KnowItAll Software Training

Creating 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 create 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
- 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

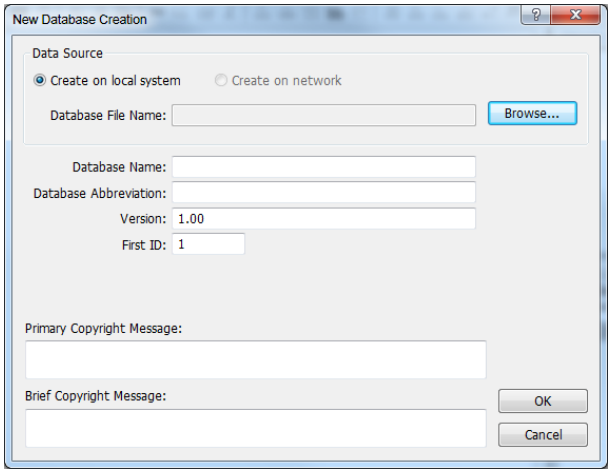
C:\Users\Public\Documents\Wiley\KnowItAll\Samples

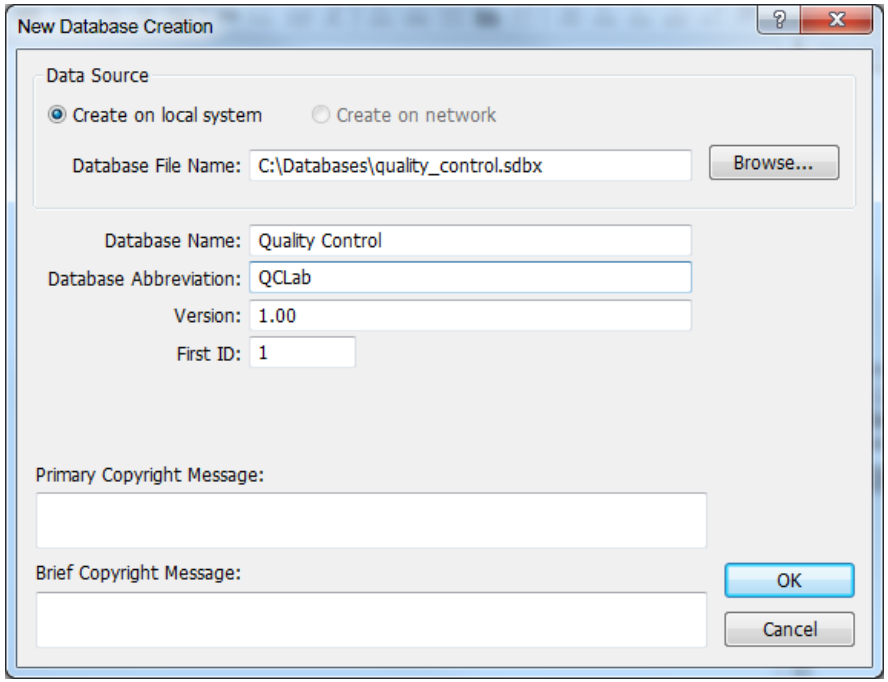
- \IR\Ethyl acetate.dx
- \Raman\Ethyl acetate.irf
- \MineIt\Import.csv
- MSDS Web Link.txt
- Ethyl acetate MSDS.pdf

KnowItAll Applications Used

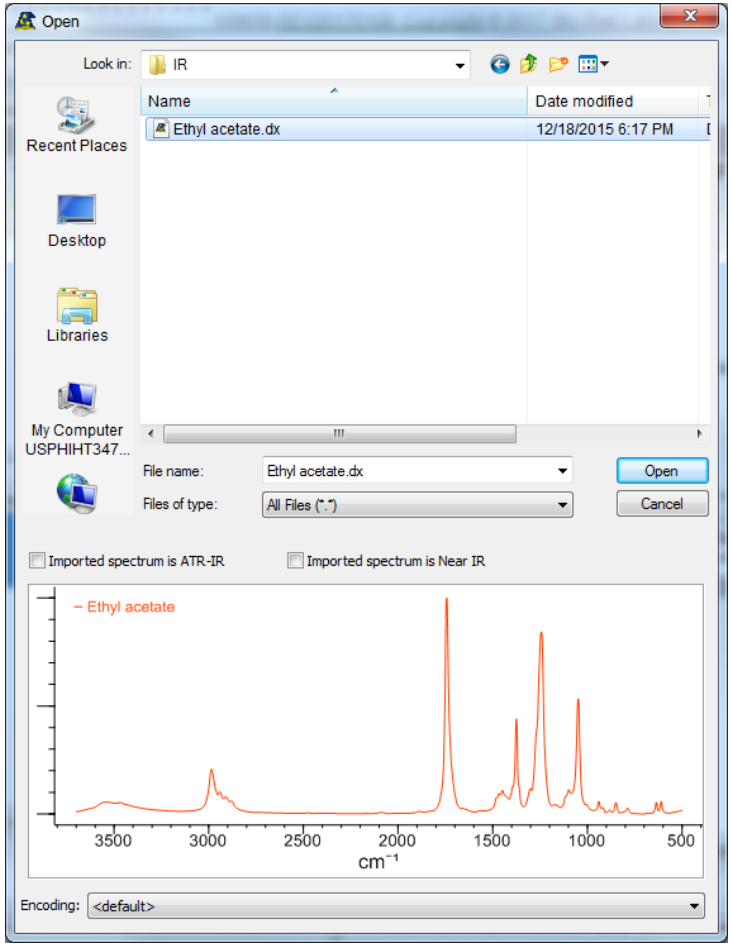
- MineIt™
- ChemWindow®
- BrowseIt™

Create a user database

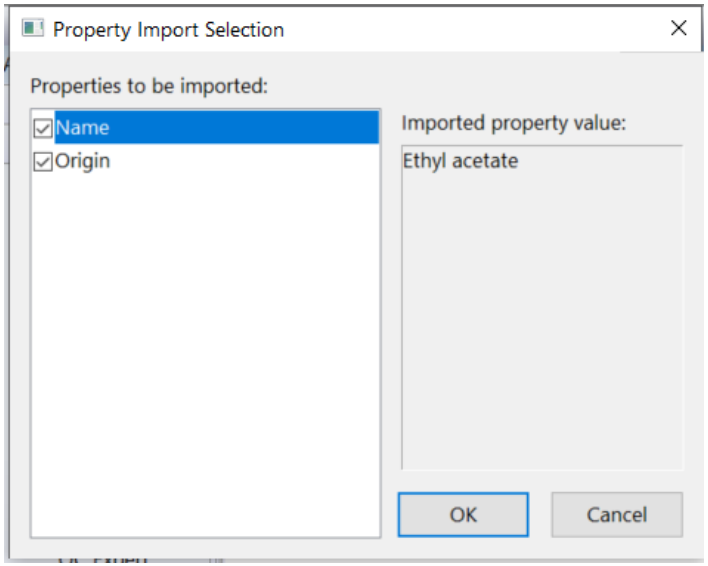
	Action	Result
1	Navigate to the **Data** toolbox and open the **MineIt** application by clicking the **MineIt/Create Database** icon.	The **MineIt** application opens.
2	Choose **Database > New**.	The **New Database Creation** dialog box opens. 
3	Select **Create on local system**.	The new database is 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 it 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.	

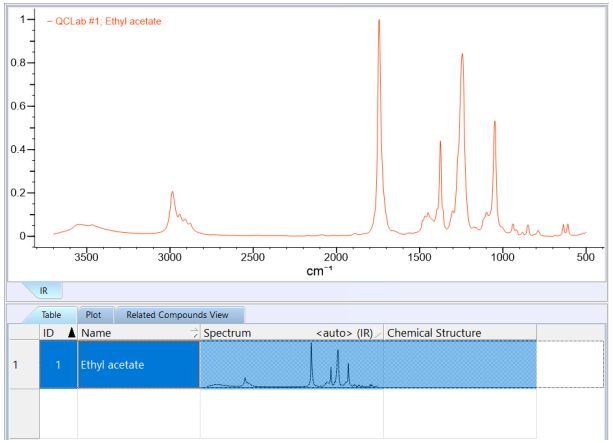
	Action	Result
6	Type **QCLab** in the **Database Abbreviation** text box. **Note**: The abbreviation must be 3-7 characters long.	
7	Enter **Version** number and the **First (starting) ID**, and type in copyright messages.	
8	Click **OK**.	The new database has been created to receive your data. The Database 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 spectrum 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 C:\Users\Public\Documents\Wiley\KnowItAll\Samples\IR folder • 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. 

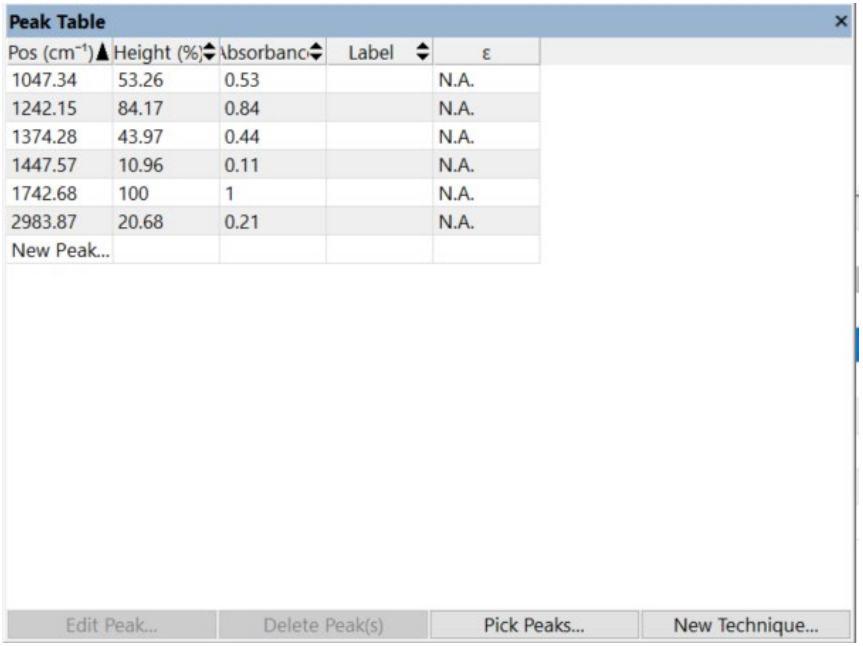
WILEY

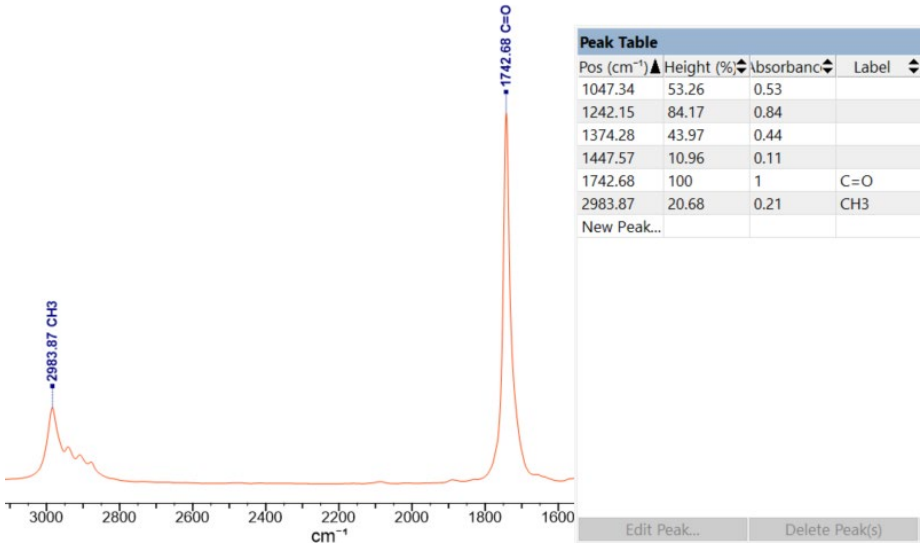
	Action	Result
2	Click **Open**.	The **Property Import Selection** dialog box opens.  This dialog box appears when you transfer information into a user database. All available properties are shown. Select each property in turn. Then use the checkboxes to define the action for each property.

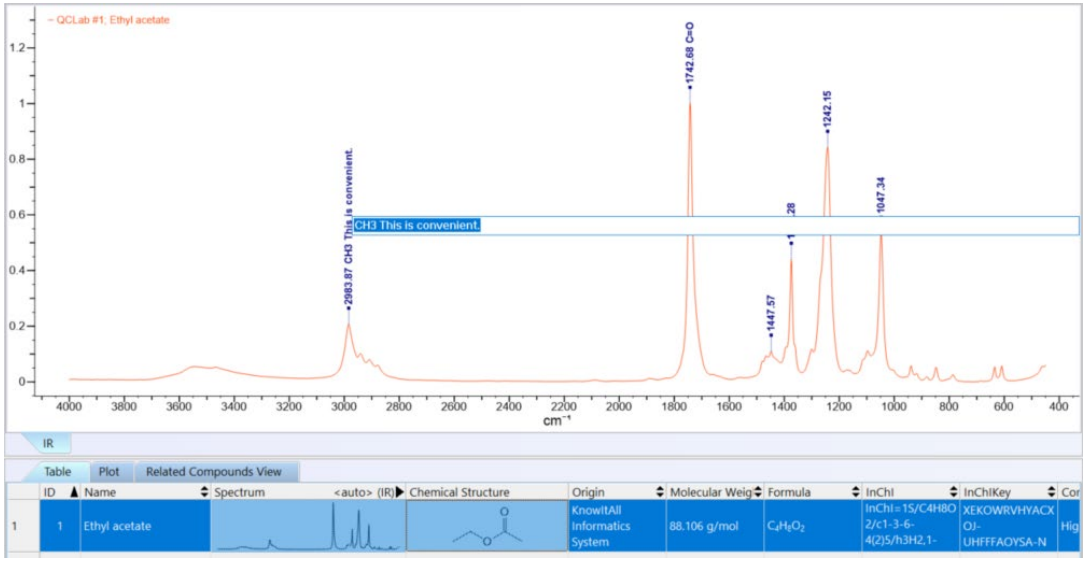
3	Click **OK**.	The dialog box closes. The spectrum has been added to the user database as the first record. 

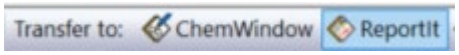
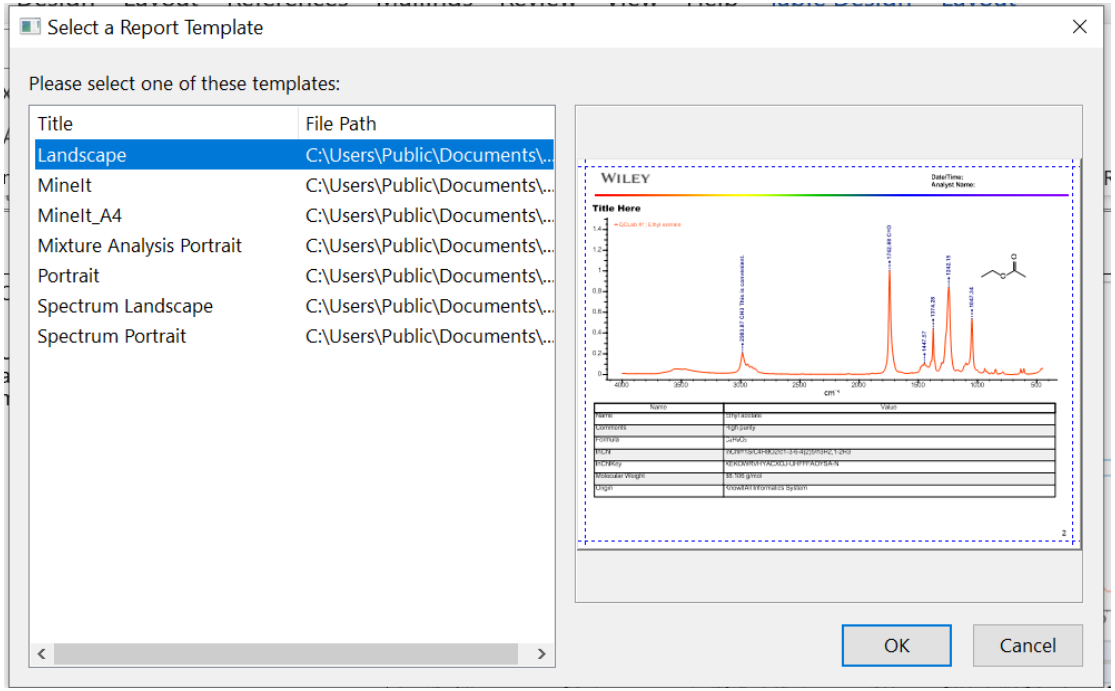
Add spectrum labels

KnowItAll 2024 release has a new feature – users can add customized peak labels.

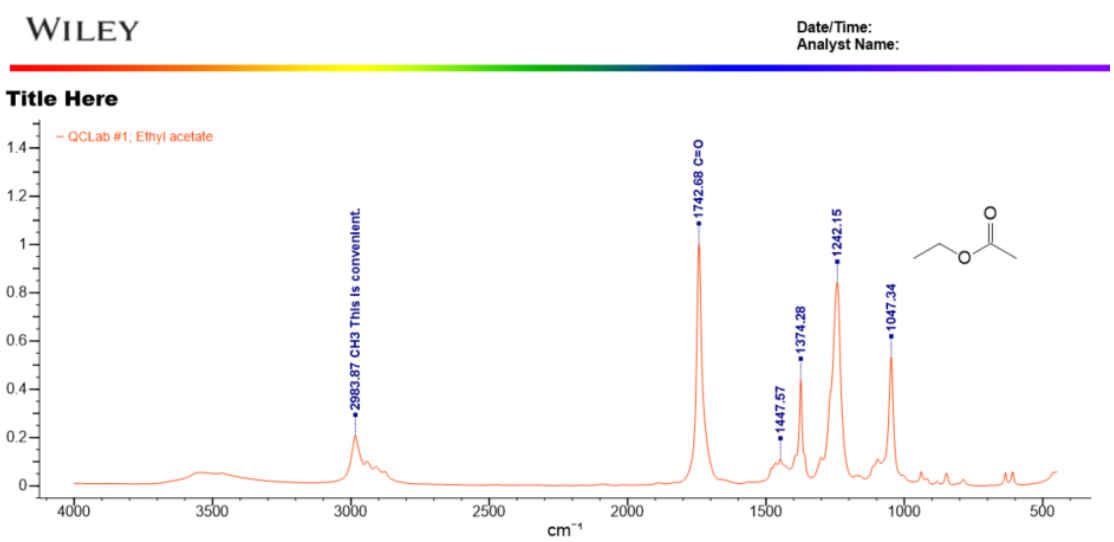
	Action	Result
1	Continue with the above example Choose **View > Windows/Tables > Peak Table** to open the spectrum peak table	**Peak Table** pops up in a window 

	Action	Result
2	One can directly type textual values into the Label column.	The labels show up in spectral pane. 

3	Close the **Peak Table** window Use the mouse to hover over a peak label and double-click would open a text box for more editing.	 Peak Label is a property of a spectrum, so it would move with the spectrum in KnowItAll, for example, be transferred to ReportIt and ProcessIt application plug-ins.

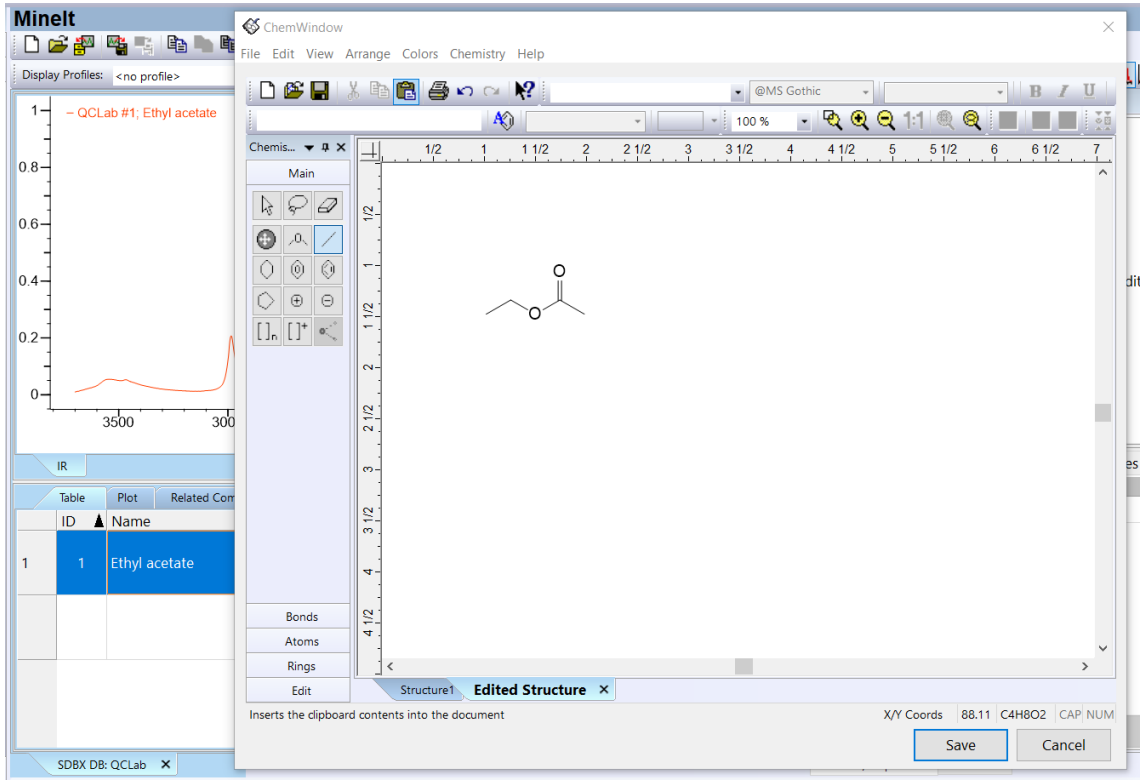
4	Select Transfer to: ReportIt  Choose the **Landscape** report template Click **OK**	

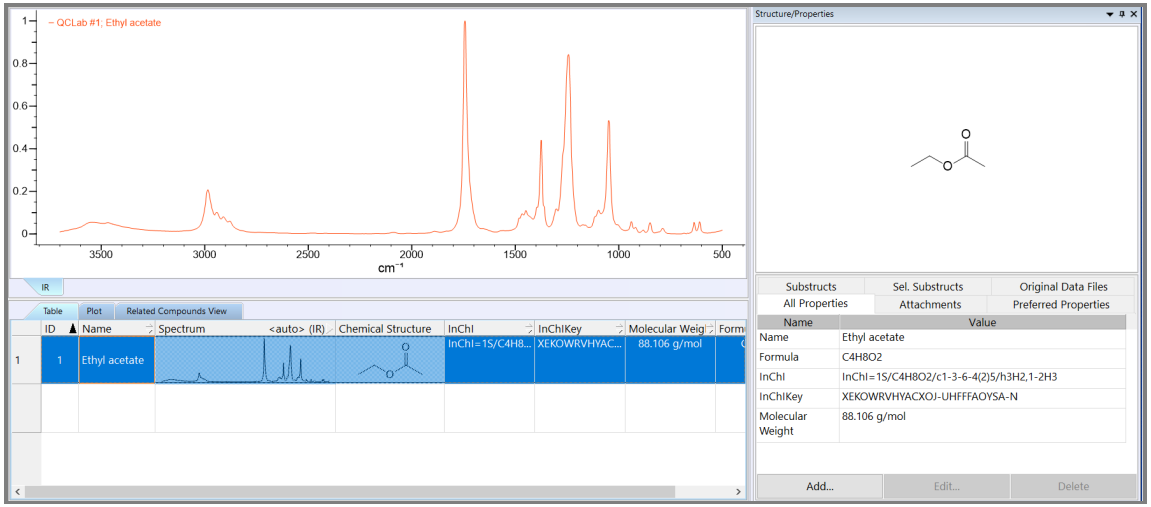
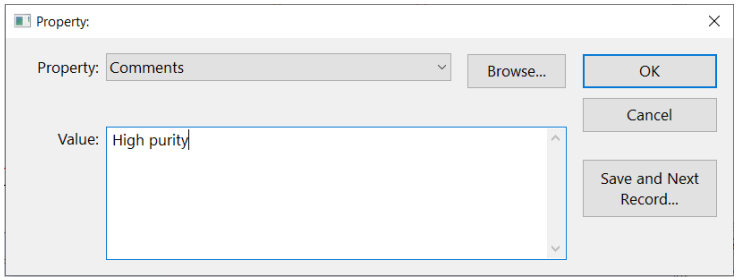
The peak labels ride along:

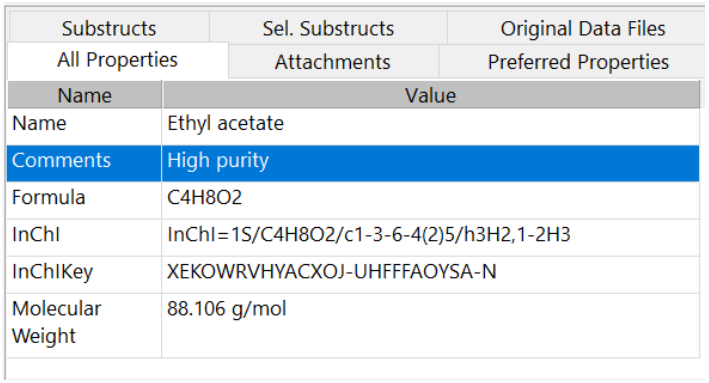


Name	Value
Name	Ethyl acetate
Comments	High purity
Formula	$C_4H_8O_2$
InChI	InChI=1S/C4H8O2/c1-3-6-4(2)5/h3H2,1-2H3
InChIKey	XEKOWRVHYACXOJ-UHFFFAOYSA-N
Molecular Weight	88.106 g/mol
Origin	KnowItAll Informatics System

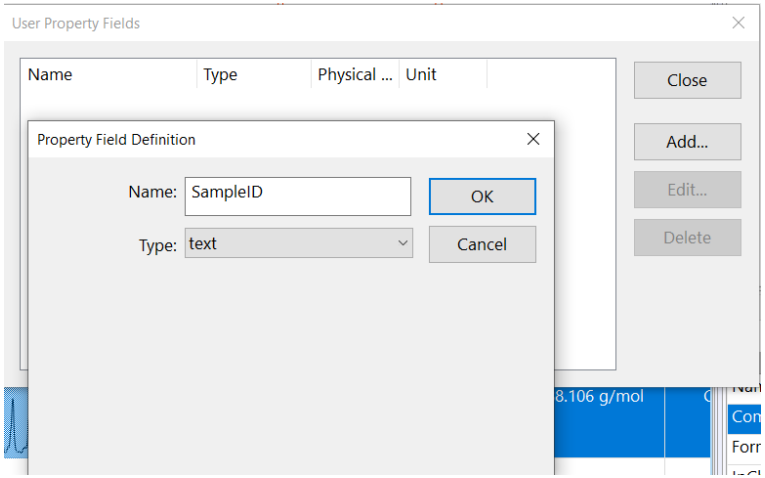
Add a chemical structure and properties to a database record

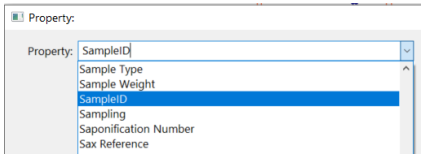
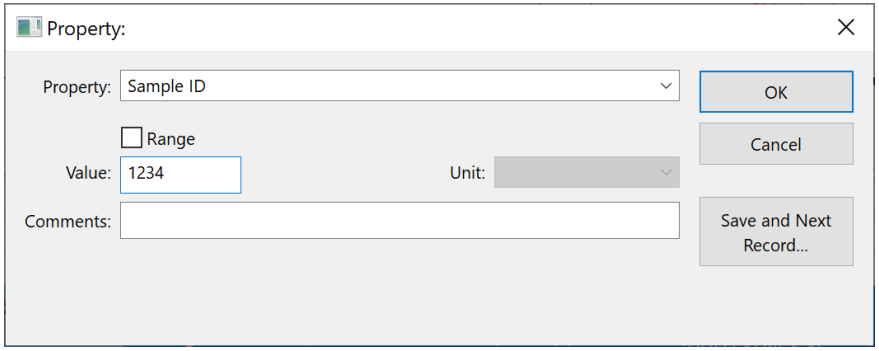
	Action	Result
1	Go back to **MineIt** With the first record selected, double-click the Structure/Properties pane at the top right of the window (**Double-click to edit structure in ChemWindow**).	The **Transfer to** ChemWindow application pops up. Alternatively, you can use **Transfer to:** to go to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

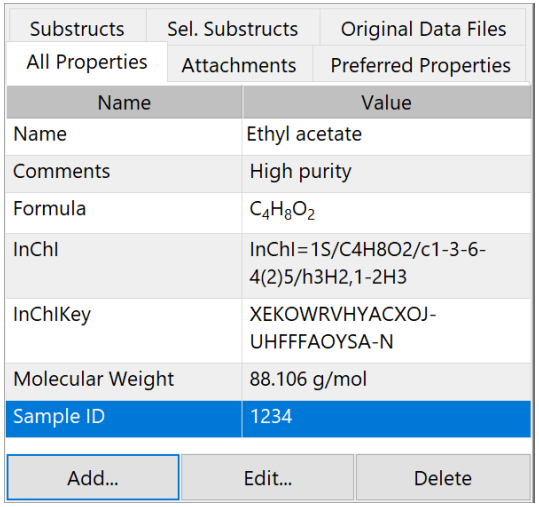
	Action	Result
3	Click **Save**.	The structure is added to the first record and is displayed both in the **Chemical Structure** column in the **Database** pane and the **Structure/Properties** pane.  **Note**: Some chemical properties such as InChI, InChIKey, Molecular Weight, etc., can be set to be automatically 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. Select **Comments**. Type **High purity** into the **Value** box.	

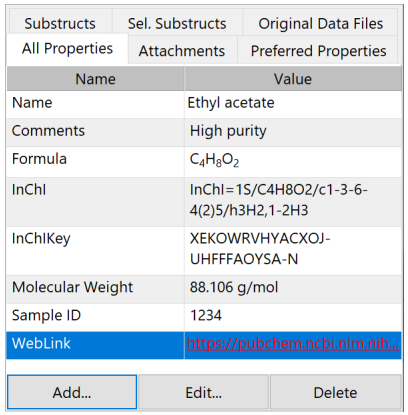
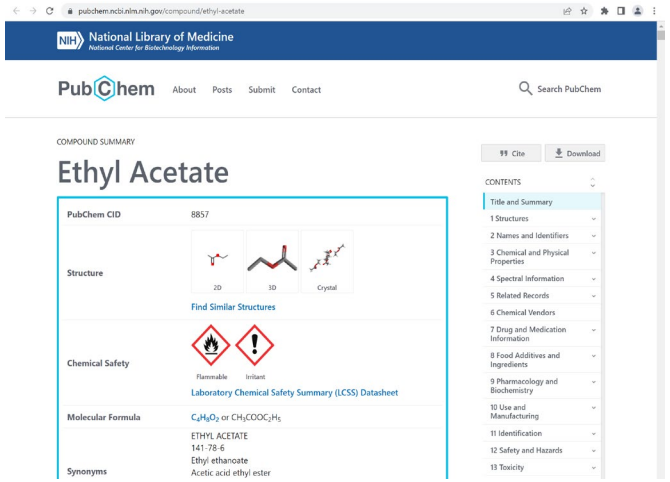
	Action	Result
6	Click **OK**.	The **Property** dialog box closes, and the name and value of the added property appears in the **Structure/Properties** pane. 
	TIP	You can select multiple database records and use the **Add** or **Edit** button at the bottom of the **Structure/Properties** pane to input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

Add user properties

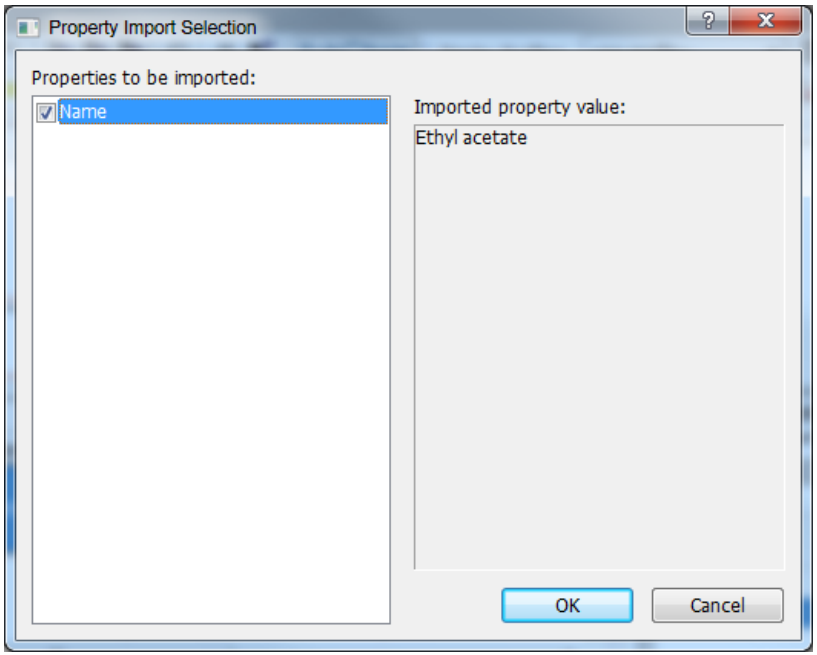
	Action	Result
1	Choose **Database > Define User Property Fields**.	The **User Property Fields** dialog box opens.
2	Click **Add**. Use the drop-down list to set **Type** to text. Enter the **Name**.	The **Property Field Definition** dialog box opens.  **Note**: Which controls are available depends on which type of field is specified: numeric, text or enumeration.
3	Click **OK.** Then click **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.

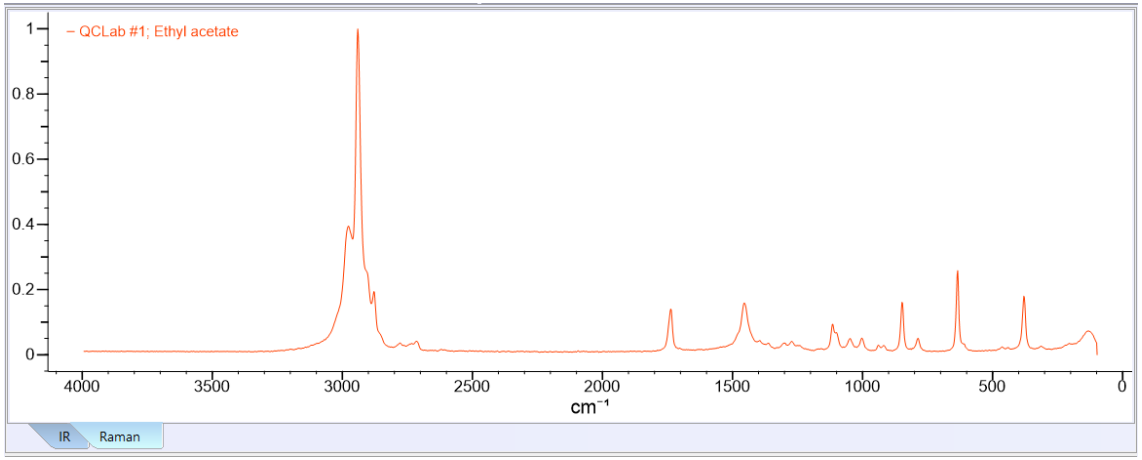
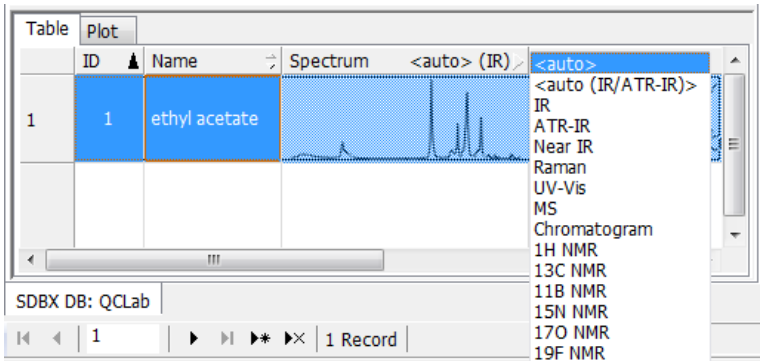
6	Select **SampleID** 	The **Value** text box is added to the dialog. **Note**: Which text boxes are added depends on whether the property is numeric, text or enumeration.
7	Type '1234' in the **Value** text box.	

8	Click **OK**.	The dialog box closes. The property **SampleID** with value 1234 is added to the **Structure/Properties** pane for the first record. 

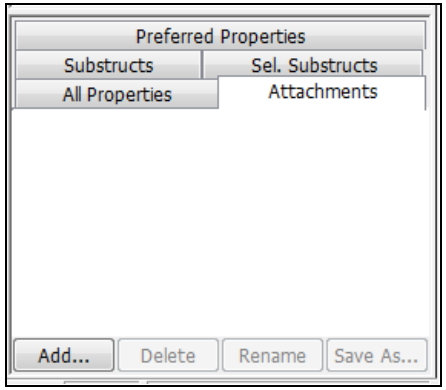
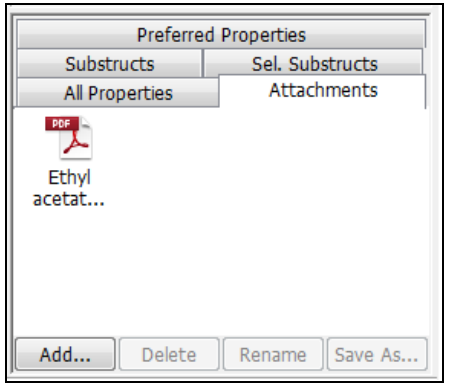
	Action	Result
9	Repeat steps 1-8 to create the user property **WebLink** and display it in the **Structure/Properties** pane. Type 'https://pubchem.ncbi.nlm.nih.gov/compound/ethyl-acetate' in the **Property** dialog box's **Value** field.	The property **WebLink** with a web address is added to the **Structure/Properties** pane for the first record. 
10	Click the web address in the **Structure/Properties** pane.	The web page opens. 
11	Click the KnowItAll **Back** button to return to the **MineIt** application.	

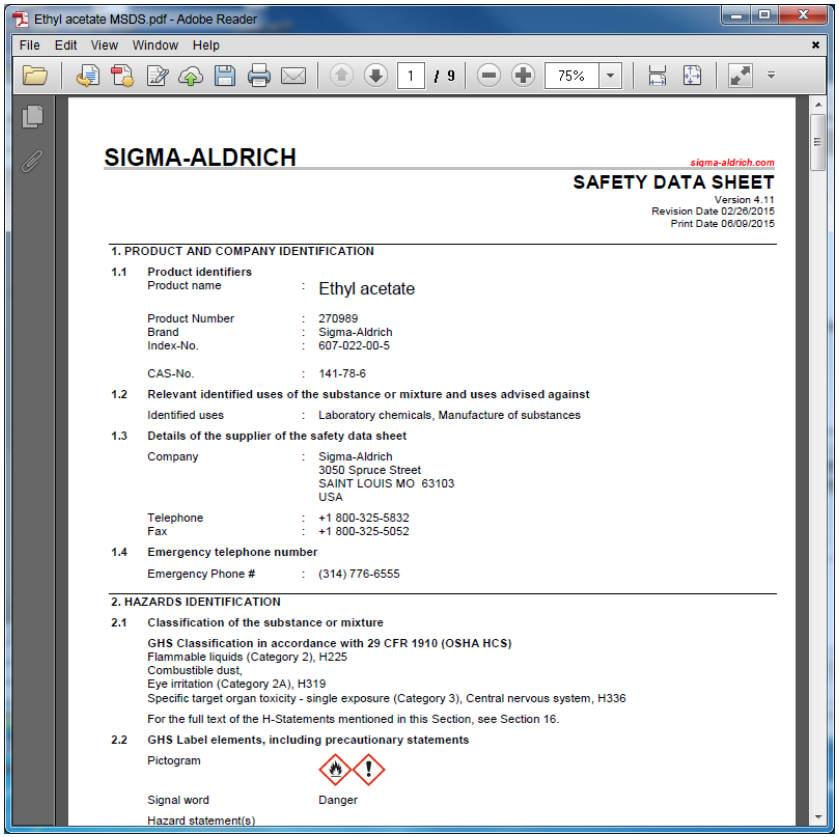
Add another spectrum (Raman) to the first database record

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

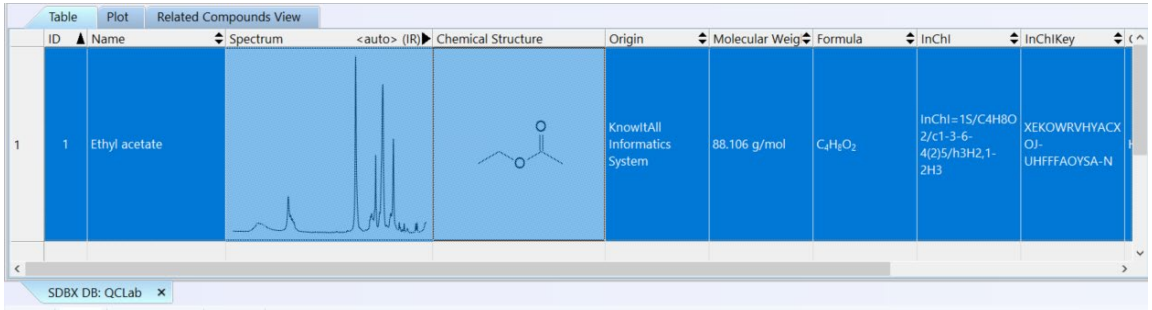
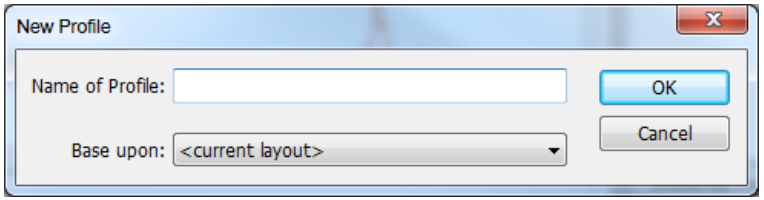
	Action	Result
3	Click **OK**.	A new **Raman** tab is added to the **Spectral** pane for the display of the Raman spectrum. 
4	Switch between spectra by using the tabs at the bottom left of the spectral pane.	
5	You can also switch between spectra by clicking the arrow in the **Database** pane's **Spectrum**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

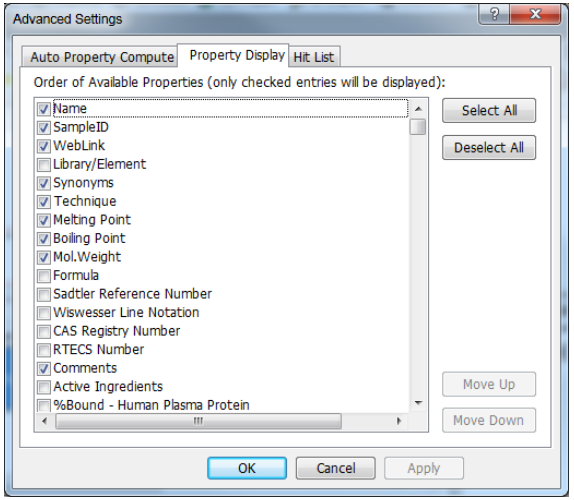
Add an attachment to the first database record

	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 C:\Users\Public\Documents\Wiley\KnowItAll\Samples\MineIt folder. Select **Ethyl acetate MSDS.pdf**. Then click **Open**.	An icon is added to the **Attachments** tab. 

	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**.

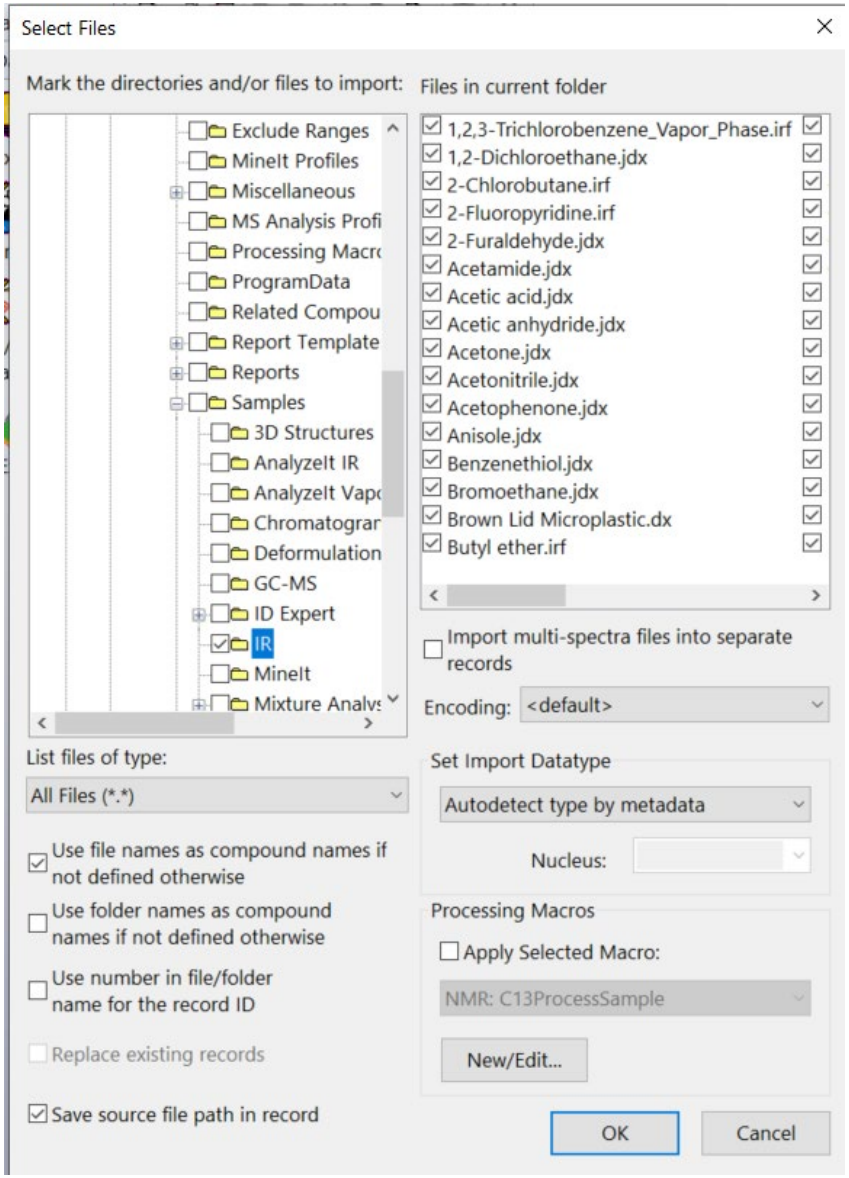
Create a new MineIt display profile

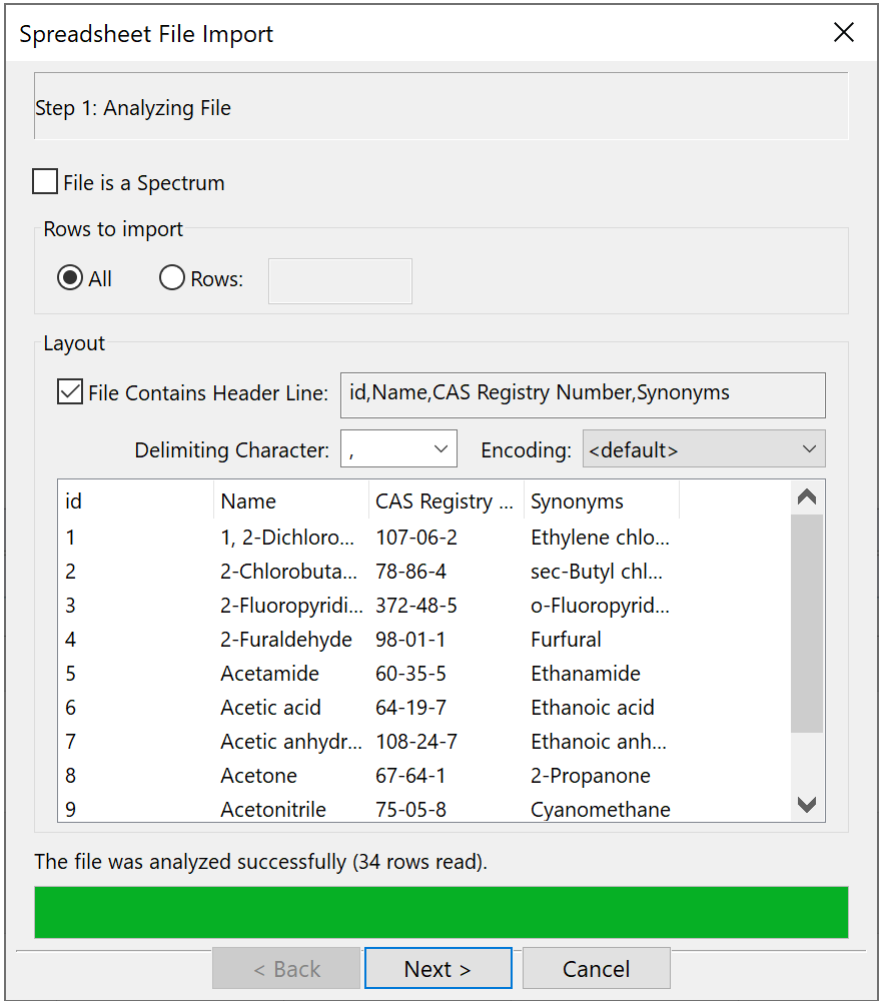
	Action	Result
1	One should the table row height to satisfactory first.	For example, make a row a lot taller: 
1	Click the **Add a New Profile** button  in the **Profile** toolbar.	The **New Profile** dialog box opens. 
2	Type in the profile name **QC Lab** and click **OK**.	This layout is now available to apply to any database or hit list display in the **MineIt** application.

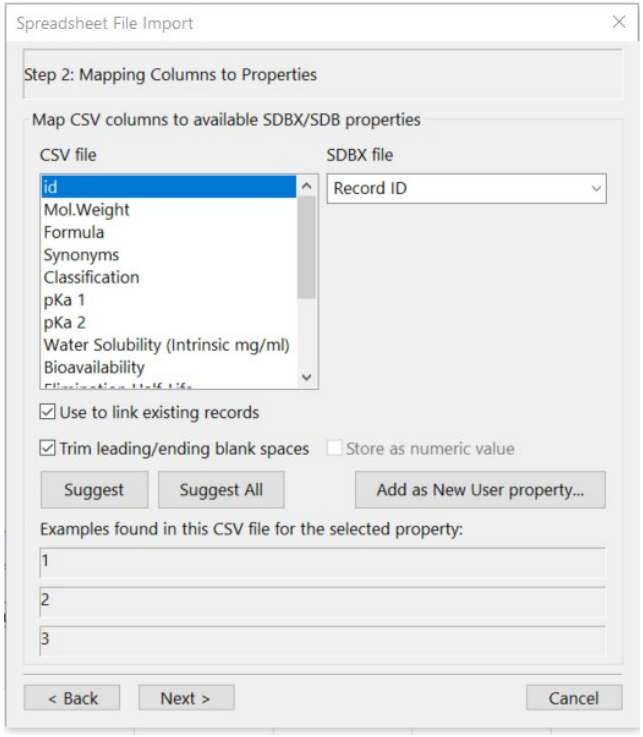
	TIP	When creating a database and to ensure individual users in your laboratory consistently enter all pertinent information into databases, you should set up preferred properties. To do so, go to **File** > **Preferences**. In the Preferences dialog, select the **Property Display** tab. Click on **Deselect 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.

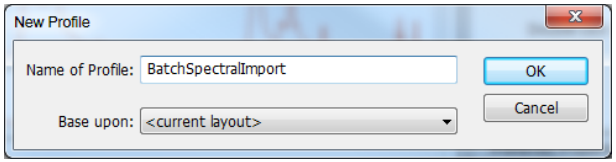
Batch Import: many spectra, many records, import properties from a spreadsheet

	Action	Result
1	Create a new empty database as in the above example.	

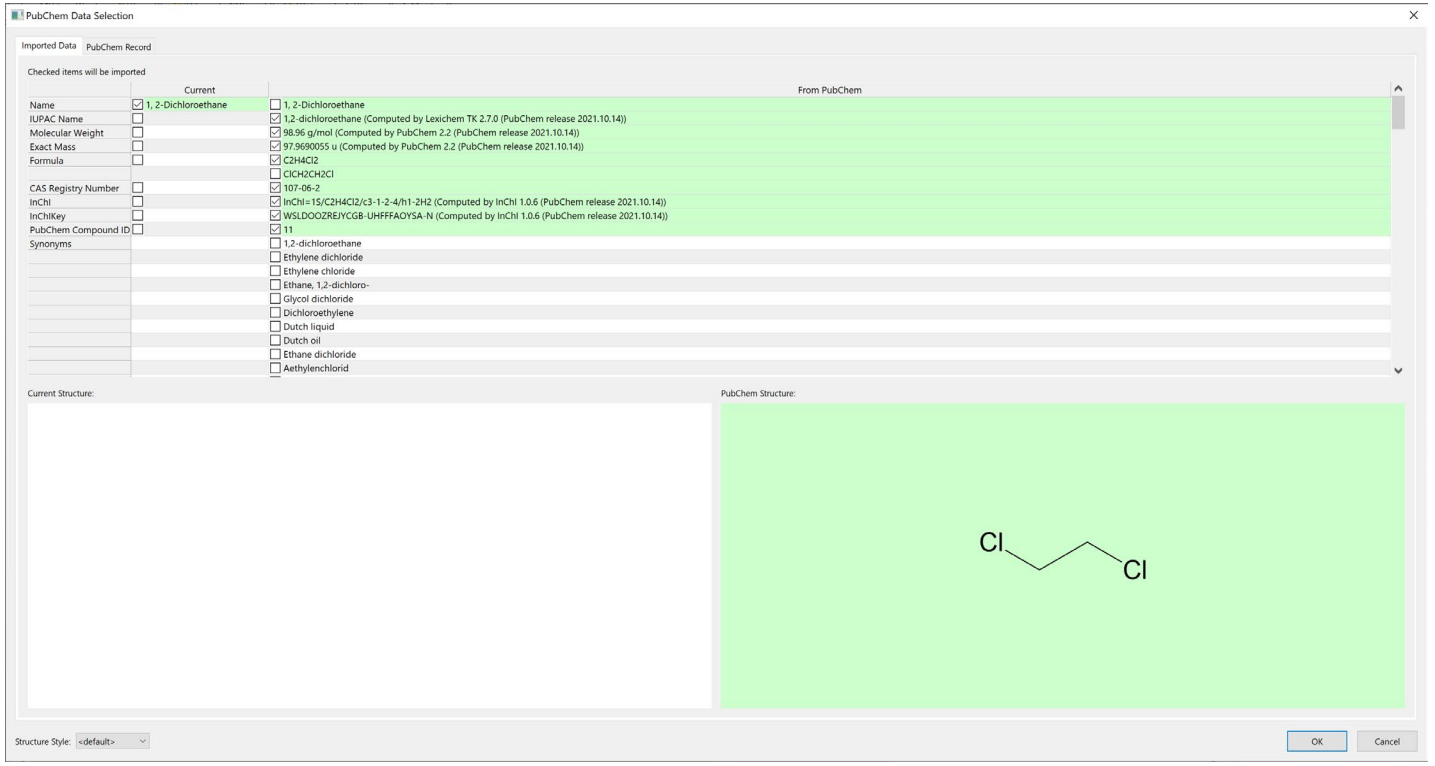
2	Choose **File > Batch Import** to open the **Select Files** dialog box. Navigate to **C:\Users\Public\Documents\Wiley\KnowItAll\Samples\IR**, select all spectral files in the folder. Check the box next to a folder name to select all files in the folder. Click **OK**	 A record is created in the new database for each spectral file.

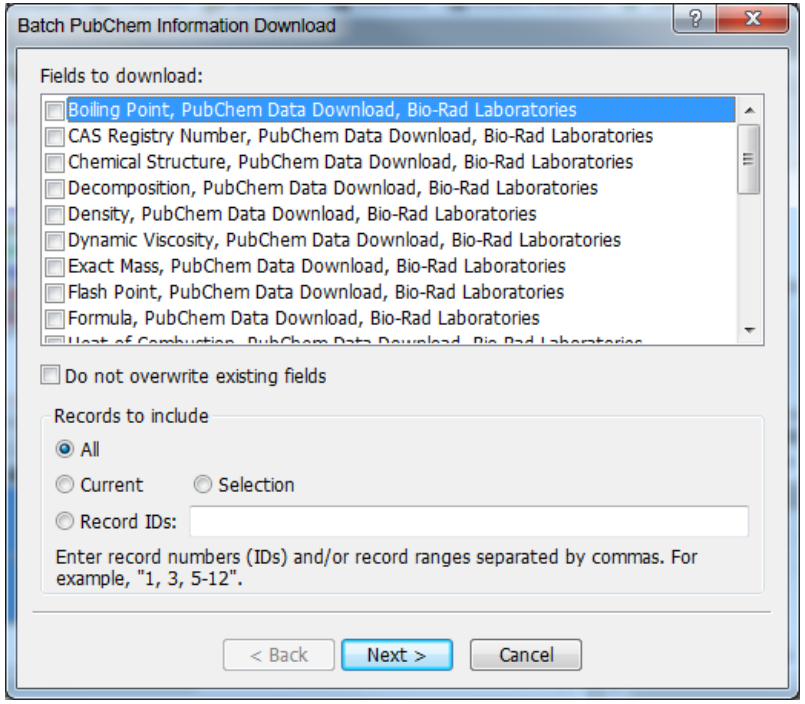
3	Choose **File > Import**. Navigate to **C:\Users\Public\Documents\Wiley\KnowItAll\Samples\MineIt** Select **BatchImportProperties.csv** to map properties to the spectrum files using a spreadsheet. Click **Open**. Make sure to check **File Contains Header Line**. Click **Next**.	The **Spreadsheet File Import** wizard opens. 

	Action	Result
4	Click **Suggest All**, then review the automatic field matches. Click on **id** in **CSV file**, confirm the SDBX file reads **Record ID**. Do the same for the others: Make sure that the CSV id field matches SDBX/SDB file Record ID field. In other words: Name=Name CAS Registry Number = CAS Registry Number Synonyms = Synonyms Check the **Use to link existing records** if not already checked. Click **Next**.	
5	Click **Finish**. You do not have to **Compact database now** at the prompt.	The database now has fields **Synonyms** and **CAS Registry Number** populated by the CSV file.

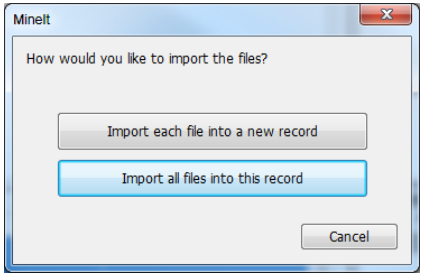
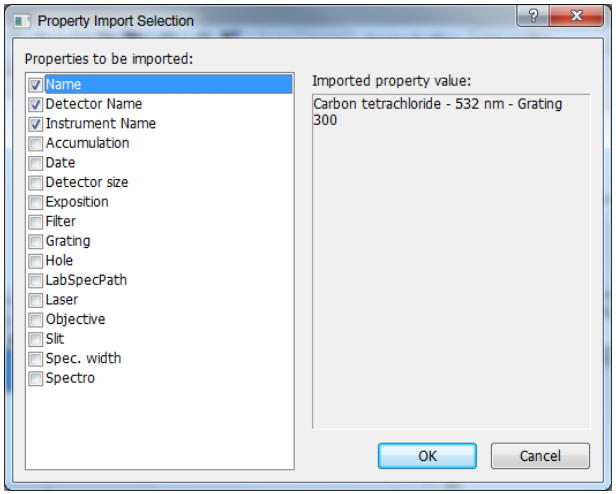
	TIP	You can rearrange the spreadsheet portion of this database (for example, to get rid of empty structure columns, right-click and choose **Delete Columns**). When edits are completed, you can save this column arrangement as a **MineIt** profile. Click **Save Current Profile** on the **Profile** toolbar, 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.

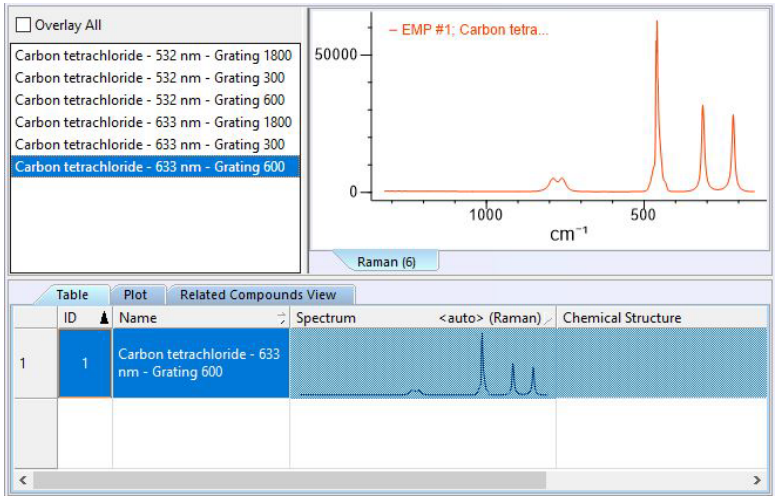
Batch Import: many spectra, many records, import properties from PubChem

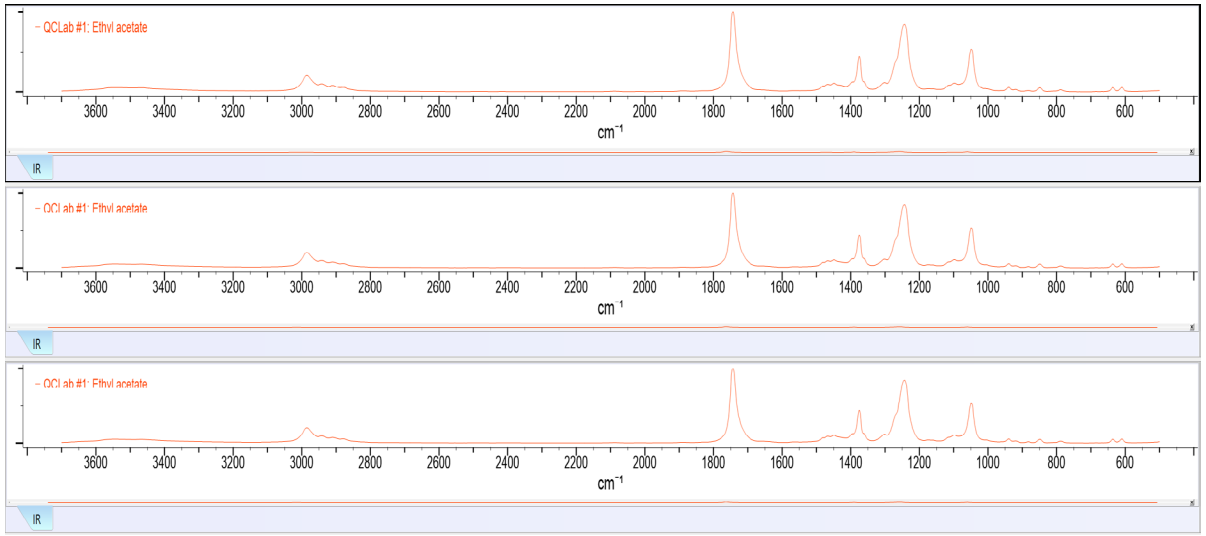
	Action	Result
1	Select the first record from the above database, click the **PubChem** toolbar button. 	**PubChem** records are searched. If information is located, the **PubChem Data Selection** dialog box opens. 

	Action	Result
2	Click **OK**.	New properties from **PubChem** are added to the first database record.
3	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. 
4	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 **C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Raman** folder Select all **.DX** 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

How to Create a Database with Structures

Purpose

This exercise demonstrates how to use 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
- 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

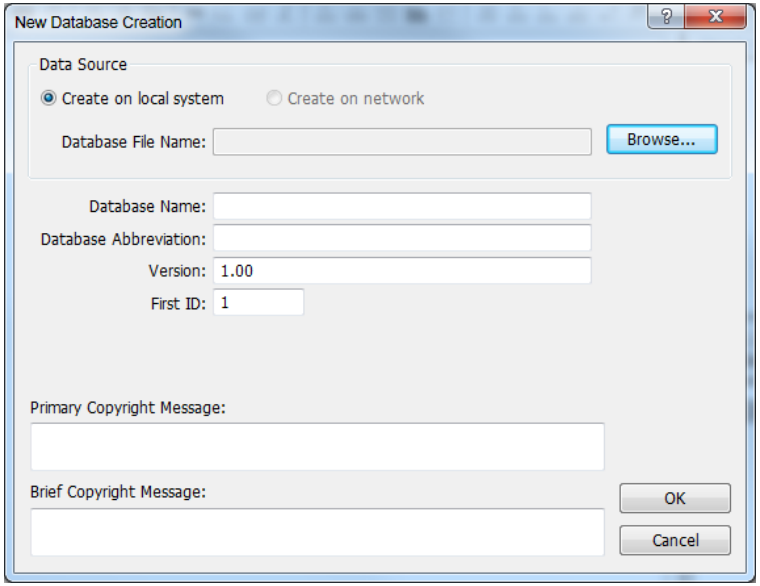
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Structures folder

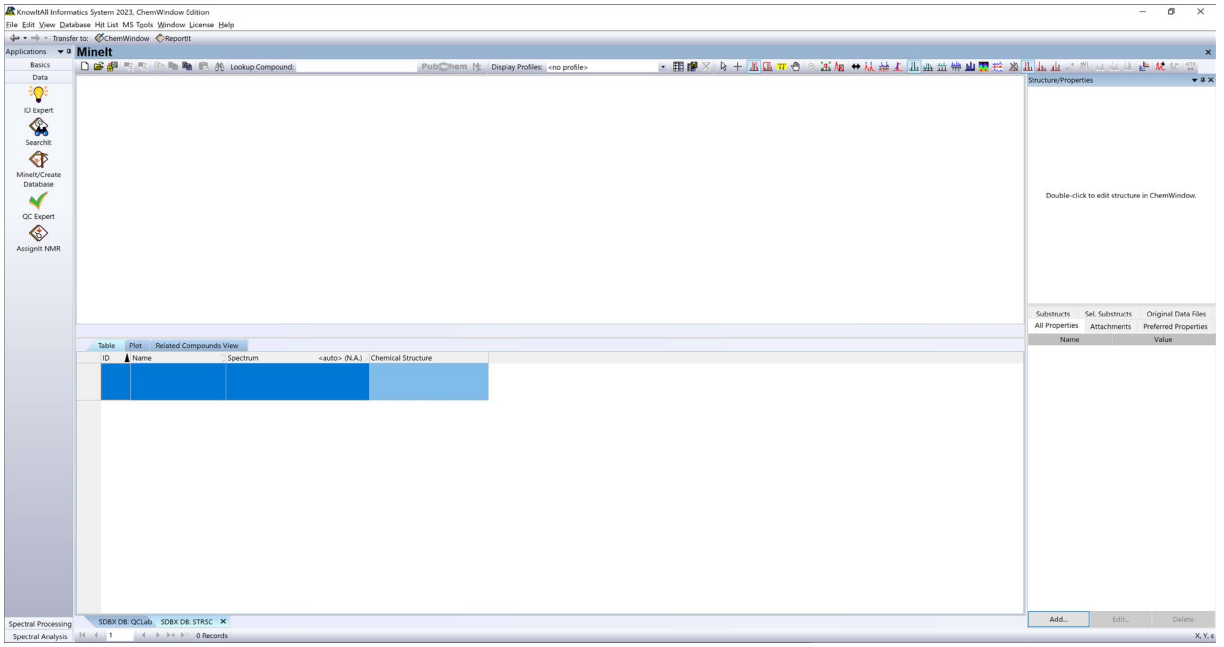
- benzylpenicillin.dsf

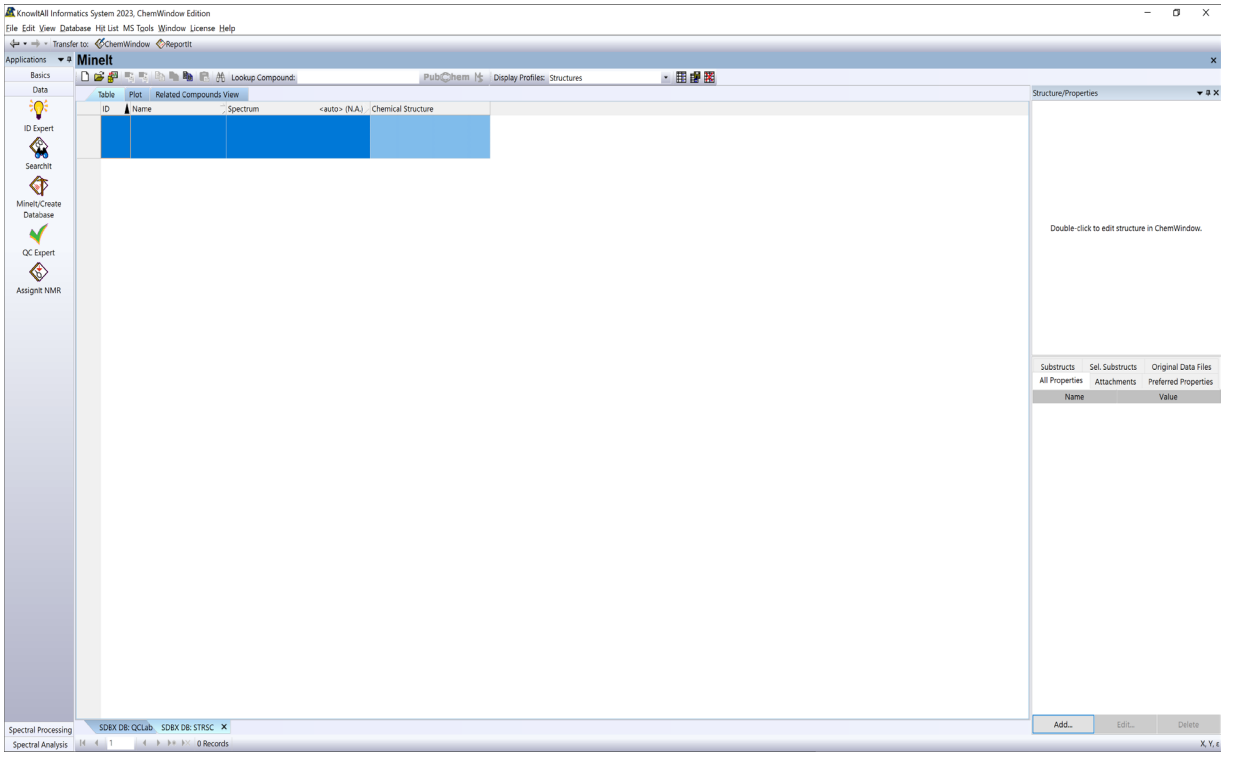
KnowItAll Applications Used

- MineIt™
- ChemWindow®

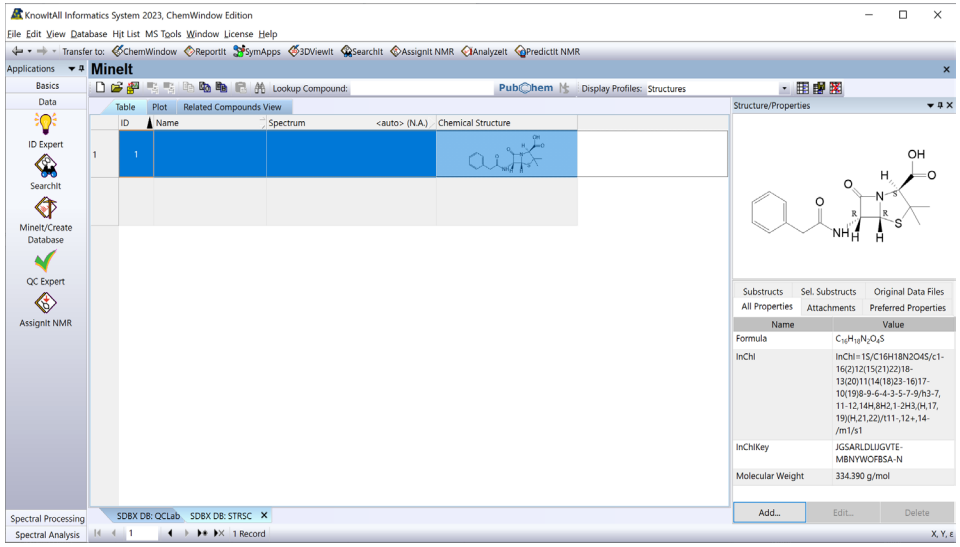
Create a user database

	Action	Result
1	In the **MineIt** application, choose **Database > New**.	The **New Database Creation** dialog box opens. 
2	Select **Create on local system**.	The new database is saved locally.
3	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.
4	Type **Structures** in the **Database Name** text box. **Note**: The file name is used if no other name is specified.	

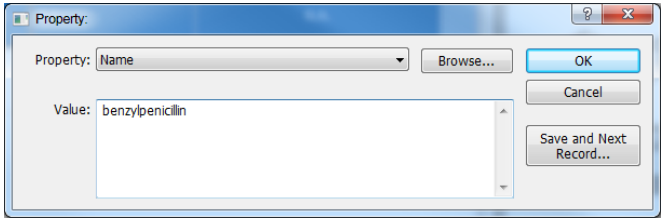
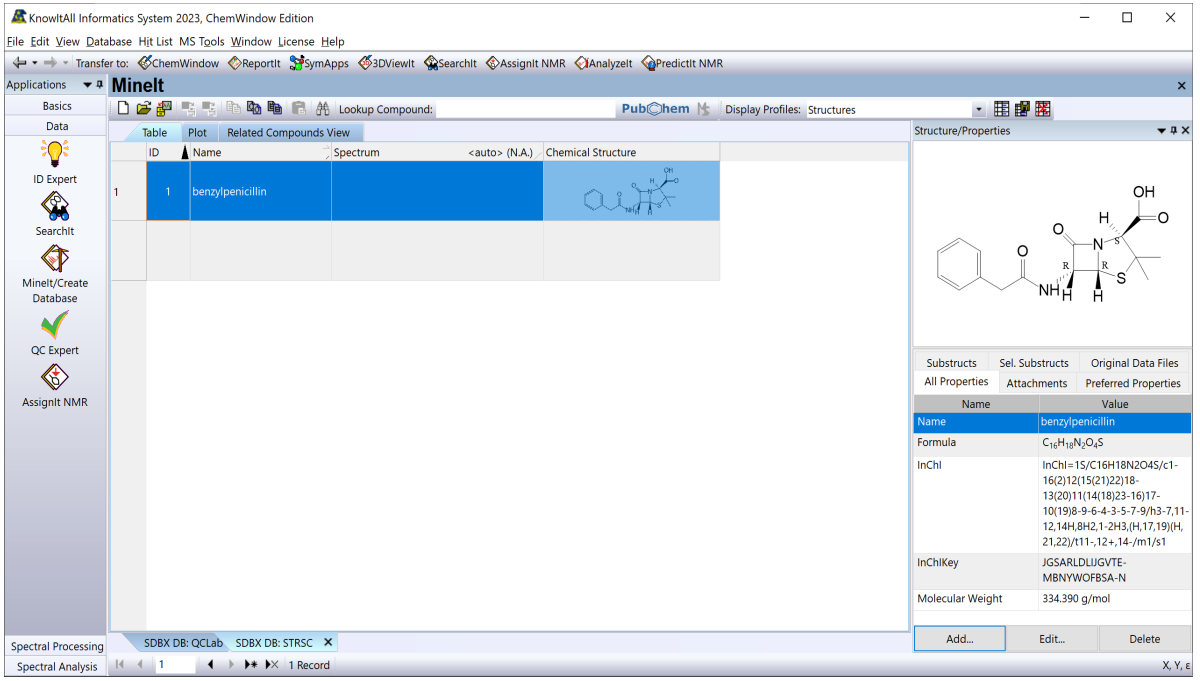
	Action	Result
5	Type ‘STRSC’ in the **Database Abbreviation** text box. **Note**: The abbreviation must be 3-7 characters long.	
6	Click **OK**.	The new database has been created to receive your data. The Database Abbreviation appears on the database tab. 
7	Choose **View > Windows/Tables > Spectrum 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
8	Click the **Add a New Profile** toolbar button  , type the name ‘Structures’ in the **New Profile** dialog box, then click **OK**.	

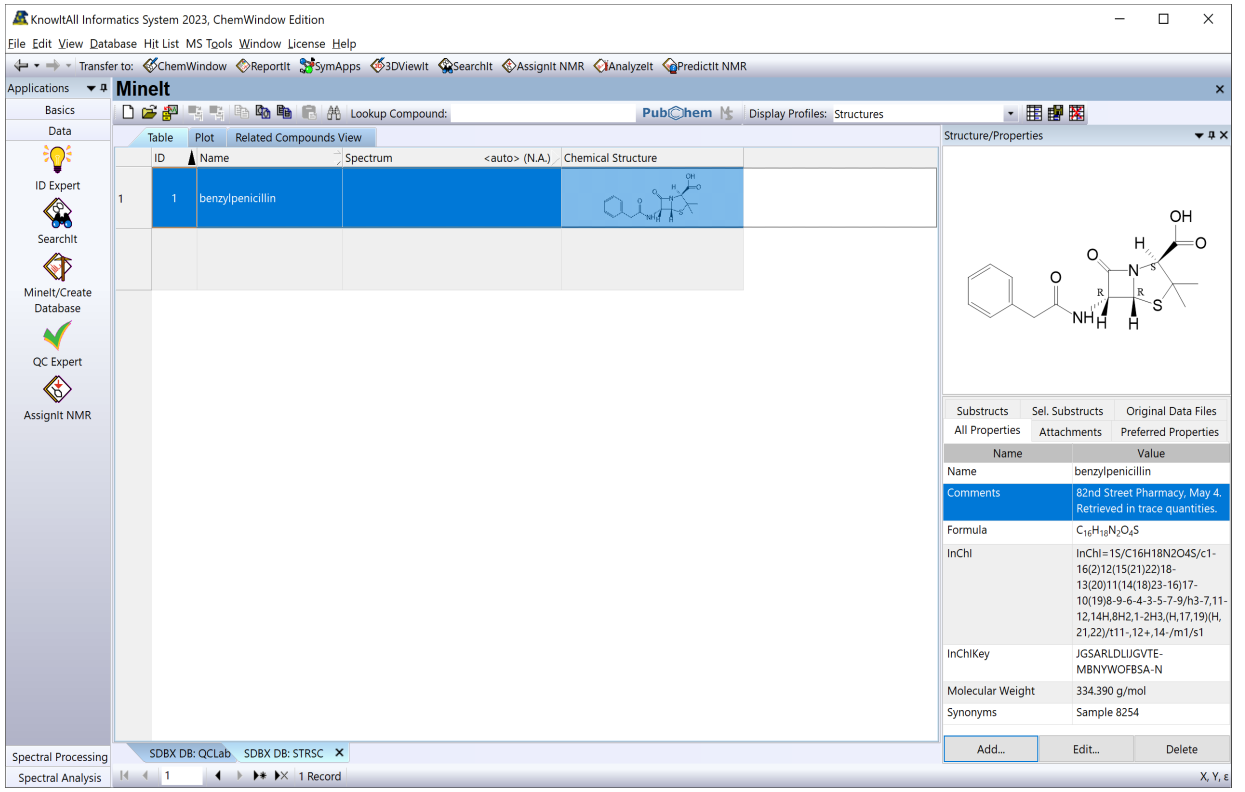
Add a structure to the first database record

	Action	Result
1	Choose **File > Import** Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Structures folder 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.

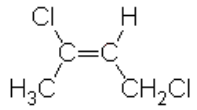
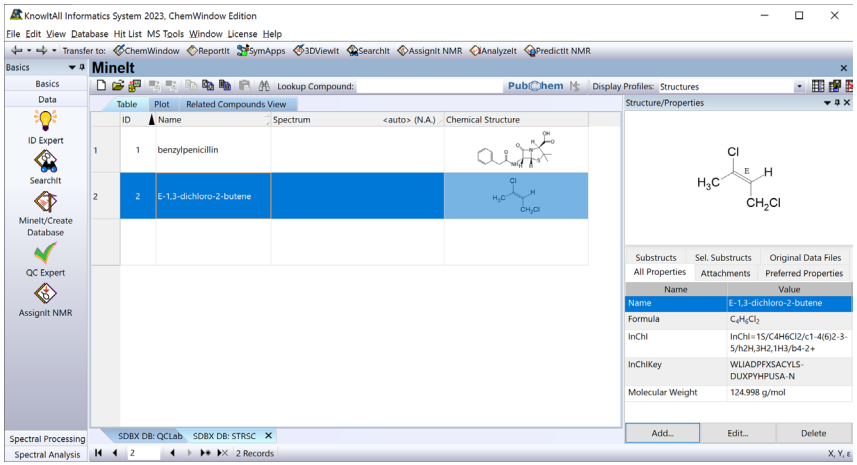
Add properties to a database record

	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. 

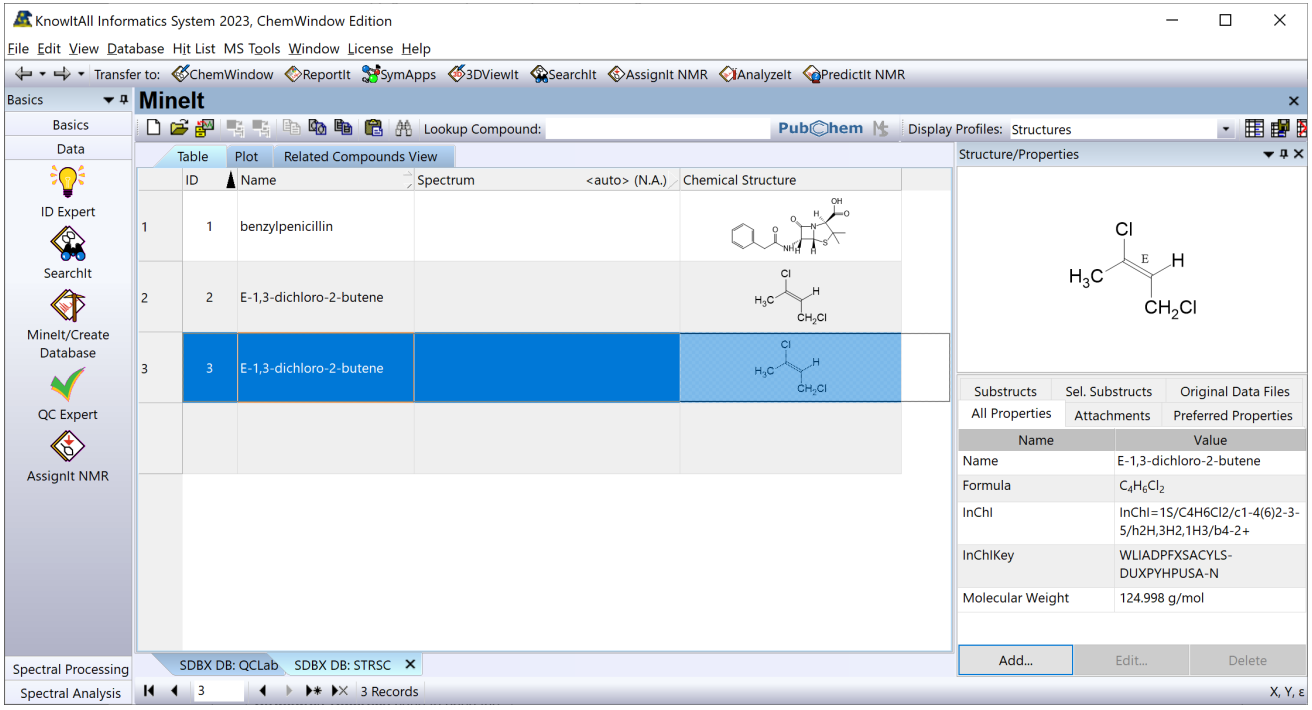
WILEY

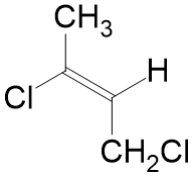
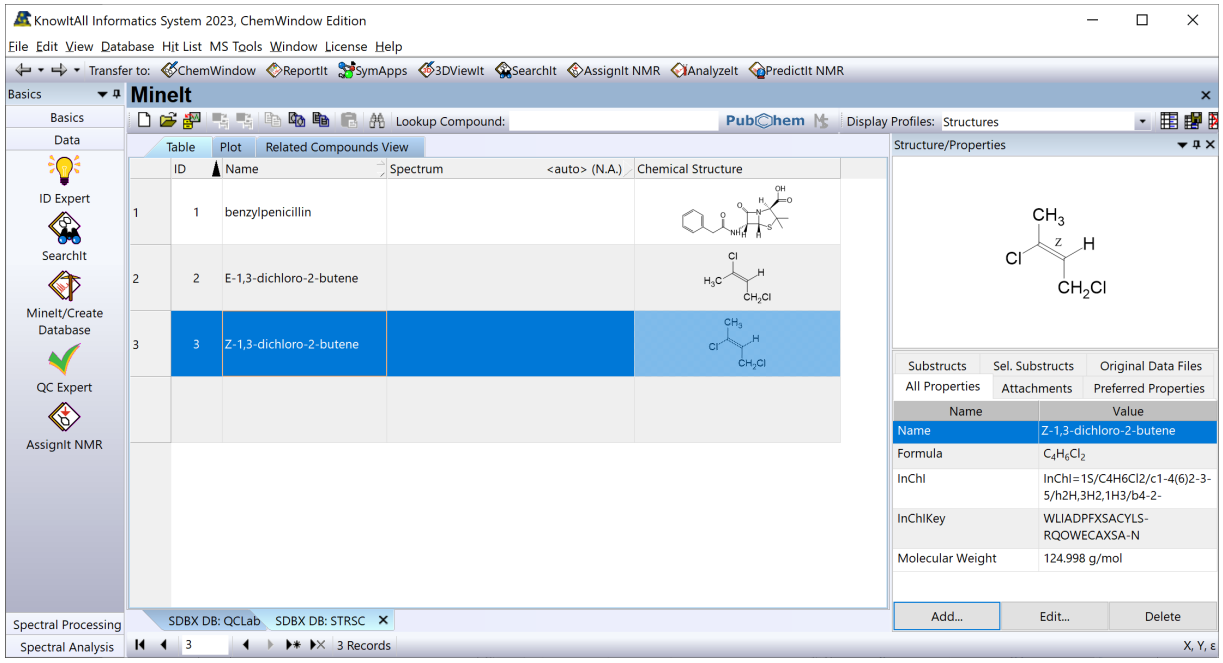
	Action	Result
4	Repeat to add the property **Synonyms** with the value 'Sample 8254.'	
5	Repeat to add the property **Comments** with the value '82nd Street Pharmacy, May 4. Retrieved in trace quantities.'	

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. ChemWindow is closed and we are back to the **MineIt** window.
5	Edit the property **Name** to 'Z-1,3-dichloro-2-butene.'	

Create Databases

How to Build User Databases Using GC-MS Data

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 filter GC-MS scans
- How to add spectra to a user database
- How to add structures to a user database

Background

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

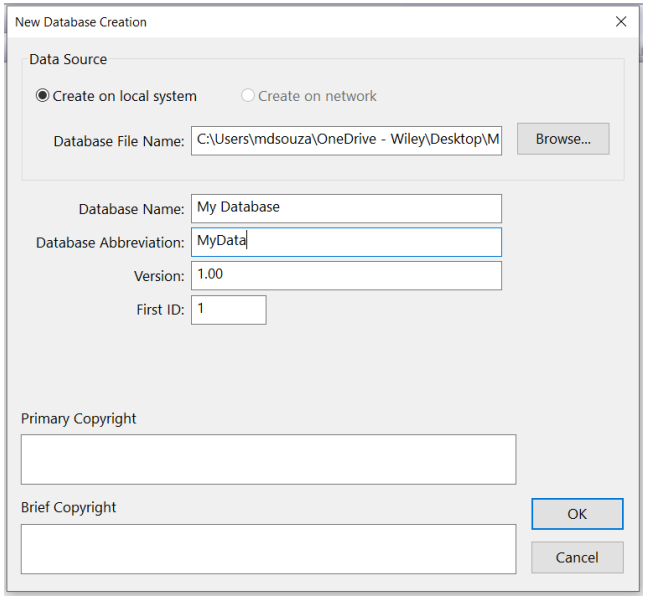
Training Files Used in This Lesson

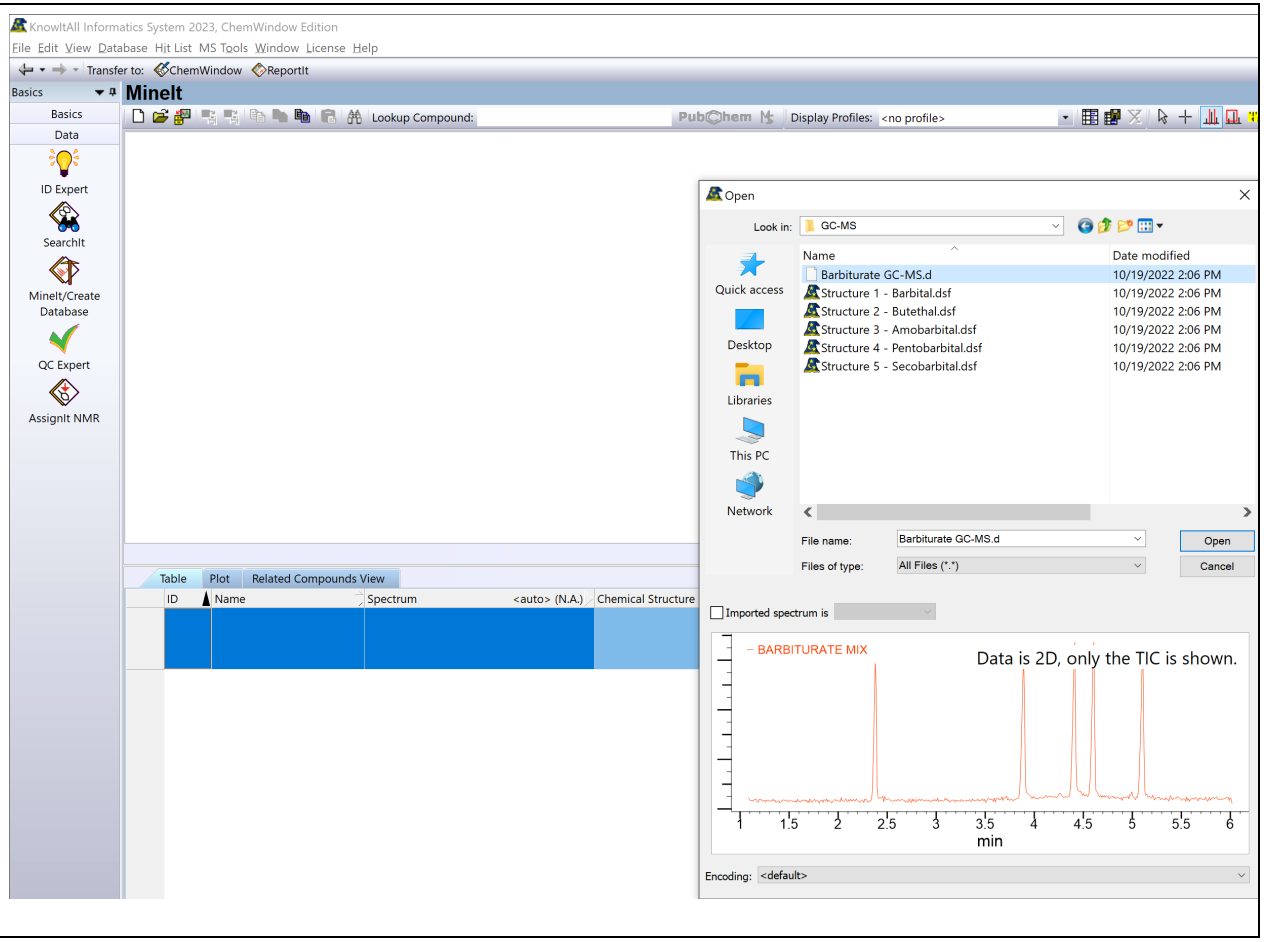
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\GC-MS folder

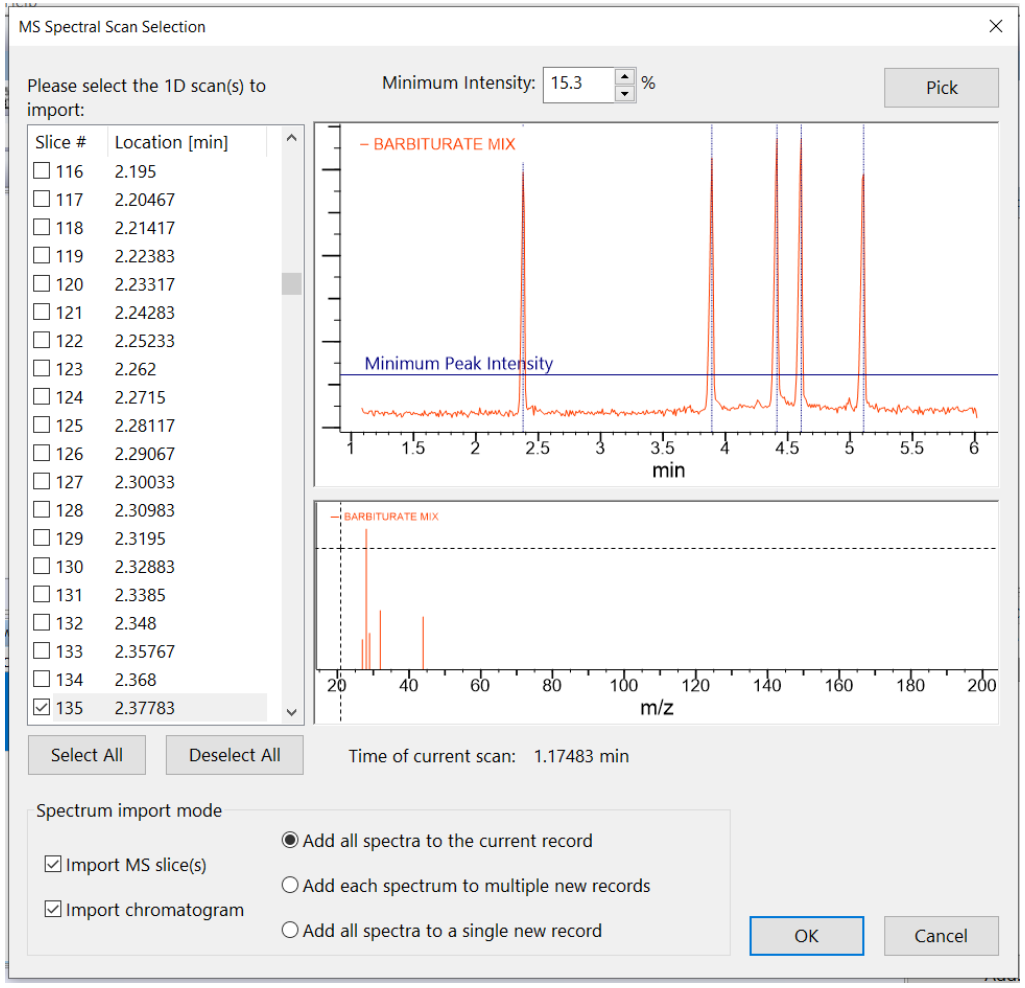
KnowItAll Applications Used

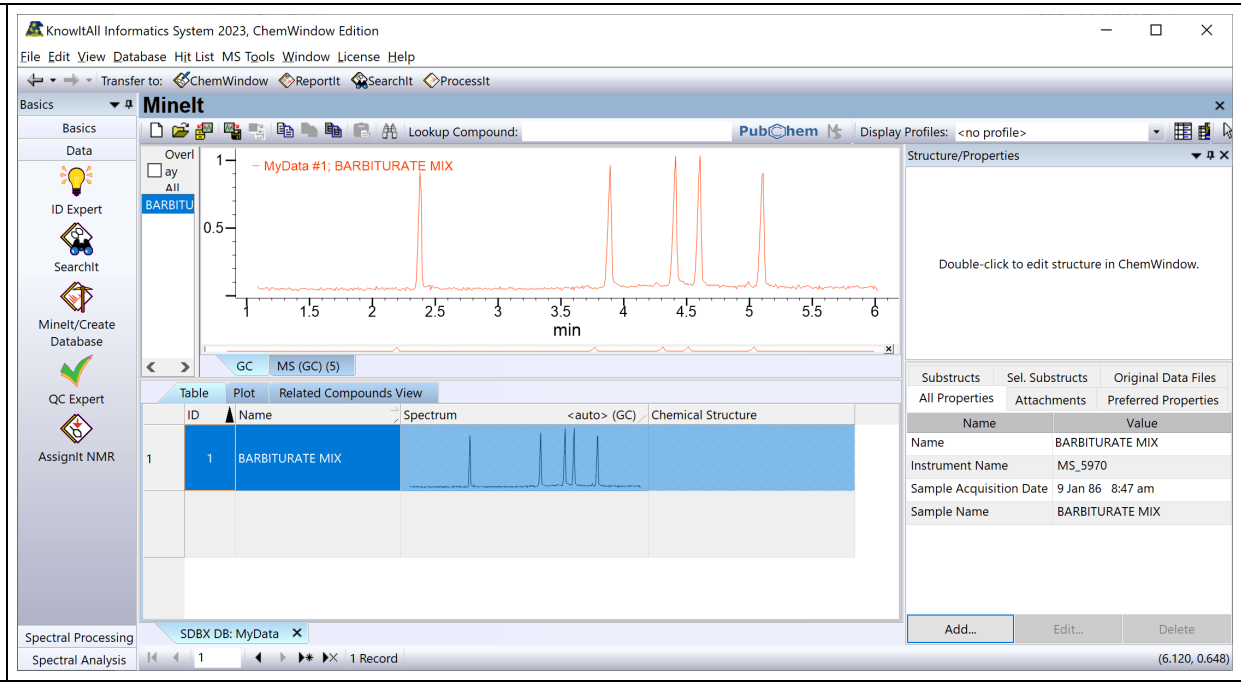
- MineIt™
- ChemWindow®
- BrowseIt™

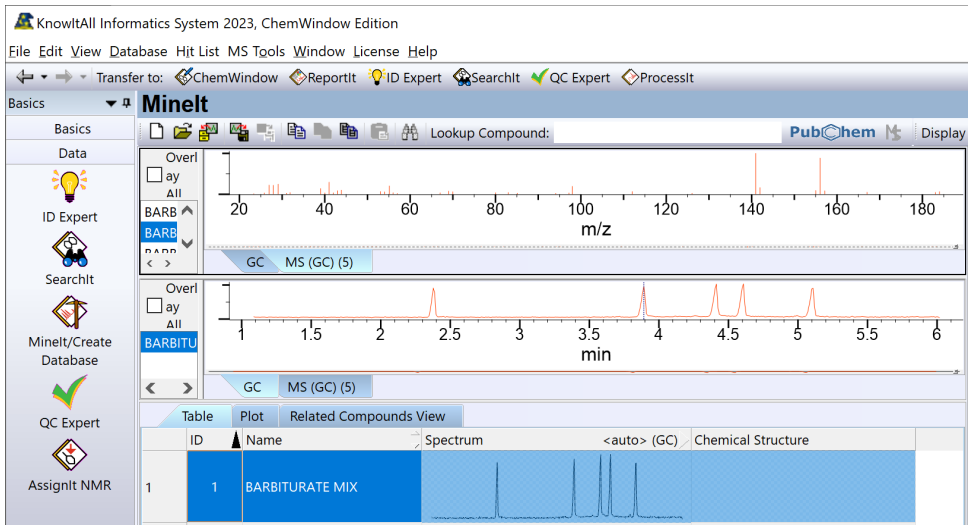
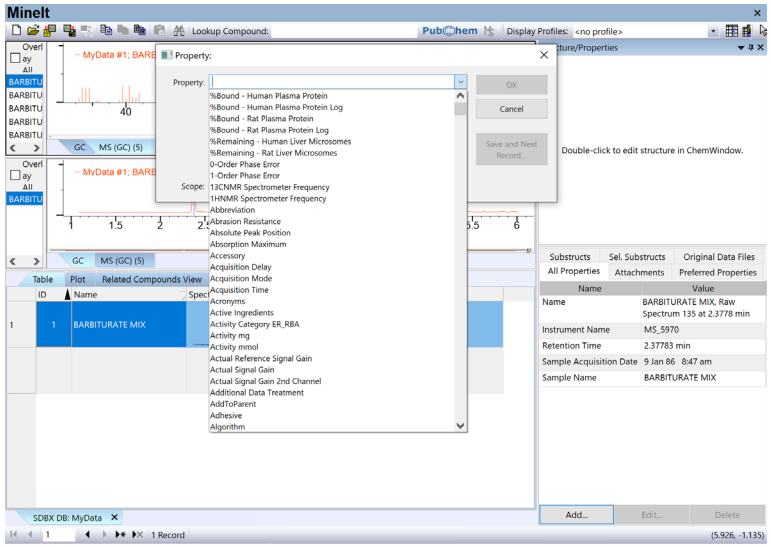
GC-MS Record Creation

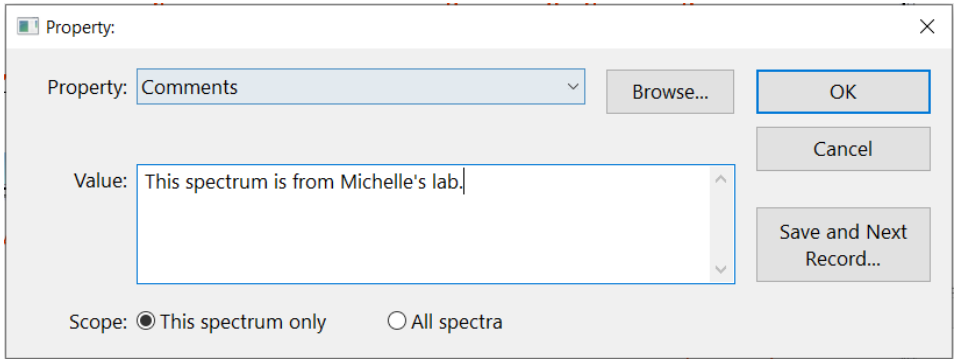
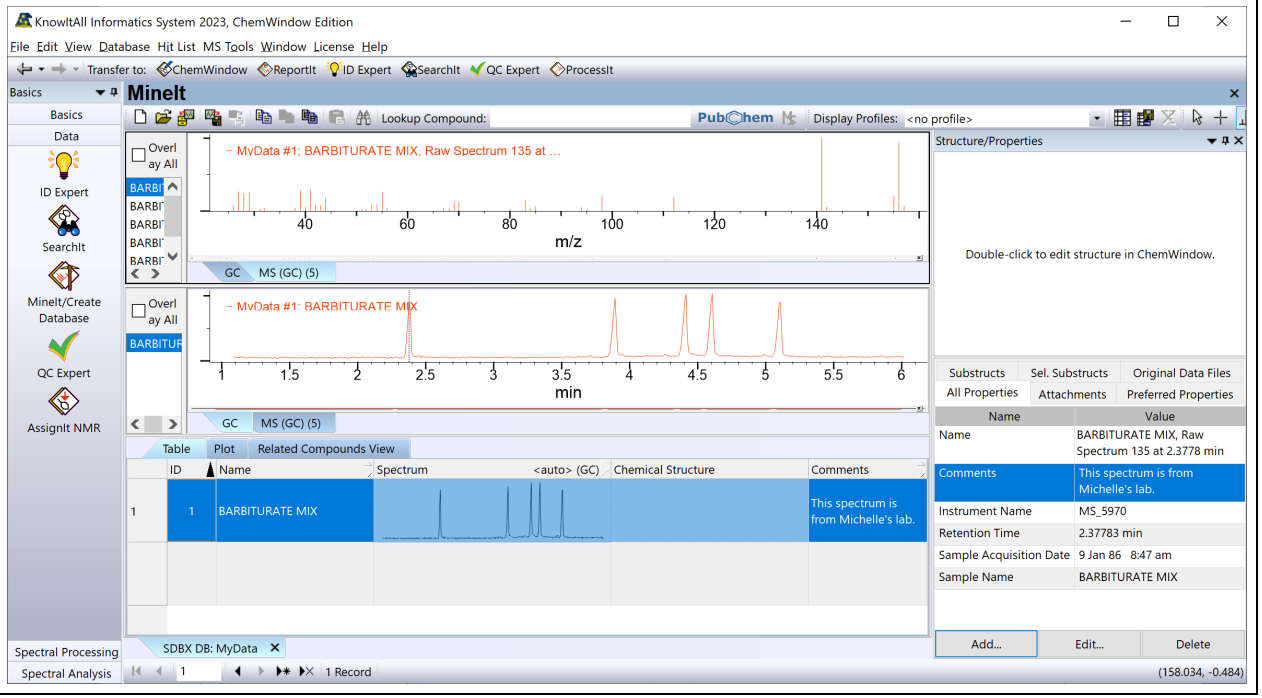
	Action	Result
1	Start **KnowItAll.** Click the **MineIt** icon. Select **Database > New**. Use **Browse** to set the hardware location for the database. Enter a tag (“MyData” etc). Click **OK**.	

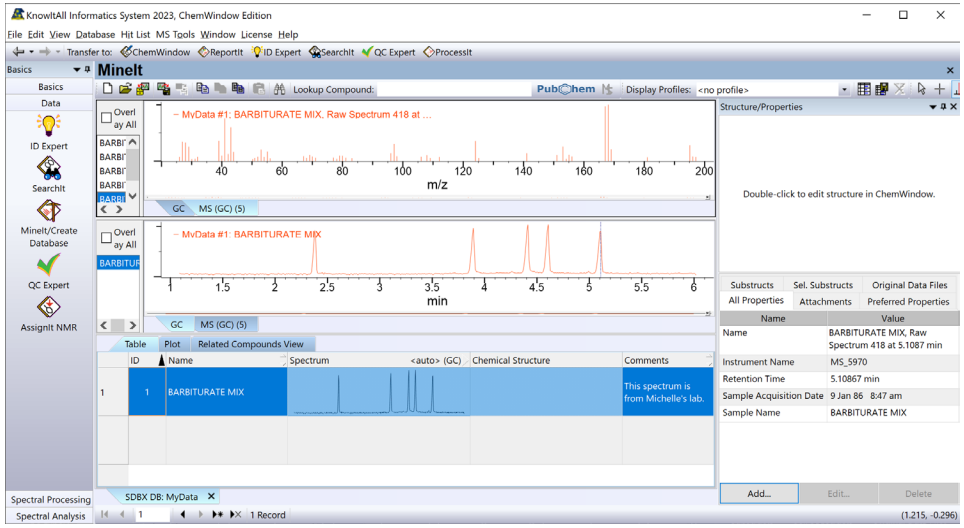
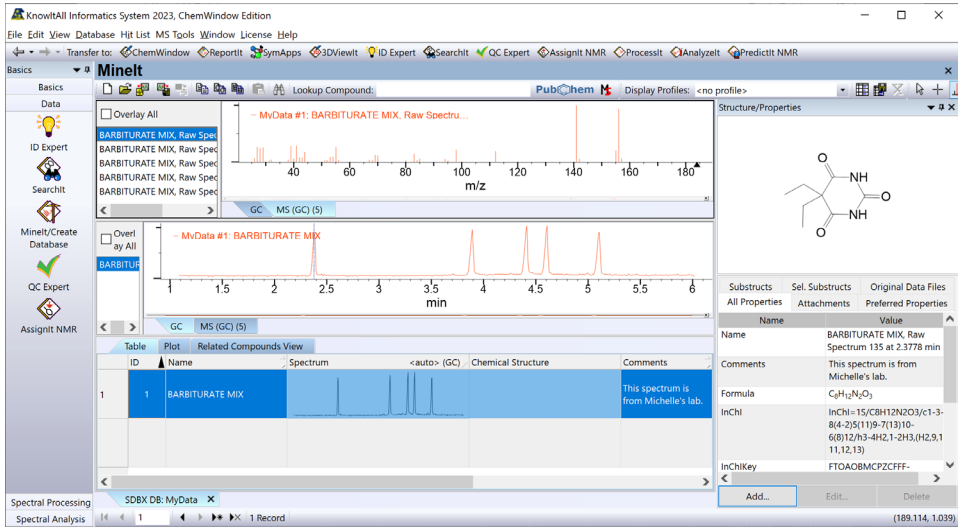
2	From the **File** menu, select **Import**. In the dialog prompt, navigate to Samples > GC-MS. Select the file **Barbiturate GC-MS.d**. Click **Open**.	

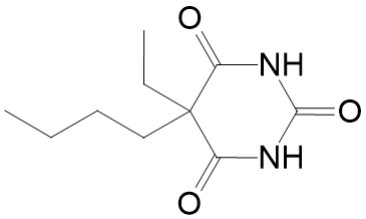
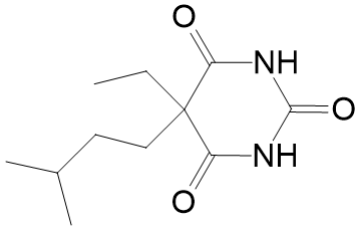
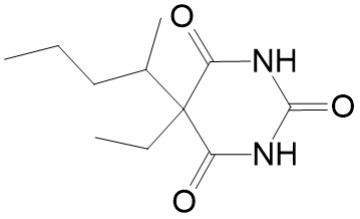
3	Select a threshold above 10% and click **Pick**. Select **Add all spectra to the current record.** Click **OK**.	

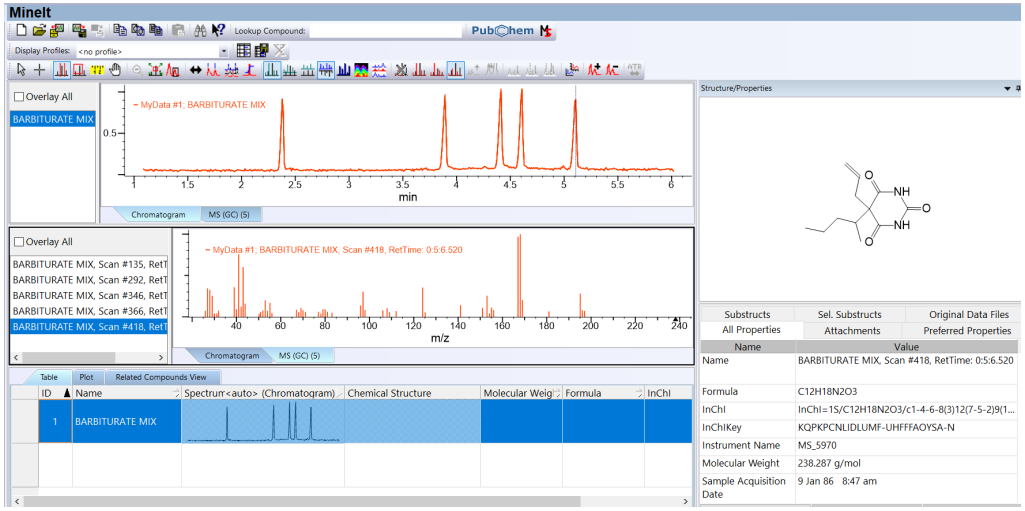
4		

5	Navigate to **Window > Split twofold**. Select **MS** to be the technique showing in the top pane and **GC** to show in bottom pane. Mouse over GC scan pane. **Right-click,** make sure mouse is in **Selection** mode. Click through GC peaks to show MS pane changing.	
6	Click the MS spectrum pane to make it selected (black bordered). Highlight the first scan (make sure it has the black border). Click the **Add button**.	

7	In the pop-up window, use the **Property** dropdown list to select a field. For example, **Comments**. Type in a value. Choose **This spectrum only**.	
8		

9	Select other MS spectrum.	
10	For MS 135, highlight the it. **File > Import**. Navigate to **C:\Users\Public\Documents\Wiley\KnowItAll\Samples\GC-MS** folder Select **Structure 1 – Barbital**. Click **Open**.	

11	For MS 292, highlight the it. **File > Import**. Select **Structure 2 – Butethal**. Click **Open**.	
12	For MS 346, highlight the it. **File > Import**. Select **Structure 3 – Amobarbital**. Click **Open**.	
13	For MS 366, highlight the it. **File > Import**. Select **Structure 4 – Pentaobarbital**. Click **Open**.	

14	For MS 418, highlight the it. **File > Import**. Select **Structure 5 – Secobarbital.** Click **Open**. Navigate MS records to see the difference.	
15	If MS Interpreter is installed: When a user database record has both MS spectrum and structure, the Transfer to MS Interpreter button is active.