

# **KnowItAll Software Training**

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## Data Mining & Analysis

# 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 Heatmap for data mining and visualization.

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### Objectives

This exercise will teach you:

- How to view and manipulate an Overlap Density Heatmap
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### 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*

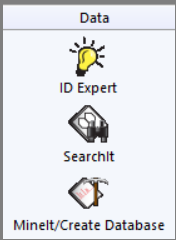
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\IR

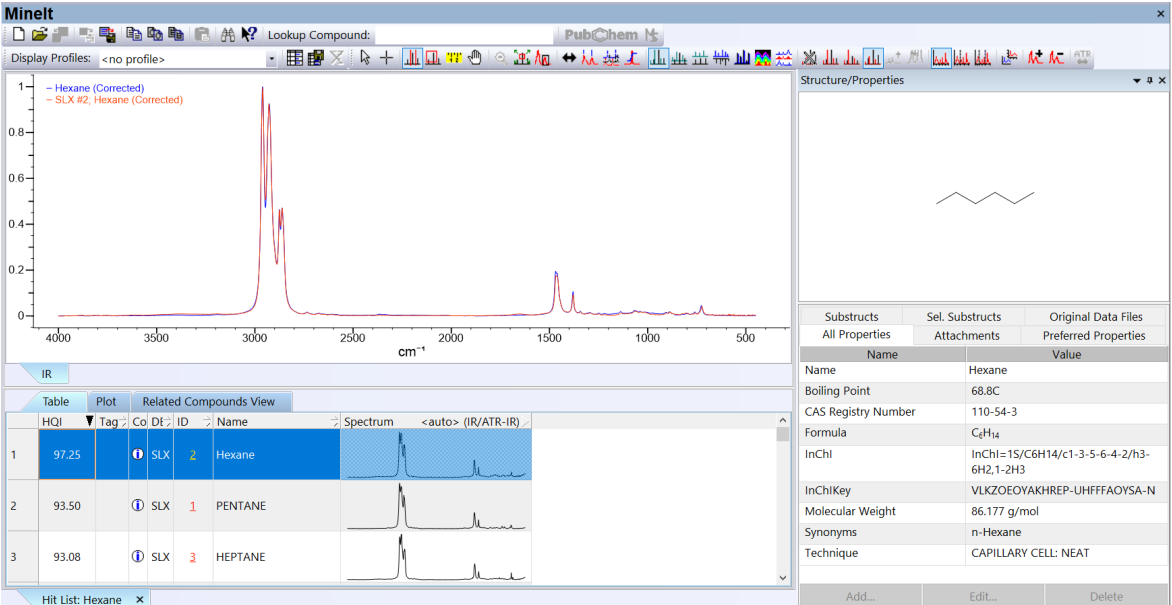
- Hexane.jdx

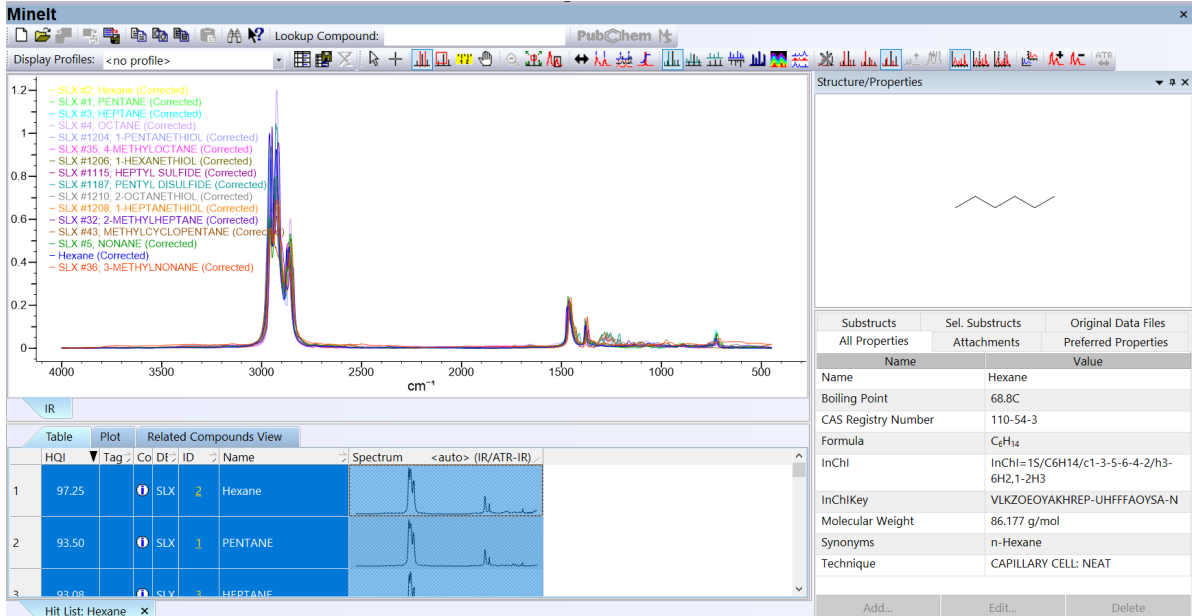
#### *KnowItAll Applications Used*

- Minelt™


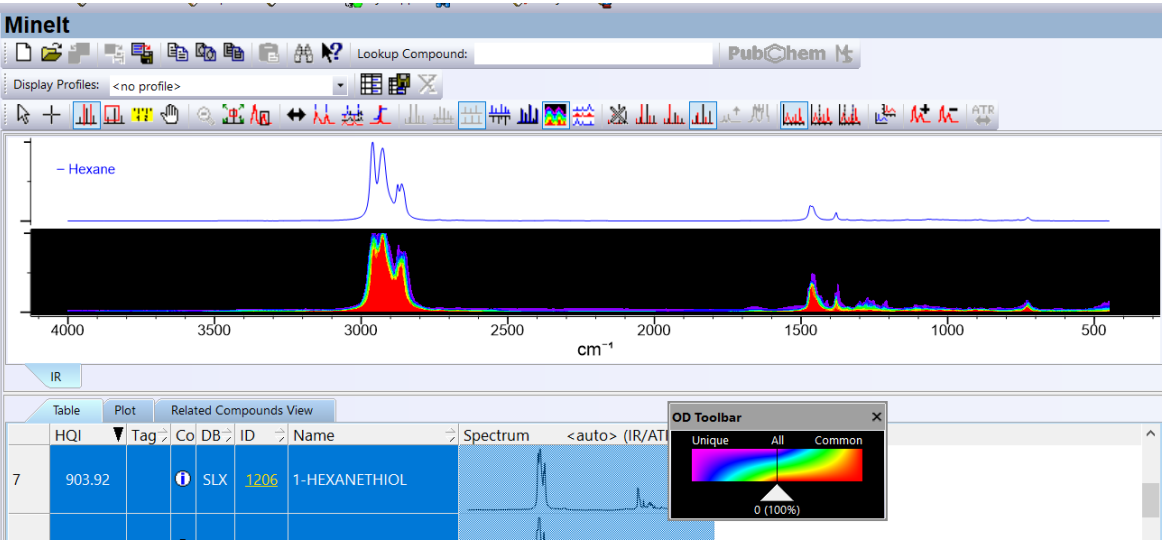
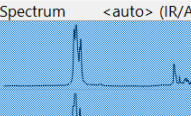
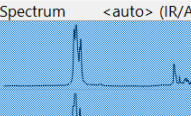
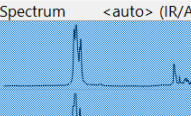
## Open a spectral hit list in the Minelt application

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

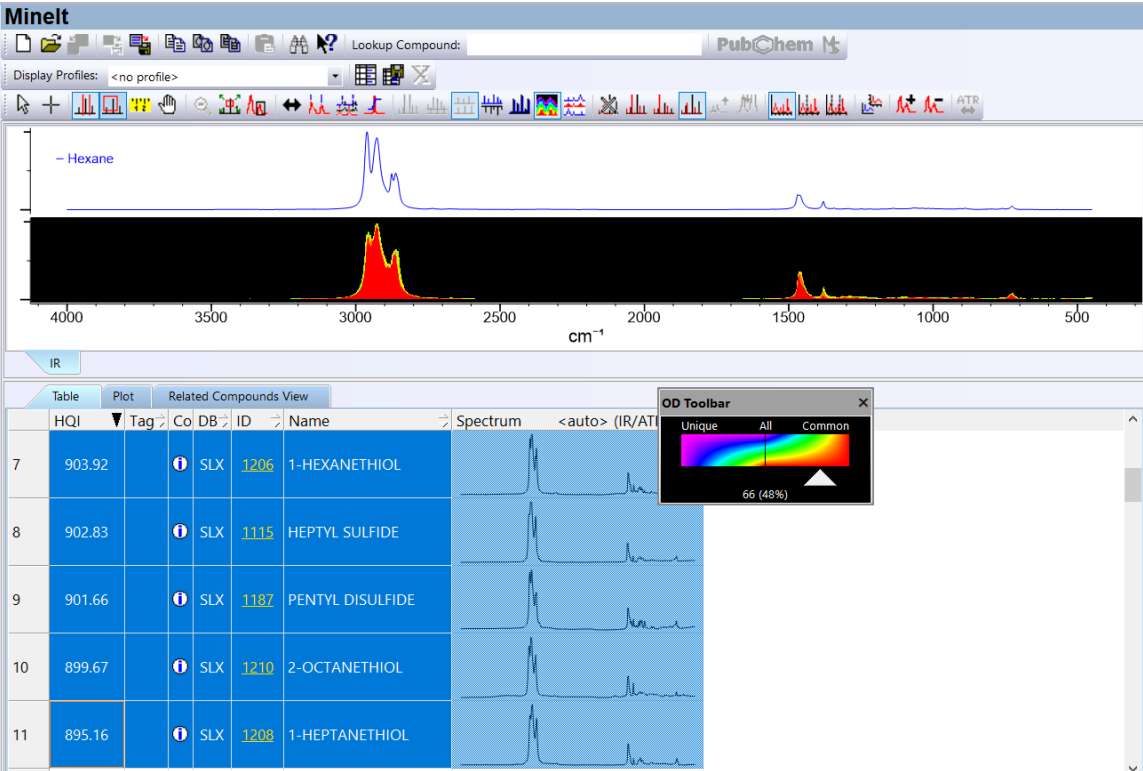
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3	Click <b>Search</b> .	<p>The results are displayed in the <b>Minelt</b> application.</p>  <p>The screenshot displays the Minelt application interface. At the top, there is a toolbar with various icons and a 'Lookup Compound:' field. Below this is a plot area showing IR spectra. The x-axis is labeled 'cm<sup>-1</sup>' and ranges from 4000 to 500. The y-axis represents intensity from 0 to 1. Two spectra are overlaid: a blue line for 'Hexane (Corrected)' and a red line for 'SLX #2; Hexane (Corrected)'. Both spectra show characteristic peaks for hexane, including a strong C-H stretching peak around 2900 cm<sup>-1</sup> and a C-C stretching peak around 1460 cm<sup>-1</sup>. To the right of the plot is a 'Structure/Properties' panel showing the skeletal structure of hexane and a table of properties.</p> <table border="1" data-bbox="1493 690 1864 987"> <thead> <tr> <th colspan="2">Substructs</th> <th colspan="2">Sel. Substructs</th> <th colspan="2">Original Data Files</th> </tr> <tr> <th colspan="2">All Properties</th> <th colspan="2">Attachments</th> <th colspan="2">Preferred Properties</th> </tr> <tr> <th>Name</th> <th></th> <th></th> <th></th> <th>Value</th> <th></th> </tr> </thead> <tbody> <tr> <td>Name</td> <td></td> <td></td> <td></td> <td>Hexane</td> <td></td> </tr> <tr> <td>Boiling Point</td> <td></td> <td></td> <td></td> <td>68.8C</td> <td></td> </tr> <tr> <td>CAS Registry Number</td> <td></td> <td></td> <td></td> <td>110-54-3</td> <td></td> </tr> <tr> <td>Formula</td> <td></td> <td></td> <td></td> <td>C<sub>6</sub>H<sub>14</sub></td> <td></td> </tr> <tr> <td>InChI</td> <td></td> <td></td> <td></td> <td>InChI=1S/C6H14/c1-3-5-6-4-2/h3-6H2,1-2H3</td> <td></td> </tr> <tr> <td>InChIKey</td> <td></td> <td></td> <td></td> <td>VLKZOEYOYAKHREP-UHFFFAOYSA-N</td> <td></td> </tr> <tr> <td>Molecular Weight</td> <td></td> <td></td> <td></td> <td>86.177 g/mol</td> <td></td> </tr> <tr> <td>Synonyms</td> <td></td> <td></td> <td></td> <td>n-Hexane</td> <td></td> </tr> <tr> <td>Technique</td> <td></td> <td></td> <td></td> <td>CAPILLARY CELL: NEAT</td> <td></td> </tr> </tbody> </table> <p>Below the plot is a 'Hit List' table with columns for HQI, Tag, Co, DE, ID, Name, and Spectrum. The table lists three hits:</p> <table border="1" data-bbox="699 776 1228 966"> <thead> <tr> <th>HQI</th> <th>Tag</th> <th>Co</th> <th>DE</th> <th>ID</th> <th>Name</th> <th>Spectrum</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>97.25</td> <td>SLX</td> <td>2</td> <td>1</td> <td>Hexane</td> <td>[Spectrum]</td> </tr> <tr> <td>2</td> <td>93.50</td> <td>SLX</td> <td>1</td> <td>2</td> <td>PENTANE</td> <td>[Spectrum]</td> </tr> <tr> <td>3</td> <td>93.08</td> <td>SLX</td> <td>3</td> <td>3</td> <td>HEPTANE</td> <td>[Spectrum]</td> </tr> </tbody> </table> <p>At the bottom of the hit list, there is a 'Hit List: Hexane' button.</p>	Substructs		Sel. Substructs		Original Data Files		All Properties		Attachments		Preferred Properties		Name				Value		Name				Hexane		Boiling Point				68.8C		CAS Registry Number				110-54-3		Formula				C <sub>6</sub> H <sub>14</sub>		InChI				InChI=1S/C6H14/c1-3-5-6-4-2/h3-6H2,1-2H3		InChIKey				VLKZOEYOYAKHREP-UHFFFAOYSA-N		Molecular Weight				86.177 g/mol		Synonyms				n-Hexane		Technique				CAPILLARY CELL: NEAT		HQI	Tag	Co	DE	ID	Name	Spectrum	1	97.25	SLX	2	1	Hexane	[Spectrum]	2	93.50	SLX	1	2	PENTANE	[Spectrum]	3	93.08	SLX	3	3	HEPTANE	[Spectrum]
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	Action	Result																																																																							
4	<p>Select the first 15 entries in the hit list.</p> <p><b>Note:</b> Select the first record, hold down the shift key, then scroll to and select the 15<sup>th</sup> entry.</p>	<p>All the selected hits are displayed in the spectral pane.</p>  <p><b>Minelt</b></p> <p>Lookup Compound: PubChem</p> <p>Display Profiles: &lt;no profile&gt;</p> <p>IR Spectrum (cm<sup>-1</sup>):</p> <ul style="list-style-type: none"> <li>- SLX #2: Hexane (Corrected)</li> <li>- SLX #1: PENTANE (Corrected)</li> <li>- SLX #3: HEPTANE (Corrected)</li> <li>- SLX #4: OCTANE (Corrected)</li> <li>- SLX #1204: 1-PENTANETHIOL (Corrected)</li> <li>- SLX #35: 4-METHYLOCTANE (Corrected)</li> <li>- SLX #1206: 1-HEXANETHIOL (Corrected)</li> <li>- SLX #1115: HEPTYL SULFIDE (Corrected)</li> <li>- SLX #1187: PENTYL DISULFIDE (Corrected)</li> <li>- SLX #1210: 2-OCTANETHIOL (Corrected)</li> <li>- SLX #1208: 1-HEPTANETHIOL (Corrected)</li> <li>- SLX #32: 2-METHYLHEPTANE (Corrected)</li> <li>- SLX #43: METHYLCYCLOPENTANE (Corrected)</li> <li>- SLX #5: NONANE (Corrected)</li> <li>- Hexane (Corrected)</li> <li>- SLX #36: 3-METHYLNONANE (Corrected)</li> </ul> <table border="1"> <thead> <tr> <th>Table</th> <th>Plot</th> <th colspan="3">Related Compounds View</th> <th>Spectrum</th> <th>&lt;auto&gt; (IR/ATR-IR)</th> </tr> <tr> <th>HQI</th> <th>Tag</th> <th>Col</th> <th>DI</th> <th>ID</th> <th>Name</th> <th></th> </tr> </thead> <tbody> <tr> <td>1</td> <td>97.25</td> <td>1</td> <td>SLX</td> <td>2</td> <td>Hexane</td> <td></td> </tr> <tr> <td>2</td> <td>93.50</td> <td>1</td> <td>SLX</td> <td>1</td> <td>PENTANE</td> <td></td> </tr> <tr> <td>3</td> <td>93.08</td> <td>1</td> <td>SLX</td> <td>3</td> <td>HEPTANE</td> <td></td> </tr> </tbody> </table> <p>Hit List: Hexane</p> <p><b>Structure/Properties</b></p> <table border="1"> <thead> <tr> <th>Substructs</th> <th>Sel. Substructs</th> <th>Original Data Files</th> </tr> <tr> <th>All Properties</th> <th>Attachments</th> <th>Preferred Properties</th> </tr> <tr> <th>Name</th> <th colspan="2">Value</th> </tr> </thead> <tbody> <tr> <td>Name</td> <td colspan="2">Hexane</td> </tr> <tr> <td>Boiling Point</td> <td colspan="2">68.8C</td> </tr> <tr> <td>CAS Registry Number</td> <td colspan="2">110-54-3</td> </tr> <tr> <td>Formula</td> <td colspan="2">C<sub>6</sub>H<sub>14</sub></td> </tr> <tr> <td>InChI</td> <td colspan="2">InChI=1S/C6H14/c1-3-5-6-4-2/h3-6H2,1-2H3</td> </tr> <tr> <td>InChIKey</td> <td colspan="2">VLKZOEYAKHREP-UHFFFAOYSA-N</td> </tr> <tr> <td>Molecular Weight</td> <td colspan="2">86.177 g/mol</td> </tr> <tr> <td>Synonyms</td> <td colspan="2">n-Hexane</td> </tr> <tr> <td>Technique</td> <td colspan="2">CAPILLARY CELL: NEAT</td> </tr> </tbody> </table>	Table	Plot	Related Compounds View			Spectrum	<auto> (IR/ATR-IR)	HQI	Tag	Col	DI	ID	Name		1	97.25	1	SLX	2	Hexane		2	93.50	1	SLX	1	PENTANE		3	93.08	1	SLX	3	HEPTANE		Substructs	Sel. Substructs	Original Data Files	All Properties	Attachments	Preferred Properties	Name	Value		Name	Hexane		Boiling Point	68.8C		CAS Registry Number	110-54-3		Formula	C <sub>6</sub> H <sub>14</sub>		InChI	InChI=1S/C6H14/c1-3-5-6-4-2/h3-6H2,1-2H3		InChIKey	VLKZOEYAKHREP-UHFFFAOYSA-N		Molecular Weight	86.177 g/mol		Synonyms	n-Hexane		Technique	CAPILLARY CELL: NEAT	
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### Change the spectral display to Overlap Density Heatmap


	Action	Result												
1	Click the <b>Overlap Density (OD) Heatmap</b> tool  in the <b>Spectral</b> toolbar.	<p>The spectral display changes, and the <b>Overlap Density (OD) Toolbar</b> 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 <b>OD Toolbar</b> 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 border="1" data-bbox="703 812 1354 950"> <thead> <tr> <th>HQI</th> <th>Tag</th> <th>Co. DB</th> <th>ID</th> <th>Name</th> <th>Spectrum</th> </tr> </thead> <tbody> <tr> <td>7</td> <td>903.92</td> <td>SLX</td> <td>1206</td> <td>1-HEXANETHIOL</td> <td></td> </tr> </tbody> </table>	HQI	Tag	Co. DB	ID	Name	Spectrum	7	903.92	SLX	1206	1-HEXANETHIOL	
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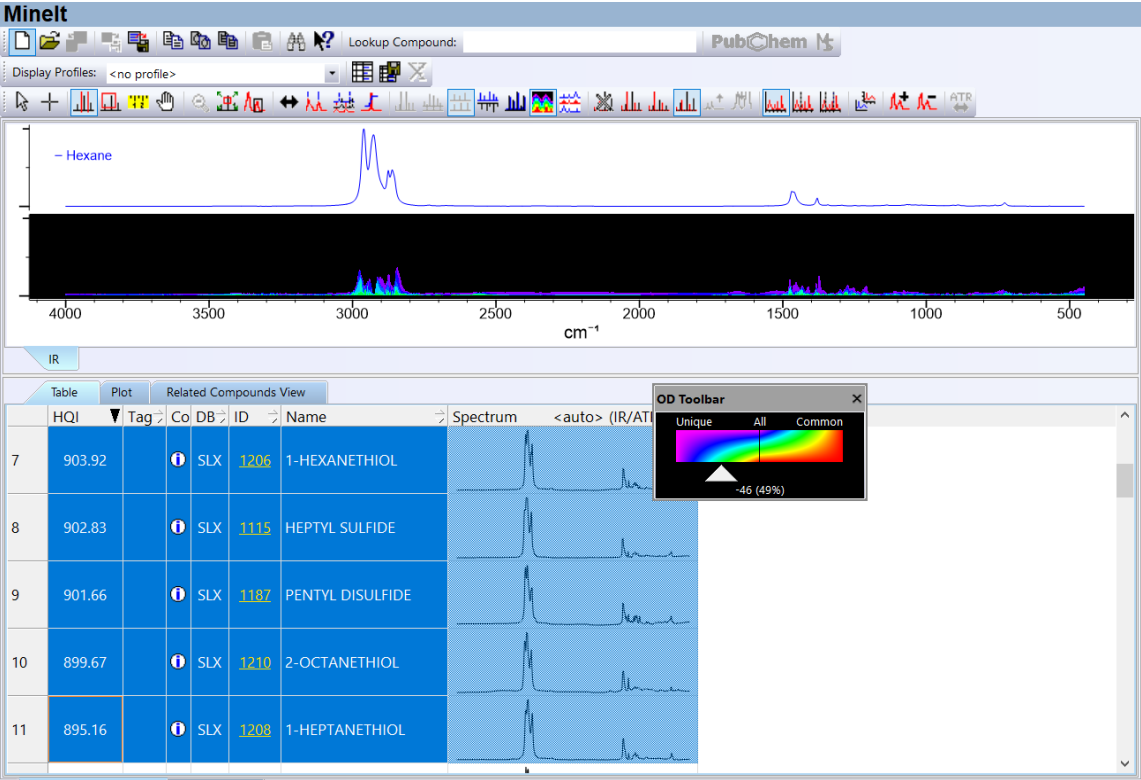


### Manipulate the Overlap Density Heatmap

	Action	Result
1	Move the slider on the <b>OD Toolbar</b> 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 Minelt software interface. At the top, there is a search bar for 'Lookup Compound' and a 'PubChem' logo. Below this is a 'Display Profiles' dropdown set to '&lt;no profile&gt;'. A toolbar with various icons is visible. The main plot area shows an IR spectrum for 'Hexane' with a wavenumber axis from 4000 to 500 cm<sup>-1</sup>. A heatmap overlay is present at the bottom of the plot. Below the plot is a table of 'Related Compounds View' with columns for HQI, Tag, Co, DB, ID, Name, and Spectrum. The table lists five compounds: 1-HEXANETHIOL, HEPTYL SULFIDE, PENTYL DISULFIDE, 2-OCTANETHIOL, and 1-HEPTANETHIOL. An 'OD Toolbar' window is overlaid on the right side of the table, showing a color scale from purple (Unique) to red (Common) and a slider set to 66 (48%).</p>

	Action	Result
2	Move the slider to the left.	<p>As the OD Level approaches -100, only the areas of lowest overlap—the unique areas—are shown.</p>  <p>The screenshot displays the Minelt software interface. At the top, there's a toolbar with various icons and a search bar. Below that, a plot shows the IR spectrum of Hexane, with the x-axis labeled in cm<sup>-1</sup> ranging from 4000 to 500. The spectrum shows several peaks, with a prominent one around 2900 cm<sup>-1</sup>. Below the plot, there's a table of related compounds with columns for HQI, Tag, Co, DB, ID, Name, and Spectrum. The table lists five compounds: 1-HEXANETHIOL, HEPTYL SULFIDE, PENTYL DISULFIDE, 2-OCTANETHIOL, and 1-HEPTANETHIOL. To the right of the table, there's an OD Toolbar with a slider and a color scale legend. The slider is positioned at -82 (28%), and the color scale ranges from purple (Unique) to red (Common).</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	Move the slider to the point where %AUC equals approximately 50%.	<p>The OD Level on the common side—or ODC—required to show 50% of the area that is most in common, is 62.</p>  <p>Another way to express this is to say that <math>ODC_{50} = 62</math>. An alternative is to say that <math>\%AUC_{42} = 50</math>.</p>

	Action	Result
4	Next, move the slider to the left to where %AUC equals approximately 50%.	<p>The OD Level on the unique side—or ODU—required to show 50% of the area that is most unique is -46.</p>  <p>Another way to express this is to say that <math>ODU_{50} = -64</math>. An alternative is to say that <math>\%AUC_{-64} = 50</math>.</p>
	<b>TIP</b>	<p>Use the <b>Horizontal Zoom</b> 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 <b>View Entire Spectrum</b> tool  to zoom out.</p>

# Data Mining & Analysis

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## 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.

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### 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

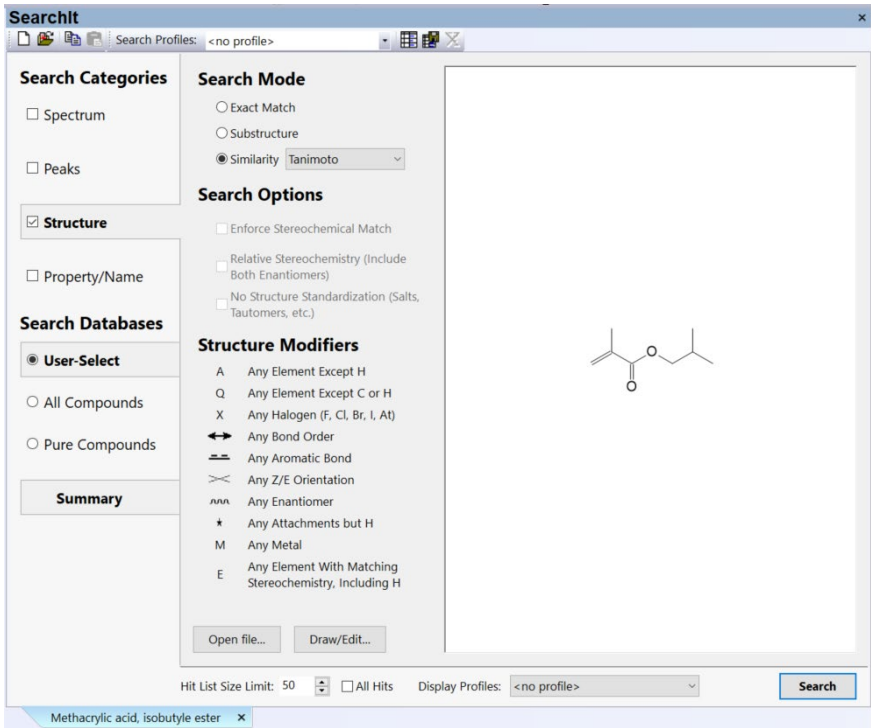
- Propiophenone Query.dsf

#### ***KnowItAll Applications Used***

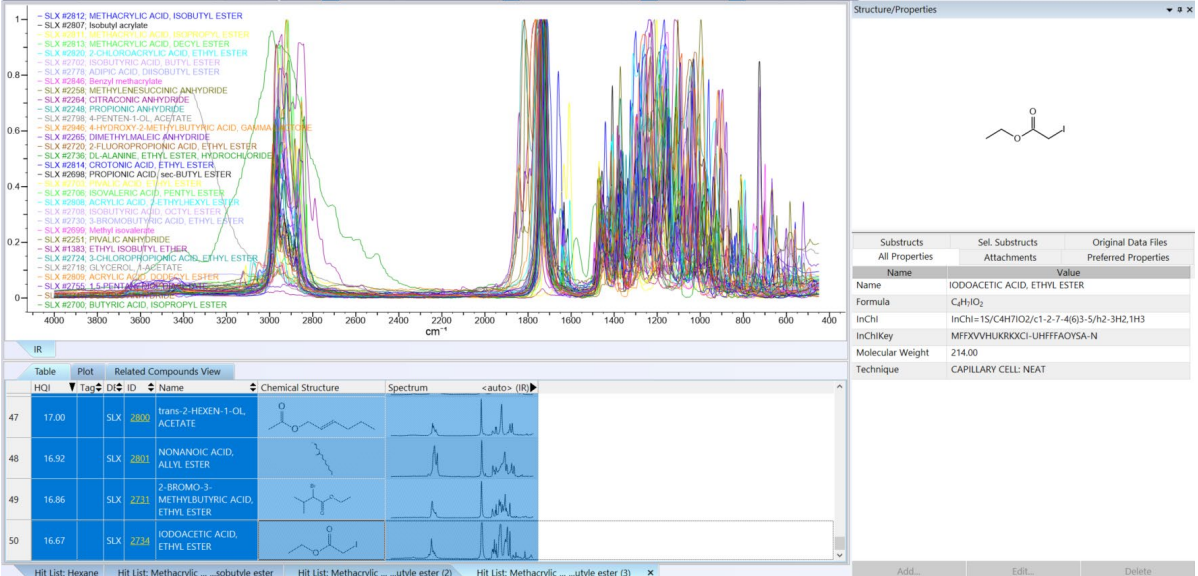
- SearchIt™
- Minelt™


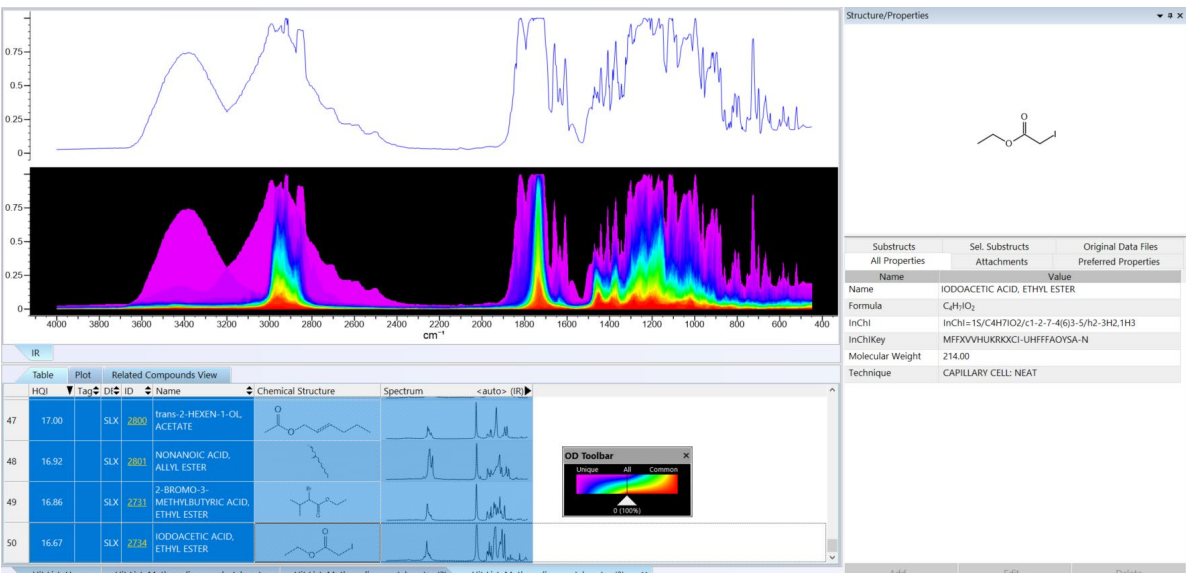
## Perform a substructure search

	Action	Result
1	<p>In the <b>SearchIt</b> application, click <b>User-select</b> under <b>Search Databases</b>.</p> <p>Under <b>Available for Searching</b>, select <b>IR - Sadtler Standards (Selected Subset) - Wiley</b> (DB Code SLX).</p> <p>Click <b>Add</b>.</p>	
2	<p>Click <b>Structure</b>.</p> <p>Click <b>Open Spectrum or Structure</b> icon.</p>	

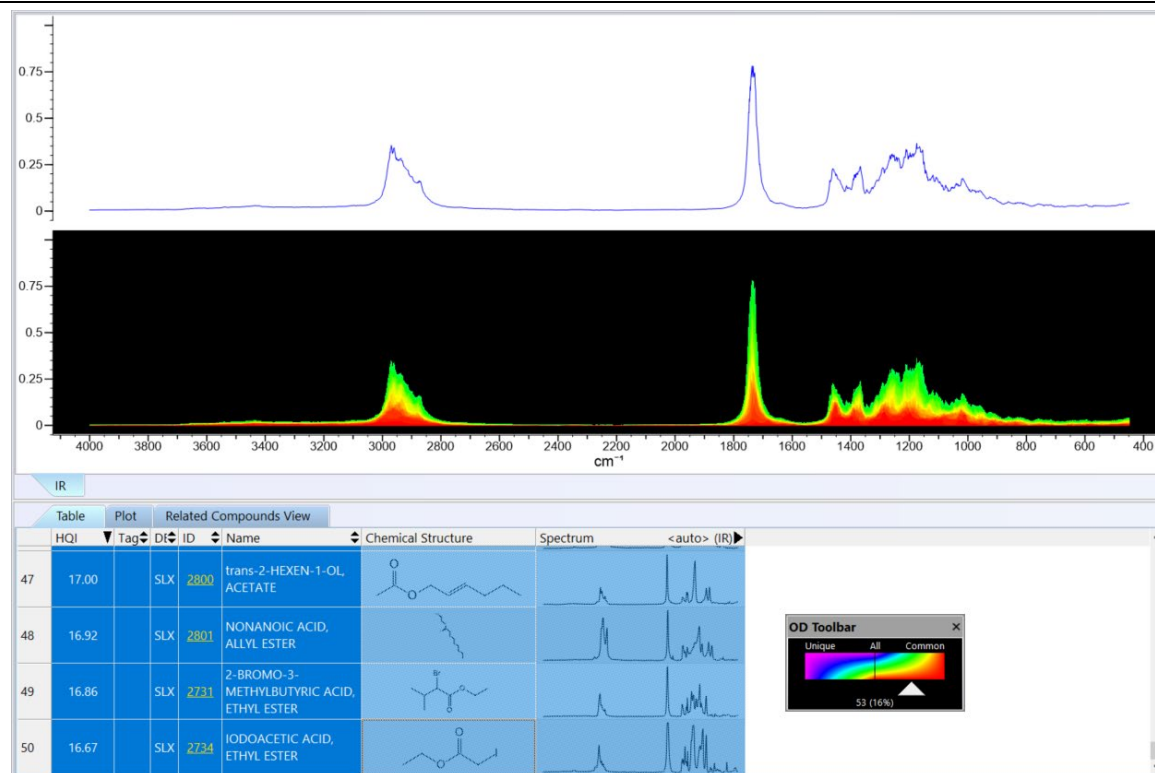
	Action	Result
3	Navigate to <b>C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Structues</b> folder.  Open <b>Methacrylic acid, isobutyle ester</b> .	The structure is displayed in the <b>Structure</b> tab.
4	Make sure <b>Search Mode</b> is set to <b>Similarity</b> , use default <b>Tanimoto</b> algorithm.  Click <b>Search</b> .	 <p>The screenshot shows the SearchIt application window. On the left, there are several sections: 'Search Categories' with 'Structure' checked; 'Search Databases' with 'User-Select' selected; and a 'Summary' button. The 'Search Mode' section has 'Similarity' selected with 'Tanimoto' as the algorithm. The 'Search Options' section has several unchecked checkboxes. The 'Structure Modifiers' section lists various options like 'Any Element Except H', 'Any Bond Order', etc. The main area displays a chemical structure of methacrylic acid isobutyle ester. At the bottom, there are controls for 'Hit List Size Limit' (50), 'All Hits' checkbox, 'Display Profiles' dropdown, and a 'Search' button. The window title bar shows 'Methacrylic acid, isobutyle ester'.</p>

### Examine the results in Minelt

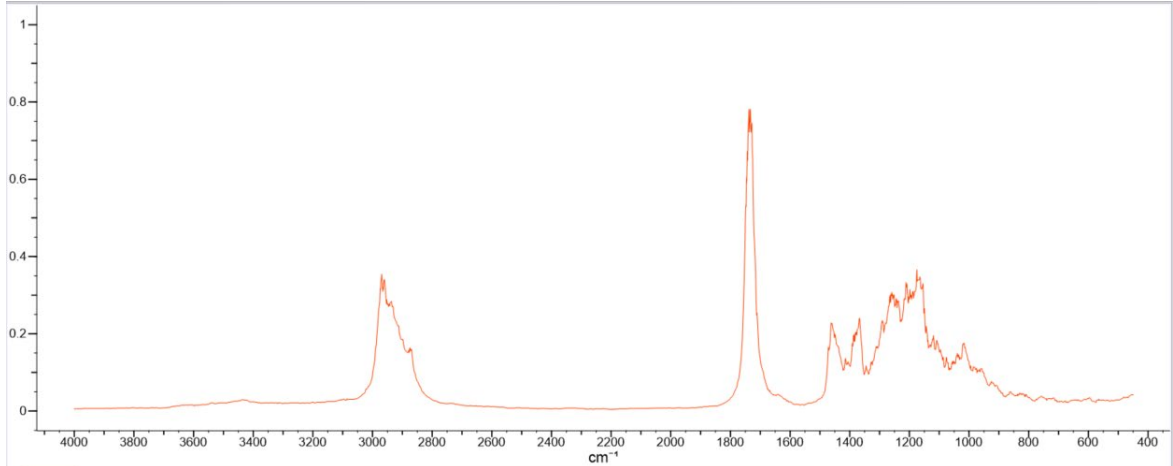
	Action	Result
1	<p>Select all eleven records in the hit list.</p> <p><b>Note:</b> Select the first record, hold down the shift key, then scroll to and select the last record.</p>	<p>All spectra are displayed in the spectral pane.</p> 
2	<p>Click the <b>OD Heatmap</b> toolbar button.</p>	

	Action	Result																																																									
3	Click the <b>OD Consensus Spectrum</b> toolbar button  .	<p>The consensus spectrum is displayed above the Overlap Density Heatmap.</p>  <p><b>Structure/Properties</b></p> <table border="1"> <thead> <tr> <th>Substructs</th> <th>Sel. Substructs</th> <th>Original Data Files</th> </tr> <tr> <th>All Properties</th> <th>Attachments</th> <th>Preferred Properties</th> </tr> <tr> <th>Name</th> <th colspan="2">Value</th> </tr> </thead> <tbody> <tr> <td>Name</td> <td colspan="2">IODOACETIC ACID, ETHYL ESTER</td> </tr> <tr> <td>Formula</td> <td colspan="2">C<sub>6</sub>H<sub>10</sub>O<sub>2</sub></td> </tr> <tr> <td>InChI</td> <td colspan="2">InChI=1S/C4H7O2/c1-2-7-4(6)-5/h2-3H2,1H3</td> </tr> <tr> <td>InChIKey</td> <td colspan="2">MFFXVHVURKXCI-UHFFFAOYSA-N</td> </tr> <tr> <td>Molecular Weight</td> <td colspan="2">214.00</td> </tr> <tr> <td>Technique</td> <td colspan="2">CAPILLARY CELL: NEAT</td> </tr> </tbody> </table> <table border="1"> <thead> <tr> <th>HQI</th> <th>Tag</th> <th>ID</th> <th>Name</th> <th>Chemical Structure</th> <th>Spectrum</th> </tr> </thead> <tbody> <tr> <td>47</td> <td>17.00</td> <td>SLX_2890</td> <td>trans-2-HEXEN-1-OL, ACETATE</td> <td></td> <td></td> </tr> <tr> <td>48</td> <td>16.92</td> <td>SLX_2891</td> <td>NONANOIC ACID, ALLYL ESTER</td> <td></td> <td></td> </tr> <tr> <td>49</td> <td>16.86</td> <td>SLX_2231</td> <td>2-BROMO-3-METHYLBUTYRIC ACID, ETHYL ESTER</td> <td></td> <td></td> </tr> <tr> <td>50</td> <td>16.67</td> <td>SLX_4236</td> <td>IODOACETIC ACID, ETHYL ESTER</td> <td></td> <td></td> </tr> </tbody> </table>	Substructs	Sel. Substructs	Original Data Files	All Properties	Attachments	Preferred Properties	Name	Value		Name	IODOACETIC ACID, ETHYL ESTER		Formula	C <sub>6</sub> H <sub>10</sub> O <sub>2</sub>		InChI	InChI=1S/C4H7O2/c1-2-7-4(6)-5/h2-3H2,1H3		InChIKey	MFFXVHVURKXCI-UHFFFAOYSA-N		Molecular Weight	214.00		Technique	CAPILLARY CELL: NEAT		HQI	Tag	ID	Name	Chemical Structure	Spectrum	47	17.00	SLX_2890	trans-2-HEXEN-1-OL, ACETATE			48	16.92	SLX_2891	NONANOIC ACID, ALLYL ESTER			49	16.86	SLX_2231	2-BROMO-3-METHYLBUTYRIC ACID, ETHYL ESTER			50	16.67	SLX_4236	IODOACETIC ACID, ETHYL ESTER		
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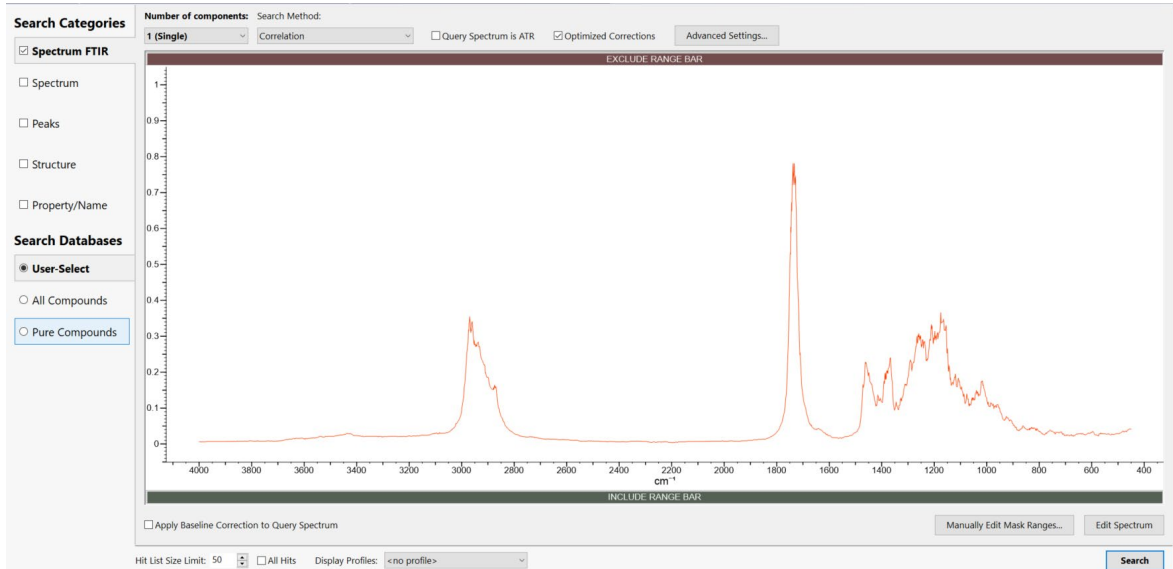
4 Move the OD Toobar to around 50 (16%)





	Action	Result
5	Click the <b>OD Heatmap</b> toolbar button again to turn off this display.	<p>The consensus spectrum remains in the display.</p> 

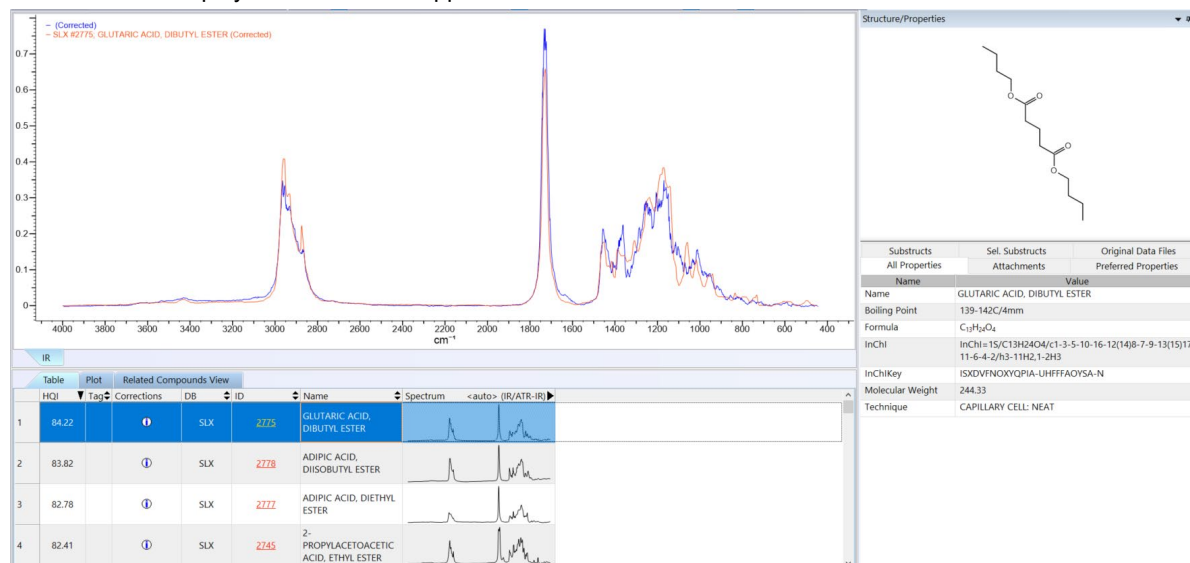
### Use the consensus spectrum to perform a search

	Action	Result
1	Click <b>SearchIt</b> in the <b>Transfer to</b> bar.	<p>The consensus spectrum is displayed on the <b>IR Spectrum</b> search tab.</p> 

2 Click the **Search** button.

**Note:** The IR - Sadtler Standards (Selected Subset) - Wiley database remains in the spectrum pane.

The results are displayed in the **Minelt** application on a new tab.



You got a hit list where hits are structurally similar to that of **Methacrylic acid, isobutyle ester**