

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


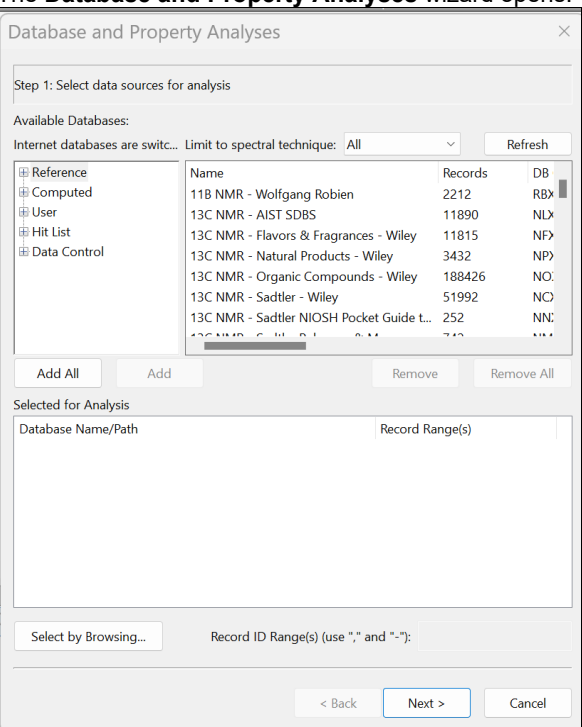
C:\Users\Public\Documents\Wiley\KnowItAll\Samples

KnowItAll Applications Used

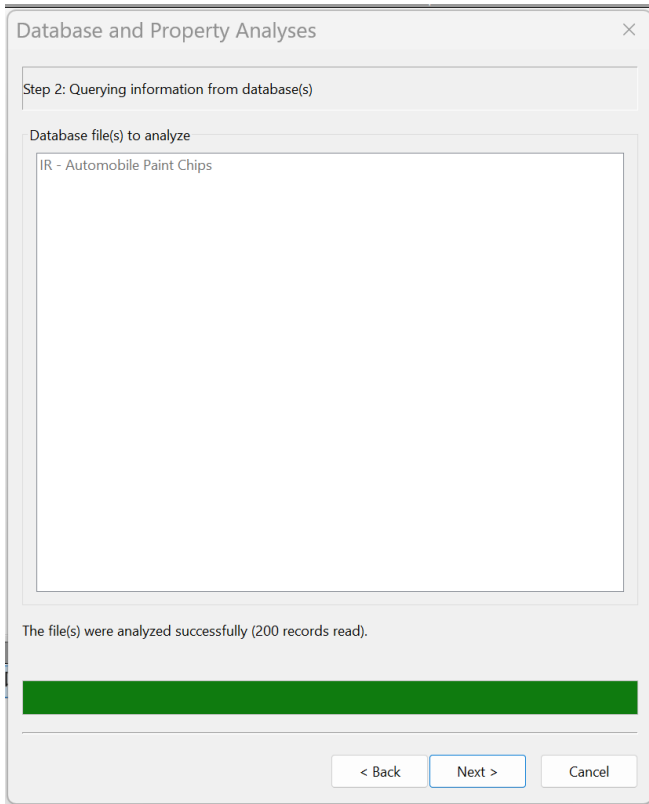
- KnowItAll Trendfinder

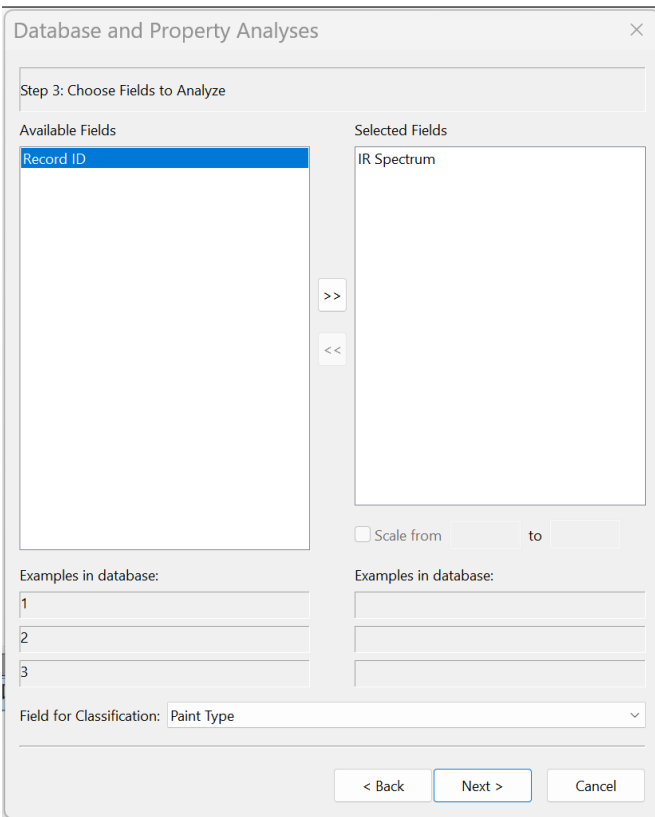
IR Example

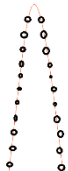
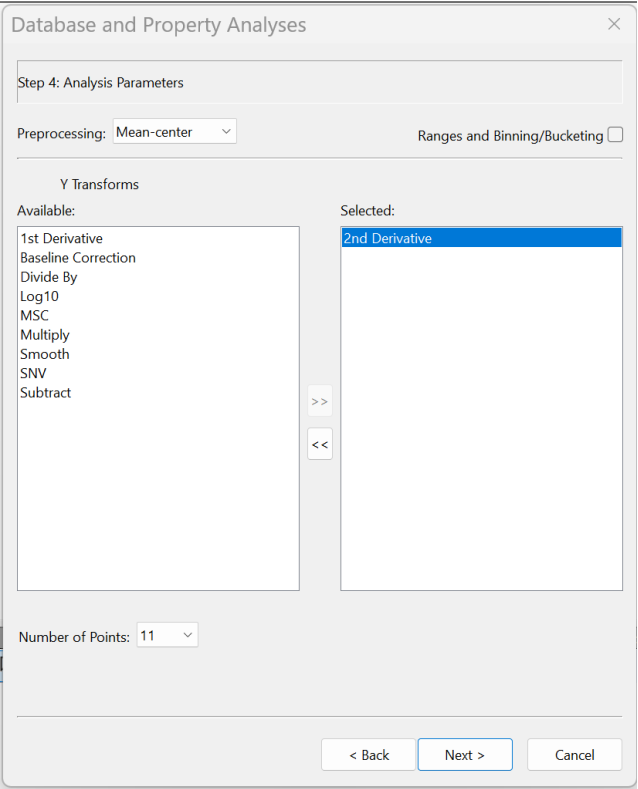
A. Principal Component Analysis (PCA) of Automobile Paint Chips

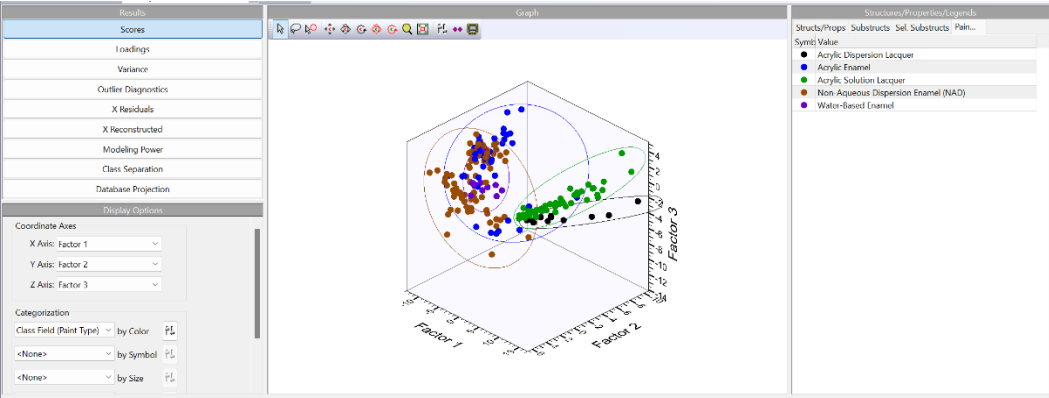
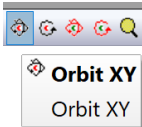
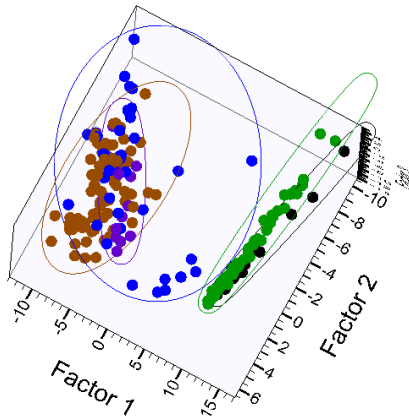
	Action	Result
1	<p>Open the Trendfinder application by clicking its icon in the Spectral Analysis toolbox.</p>  Trendfinder	The application opens.
2	Choose File > New PCA Analysis .	<p>The Database and Property Analyses wizard opens.</p> 


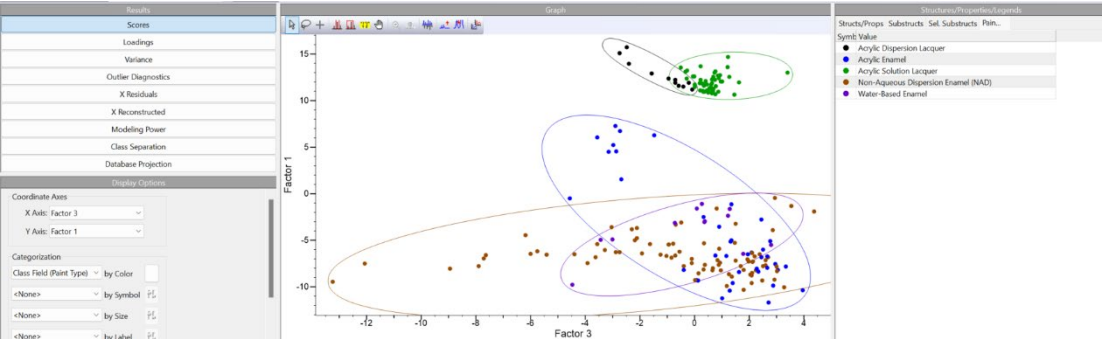
	Action	Result																																								
3	<ul style="list-style-type: none">• Select the reference database IR - Automobile Paint Chips (APX) and click Add.• Highlight the database in the Selected for Analysis box, type 1-200 in the Record ID Range field (to use the first 200 records).• Click Next >.	<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 Chemistry</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>< BackNext >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 Chemistry	527	OCX	Database Name/Path	Record Range(s)	IR - Automobile Paint Chips	1-200
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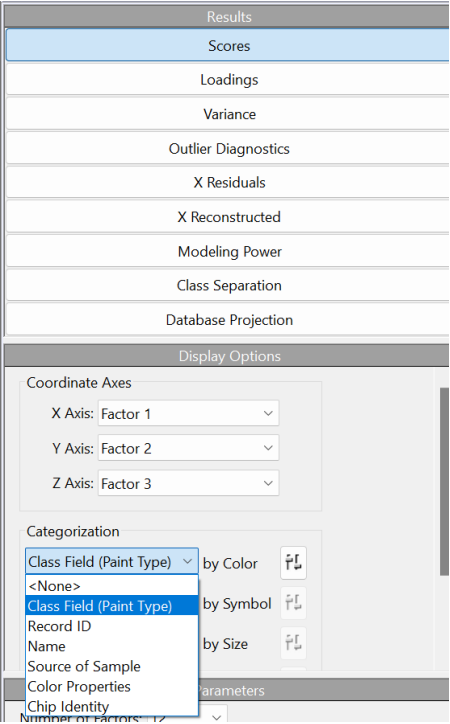
	Action	Result
4	Click Next > again.	

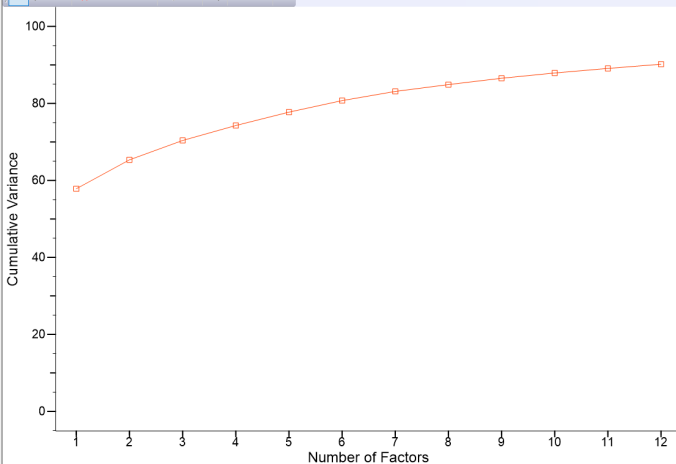
	Action	Result
5	<p>In this dialog:</p> <ul style="list-style-type: none">• Move IR Spectrum from the left box to the right one by selecting it in the left and using ">>" or double-clicking to move it to the right• Set Field for Classification to Paint Type. Click Next >.	

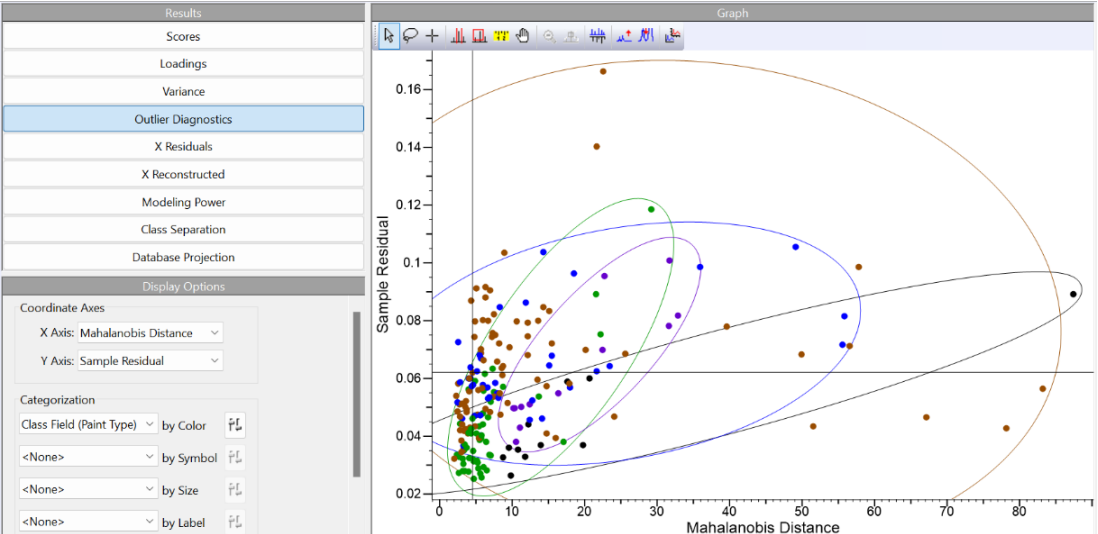
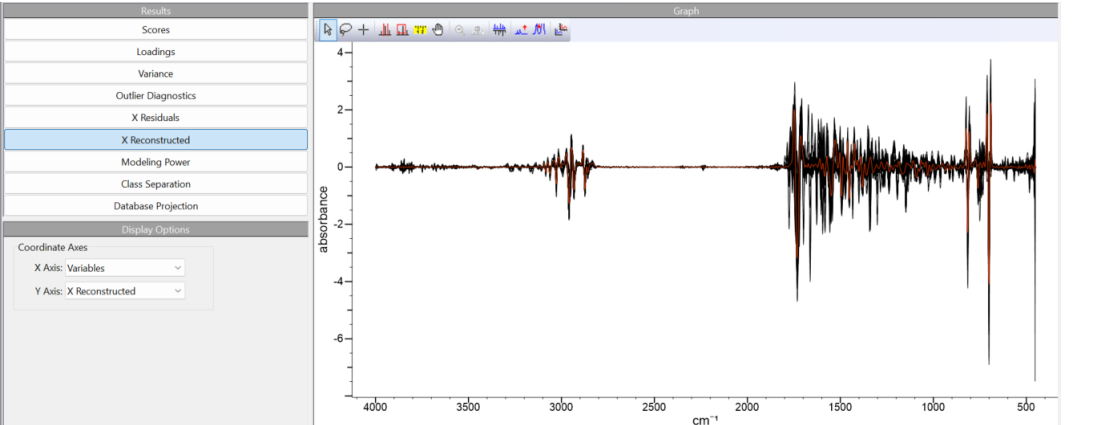
	Action	Result
6	<p>In this dialog:</p> <ul style="list-style-type: none">• Move 2nd Derivative method to the right box to perform Y Transforms on the IR spectrum.• Set the Number of Points on each side of an IR peak to be 11 (picture below as an example).  <ul style="list-style-type: none">• Click Next.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

	Action	Result
7	<p>Click Finish 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 (Trajectory) defines the boundary for a value in the Field of Classification.</p>
8	 <ul style="list-style-type: none"> Click Rotate and observe the spectra distribution in 3 factor space. 	

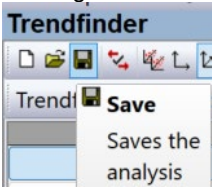
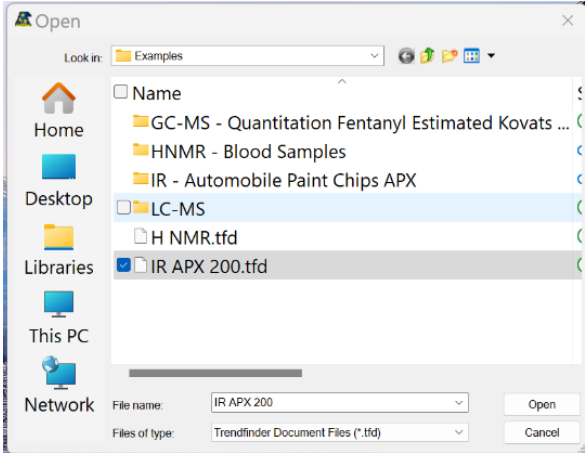
	Action	Result
9	<ul style="list-style-type: none">Click the 2D Plot toolbar button  to switch the graph display in 2 dimensions.Set the X-Axis to be Factor 3 and the Y-Axis to be Factor 1.	 <p>The lacquer types (upper) are separated from enamels (lower).</p>

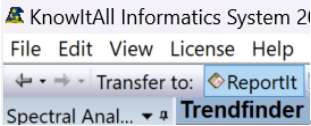
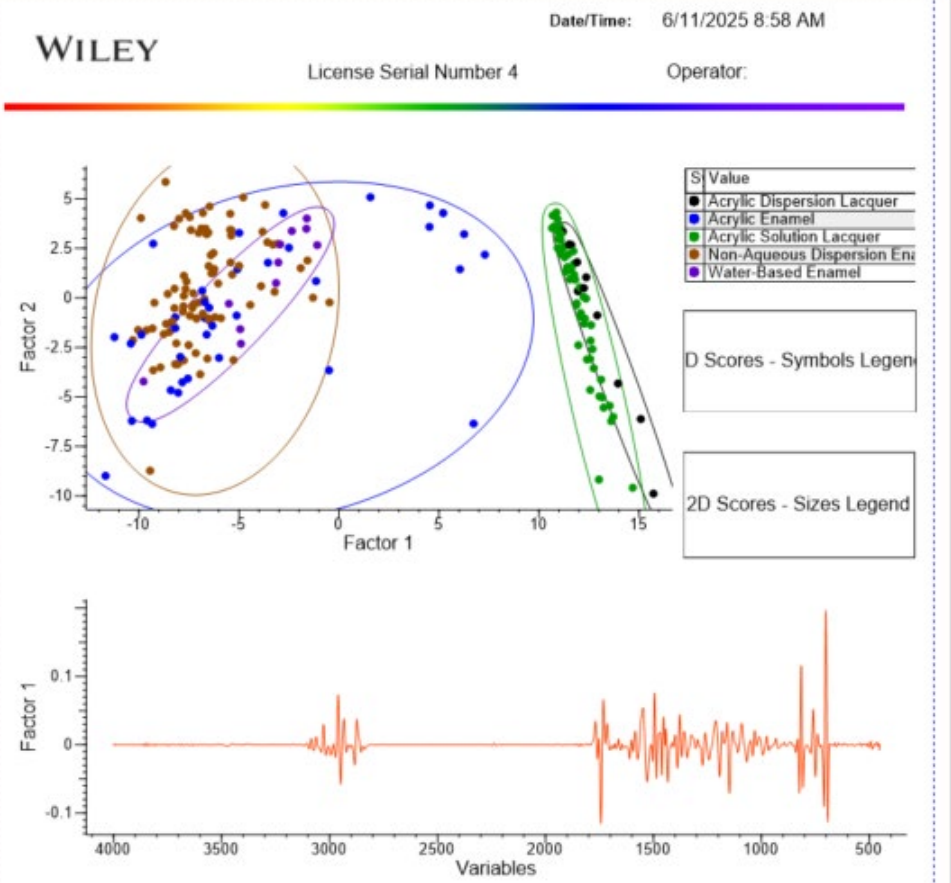
	Action	Result
10	The Categorization dropdown list allows you to see how other properties correlate to the spectral space.	

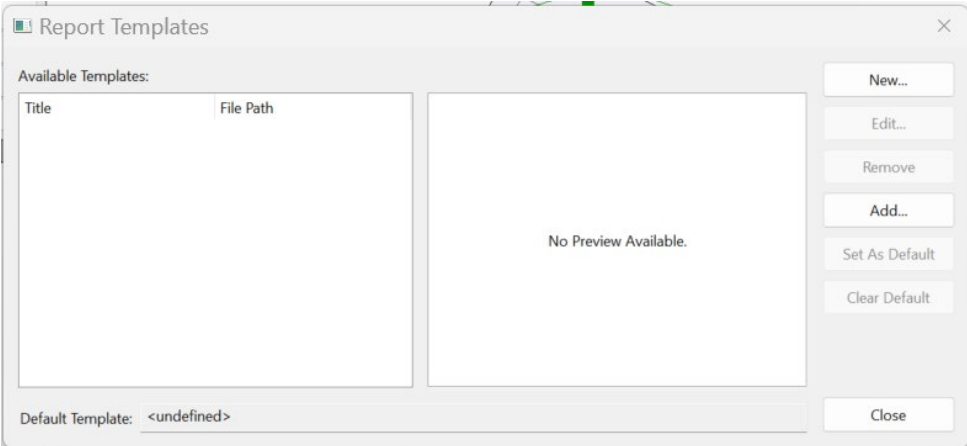
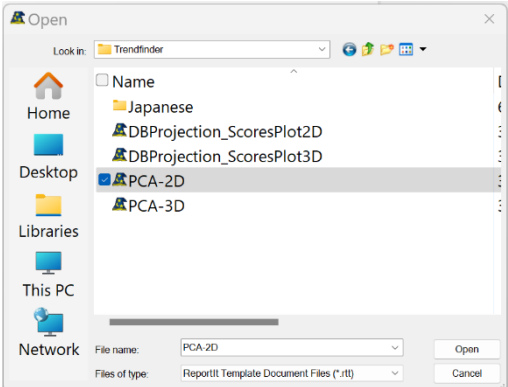
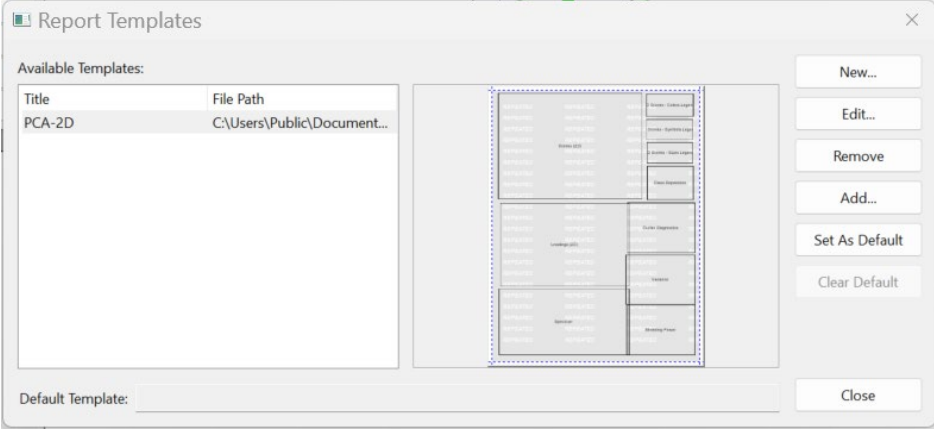
	Action	Result																										
11	Variance allows you to examine the PCA quality.	<div><div><div>Results</div><div>Scores</div><div>Loadings</div><div>Variance</div><div>Outlier Diagnostics</div><div>X Residuals</div><div>X Reconstructed</div><div>Modeling Power</div><div>Class Separation</div><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><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
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	Action	Result
12	<p>Select Outlier Diagnostics 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>X Reconstructed should look like the illustration to the right.</p>	 <p>Note: The above is a “reconstructed” 2nd derivative form of Y.</p>

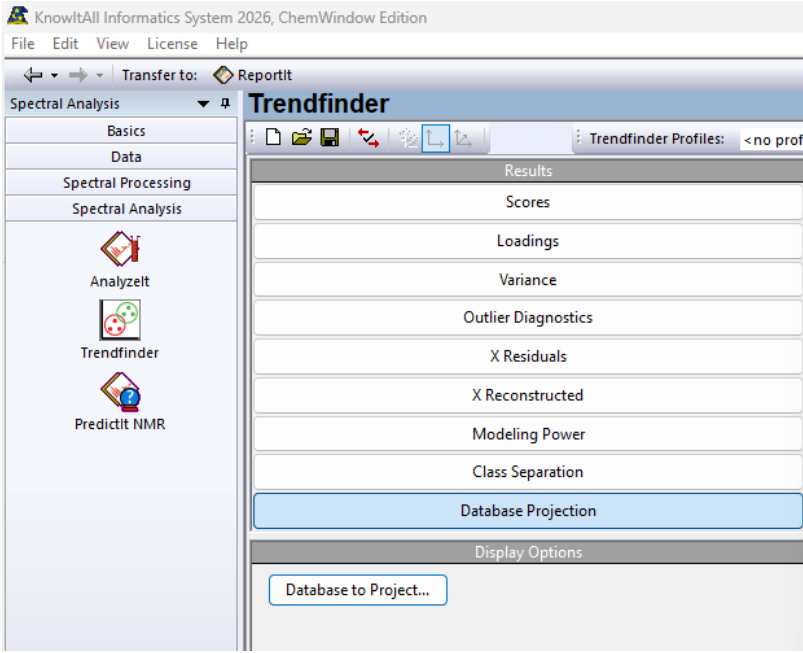
B. Save the Analysis and Create a Report

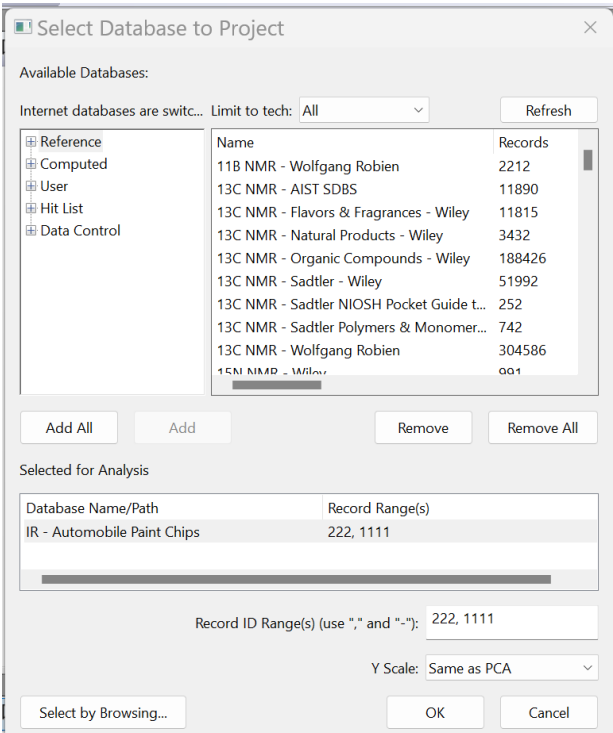
	Action	Result
1	<p>Save the analysis by:</p> <ul style="list-style-type: none">Clicking on the Save symbol  <ul style="list-style-type: none">Or by going to File>Save Analysis.Or Control + S.	

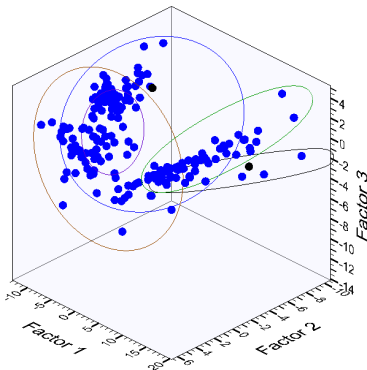
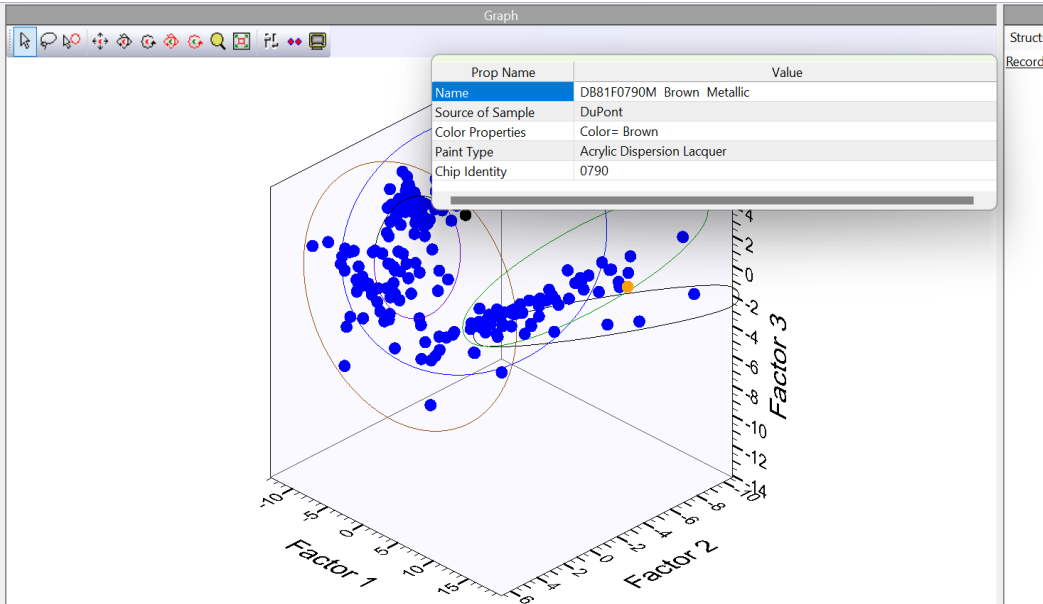
	Action	Result
2	<p>Transfer an analysis to ReportIt by:</p> <ul style="list-style-type: none"> • Selecting a group of spectra and: <ul style="list-style-type: none"> ◦ using the mouse to click a position and drag drop to another position. ◦ Or use the Lasso tool to circle points. ◦ Or Control + Click points. • Then click on ReportIt in the Transfer to <div data-bbox="388 987 697 1112">  </div> 	 <p>WILEY</p> <p>Date/Time: 6/11/2025 8:58 AM</p> <p>License Serial Number 4</p> <p>Operator:</p> <p>Factor 2</p> <p>Factor 1</p> <p>Factor 1</p> <p>Variables</p> <p>SI Value</p> <ul style="list-style-type: none"> Acrylic Dispersion Lacquer Acrylic Enamel Acrylic Solution Lacquer Non-Aqueous Dispersion Enz Water-Based Enamel <p>D Scores - Symbols Legend</p> <p>2D Scores - Sizes Legend</p>

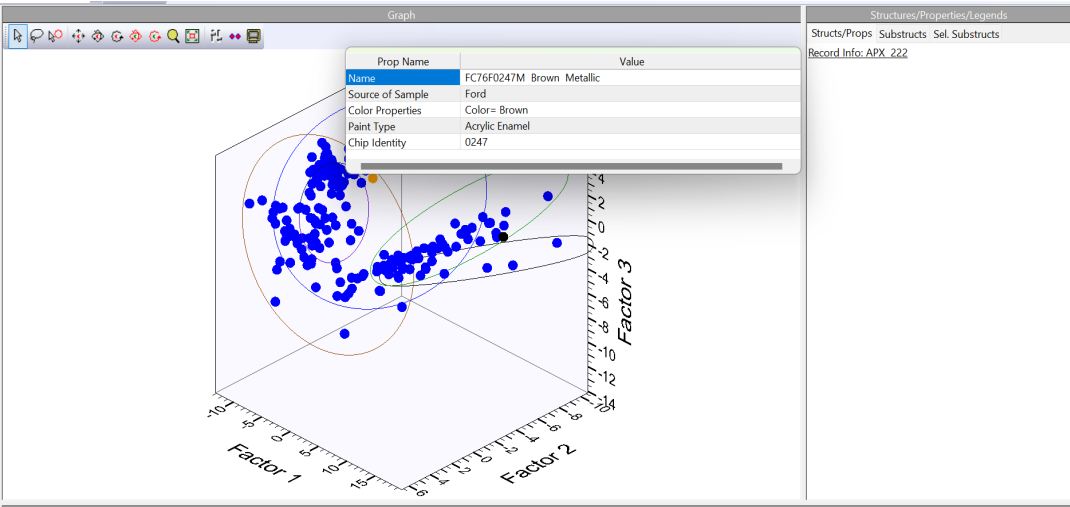
	Action	Result
<p><i>Note:</i></p> <ul style="list-style-type: none"> If a template is used for the first time, the user has to do the following before transferring data to the ReportIt application: File > Edit Report Templates Click Add button Navigate to the template file C:\Users\Public\Public Documents\Wiley\KnowItAll\Report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

C. Project Unknown Spectra to the PCA “Space”

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

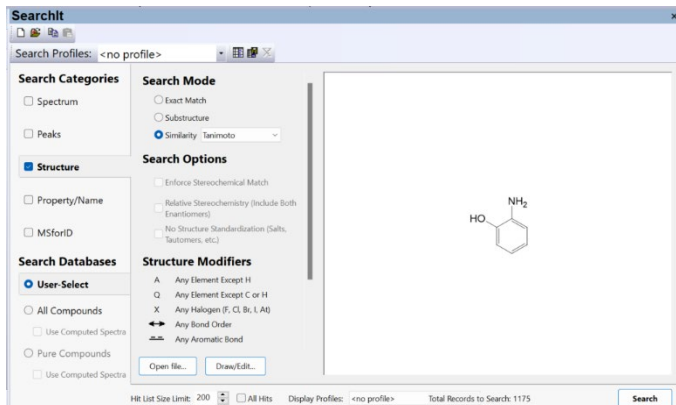
	Action	Result																																					
2	<p>Ensure the IR-Automobile Paint Chips database is selected and then:</p> <ul style="list-style-type: none">• Type in 222 and 1111 under “Record Range(s)” (use “,” and “-”) to test the classification of these unused spectra based on the first 200 spectra.• Set Y Scale: Same As PCA.• Click OK.	 <p>The screenshot shows the "Select Database to Project" dialog box. It has a title bar with a close button. Below the title bar, it says "Available Databases:". There are two sections: "Internet databases are switc..." and "Limit to tech:". The "Limit to tech:" dropdown is set to "All". There is a "Refresh" button. Below these, there is a table with three columns: "Reference", "Name", and "Records". The "Reference" column has expandable icons. The "Name" column lists various databases. The "Records" column shows the number of records for each database. The "IR - Automobile Paint Chips" database is selected. Below the table, there are buttons: "Add All", "Add", "Remove", and "Remove All". Below these buttons, it says "Selected for Analysis". There is a table with two columns: "Database Name/Path" and "Record Range(s)". The "Database Name/Path" column lists the selected databases. The "Record Range(s)" column shows the record ranges for each database. The "IR - Automobile Paint Chips" database is selected with a record range of "222, 1111". Below the table, there is a text field for "Record ID Range(s) (use \",\" and \"-\"):" with the value "222, 1111". There is also a dropdown for "Y Scale:" set to "Same as PCA". At the bottom, there are buttons: "Select by Browsing...", "OK", and "Cancel".</p> <table><thead><tr><th>Reference</th><th>Name</th><th>Records</th></tr></thead><tbody><tr><td>+</td><td>11B NMR - Wolfgang Robien</td><td>2212</td></tr><tr><td>+</td><td>13C NMR - AIST SDBS</td><td>11890</td></tr><tr><td>+</td><td>13C NMR - Flavors & Fragrances - Wiley</td><td>11815</td></tr><tr><td>+</td><td>13C NMR - Natural Products - Wiley</td><td>3432</td></tr><tr><td>+</td><td>13C NMR - Organic Compounds - Wiley</td><td>188426</td></tr><tr><td>+</td><td>13C NMR - Sadtler - Wiley</td><td>51992</td></tr><tr><td>+</td><td>13C NMR - Sadtler NIOSH Pocket Guide t...</td><td>252</td></tr><tr><td>+</td><td>13C NMR - Sadtler Polymers & Monomer...</td><td>742</td></tr><tr><td>+</td><td>13C NMR - Wolfgang Robien</td><td>304586</td></tr><tr><td>+</td><td>13C NMR - Wolfgang Robien</td><td>304586</td></tr></tbody></table> <table><thead><tr><th>Database Name/Path</th><th>Record Range(s)</th></tr></thead><tbody><tr><td>IR - Automobile Paint Chips</td><td>222, 1111</td></tr></tbody></table> <p>Record ID Range(s) (use ",\" and \"-\"):</p> <p>Y Scale:</p>	Reference	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	+	13C NMR - Wolfgang Robien	304586	Database Name/Path	Record Range(s)	IR - Automobile Paint Chips	222, 1111
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	Action	Result
3	See how two black dots fit into the PCA space (now blue).	
4	<ul style="list-style-type: none">Click one of the dots to see details for that record. (The selected dot will turn orange.)Hover over the Record Info link to see more details.	 <p>This dot is within the Acrylic Dispersion Lacquer circle .</p>

	Action	Result
5	Click on the other one dot and hover over the Record Info to see more details.	 <p>This dot is within the Acrylic Enamel circle.</p>

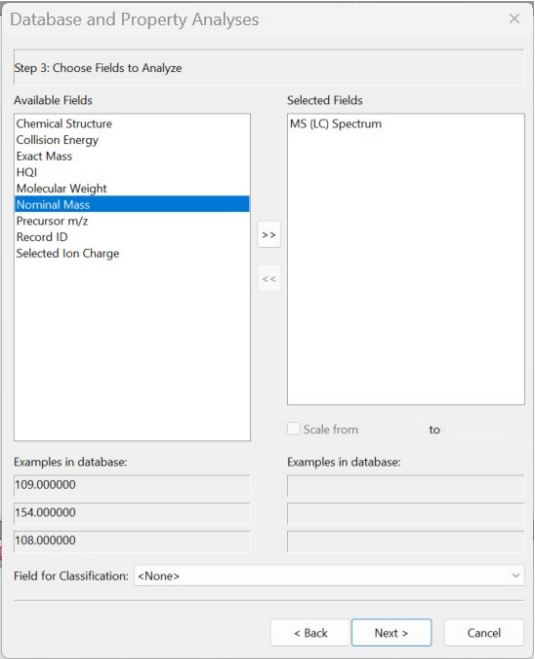
LC-MS

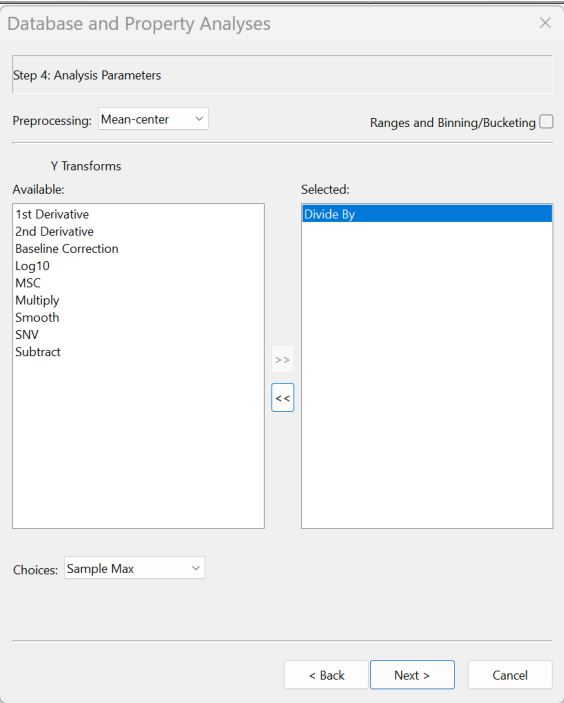
Hit List Analysis of Similar Structures

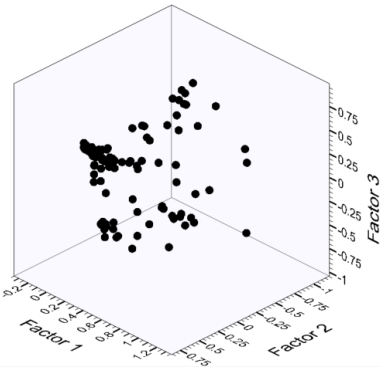
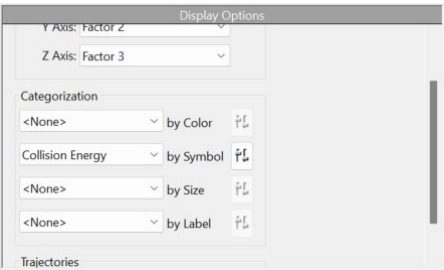
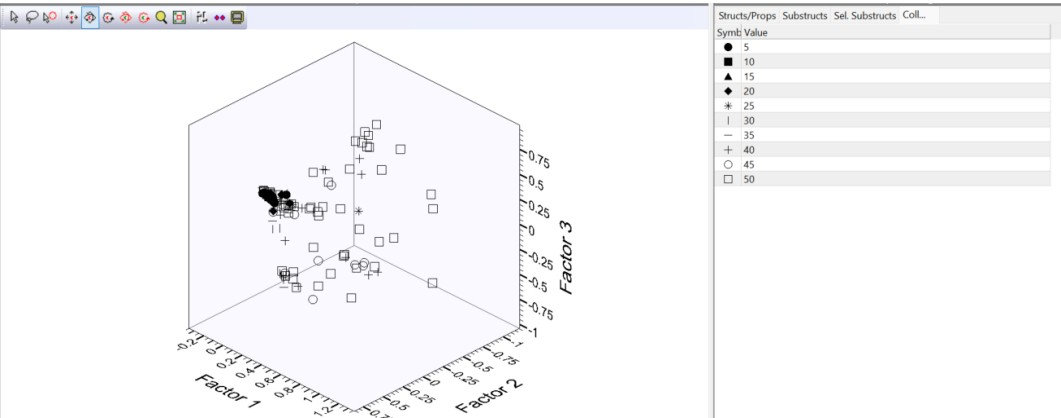
	Action	Result
1	In SearchIt , set a similarity structure search as shown in the Result column.	

	Action	Result
2	<ul style="list-style-type: none">Go to Search Databases, User-Select.Set Limit to spectral technique to MS (LC).Select the database LC-MS – Wiley Registry of Tandem Mass Spectral Data MSforID, click Add.Set Hit List Size Limit: 200.Click Search.	<div><div><div><div><div><div>Search Categories</div><div><div><input type="checkbox"/> Spectrum</div><div><input type="checkbox"/> Peaks</div><div><input checked="" type="checkbox"/> Structure</div><div><input type="checkbox"/> Property/Name</div><div><input type="checkbox"/> MSforID</div></div></div><div><div>Search Databases</div><div><div><input checked="" type="radio"/> User-Select</div><div><div><input type="radio"/> All Compounds<div><input type="checkbox"/> Use Computed Spectra</div></div><div><input type="radio"/> Pure Compounds<div><input type="checkbox"/> Use Computed Spectra</div></div></div></div></div></div><div><div>Available for Searching:</div><div><div>Internet databases are switc... Limit to spectral technique: MS (LC)</div><div><div><div><div><div><div><div>Reference</div><div>Computed</div><div>User</div><div>Hit List</div><div>Data Control</div></div></div><div><div><div>Name</div><div>Records</div><div>DB Code</div></div><div><div>LC-MS - Class Rule-Based Lipids Library</div><div>2505178</div><div>IOL</div></div><div><div>LC-MS - Class Rule-Based PFAS Library</div><div>7081</div><div>IOPF</div></div><div><div>LC-MS - Class Rule-Based Polymer Library</div><div>202752</div><div>IOPO</div></div><div><div>LC-MS - Maurer/Wissenbach/Weber LC-MSn Library of Drugs, Poisons, and Their Metab...</div><div>13027</div><div>MWW</div></div><div><div>LC-MS - MMHW LC-HR-MS/MS Library of Drugs, Poisons, and Their Metabolites, 2nd E...</div><div>5558</div><div>MMHW</div></div></div></div></div><div><div>Add All</div><div>Add</div><div>Remove</div><div>Remove All</div></div></div><div><div>Selected for Searching:</div><div><div><div><div><div>Name</div><div>Records</div><div>DB Code</div><div>Location</div></div><div><div>LC-MS - Wiley Registry of Tandem Mass Spectral Data MSforID</div><div>1175</div><div>WRTMS</div><div>C:\Use</div></div></div></div></div><div><div>Select by Browsing...</div></div></div><div><div>Hit List Size Limit: 200</div><div><input type="checkbox"/> All Hits</div><div>Display Profiles: <no profile></div><div>Search: 1175</div><div>Search</div></div></div></div></div></div></div></div>

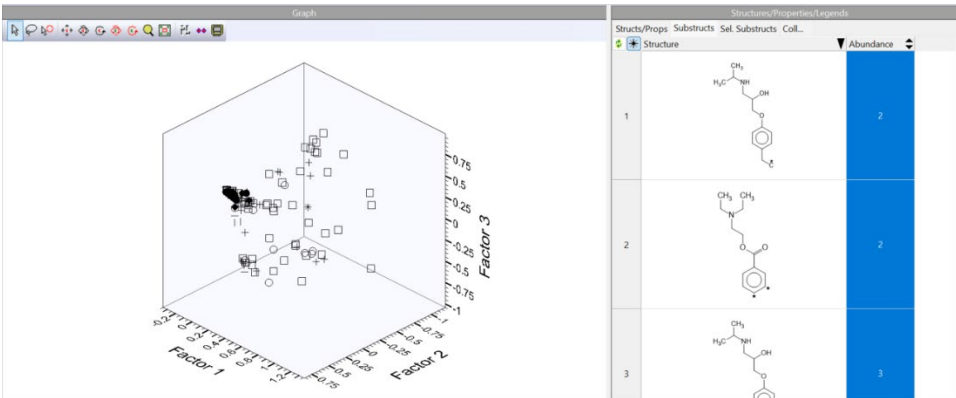
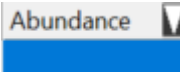
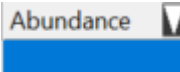
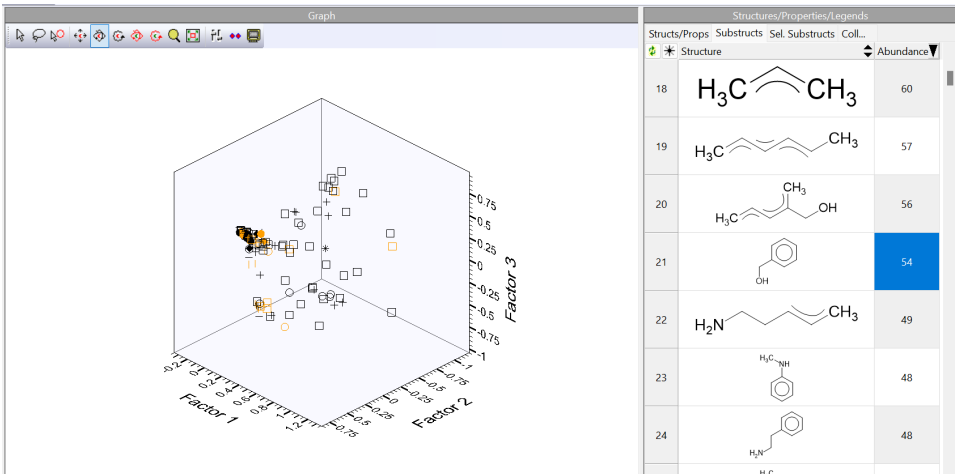
Action	Result
<div>4</div> <div>Choose Collision Energy in the Property drop down list and select all.</div>	<div><div><div><div><div><div>Overlay All</div><div>Property:</div><div>Collision Energy</div></div><div><div>10 eV</div><div>15 eV</div><div>20 eV</div><div>25 eV</div><div>30 eV</div><div>35 eV</div><div>40 eV</div></div></div></div><div><div><div><div>MS (LC) (7)</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><div><div>1000</div><div>500</div></div><div><div><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><div>m/z</div></div></div></div></div><div><div><div><div><div>100.00</div><div>20.00</div><div>19.62</div><div>19.33</div><div>17.95</div><div>14.20</div><div>14.07</div></div><div><div><div><div>WRTMS</div><div>WRTMS</div><div>WRTMS</div><div>WRTMS</div><div>WRTMS</div><div>WRTMS</div><div>WRTMS</div></div><div><div><div><div>8</div><div>643</div><div>737</div><div>1148</div><div>1149</div><div>699</div><div>986</div></div><div><div><div><div>2-Aminophenol</div><div>2-Amino-4-nitrophenol</div><div>Phenylenediamine</div><div>Salicylamide</div><div>Salicylic acid</div><div>Acetaminophen</div><div>Tyramine</div></div></div></div></div></div></div></div></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><auto> (MS (LC))</div></div><div><div><div><div>1</div><div>2</div><div>3</div><div>4</div><div>5</div><div>6</div><div>7</div></div><div><div><div><div>100.00</div><div>20.00</div><div>19.62</div><div>19.33</div><div>17.95</div><div>14.20</div><div>14.07</div></div><div><div><div><div>WRTMS</div><div>WRTMS</div><div>WRTMS</div><div>WRTMS</div><div>WRTMS</div><div>WRTMS</div><div>WRTMS</div></div><div><div><div><div>8</div><div>643</div><div>737</div><div>1148</div><div>1149</div><div>699</div><div>986</div></div><div><div><div><div>2-Aminophenol</div><div>2-Amino-4-nitrophenol</div><div>Phenylenediamine</div><div>Salicylamide</div><div>Salicylic acid</div><div>Acetaminophen</div><div>Tyramine</div></div></div></div></div></div></div></div></div></div><div><div>This database contains records with MS spectra acquired at different collision energies.</div></div></div></div></div></div></div></div></div></div></div></div></div></div></div></div></div></div></div></div></div>
<div>4</div> <div><div><div>Transfer this hit list to Trendfinder using:</div><div>Transfer to: <div>Trendfinder</div></div><div><div>Note:</div><div>To start the Trendfinder application without transferring a hit list, open it directly by clicking its icon in the Spectral Analysis toolbox.</div></div><div><div>Click Next ></div></div></div></div>	

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

	Action	Result
6	Click Next > to continue.	

	Action	Result
7	Click Finish .	 <p>Scores plot opens as above.</p>
8	<p>Under Categorization, select to show Collision Energy by Symbol:</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

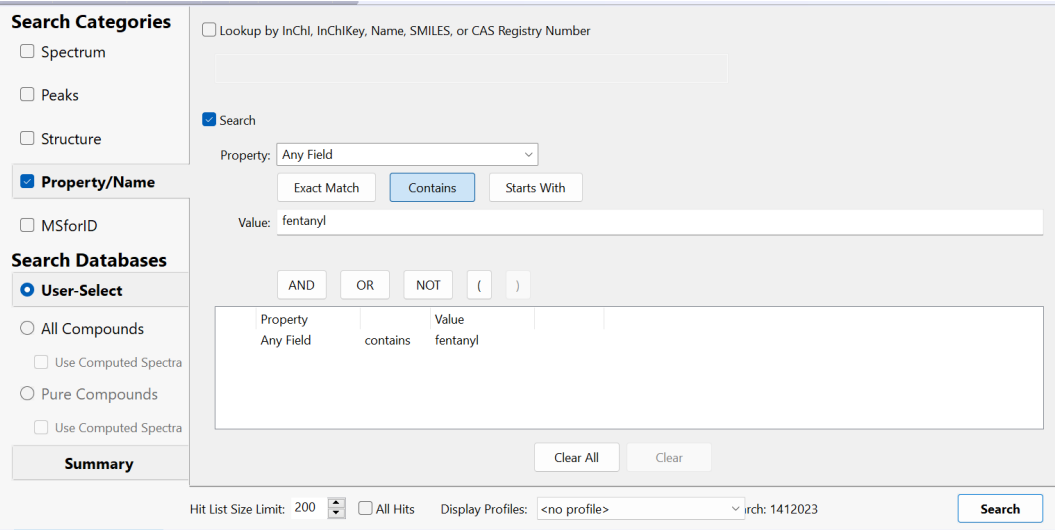
	Action	Result
1	<p>Continue with the above example.</p> <ul style="list-style-type: none">Open the Substructures tab under the Structures/Properties/Legends pane.Click Start Calculations.	<div></div> <p>The fragments and abundances (frequency to appear) within this entire dataset are shown in the right table.</p>
2	<ul style="list-style-type: none">The Abundance can be sorted by clicking  on .Select a fragment.	<div></div> <p>25 Spectra containing this fragment are highlighted in the Scores plot.</p> <p>The Sel. Substructures tab will allow the user to select a group of dots and see the fragment abundance within that group.</p>


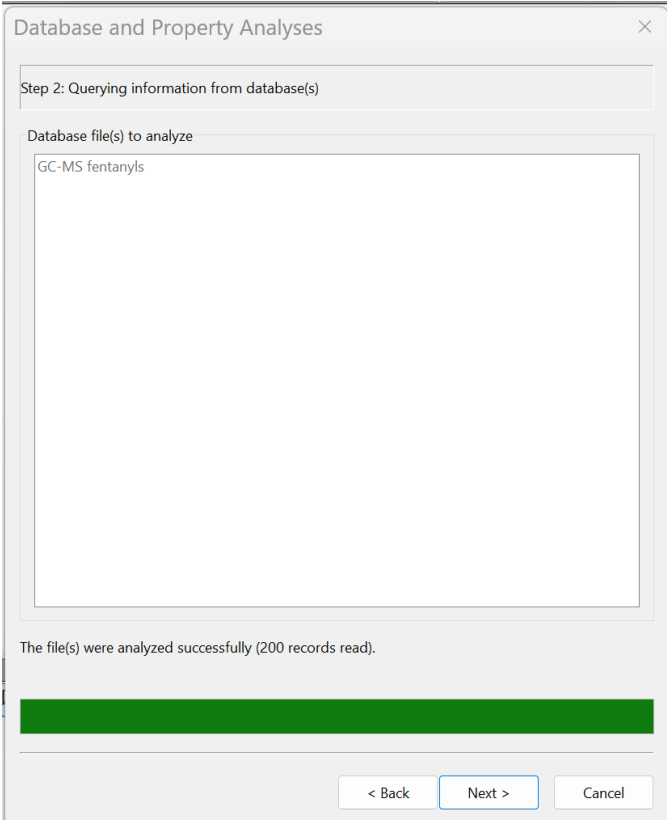
Action	Result
4 <ul style="list-style-type: none">Transfer the highlighted collection of 54 records to Minelt using the Transfer to button.The database records will open in Minelt.	<p>The screenshot displays the software interface for a mass spectral search. The top section shows a mass spectrum plot with a single prominent peak at m/z 122, labeled 'WRTMG #1149: Salicylic acid'. The x-axis is labeled 'm/z' and ranges from 60 to 130. The y-axis is labeled 'MS (LC) (10)' and ranges from 0 to 500. Below the plot is a table of results with columns for 'Hit', 'Tag', 'ID', 'Name', and 'Spectrum'. The table lists several compounds, with 'Salicylic acid' (ID 1149) highlighted in blue. To the right of the table is a 'Structure/Properties' panel showing the chemical structure of Salicylic acid (a benzene ring with a carboxylic acid group and a hydroxyl group) and a list of properties including Name, CAS Registry Number, Collision Energy, Exact Mass, Formula, InChI, InChIKey, Instrument Name, Ion Polarity, and Ionization Type. The bottom of the interface shows a 'Hit List: LC MS' with 54 records.</p>

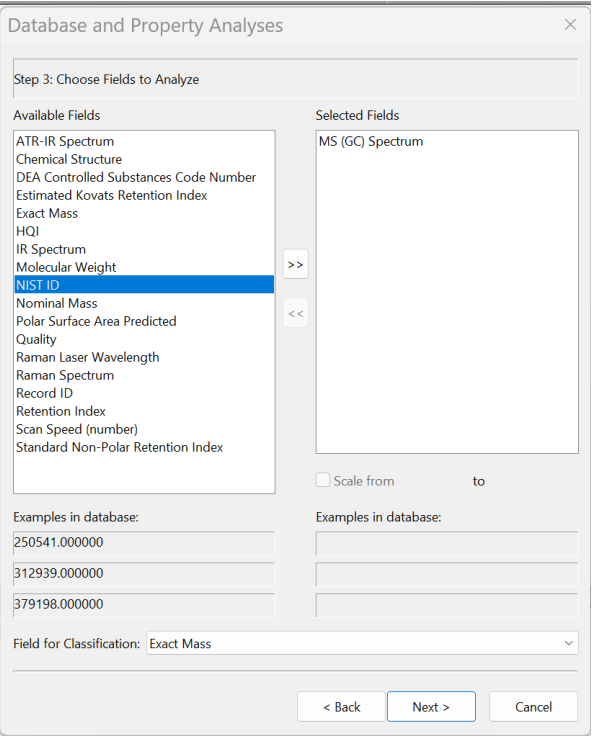
GC-MS

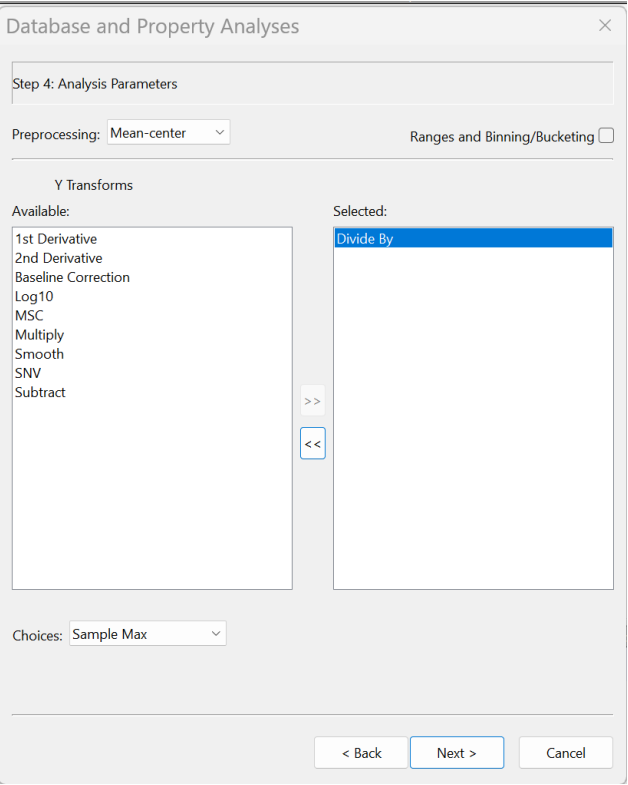
Hit List Analysis Of Fentanyl's

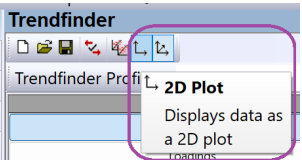
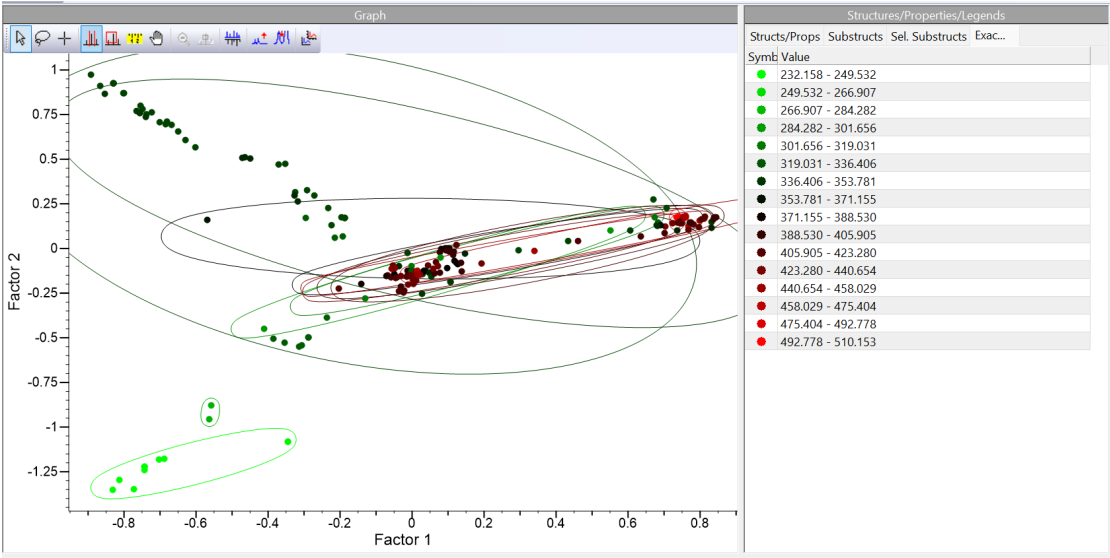
	Action	Result																																																																																																																																												
1	<ul style="list-style-type: none">In SearchIt, go to User-select.Limit to spectral technique to MS(GC) andAdd All GC-MS databases for searching.	<div><div><div><div>SearchIt</div><div><div>Search Profiles: <no profile></div><div></div></div><div><div>Search Categories</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><input checked="" type="radio"/> User-Select</div><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 switc... 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><Latest Version></td><td>25.00</td><td></td></tr><tr><td>MS - Maurer, Meyer, Pflieger, ...</td><td>10948</td><td>MMPWX</td><td><Latest Version></td><td>25.00</td><td></td></tr><tr><td>MS - NIST / EPA / NIH Mass ...</td><td>347100</td><td>MSX</td><td><Latest Version></td><td>25.00</td><td></td></tr><tr><td>MS - NIST / EPA / NIH Mass ...</td><td>46954</td><td>MSRX</td><td><Latest Version></td><td>25.00</td><td></td></tr><tr><td>MS - Sadtler NIOSH Pocket G...</td><td>476</td><td>NSX</td><td><Latest Version></td><td>25.00</td><td></td></tr><tr><td>MS - SWGDRUG Mass Spectr...</td><td>3047</td><td>SWGMSX</td><td><Latest Version></td><td>25.00</td><td></td></tr><tr><td>MS - Wiley AAFS Toxicology ...</td><td>2758</td><td>AFX</td><td><Latest Version></td><td>25.00</td><td></td></tr><tr><td>MS - Wiley Androstanes, Est...</td><td>2979</td><td>MUX</td><td><Latest Version></td><td>25.00</td><td></td></tr><tr><td>MS - Wiley Drugs</td><td>2204</td><td>MDX</td><td><Latest Version></td><td>25.00</td><td></td></tr><tr><td>MS - Wiley Geochemicals, Pet...</td><td>1093</td><td>MGX</td><td><Latest Version></td><td>25.00</td><td></td></tr><tr><td>MS - Wiley Industrial Chemi...</td><td>41110</td><td>MTX</td><td><Latest Version></td><td>25.00</td><td></td></tr><tr><td>MS - Wiley Mass Spectra of ...</td><td>36360</td><td>WDD1X</td><td><Latest Version></td><td>25.11</td><td></td></tr><tr><td>MS - Wiley Mass Spectra of ...</td><td>1300</td><td>WMP3X</td><td><Latest Version></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, Pflieger, Wilson: GC-MS Library of Dru...</td><td>10948</td><td>MMPWX</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Maurer Pflieger Wilson: 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 [MSX].sd</td></tr><tr><td>MS - Sadtler 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 - Sadtler 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 - 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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 [MSX].sd																																																																																																																																											
MS - Sadtler NIOSH Pocket Guide to Chemical Hazards Co...	476	NSX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\GC-MS\GC-MS - Sadtler 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 - Sadtler AAFS Toxicology Section Mass Spectr																																																																																																																																											
MS - Wiley Androstanes, Estrogens & other Steroids	2979	MUX	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].sdbx																																																																																																																																											
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].sdbx																																																																																																																																											
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																																																																																																																																											

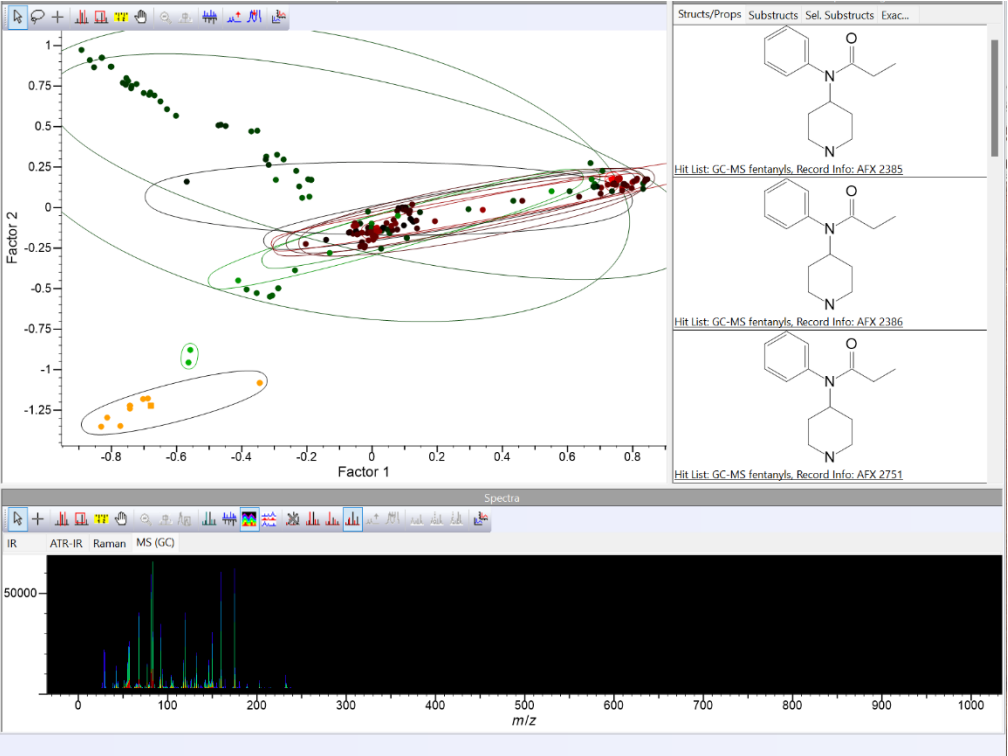
	Action	Result
2	<ul style="list-style-type: none">• Set Property/Name to search for Any Field contains “fentanyl”.• Set Hit List Size Limit: 200.• Click the Search button.	 <p>The screenshot displays the Simple Spectral Search interface. On the left, under 'Search Categories', 'Property/Name' is selected.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

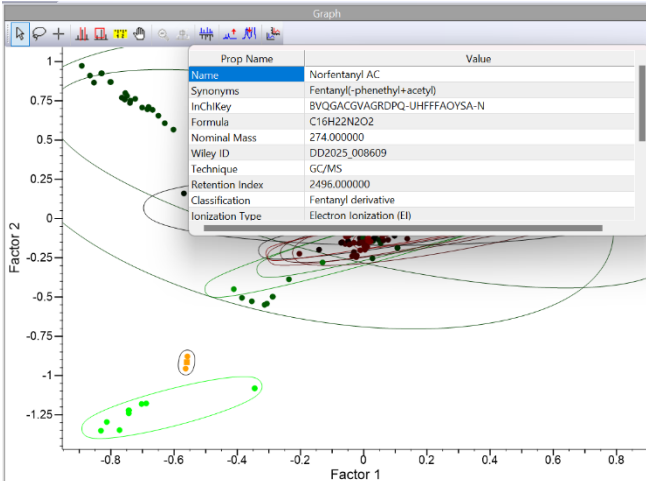
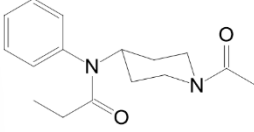
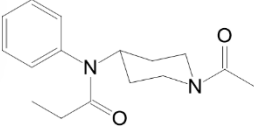
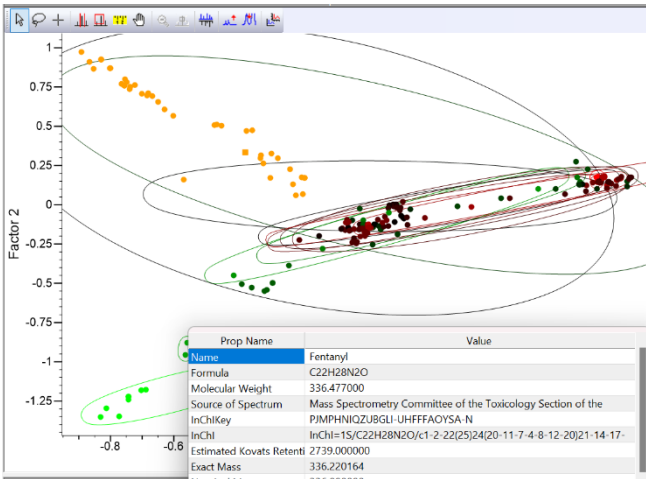
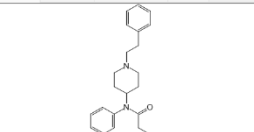
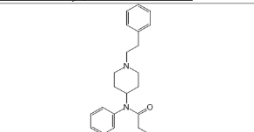
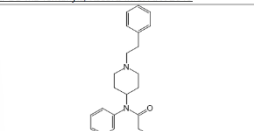
	Action	Result
3	<p>Minelt provides a hit list of various fentanyls.</p> <ul style="list-style-type: none">Transfer this hit list to Trendfinder.  <p>Note: To start the Trendfinder application without transferring a hit list, open the Trendfinder application by clicking its icon in the Spectral Analysis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

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

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

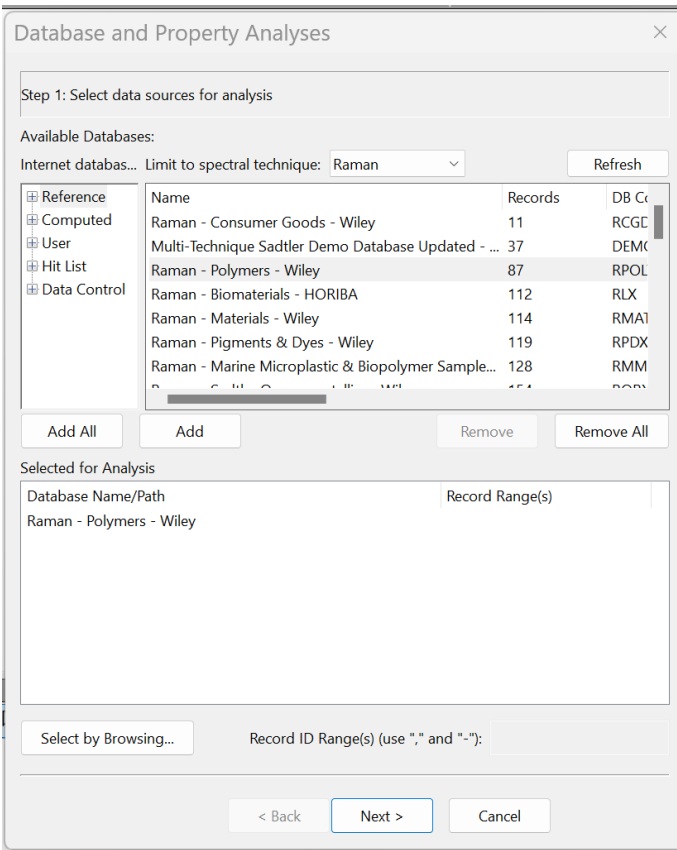
	Action	Result
6	<ul style="list-style-type: none"> Click Finish. Select 2D Scores plot view. 	 <p>You can see a group of light green (smaller mass) spectra.</p> <p>A circle (Trajectory) defines the boundary for a value in the Field of Classification.</p>

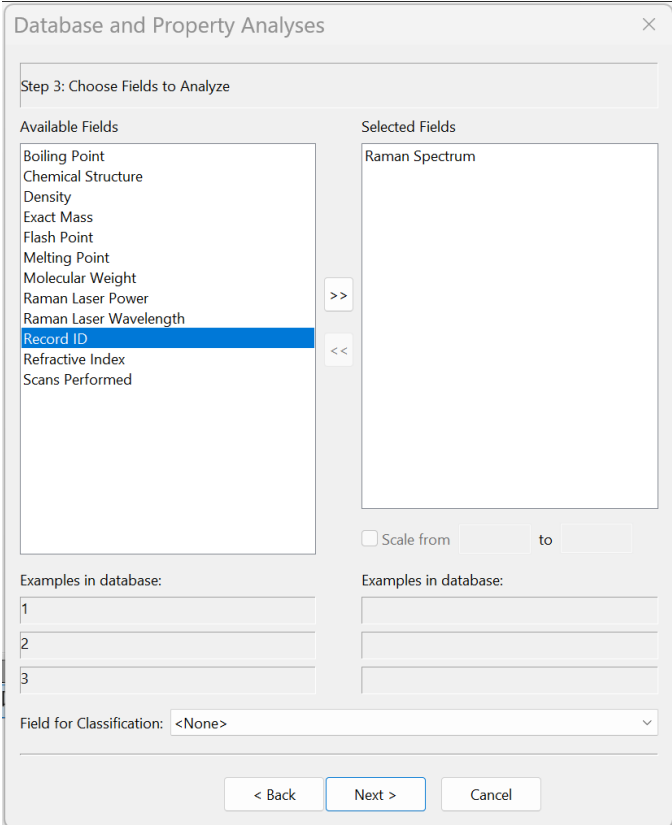
	Action	Result
7	<ul style="list-style-type: none">• Use left mouse to draw a rectangle so that the green spectra in the lower left corner are selected and turn orange.• Go to the Structs/Props tab under the Structures/Properties/Legends pane.• Click the MS (GC) tab in the bottom pane to open the spectra.	 <p>The screenshot displays the software interface for spectral analysis. 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 a list of chemical structures (norfentanyl) and their corresponding MS spectra. The bottom panel shows the MS (GC) tab selected, displaying a heatmap of the selected MS spectra.</p> <p>These are various norfentanyl MS spectra. The bottom pane shows the selected MS spectral Overlay Heatmap.</p>

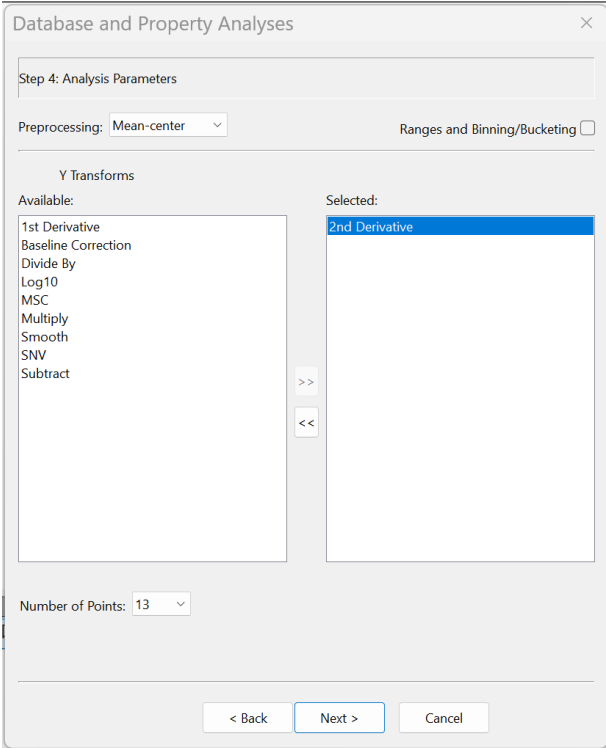
Action	Result																						
8 Selecting the two darker group dots groups the norfentanyl AC spectra.	 <table border="1"><thead><tr><th>Prop Name</th><th>Value</th></tr></thead><tbody><tr><td>Name</td><td>Norfentanyl AC</td></tr><tr><td>Synonyms</td><td>Fentanyl(-phenethyl)-acetyl</td></tr><tr><td>InChIKey</td><td>BVQGACGVAGRDQ-UHFFFAOYSA-N</td></tr><tr><td>Formula</td><td>C16H22N2O2</td></tr><tr><td>Nominal Mass</td><td>274.00000</td></tr><tr><td>Wiley ID</td><td>DD2025_008609</td></tr><tr><td>Technique</td><td>GC/MS</td></tr><tr><td>Retention Index</td><td>2496.000000</td></tr><tr><td>Classification</td><td>Fentanyl derivative</td></tr><tr><td>Ionization Type</td><td>Electron Ionization (EI)</td></tr></tbody></table>  <p>Hit List: GC-MS fentanyl, Record Info: WDD1X 8609</p>  <p>Hit List: GC-MS fentanyl, Record Info: WDD1X 9244</p>	Prop Name	Value	Name	Norfentanyl AC	Synonyms	Fentanyl(-phenethyl)-acetyl	InChIKey	BVQGACGVAGRDQ-UHFFFAOYSA-N	Formula	C16H22N2O2	Nominal Mass	274.00000	Wiley ID	DD2025_008609	Technique	GC/MS	Retention Index	2496.000000	Classification	Fentanyl derivative	Ionization Type	Electron Ionization (EI)
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9 The line of green linear dots from top left to center are fentanyls	 <table border="1"><thead><tr><th>Prop Name</th><th>Value</th></tr></thead><tbody><tr><td>Name</td><td>Fentanyl</td></tr><tr><td>Formula</td><td>C22H28N2O</td></tr><tr><td>Molecular Weight</td><td>336.477000</td></tr><tr><td>Source of Spectrum</td><td>Mass Spectrometry Committee of the Toxicology Section of the</td></tr><tr><td>InChIKey</td><td>PJMPHNIQZUBGLI-UHFFFAOYSA-N</td></tr><tr><td>InChI</td><td>InChI=1S/C22H28N2O/c1-2-22(25)24(20-11-7-4-8-12-20)21-14-17</td></tr><tr><td>Estimated Kovats Retenti</td><td>2739.000000</td></tr><tr><td>Exact Mass</td><td>336.220164</td></tr></tbody></table>  <p>Hit List: GC-MS fentanyl, Record Info: AFX 1953</p>  <p>Hit List: GC-MS fentanyl, Record Info: AFX 2019</p>  <p>Hit List: GC-MS fentanyl, Record Info: AFX 2491</p>	Prop Name	Value	Name	Fentanyl	Formula	C22H28N2O	Molecular Weight	336.477000	Source of Spectrum	Mass Spectrometry Committee of the Toxicology Section of the	InChIKey	PJMPHNIQZUBGLI-UHFFFAOYSA-N	InChI	InChI=1S/C22H28N2O/c1-2-22(25)24(20-11-7-4-8-12-20)21-14-17	Estimated Kovats Retenti	2739.000000	Exact Mass	336.220164				
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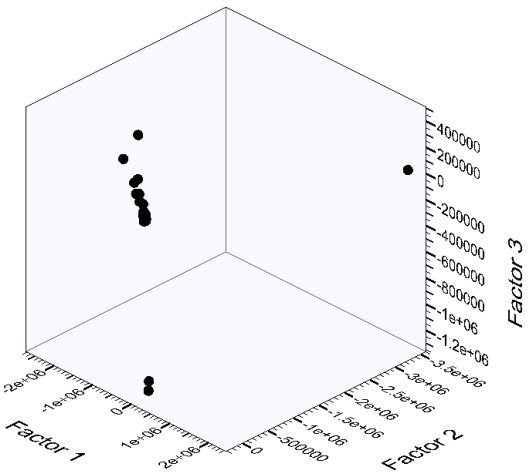
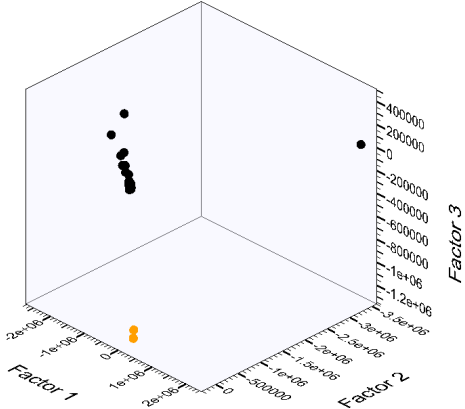
Raman

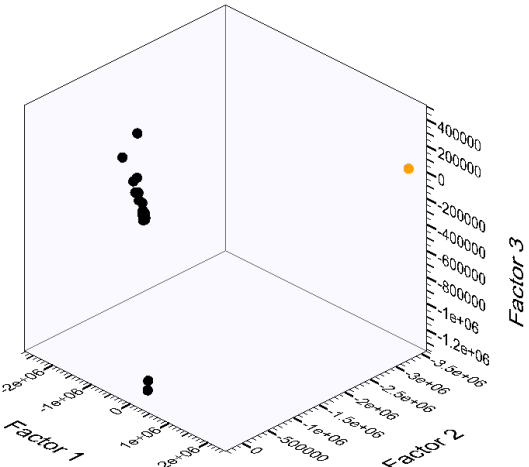
Polymer Analysis

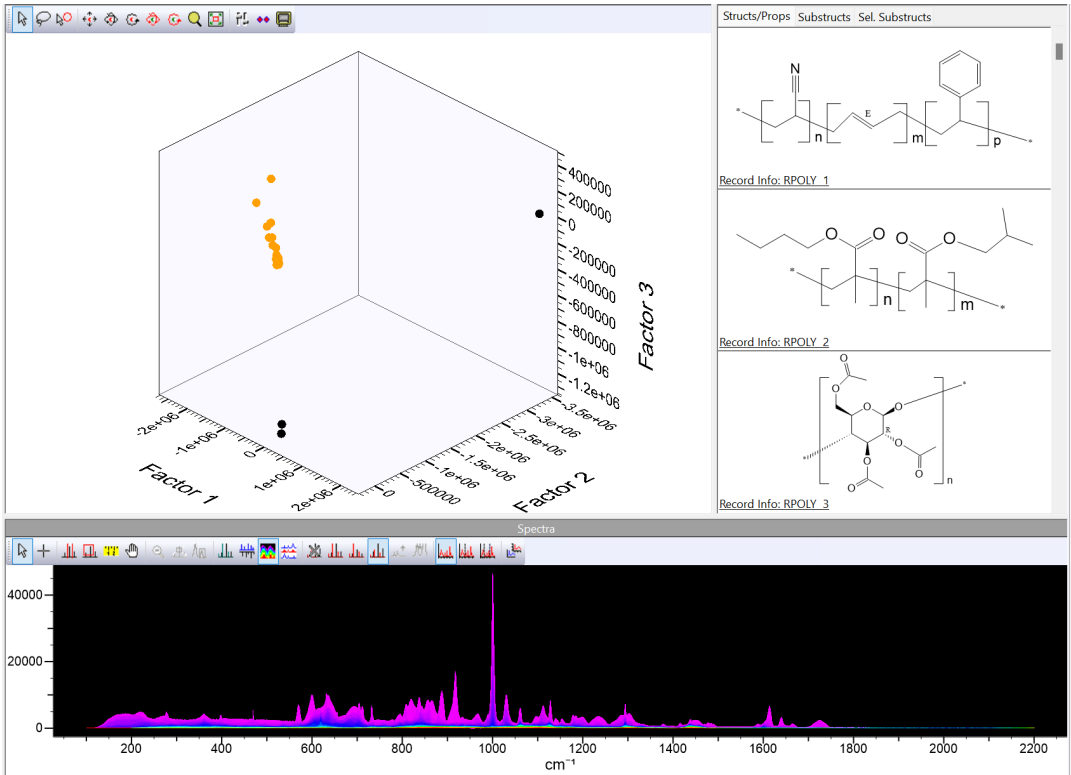
	Action	Result
1	Open the Trendfinder application by clicking its icon in the Spectral Analysis toolbox.	The application opens.
2	<ul style="list-style-type: none"> • Limit to spectral technique should be set to Raman. • Select the database Raman – Polymers – Wiley for analysis and click Add. • Click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

	Action	Result
3	<ul style="list-style-type: none">• Move Raman Spectrum to the right either by:<ul style="list-style-type: none">• Clicking >>, or• Double clicking on Raman Spectrum.• Click Next >.	 <p>Database and Property Analyses</p> <p>Step 3: Choose Fields to Analyze</p> <p>Available Fields</p> <ul style="list-style-type: none">Boiling PointChemical StructureDensityExact MassFlash PointMelting PointMolecular WeightRaman Laser PowerRaman Laser WavelengthRecord IDRefractive IndexScans Performed <p>Selected Fields</p> <ul style="list-style-type: none">Raman Spectrum <p>Scale from to</p> <p>Examples in database:</p> <p>1</p> <p>2</p> <p>3</p> <p>Field for Classification: <None></p> <p>< Back Next > Cancel</p>

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

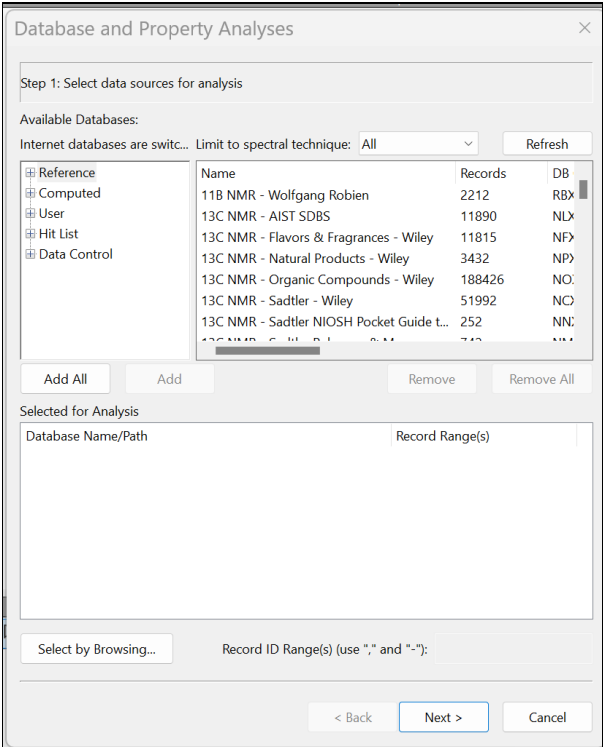
	Action	Result
6	Click Finish .	 <p>3 big groups are clearly identified.</p>
7	Use the left mouse to select a group of points.	 <div data-bbox="1470 885 1848 1372"><chem>*c1ccc(cc1)S(=O)(=O)c2ccc(cc2)Oc3ccc(cc3)*</chem><p>Record Info: RPOLY_56 Record Info: RPOLY_61</p></div>

	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">$\text{*} - \left[\text{C}_6\text{H}_4 - \text{S} \right]_n - \text{*}$</div> <div data-bbox="1428 470 1575 495">Record Info: RPOLY_57</div>

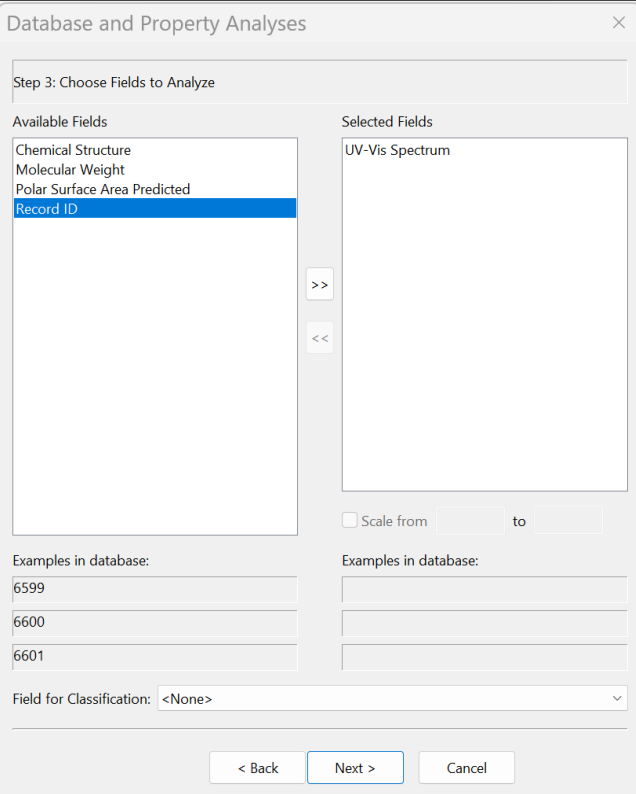
	Action	Result
9	Select another group of points by clicking and holding the left mouse button examine a different polymer.	 <p>The screenshot displays the software interface for spectral analysis. The top panel shows a 3D plot with axes labeled Factor 1, Factor 2, and Factor 3. A cluster of orange points is visible. The middle panel displays three chemical structures corresponding to different polymers, labeled Record Info: RPOLY_1, Record Info: RPOLY_2, and Record Info: RPOLY_3. The bottom panel shows an IR spectrum overlay heatmap with the x-axis labeled cm⁻¹ (ranging from 200 to 2200) and the y-axis showing intensity (ranging from 0 to 40000).</p> <p>They are quite different polymers. The bottom pane shows the Overlay Heatmap of selected spectra.</p>

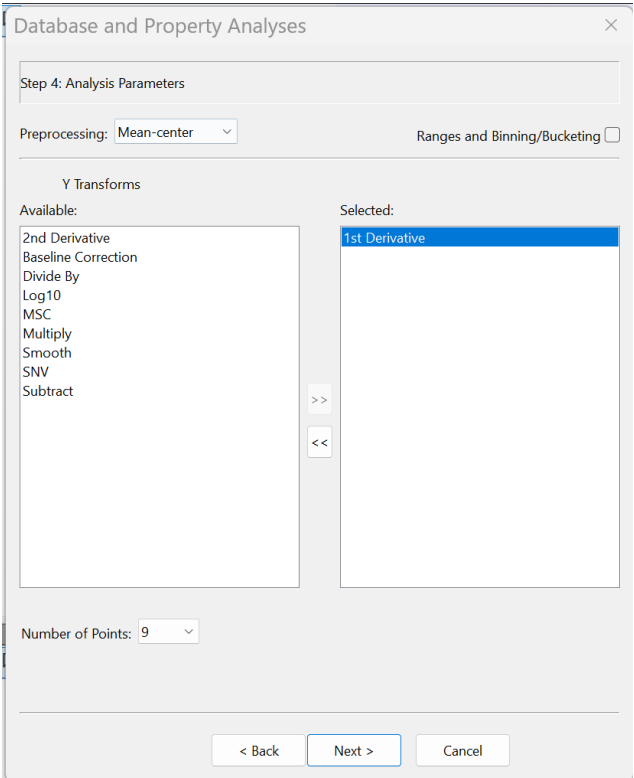
UV-Vis

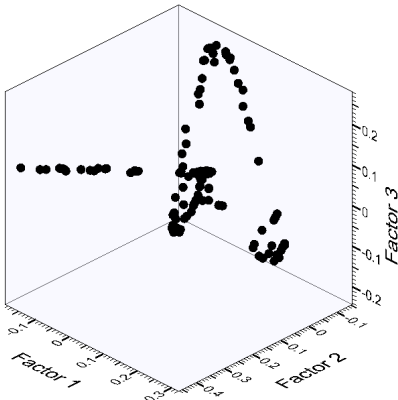
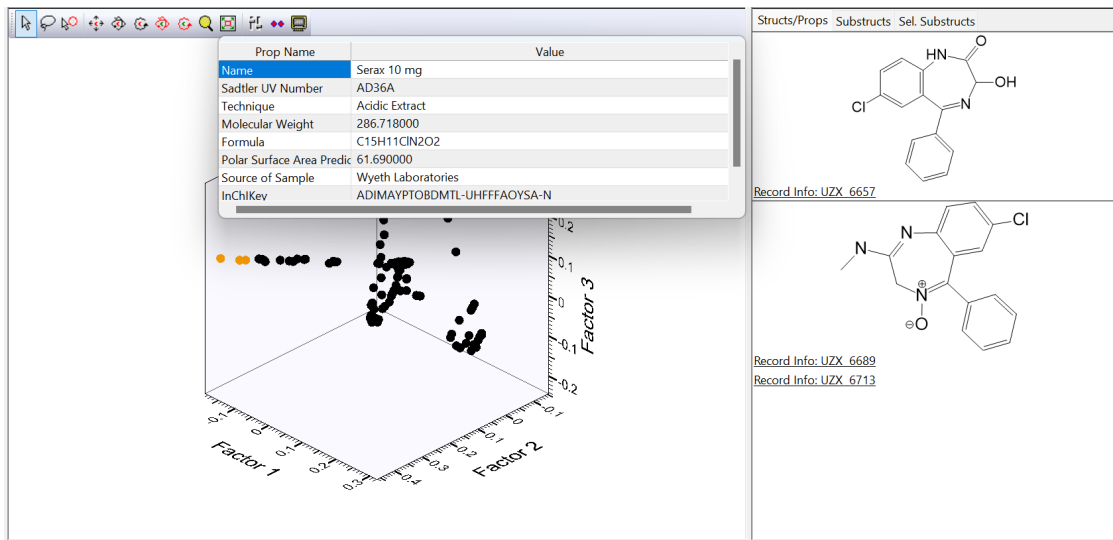
Forensic Material Analysis

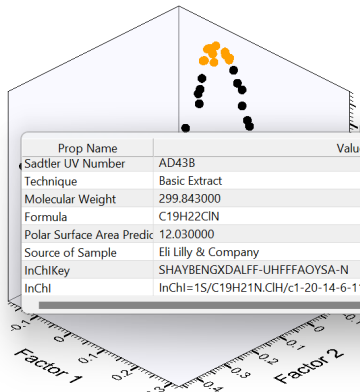
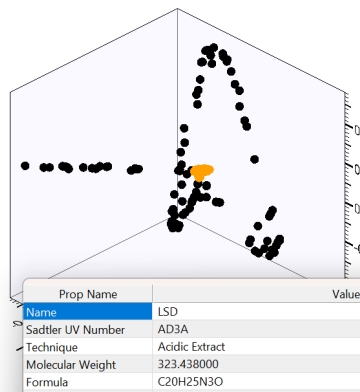
	Action	Result
1	Open the Trendfinder application by clicking its icon in the Spectral Analysis toolbox.	The application opens.
2	Choose File > New PCA Analysis .	<p>The Database and Property Analyses wizard opens</p> 

	Action	Result																						
3	<ul style="list-style-type: none">• Select the UV-Vis database UV-Vis – Sadtler Forensics 200 to 500 nm – Wiley for analysis and click Add.• Click Next >, Next >.	<div><div>Database and Property Analyses</div><div><div>Step 1: Select data sources for analysis</div><div>Available Databases: Internet databases are switc... Limit to spectral technique: UV-Vis Refresh</div><div><table><tr><td>Reference</td><td>Name</td><td>Records</td></tr><tr><td>Computed</td><td>Multi-Technique Sadtler Demo Database Updated - ...</td><td>37</td></tr><tr><td>User</td><td>UV-Vis - Sadtler 200 to 350 nm - Wiley</td><td>21660</td></tr><tr><td>Hit List</td><td>UV-Vis - Sadtler 200 to 500 nm - Wiley</td><td>6824</td></tr><tr><td>Data Control</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></div><div>Add All Add Remove Remove All</div><div>Selected for Analysis</div><div><table><tr><td>Database Name/Path</td><td>Record Range(s)</td></tr><tr><td>UV-Vis - Sadtler Forensics 200 to 500 nm - Wiley</td><td></td></tr></table></div><div>Select by Browsing... Record ID Range(s) (use "," and "-");</div><div><div>< Back</div><div>Next ></div><div>Cancel</div></div></div></div>	Reference	Name	Records	Computed	Multi-Technique Sadtler Demo Database Updated - ...	37	User	UV-Vis - Sadtler 200 to 350 nm - Wiley	21660	Hit List	UV-Vis - Sadtler 200 to 500 nm - Wiley	6824	Data Control	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	
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	Action	Result
4	<p>In this dialog:</p> <ul style="list-style-type: none">• Move UV-Vis Spectrum from the left box to the right one by selecting it in the left and using ">>" or double-clicking to move it to the right.• Click Next >.	

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

	Action	Result																		
6	Click Finish .	 <p>The above 3 factors view is returned.</p>																		
7	Use the left mouse to select box each group of points, which turn orange upon selection.	 <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>Structs/Props Substructs Sel. Substructs</p> <p>Record Info: UZX_6657</p> <p>Record Info: UZX_6689</p> <p>Record Info: UZX_6713</p>	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
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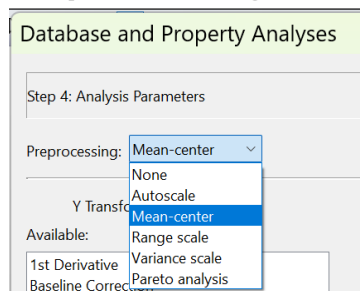
Action	Result																		
8	<div><table border="1"><thead><tr><th>Prop Name</th><th>Value</th></tr></thead><tbody><tr><td>Sadtler UV Number</td><td>AD43B</td></tr><tr><td>Technique</td><td>Basic Extract</td></tr><tr><td>Molecular Weight</td><td>299.843000</td></tr><tr><td>Formula</td><td>C19H22ClN</td></tr><tr><td>Polar Surface Area Predic</td><td>12.030000</td></tr><tr><td>Source of Sample</td><td>Eli Lilly & 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> HCl<p>Record Info: UZX 6670</p><p>Record Info: UZX 6682</p><p>Record Info: UZX 6702</p><chem>CCN(CC)c1ccc2c(c1)ccc3ccccc23</chem></div>	Prop Name	Value	Sadtler UV Number	AD43B	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
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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=C(C(=C2C(=C1)C(=C(C=C2)OC)O)N(C)CC)O</chem> H₂SO₄<p>Record Info: UZX 6601</p><chem>CC1=C(C(=C2C(=C1)C(=C(C=C2)OC)O)N(C)CC)O</chem><p>Record Info: UZX 6603</p><chem>CCN(CC)C(=O)C1=CC2=C(C=C1)C(=C(C=C2)N)C3=CC=CC=C3</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
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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 point¹.
- **Range scale:** Min-max scaling which transforms the data to fit within a specific range².
- **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 output³.

¹ Eigenvector Research Documentation Wiki (2012) *Advanced Preprocessing: Variable Centering*,

https://www.wiki.eigenvector.com/index.php?title=Advanced_Preprocessing:_Variable_Centering (accessed 2025-08-19).

² Geeks for Geeks (2025) *Normalization and Scaling*, [Normalization and Scaling – GeeksforGeeks](https://www.geeksforgeeks.org/normalization-and-scaling/) (accessed 2025-08-19).

³ 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 1st 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 Variate⁴.
- **SNV:** Standard Normal Variate⁵.
- **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.

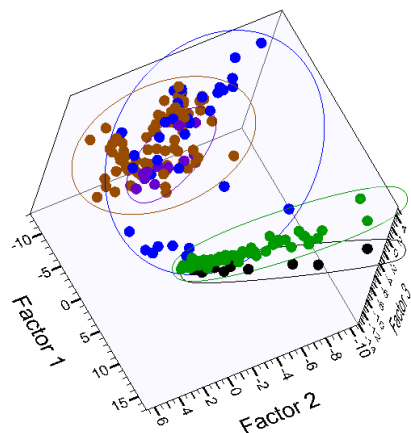
⁴ Fearn, T., Riccioli, C., Garrido-Varo, A., and Guerrero-Ginel, J.E. On the geometry of SNV and MSC, *Chemometrics and Intelligent Laboratory Systems*, **2009** 96(1), 22-26. Doi: <https://doi.org/10.1016/j.chemolab.2008.11.006>.

⁵ 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 dataset⁶. Selecting the first 200 records of the IR - Automobile Paint Chips (APX) database with the parameter **Mean-center**, results in the plot below:

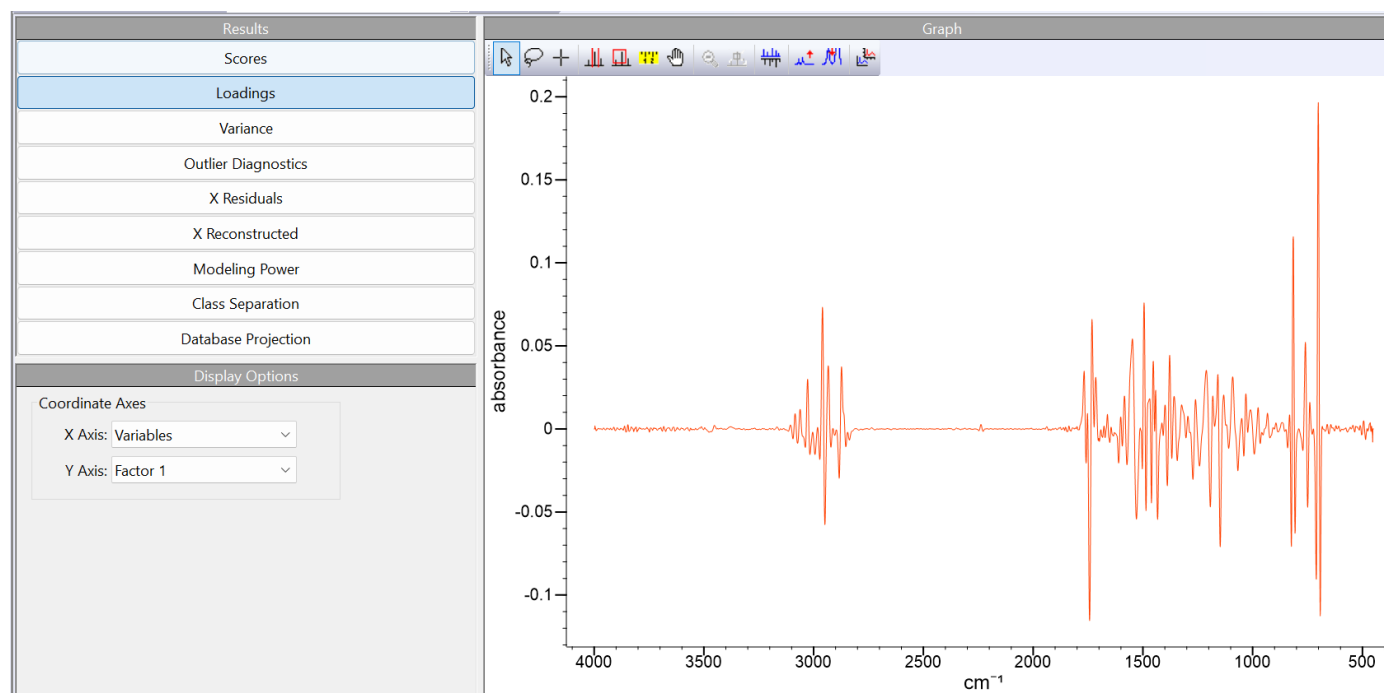


A circle (**Trajectory**) defines the boundary for a value in the **Field of Classification**).

⁶ 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

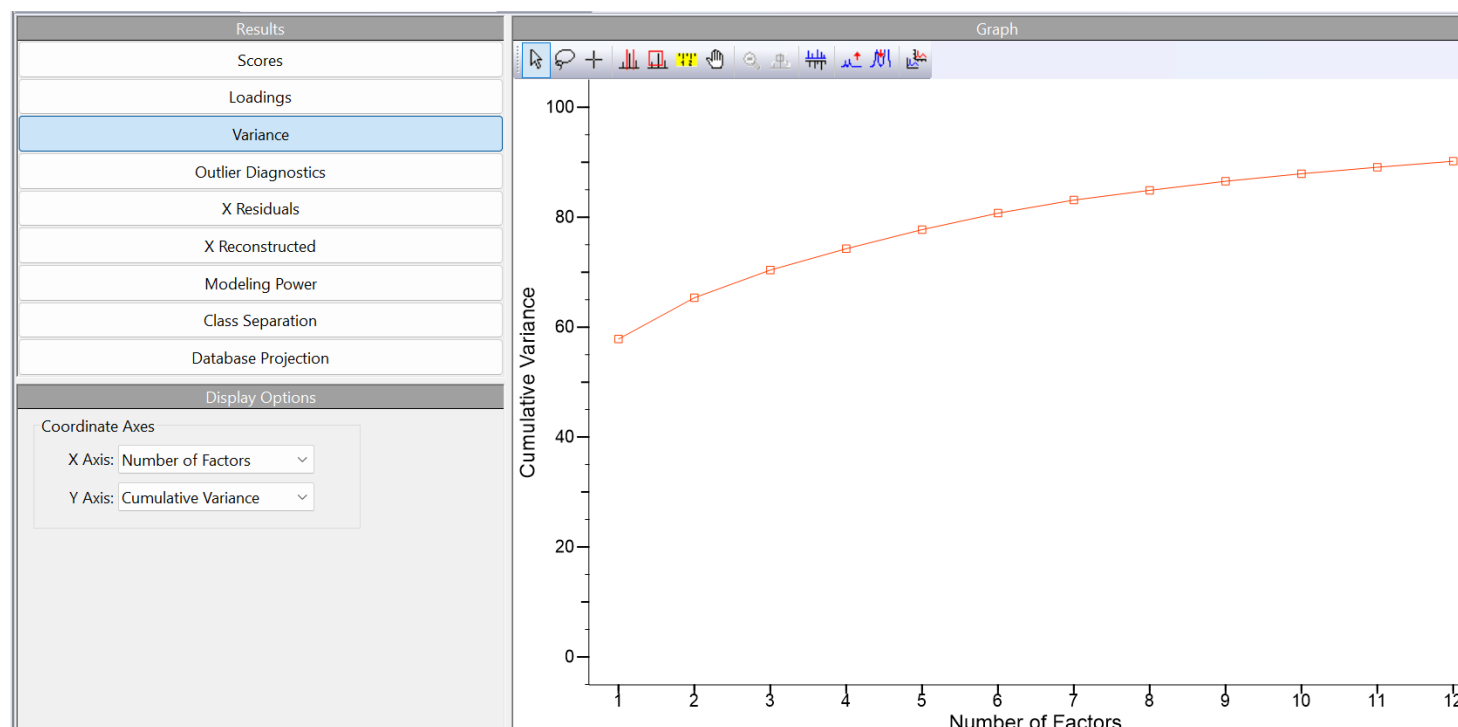
In order to show the relationship between the original variables and the principal components, it helps to understand how much each original variable contributes to the principal components and the nature of these contributions⁷. Using the above example, it would be:



⁷ 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 component⁸. 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 variance⁹ When applied to the above example, the result is:



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

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

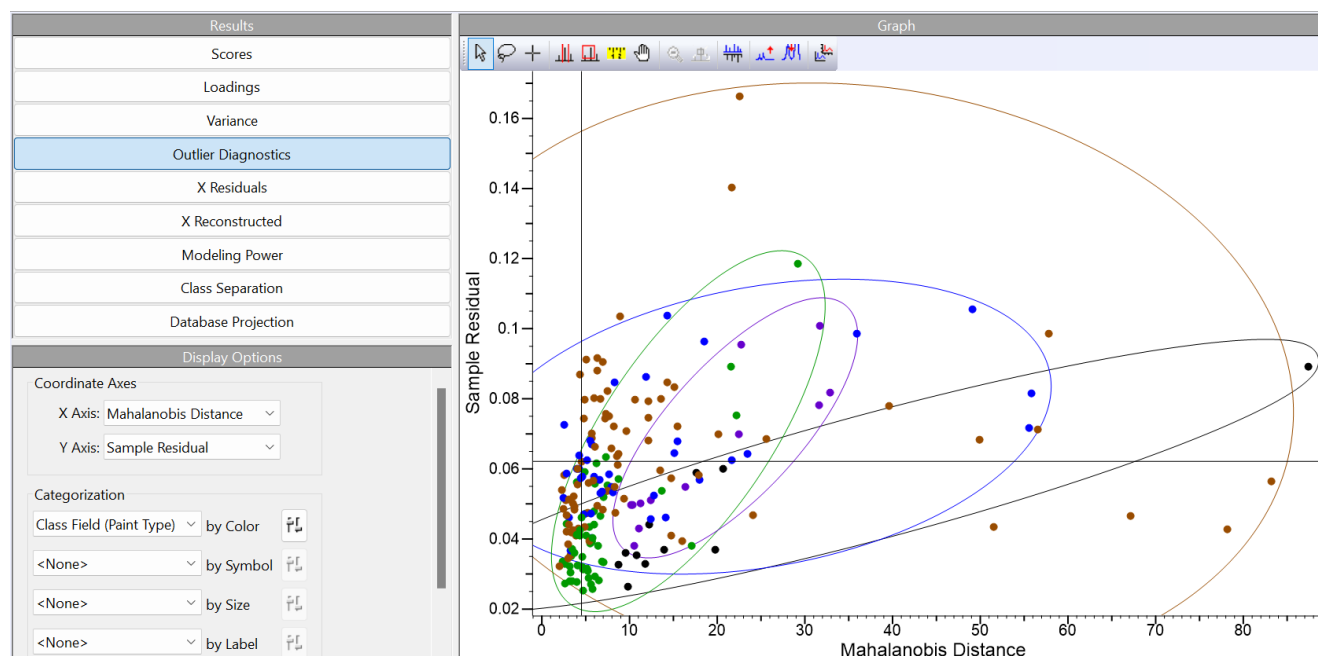
Outlier Diagnosis

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 Distance¹¹:** 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 F¹⁵.
- **Probability**

- **Record ID**

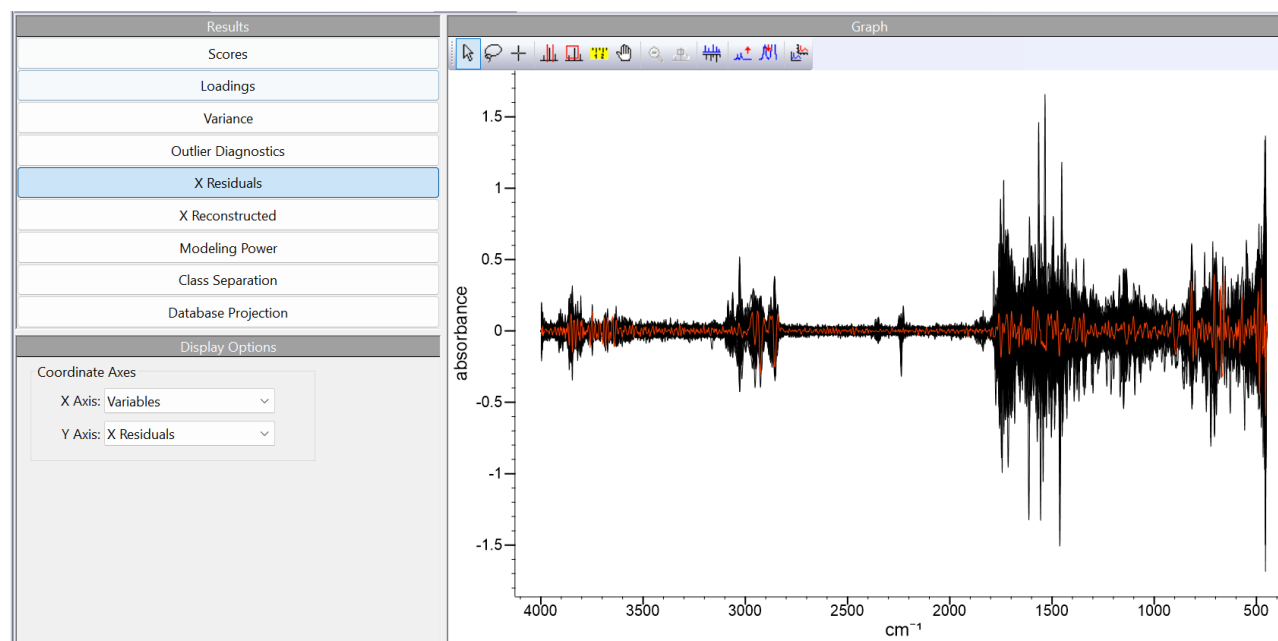
¹⁰ Datathatmatters (2024) Outlier Detection Simplified: PCA Techniques for Improved Data Analysis <https://datathatmatter.com/2024/11/03/outlier-detection-simplified-pca-techniques-for-improved-data-analysis/> (accessed 2025-08-19).

¹¹ Wikipedia (2025) Mahalanobis distance, https://en.wikipedia.org/wiki/Mahalanobis_distance (accessed 2025-08-19).

¹² 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

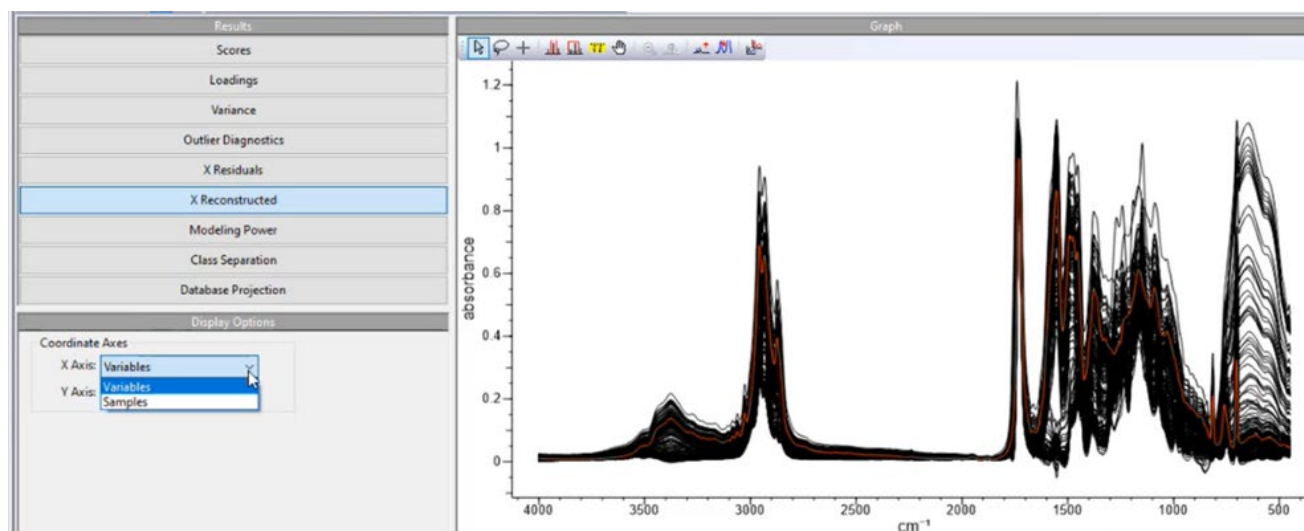
PCA residuals are calculated using the residual matrix $E = X - T P' = X - X^{\wedge}$, where X is the original matrix and $T P'$ is the PCA model. The residuals for each column in the original matrix can be calculated using the R^2 value, which gives an indication of how well the PCA model describes the data from that column. The function `pcars(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 column¹³. Using the above example, we get:



¹³ 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 component¹⁴ It can be viewed as "reverse PCA". For the above dataset, we get:



¹⁴ 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 separated¹⁵. Our particular example for the 1st 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						

¹⁵ 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).