

# **KnowItAll Software Training**

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## 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.

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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***

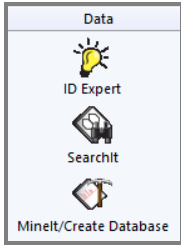
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\IR

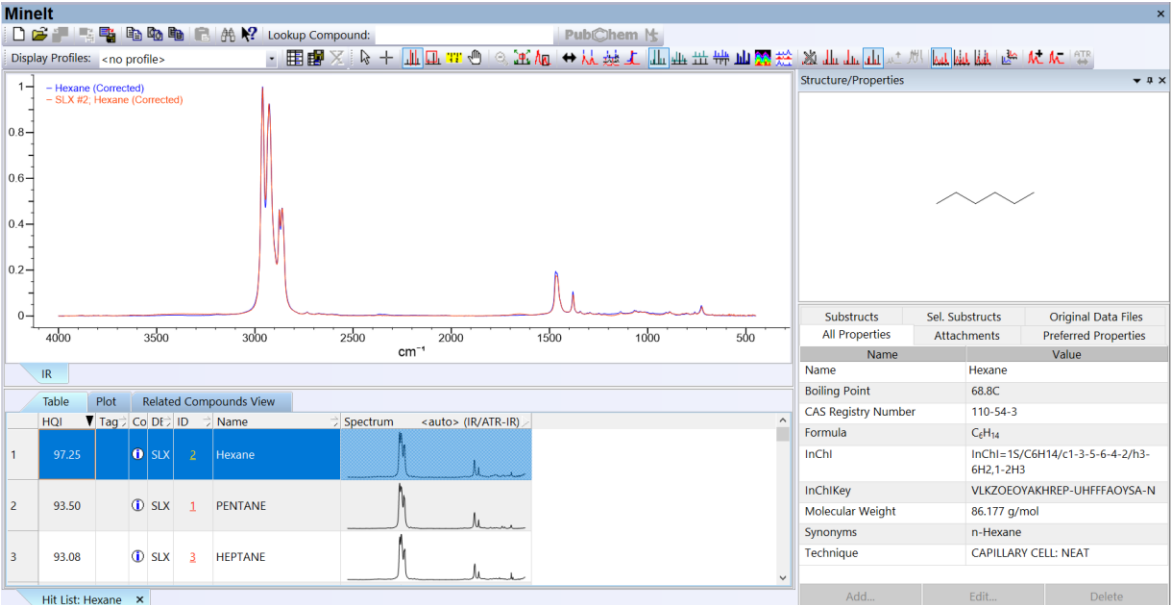
- Hexane.jdx

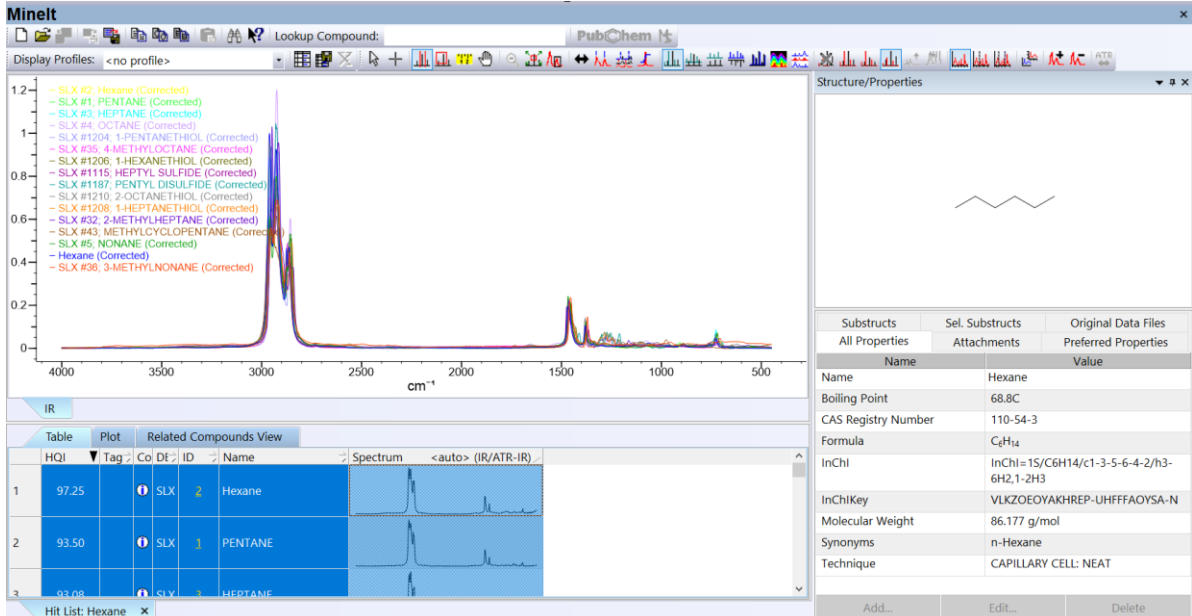
#### ***KnowItAll Applications Used***

- Minelt


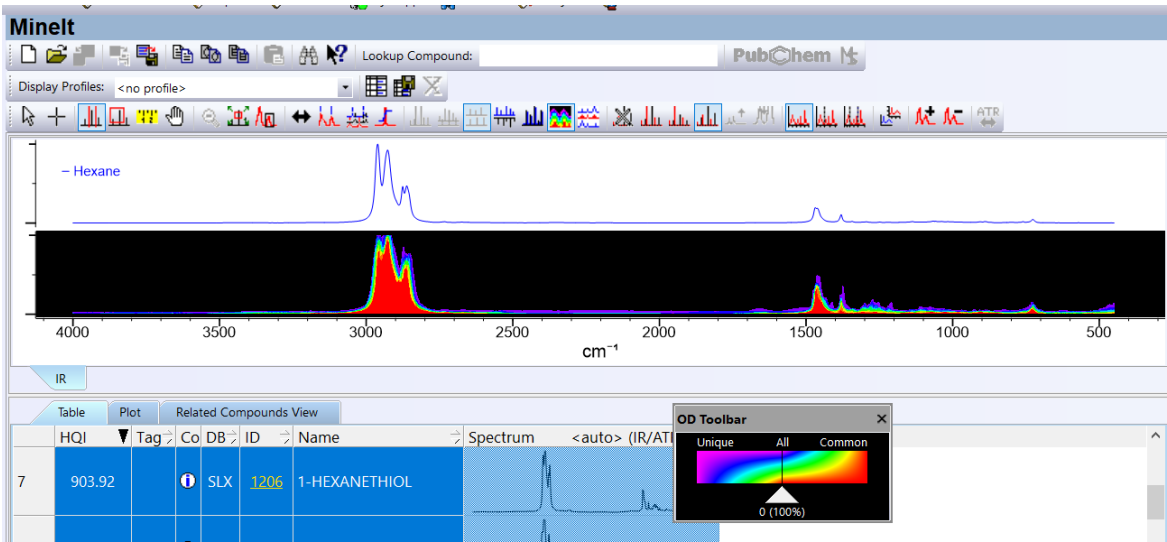
## Open a spectral hit list in the Minelt application

	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>	

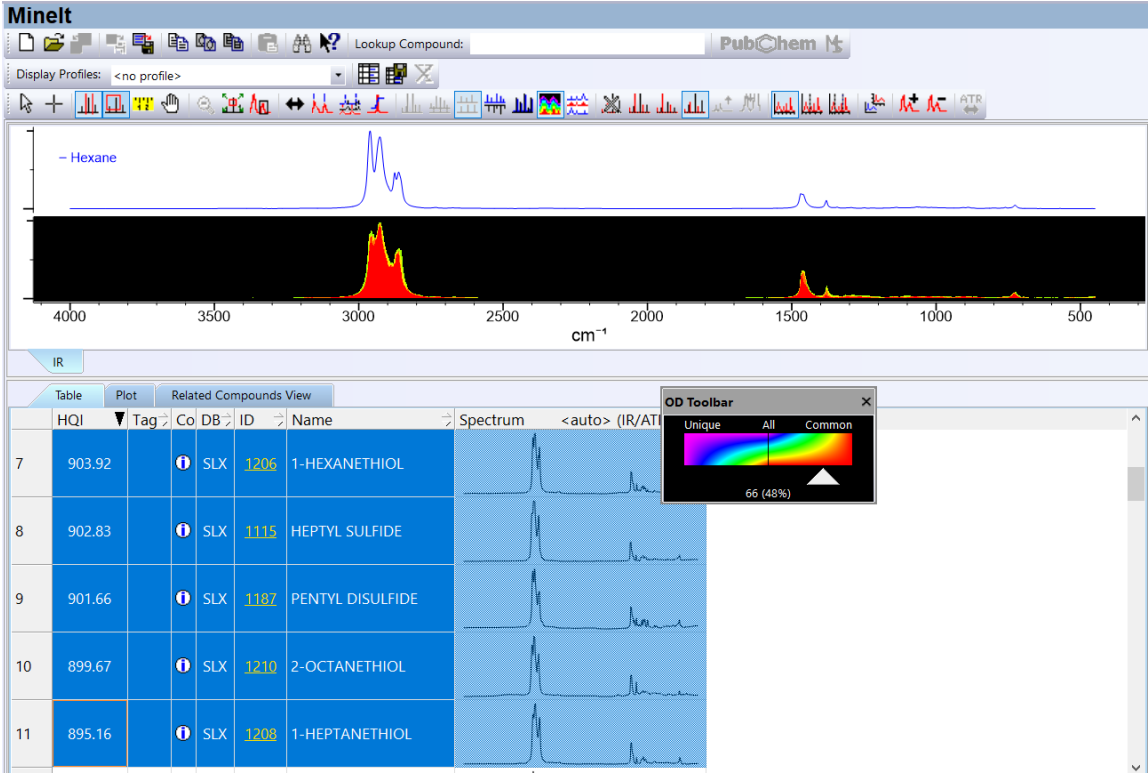
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3	Click <b>Search</b> .	<p>The results are displayed in the <b>Minelt</b> application.</p>  <p>The screenshot displays the Minelt application interface. At the top, there is a toolbar with various icons and a 'Lookup Compound:' field. Below this is an IR spectrum plot with the x-axis labeled 'cm<sup>-1</sup>' ranging from 4000 to 500 and the y-axis ranging from 0 to 1. The plot shows two traces: a blue trace for 'Hexane (Corrected)' and a red trace for 'SLX #2; Hexane (Corrected)'. Below the plot is a table with columns for 'Table', 'Plot', 'Related Compounds View', 'HQI', 'Tag', 'Co', 'DE', 'ID', 'Name', and 'Spectrum'. The table lists three results: Hexane (HQI 97.25, ID 2), PENTANE (HQI 93.50, ID 1), and HEPTANE (HQI 93.08, ID 3). To the right of the table is a 'Structure/Properties' window showing the chemical structure of Hexane and a table of its 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>Name</th> <th></th> <th>Name</th> <th>Value</th> </tr> </thead> <tbody> <tr> <td>Name</td> <td>Hexane</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>Boiling Point</td> <td>68.8C</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>CAS Registry Number</td> <td>110-54-3</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>Formula</td> <td>C<sub>6</sub>H<sub>14</sub></td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>InChI</td> <td>InChI=1S/C6H14/c1-3-5-6-4-2/h3-6H2,1-2H3</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>InChIKey</td> <td>VLKZOEYAKHREP-UHFFFAOYSA-N</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>Molecular Weight</td> <td>86.177 g/mol</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>Synonyms</td> <td>n-Hexane</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>Technique</td> <td>CAPILLARY CELL: NEAT</td> <td></td> <td></td> <td></td> <td></td> </tr> </tbody> </table>	Substructs		Sel. Substructs		Original Data Files		All Properties		Attachments		Preferred Properties		Name		Name		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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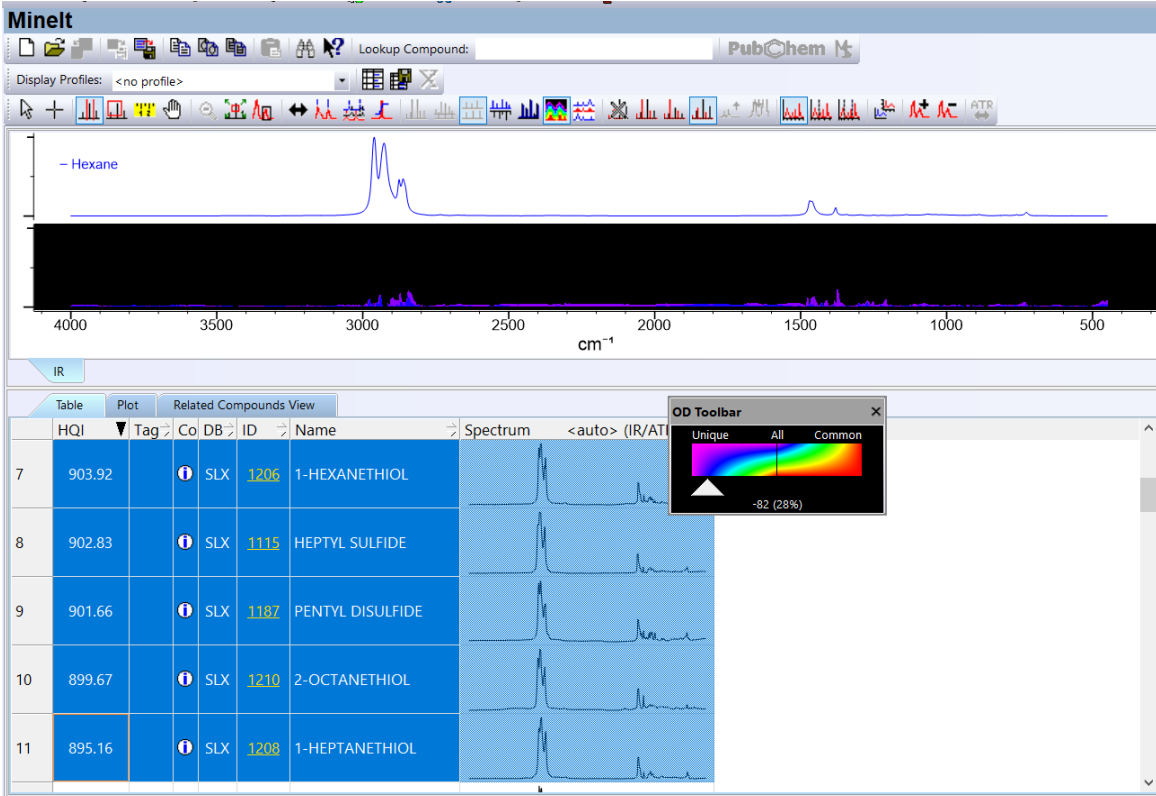
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4	<p>Select the first 15 entries in the hit list.</p> <p><b>Note:</b> Select the first record, hold down the shift key, then scroll to and select the 15<sup>th</sup> entry.</p>	<p>All the selected hits are displayed in the spectral pane.</p>  <p><b>Minelt</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="4">Related Compounds View</th> <th>Spectrum</th> </tr> <tr> <th>HQI</th> <th>Tag</th> <th>Col</th> <th>DE</th> <th>ID</th> <th>Name</th> <th>&lt;auto&gt; (IR/ATR-IR)</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>97.25</td> <td>SLX</td> <td>2</td> <td></td> <td>Hexane</td> <td></td> </tr> <tr> <td>2</td> <td>93.50</td> <td>SLX</td> <td>1</td> <td></td> <td>PENTANE</td> <td></td> </tr> <tr> <td>3</td> <td>93.08</td> <td>SLX</td> <td>3</td> <td></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	HQI	Tag	Col	DE	ID	Name	<auto> (IR/ATR-IR)	1	97.25	SLX	2		Hexane		2	93.50	SLX	1		PENTANE		3	93.08	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

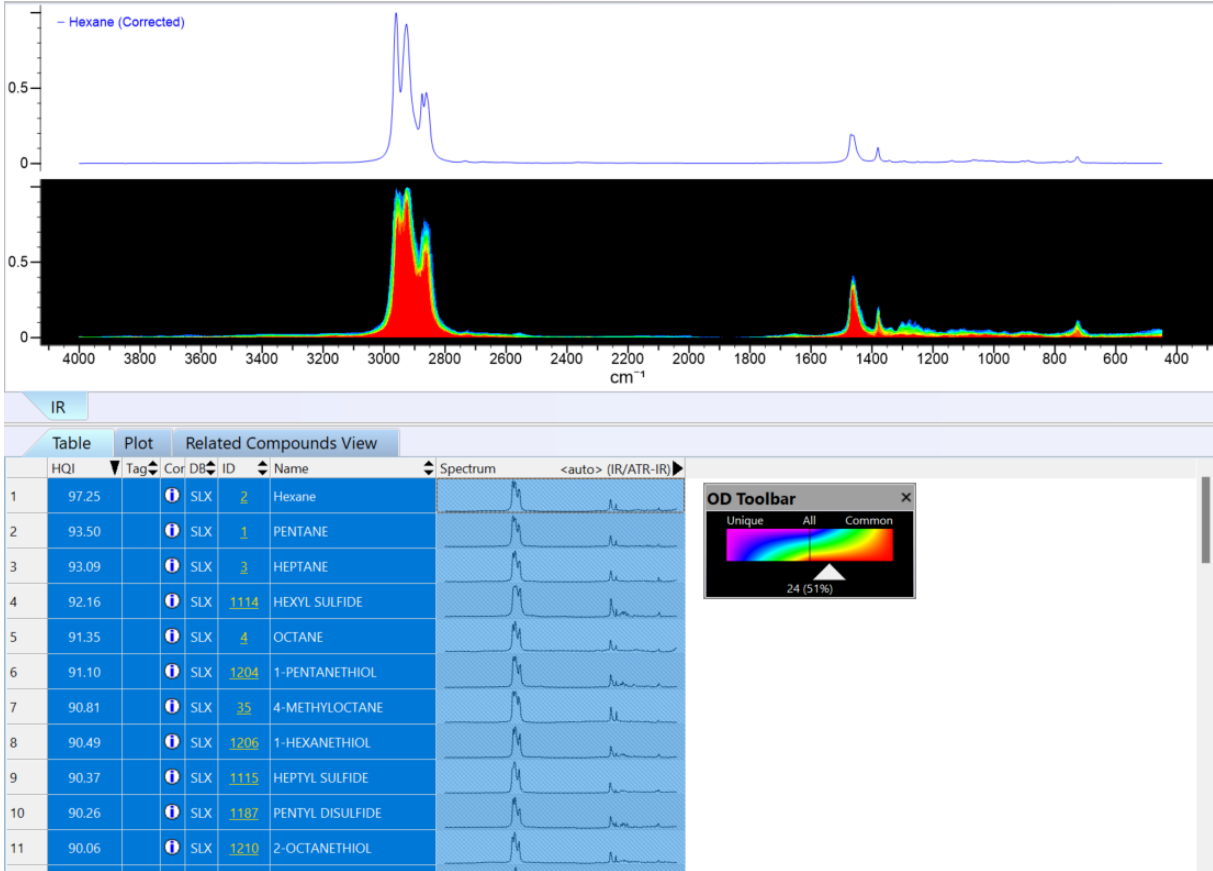
	Action	Result
1	Click the <b>Overlap Density (OD) Heatmap</b> button  in the <b>Spectral</b> toolbar.	<p>The spectral display changes, and the <b>Overlap Density (OD) Toolbar</b> is added to the display.</p>  <p>The default Overlap Density Heatmap display shows all overlap levels. High levels of overlap 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>

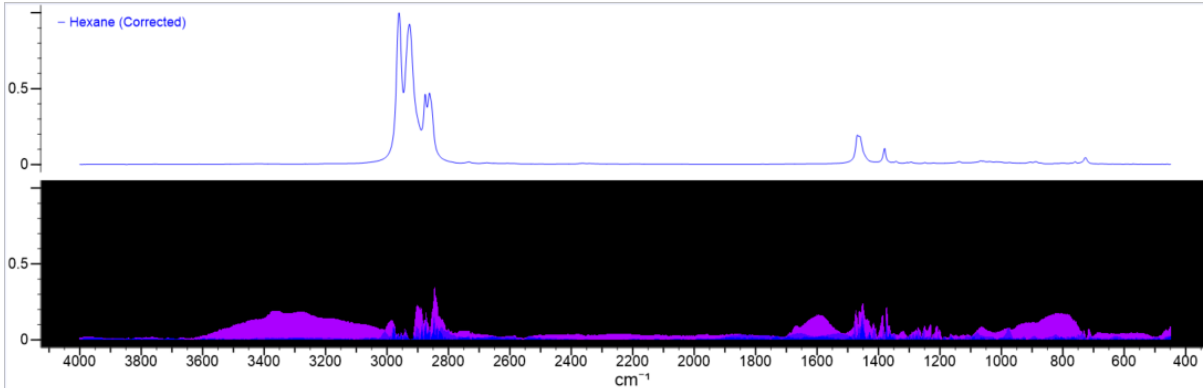
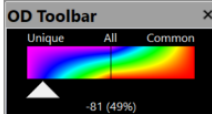
### Manipulate the Overlap Density Heatmap

	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's a toolbar with various icons and a 'Lookup Compound' field. Below that, a plot shows the IR spectrum of Hexane, with a red heatmap overlay indicating areas of overlap. The x-axis is labeled 'cm<sup>-1</sup>' and ranges from 4000 to 500. 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. An 'OD Toolbar' is overlaid on the right side of the table, showing a heatmap and a slider set to 66 (48%).</p> <table border="1" data-bbox="674 828 1375 1214"> <thead> <tr> <th>HQI</th> <th>Tag</th> <th>Co</th> <th>DB</th> <th>ID</th> <th>Name</th> <th>Spectrum</th> </tr> </thead> <tbody> <tr> <td>7</td> <td>903.92</td> <td>SLX</td> <td>1206</td> <td>1-HEXANETHIOL</td> <td>[Spectrum]</td> </tr> <tr> <td>8</td> <td>902.83</td> <td>SLX</td> <td>1115</td> <td>HEPTYL SULFIDE</td> <td>[Spectrum]</td> </tr> <tr> <td>9</td> <td>901.66</td> <td>SLX</td> <td>1187</td> <td>PENTYL DISULFIDE</td> <td>[Spectrum]</td> </tr> <tr> <td>10</td> <td>899.67</td> <td>SLX</td> <td>1210</td> <td>2-OCTANETHIOL</td> <td>[Spectrum]</td> </tr> <tr> <td>11</td> <td>895.16</td> <td>SLX</td> <td>1208</td> <td>1-HEPTANETHIOL</td> <td>[Spectrum]</td> </tr> </tbody> </table>	HQI	Tag	Co	DB	ID	Name	Spectrum	7	903.92	SLX	1206	1-HEXANETHIOL	[Spectrum]	8	902.83	SLX	1115	HEPTYL SULFIDE	[Spectrum]	9	901.66	SLX	1187	PENTYL DISULFIDE	[Spectrum]	10	899.67	SLX	1210	2-OCTANETHIOL	[Spectrum]	11	895.16	SLX	1208	1-HEPTANETHIOL	[Spectrum]
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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 shows the Minelt software interface. At the top, there's a toolbar with various icons and a 'Lookup Compound:' field. Below that, a plot shows the IR spectrum of Hexane, with the x-axis labeled 'cm<sup>-1</sup>' ranging from 4000 to 500. The spectrum shows several peaks, with the most prominent ones between 2800 and 3000 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 color scale from purple (Unique) to red (Common) and a slider set to -82 (28%).</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>



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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 24.</p>  <p>Another way to express this is to say that <math>ODC_{50} = 24</math>. An alternative is to say that <math>\%AUC_{24} = 50</math>.</p> <table border="1" data-bbox="653 829 1333 1268"> <thead> <tr> <th>HQI</th> <th>Tag</th> <th>Cor</th> <th>DB</th> <th>ID</th> <th>Name</th> <th>Spectrum</th> </tr> </thead> <tbody> <tr><td>1</td><td>97.25</td><td></td><td>SLX</td><td>2</td><td>Hexane</td><td></td></tr> <tr><td>2</td><td>93.50</td><td></td><td>SLX</td><td>1</td><td>PENTANE</td><td></td></tr> <tr><td>3</td><td>93.09</td><td></td><td>SLX</td><td>3</td><td>HEPTANE</td><td></td></tr> <tr><td>4</td><td>92.16</td><td></td><td>SLX</td><td>1114</td><td>HEXYL SULFIDE</td><td></td></tr> <tr><td>5</td><td>91.35</td><td></td><td>SLX</td><td>4</td><td>OCTANE</td><td></td></tr> <tr><td>6</td><td>91.10</td><td></td><td>SLX</td><td>1204</td><td>1-PENTANETHIOL</td><td></td></tr> <tr><td>7</td><td>90.81</td><td></td><td>SLX</td><td>35</td><td>4-METHYLOCTANE</td><td></td></tr> <tr><td>8</td><td>90.49</td><td></td><td>SLX</td><td>1206</td><td>1-HEXANETHIOL</td><td></td></tr> <tr><td>9</td><td>90.37</td><td></td><td>SLX</td><td>1115</td><td>HEPTYL SULFIDE</td><td></td></tr> <tr><td>10</td><td>90.26</td><td></td><td>SLX</td><td>1187</td><td>PENTYL DISULFIDE</td><td></td></tr> <tr><td>11</td><td>90.06</td><td></td><td>SLX</td><td>1210</td><td>2-OCTANETHIOL</td><td></td></tr> </tbody> </table>	HQI	Tag	Cor	DB	ID	Name	Spectrum	1	97.25		SLX	2	Hexane		2	93.50		SLX	1	PENTANE		3	93.09		SLX	3	HEPTANE		4	92.16		SLX	1114	HEXYL SULFIDE		5	91.35		SLX	4	OCTANE		6	91.10		SLX	1204	1-PENTANETHIOL		7	90.81		SLX	35	4-METHYLOCTANE		8	90.49		SLX	1206	1-HEXANETHIOL		9	90.37		SLX	1115	HEPTYL SULFIDE		10	90.26		SLX	1187	PENTYL DISULFIDE		11	90.06		SLX	1210	2-OCTANETHIOL	
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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 -81.</p>  <p>IR</p> <table border="1"> <thead> <tr> <th>Table</th> <th>Plot</th> <th colspan="2">Related Compounds View</th> <th>Spectrum</th> </tr> <tr> <th>HQI</th> <th>Tag</th> <th>Cor</th> <th>ID</th> <th>Name</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>97.25</td> <td>SLX</td> <td>2</td> <td>Hexane</td> </tr> <tr> <td>2</td> <td>93.50</td> <td>SLX</td> <td>1</td> <td>PENTANE</td> </tr> <tr> <td>3</td> <td>93.09</td> <td>SLX</td> <td>3</td> <td>HEPTANE</td> </tr> <tr> <td>4</td> <td>92.16</td> <td>SLX</td> <td>1114</td> <td>HEXYL SULFIDE</td> </tr> <tr> <td>5</td> <td>91.35</td> <td>SLX</td> <td>4</td> <td>OCTANE</td> </tr> <tr> <td>6</td> <td>91.10</td> <td>SLX</td> <td>1204</td> <td>1-PENTANETHIOL</td> </tr> <tr> <td>7</td> <td>90.81</td> <td>SLX</td> <td>35</td> <td>4-METHYLOCTANE</td> </tr> <tr> <td>8</td> <td>90.49</td> <td>SLX</td> <td>1206</td> <td>1-HEXANETHIOL</td> </tr> <tr> <td>9</td> <td>90.37</td> <td>SLX</td> <td>1115</td> <td>HEPTYL SULFIDE</td> </tr> <tr> <td>10</td> <td>90.26</td> <td>SLX</td> <td>1187</td> <td>PENTYL DISULFIDE</td> </tr> <tr> <td>11</td> <td>90.06</td> <td>SLX</td> <td>1210</td> <td>2-OCTANETHIOL</td> </tr> </tbody> </table>  <p>Another way to express this is to say that <math>ODU_{50} = -81</math>. An alternative is to say that <math>\%AUC_{-81} = 50</math>.</p>	Table	Plot	Related Compounds View		Spectrum	HQI	Tag	Cor	ID	Name	1	97.25	SLX	2	Hexane	2	93.50	SLX	1	PENTANE	3	93.09	SLX	3	HEPTANE	4	92.16	SLX	1114	HEXYL SULFIDE	5	91.35	SLX	4	OCTANE	6	91.10	SLX	1204	1-PENTANETHIOL	7	90.81	SLX	35	4-METHYLOCTANE	8	90.49	SLX	1206	1-HEXANETHIOL	9	90.37	SLX	1115	HEPTYL SULFIDE	10	90.26	SLX	1187	PENTYL DISULFIDE	11	90.06	SLX	1210	2-OCTANETHIOL
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**TIP**

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.

# 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

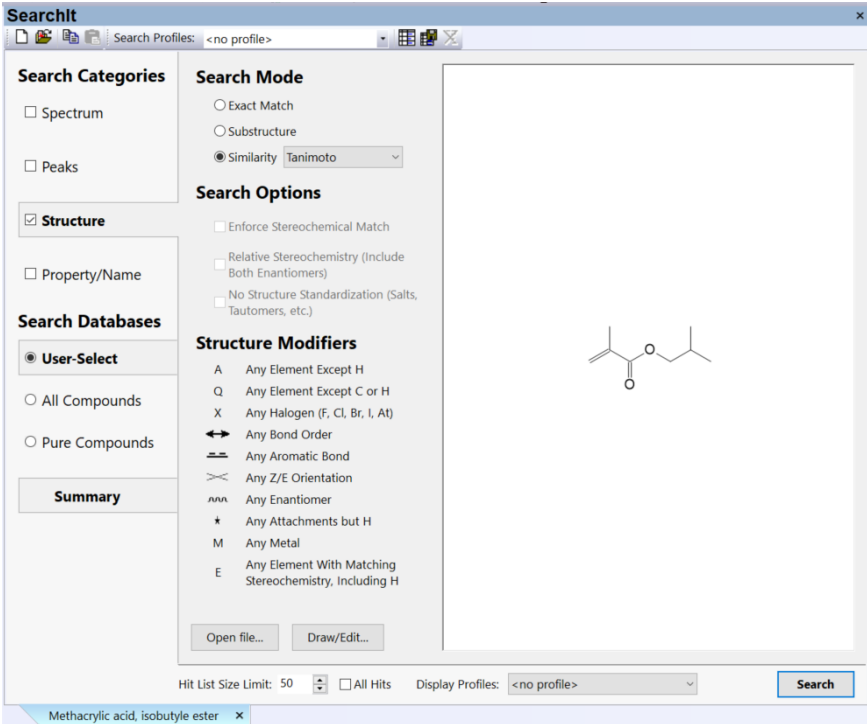
- Propiophenone Query.dsf

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

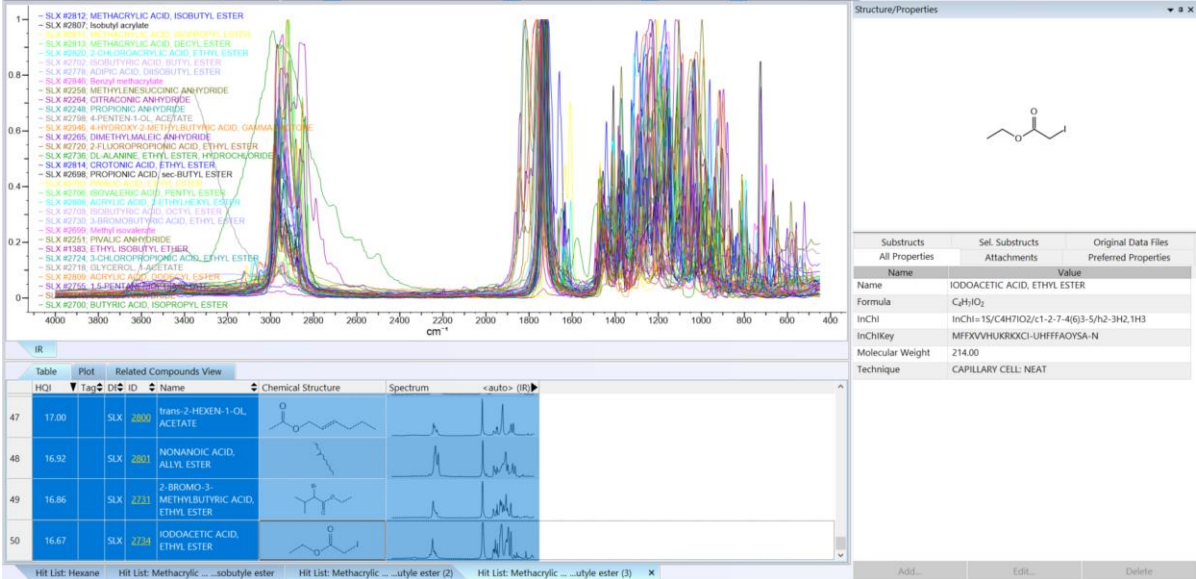

- SearchIt
- Minelt


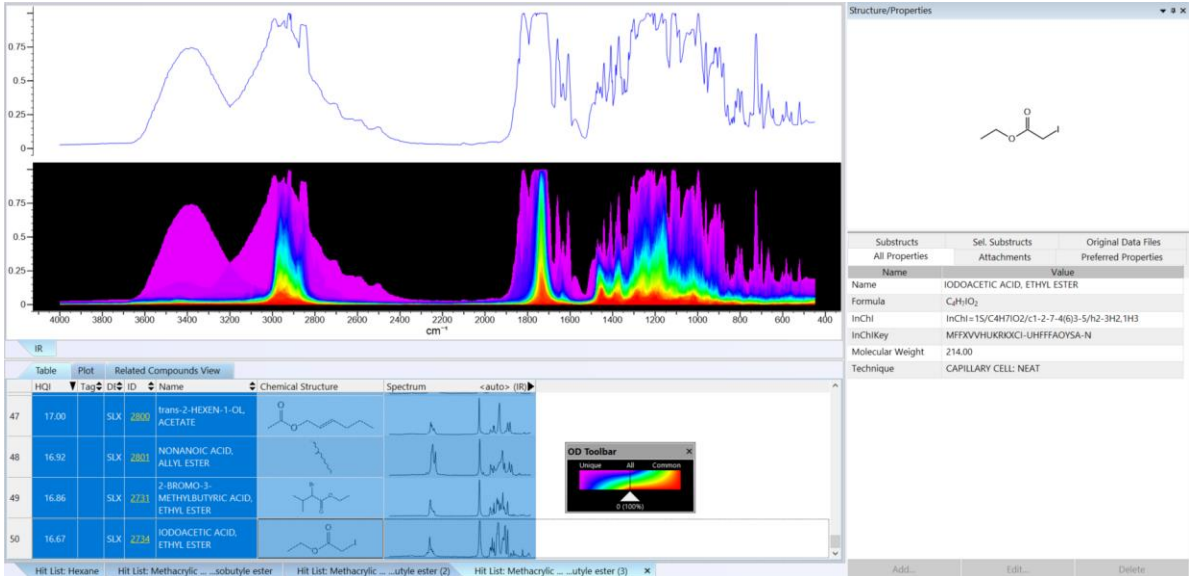
## Perform a substructure search

	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 File...</b> or Click <b>Open Spectrum or Structure</b> icon.</p>	
3	<p>Navigate to <b>C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Structures</b> folder.</p> <p>Open <b>Methacrylic acid, isobutyle ester</b>.</p>	The structure is displayed in the <b>Structure</b> tab.

	Action	Result
4	<p>Make sure <b>Search Mode</b> is set to <b>Similarity</b>, use default <b>Tanimoto</b> algorithm.</p> <p>Click <b>Search</b>.</p>	 <p>The screenshot shows the SearchIt application window. The 'Search Categories' section has 'Structure' checked. The 'Search Mode' section has 'Similarity' selected with the 'Tanimoto' algorithm chosen from a dropdown. 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 main search area displays a chemical structure of methyl acrylate. At the bottom, there are fields for 'Hit List Size Limit: 50', 'All Hits' checkbox, 'Display Profiles: &lt;no profile&gt;', and a 'Search' button. A status bar at the very bottom shows 'Methacrylic acid, isobutyle ester'.</p>

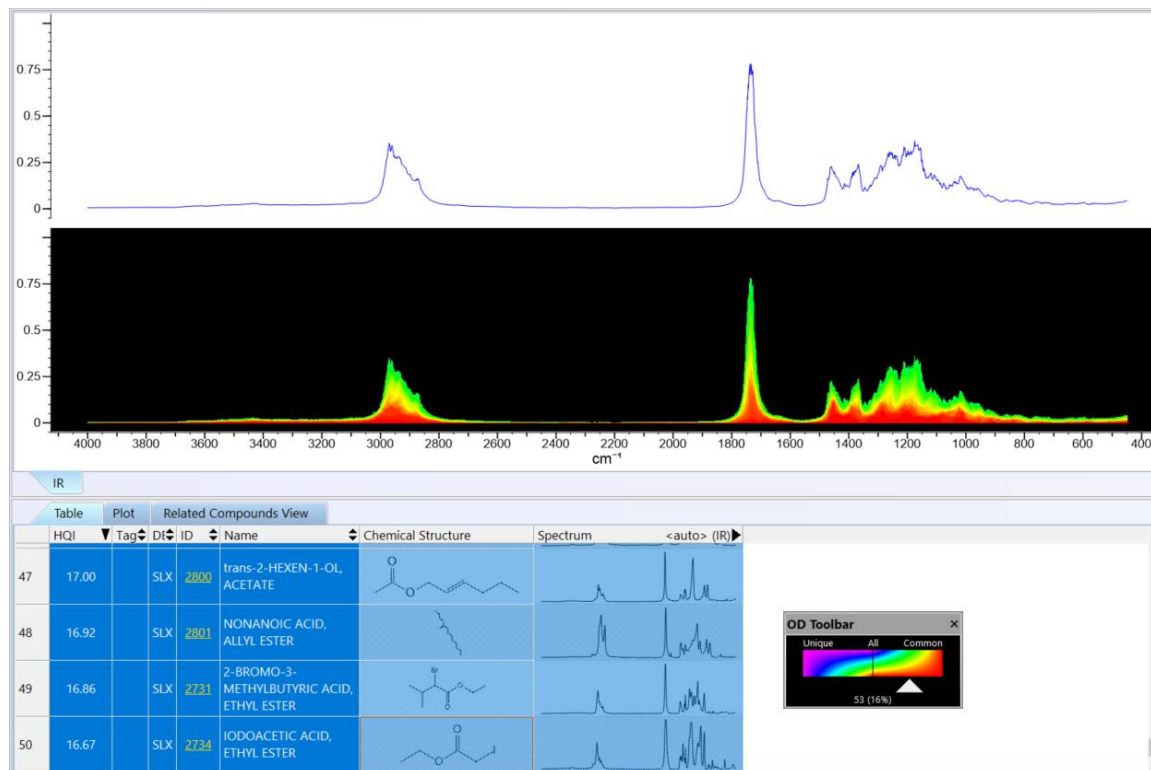
### Examine the results in Minelt

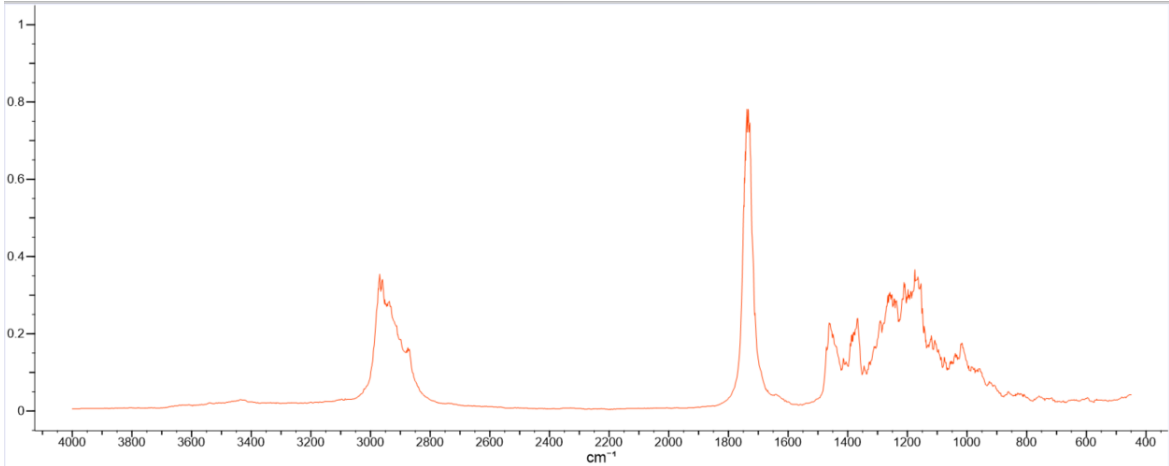
	Action	Result
1	<p>Select all records in the hit list.</p> <p><b>Note:</b> Select the first record, hold down the shift key, then scroll to and select the last record.</p>	<p>All spectra are displayed in the spectral pane.</p> 
2	<p>Click the <b>OD Heatmap</b> button  in the spectral toolbar.</p>	

	Action	Result																																																														
3	Click the <b>OD Consensus Spectrum</b> button  in the toolbar.	The consensus spectrum is displayed above the Overlap Density Heatmap.  <p>The screenshot displays the software interface with the following components:</p> <ul style="list-style-type: none"> <li><b>IR Spectrum:</b> A plot showing transmittance vs. wavenumber (cm<sup>-1</sup>) from 4000 to 400. The top trace is a single spectrum, and the bottom is an overlap density heatmap.</li> <li><b>Chemical Structure:</b> A skeletal structure of ethyl acetate is shown in the 'Structure/Properties' panel.</li> <li><b>Properties Table:</b> <table border="1"> <thead> <tr> <th colspan="2">Substructs</th> <th>Sel. Substructs</th> <th>Original Data Files</th> </tr> <tr> <th>All Properties</th> <th>Attachments</th> <th>Preferred Properties</th> <th></th> </tr> </thead> <tbody> <tr> <td>Name</td> <td colspan="2">IODOACETIC ACID, ETHYL ESTER</td> <td>Value</td> </tr> <tr> <td>Formula</td> <td colspan="2">C<sub>6</sub>H<sub>10</sub>O<sub>2</sub></td> <td></td> </tr> <tr> <td>InChI</td> <td colspan="2">InChI=1S/C4H7O2/C1-2-7-4(6)3-5/h2-3H2,1H3</td> <td></td> </tr> <tr> <td>InChIKey</td> <td colspan="2">MFXVWHUKROIC-UHFFFAOYSA-N</td> <td></td> </tr> <tr> <td>Molecular Weight</td> <td colspan="2">214.00</td> <td></td> </tr> <tr> <td>Technique</td> <td colspan="2">CAPILLARY CELL: NEAT</td> <td></td> </tr> </tbody> </table> </li> <li><b>Table:</b> A table of related compounds with columns for HQI, Tag, ID, Name, Chemical Structure, and Spectrum.                     <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 2650</td> <td>trans-2-HEXEN-1-OL, ACETATE</td> <td></td> <td></td> </tr> <tr> <td>48</td> <td>16.92</td> <td>SLX 2621</td> <td>NONANOIC ACID, ALLYL ESTER</td> <td></td> <td></td> </tr> <tr> <td>49</td> <td>16.86</td> <td>SLX 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>SLX 2734</td> <td>IODOACETIC ACID, ETHYL ESTER</td> <td></td> <td></td> </tr> </tbody> </table> </li> <li><b>OD Toolbar:</b> A small window showing a color scale for the overlap density heatmap, with 'Unique', 'All', and 'Common' options.</li> </ul>	Substructs		Sel. Substructs	Original Data Files	All Properties	Attachments	Preferred Properties		Name	IODOACETIC ACID, ETHYL ESTER		Value	Formula	C <sub>6</sub> H <sub>10</sub> O <sub>2</sub>			InChI	InChI=1S/C4H7O2/C1-2-7-4(6)3-5/h2-3H2,1H3			InChIKey	MFXVWHUKROIC-UHFFFAOYSA-N			Molecular Weight	214.00			Technique	CAPILLARY CELL: NEAT			HQI	Tag	ID	Name	Chemical Structure	Spectrum	47	17.00	SLX 2650	trans-2-HEXEN-1-OL, ACETATE			48	16.92	SLX 2621	NONANOIC ACID, ALLYL ESTER			49	16.86	SLX 2731	2-BROMO-3-METHYLBUTYRIC ACID, ETHYL ESTER			50	16.67	SLX 2734	IODOACETIC ACID, ETHYL ESTER		
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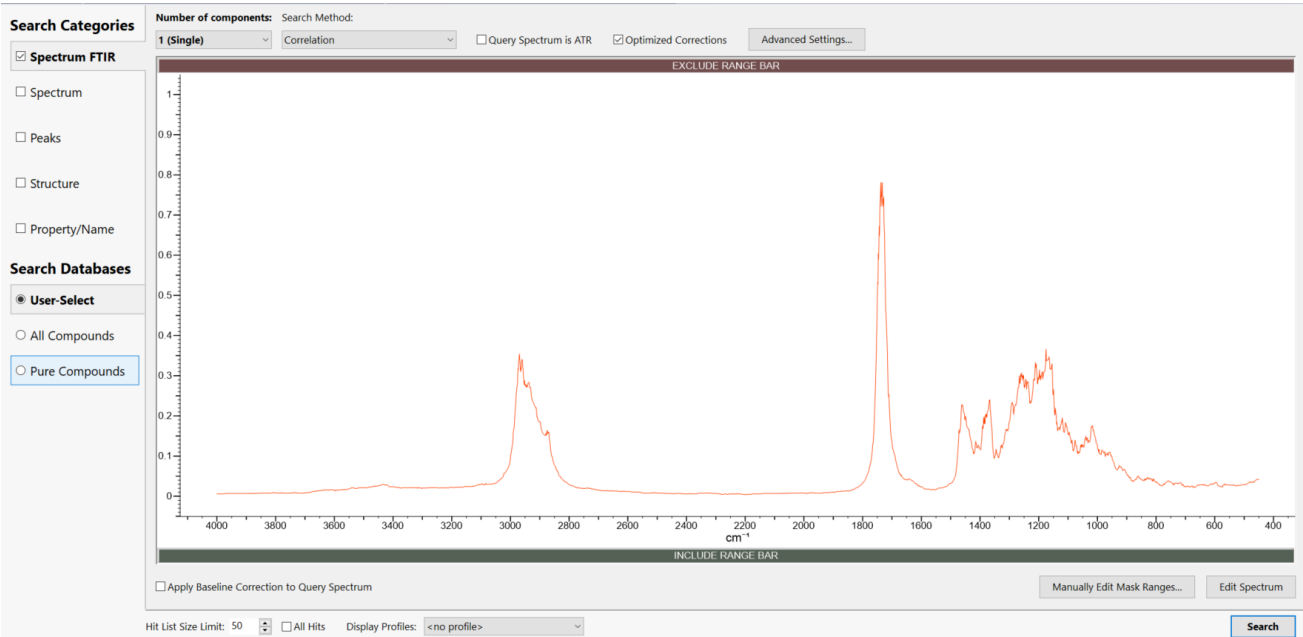


4 Move the OD Toolbar to around 50 (17%)



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

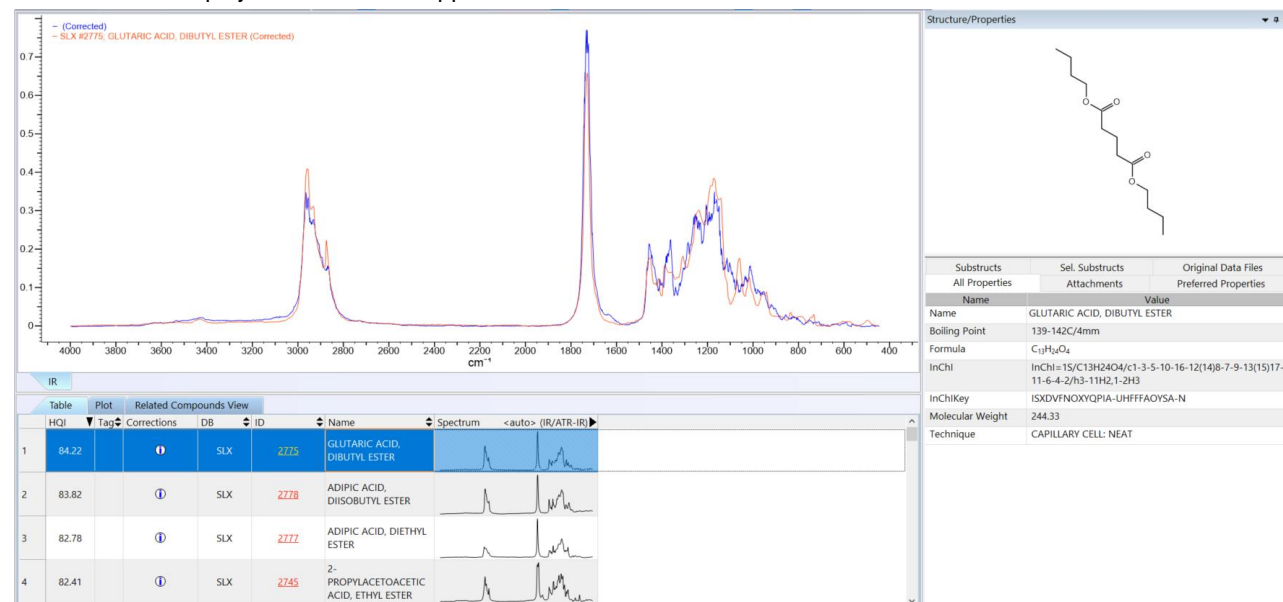
### Use the consensus spectrum to perform a search

	Action	Result
1	Click <b>SearchIt</b> in the <b>Transfer to bar</b> .	<p>The consensus spectrum is displayed on the <b>IR Spectrum</b> search tab.</p>  <p>The screenshot shows the IR Spectrum search interface. On the left, there are search categories: <b>Spectrum FTIR</b> (checked), Spectrum, Peaks, Structure, and Property/Name. Below these are search databases: <b>User-Select</b> (selected), All Compounds, and Pure Compounds. The main area displays a consensus spectrum plot with a y-axis from 0 to 1 and an x-axis from 4000 to 400 cm⁻¹. A prominent peak is visible at approximately 1700 cm⁻¹. The interface includes search parameters: Number of components: 1 (Single), Search Method: Correlation, Query Spectrum is ATR (unchecked), Optimized Corrections (checked), and Advanced Settings... At the bottom, there are options for Apply Baseline Correction to Query Spectrum (unchecked), Hit List Size Limit: 50, All Hits (unchecked), Display Profiles: &lt;no profile&gt;, and a Search button.</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 get a hit list where hits are structurally similar to that of **Methacrylic acid, isobutyle ester**.