

KnowItAll Software Training

Predicted IR

Use Predicted IR Spectra in KnowItAll

How to Use Predicted IR spectra in KnowItAll SearchIt and ID Expert

Purpose

These exercises demonstrate how to use Predicted IR spectra in KnowItAll ID Expert and SearchIt

Objectives

These exercises will teach you:

- How to use Predicted IR spectra in KnowItAll SearchIt
- How to use Predicted IR spectra in KnowItAll ID Expert

Background

Wiley has the largest quantity of experimental IR spectra, which was originally 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 Library of Predicted Infrared Spectra is an attempt to increase the catalog coverage of Wiley's IR chemical space. This does not mean to increase the chemical space, but to 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.

This library can be helpful when used as a tool 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 are not perfect. Wiley acknowledges that some results may not be entirely correct in order to convey that this library should be used as a tool to help the user classify components that are in the spectrum to characterize their unknown spectrum.

Training Files Used in This Lesson

- 5MEODIPT.SPC
- 4-(Pyridin-3-yl)-2,2,6,2-terpyridine.irf

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™

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 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 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.

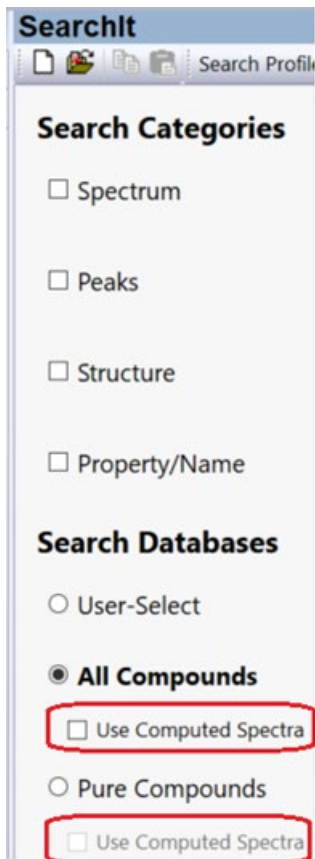
Manual corrections can be made by expert spectroscopists, but those less experienced in spectroscopy are often unaware of how to perform the necessary corrections on their sample spectrum to achieve the best search result. To address this growing concern, Wiley has introduced Optimized Corrections, a 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.

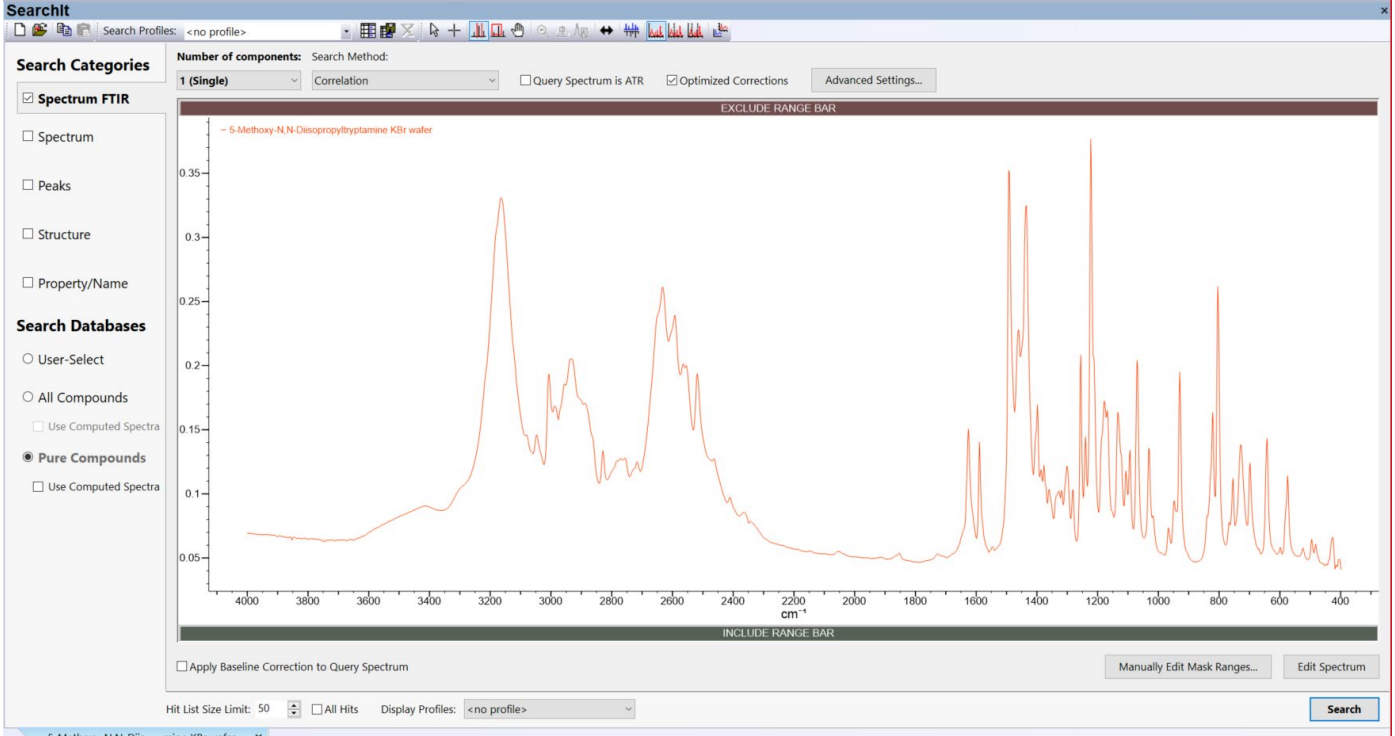
¹ E2310-04 - Standard Guide for Use of Spectral Searching by Curve Matching Algorithms with Data Recorded Using Mid-Infrared Spectroscopy, 2009. ASTM International Web Site. <http://www.astm.org/Standards/E2310.htm> (accessed March 4, 2015).

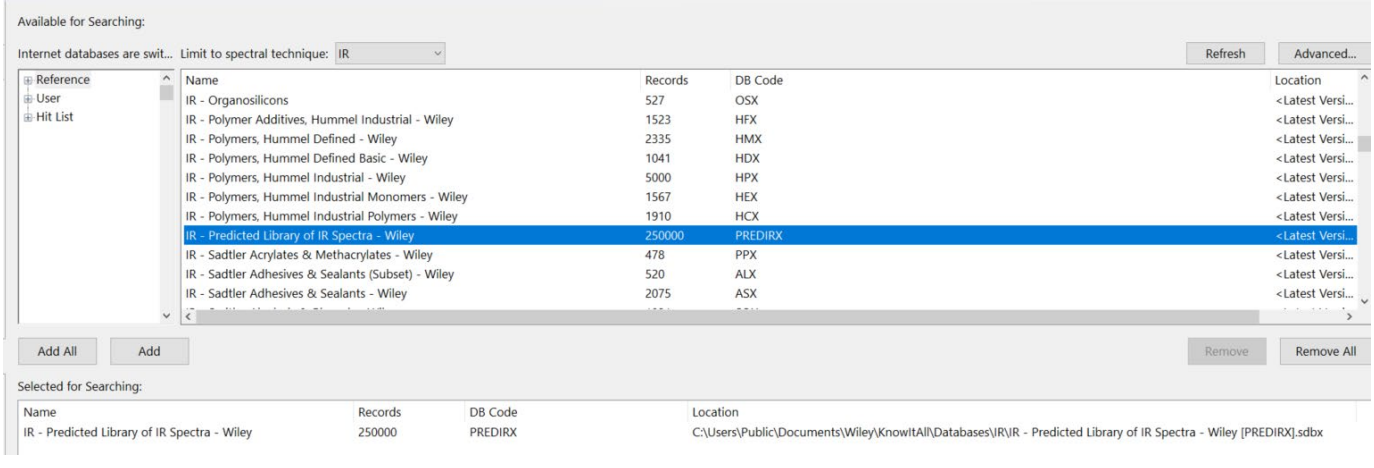
SearchIt

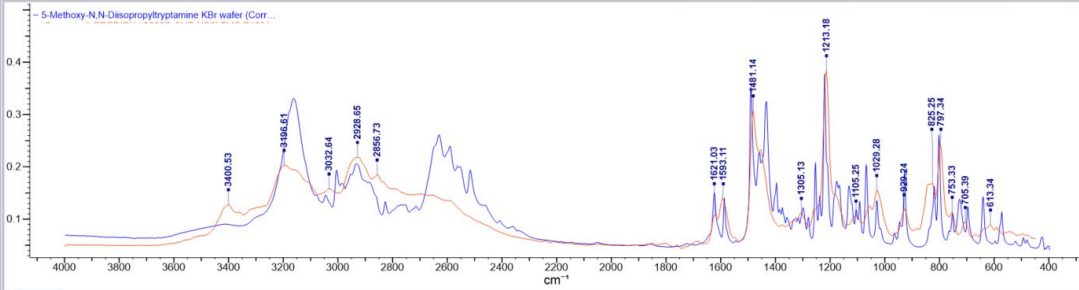
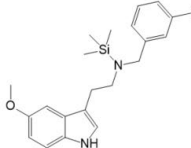
When a license contains the subscription of predicted IR spectra, it can be accessed in the **SearchIt** application > **Databases** > **All Compounds** or **Databases** > **Pure Compounds** by selecting the **Use Computed Spectra** option:



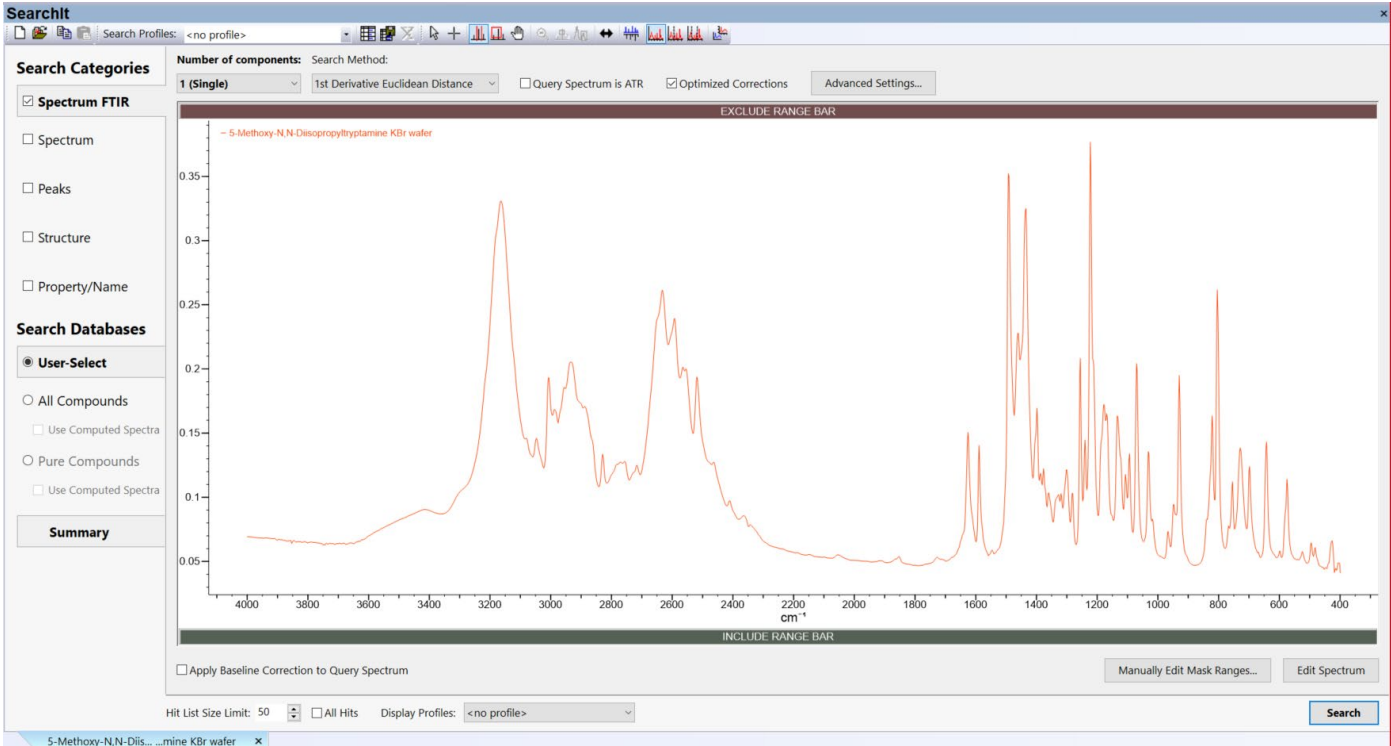
Example 1 - 5MEODIPT.SPC, Correlation Algorithm

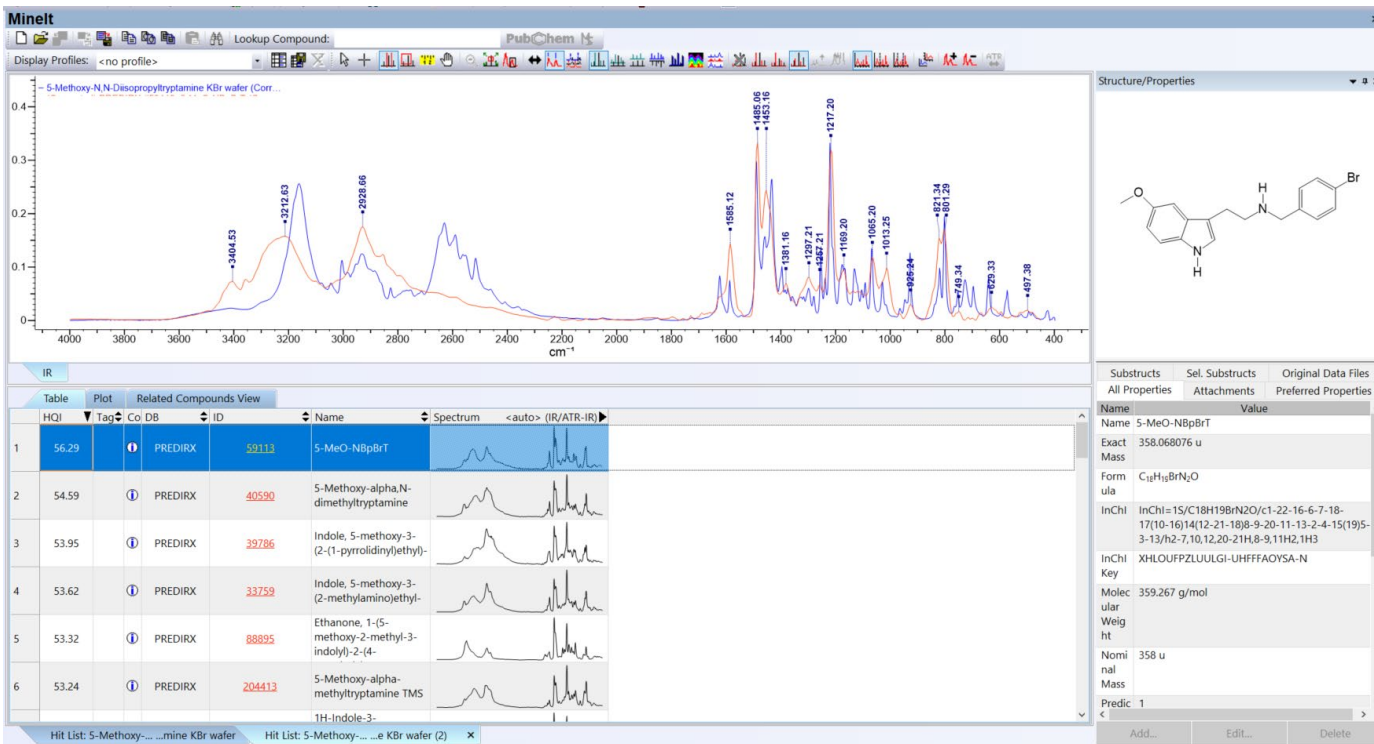
	Action	Result
1	In the SearchIt application, click Open Spectrum or Structure .	
2	Navigate to find 5MEODIPT.SPC in the Predicted IR Example Spectra folder. (Note that the training files used in this document are for example purposes only. The user should utilize their own IR spectra when following this training.) Open	 <p>The screenshot shows the SearchIt application interface. The main window displays an FTIR spectrum plot with the following details:</p> <ul style="list-style-type: none"> Search Categories: Spectrum FTIR (checked), Spectrum, Peaks, Structure, Property/Name. Search Databases: User-Select, All Compounds, Pure Compounds (selected), Use Computed Spectra. Search Method: Correlation. Number of components: 1 (Single). Plot: FTIR spectrum showing transmittance vs. wavenumber (cm⁻¹) from 4000 to 400. The plot title is "5-Methoxy-N,N-Diisopropyltryptamine KBr wafer". Buttons: Search, Edit Spectrum, Manually Edit Mask Ranges...

	Action	Result																																																																				
3	<p>Click on User-Select</p> <p>Click Remove All button</p> <p>Limit spectra technique to IR</p> <p>Select the IR – Predicted Library of IR Spectra – Wiley and click Add.</p> <p>Search</p>	 <p>Available for Searching:</p> <p>Internet databases are swit... Limit to spectral technique: IR Refresh Advanced...</p> <table border="1"> <thead> <tr> <th>Reference</th> <th>Name</th> <th>Records</th> <th>DB Code</th> <th>Location</th> </tr> </thead> <tbody> <tr><td>IR - Organosilicons</td><td></td><td>527</td><td>OSX</td><td><Latest Versi...</td></tr> <tr><td>IR - Polymer Additives, Hummel Industrial - Wiley</td><td></td><td>1523</td><td>HFX</td><td><Latest Versi...</td></tr> <tr><td>IR - Polymers, Hummel Defined - Wiley</td><td></td><td>2335</td><td>HMX</td><td><Latest Versi...</td></tr> <tr><td>IR - Polymers, Hummel Defined Basic - Wiley</td><td></td><td>1041</td><td>HDX</td><td><Latest Versi...</td></tr> <tr><td>IR - Polymers, Hummel Industrial - Wiley</td><td></td><td>5000</td><td>HPX</td><td><Latest Versi...</td></tr> <tr><td>IR - Polymers, Hummel Industrial Monomers - Wiley</td><td></td><td>1567</td><td>HEX</td><td><Latest Versi...</td></tr> <tr><td>IR - Polymers, Hummel Industrial Polymers - Wiley</td><td></td><td>1910</td><td>HCX</td><td><Latest Versi...</td></tr> <tr style="background-color: #e0f0ff;"><td>IR - Predicted Library of IR Spectra - Wiley</td><td></td><td>250000</td><td>PREDIRX</td><td><Latest Versi...</td></tr> <tr><td>IR - Sadtler Acrylates & Methacrylates - Wiley</td><td></td><td>478</td><td>PPX</td><td><Latest Versi...</td></tr> <tr><td>IR - Sadtler Adhesives & Sealants (Subset) - Wiley</td><td></td><td>520</td><td>ALX</td><td><Latest Versi...</td></tr> <tr><td>IR - Sadtler Adhesives & Sealants - Wiley</td><td></td><td>2075</td><td>ASX</td><td><Latest Versi...</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>IR - Predicted Library of IR Spectra - Wiley</td> <td>250000</td> <td>PREDIRX</td> <td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\IR - Predicted Library of IR Spectra - Wiley [PREDIRX].sdbx</td> </tr> </tbody> </table>	Reference	Name	Records	DB Code	Location	IR - Organosilicons		527	OSX	<Latest Versi...	IR - Polymer Additives, Hummel Industrial - Wiley		1523	HFX	<Latest Versi...	IR - Polymers, Hummel Defined - Wiley		2335	HMX	<Latest Versi...	IR - Polymers, Hummel Defined Basic - Wiley		1041	HDX	<Latest Versi...	IR - Polymers, Hummel Industrial - Wiley		5000	HPX	<Latest Versi...	IR - Polymers, Hummel Industrial Monomers - Wiley		1567	HEX	<Latest Versi...	IR - Polymers, Hummel Industrial Polymers - Wiley		1910	HCX	<Latest Versi...	IR - Predicted Library of IR Spectra - Wiley		250000	PREDIRX	<Latest Versi...	IR - Sadtler Acrylates & Methacrylates - Wiley		478	PPX	<Latest Versi...	IR - Sadtler Adhesives & Sealants (Subset) - Wiley		520	ALX	<Latest Versi...	IR - Sadtler Adhesives & Sealants - Wiley		2075	ASX	<Latest Versi...	Name	Records	DB Code	Location	IR - Predicted Library of IR Spectra - Wiley	250000	PREDIRX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\IR - Predicted Library of IR Spectra - Wiley [PREDIRX].sdbx
Reference	Name	Records	DB Code	Location																																																																		
IR - Organosilicons		527	OSX	<Latest Versi...																																																																		
IR - Polymer Additives, Hummel Industrial - Wiley		1523	HFX	<Latest Versi...																																																																		
IR - Polymers, Hummel Defined - Wiley		2335	HMX	<Latest Versi...																																																																		
IR - Polymers, Hummel Defined Basic - Wiley		1041	HDX	<Latest Versi...																																																																		
IR - Polymers, Hummel Industrial - Wiley		5000	HPX	<Latest Versi...																																																																		
IR - Polymers, Hummel Industrial Monomers - Wiley		1567	HEX	<Latest Versi...																																																																		
IR - Polymers, Hummel Industrial Polymers - Wiley		1910	HCX	<Latest Versi...																																																																		
IR - Predicted Library of IR Spectra - Wiley		250000	PREDIRX	<Latest Versi...																																																																		
IR - Sadtler Acrylates & Methacrylates - Wiley		478	PPX	<Latest Versi...																																																																		
IR - Sadtler Adhesives & Sealants (Subset) - Wiley		520	ALX	<Latest Versi...																																																																		
IR - Sadtler Adhesives & Sealants - Wiley		2075	ASX	<Latest Versi...																																																																		
Name	Records	DB Code	Location																																																																			
IR - Predicted Library of IR Spectra - Wiley	250000	PREDIRX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\IR - Predicted Library of IR Spectra - Wiley [PREDIRX].sdbx																																																																			

	Action	Result																																																																											
4	Locate the hit list to view predicted results.	<p>Minelt</p>  <p>Structure/Properties</p>  <p>IR</p> <table border="1"> <thead> <tr> <th>Table</th> <th>Plot</th> <th>Related Compounds View</th> </tr> <tr> <th>HQI</th> <th>Tag</th> <th>Corrections DB</th> <th>ID</th> <th>Name</th> <th>Spectrum</th> <th><auto> (IR/ATR-IR)</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>70.97</td> <td>①</td> <td>PREDIRX</td> <td>36387</td> <td>5MT-NB3I TMS P1631</td> <td></td> </tr> <tr> <td>2</td> <td>69.96</td> <td>①</td> <td>PREDIRX</td> <td>67580</td> <td>5-Methoxy-3-(2-morpholinylethyl)indole</td> <td></td> </tr> <tr> <td>3</td> <td>68.87</td> <td>①</td> <td>PREDIRX</td> <td>4072</td> <td>5-Methoxy-N,N-dipropyltryptamine</td> <td></td> </tr> <tr> <td>4</td> <td>68.22</td> <td>①</td> <td>PREDIRX</td> <td>42758</td> <td>5-METHOXYINDOLE-N,N-DIETHYL-TRYPTAMINE</td> <td></td> </tr> <tr> <td>5</td> <td>67.52</td> <td>①</td> <td>PREDIRX</td> <td>134398</td> <td>1H-Indole-3-ethanamine, 5-methoxy-N,N(or N,1)-</td> <td></td> </tr> <tr> <td>6</td> <td>67.44</td> <td>①</td> <td>PREDIRX</td> <td>62365</td> <td>5-METHOXYINDOLE-N-ETHYL-N-PROPYL-TRYPTAMINE</td> <td></td> </tr> <tr> <td></td> <td></td> <td></td> <td></td> <td></td> <td>5-METHOXYINDOLE-N-</td> <td></td> </tr> </tbody> </table> <p>Hit List: 5-Methoxy-...mine KBr wafer</p> <p>Substructs Sel. Substructs Original Data Files All Properties Attachments Preferred Properties</p> <table border="1"> <thead> <tr> <th>Name</th> <th>Value</th> </tr> </thead> <tbody> <tr> <td>Name</td> <td>5MT-NB3I TMS P1631</td> </tr> <tr> <td>Exact Mass</td> <td>478.093735 u</td> </tr> <tr> <td>Formula</td> <td>C₂₁H₂₇N₂O₂</td> </tr> <tr> <td>InChI</td> <td>InChI=1S/C21H27N2O2/c1-25-19-8-9-21-20(13-19)17(14-23-21)10-11-24(26(2,3)4)15-16-6-5-7-18(22-16/h5-9,12-14,23H,10-11,15H2,1-4H3</td> </tr> <tr> <td>InChI Key</td> <td>JIFYOVBIQULMS-UHFFFAOYSA-N</td> </tr> <tr> <td>Molecular Weight</td> <td>478.449 g/mol</td> </tr> <tr> <td>Nominal Mass</td> <td>478 u</td> </tr> </tbody> </table> <p>The similarity in the backbone across the top 10 hits indicates that KnowItAll matched a class of compound.</p>	Table	Plot	Related Compounds View	HQI	Tag	Corrections DB	ID	Name	Spectrum	<auto> (IR/ATR-IR)	1	70.97	①	PREDIRX	36387	5MT-NB3I TMS P1631		2	69.96	①	PREDIRX	67580	5-Methoxy-3-(2-morpholinylethyl)indole		3	68.87	①	PREDIRX	4072	5-Methoxy-N,N-dipropyltryptamine		4	68.22	①	PREDIRX	42758	5-METHOXYINDOLE-N,N-DIETHYL-TRYPTAMINE		5	67.52	①	PREDIRX	134398	1H-Indole-3-ethanamine, 5-methoxy-N,N(or N,1)-		6	67.44	①	PREDIRX	62365	5-METHOXYINDOLE-N-ETHYL-N-PROPYL-TRYPTAMINE							5-METHOXYINDOLE-N-		Name	Value	Name	5MT-NB3I TMS P1631	Exact Mass	478.093735 u	Formula	C ₂₁ H ₂₇ N ₂ O ₂	InChI	InChI=1S/C21H27N2O2/c1-25-19-8-9-21-20(13-19)17(14-23-21)10-11-24(26(2,3)4)15-16-6-5-7-18(22-16/h5-9,12-14,23H,10-11,15H2,1-4H3	InChI Key	JIFYOVBIQULMS-UHFFFAOYSA-N	Molecular Weight	478.449 g/mol	Nominal Mass	478 u
Table	Plot	Related Compounds View																																																																											
HQI	Tag	Corrections DB	ID	Name	Spectrum	<auto> (IR/ATR-IR)																																																																							
1	70.97	①	PREDIRX	36387	5MT-NB3I TMS P1631																																																																								
2	69.96	①	PREDIRX	67580	5-Methoxy-3-(2-morpholinylethyl)indole																																																																								
3	68.87	①	PREDIRX	4072	5-Methoxy-N,N-dipropyltryptamine																																																																								
4	68.22	①	PREDIRX	42758	5-METHOXYINDOLE-N,N-DIETHYL-TRYPTAMINE																																																																								
5	67.52	①	PREDIRX	134398	1H-Indole-3-ethanamine, 5-methoxy-N,N(or N,1)-																																																																								
6	67.44	①	PREDIRX	62365	5-METHOXYINDOLE-N-ETHYL-N-PROPYL-TRYPTAMINE																																																																								
					5-METHOXYINDOLE-N-																																																																								
Name	Value																																																																												
Name	5MT-NB3I TMS P1631																																																																												
Exact Mass	478.093735 u																																																																												
Formula	C ₂₁ H ₂₇ N ₂ O ₂																																																																												
InChI	InChI=1S/C21H27N2O2/c1-25-19-8-9-21-20(13-19)17(14-23-21)10-11-24(26(2,3)4)15-16-6-5-7-18(22-16/h5-9,12-14,23H,10-11,15H2,1-4H3																																																																												
InChI Key	JIFYOVBIQULMS-UHFFFAOYSA-N																																																																												
Molecular Weight	478.449 g/mol																																																																												
Nominal Mass	478 u																																																																												

Example 2 - 5MEODIPT.SPC, First Derivative Algorithm

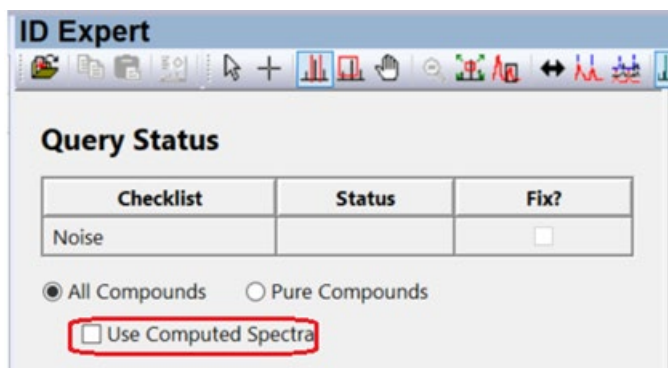
	Action	Result
1	<p>(This is a continuation of Example 1.)</p> <p>Go back to the SearchIt application.</p> <p>Reopen the file by clicking Open Spectrum or Structure > 5MEODIPT.SPA > Open > Start a new search.</p> <p>Switch Search Method to 1st Derivative Euclidean Distance.</p> <p>Click Search.</p>	

	Action	Result																																											
2	Locate the hit list to view predicted results.	 <p>The screenshot displays the MinelT interface. At the top, the title bar reads "MinelT" and "Lookup Compound: PubChem". Below this is a plot of IR spectra for "5-Methoxy-N,N-Diisopropyltryptamine KBr wafer (Corr...)". The x-axis is labeled "cm⁻¹" and ranges from 4000 to 400. The y-axis represents intensity. Several peaks are labeled with their wavenumbers: 3404.53, 3272.83, 2928.66, 1685.12, 1485.06, 1453.16, 1381.16, 1297.21, 1287.21, 1217.20, 1169.20, 1065.20, 1013.25, 926.54, 821.34, 801.29, 749.34, 629.33, and 497.38.</p> <p>Below the plot is a table of related compounds:</p> <table border="1"> <thead> <tr> <th>HQI</th> <th>Tag</th> <th>Co</th> <th>DB</th> <th>ID</th> <th>Name</th> <th>Spectrum</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>56.29</td> <td>PREDIRX</td> <td>59113</td> <td>5-MeO-NBpBrT</td> <td></td> </tr> <tr> <td>2</td> <td>54.59</td> <td>PREDIRX</td> <td>40590</td> <td>5-Methoxy-alpha,N-dimethyltryptamine</td> <td></td> </tr> <tr> <td>3</td> <td>53.95</td> <td>PREDIRX</td> <td>39786</td> <td>Indole, 5-methoxy-3-(2-(1-pyrrolidinyl)ethyl)-</td> <td></td> </tr> <tr> <td>4</td> <td>53.62</td> <td>PREDIRX</td> <td>33759</td> <td>Indole, 5-methoxy-3-(2-methylamino)ethyl-</td> <td></td> </tr> <tr> <td>5</td> <td>53.32</td> <td>PREDIRX</td> <td>88895</td> <td>Ethanone, 1-(5-methoxy-2-methyl-3-indolyl)-2-(4-</td> <td></td> </tr> <tr> <td>6</td> <td>53.24</td> <td>PREDIRX</td> <td>204413</td> <td>5-Methoxy-alpha-methyltryptamine TMS</td> <td></td> </tr> </tbody> </table> <p>At the bottom of the table, there are two tabs: "Hit List: 5-Methoxy-...mine KBr wafer" and "Hit List: 5-Methoxy-...e KBr wafer (2)".</p> <p>On the right side of the interface, the "Structure/Properties" panel shows the chemical structure of 5-MeO-NBpBrT and its properties:</p> <ul style="list-style-type: none"> Name: 5-MeO-NBpBrT Exact Mass: 358.068076 u Formula: C₁₄H₁₈BrN₂O InChI: InChI=1S/C18H19BrN2O/c1-22-16-6-7-18-17(10-16)14(12-21-18)8-9-20-11-13-2-4-15(19)5-3-13/h2-7,10,12,20-21H,8-9,11H2,1H3 InChI Key: XHLOUFPZLUULGI-UHFFFAOYSA-N Molecular Weight: 359.267 g/mol Nominal Mass: 358 u Prediction: 1 	HQI	Tag	Co	DB	ID	Name	Spectrum	1	56.29	PREDIRX	59113	5-MeO-NBpBrT		2	54.59	PREDIRX	40590	5-Methoxy-alpha,N-dimethyltryptamine		3	53.95	PREDIRX	39786	Indole, 5-methoxy-3-(2-(1-pyrrolidinyl)ethyl)-		4	53.62	PREDIRX	33759	Indole, 5-methoxy-3-(2-methylamino)ethyl-		5	53.32	PREDIRX	88895	Ethanone, 1-(5-methoxy-2-methyl-3-indolyl)-2-(4-		6	53.24	PREDIRX	204413	5-Methoxy-alpha-methyltryptamine TMS	
HQI	Tag	Co	DB	ID	Name	Spectrum																																							
1	56.29	PREDIRX	59113	5-MeO-NBpBrT																																									
2	54.59	PREDIRX	40590	5-Methoxy-alpha,N-dimethyltryptamine																																									
3	53.95	PREDIRX	39786	Indole, 5-methoxy-3-(2-(1-pyrrolidinyl)ethyl)-																																									
4	53.62	PREDIRX	33759	Indole, 5-methoxy-3-(2-methylamino)ethyl-																																									
5	53.32	PREDIRX	88895	Ethanone, 1-(5-methoxy-2-methyl-3-indolyl)-2-(4-																																									
6	53.24	PREDIRX	204413	5-Methoxy-alpha-methyltryptamine TMS																																									

The similarity in the backbone across the top 10 hits indicates that KnowItAll matched a class of compound.

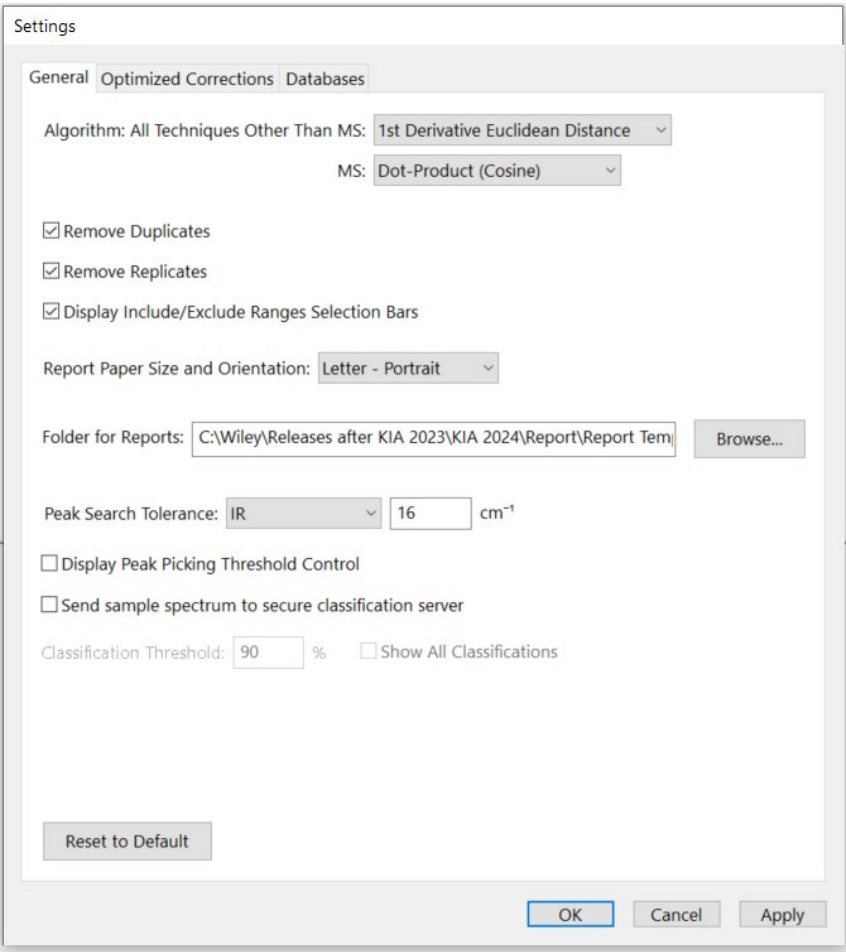
ID Expert






















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



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

	Action	Result
1	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.	The application opens and a Windows Open dialog box displays.

	Action	Result
2	<p>Close the Open dialog box, then choose File > Settings.</p> <p>Set Algorithm: All Techniques Other Than MS: 1st Derivative Euclidean Distance</p> <p>OK</p>	<p>The Settings form opens.</p> 

	Action	Result												
3	<p>New Search</p> <p>Open 4-(Pyridin-3-yl)-2-2,6,2-terpyridine.irf in the Predicted IR Example Spectra folder</p> <p>(Note that 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>Open</p>													
4	<p>Set Query Status Technique to ATR-IR.</p> <p>Check Use Computed Spectra</p>	<p>Query Status</p> <table border="1" data-bbox="604 906 1293 1089"><thead><tr><th>Checklist</th><th>Status</th><th>Fix?</th></tr></thead><tbody><tr><td>Noise</td><td> </td><td><input type="checkbox"/></td></tr><tr><td>Contaminants</td><td> </td><td></td></tr><tr><td>Technique</td><td> </td><td>ATR-IR </td></tr></tbody></table> <p><input checked="" type="radio"/> All Compounds <input type="radio"/> Pure Compounds</p> <p><input checked="" type="checkbox"/> Use Computed Spectra</p>	Checklist	Status	Fix?	Noise	 	<input type="checkbox"/>	Contaminants	 		Technique	 	ATR-IR 
Checklist	Status	Fix?												
Noise	 	<input type="checkbox"/>												
Contaminants	 													
Technique	 	ATR-IR 												

	Action	Result																																
5	View search results in the Component Table.	<div data-bbox="579 321 1871 1015"> <p>ID Expert</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>●</td> <td>i</td> </tr> <tr> <td>Contaminants</td> <td>●</td> <td>i</td> </tr> <tr> <td>Technique</td> <td>●</td> <td>i 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> <p>Optimized Corrections</p> <p>Baseline of Query, Baseline of Reference, Intensity Distortion, Vertical Clipping, Horizontal Offset i</p> <p>New Search</p> <p>Search Status</p> <p>1-Component Results: Top Hit: 61.7%</p> <p>2-Component Results: <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 61.7%, gray 61.7%);"></div></p> <p>Peak Results: Top Hit: 68.8%</p> <p>Functional Groups: 20 Functional Groups Found</p> <p>Create Report</p> <div style="border: 1px solid gray; padding: 5px;"> <p style="text-align: center;">EXCLUDE RANGE BAR</p> <p style="text-align: center;">INCLUDE RANGE BAR</p> </div> <table border="1"> <thead> <tr> <th colspan="2">1-Component Results</th> <th>Peak Results</th> <th>Functional Groups</th> </tr> <tr> <th>Score</th> <th>Info</th> <th>Name</th> <th>Spectrum</th> </tr> </thead> <tbody> <tr> <td>61.66</td> <td>i</td> <td>4'-(p-BROMOPHENYL)-2,2':6,2''-TERPYRIDINE</td> <td></td> </tr> <tr style="background-color: #e6f2ff;"> <td>60.93</td> <td>i</td> <td>4',4''-DIBROMO-(2,2':6,2'';6',2''')QUATERPYRIDINE</td> <td></td> </tr> <tr> <td>57.79</td> <td>i</td> <td>4'-(p-CHLOROPHENYL)-2,2':6,2''-TERPYRIDINE</td> <td></td> </tr> </tbody> </table> </div> <p>This search included experimental spectra and predicted ones. As we can see, both arrives to similar chemical class.</p>	Checklist	Status	Fix?	Noise	●	i	Contaminants	●	i	Technique	●	i ATR-IR	1-Component Results		Peak Results	Functional Groups	Score	Info	Name	Spectrum	61.66	i	4'-(p-BROMOPHENYL)-2,2':6,2''-TERPYRIDINE		60.93	i	4',4''-DIBROMO-(2,2':6,2'';6',2''')QUATERPYRIDINE		57.79	i	4'-(p-CHLOROPHENYL)-2,2':6,2''-TERPYRIDINE	
Checklist	Status	Fix?																																
Noise	●	i																																
Contaminants	●	i																																
Technique	●	i ATR-IR																																
1-Component Results		Peak Results	Functional Groups																															
Score	Info	Name	Spectrum																															
61.66	i	4'-(p-BROMOPHENYL)-2,2':6,2''-TERPYRIDINE																																
60.93	i	4',4''-DIBROMO-(2,2':6,2'';6',2''')QUATERPYRIDINE																																
57.79	i	4'-(p-CHLOROPHENYL)-2,2':6,2''-TERPYRIDINE																																