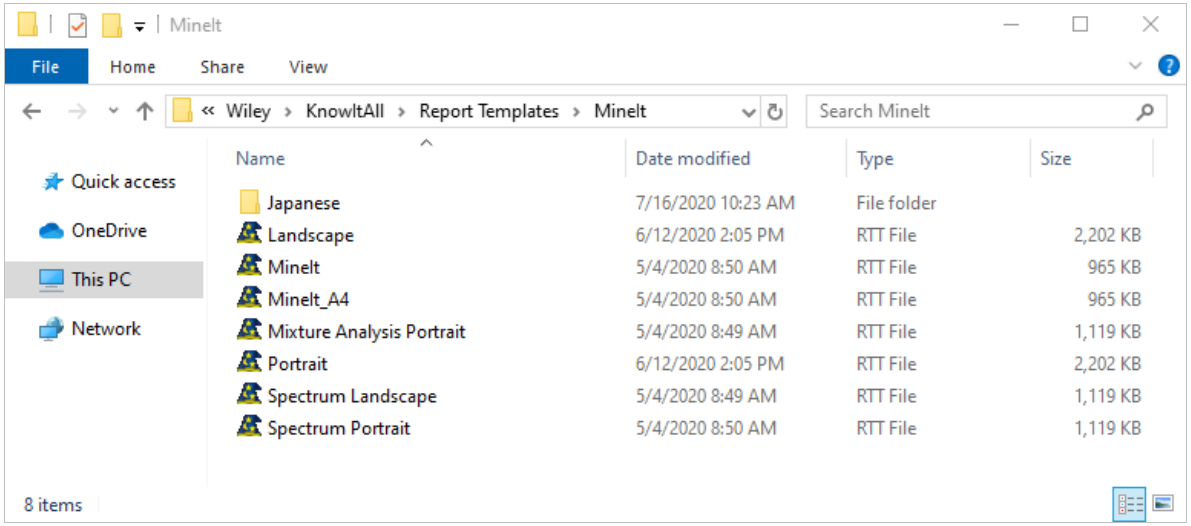
- Wiley.GIF
- Landscape.rtt

KnowItAll Applications Used

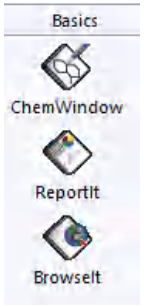
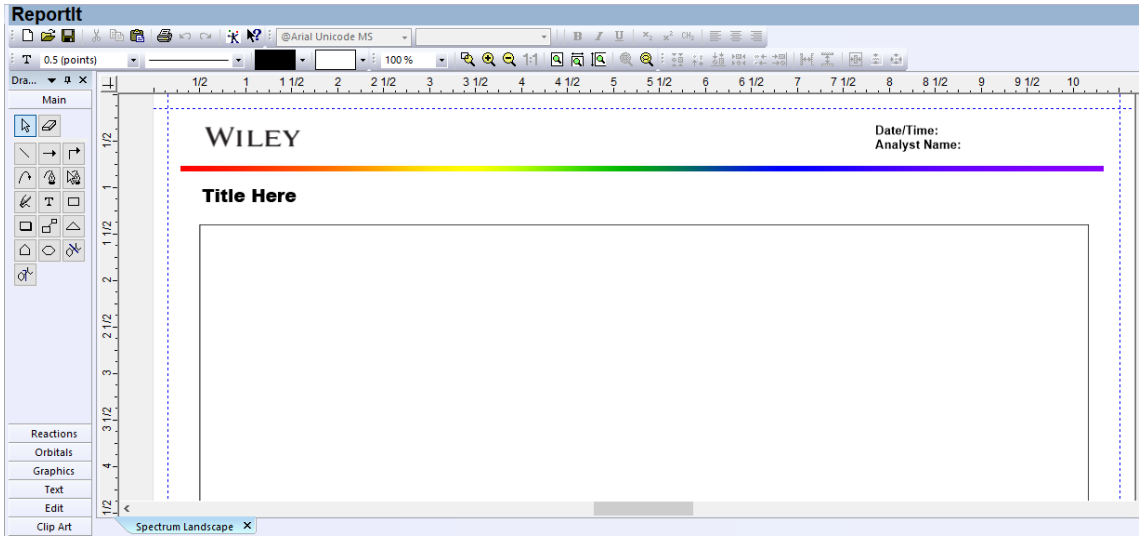
- ReportIt™
- MineIt™

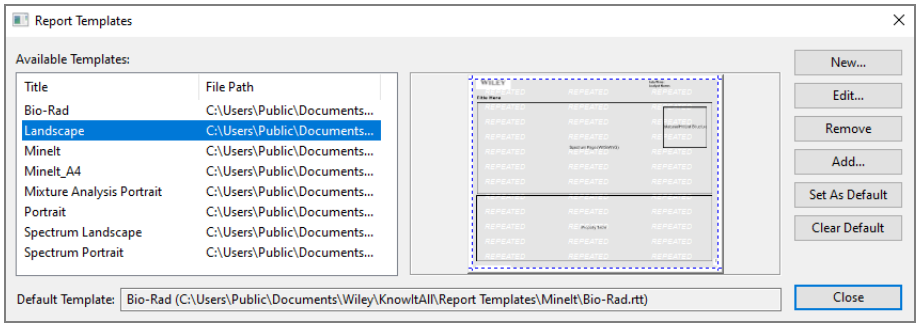
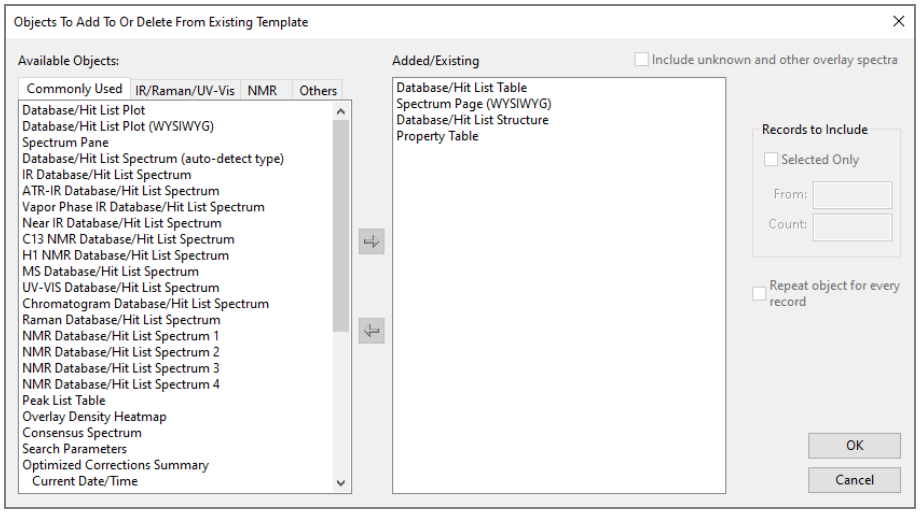
Examine predefined KnowItAll templates

	Action	Result
1	Open Windows Explorer, then navigate to **Documents > Wiley > KnowItAll > Report Templates** (Windows 10) **Note**: If you cannot find it in your version of Windows, use the Explorer search to locate it.	Each KnowItAll application has its own report templates folder: 

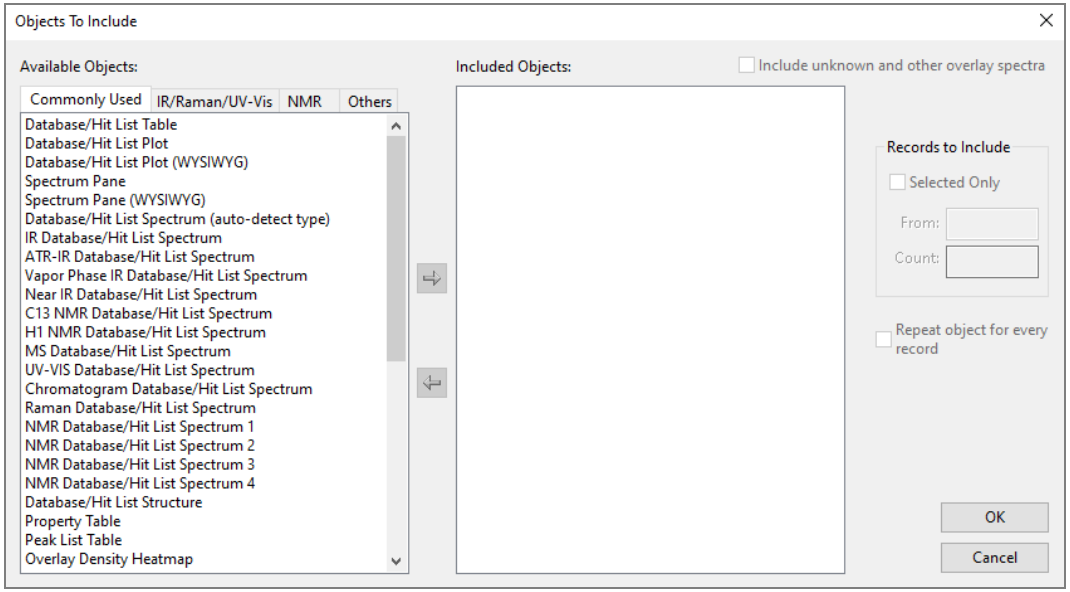
	Action	Result
2	Open the **MineIt** folder.	The **MineIt** report templates are displayed: 
3	Close Windows Explorer.	

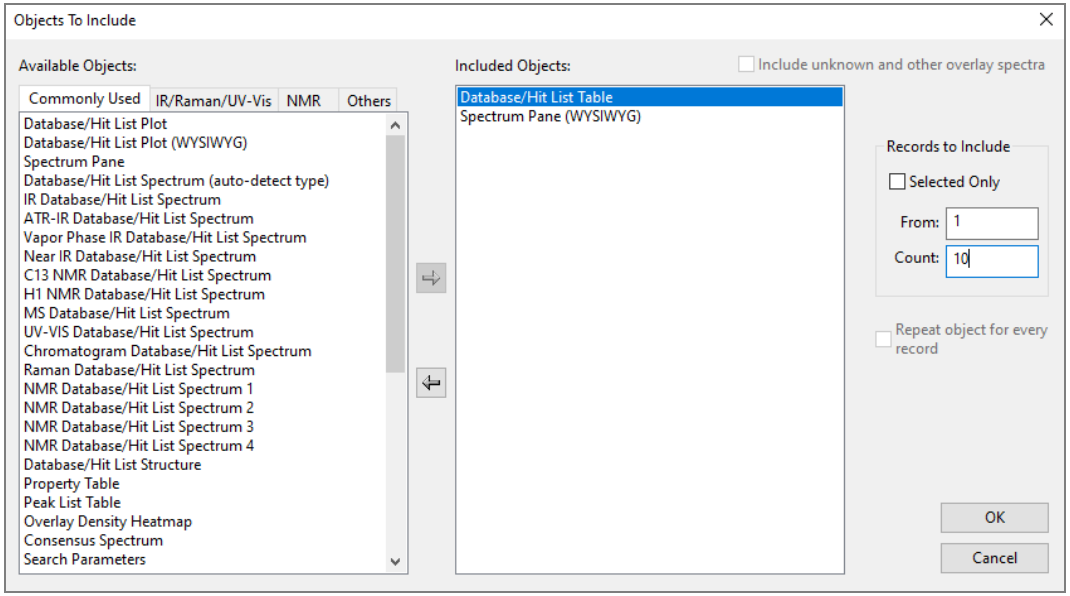
Open a predefined template in the ReportIt and MineIt applications

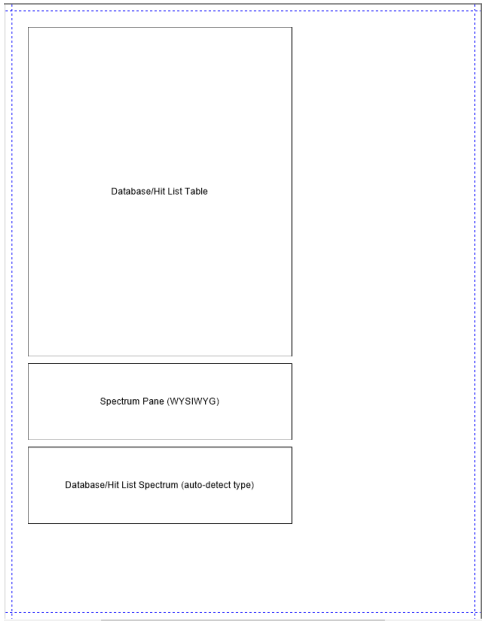
	Action	Result
1	Navigate to the **Basics** toolbox, open the **ReportIt** application by clicking its icon, then choose **File > Open**.	 An **Open** dialog box appears.
2	• Set the **Files of type** filter to ReportIt Template Document Files (*.rtt), • Navigate to **KnowItAll > Report Templates > MineIt** • Open **Spectrum Landscape.rtt** in the folder we examined earlier.	The template opens: 

	Action	Result
3	• Navigate to the **Data** toolbox • Open the **MineIt** application by clicking its icon • Choose **File > Edit Report Templates** • Select the **Landscape** template.	The **Report Templates** dialog box opens. 
4	Click **Edit**.	The **Objects to Add to Or Delete from Existing Template** dialog box opens.  Use this dialog box to see which objects are included with the template. You can also use this dialog to add or remove objects.
5	Click **Cancel**; then click **Close** on the **Report Templates** dialog box.	No changes were made to the template.

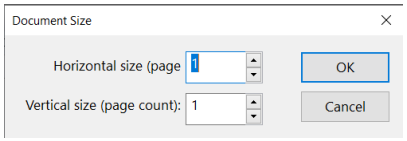
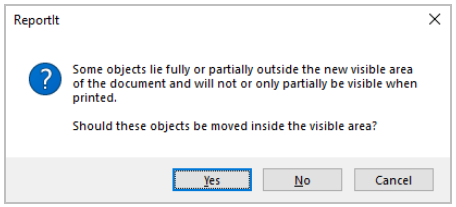
Create a new MineIt template

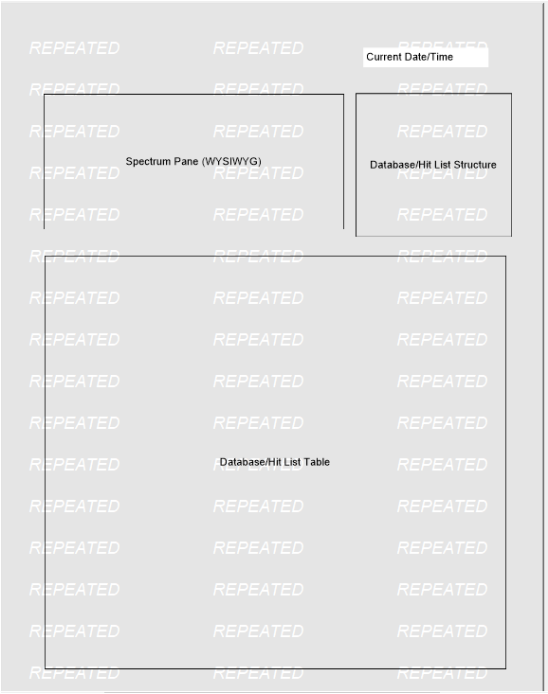
	Action	Result
1	The easiest method to create a new **Mineit** template is to start with an existing template. With the **MineIt** application open, choose **File > Edit Report Templates**; then click **New** on the **Report Templates** dialog box.	The **Objects to Include** dialog box opens: 
2	Move **Spectrum Pane (WYSIWYG)** from the list of **Available Objects** to the list of **Included Objects** by selecting it in the list on the left and clicking the right arrow available between the two lists.	
3	Move **Database/Hit List Table** from the list of **Available Objects** to the list of **Included Objects**.	

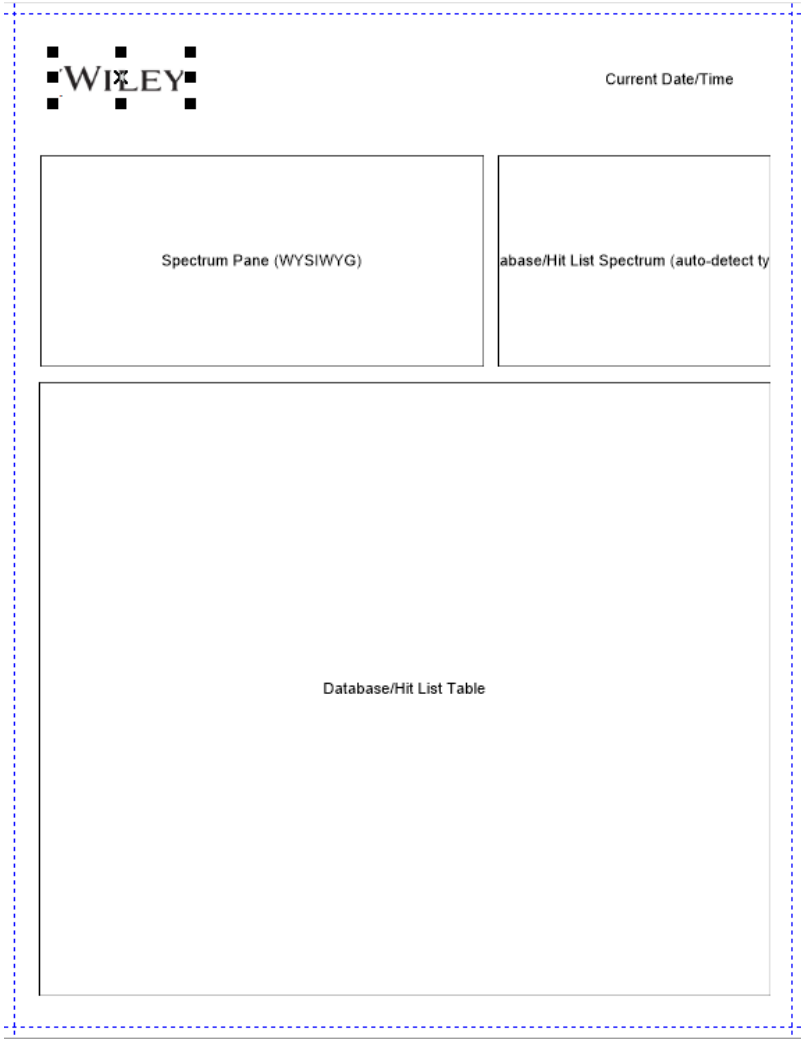
4	With **Database/Hit List Table** selected in the list of **Included Objects**, uncheck **Selected Only**, then type 1 in the **From** box and 10 in the **Count** box.	The first ten hits will be included on the template. 
5	Move **Database/Hit List Spectrum (auto-detect type)** from the list of **Available Objects** to the list of **Included Objects**, uncheck **Repeat object**… and **Selected Only**; then type 1 in the **Count** box.	The structure will be included only for the first item in the hit list.
6	Move **Property Table** from the list of **Available Objects** to the list of **Included Objects**, uncheck **Repeat object**… and **Selected Only**; then type 1 in the **Count** box.	The property table will be included only for the first item in the hit list.
7	Move **Current Date/Time** from the list of **Available Objects** to the list of **Included Objects**.	A date/time field is added to the template.

8	Click **OK**.	The new template opens in the ReportIt application.  We see object placeholders corresponding to the choices we made on the **Objects to Include** dialog box. You may have to scroll down the report template to see them all. We can now use **ReportIt** tools to arrange the placeholders and add other objects, such as images and text boxes.

Edit the template in ReportIt

	Action	Result
1	Choose **File > Document Size**.	The **Document Size** dialog box opens: 
2	Change **Horizontal size** to 2 and **Vertical size** to 1; then click **OK**.	A message box appears to tell you that some objects may no longer be completely visible. 

3	Click **Yes**. Move the database structure and property table to the second page, and re-size them as desired.	
4	• Navigate to **KnowItAll > Training Files > General Training > Files > Creating Reports** • Open **Wiley.gif** using any image editor (example MS Paint) • Select and copy the image.	

5	Return to the **ReportIt** application and choose **Edit > Paste**.	The image is added to the template: 

	Action	Result
6	Using the **Text box** tool  , draw a text box, then type 'Operator:'.	
7	Choose the **Selection** tool, then hold down the shift key and select both the Date/Time field and the text box.	
8	Choose **Arrange > Group**.	The two objects can now be moved, re-sized, etc., in exactly the same way.
9	Double click within the WYSIWYG Spectrum Page.	A spectrum toolbar opens. These tools can be used to adjust the spectral display in the template.
10	On the **Transfer to** bar, click **MineIt Database and Save**.	 A **Save As** dialog box opens.
11	Type in the new template's name (WILEY) and click **Save**.	The dialog box closes, revealing that the new template has been added to MineIt's **Report Templates** dialog box.
12	Select the new template and click **Set as Default**, then click **Close**.	Because we have set the new template as the default template, it will be used automatically whenever information is transferred from **MineIt** to **ReportIt**. Setting a default template is useful when you want to use a single template most of the time. However, you can also choose not to have a default template, and select from the list of available templates each time you transfer information to ReportIt.

KnowItAll Software Training

Data Mining & Analysis

Data Mining & Analysis

Overlap Density Heatmap Technology: A New Technology to Analyze Spectral, Chromatographic, and Other Graphical Data

Purpose

This exercise demonstrates how to use Overlap Density Heatmap technology for data mining and visualization.

Objectives

This exercise will teach you:

- How to view and manipulate an Overlap Density Heatmap.

Background

Wiley's patented Overlap Density Heatmap technology is useful for visual data mining and analysis to assess the similarities and dissimilarities in large amounts of spectral, chromatographic, and other graphical data.

This technology allows the visualization of common features of overlapped objects, such as spectra or chromatograms, by color-coding the areas from highest to lowest overlap.

Training Files Used in This Lesson

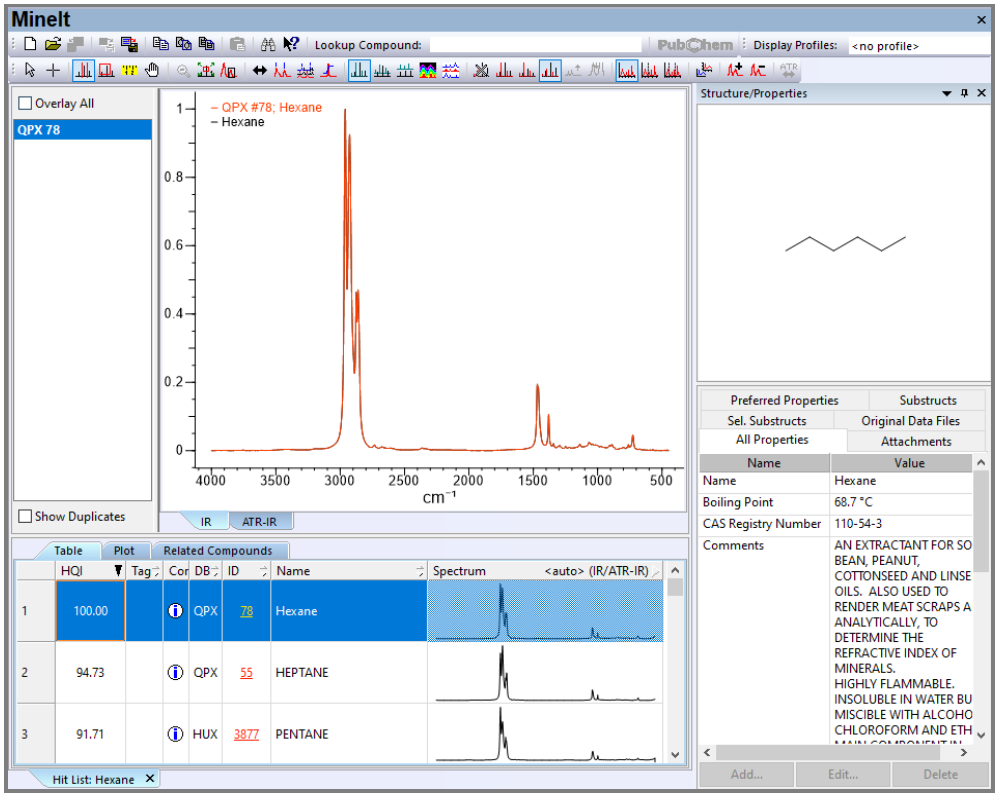
- Hexane.jdx

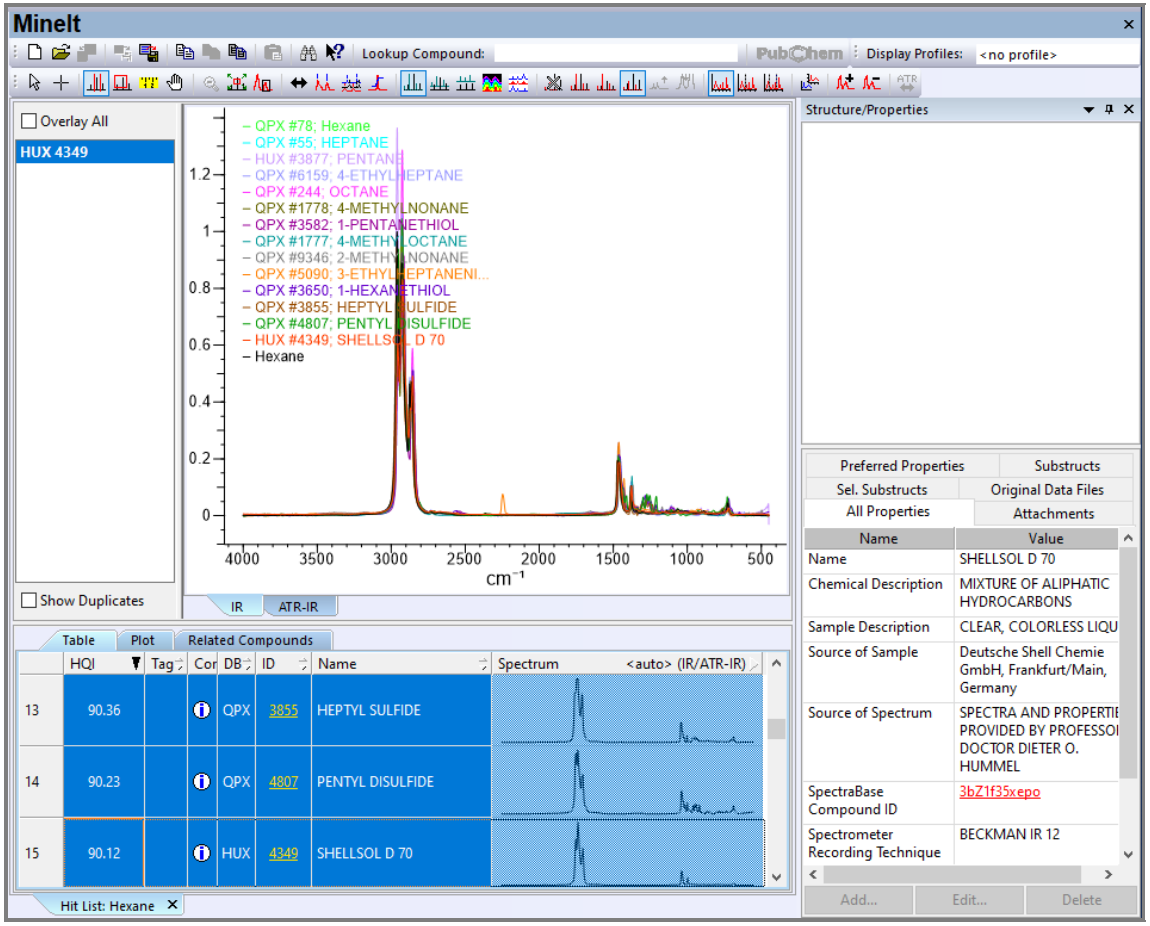
KnowItAll Applications Used

- MineIt™

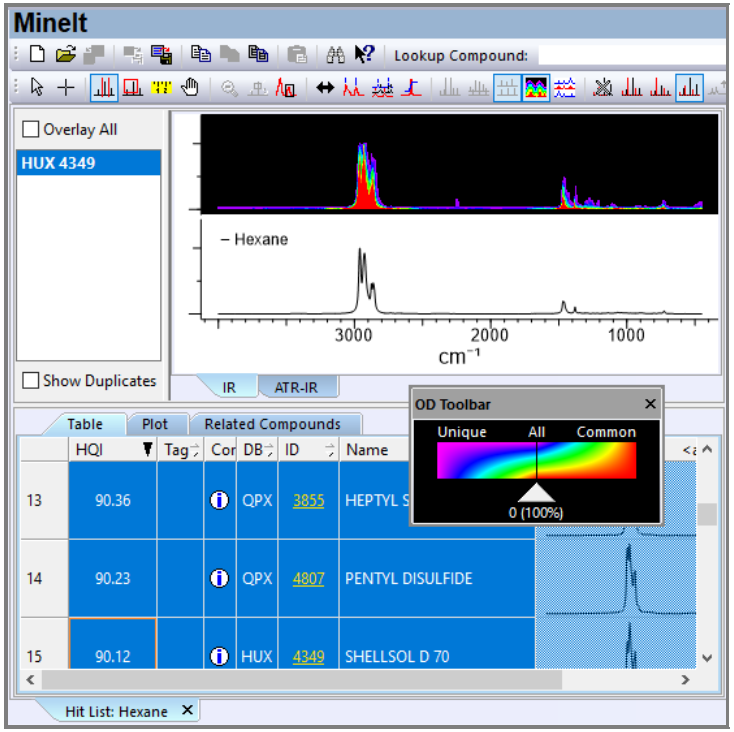
Open a spectral hit list in the MineIt application

	Action	Result
1	In the **SearchIt** application, click **User-Select** under **Search Databases**. If databases are present in the **Selected for Searching** pane, click **Remove All.** Add the **IR – Sadtler Standards (Selected Subset) – Wiley** (DB Code SLX) to the **Selected for Searching** pane.	
2	Click **Spectrum** in the **Search Categories** pane Navigate to **KnowItAll > Training Files > General Training > Files > Data Mining** Open **Hexane.jdx**.	

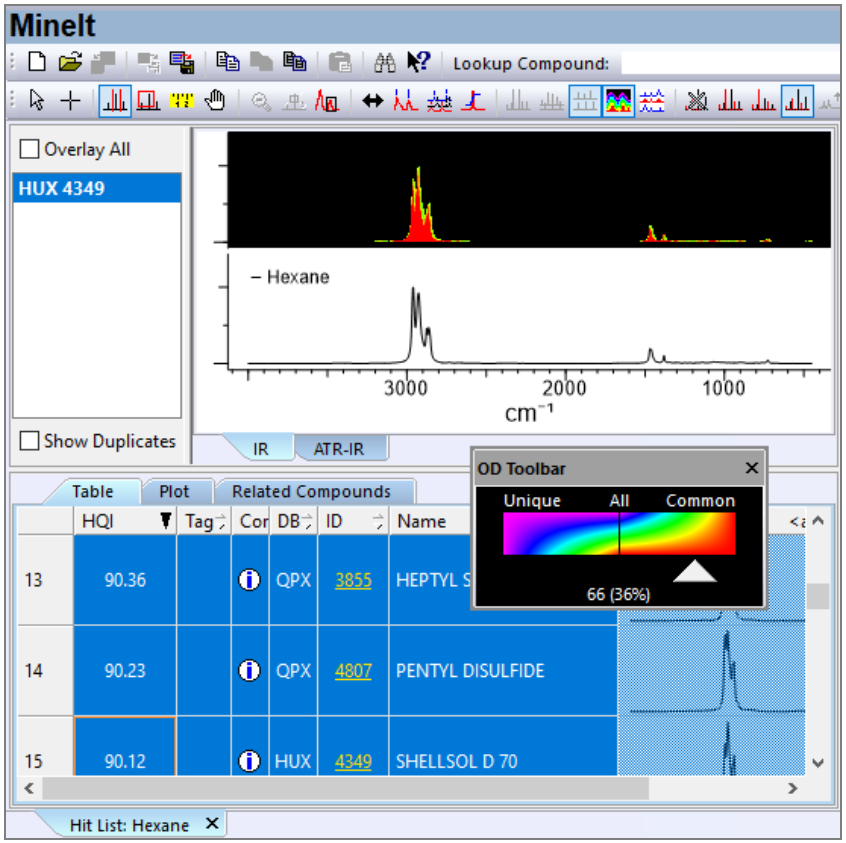
	Action	Result
3	Click **Search**.	The results are displayed in the MineIt application: 

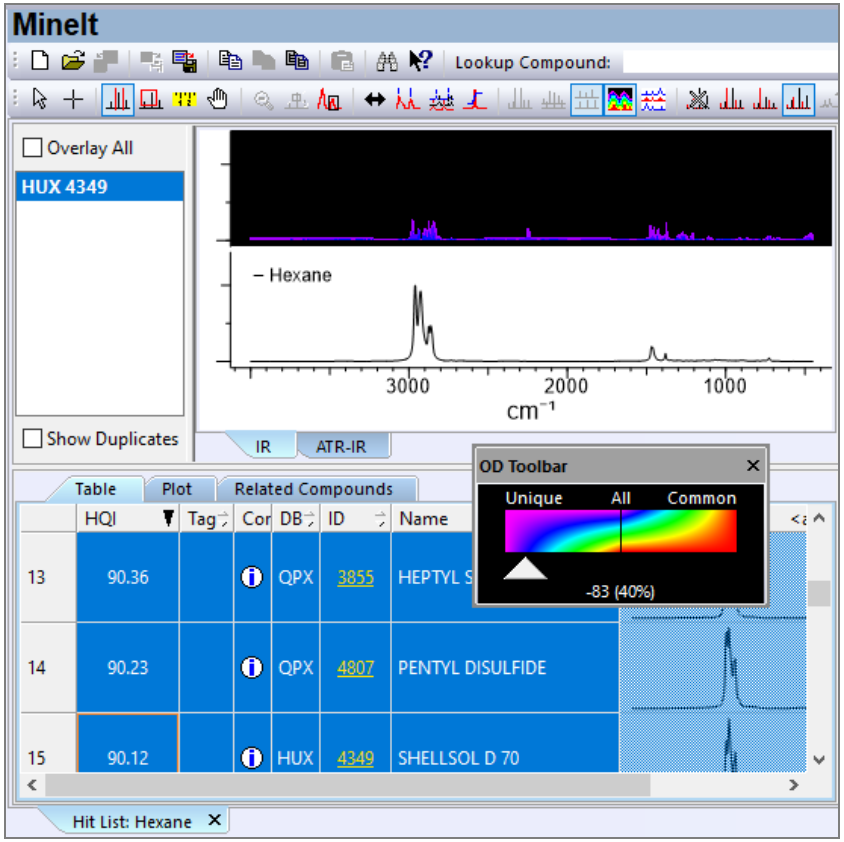
	Action	Result
4	Select the first 15 entries in the hit list. **Note**: Select the first record, hold down the shift key, then scroll to and select the 15th entry.	All the selected hits are displayed in the spectral pane. 

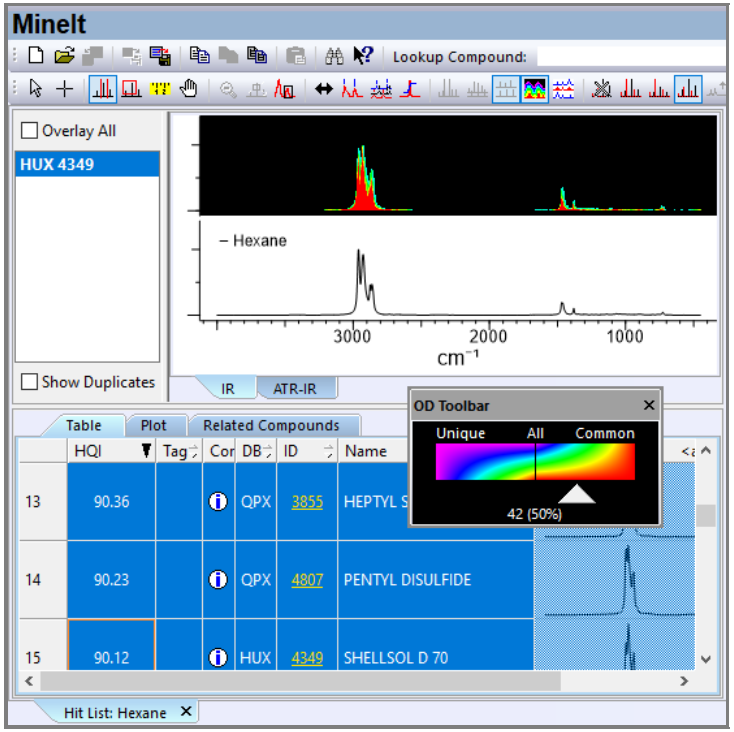
Change the spectral display to Overlap Density Heatmap

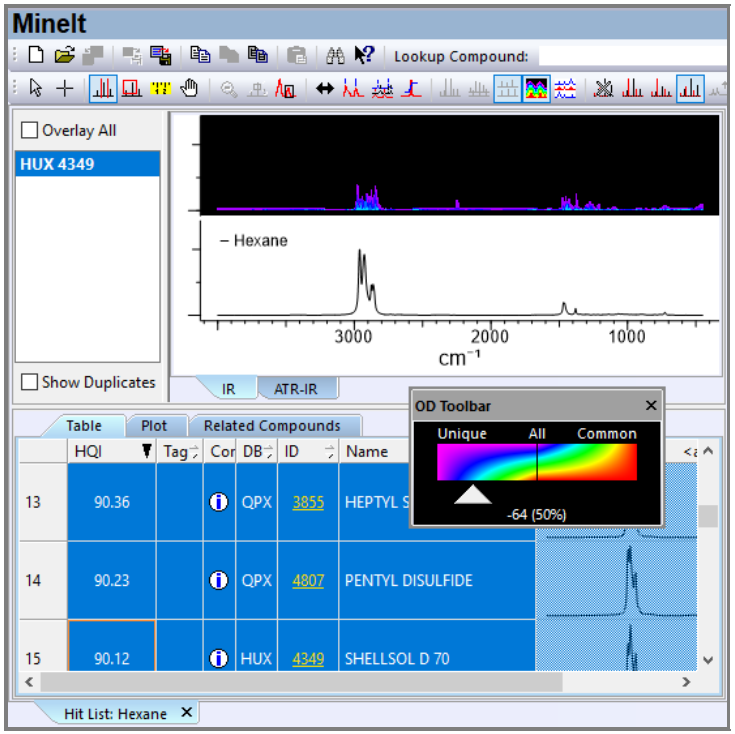
	Action	Result
1	Click the **Overlap Density (OD) Heatmap** tool in the **Spectral** toolbar.	The spectral display changes, and the **Overlap Density (OD) Toolbar** is added to the display.  The default Overlap Density Heatmap display shows all overlap levels. High levels of overlap are displayed in red; low levels are displayed in violet. The **OD Toolbar** allows you to control the amount of overlap displayed using the slider. In the default Overlap Density Heatmap, the slider is set at OD level = 0, where all colors – representing all overlap density levels – are shown.

Manipulate the Overlap Density Heatmap

	Action	Result
1	Move the slider on the **OD Toolbar** to the right.	As the slider moves to the right, the areas of common overlap are shown. Only the areas of most common overlap are shown as the OD Level approaches 100. 

	Action	Result
2	Move the slider to the left.	As the OD Level approaches -100, only the areas of lowest overlap – the unique areas – are shown.  As you move the slider to change the OD Level, a second value is shown in parentheses. This value is the percent area under the curve, or %AUC, relative to the value at OD Level = 0. In this case, %AUC = 40%. We can use the OD Level and %AUC to quantify the OD Heatmap.

	Action	Result
3	Move the slider to the point where %AUC equals approximately 50%.	The OD Level on the common side – or ODC – required to show 50% of the area that is most in common, is 42.  Another way to express this is to say that ODC_{50} = 42. An alternative is to say that $\%AUC_{42}$ = 50.

	Action	Result
4	Next, move the slider to the left to where %AUC equals approximately 50%.	The OD Level on the unique side – or ODU – required to show 50% of the area that is most unique is -57.  Another way to express this is to say that ODU_{50} = -64. An alternative is to say that $\%AUC_{-64}$ = 50.
	TIP	Use the **Horizontal Zoom** tool  to examine different regions. To do this, select the Horizontal Zoom tool, and then click and drag over an area on the spectrum to zoom in. Use the **View Entire Spectrum** tool  to zoom out.

Data Mining & Analysis

How to Create and use Overlap Density Consensus Spectra

Purpose

This exercise demonstrates how to create and use Overlap Density Consensus Spectra in the KnowItAll Informatics System.

Objectives

This exercise will teach you:

- How to view and manipulate an Overlap Density Consensus spectrum;
- How to use an Overlap Density Consensus spectrum in a search.

Background

Wiley's patented Overlap Density Heatmap technology is useful for visual data mining and analysis to assess the similarities and dissimilarities in large amounts of spectral, chromatographic, and other graphical data.

By tracing the outline of the highest level of overlap at a given OD Level, it is possible to mathematically construct a composite spectrum by using the maximum spectral y-values at each spectral x-value in the OD Heatmap. This Overlap Density Consensus Spectrum can be used in a spectral search to find similar spectra, or can be stored in a database for future use.

Training Files Used in This Lesson

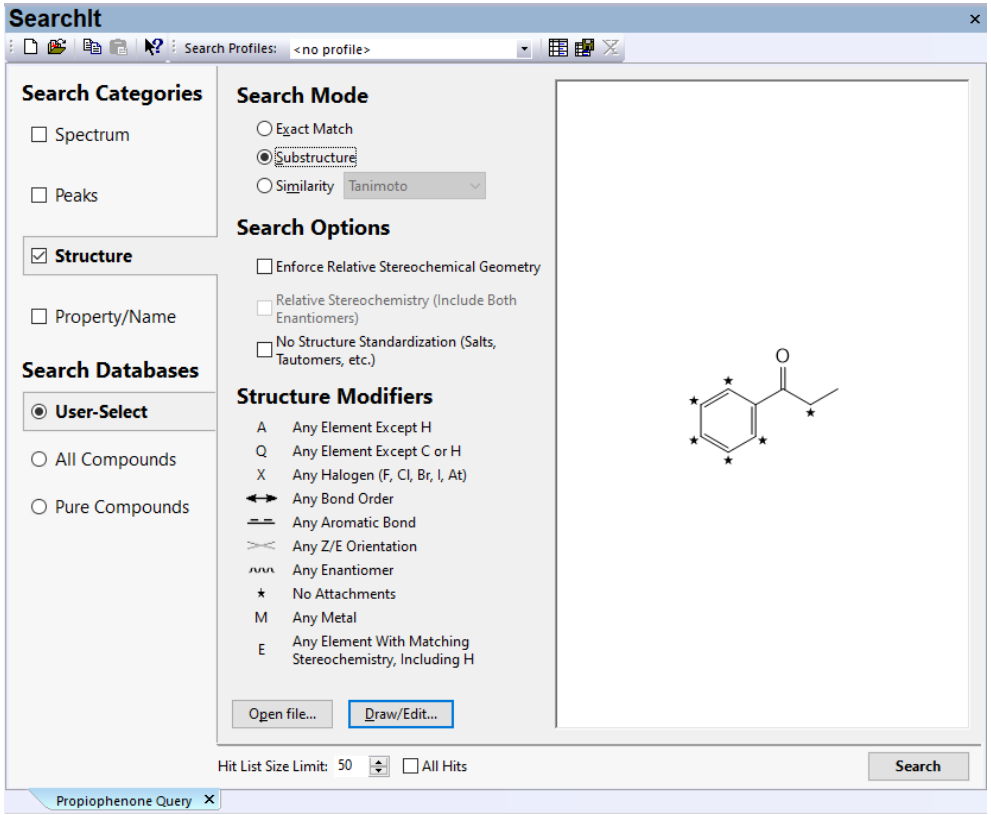
- Propiophenone Query.dsf

KnowItAll Applications Used

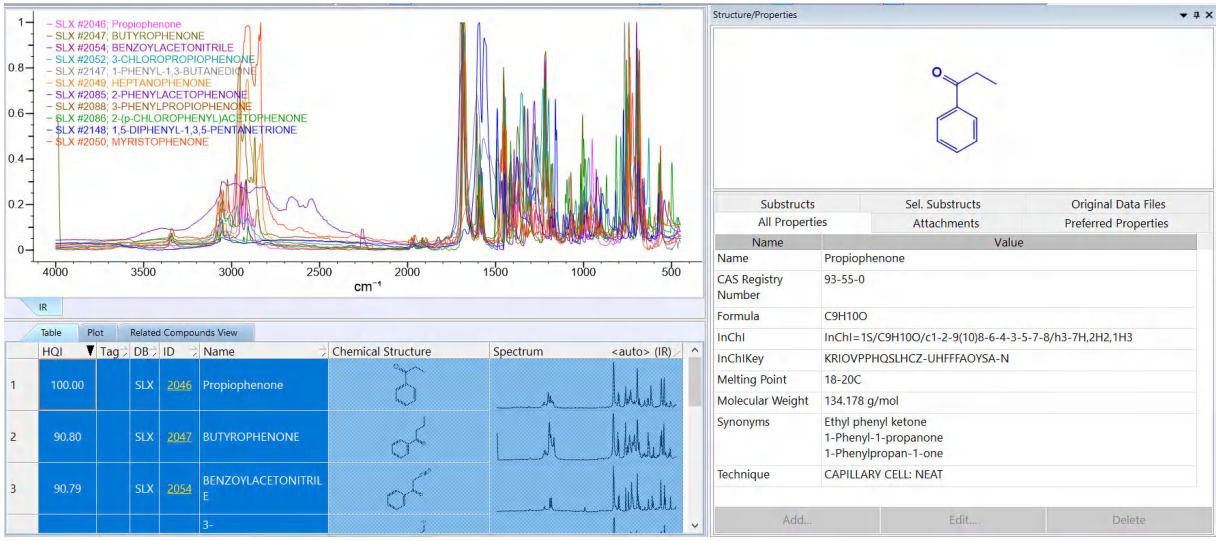
- SearchIt™
- MineIt™

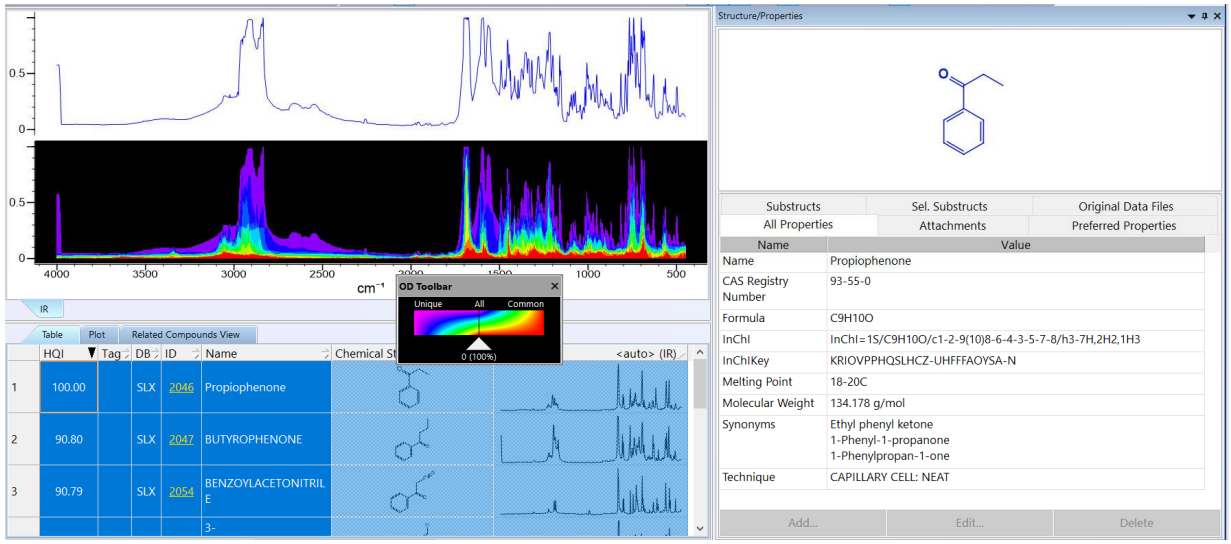
Perform a substructure search

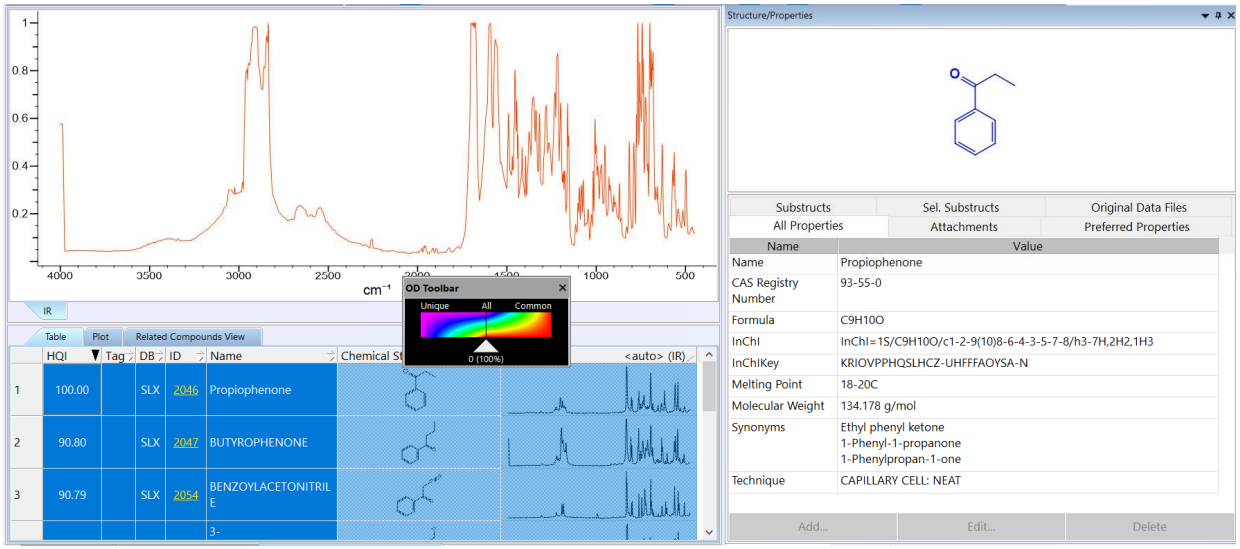
	Action	Result
1	• In the **SearchIt** application, click **User-select** under **Search Databases**. • Under **Available for Searching**, select **IR – Sadtler Standards (Selected Subset) – Wiley** (DB Code SLX) • Click **Add**	
2	• Click **Structure** button • Click **Open Spectrum or Structure** icon	

	Action	Result
3	Navigate to **KnowItAll > Training Files > General Training > Files > Data Mining** Open **Propiophenone Query.dsf**.	The structure is displayed in the **Structure** tab. 
4	Make sure **Search Mode** is set to **Substructure**. Click **Search**.	Results are displayed in the **MineIt** application.

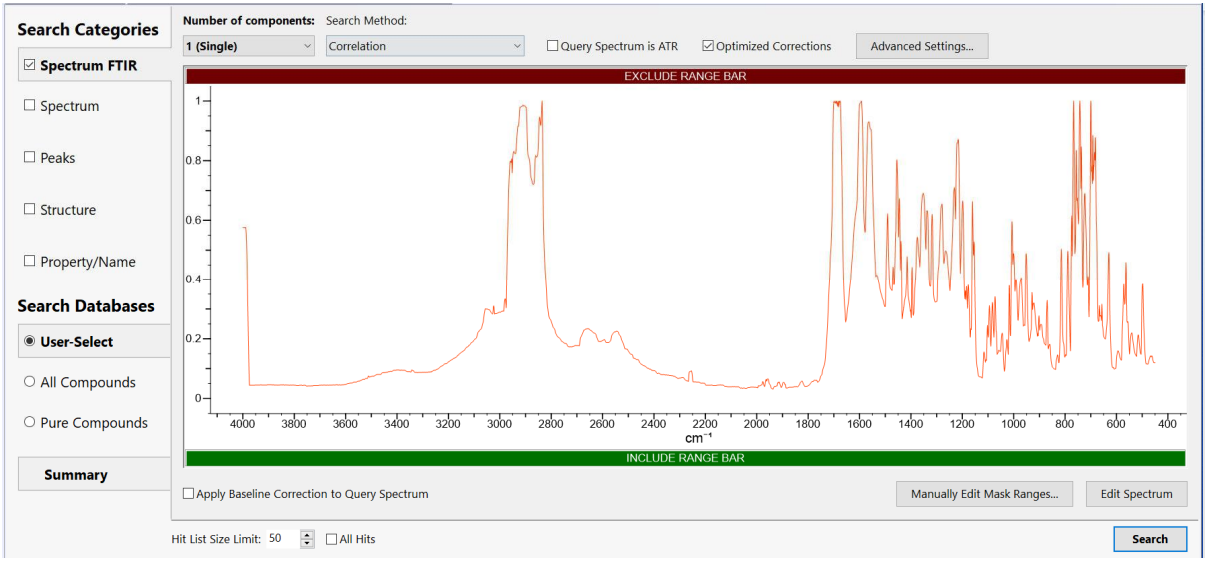
Examine the results in MineIt

	Action	Result
1	Select all eleven records in the hit list. **Note**: Select the first record, hold down the shift key, then scroll to and select the last record.	All spectra are displayed in the spectral pane: 
2	Click the **OD Heatmap** toolbar button…	

	Action	Result
3	…then click the **OD Consensus Spectrum** toolbar button  .	The consensus spectrum is displayed above the Overlap Density Heatmap: 

	Action	Result
4	Click the **OD Heatmap** toolbar button again to turn off this display.	The consensus spectrum remains in the display. 

Use the consensus spectrum to perform a search

	Action	Result
1	Click **SearchIt** in the **Transfer to** bar.	The consensus spectrum is displayed on the **IR Spectrum** search tab. 
2	Click the **Search** button. **Note**: The IR – Sadtler Standards (Selected Subset) – Wiley database remains in the spectrum pane.	The results are displayed in the **MineIt** application on a new tab: As you can see from this example, the Overlap Density Consensus Spectrum created from a hit list of spectra containing the propiophenone substructure produces a spectrum that is very similar to propiophenone itself. The use of Overlap Density Consensus Spectra, therefore, has clear applicability in structure elucidation and unknown identification.

KnowItAll Informatics Training

Quality Control Analysis with QC Expert

WILEY

QC Expert

Perform a Quality Control Comparison of a Sample Spectrum Against a Reference Spectrum

Objectives

This exercise will teach you:

- How to set up an account
- How to select a standard
- How to compare to a selected standard
- How to generate a report

Background

Wiley's KnowItAll QC Expert software performs a rapid quality check of a sample IR or Raman spectrum against a "gold standard" user spectrum to verify that a material meets control specifications.

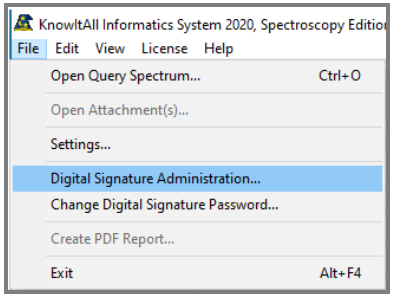
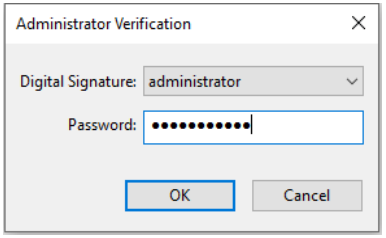
Training Files Used in This Lesson

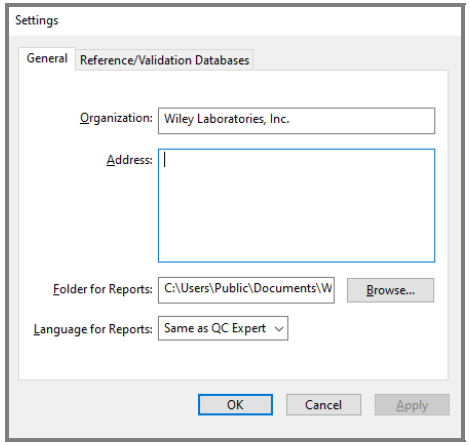
- DEET.SPA
- Epichlorohydrin Sample Spectrum.irf

KnowItAll Applications Used

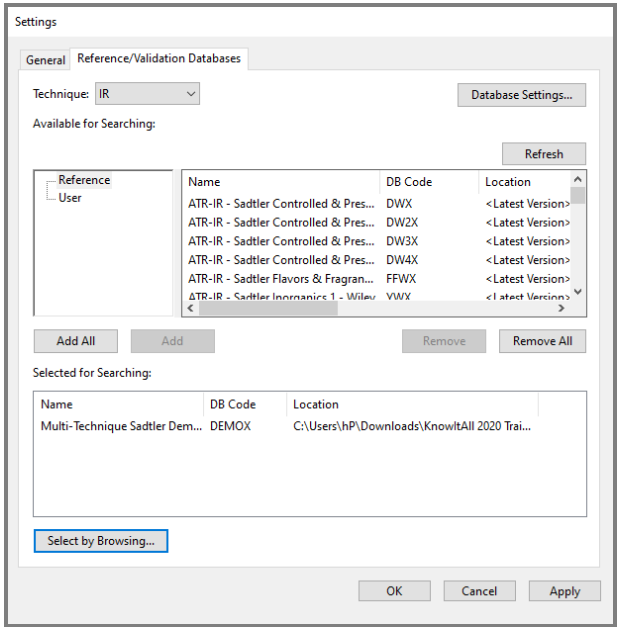
- QC Expert

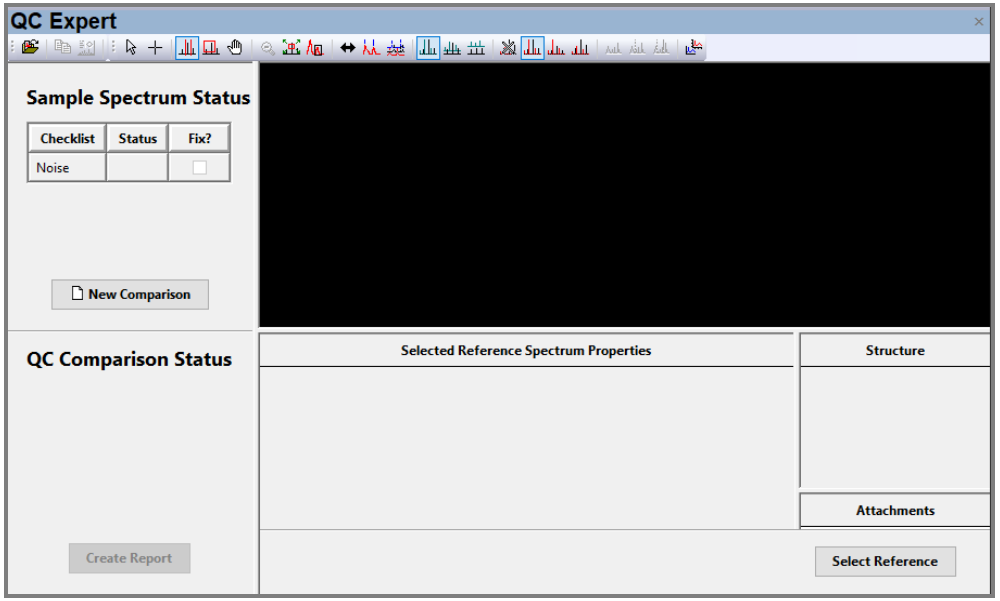
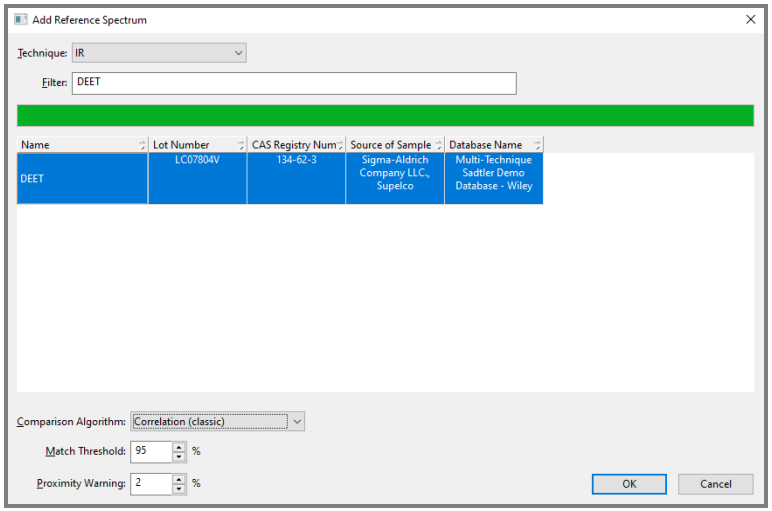
Set Up Administrator Account and Address

	Action	Result
1	Navigate to the **Data** toolbox and open the **QC Expert** application.	
2	To create an administrative account, go to **File > Digital Signature Administration…**	
3	• Enter your preferred user ID in the **Digital Signature** field • Enter preferred password in the **Password** and **Confirm Password** fields • Click **OK**	
4	In the **Administrator Verification** pop-up that appears, enter your user name and password.	

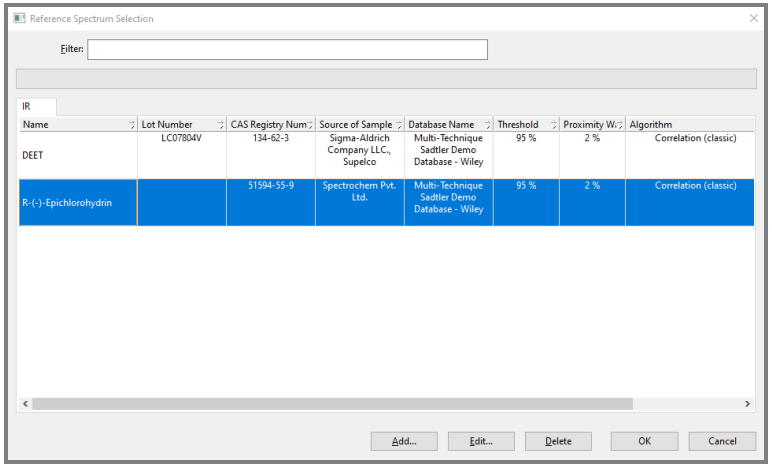
5	In **File > Settings**, set the Organization to "**Wiley Laboratories, Inc.**" and add address.	

Select Reference Database

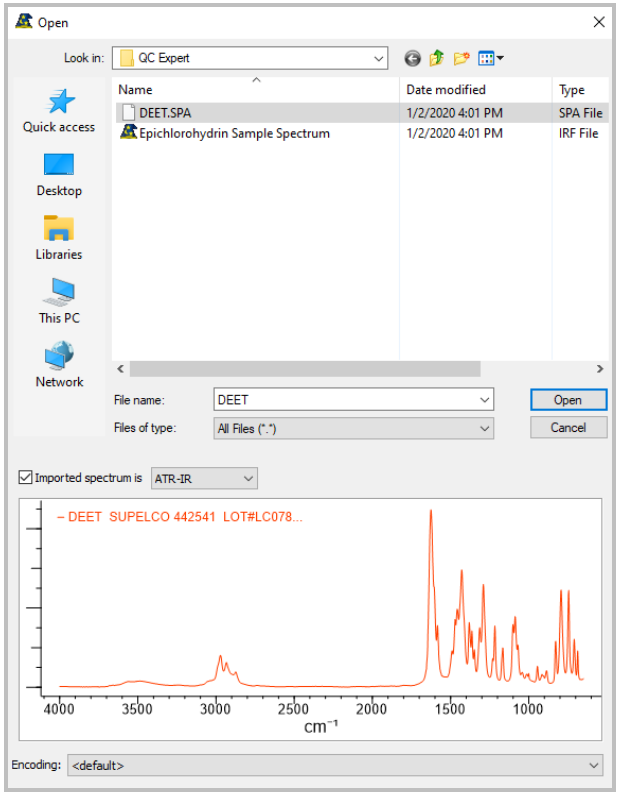
	Action	Result
1	• In the **Reference/Validation Databases** tab, click the **Select by Browsing** button • Navigate to **KnowItAll > Training Files > General Training > Databases > Samples folder** • Select the **Multi-Technique Sadtler Demo Database - Wiley [DEMO]** database.	
2	Click **OK**.	

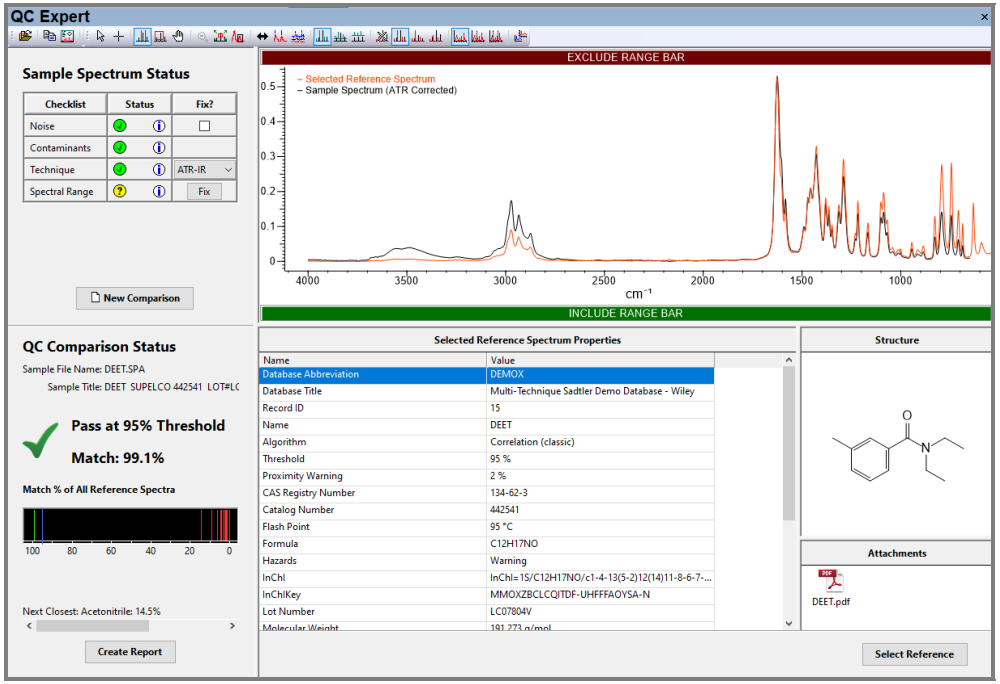
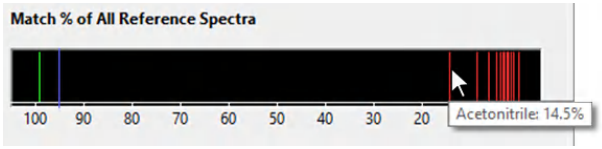
3	Click on the **Select Reference** button at the lower right of the **QC Expert** window.	
4	• At the prompt, login as administrator. The **Add Reference Spectrum** dialog box opens. • Type **deet** in the **Filter** box to search for DEET. • Point out the **Comparison Algorithm**, **Match Threshold**, and **Proximity Warning** parameters in the lower left. • Select the **Correlation (Classic)** algorithm for the demo. • Click **OK** to add the spectrum.	

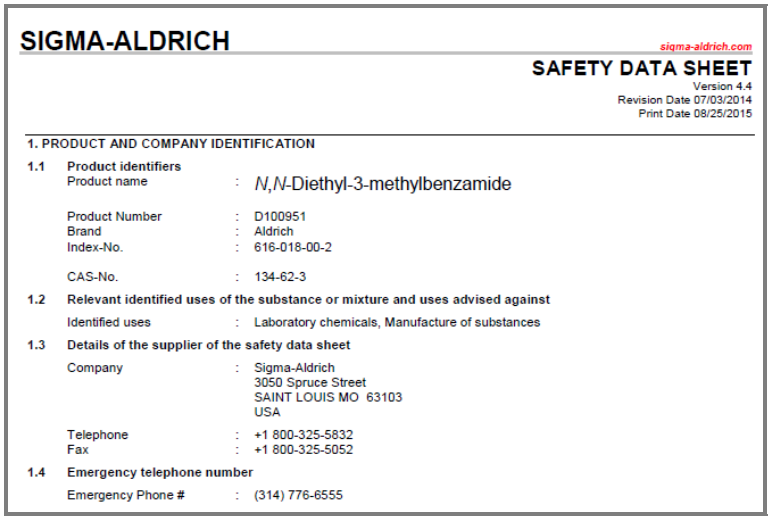
WILEY

5	• The **Reference Spectrum Selection** dialog box opens. • Click on **Add**, and type **epi** in the **Filter** box. • Select **R-(-)-Epichlorohydrin** and select the **Correlation (classic)** algorithm. • Click **OK**.	

Run QC Expert as a Non-administrator QC Analyst

	Action	Result
1	• Navigate to the **Data** toolbox and open the **QC Expert** application. • Click on the **Select Reference** button. Select the **DEET** spectrum • Click **OK.**	
2	• Click on **New Comparison** at the mid-left of the QC Expert window. • Navigate to KnowItAll > Samples > QC Expert folder and select **DEET.SPA**. • Set **Imported spectrum is** to **ATR-IR** and ensure this option is checked. • Click **Open**.	

3		The **QC Expert** window displays the **Comparison Status**.  We get an excellent match of 99.1% and a green check mark indicating that the quality control comparison passes.
4	Mouse over the green and red bars in the **Match % of All Reference Spectra** chart. **Note**: When you mouse over the various bars in the Match% Chart, you see the corresponding display in the **Spectrum Pane** at the top.	 The **Match % of All Reference Spectra** chart shows the comparison of the sample spectrum to spectra from the entire reference database. The **green bars** are for the comparison of the sample spectrum against the selected reference spectrum as well as all other reference spectra for different lots of the same compound. The **blue line** is the quality control threshold, and the **red lines** are the match % values for the comparison of the sample spectrum against all the other spectra in the database.

5	Double-click on the PDF attachment in the **Attachment** pane at the lower right.	The DEET safety datasheet and other associated information is displayed. 

SIGMA-ALDRICH sigma-aldrich.com

SAFETY DATA SHEET

Version 4.4
Revision Date 07/03/2014
Print Date 08/25/2015

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : *N,N*-Diethyl-3-methylbenzamide

Product Number : D100951
Brand : Aldrich
Index-No. : 616-018-00-2

CAS-No. : 134-62-3

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

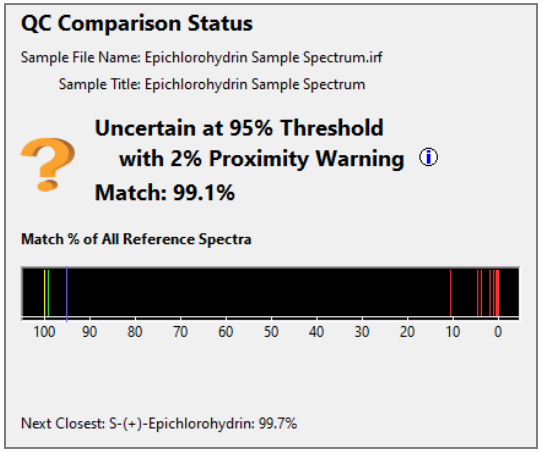
Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

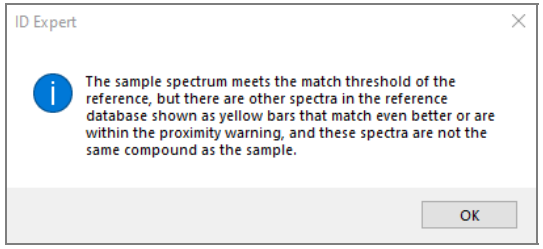
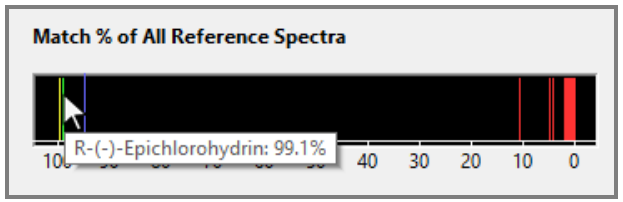
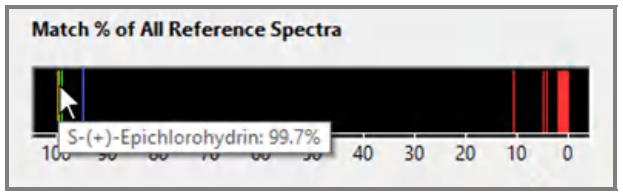
Telephone : +1 800-325-5832
Fax : +1 800-325-5052

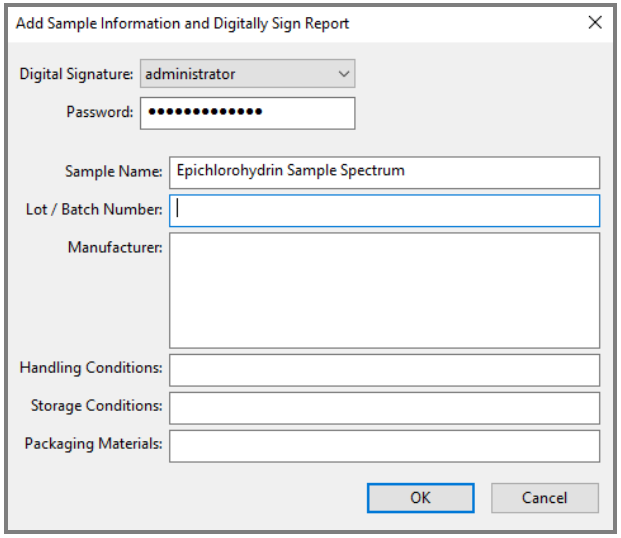
1.4 Emergency telephone number

Emergency Phone # : (314) 776-6555

Demo Protocol - QC Analyst Comparison of R-(-)-Epichlorohydrin Sample Spectrum to Reference

	Action	Result
1	• Navigate to the **Data** toolbox and open the **QC Expert** application. • Click on the **Select Reference** button. • Select the **R-(-)-Epichlorohydrin** reference spectrum. • Click **OK**.	This is to open a spectrum of a sample of **R-(-)-Epichlorohydrin** and perform a quality control comparison to make sure that the sample actually is what it is supposed to be.
2	• Click on **New Comparison** at the mid-left of the QC Expert window. • Navigate to **KnowItAll > Samples > QC Expert folder**. • Select **Epichlorohydrin Sample Spectrum.irf**. • Set **Imported spectrum is** to **ATR-IR** and ensure this option is checked. • Click **Open**.	 The Match% between the selected reference spectrum and sample spectrum is excellent at 99.1%, but the QC comparison is **Uncertain**.

3	Click on the information button ⓘ.	 An **ID Expert** pop-up says that the sample spectrum meets the match threshold, but there are other spectra that match even better or are within the proximity warning.
4	Click **OK** to close the dialog box.	
5	On the Match% chart, mouse over the bars near 100% and look at the corresponding spectra in the spectrum pane above.	There are two lines above the blue threshold line indicating two hits, one in green and one in yellow.
6	Mouse over the green bar in the Match % Chart. The hover-over text says **R-(-)-Epichlorohydrin: 99.1%**.	 The green bar in the Match % chart indicates the comparison of the sample spectrum to the reference spectrum. The match percent is 99.1%
7	Mouse over the yellow bar in the Match % Chart. The hover-over text says **S-(+)- Epichlorohydrin: 99.7%**.	 The yellow bar is for **S-(+)- Epichlorohydrin**, which is the enantiomer of the R-(-) isomer. The R and S forms of Epichlorohydrin are stereoisomers that are indistinguishable by IR.

8	Click on **Create Report** button below the Match% chart to create a digitally signed report. • Select your user name from the **Digital Signatures** drop-down. • Enter the password • Fill out the sample information..	
9	Click **OK** to view the report.	The digitally signed PDF contains the following information: Page 1 – Information about the test Page 2 – Information about the spectral comparison Page 3 – Information about the reference spectrum

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