

KnowItAll Software Training

Functional Group Analysis

Functional Group Analysis

How to Use the Knowledgebases to Identify or Differentiate Classes of Compounds by Structure or Functional Group

Purpose

This exercise demonstrates how to use the Analyzelt IR, Analyzelt Raman and Analyzelt Polymer IR Knowledgebases to identify or differentiate chemical compounds, and to correlate peaks by structure.

Objectives

This exercise will teach you:

- How to specify the Knowledgebase
- How to browse by functional group
- How to correlate a structure

Background

The IR and Raman Knowledgebases include group frequencies with over 600 band assignments, corresponding to over 200 functional groups, subdivided into general chemical classes.

Training Files Used in This Lesson

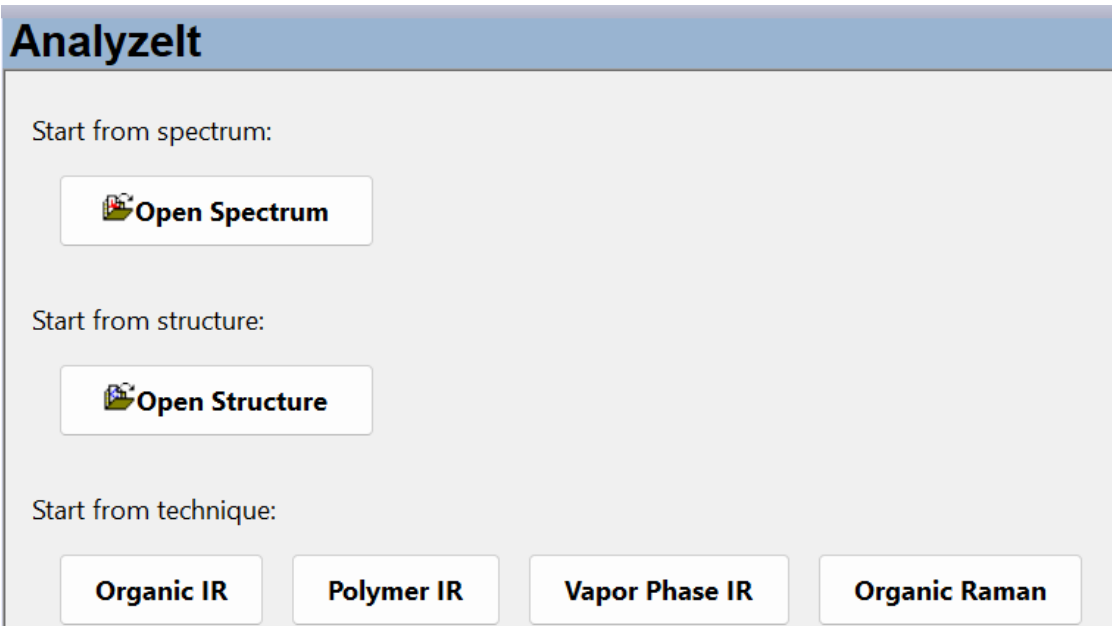
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Analyzelt IR

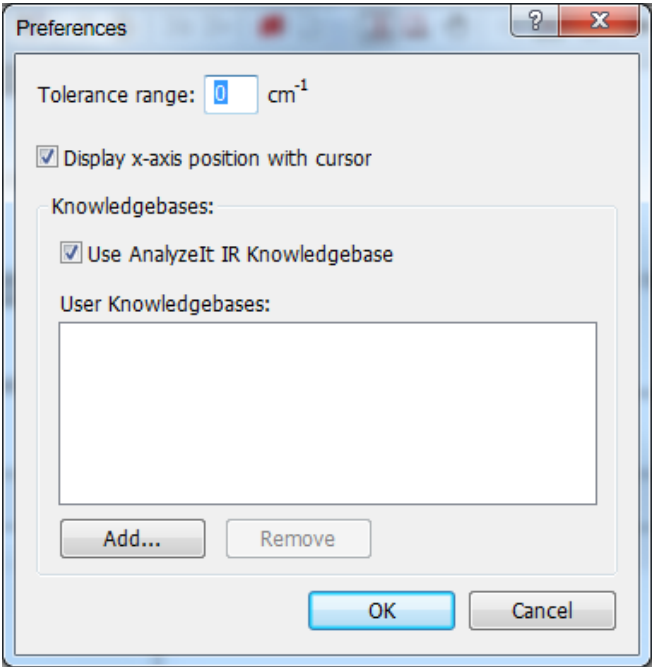
- Analyzelt IR Demo Structure.DSF

KnowItAll Applications Used

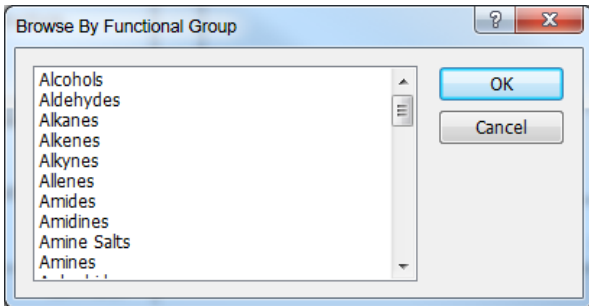
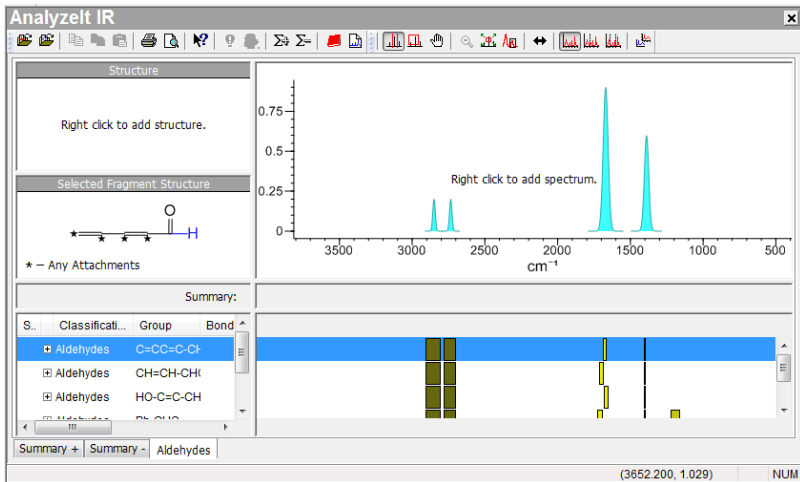
- Analyzelt

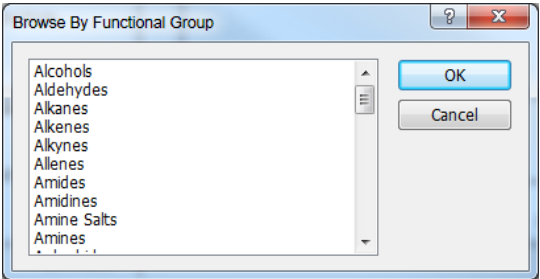
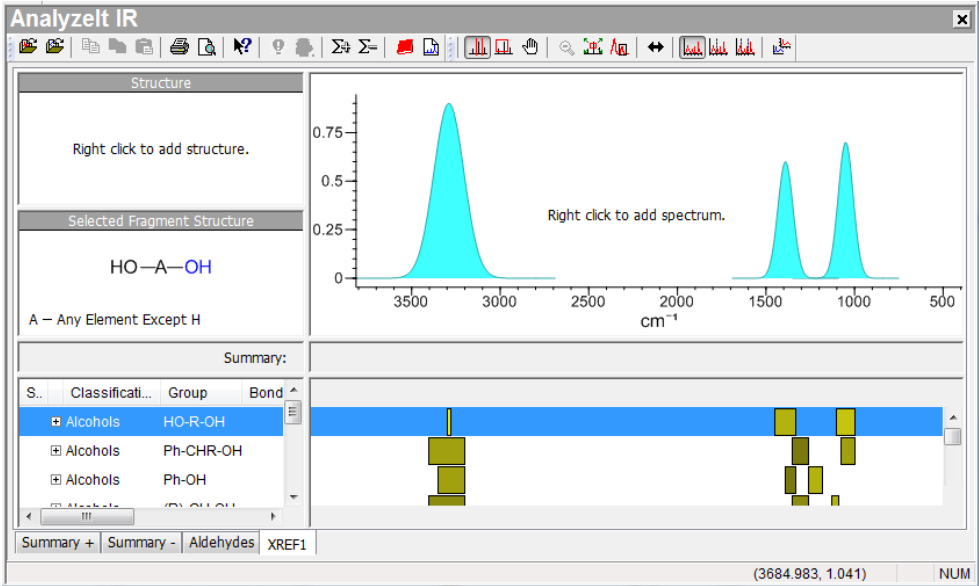
Specify the Knowledgebase

	Action	Result
1	<p>Navigate to the Spectral Analysis toolbox.</p> <p>Click Analyzelt.</p>	 <ul style="list-style-type: none"> • Open Spectrum - starts with any spectrum file. Upon selecting an IR spectrum, KnowItAll asks if it should be put into Organic IR or Polymer IR application. • Open Structure - starts with any structure file. Upon selecting a structure file, KnowItAll asks if it should be put into Organic IR or Organic Raman application. • By the same token, <ul style="list-style-type: none"> ○ IR Organic - starts a blank Analyzelt IR application. ○ Polymer IR - starts a blank Analyzelt Polymer IR application. ○ Vapor Phase IR - starts a blank Analyzelt Vapor Phase IR application ○ Raman Organic - starts a blank Analyzelt Raman application.

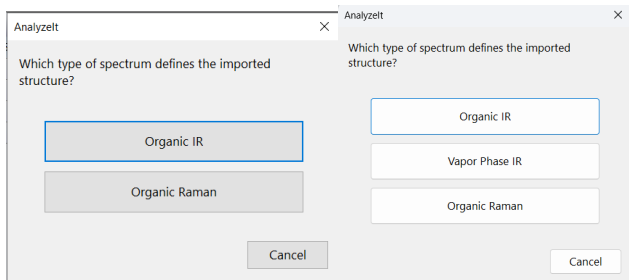
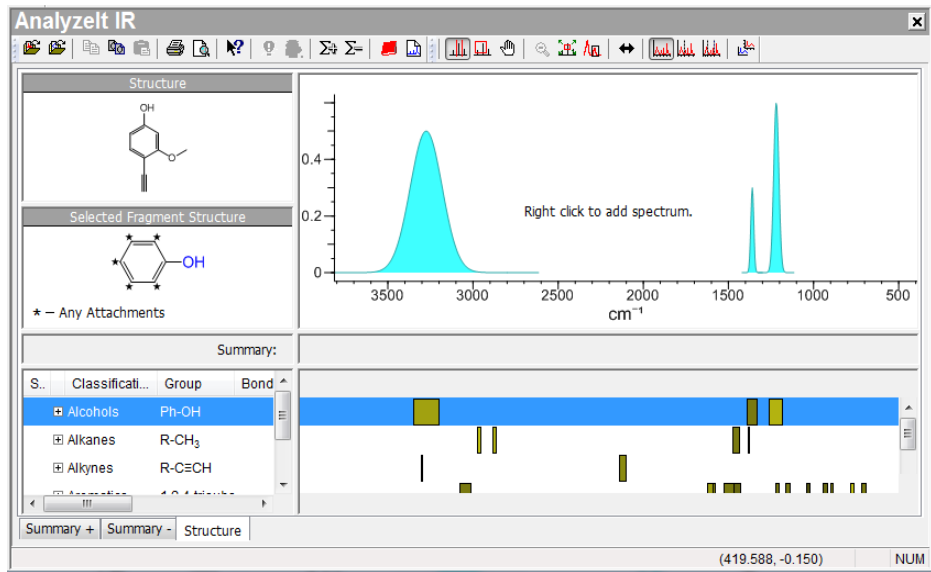
	Action	Result
2	Let's start from technique Organic IR <ul style="list-style-type: none">Click Organic IR.Choose File > Preferences.	<p>The Preferences dialog box opens.</p>  <p>Setting the Tolerance range allows you to determine how precise the matches are between your spectrum peak and the database. You can also choose to display a wavenumber (x-axis position) marker with the cursor as it moves around the Spectrum pane. Finally, use the check boxes to select the Knowledgebase you wish to use.</p>
3	Make sure Use AnalyzeIt IR Knowledgebase is selected. Click OK .	

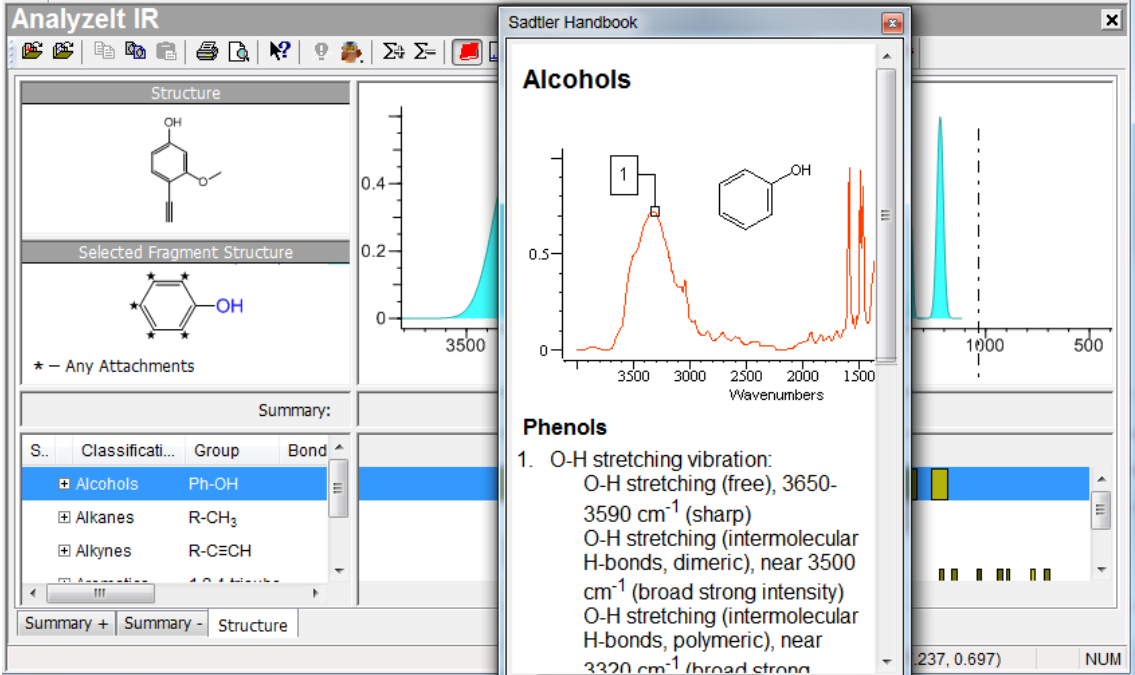
Browse by functional group

	Action	Result
1	Choose Analyze > Browse a Functional Group .	<p>The Browse By Functional Group dialog box opens.</p> 
2	Select Aldehydes and click OK .	<p>The Aldehydes tab is added to the AnalyzeIt IR display.</p>  <p>Each functional group in the aldehydes group is listed separately in the Functional Group Data pane at the lower left, and each entry includes classification, group, bond, range, intensity, mode and notes.</p> <p>Colored bars in the Bar Chart pane at the lower right represent the peaks associated with each functional group class selected in the Functional Group Data pane. The bars are intensity coded; a lighter color means greater intensity. Corresponding peaks appear in the Spectrum pane.</p>

	Action	Result
3	Choose Analyze > Browse a Functional Group again.	<p>The Browse By Functional Group dialog box opens.</p> 
4	<p>Select both Alcohols and Anhydrides, then click OK.</p> <p>Note: Select the first class, then hold down the Ctrl key and click to select a second class.</p>	<p>The XREF1 tab is added to the AnalyzeIt IR display.</p>  <p>The tab is labeled XREF1 because it is the first tab containing a combination of classes.</p>
5	Choose File > Close to clear the previous example display.	

Correlate peaks from a structure

	Action	Result
1	<p>Click Open Structure button.</p> <p>Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Analyzelt IR folder</p> <p>Open Analyzelt IR Demo Structure.DSF</p>	<p>A dialog box prompts you to choose between IR or Raman.</p> 
2	Click Organic IR .	<p>After the Knowledgebase is analyzed, the results are displayed in a Structure tab. The Functional Group Data pane includes an entry for each group found in the structure.</p> 

	Action	Result
3	Choose View > Sadtler Handbook to display the handbook information related to a particular functional group.	<p>The Sadtler Handbook pane displays information from the Sadtler Handbook of Reference Spectra - IR for the specific functional group selected in the Functional Group Data Pane.</p>  <p>Double-clicking the Sadtler Handbook pane's title bar allows you to dock and un-dock the pane with reference to the main display.</p>

Functional Group Analysis

How to Perform a Basic Spectral Analysis Using Software-Assisted Functional Group Analysis

Purpose

This exercise demonstrates how to use the Analyzelt application to perform a basic spectral analysis.

Objectives

This exercise will teach you:

- How to select peaks for correlation
- How to use the Summary+ and Summary- tabs

Background

The Analyzelt application can be used to help interpret spectra through the use of its Knowledgebases of over 200 functional groups. They can be used to obtain functional group information from a spectrum or a structure, or by browsing the chemical classes included in the Knowledgebases.

Training Files Used in This Lesson

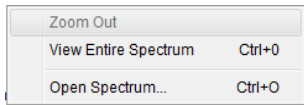
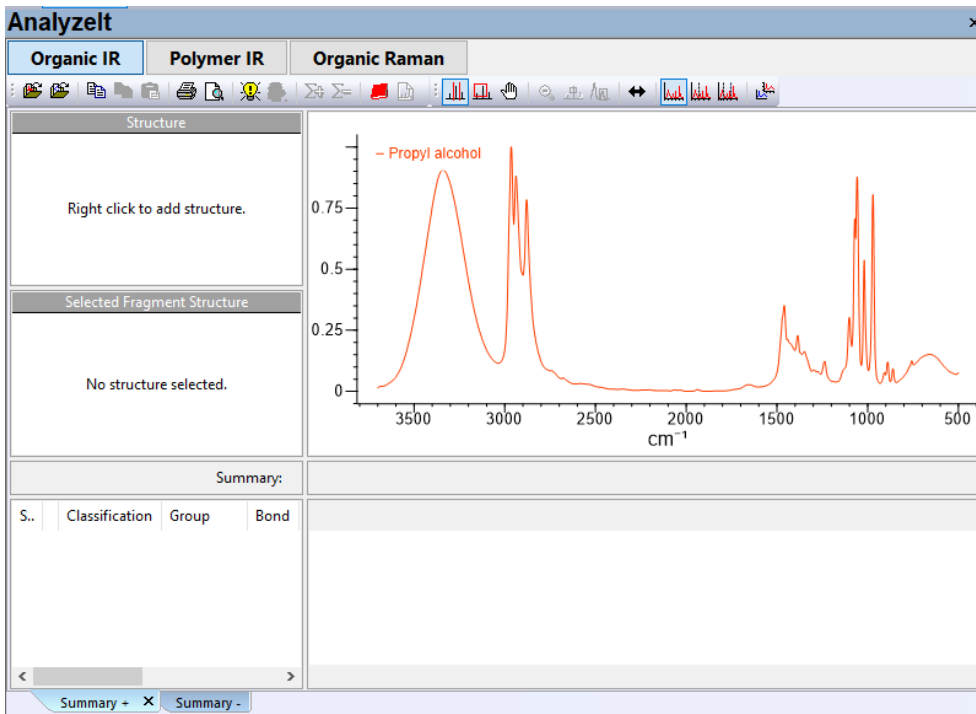
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\AnalyzeIt IR

- Peak Interpretation Example.dx (IR)


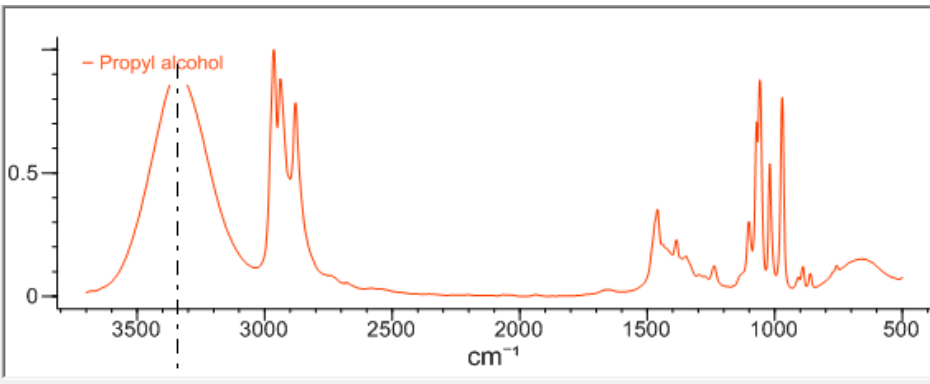
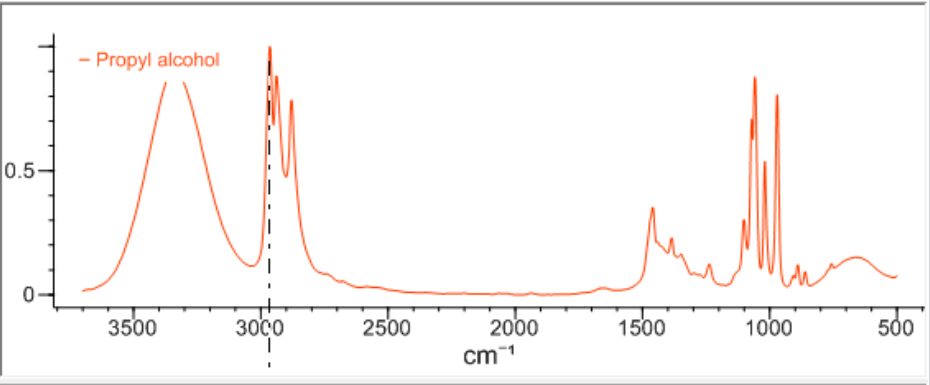
KnowItAll Applications Used


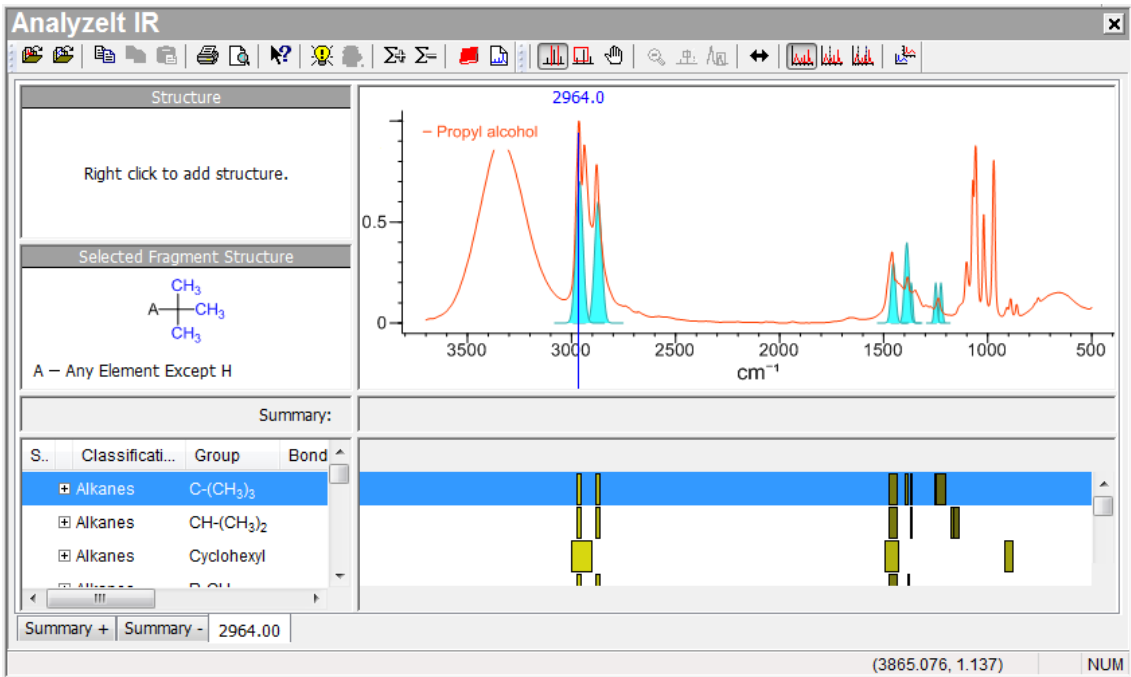
- Analyzelt

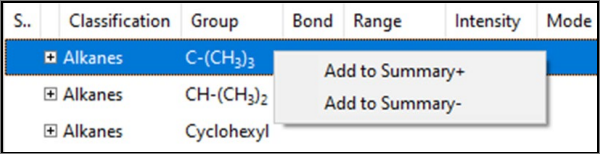
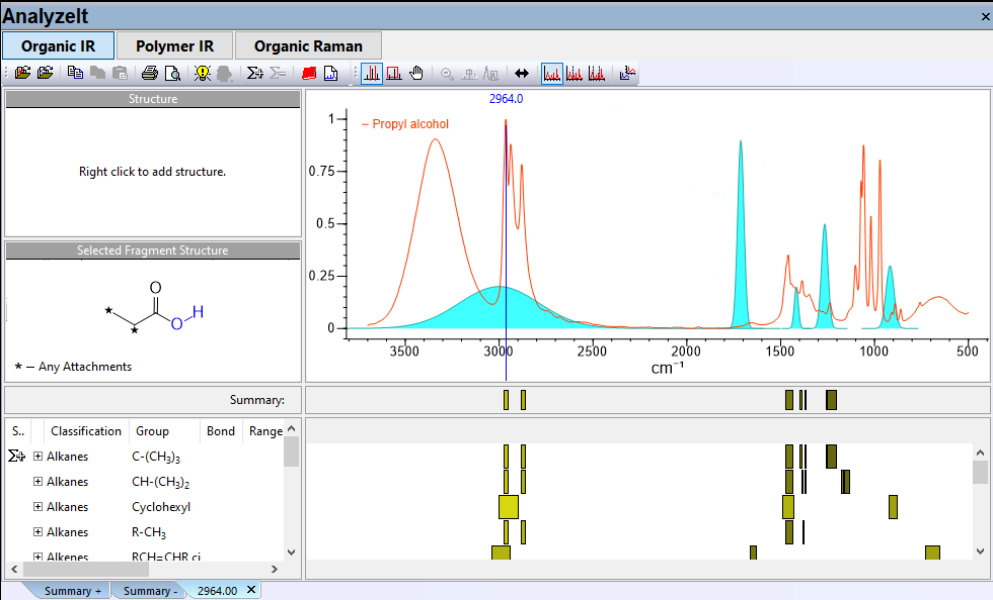
Open a spectrum

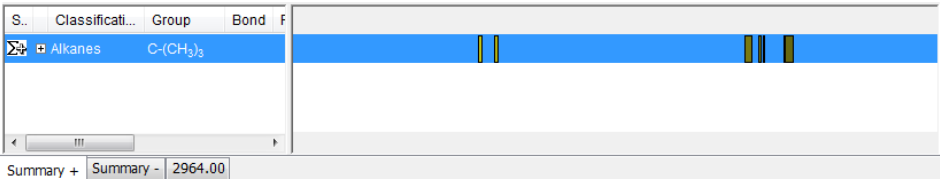
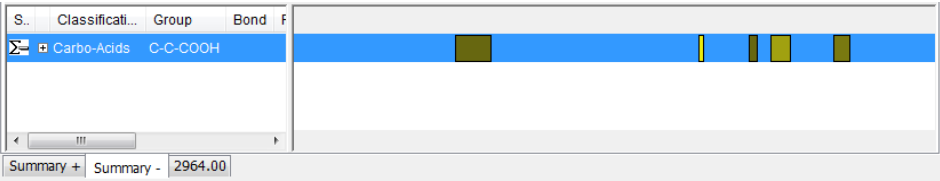
	Action	Result
1	Navigate to the Spectral Analysis toolbox, and click AnalyzeIt followed by Organic IR .	
2	Right-click in the Spectral Pane .	A pop-up menu opens. 
3	Click Open Spectrum . Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\IR folder. Open Propyl alcohol . Click OK .	The spectrum is displayed. 

Analyze the spectrum

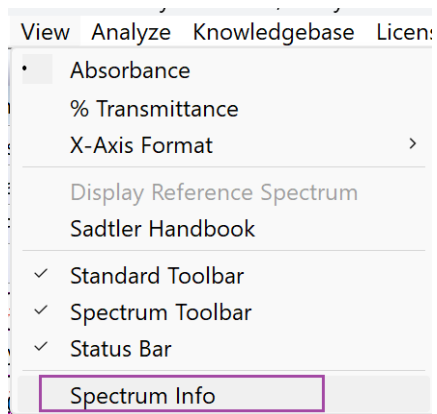
	Action	Result
1	Click the Suggest toolbar button  .	<p>The application selects a peak to analyze.</p>  <p>In general, it is best to begin a correlation with a peak above 1500 wavenumbers that is unique and strong. The AnalyzeIt application uses a set of rules to select a good starting point.</p>
2	Click the Suggest toolbar button again. Note: You can also select peaks by clicking in the spectral pane.	<p>Another peak is suggested.</p>  <p>As you click the Suggest a Peak toolbar button repeatedly, the application cycles through the suggested starting points.</p>

	Action	Result																
3	<p>Click Suggest until the second peak (at 2964) is selected and then click the Correlate button .</p>	<p>After the Knowledgebase is analyzed, the results are displayed in a tab labeled with the wavenumber.</p>  <p>The screenshot displays the Analyzelt IR software interface. The main window shows an IR spectrum with a red trace and a cyan trace. A peak at 2964.0 cm⁻¹ is highlighted. The left panel shows the chemical structure of isobutane (A) and a list of classification results. The bottom panel shows a summary of the results.</p> <p>Structure: Right click to add structure.</p> <p>Selected Fragment Structure:</p> <p>A — Any Element Except H</p> <p>Summary:</p> <table><tr><th>S..</th><th>Classificati...</th><th>Group</th><th>Bond</th></tr><tr><td>+</td><td>Alkanes</td><td>C-(CH₃)₃</td><td></td></tr><tr><td>+</td><td>Alkanes</td><td>CH-(CH₃)₂</td><td></td></tr><tr><td>+</td><td>Alkanes</td><td>Cyclohexyl</td><td></td></tr></table> <p>Summary + Summary - 2964.00</p> <p>(3865.076, 1.137) NUM</p>	S..	Classificati...	Group	Bond	+	Alkanes	C-(CH ₃) ₃		+	Alkanes	CH-(CH ₃) ₂		+	Alkanes	Cyclohexyl	
S..	Classificati...	Group	Bond															
+	Alkanes	C-(CH ₃) ₃																
+	Alkanes	CH-(CH ₃) ₂																
+	Alkanes	Cyclohexyl																

	Action	Result
4	<p>Select the alkanes entry C-(CH₃)₃ in the Functional Group Data pane.</p> <p>Right-click to open the Summary pop-up menu.</p> <p>Note: The Summary+ and Summary- tabs are created automatically and are provided to allow you to keep track of functional groups that are consistent with or inconsistent with the measured spectrum.</p>	
5	<p>Because the methyl group correlates well with the spectrum, click Add to Summary+.</p>	<p>The peaks are added to the Summary+ tab and the Summary Bar Chart pane (between the spectral display and the Bar Chart pane), and a summary plus symbol appears in the Functional Group Data pane next to this group.</p> 

6	Click the Summary+ tab to display any groups added to this tab.	
7	Click the Summary- tab to display any groups added to this tab.	
8	Choose File > Close .	The display is cleared.

Note: One can view query metadata by **View > Spectrum Info** in **AnalyzeIt** applications.



Functional Group Analysis

How to Perform a Basic Spectral Analysis Using Analyzelt for Polymer

Purpose

This exercise demonstrates how to use the Analyzelt application to perform a basic spectral analysis of polymer.

Objectives

This exercise will teach you:

- How to analyze spectra from polymer samples

Background

The Analyzelt Polymer IR Knowledgebase can provide clear and rapid verification and identification of functional groups in the mid-infrared. It features over 100 functional groups and hundreds of interpretation frequencies.

Training Files Used in This Lesson

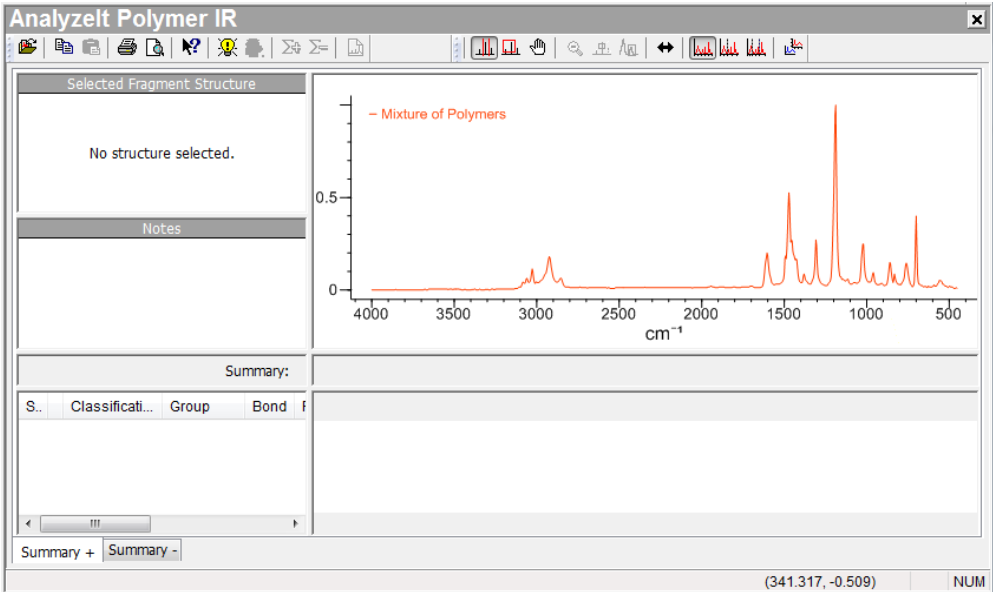
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\AnalyzeIt Polymer IR


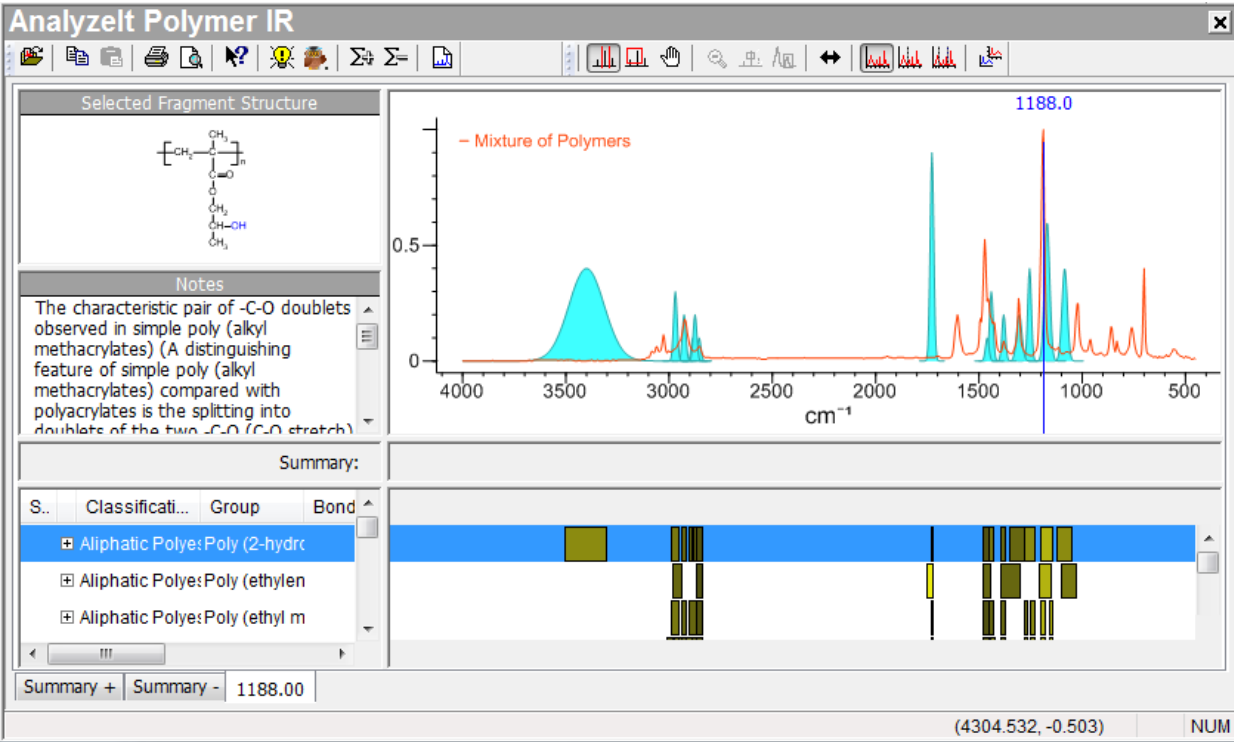
- Mixture of Polymers
- Polystyrene.irf

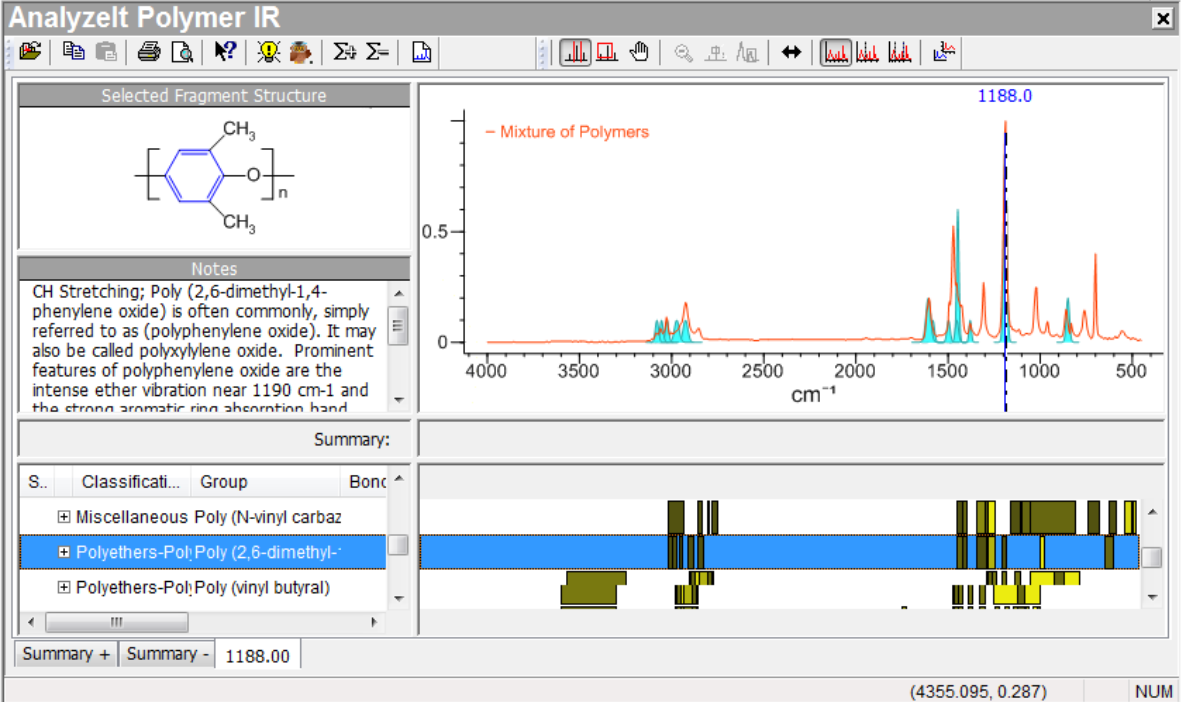
KnowItAll Applications Used


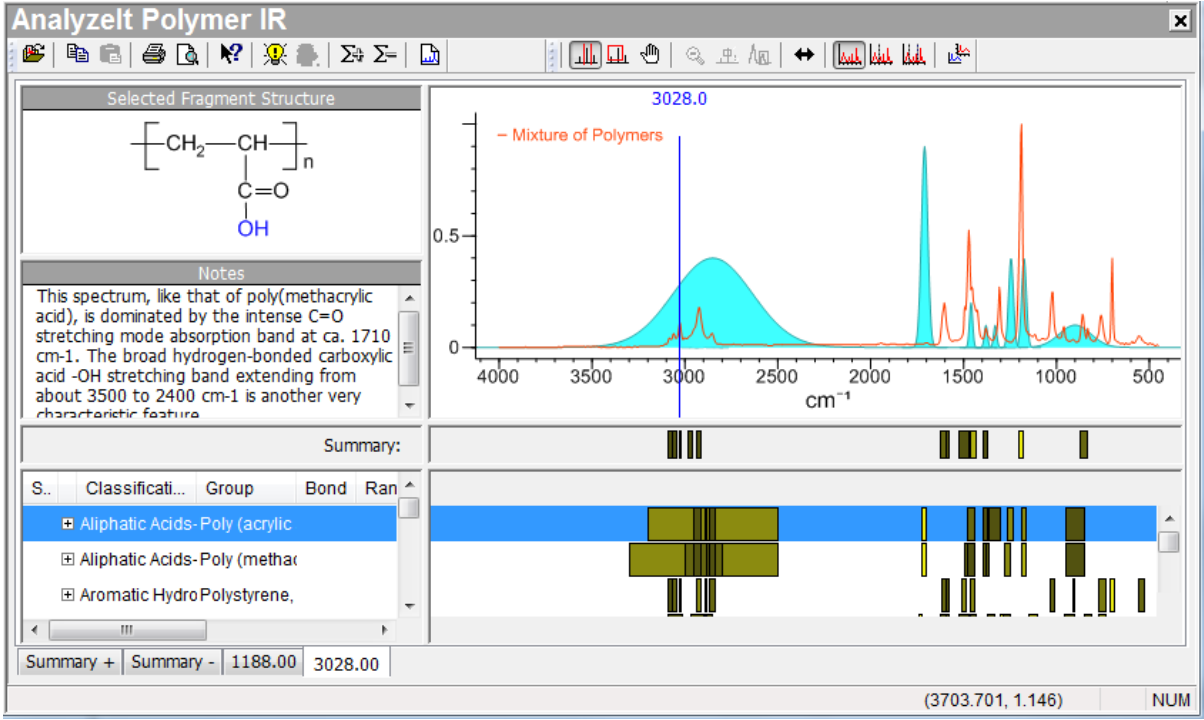
- Analyzelt

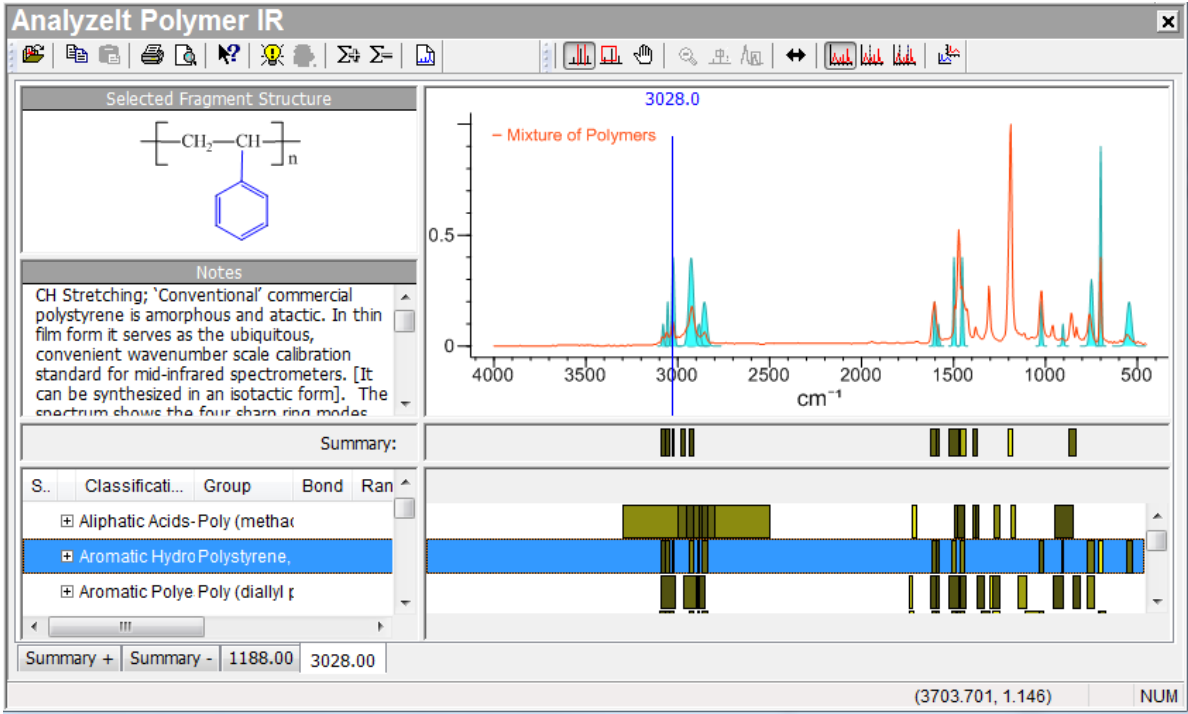
Open and analyze a mixture spectrum

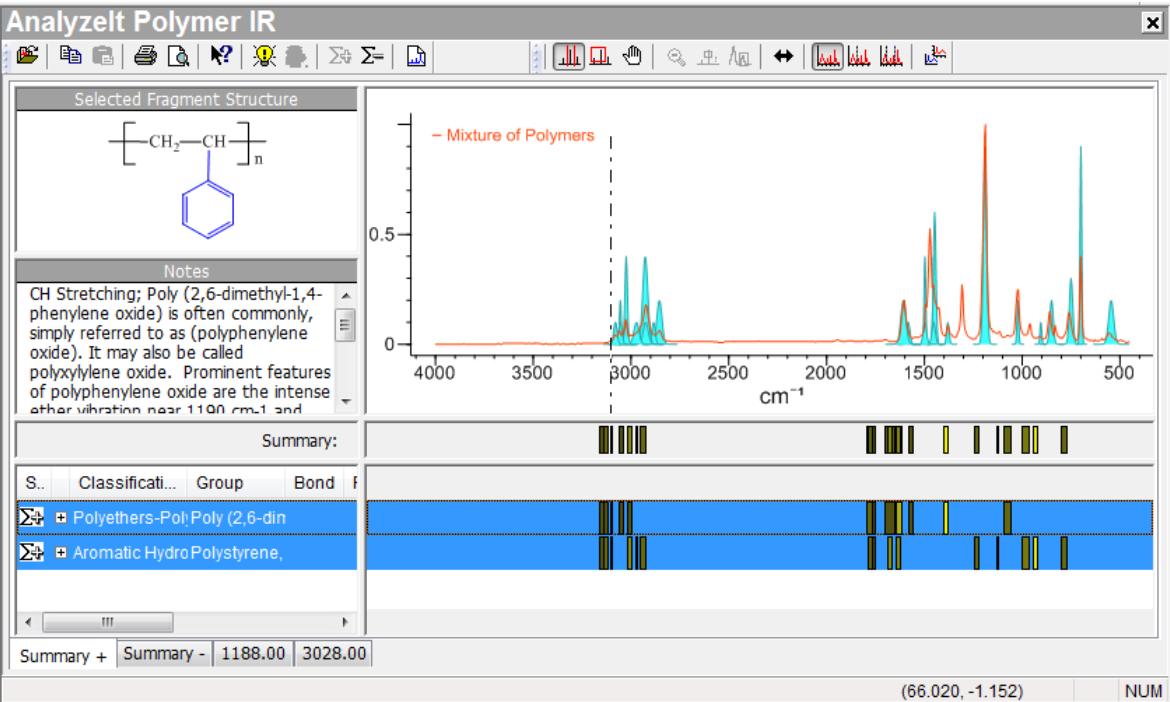
	Action	Result
1	Navigate to the Spectral Analysis toolbox and click AnalyzeIt followed by Open Spectrum .	
2	<p>Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\AnalyzeIt Polymer IR.</p> <p>Open Mixture of Polymers.irf.</p> <p>Click on the Polymer IR button in the pop-up dialog.</p> <p>Note: Use the Files of type filter to locate IRF, JCAMP and many other specific spectral files. You can also select All files (*.*).</p>	<p>The spectrum opens.</p> 

	Action	Result
3	<p>Use the Suggest button to select the tallest peak (at 1188), then click the Correlate button .</p> <p>Alternatively, you can double-click a peak to both select it and initiate searching the Knowledgebase(s) for functional group matches.</p>	<p>After the Knowledgebase is analyzed, the results are displayed in a tab labeled with the wavenumber (1188).</p> 

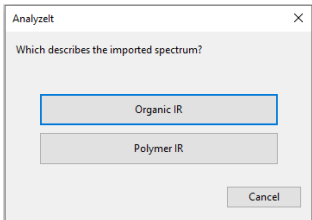
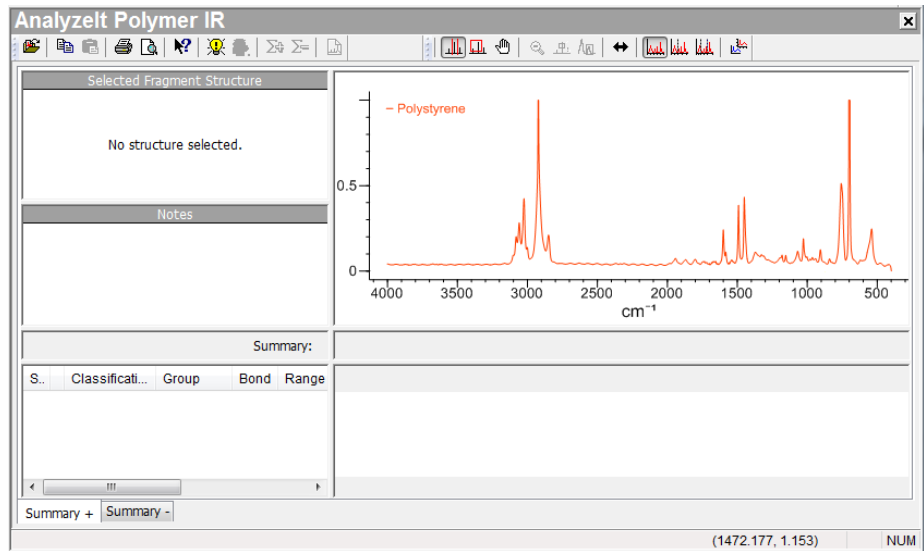
	Action	Result
4	<p>Select each entry in the Functional Group Data pane in turn.</p> <p>Note that the first Polyether-Polymer IR entry, Poly (2,6-dimethyl-1,4-phenylene oxide) is a good match.</p>	
5	<p>Right-click the entry, then select Add to Summary+.</p>	<p>The entry is added to the Summary+ tab.</p>

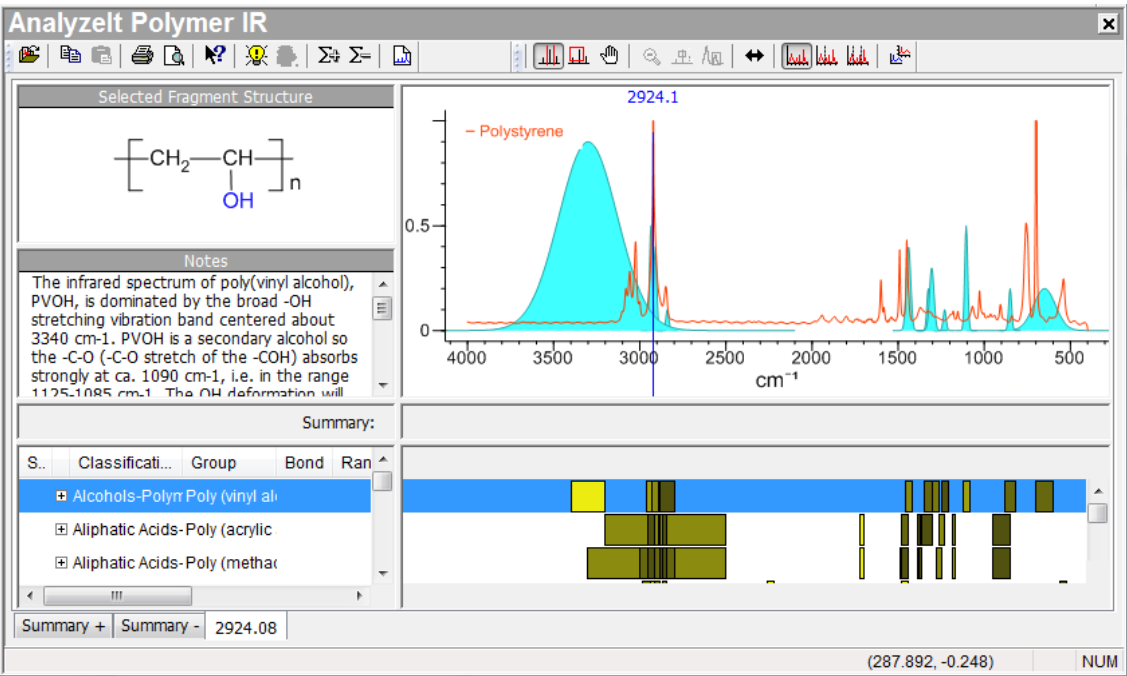
	Action	Result
6	Click the Suggest button to select the peak at 3028, then click the Correlate button  .	<p>After the Knowledgebase is analyzed, the results are displayed in a tab labeled with the wavenumber.</p>  <p>Note the detailed notes available with many Functional Group entries.</p>

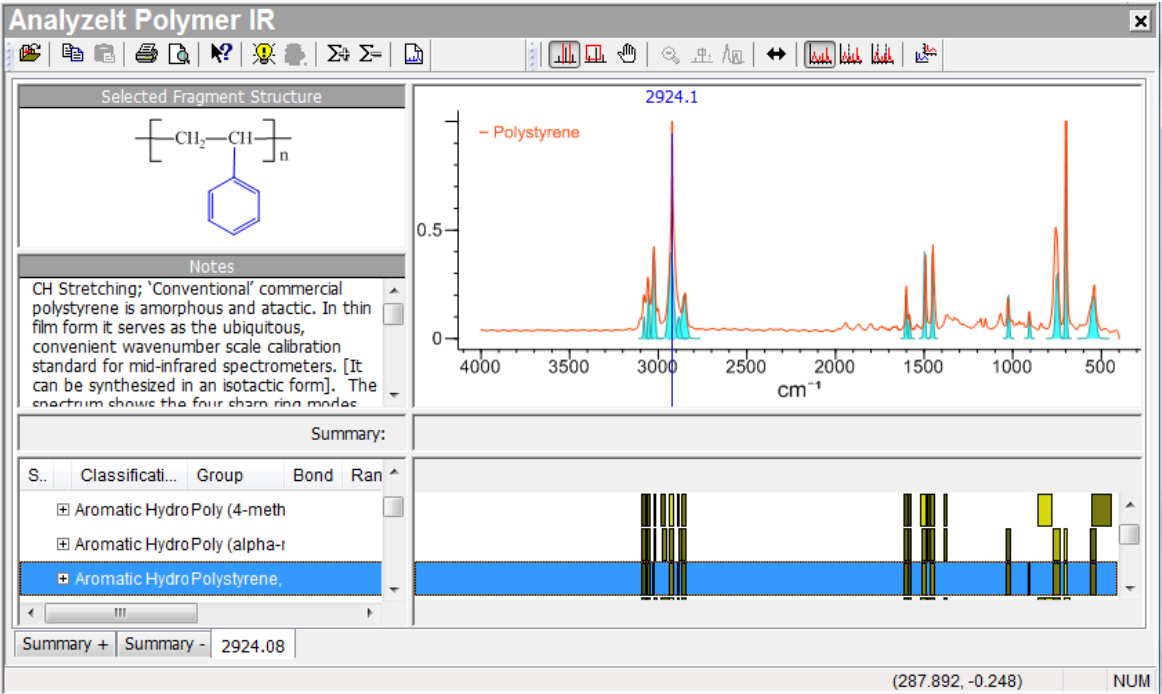
	Action	Result
7	<p>Select each entry in the Functional Group Data pane in turn.</p> <p>Note that the Aromatic Hydrocarbon (Polystyrene) entry is a good match.</p>	
8	<p>With the Aromatic Hydrocarbon (Polystyrene) entry selected, right-click, then select Add to Summary+.</p>	<p>The entry is added to the Summary+ tab.</p>

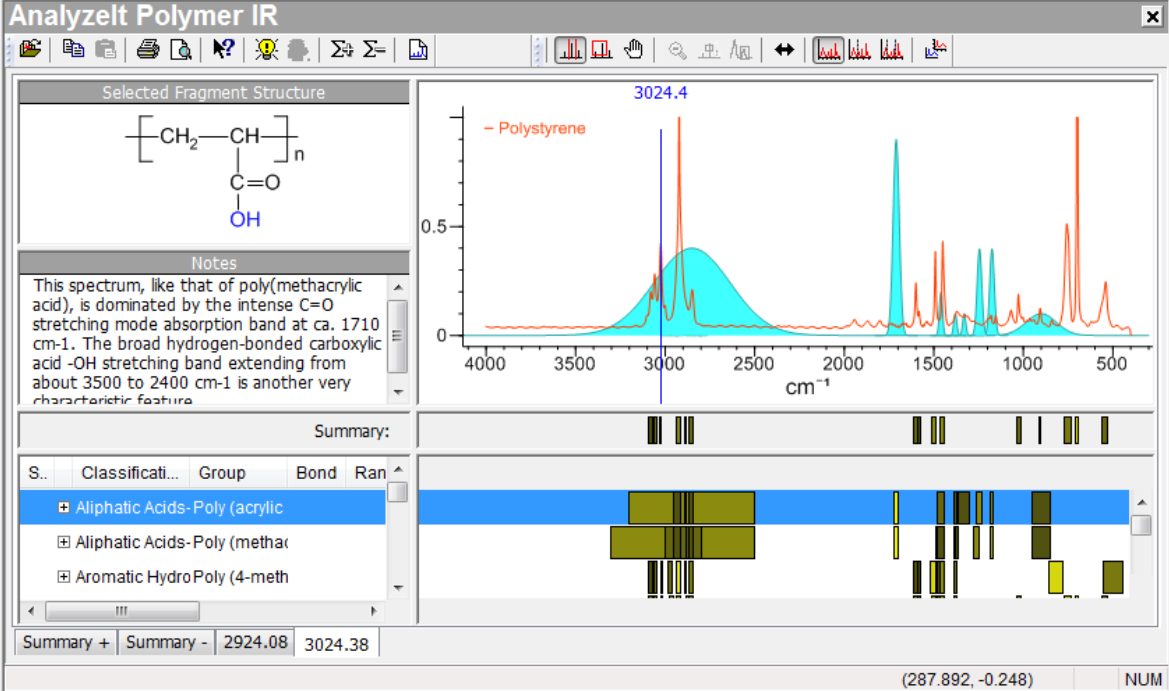
	Action	Result
9	<p>Open the Summary+ tab and select both entries.</p> <p>Note: Select the first entry, then hold down the Ctrl key and click to select the second entry.</p>	<p>We see that these functional groups account for most of the peaks in the mixture spectrum.</p> 
10	<p>Close the analysis by clicking the close button (x) in the upper right-hand corner.</p>	

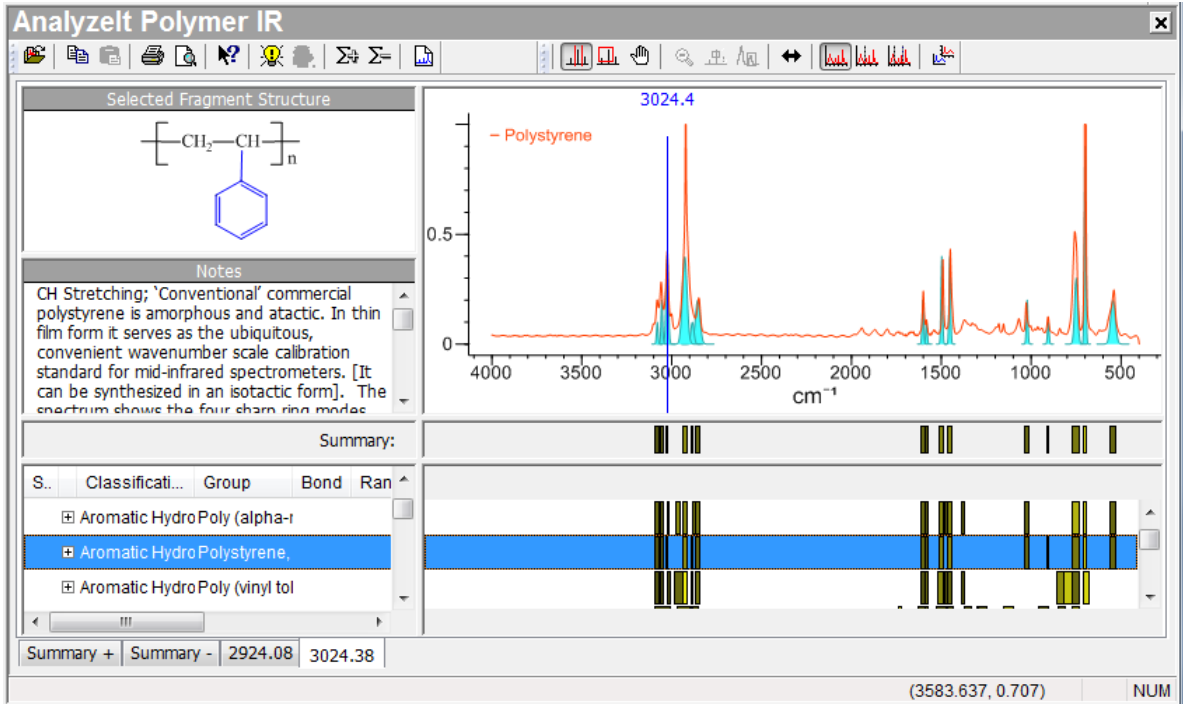
Open and analyze a single component spectrum

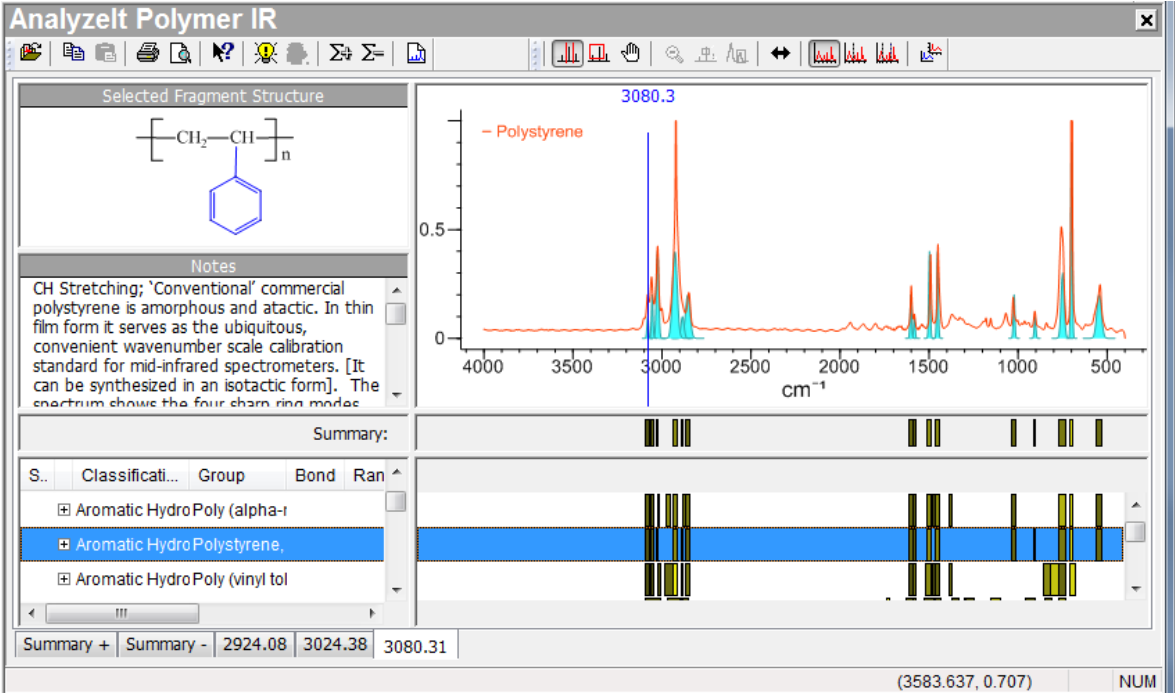
	Action	Result
1	<p>Choose File > Open Spectrum.</p> <p>Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\AnalyzeIt Polymer IR.</p> <p>Open Polystyrene.irf.</p> <p>Note: Use the Files of type filter to locate IRF, JCAMP, and many other specific spectral files. You can also select All files (*.*).</p>	<p>A pop-up dialog displays two options.</p> 
2	Click on Polymer IR .	<p>The spectrum opens.</p> 

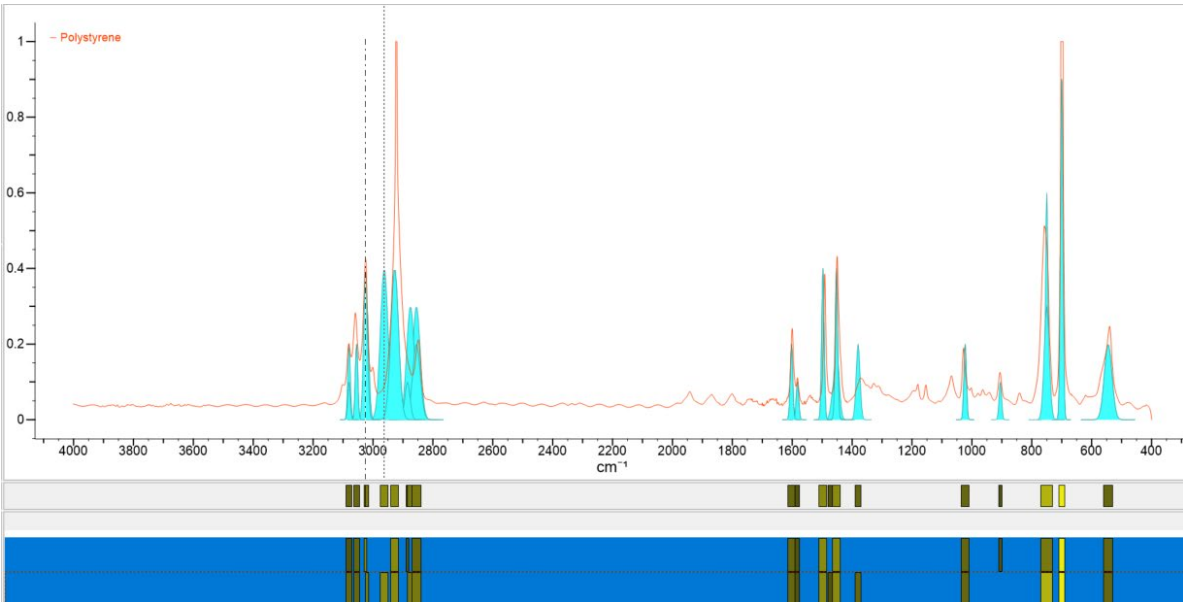
	Action	Result
3	Click the Suggest button to select the peak at 2924.1, then click the Correlate button.	<p>After the Knowledgebase is analyzed, the results are displayed in a tab labeled with the wavenumber (2924.08).</p> 

	Action	Result
4	Select each entry in the Functional Group Data pane in turn.	<p>Note that Aromatic Hydrocarbon (Polystyrene) is a good fit.</p> 
5	With the Aromatic Hydrocarbon (Polystyrene) entry selected, right-click, then select Add to Summary+ .	The functional group is added to the Summary+ tab.

	Action	Result
6	Click the Suggest a Peak toolbar button again, then click the Correlate toolbar button.	<p>After the Knowledgebase is analyzed, the results are displayed in a tab labeled with the wavenumber (3024.38).</p> 

	Action	Result
7	Select each entry in the Functional Group Data pane in turn.	<p>Note that the Aromatic Hydrocarbon (Polystyrene) is, once again, a good fit.</p> 

	Action	Result
8	<p>Repeat the process to analyze the third suggested peak (3080.3), then select each entry in the Functional Group Data pane in turn.</p>	<p>Aromatic Hydrocarbon (Polystyrene) is a good fit.</p> 

	Action	Result
9	<p>Go to the Summary + tab</p> <p>Control select both rows</p>	<p>One would see most of the spectrum peaks (red) are correlated to the functional group peaks (light blue). This means that we have a possible classification of polystyrene:</p> 

Functional Group Analysis

How to Create a User Knowledgebase

Purpose

This exercise demonstrates how to create and use user Knowledgebases in the Analyzelt applications.

Objectives

This exercise will teach you:

- How to create a user Knowledgebase
 - How to browse by functional group
 - How to correlate a structure
-

Background

Users can build their own Knowledgebases with functional groups and bands from their own data. The Knowledgebases can be used in conjunction with KnowItAll's Knowledgebases to determine the functional groups in a spectrum.

Training Files Used in This Lesson

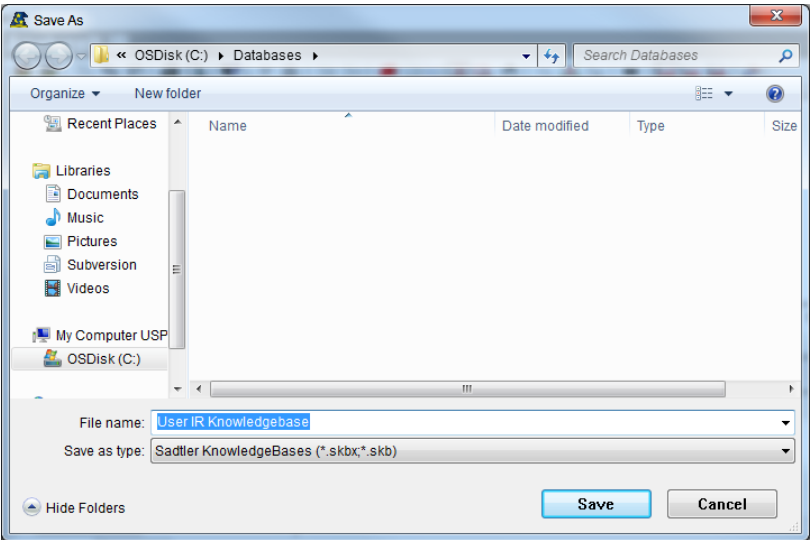
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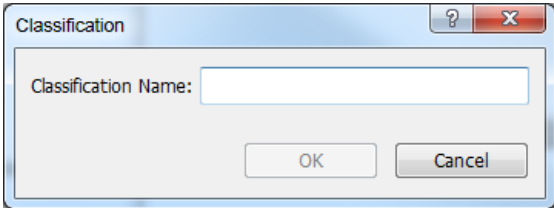
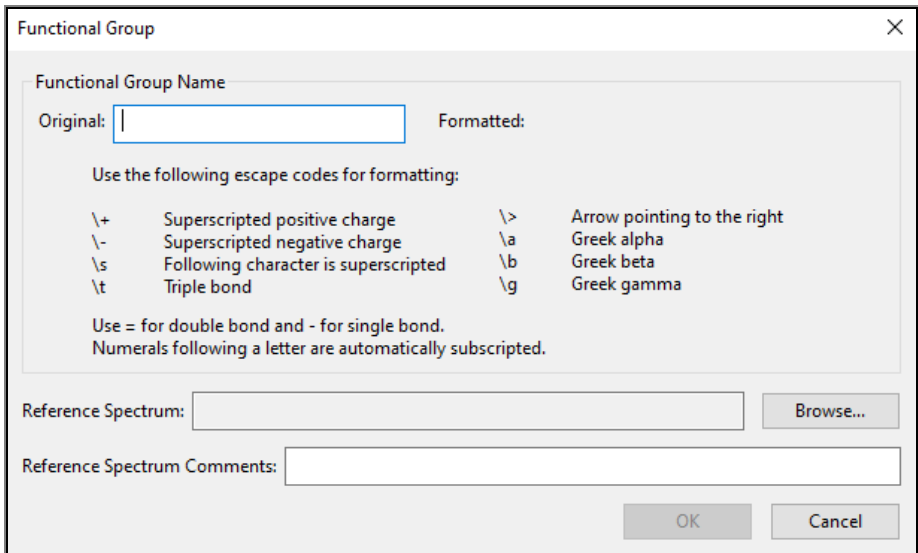
- Butylamine.jdx

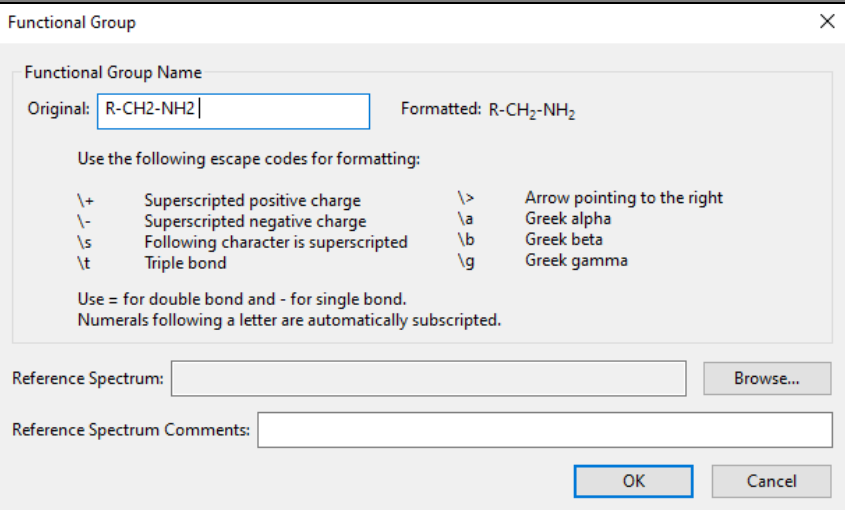
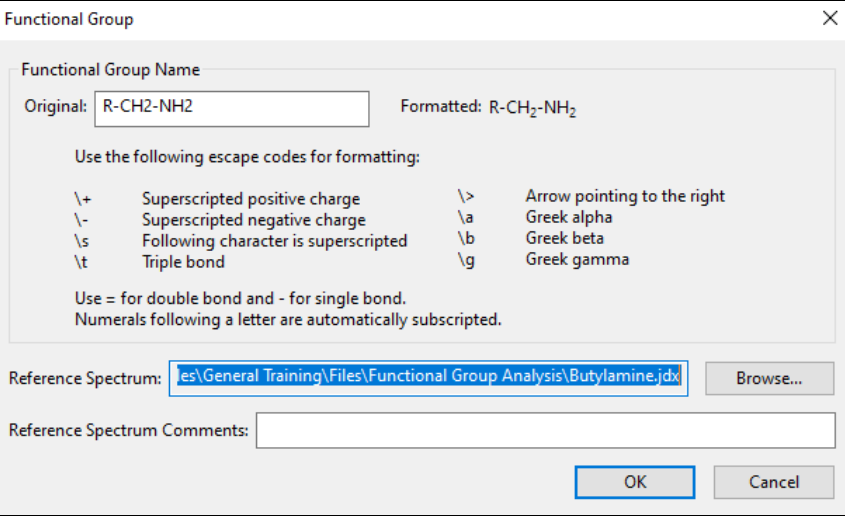
KnowItAll Applications Used

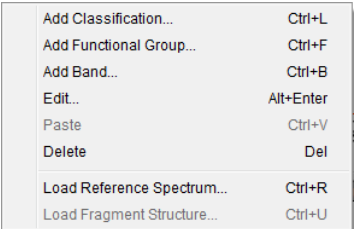
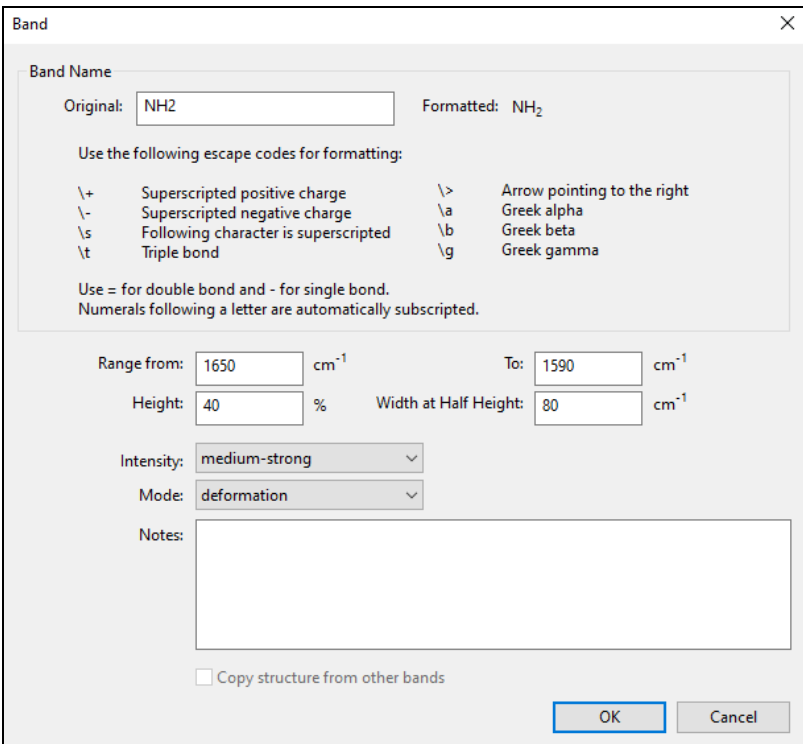
- Analyzelt

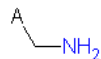
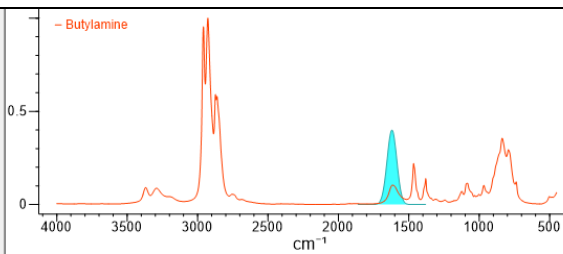



Create a user Knowledgebase

	Action	Result
1	Navigate to the Spectral Analysis toolbox and open the Analyzelt application by clicking its icon. Click the Organic IR button.	
2	Choose Knowledgebase > New .	A Save As dialog box opens.
3	Type in a name for the user Knowledgebase (such as User IR Knowledgebase) and save it to a location on your hard drive.	 <p>The file type Sadtler Knowledgebase– *.skbx or *.skb –cannot be changed.</p>

	Action	Result
4	Right-click in the Functional Group Tree pane (on the left), then select Add Classification .	<p>The Classification dialog box opens.</p>  <p>Type in AmineA and click OK.</p> <p>Note: Use a descriptive identifier to make sure the classification appears in the correct order when browsing for a functional group. Add a unique identifier to the end of the classification name to identify the Knowledgebase where the entry appears. Changes can be made easily if necessary.</p>
5	Right-click on the new classification name AmineA, then select Add Functional Group .	<p>The Functional Group dialog box opens.</p> 

	Action	Result
6	Type R-CH₂-NH₂ in the upper text box.	<p>The text is automatically formatted.</p> 
7	<p>Click Browse.</p> <p>Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\IR folder</p> <p>Select Butylamine.jdx.</p> <p>The path and file name are displayed in the Reference Spectrum text box.</p>	

	Action	Result
8	<p>Click OK to close the dialog box.</p> <p>Right-click on R-CH₂-NH₂ in the Functional Group Tree.</p>	<p>A pop-up menu opens.</p> 
9	<p>Click Add Band.</p> <p>Type in NH₂, then add other information as follows:</p> <ul style="list-style-type: none"> Range from 1650 to 1590 Height: 40 Width at Half Height: 80 Intensity: medium-strong Mode: deformation. <p>Click OK.</p>	<p>The Band dialog box opens.</p> 

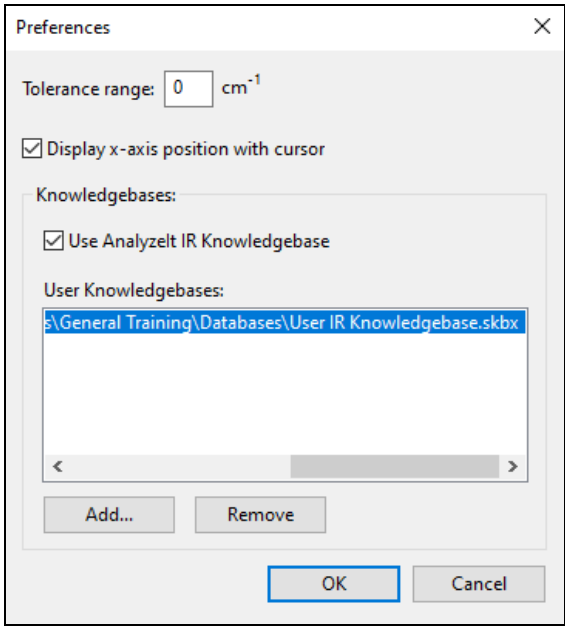
	Action	Result																				
10	Double-click in the Fragment Structure pane to open ChemWindow , then draw this structure: 																					
11	Click Save .	<p>The structure is added to the display.</p> <div><div><div><div>AmineA</div><div>R-CH₂-NH₂</div><div>NH₂ (1650-1590 cm⁻¹)</div></div></div><div><div><div>Butylamine</div></div><table><thead><tr><th>Fragment Structure</th><th>Field</th><th>Value</th></tr></thead><tbody><tr><td rowspan="8"></td><td>Bond</td><td>NH₂</td></tr><tr><td>Range From</td><td>1650 cm⁻¹</td></tr><tr><td>Range To</td><td>1590 cm⁻¹</td></tr><tr><td>Height</td><td>40 %</td></tr><tr><td>Width at Half Height</td><td>80 cm⁻¹</td></tr><tr><td>Intensity</td><td>medium-strong</td></tr><tr><td>Mode</td><td>deformation</td></tr><tr><td>Notes</td><td></td></tr></tbody></table></div></div>	Fragment Structure	Field	Value		Bond	NH ₂	Range From	1650 cm ⁻¹	Range To	1590 cm ⁻¹	Height	40 %	Width at Half Height	80 cm ⁻¹	Intensity	medium-strong	Mode	deformation	Notes	
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AmineA

R-CH₂-NH₂

- ...CN (1090-1068 cm⁻¹)
- ...NH₂ (1650-1590 cm⁻¹)
- ...NH (3400-3320 cm⁻¹)
- ...NH (3328-3250 cm⁻¹)
- ...NH (850-750 cm⁻¹)

Specify the user Knowledgebase

	Action	Result
1	Navigate to the Spectral Analysis toolbox and open the Analyzelt application by clicking its icon.	
2	Click Organic IR , Polymer IR or Organic Raman application.	
3	Choose File > Preferences .	The Preferences dialog box opens.
4	Click Add , then browse to and select the newly created user Knowledgebase.	<p>The user Knowledgebase is displayed in the Preferences dialog box.</p> 
5	Click OK to close the Preferences dialog box.	

	Action	Result
6	Choose Analyze > Browse a Functional Group .	<p>The contents of the user Knowledgebase have been added to the list of functional groups.</p> 