

# **KnowItAll Software Training**

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## SmartSpectra Databases and Classification Models

# Using SmartSpectra in KnowItAll

## Purpose

These exercises demonstrate how to use SmartSpectra in KnowItAll ID Expert and SearchIt.

## Objectives

These exercises will teach you:

- How to use SmartSpectra IR spectra in KnowItAll SearchIt
- How to use SmartSpectra Raman spectra in KnowItAll SearchIt
- How to use SmartSpectra IR spectra in KnowItAll ID Expert
- How to use SmartSpectra Raman spectra in KnowItAll ID Expert

### Training Files Used in This Lesson:

- 4-(Pyridin-3-yl)-2,2,6,2-terpyridine.irf
- 4,13-DIDECYL-1,7,10,16-TETRAOXA-4,13-DIAZACYCLOOCTADECANE.irf
- X-Phos.irf
- 1-acetyl-1234-tetrahydroquinoline.irf
- 17-Hydroxy-17-alpha-pregn-4-en-20-yn-3-one.irf

*Note:* The training files used are for example purposes only. The user should utilize their own IR spectra when following this training.

### KnowItAll Applications Used:

- KnowItAll SearchIt
- KnowItAll ID Expert

## Background

Wiley has the largest quantity of experimental IR spectra, which includes the Sadtler IR collection. Even with the continued development in the chemical industry, there is still insufficient progress to cover the newly-discovered chemical space. Sample collection is also challenging, time-consuming and costly. Wiley's IR SmartSpectra Collection is an attempt to increase the catalog coverage of Wiley's IR chemical space. This does not mean that this database will increase the chemical space, but that it will increase the amount of coverage within the bounds of our current libraries' chemical space. With the development of computer modeling technology, the feasibility of using computed IR spectra to compensate for the lack of samples was investigated and found to increase unknown compound classification.

These libraries can be helpful when used as tools for searching unknown compounds, illuminating the composition of an unknown spectrum, or accurately predicting the compound's spectrum for the associated structure and functional groups. Due to the predicted nature of this data, it should be mentioned that the results have a margin of error. Wiley acknowledges that some results may not be entirely correct. It is advised that users employ these libraries as additional tools to help the user classify components that are in the spectrum in order to characterize their unknown spectrum.

## KnowItAll IR and Raman Search Algorithms

A background in the algorithms used by KnowItAll will be beneficial. For IR and Raman spectral comparison, KnowItAll uses the following algorithms:

### Correlation

This is the default algorithm for searching in KnowItAll and it conforms to the industry standard for correlation algorithms. The Correlation algorithm is similar to the Euclidean Distance algorithm. The difference between the two is in the way the spectra are treated before the comparison. Each spectrum is mean-centered prior to performing the dot product normalization. This approach can improve search results for noisy spectra and spectra that have baseline issues, particularly with a baseline offset that is the result of a negative spike or chemical noise. It is slightly more time-consuming than the Euclidean Distance algorithm. The search speed is slower because each spectrum in the database must be mean-centered and then normalized prior to the comparison. The search results that are obtained with the Correlation algorithm are spectrally similar to the unknown, even if the unknown compound is not in the database. The Correlation algorithm is heavily weighted by peak areas. Broad features are weighted much more strongly than sharp features. The algorithm is most tolerant to peak shifts and non-linearities in relative band intensities.

### Correlation (Classic)

The Correlation algorithm that was found in all versions of KnowItAll prior to KnowItAll 2020 is similar to the Euclidean Distance algorithm. However, it did not conform to the industry standard for correlation algorithms. Beginning with KnowItAll 2020, the Correlation algorithm does conform to the industry standard and it is the default algorithm used for searching in KnowItAll. To provide backward compatibility for customers who want to reproduce prior search results, the previous correlation algorithm is now provided as Correlation (Classic).

### Euclidean Distance

The Euclidean Distance algorithm measures the point-to-point differences between a pair of spectra. The results that are obtained with the Euclidean Distance algorithm are spectrally similar to the unknown, even if the unknown compound is not in the database. This algorithm, however, can yield degraded search results when the unknown spectrum has a sloping or offset baseline. The Euclidean Distance algorithm is heavily weighted by peak areas. Broad features are weighted much more strongly than sharp features. This algorithm is most tolerant to peak shifts and non-linearities in relative band intensities.

**First Derivative Euclidean Distance**

Use this algorithm to reduce the effects of baseline slope or offset in the unknown. Although the search speed is slightly slower than with the Euclidean Distance algorithm, the First Derivative Euclidean Distance sometimes gives improved search results, especially when the unknown spectrum is a mixture of two or more compounds. The First Derivative Euclidean Distance algorithm is heavily weighted by changes in slope. Sharp features are weighted much more strongly than broad features. The algorithm is also very sensitive to peak shifts. Small shifts can make the algorithm miss a similar result.

**Second Derivative Euclidean Distance**

Use the Second Derivative Euclidean Distance algorithm to compare the second derivative of a reference spectrum to that of the query spectrum.

## **Optimized Corrections: A Breakthrough Technology for Spectral Searching**

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

According to ASTM's guide on spectral searching<sup>1</sup>, various algorithms and manual methods exist to adjust spectra to get reasonable match scores when two compared spectra of the same compound differ for various reasons. While these methods may work in selected cases, subtle discrepancies such as a shift of the X-axis are very hard to identify and correct manually. The inflexible mathematical algorithms typically employed do not compensate for these types of errors in spectra that are flawed.

Manual corrections can be made by expert spectroscopists, but those less experienced in spectroscopy are often unaware of how to perform the necessary corrections on their sample spectrum to achieve the best search result. To address this growing concern, Wiley has introduced Optimized Corrections, a breakthrough patented technology that performs a computationally complex set of multiple corrections on query and reference spectra in a search to find the optimal match between the query and each individual reference spectrum. This training guide will demonstrate how the Optimized Corrections technology yields better matches between query and reference spectra than can be attained using rigid search algorithms alone or with manual methods to optimize spectra for searching.

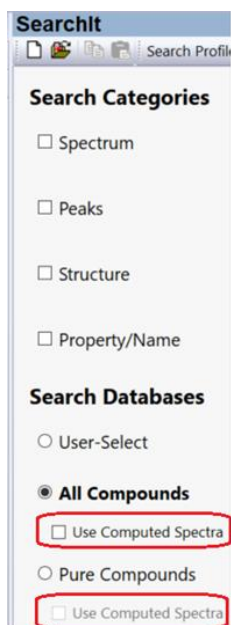
Optimized Corrections consider the full spectrum during a selected range(s) search.

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

# SearchIt


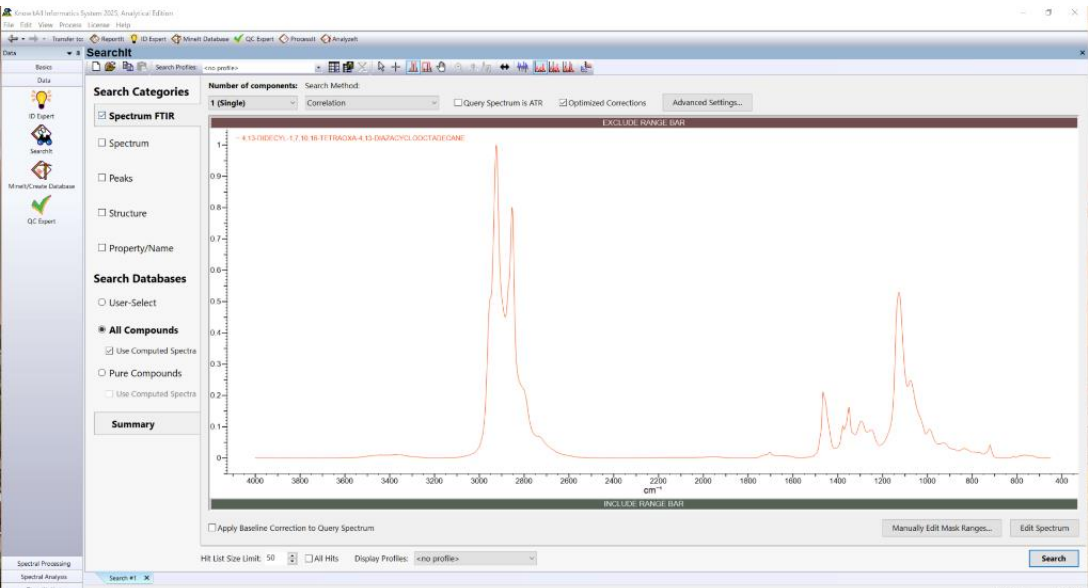
## Introduction

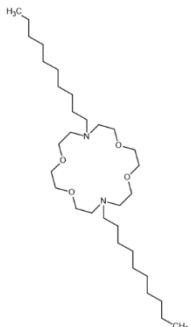
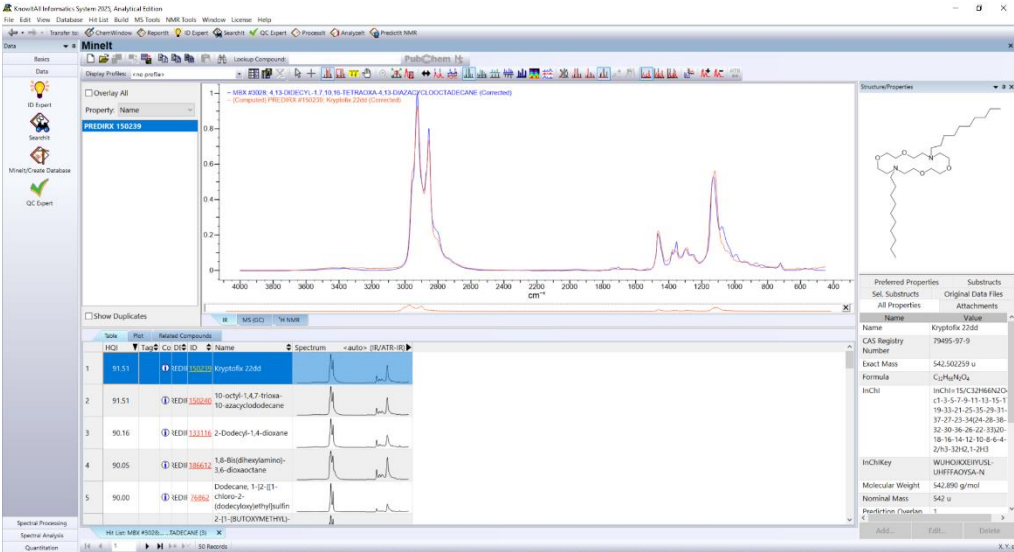
When a user license contains the subscription to SmartSpectra IR spectra, it can be accessed in the **SearchIt** application using **Search Databases > All Compounds** or **Databases > Pure Compounds** and by checking the box for the **Use Computed Spectra** option:



## Example 1

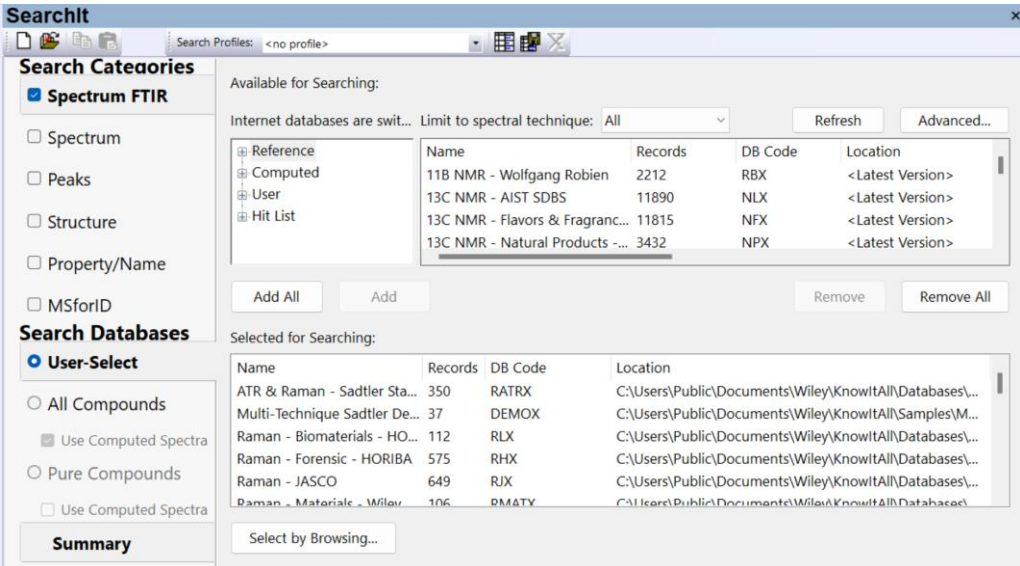
**Example File:** 4,13-DIDECYL-1,7,10,16-TETRAOXA-4,13-DIAZACYCLOOCTADECANE.irf

	Action	Result
1	In the <b>SearchIt</b> application, click <b>Open Spectrum or Structure</b> icon (  ) located on the <b>Standard Toolbar</b> .	<i>Note:</i> The training files used in this document are for example purposes only. The user should utilize their own IR spectra when following this training.
2	Navigate to find <b>4,13-DIDECYL-1,7,10,16-TETRAOXA-4,13-DIAZACYCLOOCTADECANE.irf</b> in “C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Computed Spectra\IR” folder. Click <b>Open</b> .  Confirm that the <b>Search Method</b> is set to <b>Correlation</b> algorithm. To change the method, use the dropdown menu to select it as the option. Search Method: <input type="text" value="Correlation"/>  Under the <b>Search Databases</b> section, select <b>All Compounds</b> with the ‘ <b>Use Computed Spectra</b> ’ box checked as well. <input checked="" type="radio"/> <b>All Compounds</b> <input checked="" type="checkbox"/> Use Computed Spectra  Click <b>Search</b> .	The image on this page is the correct compound structure associated with this spectrum. Upon executing the search, <b>Minelt</b> application displays the query results.  



	Action	Result
3	<p>In <b>Minelt</b>, the hit list table displays match results featuring a mix of predicted and empirical matches.</p> <p>The structure below is the correct match for the query spectrum's structure,.</p> <p>The structure below is an exact match with the predicted data which appears as the top hit in the table.</p> 	<p>The hit list results open in <b>Minelt</b>. The best match for the query appears at the top of the hit list. This top match is automatically selected and displayed:</p>  <p><b>Note:</b> Specific results will depend on the available databases in the user license.</p>


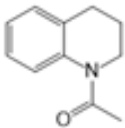
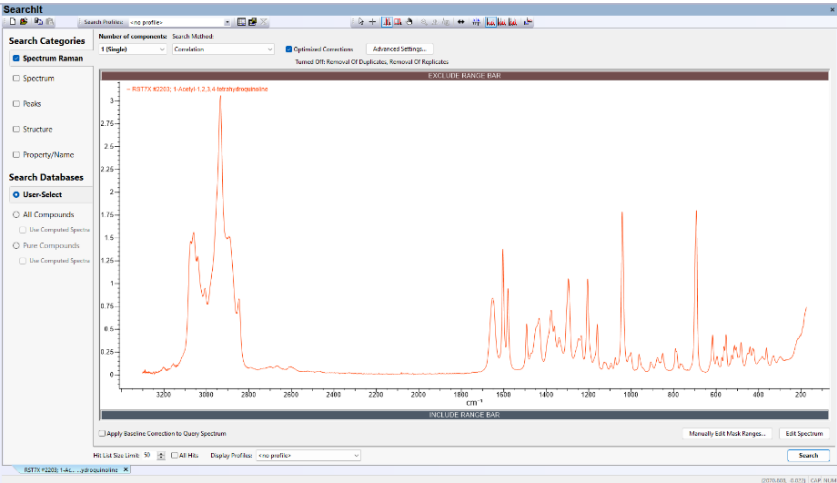
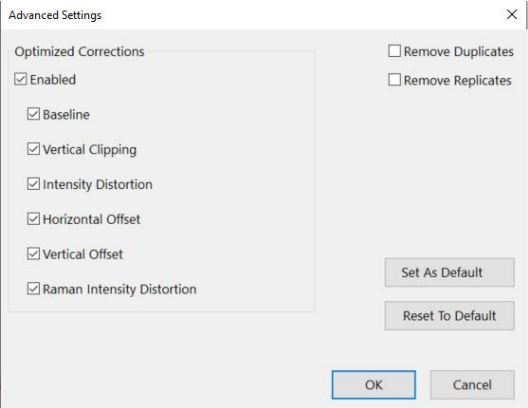
## Example 2

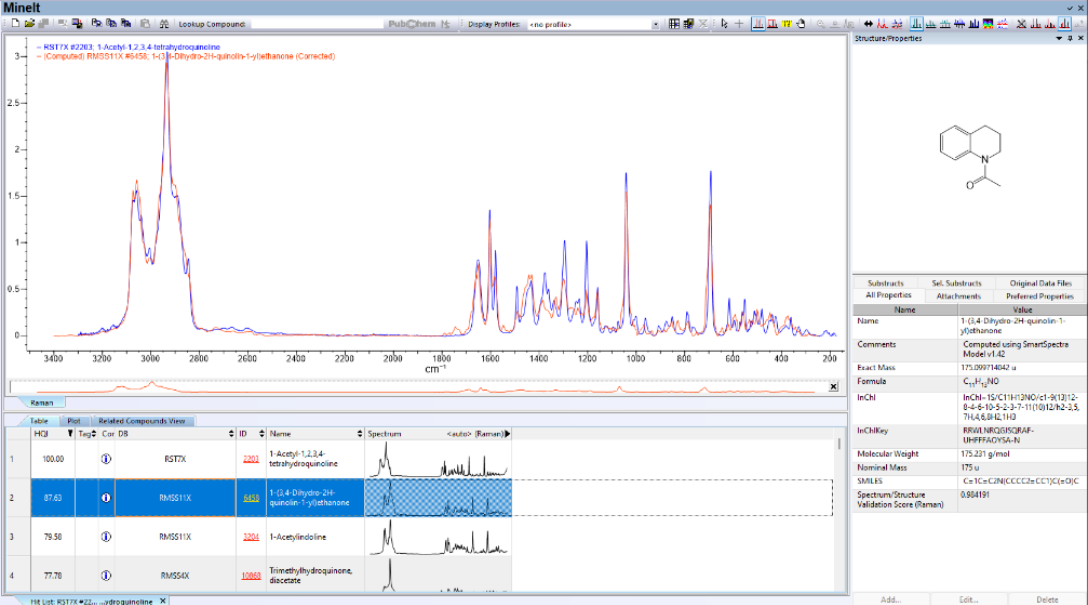
Example File: 1-acetyl-1234-tetrahydroquinoline.irf

	Action	Result																																																				
1	<p>Return to the <b>SearchIt</b> application. Clear the previous search by hitting the small <b>X</b> on the upper right-hand side of the screen (X).</p> <p>In the <b>SearchIt</b> application, click <b>User-Select</b> under the <b>Search Databases</b> section.</p>	<p>The <b>User-Select Databases</b> window is displayed:</p>  <p><b>Search Categories</b></p> <ul style="list-style-type: none"> <li><input checked="" type="checkbox"/> Spectrum FTIR</li> <li><input type="checkbox"/> Spectrum</li> <li><input type="checkbox"/> Peaks</li> <li><input type="checkbox"/> Structure</li> <li><input type="checkbox"/> Property/Name</li> <li><input type="checkbox"/> MSforID</li> </ul> <p><b>Search Databases</b></p> <ul style="list-style-type: none"> <li><input checked="" type="radio"/> User-Select</li> <li><input type="radio"/> All Compounds <ul style="list-style-type: none"> <li><input checked="" type="checkbox"/> Use Computed Spectra</li> </ul> </li> <li><input type="radio"/> Pure Compounds <ul style="list-style-type: none"> <li><input type="checkbox"/> Use Computed Spectra</li> </ul> </li> </ul> <p><b>Summary</b></p> <p>Available for Searching:</p> <p>Internet databases are swit... Limit to spectral technique: All Refresh Advanced...</p> <table border="1"> <thead> <tr> <th>Name</th> <th>Records</th> <th>DB Code</th> <th>Location</th> </tr> </thead> <tbody> <tr> <td>Reference</td> <td></td> <td></td> <td></td> </tr> <tr> <td>11B NMR - Wolfgang Robien</td> <td>2212</td> <td>RBX</td> <td>&lt;Latest Version&gt;</td> </tr> <tr> <td>13C NMR - AIST SDBS</td> <td>11890</td> <td>NLX</td> <td>&lt;Latest Version&gt;</td> </tr> <tr> <td>13C NMR - Flavors &amp; Fragranc...</td> <td>11815</td> <td>NFX</td> <td>&lt;Latest Version&gt;</td> </tr> <tr> <td>13C NMR - Natural Products -...</td> <td>3432</td> <td>NPX</td> <td>&lt;Latest Version&gt;</td> </tr> </tbody> </table> <p>Add All Add Remove Remove All</p> <p>Selected for Searching:</p> <table border="1"> <thead> <tr> <th>Name</th> <th>Records</th> <th>DB Code</th> <th>Location</th> </tr> </thead> <tbody> <tr> <td>ATR &amp; Raman - Sadtler Sta...</td> <td>350</td> <td>RATRX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\...</td> </tr> <tr> <td>Multi-Technique Sadtler De...</td> <td>37</td> <td>DEMOX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Samples\M...</td> </tr> <tr> <td>Raman - Biomaterials - HO...</td> <td>112</td> <td>RLX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\...</td> </tr> <tr> <td>Raman - Forensic - HORIBA</td> <td>575</td> <td>RHX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\...</td> </tr> <tr> <td>Raman - JASCO</td> <td>649</td> <td>RJX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\...</td> </tr> <tr> <td>Raman - Materials - Wiley</td> <td>106</td> <td>PMATY</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\...</td> </tr> </tbody> </table> <p>Select by Browsing...</p>	Name	Records	DB Code	Location	Reference				11B NMR - Wolfgang Robien	2212	RBX	<Latest Version>	13C NMR - AIST SDBS	11890	NLX	<Latest Version>	13C NMR - Flavors & Fragranc...	11815	NFX	<Latest Version>	13C NMR - Natural Products -...	3432	NPX	<Latest Version>	Name	Records	DB Code	Location	ATR & Raman - Sadtler Sta...	350	RATRX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\...	Multi-Technique Sadtler De...	37	DEMOX	C:\Users\Public\Documents\Wiley\KnowItAll\Samples\M...	Raman - Biomaterials - HO...	112	RLX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\...	Raman - Forensic - HORIBA	575	RHX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\...	Raman - JASCO	649	RJX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\...	Raman - Materials - Wiley	106	PMATY	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\...
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<p>2 Using the <b>Limit to Spectral Technique</b> dropdown menu, choose <b>Raman</b>.</p> <p>Limit to spectral technique: <input type="text" value="Raman"/></p> <p>Click <b>Reference</b> ( <b>Reference</b>) and then click <b>Add All</b> to add all licensed databases.</p> <p>After this, choose the <b>Computed</b> tab ( <b>Computed</b>) and then click <b>Add All</b> to add all SmartSpectra databases.</p>	<p>After selecting and adding the <b>References</b> and <b>Computed</b> databases, all licensed Raman libraries will be available in the <b>Selected for Searching</b> window:</p> <div data-bbox="800 383 1598 1344" style="border: 1px solid gray; padding: 5px;"> <p>Available for Searching:</p> <p>Internet databases are sw... 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	Raman - Sadtler Standards 7 - Wiley	2209	RST7X	<Latest Version>																																																																																																																																
	Raman - Semiconductor Materials ...	214	RVX	<Latest Version>																																																																																																																																
	Raman - Sigma-Aldrich Library of ...	6487	WSARX	<Latest Version>																																																																																																																																
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Raman - Sigma-Aldrich Library of Raman Spectra - Wiley	6487	WSARX																																																																																																																																		
Raman - SmartSpectra Library of Biochemicals - Wiley [RMSS1X]	59	RMSS1X																																																																																																																																		
Raman - SmartSpectra Library of Drugs - Wiley [RMSS2X]	130	RMSS2X																																																																																																																																		
Raman - SmartSpectra Library of Dyes - Wiley [RMSS3X]	36	RMSS3X																																																																																																																																		
Raman - SmartSpectra Library of Food Related Compounds - Wil...	277	RMSS5X																																																																																																																																		
Raman - SmartSpectra Library of General Compounds - Wiley [R...	24585	RMSS4X																																																																																																																																		
Raman - SmartSpectra Library of Hazmats and Explosives - Wiley ...	51	RMSS6X																																																																																																																																		
Raman - SmartSpectra Library of Hydrocarbons - Wiley [RMSS7X]	527	RMSS7X																																																																																																																																		
Raman - SmartSpectra Library of Industrial Compounds - Wiley [...]	439	RMSS8X																																																																																																																																		
Raman - SmartSpectra Library of Monomers - Wiley [RMSS9X]	152	RMSS9X																																																																																																																																		
Raman - SmartSpectra Library of Pollutants - Wiley [RMSS10X]	449	RMSS10X																																																																																																																																		
Raman - SmartSpectra Library of Standards - Wiley [RMSS11X]	6458	RMSS11X																																																																																																																																		

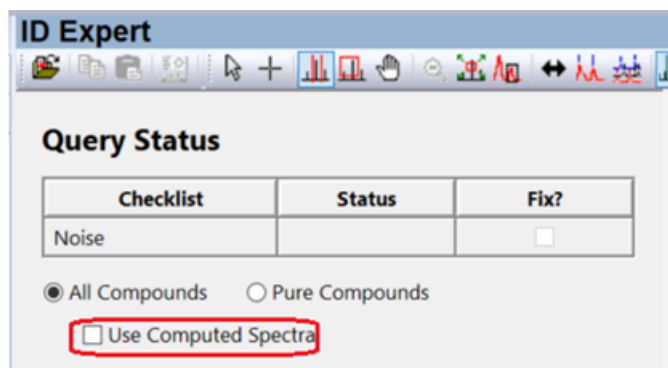
	Action	Result
3	<p>Click <b>Open Spectrum or Structure</b> icon () located on the <b>Standard Toolbar</b>.</p> <p>Navigate to find <b>1-acetyl-1234-tetrahydroquinoline.irf</b> in "<b>C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Computed Spectra\Raman</b>". Click <b>Open</b>.</p> <p><i>Note:</i> The image on this page is the correct compound structure associated with this spectrum.</p> 	<p>The selected file opens in the <b>Spectrum Search</b> window:</p> 
4	<p>In the <b>Spectrum Search</b> window, click <b>Advanced Settings</b> and deselect <b>Remove Duplicates</b> and <b>Remove Replicates</b>. Click <b>OK</b>.</p> <p>Click <b>Search</b>.</p>	<p>The <b>Advanced Settings</b> pop-up window is displayed. Upon clicking <b>OK</b> the window closes. Upon executing the search, <b>Minelt</b> loads with the query results.</p> 

	Action	Result																									
5	<p>Locate the <b>Hit List</b> to view match results featuring a mix of predicted and empirical matches.</p>	<p>The top hit in the <b>Hit List</b> is the empirical spectrum that best matches the query spectrum. The second best hit is from the SmartSpectra database.</p> <p><i>Note:</i> In this simulated test, the top hit is to be disregarded as it was used as the query spectrum, thus the SmartSpectra result is the true best match.</p>  <p>The screenshot shows the Minelt software interface. At the top, there's a title bar and a menu bar. Below that is a plot of an IR spectrum with two traces (red and blue) overlaid. The x-axis is labeled 'cm<sup>-1</sup>' and ranges from 3400 to 200. The y-axis represents intensity. Below the plot is a 'Hit List' table with the following data:</p> <table border="1"> <thead> <tr> <th>Hit#</th> <th>Cor. DB</th> <th>ID</th> <th>Name</th> <th>Spectrum</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>RSTX</td> <td>2202</td> <td>1-Acetyl-1,2,3,4-tetrahydroquinoline</td> <td></td> </tr> <tr style="background-color: #e0f0ff;"> <td>2</td> <td>RMS511X</td> <td>0810</td> <td>1-(2,4-Dihydro-2H-quinolin-1-yl)ethanone</td> <td></td> </tr> <tr> <td>3</td> <td>RMS511X</td> <td>2204</td> <td>1-Acetylindoline</td> <td></td> </tr> <tr> <td>4</td> <td>RMS50X</td> <td>1000</td> <td>Trimethylhydroquinone, diacetate</td> <td></td> </tr> </tbody> </table> <p>On the right side of the interface, there's a 'Structure Properties' panel showing the chemical structure of 1-(2,4-Dihydro-2H-quinolin-1-yl)ethanone and its properties:</p> <ul style="list-style-type: none"> <li>Name: 1-(2,4-Dihydro-2H-quinolin-1-yl)ethanone</li> <li>Comments: Computed using SmartSpectra Model v1.42</li> <li>Exact Mass: 175.09714642 u</li> <li>Formula: C<sub>11</sub>H<sub>11</sub>N</li> <li>InChI: InChI=1S=C1=CN(C)C=C1C(=O)C</li> <li>InChIKey: RRUUHRGURCAF-UHFFFAOYSA-N</li> <li>Molecular Weight: 175.231 g/mol</li> <li>Nominal Mass: 175 u</li> <li>SMILES: C=CC(=N)CCCC2=CC1C=CC=C12</li> <li>Spectrum/Structure Validation Score (Raman): 0.994191</li> </ul>	Hit#	Cor. DB	ID	Name	Spectrum	1	RSTX	2202	1-Acetyl-1,2,3,4-tetrahydroquinoline		2	RMS511X	0810	1-(2,4-Dihydro-2H-quinolin-1-yl)ethanone		3	RMS511X	2204	1-Acetylindoline		4	RMS50X	1000	Trimethylhydroquinone, diacetate	
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# ID Expert


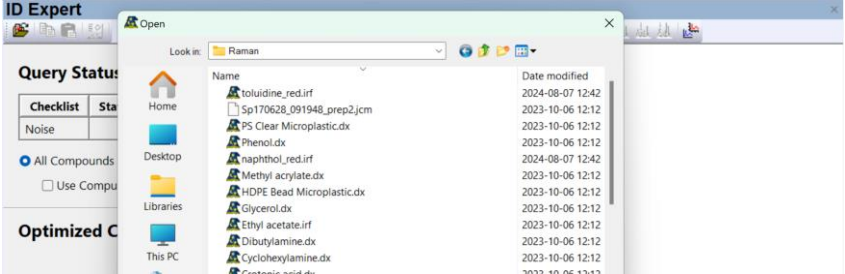
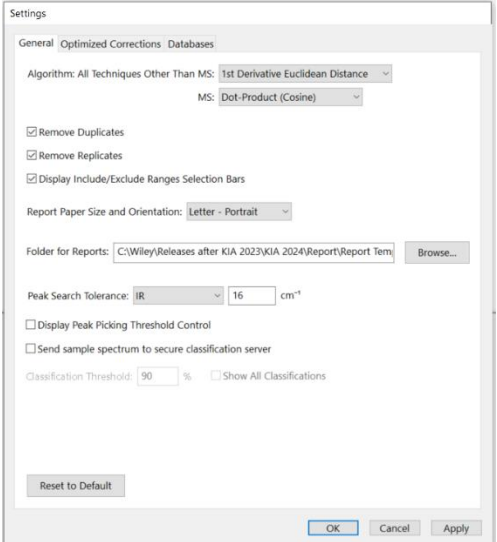
## Introduction

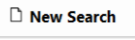
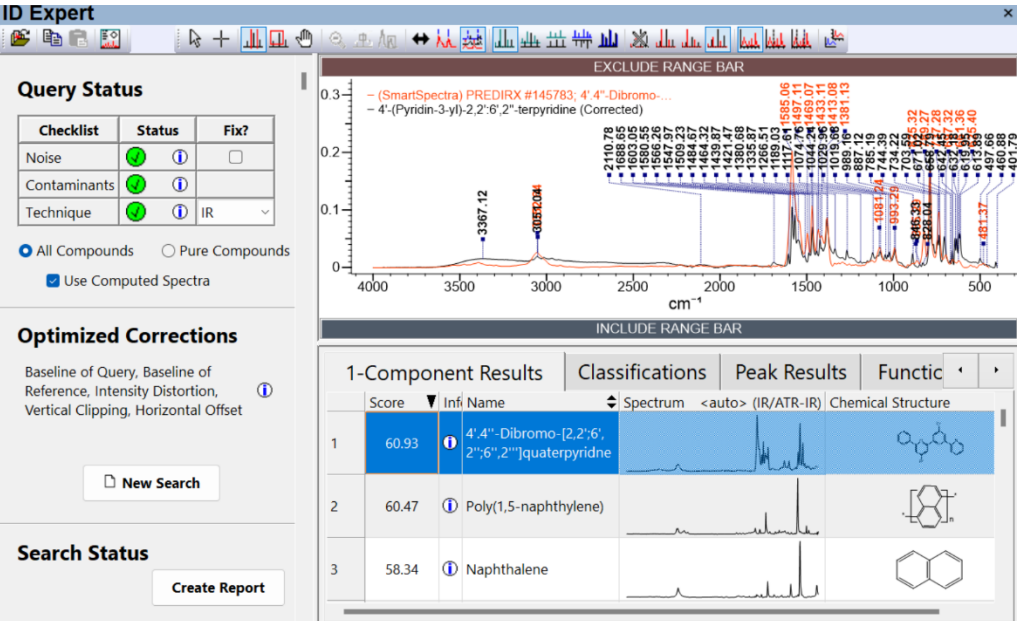
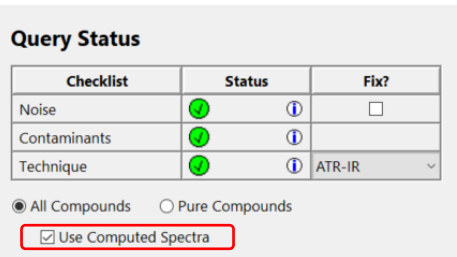
When a user's license contains the subscription for predicted IR spectra, the **ID Expert** interface **Query Status** shows the **Use Computed Spectra** option:

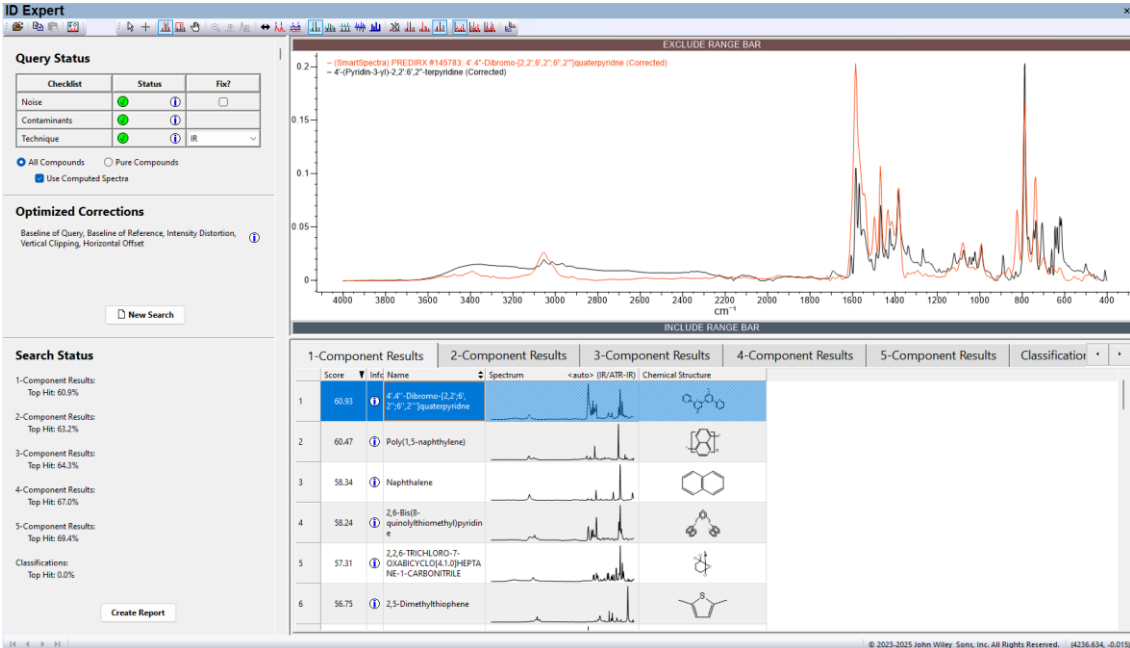



## Example 3

Example File: 4-(Pyridin-3-yl)-2-2,6,2-terpyridine.irf

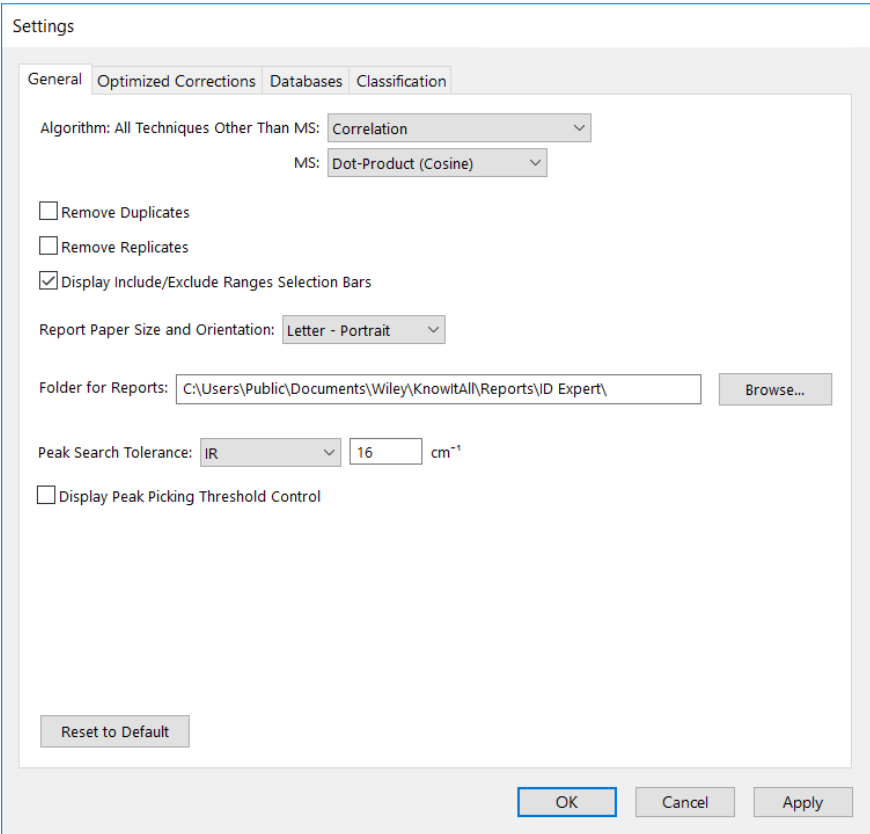
	Action	Result
1	<p>Navigate to the <b>Data</b> toolbox and open the <b>ID Expert</b> application by clicking the <b>ID Expert</b> icon (  ). Alternatively, if the desktop (standalone) application is installed, <b>ID Expert</b> can be opened directly by double-clicking on the desktop icon.</p>	<p>The application opens and an <b>Open</b> window displays:</p> 
2	<p>Click <b>Cancel</b> on the <b>Open</b> dialog window, then choose <b>File &gt; Settings</b>.</p> <p>Under <b>General</b> tab, set <b>Algorithm: All Techniques Other Than MS</b> to menu option <b>1<sup>st</sup> Derivative Euclidean Distance</b> using the dropdown menu. Select <b>Apply</b> then <b>OK</b> to apply the change.</p>	<p>Upon clicking <b>Settings</b>, the <b>Settings</b> window opens:</p> 

	Action	Result																																
3	<p>Click the <b>New Search</b> button ().</p> <p>Open <b>4-(Pyridin-3-yl)-2,2,6,2-terpyridine.irf</b> in the <b>"C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Computed Spectra\IR"</b> folder. Click <b>Open</b>.</p> <p>(Note: The training files used in this document are for example purposes only. The user should utilize their own IR spectra when following this training.)</p>	<p>Immediately upon opening the file, it begins to search for a match using the licensed databases available to the user:</p>  <p><b>Query Status</b></p> <table border="1"> <thead> <tr> <th>Checklist</th> <th>Status</th> <th>Fix?</th> </tr> </thead> <tbody> <tr> <td>Noise</td> <td><span style="color: green;">✔</span></td> <td><span style="color: blue;">i</span></td> </tr> <tr> <td>Contaminants</td> <td><span style="color: green;">✔</span></td> <td><span style="color: blue;">i</span></td> </tr> <tr> <td>Technique</td> <td><span style="color: green;">✔</span></td> <td><span style="color: blue;">i</span> IR</td> </tr> </tbody> </table> <p><input checked="" type="checkbox"/> All Compounds <input type="checkbox"/> Pure Compounds  <input checked="" type="checkbox"/> Use Computed Spectra</p> <p><b>Optimized Corrections</b></p> <p>Baseline of Query, Baseline of Reference, Intensity Distortion, Vertical Clipping, Horizontal Offset</p> <p><input type="button" value="New Search"/></p> <p><b>Search Status</b></p> <p><input type="button" value="Create Report"/></p> <p><b>1-Component Results</b></p> <table border="1"> <thead> <tr> <th>Score</th> <th>Info</th> <th>Name</th> <th>Spectrum</th> <th>Chemical Structure</th> </tr> </thead> <tbody> <tr> <td>60.93</td> <td><span style="color: blue;">i</span></td> <td>4'-4''-Dibromo-[2,2'';6',2'';6'',2''']quaterpyridine</td> <td></td> <td></td> </tr> <tr> <td>60.47</td> <td><span style="color: blue;">i</span></td> <td>Poly(1,5-naphthylene)</td> <td></td> <td></td> </tr> <tr> <td>58.34</td> <td><span style="color: blue;">i</span></td> <td>Naphthalene</td> <td></td> <td></td> </tr> </tbody> </table>	Checklist	Status	Fix?	Noise	<span style="color: green;">✔</span>	<span style="color: blue;">i</span>	Contaminants	<span style="color: green;">✔</span>	<span style="color: blue;">i</span>	Technique	<span style="color: green;">✔</span>	<span style="color: blue;">i</span> IR	Score	Info	Name	Spectrum	Chemical Structure	60.93	<span style="color: blue;">i</span>	4'-4''-Dibromo-[2,2'';6',2'';6'',2''']quaterpyridine			60.47	<span style="color: blue;">i</span>	Poly(1,5-naphthylene)			58.34	<span style="color: blue;">i</span>	Naphthalene		
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4	<p>Under <b>Query Status</b>, change <b>Technique</b> to <b>ATR-IR</b>.</p> <p>Check <b>Use Computed Spectra</b> checkbox.</p> <p><input checked="" type="checkbox"/> Use Computed Spectra</p>	<p>The modified <b>Query Status</b> settings are displayed. <b>ID Expert</b> updates the search with the modified settings.</p>  <p><b>Query Status</b></p> <table border="1"> <thead> <tr> <th>Checklist</th> <th>Status</th> <th>Fix?</th> </tr> </thead> <tbody> <tr> <td>Noise</td> <td><span style="color: green;">✔</span></td> <td><span style="color: blue;">i</span></td> </tr> <tr> <td>Contaminants</td> <td><span style="color: green;">✔</span></td> <td><span style="color: blue;">i</span></td> </tr> <tr> <td>Technique</td> <td><span style="color: green;">✔</span></td> <td><span style="color: blue;">i</span> ATR-IR</td> </tr> </tbody> </table> <p><input checked="" type="radio"/> All Compounds <input type="radio"/> Pure Compounds  <input checked="" type="checkbox"/> Use Computed Spectra</p>	Checklist	Status	Fix?	Noise	<span style="color: green;">✔</span>	<span style="color: blue;">i</span>	Contaminants	<span style="color: green;">✔</span>	<span style="color: blue;">i</span>	Technique	<span style="color: green;">✔</span>	<span style="color: blue;">i</span> ATR-IR																				
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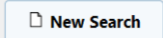
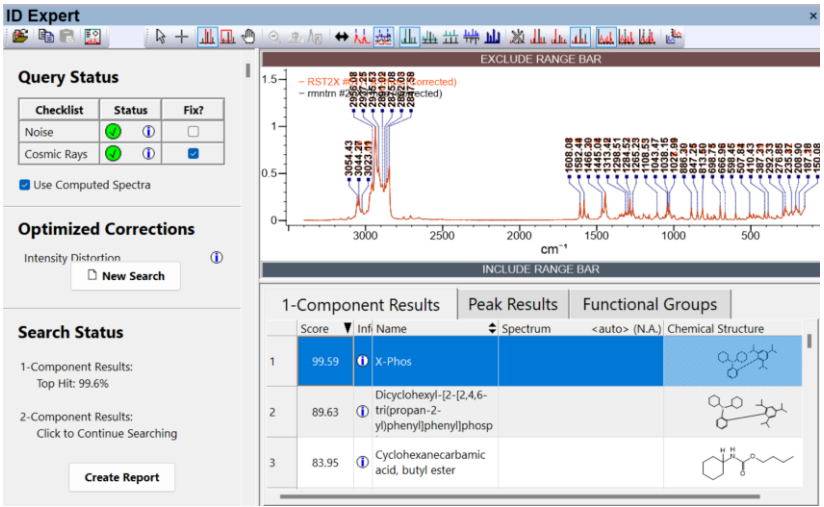
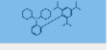
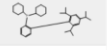
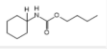
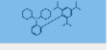
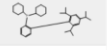
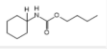
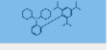
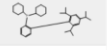
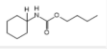
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5	View the search results in the <b>Component Table</b> .	<p>This search results include experimental and predicted spectra.</p>  <p><b>Query Status</b></p> <table border="1"> <thead> <tr> <th>Checklist</th> <th>Status</th> <th>Fix?</th> </tr> </thead> <tbody> <tr> <td>Noise</td> <td>●</td> <td>ⓘ</td> </tr> <tr> <td>Contaminants</td> <td>●</td> <td>ⓘ</td> </tr> <tr> <td>Technique</td> <td>●</td> <td>ⓘ IR</td> </tr> </tbody> </table> <p> <input checked="" type="radio"/> All Compounds   <input type="radio"/> Pure Compounds  <input checked="" type="checkbox"/> Use Computed Spectra   </p> <p><b>Optimized Corrections</b>    Baseline of Query, Baseline of Reference, Intensity Distortion, Vertical Clipping, Horizontal Offset ⓘ</p> <p><input type="button" value="New Search"/></p> <p><b>Search Status</b></p> <p>1-Component Results: Top Hit: 60.9%</p> <p>2-Component Results: Top Hit: 63.2%</p> <p>3-Component Results: Top Hit: 64.3%</p> <p>4-Component Results: Top Hit: 67.0%</p> <p>5-Component Results: Top Hit: 69.4%</p> <p>Classifications: Top Hit: 0.0%</p> <p><input type="button" value="Create Report"/></p> <p><b>Component Table</b></p> <table border="1"> <thead> <tr> <th>Score</th> <th>Infid</th> <th>Name</th> <th>Spectrum</th> <th>(IR/ATR-IR)</th> <th>Chemical Structure</th> </tr> </thead> <tbody> <tr> <td>60.93</td> <td>ⓘ</td> <td>4,4'-Dibromo-2,2',5,5'-tetrakispyridine</td> <td></td> <td></td> <td></td> </tr> <tr> <td>60.47</td> <td>ⓘ</td> <td>Poly(1,5-naphthylene)</td> <td></td> <td></td> <td></td> </tr> <tr> <td>58.34</td> <td>ⓘ</td> <td>Naphthalene</td> <td></td> <td></td> <td></td> </tr> <tr> <td>58.24</td> <td>ⓘ</td> <td>2,6-Bis(2-quinolylthiomethyl)pyridine</td> <td></td> <td></td> <td></td> </tr> <tr> <td>57.31</td> <td>ⓘ</td> <td>2,2,6-TRICHLORO-7-OXABICYCLO[4.1.0]HEPTANE-1-CARBONITRILE</td> <td></td> <td></td> <td></td> </tr> <tr> <td>56.75</td> <td>ⓘ</td> <td>2,5-Dimethylthiophene</td> <td></td> <td></td> <td></td> </tr> </tbody> </table>	Checklist	Status	Fix?	Noise	●	ⓘ	Contaminants	●	ⓘ	Technique	●	ⓘ IR	Score	Infid	Name	Spectrum	(IR/ATR-IR)	Chemical Structure	60.93	ⓘ	4,4'-Dibromo-2,2',5,5'-tetrakispyridine				60.47	ⓘ	Poly(1,5-naphthylene)				58.34	ⓘ	Naphthalene				58.24	ⓘ	2,6-Bis(2-quinolylthiomethyl)pyridine				57.31	ⓘ	2,2,6-TRICHLORO-7-OXABICYCLO[4.1.0]HEPTANE-1-CARBONITRILE				56.75	ⓘ	2,5-Dimethylthiophene			
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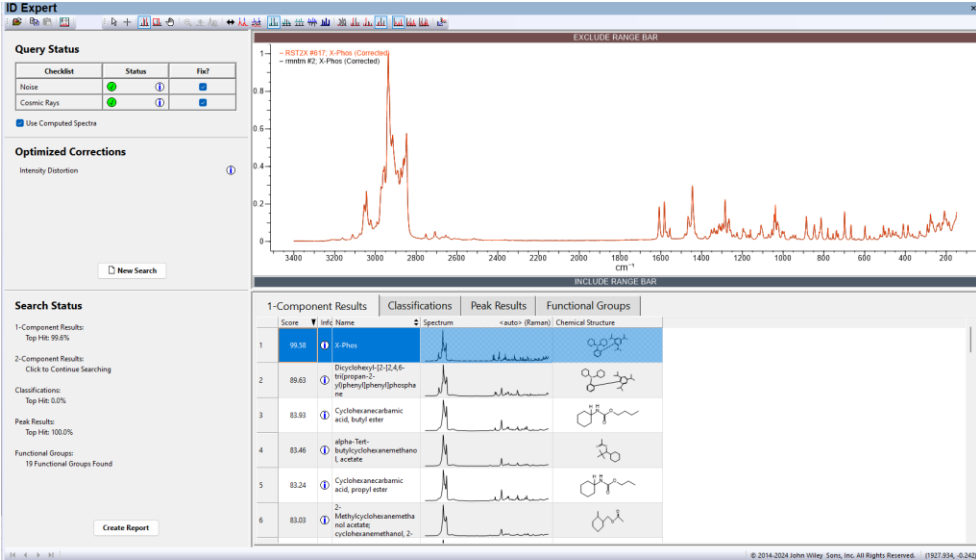

## Example 4

Example File: X-Phos.irf

	Action	Result
1	<p>Close the <b>Open</b> window (if open), then choose <b>File &gt; Settings</b>.</p> <p>In the <b>Settings</b> pop-up window, under the <b>General</b> tab, set <b>Algorithm: All Techniques Other Than MS</b> to menu option <b>Correlation</b> using the dropdown menu.</p> <p>Uncheck <b>Remove Duplicates</b> and <b>Remove Replicates</b>.</p> <p>Click <b>Apply</b> the <b>OK</b> to apply the change.</p>	 <p>Settings</p> <p>General   Optimized Corrections   Databases   Classification</p> <p>Algorithm: All Techniques Other Than MS: Correlation</p> <p>MS: Dot-Product (Cosine)</p> <p><input type="checkbox"/> Remove Duplicates</p> <p><input type="checkbox"/> Remove Replicates</p> <p><input checked="" type="checkbox"/> Display Include/Exclude Ranges Selection Bars</p> <p>Report Paper Size and Orientation: Letter - Portrait</p> <p>Folder for Reports: C:\Users\Public\Documents\Wiley\KnowItAll\Reports\ID Expert\ Browse...</p> <p>Peak Search Tolerance: IR 16 cm<sup>-1</sup></p> <p><input type="checkbox"/> Display Peak Picking Threshold Control</p> <p>Reset to Default</p> <p>OK Cancel Apply</p>



	Action	Result																
2	<p>Click the <b>New Search</b> button (  ).</p> <p>Open <b>X-Phos.irf</b> in “C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Computed Spectra\Raman”. Click <b>Open</b>.</p> <p>In the <b>Query Status</b> panel, check the <b>Use Computer Spectra</b> box.</p> <p>Checking the <b>Use Computer Spectra</b> checkbox adds SmartSpectra data to <b>ID Expert's</b> library search. When not checked, SmartSpectra will not be searched.</p> <p>(<i>Note:</i> The training files used in this document are for example purposes only. The user should utilize their own Raman spectra when following this training.)</p>	<p>Immediately upon opening the file, it begins to search for a match using the licensed databases available to the user:</p>  <p>The screenshot shows the ID Expert interface. The top panel displays the Raman spectrum with an 'EXCLUDE RANGE BAR' and an 'INCLUDE RANGE BAR'. The spectrum shows several peaks, with the most prominent one at approximately 3000 cm<sup>-1</sup>. The search results are displayed in a table below the spectrum:</p> <table border="1"> <thead> <tr> <th>Score</th> <th>Inf Name</th> <th>Spectrum</th> <th>Chemical Structure</th> </tr> </thead> <tbody> <tr> <td>99.59</td> <td>X-Phos</td> <td></td> <td></td> </tr> <tr> <td>89.63</td> <td>Dicyclohexyl-[2-(2,4,6-tri(propan-2-yl)phenyl)phenyl]phosp</td> <td></td> <td></td> </tr> <tr> <td>83.95</td> <td>Cyclohexanecarbamic acid, butyl ester</td> <td></td> <td></td> </tr> </tbody> </table>	Score	Inf Name	Spectrum	Chemical Structure	99.59	X-Phos			89.63	Dicyclohexyl-[2-(2,4,6-tri(propan-2-yl)phenyl)phenyl]phosp			83.95	Cyclohexanecarbamic acid, butyl ester		
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	Action	Result
3	View search results in the <b>Component Results</b> table.	<p>The top hit in the <b>Hit List</b> is the empirical spectrum that best matches the query spectrum. The second best hit is from the SmartSpectra database.</p> <p><i>Note:</i> In this simulated test, the top hit is to be disregarded as it was used as the query spectrum, thus the SmartSpectra result is the true best match.</p> 
4	Close the active search by selecting the <b>X</b> icon (  ) in the top right-hand corner.	

# Classification Models

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## Purpose

These exercises demonstrate how to use classification models in KnowItAll ID Expert and Minelt.

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## Objectives

These exercises will teach you:

- How to use the KnowItAll Classification models in ID Expert
- How to use the KnowItAll Classification models in Minelt

Training Files Used in This Lesson:

- 17-Hydroxy-17-alpha-pregn-4-en-20-yn-3-one.irf
- SmartSpectraFTIROxycodone.irf
- SmartSpectraRamanAndrosteroneacetate.irf

*Note:* The training files used are for example purposes only. The user should utilize their own IR spectra when following this training.

KnowItAll Applications Used:



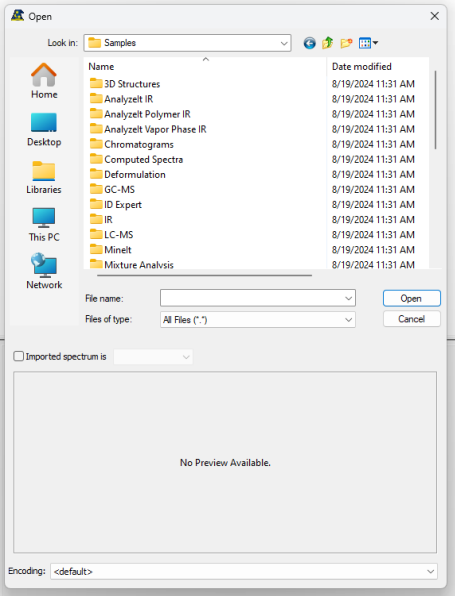
- KnowItAll ID Expert
  - KnowItAll Minelt
-

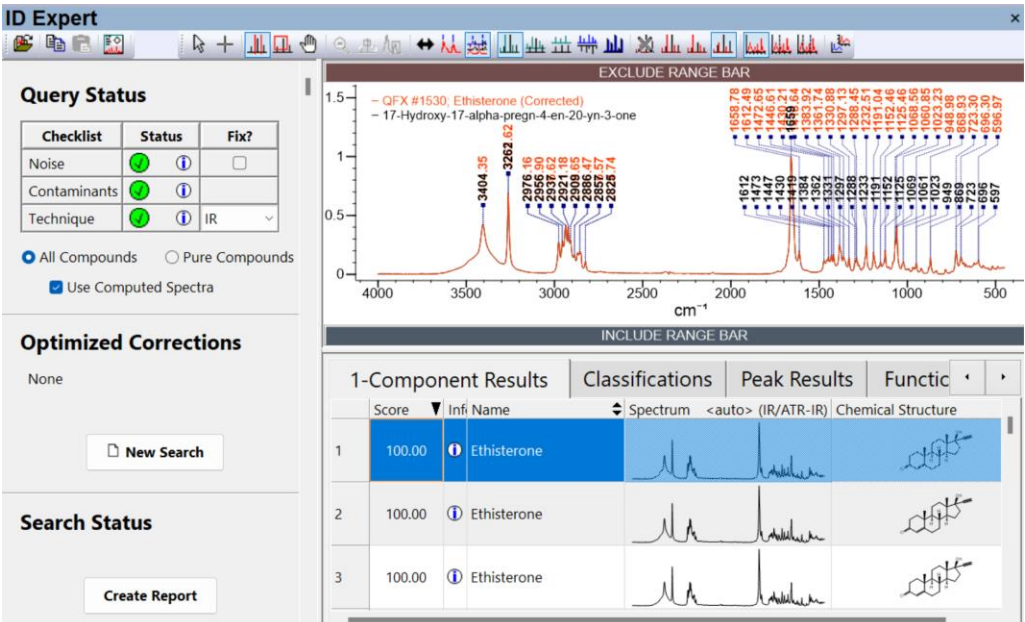
## Background

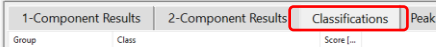
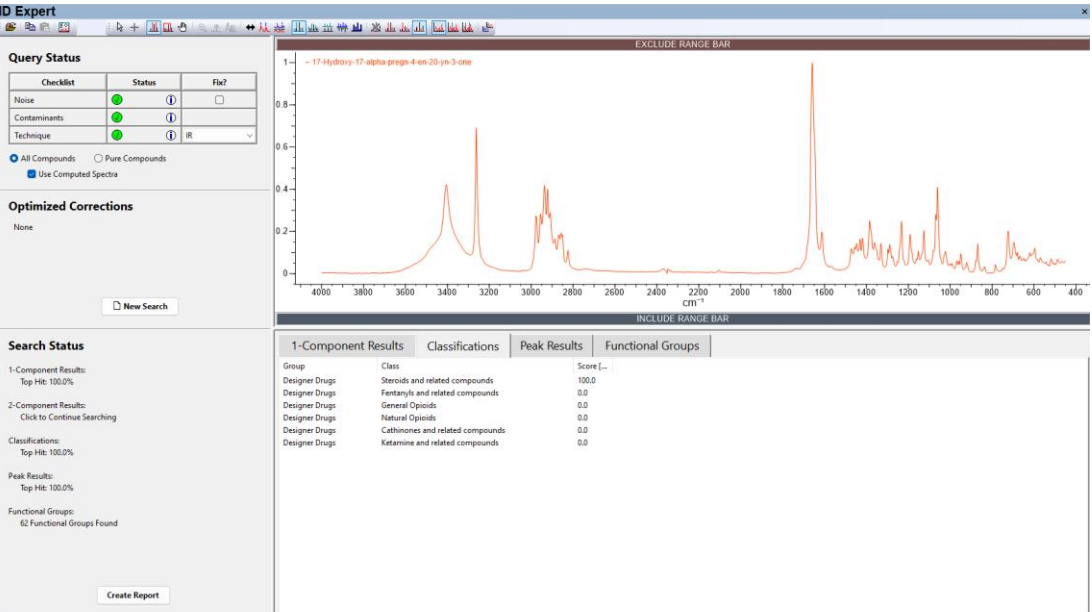
Classification models are a type of supervised learning used to label or categorize data into predefined classes or groups. These models predict the said label based on feature data. The model must be trained on labeled data or have an architecture that leads to the data being trained on to be self labelled by the model. Our models are binary classifiers that involve either a true or false result. The model also uses the neural network algorithm architecture, which has gained much popularity in recent years. The models have been optimized for FT-IR, Raman and GC-MS techniques within KnowItAll's ID Expert and Minelt applications.

## ID Expert

**Example File:** 17-Hydroxy-17-alpha-pregn-4-en-20-yn-3-one.irf

	Action	Result
1	<p>Open <b>ID Expert</b> (  ).</p> <p>If the <b>Open</b> window does not appear, then click <b>New Search</b> button (  ) to manually launch the dialog window.</p>	<p>The <b>Open</b> window appears for file selection:</p> 


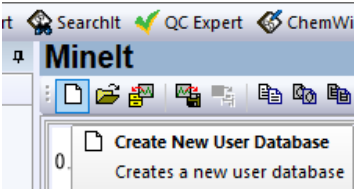
	Action	Result
2	<p>Open <b>17-Hydroxy-17-alpha-pregn-4-en-20-yn-3-one.irf</b> in the “C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Mixture Analysis\IR Examples\Components” folder.</p> <p>Click <b>Open</b>.</p>	<p>Immediately upon opening the file, it begins to search for a match using the licensed databases available to the user:</p> 
3	<p>Click <b>File &gt; Settings</b>.</p> <p>Under the <b>Classification</b> tab of the <b>Settings</b> window, check the <b>Show All Classifications</b> checkbox. Click <b>OK</b> to save the changes.</p> <p><input checked="" type="checkbox"/> Show All Classifications</p>	<p>Upon clicking <b>OK</b>, the Settings window is closed.</p>

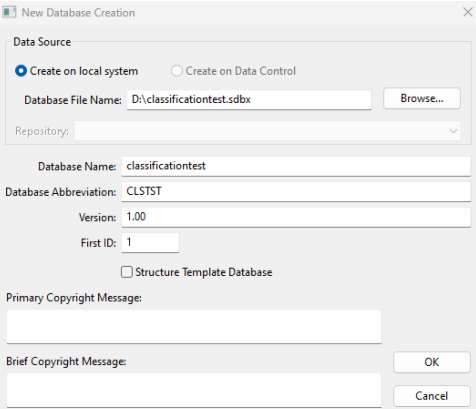
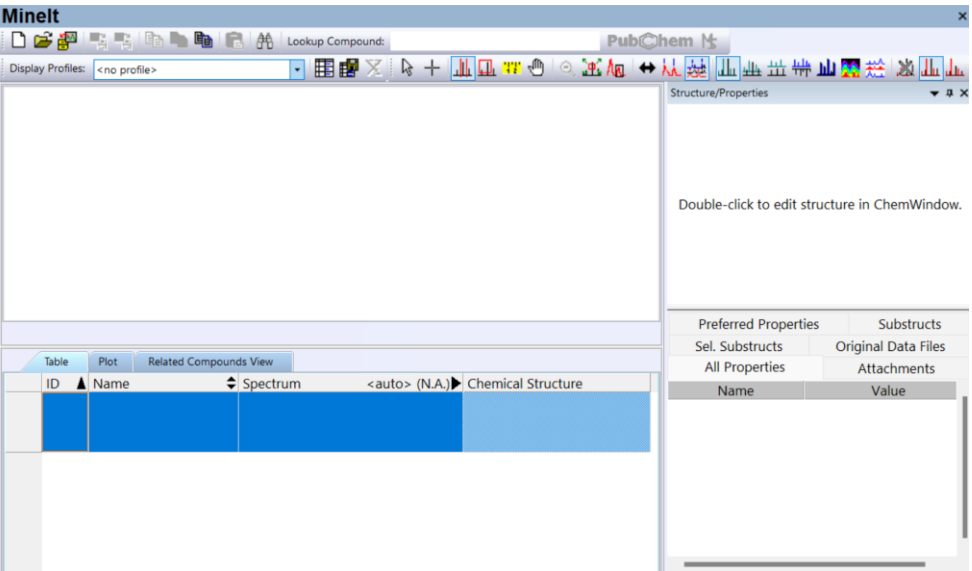
	Action	Result																																	
4	<p>Click the <b>Classifications</b> tab just right of the <b>Component Results</b> tab.</p> <p><i>Note:</i> If there is a situation where there are multiple components detected in the sample (<i>i.e.</i>, &gt;1), the tab is located to the right of the last component result as seen in the image below.</p> 	<p><b>ID Expert</b> displays the classification results for the classification models available in the user license. In this case, the sample is identified to be a <b>Steroid</b>:</p>  <p>The screenshot shows the ID Expert interface with the following sections:</p> <ul style="list-style-type: none"> <li><b>Query Status:</b> A table with columns 'Checklist', 'Status', and 'Fix?'.             <table border="1"> <tr> <td>Noise</td> <td>Green circle</td> <td>Down arrow</td> <td><input type="checkbox"/></td> </tr> <tr> <td>Contaminants</td> <td>Green circle</td> <td>Down arrow</td> <td><input type="checkbox"/></td> </tr> <tr> <td>Technique</td> <td>Green circle</td> <td>Down arrow</td> <td>IR</td> </tr> </table> </li> <li><b>Optimized Corrections:</b> None</li> <li><b>Search Status:</b> <ul style="list-style-type: none"> <li>1-Component Results: Top Hit: 100.0%</li> <li>2-Component Results: Click to Continue Searching</li> <li>Classifications: Top Hit: 100.0%</li> <li>Peak Results: Top Hit: 100.0%</li> <li>Functional Groups: 62 Functional Groups Found</li> </ul> </li> <li><b>IR Spectrum:</b> A plot of transmittance vs. wavenumber (cm⁻¹) from 4000 to 400. The title is '-17-Hydroxy-17-alpha-pregn-4-en-20-one'. The x-axis is labeled 'INCLUDE RANGE BAR' and the y-axis is labeled 'EXCLUDE RANGE BAR'.</li> <li><b>Classification Results Table:</b> <table border="1"> <thead> <tr> <th>Group</th> <th>Class</th> <th>Score [..]</th> </tr> </thead> <tbody> <tr> <td>Designer Drugs</td> <td>Steroids and related compounds</td> <td>100.0</td> </tr> <tr> <td>Designer Drugs</td> <td>Fentanyl and related compounds</td> <td>0.0</td> </tr> <tr> <td>Designer Drugs</td> <td>General Opioids</td> <td>0.0</td> </tr> <tr> <td>Designer Drugs</td> <td>Natural Opioids</td> <td>0.0</td> </tr> <tr> <td>Designer Drugs</td> <td>Cathinones and related compounds</td> <td>0.0</td> </tr> <tr> <td>Designer Drugs</td> <td>Ketamine and related compounds</td> <td>0.0</td> </tr> </tbody> </table> </li> </ul>	Noise	Green circle	Down arrow	<input type="checkbox"/>	Contaminants	Green circle	Down arrow	<input type="checkbox"/>	Technique	Green circle	Down arrow	IR	Group	Class	Score [..]	Designer Drugs	Steroids and related compounds	100.0	Designer Drugs	Fentanyl and related compounds	0.0	Designer Drugs	General Opioids	0.0	Designer Drugs	Natural Opioids	0.0	Designer Drugs	Cathinones and related compounds	0.0	Designer Drugs	Ketamine and related compounds	0.0
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## Classification Batch Property Calculation in Minelt

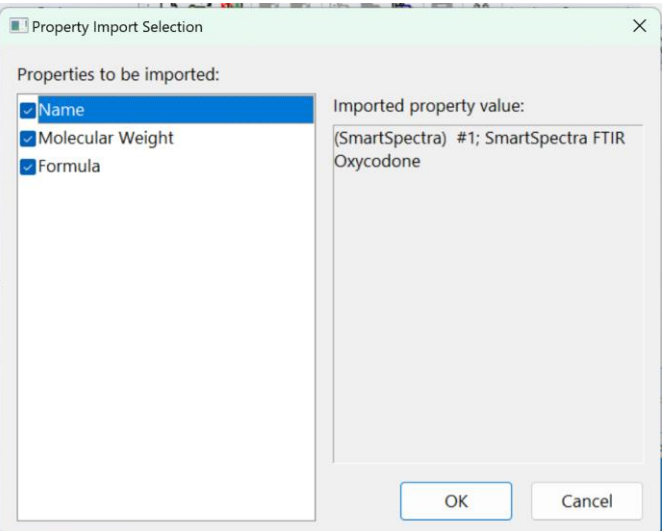
**Example Files:** SmartSpectraFTIROxycodone.irf, SmartSpectraRamanAndrosteroneacetate.irf

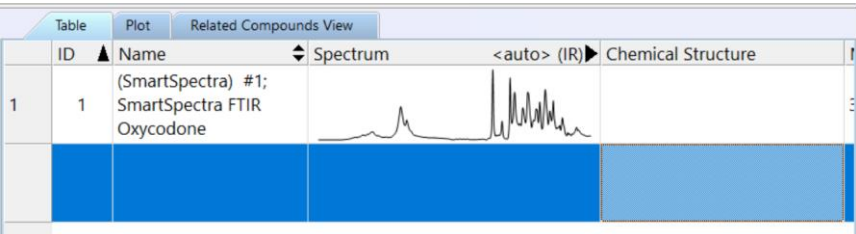



Batch property calculation is a calculation that will be applied to a series of compounds at one time. In this exercise, an unlocked user database will be created that to simulate executing a batch property calculation. This workflow can only be performed using unlocked (user) databases.

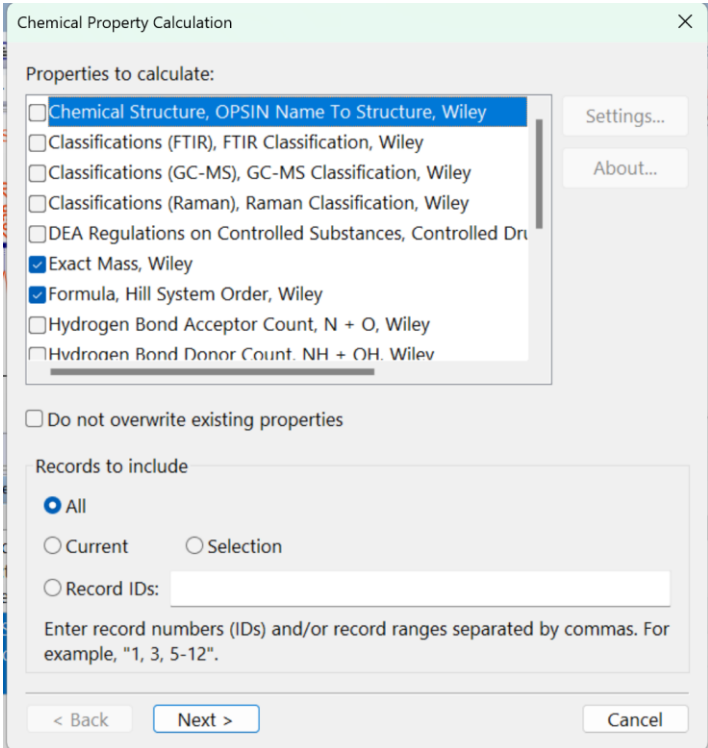
	Action	Result
1	<p>Navigate to the <b>Minelt</b> application (  ).</p> <p>To use the <b>Batch Property Calculation</b> tools in <b>Minelt</b>, a user database must be created.</p> <p><i>Note:</i> Creating a user database creates an unlocked database. Licensed KnowItAll databases are locked databases.</p> <p>Select the <b>Create New User Database</b> icon on the <b>Standard Toolbar</b>.</p>	
2	<p>In the <b>New Database Creation</b> window, choose a location to save the file by using the <b>Browse</b> button. Click <b>OK</b> to save.</p> <p>In the <b>New Database Creation</b> window, fill out the <b>Database Name</b> and <b>Database Abbreviation</b>.</p>	<p>The <b>New Database Creation</b> window is launched.</p>

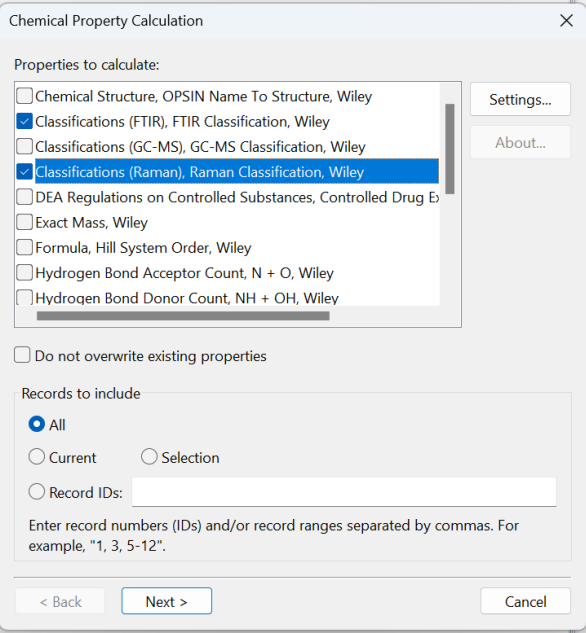
	Action	Result
		
3	Click <b>OK</b> to create the database.	<p>A blank user database is opened in <b>Minelt</b>.</p> 
4	Navigate to the <b>File &gt; Import</b> to import spectral files.	The <b>Open</b> window is launched.

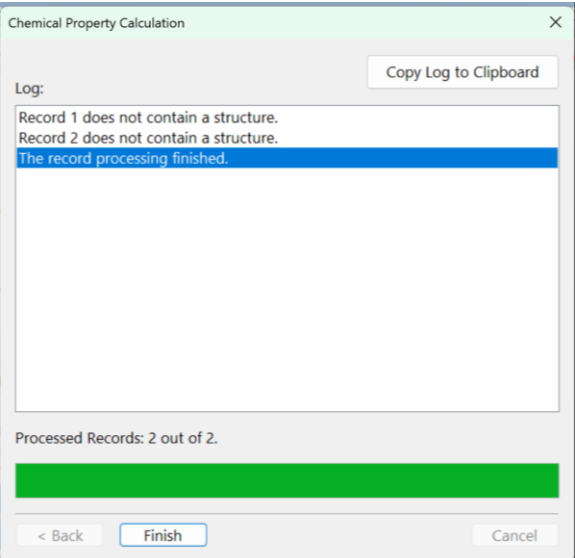


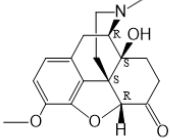
	Action	Result																												
5	<p>Open <b>SmartSpectraFTIROxycodone.irf</b> in the  <b>“C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Computed Spectra\IR”</b> folder.</p> <p>Click <b>Open</b>.</p>	<p>The <b>Property Import Selection</b> window is launched:</p> 																												
6	<p>Click <b>OK</b> on the <b>Property Import Selection</b> window.</p>	<p>The <b>Property Import Selection</b> window is closed and the properties are imported in the <b>Structure/Properties</b> panel.</p> <table border="1" data-bbox="772 963 1207 1252"> <thead> <tr> <th colspan="2">Preferred Properties</th> <th colspan="2">Substructs</th> </tr> <tr> <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> </tr> <tr> <th>Name</th> <th colspan="3">Value</th> </tr> </thead> <tbody> <tr> <td>Name</td> <td colspan="3">(SmartSpectra) #1; SmartSpectra FTIR Oxycodone</td> </tr> <tr> <td>Formula</td> <td colspan="3">C<sub>18</sub>H<sub>21</sub>NO<sub>4</sub></td> </tr> <tr> <td>Molecular Weight</td> <td colspan="3">315.369 g/mol</td> </tr> </tbody> </table>	Preferred Properties		Substructs		Sel. Substructs		Original Data Files		All Properties		Attachments		Name	Value			Name	(SmartSpectra) #1; SmartSpectra FTIR Oxycodone			Formula	C <sub>18</sub> H <sub>21</sub> NO <sub>4</sub>			Molecular Weight	315.369 g/mol		
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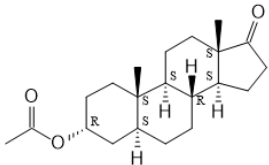
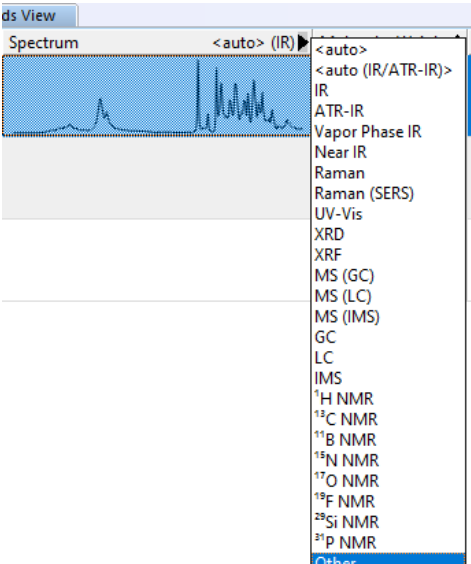
	Action	Result								
7	Click on the row below the first record in the <b>Table</b> .	<p>The second row is shaded in the <b>Table</b>:</p>  <p>The screenshot shows a software window with tabs for 'Table', 'Plot', and 'Related Compounds View'. The 'Table' tab is active, displaying a table with the following content:</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>(SmartSpectra) #1; SmartSpectra FTIR Oxycodone</td> <td></td> <td></td> </tr> </tbody> </table> <p>The second row of the table is highlighted in blue.</p>	ID	Name	Spectrum	Chemical Structure	1	(SmartSpectra) #1; SmartSpectra FTIR Oxycodone		
ID	Name	Spectrum	Chemical Structure							
1	(SmartSpectra) #1; SmartSpectra FTIR Oxycodone									
8	Navigate to the <b>File</b> tab and select <b>Import</b> to import a second file into the user database.	The <b>Open</b> dialog window is launched.								
9	Repeat steps 4 through 8 using <b>SmartSpectraRamanAndrosteroneacetate.irf</b> in the “C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Computed Spectra\Raman” folder.	The <b>Property Import Selection</b> window is launched. The Raman sample file is imported into the user database.								

	Action	Result
10	Navigate to <b>Database &gt; Batch Property Calculation</b> .	<p>The <b>Batch Property Calculation</b> window is launched:</p>  <p>Chemical Property Calculation</p> <p>Properties to calculate:</p> <ul style="list-style-type: none"><li><input type="checkbox"/> Chemical Structure, OPSIN Name To Structure, Wiley</li><li><input type="checkbox"/> Classifications (FTIR), FTIR Classification, Wiley</li><li><input type="checkbox"/> Classifications (GC-MS), GC-MS Classification, Wiley</li><li><input type="checkbox"/> Classifications (Raman), Raman Classification, Wiley</li><li><input type="checkbox"/> DEA Regulations on Controlled Substances, Controlled Dr</li><li><input checked="" type="checkbox"/> Exact Mass, Wiley</li><li><input checked="" type="checkbox"/> Formula, Hill System Order, Wiley</li><li><input type="checkbox"/> Hydrogen Bond Acceptor Count, N + O, Wiley</li><li><input type="checkbox"/> Hydrogen Bond Donor Count, NH + OH, Wiley</li></ul> <p><input type="checkbox"/> Do not overwrite existing properties</p> <p>Records to include</p> <p><input checked="" type="radio"/> All <input type="radio"/> Current <input type="radio"/> Selection</p> <p><input type="radio"/> Record IDs: <input type="text"/></p> <p>Enter record numbers (IDs) and/or record ranges separated by commas. For example, "1, 3, 5-12".</p> <p>&lt; Back Next &gt; Cancel</p>

	Action	Result
11	<p>Click to select the <b>Classifications</b> models for IR and Raman:</p> <ul style="list-style-type: none"><li>▪ <b>Classifications (FTIR), FTIR Classification, Wiley</b></li><li>▪ <b>Classifications (Raman), Raman Classification, Wiley</b></li></ul> <p><i>Note:</i> It is recommended to execute the models one at a time for their specific technique, but it is possible to run all classification engines at once on the different spectral records.</p>	<p>The <b>Chemical Property Calculation</b> window is shown below with the selected <b>Classifications</b> models selected:</p>  <p>The screenshot shows a dialog box titled "Chemical Property Calculation". It has a close button (X) in the top right. Under "Properties to calculate:", there is a list of checkboxes. The following are checked: "Classifications (FTIR), FTIR Classification, Wiley" and "Classifications (Raman), Raman Classification, Wiley". Other unchecked items include "Chemical Structure, OPSIN Name To Structure, Wiley", "Classifications (GC-MS), GC-MS Classification, Wiley", "DEA Regulations on Controlled Substances, Controlled Drug B", "Exact Mass, Wiley", "Formula, Hill System Order, Wiley", "Hydrogen Bond Acceptor Count, N + O, Wiley", and "Hydrogen Bond Donor Count, NH + OH, Wiley". There are "Settings..." and "About..." buttons to the right. Below this list is a checkbox for "Do not overwrite existing properties". Under "Records to include", the "All" radio button is selected. There are also "Current" and "Selection" radio buttons, and a "Record IDs:" text input field. A note below the input field says: "Enter record numbers (IDs) and/or record ranges separated by commas. For example, '1, 3, 5-12'." At the bottom, there are "&lt; Back", "Next &gt;", and "Cancel" buttons.</p>
12	<p>Under <b>Records to Include</b>, ensure <b>All</b> is selected. Then click <b>Next &gt;</b> to execute the <b>Batch Property Calculations</b>.</p>	

	Action	Result
13	Allow the <b>Batch Property Calculation</b> to execute entirely, where progress can be tracked using the green colored <b>Status Bar</b> .	Upon completion of the <b>Batch Property Calculations</b> , the <b>Log</b> box will read "The record processing finished". The <b>Status Bar</b> will be entirely colored in green: 
14	Click <b>Finish</b> on the <b>Chemical Property Calculation</b> window to return to <b>Minelt</b> .	The <b>Chemical Property Calculation</b> window is closed.

	Action	Result																																																
15	The resulting classification can be found in the <b>Structure/Properties</b> panel for the selected record.	<p>Record ID 1 has results <b>Classifications (FTIR)</b> “General Opioids (100.0%)” and “Natural Opioids (100.0%)”.</p> <table border="1" data-bbox="772 397 1077 743"> <thead> <tr> <th colspan="2">Preferred Properties</th> <th>Substructs</th> </tr> <tr> <th colspan="2">Sel. Substructs</th> <th>Original Data Files</th> </tr> <tr> <th colspan="2">All Properties</th> <th>Attachments</th> </tr> <tr> <th>Name</th> <th colspan="2">Value</th> </tr> </thead> <tbody> <tr> <td>Name</td> <td colspan="2">(SmartSpectra) #1; SmartSpectra FTIR Oxycodone</td> </tr> <tr> <td>Classifications</td> <td colspan="2">General Opioids (100.0%) Natural Opioids (100.0%)</td> </tr> <tr> <td>Formula</td> <td colspan="2">C<sub>18</sub>H<sub>21</sub>NO<sub>4</sub></td> </tr> <tr> <td>Molecular Weight</td> <td colspan="2">315.369 g/mol</td> </tr> </tbody> </table> <p>Record ID 2 has results <b>Classifications (Raman)</b> “Steroids and related compounds (100.0%)”.</p> <table border="1" data-bbox="772 836 1098 1182"> <thead> <tr> <th colspan="2">Preferred Properties</th> <th>Substructs</th> </tr> <tr> <th colspan="2">Sel. Substructs</th> <th>Original Data Files</th> </tr> <tr> <th colspan="2">All Properties</th> <th>Attachments</th> </tr> <tr> <th>Name</th> <th colspan="2">Value</th> </tr> </thead> <tbody> <tr> <td>Name</td> <td colspan="2">#2; SmartSpectra Raman Androsterone Acetate</td> </tr> <tr> <td>Classifications</td> <td colspan="2">Steroids and related compounds (100.0%)</td> </tr> <tr> <td>Formula</td> <td colspan="2">C<sub>21</sub>H<sub>32</sub>O<sub>3</sub></td> </tr> <tr> <td>Molecular Weight</td> <td colspan="2">332.484 g/mol</td> </tr> </tbody> </table>	Preferred Properties		Substructs	Sel. Substructs		Original Data Files	All Properties		Attachments	Name	Value		Name	(SmartSpectra) #1; SmartSpectra FTIR Oxycodone		Classifications	General Opioids (100.0%) Natural Opioids (100.0%)		Formula	C <sub>18</sub> H <sub>21</sub> NO <sub>4</sub>		Molecular Weight	315.369 g/mol		Preferred Properties		Substructs	Sel. Substructs		Original Data Files	All Properties		Attachments	Name	Value		Name	#2; SmartSpectra Raman Androsterone Acetate		Classifications	Steroids and related compounds (100.0%)		Formula	C <sub>21</sub> H <sub>32</sub> O <sub>3</sub>		Molecular Weight	332.484 g/mol	
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Name	#2; SmartSpectra Raman Androsterone Acetate																																																	
Classifications	Steroids and related compounds (100.0%)																																																	
Formula	C <sub>21</sub> H <sub>32</sub> O <sub>3</sub>																																																	
Molecular Weight	332.484 g/mol																																																	
16	The final compound structures are provided in the <b>Results</b> cell for reference. These are the structural representations of the two spectra used in the batch property calculations added for comparison to show that they are classified correctly.	<p><b>Record ID 1:</b> (SmartSpectra) #1; SmartSpectra FTIR Oxycodone.</p>  <p>The image shows the chemical structure of Oxycodone, a semi-synthetic opioid. It features a pentacyclic ring system with a morphine-like core, a methoxy group at the 3-position, and a hydroxyl group at the 6-position. Stereochemistry is indicated with wedges and dashes at the 5 and 6 positions.</p>																																																

Action	Result
<p>To view all the different spectral techniques in the database spectrum pane, select the black triangle to the right of '&lt;auto&gt; (IR)' or '&lt;auto&gt; (Raman)' part of the pane.</p> <p>When the dropdown appears, select the technique you would like to view.</p>	<p><b>Record ID 2: #2; SmartSpectra Raman Androsterone Acetate.</b></p>  <p>The chemical structure shows a steroid nucleus with an acetate group at C-3, a ketone at C-20, and a methyl group at C-19. Stereochemistry is indicated with wedges and dashes.</p>  <p>The screenshot shows the 'ds View' pane with a 'Spectrum' dropdown menu. The menu is open, displaying a list of spectral techniques. The current selection is '&lt;auto&gt; (IR)'. The list includes: &lt;auto&gt;, &lt;auto&gt; (IR/ATR-IR)&gt;, IR, ATR-IR, Vapor Phase IR, Near IR, Raman, Raman (SERS), UV-Vis, XRD, XRF, MS (GC), MS (LC), MS (IMS), GC, LC, IMS, <sup>1</sup>H NMR, <sup>13</sup>C NMR, <sup>11</sup>B NMR, <sup>15</sup>N NMR, <sup>17</sup>O NMR, <sup>19</sup>F NMR, <sup>29</sup>Si NMR, <sup>31</sup>P NMR, and Other... The 'Other...' option is highlighted at the bottom.</p>