

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, scientists can improve their analyses.

Training Files Used in This Lesson

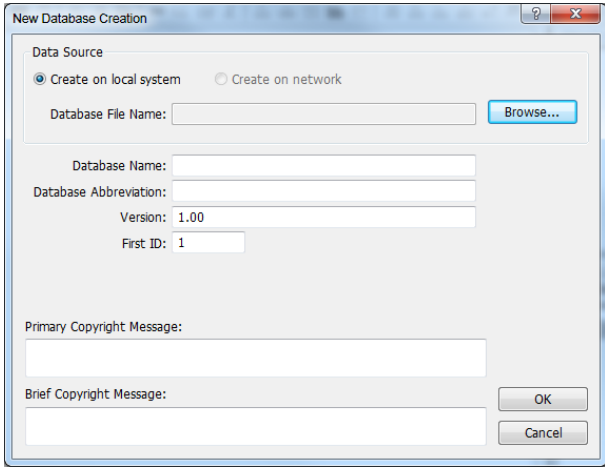
C:\Users\Public\Documents\Wiley\KnowItAll\Samples

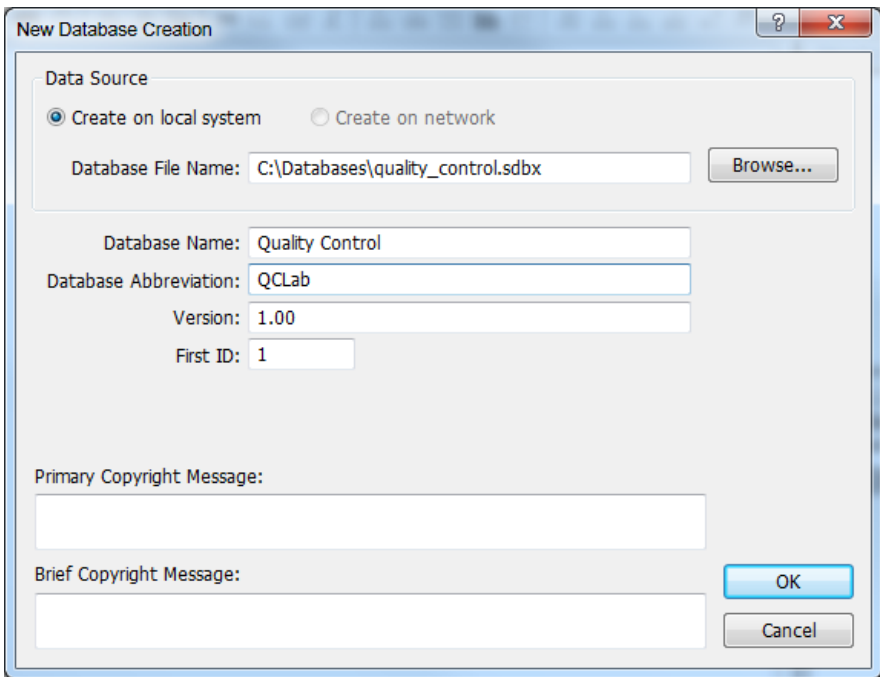
- \IR\Ethyl acetate.dx
- \Raman\Ethyl acetate.irf
- \Minelt\Import.csv
- MSDS Web Link.txt
- Ethyl acetate MSDS.pdf

KnowItAll Applications Used

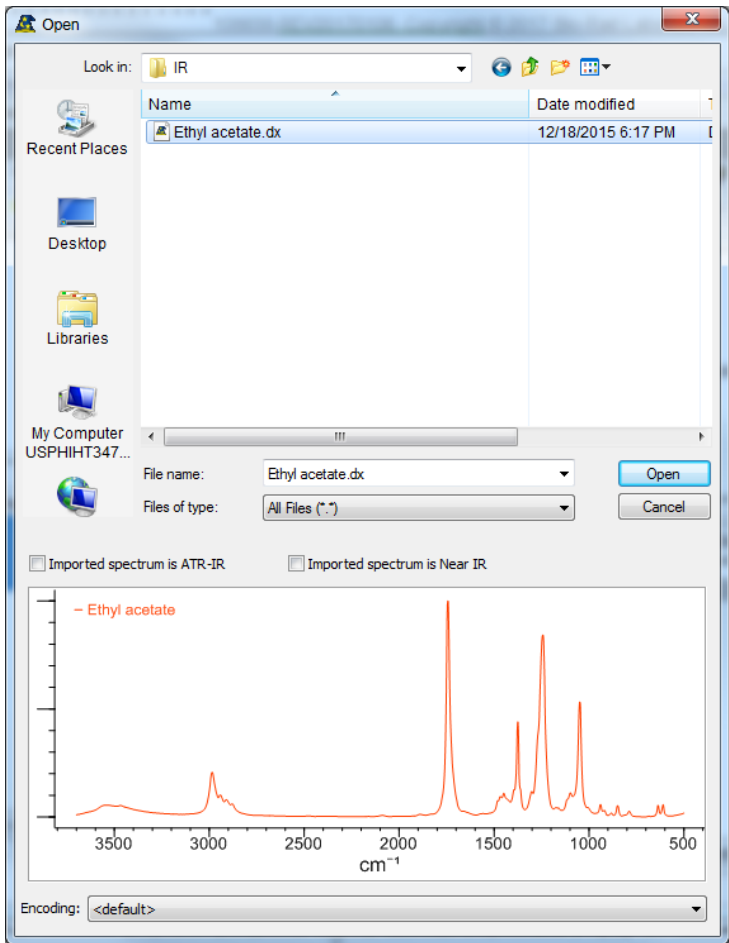
- Minelt
- ChemWindow®
- Browselt

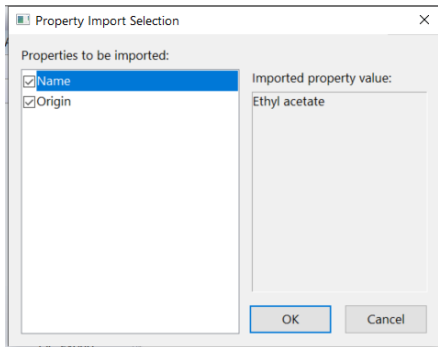
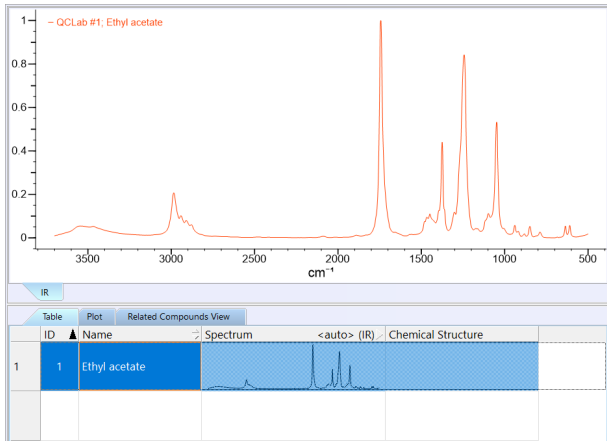
Create a user database

	Action	Result
1	Navigate to the 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 .	
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>The new database is saved locally.</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>

	Action	Result
5	Type Quality Control in the Database Name text box. Note: The file name is used if no other name is specified.	
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).

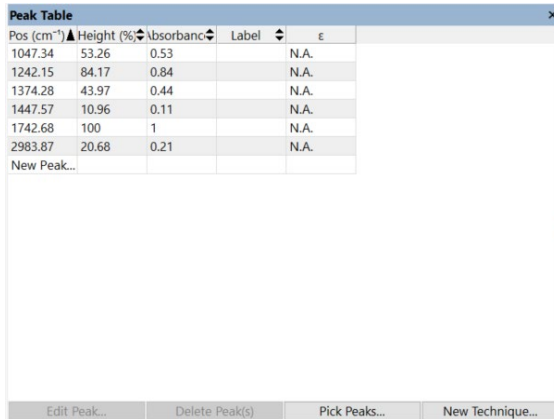
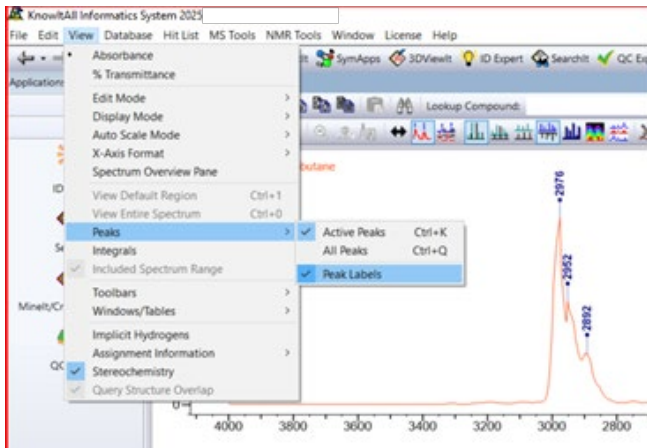
Add the first spectrum record to the user database

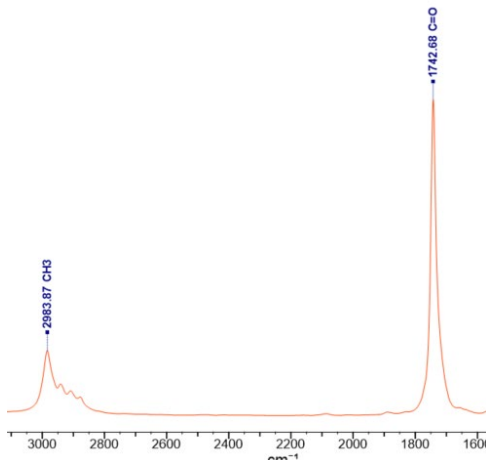
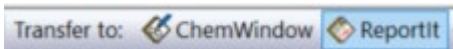
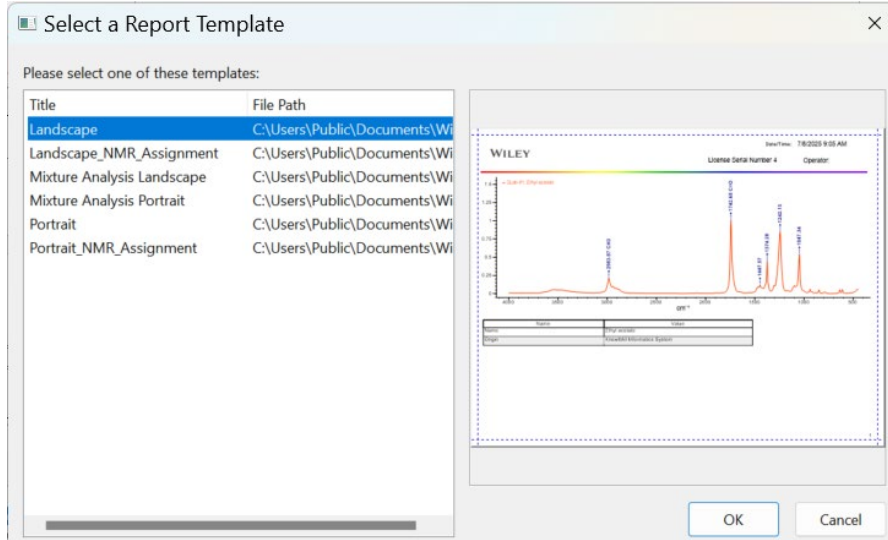
	Action	Result
1	<p>Create the first database record by importing a spectrum:</p> <ul style="list-style-type: none">Choose File > Import or press Ctrl+I.Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\IR folderOpen Ethyl acetate.dx. <p>Note: Use the Files of type filter to locate IRF, JCAMP 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:' dropdown 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 contains 'Ethyl acetate.dx' and the 'Files of type:' dropdown is set to 'All Files (*.*)'. At the bottom, there is a preview of the IR spectrum for 'Ethyl acetate', showing a plot of transmittance versus wavenumber (cm⁻¹) from 3500 to 500. The spectrum shows several characteristic peaks, including a broad one around 3000 cm⁻¹ and sharp ones in the fingerprint region. There are also checkboxes for 'Imported spectrum is ATR-IR' and 'Imported spectrum is Near IR', both of which are currently unchecked. An 'Encoding:' dropdown is set to '<default>'.</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. Use the checkboxes to define whether a property should be imported into the database or not.</p>
3	Click OK .	<p>The dialog box closes. The spectrum has been added to the user database as the first record.</p> 

Add spectrum labels


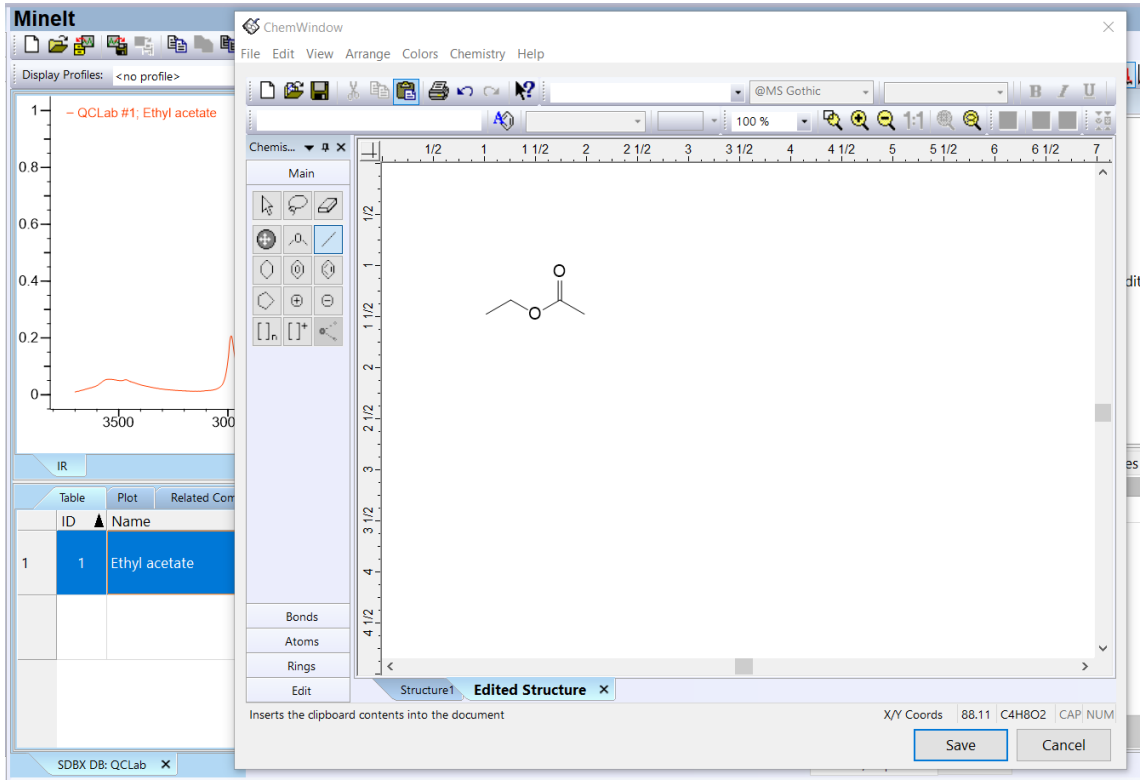
KnowItAll 2025 release allowed users to add customized peak labels.

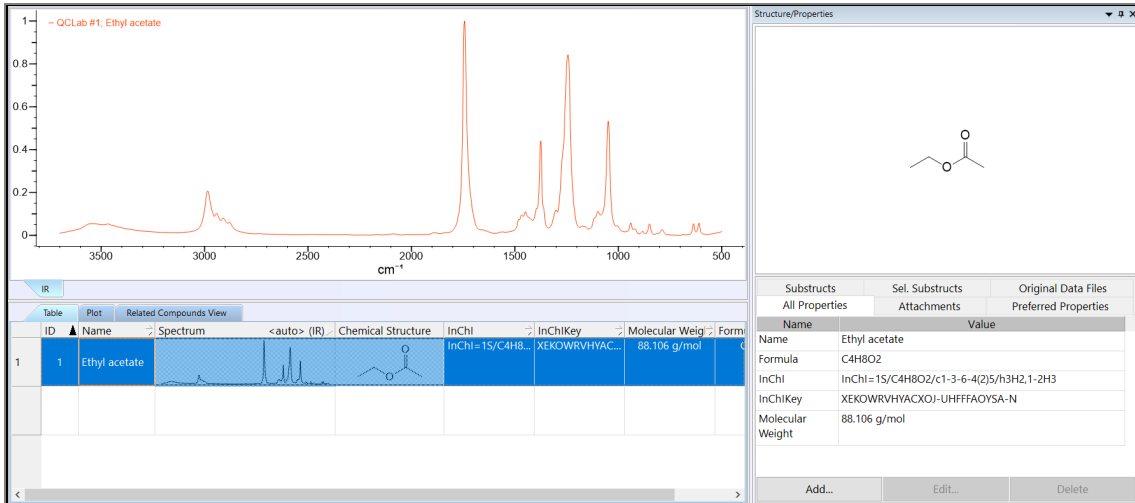
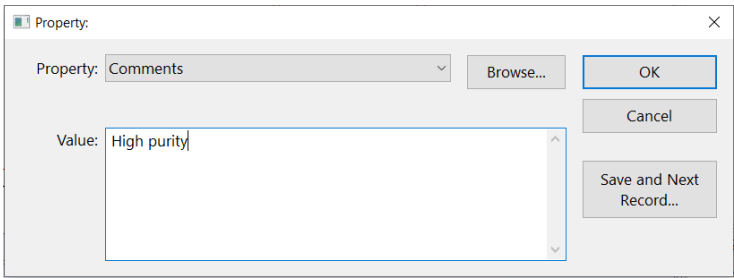
	Action	Result																																								
1	<p>Continue with the above example</p> <p>Choose View > Windows/Tables > Peak Table to open the spectrum peak table</p>	<p>Peak Table pops up in a window</p>  <table><thead><tr><th>Pos (cm⁻¹)</th><th>Height (%)</th><th>Absorbance</th><th>Label</th><th>ε</th></tr></thead><tbody><tr><td>1047.34</td><td>53.26</td><td>0.53</td><td>N.A.</td><td></td></tr><tr><td>1242.15</td><td>84.17</td><td>0.84</td><td>N.A.</td><td></td></tr><tr><td>1374.28</td><td>43.97</td><td>0.44</td><td>N.A.</td><td></td></tr><tr><td>1447.57</td><td>10.96</td><td>0.11</td><td>N.A.</td><td></td></tr><tr><td>1742.68</td><td>100</td><td>1</td><td>N.A.</td><td></td></tr><tr><td>2983.87</td><td>20.68</td><td>0.21</td><td>N.A.</td><td></td></tr><tr><td colspan="5">New Peak...</td></tr></tbody></table>	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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New Peak...																																										
2	<p>TIP: To ensure Peak Labels are visible in the spectrum, perform the following step:</p> <p>Choose View > Peaks > Peak Labels and make sure Peak Labels is selected.</p>																																									

	Action	Result																																
3	One can directly type textual values into the Label column.	<div>The labels show up in spectral pane.</div> <div><table border="1" data-bbox="1226 396 1520 574"><caption>Peak Table</caption><thead><tr><th>Pos (cm⁻¹)</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><div data-bbox="1226 810 1520 828">Edit Peak... Delete Peak(s)</div></div>	Pos (cm ⁻¹)	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	<div>Select Transfer to: ReportIt</div> <div></div> <div>Choose the Landscape report template</div> <div>Click OK</div>	<div></div>																																

Action	Result						
	<p>The peak labels are also transferred over:</p> <p>WILEY</p> <p>Date/Time: 7/8/2025 9:06 AM</p> <p>License Serial Number 4 Operator:</p> <p>— QLab #1; Ethyl acetate</p> <p>cm⁻¹</p> <table><thead><tr><th>Name</th><th>Value</th></tr></thead><tbody><tr><td>Name</td><td>Ethyl acetate</td></tr><tr><td>Origin</td><td>KnowItAll Informatics System</td></tr></tbody></table>	Name	Value	Name	Ethyl acetate	Origin	KnowItAll Informatics System
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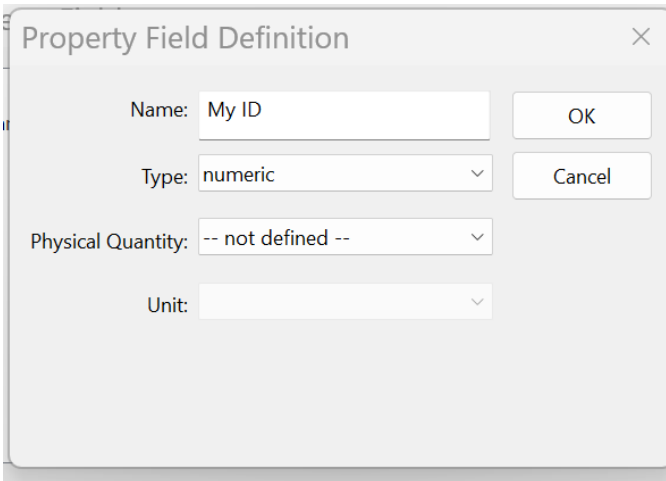
Add a chemical structure and properties to a database record

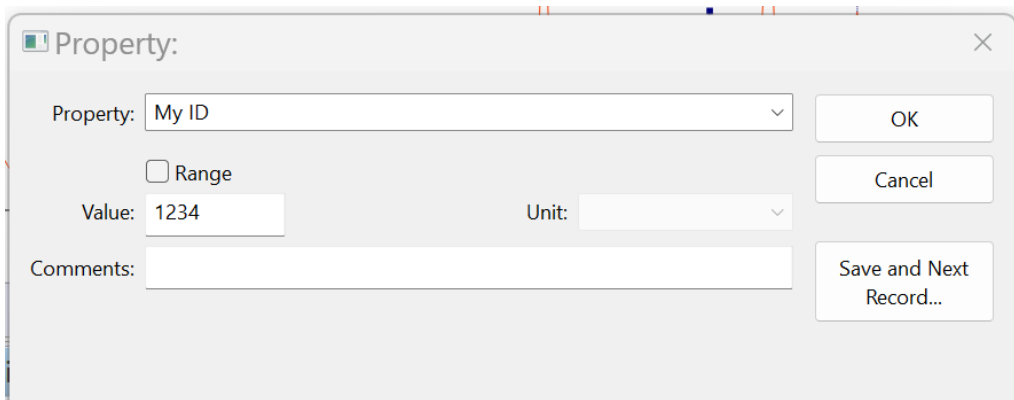
	Action	Result
1	<p>Go back to Minelt</p> <p>With the first record selected, double-click the Structure/Properties pane at the top right of the window (Double-click to edit structure in ChemWindow).</p>	<p>The Transfer to ChemWindow application pops up. Alternatively, you can use Transfer to: to go to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

	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	<p>Use the drop-down list to select the property you wish to add. Select Comments.</p> <p>Type High purity into the Value box.</p>	

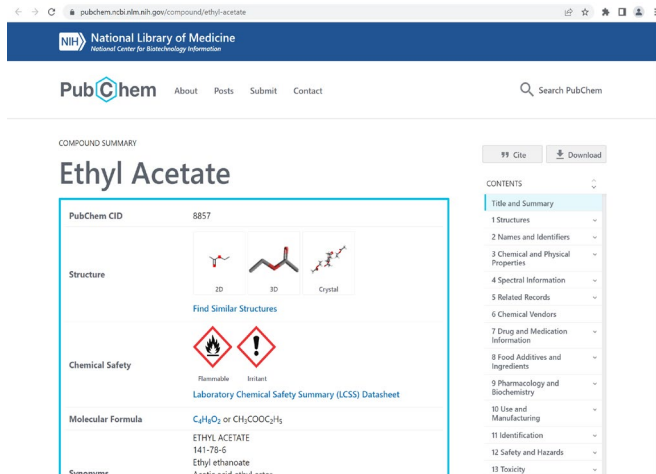
	Action	Result																											
6	Click OK .	<p>The Property dialog box closes, and the name and value of the added property appears in the Structure/Properties pane.</p> <table border="1"> <tr> <td>Substructs</td><td>Sel. Substructs</td><td>Original Data Files</td></tr> <tr> <td>All Properties</td><td>Attachments</td><td>Preferred Properties</td></tr> <tr> <th>Name</th><th colspan="2">Value</th></tr> <tr> <td>Name</td><td colspan="2">Ethyl acetate</td></tr> <tr> <td>Comments</td><td colspan="2">High purity</td></tr> <tr> <td>Formula</td><td colspan="2">C4H8O2</td></tr> <tr> <td>InChI</td><td colspan="2">InChI=1S/C4H8O2/c1-3-6-4(2)5/h3H2,1-2H3</td></tr> <tr> <td>InChIKey</td><td colspan="2">XEKOWRVHYACXOJ-UHFFFAOYSA-N</td></tr> <tr> <td>Molecular Weight</td><td colspan="2">88.106 g/mol</td></tr> </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

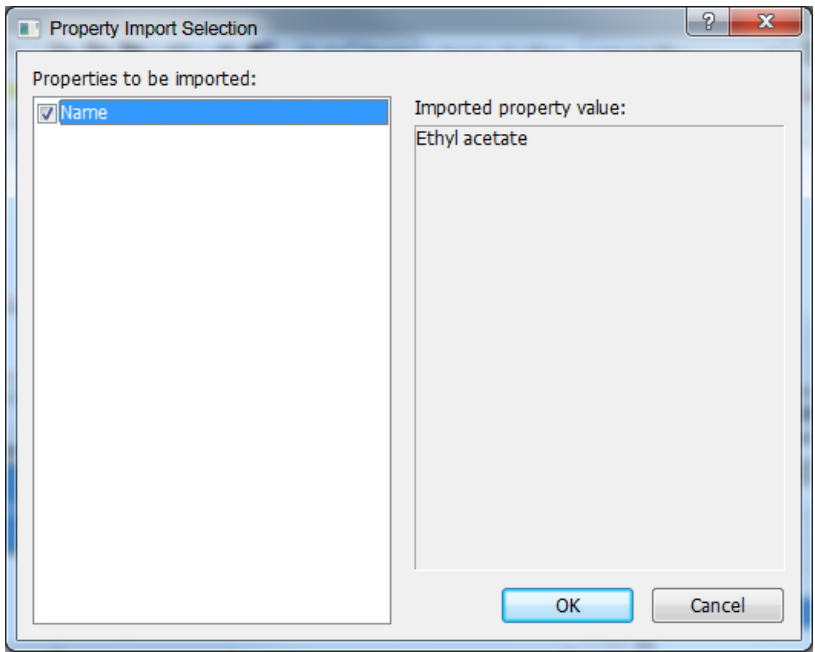
	Action	Result
1	Choose Database > Define User Property Fields .	The User Property Fields dialog box opens.
2	Click Add . Use the drop-down list to set Type to text. Enter the Name .	<p>The Property Field Definition dialog box opens.</p>  <p>Note: Which controls are available depends on which type of 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.
6	Select Sample ID	<p>The Value text box is added to the dialog.</p> <p>Note: Which text boxes are added depends on whether the property is numeric, text or enumeration.</p>

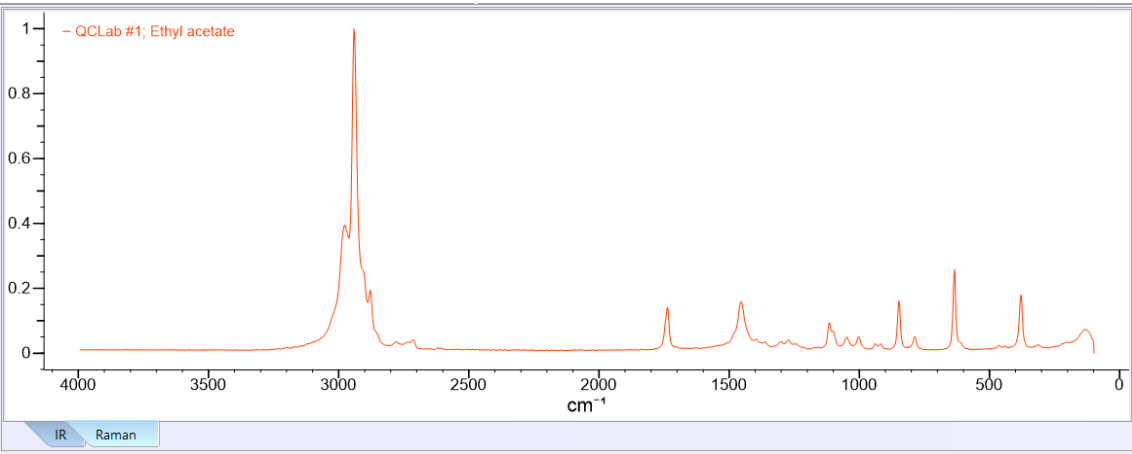
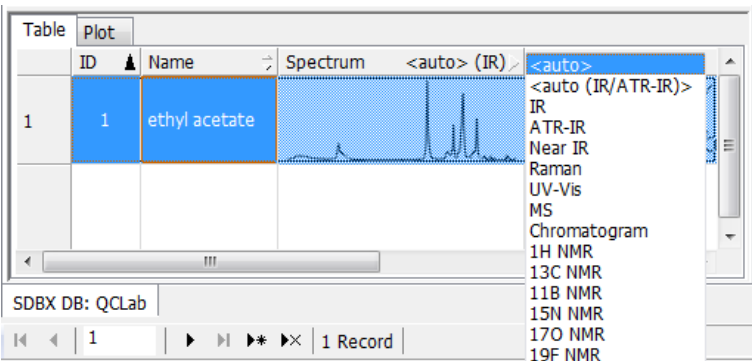
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7	Type '1234' in the Value text box.																																													
8	Click OK .	<p>The dialog box closes. The property SampleID with value 1234 is added to the Structure/Properties pane for the first record.</p> <table><tr><th>Substructs</th><th>Sel. Substructs</th><th>Original Data Files</th><th>History</th></tr><tr><td>All Properties</td><td>Attachments</td><td>Preferred Properties</td><td></td></tr><tr><th colspan="2">Name</th><th colspan="2">Value</th></tr><tr><td colspan="2">Name</td><td colspan="2">Ethyl acetate</td></tr><tr><td colspan="2">Comments</td><td colspan="2">High purity</td></tr><tr><td colspan="2">Formula</td><td colspan="2">C₄H₈O₂</td></tr><tr><td colspan="2">InChI</td><td colspan="2">InChI=1S/C4H8O2/c1-3-6-4(2)5/h3H2,1-2H3</td></tr><tr><td colspan="2">InChIKey</td><td colspan="2">XEKOWRVHYACXOJ-UHFFFAOYSA-N</td></tr><tr><td colspan="2">Molecular Weight</td><td colspan="2">88.106 g/mol</td></tr><tr><td colspan="2">My ID</td><td colspan="2">1234</td></tr><tr><td colspan="2">Origin</td><td colspan="2">KnowItAll Informatics System</td></tr></table>	Substructs	Sel. Substructs	Original Data Files	History	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		My ID		1234		Origin		KnowItAll Informatics System	
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Action	Result																						
<p>Note: in KnowItAll 2026 release, you can change a property to another by</p> <ul style="list-style-type: none">Click the Rename buttonKnowItAll would provide a list of properties of matching types for user to select	<div><div>All PropertiesAttachmentsPreferred PropertiesSubstructsSel. SubstructsOriginal Data FilesHistory</div><table><thead><tr><th>Name</th><th>Value</th></tr></thead><tbody><tr><td>Name</td><td>Amphetamine</td></tr><tr><td>CAS Registry Number</td><td>300-62-9</td></tr><tr><td>Exact Mass</td><td>135.104799419 u (Computed by PubChem 2.2 (PubChem release 2025.04.14))</td></tr><tr><td>Formula</td><td>C₉H₁₃N</td></tr><tr><td>InChI</td><td>InChI=1S/C9H13N/c1-8(10)7-9-5-3-2-4-6-9/h2-6,8H,7,10H2,1H3</td></tr><tr><td>InChIKey</td><td>KWTSXDURSIMDCE-UHFFFAOYSA-N</td></tr><tr><td>IUPAC Name</td><td>1-phenylpropan-2-amine</td></tr><tr><td>Molecular Weight</td><td>135.21 g/mol (Computed by PubChem 2.2 (PubChem release 2025.04.14))</td></tr><tr><td>PubChem Compound ID</td><td>3007</td></tr><tr><td>Retention Time</td><td>3.7 min</td></tr></tbody></table><div><div>Rename Property</div><div>Property: <div>Equivalent Molecular Weight</div><div>Nominal Mass</div></div><div><div>OK</div><div>Cancel</div></div></div><div><div>Add...</div><div>Edit...</div><div>Delete</div><div>Rename...</div></div></div>	Name	Value	Name	Amphetamine	CAS Registry Number	300-62-9	Exact Mass	135.104799419 u (Computed by PubChem 2.2 (PubChem release 2025.04.14))	Formula	C ₉ H ₁₃ N	InChI	InChI=1S/C9H13N/c1-8(10)7-9-5-3-2-4-6-9/h2-6,8H,7,10H2,1H3	InChIKey	KWTSXDURSIMDCE-UHFFFAOYSA-N	IUPAC Name	1-phenylpropan-2-amine	Molecular Weight	135.21 g/mol (Computed by PubChem 2.2 (PubChem release 2025.04.14))	PubChem Compound ID	3007	Retention Time	3.7 min
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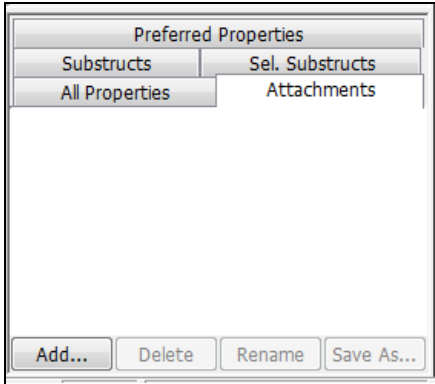
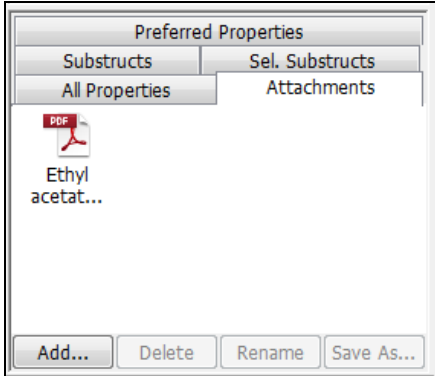
	Action	Result																																				
9	<p>Repeat steps 1-8 to create the user property WebLink (text field) and display it in the Structure/Properties pane.</p> <p>Type 'https://pubchem.ncbi.nlm.nih.gov/compound/ethyl-acetate' in the Property dialog box's Value field.</p>	<p>The property WebLink with a web address is added to the Structure/Properties pane for the first record.</p> <table><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><td colspan="2">Name</td><td>Value</td></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">WebLink</td><td>https://pubchem.ncbi.nlm.nih.gov/compound/ethyl-acetate</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	WebLink		https://pubchem.ncbi.nlm.nih.gov/compound/ethyl-acetate	Add...		Edit... Delete
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Add...		Edit... Delete																																				
10	<p>Click the web address in the Structure/Properties pane.</p>	<p>The web page opens.</p> 																																				

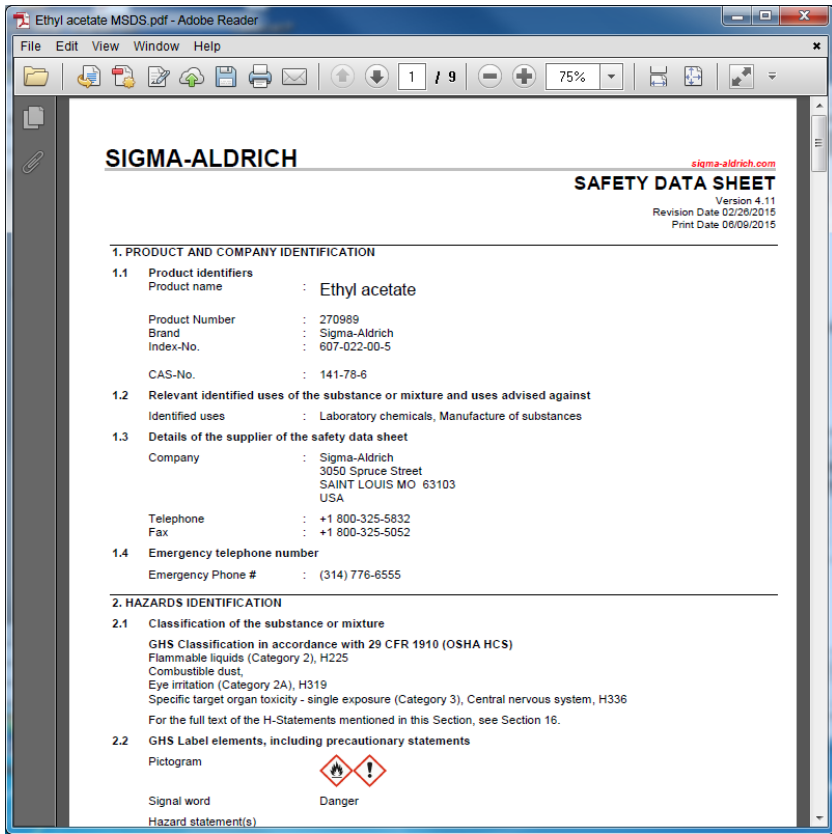
Add another spectrum (Raman) to the first database record

	Action	Result
1	Make sure the first database record is selected, then choose 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 .	<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.</p>

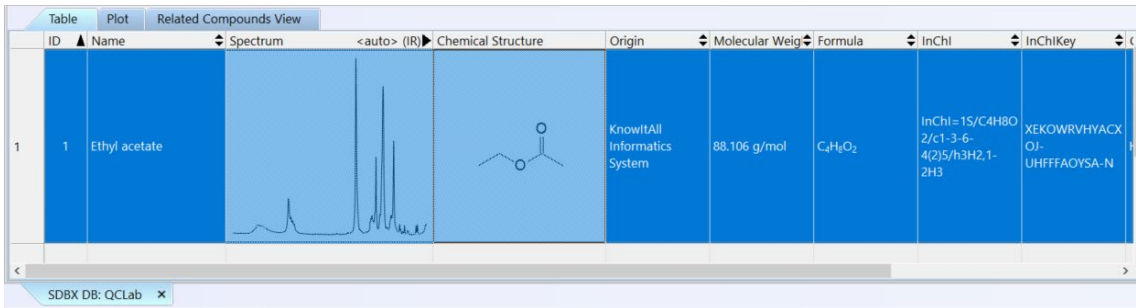

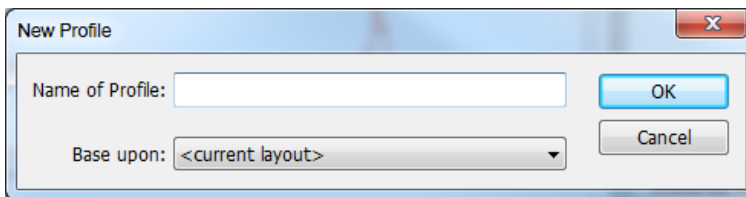

	Action	Result
3	Click OK .	<p>A new Raman tab is added to the Spectral pane for the display of the Raman spectrum.</p> 
4	Switch between spectra by using the tabs at the bottom left of the spectral pane.	
5	You can also switch between spectra by clicking the arrow in the Database pane's Spectrum column.	

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.	<p>The Attachments tab is empty.</p> 
2	Choose File > Import Attachment(s) .	A Windows Open dialog box is displayed.
3	<p>Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Minelt folder.</p> <p>Select Ethyl acetate MSDS.pdf. Then click Open.</p>	<p>An icon is added to the Attachments tab.</p> 

	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>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.</p>

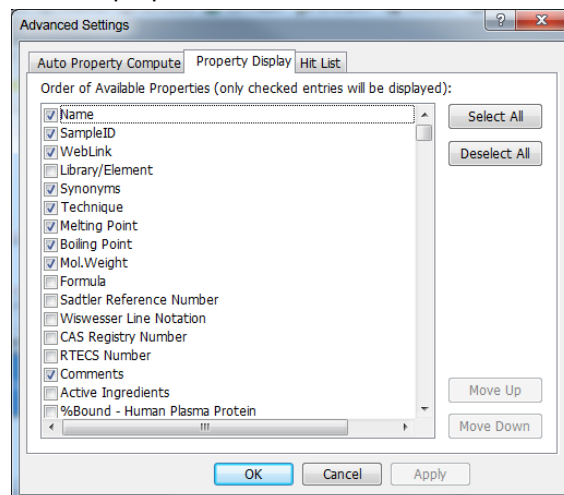
Create a new Minelt display profile

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

TIP

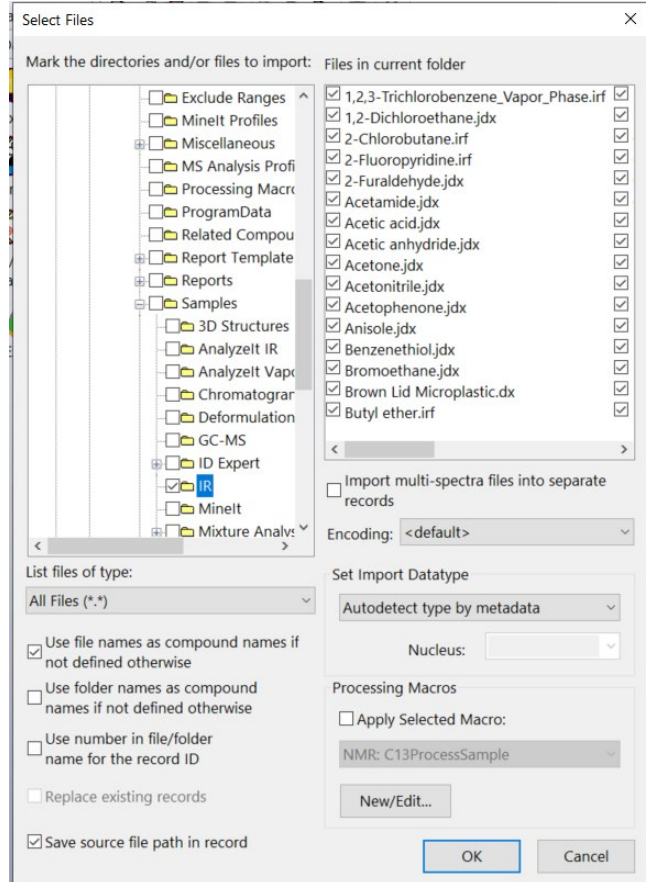
When creating a database and to ensure individual users in your laboratory consistently enter all pertinent information into databases, you should set up preferred properties.

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

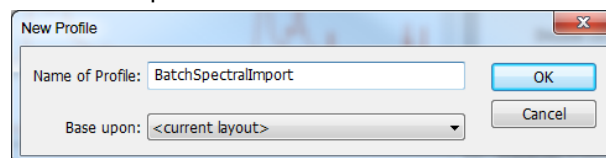
	Action	Result
1	Create a new empty database as in the above example.	
2	<p>Choose File > Batch Import to open the Select Files dialog box.</p> <p>Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\IR, select all spectral files in the folder.</p> <p>Check the box next to a folder name to select all files in the folder.</p> <p>Click OK</p>	 <p>A record is created in the new database for each spectral file.</p>

	Action	Result																																								
3	<p>Choose File > Import.</p> <p>Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Minelt</p> <p>Select BatchImportProperties.csv to map properties to the spectrum files using a spreadsheet.</p> <p>Click Open.</p> <p>Make sure to check File Contains Header Line.</p> <p>Click Next.</p>	<p>The Spreadsheet File Import wizard opens.</p> <div><div>Spreadsheet File Import</div><div><div>Step 1: Analyzing File</div><div><div><input type="checkbox"/> File is a Spectrum</div><div>Rows to import<div><div><input checked="" type="radio"/> All</div><div><input type="radio"/> Rows: <div></div></div></div></div><div>Layout<div><div><input checked="" type="checkbox"/> File Contains Header Line: id,Name,CAS Registry Number,Synonyms</div><div>Delimiting Character: , Encoding: <default></div><table><tr><th>id</th><th>Name</th><th>CAS Registry ...</th><th>Synonyms</th></tr><tr><td>1</td><td>1, 2-Dichloro...</td><td>107-06-2</td><td>Ethylene chlo...</td></tr><tr><td>2</td><td>2-Chlorobuta...</td><td>78-86-4</td><td>sec-Butyl chl...</td></tr><tr><td>3</td><td>2-Fluoropyridi...</td><td>372-48-5</td><td>o-Fluoropyrid...</td></tr><tr><td>4</td><td>2-Furaldehyde</td><td>98-01-1</td><td>Furfural</td></tr><tr><td>5</td><td>Acetamide</td><td>60-35-5</td><td>Ethanamide</td></tr><tr><td>6</td><td>Acetic acid</td><td>64-19-7</td><td>Ethanoic acid</td></tr><tr><td>7</td><td>Acetic anhydr...</td><td>108-24-7</td><td>Ethanoic anh...</td></tr><tr><td>8</td><td>Acetone</td><td>67-64-1</td><td>2-Propanone</td></tr><tr><td>9</td><td>Acetonitrile</td><td>75-05-8</td><td>Cyanomethane</td></tr></table></div></div><div><div>The file was analyzed successfully (34 rows read).</div><div><div>< Back</div><div>Next ></div><div>Cancel</div></div></div></div></div></div>	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
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8	Acetone	67-64-1	2-Propanone																																							
9	Acetonitrile	75-05-8	Cyanomethane																																							

	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> <ul style="list-style-type: none">• Highlight the id field• Check the “Use to link existing records” if not already checked. <p>Click Next.</p>	
5	<p>Click Finish.</p> <p>You do not have to Compact database now at the prompt.</p>	The database now has fields Synonyms and CAS Registry Number populated by the CSV file.


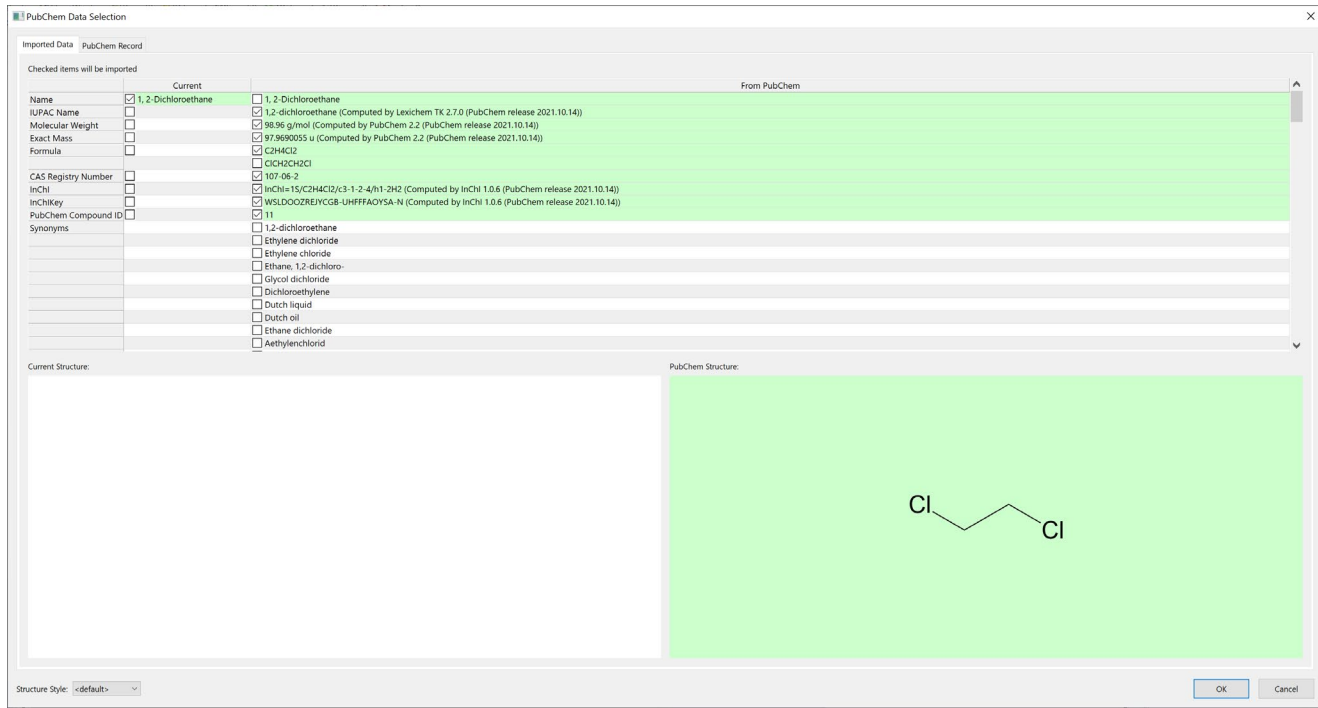
TIP

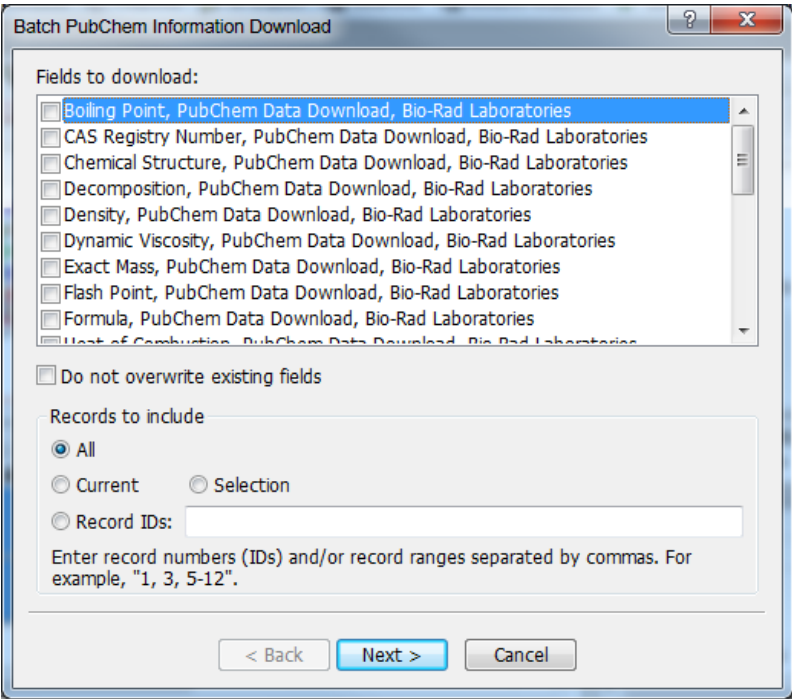
You can rearrange the table portion of this database (for example, to get rid of empty structure columns, right-click and choose **Delete Columns**). When edits are completed, you can save this column arrangement as a **Minelt** profile. Click **Save Current Profile** on the **Profile** toolbar, then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

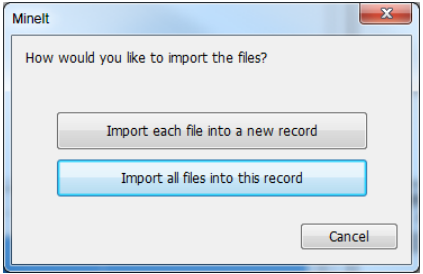
Batch Import: many spectra, many records, import properties from PubChem

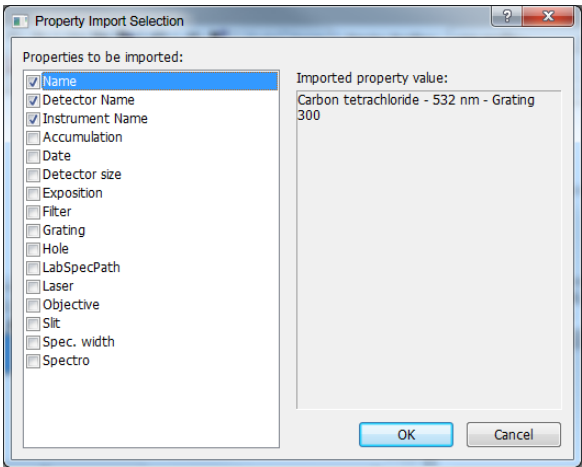
	Action	Result
1	<p>Select the first record from the above database, click the PubChem toolbar button.</p> 	<p>PubChem records are searched. If information is located, the PubChem Data Selection dialog box opens.</p> 

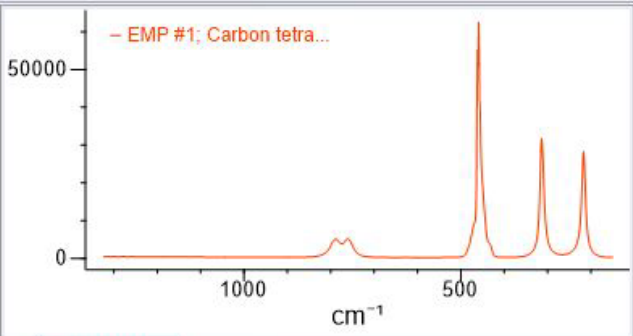



	Action	Result
2	Click OK .	New properties from PubChem are added to the first database record.
3	Select the remaining database records by holding the Shift key, then choose Database > Batch PubChem Information Download .	<p>The Batch PubChem Information Download dialog box opens.</p> 
4	Check the property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

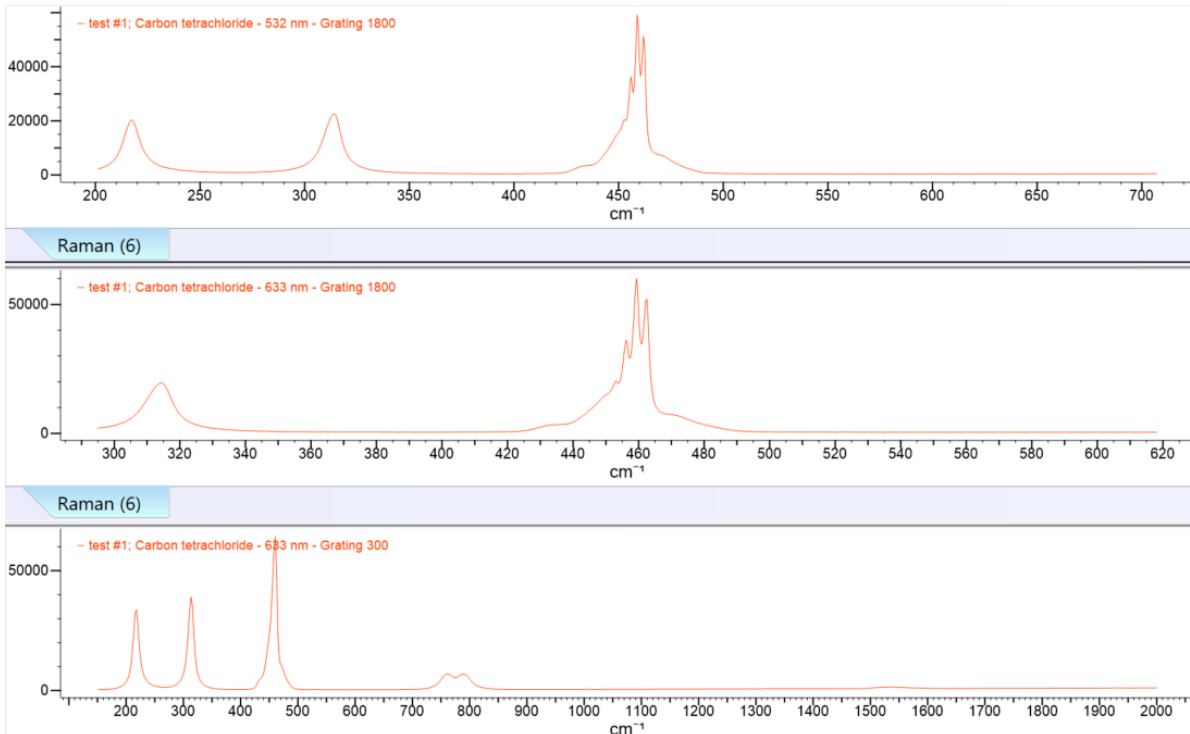
TIP: Sometimes one may get error saying compounds not being found, because PubChem do not have them.

Batch Import: many spectra, one record

	Action	Result
1	Create a new empty database as in the above example.	
2	<p>Choose File > Import.</p> <p>Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Raman folder</p> <p>Select Carbon tetrachloride files in the folder.</p> <p>Click Open.</p>	<p>A dialog box opens and asks how you want to import the files.</p> 

	Action	Result
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> <div><div><div><input type="checkbox"/> Overlay All</div><div>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</div></div><div><p>– EMP #1; Carbon tetra...</p><p>Raman (6)</p></div></div> <div><div>TablePlotRelated Compounds View</div><table><tr><th></th><th>ID</th><th>Name</th><th>Spectrum</th><th>Chemical Structure</th></tr><tr><td>1</td><td>1</td><td>Carbon tetrachloride - 633 nm - Grating 600</td><td></td><td></td></tr><tr><td></td><td></td><td></td><td></td><td></td></tr></table></div>		ID	Name	Spectrum	Chemical Structure	1	1	Carbon tetrachloride - 633 nm - Grating 600							
	ID	Name	Spectrum	Chemical Structure													
1	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, scientists can improve their analyses.

Training Files Used in This Lesson

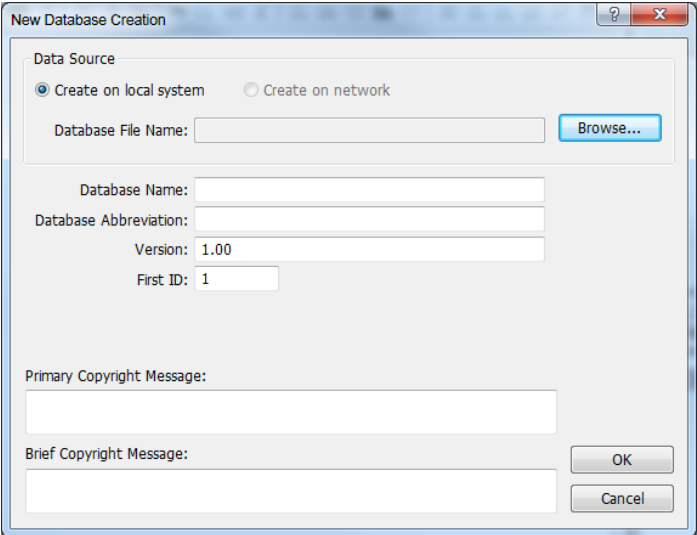
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Structures folder

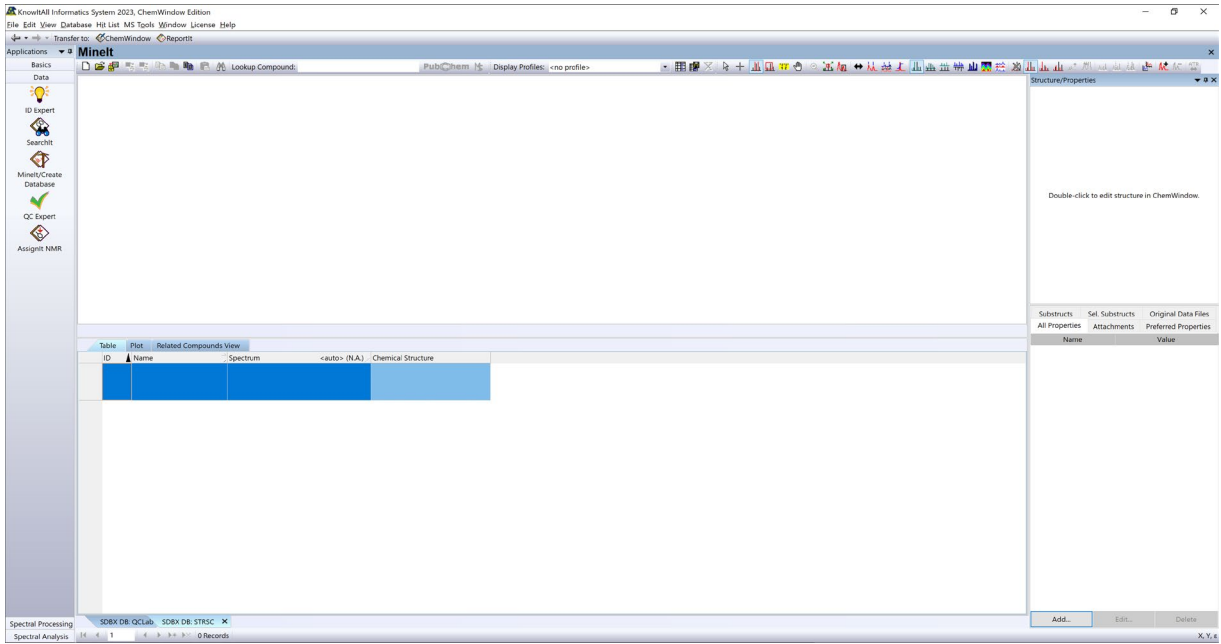
- benzylpenicillin.dsf


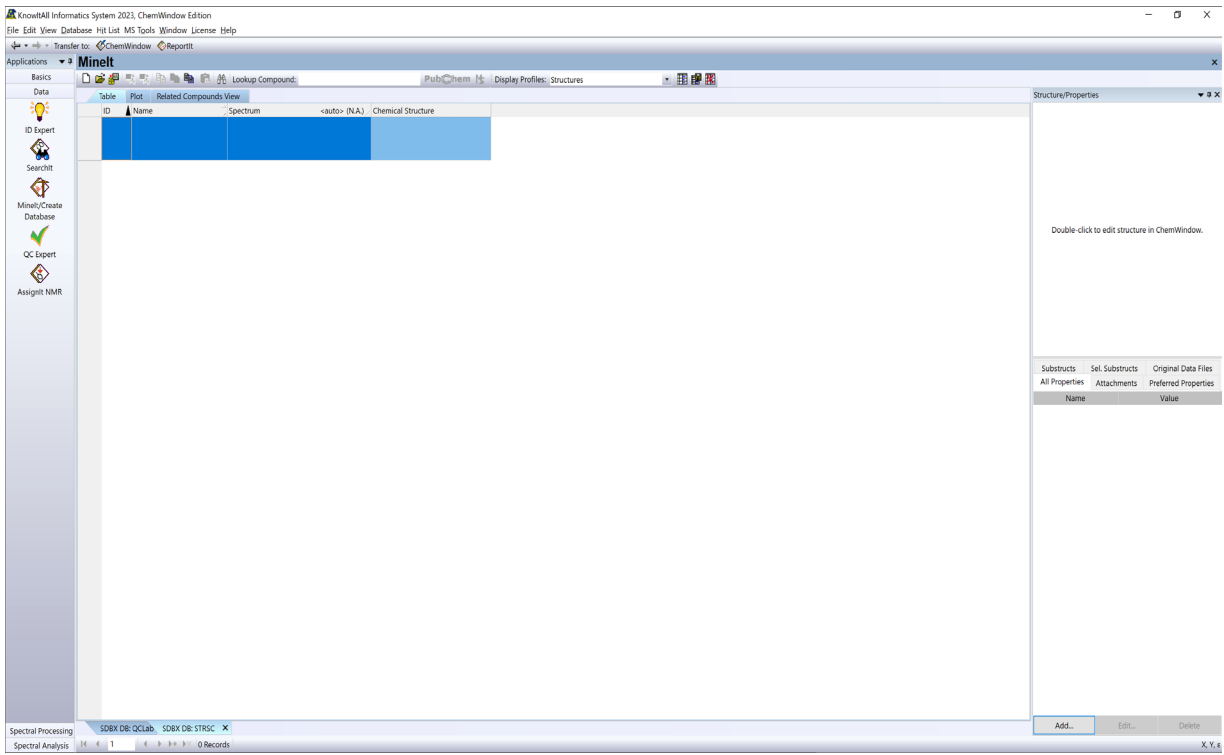
KnowItAll Applications Used

- Minelt
- ChemWindow®

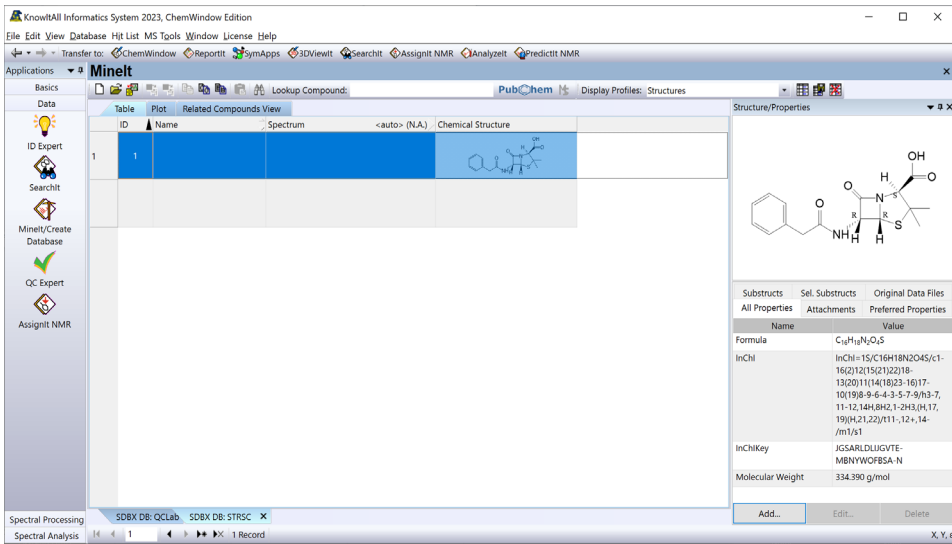
Create a user database

	Action	Result
1	In the 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>	

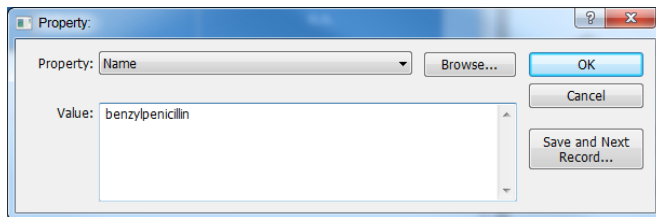
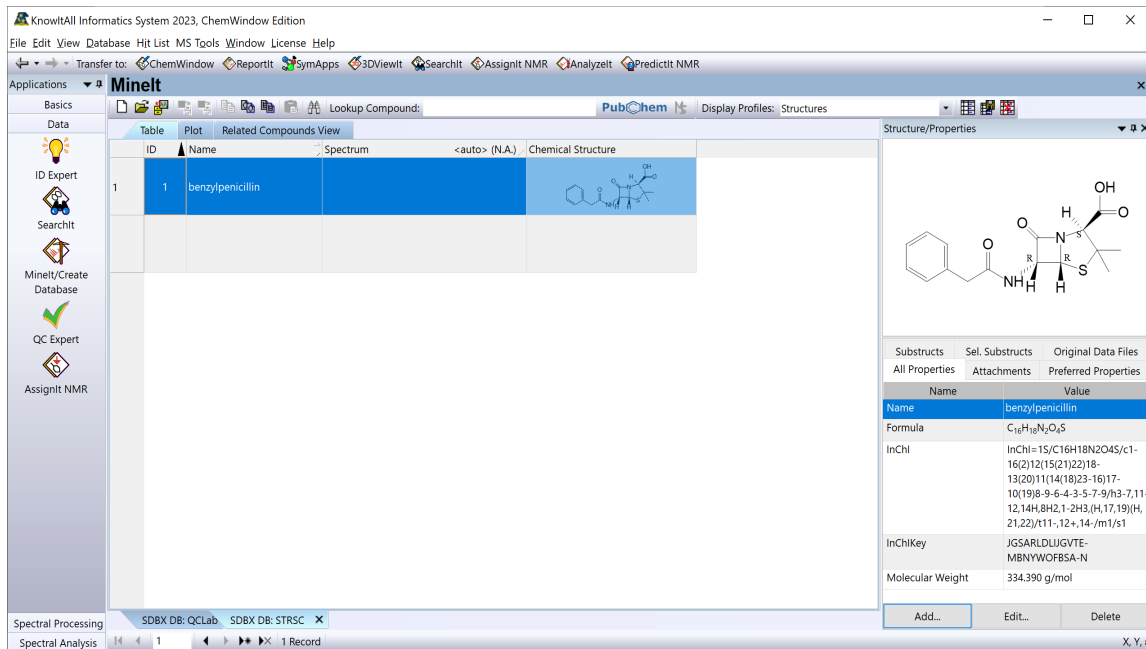
	Action	Result
5	Type 'STRSC' in the Database Abbreviation text box. Note: The abbreviation must be 3-7 characters long.	
6	Click OK .	<p>The new database has been created to receive your data. The Database Abbreviation appears on the database tab.</p> 
7	Choose View > Windows/Tables > Spectrum Pane to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

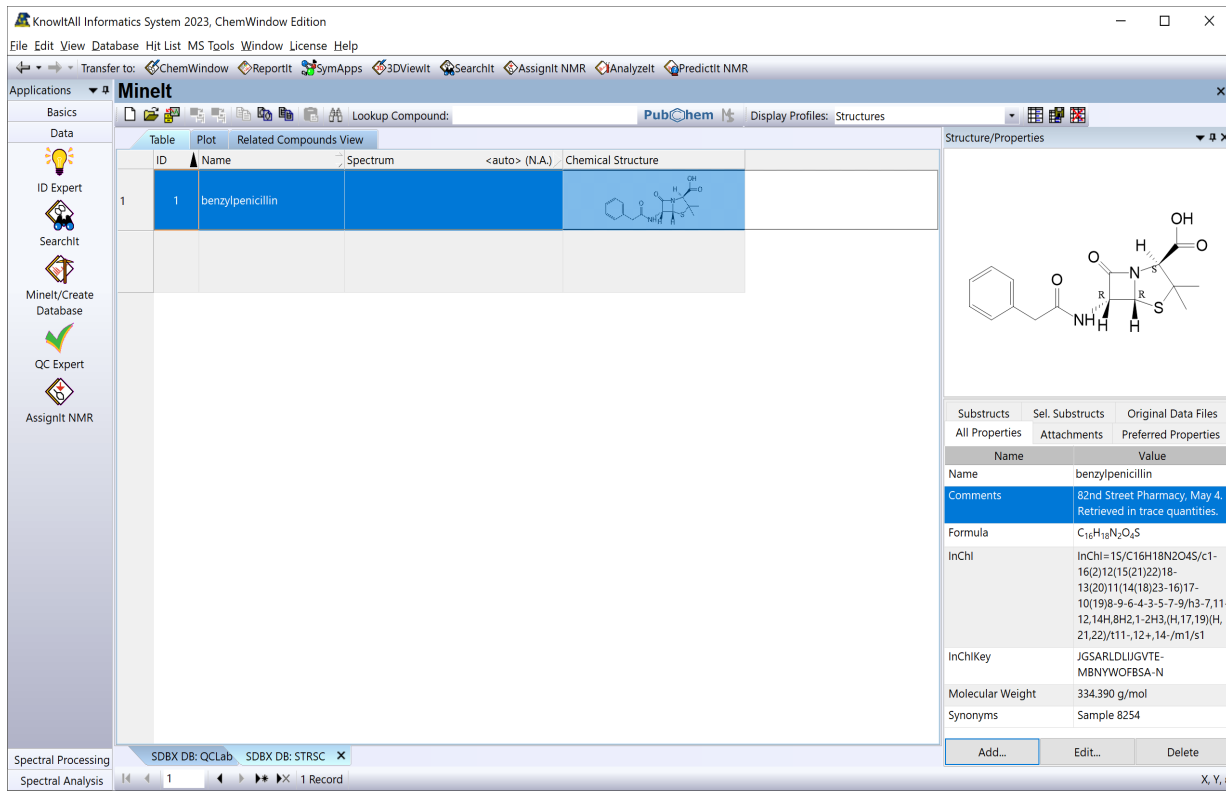
	Action	Result
8	Click the Add a New Profile toolbar button  , type the name 'Structures' in the New Profile dialog box, then click OK .	

Add a structure to the first database record

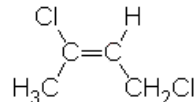
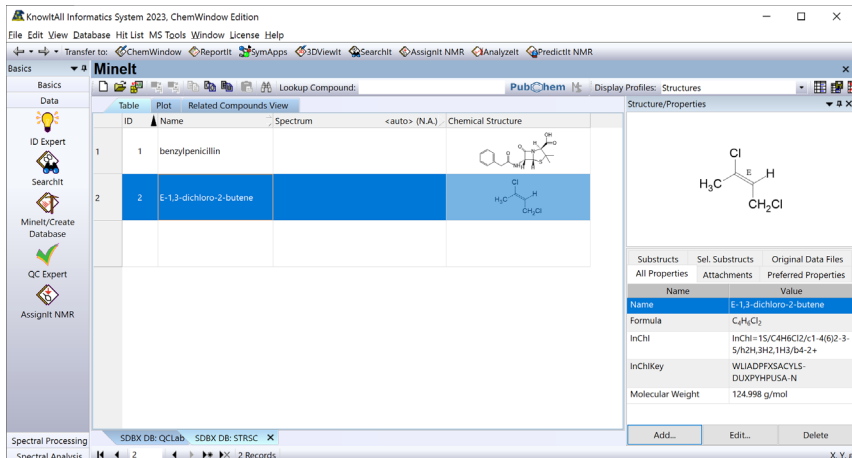
	Action	Result
1	<p>Choose File > Import</p> <p>Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Structures folder</p> <p>Open the structure file Benzylpenicillin.dsf.</p>	<p>The structure is displayed in the Structure/Properties pane.</p>  <p>The screenshot shows the KnowItAll Informatics System 2023, ChemWindow Edition interface. The main window displays a table with one record (ID 1) and a chemical structure of Benzylpenicillin. The Structure/Properties pane on the right shows the chemical structure and its properties, including the formula C₁₆H₁₈N₂O₅S, InChI string, InChIKey, and Molecular Weight (334.390 g/mol).</p>
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 .	The Property dialog box closes, and the added property Name appears in the Structure/Properties pane.  <table><tr><th colspan="2">Substructures</th><th colspan="2">Sel. Substructures</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>Name</th><th>Value</th><th colspan="4"></th></tr><tr><td>Name</td><td>benzylpenicillin</td><td colspan="4"></td></tr><tr><td>Formula</td><td>C₁₆H₁₈N₂O₄S</td><td colspan="4"></td></tr><tr><td>InChI</td><td>InChI=1S/C16H18N2O4S/c1-16(2)12(15(2)22)18-13(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)/t11-,12+,14-/m1/s1</td><td colspan="4"></td></tr><tr><td>InChIKey</td><td>JGSARLDLUGVTE-MBNYWOFBSA-N</td><td colspan="4"></td></tr><tr><td>Molecular Weight</td><td>334.390 g/mol</td><td colspan="4"></td></tr></table>	Substructures		Sel. Substructures		Original Data Files		All Properties		Attachments		Preferred Properties		Name	Value					Name	benzylpenicillin					Formula	C ₁₆ H ₁₈ N ₂ O ₄ S					InChI	InChI=1S/C16H18N2O4S/c1-16(2)12(15(2)22)18-13(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)/t11-,12+,14-/m1/s1					InChIKey	JGSARLDLUGVTE-MBNYWOFBSA-N					Molecular Weight	334.390 g/mol				
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All Properties		Attachments		Preferred Properties																																														
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Name	benzylpenicillin																																																	
Formula	C ₁₆ H ₁₈ N ₂ O ₄ S																																																	
InChI	InChI=1S/C16H18N2O4S/c1-16(2)12(15(2)22)18-13(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)/t11-,12+,14-/m1/s1																																																	
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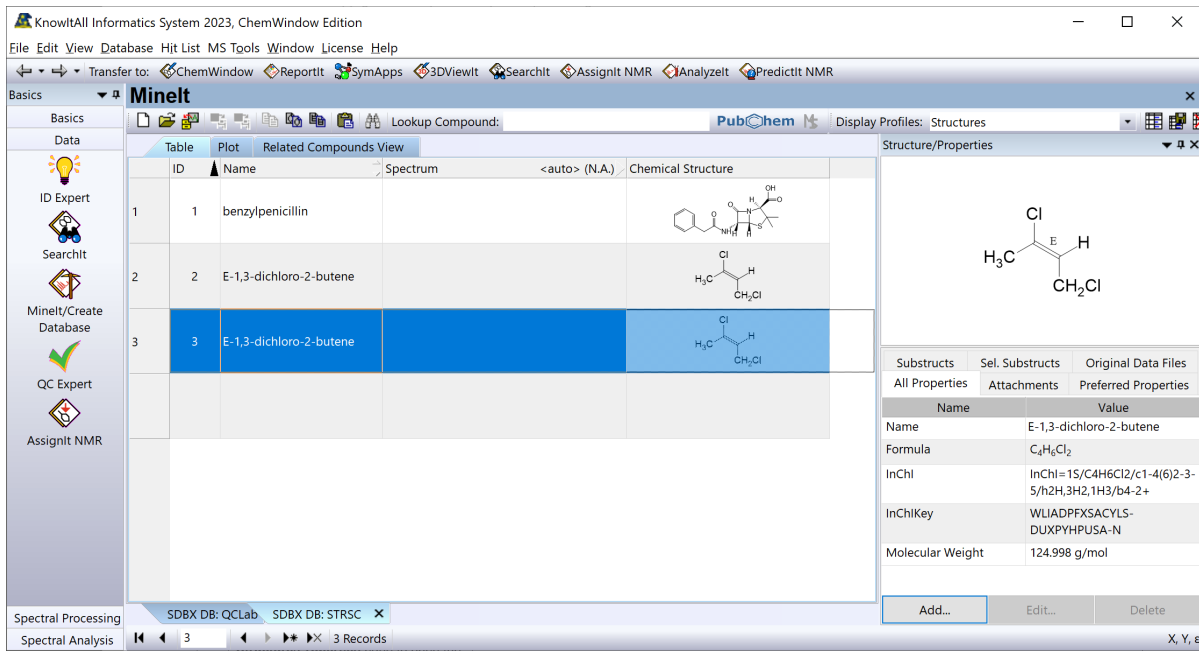
	Action	Result																
4	Repeat to add the property Synonyms with the value 'Sample 8254.'																	
5	Repeat to add the property Comments with the value '82 nd Street Pharmacy, May 4. Retrieved in trace quantities.'	 <p>The screenshot shows the KnowItAll Informatics System 2023, ChemWindow Edition interface. The main window displays a table with one entry: ID 1, Name benzylpenicillin. The right pane shows the chemical structure of benzylpenicillin and a list of properties including Name, Comments, Formula, InChI, InChIKey, Molecular Weight, and Synonyms.</p> <table><tr><th>Name</th><th>Value</th></tr><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>C₁₆H₁₈N₂O₅S</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/h3-7,11-12,14H,8H2,1-2H3,(H,17,19)(H,21,22)/t11-,12-,14-/m1/s1</td></tr><tr><td>InChIKey</td><td>JQSARLDLJGVTE-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></table>	Name	Value	Name	benzylpenicillin	Comments	82 nd Street Pharmacy, May 4. Retrieved in trace quantities.	Formula	C ₁₆ 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/h3-7,11-12,14H,8H2,1-2H3,(H,17,19)(H,21,22)/t11-,12-,14-/m1/s1	InChIKey	JQSARLDLJGVTE-MBNYWOFBSA-N	Molecular Weight	334.390 g/mol	Synonyms	Sample 8254
Name	Value																	
Name	benzylpenicillin																	
Comments	82 nd Street Pharmacy, May 4. Retrieved in trace quantities.																	
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InChIKey	JQSARLDLJGVTE-MBNYWOFBSA-N																	
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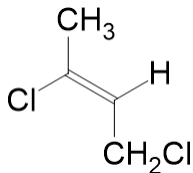
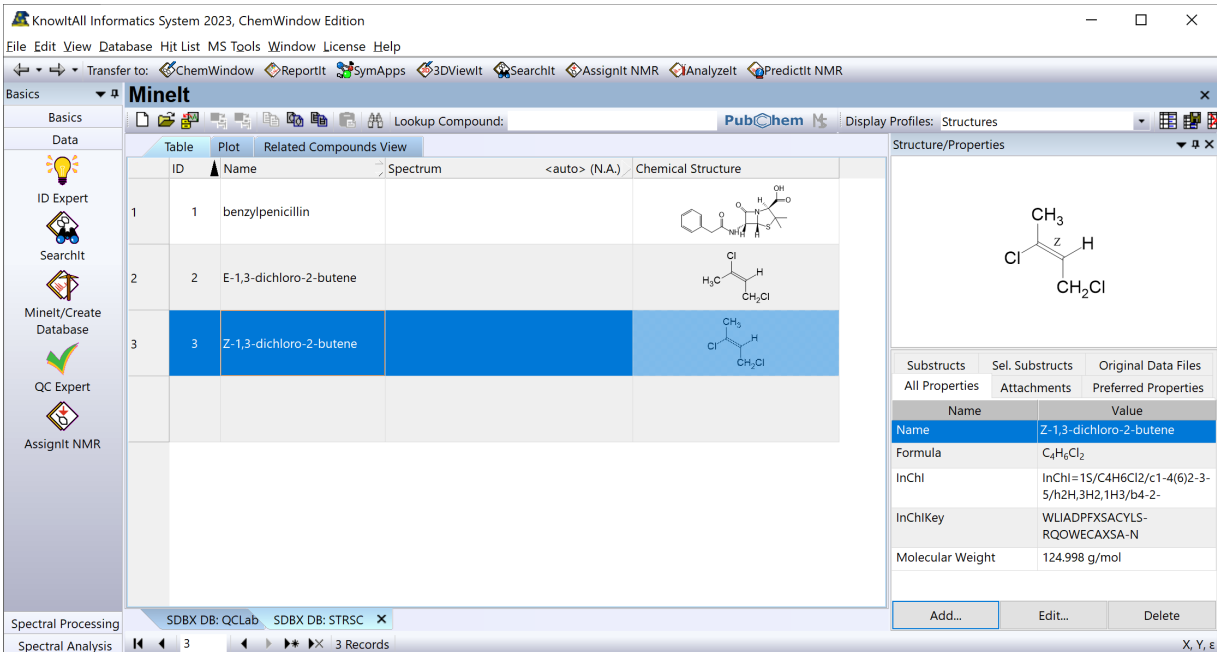
Add a second database record

	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: 													
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>  <table><tr><th>Name</th><th>Value</th></tr><tr><td>Name</td><td>(E)-1,3-dichloro-2-butene</td></tr><tr><td>Formula</td><td>C₄H₂Cl₂</td></tr><tr><td>InChI</td><td>InChI=1S/C4H4Cl2/c1-4/b2-3-5/r2H,3H2,1H3/b4-2+</td></tr><tr><td>InChIKey</td><td>WUADPFXSACYLS-DUXPHYPUA-N</td></tr><tr><td>Molecular Weight</td><td>124.998 g/mol</td></tr></table>	Name	Value	Name	(E)-1,3-dichloro-2-butene	Formula	C ₄ H ₂ Cl ₂	InChI	InChI=1S/C4H4Cl2/c1-4/b2-3-5/r2H,3H2,1H3/b4-2+	InChIKey	WUADPFXSACYLS-DUXPHYPUA-N	Molecular Weight	124.998 g/mol
Name	Value													
Name	(E)-1,3-dichloro-2-butene													
Formula	C ₄ H ₂ Cl ₂													
InChI	InChI=1S/C4H4Cl2/c1-4/b2-3-5/r2H,3H2,1H3/b4-2+													
InChIKey	WUADPFXSACYLS-DUXPHYPUA-N													
Molecular Weight	124.998 g/mol													

	Action	Result
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 window. The main table has columns: ID, Name, Spectrum, and Chemical Structure. The third record is highlighted in blue. The 'Structure/Properties' pane on the right displays the chemical structure of E-1,3-dichloro-2-butene and its properties.</p> <table border="1"> <thead> <tr> <th colspan="2">Substructures</th> <th>Original Data Files</th> </tr> <tr> <th>All Properties</th> <th>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">E-1,3-dichloro-2-butene</td> </tr> <tr> <td>Formula</td> <td colspan="2">C₄H₆Cl₂</td> </tr> <tr> <td>InChi</td> <td colspan="2">InChi=1S/C4H6Cl2/c1-4(6)2-3-5/h2H,3H2,1H3/b4-2+</td> </tr> <tr> <td>InChiKey</td> <td colspan="2">WLIADPFXSACYLS-DUXPHYPUA-N</td> </tr> <tr> <td>Molecular Weight</td> <td colspan="2">124.998 g/mol</td> </tr> </tbody> </table>	Substructures		Original Data Files	All Properties	Attachments	Preferred Properties	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-DUXPHYPUA-N		Molecular Weight	124.998 g/mol	
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InChiKey	WLIADPFXSACYLS-DUXPHYPUA-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	<p>Edit the structure as shown, then click Return to Minelt Database and Save.</p> 	<p>The structure is added to the third database record.</p> <p>ChemWindow is closed and we are back to the Minelt window.</p>																
5	<p>Edit the property Name to 'Z-1,3-dichloro-2-butene.'</p>	 <table><thead><tr><th colspan="2">Structure/Properties</th></tr><tr><th colspan="2">Substructures</th></tr><tr><th>All Properties</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>	Structure/Properties		Substructures		All Properties	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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InChIKey	WLIADPFXSACYLS-RQOWECAXSA-N																	
Molecular Weight	124.998 g/mol																	

Note: In the KnowItAll 2026 release, to be compliant with 21 CFR Part 11, we added history information for modifications to the database records. You can check the record history by clicking on its History button:

All Properties	Attachments	Preferred Properties	Substructs	Sel. Substructs	Original Data File	History
Date/Time		Object		Modification		
6/30/2025 1:26 PM		Name		Added		
6/30/2025 1:27 PM		Name		Modified		
6/30/2025 1:27 PM		IUPAC Name		Added		
6/30/2025 1:27 PM		Molecular Weight		Added		

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, scientists can improve their analyses.

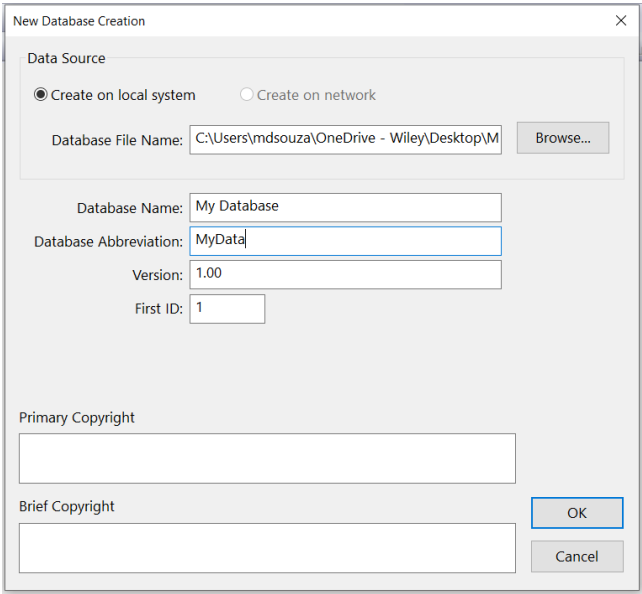
Training Files Used in This Lesson

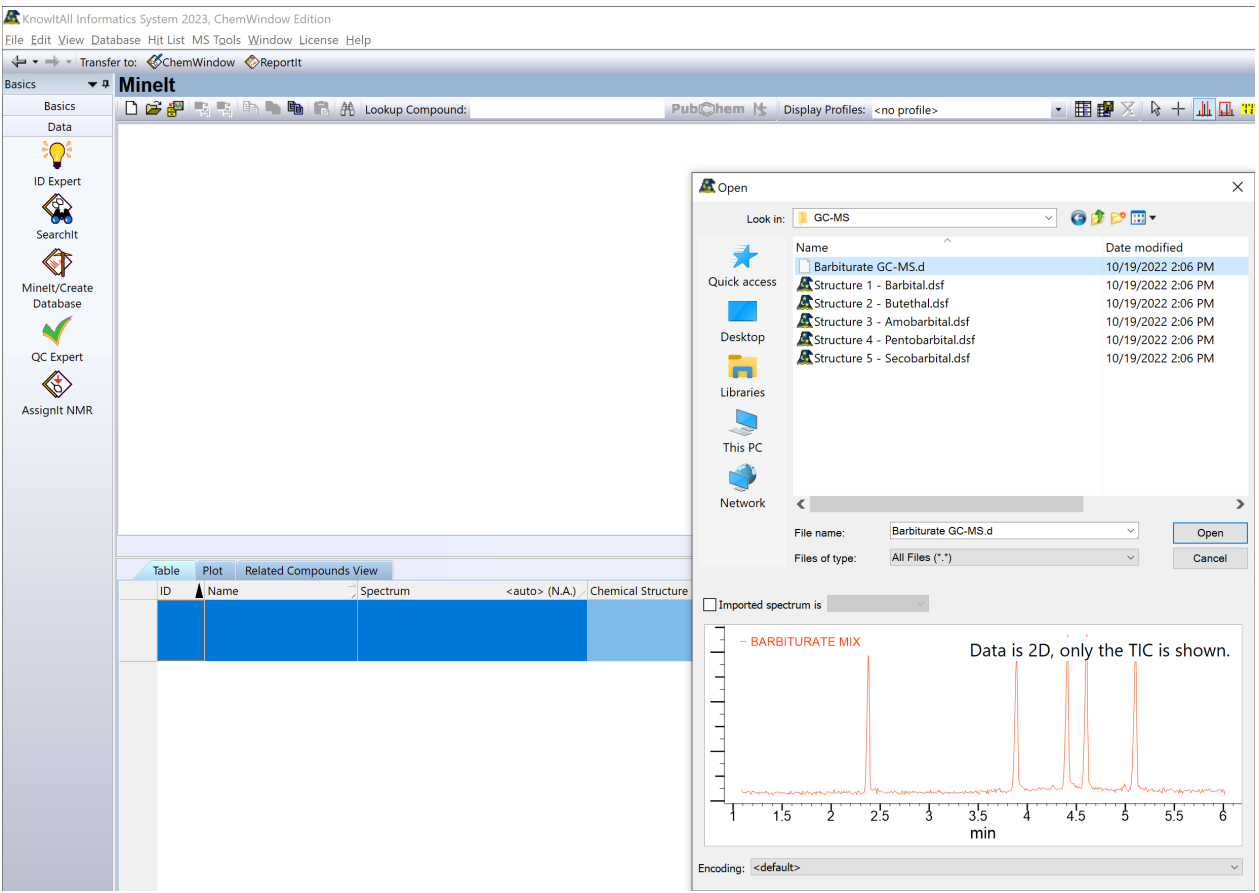
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\GC-MS folder

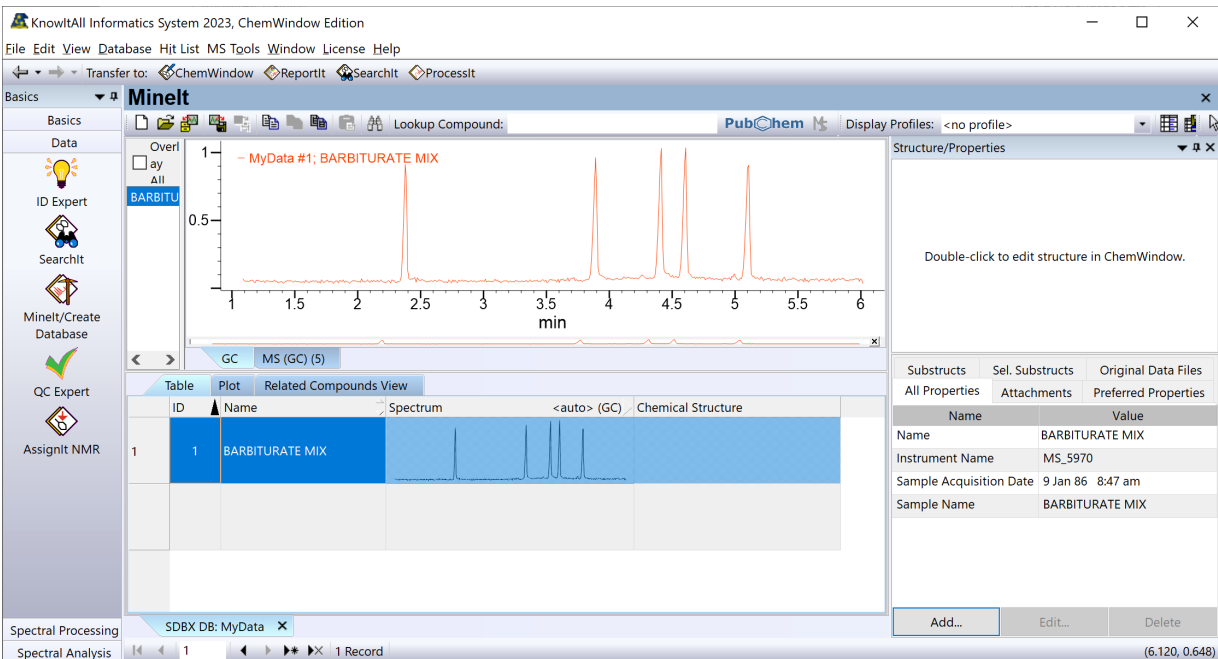
KnowItAll Applications Used

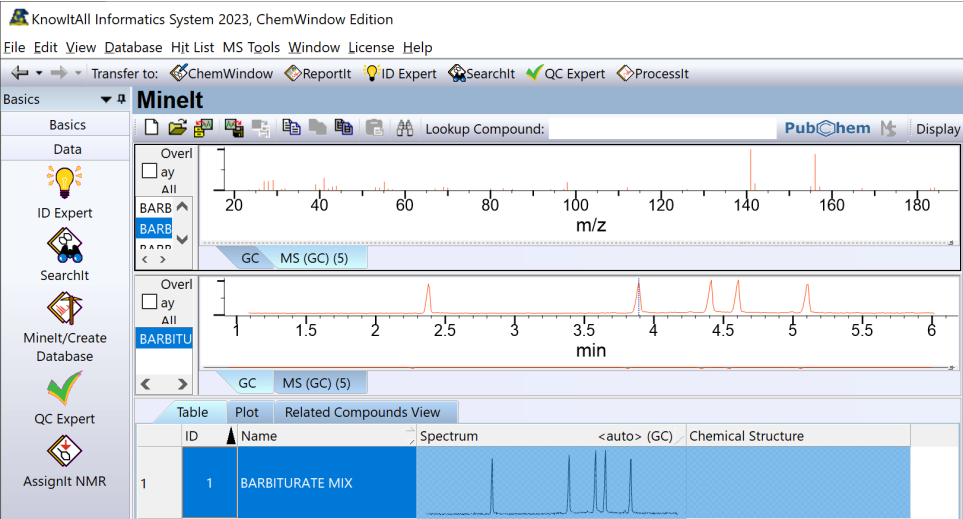
- Minelt
- ChemWindow®
- Browselt

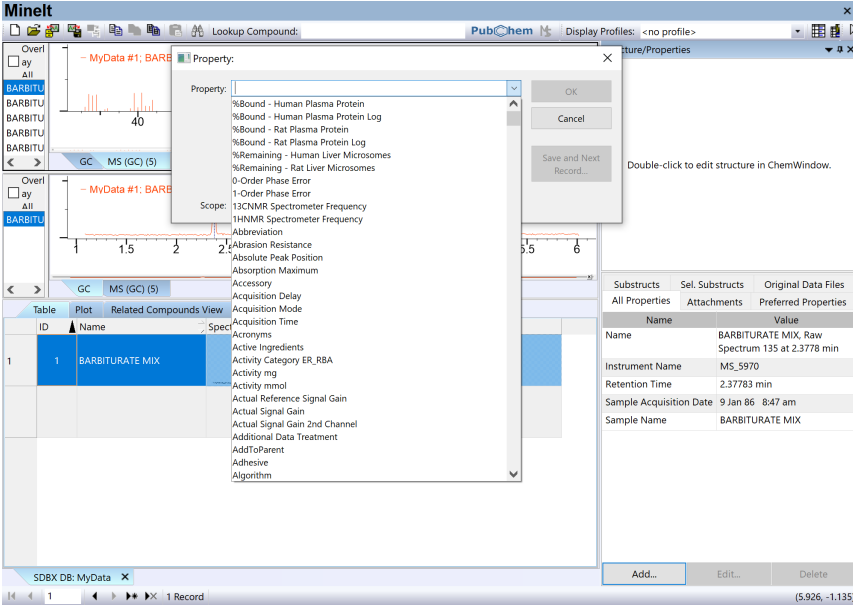
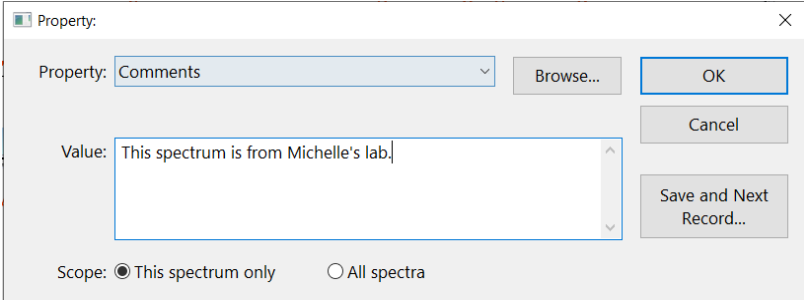
GC-MS Record Creation

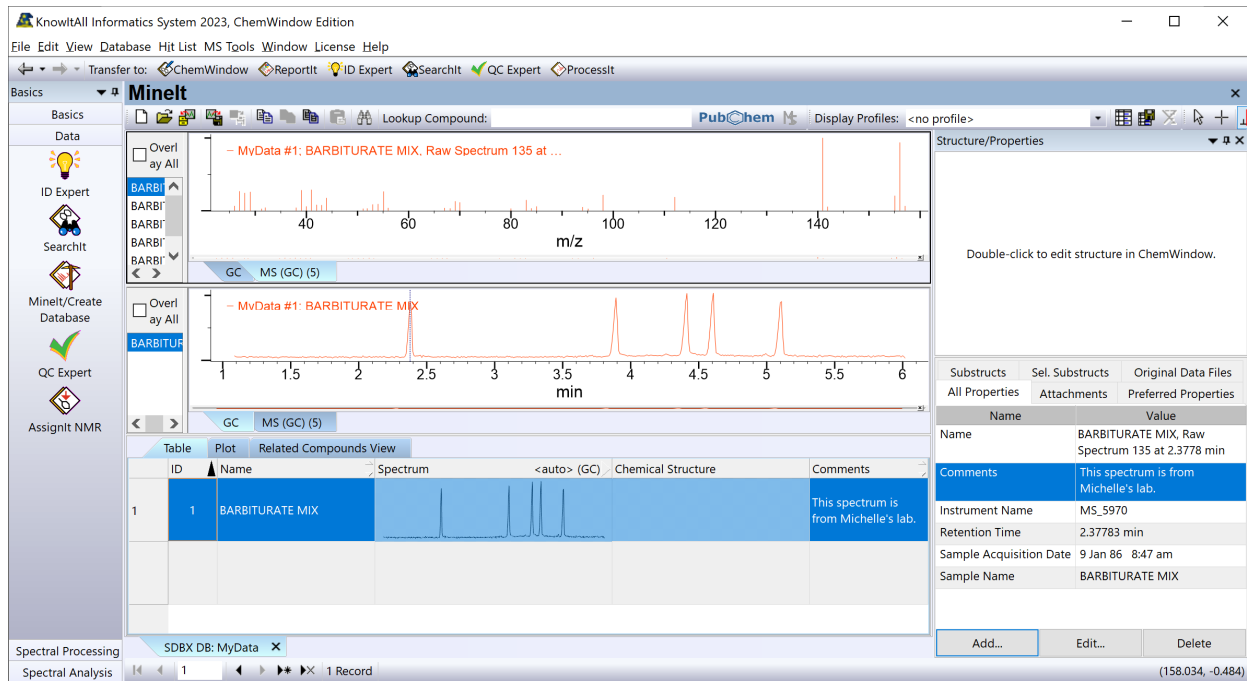
	Action	Result
1	<p>Start KnowItAll.</p> <p>Click the Minelt icon.</p> <p>Select Database > New.</p> <p>Use Browse to set the hardware location for the database.</p> <p>Enter a Database Name.</p> <p>Enter a Database Abbreviation ("MyData" etc).</p> <p>Click OK.</p>	

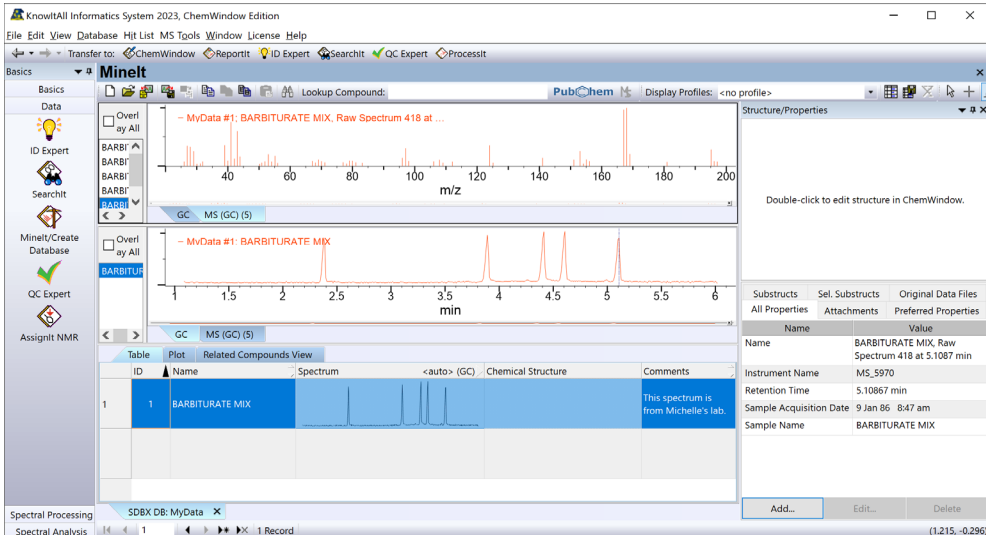
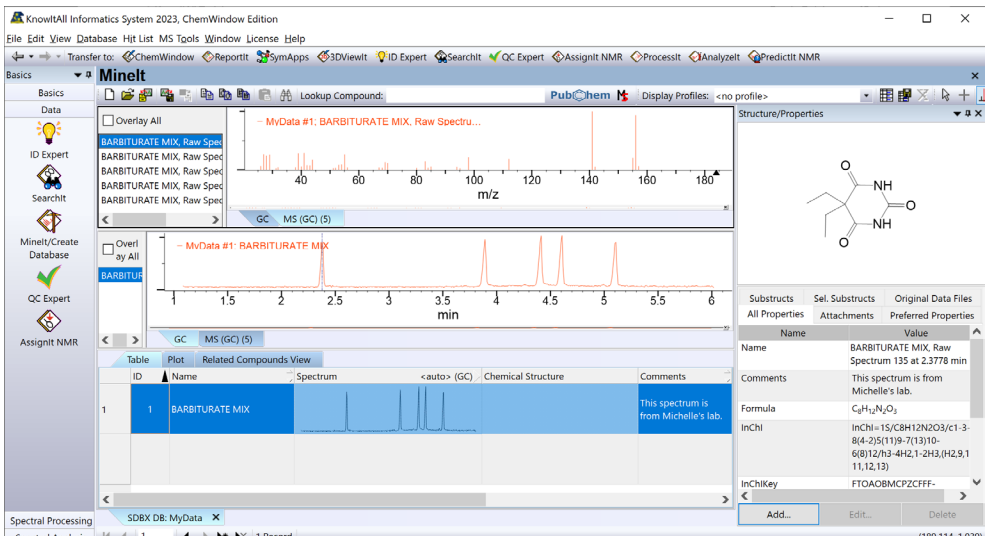
	Action	Result								
2	<p>From the File menu, select Import.</p> <p>In the dialog prompt, navigate to Samples > GC-MS.</p> <p>Select the file Barbiturate GC-MS.d.</p> <p>Click Open.</p>	 <p>KnowItAll Informatics System 2023, ChemWindow Edition</p> <p>File Edit View Database Hit List MS Tools Window License Help</p> <p>Transfer to: ChemWindow ReportIt</p> <p>Basics Minelt</p> <p>Basics Data ID Expert SearchIt Minelt/Create Database QC Expert AssignIt NMR</p> <p>Table Plot Related Compounds View</p> <table border="1"><thead><tr><th>ID</th><th>Name</th><th>Spectrum</th><th>Chemical Structure</th></tr></thead><tbody><tr><td></td><td></td><td></td><td></td></tr></tbody></table> <p>File name: Barbiturate GC-MS.d</p> <p>Files of type: All Files (*.*)</p> <p>Open Cancel</p> <p>Imported spectrum is</p> <p>BARBITURATE MIX</p> <p>Data is 2D, only the TIC is shown.</p> <p>min</p> <p>Encoding: <default></p>	ID	Name	Spectrum	Chemical Structure				
ID	Name	Spectrum	Chemical Structure							

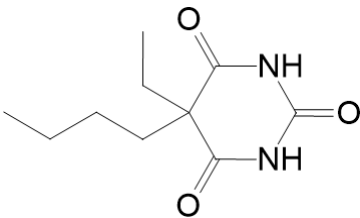
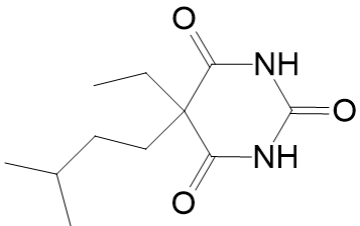
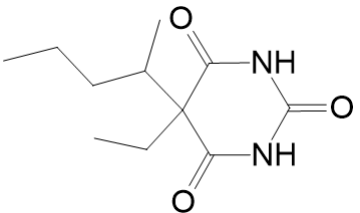
Action	Result																					
4	 <p>KnowItAll Informatics System 2023, ChemWindow Edition</p> <p>File Edit View Database Hit List MS Tools Window License Help</p> <p>Transfer to: ChemWindow Reportit Searchit Processit</p> <p>Basics</p> <p>Basics Data ID Expert Searchit Minelt/Create Database QC Expert Assignit NMR</p> <p>Minelt</p> <p>Lookup Compound: PubChem Display Profiles: <no profile></p> <p>Structure/Properties</p> <p>Double-click to edit structure in ChemWindow.</p> <table border="1"><thead><tr><th>Substructs</th><th>Sel. Substructs</th><th>Original Data Files</th></tr><tr><th>All Properties</th><th>Attachments</th><th>Preferred Properties</th></tr><tr><th>Name</th><th>Value</th><th></th></tr></thead><tbody><tr><td>Name</td><td>BARBITURATE MIX</td><td></td></tr><tr><td>Instrument Name</td><td>MS_5970</td><td></td></tr><tr><td>Sample Acquisition Date</td><td>9 Jan 86 8:47 am</td><td></td></tr><tr><td>Sample Name</td><td>BARBITURATE MIX</td><td></td></tr></tbody></table> <p>Add... Edit... Delete</p> <p>(6.120, 0.648)</p> <p>Spectral Processing SDBX DB: MyData</p> <p>Spectral Analysis 1 1 Record</p>	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	
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Sample Name	BARBITURATE MIX																					

	Action	Result
5	<p>Navigate to Window > Split twofold.</p> <p>Select MS to be the technique showing in the top pane and GC to show in bottom pane.</p> <p>Mouse over GC scan pane.</p> <p>Right-click, make sure mouse is in Selection mode.</p> <p>Click through GC peaks to show MS pane changing.</p>	

	Action	Result
6	<p>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 Add button.</p>	 <p>The screenshot shows the Minelt software interface. The 'MS (GC) (5)' pane is selected and has a black border. The first scan is highlighted. The 'Add' button is highlighted in the bottom right corner of the interface.</p>
7	<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>The screenshot shows the 'Property' pop-up window. The 'Property' dropdown is set to 'Comments'. The 'Value' text box contains the text 'This spectrum is from Michelle's lab.'. The 'Scope' section has the 'This spectrum only' radio button selected.</p>

Action	Result																											
8	 <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</p> <p>Minelt</p> <p>PubChem Display Profiles: <no profile></p> <p>Structure/Properties</p> <p>Double-click to edit structure in ChemWindow.</p> <table border="1"><thead><tr><th>Substructs</th><th>Sel. Substructs</th><th>Original Data Files</th></tr><tr><th>All Properties</th><th>Attachments</th><th>Preferred Properties</th></tr></thead><tbody><tr><td>Name</td><td>Value</td><td></td></tr><tr><td>Name</td><td>BARBITURATE MIX, Raw Spectrum 135 at 2.3778 min</td><td></td></tr><tr><td>Comments</td><td>This spectrum is from Michelle's lab.</td><td></td></tr><tr><td>Instrument Name</td><td>MS_5970</td><td></td></tr><tr><td>Retention Time</td><td>2.37783 min</td><td></td></tr><tr><td>Sample Acquisition Date</td><td>9 Jan 86 8:47 am</td><td></td></tr><tr><td>Sample Name</td><td>BARBITURATE MIX</td><td></td></tr></tbody></table> <p>Add... Edit... Delete</p> <p>(158.034, -0.484)</p>	Substructs	Sel. Substructs	Original Data Files	All Properties	Attachments	Preferred Properties	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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	Action	Result
9	Select another MS spectrum.	
10	<p>Highlight MS 135 from the available list.</p> <p>File > Import.</p> <p>Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\GC-MS folder</p> <p>Select Structure 1 – Barbitol.</p> <p>Click Open.</p>	

	Action	Result
11	Highlight MS 292 from the available list. File > Import. Select Structure 2 – Butethal. Click Open.	
12	Highlight MS 346 from available list. File > Import. Select Structure 3 – Amobarbital. Click Open.	
13	Highlight MS 366 from the available list. File > Import. Select Structure 4 – Pentaobarbital. Click Open.	

Report Data Related Issues

KnowItAll users can submit feedback on data in **Minelt** if a user database is open.

	Action	Result
1	Open the KnowItAll Informatics System by double-clicking its icon on the desktop.	<p>The KnowItAll Informatics System automatically opens to the Browselt 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 Minelt/Create Database application in Data toolbox	
3	Use the Help > Submit Feedback menu-item	
4	<p>A dialog box pops up</p> <ul style="list-style-type: none"> • Enter your feedback • Check the agreement box • Submit 	<p>KnowItAll confirms the message submission:</p> 