

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 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.

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, researchers can improve their analyses.

Training Files Used in This Lesson

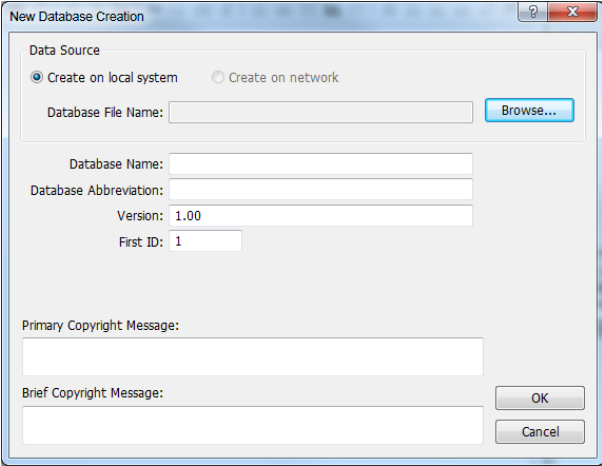
C:\Users\Public\Documents\Wiley\KnowItAll\Samples

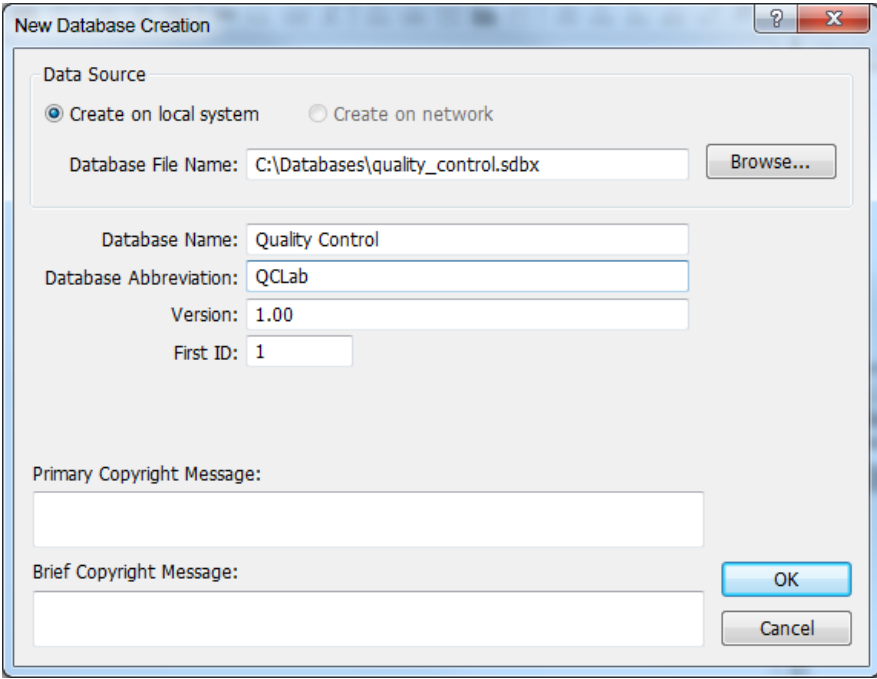
- \IR\Ethyl acetate.dx
- \Raman\Ethyl acetate.irf
- \Minelt\Import.csv
- MSDS Web Link.txt
- Ethyl acetate MSDS.pdf

KnowItAll Applications Used

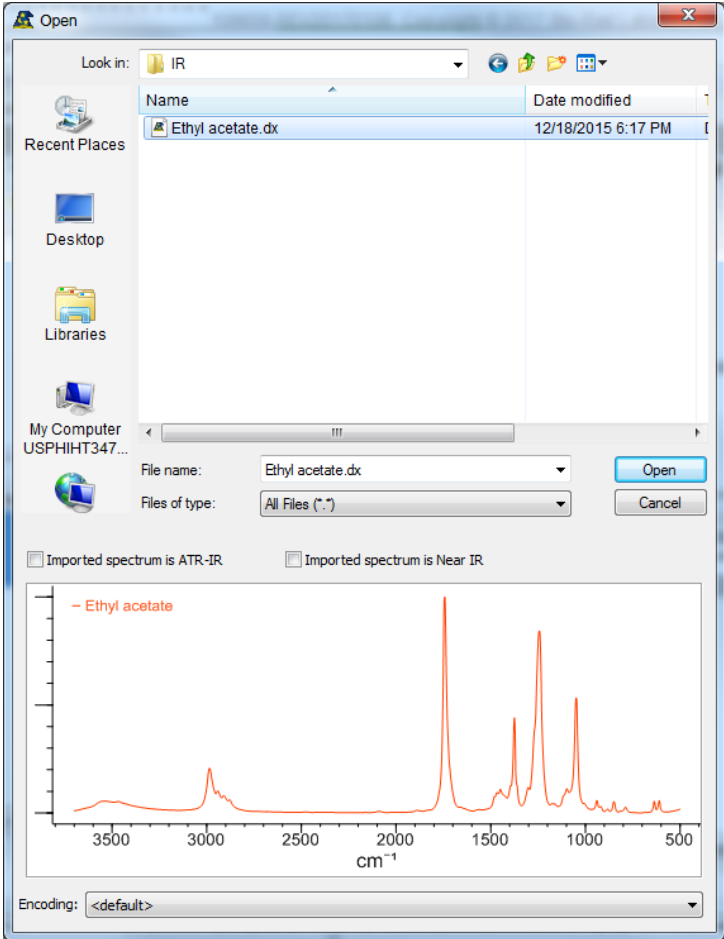
- Minelt™
- ChemWindow®
- Browselt™

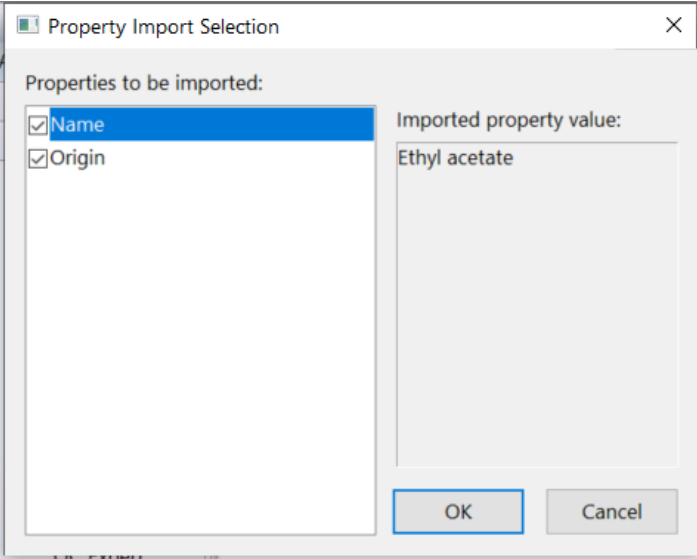
Create a user database

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

	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).

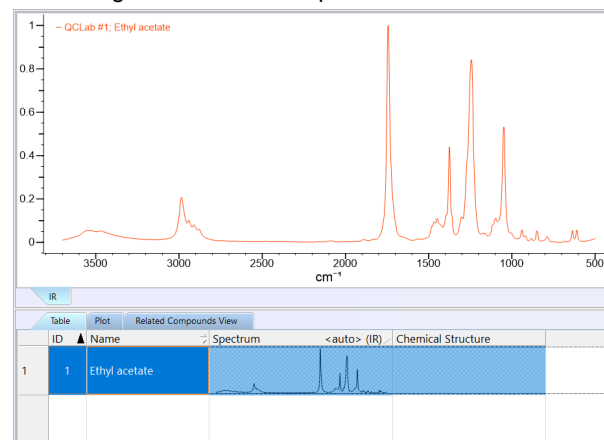
Add the first spectrum record to the user database

	Action	Result
1	<p>Create the first database record by importing a spectrum:</p> <ul style="list-style-type: none">• Choose File > Import or press Ctrl+I.• Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Sample s\IR folder• Open Ethyl acetate.dx. <p>Note: Use the Files of type filter to locate IRF, JCAMP and many other specific spectral files.</p>	<p>A Windows Open dialog box appears.</p>  <p>The screenshot shows a Windows 'Open' dialog box. The 'Look in:' field is set to 'IR'. The file list contains one entry: 'Ethyl acetate.dx' with a date modified of '12/18/2015 6:17 PM'. The 'File name:' field is filled with 'Ethyl acetate.dx' and the 'Files of type:' dropdown is set to 'All Files (*.*)'. Below the file list, there are two checkboxes: 'Imported spectrum is ATR-IR' and 'Imported spectrum is Near IR', both of which are unchecked. At the bottom of the dialog, there is a plot of the IR spectrum for 'Ethyl acetate'. The x-axis is labeled 'cm⁻¹' and ranges from 3500 to 500. The y-axis represents transmittance. The spectrum shows several characteristic absorption bands, including a sharp peak around 1735 cm⁻¹ and a strong, broad peak around 1100 cm⁻¹.</p>

	Action	Result
2	Click Open .	<p>The Property Import Selection 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>

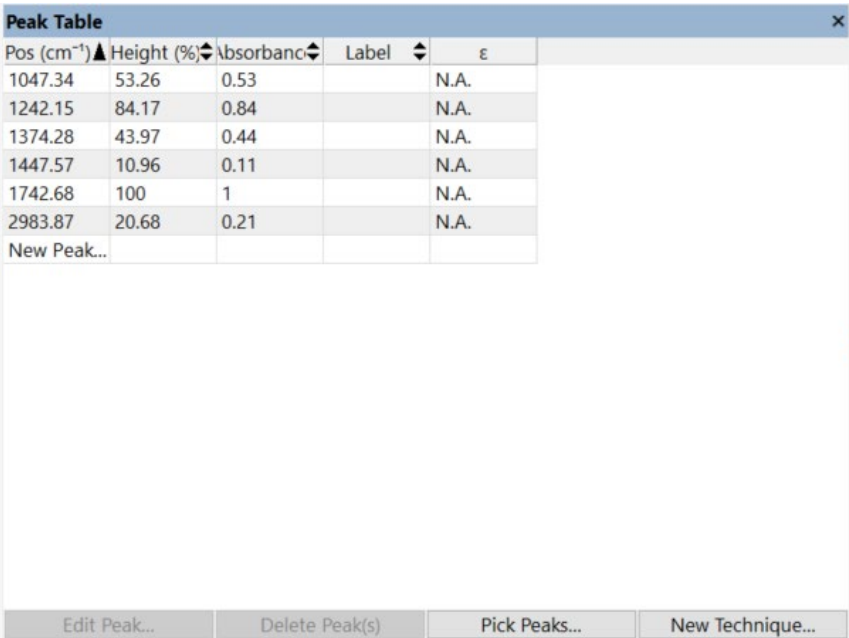
3 Click **OK**.

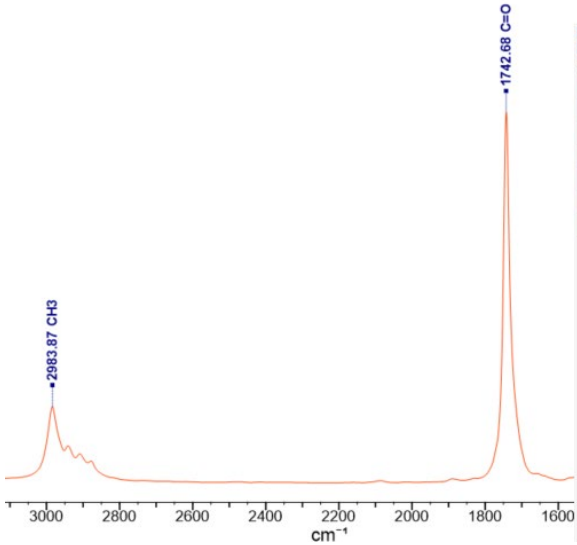
The dialog box closes. The spectrum has been added to the user database as the first record.



Add spectrum labels

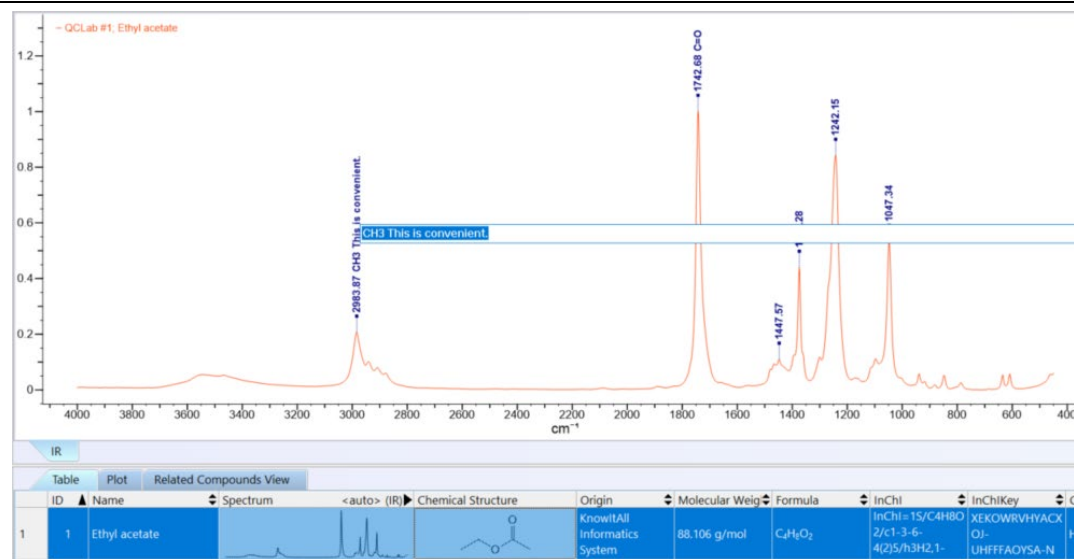
KnowItAll 2024 release has a new feature – users can add customized peak labels.

	Action	Result																																								
1	Continue with the above example Choose View > Windows/Tables > Peak Table to open the spectrum peak table	<p>Peak Table pops up in a window</p>  <table border="1"><thead><tr><th>Pos (cm⁻¹)</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> <p>Buttons: Edit Peak... Delete Peak(s) Pick Peaks... New Technique...</p>	Pos (cm ⁻¹)	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	One can directly type textual values into the Label column.	<p>The labels show up in spectral pane.</p>  <table border="1" data-bbox="1289 483 1629 690"> <caption>Peak Table</caption> <thead> <tr> <th>Pos (cm⁻¹)</th> <th>Height (%)</th> <th>Absorbanc</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> </tbody> </table> <p>New Peak...</p> <p>Edit Peak... Delete Peak(s)</p>	Pos (cm ⁻¹)	Height (%)	Absorbanc	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
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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

Transfer to: ChemWindow ReportIt

Choose the **Landscape** report template

Click **OK**

Select a Report Template X

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\...

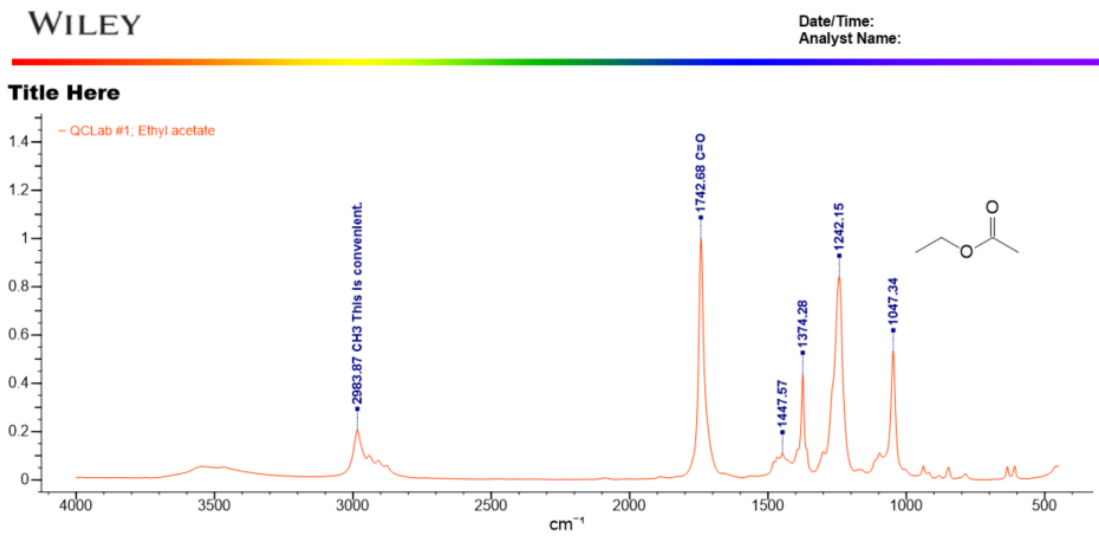
WILEY

Title Here Date/Time: Analyt Name

Name	Value
Formula	C ₁₀ H ₁₈ O
MW	158.25
Structure	C:\Users\Public\Documents\...
Reference Weight	158.25


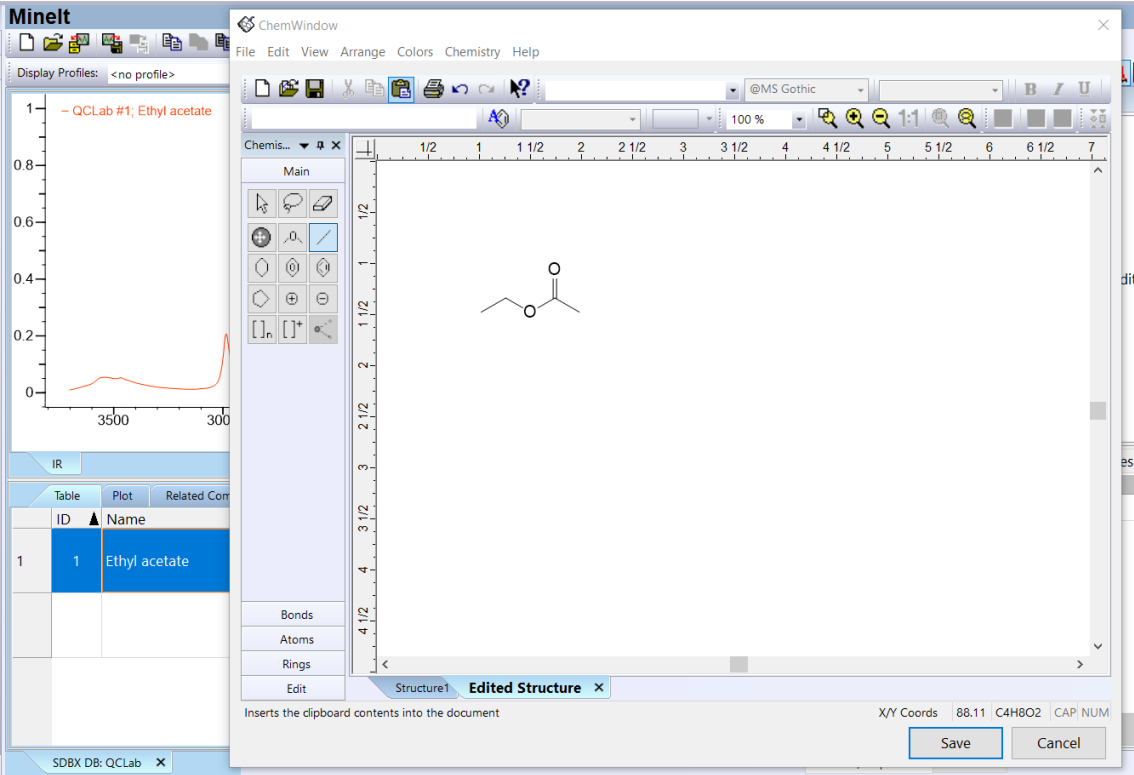
OK
Cancel

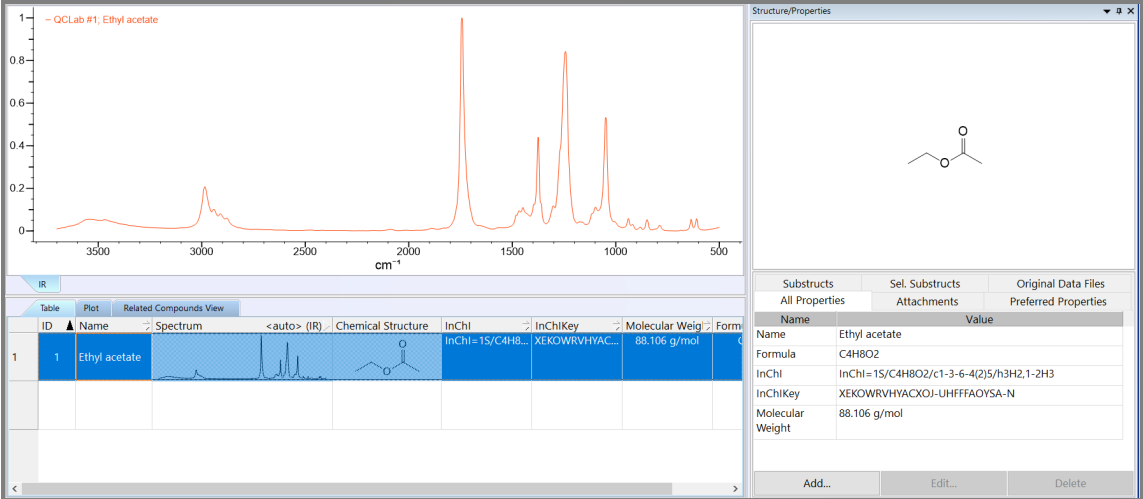
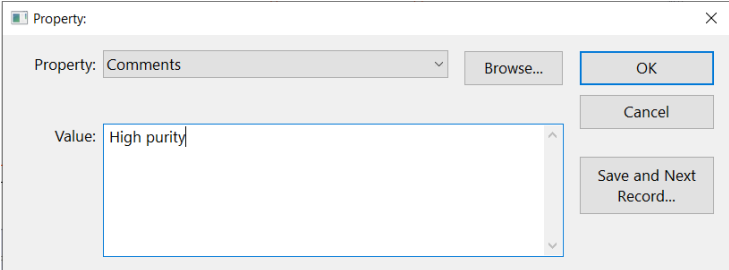
The peak labels ride along:



Name	Value
Name	Ethyl acetate
Comments	High purity
Formula	C ₄ H ₈ O 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

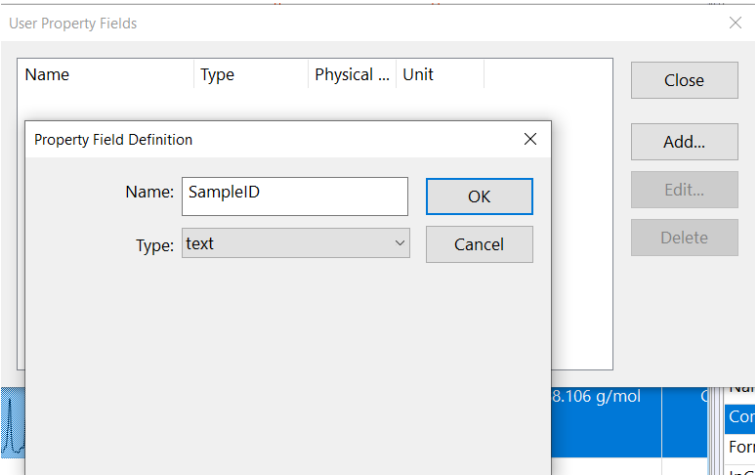
Add a chemical structure and properties to a database record

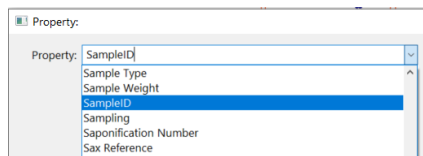
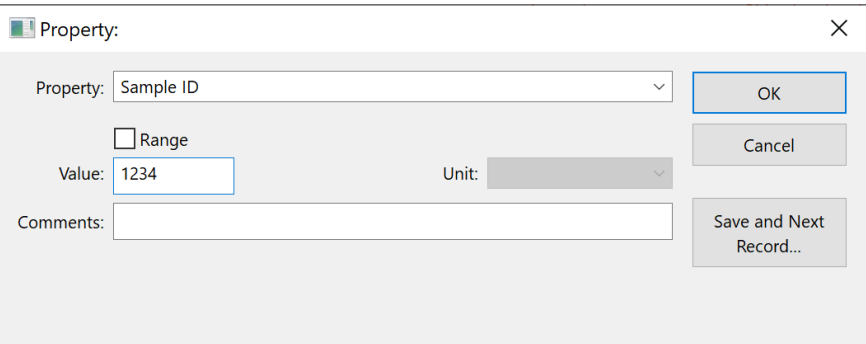
	Action	Result
1	<p>Go back to Minelt</p> <p>With the first record selected, double-click the Structure/Properties pane at the top right of the window (Double-click to edit structure in ChemWindow).</p>	<p>The Transfer to ChemWindow application pops up. Alternatively, you can use Transfer to: to go to the ChemWindow application.</p> 
2	<p>Use the drawing tools to create this structure.</p>	 <p>The screenshot shows the ChemWindow application with the chemical structure of ethyl acetate (<chem>CC(=O)OCC</chem>) displayed in the main drawing area. The interface includes a toolbar with drawing tools, a table with one record for 'Ethyl acetate', and an IR spectrum plot. The table has columns for ID and Name, with the first record having ID 1 and Name Ethyl acetate.</p>

	Action	Result
3	Click Save .	<p>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.</p>  <p>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.</p>
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.	

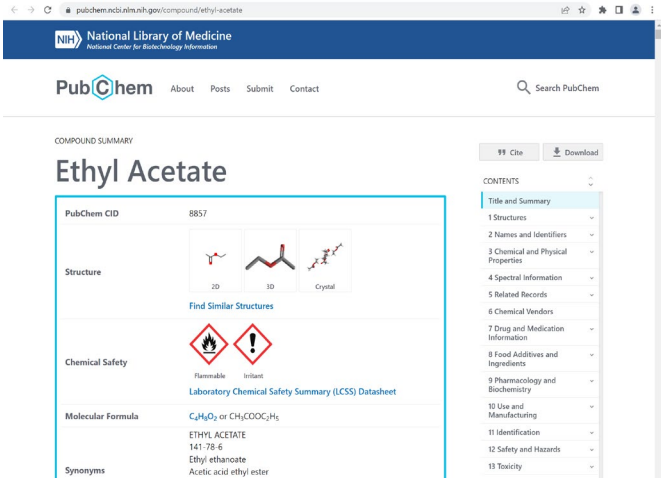
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6	Click OK .	<p>The Property dialog box closes, and the name and value of the added property appears in the Structure/Properties pane.</p> <table border="1" data-bbox="701 440 1394 808"> <thead> <tr> <th colspan="2" data-bbox="701 440 1394 472">Substructs</th> <th colspan="2" data-bbox="701 472 1394 505">Sel. Substructs</th> <th colspan="2" data-bbox="701 505 1394 537">Original Data Files</th> </tr> <tr> <th colspan="2" data-bbox="701 537 919 570">All Properties</th> <th colspan="2" data-bbox="919 537 1138 570">Attachments</th> <th colspan="2" data-bbox="1138 537 1394 570">Preferred Properties</th> </tr> <tr> <th data-bbox="701 570 856 602">Name</th> <th colspan="5" data-bbox="856 570 1394 602">Value</th> </tr> </thead> <tbody> <tr> <td data-bbox="701 602 856 634">Name</td> <td colspan="5" data-bbox="856 602 1394 634">Ethyl acetate</td> </tr> <tr> <td data-bbox="701 634 856 667">Comments</td> <td colspan="5" data-bbox="856 634 1394 667">High purity</td> </tr> <tr> <td data-bbox="701 667 856 699">Formula</td> <td colspan="5" data-bbox="856 667 1394 699">C4H8O2</td> </tr> <tr> <td data-bbox="701 699 856 732">InChI</td> <td colspan="5" data-bbox="856 699 1394 732">InChI=1S/C4H8O2/c1-3-6-4(2)5/h3H2,1-2H3</td> </tr> <tr> <td data-bbox="701 732 856 764">InChIKey</td> <td colspan="5" data-bbox="856 732 1394 764">XEKOWRVHYACXOJ-UHFFFAOYSA-N</td> </tr> <tr> <td data-bbox="701 764 856 797">Molecular Weight</td> <td colspan="5" data-bbox="856 764 1394 797">88.106 g/mol</td> </tr> </tbody> </table>	Substructs		Sel. Substructs		Original Data Files		All Properties		Attachments		Preferred Properties		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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	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

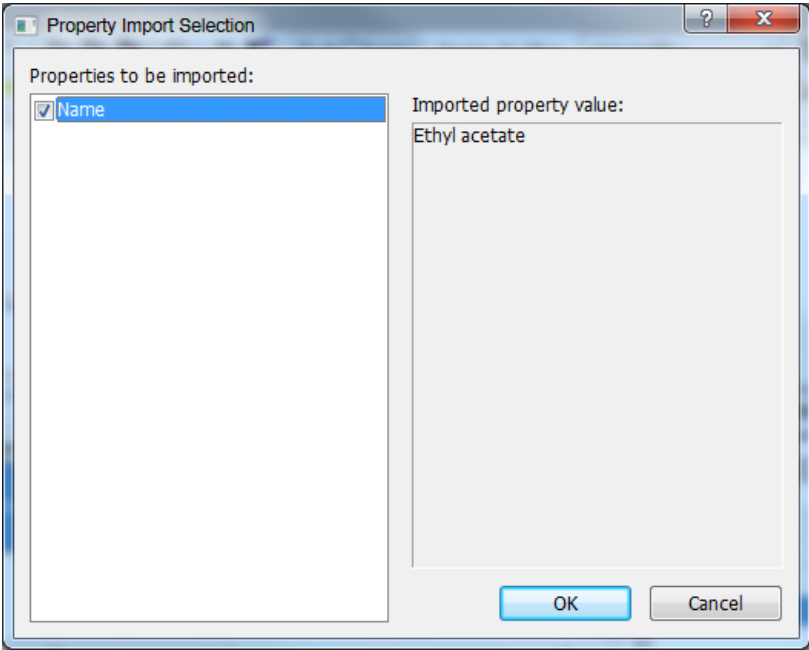
	Action	Result
1	Choose Database > Define User Property Fields .	The User Property Fields dialog box opens.
2	Click Add . Use the drop-down list to set Type to text. Enter the Name .	<p>The Property Field Definition dialog box opens.</p>  <p>Note: Which controls are available depends on which type of field is specified: numeric, text or enumeration.</p>
3	Click OK . Then click Close .	
4	Click Add in the Structure/Properties pane.	<p>The Property dialog box opens.</p> <p>Note: Choose View > Windows/Tables > Structure/Properties Table or press Alt+3 if the pane is not visible.</p>
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.

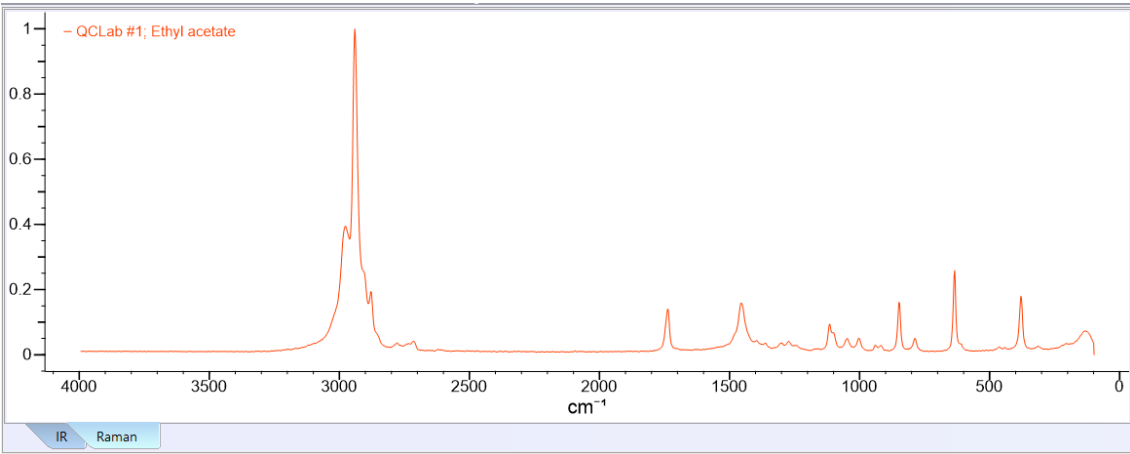
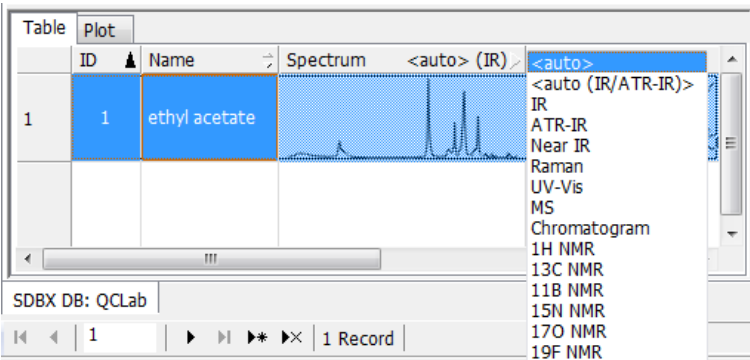
<p>6</p>	<p>Select SampleID</p> 	<p>The Value text box is added to the dialog. Note: Which text boxes are added depends on whether the property is numeric, text or enumeration.</p>
<p>7</p>	<p>Type '1234' in the Value text box.</p>	

8	Click OK .	<p>The dialog box closes. The property SampleID with value 1234 is added to the Structure/Properties pane for the first record.</p> <table border="1" data-bbox="703 373 1228 868"><tr><td>Substructs</td><td>Sel. Substructs</td><td>Original Data Files</td></tr><tr><td>All Properties</td><td>Attachments</td><td>Preferred Properties</td></tr><tr><th colspan="2">Name</th><th>Value</th></tr><tr><td colspan="2">Name</td><td>Ethyl acetate</td></tr><tr><td colspan="2">Comments</td><td>High purity</td></tr><tr><td colspan="2">Formula</td><td>C₄H₈O₂</td></tr><tr><td colspan="2">InChI</td><td>InChI=1S/C4H8O2/c1-3-6-4(2)5/h3H2,1-2H3</td></tr><tr><td colspan="2">InChIKey</td><td>XEKOWRVHYACXOJ-UHFFFAOYSA-N</td></tr><tr><td colspan="2">Molecular Weight</td><td>88.106 g/mol</td></tr><tr><td colspan="2">Sample ID</td><td>1234</td></tr><tr><td colspan="2">Add...</td><td>Edit... Delete</td></tr></table>	Substructs	Sel. Substructs	Original Data Files	All Properties	Attachments	Preferred Properties	Name		Value	Name		Ethyl acetate	Comments		High purity	Formula		C ₄ H ₈ O ₂	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	Add...		Edit... Delete
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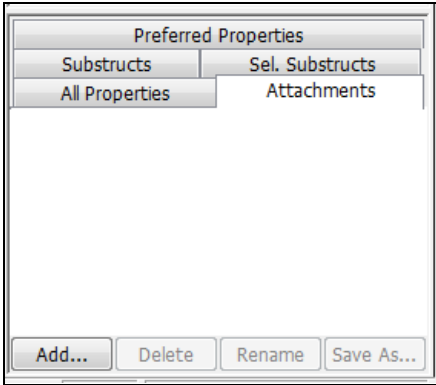
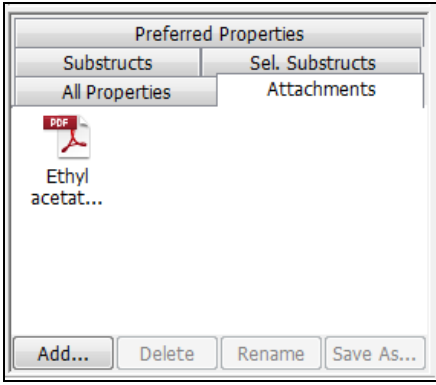
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9	<p>Repeat steps 1-8 to create the user property WebLink and display it in the Structure/Properties pane.</p> <p>Type 'https://pubchem.ncbi.nlm.nih.gov/compound/ethyl-acetate' in the Property dialog box's Value field.</p>	<p>The property WebLink with a web address is added to the Structure/Properties pane for the first record.</p> <table border="1" data-bbox="697 402 1092 808"> <thead> <tr> <th colspan="2">Substances</th> </tr> <tr> <th>Name</th> <th>Value</th> </tr> </thead> <tbody> <tr> <td>Name</td> <td>Ethyl acetate</td> </tr> <tr> <td>Comments</td> <td>High purity</td> </tr> <tr> <td>Formula</td> <td>C₄H₈O₂</td> </tr> <tr> <td>InChI</td> <td>InChI=1S/C4H8O2/c1-3-6-4(2)5/h3H2,1-2H3</td> </tr> <tr> <td>InChIKey</td> <td>XEKOWRVHYACXOJ-UHFFFAOYSA-N</td> </tr> <tr> <td>Molecular Weight</td> <td>88.106 g/mol</td> </tr> <tr> <td>Sample ID</td> <td>1234</td> </tr> <tr> <td>WebLink</td> <td>https://pubchem.ncbi.nlm.nih.gov/compound/ethyl-acetate</td> </tr> </tbody> </table>	Substances		Name	Value	Name	Ethyl acetate	Comments	High purity	Formula	C ₄ H ₈ O ₂	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
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10	<p>Click the web address in the Structure/Properties pane.</p>	<p>The web page opens.</p> 																				
11	<p>Click the KnowItAll Back button to return to the Minelt application.</p>																					

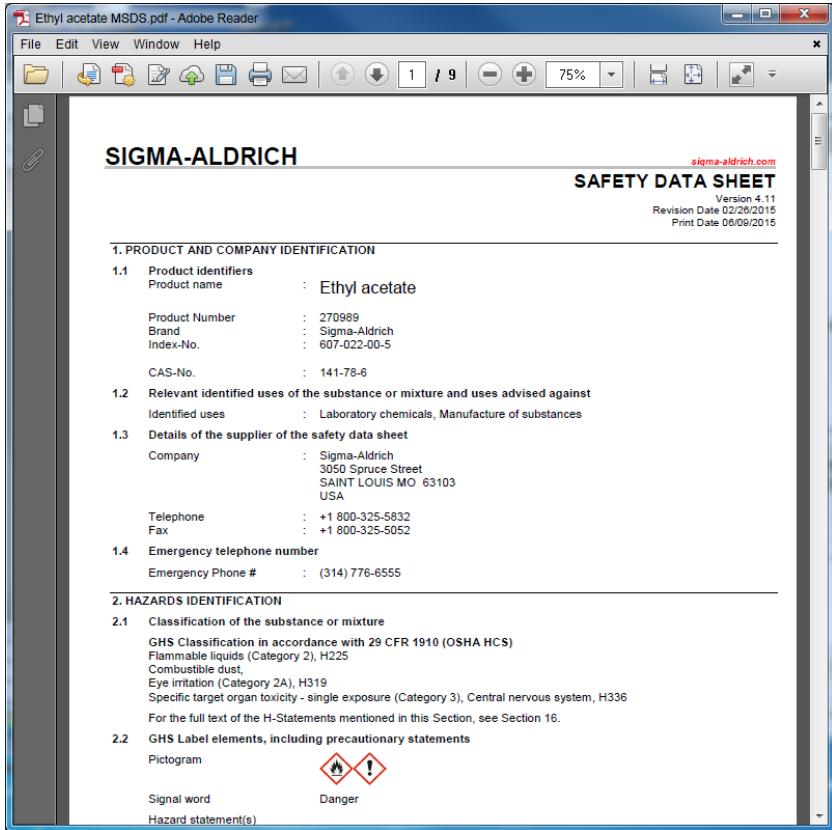

Add another spectrum (Raman) to the first database record

	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.  <p>This dialog box appears when you transfer information into a user database. All available properties are shown.</p>

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

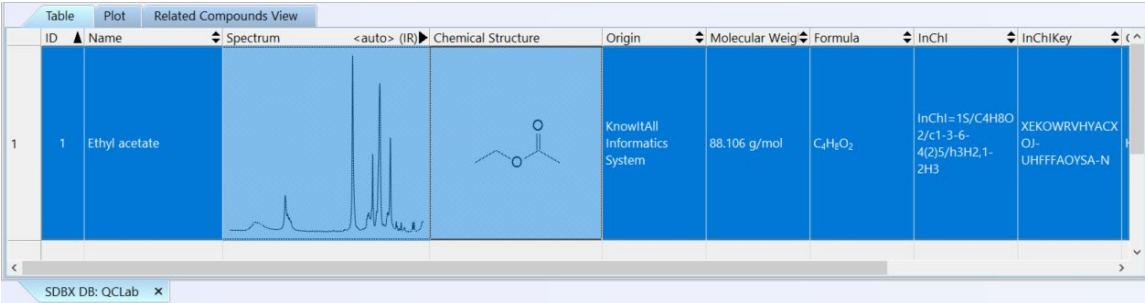

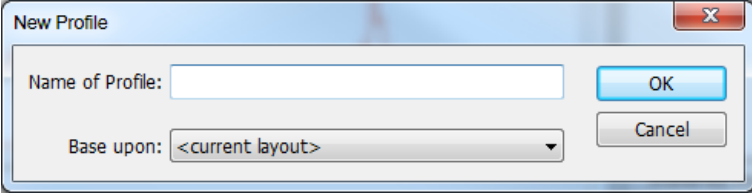
Add an attachment to the first database record

	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\Minelt 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.	<p>The document opens in its native application—in this case, Adobe Acrobat.</p>  <p>SIGMA-ALDRICH <small>sigma-aldrich.com</small> SAFETY DATA SHEET Version 4.11 Revision Date 02/26/2015 Print Date 06/06/2015</p> <p>1. PRODUCT AND COMPANY IDENTIFICATION</p> <p>1.1 Product Identifiers Product name : Ethyl acetate Product Number : 270989 Brand : Sigma-Aldrich Index-No. : 607-022-00-5 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 Telephone : +1 800-325-5832 Fax : +1 800-325-5052</p> <p>1.4 Emergency telephone number Emergency Phone # : (314) 776-6555</p> <p>2. HAZARDS IDENTIFICATION</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  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**.

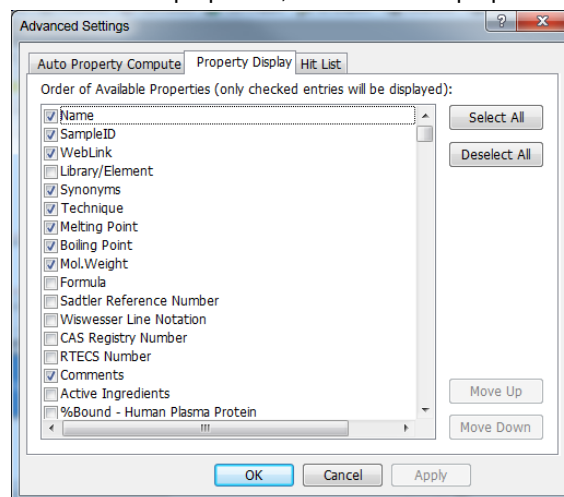
Create a new Minelt display profile

	Action	Result
1	One should the table row height to satisfactory first.	<p>For example, make a row a lot taller:</p> 
1	Click the Add a New Profile button  in the Profile toolbar.	<p>The New Profile dialog box opens.</p> 
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 Minelt 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

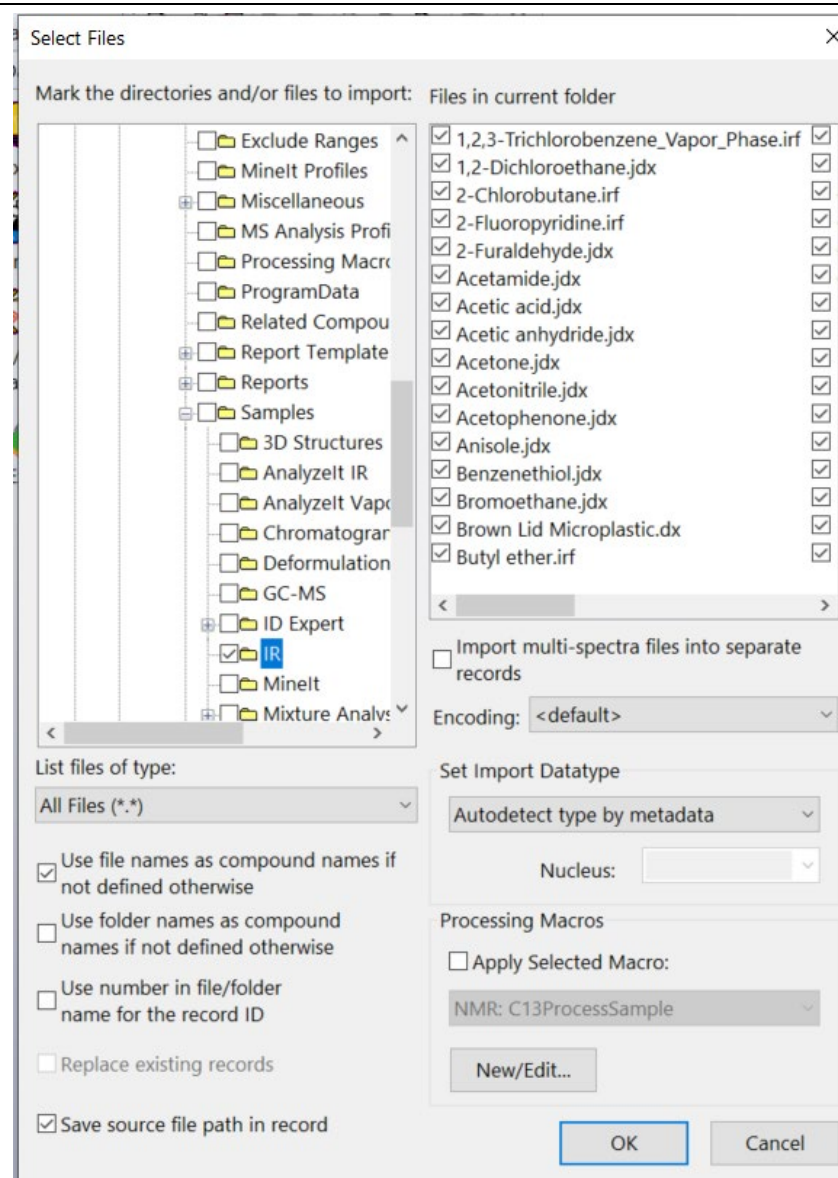
	Action	Result
1	Create a new empty database as in the above example.	

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\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:

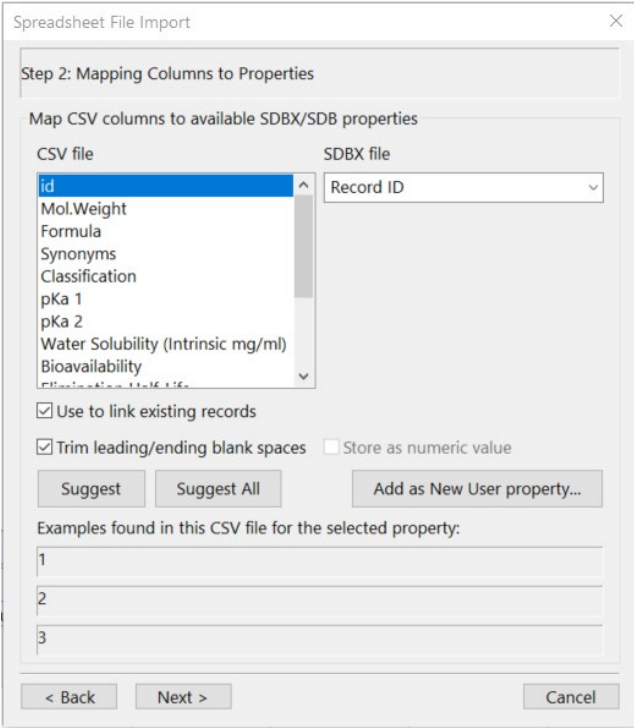
Layout

File Contains Header Line:

Delimiting Character: Encoding:

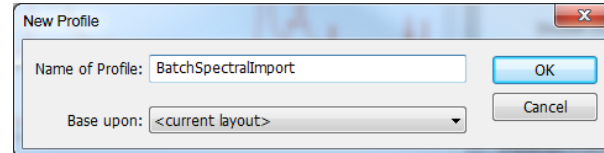
id	Name	CAS Registry ...	Synonyms
1	1, 2-Dichloro...	107-06-2	Ethylene chlo...
2	2-Chlorobuta...	78-86-4	sec-Butyl chl...
3	2-Fluoropyridi...	372-48-5	o-Fluoropyrid...
4	2-Furaldehyde	98-01-1	Furfural
5	Acetamide	60-35-5	Ethanamide
6	Acetic acid	64-19-7	Ethanoic acid
7	Acetic anhydr...	108-24-7	Ethanoic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

The file was analyzed successfully (34 rows read).

	Action	Result
4	<p>Click Suggest All, then review the automatic field matches.</p> <p>Click on id in CSV file, confirm the SDBX file reads Record ID. 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 Use to link existing records if not already checked.</p> <p>Click Next.</p>	
5	<p>Click Finish.</p> <p>You do not have to Compact database now at the prompt.</p>	<p>The database now has fields Synonyms and CAS Registry Number populated by the CSV file.</p>


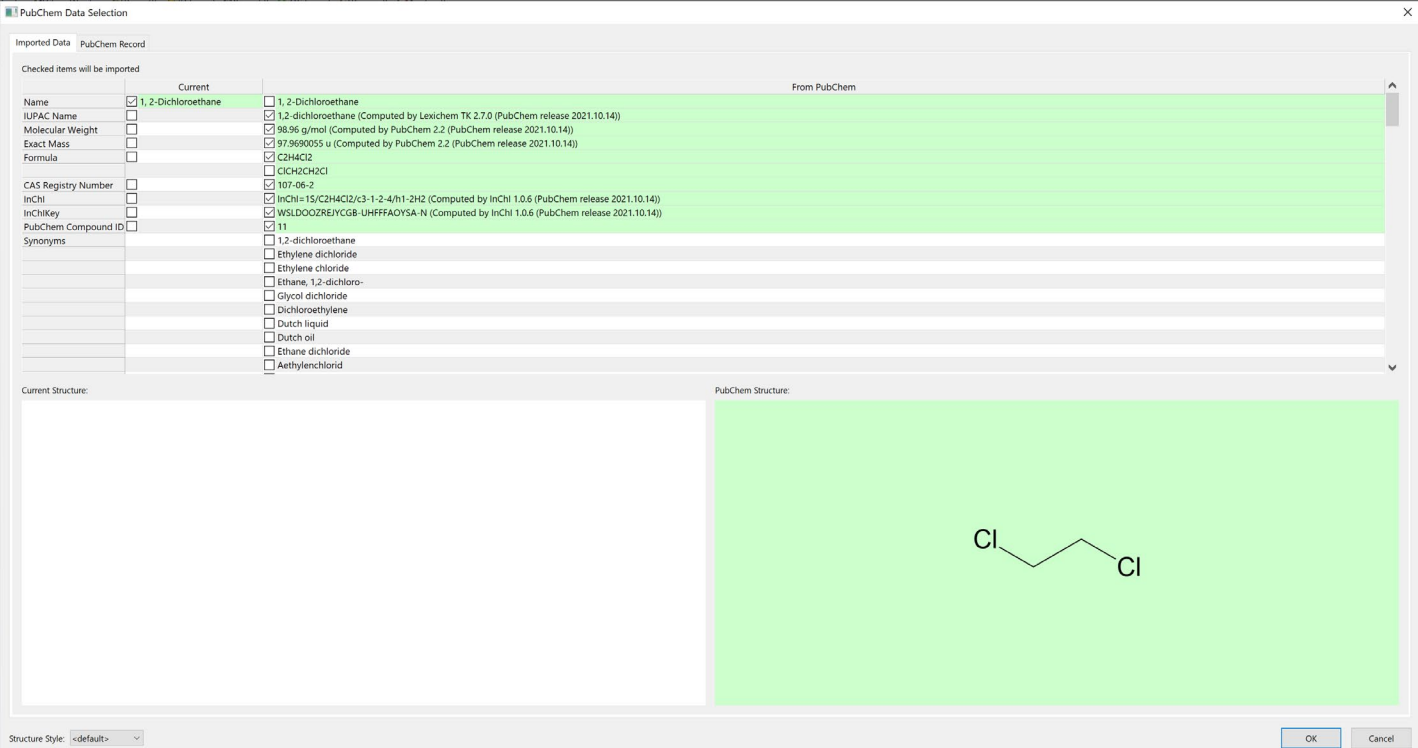
TIP

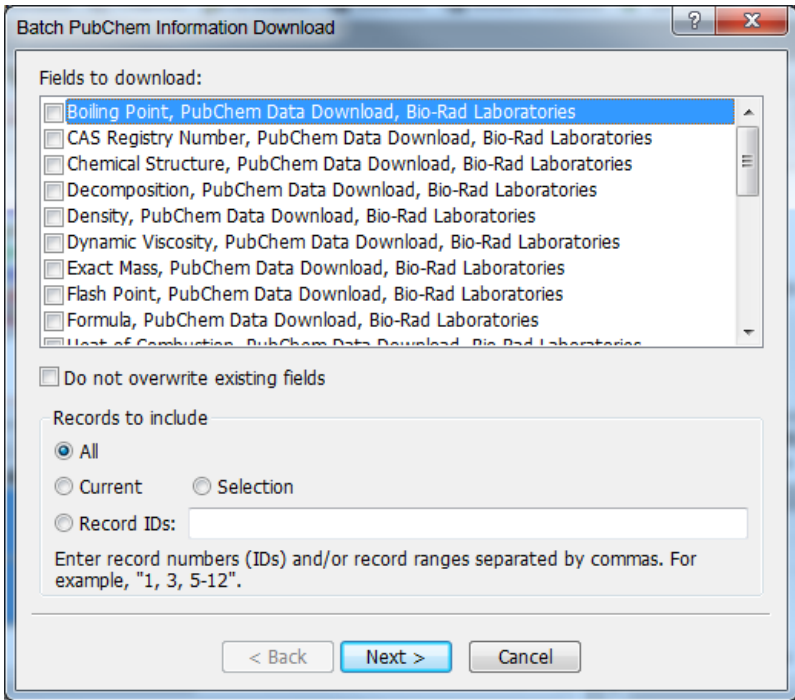
You can rearrange the spreadsheet portion of this database (for example, to get rid of empty structure columns, right-click and choose **Delete Columns**). When edits are completed, you can save this column arrangement as a **Minelt** profile. Click **Save Current Profile** on the **Profile** toolbar,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



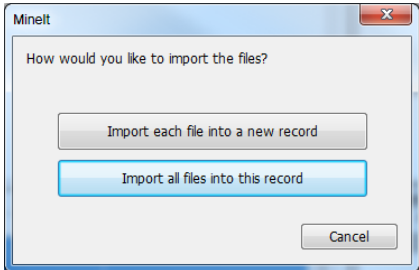
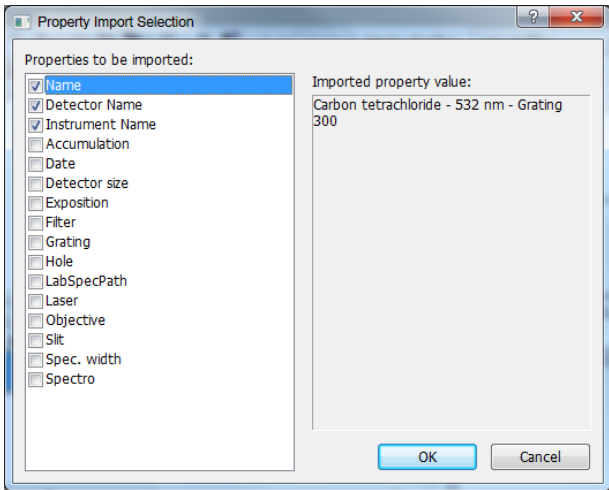
This profile will be linked with this database. It can also be selected for use with other databases.

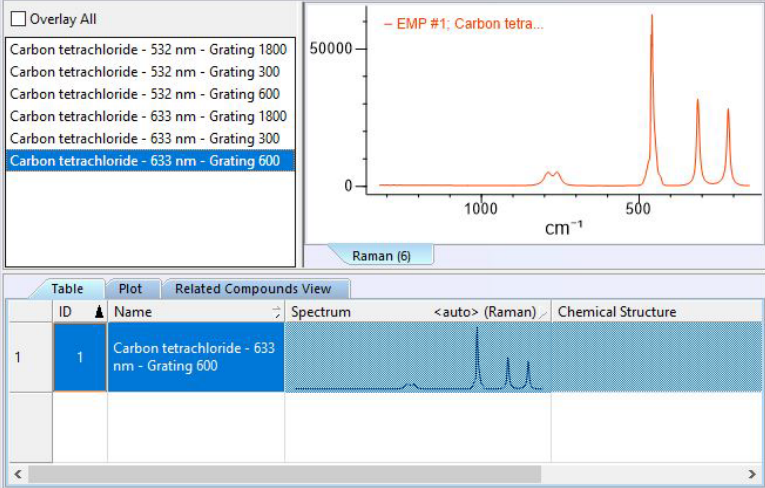
Batch Import: many spectra, many records, import properties from PubChem

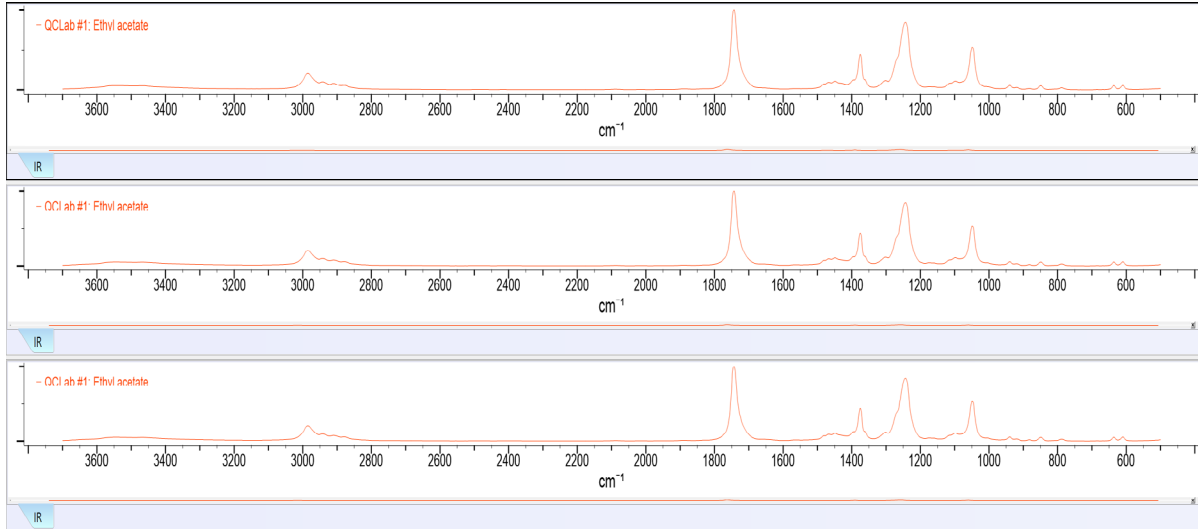
	Action	Result
1	<p>Select the first record from the above database, click the PubChem toolbar button.</p> 	<p>PubChem records are searched. If information is located, the PubChem Data Selection dialog box opens.</p> 

	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 .	<p>The Batch PubChem Information Download dialog box opens.</p> 
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	<p>Choose File > Import.</p> <p>Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Raman folder</p> <p>Select all .DX files in the folder.</p> <p>Click Open.</p>	<p>A dialog box opens and asks how you want to import the files.</p> 
3	Click Import all files into this record .	<p>The Property Import Selection dialog opens.</p>  <p>Check the properties you wish to import.</p>

	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.	<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"> Carbon tetrachloride - 532 nm - Grating 1800 Carbon tetrachloride - 532 nm - Grating 300 Carbon tetrachloride - 532 nm - Grating 600 Carbon tetrachloride - 633 nm - Grating 1800 Carbon tetrachloride - 633 nm - Grating 300 Carbon tetrachloride - 633 nm - Grating 600 (highlighted) <p>The plot shows a Raman spectrum for Carbon tetrachloride with a y-axis labeled '50000' and an x-axis labeled 'cm⁻¹'. The plot title is '- EMP #1: Carbon tetra...'. The plot shows several peaks, with the most prominent one around 500 cm⁻¹.</p> <p>Below the plot is a table with the following columns: ID, Name, Spectrum, <auto> (Raman), and Chemical Structure. The first row is highlighted and contains the following data:</p> <table border="1"> <thead> <tr> <th>ID</th> <th>Name</th> <th>Spectrum</th> <th><auto> (Raman)</th> <th>Chemical Structure</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>Carbon tetrachloride - 633 nm - Grating 600</td> <td></td> <td></td> <td></td> </tr> </tbody> </table>	ID	Name	Spectrum	<auto> (Raman)	Chemical Structure	1	Carbon tetrachloride - 633 nm - Grating 600			
ID	Name	Spectrum	<auto> (Raman)	Chemical Structure								
1	Carbon tetrachloride - 633 nm - Grating 600											
6	Click the name of a spectrum in the left pane to display it.											

	Action	Result
7	Choose Window > Split Threefold .	<p>The Spectral 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.

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

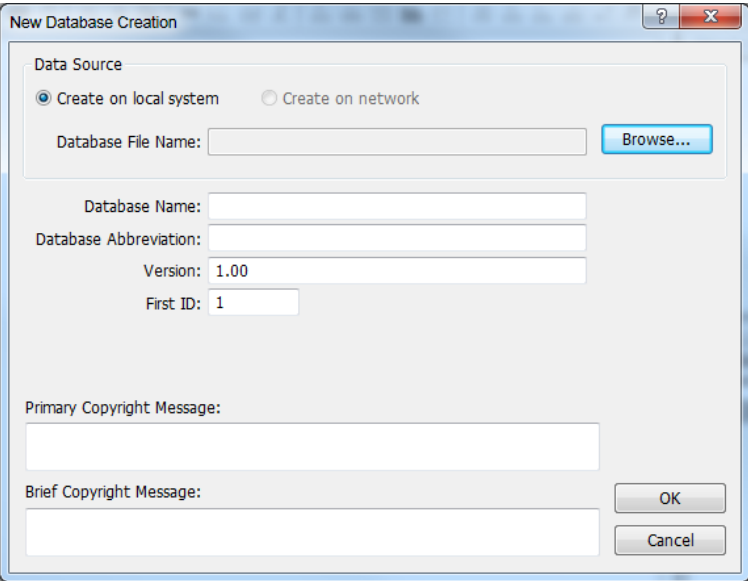
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Structures folder

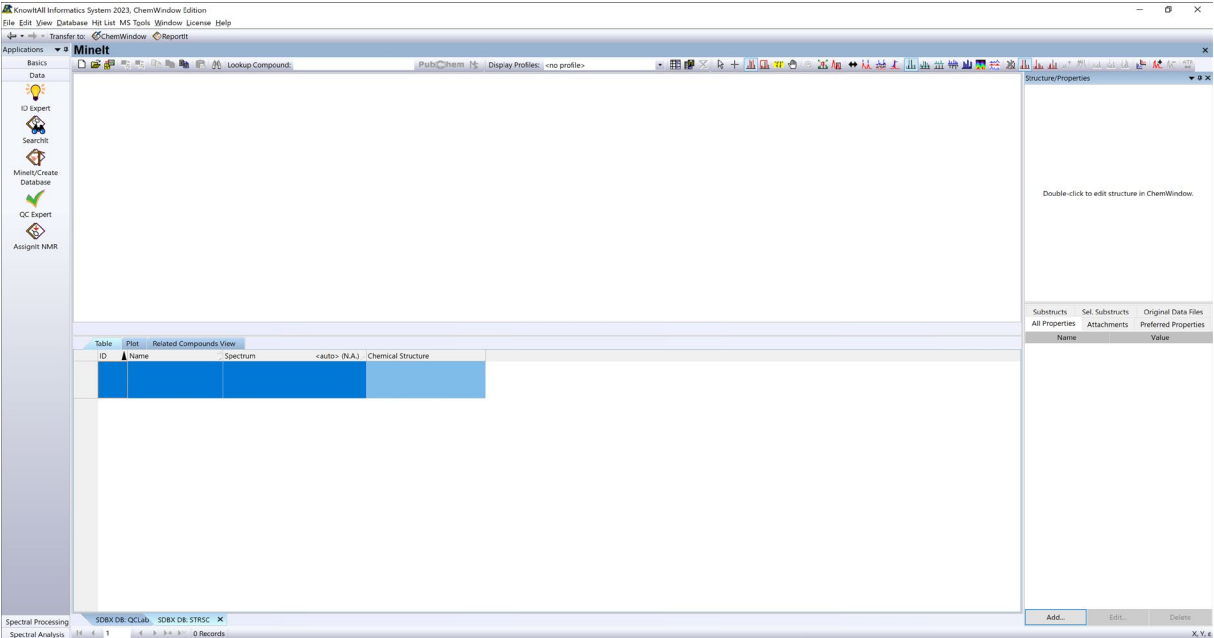
- benzylpenicillin.dsf


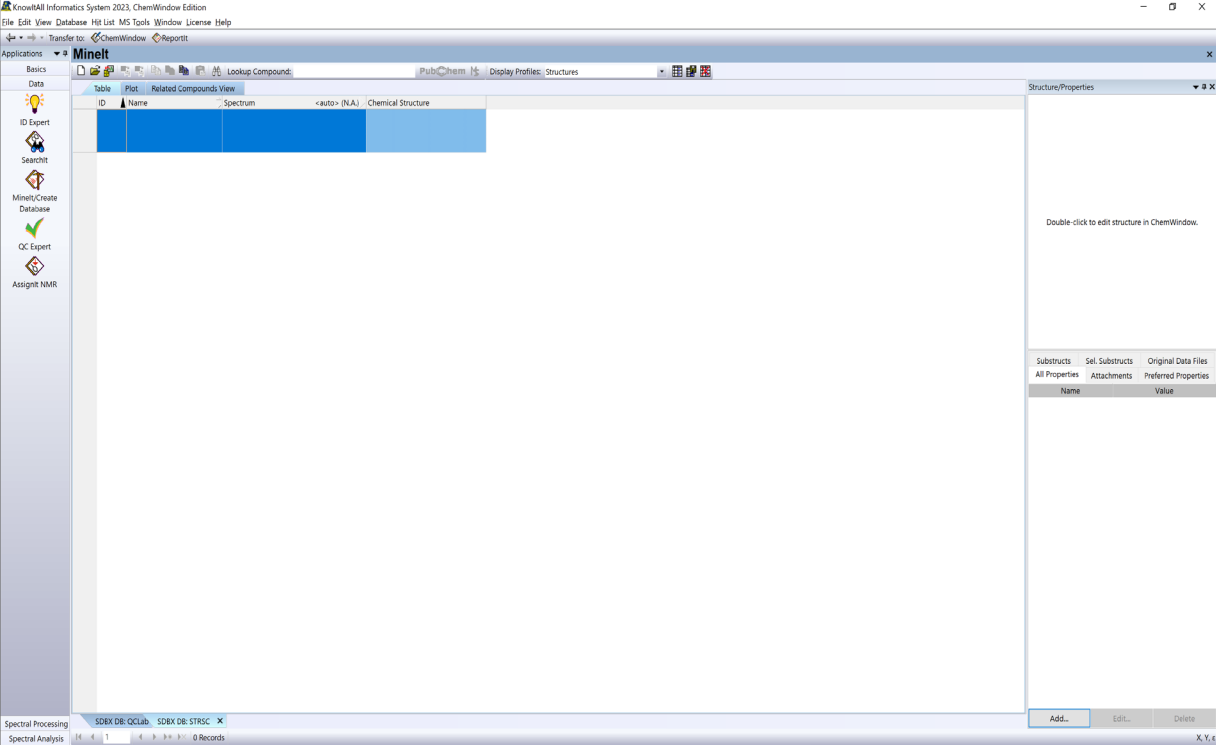
KnowItAll Applications Used

- Minelt™
- ChemWindow®

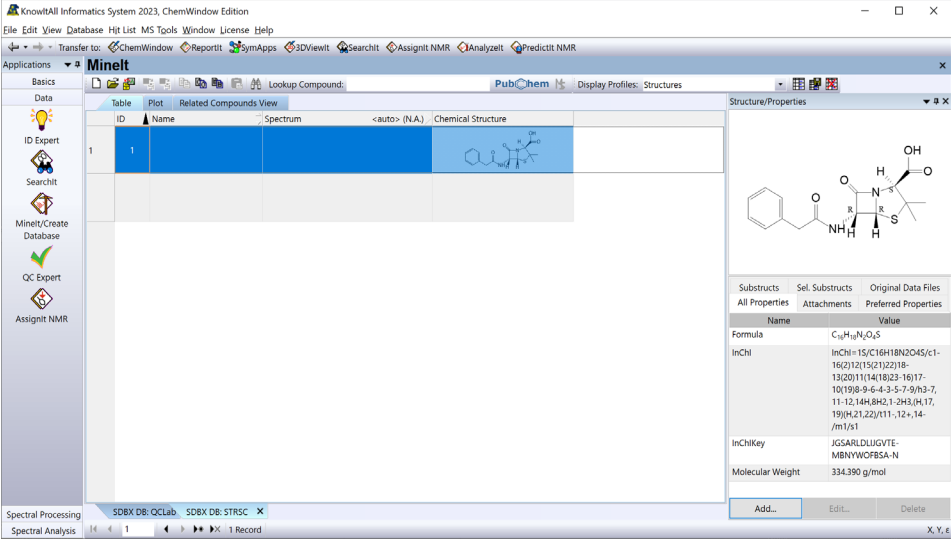
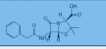
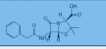
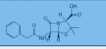
Create a user database

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

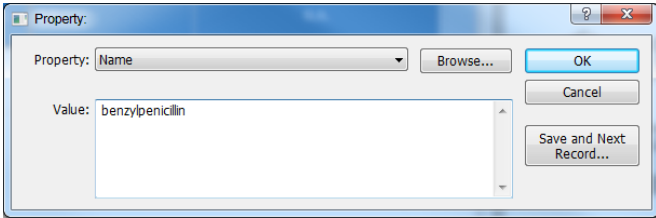
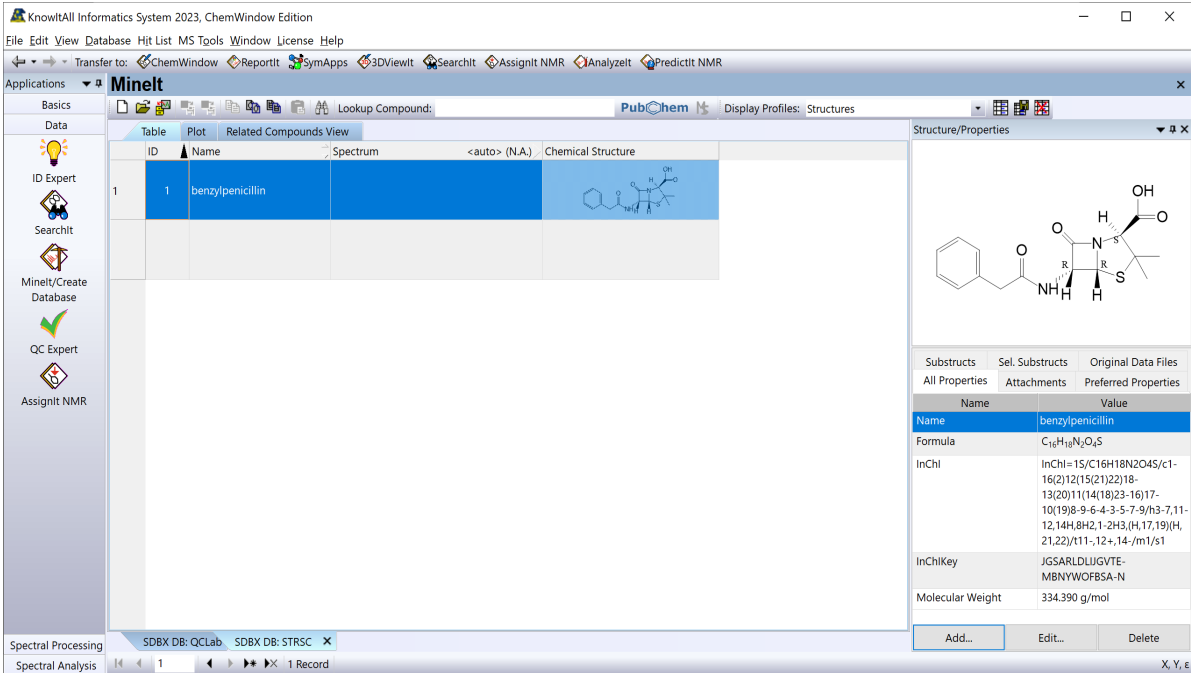
	Action	Result
5	Type 'STRSC' in the Database Abbreviation text box. Note: The abbreviation must be 3-7 characters long.	
6	Click OK .	<p>The new database has been created to receive your data. The Database Abbreviation appears on the database tab.</p> 
7	Choose View > Windows/Tables > Spectrum Pane to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

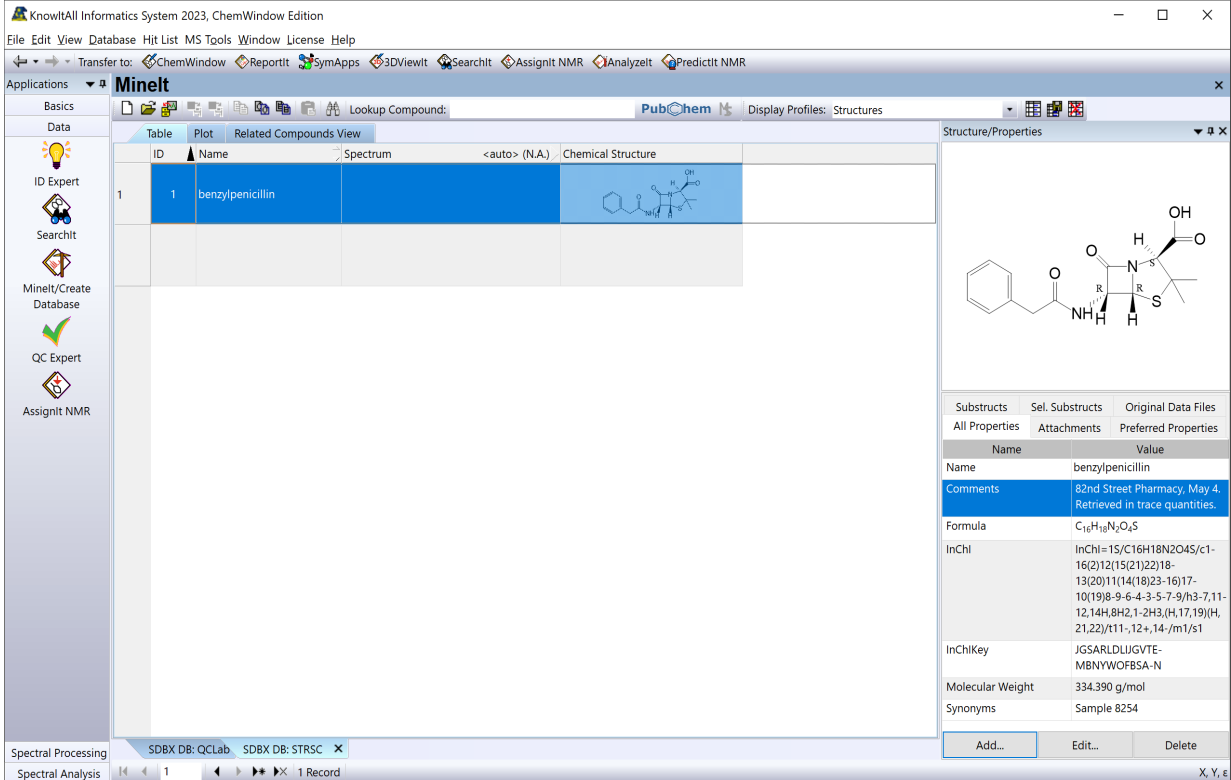
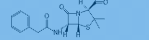
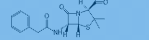
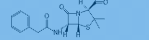
	Action	Result
8	<p>Click the Add a New Profile toolbar button , type the name 'Structures' in the New Profile dialog box, then click OK.</p>	 <p>The screenshot displays the KnowItAll Informatics System 2023, ChemWindow Edition interface. The main window shows a table with columns 'ID', 'Name', and 'Spectrum'. The 'Name' column is highlighted in blue. The status bar at the bottom indicates 'SDBX DB: OCLab' and 'SDBX DB: STRSC'. The 'Add...' button is visible in the bottom right corner.</p>

Add a structure to the first database record

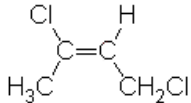
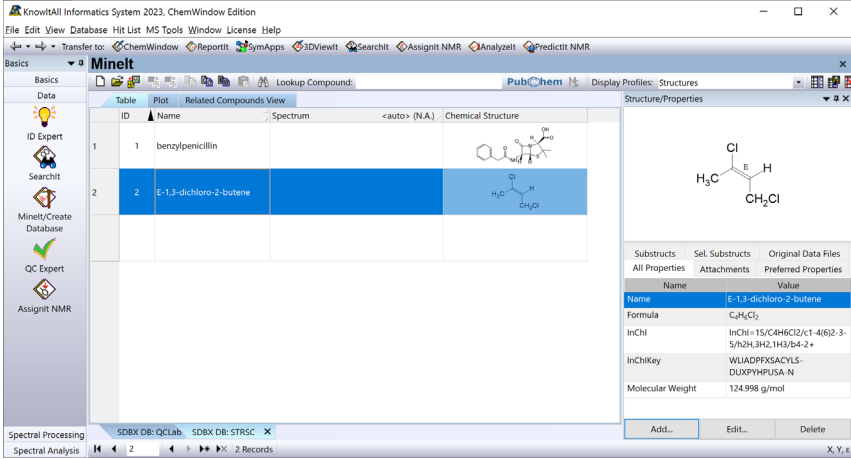
	Action	Result																		
1	<p>Choose File > Import</p> <p>Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Structures folder</p> <p>Open the structure file Benzylpenicillin.dsf.</p>	<p>The structure is displayed in the Structure/Properties pane.</p>  <p>The screenshot shows the 'Minelt' application window. The main area contains a table with the following data:</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></td> <td></td> <td></td> </tr> </tbody> </table> <p>The right-hand pane, titled 'Structure/Properties', displays the chemical structure of Benzylpenicillin and its properties:</p> <table border="1"> <thead> <tr> <th>Name</th> <th>Value</th> </tr> </thead> <tbody> <tr> <td>Formula</td> <td>C₁₆H₁₈N₂O₅S</td> </tr> <tr> <td>InChI</td> <td>InChI=1S/C16H18N2O5/c1-16(2)12(15)2(1)2(1)8-13(20)11(14)18(23-16)17-10(19)8-9-6-4-3-5-7-9/h3-7,11-12,14H,8H2,1-2H3,(H,17,19)(H,21,22)(H11-12-,14-m)1/51</td> </tr> <tr> <td>InChIKey</td> <td>JCSARLDLUGVTE-MBNYWOFBSA-N</td> </tr> <tr> <td>Molecular Weight</td> <td>334.390 g/mol</td> </tr> </tbody> </table>	ID	Name	Spectrum	Chemical Structure	1				Name	Value	Formula	C ₁₆ H ₁₈ N ₂ O ₅ S	InChI	InChI=1S/C16H18N2O5/c1-16(2)12(15)2(1)2(1)8-13(20)11(14)18(23-16)17-10(19)8-9-6-4-3-5-7-9/h3-7,11-12,14H,8H2,1-2H3,(H,17,19)(H,21,22)(H11-12-,14-m)1/51	InChIKey	JCSARLDLUGVTE-MBNYWOFBSA-N	Molecular Weight	334.390 g/mol
ID	Name	Spectrum	Chemical Structure																	
1																				
Name	Value																			
Formula	C ₁₆ H ₁₈ N ₂ O ₅ S																			
InChI	InChI=1S/C16H18N2O5/c1-16(2)12(15)2(1)2(1)8-13(20)11(14)18(23-16)17-10(19)8-9-6-4-3-5-7-9/h3-7,11-12,14H,8H2,1-2H3,(H,17,19)(H,21,22)(H11-12-,14-m)1/51																			
InChIKey	JCSARLDLUGVTE-MBNYWOFBSA-N																			
Molecular Weight	334.390 g/mol																			
2	<p>Open the View menu and check Stereochemistry if it is not already checked.</p>	<p>Stereochemical descriptors are shown on the structure when Stereochemistry is enabled on the View menu.</p>																		

Add properties to a database record

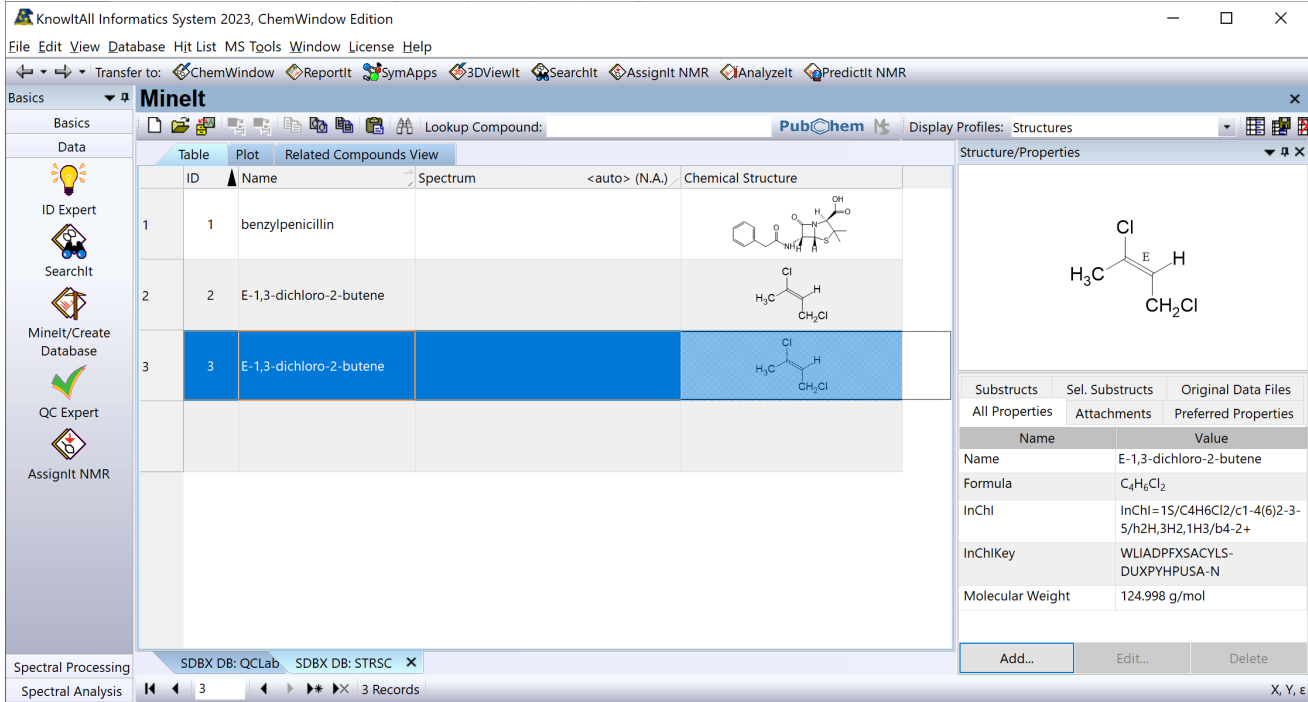
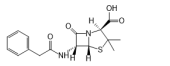
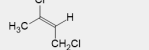
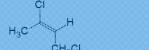
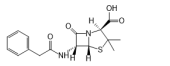
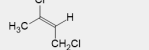
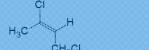
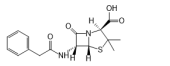
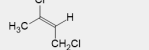
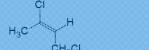
	Action	Result																		
1	Click Add in the Structure/Properties pane.	The Property dialog box opens.																		
2	Select the property Name , then type 'benzylpenicillin' in the Value text box.																			
3	Click OK .	<p>The Property dialog box closes, and the added property Name appears in the Structure/Properties pane.</p>  <table border="1" data-bbox="1591 1068 1871 1360"> <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>C₁₈H₁₆N₂O₄S</td> <td></td> </tr> <tr> <td>InChI</td> <td>InChI=1S/C16H18N2O4S/c1-16(2)2(15(2)2)18-13(20)1(14(18)23-16)17-10(19)8-9-6-4-3-5-7-9/h3-7,11-12,14h,8h2,1-2h3,(4,17,19)/H,21,22/11-,12+,-/m/1/s1</td> <td></td> </tr> <tr> <td>InChIKey</td> <td>JGSARLDLJGVTI-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 ₁₈ H ₁₆ N ₂ O ₄ S		InChI	InChI=1S/C16H18N2O4S/c1-16(2)2(15(2)2)18-13(20)1(14(18)23-16)17-10(19)8-9-6-4-3-5-7-9/h3-7,11-12,14h,8h2,1-2h3,(4,17,19)/H,21,22/11-,12+,-/m/1/s1		InChIKey	JGSARLDLJGVTI-MBNYWOFBSA-N		Molecular Weight	334.390 g/mol	
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Molecular Weight	334.390 g/mol																			

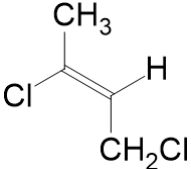
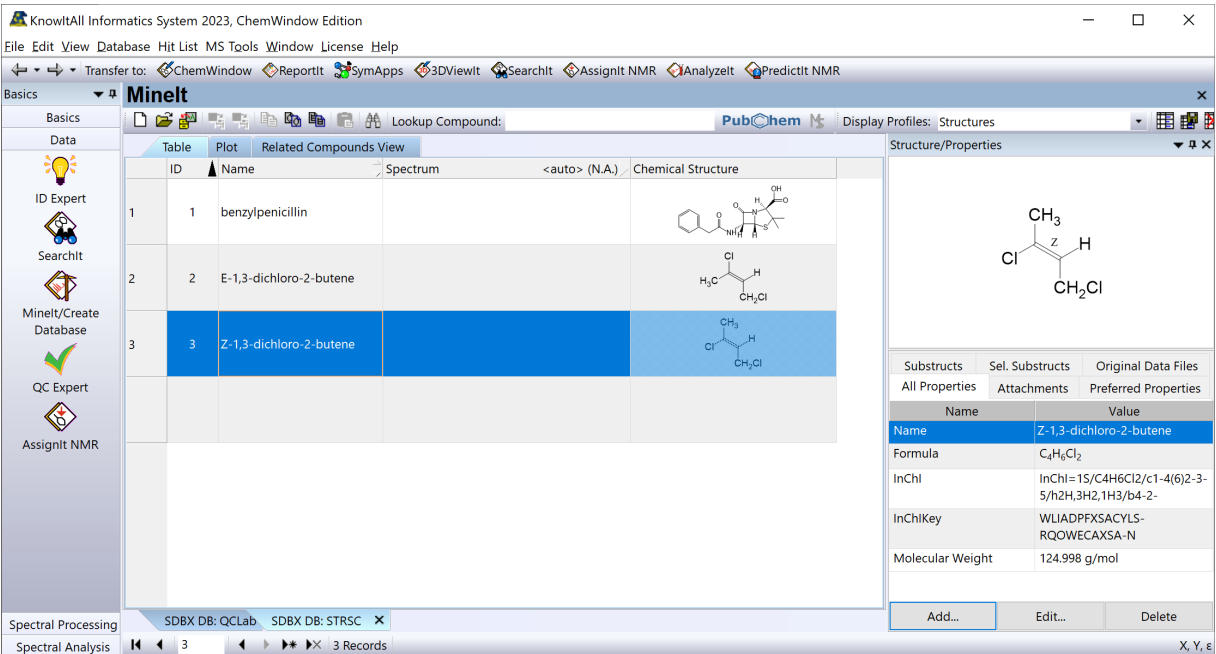
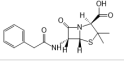
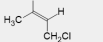
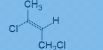
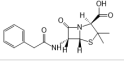
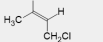
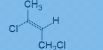
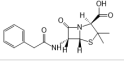
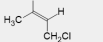
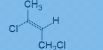
	Action	Result																								
4	Repeat to add the property Synonyms with the value 'Sample 8254.'																									
5	Repeat to add the property Comments with the value '82 nd Street Pharmacy, May 4. Retrieved in trace quantities.'	 <p>The screenshot shows the 'Minelt' application window. The table view displays the following data:</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>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"> <thead> <tr> <th>Name</th> <th>Value</th> </tr> </thead> <tbody> <tr> <td>Name</td> <td>benzylpenicillin</td> </tr> <tr> <td>Comments</td> <td>82nd Street Pharmacy, May 4. Retrieved in trace quantities.</td> </tr> <tr> <td>Formula</td> <td>C₁₈H₁₈N₂O₅S</td> </tr> <tr> <td>InChI</td> <td>InChI=1S/C16H18N2O4S/c1-16(2)12(15(21)22)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-MBXYWOFBSA-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 nd Street Pharmacy, May 4. Retrieved in trace quantities.	Formula	C ₁₈ H ₁₈ N ₂ O ₅ S	InChI	InChI=1S/C16H18N2O4S/c1-16(2)12(15(21)22)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-MBXYWOFBSA-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 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: <div style="text-align: center;">  </div>	
3	Use the Selection tool to select the structure, then choose Edit > Copy .	
4	Use the KnowItAll Back button to return to the Minelt 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 .	<p>The structure is added to the second record.</p> 
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	<p>Select the third database record and choose Edit > Paste.</p> <p>A message box asks, "Would you like to append the new data as a new record?"</p> <p>Click OK.</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 the following data:</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>benzylpenicillin</td> <td><auto> (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> <p>The 'Structure/Properties' pane on the right shows the following information for the selected record:</p> <table border="1"> <thead> <tr> <th>Name</th> <th>Value</th> </tr> </thead> <tbody> <tr> <td>Name</td> <td>E-1,3-dichloro-2-butene</td> </tr> <tr> <td>Formula</td> <td>C₄H₆Cl₂</td> </tr> <tr> <td>InChI</td> <td>InChI=1S/C4H6Cl2/c1-4(6)2-3-5/h2H,3H2,1H3/b4-2+</td> </tr> <tr> <td>InChIKey</td> <td>WLIADPFXSACYLS-DUXPYHPUSA-N</td> </tr> <tr> <td>Molecular Weight</td> <td>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			Name	Value	Name	E-1,3-dichloro-2-butene	Formula	C ₄ H ₆ Cl ₂	InChI	InChI=1S/C4H6Cl2/c1-4(6)2-3-5/h2H,3H2,1H3/b4-2+	InChIKey	WLIADPFXSACYLS-DUXPYHPUSA-N	Molecular Weight	124.998 g/mol
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InChIKey	WLIADPFXSACYLS-DUXPYHPUSA-N																													
Molecular Weight	124.998 g/mol																													
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 Minelt Database and Save. 	The structure is added to the third database record. ChemWindow is closed and we are back to the Minelt window.																												
5	Edit the property Name to 'Z-1,3-dichloro-2-butene.'	 <p>The screenshot shows the Minelt software interface. The main window displays a table with the following data:</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>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> <p>The right-hand pane shows the chemical structure and its properties:</p> <table border="1"> <thead> <tr> <th>Name</th> <th>Value</th> </tr> </thead> <tbody> <tr> <td>Name</td> <td>Z-1,3-dichloro-2-butene</td> </tr> <tr> <td>Formula</td> <td>C₄H₆Cl₂</td> </tr> <tr> <td>InChI</td> <td>InChI=1S/C4H6Cl2/c1-4(6)2-3-5/h2H,3H2,1H3/b4-2-</td> </tr> <tr> <td>InChIKey</td> <td>WLIADPFXSACYLS-RQOWECAXSA-N</td> </tr> <tr> <td>Molecular Weight</td> <td>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			Name	Value	Name	Z-1,3-dichloro-2-butene	Formula	C ₄ H ₆ Cl ₂	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

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, researchers can improve their analyses.

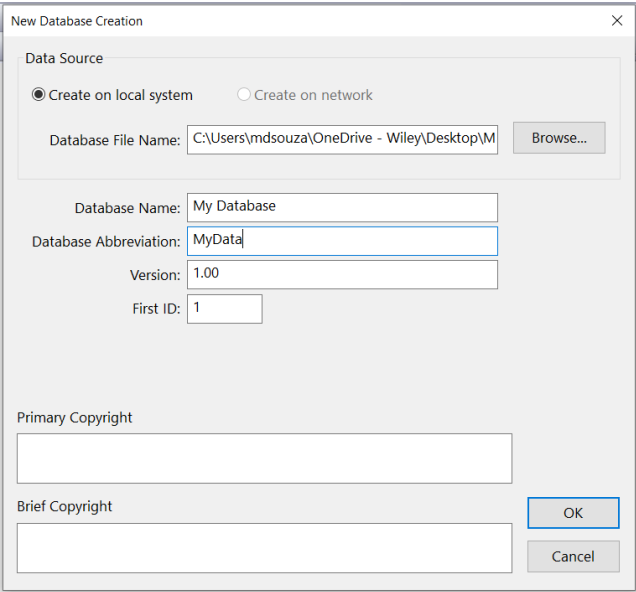
Training Files Used in This Lesson

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 KnowItAll.</p> <p>Click the Minelt icon.</p> <p>Select Database > New.</p> <p>Use Browse to set the hardware location for the database.</p> <p>Enter a tag ("MyData" etc).</p> <p>Click OK.</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**.

The screenshot displays the Minelt software interface. The 'Open' dialog box is open, showing the file 'Barbiturate GC-MS.d' selected in the 'GC-MS' directory. Below the dialog, a chromatogram plot is visible, showing a signal labeled 'BARBITURATE MIX' with several peaks. The x-axis is labeled 'min' and ranges from 1 to 6. A note on the plot states 'Data is 2D, only the TIC is shown.'

ID	Name	Spectrum	Chemical Structure

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
<input type="checkbox"/>	127 2.30033
<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
- Import chromatogram Add each spectrum to multiple new records
- Add all spectra to a single new record

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

Lookup Compound: PubChem Display Profiles: <no profile>

GC MS (GC) (5)

ID	Name	Spectrum	<auto> (GC)	Chemical Structure
1	BARBITURATE MIX			

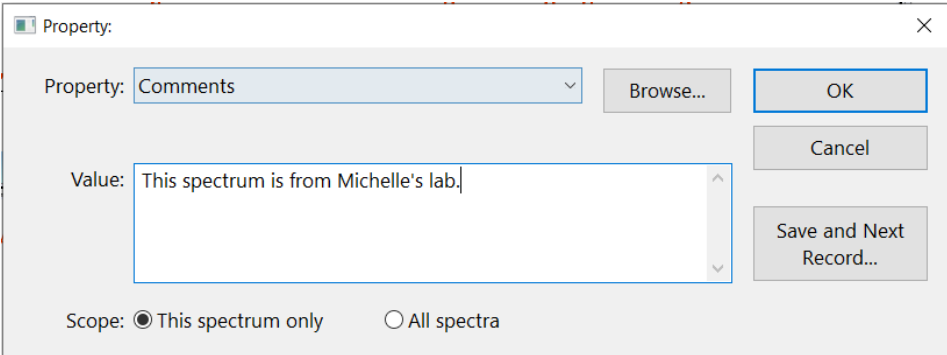
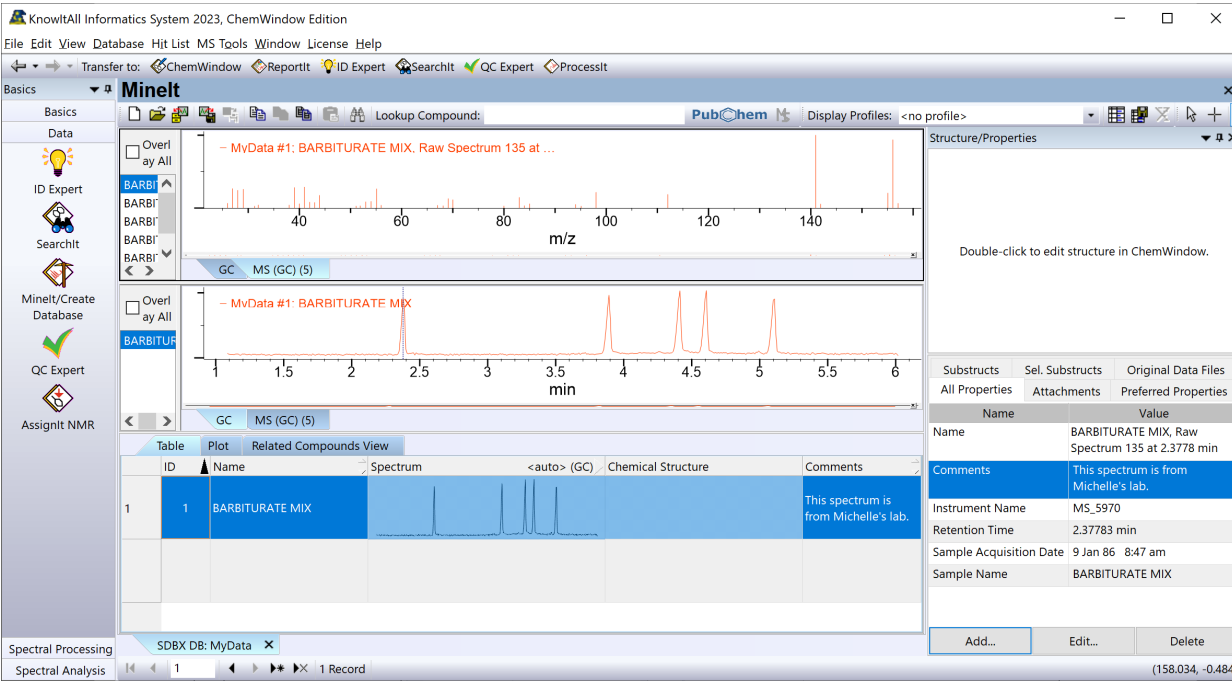
SDBX DB: MyData

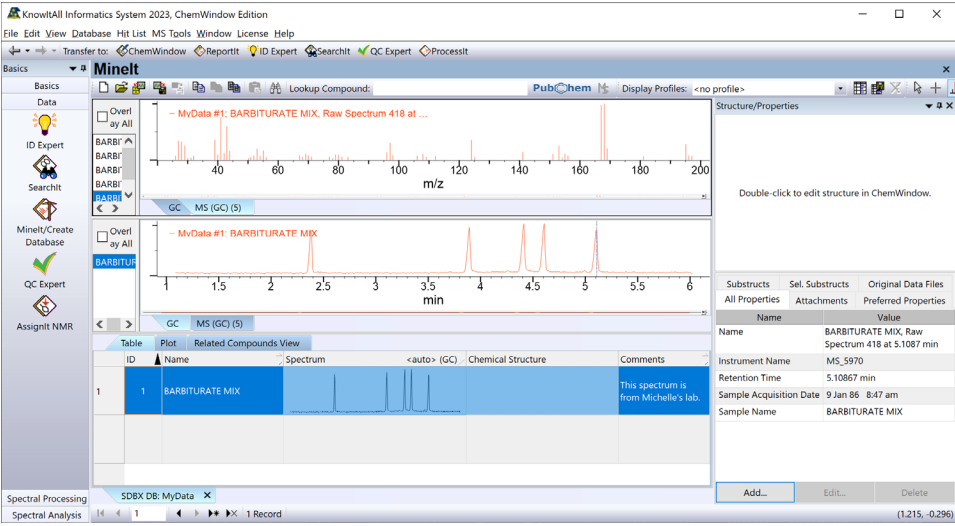
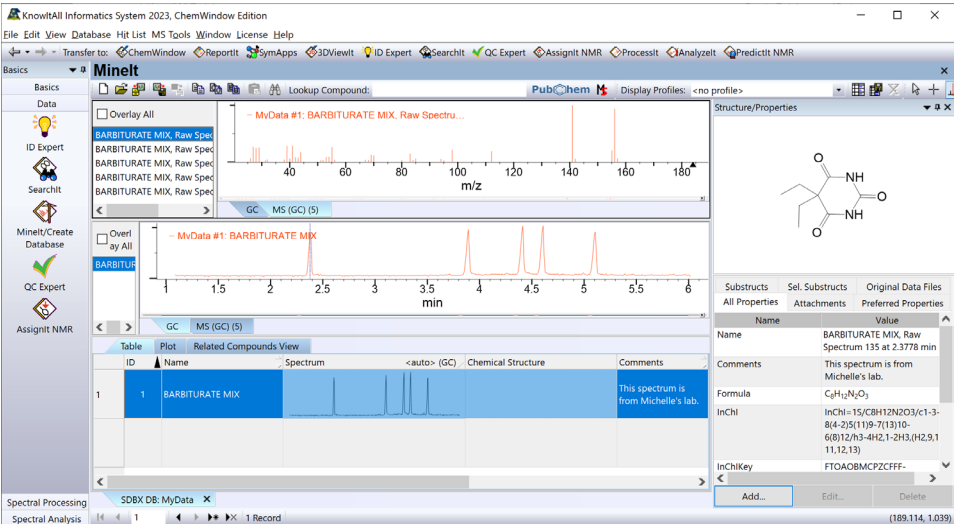
Spectral Processing Spectral Analysis 1 Record (6.120, 0.648)

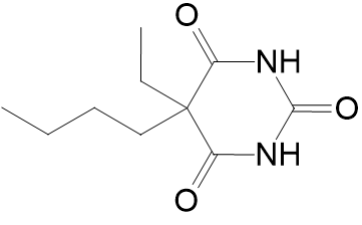
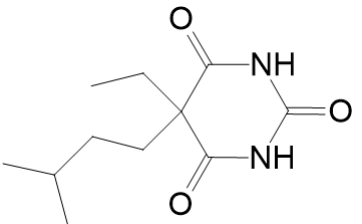
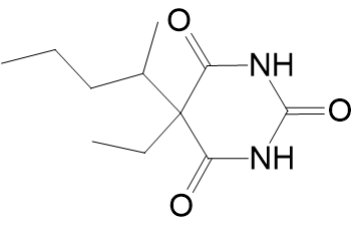
Structure/Properties

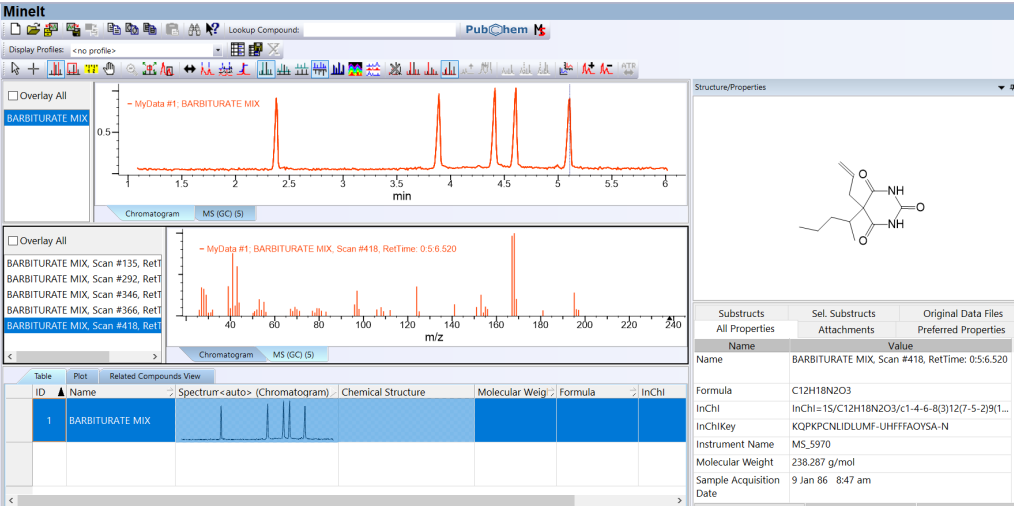
Double-click to edit structure in ChemWindow.

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

<p>7</p>	<p>In the pop-up window, use the Property dropdown list to select a field. For example, Comments.</p> <p>Type in a value.</p> <p>Choose This spectrum only.</p>															
<p>8</p>		 <table border="1" data-bbox="1514 1008 1822 1300"> <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</p>	<p>Select other MS spectrum.</p>	
<p>10</p>	<p>For MS 135, highlight the it.</p> <p>File > Import.</p> <p>Navigate to C:\Users\Public\Documents Wiley\KnowItAll\Samples\G C-MS folder</p> <p>Select Structure 1 – Barbital.</p> <p>Click Open.</p>	

11	<p>For MS 292, highlight the it.</p> <p>File > Import.</p> <p>Select Structure 2 – Butethal.</p> <p>Click Open.</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) attached. The central carbon is also bonded to a butyl group (CH₂CH₂CH₂CH₃) and an ethyl group (CH₂CH₃).</p>
12	<p>For MS 346, highlight the it.</p> <p>File > Import.</p> <p>Select Structure 3 – Amobarbital.</p> <p>Click Open.</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) attached. The central carbon is also bonded to an isopropyl group (CH(CH₃)₂) and a propyl group (CH₂CH₂CH₃).</p>
13	<p>For MS 366, highlight the it.</p> <p>File > Import.</p> <p>Select Structure 4 – Pentaobarbital.</p> <p>Click Open.</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) attached. The central carbon is also bonded to a propyl group (CH₂CH₂CH₃) and an ethyl group (CH₂CH₃).</p>

<p>14</p>	<p>For MS 418, highlight the it.</p> <p>File > Import.</p> <p>Select Structure 5 – Secobarbital.</p> <p>Click Open.</p> <p>Navigate MS records to see the difference.</p>	 <table border="1" data-bbox="1283 578 1604 781"> <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="2">Value</th> <th colspan="2"></th> </tr> </thead> <tbody> <tr> <td>Name</td> <td>BARBITURATE MIX, Scan #418, RetTime: 0:5:6.520</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>Formula</td> <td>C12H18N2O3</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>InChI</td> <td>InChI=1S/C12H18N2O3(c1-4-6-8(3)12(7-5-2)9(1...</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>InChIKey</td> <td>KQPKCNLIDLUMF-UHFFFAOYSA-N</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>Instrument Name</td> <td>MS_5970</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>Molecular Weight</td> <td>238.287 g/mol</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>Sample Acquisition Date</td> <td>9 Jan 86 8:47 am</td> <td></td> <td></td> <td></td> <td></td> </tr> </tbody> </table>	Substructs		Sel. Substructs		Original Data Files		All Properties		Attachments		Preferred Properties		Name		Value				Name	BARBITURATE MIX, Scan #418, RetTime: 0:5:6.520					Formula	C12H18N2O3					InChI	InChI=1S/C12H18N2O3(c1-4-6-8(3)12(7-5-2)9(1...					InChIKey	KQPKCNLIDLUMF-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>	