

# **KnowItAll Software Training**

---

## Chemometrics Analysis with KnowItAll Trendfinder

# Spectrum Analysis

## How to Use KnowItAll Trendfinder to Perform Chemometrics Analysis

### Purpose

These exercises demonstrate how to use KnowItAll Trendfinder to perform Chemometrics analysis on various spectra.

### Objectives

These exercises will teach you to apply KnowItAll Trendfinder to

- IR
- LC-MS
- GC-MS
- Raman
- UV-Vis

### Background

The KnowItAll Trendfinder application allows one to perform Chemometrics analysis of spectral and chromatographic data.

#### *Training Files Used in This Lesson*


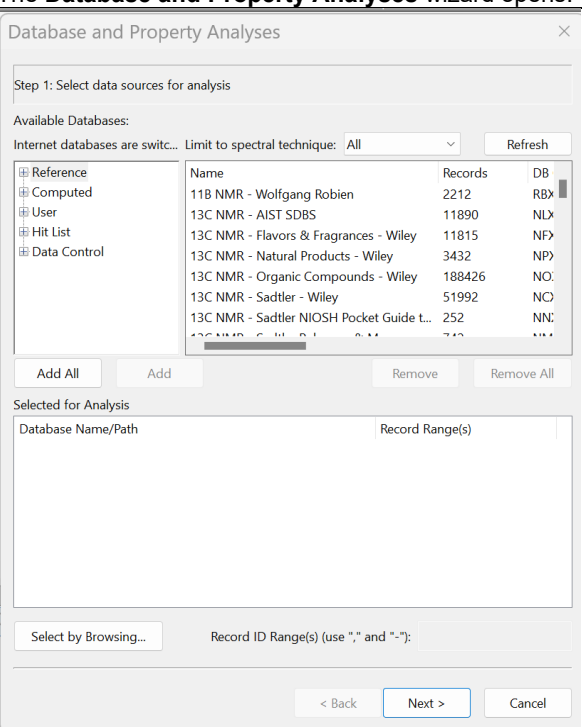
C:\Users\Public\Documents\Wiley\KnowItAll\Samples

#### *KnowItAll Applications Used*

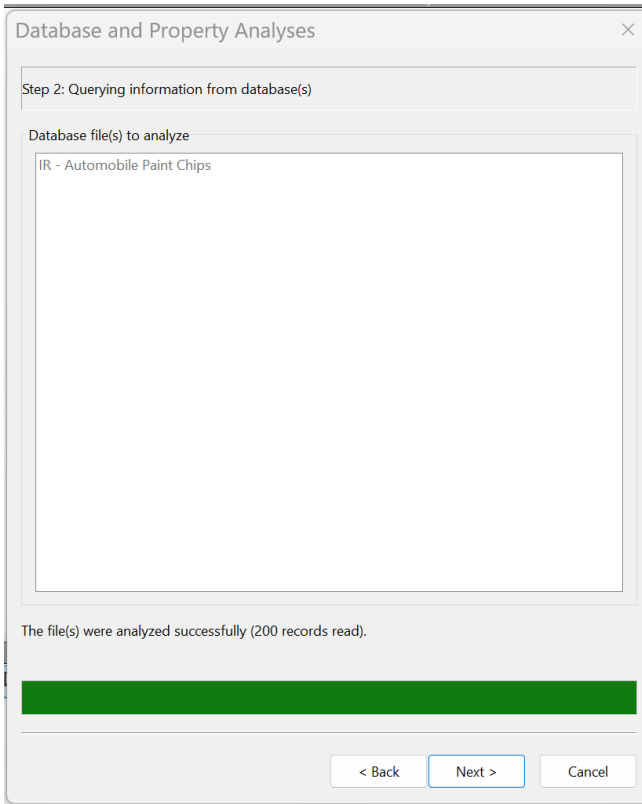
- KnowItAll Trendfinder

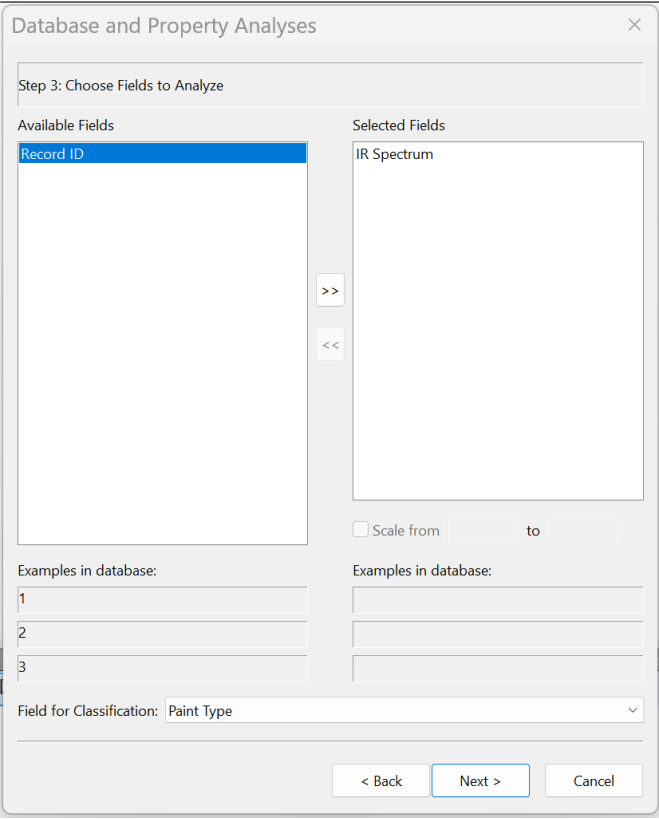
## IR Example

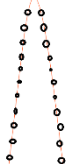
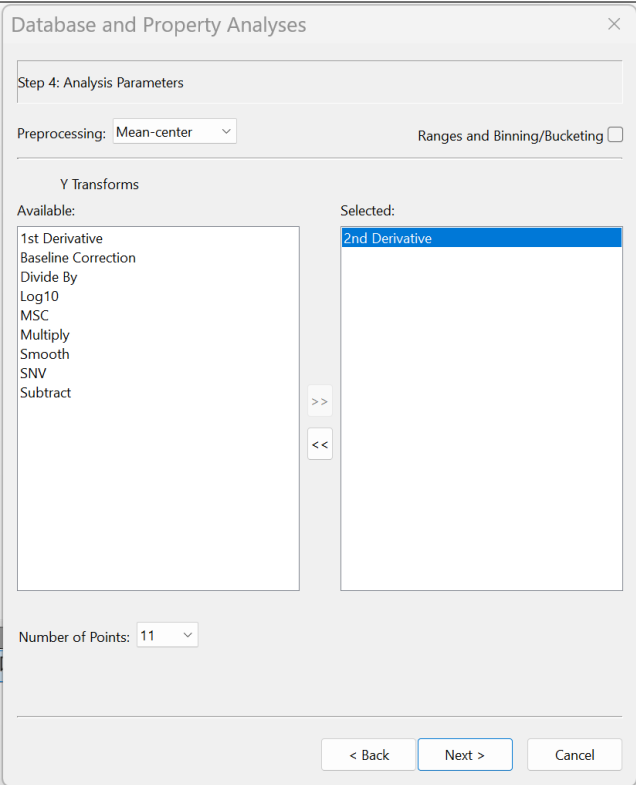
### A. Principal Component Analysis (PCA) of Automobile Paint Chips

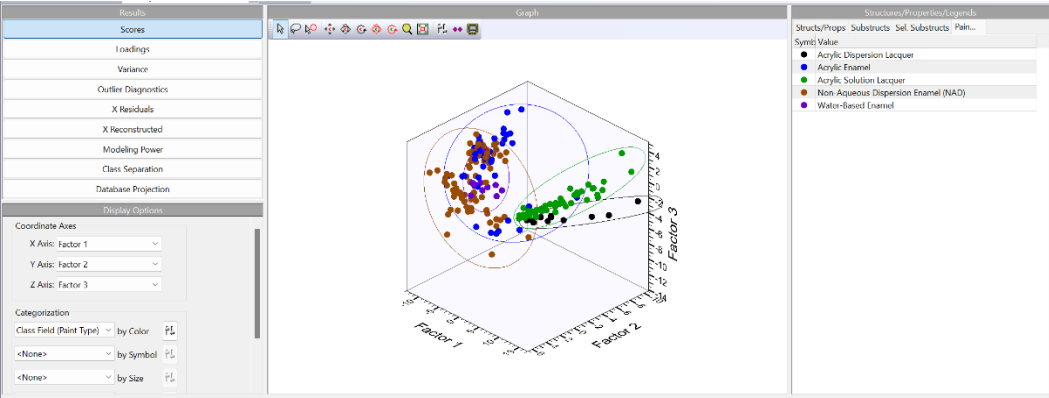
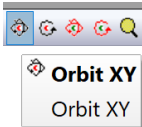
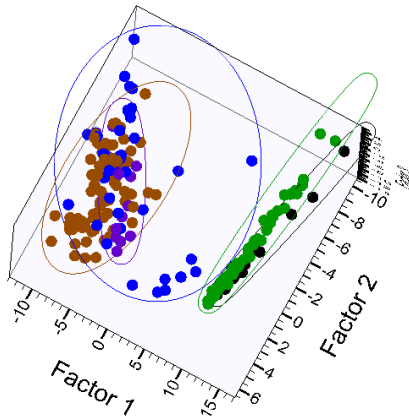
	Action	Result
1	Open the <b>Trendfinder</b> application by clicking its icon in the <b>Spectral Analysis</b> toolbox.  Trendfinder	The application opens.
2	Choose <b>File &gt; New PCA Analysis</b> .	The <b>Database and Property Analyses</b> wizard opens. 

	Action	Result																																								
3	<ul style="list-style-type: none"><li>• Select the reference database <b>IR - Automobile Paint Chips (APX)</b> and click <b>Add</b>.</li><li>• Highlight the database in the Selected for Analysis box, type <b>1-200</b> in the <b>Record ID Range</b> field (to use the first 200 records).</li><li>• Click <b>Next &gt;</b>.</li></ul>	<div><div>Database and Property Analyses</div><div><div>Step 1: Select data sources for analysis</div><div>Available Databases: Internet databases are swit... Limit to spectral technique: IR Refresh</div><div><table><tr><td><input checked="" type="checkbox"/> Reference</td><td>Name</td><td>Records</td><td>DB</td></tr><tr><td><input checked="" type="checkbox"/> Computed</td><td>IR - Automobile Paint Chips</td><td>1991</td><td>APX</td></tr><tr><td><input checked="" type="checkbox"/> User</td><td>IR - Canadian Forensics</td><td>3495</td><td>CFX</td></tr><tr><td><input checked="" type="checkbox"/> Hit List</td><td>IR - Georgia State Crime Lab</td><td>1910</td><td>DLX</td></tr><tr><td><input checked="" type="checkbox"/> Data Control</td><td>IR - Industrial Chemicals, Basic Organic Co...</td><td>1000</td><td>HLX</td></tr><tr><td></td><td>IR - Industrial Chemicals, Pure Organic Co...</td><td>20316</td><td>HIX</td></tr><tr><td></td><td>IR - Microplastic Classifications - Wiley</td><td>9</td><td>MPX</td></tr><tr><td></td><td>IR - Minerals - Wiley</td><td>262</td><td>IMX</td></tr><tr><td></td><td>IR - Organic Chemicals - Wiley</td><td>527</td><td>OCX</td></tr></table></div><div>Add AllAddRemoveRemove All</div><div>Selected for Analysis</div><div><table><tr><td>Database Name/Path</td><td>Record Range(s)</td></tr><tr><td>IR - Automobile Paint Chips</td><td>1-200</td></tr></table></div><div>Select by Browsing...Record ID Range(s) (use "," and "-"): 1-200</div><div>&lt; BackNext &gt;Cancel</div></div></div>	<input checked="" type="checkbox"/> Reference	Name	Records	DB	<input checked="" type="checkbox"/> Computed	IR - Automobile Paint Chips	1991	APX	<input checked="" type="checkbox"/> User	IR - Canadian Forensics	3495	CFX	<input checked="" type="checkbox"/> Hit List	IR - Georgia State Crime Lab	1910	DLX	<input checked="" type="checkbox"/> Data Control	IR - Industrial Chemicals, Basic Organic Co...	1000	HLX		IR - Industrial Chemicals, Pure Organic Co...	20316	HIX		IR - Microplastic Classifications - Wiley	9	MPX		IR - Minerals - Wiley	262	IMX		IR - Organic Chemicals - Wiley	527	OCX	Database Name/Path	Record Range(s)	IR - Automobile Paint Chips	1-200
<input checked="" type="checkbox"/> Reference	Name	Records	DB																																							
<input checked="" type="checkbox"/> Computed	IR - Automobile Paint Chips	1991	APX																																							
<input checked="" type="checkbox"/> User	IR - Canadian Forensics	3495	CFX																																							
<input checked="" type="checkbox"/> Hit List	IR - Georgia State Crime Lab	1910	DLX																																							
<input checked="" type="checkbox"/> Data Control	IR - Industrial Chemicals, Basic Organic Co...	1000	HLX																																							
	IR - Industrial Chemicals, Pure Organic Co...	20316	HIX																																							
	IR - Microplastic Classifications - Wiley	9	MPX																																							
	IR - Minerals - Wiley	262	IMX																																							
	IR - Organic Chemicals - Wiley	527	OCX																																							
Database Name/Path	Record Range(s)																																									
IR - Automobile Paint Chips	1-200																																									


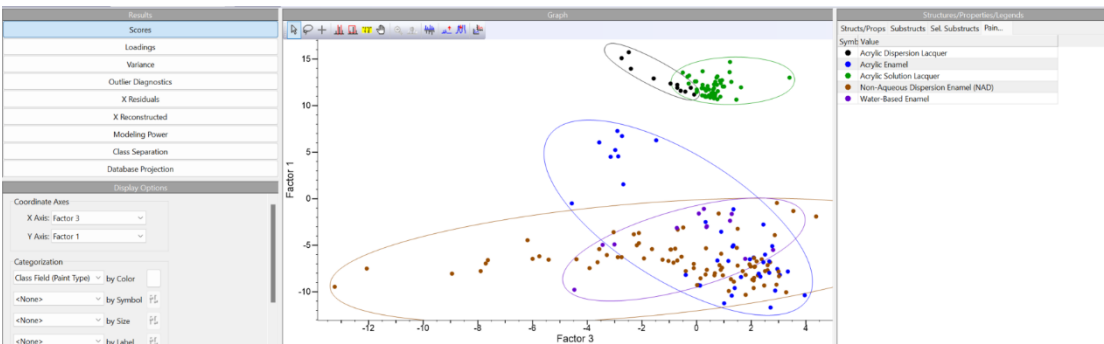
	Action	Result
4	Click <b>Next &gt;</b> again.	

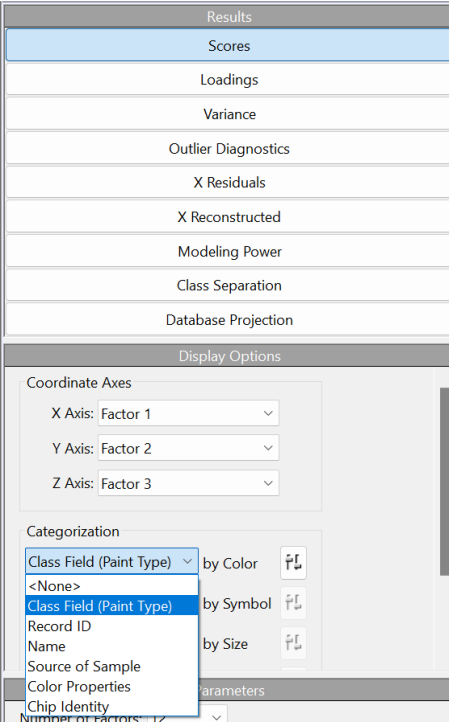
	Action	Result
5	<p>In this dialog:</p> <ul style="list-style-type: none"><li>• Move <b>IR Spectrum</b> from the left box to the right one by selecting it in the left and using "&gt;&gt;" or double-clicking to move it to the right</li><li>• Set <b>Field for Classification</b> to <b>Paint Type</b>. Click <b>Next &gt;</b>.</li></ul>	 <p>The screenshot shows a dialog box titled "Database and Property Analyses" with a close button (X) in the top right corner. The dialog is at "Step 3: Choose Fields to Analyze". It features two list boxes: "Available Fields" on the left and "Selected Fields" on the right. "Available Fields" contains "Record ID". "Selected Fields" contains "IR Spectrum". Between the lists are "&gt;&gt;" and "&lt;&lt;" buttons. Below the lists is a "Scale from" checkbox and a "to" label. At the bottom, there are two "Examples in database:" sections, each with three input fields numbered 1, 2, and 3. A "Field for Classification:" dropdown menu is set to "Paint Type". At the very bottom are three buttons: "&lt; Back", "Next &gt;" (which is highlighted with a blue border), and "Cancel".</p>

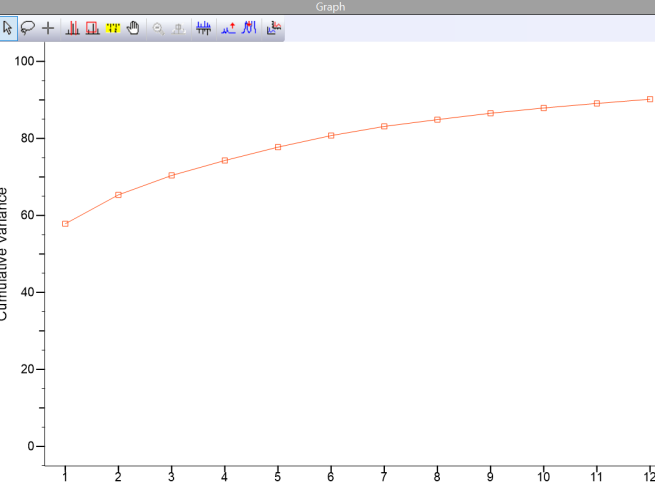
	Action	Result
6	<p>In this dialog:</p> <ul style="list-style-type: none"> <li>Move <b>2<sup>nd</sup> Derivative</b> method to the right box to perform <b>Y Transforms</b> on the IR spectrum.</li> <li>Set the <b>Number of Points</b> on each side of an IR peak to be 11 (picture below as an example).</li> </ul>  <ul style="list-style-type: none"> <li>Click <b>Next</b>.</li> </ul> <p><i>Note: 1<sup>st</sup> derivative pinpoints an apex, 2<sup>nd</sup> derivative nails down peak shoulders.</i></p>	

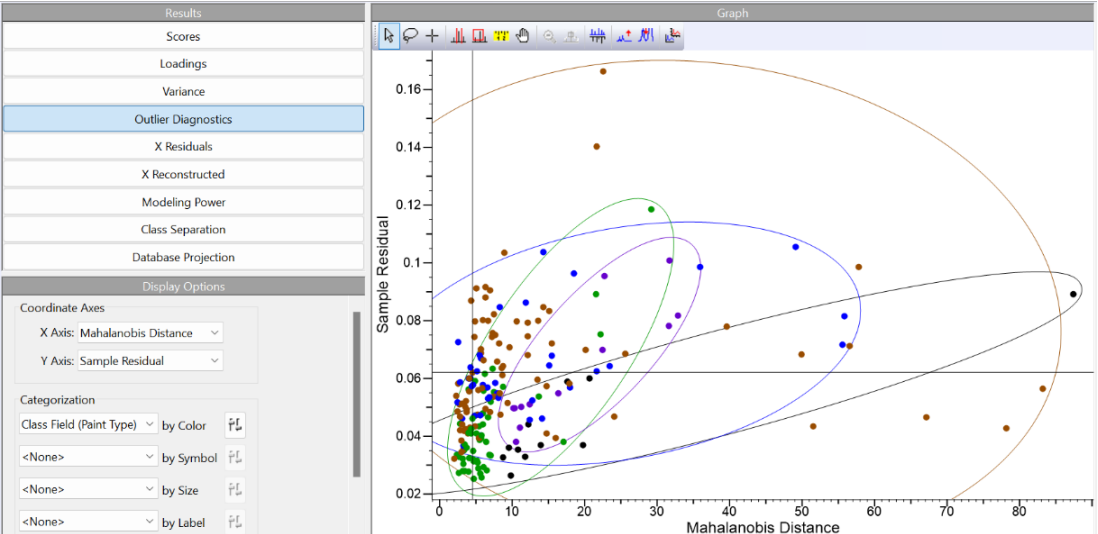
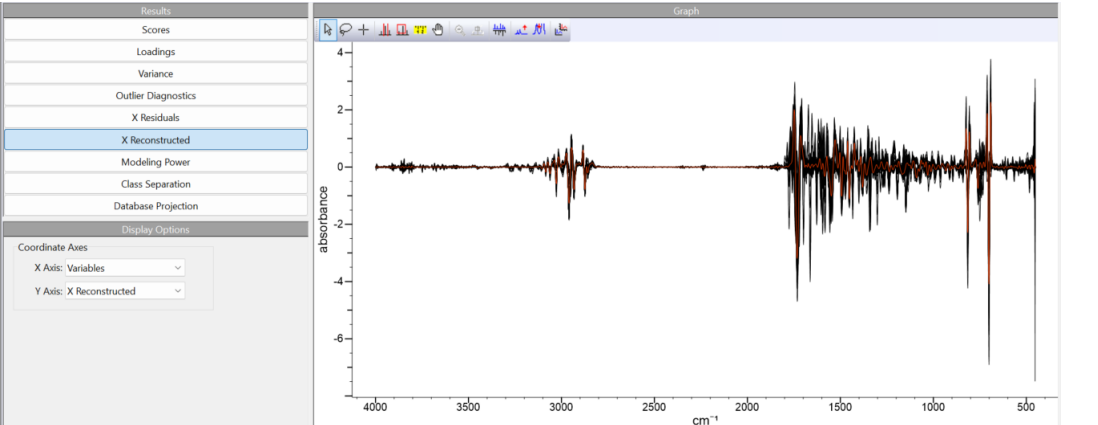
	Action	Result
7	<p>Click <b>Finish</b> when the analysis is done.</p> <p><i>Note: Factors are mathematical axis' orthogonal to each other.</i></p>	 <p>This is a 3 factors view of the analysis, showing the distribution of different type of paint. A circle (<b>Trajectory</b>) defines the boundary for a value in the <b>Field of Classification</b>.</p>
8	 <ul style="list-style-type: none"> <li>Click</li> <li>Rotate and observe the spectra distribution in 3 factor space.</li> </ul>	



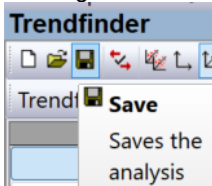
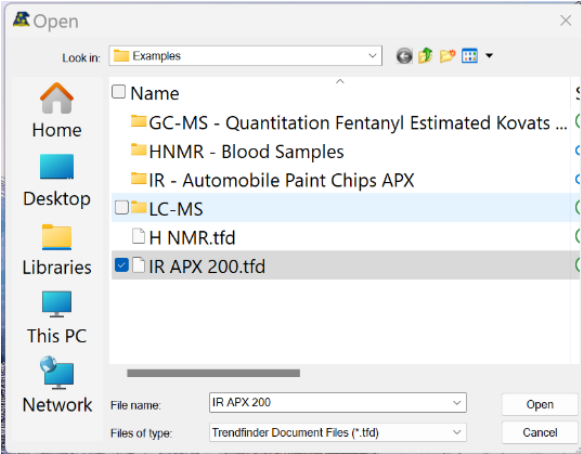
	Action	Result
9	<ul style="list-style-type: none"><li>Click the <b>2D Plot</b> toolbar button  to switch the graph display in 2 dimensions.</li><li>Set the <b>X-Axis</b> to be <b>Factor 3</b> and the <b>Y-Axis</b> to be <b>Factor 1</b>.</li></ul>	 <p>The lacquer types (upper) are separated from enamels (lower).</p>

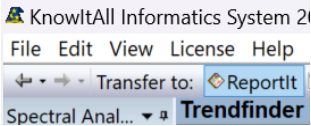
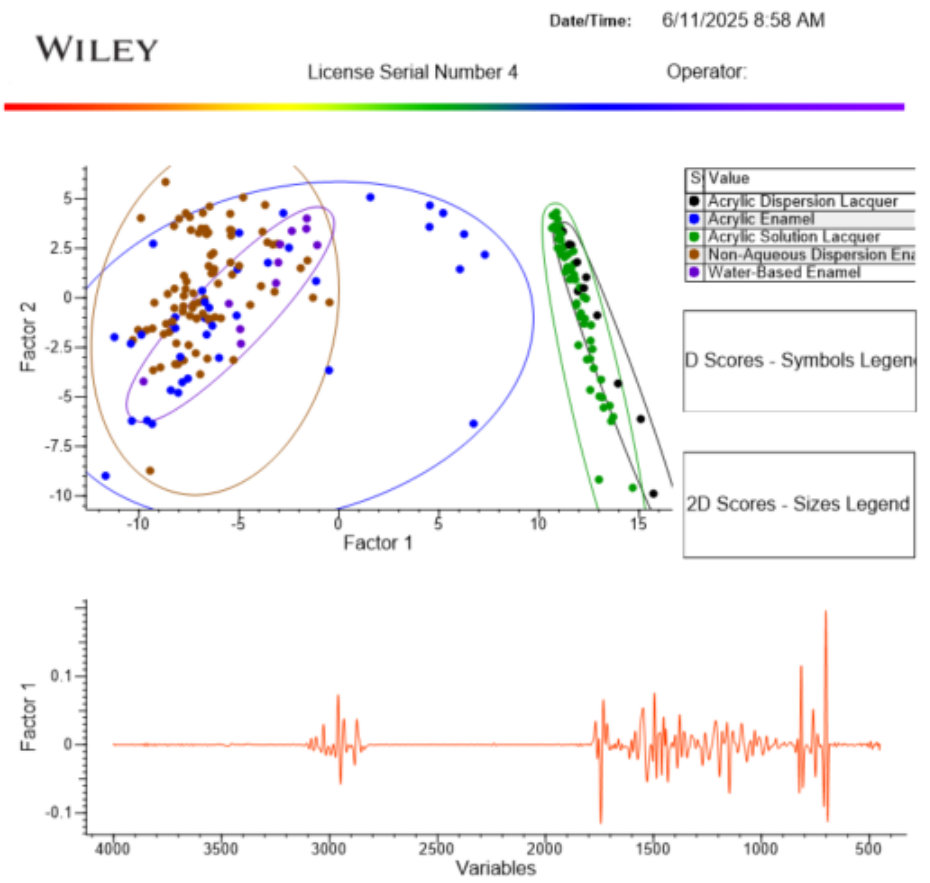
	Action	Result
10	The <b>Categorization</b> dropdown list allows you to see how other properties correlate to the spectral space.	

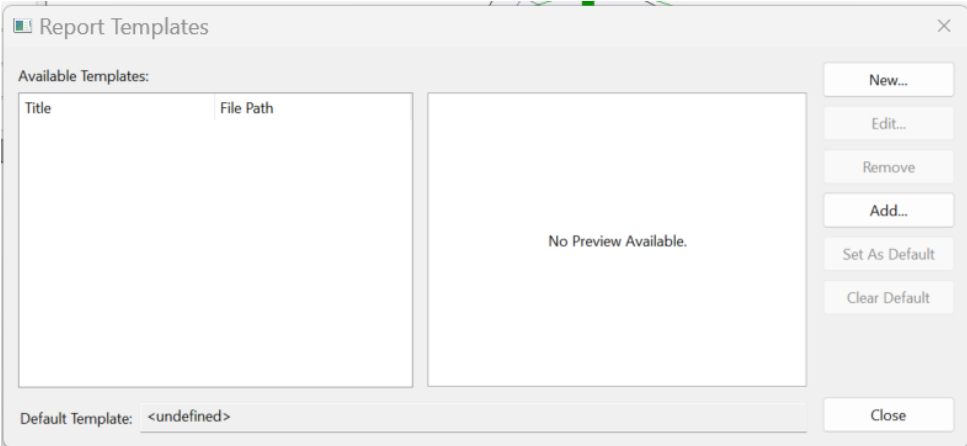
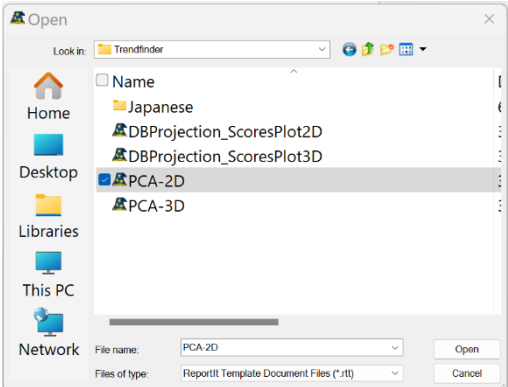
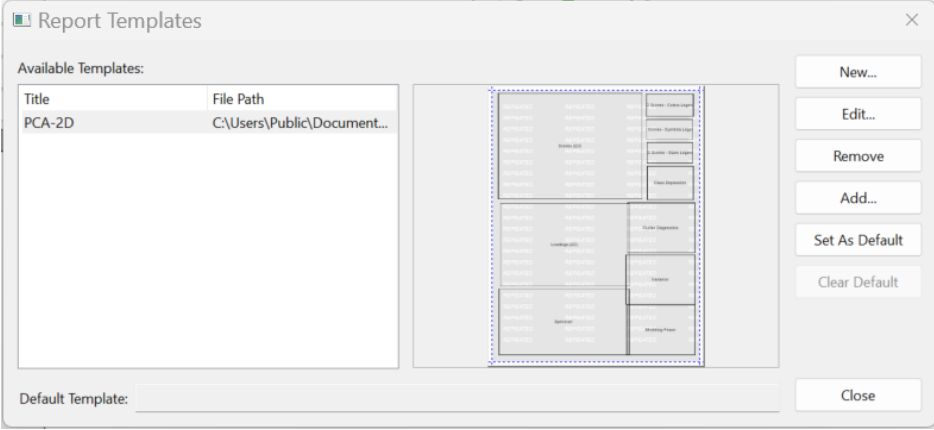
	Action	Result																										
11	<b>Variance</b> allows you to examine the PCA quality.	<div><div><div>Results</div><div>Scores</div><div>Loadings</div><div>Variance</div><div>Outlier Diagnostics</div><div>X Residuals</div><div>X Reconstructed</div><div>Modeling Power</div><div>Class Separation</div><div>Database Projection</div></div><div><div>Display Options</div><div>Coordinate Axes</div><div>X Axis: Number of Factors</div><div>Y Axis: Cumulative Variance</div></div></div> <div><div>Graph</div><table><caption>Cumulative Variance Data</caption><tr><th>Number of Factors</th><th>Cumulative Variance (%)</th></tr><tr><td>1</td><td>58</td></tr><tr><td>2</td><td>65</td></tr><tr><td>3</td><td>70</td></tr><tr><td>4</td><td>74</td></tr><tr><td>5</td><td>77</td></tr><tr><td>6</td><td>80</td></tr><tr><td>7</td><td>82</td></tr><tr><td>8</td><td>84</td></tr><tr><td>9</td><td>86</td></tr><tr><td>10</td><td>87</td></tr><tr><td>11</td><td>88</td></tr><tr><td>12</td><td>89</td></tr></table></div> <p>As shown above, 6 factors can explain over 80% of the case.</p>	Number of Factors	Cumulative Variance (%)	1	58	2	65	3	70	4	74	5	77	6	80	7	82	8	84	9	86	10	87	11	88	12	89
Number of Factors	Cumulative Variance (%)																											
1	58																											
2	65																											
3	70																											
4	74																											
5	77																											
6	80																											
7	82																											
8	84																											
9	86																											
10	87																											
11	88																											
12	89																											

	Action	Result
12	<p>Select <b>Outlier Diagnostics</b> to examine potential outliers.</p> <p><i>Manhalanobis Distance is the most common measure to determine if a sample is an outlier.</i></p>	 <p>The right most black dot (spectrum sample) is an obvious outlier of the group – it is deviating almost 100% from the center of distribution.</p>
13	<p><b>X Reconstructed</b> should look like the illustration to the right.</p>	 <p>Note: The above is a “reconstructed” 2<sup>nd</sup> derivative form of Y.</p>

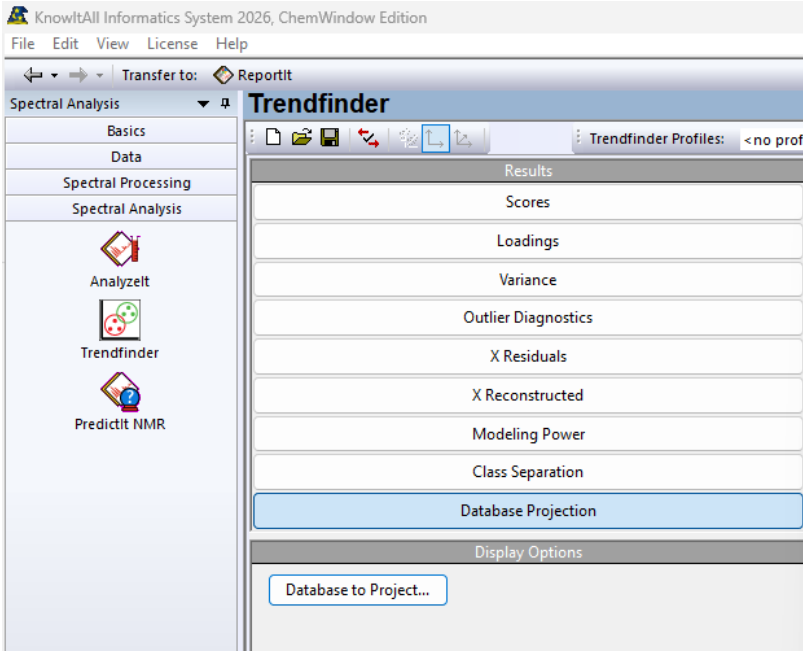
## B. Save the Analysis and Create a Report

	Action	Result
1	<p>Save the analysis by:</p> <ul style="list-style-type: none"><li>Clicking on the Save symbol</li></ul>  <ul style="list-style-type: none"><li>Or by going to File&gt;Save Analysis.</li><li>Or <b>Control + S</b>.</li></ul>	

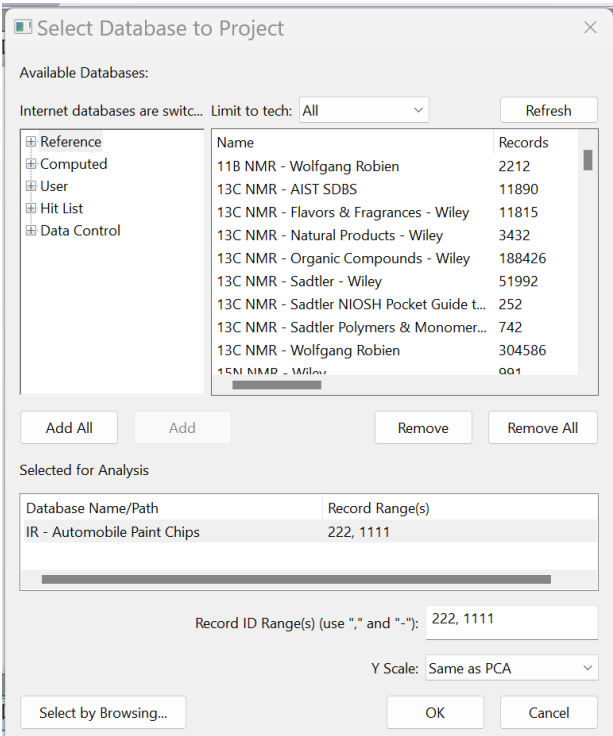
	Action	Result
2	<p>Transfer an analysis to <b>ReportIt</b> by:</p> <ul style="list-style-type: none"> <li>Selecting a group of spectra and: <ul style="list-style-type: none"> <li>using the mouse to click a position and drag drop to another position.</li> </ul> </li> <li>Or use the Lasso tool to circle points.</li> <li>Or <b>Control + Click</b> points.</li> <li>Then click on <b>ReportIt</b> in the <b>Transfer to</b> <div data-bbox="388 987 697 1112">  </div> </li> </ul>	 <p>The screenshot displays the WILEY software interface. At the top, it shows the 'WILEY' logo, 'License Serial Number 4', and the 'Date/Time: 6/11/2025 8:58 AM'. Below this is a color calibration bar. The main plot is a 2D Factor 1 vs Factor 2 plot. The x-axis is labeled 'Factor 1' and ranges from -10 to 15. The y-axis is labeled 'Factor 2' and ranges from -10 to 5. Data points are categorized by material type: Acrylic Dispersion Lacquer (black), Acrylic Enamel (blue), Acrylic Solution Lacquer (green), Non-Aqueous Dispersion Enz (orange), and Water-Based Enamel (purple). A Lasso Selection Mode tooltip is visible, showing a selection tool and the text 'Lasso Selection Mode' and 'Lasso selection mode'. Below the plot is a spectral plot of Factor 1 vs Variables, with the x-axis labeled 'Variables' ranging from 4000 to 500 and the y-axis labeled 'Factor 1' ranging from -0.1 to 0.1.</p>

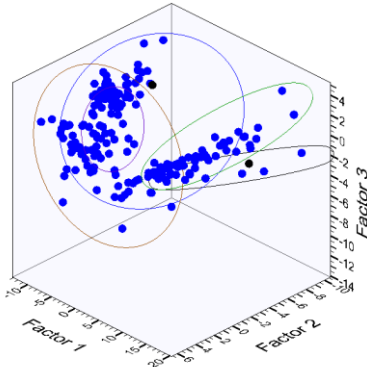
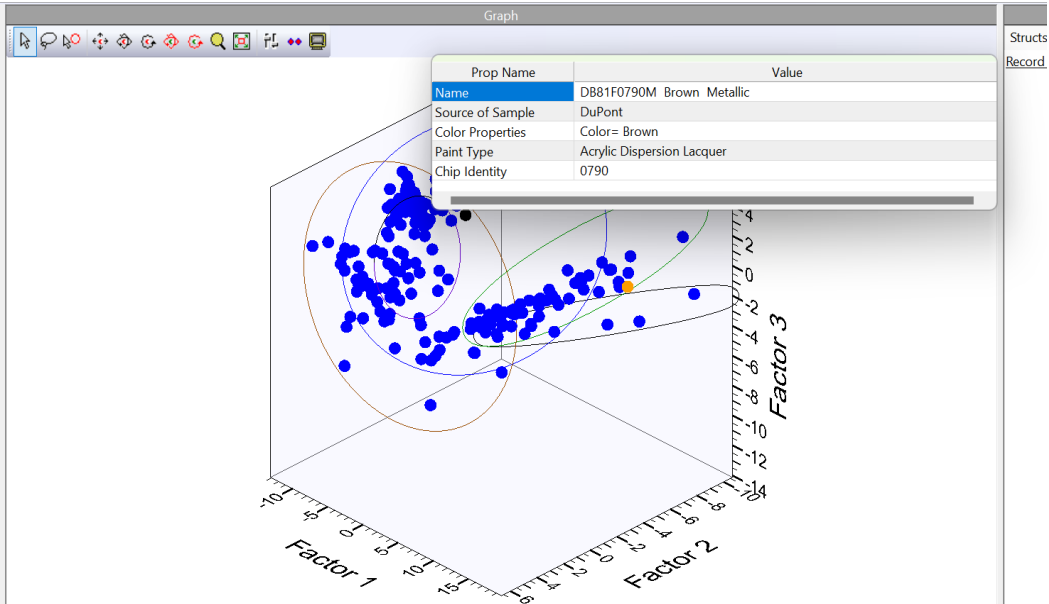
	Action	Result
<p><i>Note:</i></p> <ul style="list-style-type: none"> <li>If a template is used for the first time, the user has to do the following before transferring data to the <b>ReportIt</b> application: <b>File &gt; Edit Report Templates</b></li> <li>Click <b>Add button</b></li> <li>Navigate to the template file <b>C:\Users\Public\Public Documents\Wiley\KnowItAll\Report Templates\Trendfinder</b> to see the options.</li> <li>Click <b>Open</b> to add.</li> </ul>		
3	<p>Add as many templates as desired and click <b>Close</b> when finished.</p> 	

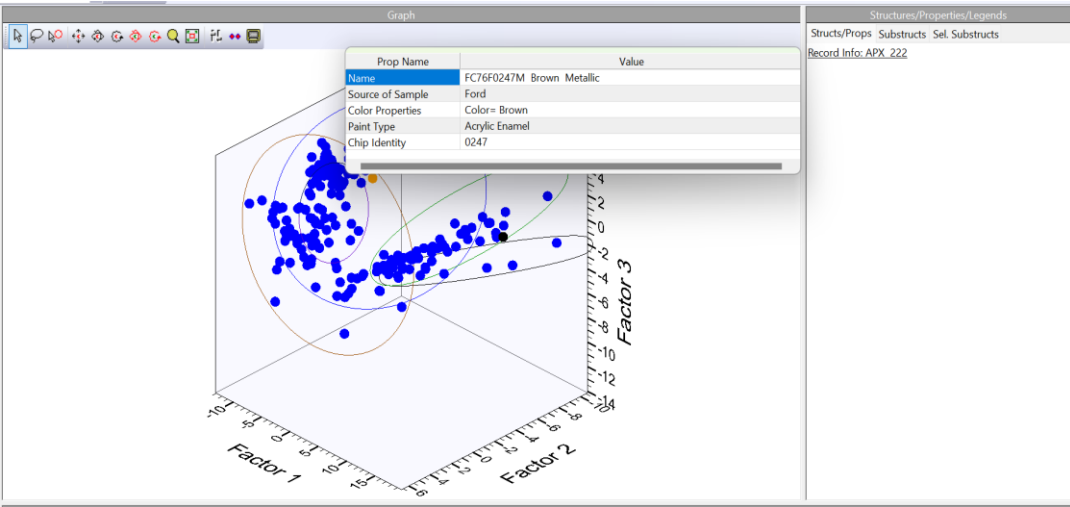
### C. Project Unknown Spectra to the PCA “Space”

	Action	Result
1	Using the same data as before, click the <b>Database Projection</b> button under the <b>Results</b> section.	



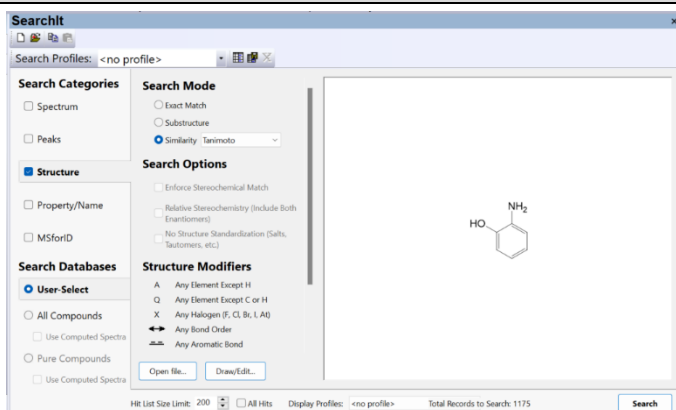
	Action	Result																										
2	<p>Ensure the IR-Automobile Paint Chips database is selected and then:</p> <ul style="list-style-type: none"><li>• Type in 222 and 1111 under “<b>Record Range(s)</b>” (use “,” and “-”) to test the classification of these unused spectra based on the first 200 spectra.</li><li>• Set <b>Y Scale: Same As PCA</b>.</li><li>• Click <b>OK</b>.</li></ul>	 <p>The screenshot shows the 'Select Database to Project' dialog box. It has a title bar with a close button. Below the title bar, there's a section 'Available Databases:' with a sub-label 'Internet databases are switch...'. There's a 'Limit to tech:' dropdown set to 'All' and a 'Refresh' button. A list of databases is shown with columns for 'Name' and 'Records'. The 'Selected for Analysis' section has a table with 'Database Name/Path' and 'Record Range(s)'. The 'IR - Automobile Paint Chips' database is selected with a record range of '222, 1111'. Below this, there's a 'Record ID Range(s) (use ", " and "-"):' field with '222, 1111' entered. There's also a 'Y Scale:' dropdown set to 'Same as PCA'. At the bottom, there are buttons for 'Select by Browsing...', 'OK', and 'Cancel'.</p> <table><tr><th>Name</th><th>Records</th></tr><tr><td>11B NMR - Wolfgang Robien</td><td>2212</td></tr><tr><td>13C NMR - AIST SDBS</td><td>11890</td></tr><tr><td>13C NMR - Flavors &amp; Fragrances - Wiley</td><td>11815</td></tr><tr><td>13C NMR - Natural Products - Wiley</td><td>3432</td></tr><tr><td>13C NMR - Organic Compounds - Wiley</td><td>188426</td></tr><tr><td>13C NMR - Sadtler - Wiley</td><td>51992</td></tr><tr><td>13C NMR - Sadtler NIOSH Pocket Guide t...</td><td>252</td></tr><tr><td>13C NMR - Sadtler Polymers &amp; Monomer...</td><td>742</td></tr><tr><td>13C NMR - Wolfgang Robien</td><td>304586</td></tr><tr><td>15N NMR - Wiley</td><td>901</td></tr></table> <table><tr><th>Database Name/Path</th><th>Record Range(s)</th></tr><tr><td>IR - Automobile Paint Chips</td><td>222, 1111</td></tr></table> <p>Record ID Range(s) (use ", " and "-"): 222, 1111</p> <p>Y Scale: Same as PCA</p>	Name	Records	11B NMR - Wolfgang Robien	2212	13C NMR - AIST SDBS	11890	13C NMR - Flavors & Fragrances - Wiley	11815	13C NMR - Natural Products - Wiley	3432	13C NMR - Organic Compounds - Wiley	188426	13C NMR - Sadtler - Wiley	51992	13C NMR - Sadtler NIOSH Pocket Guide t...	252	13C NMR - Sadtler Polymers & Monomer...	742	13C NMR - Wolfgang Robien	304586	15N NMR - Wiley	901	Database Name/Path	Record Range(s)	IR - Automobile Paint Chips	222, 1111
Name	Records																											
11B NMR - Wolfgang Robien	2212																											
13C NMR - AIST SDBS	11890																											
13C NMR - Flavors & Fragrances - Wiley	11815																											
13C NMR - Natural Products - Wiley	3432																											
13C NMR - Organic Compounds - Wiley	188426																											
13C NMR - Sadtler - Wiley	51992																											
13C NMR - Sadtler NIOSH Pocket Guide t...	252																											
13C NMR - Sadtler Polymers & Monomer...	742																											
13C NMR - Wolfgang Robien	304586																											
15N NMR - Wiley	901																											
Database Name/Path	Record Range(s)																											
IR - Automobile Paint Chips	222, 1111																											

	Action	Result
3	See how two black dots fit into the PCA space (now blue).	
4	<ul style="list-style-type: none"><li>Click one of the dots to see details for that record. (The selected dot will turn orange.)</li><li>Hover over the <b>Record Info</b> link to see more details.</li></ul>	 <p>This dot is within the Acrylic Dispersion Lacquer circle .</p>

	Action	Result
5	Click on the other one dot and hover over the <b>Record Info</b> to see more details.	 <p data-bbox="800 834 1247 862">This dot is within the Acrylic Enamel circle.</p>

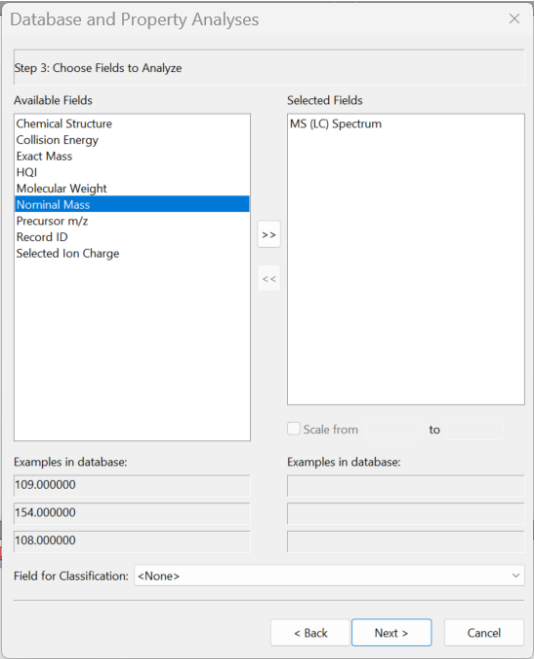
## LC-MS

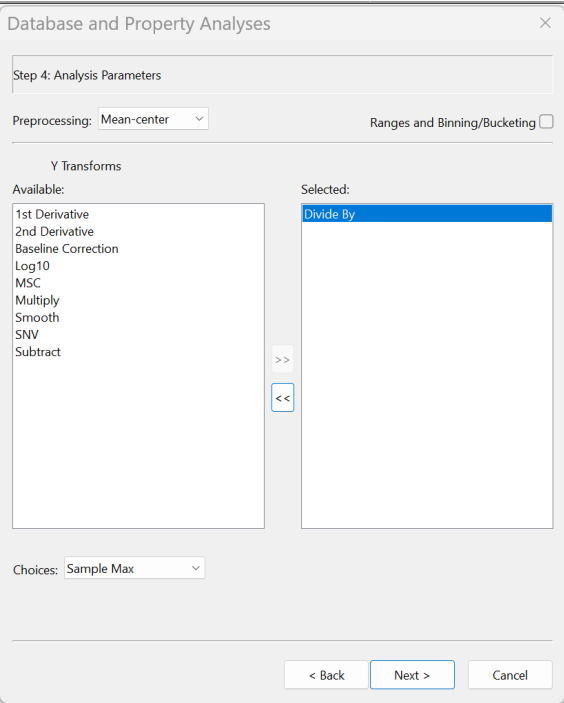
### Hit List Analysis of Similar Structures

	Action	Result
1	In <b>SearchIt</b> , set a <b>similarity</b> structure search as shown in the Result column.	

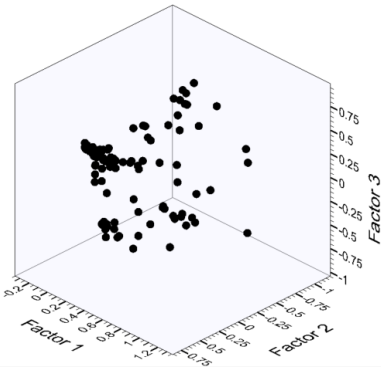
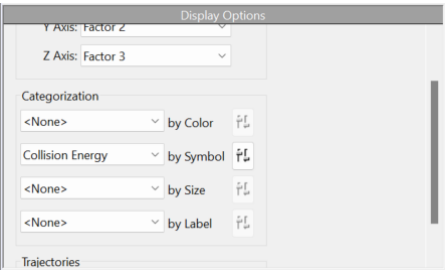
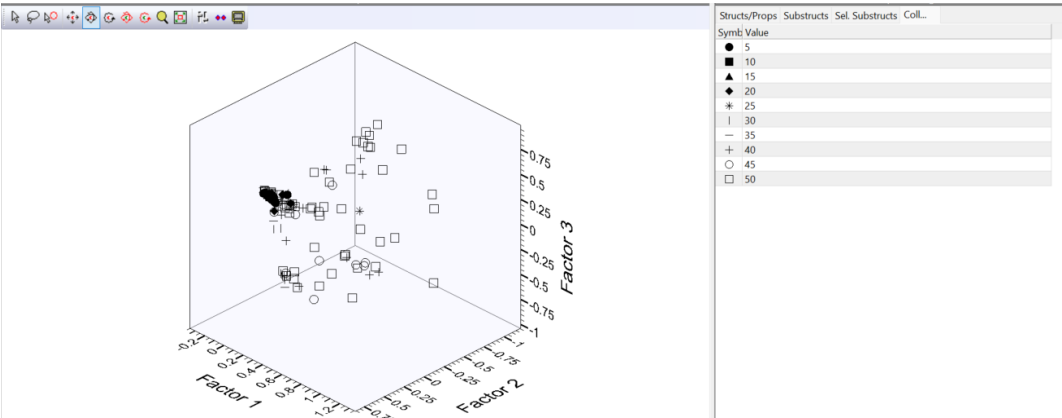


Action	Result
<div>4</div> <div>Choose <b>Collision Energy</b> in the <b>Property</b> drop down list and select all.</div>	<div><div><div><div><div><div>Overlay All</div></div><div>Property:</div><div>Collision Energy</div></div><div><div>10 eV</div><div>15 eV</div><div>20 eV</div><div>25 eV</div><div>30 eV</div><div>35 eV</div><div>40 eV</div></div></div><div><div><div>MS (LC) (7)</div></div></div></div><div><div><div><div><div>WRTMS #8: 2-Aminophenol</div><div>WRTMS #8: 2-Aminophenol</div><div>WRTMS #8: 2-Aminophenol</div><div>WRTMS #8: 2-Aminophenol</div><div>WRTMS #8: 2-Aminophenol</div><div>WRTMS #8: 2-Aminophenol</div><div>WRTMS #8: 2-Aminophenol</div></div><div><div><div>1000</div><div>500</div></div><div><div><div>50</div><div>55</div><div>60</div><div>65</div><div>70</div><div>75</div><div>80</div><div>85</div><div>90</div><div>95</div><div>100</div><div>105</div><div>110</div></div><div><div>m/z</div></div></div></div></div><div><div>Table</div><div>Plot</div><div>Related Compounds View</div></div><div><div><div>HQI</div><div>Tag</div><div>DB</div><div>ID</div><div>Name</div><div>Chemical Structure</div><div>Spectrum</div><div>&lt;auto&gt; (MS (LC))</div></div><div><div>1</div><div>100.00</div><div></div><div>WRTMS</div><div>8</div><div>2-Aminophenol</div><div><div><div><div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div></div></div></div></div></div></div></div></div>

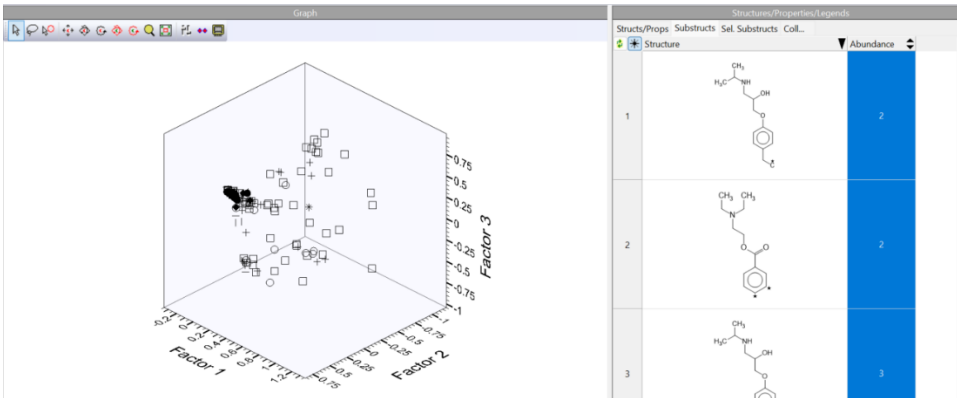
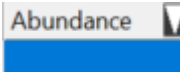
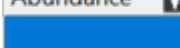
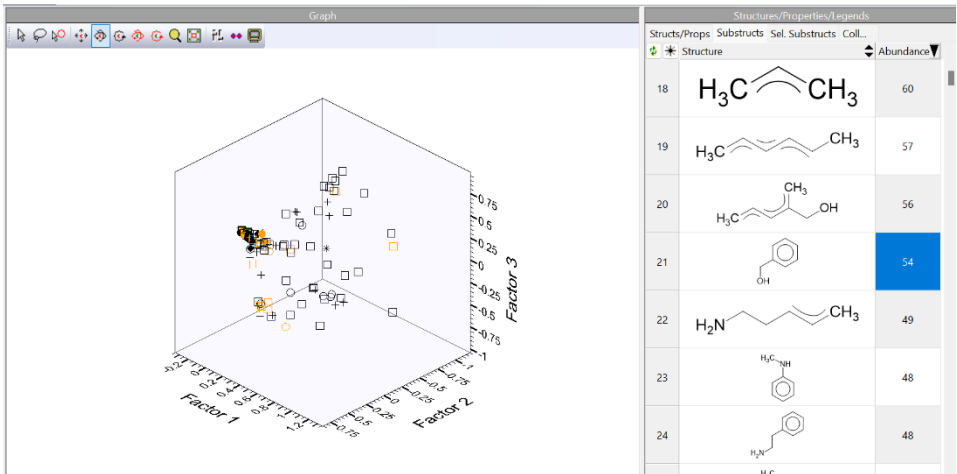
	Action	Result
5	<ul style="list-style-type: none"> <li>• Select <b>MS (LC) Spectrum</b> to analyze.</li> <li>• Click <b>Next &gt;</b>.</li> </ul>	
	<p><b>Tip:</b> Based on experience, selecting <b>Divide By</b> from the <b>Available</b> list in the <b>Y Transform</b> and <b>Sample Max</b> from the Choices drop down is effective for MS spectra.</p>	

	Action	Result
6	Click <b>Next &gt;</b> to continue.	 <p>Database and Property Analyses</p> <p>Step 4: Analysis Parameters</p> <p>Preprocessing: Mean-center <input type="button" value="v"/> Ranges and Binning/Bucketing <input type="checkbox"/></p> <p>Y Transforms</p> <p>Available:</p> <ul style="list-style-type: none"><li>1st Derivative</li><li>2nd Derivative</li><li>Baseline Correction</li><li>Log10</li><li>MSC</li><li>Multiply</li><li>Smooth</li><li>SNV</li><li>Subtract</li></ul> <p>Selected:</p> <ul style="list-style-type: none"><li>Divide By</li></ul> <p>Choices: Sample Max <input type="button" value="v"/></p> <p>&lt; Back Next &gt; Cancel</p>



	Action	Result
7	Click <b>Finish</b> .	 <p>Scores plot opens as above.</p>
8	<p>Under <b>Categorization</b>, select to show <b>Collision Energy by Symbol</b>:</p> 	 <p>This plot is an interesting way of looking at this set of data. High collision energy breaks molecules more thoroughly resulting in differences in their spectra!</p>
9	Select a particular spot (*)	

## Common Fragments

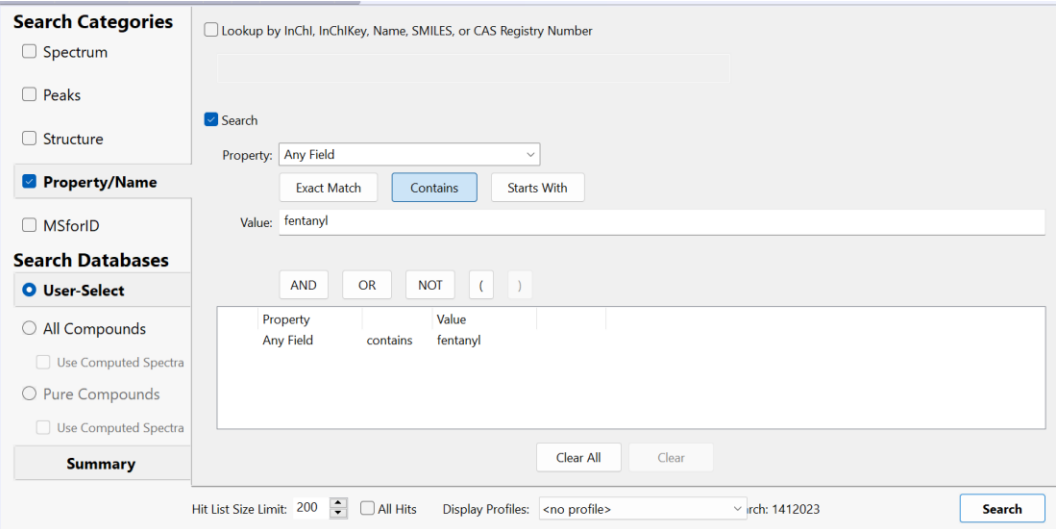
	Action	Result																		
1	<p>Continue with the above example.</p> <ul style="list-style-type: none"><li>Open the <b>Substructures</b> tab under the <b>Structures/Properties/Legends</b> pane.</li><li>Click <b>Start Calculations</b>.</li></ul>	<div></div> <p>The fragments and abundances (frequency to appear) within this entire dataset are shown in the right table.</p> <table><tr><th>Structure</th><th>Abundance</th></tr><tr><td><chem>CC(C)C(O)C1=CC=C(C=C1)C=C</chem></td><td>2</td></tr><tr><td><chem>CC(C)C(=O)OC1=CC=C(C=C1)C=C</chem></td><td>2</td></tr><tr><td><chem>CC(C)C(O)C1=CC=C(C=C1)C=C</chem></td><td>1</td></tr></table>	Structure	Abundance	<chem>CC(C)C(O)C1=CC=C(C=C1)C=C</chem>	2	<chem>CC(C)C(=O)OC1=CC=C(C=C1)C=C</chem>	2	<chem>CC(C)C(O)C1=CC=C(C=C1)C=C</chem>	1										
Structure	Abundance																			
<chem>CC(C)C(O)C1=CC=C(C=C1)C=C</chem>	2																			
<chem>CC(C)C(=O)OC1=CC=C(C=C1)C=C</chem>	2																			
<chem>CC(C)C(O)C1=CC=C(C=C1)C=C</chem>	1																			
2	<ul style="list-style-type: none"><li>The <b>Abundance</b> can be sorted by clicking  on </li><li>Select a fragment.</li></ul>	<div></div> <p>25 Spectra containing this fragment are highlighted in the <b>Scores</b> plot.</p> <p>The <b>Sel. Substructures</b> tab will allow the user to select a group of dots and see the fragment abundance within that group.</p> <table><tr><th>Structure</th><th>Abundance</th></tr><tr><td><chem>CC(=C)C</chem></td><td>60</td></tr><tr><td><chem>CC=CC=CC</chem></td><td>57</td></tr><tr><td><chem>CC(C)=CCO</chem></td><td>56</td></tr><tr><td><chem>CC1=CC=CC=C1O</chem></td><td>54</td></tr><tr><td><chem>CCNCCC=CC</chem></td><td>49</td></tr><tr><td><chem>CC(N)C1=CC=CC=C1</chem></td><td>48</td></tr><tr><td><chem>CC(N)C1=CC=CC=C1</chem></td><td>48</td></tr><tr><td><chem>CC(N)C1=CC=CC=C1</chem></td><td>48</td></tr></table>	Structure	Abundance	<chem>CC(=C)C</chem>	60	<chem>CC=CC=CC</chem>	57	<chem>CC(C)=CCO</chem>	56	<chem>CC1=CC=CC=C1O</chem>	54	<chem>CCNCCC=CC</chem>	49	<chem>CC(N)C1=CC=CC=C1</chem>	48	<chem>CC(N)C1=CC=CC=C1</chem>	48	<chem>CC(N)C1=CC=CC=C1</chem>	48
Structure	Abundance																			
<chem>CC(=C)C</chem>	60																			
<chem>CC=CC=CC</chem>	57																			
<chem>CC(C)=CCO</chem>	56																			
<chem>CC1=CC=CC=C1O</chem>	54																			
<chem>CCNCCC=CC</chem>	49																			
<chem>CC(N)C1=CC=CC=C1</chem>	48																			
<chem>CC(N)C1=CC=CC=C1</chem>	48																			
<chem>CC(N)C1=CC=CC=C1</chem>	48																			


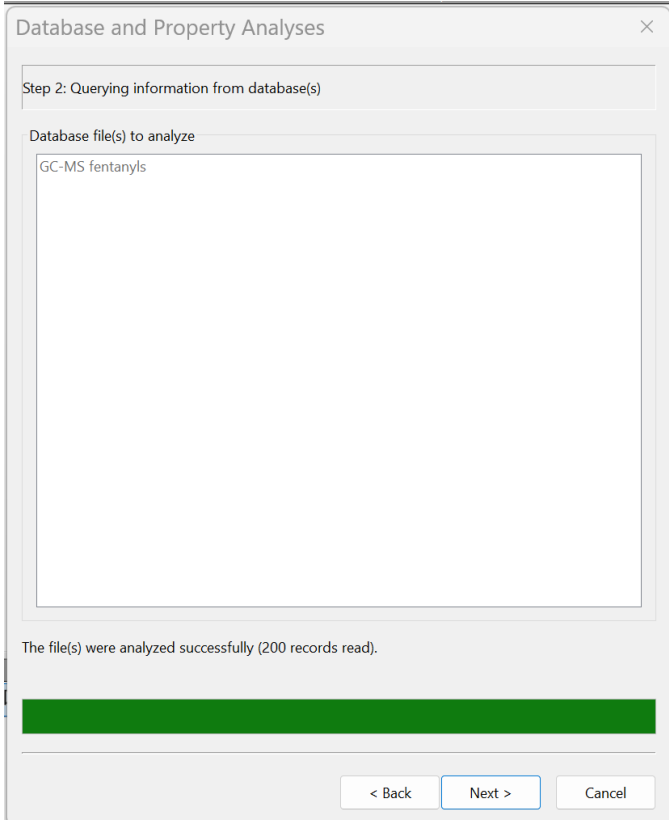
Action	Result																								
4 <ul style="list-style-type: none"><li>Transfer the highlighted collection of 54 records to Minelt using the <b>Transfer to</b> button.</li><li>The database records will open in Minelt.</li></ul>	<p>The screenshot displays the software interface for a mass spectral search. The top section shows a mass spectrum plot with a base peak at m/z 110. The plot is labeled "MS (LC) (10)". Below the plot is a table of results with columns for Hit, Name, and Spectrum. The first row is highlighted in blue and corresponds to Salicylic acid. The table lists 7 hits, all with a 100.00% match. The chemical structure of Salicylic acid is shown on the right. The structure is a benzene ring with a carboxylic acid group (-COOH) and a hydroxyl group (-OH) in the ortho position. The bottom right panel shows the properties of the selected compound, including Name, CAS Registry Number, Collision Energy, Exact Mass, Formula, InChI, InChIKey, Instrument Name, Ion Polarity, and Ionization Type.</p> <table border="1"><thead><tr><th>Hit</th><th>Name</th><th>Spectrum</th></tr></thead><tbody><tr><td>1</td><td>1149 Salicylic acid</td><td></td></tr><tr><td>2</td><td>548 Methyl 4-aminobenzoate</td><td></td></tr><tr><td>3</td><td>91 Benzoic acid</td><td></td></tr><tr><td>4</td><td>1105 Monobenzone</td><td></td></tr><tr><td>5</td><td>1127 Phenyl salicylate</td><td></td></tr><tr><td>6</td><td>650 Norepinephrine</td><td></td></tr><tr><td>7</td><td>1113 Methylparaben</td><td></td></tr></tbody></table> <p>Hit List: LC MS Hit List: LC MS Hit List: LC MS Hit List: Search #1 Hit List: PCA2</p> <p>54 Records (89454, 818.692)</p>	Hit	Name	Spectrum	1	1149 Salicylic acid		2	548 Methyl 4-aminobenzoate		3	91 Benzoic acid		4	1105 Monobenzone		5	1127 Phenyl salicylate		6	650 Norepinephrine		7	1113 Methylparaben	
Hit	Name	Spectrum																							
1	1149 Salicylic acid																								
2	548 Methyl 4-aminobenzoate																								
3	91 Benzoic acid																								
4	1105 Monobenzone																								
5	1127 Phenyl salicylate																								
6	650 Norepinephrine																								
7	1113 Methylparaben																								

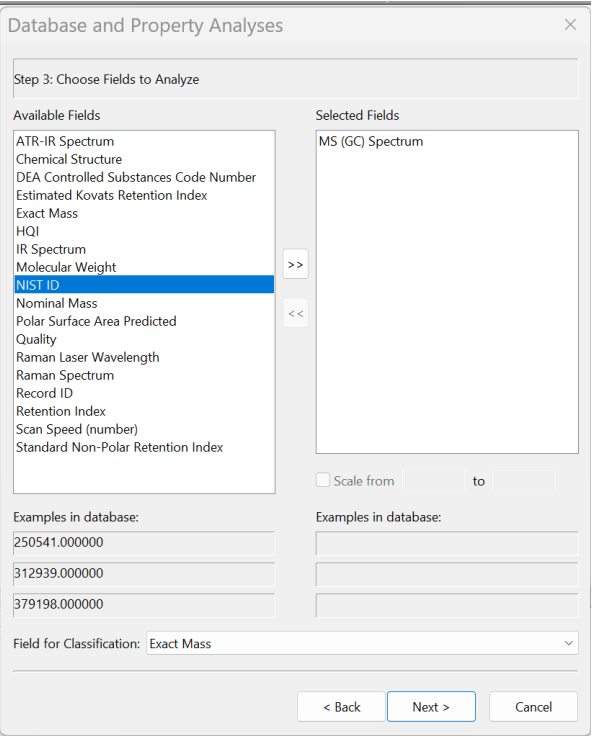
## GC-MS

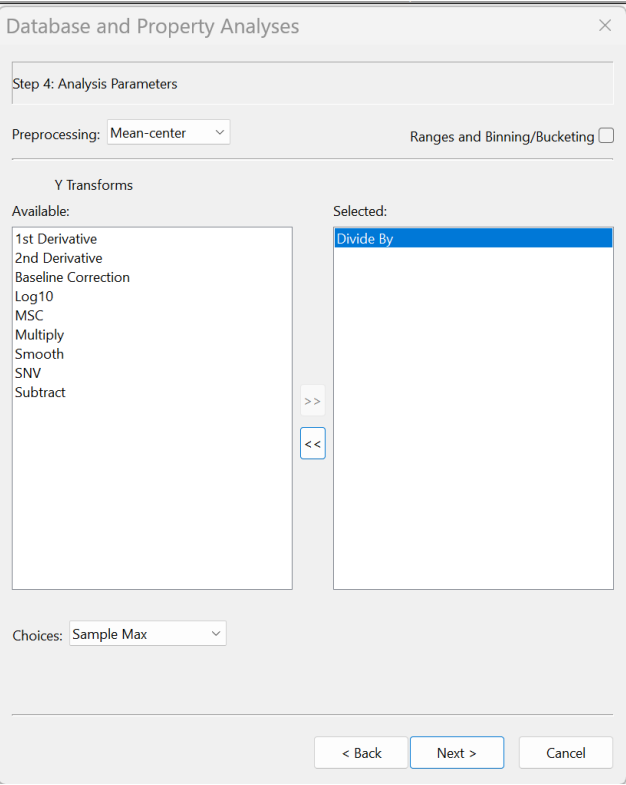
### Hit List Analysis Of Fentanyl's

	Action	Result																																																																																																																																												
1	<ul style="list-style-type: none"><li>• In SearchIt, go to <b>User-select</b>.</li><li>• <b>Limit to spectral technique to MS(GC)</b> and</li><li>• <b>Add All GC-MS databases for searching.</b></li></ul>	<div><div><div><div>SearchIt</div><div><div>Search Profiles: &lt;no profile&gt;</div><div><div>Search Categories</div><div><div><div><div><input type="checkbox"/> Spectrum</div><div><input type="checkbox"/> Peaks</div><div><input type="checkbox"/> Structure</div><div><input type="checkbox"/> Property/Name</div><div><input type="checkbox"/> MSforID</div></div><div><div>Search Databases</div><div><div><div><input checked="" type="radio"/> User-Select</div><div><input type="radio"/> All Compounds</div><div><input type="radio"/> Pure Compounds</div><div><input type="checkbox"/> Use Computed Spectra</div></div></div></div></div><div><div>Available for Searching:</div><div><div>Internet databases are switched to: Limit to spectral technique: MS (GC)</div><table><thead><tr><th>Name</th><th>Records</th><th>DB Code</th><th>Location</th><th>Version</th><th>Lock Owner</th></tr></thead><tbody><tr><td>MS - Food, Flavors, Fragranc...</td><td>13677</td><td>WFCX</td><td>&lt;Latest Version&gt;</td><td>25.00</td><td></td></tr><tr><td>MS - Maurer, Meyer, Pfeig...</td><td>10948</td><td>MMPWX</td><td>&lt;Latest Version&gt;</td><td>25.00</td><td></td></tr><tr><td>MS - NIST / EPA / NIH Mass ...</td><td>347100</td><td>MSX</td><td>&lt;Latest Version&gt;</td><td>25.00</td><td></td></tr><tr><td>MS - NIST / EPA / NIH Mass ...</td><td>46954</td><td>MSRX</td><td>&lt;Latest Version&gt;</td><td>25.00</td><td></td></tr><tr><td>MS - Sadler NIOSH Pocket G...</td><td>476</td><td>NSX</td><td>&lt;Latest Version&gt;</td><td>25.00</td><td></td></tr><tr><td>MS - SWGDRUG Mass Spectr...</td><td>3047</td><td>SWGMSX</td><td>&lt;Latest Version&gt;</td><td>25.00</td><td></td></tr><tr><td>MS - Wiley AAFS Toxicology ...</td><td>2758</td><td>AFX</td><td>&lt;Latest Version&gt;</td><td>25.00</td><td></td></tr><tr><td>MS - Wiley Androstanes, Est...</td><td>2979</td><td>MDX</td><td>&lt;Latest Version&gt;</td><td>25.00</td><td></td></tr><tr><td>MS - Wiley Drugs</td><td>2204</td><td>MDX</td><td>&lt;Latest Version&gt;</td><td>25.00</td><td></td></tr><tr><td>MS - Wiley Geochemicals, Pet...</td><td>1093</td><td>MGX</td><td>&lt;Latest Version&gt;</td><td>25.00</td><td></td></tr><tr><td>MS - Wiley Industrial Chemi...</td><td>41110</td><td>MTX</td><td>&lt;Latest Version&gt;</td><td>25.00</td><td></td></tr><tr><td>MS - Wiley Mass Spectra of ...</td><td>36360</td><td>WDD1X</td><td>&lt;Latest Version&gt;</td><td>25.11</td><td></td></tr><tr><td>MS - Wiley Mass Spectra of ...</td><td>1300</td><td>WMP3X</td><td>&lt;Latest Version&gt;</td><td>25.00</td><td></td></tr></tbody></table><div><div>Add All</div><div>Add</div><div>Remove</div><div>Remove All</div></div></div></div><div><div>Selected for Searching:</div><table><thead><tr><th>Name</th><th>Records</th><th>DB Code</th><th>Location</th></tr></thead><tbody><tr><td>MS - Food, Flavors, Fragrances, and Related Compounds...</td><td>13677</td><td>WFCX</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Food, Flavors, Fragrances, and Related Comp...</td></tr><tr><td>MS - Maurer, Meyer, Pfeiffer, Weber: GC-MS Library of Drugs...</td><td>10948</td><td>MMPWX</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Maurer Pfeiffer Weber: GCMS of Drugs... an</td></tr><tr><td>MS - NIST / EPA / NIH Mass Spectral Library 2023 - Main L...</td><td>347100</td><td>MSX</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - NIST EPA NIH Mass Spectral Library [MSX].sd</td></tr><tr><td>MS - NIST / EPA / NIH Mass Spectral Library 2023 - Replica...</td><td>46954</td><td>MSRX</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - NIST EPA NIH Mass Spectral Library [MSRX].sd</td></tr><tr><td>MS - Sadler NIOSH Pocket Guide to Chemical Hazards Co...</td><td>476</td><td>NSX</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Sadler NIOSH Pocket Guide to Chemical Haz</td></tr><tr><td>MS - SWGDRUG Mass Spectral Library - Wiley</td><td>3047</td><td>SWGMSX</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - SWGDRUG Mass Spectral Library - Wiley [SW</td></tr><tr><td>MS - Wiley AAFS Toxicology Section Mass Spectra of Drugs</td><td>2758</td><td>AFX</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Sadler AAFS Toxicology Section Mass Spect</td></tr><tr><td>MS - Wiley Androstanes, Estrogens &amp; other Steroids</td><td>2979</td><td>MDX</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Wiley Androstanes, Estrogens &amp; other Steroi</td></tr><tr><td>MS - Wiley Drugs</td><td>2204</td><td>MDX</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Wiley Drugs [MDX].sd</td></tr><tr><td>MS - Wiley Geochemicals, Petrochemicals &amp; Biomarkers</td><td>1093</td><td>MGX</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Wiley Geochemicals, Petrochemicals &amp; Biome</td></tr><tr><td>MS - Wiley Industrial Chemicals</td><td>41110</td><td>MTX</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Wiley Industrial Chemicals [MTX].sd</td></tr><tr><td>MS - Wiley Mass Spectra of Designer Drugs 2025</td><td>36360</td><td>WDD1X</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Wiley Mass Spectra of Designer Drugs [WDC</td></tr><tr><td>MS - Wiley Mass Spectra of Pesticides with Retention Indic...</td><td>1300</td><td>WMP3X</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Wiley Mass Spectra of Pesticides with Retenti</td></tr></tbody></table><div><div>Select by Browsing...</div></div></div><div><div>Hit List Size Limit: 100</div><div><input type="checkbox"/> All Hits</div><div>Display Profiles: &lt;no profile&gt;</div><div>Total Records to Search: 1412023</div><div>Search</div></div></div></div></div></div></div></div>	Name	Records	DB Code	Location	Version	Lock Owner	MS - Food, Flavors, Fragranc...	13677	WFCX	<Latest Version>	25.00		MS - Maurer, Meyer, Pfeig...	10948	MMPWX	<Latest Version>	25.00		MS - NIST / EPA / NIH Mass ...	347100	MSX	<Latest Version>	25.00		MS - NIST / EPA / NIH Mass ...	46954	MSRX	<Latest Version>	25.00		MS - Sadler NIOSH Pocket G...	476	NSX	<Latest Version>	25.00		MS - SWGDRUG Mass Spectr...	3047	SWGMSX	<Latest Version>	25.00		MS - Wiley AAFS Toxicology ...	2758	AFX	<Latest Version>	25.00		MS - Wiley Androstanes, Est...	2979	MDX	<Latest Version>	25.00		MS - Wiley Drugs	2204	MDX	<Latest Version>	25.00		MS - Wiley Geochemicals, Pet...	1093	MGX	<Latest Version>	25.00		MS - Wiley Industrial Chemi...	41110	MTX	<Latest Version>	25.00		MS - Wiley Mass Spectra of ...	36360	WDD1X	<Latest Version>	25.11		MS - Wiley Mass Spectra of ...	1300	WMP3X	<Latest Version>	25.00		Name	Records	DB Code	Location	MS - Food, Flavors, Fragrances, and Related Compounds...	13677	WFCX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Food, Flavors, Fragrances, and Related Comp...	MS - Maurer, Meyer, Pfeiffer, Weber: GC-MS Library of Drugs...	10948	MMPWX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Maurer Pfeiffer Weber: GCMS of Drugs... an	MS - NIST / EPA / NIH Mass Spectral Library 2023 - Main L...	347100	MSX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - NIST EPA NIH Mass Spectral Library [MSX].sd	MS - NIST / EPA / NIH Mass Spectral Library 2023 - Replica...	46954	MSRX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - NIST EPA NIH Mass Spectral Library [MSRX].sd	MS - Sadler NIOSH Pocket Guide to Chemical Hazards Co...	476	NSX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Sadler NIOSH Pocket Guide to Chemical Haz	MS - SWGDRUG Mass Spectral Library - Wiley	3047	SWGMSX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - SWGDRUG Mass Spectral Library - Wiley [SW	MS - Wiley AAFS Toxicology Section Mass Spectra of Drugs	2758	AFX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Sadler AAFS Toxicology Section Mass Spect	MS - Wiley Androstanes, Estrogens & other Steroids	2979	MDX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Wiley Androstanes, Estrogens & other Steroi	MS - Wiley Drugs	2204	MDX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Wiley Drugs [MDX].sd	MS - Wiley Geochemicals, Petrochemicals & Biomarkers	1093	MGX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Wiley Geochemicals, Petrochemicals & Biome	MS - Wiley Industrial Chemicals	41110	MTX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Wiley Industrial Chemicals [MTX].sd	MS - Wiley Mass Spectra of Designer Drugs 2025	36360	WDD1X	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Wiley Mass Spectra of Designer Drugs [WDC	MS - Wiley Mass Spectra of Pesticides with Retention Indic...	1300	WMP3X	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Wiley Mass Spectra of Pesticides with Retenti
Name	Records	DB Code	Location	Version	Lock Owner																																																																																																																																									
MS - Food, Flavors, Fragranc...	13677	WFCX	<Latest Version>	25.00																																																																																																																																										
MS - Maurer, Meyer, Pfeig...	10948	MMPWX	<Latest Version>	25.00																																																																																																																																										
MS - NIST / EPA / NIH Mass ...	347100	MSX	<Latest Version>	25.00																																																																																																																																										
MS - NIST / EPA / NIH Mass ...	46954	MSRX	<Latest Version>	25.00																																																																																																																																										
MS - Sadler NIOSH Pocket G...	476	NSX	<Latest Version>	25.00																																																																																																																																										
MS - SWGDRUG Mass Spectr...	3047	SWGMSX	<Latest Version>	25.00																																																																																																																																										
MS - Wiley AAFS Toxicology ...	2758	AFX	<Latest Version>	25.00																																																																																																																																										
MS - Wiley Androstanes, Est...	2979	MDX	<Latest Version>	25.00																																																																																																																																										
MS - Wiley Drugs	2204	MDX	<Latest Version>	25.00																																																																																																																																										
MS - Wiley Geochemicals, Pet...	1093	MGX	<Latest Version>	25.00																																																																																																																																										
MS - Wiley Industrial Chemi...	41110	MTX	<Latest Version>	25.00																																																																																																																																										
MS - Wiley Mass Spectra of ...	36360	WDD1X	<Latest Version>	25.11																																																																																																																																										
MS - Wiley Mass Spectra of ...	1300	WMP3X	<Latest Version>	25.00																																																																																																																																										
Name	Records	DB Code	Location																																																																																																																																											
MS - Food, Flavors, Fragrances, and Related Compounds...	13677	WFCX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Food, Flavors, Fragrances, and Related Comp...																																																																																																																																											
MS - Maurer, Meyer, Pfeiffer, Weber: GC-MS Library of Drugs...	10948	MMPWX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Maurer Pfeiffer Weber: GCMS of Drugs... an																																																																																																																																											
MS - NIST / EPA / NIH Mass Spectral Library 2023 - Main L...	347100	MSX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - NIST EPA NIH Mass Spectral Library [MSX].sd																																																																																																																																											
MS - NIST / EPA / NIH Mass Spectral Library 2023 - Replica...	46954	MSRX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - NIST EPA NIH Mass Spectral Library [MSRX].sd																																																																																																																																											
MS - Sadler NIOSH Pocket Guide to Chemical Hazards Co...	476	NSX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Sadler NIOSH Pocket Guide to Chemical Haz																																																																																																																																											
MS - SWGDRUG Mass Spectral Library - Wiley	3047	SWGMSX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - SWGDRUG Mass Spectral Library - Wiley [SW																																																																																																																																											
MS - Wiley AAFS Toxicology Section Mass Spectra of Drugs	2758	AFX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Sadler AAFS Toxicology Section Mass Spect																																																																																																																																											
MS - Wiley Androstanes, Estrogens & other Steroids	2979	MDX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Wiley Androstanes, Estrogens & other Steroi																																																																																																																																											
MS - Wiley Drugs	2204	MDX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Wiley Drugs [MDX].sd																																																																																																																																											
MS - Wiley Geochemicals, Petrochemicals & Biomarkers	1093	MGX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Wiley Geochemicals, Petrochemicals & Biome																																																																																																																																											
MS - Wiley Industrial Chemicals	41110	MTX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Wiley Industrial Chemicals [MTX].sd																																																																																																																																											
MS - Wiley Mass Spectra of Designer Drugs 2025	36360	WDD1X	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Wiley Mass Spectra of Designer Drugs [WDC																																																																																																																																											
MS - Wiley Mass Spectra of Pesticides with Retention Indic...	1300	WMP3X	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Wiley Mass Spectra of Pesticides with Retenti																																																																																																																																											

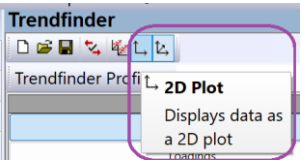
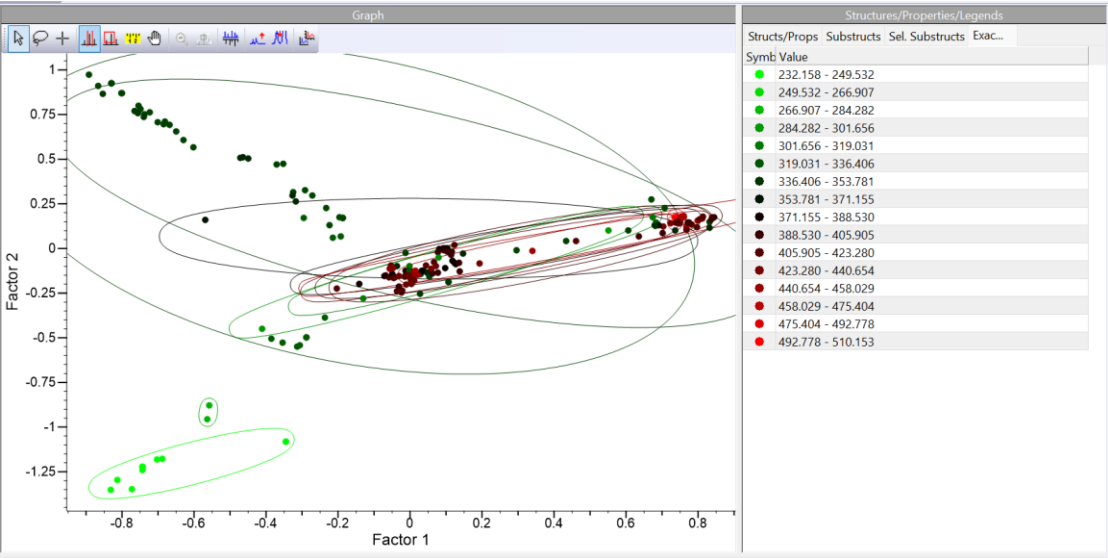
	Action	Result
2	<ul style="list-style-type: none"><li>• Set <b>Property/Name</b> to search for <b>Any Field</b> contains “<b>fentanyl</b>”.</li><li>• Set <b>Hit List Size Limit</b>: 200.</li><li>• Click the <b>Search</b> button.</li></ul>	 <p>The screenshot displays the Simple Spectral Search interface. On the left, under 'Search Categories', 'Property/Name' is selected. Under 'Search Databases', 'User-Select' is chosen, with 'All Compounds' selected. The main search area shows 'Property: Any Field' and 'Value: fentanyl' with the 'Contains' operator. The 'Hit List Size Limit' is set to 200. The 'Search' button is visible at the bottom right.</p>

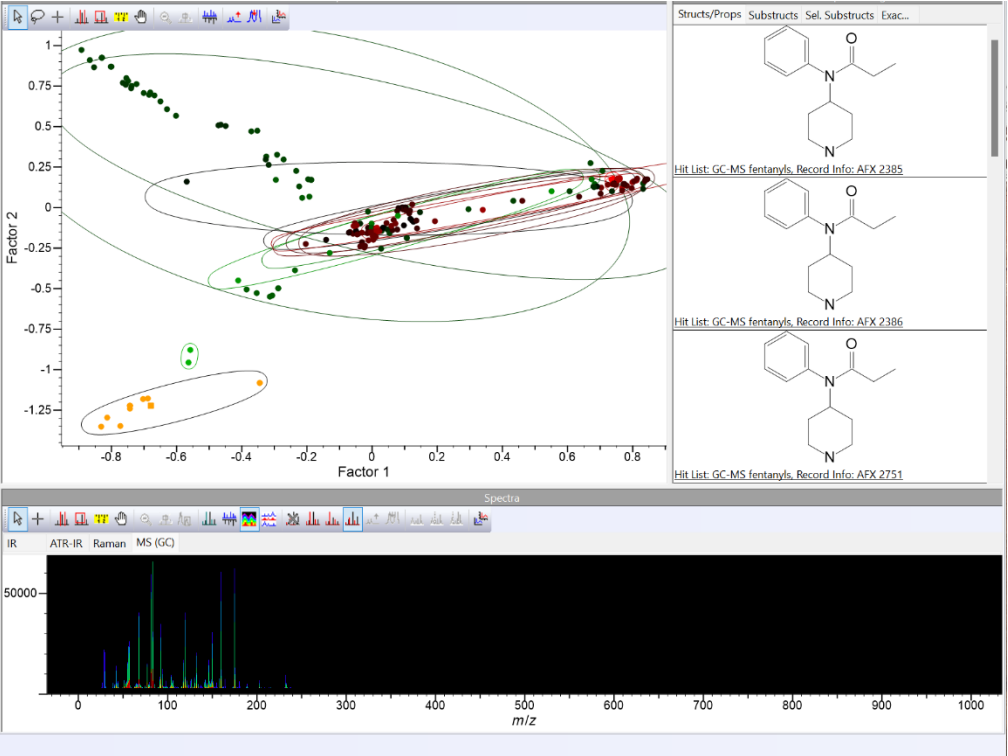
	Action	Result
3	<p><b>Minelt</b> provides a hit list of various <b>fentanyl</b>s.</p> <ul style="list-style-type: none"><li>Transfer this hit list to Trendfinder. </li></ul> <p><b>Note:</b> To start the Trendfinder application without transferring a hit list, open the Trendfinder application by clicking its icon in the Spectral Analysis toolbox.</p> <ul style="list-style-type: none"><li>Click <b>Next &gt;</b> at the prompt.</li></ul>	

	Action	Result
4	<ul style="list-style-type: none"><li>• Move <b>MS (GC) Spectrum</b> to <b>Selected Fields</b> for analysis.</li><li>• Select <b>Exact Mass</b> as <b>Field for Classification</b>.</li><li>• Click <b>Next &gt;</b>.</li></ul>	

	Action	Result
5	<ul style="list-style-type: none"><li>Choose <b>Divide By</b> in <b>Y Transform</b> and <b>Sample Max</b> in <b>Choices</b> to obtain the best results for MS spectra.</li><li>Click <b>Next &gt;</b>.</li></ul>	



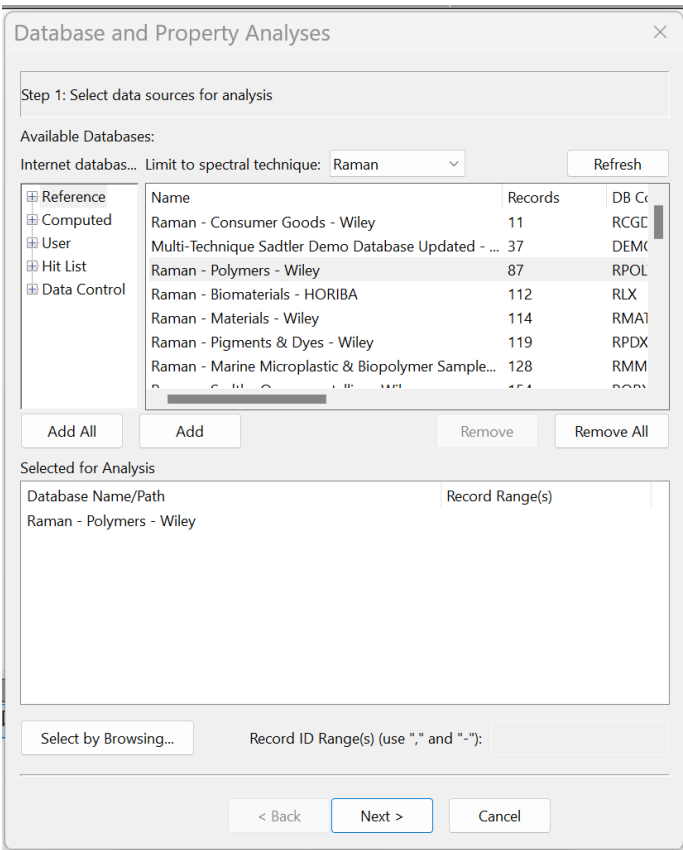
	Action	Result
6	<ul style="list-style-type: none"> <li>Click <b>Finish</b>.</li> <li>Select <b>2D Scores</b> plot view.</li> </ul> 	 <p>You can see a group of light green (smaller mass) spectra.</p> <p>A circle (<b>Trajectory</b>) defines the boundary for a value in the <b>Field of Classification</b>.</p>

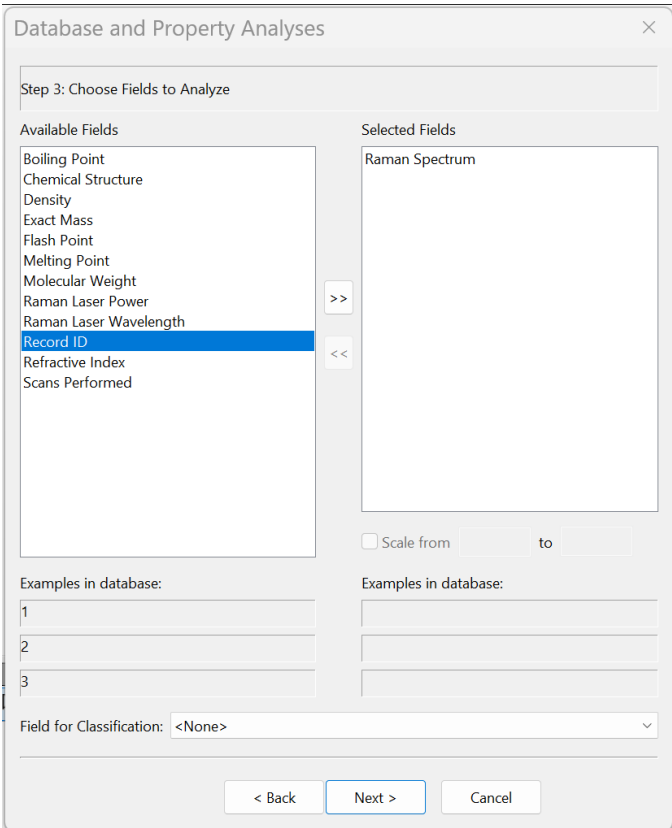
	Action	Result
7	<ul style="list-style-type: none"><li>• Use <b>left mouse</b> to draw a rectangle so that the green spectra in the lower left corner are selected and turn orange.</li><li>• Go to the <b>Structs/Props</b> tab under the <b>Structures/Properties/Legends</b> pane.</li><li>• Click the <b>MS (GC)</b> tab in the bottom pane to open the spectra.</li></ul>	 <p>The screenshot displays the KnowItAll software interface. The top panel shows a PCA plot with Factor 1 on the x-axis and Factor 2 on the y-axis. Data points are colored green, red, and orange, with green points clustered in the lower left. The right panel shows the 'Structs/Props' tab with three chemical structures of norfentanyl and their corresponding hit lists: 'Hit List: GC-MS fentanyl, Record Info: AFX 2385', 'Hit List: GC-MS fentanyl, Record Info: AFX 2386', and 'Hit List: GC-MS fentanyl, Record Info: AFX 2751'. The bottom panel shows the 'Spectra' tab with an 'MS (GC)' overlay heatmap showing intensity versus m/z from 0 to 1000.</p> <p>These are various <b>norfentanyl</b> MS spectra. The bottom pane shows the selected MS spectral <b>Overlay Heatmap</b>.</p>

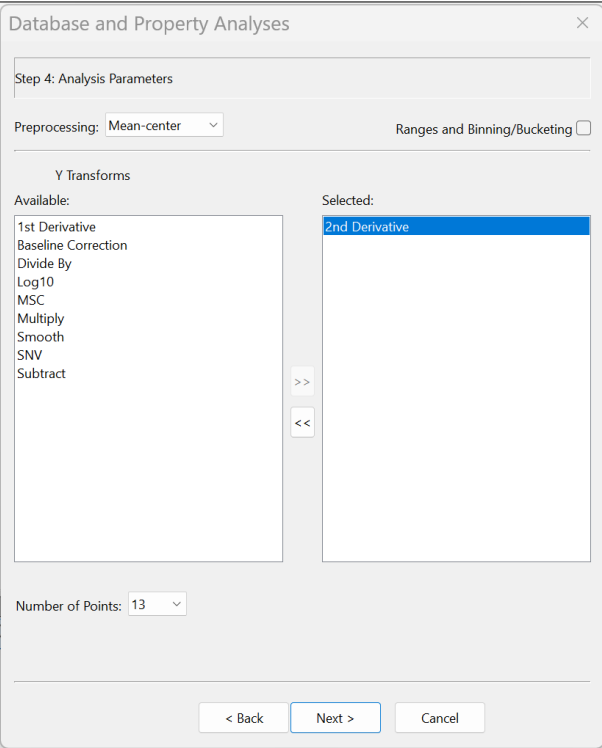


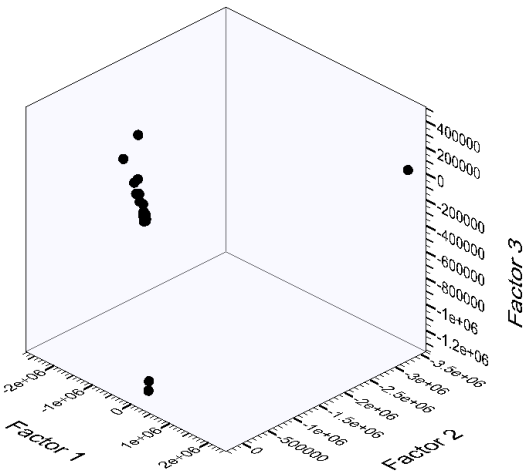
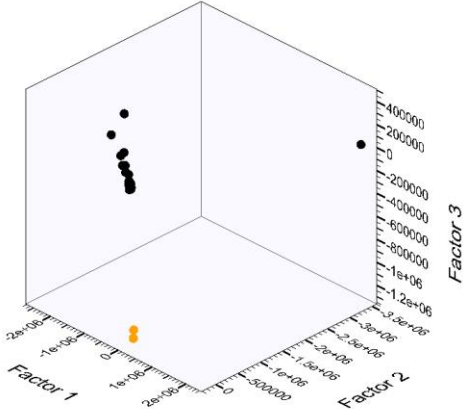
## Raman

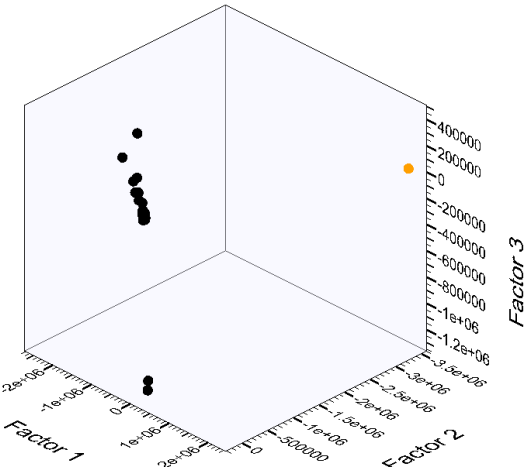
### Polymer Analysis

	Action	Result
1	Open the <b>Trendfinder</b> application by clicking its icon in the <b>Spectral Analysis</b> toolbox.	The application opens.
2	<ul style="list-style-type: none"> <li>• <b>Limit to spectral technique</b> should be set to Raman.</li> <li>• Select the database <b>Raman – Polymers – Wiley</b> for analysis and click <b>Add</b>.</li> <li>• Click <b>Next &gt;</b>, <b>Next &gt;</b>.</li> </ul>	

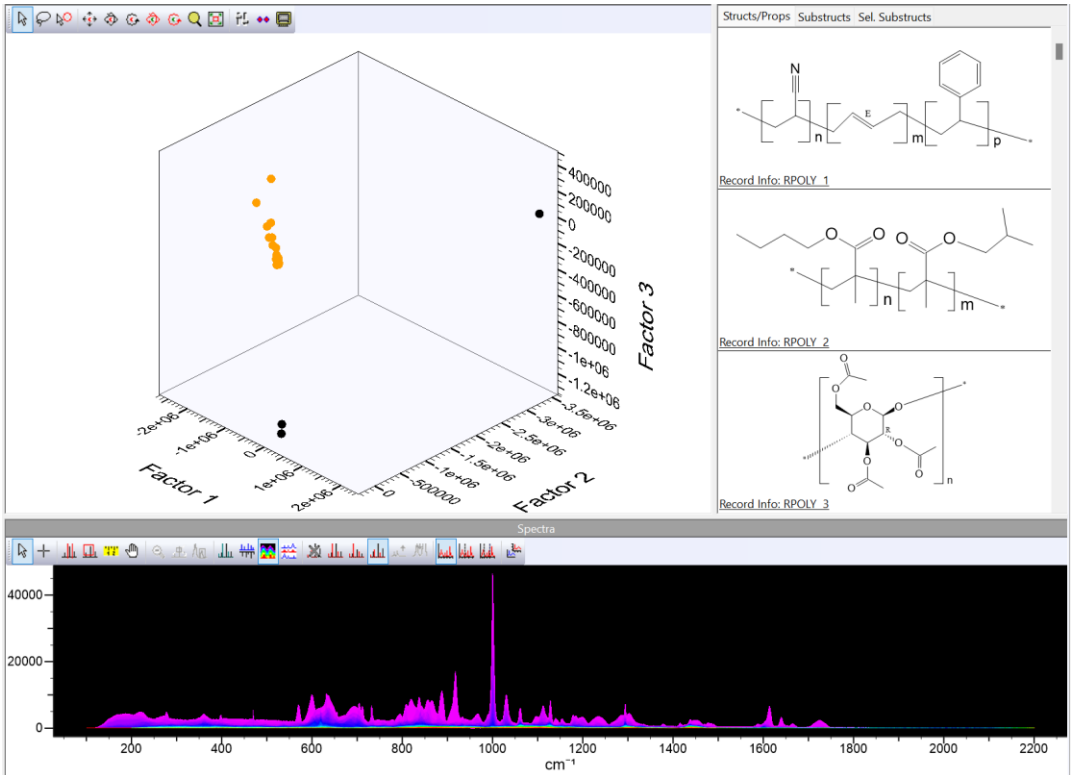
	Action	Result
3	<ul style="list-style-type: none"><li>• Move <b>Raman Spectrum</b> to the right either by:<ul style="list-style-type: none"><li>• Clicking &gt;&gt;, or</li><li>• Double clicking on <b>Raman Spectrum</b>.</li></ul></li><li>• Click <b>Next &gt;</b>.</li></ul>	 <p>Database and Property Analyses</p> <p>Step 3: Choose Fields to Analyze</p> <p>Available Fields</p> <ul style="list-style-type: none"><li>Boiling Point</li><li>Chemical Structure</li><li>Density</li><li>Exact Mass</li><li>Flash Point</li><li>Melting Point</li><li>Molecular Weight</li><li>Raman Laser Power</li><li>Raman Laser Wavelength</li><li><b>Record ID</b></li><li>Refractive Index</li><li>Scans Performed</li></ul> <p>Selected Fields</p> <ul style="list-style-type: none"><li>Raman Spectrum</li></ul> <p>Scale from to</p> <p>Examples in database:</p> <p>1</p> <p>2</p> <p>3</p> <p>Field for Classification: &lt;None&gt;</p> <p>&lt; Back Next &gt; Cancel</p>

	Action	Result
4	<ul style="list-style-type: none"><li>• Select <b>2<sup>nd</sup> Derivative</b> in the <b>Y Transform Available</b> list.</li><li>• <b>Set Number of Points to 13.</b></li></ul>	
5	Click <b>Next &gt;</b> .	

	Action	Result
6	Click <b>Finish</b> .	 <p>3 big groups are clearly identified.</p>
7	Use the <b>left mouse</b> to select a group of points.	 <div data-bbox="1470 885 1848 1372"><chem>*c1ccc(cc1)S(=O)(=O)c2ccc(cc2)Oc3ccc(cc3)*</chem><p><a href="#">Record Info: RPOLY_56</a> <a href="#">Record Info: RPOLY_61</a></p></div>

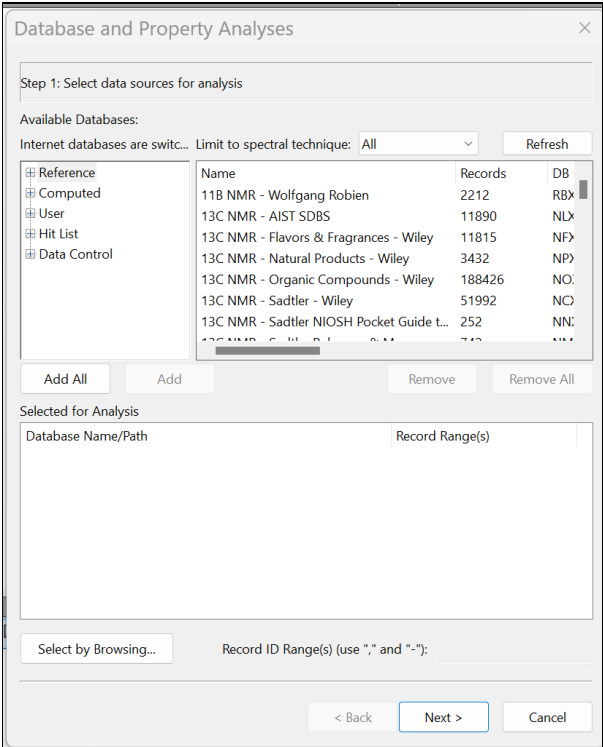
	Action	Result
8	Move to another point to examine a different polymer.	<div data-bbox="766 373 1291 836"></div> <div data-bbox="1428 332 1827 438"><math display="block">\text{*} - \left[ \text{C}_6\text{H}_4 - \text{S} \right]_n - \text{*}</math></div> <div data-bbox="1428 470 1575 495">Record Info: RPOLY_57</div>

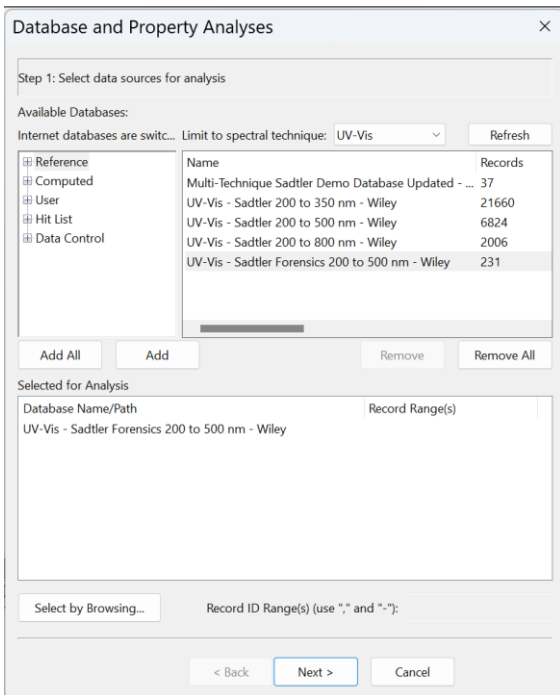


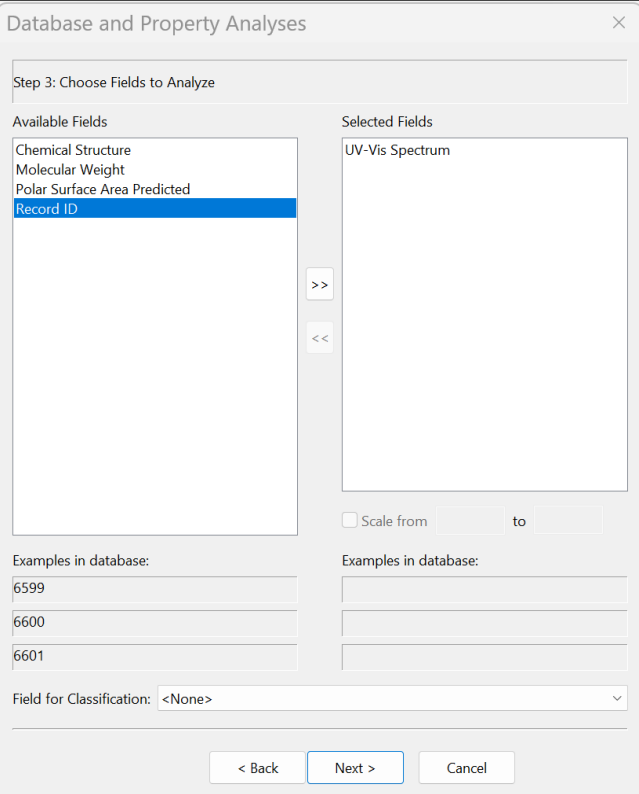
	Action	Result
9	Select another group of points by clicking and holding the left mouse button examine a different polymer.	 <p>The screenshot displays the software interface for spectral analysis. The top panel shows a 3D plot with axes labeled Factor 1, Factor 2, and Factor 3. A cluster of orange points is visible. The right panel shows three chemical structures labeled Record Info: RPOLY_1, Record Info: RPOLY_2, and Record Info: RPOLY_3. The bottom panel shows an IR spectrum plot with the x-axis labeled cm<sup>-1</sup> and the y-axis showing intensity. The spectrum shows a prominent peak around 1000 cm<sup>-1</sup>.</p> <p>They are quite different polymers. The bottom pane shows the <b>Overlay Heatmap</b> of selected spectra.</p>

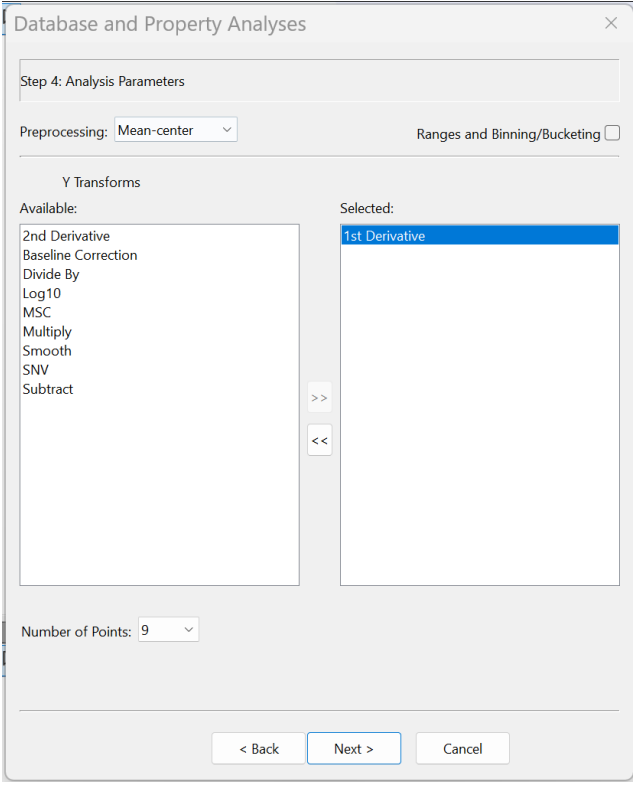
## UV-Vis

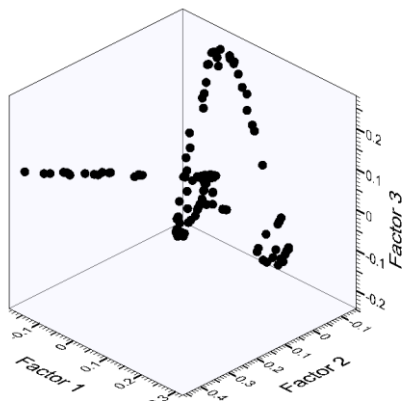
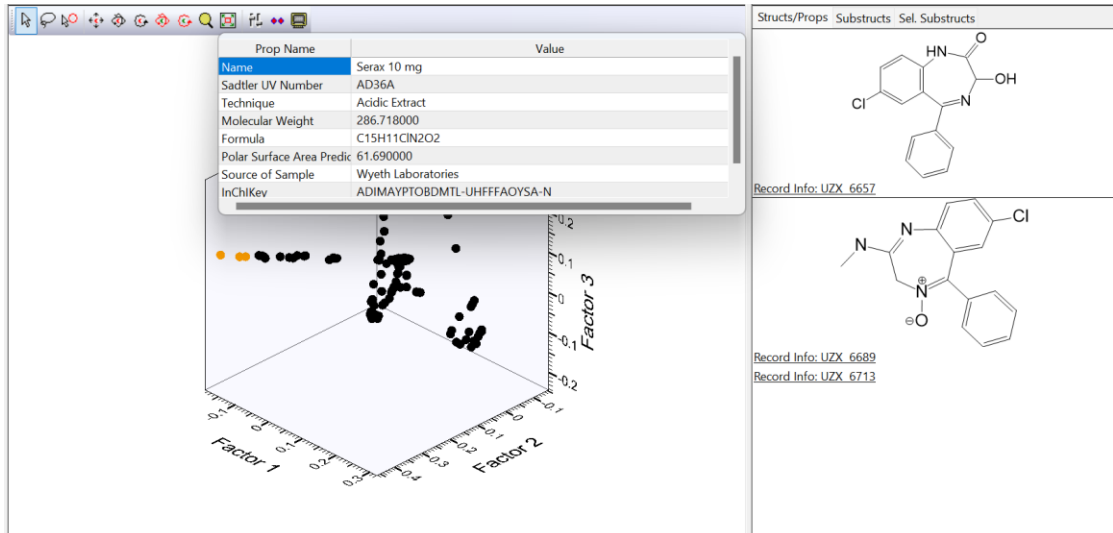
### Forensic Material Analysis

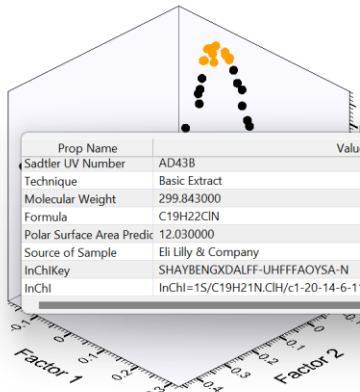
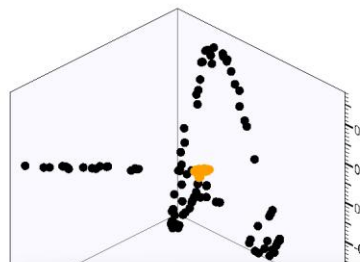
	Action	Result
1	Open the <b>Trendfinder</b> application by clicking its icon in the <b>Spectral Analysis</b> toolbox.	The application opens.
2	Choose <b>File &gt; New PCA Analysis</b> .	<p>The <b>Database and Property Analyses</b> wizard opens</p> 

	Action	Result																						
3	<ul style="list-style-type: none"><li>• Select the <b>UV-Vis</b> database <b>UV-Vis – Sadtler Forensics 200 to 500 nm – Wiley</b> for analysis and click <b>Add</b>.</li><li>• Click <b>Next &gt;</b>, <b>Next &gt;</b>.</li></ul>	 <p>Database and Property Analyses</p> <p>Step 1: Select data sources for analysis</p> <p>Available Databases:</p> <p>Internet databases are switc... Limit to spectral technique: UV-Vis Refresh</p> <table><tr><th>Reference</th><th>Name</th><th>Records</th></tr><tr><td>+</td><td>Multi-Technique Sadtler Demo Database Updated - ...</td><td>37</td></tr><tr><td>+</td><td>UV-Vis - Sadtler 200 to 350 nm - Wiley</td><td>21660</td></tr><tr><td>+</td><td>UV-Vis - Sadtler 200 to 500 nm - Wiley</td><td>6824</td></tr><tr><td>+</td><td>UV-Vis - Sadtler 200 to 800 nm - Wiley</td><td>2006</td></tr><tr><td>+</td><td>UV-Vis - Sadtler Forensics 200 to 500 nm - Wiley</td><td>231</td></tr></table> <p>Add All Add Remove Remove All</p> <p>Selected for Analysis</p> <table><tr><th>Database Name/Path</th><th>Record Range(s)</th></tr><tr><td>UV-Vis - Sadtler Forensics 200 to 500 nm - Wiley</td><td></td></tr></table> <p>Select by Browsing... Record ID Range(s) (use "," and "-");</p> <p>&lt; Back Next &gt; Cancel</p>	Reference	Name	Records	+	Multi-Technique Sadtler Demo Database Updated - ...	37	+	UV-Vis - Sadtler 200 to 350 nm - Wiley	21660	+	UV-Vis - Sadtler 200 to 500 nm - Wiley	6824	+	UV-Vis - Sadtler 200 to 800 nm - Wiley	2006	+	UV-Vis - Sadtler Forensics 200 to 500 nm - Wiley	231	Database Name/Path	Record Range(s)	UV-Vis - Sadtler Forensics 200 to 500 nm - Wiley	
Reference	Name	Records																						
+	Multi-Technique Sadtler Demo Database Updated - ...	37																						
+	UV-Vis - Sadtler 200 to 350 nm - Wiley	21660																						
+	UV-Vis - Sadtler 200 to 500 nm - Wiley	6824																						
+	UV-Vis - Sadtler 200 to 800 nm - Wiley	2006																						
+	UV-Vis - Sadtler Forensics 200 to 500 nm - Wiley	231																						
Database Name/Path	Record Range(s)																							
UV-Vis - Sadtler Forensics 200 to 500 nm - Wiley																								

	Action	Result
4	<p>In this dialog:</p> <ul style="list-style-type: none"><li>• Move <b>UV-Vis Spectrum</b> from the left box to the right one by selecting it in the left and using "&gt;&gt;" or double-clicking to move it to the right.</li><li>• Click <b>Next &gt;</b>.</li></ul>	

	Action	Result
5	<p>In this dialog:</p> <ul style="list-style-type: none"><li>• Move <b>1st Derivative</b> method to the right box to perform <b>Y Transforms</b> on the IR spectrum.</li><li>• Set the <b>Number of Points</b> on each side of an IR peak to be 9.</li><li>• Click <b>Next</b>.</li></ul> <p><i>Note: For UV-Vis, 1<sup>st</sup> derivative, which locates the peak top position is sufficient.</i></p>	

	Action	Result																		
6	Click <b>Finish</b> .	 <p>The above 3 factors view is returned.</p>																		
7	Use the <b>left mouse</b> to select box each group of points, which turn orange upon selection.	 <p>Properties of the selected point:</p> <table><tr><th>Prop Name</th><th>Value</th></tr><tr><td>Name</td><td>Serax 10 mg</td></tr><tr><td>Sadtler UV Number</td><td>AD36A</td></tr><tr><td>Technique</td><td>Acidic Extract</td></tr><tr><td>Molecular Weight</td><td>286.718000</td></tr><tr><td>Formula</td><td>C15H11ClN2O2</td></tr><tr><td>Polar Surface Area Predic</td><td>61.690000</td></tr><tr><td>Source of Sample</td><td>Wyeth Laboratories</td></tr><tr><td>InChIKey</td><td>ADIMAYPTOBDMTL-UHFFFAOYSA-N</td></tr></table> <p>Chemical structures and record information:</p> <ul style="list-style-type: none"><li>Record Info: UZX_6657</li><li>Record Info: UZX_6689</li><li>Record Info: UZX_6713</li></ul>	Prop Name	Value	Name	Serax 10 mg	Sadtler UV Number	AD36A	Technique	Acidic Extract	Molecular Weight	286.718000	Formula	C15H11ClN2O2	Polar Surface Area Predic	61.690000	Source of Sample	Wyeth Laboratories	InChIKey	ADIMAYPTOBDMTL-UHFFFAOYSA-N
Prop Name	Value																			
Name	Serax 10 mg																			
Sadtler UV Number	AD36A																			
Technique	Acidic Extract																			
Molecular Weight	286.718000																			
Formula	C15H11ClN2O2																			
Polar Surface Area Predic	61.690000																			
Source of Sample	Wyeth Laboratories																			
InChIKey	ADIMAYPTOBDMTL-UHFFFAOYSA-N																			

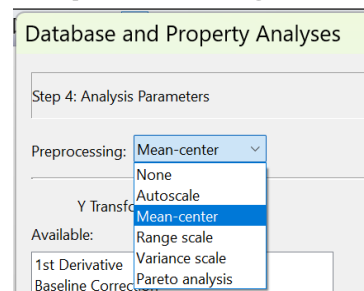
Action	Result																		
8	<div><table border="1"><thead><tr><th>Prop Name</th><th>Value</th></tr></thead><tbody><tr><td>Sadtler UV Number</td><td>AD438</td></tr><tr><td>Technique</td><td>Basic Extract</td></tr><tr><td>Molecular Weight</td><td>299.843000</td></tr><tr><td>Formula</td><td>C19H22ClN</td></tr><tr><td>Polar Surface Area Predic</td><td>12.030000</td></tr><tr><td>Source of Sample</td><td>Eli Lilly &amp; Company</td></tr><tr><td>InChIKey</td><td>SHAYBENGXDALFF-UHFFFAOYSA-N</td></tr><tr><td>InChI</td><td>InChI=1S/C19H21N.ClH/c1-20-14-6-11-19-17-9-4-2-7-15(17)12-13-16</td></tr></tbody></table></div> <div><p>Structs/Props Substructs Sel. Substructs</p><p>Record Info: UZX_6644</p><chem>CC(N)Cc1ccc2c(c1)OCO2</chem><p>Record Info: UZX_6654</p><chem>CNCCc1ccc2c(c1)ccc3ccccc23</chem><p>HCl</p><p>Record Info: UZX_6670</p><p>Record Info: UZX_6682</p><p>Record Info: UZX_6702</p><chem>CCN(CC1=CC=CC=C1)C2=CC=CC=C2</chem></div>	Prop Name	Value	Sadtler UV Number	AD438	Technique	Basic Extract	Molecular Weight	299.843000	Formula	C19H22ClN	Polar Surface Area Predic	12.030000	Source of Sample	Eli Lilly & Company	InChIKey	SHAYBENGXDALFF-UHFFFAOYSA-N	InChI	InChI=1S/C19H21N.ClH/c1-20-14-6-11-19-17-9-4-2-7-15(17)12-13-16
Prop Name	Value																		
Sadtler UV Number	AD438																		
Technique	Basic Extract																		
Molecular Weight	299.843000																		
Formula	C19H22ClN																		
Polar Surface Area Predic	12.030000																		
Source of Sample	Eli Lilly & Company																		
InChIKey	SHAYBENGXDALFF-UHFFFAOYSA-N																		
InChI	InChI=1S/C19H21N.ClH/c1-20-14-6-11-19-17-9-4-2-7-15(17)12-13-16																		
9	<div><table border="1"><thead><tr><th>Prop Name</th><th>Value</th></tr></thead><tbody><tr><td>Name</td><td>LSD</td></tr><tr><td>Sadtler UV Number</td><td>AD3A</td></tr><tr><td>Technique</td><td>Acidic Extract</td></tr><tr><td>Molecular Weight</td><td>323.438000</td></tr><tr><td>Formula</td><td>C20H25N3O</td></tr><tr><td>Polar Surface Area Predic</td><td>36.440000</td></tr><tr><td>CAS Registry Number</td><td>50-37-3</td></tr><tr><td>Synonyms</td><td>Lysergic acid, diethylamide</td></tr></tbody></table></div> <div><p>Structs/Props Substructs Sel. Substructs</p><p>Record Info: UZX_6599</p><chem>CC1=CC=C2C3=C1OC(=O)C4=CC=CC=C4N3C2=CC=C1</chem><p>H<sub>2</sub>SO<sub>4</sub></p><p>Record Info: UZX_6601</p><chem>CC1=CC=C2C3=C1OC(=O)C4=CC=CC=C4N3C2=CC=C1</chem><p>Record Info: UZX_6603</p><chem>CCN(CC1=CC=CC=C1)C2=CC=CC=C2</chem></div>	Prop Name	Value	Name	LSD	Sadtler UV Number	AD3A	Technique	Acidic Extract	Molecular Weight	323.438000	Formula	C20H25N3O	Polar Surface Area Predic	36.440000	CAS Registry Number	50-37-3	Synonyms	Lysergic acid, diethylamide
Prop Name	Value																		
Name	LSD																		
Sadtler UV Number	AD3A																		
Technique	Acidic Extract																		
Molecular Weight	323.438000																		
Formula	C20H25N3O																		
Polar Surface Area Predic	36.440000																		
CAS Registry Number	50-37-3																		
Synonyms	Lysergic acid, diethylamide																		

# Principal Component Analysis (PCA) Theory

Principal Component Analysis (PCA) is a process which performs dimensionality reduction. Thus, it transforms a large set of variables into a smaller set of uncorrelated variables (principal components). At the same time, it retains most of the original data's variance. This portion of training will explain how it is applied to spectral data analysis by KnowItAll.

## Parameters

### *Preprocessing*



- **None:** No preprocessing occurs.
- **Autoscale:**  
In Principal Component Analysis (PCA), "autoscale" refers to a preprocessing step where each variable in the dataset is standardized. This involves two main actions:
  1. **Centering:** Subtracting the mean of each variable so that the mean of the transformed variable is zero.
  2. **Scaling:** Dividing each variable by its standard deviation so that the variance of the transformed variable is one.Autoscaling ensures that all variables contribute equally to the PCA, regardless of their original scales or units. This is crucial because PCA identifies directions of maximum variance, and without autoscaling, variables with larger scales could dominate the analysis.
- **Mean-center:** Centers the data relative to a reference point<sup>1</sup>.
- **Range scale:** Min-max scaling which transforms the data to fit within a specific range<sup>2</sup>.
- **Variance scale:** First, the variance for each variable is calculated. Then, each variable is divided by the standard deviation.



- **Pareto analysis:** Pareto analysis is a decision-making tool based on the idea that 80% of a project's benefit can be achieved by doing 20% of the work, or conversely, 80% of problems can be traced to 20% of the causes. In other words, it posits that not all inputs have the same or even proportional impact on a given output<sup>3</sup>.

<sup>1</sup> Eigenvector Research Documentation Wiki (2012) *Advanced Preprocessing: Variable Centering*,

[https://www.wiki.eigenvector.com/index.php?title=Advanced\\_Preprocessing:\\_Variable\\_Centering](https://www.wiki.eigenvector.com/index.php?title=Advanced_Preprocessing:_Variable_Centering) (accessed 2025-08-19).

<sup>2</sup> Geeks for Geeks (2025) *Normalization and Scaling*, [Normalization and Scaling – GeeksforGeeks](#) (accessed 2025-08-19).

<sup>3</sup> Kenton, W. (2025) *Pareto Analysis: Definition, How to Create a Pareto Chart, and Example*, <https://www.investopedia.com/terms/p/pareto-analysis.asp> (accessed 2025-08-19).

## Y-Transforms

Database and Property Analyses

Step 4: Analysis Parameters

Preprocessing: Mean-center Ranges and Binning/Bucketing ☐

Y Transforms

Available:

- 1st Derivative
- Baseline Correction
- Divide By
- Log10
- MSC
- Multiply
- Smooth
- SNV
- Subtract

Selected:

- 2nd Derivative

Number of Points: 11

< Back Next > Cancel

- **1st Derivative:** parameter “Number of points” is the number of points on each side of a bell curve (peak).
- **2nd Derivative:** parameter “Number of Points” definition like 1<sup>st</sup> derivative.
- **Baseline Correction:** to correct the baseline.
- **Divide By:** Various data matrix transformation and normalization methods.
  - **Sample 1-norm:** area normalization.

- **Sample 2-norm:** vector length normalization.
- **Sample Max:** sample max value (suitable for MS spectra).
- **Sample Range:** consider various instrument measurement differences.
- **Value at Variable:** normalize to the value at a particular variable n.
- **Log10:** Applies  $\log^{10}$  to scale Y values.
- **MSC:** Multiple Scatter Variate<sup>4</sup>.
- **SNV:** Standard Normal Variate<sup>5</sup>.
- **Multiply:** Multiple Y by an editable numerical value.
- **Smoothing:** Uses our standard Savitzky-Golay algorithm to smooth noisy data.
- **Subtract:** The user can define the value to subtract.

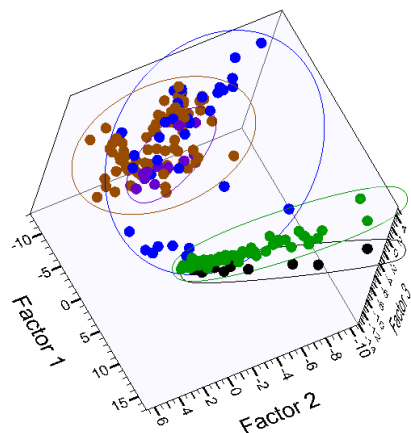
<sup>4</sup> Fearn, T., Riccioli, C., Garrido-Varo, A., and Guerrero-Ginel, J.E. On the geometry of SNV and MSC, *Chemometrics and Intelligent Laboratory Systems*, **2009** 96(1), 22-26. Doi: <https://doi.org/10.1016/j.chemolab.2008.11.006>.

<sup>5</sup> Standard Normal Variate (2025) [Standard Normal Variate - an overview | ScienceDirect Topics](#), ScienceDirect (accessed 2025-08-19).

## Result

### Scores (plot)

A graphical representation that displays the scores of the first 2 or 3 principal components as Factors, mathematical axis' orthogonal to each other, allowing for the visualization of the relationships between observations in a dataset<sup>6</sup>. Selecting the first 200 records of the IR - Automobile Paint Chips (APX) database with the parameter **Mean-center**, results in the plot below:

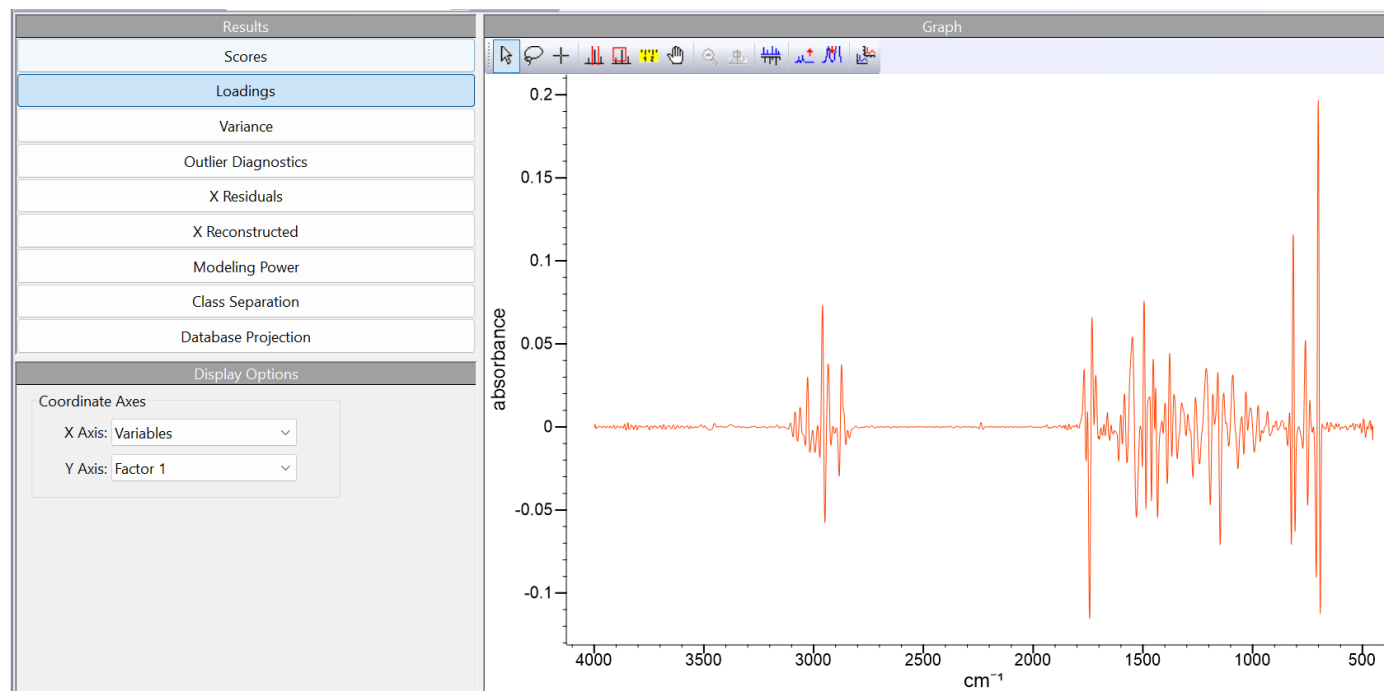


A circle (**Trajectory**) defines the boundary for a value in the **Field of Classification**).

<sup>6</sup> Dunn, K.G. (2025) Latent Variable Modelling in *Process Improvement using Data*, (<https://learnche.org/pid/latent-variable-modelling/principal-component-analysis/interpreting-score-plots-and-loading-plots>) (accessed 2025-08-19).

### Loadings

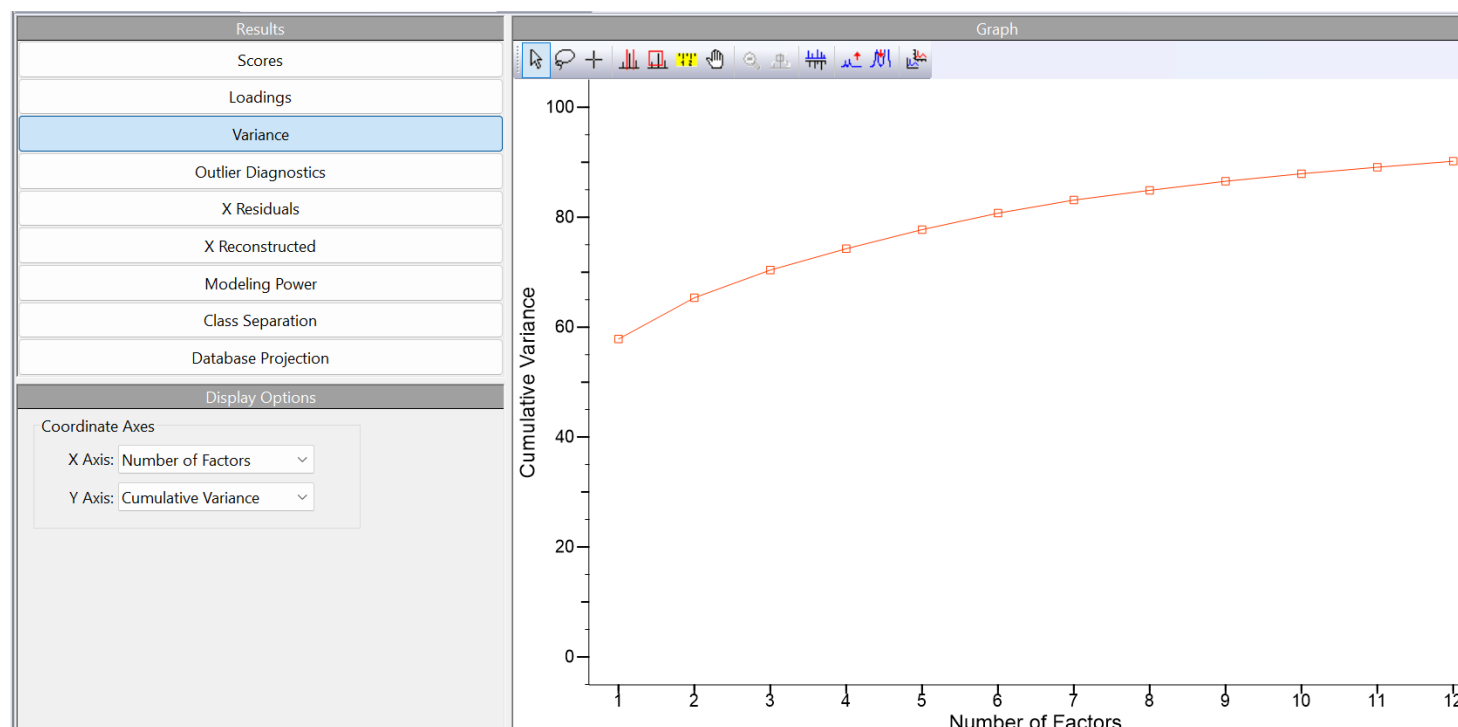
In order to show the relationship between the original variables and the principal components, it helps to understand how much each original variable contributes to the principal components and the nature of these contributions<sup>7</sup>. Using the above example, it would be:



<sup>7</sup> Schork, J. (2025) What are Loadings in PCA? *Statistics Global* (<https://statisticsglobe.com/what-are-loadings-pca#loadings-in-pca>) (accessed 2025-08-19).

## Variance

Variance refers to the proportion of the total variance attributed to each principal component<sup>8</sup>. It helps us understand how much information is retained after dimensionality reduction. The fraction of variance explained by a principal component is the ratio between the variance of that principal component and the total variance<sup>9</sup> When applied to the above example, the result is:



<sup>8</sup> Chouinard, J.C. (2023) What is the Explained Variance in PCA (Python Example), <https://www.jcchouinard.com/pca-explained-variance/> (accessed 2025-08-19).

<sup>9</sup> Cheplyaka, R. (2017) Explained variance in PCA, <https://ro-che.info/articles/2017-12-11-pca-explained-variance> (accessed 2025-08-19).

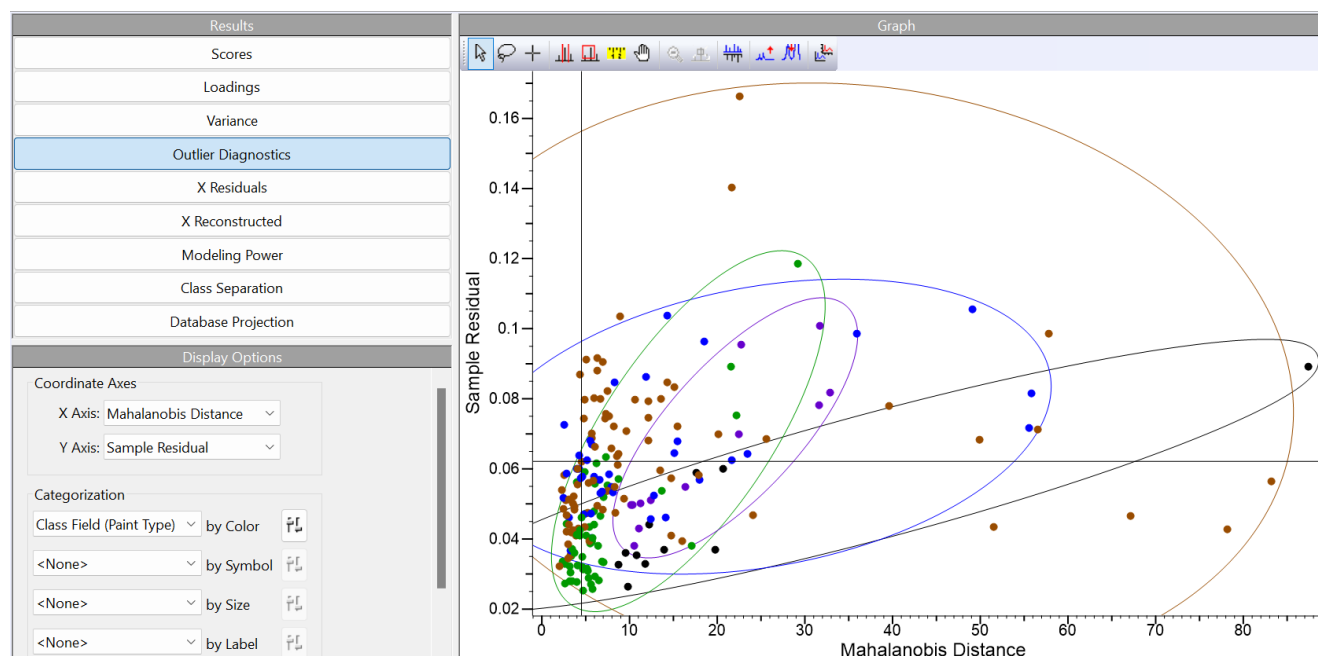
## Outlier Diagnosis

It identify outliers by reducing dimensionality and visualizing data on scores plots. Here are the terms used in KnowItAll under the Outlier Diagnostics pane:

- Mahalanobis Distance<sup>11</sup>:** Measures a distance between 2 points. It is a multivariate generalization of the square of the standard score  $z=(x-\mu)/\sigma$ : how many standard deviations away P is from the mean of D. This distance is zero for P at the mean of D and grows as P moves away from the mean along each principal component axis. If each of these axes is re-scaled to have unit variance, then the Mahalanobis distance corresponds to standard Euclidean distance in the transformed space. The Mahalanobis distance is thus unitless, scale-invariant, and takes into account the correlations of the data set. In short, **it measures how far a point is from the center of the data**

**distribution, considering the covariance structure.** PCA can be used to compute this distance in the reduced feature space. The following steps apply:

- Apply PCA to reduce dimensionality.
- Compute the Mahalanobis distance for each data point in the reduced space.
- Identify points with distances exceeding a threshold (e.g., based on a chi-squared distribution) as outliers. Using the above example, the result is:



- **Samples:** The ID of each sample (i.e., 1 to number of rows/spectra).
- **Sample residual**
- **F Ratio:** This is the statistic for evaluating whether two variances or standard deviations are significantly different. It is calculated by dividing one variance by another variance. If the null hypothesis is true, you expect F to have a value close to 1.0 most of the time. A large F ratio means that the variation among group means is more than you'd expect to see by chance. The F-distribution or F-ratio is a continuous probability distribution that arises frequently as the null distribution of a test statistic, most notably in the analysis of variance (ANOVA) and other F<sup>15</sup>.
- **Probability**

- **Record ID**

<sup>10</sup> Datathatmatters (2024) Outlier Detection Simplified: PCA Techniques for Improved Data Analysis <https://datathatmatter.com/2024/11/03/outlier-detection-simplified-pca-techniques-for-improved-data-analysis/> (accessed 2025-08-19).

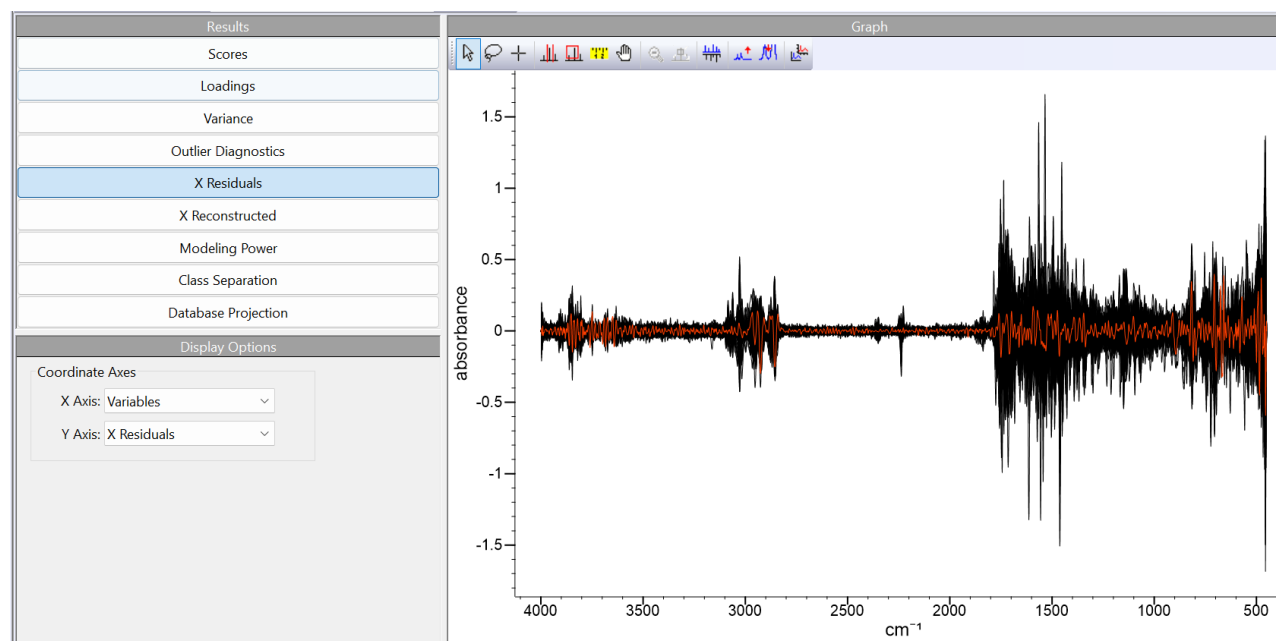
<sup>11</sup> Wikipedia (2025) Mahalanobis distance, [https://en.wikipedia.org/wiki/Mahalanobis\\_distance](https://en.wikipedia.org/wiki/Mahalanobis_distance) (accessed 2025-08-19).

<sup>12</sup> GraphPad Software, LLC.(2025) Interpreting results: One-way ANOVA, [https://www.graphpad.com/guides/prism/latest/statistics/f\\_ratio\\_and\\_anova\\_table\\_\(one-way\\_anova\).htm](https://www.graphpad.com/guides/prism/latest/statistics/f_ratio_and_anova_table_(one-way_anova).htm) (accessed 2025-08-19).

## ***X Residuals***

PCA residuals are calculated using the residual matrix  $E = X - T P' = X - X^{\wedge}$ , where  $X$  is the original matrix and  $T P'$  is the PCA model. The residuals for each column in the original matrix can be calculated using the  $R^2$  value, which gives an indication of how well the PCA model describes the data from that column. The function `pcares(X, ndim)` returns the residuals obtained by retaining `ndim` principal components of the  $n$ -by- $p$  matrix  $X$ . PCA of a model residuals is based on how well the model translates the effect of variables in  $Z Z$  on the data we are analyzing. Using the **residual** matrix  $E = X - T P' = X - X^{\wedge}$ , we can calculate the **residuals** for each column in the original matrix. This is summarized by the  $R^2$  value for each column in  $X$  and gives an indication of how well the **PCA** model describes the data from that column<sup>13</sup>. Using the above example, we get:

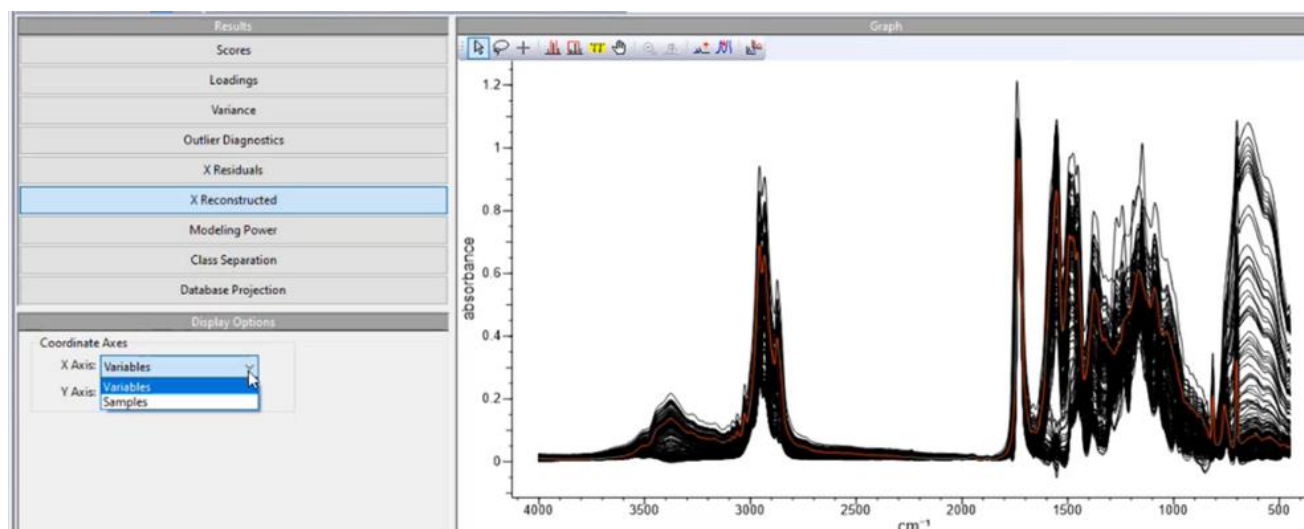




<sup>13</sup> Dunn, K.G. (2025) Latent Variable Modelling in *Process Improvement using Data*, <https://learnche.org/pid/latent-variable-modelling/principal-component-analysis/interpreting-the-residuals> (accessed 2025-08-19).

## ***X-reconstructed***

Reconstruct the original variables from a principal component<sup>14</sup> It can be viewed as "reverse PCA". For the above dataset, we get:



<sup>14</sup> Stack Exchange (2025) How to reverse PCA and reconstruct original variables from several principal components? <https://stats.stackexchange.com/questions/229092/how-to-reverse-pca-and-reconstruct-original-variables-from-several-principal-com> (accessed 2025-08-19).

## Modeling power

## Class Separation

It measures how well different class are separated<sup>15</sup>. Our particular example for the 1<sup>st</sup> 1000 spectra:

Results	Matrix					
Scores	Paint Type	Non-Aqueous Dispersion Enamel (NAD)	Acrylic Solution Lacquer	Water-Based Enamel	Acrylic Enamel	Acrylic Dispersion Lacquer
Loadings	Non-Aqueous Dispersion Enamel (NAD)		7.27	3.99	0.00	4.80
Variance	Acrylic Solution Lacquer	7.27		6.42	7.13	1.04
Outlier Diagnostics	Water-Based Enamel	3.99	6.42		3.51	5.47
X Residuals	Acrylic Enamel	0.00	7.13	3.51		4.58
X Reconstructed	Acrylic Dispersion Lacquer	4.80	1.04	5.47	4.58	
Modeling Power						
Class Separation						

<sup>15</sup> Stack Exchange (2025) Measures of class separability in classification problems, <https://stats.stackexchange.com/questions/46780/measures-of-class-separability-in-classification-problems> (accessed 2025-08-19).