

KnowItAll Software Training

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 searching¹, 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.

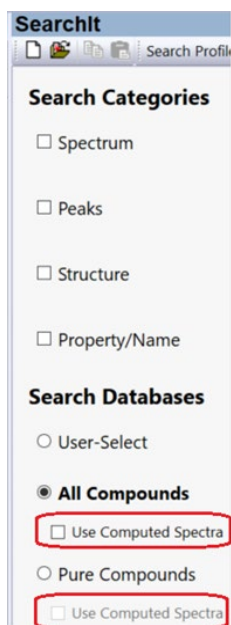
Optimized Corrections consider the full spectrum during a selected range(s) search.

¹ 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


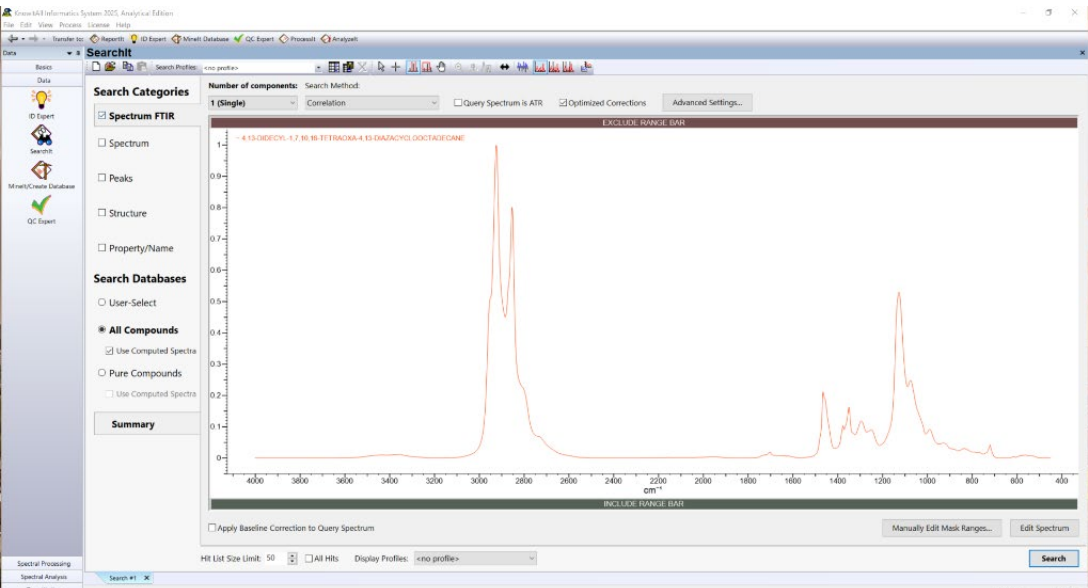
Introduction

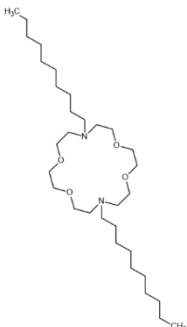
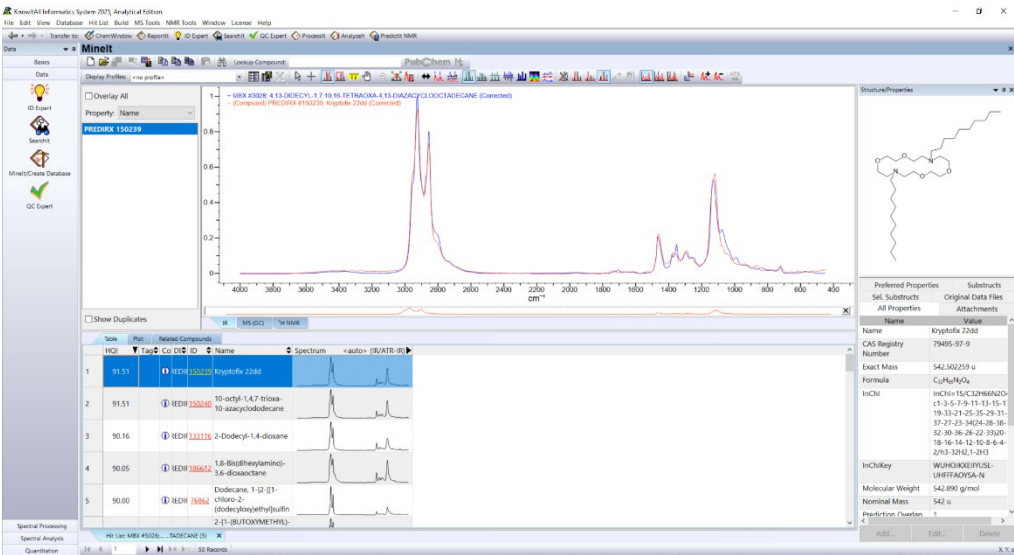
When a user license contains the subscription to SmartSpectra IR spectra, it can be accessed in the **SearchIt** application using **Search Databases > All Compounds** or **Databases > Pure Compounds** and by checking the box for the **Use Computed Spectra** option:



Example 1

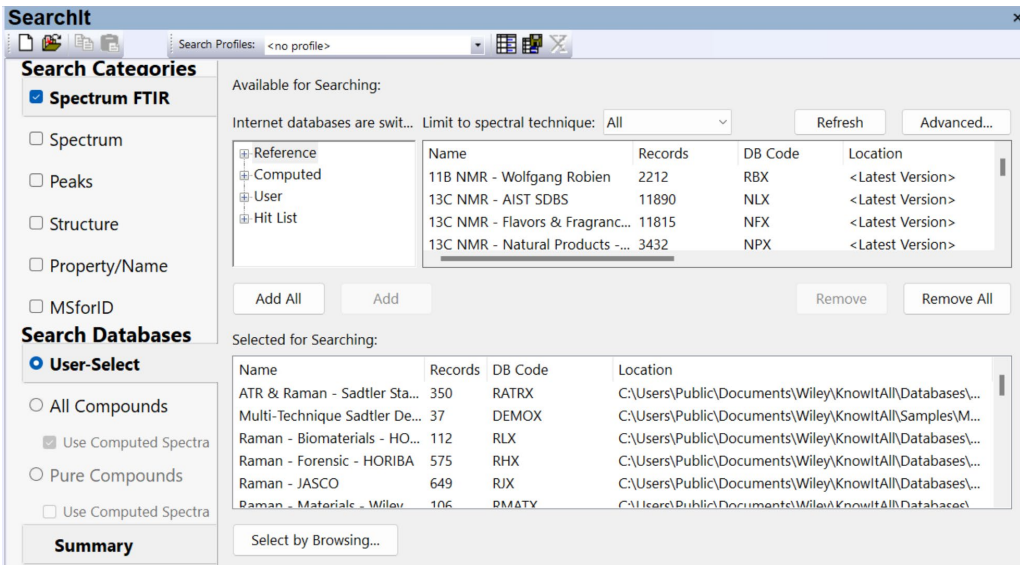
Example File: 4,13-DIDECYL-1,7,10,16-TETRAOXA-4,13-DIAZACYCLOOCTADECANE.irf

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


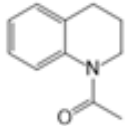
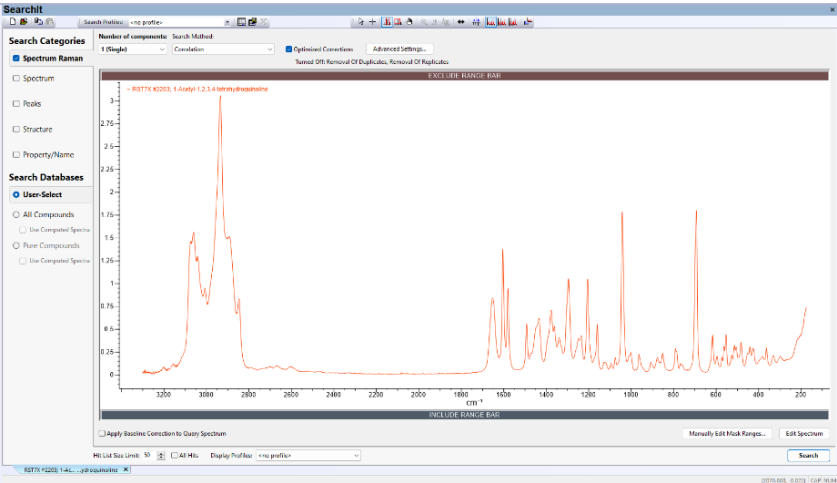
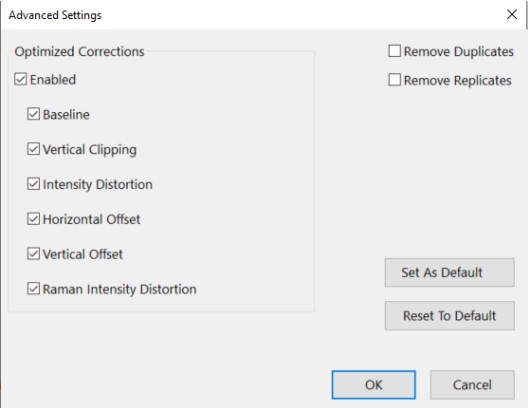
	Action	Result
3	<p>In Minelt, the hit list table displays match results featuring a mix of predicted and empirical matches.</p> <p>The structure below is the correct match for the query spectrum's structure,.</p> <p>The structure below is an exact match with the predicted data which appears as the top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

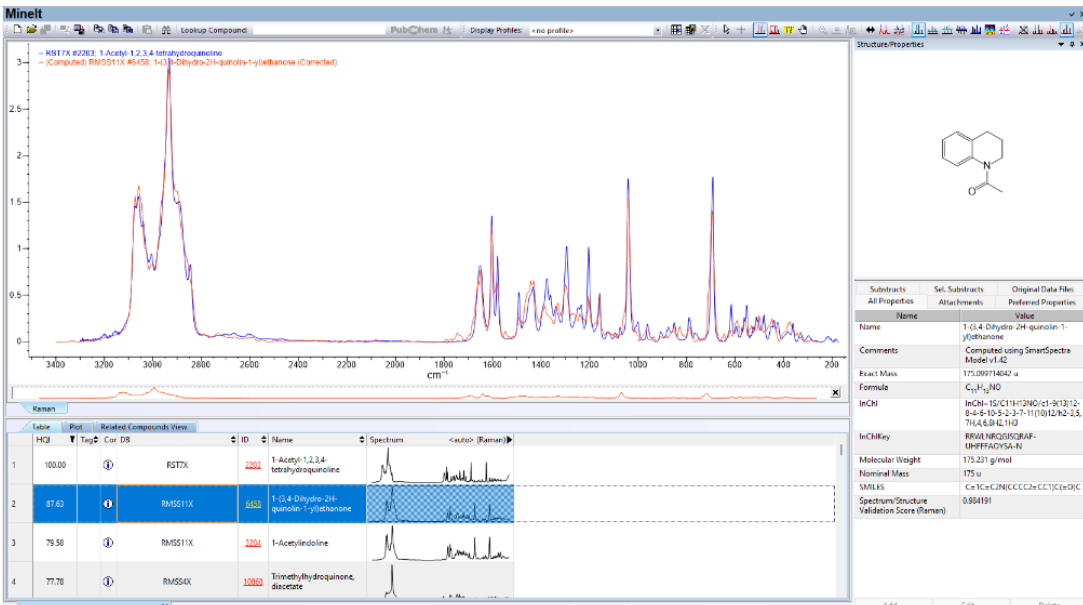
Example 2

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

	Action	Result																																																
1	<p>Return to the SearchIt application. Clear the previous search by hitting the small X on the upper right-hand side of the screen (X).</p> <p>In the SearchIt application, click User-Select under the Search Databases section.</p>	<p>The User-Select Databases window is displayed:</p>  <p>Search Categories</p> <ul style="list-style-type: none"><input checked="" type="checkbox"/> Spectrum FTIR<input type="checkbox"/> Spectrum<input type="checkbox"/> Peaks<input type="checkbox"/> Structure<input type="checkbox"/> Property/Name<input type="checkbox"/> MSforID <p>Search Databases</p> <ul style="list-style-type: none"><input checked="" type="radio"/> User-Select<input type="radio"/> All Compounds<ul style="list-style-type: none"><input checked="" type="checkbox"/> Use Computed Spectra<input type="radio"/> Pure Compounds<ul style="list-style-type: none"><input type="checkbox"/> Use Computed Spectra <p>Summary</p> <p>Available for Searching:</p> <p>Internet databases are swit... Limit to spectral technique: All Refresh Advanced...</p> <table><thead><tr><th>Name</th><th>Records</th><th>DB Code</th><th>Location</th></tr></thead><tbody><tr><td>11B NMR - Wolfgang Robien</td><td>2212</td><td>RBX</td><td><Latest Version></td></tr><tr><td>13C NMR - AIST SDBS</td><td>11890</td><td>NLX</td><td><Latest Version></td></tr><tr><td>13C NMR - Flavors & Fragranc...</td><td>11815</td><td>NFX</td><td><Latest Version></td></tr><tr><td>13C NMR - Natural Products -...</td><td>3432</td><td>NPX</td><td><Latest Version></td></tr></tbody></table> <p>Add All Add Remove Remove All</p> <p>Selected for Searching:</p> <table><thead><tr><th>Name</th><th>Records</th><th>DB Code</th><th>Location</th></tr></thead><tbody><tr><td>ATR & 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 - Wilov...</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	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 - Wilov...	106	PMATY	C:\Users\Public\Documents\Wiley\KnowitAll\Databases\...
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Raman - Sadtler Standards 6 - Wiley	1000	RST6X																																																																																																																																							
Raman - Sadtler Standards 7 - Wiley	2209	RST7X																																																																																																																																							
Raman - Semiconductor Materials - HORIBA	214	RVX																																																																																																																																							
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																																																																																																																																							

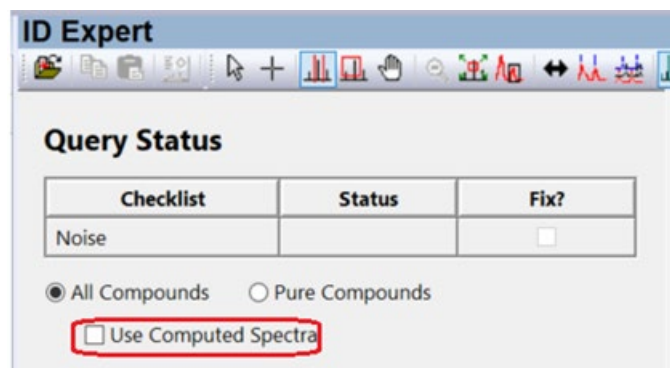
	Action	Result
3	<p>Click Open Spectrum or Structure icon () located on the Standard Toolbar.</p> <p>Navigate to find 1-acetyl-1234-tetrahydroquinoline.irf in “C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Computed Spectra\Raman”. Click Open.</p> <p><i>Note:</i> The image on this page is the correct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

	Action	Result
5	Locate the Hit List to view match results featuring a mix of predicted and empirical matches.	<p>The top hit in the Hit List 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> <div><div><p>Minell</p></div></div>

ID Expert


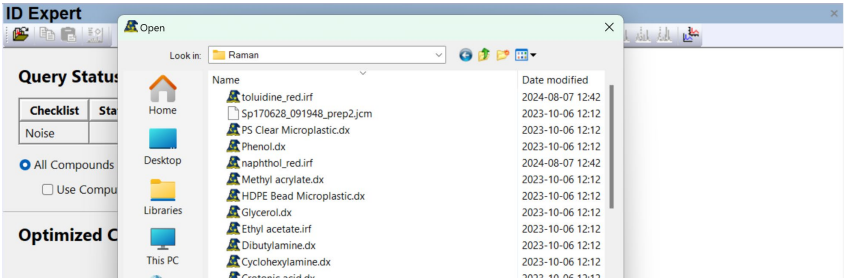
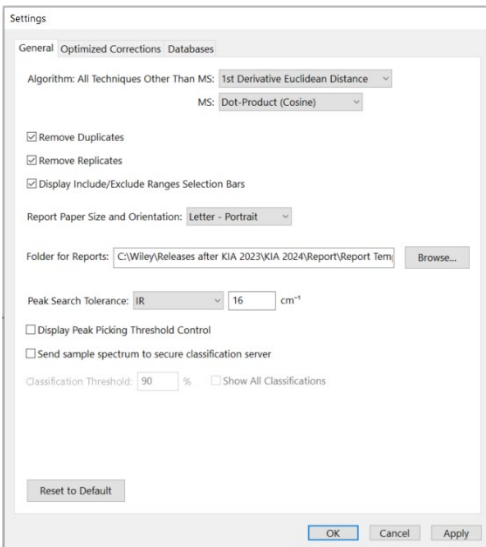
Introduction

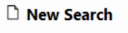
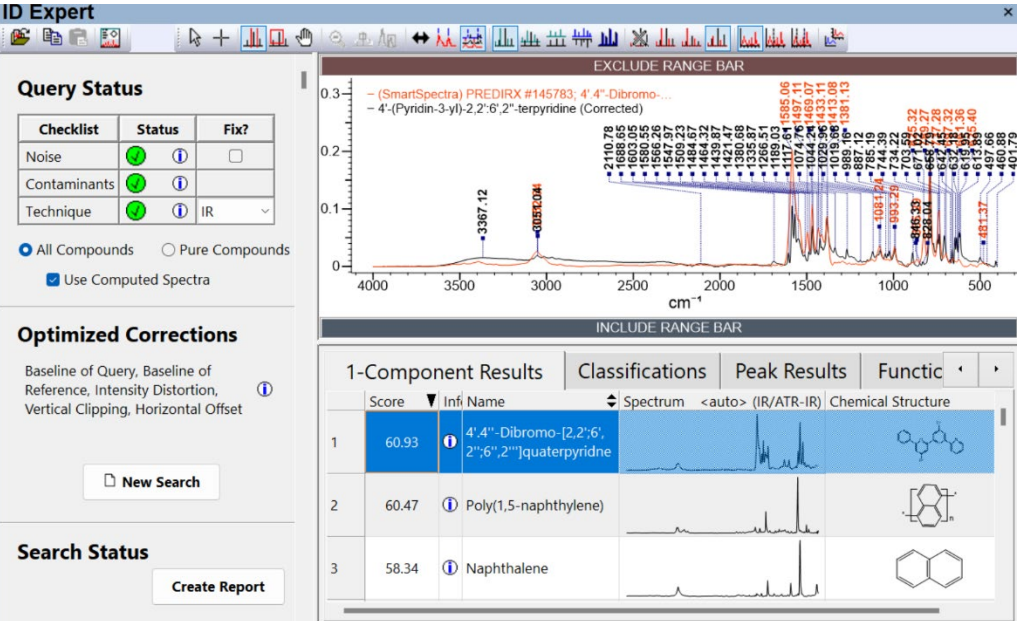
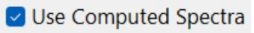
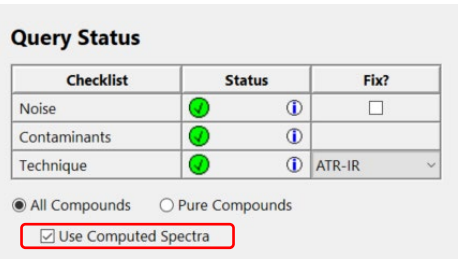
When a user's license contains the subscription for predicted IR spectra, the **ID Expert** interface **Query Status** shows the **Use Computed Spectra** option:



Example 3

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

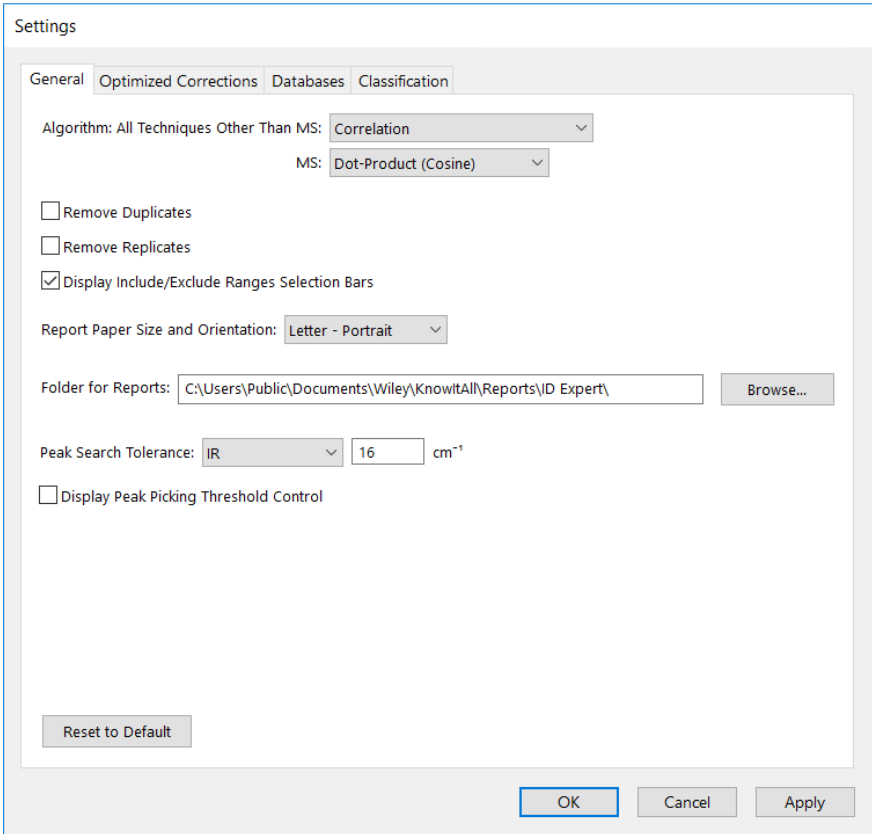
	Action	Result
1	<p>Navigate to the Data toolbox and open the ID Expert application by clicking the ID Expert icon (). Alternatively, if the desktop (standalone) application is installed, ID Expert can be opened directly by double-clicking on the desktop icon.</p>	<p>The application opens and an Open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


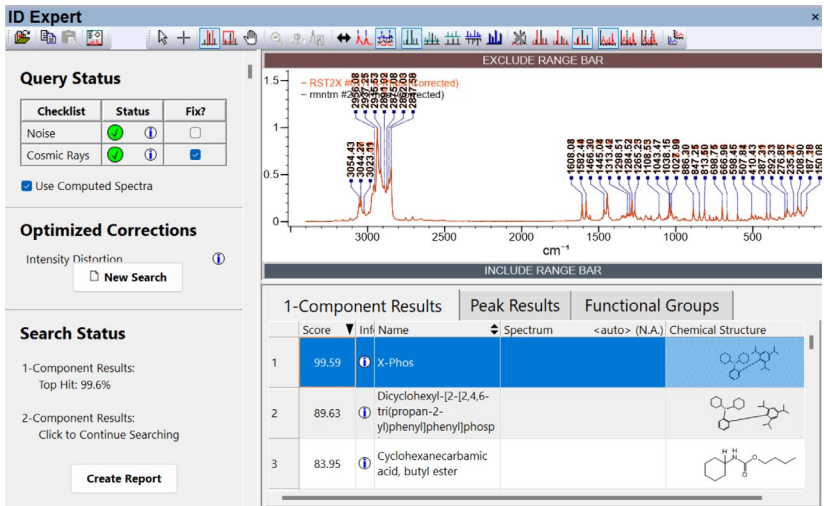
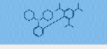
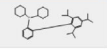
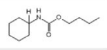
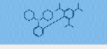
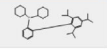
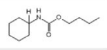
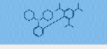
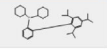
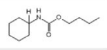
	Action	Result
3	<p>Click the New Search button</p> <p>().</p> <p>Open 4-(Pyridin-3-yl)-2-2,6,2-terpyridine.irf in the “C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Computed Spectra\IR” folder. Click Open.</p> <p>(Note: The training files used in this document are for example purposes only. The user 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> 
4	<p>Under Query Status, change Technique to ATR-IR.</p> <p>Check Use Computed Spectra checkbox.</p> <p></p>	<p>The modified Query Status settings are displayed. ID Expert updates the search with the modified settings.</p> 

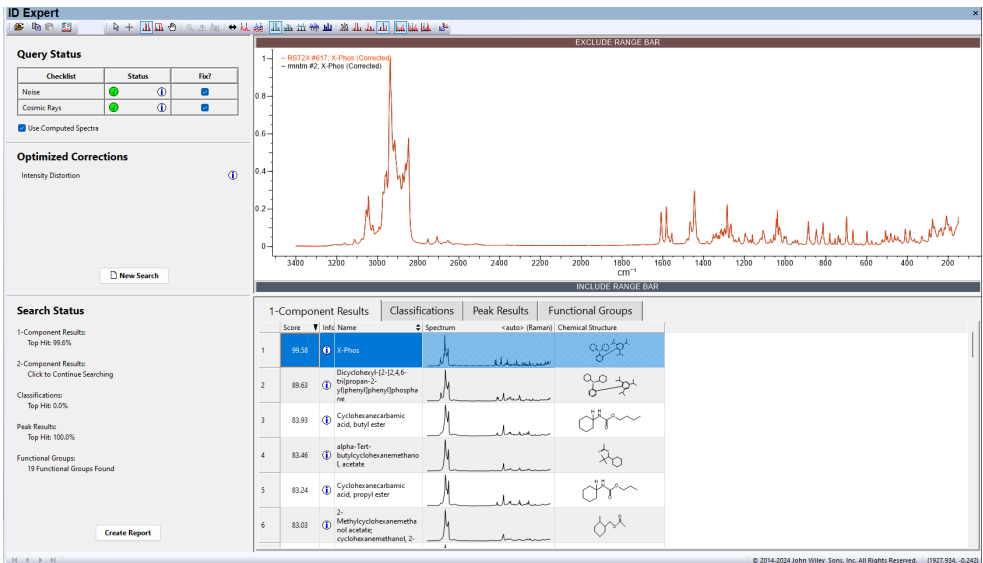

	Action	Result																																								
5	View the search results in the Component Table .	<div>This search results include experimental and predicted spectra.</div> <div><div><div><div><div><div>EXCLUDE RANGE BAR</div><div></div><div>INCLUDE RANGE BAR</div></div><div><div>1-Component Results</div><div>2-Component Results</div><div>3-Component Results</div><div>4-Component Results</div><div>5-Component Results</div><div>Classification</div></div><table><thead><tr><th>Score</th><th>Info Name</th><th>Spectrum</th><th>Chemical Structure</th></tr></thead><tbody><tr><td>60.93</td><td>4,4'-Dibromo-2,2',5,5'-terpyridine</td><td></td><td></td></tr><tr><td>60.47</td><td>Poly(1,5-naphthylene)</td><td></td><td></td></tr><tr><td>58.34</td><td>Naphthalene</td><td></td><td></td></tr><tr><td>58.24</td><td>2,6-Bis(quinolylthiomethyl)pyridine</td><td></td><td></td></tr><tr><td>57.31</td><td>2,2,6-TRICHLORO-7-OXABICYCLO[4.1.0]HEPTANE-1-CARBONITRILE</td><td></td><td></td></tr><tr><td>56.75</td><td>2,5-Dimethylthiophene</td><td></td><td></td></tr></tbody></table></div></div><div><div><div><div>Query Status</div><table><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><div><div><input checked="" type="radio"/> All Compounds</div><div><input type="radio"/> Pure Compounds</div></div><div><input checked="" type="checkbox"/> Use Computed Spectra</div></div><div><div>Optimized Corrections</div><div>Baseline of Query, Baseline of Reference, Intensity Distortion, Vertical Clipping, Horizontal Offset ⓘ</div><div><div>New Search</div></div></div><div><div>Search Status</div><div>1-Component Results: Top Hit: 60.9%</div><div>2-Component Results: Top Hit: 63.2%</div><div>3-Component Results: Top Hit: 64.3%</div><div>4-Component Results: Top Hit: 67.0%</div><div>5-Component Results: Top Hit: 69.4%</div><div>Classifications: Top Hit: 0.0%</div><div><div>Create Report</div></div></div></div></div></div></div>	Score	Info Name	Spectrum	Chemical Structure	60.93	4,4'-Dibromo-2,2',5,5'-terpyridine			60.47	Poly(1,5-naphthylene)			58.34	Naphthalene			58.24	2,6-Bis(quinolylthiomethyl)pyridine			57.31	2,2,6-TRICHLORO-7-OXABICYCLO[4.1.0]HEPTANE-1-CARBONITRILE			56.75	2,5-Dimethylthiophene			Checklist	Status	Fix?	Noise	●	ⓘ	Contaminants	●	ⓘ	Technique	●	ⓘ IR
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6	Close the active search by selecting the X icon () in the top right-hand corner.																																									

Example 4

Example File: X-Phos.irf

	Action	Result
1	<p>Close the Open window (if open), then choose File > Settings.</p> <p>In the Settings pop-up window, under the General tab, set Algorithm: All Techniques Other Than MS to menu option Correlation using the dropdown menu.</p> <p>Uncheck Remove Duplicates and Remove Replicates.</p> <p>Click Apply the OK to apply the change.</p>	

	Action	Result																										
2	<p>Click the New Search button ( New Search).</p> <p>Open X-Phos.irf in “C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Computed Spectra\Raman”. Click Open.</p> <p>In the Query Status panel, check the Use Computer Spectra box.</p> <p>Checking the Use Computer Spectra checkbox adds SmartSpectra data to ID Expert's library search. When not checked, SmartSpectra will not be searched.</p> <p>(Note: 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 software interface. The top panel displays a Raman spectrum with peaks labeled with wavenumbers (cm⁻¹). The bottom panel shows the search results table.</p> <table><tr><th colspan="4">1-Component Results</th><th>Peak Results</th><th>Functional Groups</th></tr><tr><th>Score</th><th>Inf Name</th><th>Spectrum</th><th><auto> (N.A.)</th><th>Chemical Structure</th></tr><tr><td>99.59</td><td>X-Phos</td><td></td><td></td><td></td></tr><tr><td>89.63</td><td>Dicyclohexyl-[2-(2,4,6-tri(phenyl-2-yl)phenyl)phenyl]phosph</td><td></td><td></td><td></td></tr><tr><td>83.95</td><td>Cyclohexanecarboxylic acid, butyl ester</td><td></td><td></td><td></td></tr></table>	1-Component Results				Peak Results	Functional Groups	Score	Inf Name	Spectrum	<auto> (N.A.)	Chemical Structure	99.59	X-Phos				89.63	Dicyclohexyl-[2-(2,4,6-tri(phenyl-2-yl)phenyl)phenyl]phosph				83.95	Cyclohexanecarboxylic acid, butyl ester			
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	Action	Result
3	View search results in the Component Results table.	<p>The top hit in the Hit List 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 X icon () in the top right-hand corner.	

Classification Models

Purpose

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

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:



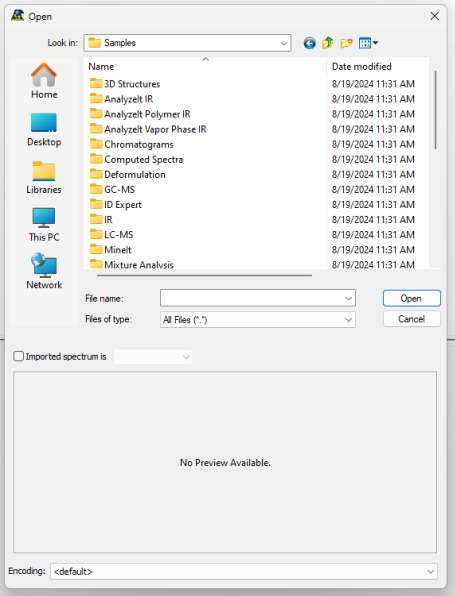
- KnowItAll ID Expert
- KnowItAll Minelt

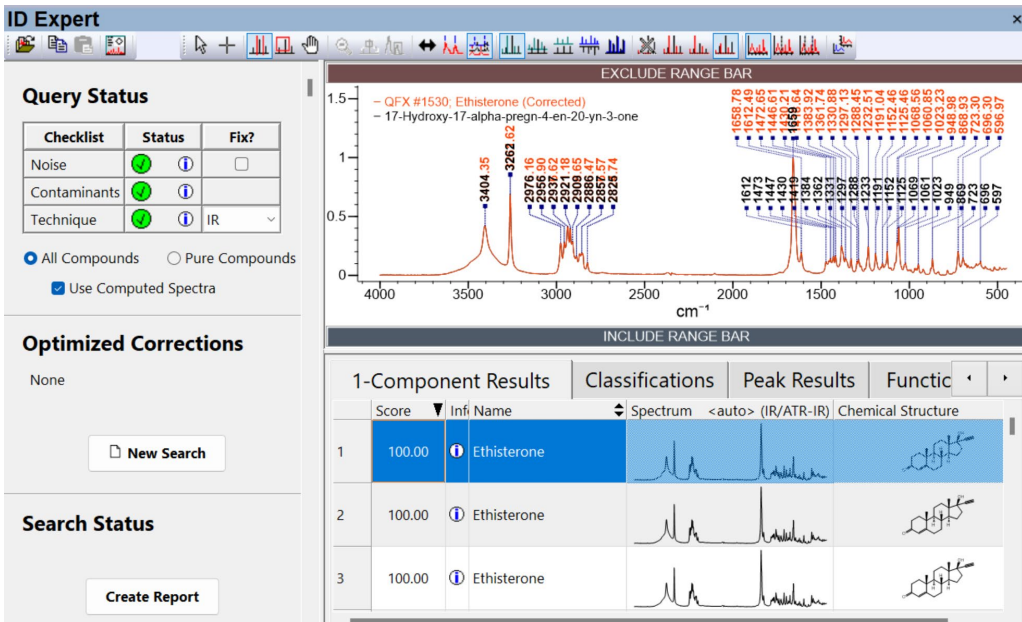
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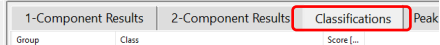
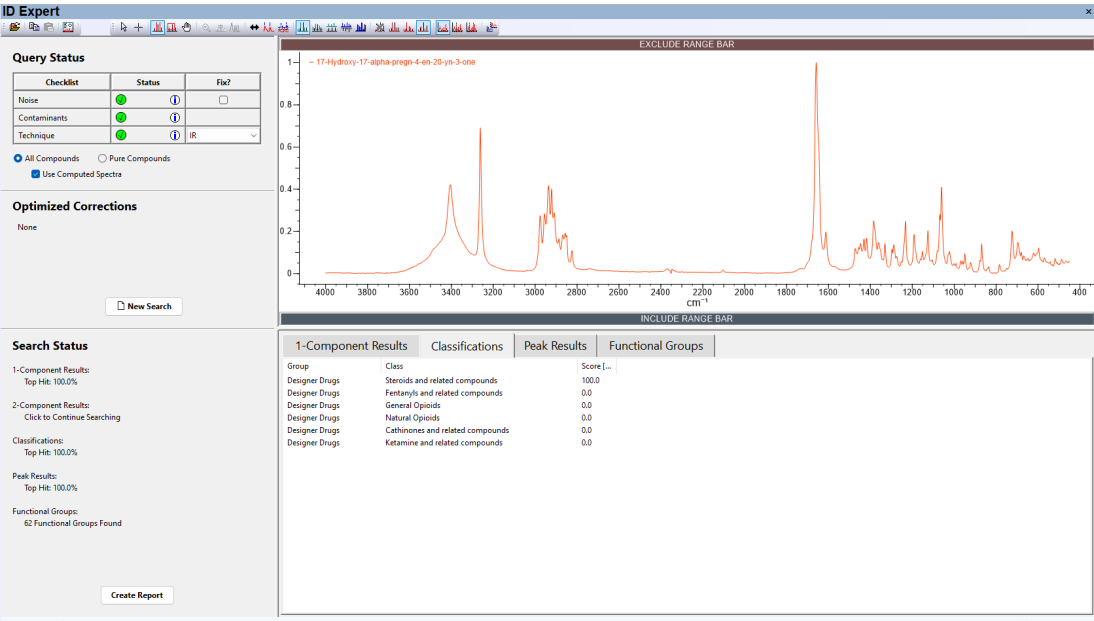
Classification models are a type of supervised learning used to label or categorize data into predefined classes or groups. These models predict the said label based on feature data. The model must be trained on labeled data or have an architecture that leads to the data being trained on to be self labelled 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 ID Expert ().</p> <p>If the Open window does not appear, then click New Search button () to manually launch the dialog window.</p>	<p>The Open window appears for file selection:</p> 


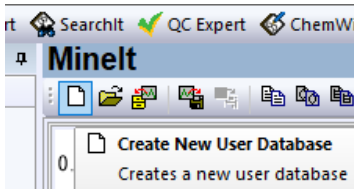
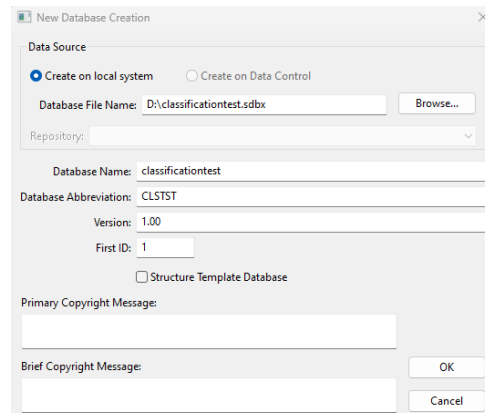
	Action	Result																
2	<p>Open 17-Hydroxy-17-alpha-pregn-4-en-20-yn-3-one.irf in the “C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Mixture Analysis\IR Examples\Components” folder.</p> <p>Click Open.</p>	<p>Immediately upon opening the file, it begins to search for a match using the licensed databases available to the user:</p>  <p>The screenshot displays the ID Expert software window. On the left, the Query Status section shows a checklist with 'Noise', 'Contaminants', and 'Technique' (set to IR). Below this, the Optimized Corrections section shows 'None'. The Search Status section includes 'New Search' and 'Create Report' buttons. The main area shows an IR spectrum plot with peaks labeled with wavenumbers. Below the plot, the 1-Component Results table lists three matches for Ethisterone, all with a score of 100.00. The Classifications tab is selected, showing the spectrum and chemical structure for each match.</p> <table><thead><tr><th>Score</th><th>Inf Name</th><th>Spectrum</th><th>Chemical Structure</th></tr></thead><tbody><tr><td>100.00</td><td>Ethisterone</td><td></td><td></td></tr><tr><td>100.00</td><td>Ethisterone</td><td></td><td></td></tr><tr><td>100.00</td><td>Ethisterone</td><td></td><td></td></tr></tbody></table>	Score	Inf Name	Spectrum	Chemical Structure	100.00	Ethisterone			100.00	Ethisterone			100.00	Ethisterone		
Score	Inf Name	Spectrum	Chemical Structure															
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3	<p>Click File > Settings.</p> <p>Under the Classification tab of the Settings window, check the Show All Classifications checkbox. Click OK to save the changes.</p> <p><input checked="" type="checkbox"/> Show All Classifications</p>	<p>Upon clicking OK, the Settings window is closed.</p>																

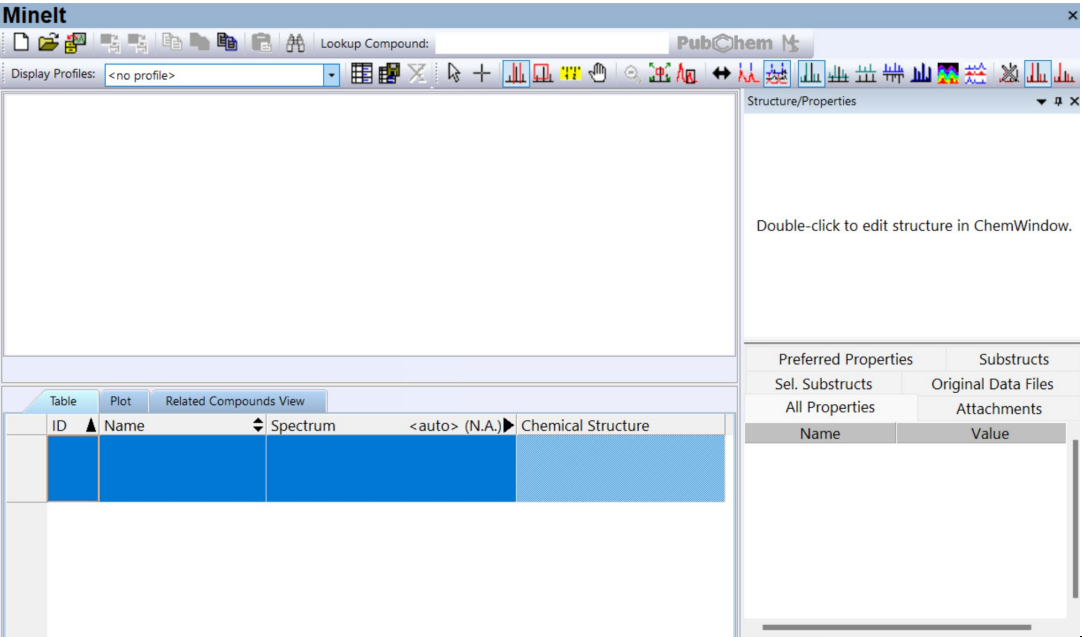
	Action	Result																																												
4	<p>Click the Classifications tab just right of the Component Results tab.</p> <p><i>Note:</i> If there is a situation where there are multiple components detected in the sample (<i>i.e.</i>, >1), the tab is located to the right of the last component result as seen in the image below.</p> 	<p>ID Expert displays the classification results for the classification models available in the user license. In this case, the sample is identified to be a Steroid:</p>  <p>Query Status</p> <table border="1"> <thead> <tr> <th>Checklist</th> <th>Status</th> <th>Fix?</th> </tr> </thead> <tbody> <tr> <td>Noise</td> <td>Green circle</td> <td>Down arrow</td> </tr> <tr> <td>Contaminants</td> <td>Green circle</td> <td>Down arrow</td> </tr> <tr> <td>Technique</td> <td>Green circle</td> <td>Down arrow</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>Optimized Corrections</p> <p>None</p> <p><input type="button" value="New Search"/></p> <p>Search Status</p> <p>1-Component Results: Top Hit: 100.0%</p> <p>2-Component Results: Click to Continue Searching</p> <p>Classifications: Top Hit: 100.0%</p> <p>Peak Results: Top Hit: 100.0%</p> <p>Functional Groups: 62 Functional Groups Found</p> <p><input type="button" value="Create Report"/></p> <table border="1"> <thead> <tr> <th>1-Component Results</th> <th>Classifications</th> <th>Peak Results</th> <th>Functional Groups</th> </tr> </thead> <tbody> <tr> <td>Group</td> <td>Class</td> <td>Score [...]</td> <td></td> </tr> <tr> <td>Designer Drugs</td> <td>Steroids and related compounds</td> <td>100.0</td> <td></td> </tr> <tr> <td>Designer Drugs</td> <td>Fentanyl and related compounds</td> <td>0.0</td> <td></td> </tr> <tr> <td>Designer Drugs</td> <td>General Opioids</td> <td>0.0</td> <td></td> </tr> <tr> <td>Designer Drugs</td> <td>Natural Opioids</td> <td>0.0</td> <td></td> </tr> <tr> <td>Designer Drugs</td> <td>Cathinones and related compounds</td> <td>0.0</td> <td></td> </tr> <tr> <td>Designer Drugs</td> <td>Ketamine and related compounds</td> <td>0.0</td> <td></td> </tr> </tbody> </table>	Checklist	Status	Fix?	Noise	Green circle	Down arrow	Contaminants	Green circle	Down arrow	Technique	Green circle	Down arrow	1-Component Results	Classifications	Peak Results	Functional Groups	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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Designer Drugs	Ketamine and related compounds	0.0																																												

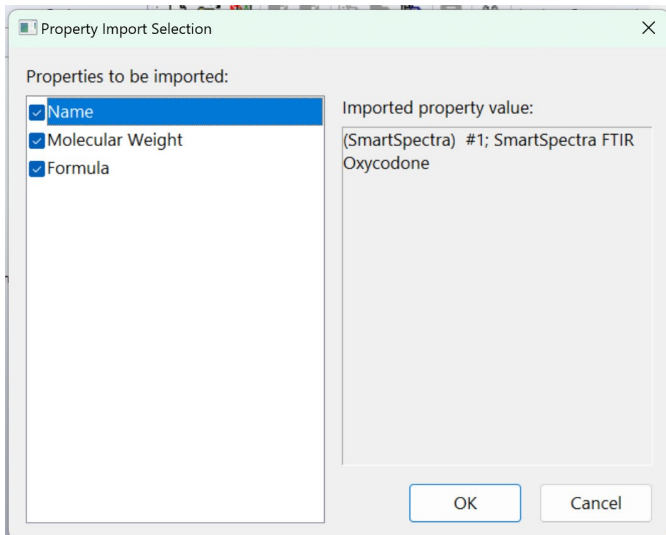
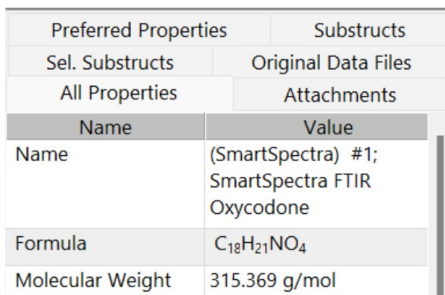
Classification Batch Property Calculation in Minelt

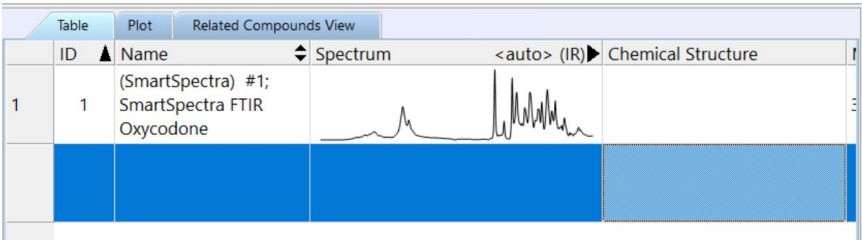
Example Files: SmartSpectraFTIROxycodone.irf, SmartSpectraRamanAndrosteroneacetate.irf

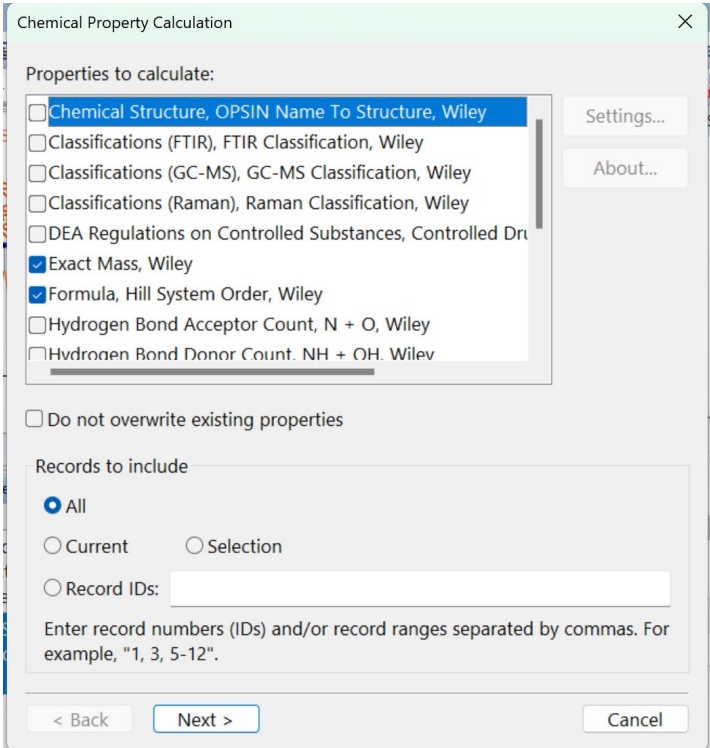
Batch property calculation is a calculation that will be applied to a series of compounds at one time. In this exercise, an unlocked user database will be created that to simulate executing a batch property calculation. This workflow can only be performed using unlocked (user) databases.

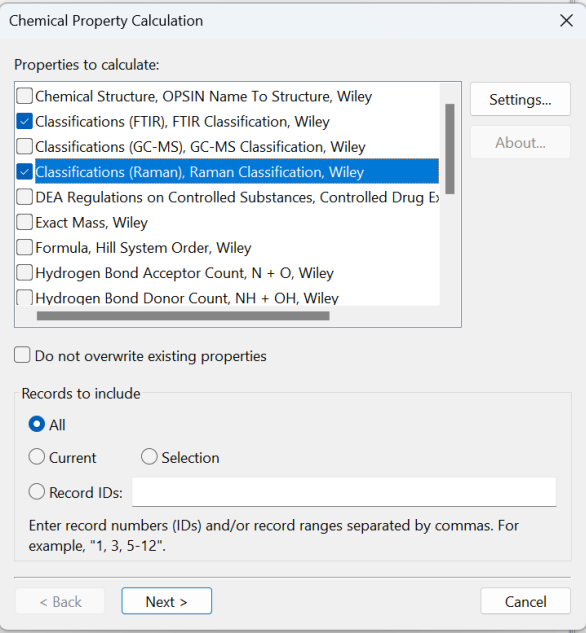
	Action	Result
1	<p>Navigate to the Minelt application ().</p> <p>To use the Batch Property Calculation tools in Minelt, a user database must be created.</p> <p><i>Note:</i> Creating a user database creates an unlocked database. Licensed KnowItAll databases are locked databases.</p> <p>Select the Create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

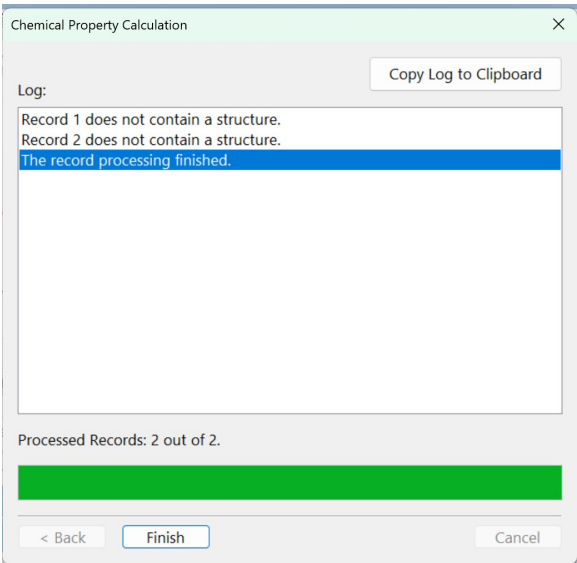
	Action	Result
3	Click OK to create the database.	<p>A blank user database is opened in Minelt.</p>  <p>The screenshot shows the Minelt application window. At the top is a menu bar with 'File', 'Edit', 'View', 'Tools', 'Window', and 'Help'. Below the menu bar is a toolbar with various icons for file operations, editing, and viewing. The main workspace is a large empty area. On the right side, there is a 'Structure/Properties' panel with a 'Double-click to edit structure in ChemWindow.' message. Below the workspace, there is a 'Table' view with columns: ID, Name, Spectrum, and Chemical Structure. The 'Table' tab is selected, and the table is currently empty.</p>
4	Navigate to the File > Import to import spectral files.	The Open window is launched.

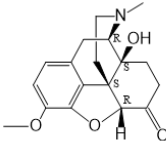
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5	<p>Open SmartSpectraFTIROxycodone.irf in the “C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Computed Spectra\IR” folder.</p> <p>Click Open.</p>	<p>The Property Import Selection window is launched:</p> 																												
6	<p>Click OK on the Property Import Selection window.</p>	<p>The Property Import Selection window is closed and the properties are imported in the Structure/Properties panel.</p>  <table><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>Value</th><th></th><th></th></tr><tr><td>Name</td><td>(SmartSpectra) #1; SmartSpectra FTIR Oxycodone</td><td></td><td></td></tr><tr><td>Formula</td><td>C₁₈H₂₁NO₄</td><td></td><td></td></tr><tr><td>Molecular Weight</td><td>315.369 g/mol</td><td></td><td></td></tr></table>	Preferred Properties		Substructs		Sel. Substructs		Original Data Files		All Properties		Attachments		Name	Value			Name	(SmartSpectra) #1; SmartSpectra FTIR Oxycodone			Formula	C ₁₈ H ₂₁ NO ₄			Molecular Weight	315.369 g/mol		
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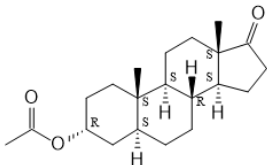
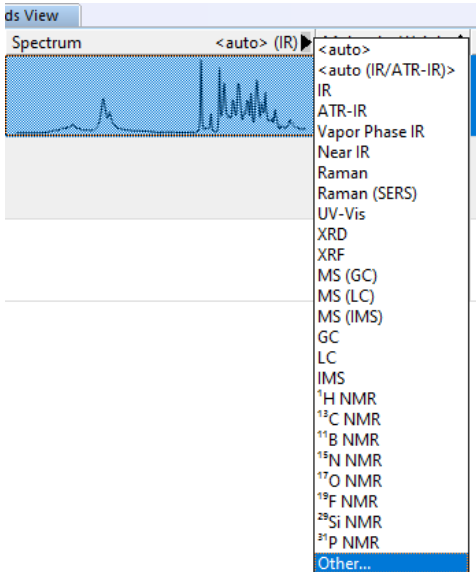
	Action	Result
7	Click on the row below the first record in the Table .	<p>The second row is shaded in the Table:</p> 
8	Navigate to the File tab and select Import to import a second file into the user database.	The Open dialog window is launched.
9	Repeat steps 4 through 8 using SmartSpectraRamanAndrosteroneacetate.irf in the "C:\Users\Public\Documents\Wiley\KnowItAll\Samples\ Computed Spectra\Raman" folder.	The Property Import Selection window is launched. The Raman sample file is imported into the user database.

	Action	Result
10	Navigate to Database > Batch Property Calculation .	<p>The Batch Property Calculation window is launched:</p>  <p>Chemical Property Calculation</p> <p>Properties to calculate:</p> <ul style="list-style-type: none"><input type="checkbox"/> Chemical Structure, OPSIN Name To Structure, Wiley<input type="checkbox"/> Classifications (FTIR), FTIR Classification, Wiley<input type="checkbox"/> Classifications (GC-MS), GC-MS Classification, Wiley<input type="checkbox"/> Classifications (Raman), Raman Classification, Wiley<input type="checkbox"/> DEA Regulations on Controlled Substances, Controlled Dr<input checked="" type="checkbox"/> Exact Mass, Wiley<input checked="" type="checkbox"/> Formula, Hill System Order, Wiley<input type="checkbox"/> Hydrogen Bond Acceptor Count, N + O, Wiley<input type="checkbox"/> Hydrogen Bond Donor Count, NH + OH, Wiley <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>< Back Next > Cancel</p>

	Action	Result
11	<p>Click to select the Classifications models for IR and Raman:</p> <ul style="list-style-type: none"> ▪ Classifications (FTIR), FTIR Classification, Wiley ▪ Classifications (Raman), Raman Classification, Wiley <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 Chemical Property Calculation window is shown below with the selected Classifications models selected:</p> 
12	<p>Under Records to Include, ensure All is selected. Then click Next > to execute the Batch Property Calculations.</p>	

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

	Action	Result																																
15	The resulting classification can be found in the Structure/Properties panel for the selected record.	<p>Record ID 1 has results Classifications (FTIR) “General Opioids (100.0%)” and “Natural Opioids (100.0%)”.</p> <table><tr><td>Preferred Properties</td><td>Substructs</td></tr><tr><td>Sel. Substructs</td><td>Original Data Files</td></tr><tr><td>All Properties</td><td>Attachments</td></tr><tr><th>Name</th><th>Value</th></tr><tr><td>Name</td><td>(SmartSpectra) #1; SmartSpectra FTIR Oxycodone</td></tr><tr><td>Classifications</td><td>General Opioids (100.0%) Natural Opioids (100.0%)</td></tr><tr><td>Formula</td><td>C₁₈H₂₁NO₄</td></tr><tr><td>Molecular Weight</td><td>315.369 g/mol</td></tr></table> <p>Record ID 2 has results Classifications (Raman) “Steroids and related compounds (100.0%)”.</p> <table><tr><td>Preferred Properties</td><td>Substructs</td></tr><tr><td>Sel. Substructs</td><td>Original Data Files</td></tr><tr><td>All Properties</td><td>Attachments</td></tr><tr><th>Name</th><th>Value</th></tr><tr><td>Name</td><td>#2; SmartSpectra Raman Androsterone Acetate</td></tr><tr><td>Classifications</td><td>Steroids and related compounds (100.0%)</td></tr><tr><td>Formula</td><td>C₂₁H₃₂O₃</td></tr><tr><td>Molecular Weight</td><td>332.484 g/mol</td></tr></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 ₁₈ H ₂₁ NO ₄	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 ₂₁ H ₃₂ O ₃	Molecular Weight	332.484 g/mol
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16	The final compound structures are provided in the Results 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>Record ID 1: (SmartSpectra) #1; SmartSpectra FTIR Oxycodone.</p> 																																

Action	Result
<p>To view all the different spectral techniques in the database spectrum pane, select the black triangle to the right of '<auto> (IR)' or '<auto> (Raman)' part of the pane.</p> <p>When the dropdown appears, select the technique you would like to view.</p>	<p>Record ID 2: #2; SmartSpectra Raman Androsterone Acetate.</p>  <p>The chemical structure of Androsterone Acetate is shown, featuring a steroid nucleus with an acetate group at C3 and a ketone at C20. Stereochemistry is indicated with wedges and dashes.</p>  <p>The screenshot displays the 'ds View' pane. The 'Spectrum' section has a dropdown menu open, showing a list of spectral techniques. The current selection is '<auto> (IR)'. The dropdown menu includes the following options: '<auto>', '<auto> (IR/ATR-IR)>', 'IR', 'ATR-IR', 'Vapor Phase IR', 'Near IR', 'Raman', 'Raman (SERS)', 'UV-Vis', 'XRD', 'XRF', 'MS (GC)', 'MS (LC)', 'MS (IMS)', 'GC', 'LC', 'IMS', '¹H NMR', '¹³C NMR', '¹¹B NMR', '¹⁵N NMR', '¹⁷O NMR', '¹⁹F NMR', '²⁹Si NMR', '³¹P NMR', and 'Other...'. The 'Other...' option is highlighted at the bottom.</p>