

KnowItAll Software Training

Data Mining & Analysis

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Overlap Density Heatmap: A Technology to Analyze Spectral, Chromatographic, and Other Graphical Data

Purpose

This exercise demonstrates how to use Overlap Density (OD) Heatmap for data mining and visualization.

Objectives

This exercise will teach you:

- How to view and manipulate an Overlap Density Heatmap
-

Background

Wiley's patented Overlap Density Heatmap is useful for visual data mining and analysis to assess the similarities and dissimilarities in large amounts of spectral, chromatographic, and other graphical data.

This technology allows the visualization of common features of overlapped objects, such as spectra or chromatograms, by color-coding the areas from highest to lowest overlap.

Training Files Used in This Lesson

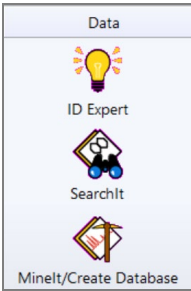
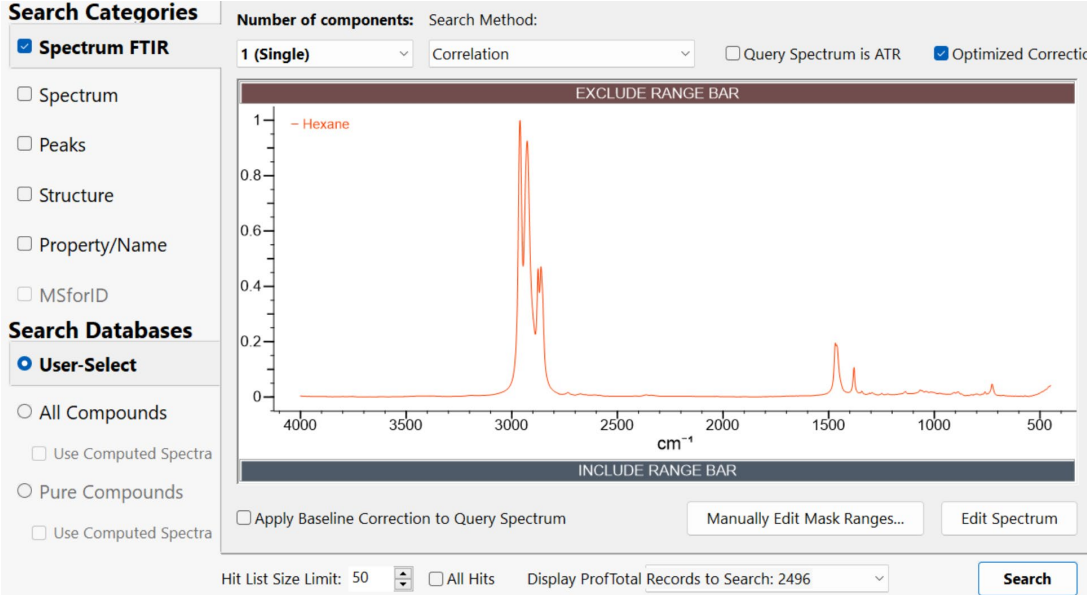
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\IR

- Hexane.jdx

KnowItAll Applications Used

- Minelt


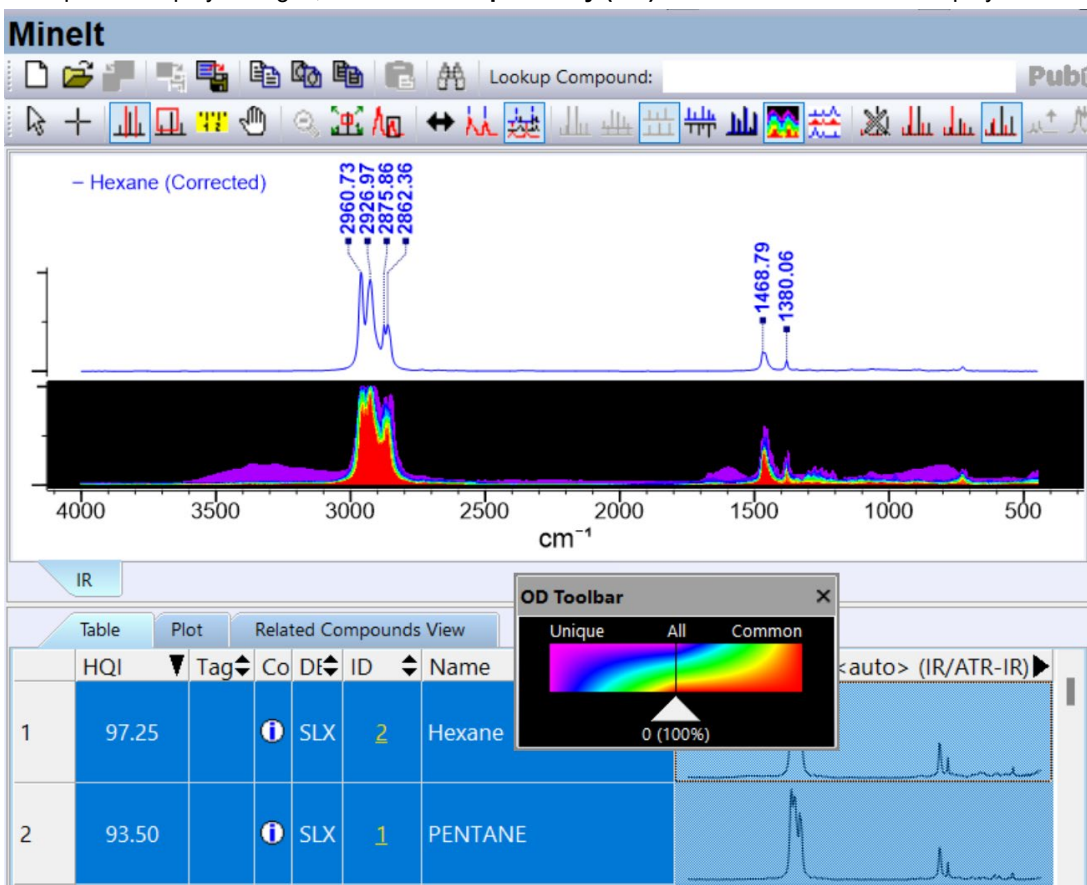






Open a spectral hit list in the Minelt application

	Action	Result
1	<p>In the SearchIt application, click User-Select under Search Databases.</p> <p><input type="radio"/> User-Select</p> <p>If databases are present in the Selected for Searching pane, click Remove All.</p> <p><input type="button" value="Remove All"/></p> <p>Add the IR - Sadtler Standards (Selected Subset) - Wiley (DB Code SLX) to the Selected for Searching pane.</p>	
2	<p>Click Spectrum in the Search Categories pane.</p> <p><input type="checkbox"/> Spectrum</p> <p>Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\IR folder.</p> <p>Open Hexane.jdx.</p>	

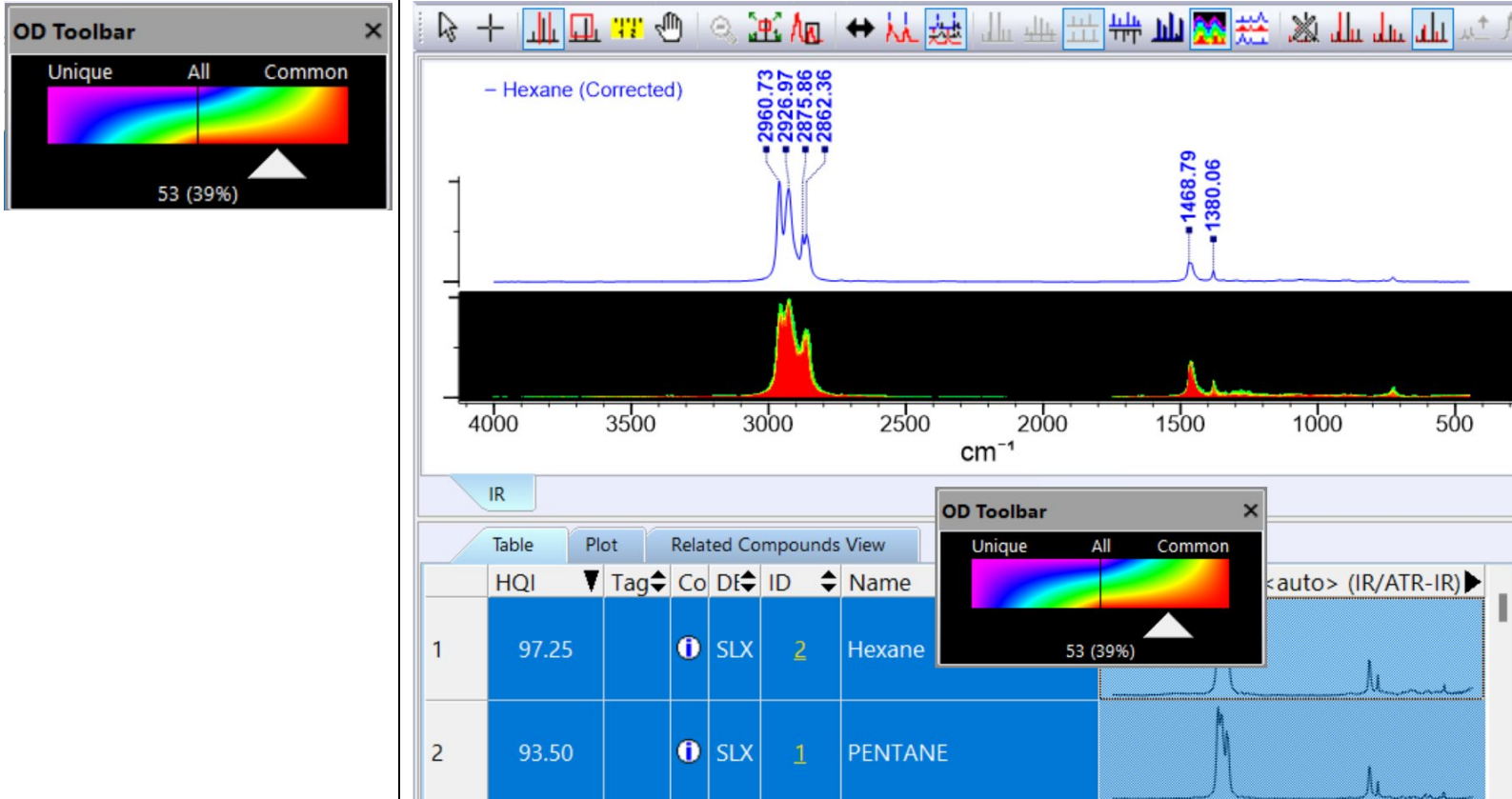
Action	Result
3 Click Search .	<p>The results are displayed in the Minelt application.</p> <div><div><div><div>Minelt</div><div><div>Lookup Compound:</div><div>PubChem</div><div>Display Profiles: <no 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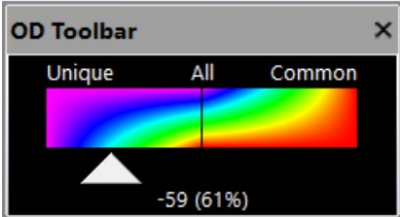
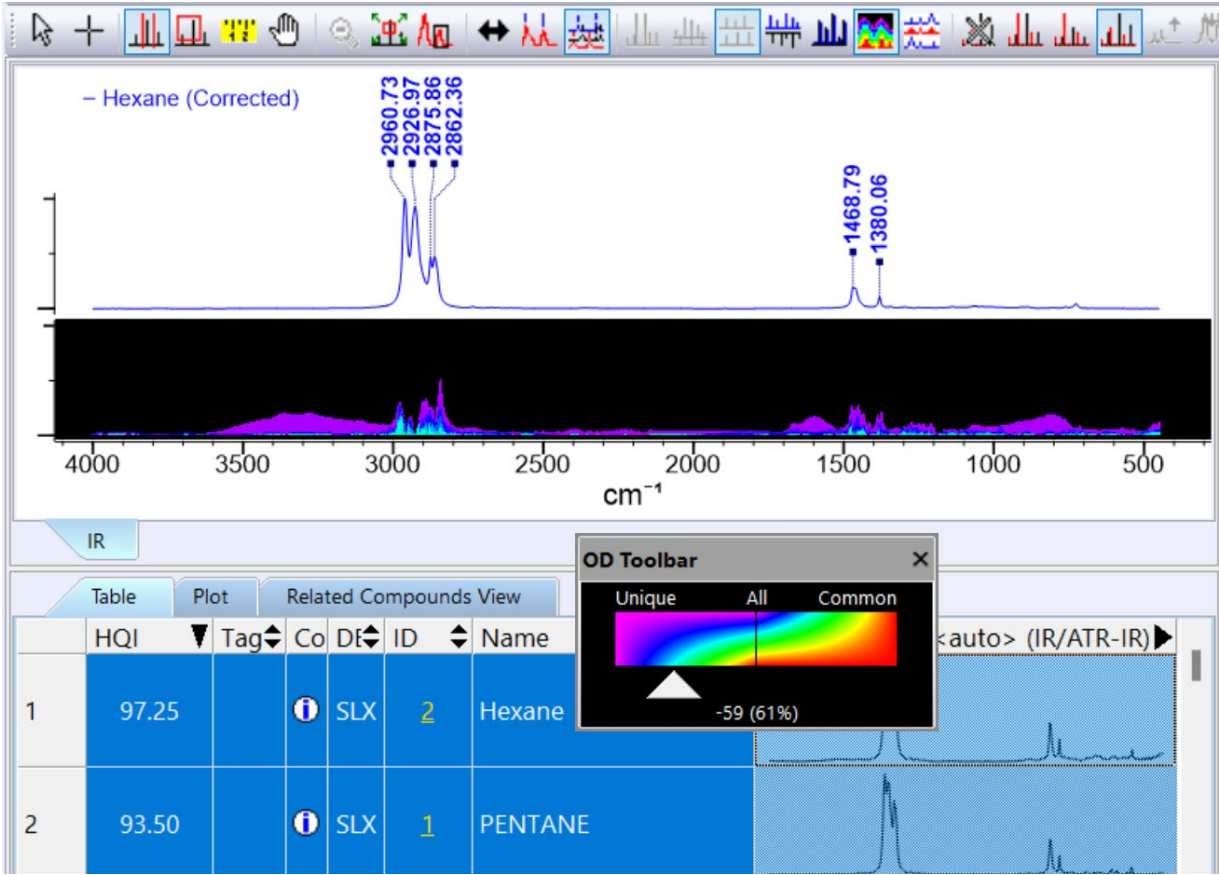
	Action	Result
4	<p>Select the first 15 entries in the hit list.</p> <p>Note: Select the first record, hold down the shift key, then scroll to and select the 15th entry.</p>	<p>All the selected hits are displayed in the spectral pane.</p> <div><div><div><div><div>Minelt</div><div><div>Lookup Compound:</div><div>PubChem</div><div>Display Profiles: <no profile></div></div><div><div><div><div><div><div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div>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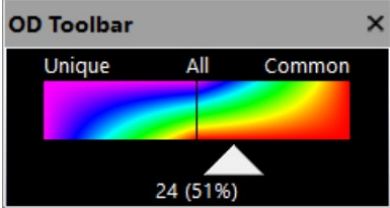
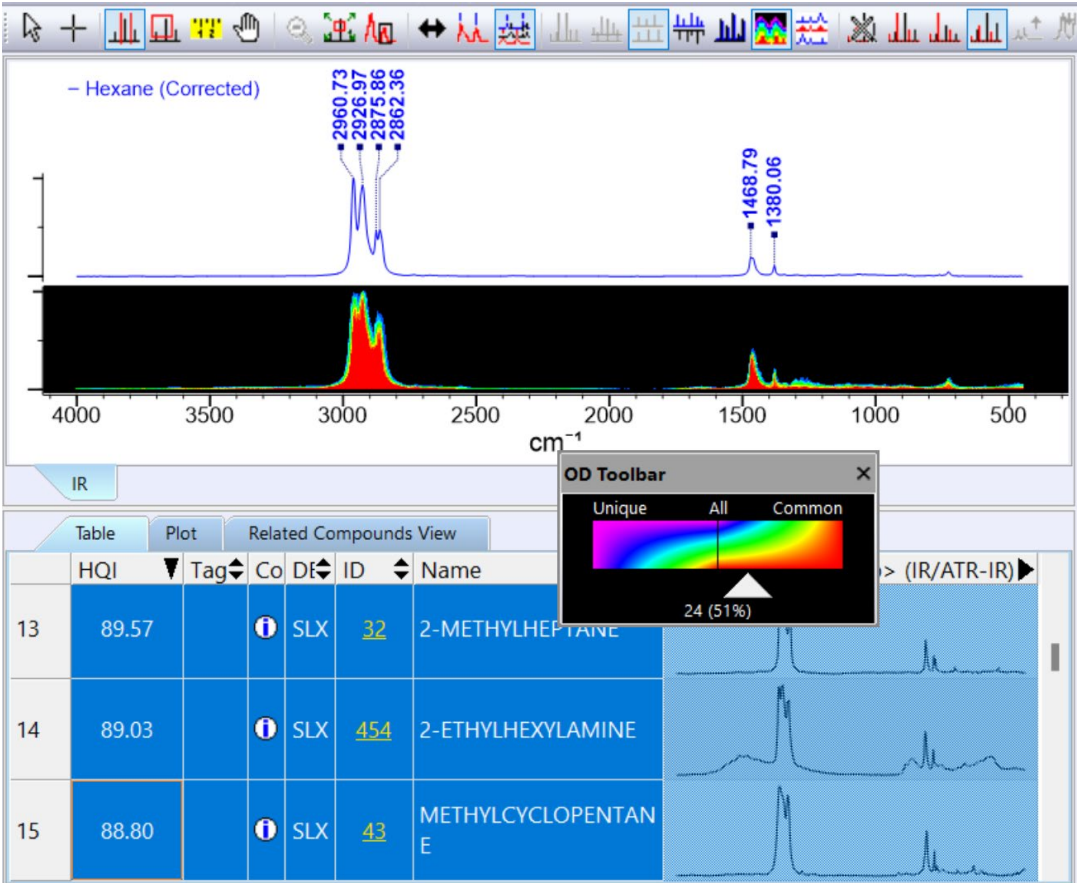
Change the spectral display to Overlap Density Heatmap

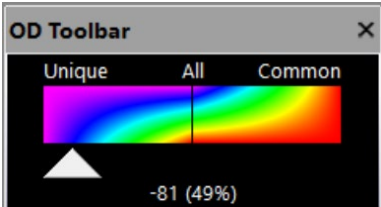
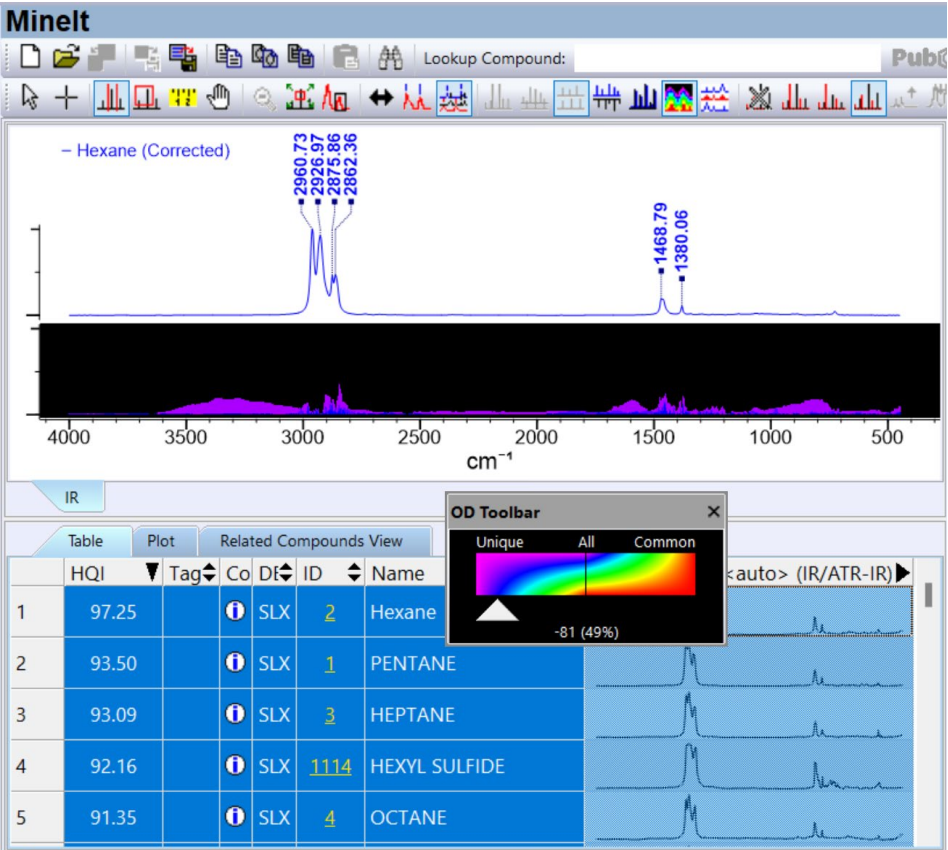


	Action	Result																					
1	Click the Overlap Density (OD) Heatmap button  in the Spectrum Toolbar .	<p>The spectral display changes, and the Overlap Density (OD) Toolbar is added to the display.</p>  <p>The default Overlap Density Heatmap display shows all overlap levels. High levels of overlap are displayed in red; low levels are displayed in violet. The OD Toolbar allows you to control the amount of overlap displayed using the slider. In the default Overlap Density Heatmap, the slider is set at OD level = 0, where all colors—representing all overlap density levels—are shown.</p> <table><tr><th></th><th>HQI</th><th>Tag</th><th>Co</th><th>DI</th><th>ID</th><th>Name</th></tr><tr><td>1</td><td>97.25</td><td></td><td></td><td>SLX</td><td>2</td><td>Hexane</td></tr><tr><td>2</td><td>93.50</td><td></td><td></td><td>SLX</td><td>1</td><td>PENTANE</td></tr></table>		HQI	Tag	Co	DI	ID	Name	1	97.25			SLX	2	Hexane	2	93.50			SLX	1	PENTANE
	HQI	Tag	Co	DI	ID	Name																	
1	97.25			SLX	2	Hexane																	
2	93.50			SLX	1	PENTANE																	

Manipulate the Overlap Density Heatmap

	Action	Result																			
1	Move the slider on the OD Toolbar to the right.	<p>As the slider moves to the right, the areas of common overlap are shown. Only the areas of most common overlap are shown as the OD Level approaches 100.</p>  <p>The screenshot displays the software interface for manipulating the Overlap Density (OD) heatmap. The OD Toolbar is visible in the top left and bottom right, showing a color gradient from purple (Unique) to red (Common) with a slider set at 53 (39%). The main window shows the IR spectra of Hexane (Corrected) and PENTANE. The x-axis represents wavenumber in cm^{-1}, ranging from 4000 to 500. The y-axis represents intensity. The spectra show characteristic peaks for Hexane (Corrected) at 2960.73, 2926.97, 2875.86, and 2862.36 cm^{-1}, and for PENTANE at 1468.79 and 1380.06 cm^{-1}. The OD heatmap is overlaid on the spectra, showing the areas of common overlap. The bottom right corner shows a table of results:</p> <table><tr><th></th><th>HQI</th><th>Tag</th><th>Co</th><th>DE</th><th>ID</th><th>Name</th></tr><tr><td>1</td><td>97.25</td><td></td><td>SLX</td><td>2</td><td>Hexane</td></tr><tr><td>2</td><td>93.50</td><td></td><td>SLX</td><td>1</td><td>PENTANE</td></tr></table>		HQI	Tag	Co	DE	ID	Name	1	97.25		SLX	2	Hexane	2	93.50		SLX	1	PENTANE
	HQI	Tag	Co	DE	ID	Name															
1	97.25		SLX	2	Hexane																
2	93.50		SLX	1	PENTANE																

	Action	Result
2	<p>Move the slider to the left.</p> 	<p>As the OD Level approaches -100, only the areas of lowest overlap – the unique areas – are shown.</p>  <p>As you move the slider to change the OD Level, a second value is shown in parentheses. This value is the percent area under the curve, or %AUC, relative to the value at OD Level = 0.</p>

	Action	Result
3	<p>Move the slider to the point where %AUC equals approximately 50%.</p> 	<p>The OD Level on the common side – or ODC – required to show 50% of the area that is most in common, is ~24.</p>  <p>Another way to express this is to say that $ODC_{50} = 24$. An alternative is to say that $\%AUC_{24} = 50$.</p>

	Action	Result
4	<p>Next, move the slider to the left to where %AUC equals approximately 50%.</p> 	<p>The OD Level on the unique side—or ODU—required to show 50% of the area that is most unique is -81.</p>  <p>Another way to express this is to say that $ODU_{50} = -81$. An alternative is to say that $\%AUC_{-81} = 50$.</p>
	<p>TIP</p>	<p>Use the Horizontal Zoom tool  to examine different regions. To do this, select the Horizontal Zoom tool, and then click and drag over an area on the spectrum to zoom in. Use the View Entire Spectrum tool  to zoom out.</p>

Data Mining & Analysis

How to Create and Use Overlap Density Consensus Spectra

Purpose

This exercise demonstrates how to create and use Overlap Density Consensus Spectra in the KnowItAll Informatics System.

Objectives

This exercise will teach you:

- How to view and manipulate an Overlap Density Consensus spectrum
- How to use an Overlap Density Consensus spectrum in a search

Background

Wiley's patented Overlap Density Heatmap technology is useful for visual data mining and analysis to assess the similarities and dissimilarities in large amounts of spectral, chromatographic, and other graphical data.

By tracing the outline of the highest level of overlap at a given OD Level, it is possible to mathematically construct a composite spectrum by using the maximum spectral y-values at each spectral x-value in the OD Heatmap. This Overlap Density Consensus Spectrum can be used in a spectral search to find similar spectra or can be stored in a database for future use.

Training Files Used in This Lesson


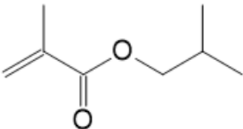
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\IR

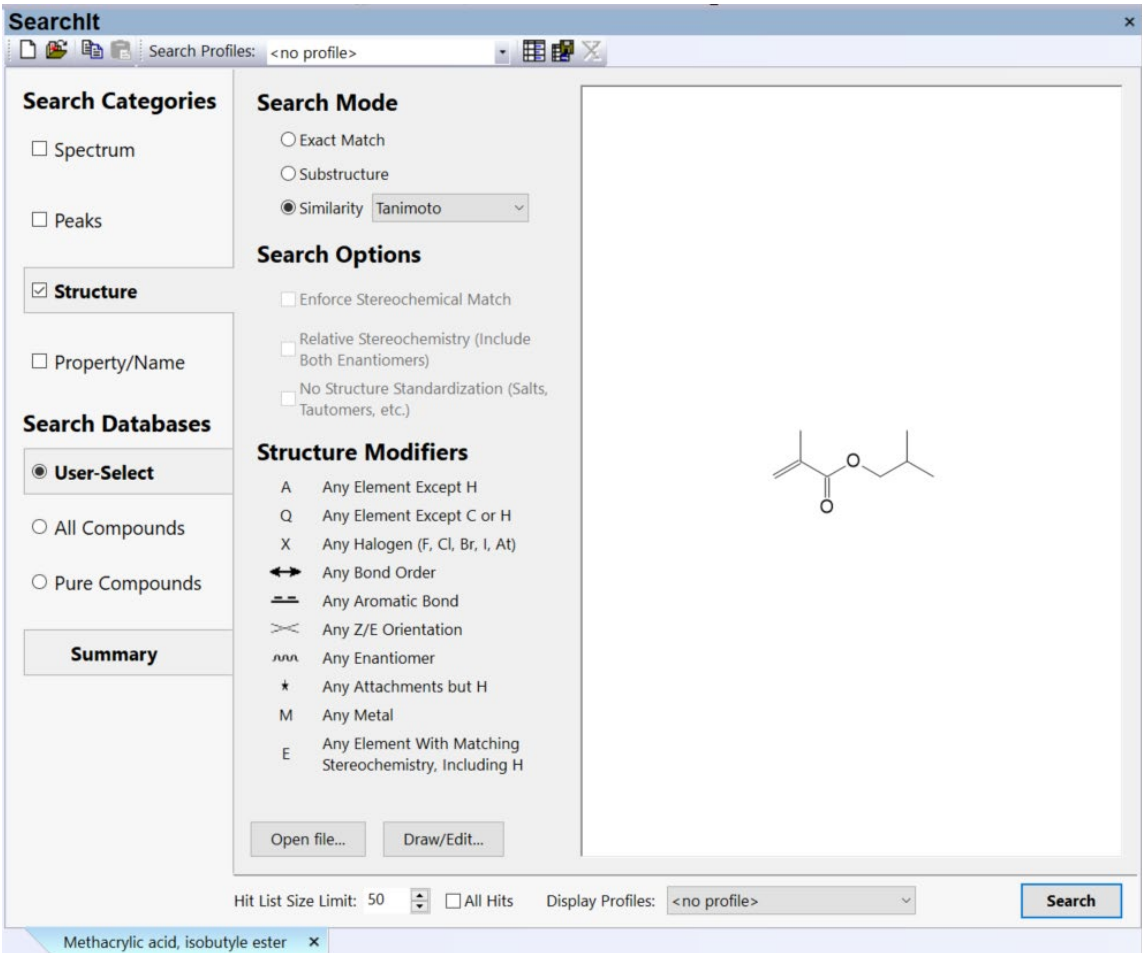
- Propiophenone Query.dsf

KnowItAll Applications Used

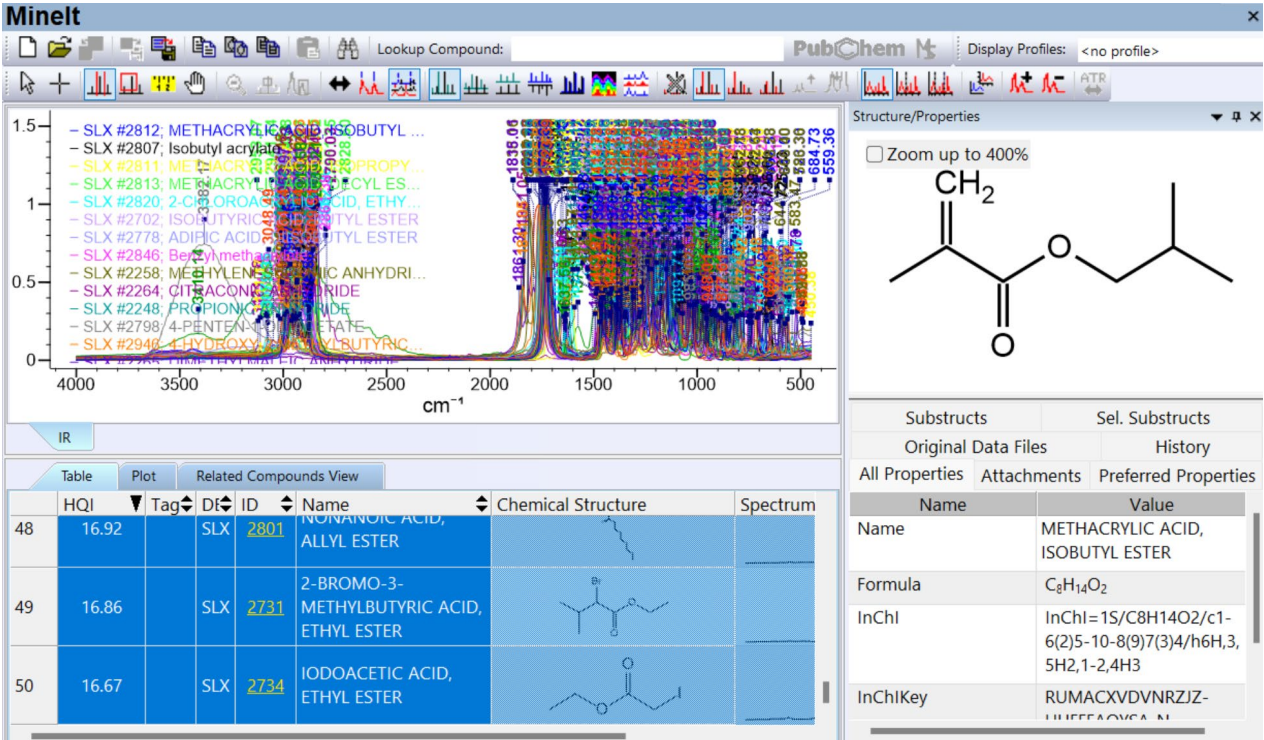

- SearchIt
- MinIt


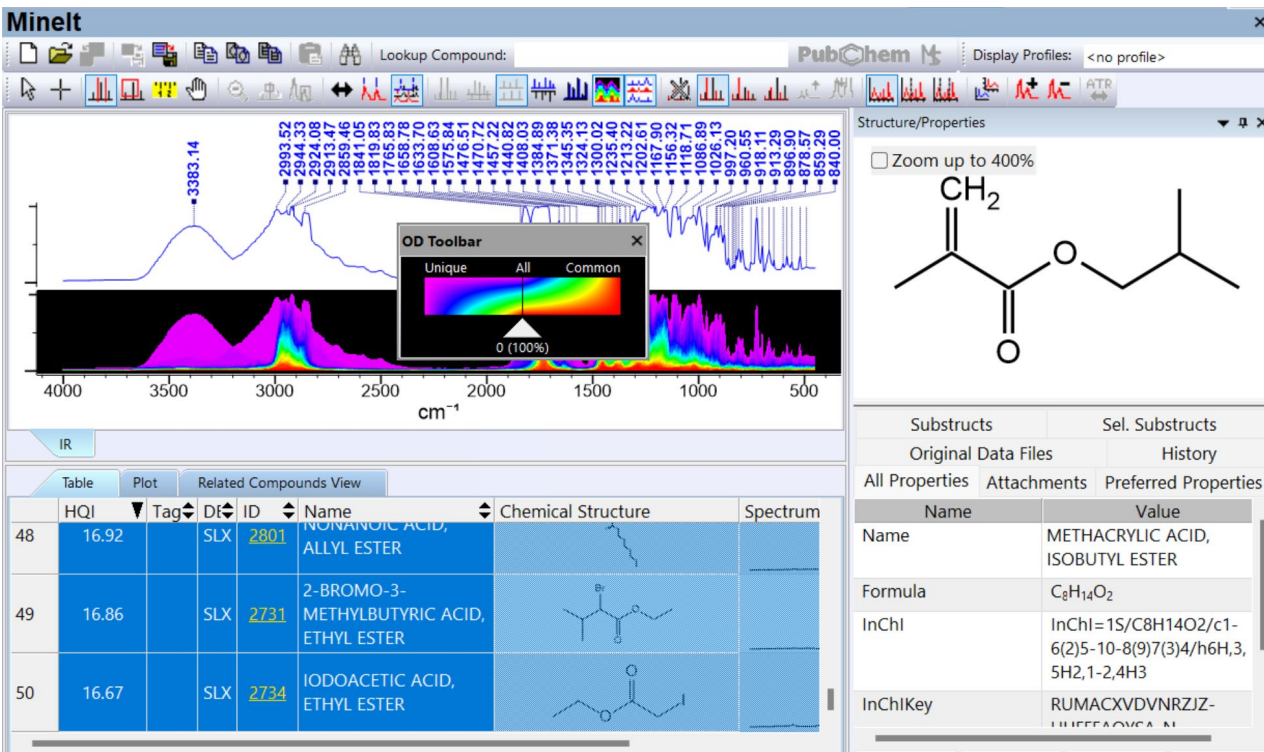
Perform a substructure search

	Action	Result
1	<p>In the SearchIt application, click User-select under Search Databases.</p> <p><input type="radio"/> User-Select</p> <p>Under Available for Searching, select IR - Sadtler Standards (Selected Subset) - Wiley (DB Code SLX).</p> <p>Available for Searching:</p> <p>Click Add.</p> <p><input type="button" value="Add"/></p>	
2	<p>Click Structure.</p> <p><input type="checkbox"/> Structure</p> <p>Click Open File... or Click Open Spectrum or Structure icon .</p>	
3	<p>Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Structures folder.</p> <p>Open Methacrylic acid, isobutyle ester.</p>	<p>The structure is displayed in the Structure window.</p>  <chem>CC(C)COC(=O)C(=C)C</chem>


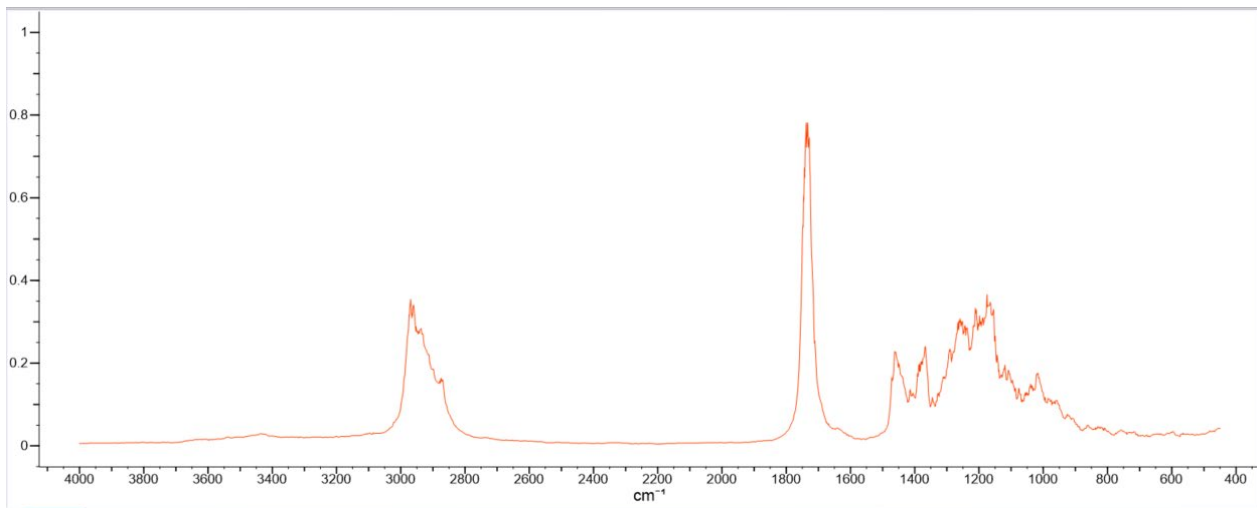
	Action	Result
4	<p>Make sure Search Mode is set to Similarity, use default Tanimoto algorithm.</p> <p>Click Search.</p>	 <p>The screenshot shows the SearchIt software interface. The 'Search Categories' section on the left has 'Structure' checked. The 'Search Mode' section has 'Similarity' selected with 'Tanimoto' as the algorithm. The 'Search Options' section has 'Enforce Stereochemical Match' checked. The 'Structure Modifiers' section lists various options like 'Any Element Except H', 'Any Bond Order', etc. The 'Search Databases' section has 'User-Select' selected. The 'Summary' button is visible. The 'Hit List Size Limit' is set to 50. The 'Display Profiles' dropdown is set to '<no profile>'. The 'Search' button is highlighted. The chemical structure of Methacrylic acid, isobutyle ester is displayed in the main window.</p>

Examine the results in Minelt

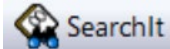
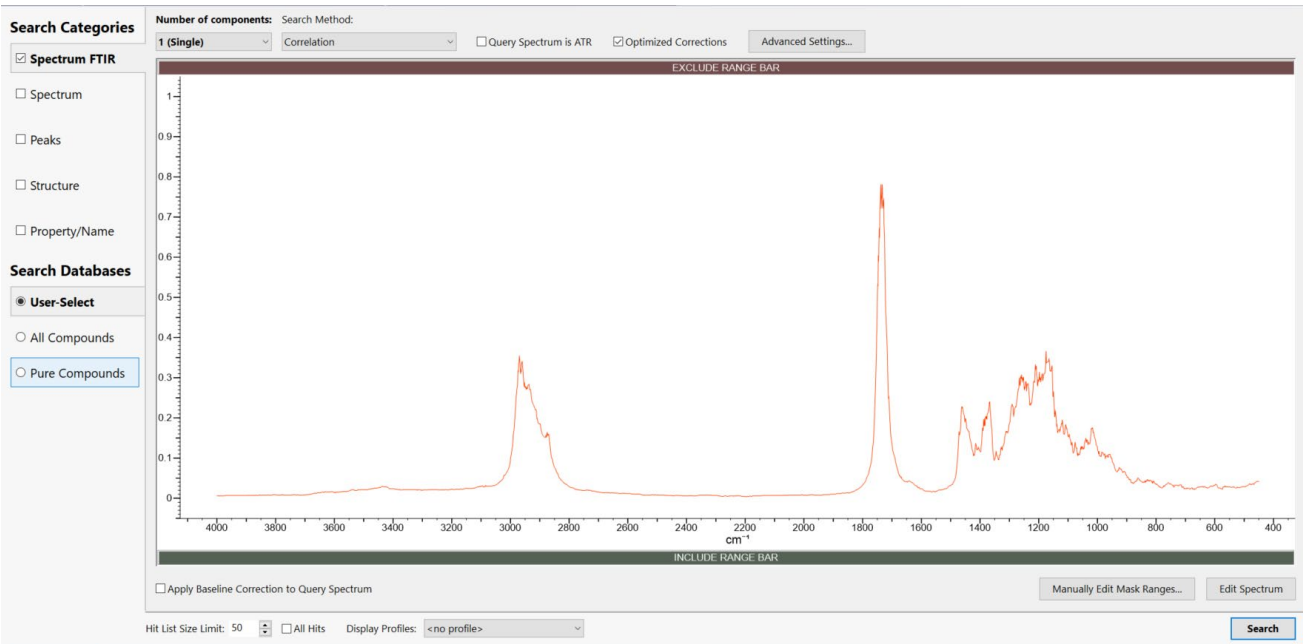
	Action	Result
1	<p>Select all records in the hit list.</p> <p>Note: Select the first record, hold down the shift key, then scroll to and select the last record.</p>	<p>All spectra are displayed in the spectral pane.</p> 
2	<p>Click the OD Heatmap button  in the Spectrum Toolbar.</p>	

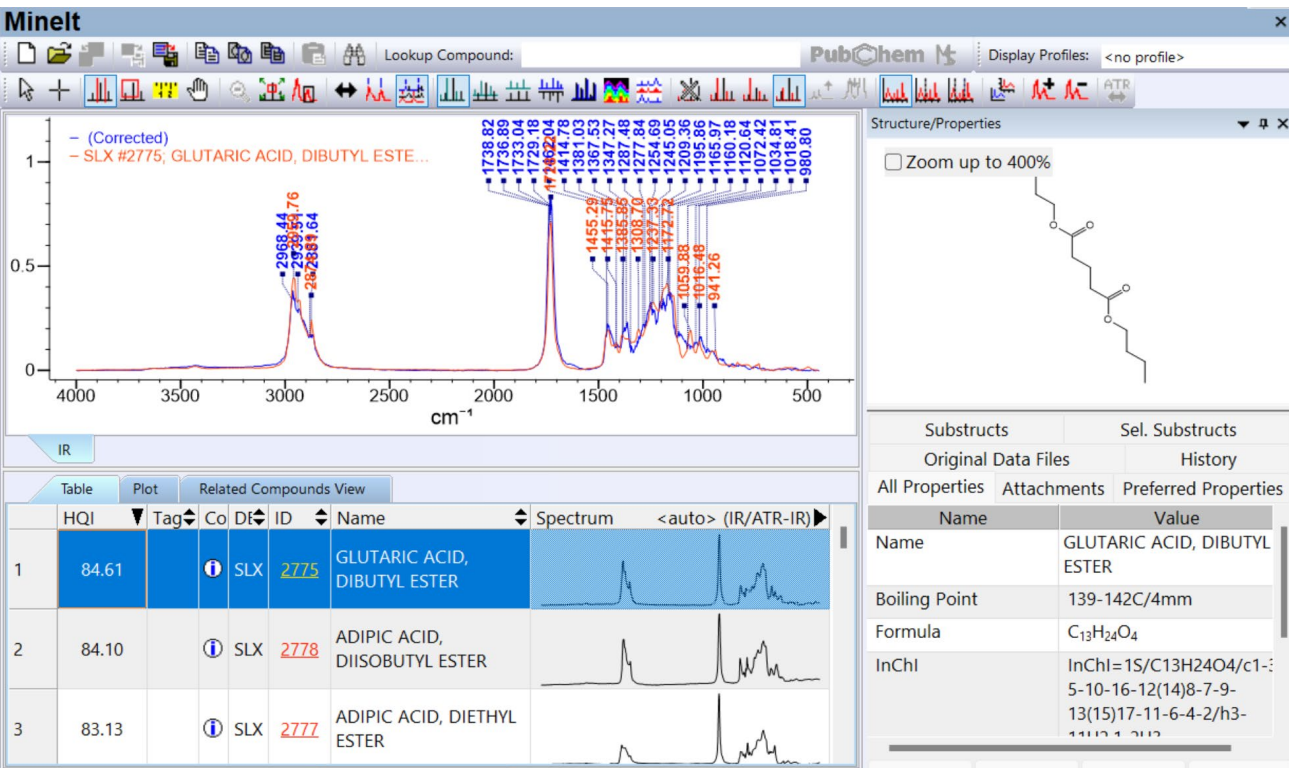
	Action	Result																																																																				
3	Click the OD Consensus Spectrum button  in the Spectrum Toolbar .	<p>The consensus spectrum is displayed above the Overlap Density Heatmap.</p>  <p>Minelt</p> <p>Lookup Compound: PubChem Display Profiles: <no profile></p> <p>Structure/Properties</p> <p><input type="checkbox"/> Zoom up to 400%</p> <p><chem>CC(=C)C(=O)OCC(C)C</chem></p> <table border="1"> <thead> <tr> <th colspan="2">Substructures</th> <th colspan="2">Sel. Substructures</th> </tr> <tr> <th colspan="2">Original Data Files</th> <th colspan="2">History</th> </tr> <tr> <th colspan="2">All Properties</th> <th colspan="2">Attachments</th> </tr> <tr> <th colspan="2">Preferred Properties</th> <th colspan="2"></th> </tr> <tr> <th>Name</th> <th>Value</th> <th></th> <th></th> </tr> <tr> <td>Name</td> <td>METHACRYLIC ACID, ISOBUTYL ESTER</td> <td></td> <td></td> </tr> <tr> <td>Formula</td> <td>C₈H₁₄O₂</td> <td></td> <td></td> </tr> <tr> <td>InChI</td> <td>InChI=1S/C8H14O2/c1-6(2)5-10-8(9)7(3)4/h6H,3,5H2,1-2,4H3</td> <td></td> <td></td> </tr> <tr> <td>InChIKey</td> <td>RUMACXVDVNRZJZ-UBFFACVCA-N</td> <td></td> <td></td> </tr> </thead></table> <p>Table Plot Related Compounds View</p> <table border="1"> <thead> <tr> <th></th> <th>HQI</th> <th>Tag</th> <th>DI</th> <th>ID</th> <th>Name</th> <th>Chemical Structure</th> <th>Spectrum</th> </tr> </thead> <tbody> <tr> <td>48</td> <td>16.92</td> <td></td> <td>SLX</td> <td>2801</td> <td>NONANOIC ACID, ALLYL ESTER</td> <td></td> <td></td> </tr> <tr> <td>49</td> <td>16.86</td> <td></td> <td>SLX</td> <td>2731</td> <td>2-BROMO-3-METHYLBUTYRIC ACID, ETHYL ESTER</td> <td></td> <td></td> </tr> <tr> <td>50</td> <td>16.67</td> <td></td> <td>SLX</td> <td>2734</td> <td>IDOACETIC ACID, ETHYL ESTER</td> <td></td> <td></td> </tr> </tbody> </table>	Substructures		Sel. Substructures		Original Data Files		History		All Properties		Attachments		Preferred Properties				Name	Value			Name	METHACRYLIC ACID, ISOBUTYL ESTER			Formula	C ₈ H ₁₄ O ₂			InChI	InChI=1S/C8H14O2/c1-6(2)5-10-8(9)7(3)4/h6H,3,5H2,1-2,4H3			InChIKey	RUMACXVDVNRZJZ-UBFFACVCA-N				HQI	Tag	DI	ID	Name	Chemical Structure	Spectrum	48	16.92		SLX	2801	NONANOIC ACID, ALLYL ESTER			49	16.86		SLX	2731	2-BROMO-3-METHYLBUTYRIC ACID, ETHYL ESTER			50	16.67		SLX	2734	IDOACETIC ACID, ETHYL ESTER		
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4 Move the OD Toolbar to around 50 (17%)	<p>The screenshot displays the software interface with the IR spectrum plot at the top. The x-axis is labeled cm^{-1} and ranges from 4000 to 500. The y-axis represents intensity. A toolbar is visible at the top of the plot area. Below the plot, there is a table with columns: HQI, Tag, DE, ID, Name, and Spectrum. The table lists three entries: 48 (NONANOIC ACID ALLYL ESTER), 49 (2-BROMO-3-METHYLBUTYRIC ACID, ETHYL ESTER), and 50 (IODOACETIC ACID, ETHYL ESTER). The OD Toolbar is shown in two positions: one at the top left and one at the bottom right, both indicating the 50 (17%) position.</p> <table border="1"><thead><tr><th>HQI</th><th>Tag</th><th>DE</th><th>ID</th><th>Name</th><th>Spectrum</th></tr></thead><tbody><tr><td>16.92</td><td></td><td>SLX</td><td>2801</td><td>NONANOIC ACID ALLYL ESTER</td><td></td></tr><tr><td>16.86</td><td></td><td>SLX</td><td>2731</td><td>2-BROMO-3-METHYLBUTYRIC ACID, ETHYL ESTER</td><td></td></tr><tr><td>16.67</td><td></td><td>SLX</td><td>2734</td><td>IODOACETIC ACID, ETHYL ESTER</td><td></td></tr></tbody></table>	HQI	Tag	DE	ID	Name	Spectrum	16.92		SLX	2801	NONANOIC ACID ALLYL ESTER		16.86		SLX	2731	2-BROMO-3-METHYLBUTYRIC ACID, ETHYL ESTER		16.67		SLX	2734	IODOACETIC ACID, ETHYL ESTER	
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	Action	Result
5	<p>Click the OD Heatmap button</p> <p>() in the Spectrum Toolbar again to turn off this display.</p>	<p>The consensus spectrum remains in the display.</p> 

Use the consensus spectrum to perform a search

	Action	Result
1	<p>Continuing with the previous result in Minelt above, use the Transfer to bar to select SearchIt.</p>  <p>Deselect Structure in SearchIt Search Categories.</p>	<p>The consensus spectrum is displayed on the IR Spectrum search tab.</p> 

	Action	Result
2	<p>Click the Search button.</p> <p>Note: The IR - Sadtler Standards (Selected Subset) - Wiley (SLX) database remains in the spectrum pane.</p>	<p>The results are displayed in the Minelt application on a new tab.</p>  <p>The screenshot shows the Minelt application interface. At the top, there's a toolbar with various icons and a 'Lookup Compound:' field. Below this is a large IR spectrum plot with two traces: a blue trace labeled '(Corrected)' and a red trace labeled 'SLX #2775, GLUTARIC ACID, DIBUTYL ESTER...'. The x-axis is labeled 'cm⁻¹' and ranges from 4000 to 500. The y-axis ranges from 0 to 1. Numerous peaks are labeled with their wavenumbers. To the right of the plot is a 'Structure/Properties' panel showing the chemical structure of glutaric acid, dibutyl ester and a table of properties. Below the plot is a 'Table' tab with a hit list. The hit list has columns for HQI, Tag, Co, ID, Name, and Spectrum. It lists three hits: 1. GLUTARIC ACID, DIBUTYL ESTER (HQI 84.61, ID 2775), 2. ADIPIC ACID, DIISOBUTYL ESTER (HQI 84.10, ID 2778), and 3. ADIPIC ACID, DIETHYL ESTER (HQI 83.13, ID 2777). Each hit has a small spectrum preview. At the bottom, a text box states: 'You get a hit list where hits are structurally similar to that of Methacrylic acid, isobutyle ester.'</p>