

# **KnowItAll Software Training**

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## Creating Databases

# Create Databases

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## How to Build Your Own User Databases of Multiple Analytical Techniques

### Purpose

This exercise demonstrates how to use KnowItAll's Minelt 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.

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### 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 Minelt display profile

### Background

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

#### ***Training Files Used in This Lesson***

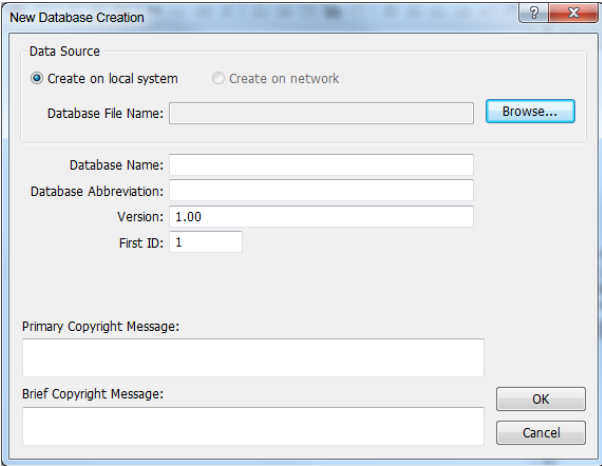
C:\Users\Public\Documents\Wiley\KnowItAll\Samples

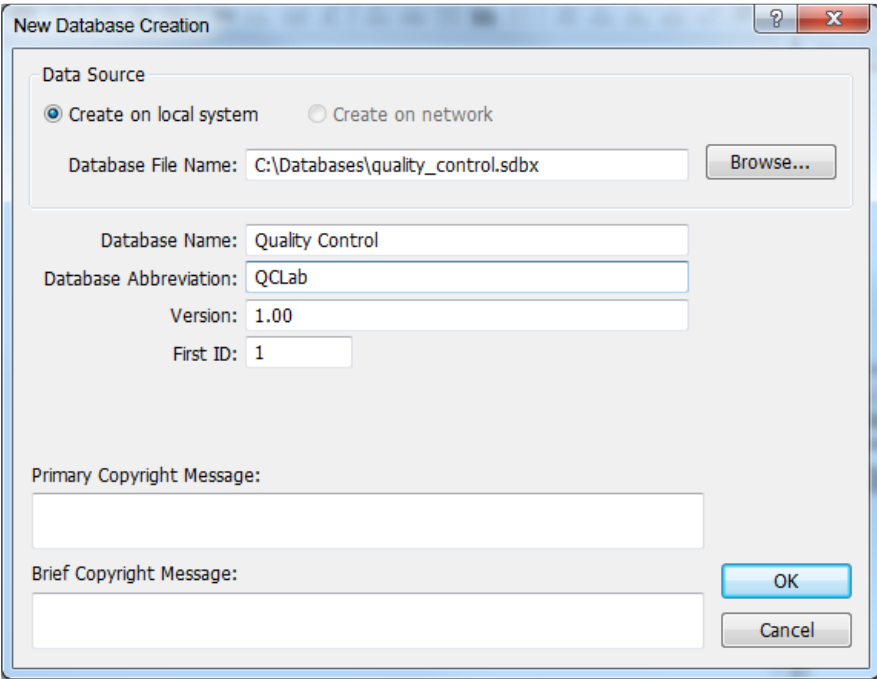
- \IR\Ethyl acetate.dx
- \Raman\Ethyl acetate.irf
- \Minelt\Import.csv
- MSDS Web Link.txt
- Ethyl acetate MSDS.pdf

#### ***KnowItAll Applications Used***

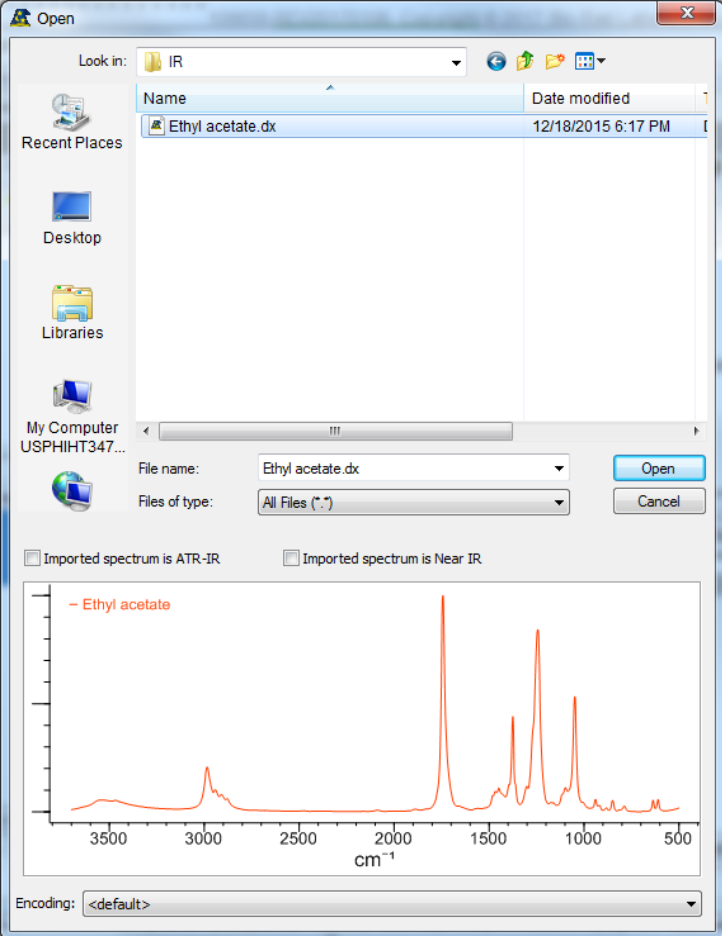
- Minelt
- ChemWindow®
- Browselt

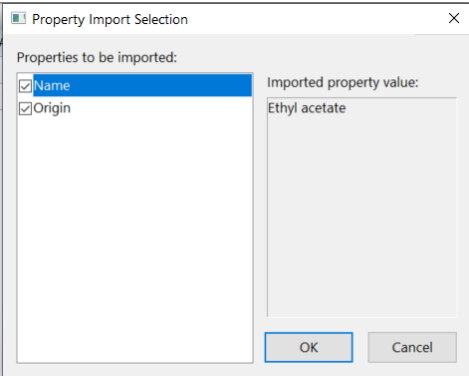
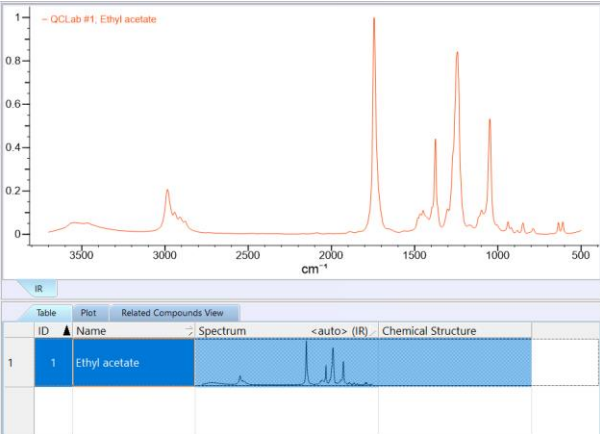
### Create a user database

	Action	Result
1	Navigate to the <b>Data</b> toolbox and open the <b>Minelt</b> application by clicking the <b>Minelt/Create Database</b> icon.	The <b>Minelt</b> application opens.
2	Choose <b>Database &gt; New</b> .	<p>The <b>New Database Creation</b> dialog box opens.</p> 
3	Select <b>Create on local system</b> .	
4	<p>Click <b>Browse</b>.</p> <p>Create a folder named <b>Databases</b> on a local drive.</p> <p>Open the folder, then type in the file name <b>quality_control</b>.</p> <p>Click <b>Save</b>.</p>	<p>The *.sdbx extension is added automatically.</p> <p>The new database is saved locally.</p> <p><b>Note:</b> 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.</p>
5	<p>Type <b>Quality Control</b> in the <b>Database Name</b> text box.</p> <p><b>Note:</b> The file name is used if no other name is specified.</p>	

	Action	Result
6	Type <b>QCLab</b> in the <b>Database Abbreviation</b> text box. <b>Note:</b> The abbreviation must be 3-7 characters long.	
7	Enter <b>Version</b> number and the <b>First (starting) ID</b> , and type in copyright messages.	
8	Click <b>OK</b> .	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).

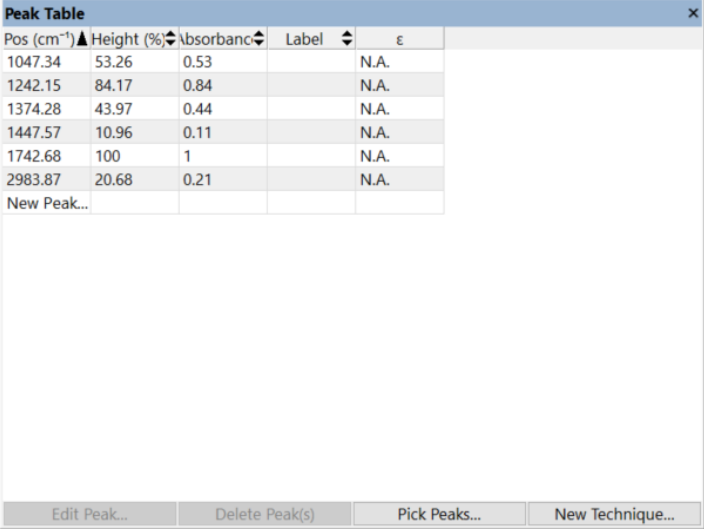
## Add the first spectrum record to the user database

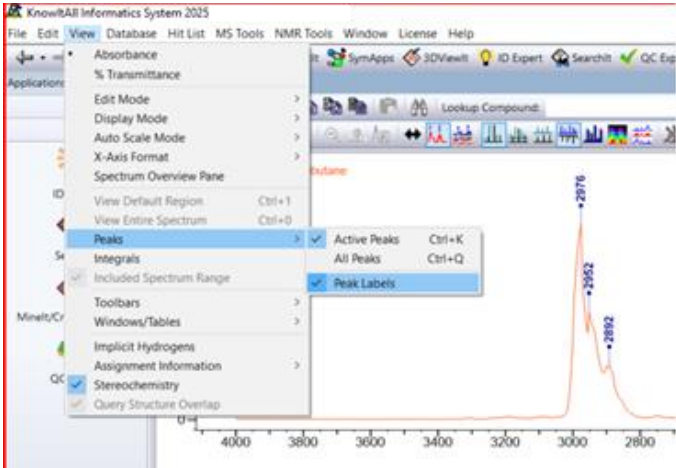
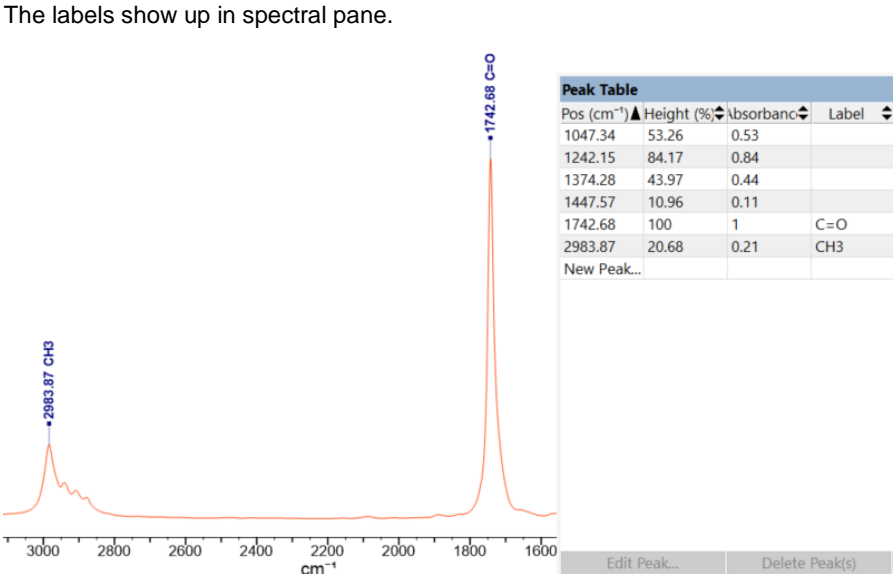
	Action	Result
1	<p>Create the first database record by importing a spectrum:</p> <ul style="list-style-type: none"><li>Choose <b>File &gt; Import</b> or press Ctrl+I.</li><li>Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\IR folder</li><li>Open <b>Ethyl acetate.dx</b>.</li></ul> <p><b>Note:</b> Use the <b>Files of type</b> filter to locate IRF, JCAMP and many other specific spectral files.</p>	<p>A Windows <b>Open</b> dialog box appears.</p>  <p>The screenshot shows a Windows 'Open' dialog box with the following details:</p> <ul style="list-style-type: none"><li><b>Look in:</b> IR</li><li><b>Name:</b> Ethyl acetate.dx</li><li><b>Date modified:</b> 12/18/2015 6:17 PM</li><li><b>File name:</b> Ethyl acetate.dx</li><li><b>Files of type:</b> All Files (*.*)</li><li><b>Encoding:</b> &lt;default&gt;</li><li><b>Options:</b> <input type="checkbox"/> Imported spectrum is ATR-IR, <input type="checkbox"/> Imported spectrum is Near IR</li><li><b>Spectrum Plot:</b> Shows an IR spectrum for Ethyl acetate with a y-axis for intensity and an x-axis for wavenumber (cm<sup>-1</sup>) ranging from 3500 to 500. The plot shows several characteristic absorption bands, including a sharp peak around 1735 cm<sup>-1</sup> and a strong, broad peak around 1100 cm<sup>-1</sup>.</li></ul>

	Action	Result
2	Click <b>Open</b> .	<p>The <b>Property Import Selection</b> dialog box opens.</p>  <p>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.</p>
3	Click <b>OK</b> .	<p>The dialog box closes. The spectrum has been added to the user database as the first record.</p> 

## Add spectrum labels

KnowItAll 2025 release has a new feature – users can add customized peak labels.

	Action	Result																																								
1	Continue with the above example Choose <b>View &gt; Windows/Tables &gt; Peak Table</b> to open the spectrum peak table	<p><b>Peak Table</b> pops up in a window</p>  <table border="1"><thead><tr><th>Pos (cm<sup>-1</sup>)</th><th>Height (%)</th><th>Absorbance</th><th>Label</th><th>ε</th></tr></thead><tbody><tr><td>1047.34</td><td>53.26</td><td>0.53</td><td></td><td>N.A.</td></tr><tr><td>1242.15</td><td>84.17</td><td>0.84</td><td></td><td>N.A.</td></tr><tr><td>1374.28</td><td>43.97</td><td>0.44</td><td></td><td>N.A.</td></tr><tr><td>1447.57</td><td>10.96</td><td>0.11</td><td></td><td>N.A.</td></tr><tr><td>1742.68</td><td>100</td><td>1</td><td></td><td>N.A.</td></tr><tr><td>2983.87</td><td>20.68</td><td>0.21</td><td></td><td>N.A.</td></tr><tr><td colspan="5">New Peak...</td></tr></tbody></table>	Pos (cm <sup>-1</sup> )	Height (%)	Absorbance	Label	ε	1047.34	53.26	0.53		N.A.	1242.15	84.17	0.84		N.A.	1374.28	43.97	0.44		N.A.	1447.57	10.96	0.11		N.A.	1742.68	100	1		N.A.	2983.87	20.68	0.21		N.A.	New Peak...				
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2	<p><b>TIP:</b> To ensure Peak Labels are visible in the spectrum, perform the following step:</p> <p>Choose <b>View &gt; Peaks &gt; Peak Labels</b> and make sure Peak Labels is selected.</p>	 <p>The screenshot shows the 'View' menu with 'Peaks' selected, and a sub-menu where 'Peak Labels' is checked. The background spectrum shows three peaks labeled with their wavenumbers: 2983.87, 2952, and 2892.</p>																																
3	<p>One can directly type textual values into the Label column.</p>	<p>The labels show up in spectral pane.</p>  <p>The screenshot shows a zoomed-in view of the spectrum with two peaks labeled: 2983.87 CH3 and 1742.68 C=O. To the right, a 'Peak Table' is displayed with the following data:</p> <table border="1" data-bbox="1264 922 1596 1123"> <thead> <tr> <th>Pos (cm<sup>-1</sup>)</th> <th>Height (%)</th> <th>Absorbance</th> <th>Label</th> </tr> </thead> <tbody> <tr> <td>1047.34</td> <td>53.26</td> <td>0.53</td> <td></td> </tr> <tr> <td>1242.15</td> <td>84.17</td> <td>0.84</td> <td></td> </tr> <tr> <td>1374.28</td> <td>43.97</td> <td>0.44</td> <td></td> </tr> <tr> <td>1447.57</td> <td>10.96</td> <td>0.11</td> <td></td> </tr> <tr> <td>1742.68</td> <td>100</td> <td>1</td> <td>C=O</td> </tr> <tr> <td>2983.87</td> <td>20.68</td> <td>0.21</td> <td>CH3</td> </tr> <tr> <td colspan="4">New Peak...</td> </tr> </tbody> </table> <p>Buttons for 'Edit Peak...' and 'Delete Peak(s)' are visible at the bottom of the table.</p>	Pos (cm <sup>-1</sup> )	Height (%)	Absorbance	Label	1047.34	53.26	0.53		1242.15	84.17	0.84		1374.28	43.97	0.44		1447.57	10.96	0.11		1742.68	100	1	C=O	2983.87	20.68	0.21	CH3	New Peak...			
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4 Select **Transfer to:** ReportIt

Transfer to:

 ChemWindow
 ReportIt

Choose the **Landscape** report template

Click **OK**

Select a Report Template
✕

Please select one of these templates:

Title	File Path
Landscape	C:\Users\Public\Documents\...
Minelt	C:\Users\Public\Documents\...
Minelt_A4	C:\Users\Public\Documents\...
Mixture Analysis Portrait	C:\Users\Public\Documents\...
Portrait	C:\Users\Public\Documents\...
Spectrum Landscape	C:\Users\Public\Documents\...
Spectrum Portrait	C:\Users\Public\Documents\...

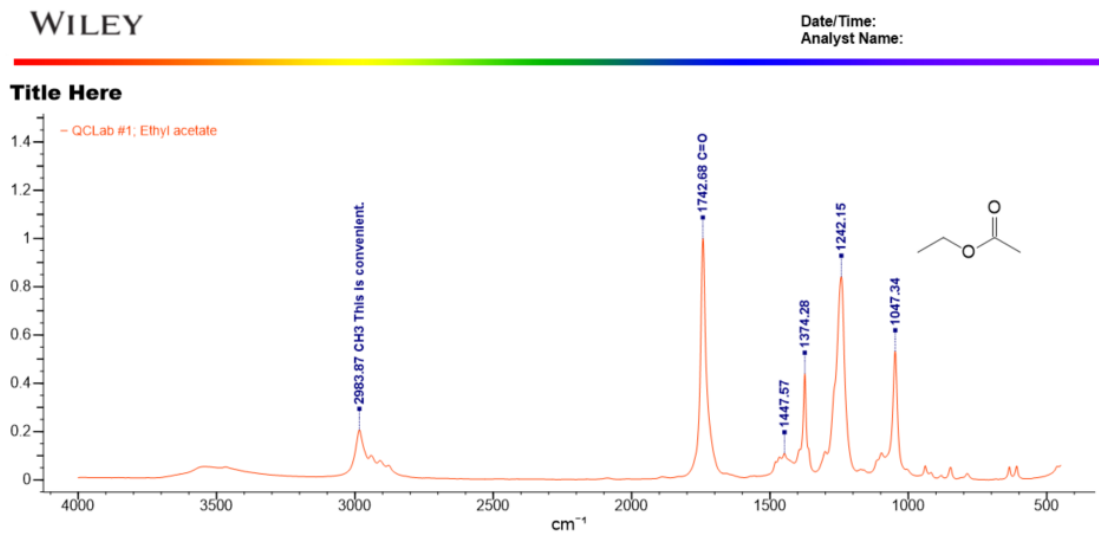
WILEY
DataTime:  
Analysis Name:

**Title Here**

Name	Value
NAME	IR Spectrum
INSTRUMENT	IR Spectrum
POSITION	IR Spectrum
FILE	IR Spectrum
TECHNIQUE	IR Spectrum
ANALYST	IR Spectrum
DATE	IR Spectrum


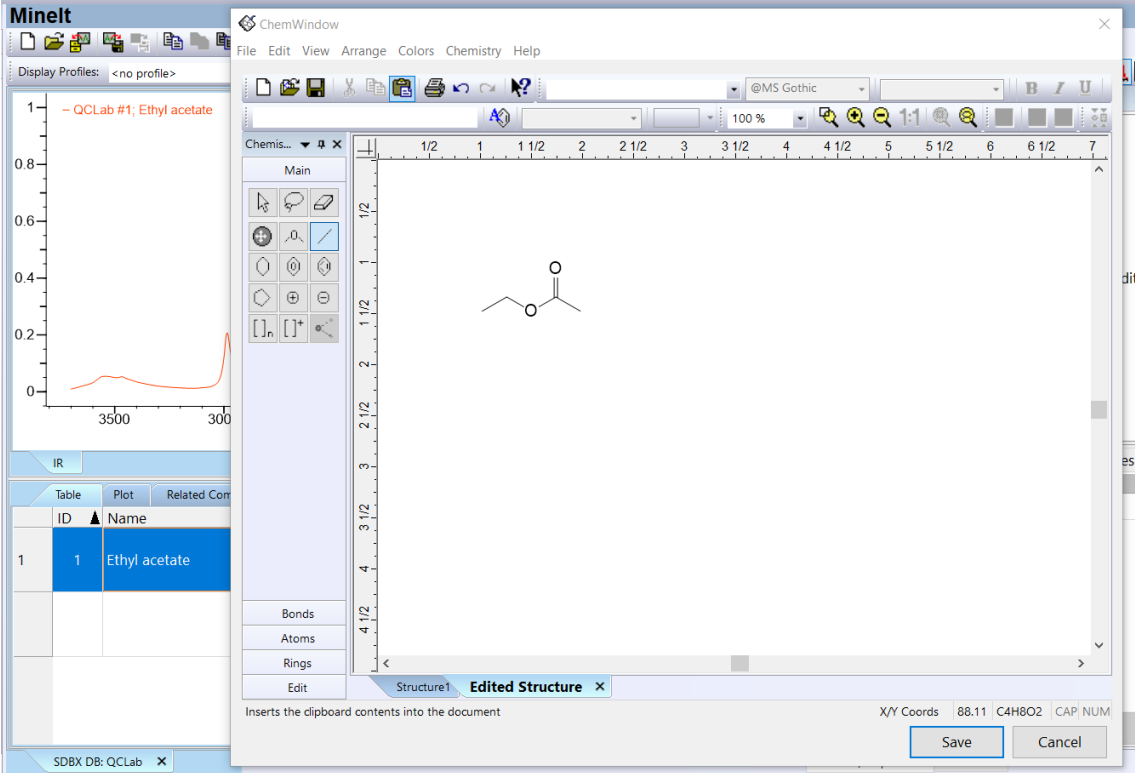
OK
Cancel

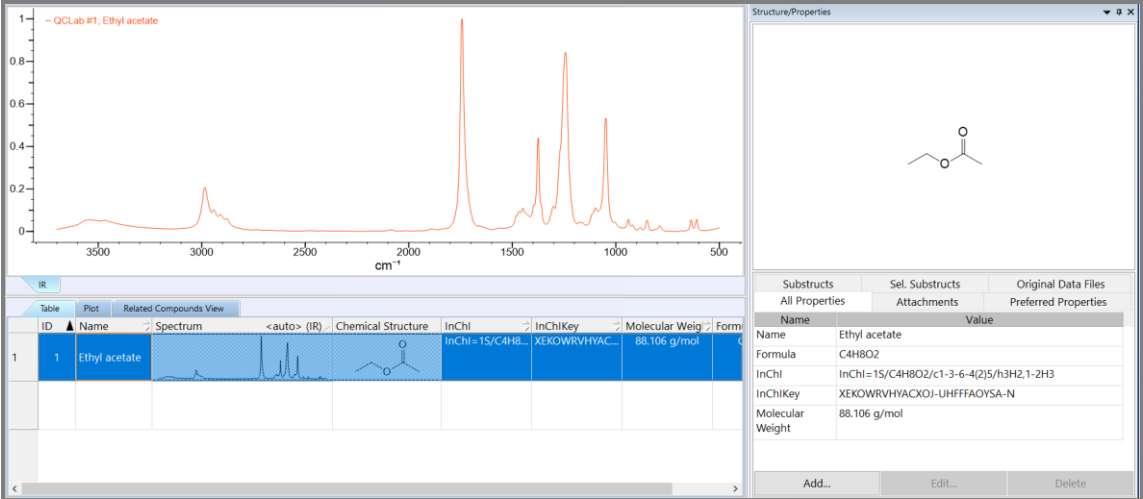
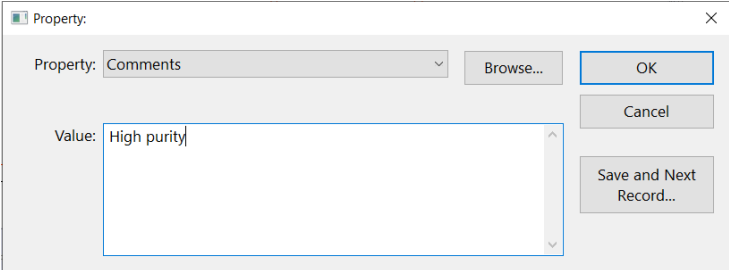
The peak labels are also transferred over:



Name	Value
Name	Ethyl acetate
Comments	High purity
Formula	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>
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

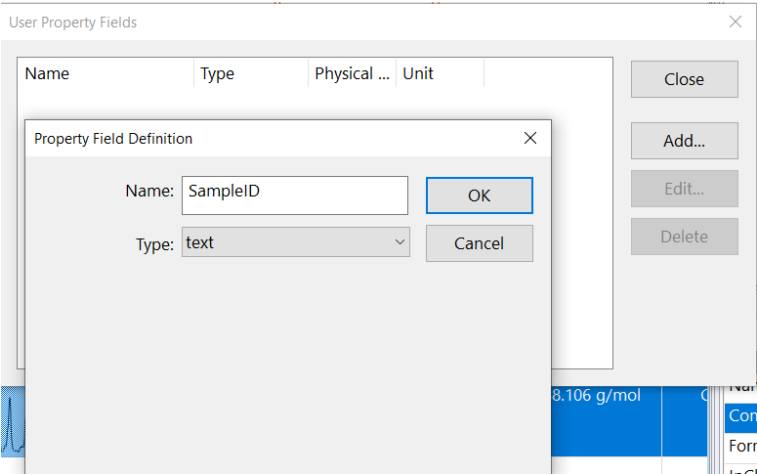
## Add a chemical structure and properties to a database record

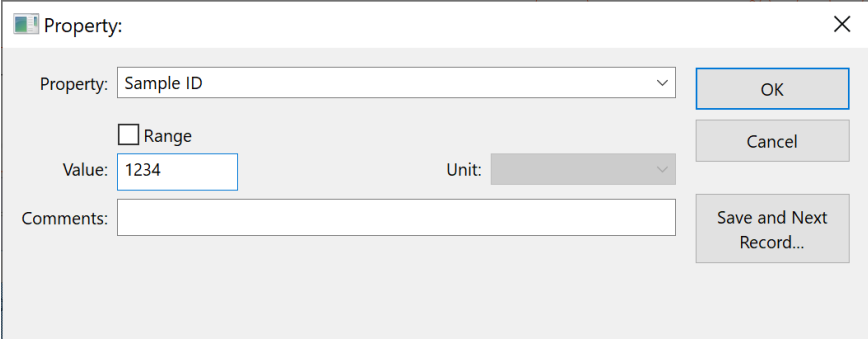
	Action	Result
1	<p>Go back to <b>Minelt</b></p> <p>With the first record selected, double-click the Structure/Properties pane at the top right of the window (<b>Double-click to edit structure in ChemWindow</b>).</p>	<p>The <b>Transfer to ChemWindow</b> application pops up. Alternatively, you can use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

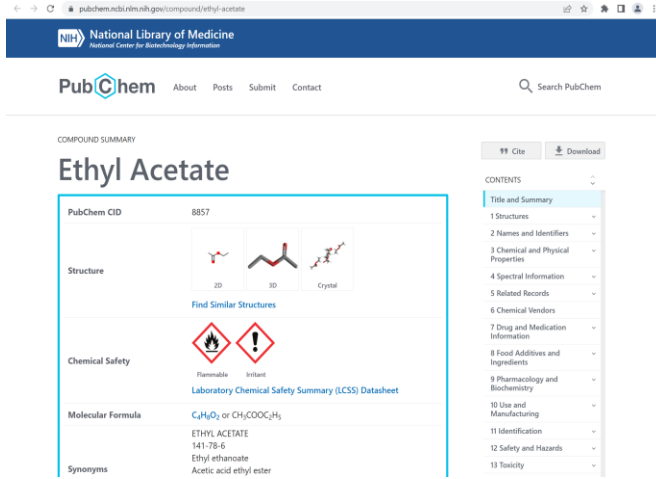
	Action	Result
3	Click <b>Save</b> .	<p>The structure is added to the first record and is displayed both in the <b>Chemical Structure</b> column in the <b>Database</b> pane and the <b>Structure/Properties</b> pane.</p>  <p><b>Note:</b> Some chemical properties such as InChI, InChIKey, Molecular Weight,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

	Action	Result														
6	Click <b>OK</b> .	<p>The <b>Property</b> dialog box closes, and the name and value of the added property appears in the <b>Structure/Properties</b> pane.</p> <table border="1" data-bbox="701 440 1394 808"> <thead> <tr> <th data-bbox="701 513 856 542">Name</th> <th data-bbox="856 513 1394 542">Value</th> </tr> </thead> <tbody> <tr> <td data-bbox="701 542 856 571">Name</td> <td data-bbox="856 542 1394 571">Ethyl acetate</td> </tr> <tr> <td data-bbox="701 571 856 600">Comments</td> <td data-bbox="856 571 1394 600">High purity</td> </tr> <tr> <td data-bbox="701 600 856 630">Formula</td> <td data-bbox="856 600 1394 630">C4H8O2</td> </tr> <tr> <td data-bbox="701 630 856 659">InChI</td> <td data-bbox="856 630 1394 659">InChI=1S/C4H8O2/c1-3-6-4(2)5/h3H2,1-2H3</td> </tr> <tr> <td data-bbox="701 659 856 688">InChIKey</td> <td data-bbox="856 659 1394 688">XEKOWRVHYACXOJ-UHFFFAOYSA-N</td> </tr> <tr> <td data-bbox="701 688 856 789">Molecular Weight</td> <td data-bbox="856 688 1394 789">88.106 g/mol</td> </tr> </tbody> </table>	Name	Value	Name	Ethyl acetate	Comments	High purity	Formula	C4H8O2	InChI	InChI=1S/C4H8O2/c1-3-6-4(2)5/h3H2,1-2H3	InChIKey	XEKOWRVHYACXOJ-UHFFFAOYSA-N	Molecular Weight	88.106 g/mol
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InChIKey	XEKOWRVHYACXOJ-UHFFFAOYSA-N															
Molecular Weight	88.106 g/mol															
	<b>TIP</b>	You can select multiple database records and use the <b>Add</b> or <b>Edit</b> button at the bottom of the <b>Structure/Properties</b> pane to input the same value for a field.														

## Add user properties

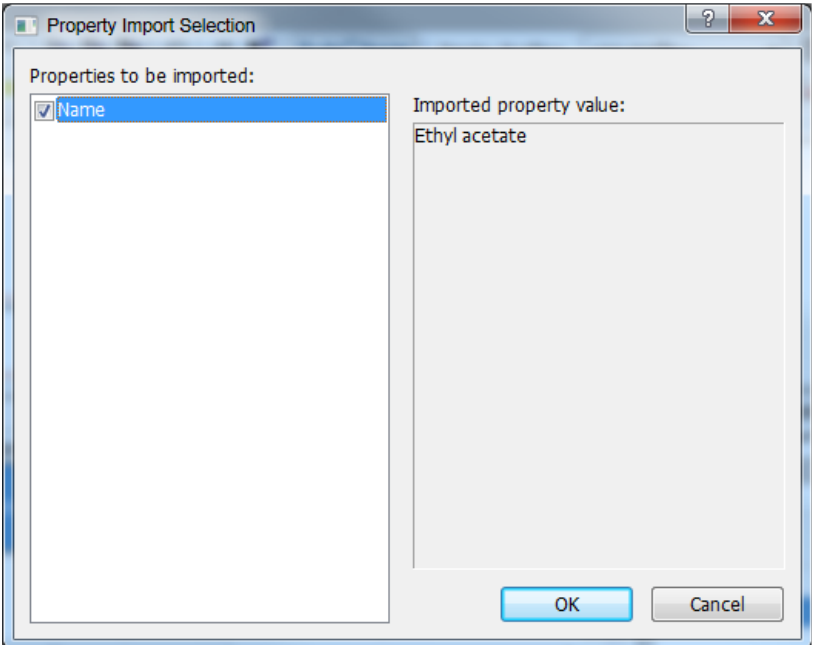
	Action	Result
1	Choose <b>Database &gt; Define User Property Fields</b> .	The <b>User Property Fields</b> dialog box opens.
2	Click <b>Add</b> .  Use the drop-down list to set <b>Type</b> to text.  Enter the <b>Name</b> .	The <b>Property Field Definition</b> dialog box opens.   <p><b>Note:</b> Which controls are available depends on which type of field is specified: numeric, text or enumeration.</p>
3	Click <b>OK</b> . Then click <b>Close</b> .	
4	Click <b>Add</b> in the <b>Structure/Properties</b> pane.	The <b>Property</b> dialog box opens.  <b>Note:</b> Choose <b>View &gt; Windows/Tables &gt; Structure/Properties Table</b> 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 <b>Sample ID</b>	The <b>Value</b> text box is added to the dialog.  <b>Note:</b> Which text boxes are added depends on whether the property is numeric, text or enumeration.

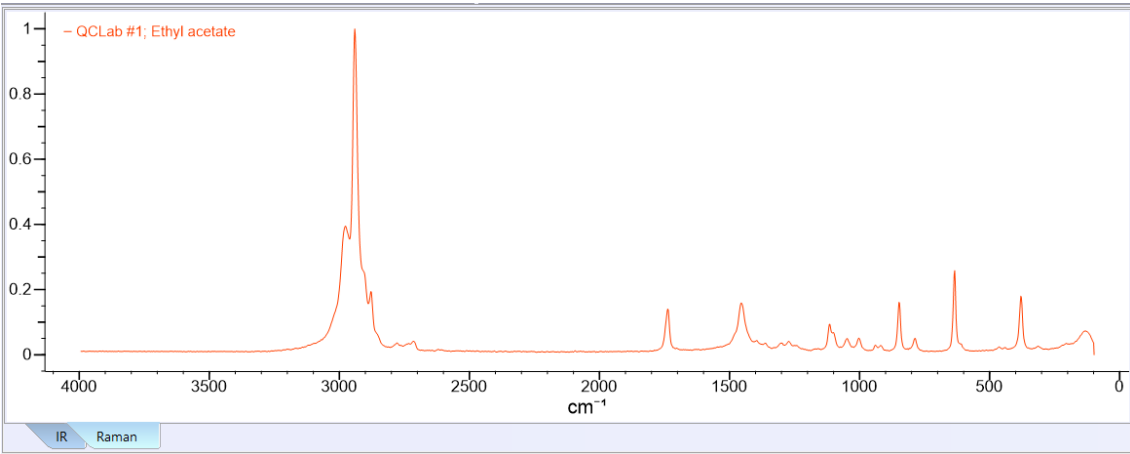
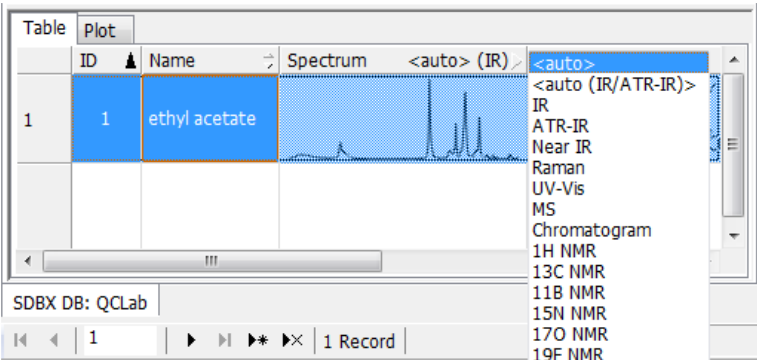
7	Type '1234' in the <b>Value</b> text box.																																																													
8	Click <b>OK</b> .	<p>The dialog box closes. The property <b>SampleID</b> with value 1234 is added to the <b>Structure/Properties</b> pane for the first record.</p> <table border="1" data-bbox="699 732 1226 1227"><thead><tr><th colspan="2">Substructs</th><th colspan="2">Sel. Substructs</th><th colspan="2">Original Data Files</th></tr><tr><th colspan="2">All Properties</th><th colspan="2">Attachments</th><th colspan="2">Preferred Properties</th></tr><tr><th colspan="2">Name</th><th colspan="4">Value</th></tr></thead><tbody><tr><td colspan="2">Name</td><td colspan="4">Ethyl acetate</td></tr><tr><td colspan="2">Comments</td><td colspan="4">High purity</td></tr><tr><td colspan="2">Formula</td><td colspan="4">C<sub>4</sub>H<sub>8</sub>O<sub>2</sub></td></tr><tr><td colspan="2">InChI</td><td colspan="4">InChI=1S/C4H8O2/c1-3-6-4(2)5/h3H2,1-2H3</td></tr><tr><td colspan="2">InChIKey</td><td colspan="4">XEKOWRVHYACXOJ-UHFFFAOYSA-N</td></tr><tr><td colspan="2">Molecular Weight</td><td colspan="4">88.106 g/mol</td></tr><tr><td colspan="2">Sample ID</td><td colspan="4">1234</td></tr></tbody></table> <p>Buttons: Add... Edit... Delete</p>	Substructs		Sel. Substructs		Original Data Files		All Properties		Attachments		Preferred Properties		Name		Value				Name		Ethyl acetate				Comments		High purity				Formula		C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>				InChI		InChI=1S/C4H8O2/c1-3-6-4(2)5/h3H2,1-2H3				InChIKey		XEKOWRVHYACXOJ-UHFFFAOYSA-N				Molecular Weight		88.106 g/mol				Sample ID		1234			
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	Action	Result																																																																								
9	<p>Repeat steps 1-8 to create the user property <b>WebLink</b> and display it in the <b>Structure/Properties</b> pane.</p> <p>Type 'https://pubchem.ncbi.nlm.nih.gov/compound/ethyl-acetate' in the <b>Property</b> dialog box's <b>Value</b> field.</p>	<p>The property <b>WebLink</b> with a web address is added to the <b>Structure/Properties</b> pane for the first record.</p> <table border="1" data-bbox="695 402 1094 808"> <thead> <tr> <th colspan="2">Substances</th> <th colspan="2">Sel. Substances</th> <th colspan="2">Original Data Files</th> </tr> <tr> <th colspan="2">All Properties</th> <th colspan="2">Attachments</th> <th colspan="2">Preferred Properties</th> </tr> <tr> <th colspan="2">Name</th> <th colspan="2">Value</th> <th colspan="2"></th> </tr> </thead> <tbody> <tr> <td colspan="2">Name</td> <td colspan="2">Ethyl acetate</td> <td colspan="2"></td> </tr> <tr> <td colspan="2">Comments</td> <td colspan="2">High purity</td> <td colspan="2"></td> </tr> <tr> <td colspan="2">Formula</td> <td colspan="2">C<sub>4</sub>H<sub>8</sub>O<sub>2</sub></td> <td colspan="2"></td> </tr> <tr> <td colspan="2">InChI</td> <td colspan="2">InChI=1S/C4H8O2/c1-3-6-4(2)5/h3H2,1-2H3</td> <td colspan="2"></td> </tr> <tr> <td colspan="2">InChIKey</td> <td colspan="2">XEKOWRVHYACXOJ-UHFFFAOYSA-N</td> <td colspan="2"></td> </tr> <tr> <td colspan="2">Molecular Weight</td> <td colspan="2">88.106 g/mol</td> <td colspan="2"></td> </tr> <tr> <td colspan="2">Sample ID</td> <td colspan="2">1234</td> <td colspan="2"></td> </tr> <tr> <td colspan="2">WebLink</td> <td colspan="2">https://pubchem.ncbi.nlm.nih.gov/compound/ethyl-acetate</td> <td colspan="2"></td> </tr> <tr> <td colspan="2">Add...</td> <td colspan="2">Edit...</td> <td colspan="2">Delete</td> </tr> </tbody> </table>	Substances		Sel. Substances		Original Data Files		All Properties		Attachments		Preferred Properties		Name		Value				Name		Ethyl acetate				Comments		High purity				Formula		C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>				InChI		InChI=1S/C4H8O2/c1-3-6-4(2)5/h3H2,1-2H3				InChIKey		XEKOWRVHYACXOJ-UHFFFAOYSA-N				Molecular Weight		88.106 g/mol				Sample ID		1234				WebLink		https://pubchem.ncbi.nlm.nih.gov/compound/ethyl-acetate				Add...		Edit...		Delete	
Substances		Sel. Substances		Original Data Files																																																																						
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10	<p>Click the web address in the <b>Structure/Properties</b> pane.</p>	<p>The web page opens.</p> 																																																																								

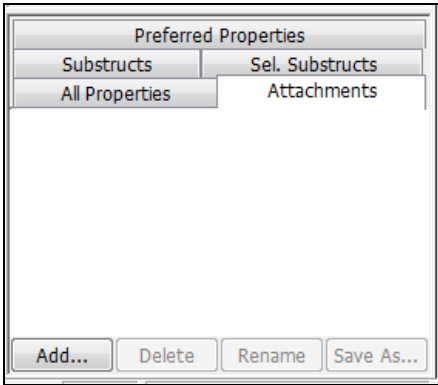
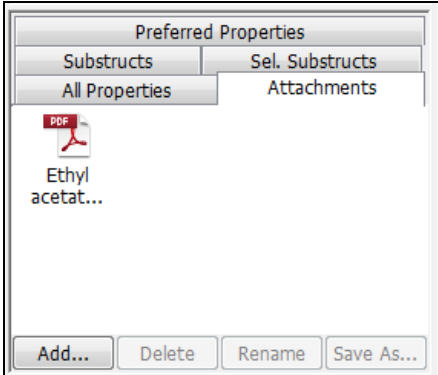


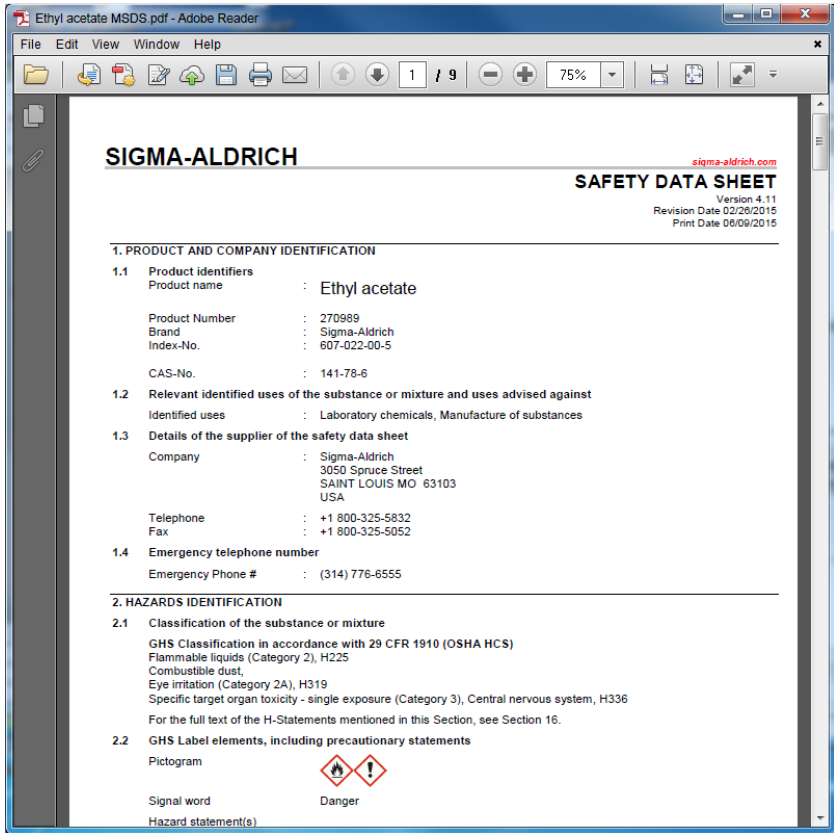

## Add another spectrum (Raman) to the first database record

	Action	Result
1	Make sure the first database record is selected, then choose <b>File &gt; Import</b> .	The <b>Open</b> dialog box with preview pane appears.
2	Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Raman folder.  Open <b>Ethyl acetate.irf</b> .	<p>The <b>Property Import Selection</b> dialog box opens.</p>  <p>This dialog box appears when you transfer information into a user database. All available properties are shown.</p>

	Action	Result
3	Click <b>OK</b> .	<p>A new <b>Raman</b> tab is added to the <b>Spectral</b> pane for the display of the Raman spectrum.</p> 
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 <b>Database</b> pane's <b>Spectrum</b> column.	

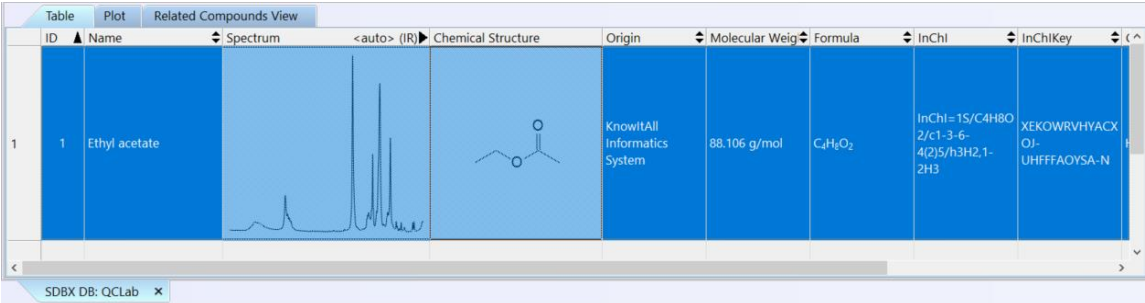

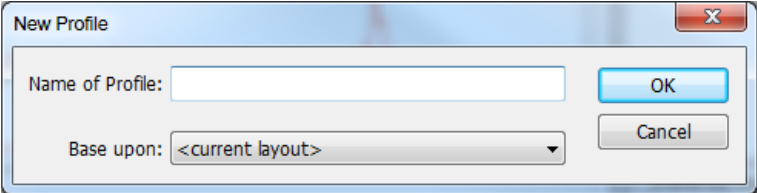
## Add an attachment to the first database record

	Action	Result
1	With the first database record selected, click the <b>Attachments</b> tab in the <b>Structure/Properties</b> pane.	The <b>Attachments</b> tab is empty. 
2	Choose <b>File &gt; Import Attachment(s)</b> .	A Windows <b>Open</b> dialog box is displayed.
3	Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Minelt folder.  Select <b>Ethyl acetate MSDS.pdf</b> . Then click <b>Open</b> .	An icon is added to the <b>Attachments</b> tab. 

	Action	Result
4	Double click the icon in the <b>Attachments</b> tab.	<p>The document opens in its native application—in this case, Adobe Acrobat.</p>  <p><b>ETHYL ACETATE MSDS.pdf - Adobe Reader</b></p> <p>File Edit View Window Help</p> <p>1 / 9 75%</p> <p><b>SIGMA-ALDRICH</b> <small>sigma-aldrich.com</small></p> <p><b>SAFETY DATA SHEET</b> Version 4.11 Revision Date 02/26/2015 Print Date 06/06/2015</p> <p><b>1. PRODUCT AND COMPANY IDENTIFICATION</b></p> <p>1.1 Product Identifiers Product name : Ethyl acetate</p> <p>Product Number : 270989 Brand : Sigma-Aldrich Index-No. : 607-022-00-5</p> <p>CAS-No. : 141-78-6</p> <p>1.2 Relevant identified uses of the substance or mixture and uses advised against Identified uses : Laboratory chemicals, Manufacture of substances</p> <p>1.3 Details of the supplier of the safety data sheet Company : Sigma-Aldrich 3050 Spruce Street SAINT LOUIS MO 63103 USA</p> <p>Telephone : +1 800-325-5832 Fax : +1 800-325-5052</p> <p>1.4 Emergency telephone number Emergency Phone # : (314) 776-6555</p> <p><b>2. HAZARDS IDENTIFICATION</b></p> <p>2.1 Classification of the substance or mixture GHS Classification in accordance with 29 CFR 1910 (OSHA HCS) Flammable liquids (Category 2), H225 Combustible dust, Eye irritation (Category 2A), H319 Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336 For the full text of the H-Statements mentioned in this Section, see Section 16.</p> <p>2.2 GHS Label elements, including precautionary statements Pictogram </p> <p>Signal word : Danger Hazard statement(s)</p>

**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**.

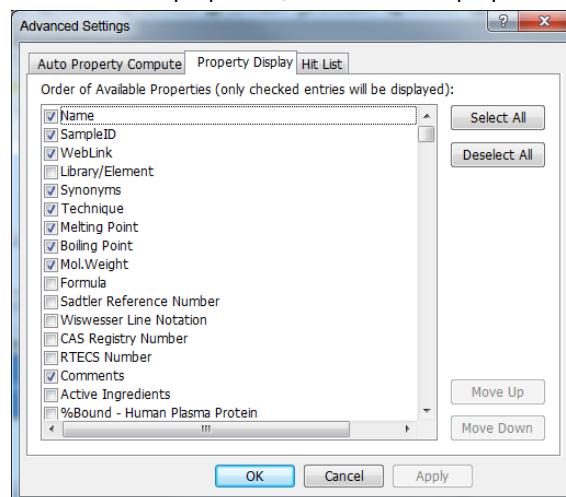
## Create a new Minelt display profile

	Action	Result
1	Adapt the table row height to a satisfactory height first.	<p>For example, the row is taller:</p> 
2	Click the <b>Add a New Profile</b> button  in the <b>Profile</b> toolbar.	<p>The <b>New Profile</b> dialog box opens.</p> 
3	Type in the profile name <b>QC Lab</b> and click <b>OK</b> .	This layout is now available to apply to any database or hit list display in the <b>Minelt</b> 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.

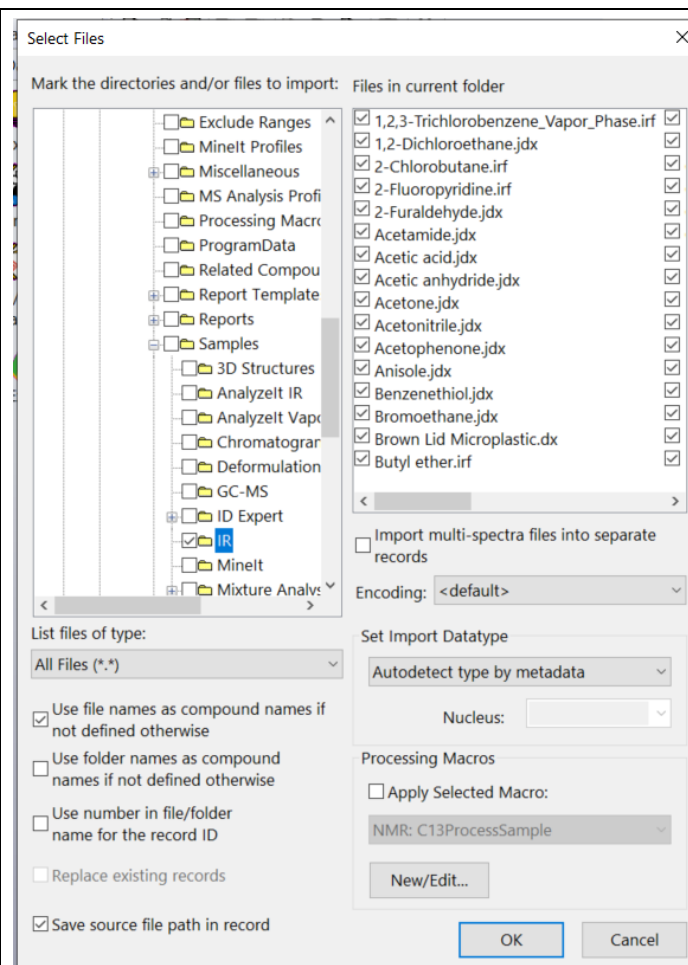
To do so, go to **File > Preferences**. In the Preferences dialog, select the **Property Display** tab. Click on **Deselect All** to clear the properties; then select the properties that you want entered and the order of those properties.



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.	

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



3 Choose **File > Import**.

Navigate to **C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Minelt**

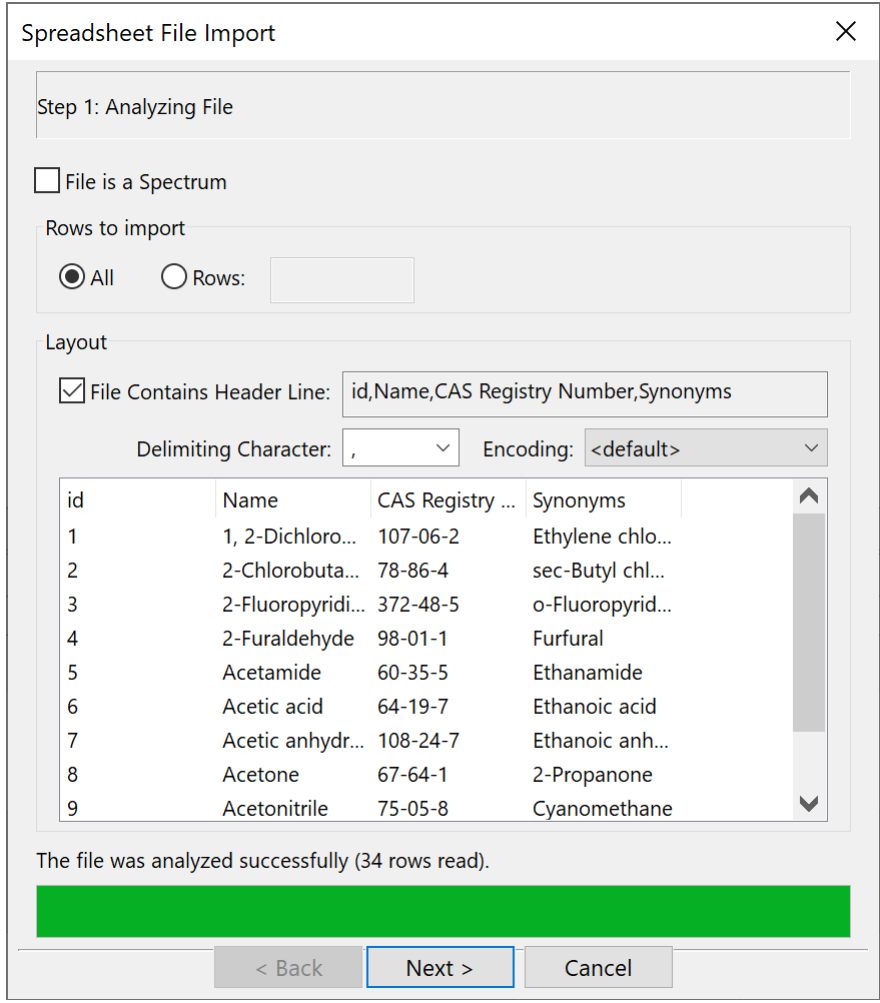
Select **BatchImportProperties.csv** to map properties to the spectrum files using a spreadsheet.

Click **Open**.

Make sure to check **File Contains Header Line**.

Click **Next**.

The **Spreadsheet File Import** wizard opens.



Spreadsheet File Import

Step 1: Analyzing File

File is a Spectrum

Rows to import

All  Rows:

Layout

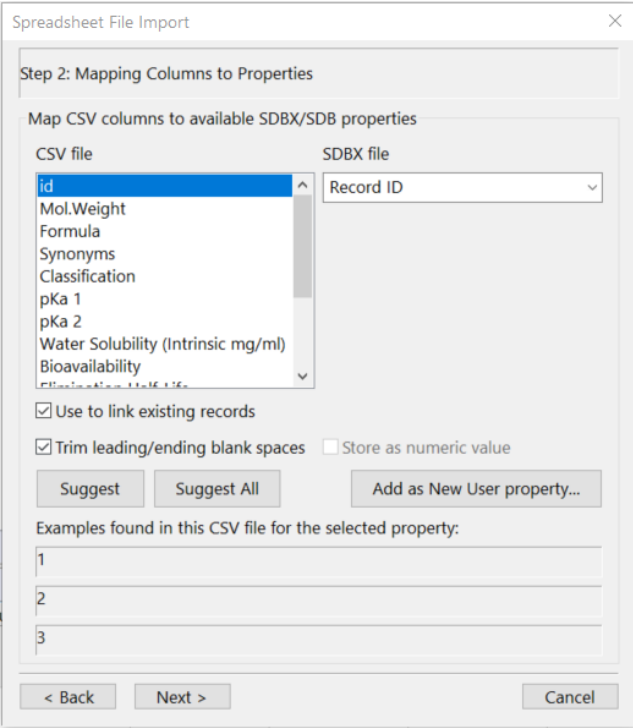
File Contains Header Line: id,Name,CAS Registry Number,Synonyms

Delimiting Character: , Encoding: <default>

id	Name	CAS Registry ...	Synonyms
1	1, 2-Dichloro...	107-06-2	Ethylene chlo...
2	2-Chlorobuta...	78-86-4	sec-Butyl chl...
3	2-Fluoropyridi...	372-48-5	o-Fluoropyrid...
4	2-Furaldehyde	98-01-1	Furfural
5	Acetamide	60-35-5	Ethanamide
6	Acetic acid	64-19-7	Ethanoic acid
7	Acetic anhydr...	108-24-7	Ethanoic anh...
8	Acetone	67-64-1	2-Propanone
9	Acetonitrile	75-05-8	Cyanomethane

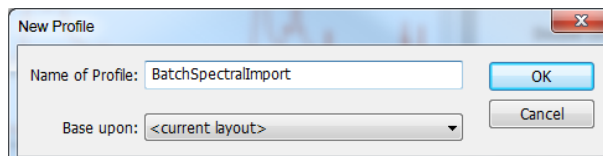
The file was analyzed successfully (34 rows read).

< Back Next > Cancel

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


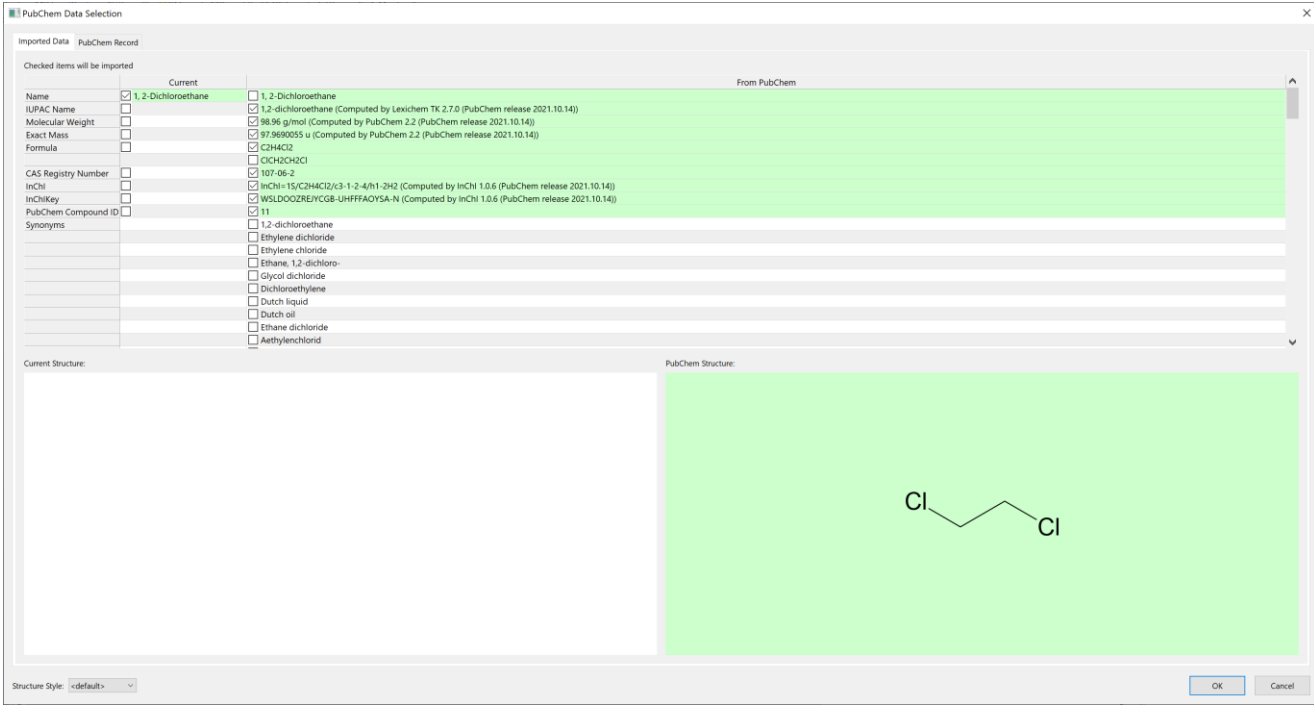
**TIP**

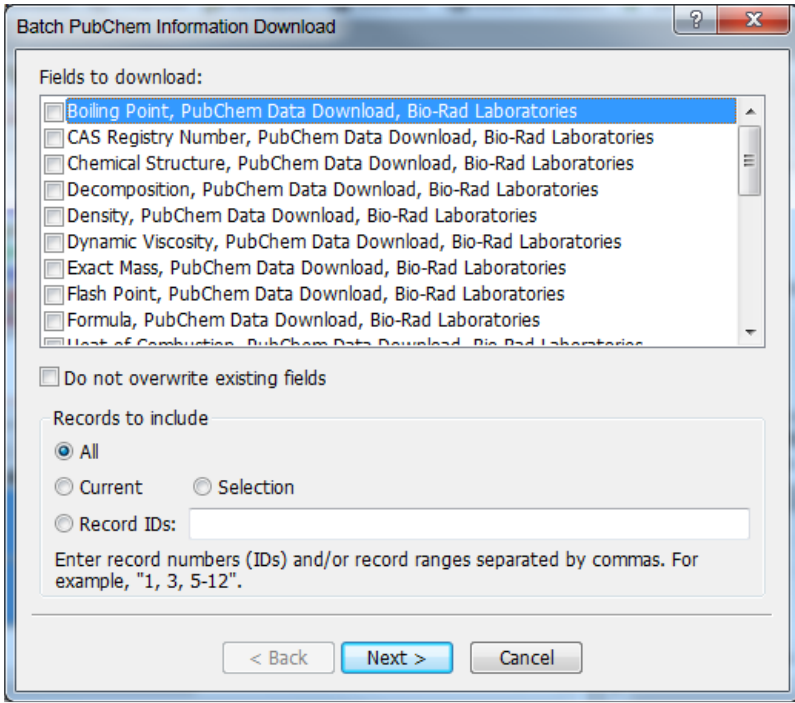
You can rearrange the table portion of this database (for example, to get rid of empty structure columns, right-click and choose **Delete Columns**). When edits are completed, you can save this column arrangement as a **Minelt** profile. Click **Save Current Profile** on the **Profile** toolbar, then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

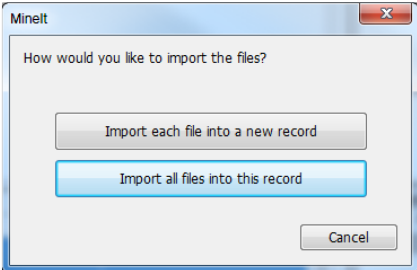
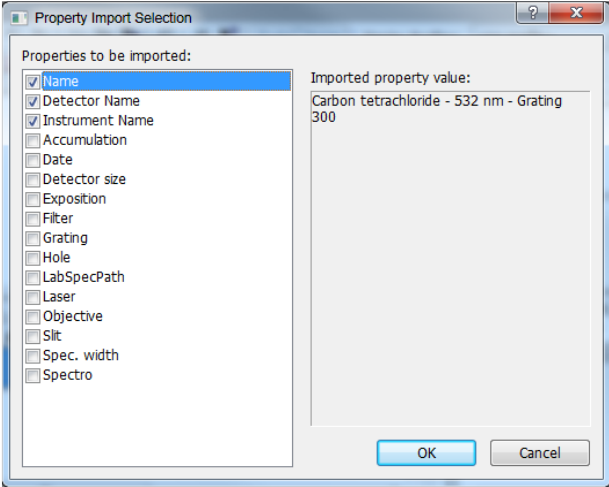
**Batch Import: many spectra, many records, import properties from PubChem**

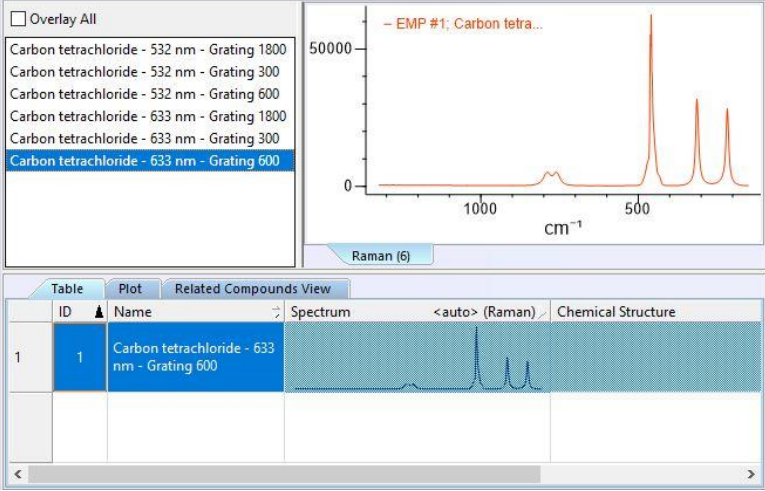
	Action	Result
1	<p>Select the first record from the above database, click the <b>PubChem</b> toolbar button.</p> 	<p>PubChem records are searched. If information is located, the <b>PubChem Data Selection</b> dialog box opens.</p>  <p>The dialog box displays a list of properties for 1,2-Dichloroethane, with the following items checked:</p> <ul style="list-style-type: none"><li>Name: 1,2-Dichloroethane</li><li>IUPAC Name: 1,2-dichloroethane (Computed by Lexichem TK 2.7.0 (PubChem release 2021.10.14))</li><li>Molecular Weight: 98.96 g/mol (Computed by PubChem 2.2 (PubChem release 2021.10.14))</li><li>Exact Mass: 97.969055 u (Computed by PubChem 2.2 (PubChem release 2021.10.14))</li><li>Formula: C<sub>2</sub>H<sub>4</sub>Cl<sub>2</sub></li><li>CAS Registry Number: 107-06-2</li><li>InChI: InChI=1S/C2H4Cl2/c3-1-2-4/h1-2H2 (Computed by InChI 1.0.6 (PubChem release 2021.10.14))</li><li>InChIKey: WSLD00ZREJYCGB-UHFFFAOYSA-N (Computed by InChI 1.0.6 (PubChem release 2021.10.14))</li><li>PubChem Compound ID: 11</li></ul> <p>The PubChem Structure panel shows the chemical structure of 1,2-dichloroethane: <chem>ClCCl</chem>.</p>

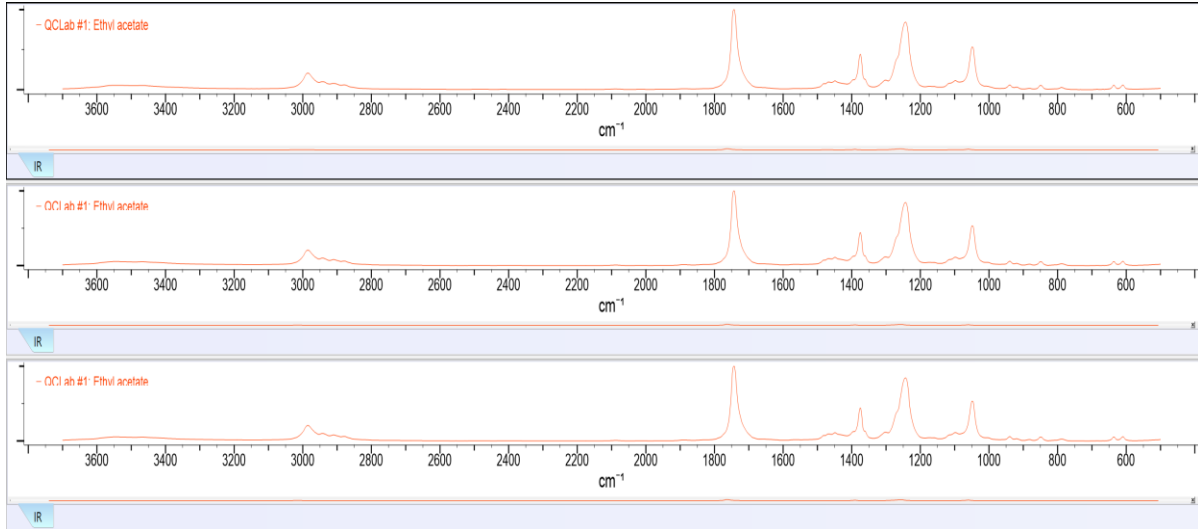
	Action	Result
2	Click <b>OK</b> .	New properties from <b>PubChem</b> are added to the first database record.
3	Select the remaining database records by holding the Shift key, then choose <b>Database &gt; Batch PubChem Information Download</b> .	<p>The <b>Batch PubChem Information Download</b> dialog box opens.</p> 
4	Check the property fields you wish to add to the database records, then click <b>Next</b> .	<p>New properties from PubChem are added to the remaining database records.</p> <p><b>TIP:</b> This process can take several minutes.</p>

**TIP:** Sometimes one may get error saying compounds not being found, because PubChem do not have them.

### Batch Import: many spectra, one record

	Action	Result
1	Create a new empty database as in the above example.	
2	<p>Choose <b>File &gt; Import</b>.</p> <p>Navigate to <b>C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Raman</b> folder</p> <p>Select all files in the folder.</p> <p>Click <b>Open</b>.</p>	<p>A dialog box opens and asks how you want to import the files.</p> 
3	Click <b>Import all files into this record</b> .	<p>The <b>Property Import Selection</b> dialog opens.</p>  <p>Check the properties you wish to import.</p>

	Action	Result								
4	Click <b>OK</b> each time the dialog appears.	The dialog box appears once for each spectrum in the record.								
5	With the first record selected, observe the <b>Spectrum</b> pane.	<p>The tab shows that there are 6 Raman spectra associated with the first record.</p>  <p>The screenshot displays a software window with a list of Raman spectra on the left and a plot on the right. The list includes:</p> <ul style="list-style-type: none"> <li>Carbon tetrachloride - 532 nm - Grating 1800</li> <li>Carbon tetrachloride - 532 nm - Grating 300</li> <li>Carbon tetrachloride - 532 nm - Grating 600</li> <li>Carbon tetrachloride - 633 nm - Grating 1800</li> <li>Carbon tetrachloride - 633 nm - Grating 300</li> <li>Carbon tetrachloride - 633 nm - Grating 600 (highlighted)</li> </ul> <p>The plot shows a Raman spectrum for the selected entry, with a y-axis ranging from 0 to 50000 and an x-axis labeled <math>\text{cm}^{-1}</math> with markers at 1000 and 500. The plot title is '- EMP #1; Carbon tetra...'. Below the plot is a table with the following structure:</p> <table border="1"> <thead> <tr> <th>ID</th> <th>Name</th> <th>Spectrum</th> <th>Chemical Structure</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>Carbon tetrachloride - 633 nm - Grating 600</td> <td>&lt;auto&gt; (Raman)</td> <td></td> </tr> </tbody> </table>	ID	Name	Spectrum	Chemical Structure	1	Carbon tetrachloride - 633 nm - Grating 600	<auto> (Raman)	
ID	Name	Spectrum	Chemical Structure							
1	Carbon tetrachloride - 633 nm - Grating 600	<auto> (Raman)								
6	Click the name of a spectrum in the left pane to display it.									

	Action	Result
7	Choose <b>Window &gt; Split Threefold</b> .	<p>The <b>Spectral</b> pane is split into 3 panes displaying 3 of the 6 spectra.</p> 



# Creating Databases

---

## How to Create a Database with Structures

### Purpose

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

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### 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, scientists can improve their analyses.

#### ***Training Files Used in This Lesson***

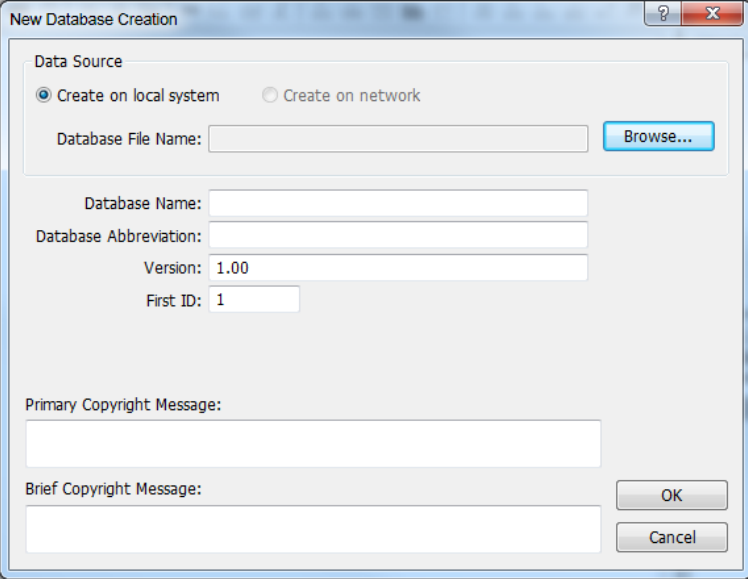
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Structures folder

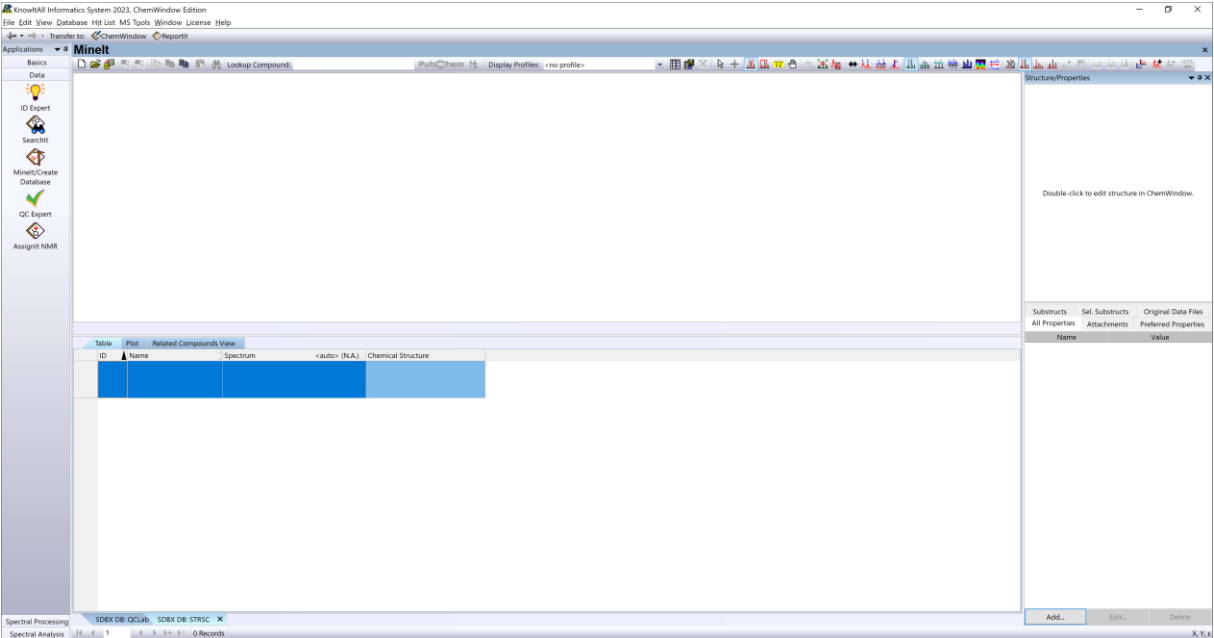
- benzylpenicillin.dsf


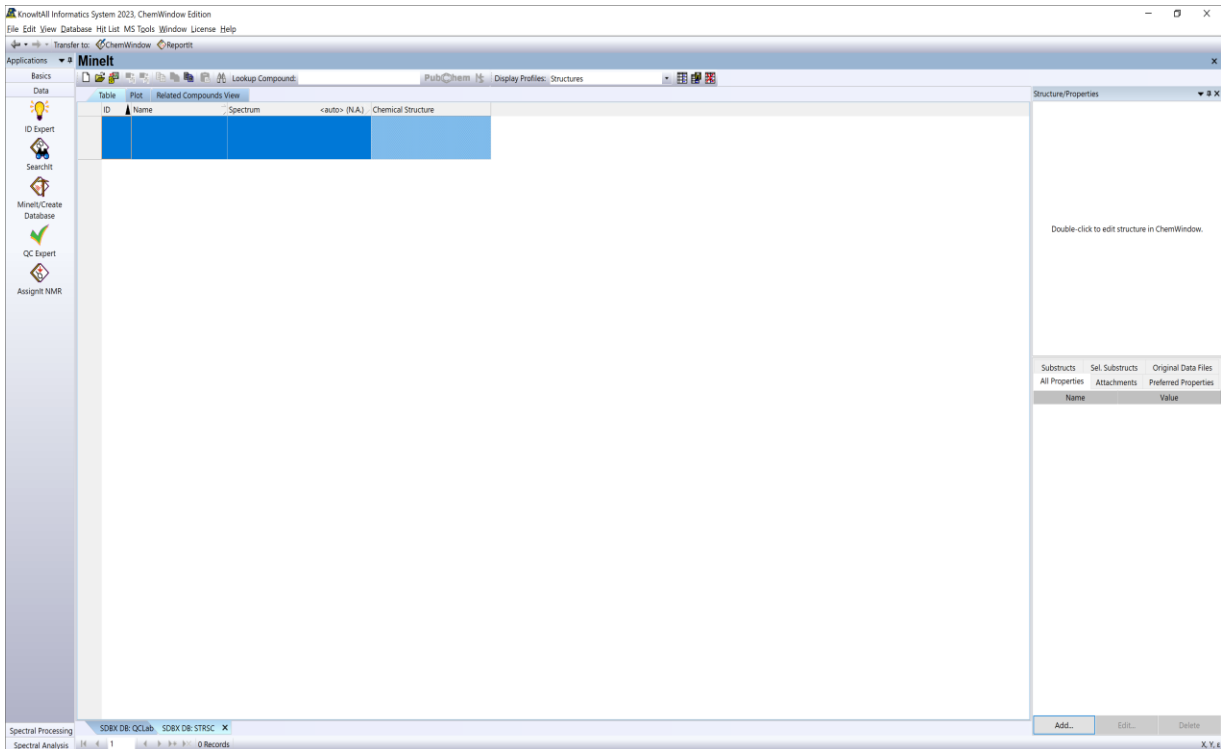
#### ***KnowItAll Applications Used***

- Minelt
- ChemWindow®

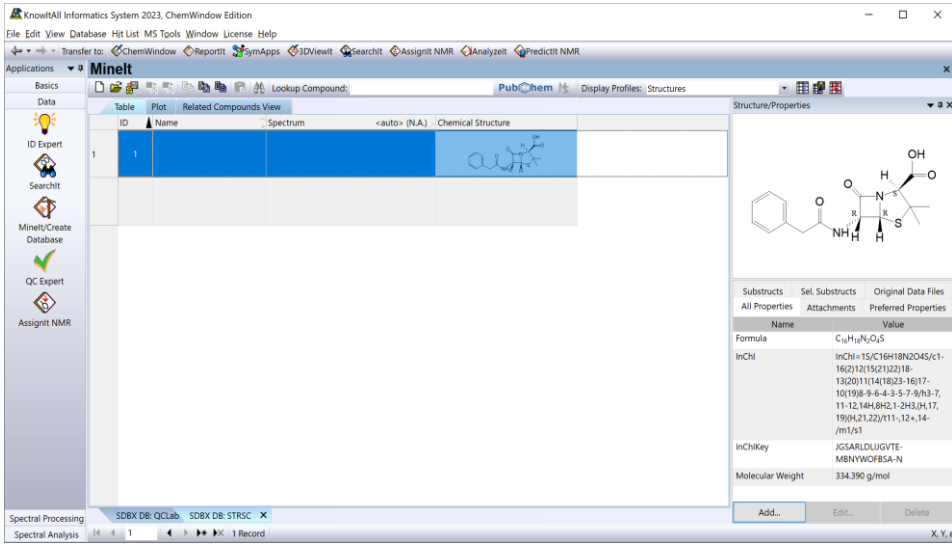
## Create a user database

	Action	Result
1	In the <b>Minelt</b> application, choose <b>Database &gt; New</b> .	<p>The <b>New Database Creation</b> dialog box opens.</p> 
2	Select <b>Create on local system</b> .	The new database is saved locally.
3	<p>Click <b>Browse</b>.</p> <p>Navigate to the <b>Databases</b> folder you created earlier,</p> <p>Type <b>structures-sc</b> in the <b>Database File Name</b></p> <p>Click <b>Save</b>.</p>	<p>The *.sdbx extension is added automatically.</p> <p><b>Note:</b> 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.</p>
4	<p>Type <b>Structures</b> in the <b>Database Name</b> text box.</p> <p><b>Note:</b> The file name is used if no other name is specified.</p>	

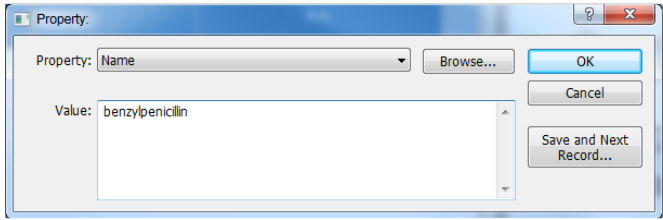
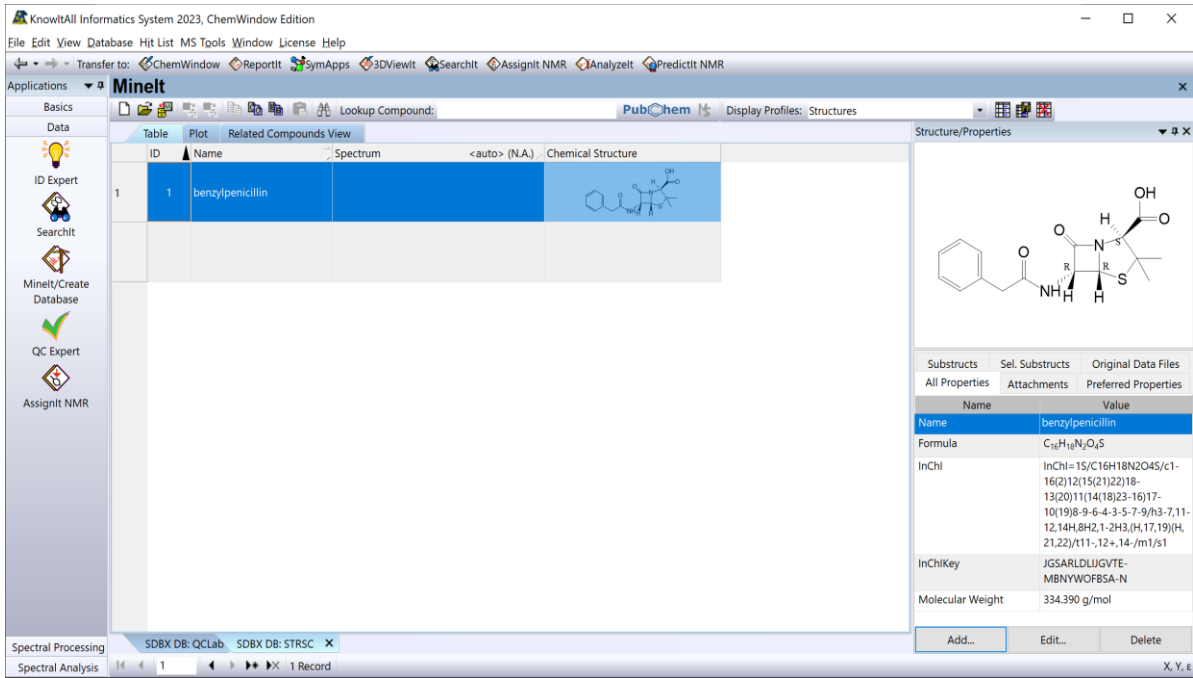
	Action	Result
5	Type 'STRSC' in the <b>Database Abbreviation</b> text box. <b>Note:</b> The abbreviation must be 3-7 characters long.	
6	Click <b>OK</b> .	<p>The new database has been created to receive your data. The Database Abbreviation appears on the database tab.</p> 
7	Choose <b>View &gt; Windows/Tables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

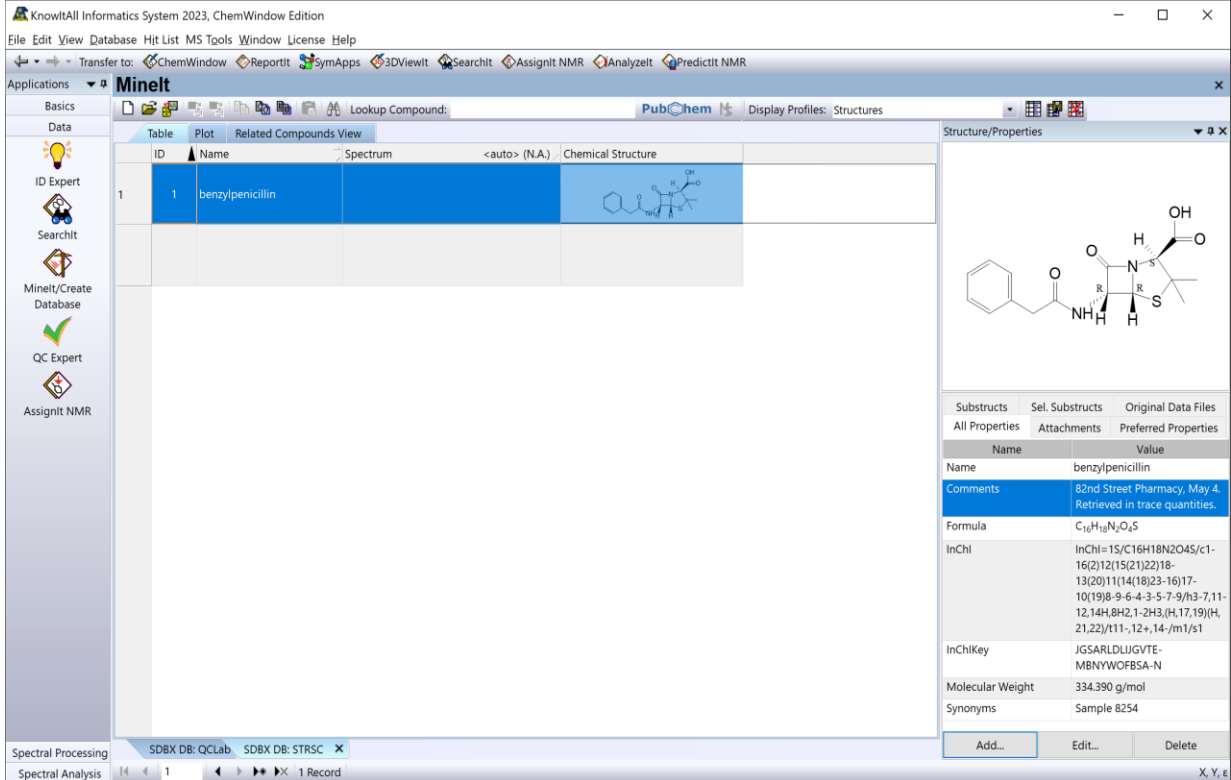
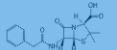
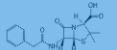
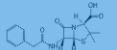
	Action	Result
8	<p>Click the <b>Add a New Profile</b> toolbar button , type the name 'Structures' in the <b>New Profile</b> dialog box, then click <b>OK</b>.</p>	 <p>The screenshot shows the Minelt software interface. The main window displays a table with the following columns: ID, Name, and Spectrum. The table is currently empty. The interface includes a toolbar on the left with various icons, a menu bar at the top, and a status bar at the bottom showing 'Spectral Processing' and 'Spectral Analysis'.</p>

## Add a structure to the first database record

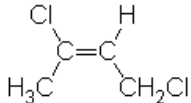
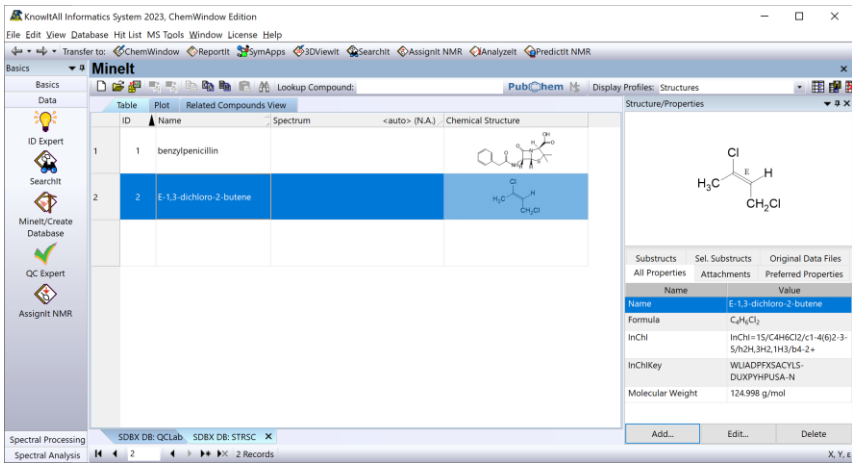
	Action	Result
1	<p>Choose <b>File &gt; Import</b></p> <p>Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Structures folder</p> <p>Open the structure file <b>Benzylpenicillin.dsf</b>.</p>	<p>The structure is displayed in the <b>Structure/Properties</b> pane.</p> 
2	<p>Open the <b>View</b> menu and check <b>Stereochemistry</b> if it is not already checked.</p>	<p>Stereochemical descriptors are shown on the structure when <b>Stereochemistry</b> is enabled on the <b>View</b> menu.</p>

## Add properties to a database record

	Action	Result																		
1	Click <b>Add</b> in the <b>Structure/Properties</b> pane.	The <b>Property</b> dialog box opens.																		
2	Select the property <b>Name</b> , then type 'benzylpenicillin' in the <b>Value</b> text box.																			
3	Click <b>OK</b> .	<p>The <b>Property</b> dialog box closes, and the added property <b>Name</b> appears in the <b>Structure/Properties</b> pane.</p>  <table border="1" data-bbox="1591 1068 1873 1351"> <thead> <tr> <th colspan="2">Name</th> <th>Value</th> </tr> </thead> <tbody> <tr> <td>Name</td> <td>benzylpenicillin</td> <td></td> </tr> <tr> <td>Formula</td> <td>C<sub>16</sub>H<sub>18</sub>N<sub>2</sub>O<sub>5</sub>S</td> <td></td> </tr> <tr> <td>InChI</td> <td>InChI=1S/C16H18N2O4S/c1-16(2)12(15(2)2)18-13(20)11(4)18(23-16)17-10(19)8-9-6-4-3-5-7-9/h3-7,11-12,14,8,42,1-2H2,(H,17,19)(H,21,22)/t11-12,+14-/m1/s1</td> <td></td> </tr> <tr> <td>InChIKey</td> <td>JGSARLDLUGVTE-MBNYWOFBSA-N</td> <td></td> </tr> <tr> <td>Molecular Weight</td> <td>334.390 g/mol</td> <td></td> </tr> </tbody> </table>	Name		Value	Name	benzylpenicillin		Formula	C <sub>16</sub> H <sub>18</sub> N <sub>2</sub> O <sub>5</sub> S		InChI	InChI=1S/C16H18N2O4S/c1-16(2)12(15(2)2)18-13(20)11(4)18(23-16)17-10(19)8-9-6-4-3-5-7-9/h3-7,11-12,14,8,42,1-2H2,(H,17,19)(H,21,22)/t11-12,+14-/m1/s1		InChIKey	JGSARLDLUGVTE-MBNYWOFBSA-N		Molecular Weight	334.390 g/mol	
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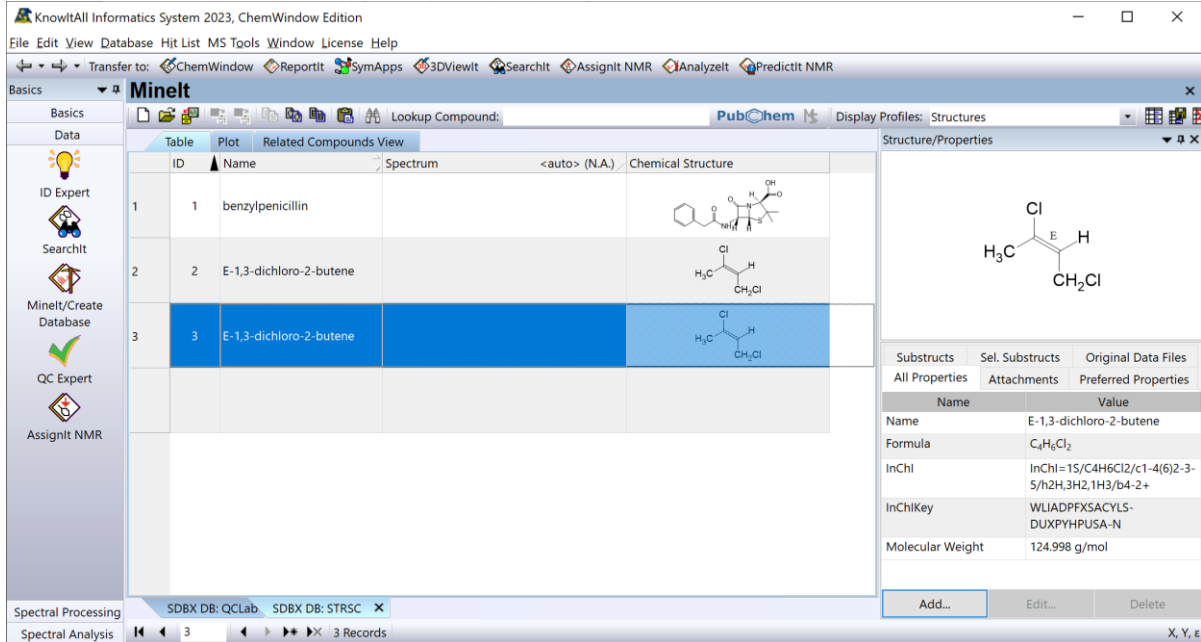
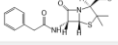


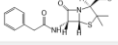


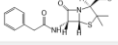


	Action	Result																								
4	Repeat to add the property <b>Synonyms</b> with the value 'Sample 8254.'																									
5	Repeat to add the property <b>Comments</b> with the value '82 <sup>nd</sup> Street Pharmacy, May 4. Retrieved in trace quantities.'	 <p>The screenshot shows the 'Minelt' application window. The table below is visible in the main view:</p> <table border="1" data-bbox="798 532 1617 673"> <thead> <tr> <th>ID</th> <th>Name</th> <th>Spectrum</th> <th>Chemical Structure</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>benzylpenicillin</td> <td></td> <td></td> </tr> </tbody> </table> <p>The 'Structure/Properties' pane on the right shows the following details:</p> <table border="1" data-bbox="1627 787 1900 1128"> <thead> <tr> <th>Name</th> <th>Value</th> </tr> </thead> <tbody> <tr> <td>Name</td> <td>benzylpenicillin</td> </tr> <tr> <td>Comments</td> <td>82<sup>nd</sup> Street Pharmacy, May 4. Retrieved in trace quantities.</td> </tr> <tr> <td>Formula</td> <td>C<sub>18</sub>H<sub>18</sub>N<sub>2</sub>O<sub>5</sub>S</td> </tr> <tr> <td>InChI</td> <td>InChI=1S/C16H18N2O4S/c1-16(2)12(15(2)12)18-13(20)11(14)18(23-16)17-10(19)8-9-6-4-3-5-7-9/h3-7,11-12,14,8,2,1-2H3,(H,17,19)(H,21,22)/t11-,12+,-,14-/m1/s1</td> </tr> <tr> <td>InChIKey</td> <td>JGSARLDLJGVTE-MBNYWOFBSA-N</td> </tr> <tr> <td>Molecular Weight</td> <td>334.390 g/mol</td> </tr> <tr> <td>Synonyms</td> <td>Sample 8254</td> </tr> </tbody> </table>	ID	Name	Spectrum	Chemical Structure	1	benzylpenicillin			Name	Value	Name	benzylpenicillin	Comments	82 <sup>nd</sup> Street Pharmacy, May 4. Retrieved in trace quantities.	Formula	C <sub>18</sub> H <sub>18</sub> N <sub>2</sub> O <sub>5</sub> S	InChI	InChI=1S/C16H18N2O4S/c1-16(2)12(15(2)12)18-13(20)11(14)18(23-16)17-10(19)8-9-6-4-3-5-7-9/h3-7,11-12,14,8,2,1-2H3,(H,17,19)(H,21,22)/t11-,12+,-,14-/m1/s1	InChIKey	JGSARLDLJGVTE-MBNYWOFBSA-N	Molecular Weight	334.390 g/mol	Synonyms	Sample 8254
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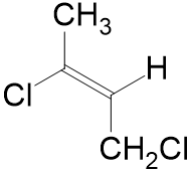
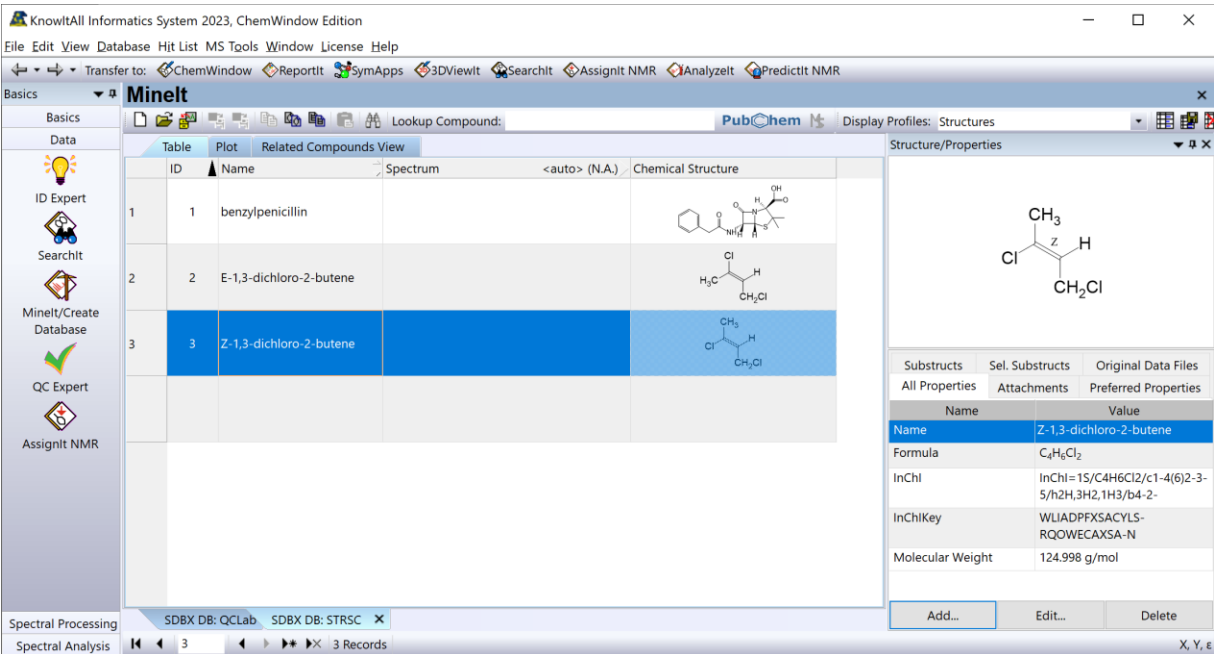
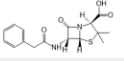
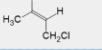
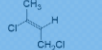
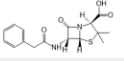
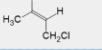
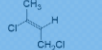
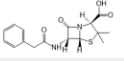
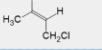
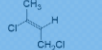
## Add a second database record

	Action	Result
1	Navigate to the <b>Basics</b> toolbox, then open the ChemWindow application by clicking its icon. <b>Note:</b> Do not use the <b>Transfer to</b> bar in this case.	
2	Draw this structure: <div style="text-align: center;">  </div>	
3	Use the <b>Selection</b> tool to select the structure, then choose <b>Edit &gt; Copy</b> .	
4	Use the KnowItAll <b>Back</b> button to return to the <b>Minelt</b> application.	
5	With the second database entry selected, choose <b>Edit &gt; Paste</b> . A message box asks, "Would you like to append the new data as a new record?" Click <b>OK</b> .	<p>The structure is added to the second record.</p> 
6	Add the property <b>Name</b> 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 <b>Edit &gt; Copy Structure</b> .																																																	
2	<p>Select the third database record and choose <b>Edit &gt; Paste</b>.</p> <p>A message box asks, "Would you like to append the new data as a new record?"</p> <p>Click <b>OK</b>.</p>	<p>The structure and properties are added to the third database record.</p>  <p>The screenshot shows the Minelt software interface. The main window displays a table with three records. The third record, 'E-1,3-dichloro-2-butene', is selected. The 'Structure/Properties' pane on the right shows the chemical structure and associated data.</p> <table border="1" data-bbox="814 662 1556 946"> <thead> <tr> <th>ID</th> <th>Name</th> <th>Spectrum</th> <th>Chemical Structure</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>benzylpenicillin</td> <td>&lt;auto&gt; (N.A.)</td> <td></td> </tr> <tr> <td>2</td> <td>E-1,3-dichloro-2-butene</td> <td></td> <td></td> </tr> <tr> <td>3</td> <td>E-1,3-dichloro-2-butene</td> <td></td> <td></td> </tr> </tbody> </table> <table border="1" data-bbox="1564 857 1881 1073"> <thead> <tr> <th colspan="2">Substructs</th> <th>Sel. Substructs</th> <th>Original Data Files</th> </tr> <tr> <th colspan="2">All Properties</th> <th>Attachments</th> <th>Preferred Properties</th> </tr> <tr> <th>Name</th> <th colspan="3">Value</th> </tr> </thead> <tbody> <tr> <td>Name</td> <td colspan="3">E-1,3-dichloro-2-butene</td> </tr> <tr> <td>Formula</td> <td colspan="3">C<sub>4</sub>H<sub>6</sub>Cl<sub>2</sub></td> </tr> <tr> <td>InChi</td> <td colspan="3">InChi=1S/C4H6Cl2/c1-4(6)2-3-5/h2H,3H2,1H3/b4-2+</td> </tr> <tr> <td>InChiKey</td> <td colspan="3">WLIADPFXSACYLS-DUXPHYPUA-N</td> </tr> <tr> <td>Molecular Weight</td> <td colspan="3">124.998 g/mol</td> </tr> </tbody> </table>	ID	Name	Spectrum	Chemical Structure	1	benzylpenicillin	<auto> (N.A.)		2	E-1,3-dichloro-2-butene			3	E-1,3-dichloro-2-butene			Substructs		Sel. Substructs	Original Data Files	All Properties		Attachments	Preferred Properties	Name	Value			Name	E-1,3-dichloro-2-butene			Formula	C <sub>4</sub> H <sub>6</sub> Cl <sub>2</sub>			InChi	InChi=1S/C4H6Cl2/c1-4(6)2-3-5/h2H,3H2,1H3/b4-2+			InChiKey	WLIADPFXSACYLS-DUXPHYPUA-N			Molecular Weight	124.998 g/mol		
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3	With the third database record selected, double click in the <b>Structure/Properties</b> pane to open the structure in <b>ChemWindow</b> .																																																	

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4	Edit the structure as shown, then click <b>Return to Minelt Database and Save.</b> 	The structure is added to the third database record.  ChemWindow is closed and we are back to the <b>Minelt</b> window.																																																																
5	Edit the property <b>Name</b> to 'Z-1,3-dichloro-2-butene.'	 <table border="1" data-bbox="821 732 1528 1036"> <thead> <tr> <th>ID</th> <th>Name</th> <th>Spectrum</th> <th>Chemical Structure</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>benzylpenicillin</td> <td></td> <td></td> </tr> <tr> <td>2</td> <td>E-1,3-dichloro-2-butene</td> <td></td> <td></td> </tr> <tr> <td>3</td> <td>Z-1,3-dichloro-2-butene</td> <td></td> <td></td> </tr> </tbody> </table> <table border="1" data-bbox="1581 946 1906 1166"> <thead> <tr> <th colspan="2">Substructs</th> <th colspan="2">Sel. Substructs</th> <th colspan="2">Original Data Files</th> </tr> <tr> <th colspan="2">All Properties</th> <th colspan="2">Attachments</th> <th colspan="2">Preferred Properties</th> </tr> <tr> <th colspan="2">Name</th> <th colspan="4">Value</th> </tr> </thead> <tbody> <tr> <td colspan="2">Name</td> <td colspan="4">Z-1,3-dichloro-2-butene</td> </tr> <tr> <td colspan="2">Formula</td> <td colspan="4">C<sub>4</sub>H<sub>6</sub>Cl<sub>2</sub></td> </tr> <tr> <td colspan="2">InChI</td> <td colspan="4">InChI=1S/C4H6Cl2/c1-4(6)2-3-5/h2H,3H2,1H3/b4-2-</td> </tr> <tr> <td colspan="2">InChIKey</td> <td colspan="4">WLIADPFXSACYLS-RQOWECAXSA-N</td> </tr> <tr> <td colspan="2">Molecular Weight</td> <td colspan="4">124.998 g/mol</td> </tr> </tbody> </table>	ID	Name	Spectrum	Chemical Structure	1	benzylpenicillin			2	E-1,3-dichloro-2-butene			3	Z-1,3-dichloro-2-butene			Substructs		Sel. Substructs		Original Data Files		All Properties		Attachments		Preferred Properties		Name		Value				Name		Z-1,3-dichloro-2-butene				Formula		C <sub>4</sub> H <sub>6</sub> Cl <sub>2</sub>				InChI		InChI=1S/C4H6Cl2/c1-4(6)2-3-5/h2H,3H2,1H3/b4-2-				InChIKey		WLIADPFXSACYLS-RQOWECAXSA-N				Molecular Weight		124.998 g/mol			
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# Create Databases

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## How to Build User Databases Using GC-MS Data

### Purpose

This exercise demonstrates how to use KnowItAll's Minelt 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, scientists can improve their analyses.

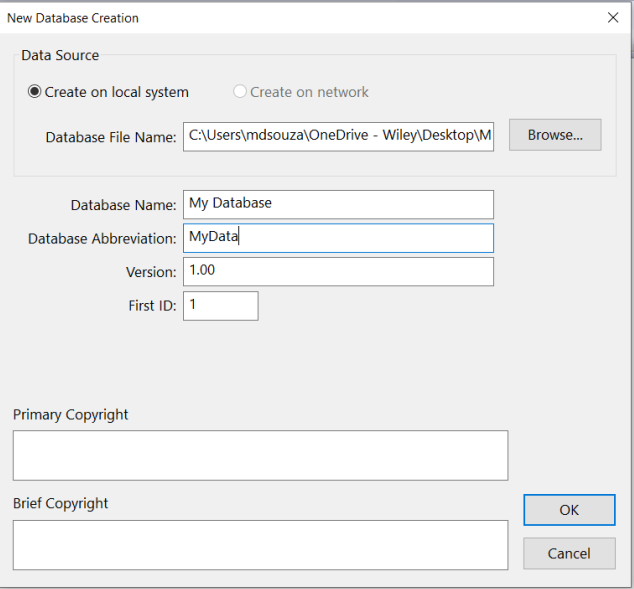
#### ***Training Files Used in This Lesson***

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

#### ***KnowItAll Applications Used***

- Minelt
- ChemWindow®
- Browselt

### GC-MS Record Creation

	Action	Result
1	<p>Start <b>KnowItAll</b>.</p> <p>Click the <b>Minelt</b> icon.</p> <p>Select <b>Database &gt; New</b>.</p> <p>Use <b>Browse</b> to set the hardware location for the database.</p> <p>Enter a Database Name.</p> <p>Enter a Database Abbreviation ("MyData" etc).</p> <p>Click <b>OK</b>.</p>	

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**.

KnowItAll Informatics System 2023, ChemWindow Edition  
File Edit View Database Hit List MS Tools Window License Help

Transfer to: ChemWindow ReportIt

Basics Minelt

Lookup Compound: PubChem Display Profiles: <no profile>

Basics

Data

ID Expert

SearchIt

Minelt/Create Database

QC Expert

AssignIt NMR

ID	Name	Spectrum	Chemical Structure

Open

Look in: GC-MS

Name	Date modified
Barbiturate GC-MS.d	10/19/2022 2:06 PM
Structure 1 - Barbitol.dsf	10/19/2022 2:06 PM
Structure 2 - Butethal.dsf	10/19/2022 2:06 PM
Structure 3 - Amobarbital.dsf	10/19/2022 2:06 PM
Structure 4 - Pentobarbital.dsf	10/19/2022 2:06 PM
Structure 5 - Secobarbital.dsf	10/19/2022 2:06 PM

File name: Barbiturate GC-MS.d

Files of type: All Files (\*.\*)

Imported spectrum is

BARBITURATE MIX

Data is 2D, only the TIC is shown.

min

Encoding: <default>

3 Select a threshold above 10% and click **Pick**.

Select **Add all spectra to the current record**.

Click **OK**.

MS Spectral Scan Selection

Please select the 1D scan(s) to import: Minimum Intensity: 15.3 % Pick

Slice #	Location [min]
<input type="checkbox"/>	116 2.195
<input type="checkbox"/>	117 2.20467
<input type="checkbox"/>	118 2.21417
<input type="checkbox"/>	119 2.22383
<input type="checkbox"/>	120 2.23317
<input type="checkbox"/>	121 2.24283
<input type="checkbox"/>	122 2.25233
<input type="checkbox"/>	123 2.262
<input type="checkbox"/>	124 2.2715
<input type="checkbox"/>	125 2.28117
<input type="checkbox"/>	126 2.29067
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<input type="checkbox"/>	128 2.30983
<input type="checkbox"/>	129 2.3195
<input type="checkbox"/>	130 2.32883
<input type="checkbox"/>	131 2.3385
<input type="checkbox"/>	132 2.348
<input type="checkbox"/>	133 2.35767
<input type="checkbox"/>	134 2.368
<input checked="" type="checkbox"/>	135 2.37783

Select All Deselect All Time of current scan: 1.17483 min

Spectrum import mode

- Import MS slice(s)
  - Add all spectra to the current record
  - Add each spectrum to multiple new records
  - Add all spectra to a single new record
- Import chromatogram

OK Cancel

4

KnowItAll Informatics System 2023, ChemWindow Edition

File Edit View Database Hit List MS Tools Window License Help

Transfer to: ChemWindow ReportIt SearchIt ProcessIt

Basics

Minelt

PubChem Display Profiles: <no profile>

Structure/Properties

Double-click to edit structure in ChemWindow.

Substructs Sel. Substructs Original Data Files

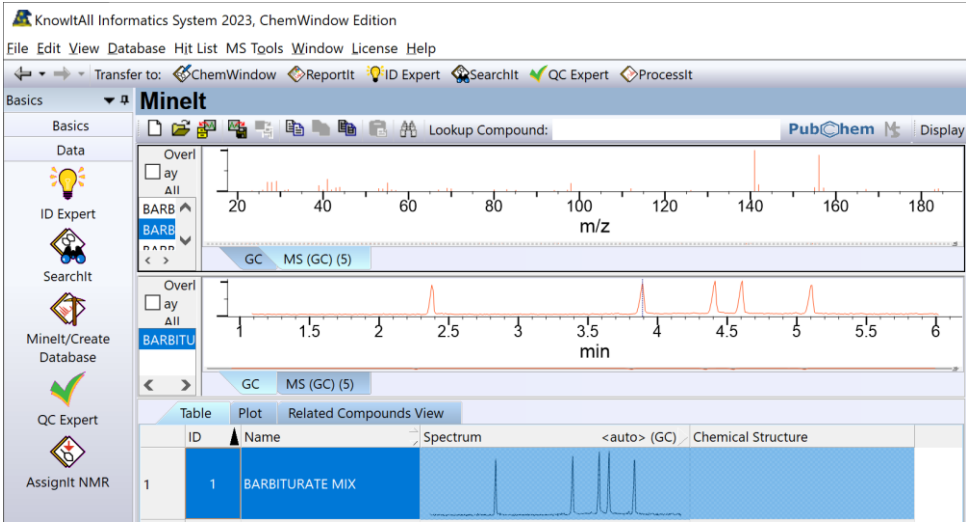
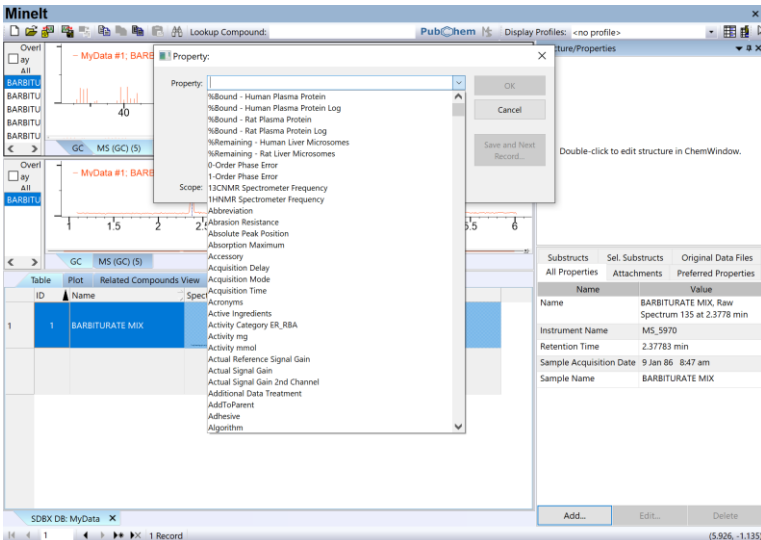
All Properties	Attachments	Preferred Properties
Name	Value	
Name	BARBITURATE MIX	
Instrument Name	MS_5970	
Sample Acquisition Date	9 Jan 86 8:47 am	
Sample Name	BARBITURATE MIX	

Add... Edit... Delete

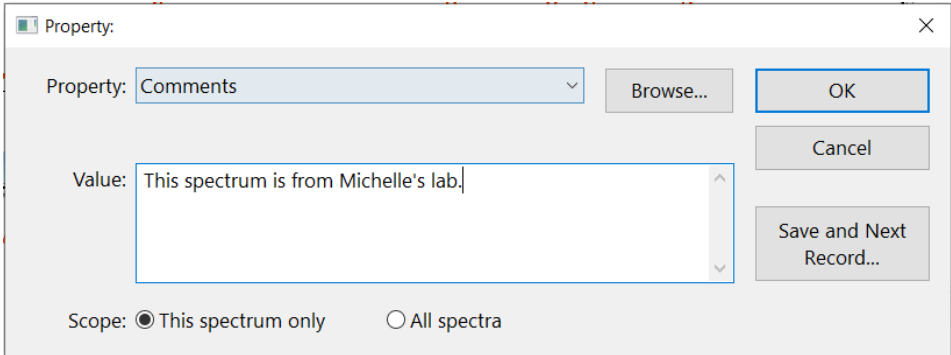
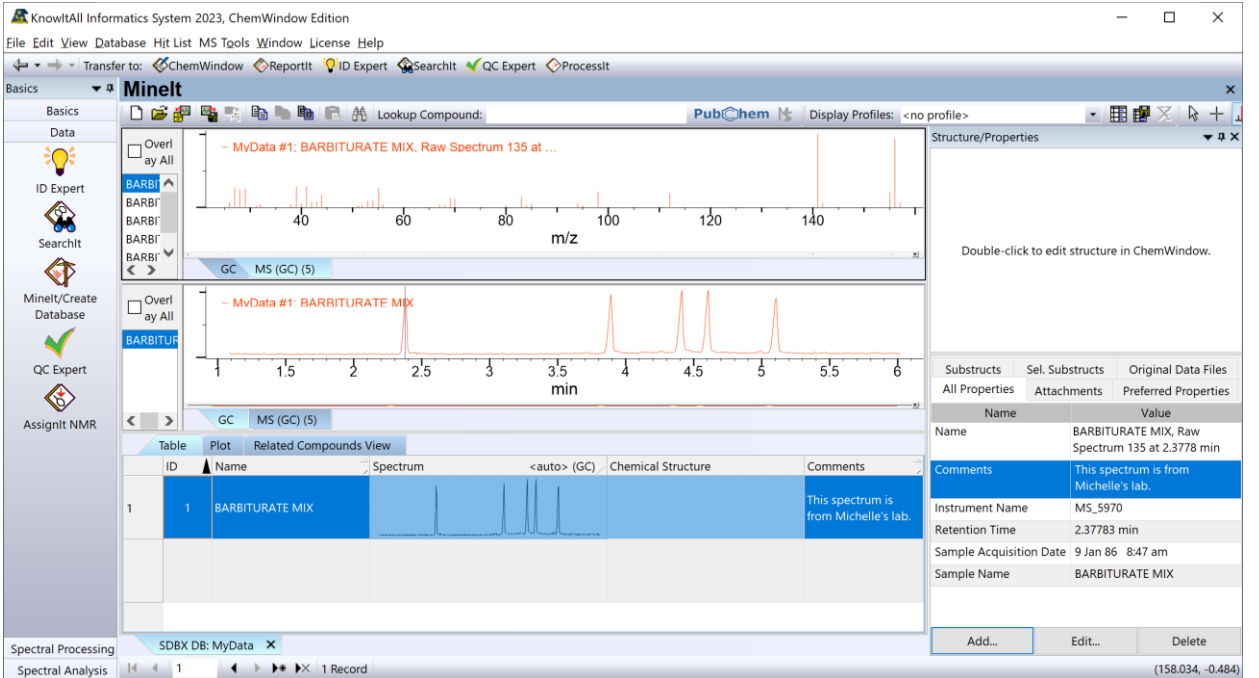
(6,120, 0,648)

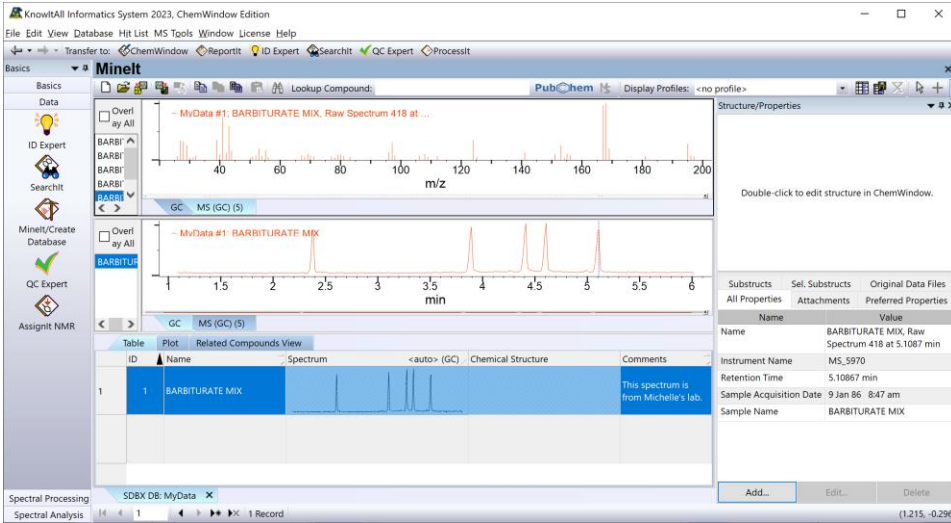
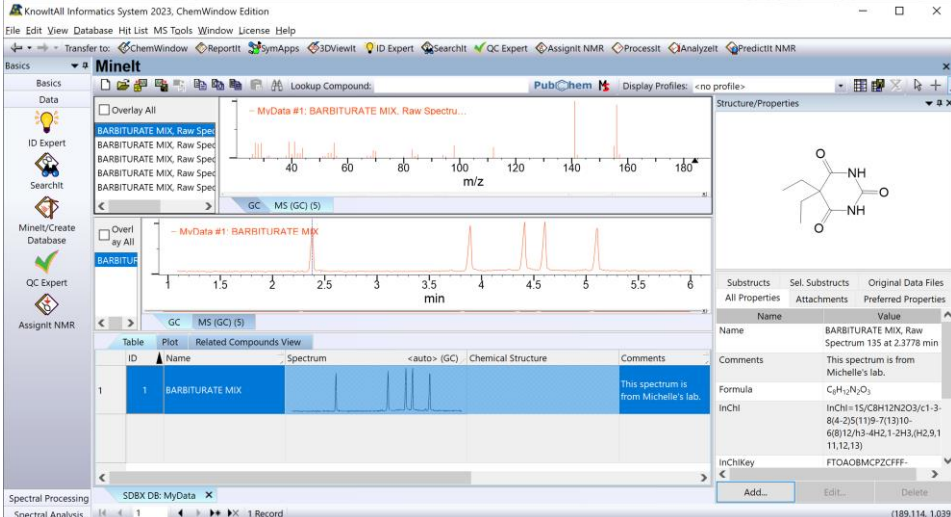
Spectral Processing SDBX DB: MyData

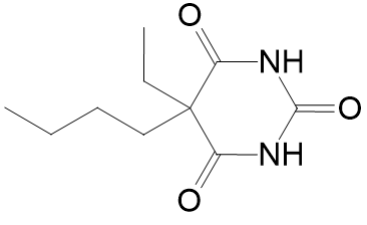
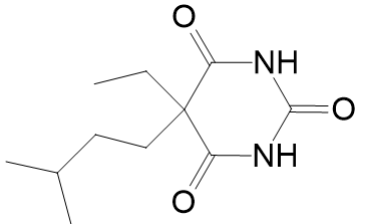
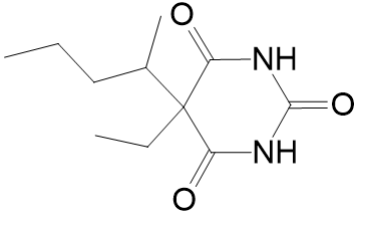
Spectral Analysis 1 1 Record

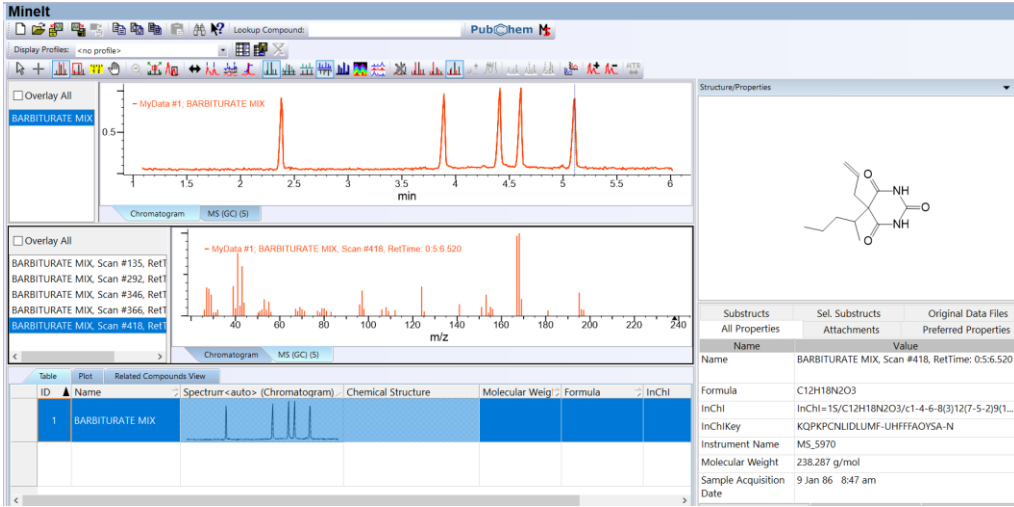
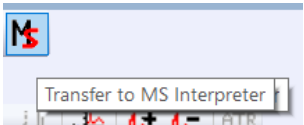
<p>5 Navigate to <b>Window &gt; Split twofold</b>.</p> <p>Select <b>MS</b> to be the technique showing in the top pane and <b>GC</b> to show in bottom pane.</p> <p>Mouse over GC scan pane.</p> <p><b>Right-click</b>, make sure mouse is in <b>Selection</b> mode.</p> <p>Click through GC peaks to show MS pane changing.</p>	 <p>KnowItAll Informatics System 2023, ChemWindow Edition</p> <p>File Edit View Database Hit List MS Tools Window License Help</p> <p>Transfer to: ChemWindow ReportIt ID Expert SearchIt QC Expert ProcessIt</p> <p>Basics Minelt</p> <p>Lookup Compound: PubChem Display</p> <p>Overlaid: GC MS (GC) (5)</p> <p>Overlaid: GC MS (GC) (5)</p> <table border="1"> <thead> <tr> <th>ID</th> <th>Name</th> <th>Spectrum</th> <th>&lt;auto&gt; (GC)</th> <th>Chemical Structure</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>BARBITURATE MIX</td> <td></td> <td></td> <td></td> </tr> </tbody> </table>	ID	Name	Spectrum	<auto> (GC)	Chemical Structure	1	BARBITURATE MIX					
ID	Name	Spectrum	<auto> (GC)	Chemical Structure									
1	BARBITURATE MIX												
<p>6 Click the MS spectrum pane to make it selected (black bordered).</p> <p>Highlight the first scan (make sure it has the black border).</p> <p>Click the <b>Add</b> button.</p>	 <p>Minelt</p> <p>Lookup Compound: PubChem Display Profiles: &lt;no profiles&gt;</p> <p>Property:</p> <ul style="list-style-type: none"> <li>%Bound - Human Plasma Protein</li> <li>%Bound - Human Plasma Protein Log</li> <li>%Bound - Rat Plasma Protein</li> <li>%Bound - Rat Plasma Protein Log</li> <li>%Remaining - Human Liver Microsomes</li> <li>%Remaining - Rat Liver Microsomes</li> <li>0-Order Phase Error</li> <li>1-Order Phase Error</li> <li>13CNMR Spectrometer Frequency</li> <li>1HNMR Spectrometer Frequency</li> <li>Abbreviation</li> <li>Adsorption Resistance</li> <li>Absolute Peak Position</li> <li>Absorption Maximum</li> <li>Accessory</li> <li>Acquisition Delay</li> <li>Acquisition Mode</li> <li>Acquisition Time</li> <li>Acronym</li> <li>Active Ingredients</li> <li>Activity Category ER_RBA</li> <li>Activity mg</li> <li>Activity mmol</li> <li>Actual Reference Signal Gain</li> <li>Actual Signal Gain</li> <li>Actual Signal Gain 2nd Channel</li> <li>Additional Data Treatment</li> <li>AddToParent</li> <li>Adhesive</li> <li>Algorithm</li> </ul> <table border="1"> <thead> <tr> <th>Name</th> <th>Value</th> </tr> </thead> <tbody> <tr> <td>Name</td> <td>BARBITURATE MIX, Raw Spectrum 135 at 2.3778 min</td> </tr> <tr> <td>Instrument Name</td> <td>MS_5970</td> </tr> <tr> <td>Retention Time</td> <td>2.37783 min</td> </tr> <tr> <td>Sample Acquisition Date</td> <td>9 Jan 86 8:47 am</td> </tr> <tr> <td>Sample Name</td> <td>BARBITURATE MIX</td> </tr> </tbody> </table> <p>SDBX DB: MyData X</p> <p>1 Record (5,926, -1,135)</p>	Name	Value	Name	BARBITURATE MIX, Raw Spectrum 135 at 2.3778 min	Instrument Name	MS_5970	Retention Time	2.37783 min	Sample Acquisition Date	9 Jan 86 8:47 am	Sample Name	BARBITURATE MIX
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Sample Name	BARBITURATE MIX												



<p>7</p>	<p>In the pop-up window, use the <b>Property</b> dropdown list to select a field. For example, <b>Comments</b>.</p> <p>Type in a value.</p> <p>Choose <b>This spectrum only</b>.</p>															
<p>8</p>		 <table border="1" data-bbox="1591 1008 1906 1325"> <thead> <tr> <th>Name</th> <th>Value</th> </tr> </thead> <tbody> <tr> <td>Name</td> <td>BARBITURATE MIX, Raw Spectrum 135 at 2.3778 min</td> </tr> <tr> <td>Comments</td> <td>This spectrum is from Michelle's lab.</td> </tr> <tr> <td>Instrument Name</td> <td>MS_5970</td> </tr> <tr> <td>Retention Time</td> <td>2.37783 min</td> </tr> <tr> <td>Sample Acquisition Date</td> <td>9 Jan 86 8:47 am</td> </tr> <tr> <td>Sample Name</td> <td>BARBITURATE MIX</td> </tr> </tbody> </table>	Name	Value	Name	BARBITURATE MIX, Raw Spectrum 135 at 2.3778 min	Comments	This spectrum is from Michelle's lab.	Instrument Name	MS_5970	Retention Time	2.37783 min	Sample Acquisition Date	9 Jan 86 8:47 am	Sample Name	BARBITURATE MIX
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Sample Name	BARBITURATE MIX															

<p>9 Select another MS spectrum.</p>	
<p>10 Highlight MS 135 from the available list.</p> <p><b>File &gt; Import.</b></p> <p>Navigate to <b>C:\Users\Public\Documents\Wiley\KnowItAll\Samples\GC-MS</b> folder</p> <p>Select <b>Structure 1 – Barbital.</b></p> <p>Click <b>Open.</b></p>	

11	<p>Highlight MS 292 from the available list.</p> <p><b>File &gt; Import.</b></p> <p>Select <b>Structure 2 – Butethal.</b></p> <p>Click <b>Open.</b></p>	 <p>The chemical structure of Butethal is a barbiturate derivative. It features a central carbon atom bonded to two nitrogen atoms, each with a carbonyl group (C=O). The central carbon is also bonded to a butyl group (CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>) and an ethyl group (CH<sub>2</sub>CH<sub>3</sub>).</p>
12	<p>Highlight MS 346 from available list.</p> <p><b>File &gt; Import.</b></p> <p>Select <b>Structure 3 – Amobarbital.</b></p> <p>Click <b>Open.</b></p>	 <p>The chemical structure of Amobarbital is a barbiturate derivative. It features a central carbon atom bonded to two nitrogen atoms, each with a carbonyl group (C=O). The central carbon is also bonded to an isopropyl group (CH(CH<sub>3</sub>)<sub>2</sub>) and a propyl group (CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>).</p>
13	<p>Highlight MS 366 from the available list.</p> <p><b>File &gt; Import.</b></p> <p>Select <b>Structure 4 – Pentaobarbital.</b></p> <p>Click <b>Open.</b></p>	 <p>The chemical structure of Pentaobarbital is a barbiturate derivative. It features a central carbon atom bonded to two nitrogen atoms, each with a carbonyl group (C=O). The central carbon is also bonded to a propyl group (CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>) and a butyl group (CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>).</p>

<p>14</p>	<p>Highlight MS 418 from the available list.</p> <p><b>File &gt; Import.</b></p> <p>Select <b>Structure 5 – Secobarbital.</b></p> <p>Click <b>Open.</b></p> <p>Navigate MS records to see the difference.</p>	 <p>The screenshot shows the Minelit software interface. At the top, there is a 'PubChem' logo and a 'Lookup Compound' field. Below this, there are two chromatograms. The top one is labeled '-MyData #1, BARBITURATE MIX' and shows a peak at approximately 2.5 minutes. The bottom one is labeled '-MyData #1, BARBITURATE MIX, Scan #418, RetTime: 0.5.6.529' and shows a peak at approximately 160 m/z. To the right, there is a 'Structure/Properties' panel showing the chemical structure of Secobarbital and a table of properties.</p> <table border="1" data-bbox="1360 576 1675 781"> <thead> <tr> <th colspan="2">Substructs</th> <th>Original Data Files</th> </tr> <tr> <th>All Properties</th> <th>Sel. Substructs Attachments</th> <th>Preferred Properties</th> </tr> <tr> <th>Name</th> <th colspan="2">Value</th> </tr> </thead> <tbody> <tr> <td>Name</td> <td colspan="2">BARBITURATE MIX, Scan #418, RetTime: 0.5.6.529</td> </tr> <tr> <td>Formula</td> <td colspan="2">C12H18N2O3</td> </tr> <tr> <td>InChI</td> <td colspan="2">InChI=1S/C12H18N2O3/c1-4-6-8(3)12(7-5-2)9(1...</td> </tr> <tr> <td>InChIKey</td> <td colspan="2">KQPKPCNLIDLUMF-UHFFFAOYSA-N</td> </tr> <tr> <td>Instrument Name</td> <td colspan="2">MS_5970</td> </tr> <tr> <td>Molecular Weight</td> <td colspan="2">238.287 g/mol</td> </tr> <tr> <td>Sample Acquisition Date</td> <td colspan="2">9 Jan 86 8:47 am</td> </tr> </tbody> </table>	Substructs		Original Data Files	All Properties	Sel. Substructs Attachments	Preferred Properties	Name	Value		Name	BARBITURATE MIX, Scan #418, RetTime: 0.5.6.529		Formula	C12H18N2O3		InChI	InChI=1S/C12H18N2O3/c1-4-6-8(3)12(7-5-2)9(1...		InChIKey	KQPKPCNLIDLUMF-UHFFFAOYSA-N		Instrument Name	MS_5970		Molecular Weight	238.287 g/mol		Sample Acquisition Date	9 Jan 86 8:47 am	
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<p>15</p>	<p>If MS Interpreter is installed: When a user database record has both MS spectrum and structure, the Transfer to MS Interpreter button is active.</p>	 <p>The screenshot shows a small window with a 'Transfer to MS Interpreter' button. The button is highlighted, indicating it is active.</p>																														

## Report Data Related Issues

In the 2025 release, KnowItAll users can submit feedback on data in **Minelt** if a user database is open.

	Action	Result
1	Open the <b>KnowItAll Informatics System</b> by double-clicking its icon on the desktop.	<p>The KnowItAll Informatics System automatically opens to the <b>Browselt</b> application. This application offers access to a web community designed especially for KnowItAll users and access to training movies and other information.</p> <p>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.</p> <p>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 Applications toolboxes).</p>
2	Click the <b>Minelt/Create Database</b> application in <b>Data</b> toolbox	
3	Use the <b>Help &gt; Submit Feedback</b> menu-item	
4	<p>A dialog box pops up</p> <ul style="list-style-type: none"> <li>• Enter your feedback</li> <li>• Check the agreement box</li> <li>• Submit</li> </ul>	<p>KnowItAll confirms the message submission:</p> 