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 AnalyzeIt IR, AnalyzeIt Raman and AnalyzeIt 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\AnalyzeIt IR

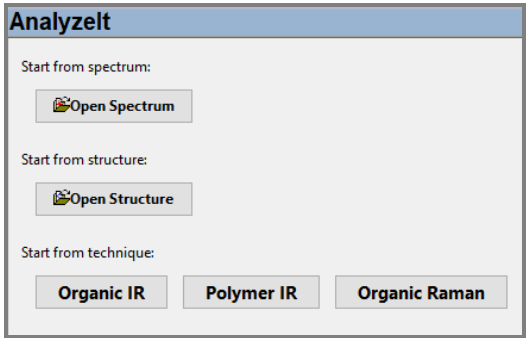
- AnalyzeIt IR Demo Structure.DSF

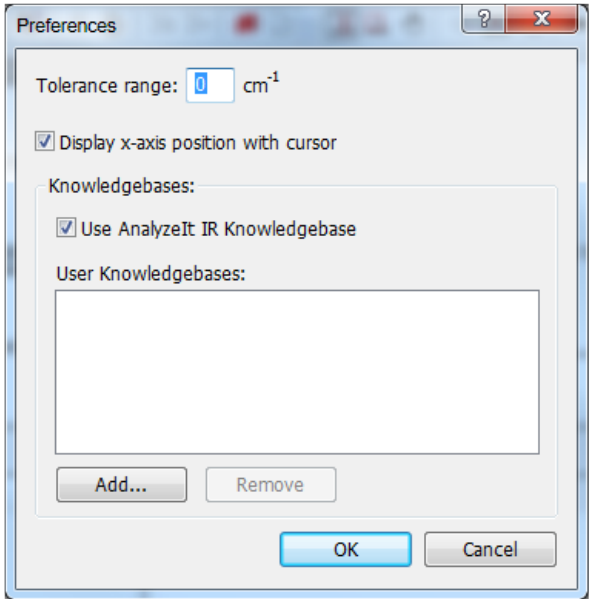
KnowItAll Applications Used

- AnalyzeIt

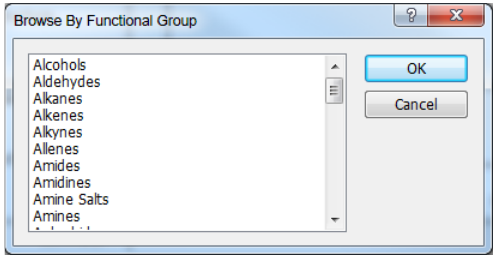
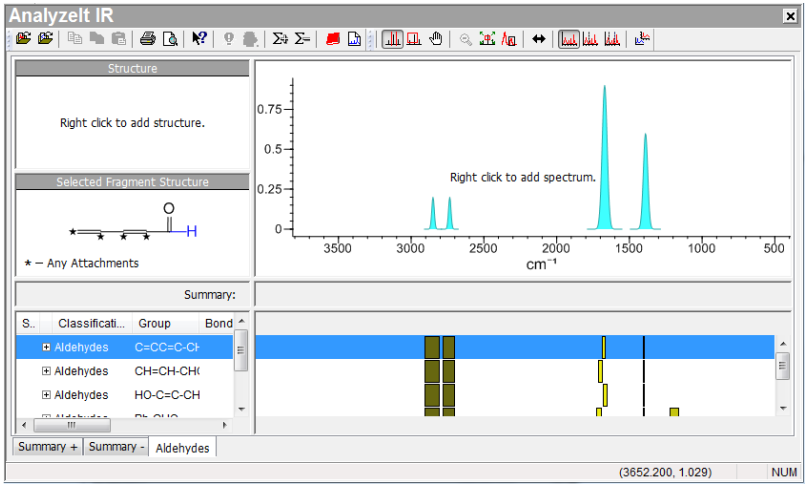
Specify the Knowledgebase

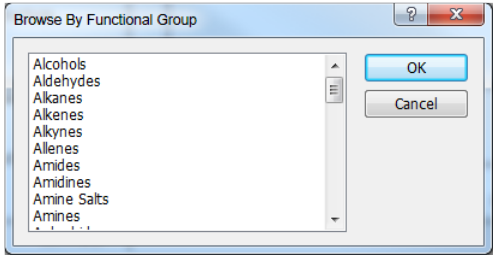
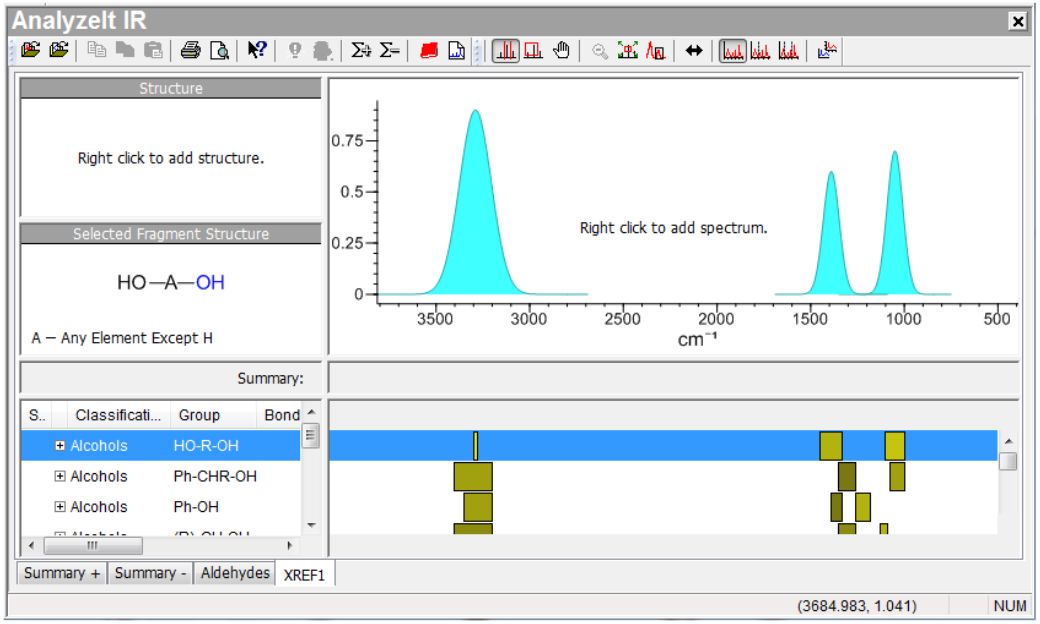
	Action	Result

1	Navigate to the **Spectral Analysis** toolbox.
	
	Click **AnalyzeIt**.
		
		• **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,
		  ○ **IR Organic** - starts a blank **AnalyzeIt IR** application.
		  ○ **Polymer IR** - starts a blank **AnalyzeIt Polymer IR** application.
		• **Raman Organic** - starts a blank **AnalyzeIt Raman** application.

2	Let's start from technique **Organic IR** • Click **Organic IR**. • Choose **File > Preferences**.	The **Preferences** dialog box opens.  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.
3	Make sure **Use AnalyzeIt IR Knowledgebase** is selected. Click **OK**.	

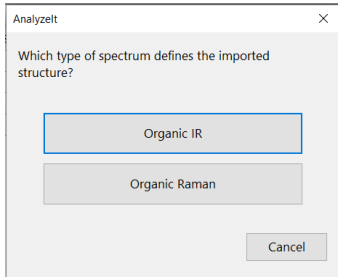
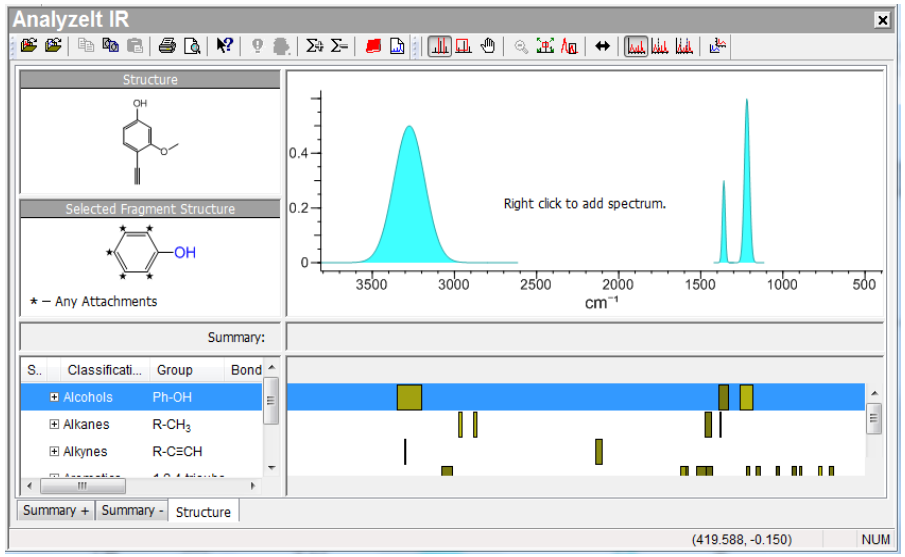
Browse by functional group

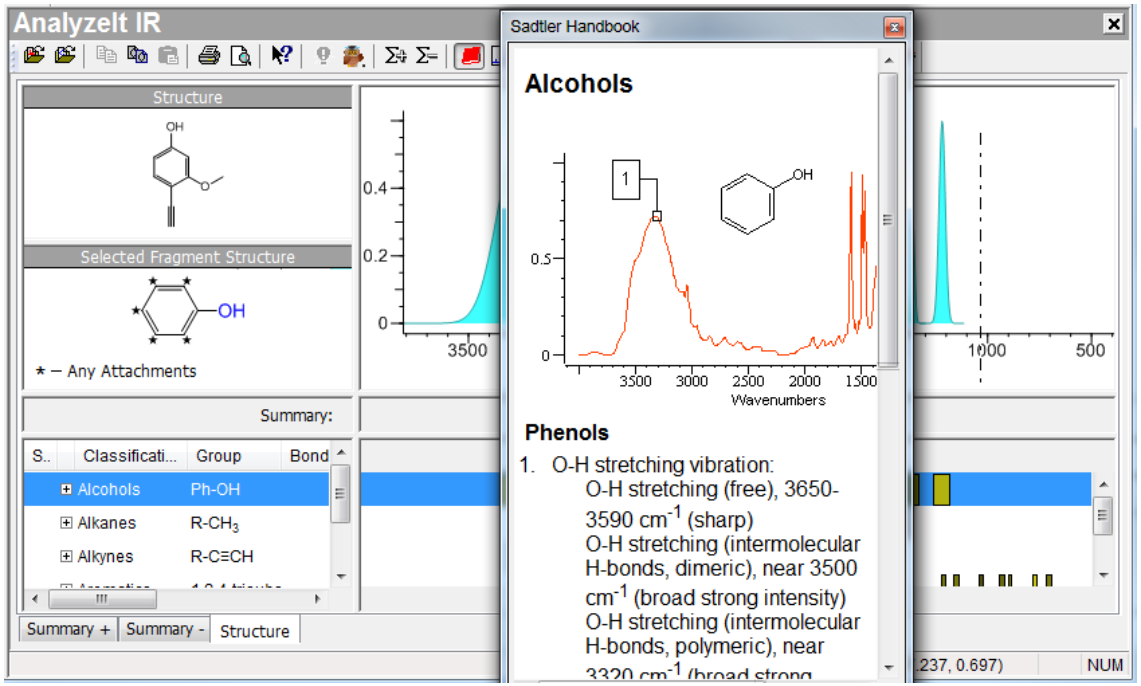
	Action	Result
1	Choose **Analyze > Browse a Functional Group**.	The **Browse By Functional Group** dialog box opens. 
2	Select **Aldehydes** and click **OK**.	The **Aldehydes** tab is added to the **AnalyzeIt IR** display.  Each functional group in the aldehydes group is listed separately in the **Functional Group Data** pane at the lower left, and each entry includes classification, group, bond, range, intensity, mode and notes. 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.

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

5	Choose **File > Close** to clear the previous example display.	

Correlate peaks from a structure

	Action	Result
1	Click **Open Structure** button. Navigate to **C:\Users\Public\Documents\Wiley\KnowItAll\Samples\AnalyzeIt IR** folder Open **AnalyzeIt IR Demo Structure.DSF**	A dialog box prompts you to choose between IR or Raman. 
2	Click **Organic IR**.	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. 

	Action	Result
3	Choose **View > Sadtler Handbook** to display the handbook information related to a particular functional group.	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**.  Double-clicking the **Sadtler Handbook** pane's title bar allows you to dock and un-dock the pane with reference to the main display.

Functional Group Analysis

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

Purpose

This exercise demonstrates how to use the AnalyzeIt 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 AnalyzeIt 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

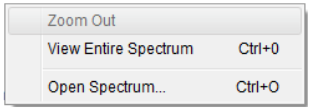
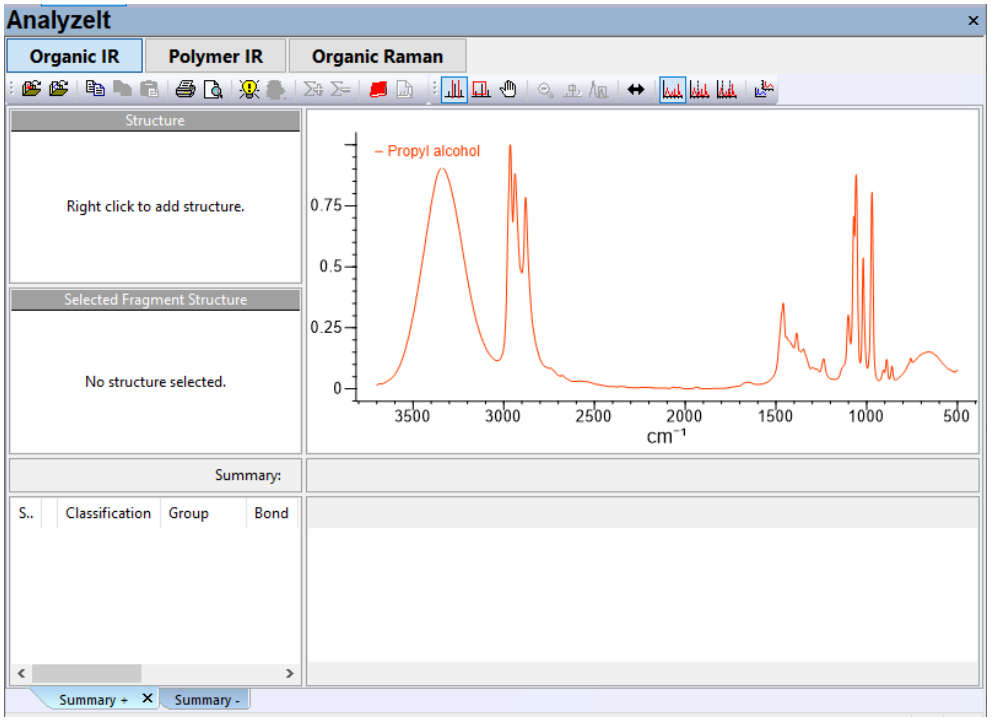
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\AnalyzeIt IR

- Peak Interpretation Example.dx (IR)

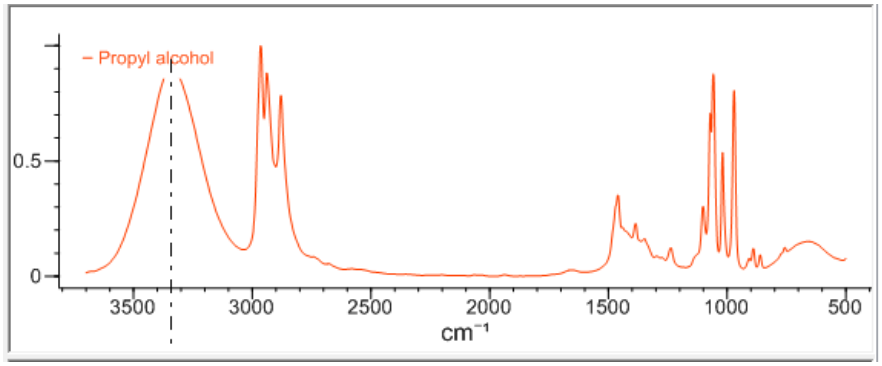
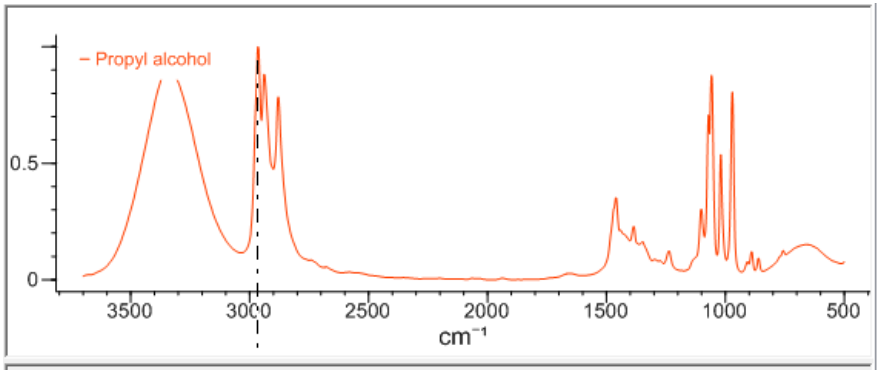
KnowItAll Applications Used

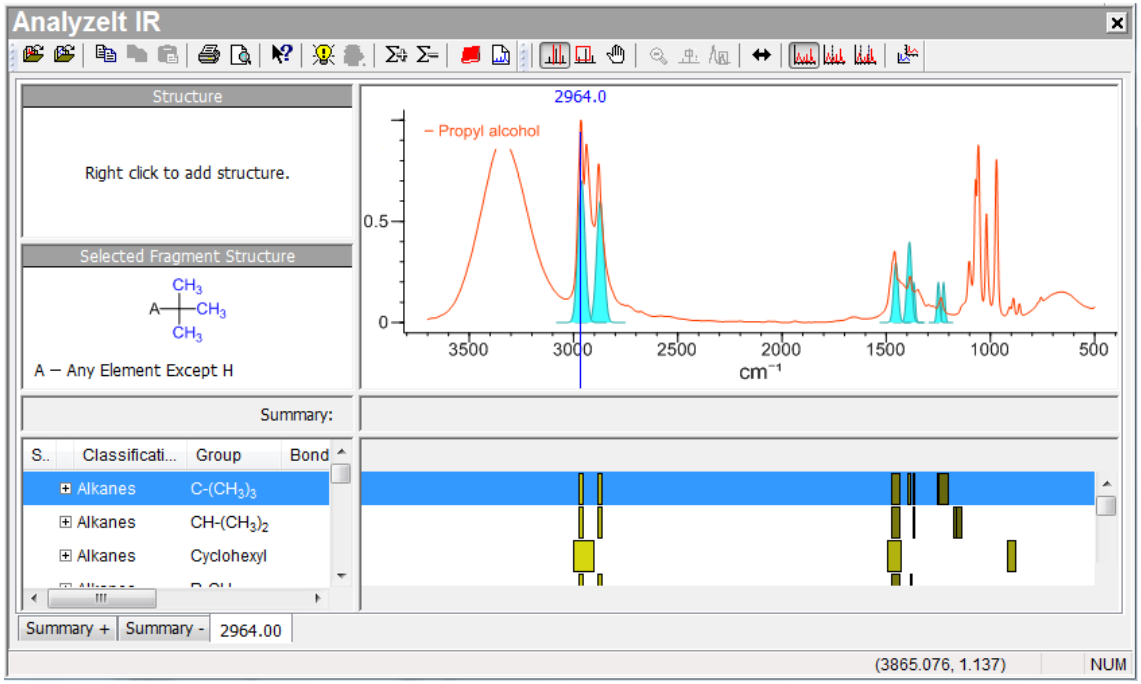
- AnalyzeIt

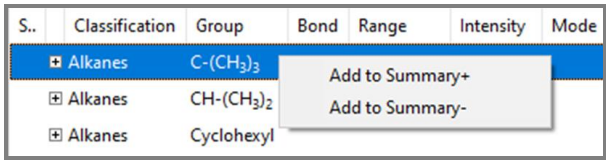
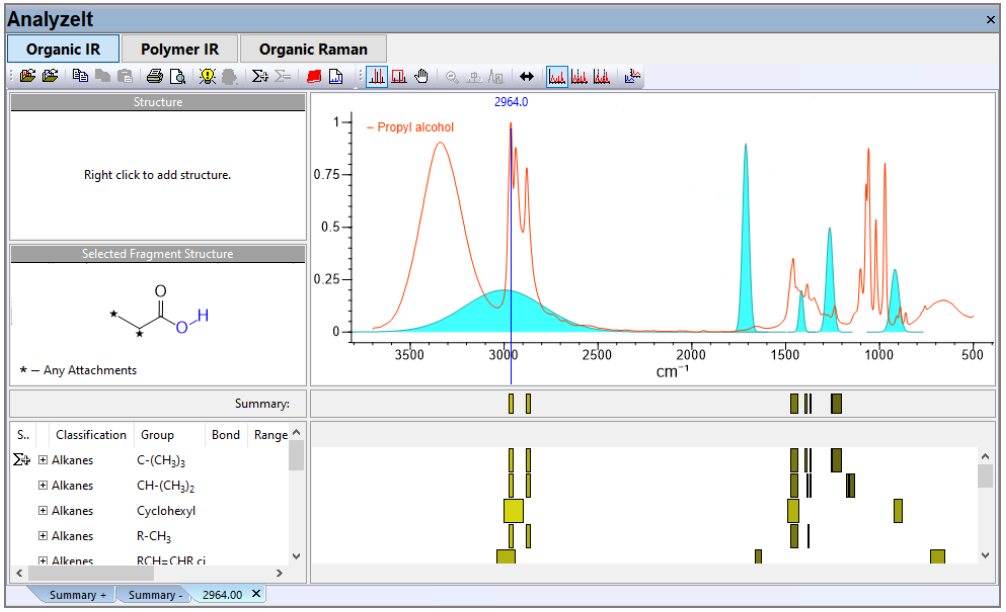
Open a spectrum

	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  .	The application selects a peak to analyze.  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.
2	Click the **Suggest** toolbar button again. **Note**: You can also select peaks by clicking in the spectral pane.	Another peak is suggested.  As you click the **Suggest a Peak** toolbar button repeatedly, the application cycles through the suggested starting points.

	Action	Result
3	Click **Suggest** until the second peak (at 2964) is selected and then click the **Correlate** button  .	After the Knowledgebase is analyzed, the results are displayed in a tab labeled with the wavenumber. 

	Action	Result
4	Select the alkanes entry C-$(CH_3)_3$ in the **Functional Group Data** pane. Right-click to open the **Summary** pop-up menu. **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.	
5	Because the methyl group correlates well with the spectrum, click **Add to Summary+**.	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. 

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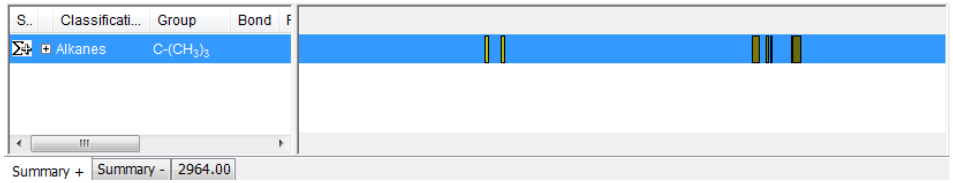
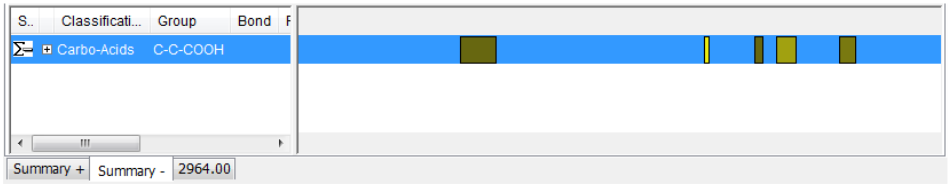
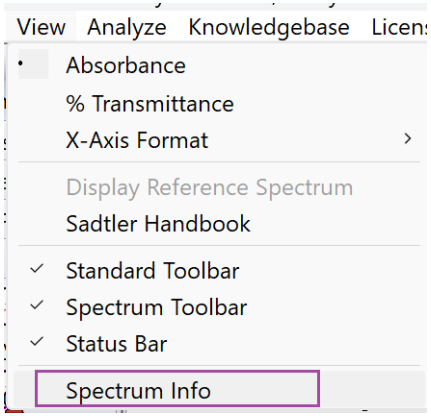
6	Click the **Summary+** tab to display any groups added to this tab.	
7	Click the **Summary-** tab to display any groups added to this tab.	
8	Choose **File > Close**.	The display is cleared.

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



Functional Group Analysis

How to Perform a Basic Spectral Analysis Using AnalyzeIt for Polymer

Purpose

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

Objectives

This exercise will teach you:

- How to analyze spectra from polymer samples

Background

The AnalyzeIt 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

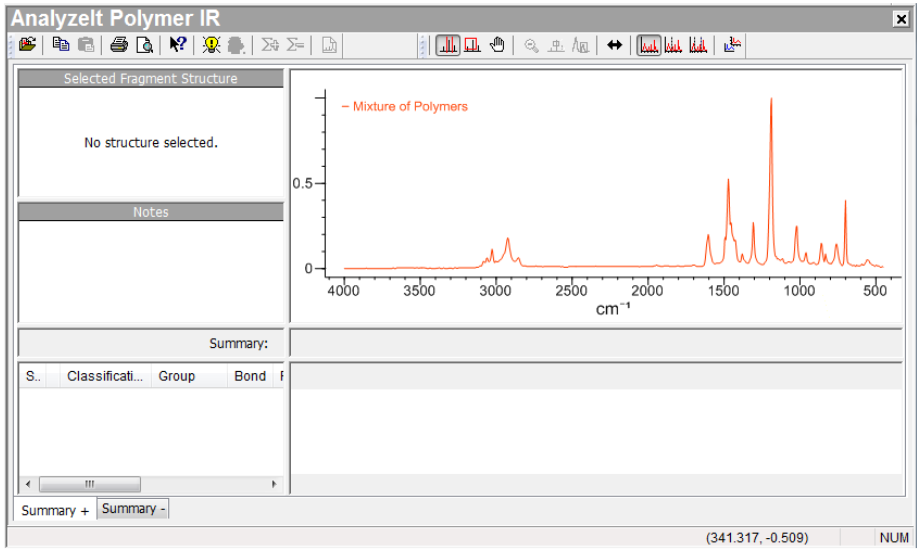
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\AnalyzeIt Polymer IR

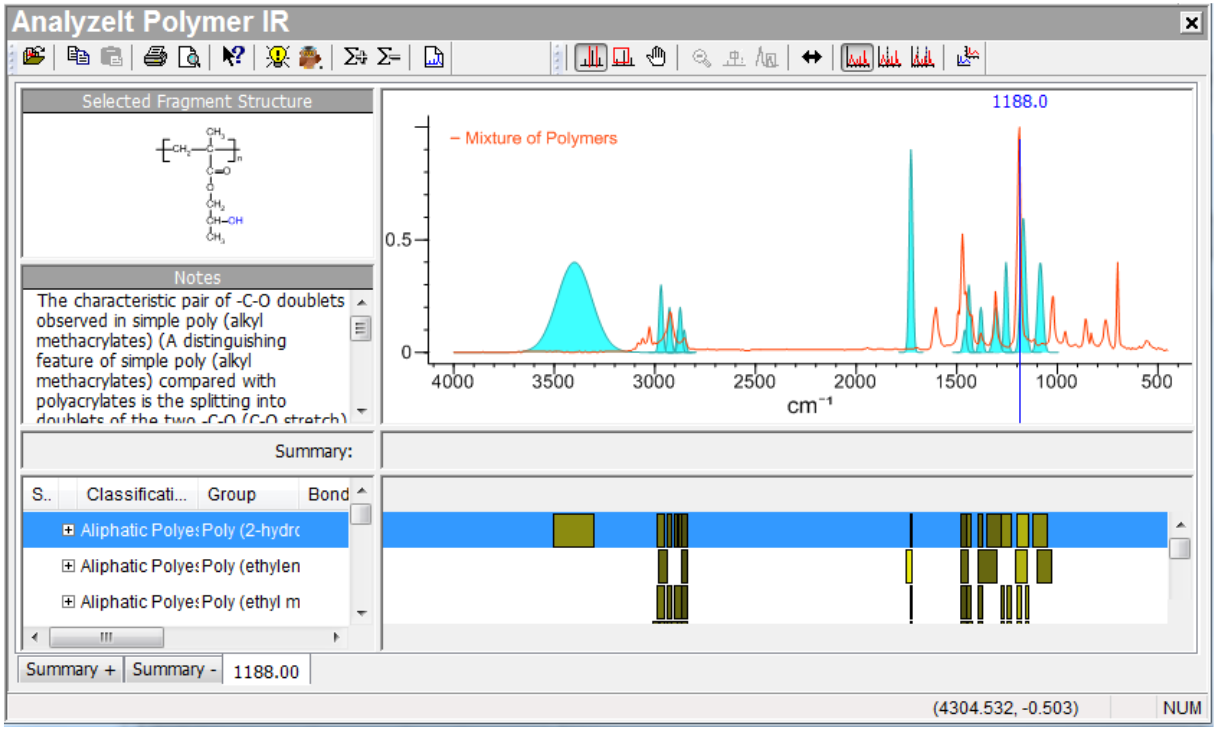
- Mixture of Polymers
- Polystyrene.irf

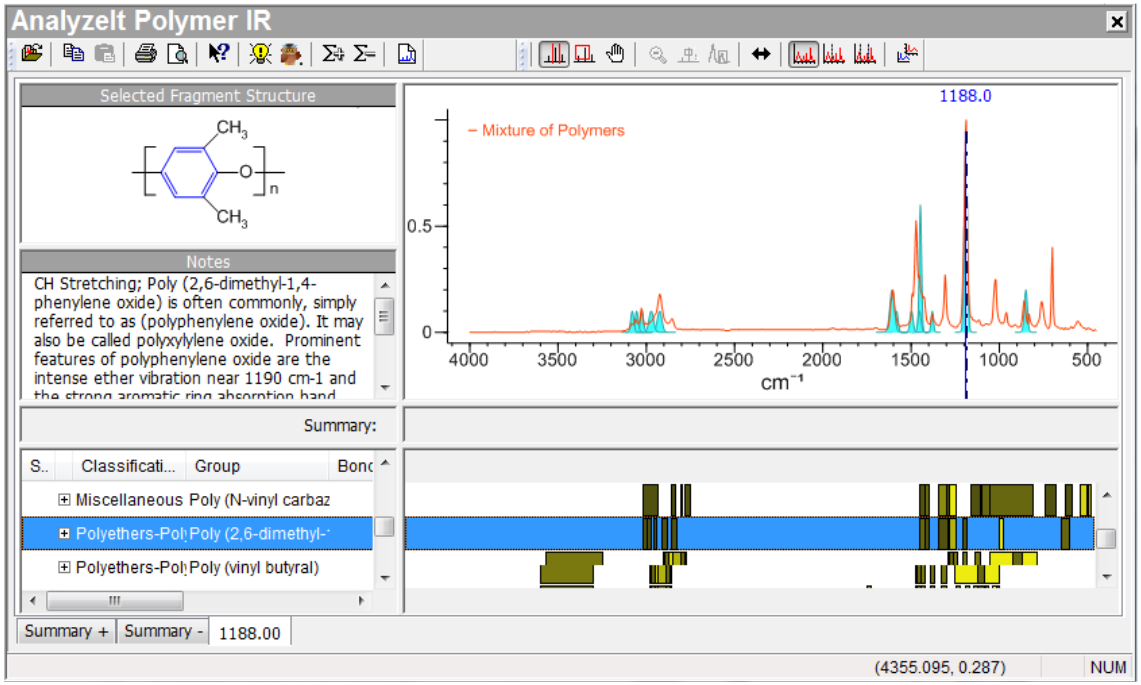
KnowItAll Applications Used

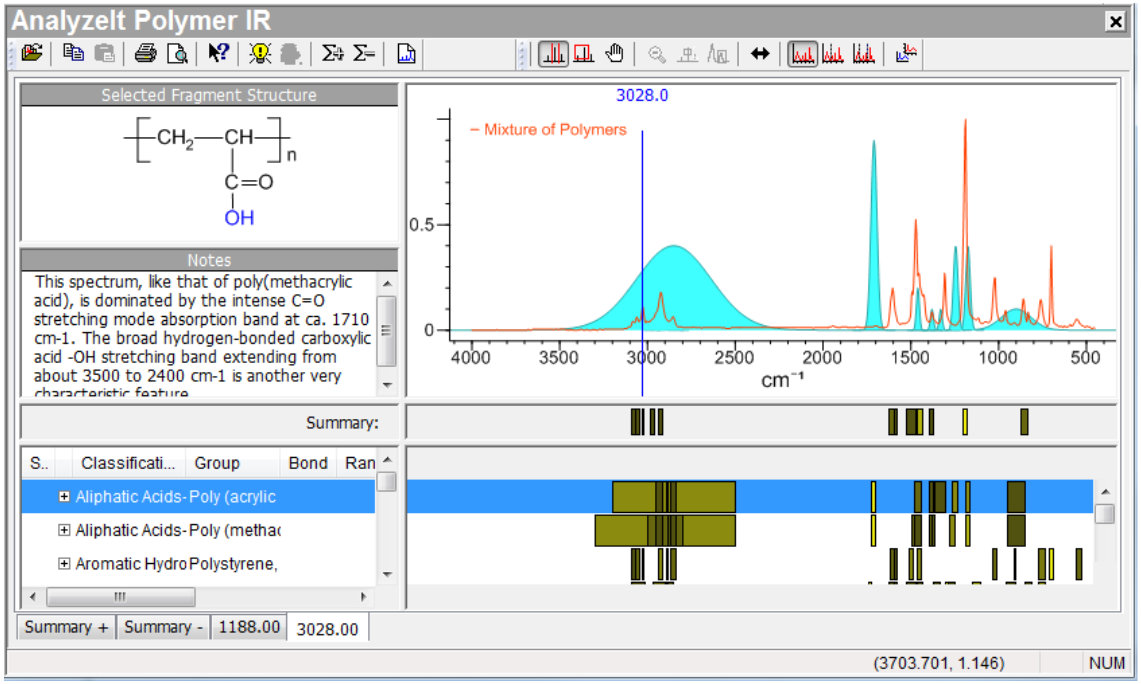
- AnalyzeIt

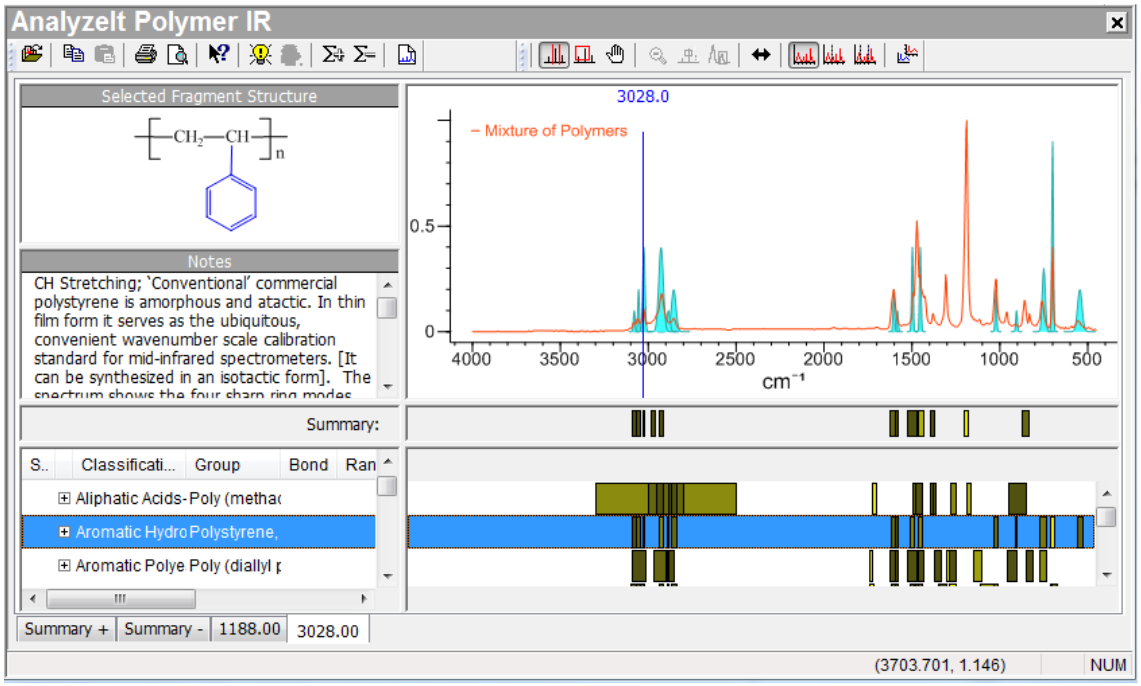
Open and analyze a mixture spectrum

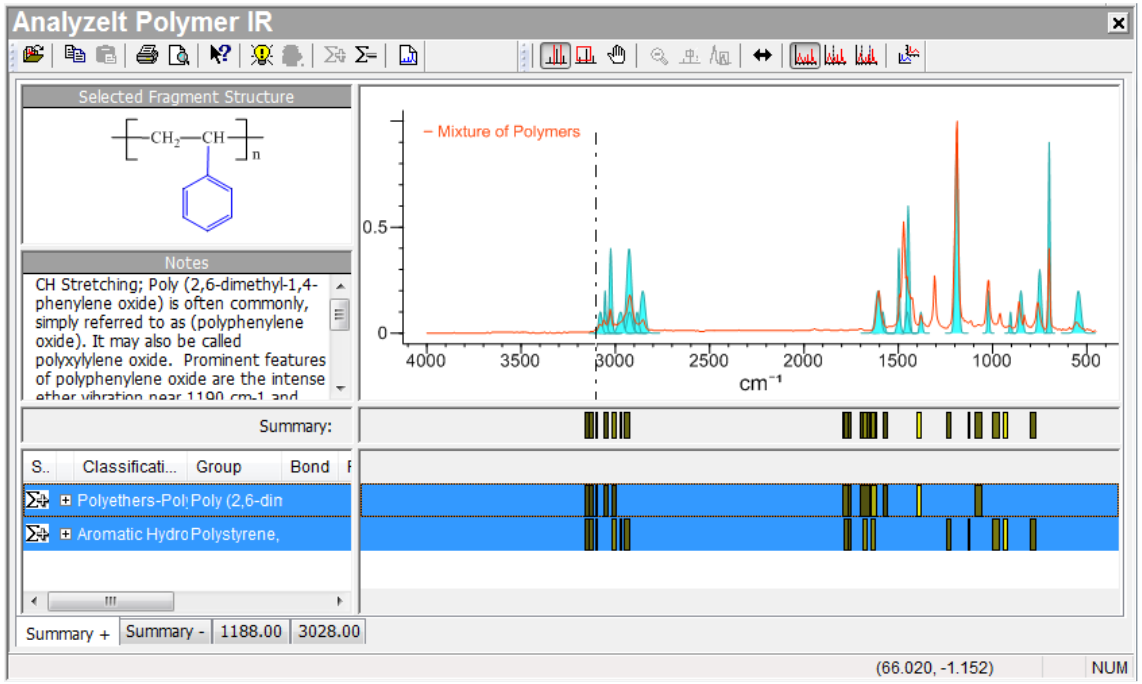
	Action	Result
1	Navigate to the **Spectral Analysis** toolbox and click **AnalyzeIt** followed by **Open Spectrum**.	
2	Navigate to **C:\Users\Public\Documents\Wiley\KnowItAll\Samples\AnalyzeIt Polymer IR**. Open **Mixture of Polymers.irf**. Click on the **Polymer IR** button in the pop-up dialog. **Note**: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

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

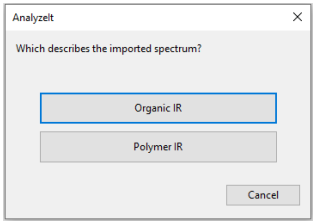
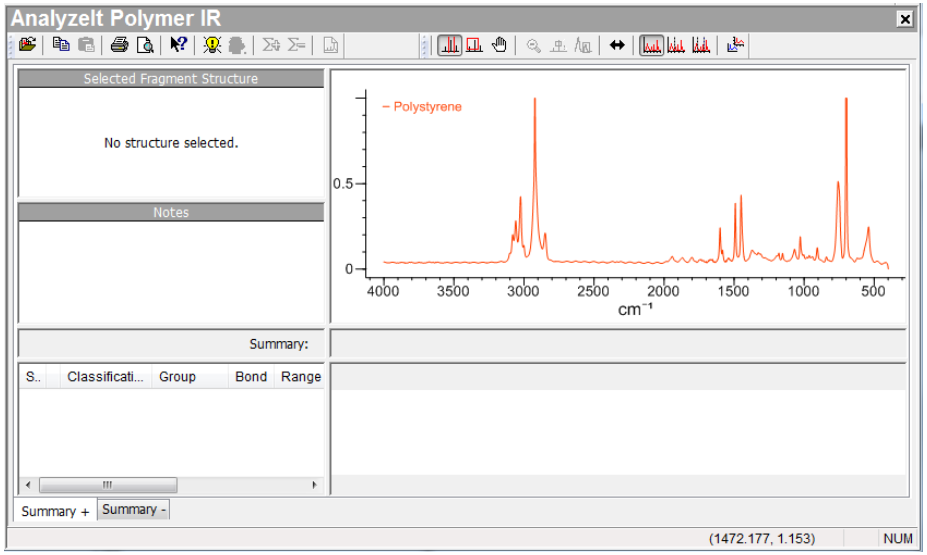
	Action	Result
4	Select each entry in the **Functional Group Data** pane in turn. Note that the first Polyether-Polymer IR entry, Poly (2,6-dimethyl-1,4-phenylene oxide) is a good match.	
5	Right-click the entry, then select **Add to Summary+**.	The entry is added to the **Summary+** tab.

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

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

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

Open and analyze a single component spectrum

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

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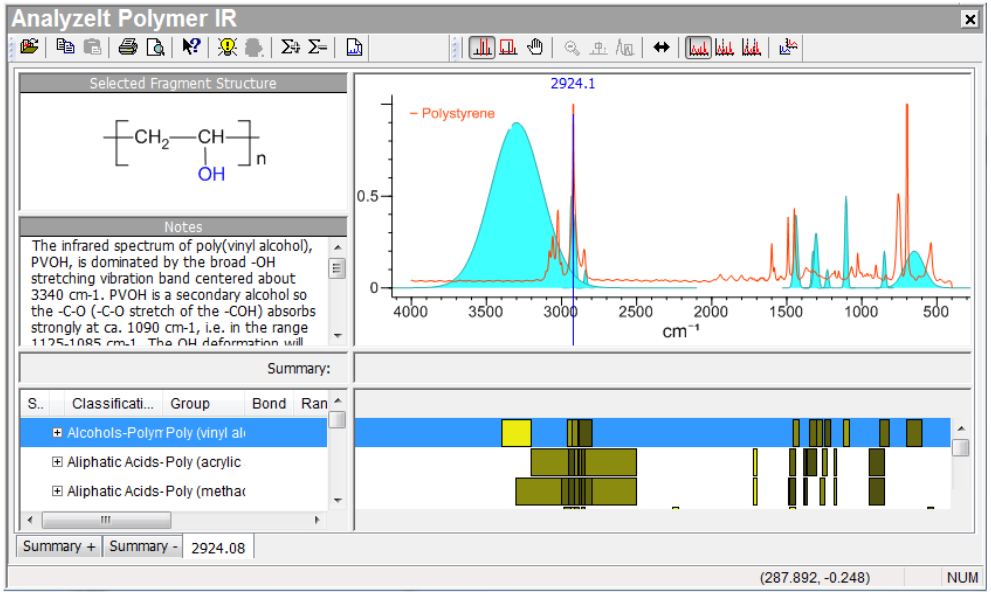
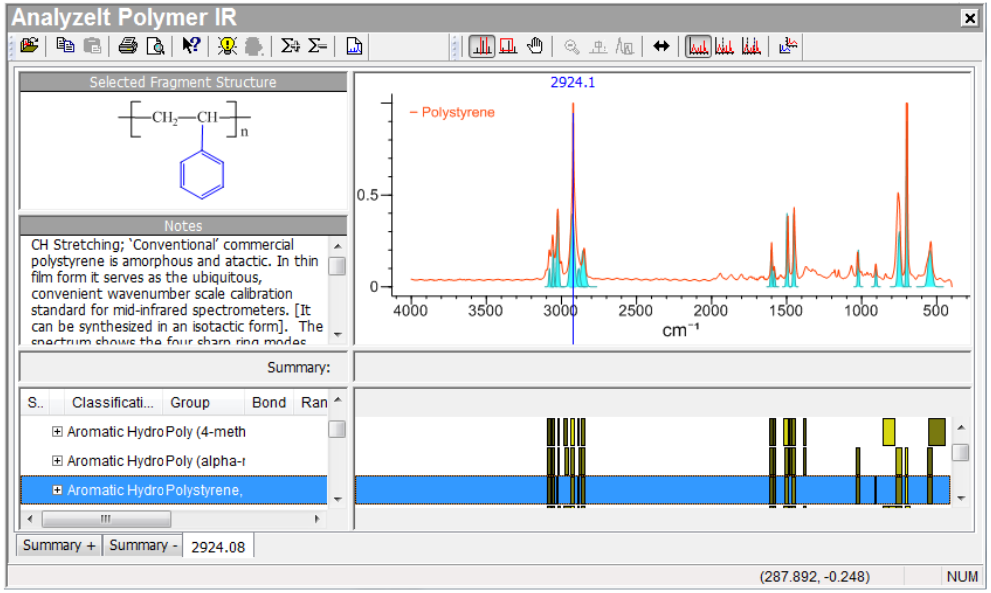
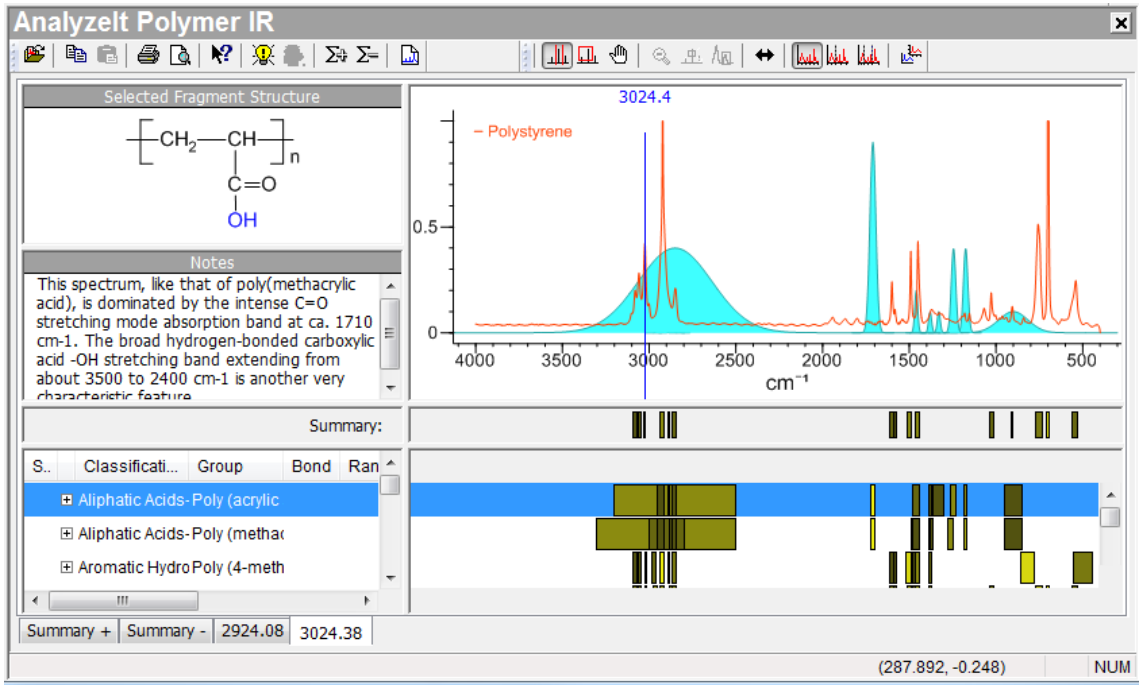
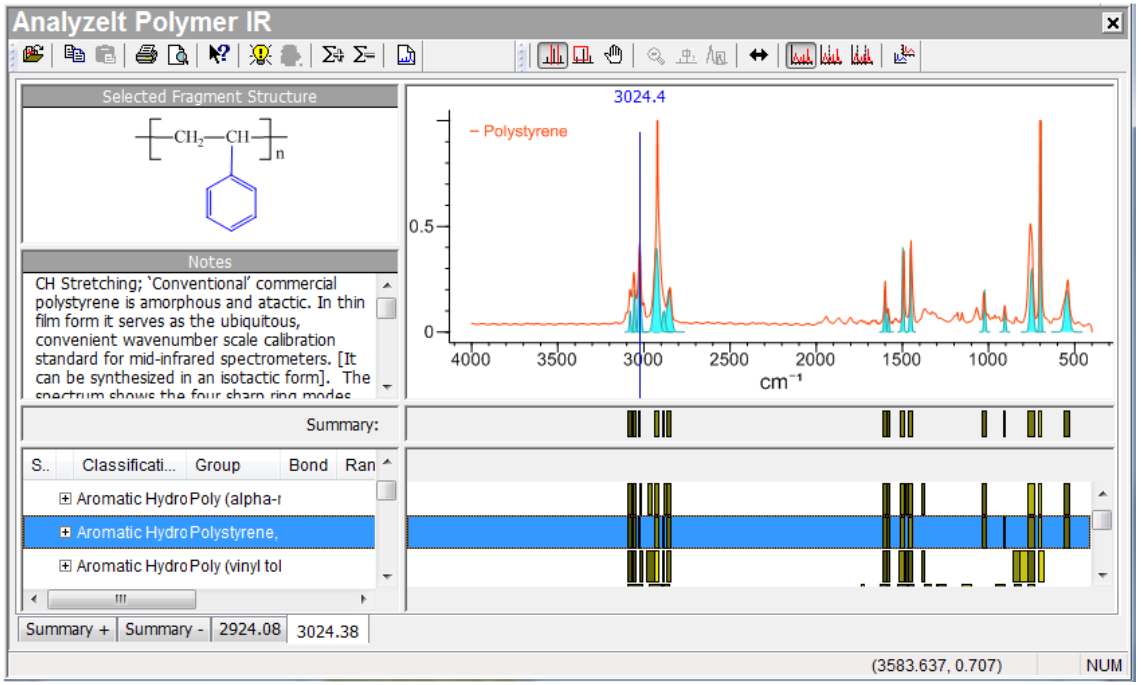
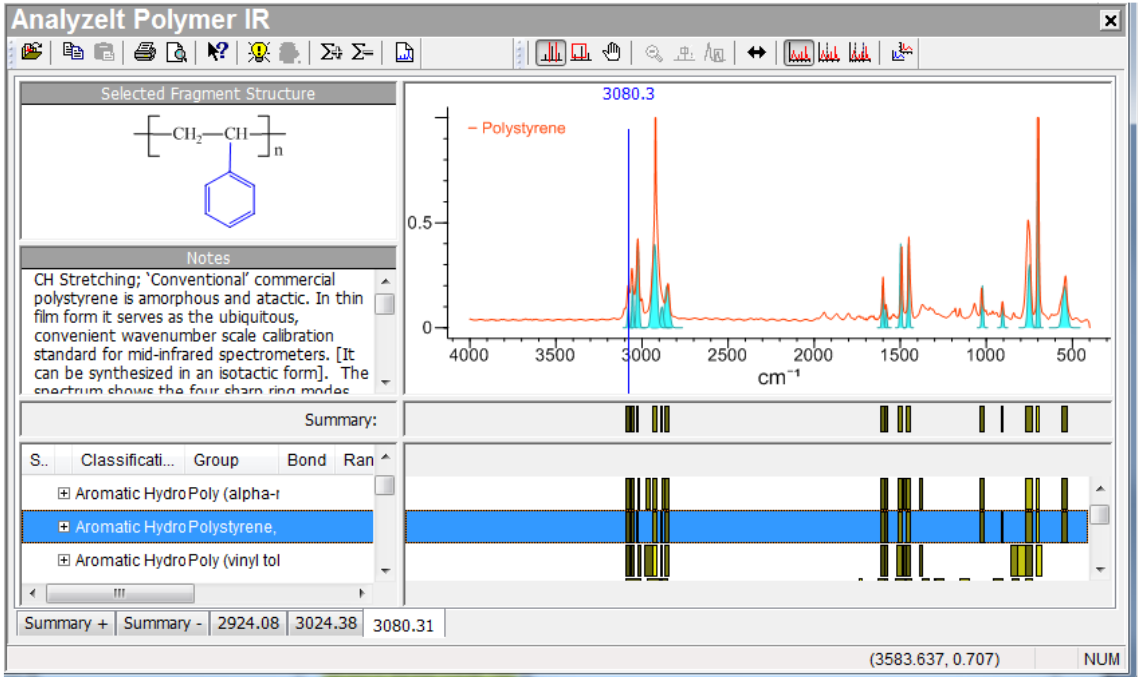
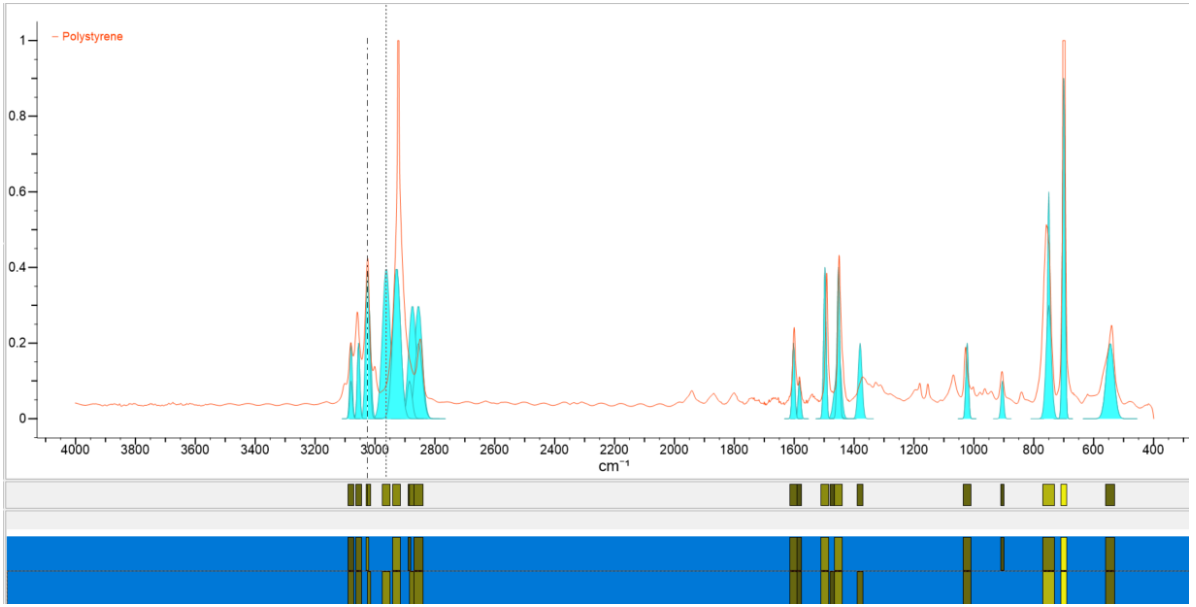
3	Click the **Suggest** button to select the peak at 2924.1, then click the **Correlate** button.	After the Knowledgebase is analyzed, the results are displayed in a tab labeled with the wavenumber (2924.08). 

	Action	Result
4	Select each entry in the **Functional Group Data** pane in turn.	Note that Aromatic Hydrocarbon (Polystyrene) is a good fit. 
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.	After the Knowledgebase is analyzed, the results are displayed in a tab labeled with the wavenumber (3024.38). 

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

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

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

Functional Group Analysis

How to Create a User Knowledgebase

Purpose

This exercise demonstrates how to create and use user Knowledgebases in the AnalyzeIt 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

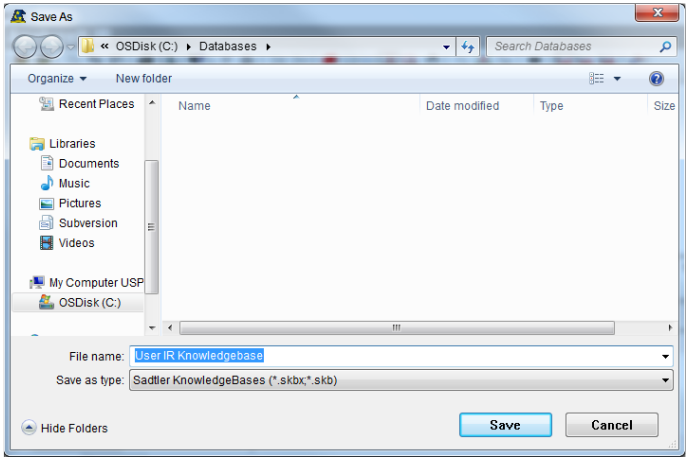
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\IR

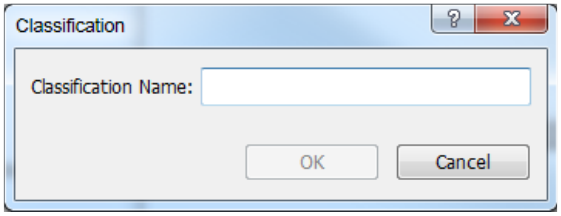
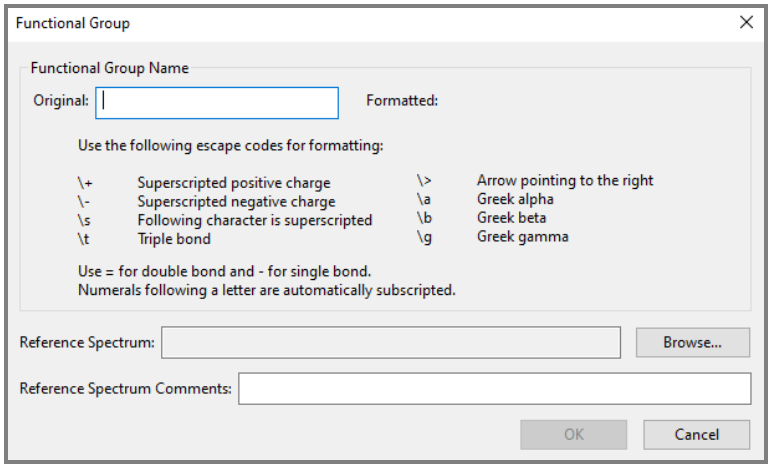
- Butylamine.jdx

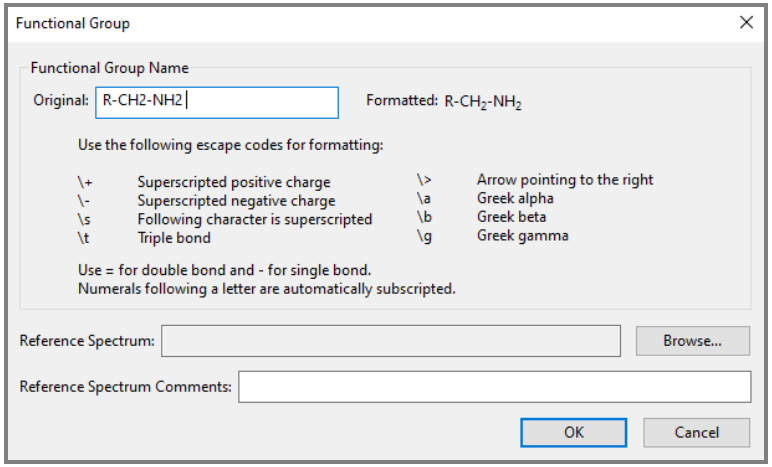
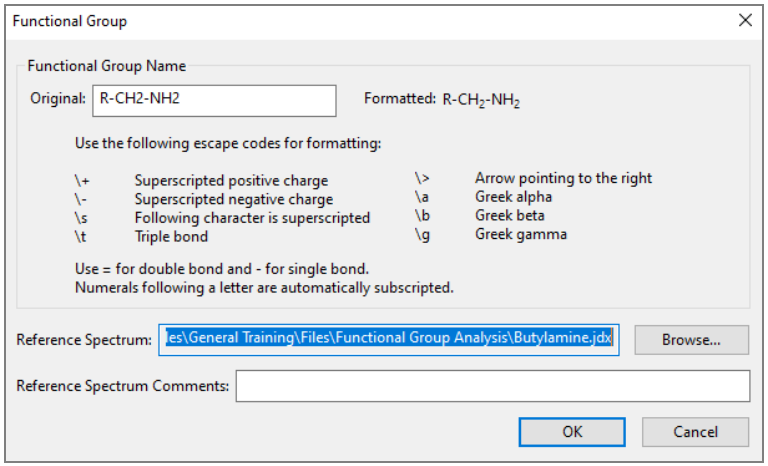
KnowItAll Applications Used

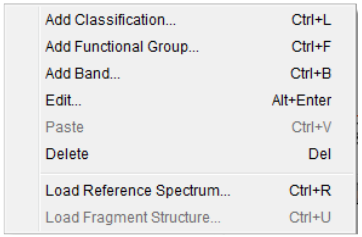
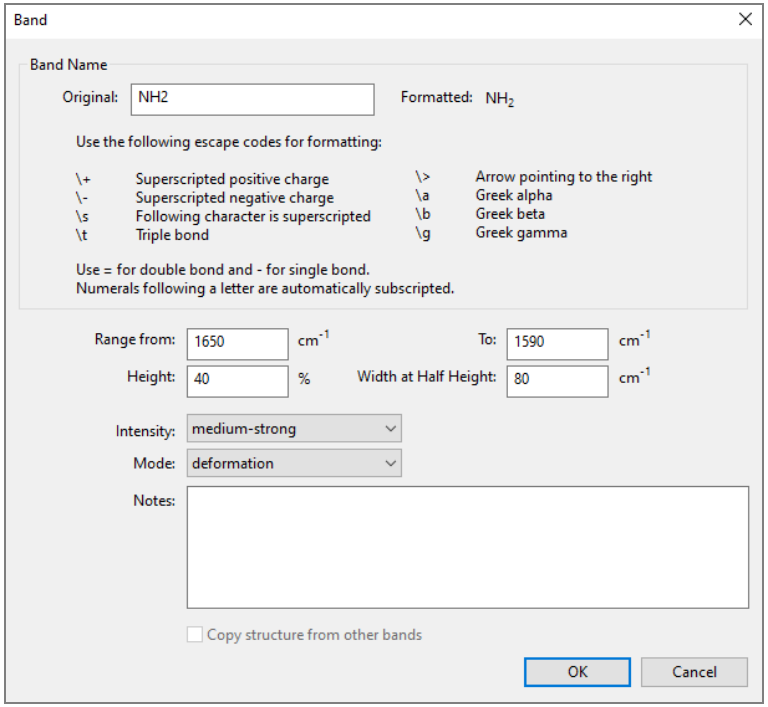
- AnalyzeIt

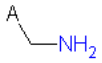
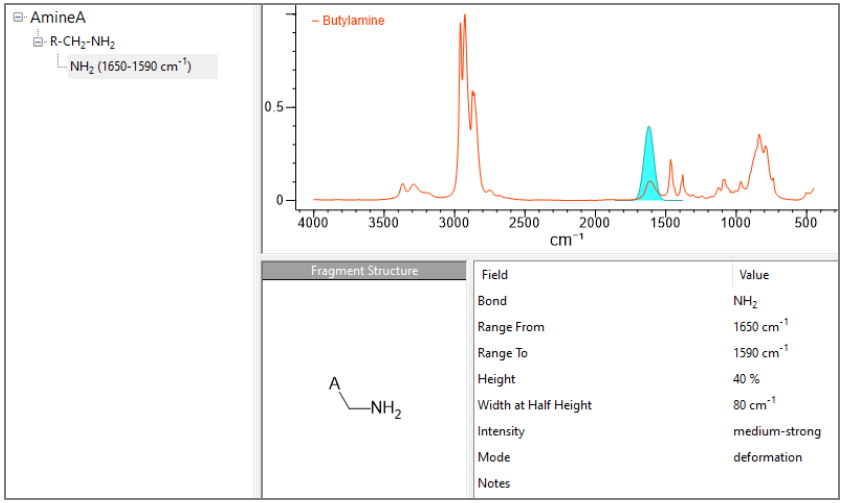
Create a user Knowledgebase

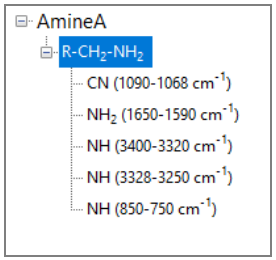
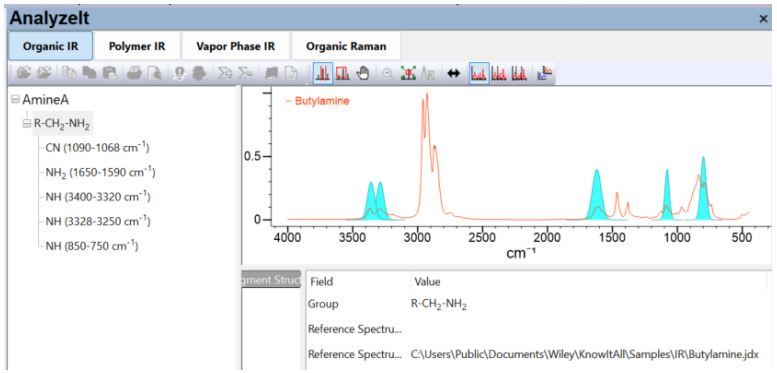
	Action	Result
1	Navigate to the **Spectral Analysis** toolbox and open the **AnalyzeIt** application by clicking its icon. Click the **Organic IR** button.	
2	Choose **Knowledgebase > New**.	A **Save As** dialog box opens.
3	Type in a name for the user Knowledgebase (such as **User IR Knowledgebase**)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

4	Right-click in the **Functional Group Tree** pane (on the left), then select **Add Classification**.	The **Classification** dialog box opens.  Type in AmineA and click **OK**. **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.
5	Right-click on the new classification name AmineA, then select **Add Functional Group**.	The **Functional Group** dialog box opens. 

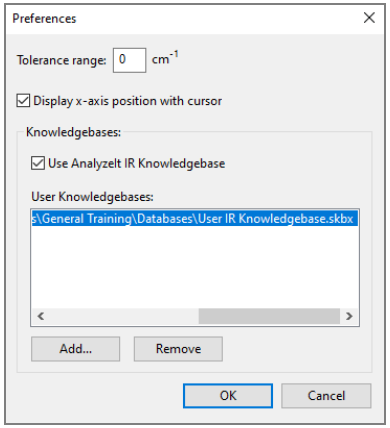
6	Type **R-CH2-NH2** in the upper text box.	The text is automatically formatted. 
7	Click **Browse**. Navigate to **C:\Users\Public\Documents\Wiley\KnowItAll\Samples\IR folder** Select **Butylamine.jdx.** The path and file name are displayed in the **Reference Spectrum** text box.	

	Action	Result
8	Click **OK** to close the dialog box. Right-click on **R-CH_2-NH_2** in the **Functional Group Tree**.	A pop-up menu opens. 
9	Click **Add Band**. Type in **NH2**, then add other information as follows: • **Range from** 1650 to 1590 **Height**: 40 **Width at Half Height**: 80 **Intensity**: medium-strong **Mode**: deformation. Click **OK**.	The **Band** dialog box opens. 

	Action	Result
10	Double-click in the **Fragment Structure** pane to open **ChemWindow**, then draw this structure: 	
11	Click **Save**.	The structure is added to the display. 

<table>
<tr><th></th><th>Action</th><th>Result</th></tr>
<tr><td>12</td><td>Continue the process to add additional bands.
<table>
<tr><th>Band</th><th>Position</th><th>Height</th><th>Width at Half Height</th><th>Intensity</th><th>Mode</th></tr>
<tr><td>NH</td><td>3400-3320</td><td>30</td><td>65</td><td>medium</td><td>antisymmetric stretching</td></tr>
<tr><td>NH</td><td>3328-3250</td><td>30</td><td>65</td><td>medium</td><td>symmetric stretching</td></tr>
<tr><td>CN</td><td>1090-1068</td><td>40</td><td>40</td><td>medium-weak</td><td>stretching</td></tr>
<tr><td>NH</td><td>850-750</td><td>50</td><td>49</td><td>strong</td><td>wagging</td></tr>
</table></td><td>Knowledgebase information is saved automatically.
 
</td></tr>
<tr><td>13</td><td>By highlighting R-CH2-NH2, you would see the peaks for this functional group</td><td> 
</td></tr>
<tr><td>14</td><td>Click ✕ in the upper right corner to close the Knowledgebase.</td><td></td></tr>
</table>

Specify the user Knowledgebase

	Action	Result
1	Navigate to the **Spectral Analysis** toolbox and open the **AnalyzeIt** 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.	The user Knowledgebase is displayed in the **Preferences** dialog box. 
5	Click **OK** to close the **Preferences** dialog box.	

6	Choose **Analyze** > **Browse a Functional Group**.	The contents of the user Knowledgebase have been added to the list of functional groups.