

KnowItAll Software Training

Mass Spectrometry Search

Mass Spectrometry Spectral Searching

How to Perform a Mass Spectrometry Spectral Search

Purpose

This exercise demonstrates how to perform a mass spectrometry spectral search.

Objectives

This exercise will teach you:

- How to perform a straightforward search
- How to perform a reverse search
- How to complete a mixture analysis
- How to perform an adaptive search (similar compound search)
- How to perform simultaneous multiple MS spectra search

Background

Spectral searching against reference databases is frequently used in the analysis of unknown compounds. KnowItAll has full-featured MS spectrum comparison tools for this purpose.

Training Files Used in This Lesson

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

- \MS\1,1,1-Trichlorobutane - Adaptive Search demo
- \MS\2-Hydroxybenzoic acid
- \Mixture Analysis\MS Examples\MS Mixture of Two 1
- \Mixture Analysis\MS Examples\MS Mixture of Two 2
- \Mixture Analysis\MS Examples\MS Mixture of Three
- \GC-MS\Barbiturate GC-MS.d
- \Mixture Analysis\MS Examples\Components.SDBX

KnowItAll Applications Used

- SearchIt
- MinIt

Algorithms

Research article

Journal of
MASS
SPECTROMETRY

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Evaluation of mass spectral library search algorithms implemented in commercial software

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MS SEARCH

Composite algorithm

$$SI = \frac{N_U \cdot \left[\frac{\left(\sum W_L \cdot W_U \right)^2}{\sum W_L^2 \cdot \sum W_U^2} \right] + \left[\sum \left(\frac{R_U}{R_L} \right)^n \right]}{N_U + N_{U\&L}}$$

Dot-product algorithm

$$SI = \frac{\left(\sum W_L \cdot W_U \right)^2}{\sum W_L^2 \cdot \sum W_U^2}$$

Spectrum search type – identity (normal)

Presearch – default

Included Libs – MainLib

Apply limits – unchecked

Use constraints – unchecked

Spectrum search type – similarity (simple)

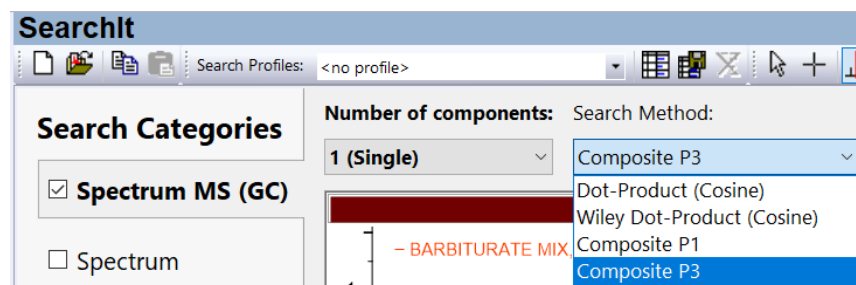
Presearch – default

Included Libs – MainLib

Apply limits – unchecked

Use constraints – unchecked

A. Samokhin, K. Sotnezova, V. Lashin, I. Revelsky. Evaluation of mass spectral library search algorithms implemented in commercial software. *Journal of Mass Spectrometry*. 2015, 50, 820-825.

**Search Methods:**

- Dot-Product (Cosine): second equation in above figure
- Wiley Dot-Product (Cosine): the Finnigan algorithm that verified at least 12 of the largest 16 peaks and the base peak match before continuing with the dot-product calculation
- Composite P1: first equation in above figure
- Composite P3: first equation in above figure
P1 and P3 are different by the power applied to the weighted intensity of peak.

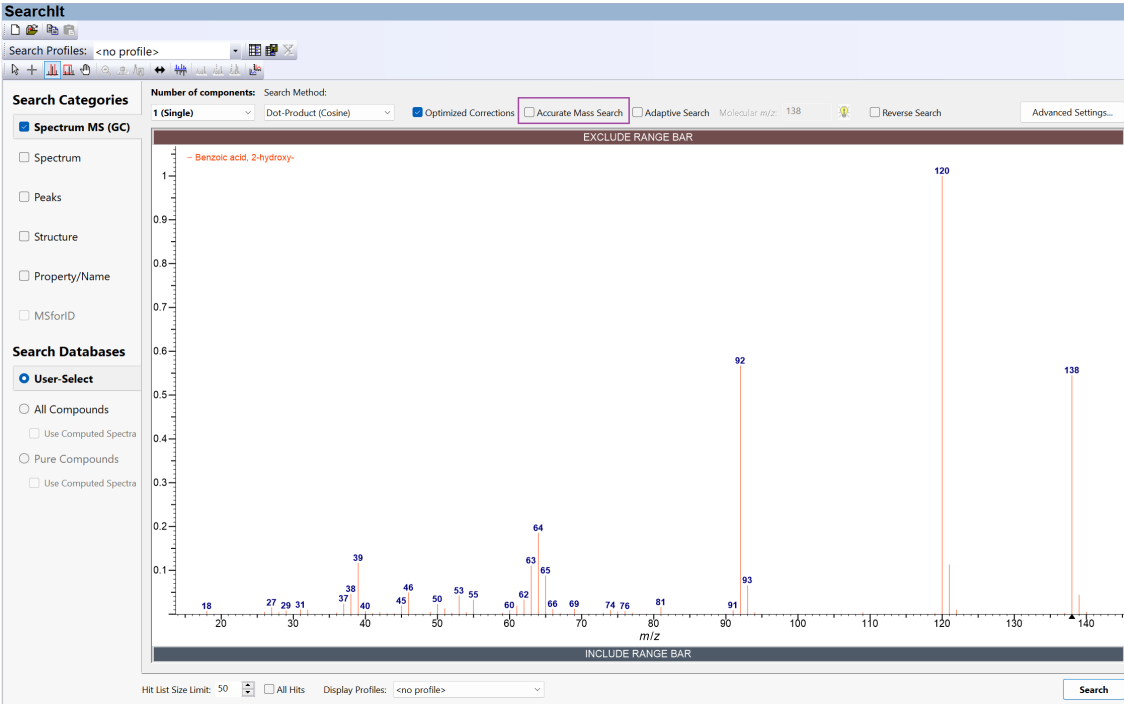
Optimized Corrections:

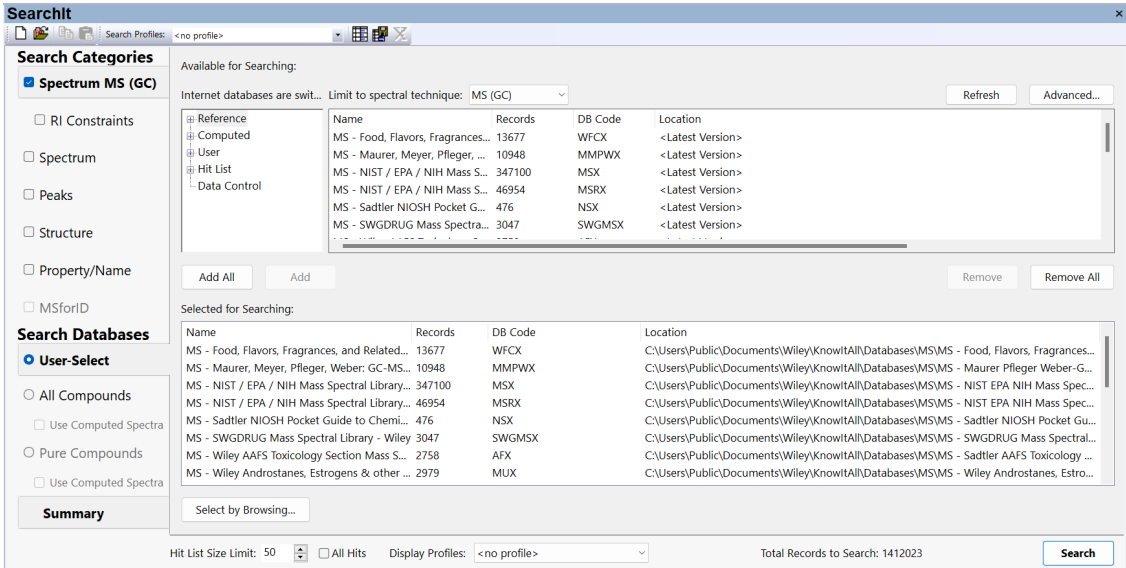
- Mass Defection is the difference between a compound's exact mass and its nominal mass. It is automatically applied for a MS search.
Examples:
 - For hydrocarbon compounds, when m/z value is over 500, use 0.99888.
 - For polybrominated compounds, when there are more than 5 Br atoms and m/z value is over 800, use 1.00087.
- Spectral Skewing is caused by analyte's concentration changing during scan. A linear compensation factor (positive for ascending or negative for descending slope) is calculated for each search match. This factor corrects the intensities as follows:


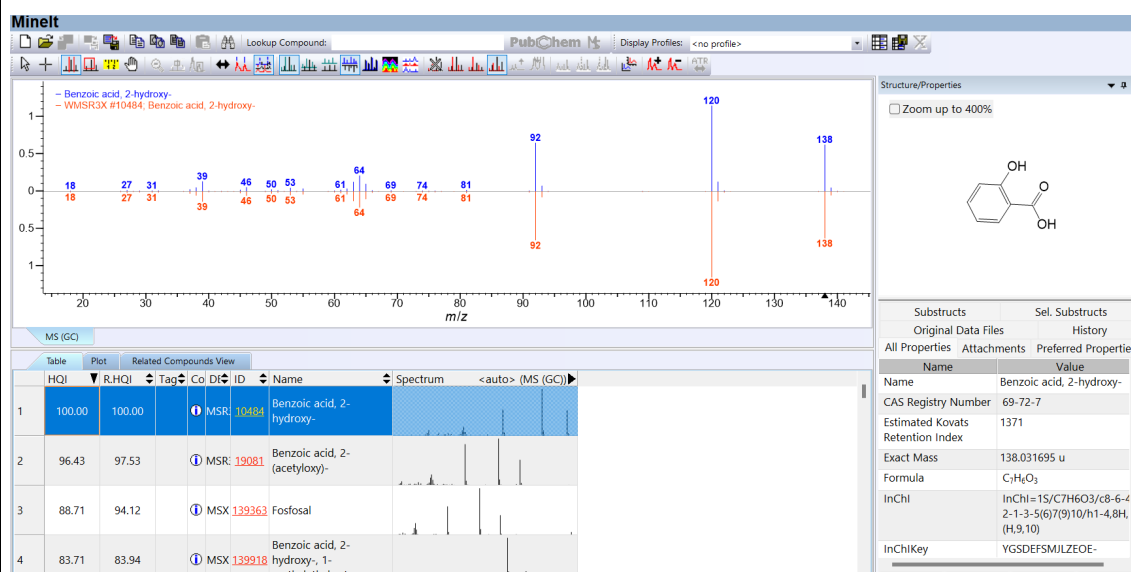
$$I(\text{corrected}) = I * f * m,$$

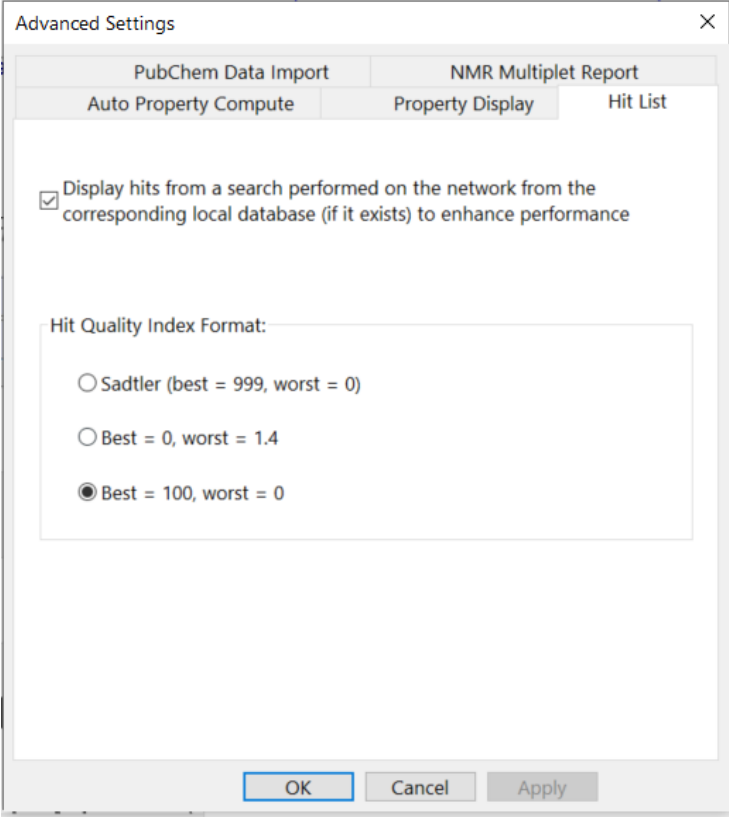
where I =intensity, f =OC factor, and m = m/z value

Straightforward Search

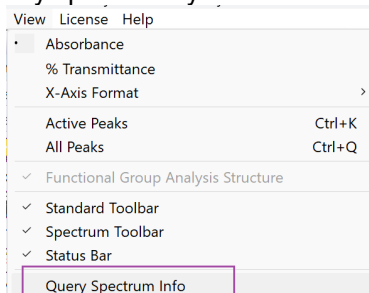
	Action	Result
1	<p>Open the KnowItAll SearchIt application by clicking its icon in the KnowItAll application.</p> <p>Check Spectrum and navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\MS folder.</p> <p>Select the file 2-Hydroxybenzoic acid.</p> <p>Click Open.</p> <p>Ensure Adaptive Search or Reverse Search is unchecked.</p>	 <p>The screenshot shows the SearchIt application window. The 'Search Profiles' dropdown is set to '<no profile>'. The 'Search Categories' panel on the left has 'Spectrum MS (GC)' selected. The 'Search Method' is 'Dot-Product (Cosine)'. The 'Number of components' is '1 (Single)'. The 'Accurate Mass Search' checkbox is highlighted with a pink box. The 'Molecular m/z' is '138'. The 'Reverse Search' checkbox is unchecked. The mass spectrum plot shows relative intensity on the y-axis (0 to 1) and m/z on the x-axis (20 to 140). The base peak is at m/z 120. Other significant peaks are at m/z 92 and 138. The spectrum is labeled 'Benzoic acid, 2-hydroxy-'.</p> <p>Note: Since the KnowItAll 2025 release, one can perform accurate mass search in addition to the default unit mass search (check highlighted box above).</p>

Action	Result
<p>2 Click User-Select.</p> <p>Search Databases</p> <p>User-Select</p> <p>Use Remove All to clean selected databases.</p> <p>Remove All</p> <p>Use Limit to spectral technique to select MS (GC).</p> <p>Limit to spectral technique: MS (GC)</p> <p>Use Add All to add all MS (GC) databases.</p> <p>Add All</p> <p>Click Search.</p> <p>Search</p>	<p>After selecting Add All for the MS (GC) databases, the full GC-MS database collection is selected for searching:</p> 

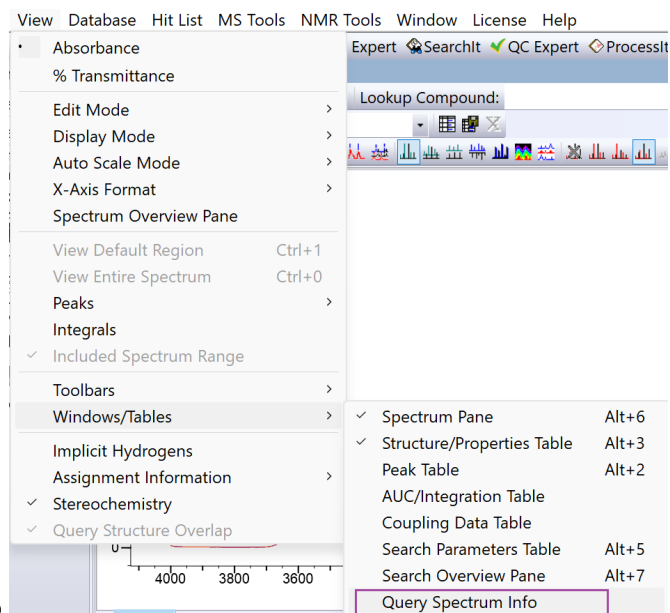
Action	Result
<div>3</div> <div>Click the Butterfly view icon  to place the unknown and reference spectrum in the opposite Y-direction.</div>	<div>A target from a database is found:</div> <div></div> <div>Hits are initially sorted by the Hit Quality Index (HQI). Reverse Hit Quality Index (R.HQI) is also calculated for each reference spectrum.</div>

	Action	Result
4	Note: HQI (Hit Quality Index)	<p>The HQI value measures how close the reference spectrum is to that of the query. The default scale of HQI is 0-100. You can change the scale from Minelt > File > Preferences > Hit List.</p>  <p>Note: Reverse Search ignores peaks that are in unknown but not in reference. One scenario is that the unknown spectrum might be a mixture and the reference spectrum might be a component.</p>

Note: One can view the metadata of query spectrum by


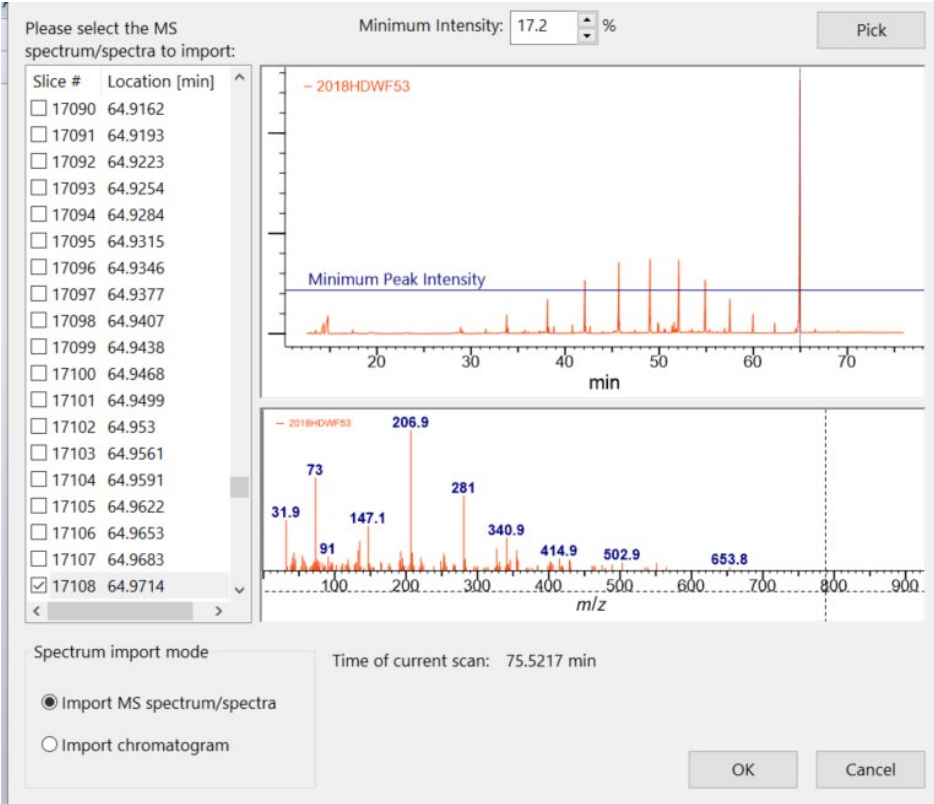


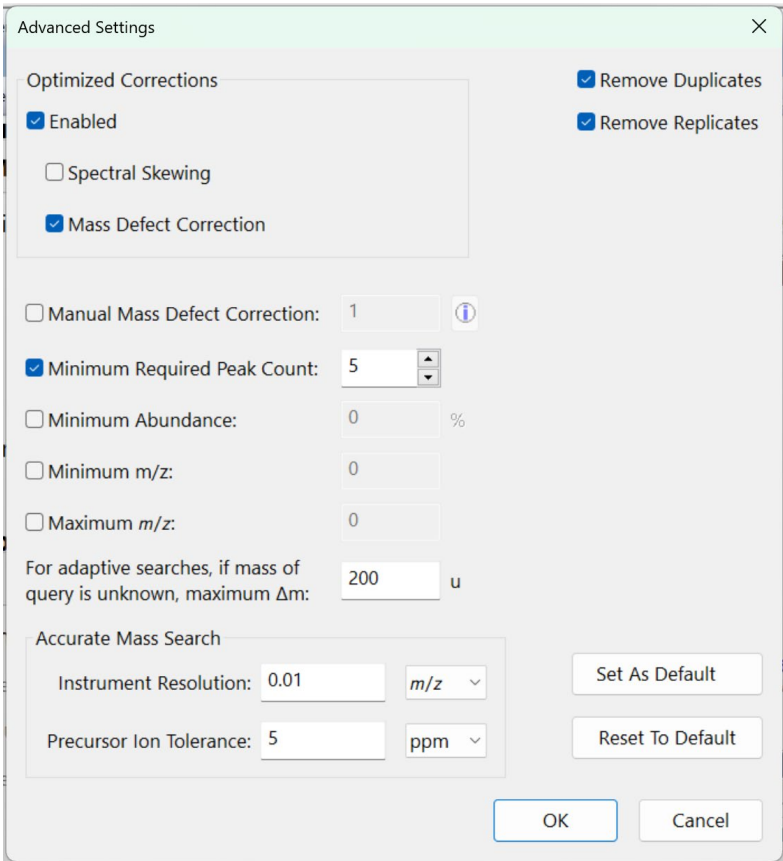
- **View > Query Spectrum Info** in **SearchIt** and

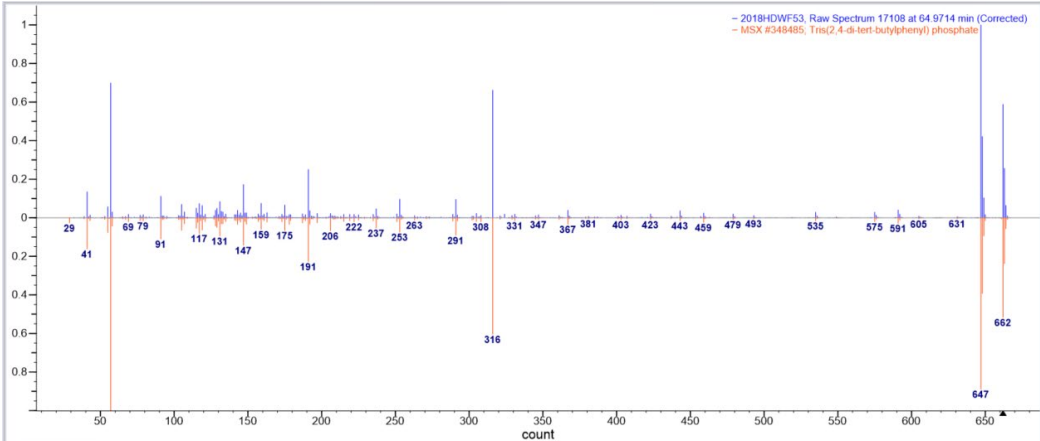
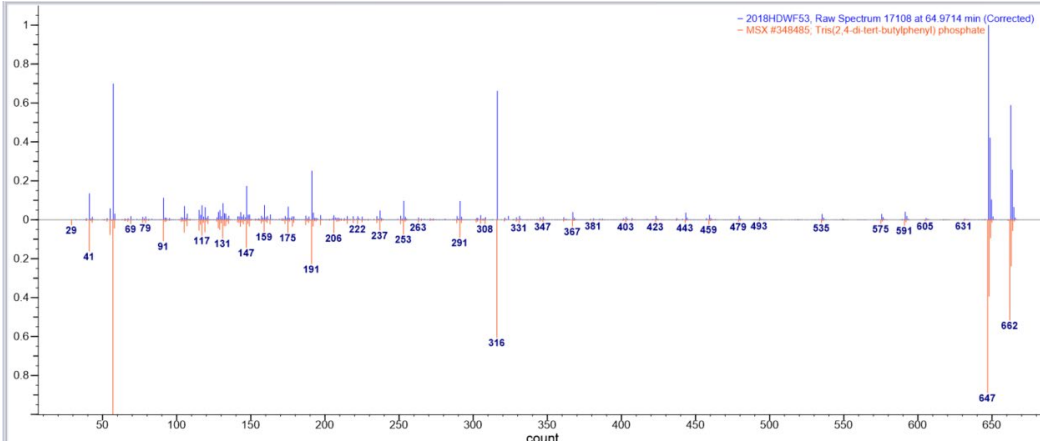


- **View > Windows/Tables > Query Spectrum Info** in a **MinIt** hit list.

Optimized Corrections

	Action	Result
1	<p>Go back to SearchIt.</p> <p>Click  to start a new search.</p> <p>Click Spectrum and navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\MS.</p> <p>Select the file Mass defect correction example.ms. Click Open.</p> <p>Click OK (use the default MS 17108).</p>	<p>Upon selecting the Mass defect correction example.ms, the MS Spectrum Selection dialog appears to prompt for spectrum import selection:</p> 

Action	Result
<p>2 Optimized Corrections for MS spectrum is the default to be checked.</p> <p><input checked="" type="checkbox"/> Optimized Corrections</p> <p>Click Advanced Setting button.</p> <p>Advanced Settings...</p> <p>Click OK to close this dialog.</p> <p>OK</p> <p>Click the Search button.</p> <p>Search</p>	<p>One can see that Mass Defection Correction (the difference between a compound's exact mass and its nominal mass) is automatically applied. Many other criterion, such as Spectral Skewing (analyte's concentration changing during scan), can be applied by users choice to improve a search.</p> 

	Action	Result
3	View the search results.	 <p>Mass spectrum plot showing relative intensity (0 to 1) versus m/z (0 to 650). The plot displays two overlapping spectra: a blue line representing the '2018HDWF53, Raw Spectrum 17108 at 64.9714 min (Corrected)' and an orange line representing the 'MSX #348485, Tris(2,4-di-tert-butylphenyl) phosphate' reference. The x-axis is labeled 'count' and the y-axis is labeled 'count'. The spectra show a base peak at m/z 662 and a significant peak at m/z 647. Other labeled peaks include 29, 41, 69, 79, 91, 117, 131, 147, 159, 175, 191, 206, 222, 237, 253, 263, 291, 308, 316, 331, 347, 367, 381, 403, 423, 443, 459, 479, 493, 535, 575, 591, 605, and 631.</p> <p>We can see analyte MS and reference MS are perfectly aligned at m/z 662.</p>
4	<p>Go back to SearchIt.</p> <p>Check off Optimized Corrections.</p> <p><input type="checkbox"/> Optimized Corrections</p> <p>Search again.</p> <p>Search</p>	 <p>Mass spectrum plot showing relative intensity (0 to 1) versus m/z (0 to 650). The plot displays two overlapping spectra: a blue line representing the '2018HDWF53, Raw Spectrum 17108 at 64.9714 min (Corrected)' and an orange line representing the 'MSX #348485, Tris(2,4-di-tert-butylphenyl) phosphate' reference. The x-axis is labeled 'count' and the y-axis is labeled 'count'. The spectra show a base peak at m/z 662 and a significant peak at m/z 647. Other labeled peaks include 29, 41, 69, 79, 91, 117, 131, 147, 159, 175, 191, 206, 222, 237, 253, 263, 291, 308, 316, 331, 347, 367, 381, 403, 423, 443, 459, 479, 493, 535, 575, 591, 605, and 631.</p> <p>At high m/z range, analyte peaks and reference peaks are not aligned nicely.</p>

Combined Retention Index (RI) Search

In KnowItAll 2026 release, you can add RI search to the MS spectral search. When a MS spectrum is read in SearchIt, the RI Constraints check

Search Categories

☒ Spectrum MS (GC)

☐ RI Constraints

shows up:

SearchIt

Search Profiles: <no profile>

Search Categories

☒ Spectrum MS (GC)

☒ RI Constraints

Property: Retention Index

Low: 1592 High: 1594

Tolerance: %

Open this box, select a RI field and enter the value range.

Partial MS Search

Also new in KnowItAll 2026, you can choose the MS partial spectrum search.

- The partial spectrum search HQI (P.HQI) will not penalize peaks that are found in the database spectrum but not in the query.
- Partial spectrum search and reverse search cannot be used together.

Search Categories

☒ Spectrum MS (GC)


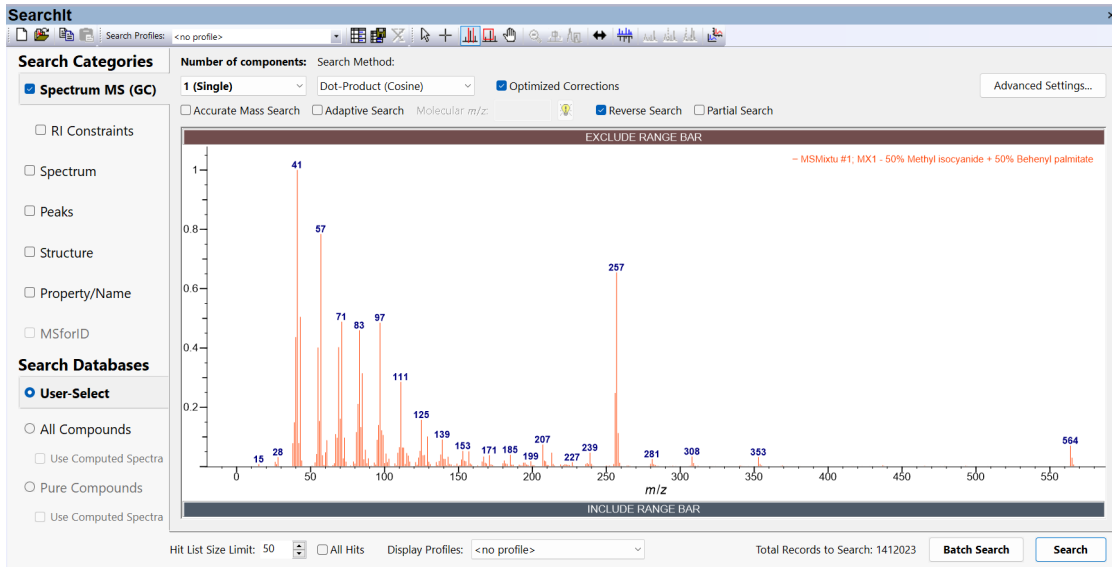
Number of components: 1 (Single) Search Method: Dot-Product (Cosine)

☒ Optimized Corrections ☐ Accurate Mass Search ☐ Adaptive Search Molecular m/z: 210

☐ Reverse Search ☒ Partial Search Advanced Settings...




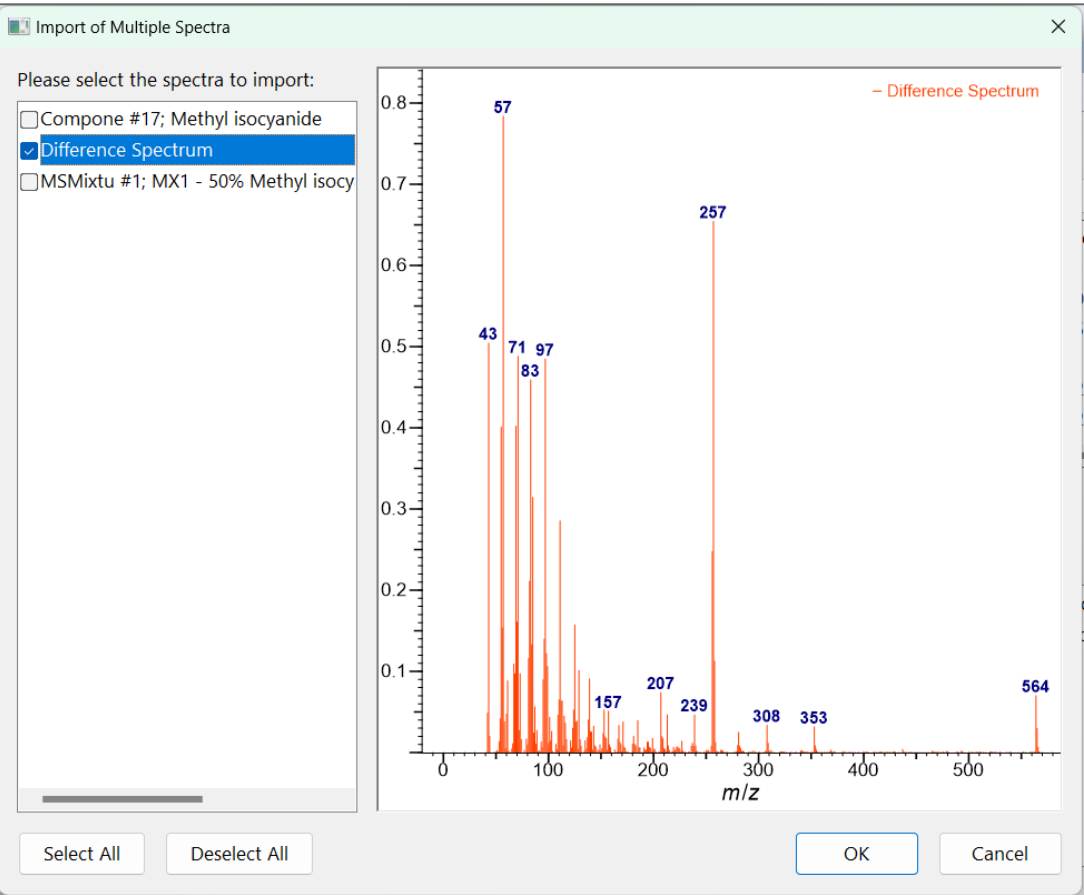
Reverse Search

This search ignores peaks that are in unknown but not in reference.

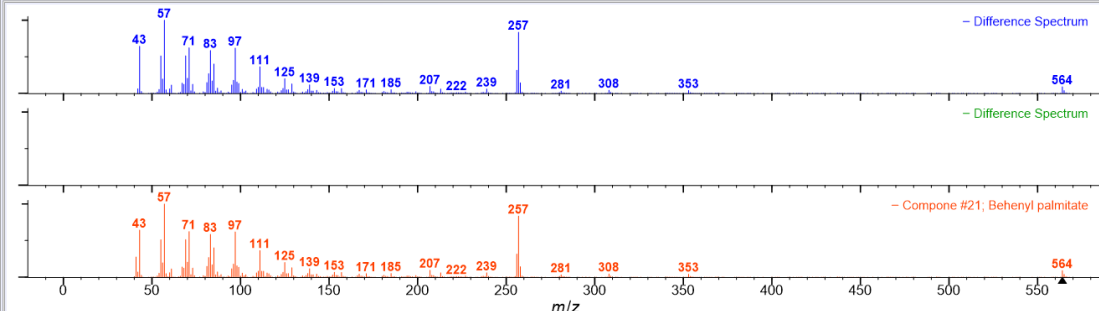
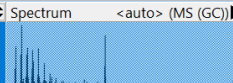
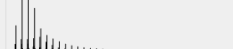
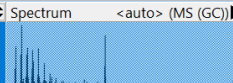
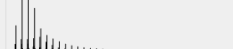
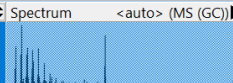
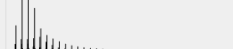
	Action	Result
1	<p>Go back to SearchIt.</p> <p>Click  to start a new search.</p> <p>Click Spectrum and navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Mixture Analysis\MS Examples folder.</p> <p>Select MS Mixture of Two 1 to open.</p> <p>Check Reverse Search.</p> <p><input checked="" type="checkbox"/> Reverse Search</p>	 <p>The screenshot shows the SearchIt software interface. On the left, the 'Search Categories' panel has 'Spectrum MS (GC)' selected. Below it, 'Search Databases' has 'User-Select' selected. The main area displays a mass spectrum plot with the x-axis labeled 'm/z' ranging from 0 to 550 and the y-axis representing relative intensity from 0 to 1.0. The plot shows several peaks, with the base peak at m/z 41. Other labeled peaks include 15, 28, 57, 71, 83, 97, 111, 125, 139, 153, 171, 185, 199, 207, 227, 239, 257, 281, 308, 353, and 564. Above the plot, search settings are visible: 'Number of components: 1 (Single)', 'Search Method: Dot-Product (Cosine)', 'Optimized Corrections' checked, 'Reverse Search' checked, and 'Partial Search' unchecked. At the bottom of the interface, there are fields for 'Hit List Size Limit: 50', 'All Hits' checkbox, 'Display Profiles: <no profile>', 'Total Records to Search: 1412023', and 'Batch Search' and 'Search' buttons.</p>

Action	Result																																											
<div>2 Click User-Select button.</div> <div><div>Search Databases</div><div><div>User-Select</div></div></div> <div>Use button Remove All to clean current database selection.</div> <div><div>Remove All</div></div> <div>Then, use Select by Browsing button to add the example database: C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Mixture Analysis\MS Examples\Components.SDBX.</div> <div>Click Search.</div> <div><div>Search</div></div>	<div><div>SearchIt</div><div><div><div>Search Categories</div><div><div><div><input checked="" type="checkbox"/> Spectrum MS (GC)</div><div><input type="checkbox"/> RI Constraints</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"/> Use Computed Spectra</div><div><input type="radio"/> Pure Compounds</div><div><input type="radio"/> Use Computed Spectra</div></div></div></div></div><div><div>Available for Searching:</div><div><div>Internet databases are swit... Limit to spectral technique: All</div><div><table><tr><th>Reference</th><th>Name</th><th>Records</th><th>DB Code</th><th>Location</th></tr><tr><td><input checked="" type="checkbox"/> User</td><td>11B NMR - Wolfgang Robien</td><td>2212</td><td>RBX</td><td><Latest Version></td></tr><tr><td><input checked="" type="checkbox"/> Hit List</td><td>13C NMR - AIST SDBS</td><td>11890</td><td>NLX</td><td><Latest Version></td></tr><tr><td><input type="checkbox"/> Data Control</td><td>13C NMR - Flavors & Fragranc...</td><td>11815</td><td>NFX</td><td><Latest Version></td></tr><tr><td></td><td>13C NMR - Natural Products ...</td><td>3432</td><td>NPX</td><td><Latest Version></td></tr><tr><td></td><td>13C NMR - Organic Compoun...</td><td>188426</td><td>NOX</td><td><Latest Version></td></tr><tr><td></td><td>13C NMR - Sadtler - Wiley</td><td>51992</td><td>NCX</td><td><Latest Version></td></tr></table></div><div><div>Add All</div><div>Add</div><div>Remove</div><div>Remove All</div></div></div></div><div><div>Selected for Searching:</div><div><table><tr><th>Name</th><th>Records</th><th>DB Code</th><th>Location</th></tr><tr><td>Components</td><td>44</td><td>Compone</td><td>C:\Users\Public\Documents\Wiley\KnowitAll\Samples\Mixture Analysis\MS Examples\Com...</td></tr></table></div><div><div>Select by Browsing...</div></div></div><div><div>Hit List Size Limit: 50</div><div><input type="checkbox"/> All Hits</div><div>Display Profiles: <no profile></div><div>Total Records to Search: 0</div><div><div>Batch Search</div><div>Search</div></div></div></div></div></div>	Reference	Name	Records	DB Code	Location	<input checked="" type="checkbox"/> User	11B NMR - Wolfgang Robien	2212	RBX	<Latest Version>	<input checked="" type="checkbox"/> Hit List	13C NMR - AIST SDBS	11890	NLX	<Latest Version>	<input type="checkbox"/> Data Control	13C NMR - Flavors & Fragranc...	11815	NFX	<Latest Version>		13C NMR - Natural Products ...	3432	NPX	<Latest Version>		13C NMR - Organic Compoun...	188426	NOX	<Latest Version>		13C NMR - Sadtler - Wiley	51992	NCX	<Latest Version>	Name	Records	DB Code	Location	Components	44	Compone	C:\Users\Public\Documents\Wiley\KnowitAll\Samples\Mixture Analysis\MS Examples\Com...
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Components	44	Compone	C:\Users\Public\Documents\Wiley\KnowitAll\Samples\Mixture Analysis\MS Examples\Com...																																									

Action	Result
<p>3 In Minelt, make sure that Subtract View (circled) is selected.</p> <p>In the spectrum pane, the first row is the unknown, the last row is the reference spectrum, and the middle row is the difference between the two.</p>	<div><div><div><div><div><div>Minelt</div><div><div>Lookup Compound:</div><div>PubChem</div><div>Display Profiles: <no profile></div></div><div><div><div><div><div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div>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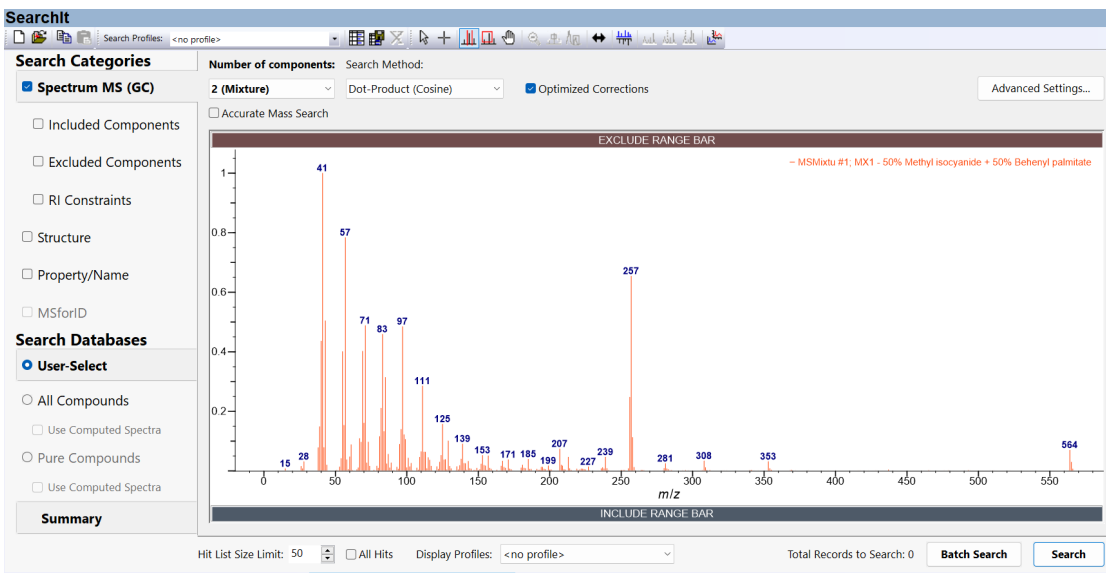
Action	Result
<p>4 Transfer spectra in spectrum pane to SearchIt using the Transfer to: menu at the top of the application.</p> <p>Transfer to:  ReportIt  ID Expert  SearchIt</p> <p>Select to transfer only the Difference Spectrum. Click OK.</p> <p>When prompted by SearchIt, choose Start a new search.</p> <p>Start a new search</p>	<p>Upon transferring the Difference Spectrum to SearchIt, the Import of Multiple Spectra dialog is prompted:</p> 

Action	Result
<div>5 Click Search.</div> <div><div>Search</div></div>	<div><div>SearchIt</div><div><div><div>Search Profiles: <no profile></div><div><div>Search Categories</div><div><div><div><input checked="" type="checkbox"/> Spectrum MS (GC)</div><div><input type="checkbox"/> RI Constraints</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="checkbox"/> Use Computed Spectra</div></div><div><div><input type="radio"/> Pure Compounds</div><div><input type="checkbox"/> Use Computed Spectra</div></div></div><div><div>Summary</div></div></div></div><div><div>Number of components: 1 (Single)</div><div>Search Method: Dot-Product (Cosine)</div><div><input checked="" type="checkbox"/> Optimized Corrections</div><div><input type="checkbox"/> Accurate Mass Search</div><div><input type="checkbox"/> Adaptive Search</div><div>Molecular m/z</div><div><input type="checkbox"/> Reverse Search</div><div><input type="checkbox"/> Partial Search</div><div>Advanced Settings...</div></div><div><div>EXCLUDE RANGE BAR</div><div><div><div>1</div><div>0.8</div><div>0.6</div><div>0.4</div><div>0.2</div><div>0</div></div><div><div>43</div><div>57</div><div>71</div><div>83</div><div>97</div><div>111</div><div>125</div><div>139</div><div>153</div><div>171</div><div>185</div><div>199</div><div>207</div><div>227</div><div>239</div><div>257</div><div>281</div><div>308</div><div>353</div><div>564</div></div><div><div>m/z</div></div></div><div><div>INCLUDE RANGE BAR</div></div></div><div><div>Hit List Size Limit: 50</div><div><input type="checkbox"/> All Hits</div><div>Display Profiles: <no profile></div><div>Total Records to Search: 44</div><div><div>Batch Search</div><div>Search</div></div></div></div></div></div></div>

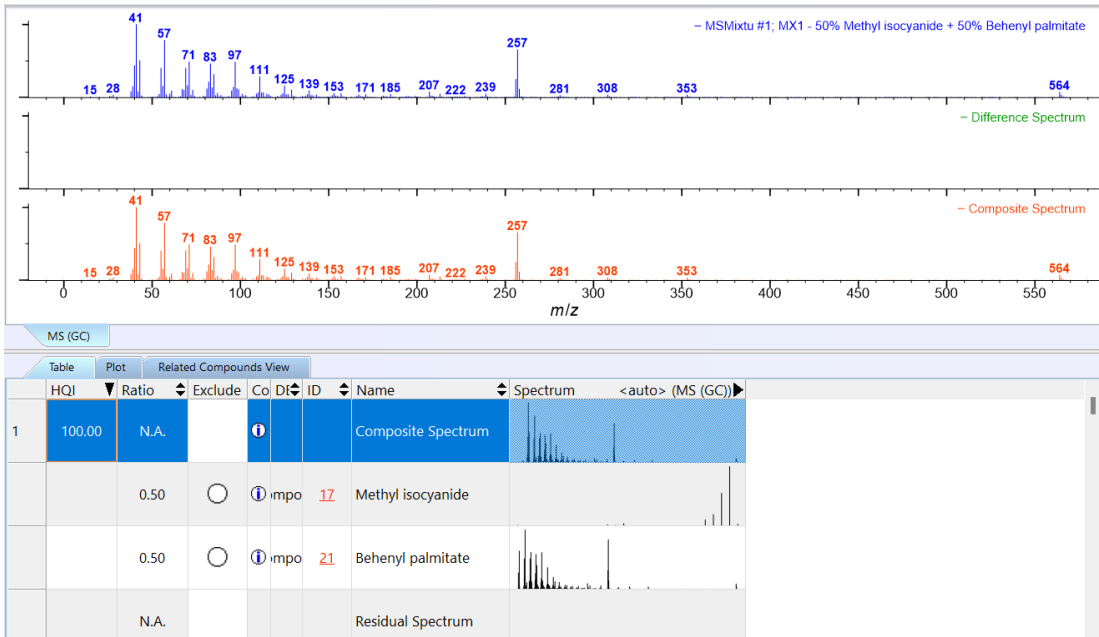
Action	Result																											
6 Analyze the search results in Minelt.	<div><p>Minelt</p><p>Lookup Compound: PubChem Display Profiles: <no profile></p><p>MS (GC)</p><table><tr><th></th><th>HQI</th><th>R.HQI</th><th>Tag</th><th>Co</th><th>Di</th><th>ID</th><th>Name</th><th>Spectrum</th></tr><tr><td>1</td><td>99.23</td><td>99.23</td><td>mpo</td><td>21</td><td></td><td></td><td>Behenyl palmitate</td><td></td></tr><tr><td>2</td><td>45.45</td><td>68.48</td><td>mpo</td><td>38</td><td></td><td></td><td>Octatriacontane</td><td></td></tr></table></div> <p>A second component is identified.</p> <p>Notice that the Difference Spectrum is empty, which means there are no more components.</p>		HQI	R.HQI	Tag	Co	Di	ID	Name	Spectrum	1	99.23	99.23	mpo	21			Behenyl palmitate		2	45.45	68.48	mpo	38			Octatriacontane	
	HQI	R.HQI	Tag	Co	Di	ID	Name	Spectrum																				
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Mixture Analysis


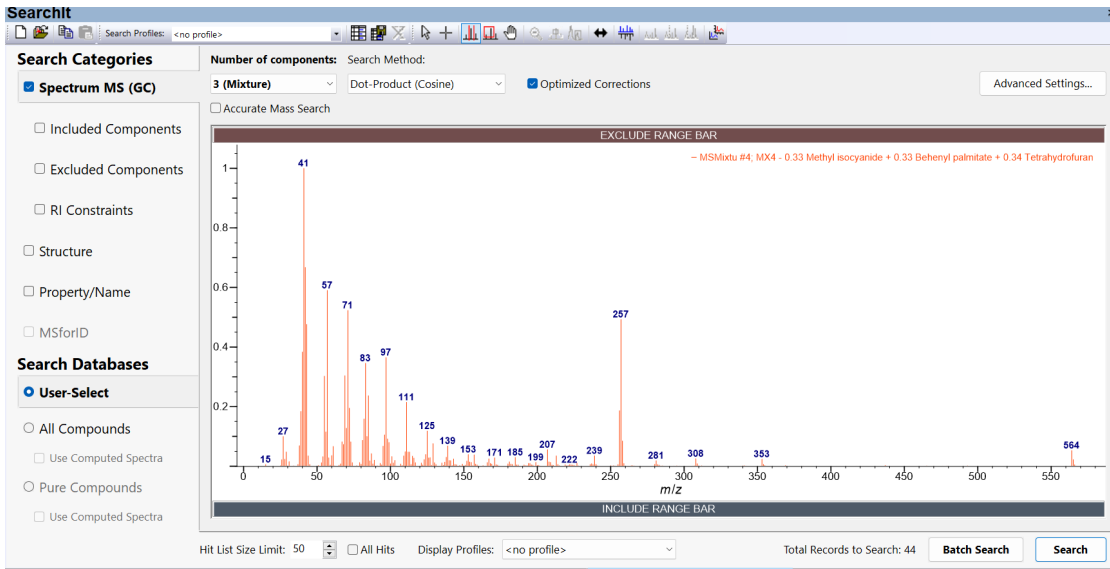
A mixture wherein two-component MS spectra have limited overlap, and one of them has a large MS range.

	Action	Result
1	<p>Go back to SearchIt.</p> <p>Start a new search by clicking .</p> <p>Select MS Mixture of Two 1.</p> <p>Ensure Reverse Search or Adaptive Search is unchecked.</p> <p>Use the drop-down menu to set the Number of components to 2.</p> <p>Number of components:</p> <p>2 (Mixture)</p>	

	Action	Result																																																
2	<p>Click on User-Select.</p> <p>Search Databases</p> <div><div>User-Select</div></div> <p>Make sure Components database is selected to use.</p> <p>Click Search.</p> <div><div>Search</div></div>	<div><div><div><div>Search Categories</div><div><div><div><input checked="" type="checkbox"/> Spectrum MS (GC)</div><div><input type="checkbox"/> Included Components</div><div><input type="checkbox"/> Excluded Components</div><div><input type="checkbox"/> RI Constraints</div><div><input 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><div><input checked="" type="radio"/> User-Select</div><div><input type="radio"/> All Compounds</div><div><input type="checkbox"/> Use Computed Spectra</div><div><input type="radio"/> Pure Compounds</div><div><input type="checkbox"/> Use Computed Spectra</div></div></div><div><div>Summary</div></div></div></div><div><div><div>SearchIt</div><div><div>Search Profiles: <no profile></div><div>Available for Searching:</div><div>Internet databases are swit... Limit to spectral technique: All</div><div><table><thead><tr><th></th><th>Name</th><th>Records</th><th>DB Code</th><th>Location</th></tr></thead><tbody><tr><td><input checked="" type="checkbox"/></td><td>Reference</td><td></td><td></td><td></td></tr><tr><td><input checked="" type="checkbox"/></td><td>Computed</td><td>11B NMR - Wolfgang Robien</td><td>2212</td><td>RBX</td></tr><tr><td><input checked="" type="checkbox"/></td><td>User</td><td>13C NMR - AIST SDBS</td><td>11890</td><td>NLX</td></tr><tr><td><input checked="" type="checkbox"/></td><td>Hit List</td><td>13C NMR - Flavors & Fragranc...</td><td>11815</td><td>NFX</td></tr><tr><td><input checked="" type="checkbox"/></td><td>Data Control</td><td>13C NMR - Natural Products ~...</td><td>3432</td><td>NPX</td></tr><tr><td></td><td></td><td>13C NMR - Organic Compoun...</td><td>188426</td><td>NOX</td></tr><tr><td></td><td></td><td>13C NMR - Sadtler - Wiley</td><td>51992</td><td>NCX</td></tr></tbody></table></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><table><thead><tr><th>Name</th><th>Records</th><th>DB Code</th><th>Location</th></tr></thead><tbody><tr><td>Components</td><td>44</td><td>Compone</td><td>C:\Users\Public\Documents\Wiley\KnowitAll\Samples\Mi...</td></tr></tbody></table></div><div><div>Select by Browsing...</div></div></div><div><div>Hit List Size Limit: 50</div><div><input type="checkbox"/> All Hits</div><div>Display Profiles: <no profile></div><div>Total Records to Search: 0</div><div><div>Batch Search</div><div>Search</div></div></div></div></div></div></div>		Name	Records	DB Code	Location	<input checked="" type="checkbox"/>	Reference				<input checked="" type="checkbox"/>	Computed	11B NMR - Wolfgang Robien	2212	RBX	<input checked="" type="checkbox"/>	User	13C NMR - AIST SDBS	11890	NLX	<input checked="" type="checkbox"/>	Hit List	13C NMR - Flavors & Fragranc...	11815	NFX	<input checked="" type="checkbox"/>	Data Control	13C NMR - Natural Products ~...	3432	NPX			13C NMR - Organic Compoun...	188426	NOX			13C NMR - Sadtler - Wiley	51992	NCX	Name	Records	DB Code	Location	Components	44	Compone	C:\Users\Public\Documents\Wiley\KnowitAll\Samples\Mi...
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Components	44	Compone	C:\Users\Public\Documents\Wiley\KnowitAll\Samples\Mi...																																															

	Action	Result
3	Analyze the search results in Minelt .	<div></div> <p>KnowItAll presents a 2-component search result. The top spectrum is unknown; the bottom spectrum is the composite spectrum of 2 components. The middle spectrum is the difference between the two. In this case, it is next to nothing, indicating that there are no more residual peaks.</p> <p>Note: This is an example wherein the two-component MS spectra have limited overlap, but one of them has large MS range.</p>

A more complex example


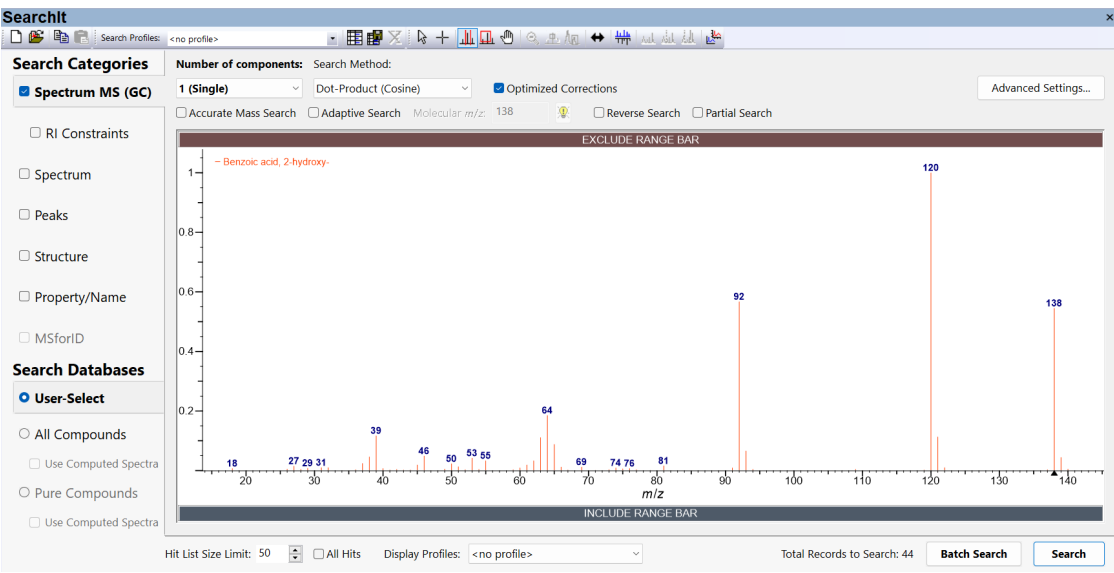
	Action	Result
1	<p>Go back to SearchIt.</p> <p>Start a new search by clicking .</p> <p>Select the file MS Mixture of Three.</p> <p>Use the drop-down menu to set the Number of components to 3 (Mixture).</p> <p>Number of components:</p> <p>3 (Mixture)</p>	 <p>The screenshot shows the SearchIt software interface. On the left, the 'Search Categories' panel has 'Spectrum MS (GC)' selected. Below it, 'Search Databases' has 'User-Select' selected. The 'Number of components' is set to '3 (Mixture)'. The 'Search Method' is 'Dot-Product (Cosine)'. The 'Accurate Mass Search' checkbox is unchecked. The main area displays a mass spectrum plot with the x-axis labeled 'm/z' ranging from 0 to 550. The y-axis represents relative intensity from 0 to 1.0. The spectrum shows several peaks, with the base peak at m/z 41. Other labeled peaks include 15, 27, 57, 71, 83, 97, 111, 125, 139, 153, 171, 185, 199, 207, 222, 239, 257, 281, 308, 353, and 564. A legend at the top right of the plot area indicates the mixture composition: 'MSMixture #4, MX4 - 0.33 Methyl isocyanide + 0.33 Behenyl palmitate + 0.34 Tetrahydrofuran'. At the bottom, there are controls for 'Hit List Size Limit' (50), 'All Hits' checkbox, 'Display Profiles' dropdown, 'Total Records to Search' (44), and 'Batch Search' and 'Search' buttons.</p>


	Action	Result
3	Analyze the search results in Minelt .	<div><div><div><div><div><div>Minelt</div><div>Lookup Compound: PubChem</div><div>Display Profiles: <no profile></div></div><div><div><div><div><div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div>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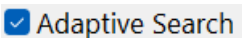


Adaptive Search

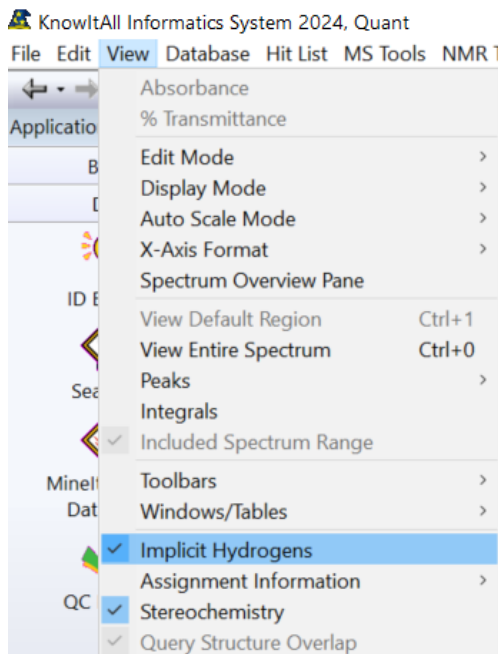

This search finds similar compounds where a fragment group can be present or missing compared to the unknown. The presence/absence of a fragment causes some peak positions in reference MS differing to that of unknown by a delta mass (Δm). KnowItAll shifts some peaks by the Δm to achieve a better matching score. Because of the better matching score, similar compounds come atop of the hit list. To clearly mark the shifts done by Adaptive Search, dotted lines are used to show reference spectrum before and after shifting in the pop-up window when you click on the (i) button in a hit.


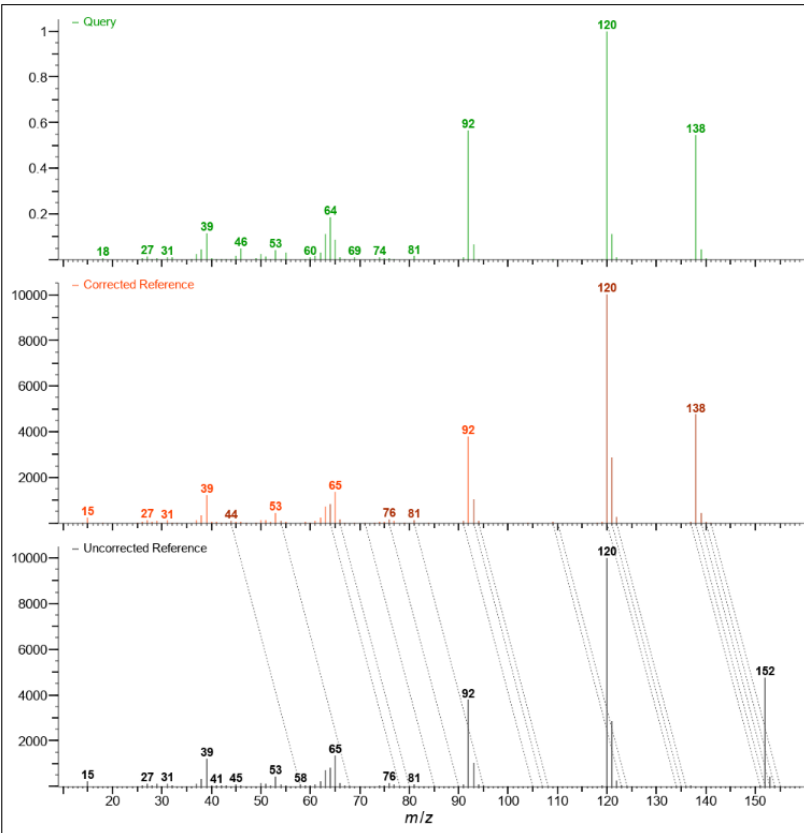
Example wherein exact mass is in a spectrum

	Action	Result
1	<p>In SearchIt, start a new search by clicking .</p> <p>Click Spectrum to navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\MS folder.</p> <p>Select the file 2-Hydroxybenzoic acid.</p> <p>Use the drop-down menu to set the Number of components to 1 (Single).</p> <p>Number of components: 1 (Single)</p> <p>Ensure that either Adaptive Search or Reverse Search is unchecked.</p>	 <p>This spectrum file contains a molecular ion mass of 138. KnowItAll will use this value for the Adaptive Search.</p>

Action	Result
3 Click the Butterfly view icon  .	 <p>The screenshot displays the Minelt software interface. The top section shows a mass spectrum plot with m/z on the x-axis (20 to 140) and relative intensity on the y-axis (0 to 1). Two spectra are overlaid: a blue spectrum for Benzoic acid, 2-hydroxy- and a red spectrum for WMS3X #28574, Salicylic acid. The blue spectrum has major peaks at m/z 92, 120, and 138. The red spectrum has major peaks at m/z 92, 120, and 138. The bottom section shows a table of results with columns for HQI, R.HQI, Tag, Co, DI, ID, Name, and Spectrum. The table lists four entries: 1. Salicylic acid (HQI 97.52, R.HQI 99.29, ID /MS3 28574), 2. Fosfosal (HQI 88.44, R.HQI 93.84, ID /MS3 176449), 3. Benzoic acid, 2-(acetyloxy)- (HQI 86.88, R.HQI 88.83, ID /MS3 93558), and 4. Benzoic acid, 2-(acetyloxy)- (HQI 85.66, R.HQI 90.37, ID /MS3 93559). The right sidebar shows the chemical structure of Salicylic acid and a table of properties including Name, Estimated Kovats Retention Index, Exact Mass, Formula, InChI, and InChIKey.</p>


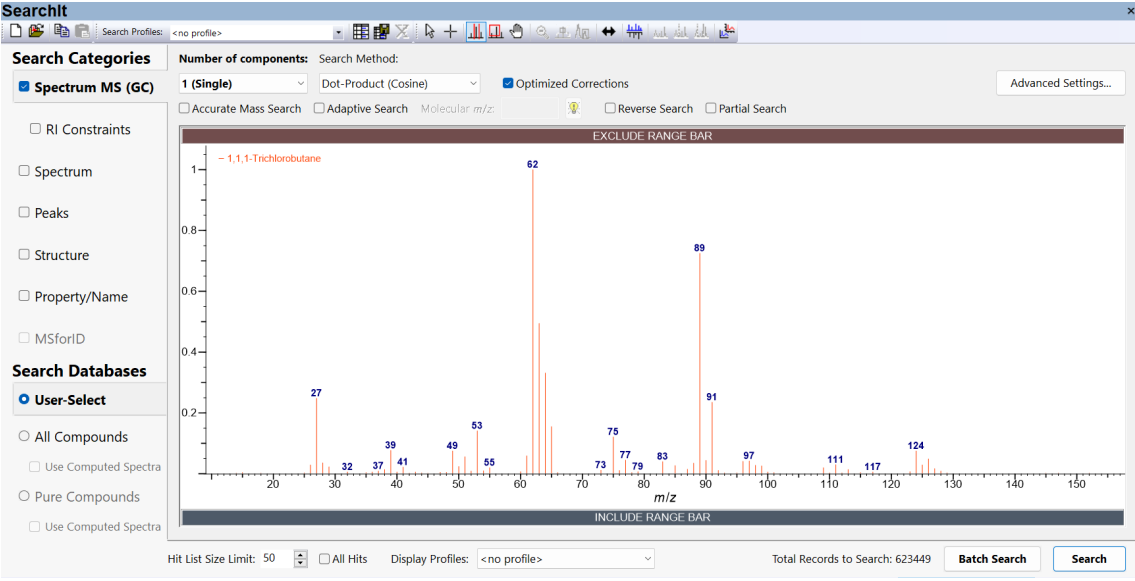
	Action	Result
5	<p>Go back to SearchIt.</p> <p>Click Spectrum MS(GC).</p> <p></p> <p>Check Adaptive Search.</p> <p></p> <p>Click Search.</p> <p></p>	 <ul style="list-style-type: none"> • If a spectrum file contains the molecular ion mass, it will be displayed in the “Molecular <i>m/z</i>” box, and a solid triangle marks this position in the spectrum pane. • You can type in an appropriate value as well. This value is used to assist Adaptive Search. • Or, you can ask KnowItAll to estimate a molecular mass for you by clicking the bulb icon. • However, if molecular ion mass is unknown, this box would be empty. KnowItAll Adaptive Search will estimate this value from the input unknown MS spectrum.


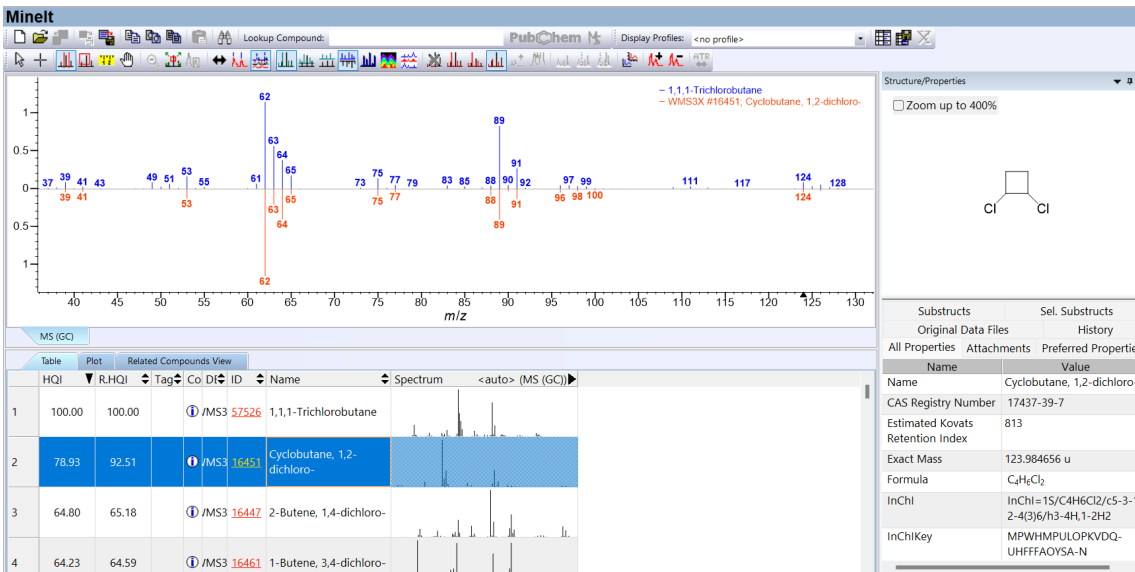
Action	Result
<p>6 Ignore the 1st hit and move to the 2nd hit.</p> <p>Make sure KnowItAll displays implicit Hydrogens. Go to the View menu and check Implicit Hydrogens.</p> 	 <p>The result looks good. Δm of -14 suggests a few possibilities wherein the unknown's molecular ion mass (m/z) is 14 unit less than that of the reference. One of them is "In unknown, Benzene replaces Toluene in reference."</p> <p>Columns of interest:</p> <ul style="list-style-type: none"> • Δm: the molecular ion mass of unknown minus that of the reference • Δm Info: details on reference peak shifts to make the match • Replacement: suggestions of possible group exchange which would cause the difference between unknown and reference molecular ion masses


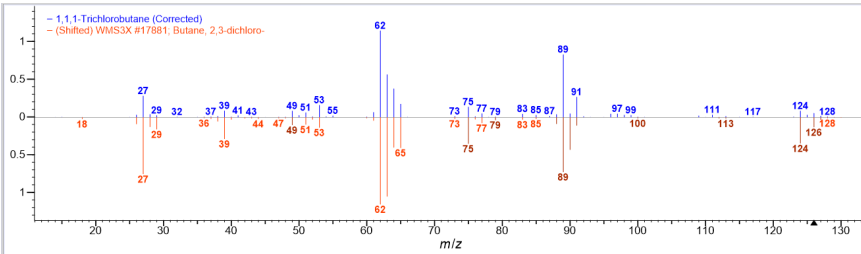



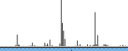

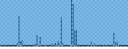

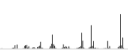

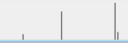

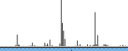

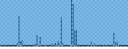

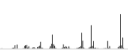

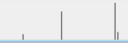

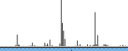

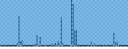

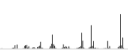

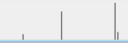

	Action	Result
7	Click (i) icon () in the Δm Info column. This brings up the Adaptive Corrections html page which explains how selective peaks have been shifted to obtain good Hit Quality Index (HQI) .	<h3 style="text-align: center;">Adaptive Corrections</h3> <hr/> <p>The following correction was applied to the reference spectrum to get optimal results:</p> <p>Some peaks in the reference spectrum were offset horizontally by -14 u</p> <p>The top spectrum is the unknown spectrum, the bottom spectrum is the unshifted reference spectrum, and the middle one is the shifted spectrum. In the shifted spectrum, the darker red peaks are additions of unshifted peaks and shifted peaks. Dotted lines between shifted and reference spectrum link shifted peaks to their original positions.</p>
8	Analyze the information in the popup for Optimized Corrections .	


	Action	Result
		<ul style="list-style-type: none">• The top spectrum is the unknown• The bottom spectrum is the unshifted reference• The middle “spectrum” contains shifted peaks• Dotted lines indicate what peaks have been moved by an Δm• In the middle “spectrum,” darker red peaks are the additions of existing peaks and moved ones


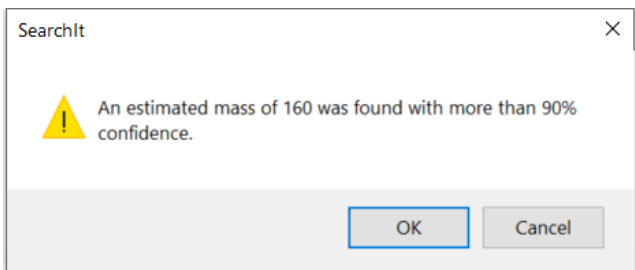

Example wherein exact mass is NOT in a spectrum

	Action	Result
1	<p>Start a new search by clicking .</p> <p>Click Spectrum and navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\MS folder.</p> <p>Select file 1,1,1-Trichlorobutane.</p> <p>Use the drop-down menu to set the Number of components to 1 (Single).</p> <p>Number of components: 1 (Single)</p> <p>Ensure either Adaptive Search or Reverse Search is unchecked.</p> <p>Click User-Select.</p> <p>Use Remove All to clean selected databases.</p> <p>Use Add to add MS (GC) databases by codes: WMS3X.</p> <p>Click Search.</p>	 <p>As we can see, this spectrum does not contain molecular ion mass. KnowItAll will estimate this value and use it for Adaptive Search.</p>

Action	Result
<div>2</div> <div>Click the Butterfly view icon .</div> <div>Go to the 2nd hit since the 1st hit is the exact match (pretend that we do not have the exact match in our databases).</div>	<div></div> <div>We are not sure by looking at the HQI that we have a hit that is structurally similar to our unknown.</div>

Action	Result																																																																																						
<p>3 Go back to SearchIt.</p> <p>Check Adaptive Search.</p> <p><input checked="" type="checkbox"/> Adaptive Search Molecular m/z: <input type="text"/></p> <p>Click Search.</p> <p>Search</p> <p>In Minelt, Click the Butterfly view icon .</p> <p>Go to the 2nd hit (1st being the unknown which is already in a database).</p>	 <p>Structure/Properties  </p> <p><input type="checkbox"/> Zoom up to 400%</p>  <table border="1"> <thead> <tr> <th colspan="2">Substructs</th> <th>Sel. Substructs</th> </tr> <tr> <th colspan="2">Original Data Files</th> <th>History</th> </tr> <tr> <th>All Properties</th> <th>Attachments</th> <th>Preferred Properties</th> </tr> <tr> <th>Name</th> <th colspan="2">Value</th> </tr> </thead> <tbody> <tr> <td>Name</td> <td colspan="2">Butane, 2,3-dichloro-</td> </tr> <tr> <td>CAS Registry Number</td> <td colspan="2">7581-97-7</td> </tr> <tr> <td>Estimated Kovats Retention Index</td> <td colspan="2">700</td> </tr> <tr> <td>Exact Mass</td> <td colspan="2">126.000306 u</td> </tr> <tr> <td>Formula</td> <td colspan="2">C₄H₉Cl₂</td> </tr> <tr> <td>InChi</td> <td colspan="2">InChi=1S/C4H8Cl2/c1-3(5)4(2)6/h3-4H,1-2H3</td> </tr> <tr> <td>InChiKey</td> <td colspan="2">RMISVOPUIFJTEO-UHFFFAOYSA-N</td> </tr> </tbody> </table> <table border="1"> <thead> <tr> <th>Table</th> <th>Plot</th> <th>Related Compounds View</th> </tr> <tr> <th>HQI</th> <th>R.HQI</th> <th>Tag</th> <th>ID</th> <th>Name</th> <th>Spectrum</th> <th><auto> (MS (GC))</th> <th>Δm [u]</th> <th>Δm Info</th> <th>Replacement</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>100.00</td> <td>100.00</td> <td>/MS3 57526</td> <td>1,1,1-Trichlorobutane</td> <td></td> <td></td> <td>0</td> <td></td> <td></td> </tr> <tr> <td>2</td> <td>82.79</td> <td>67.26</td> <td>/MS3 17881</td> <td>Butane, 2,3-dichloro-</td> <td></td> <td></td> <td>34</td> <td></td> <td>In unknown, Chlorine replaces Hydrogen in reference. In unknown, -CF3 group replaces</td> </tr> <tr> <td>3</td> <td>80.65</td> <td>24.63</td> <td>/MS3 78912</td> <td>Benzenamine, 4-chloro-2-nitro-</td> <td></td> <td></td> <td>-37</td> <td></td> <td></td> </tr> <tr> <td>4</td> <td>80.59</td> <td>63.52</td> <td>/MS3 16455</td> <td>(2Z)-1,3-Dichloro-2-butene</td> <td></td> <td></td> <td>9</td> <td></td> <td></td> </tr> </tbody> </table> <p>One of the suggestions in the Replacement cell makes sense. The unknown should have 1 more Chlorine for a delta mass of 34.</p>	Substructs		Sel. Substructs	Original Data Files		History	All Properties	Attachments	Preferred Properties	Name	Value		Name	Butane, 2,3-dichloro-		CAS Registry Number	7581-97-7		Estimated Kovats Retention Index	700		Exact Mass	126.000306 u		Formula	C ₄ H ₉ Cl ₂		InChi	InChi=1S/C4H8Cl2/c1-3(5)4(2)6/h3-4H,1-2H3		InChiKey	RMISVOPUIFJTEO-UHFFFAOYSA-N		Table	Plot	Related Compounds View	HQI	R.HQI	Tag	ID	Name	Spectrum	<auto> (MS (GC))	Δm [u]	Δm Info	Replacement	1	100.00	100.00	/MS3 57526	1,1,1-Trichlorobutane			0			2	82.79	67.26	/MS3 17881	Butane, 2,3-dichloro-			34		In unknown, Chlorine replaces Hydrogen in reference. In unknown, -CF3 group replaces	3	80.65	24.63	/MS3 78912	Benzenamine, 4-chloro-2-nitro-			-37			4	80.59	63.52	/MS3 16455	(2Z)-1,3-Dichloro-2-butene			9		
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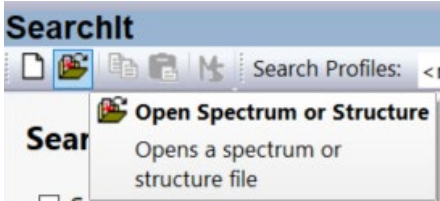
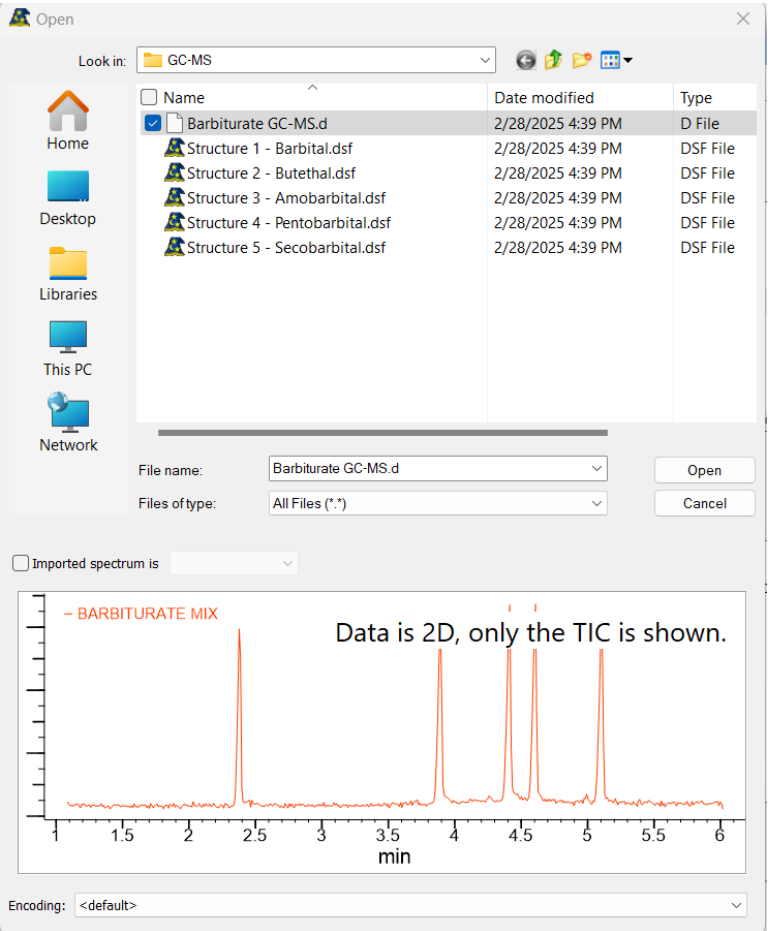
Alternatively, one can use the molecular ion mass estimation icon  to estimate the molecular ion mass:

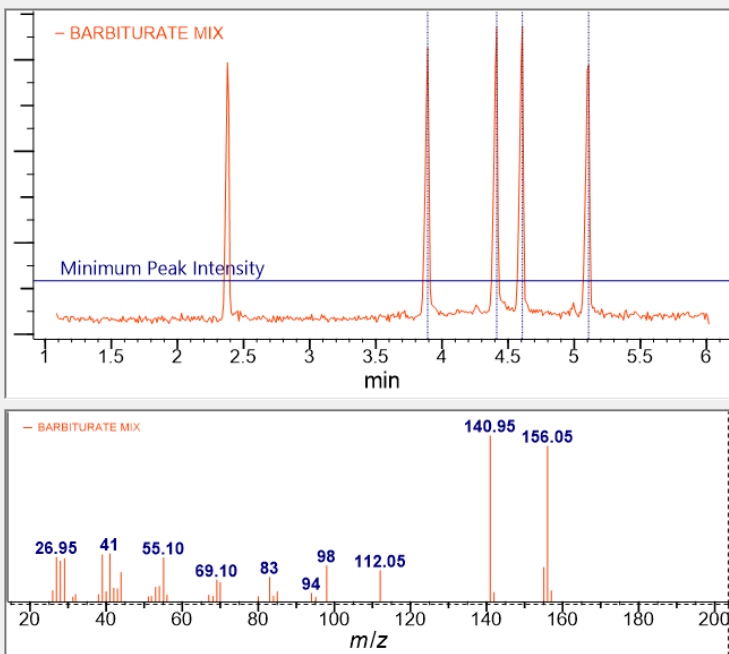
	Action	Result
1	Go Back to SearchIt . Click the  icon. Let the calculation complete.	
2	Click OK button	The estimated molecular ion mass value fills the box 

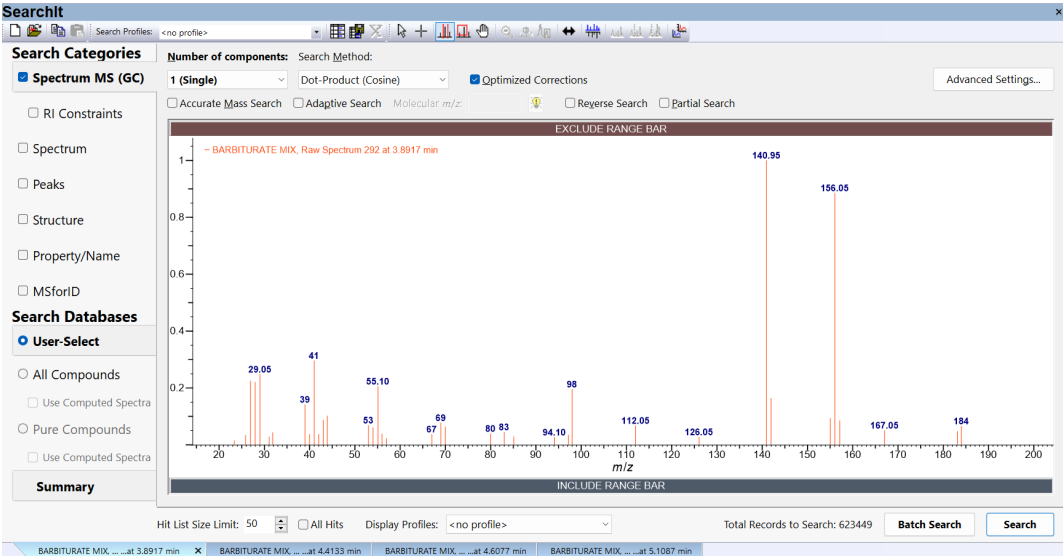
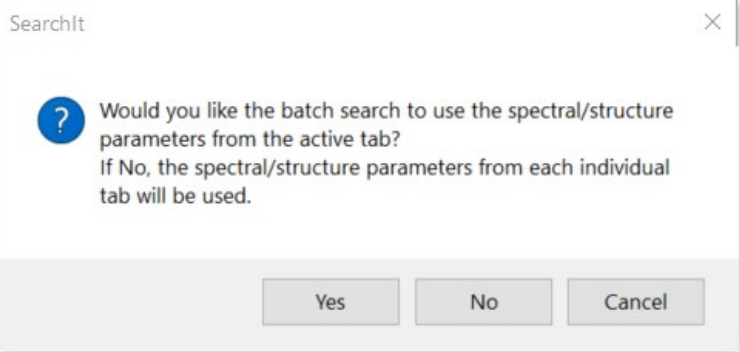
NOTE: KnowItAll runs an adaptive search of the unknown against all of our MS databases. The resulting hit list is then analyzed in steps. The mass of every hit list entry is calculated as the nominal mass of the compound in the database record plus the Δm found for the match. Matches of equal mass are then grouped together into clusters. The higher the found HQL, the higher the score for an individual match. Scores for clusters are then calculated as a combination of individual match scores with additional information such as the number of entries in the cluster and the separation from the next best cluster. The cluster with the best score determines the found mass. As side information of this procedure, information on confidence that the found mass will be correct is reported.

The confidence values found by the algorithm were determined by running statistics with thousands of very diverse compound spectra run against our MS data.

Simultaneous Multiple MS Spectra Search

	Action	Result
1	<p>In SearchIt, select Open Spectrum or Structure</p>  <p>Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\GC-MS\Barbiturate GC-MS.d</p> <p>Click Open in previous dialog.</p>	 <p>The 'Open' dialog shows the file 'Barbiturate GC-MS.d' selected in the 'Look in: GC-MS' folder. The file list includes 'Structure 1 - Barbitol.dsf', 'Structure 2 - Butethal.dsf', 'Structure 3 - Amobarbital.dsf', 'Structure 4 - Pentobarbital.dsf', and 'Structure 5 - Secobarbital.dsf'. The 'File name' field contains 'Barbiturate GC-MS.d' and 'Files of type' is set to 'All Files (*.*)'. Below the dialog, a chromatogram plot shows a baseline with several sharp peaks. The first peak is labeled 'BARBITURATE MIX'. The x-axis is labeled 'min' and ranges from 1 to 6. The y-axis is unlabeled. The plot title is 'Data is 2D, only the TIC is shown.'</p>

	Action	Result																																																												
2	<p>Pick multiple MS spectrum in the MS Spectra Scan Selection dialog.</p> <p>For example, 292, 346, 366.</p> <p>Click OK button.</p>	<p>Please select the MS spectrum/spectra to import:</p> <p>Minimum Intensity: 14.5 % Pick</p> <p>Spectr... Location [min]</p> <table><tbody><tr><td><input type="checkbox"/></td><td>354</td><td>4.49167</td></tr><tr><td><input type="checkbox"/></td><td>355</td><td>4.50133</td></tr><tr><td><input type="checkbox"/></td><td>356</td><td>4.51083</td></tr><tr><td><input type="checkbox"/></td><td>357</td><td>4.5205</td></tr><tr><td><input type="checkbox"/></td><td>358</td><td>4.53</td></tr><tr><td><input type="checkbox"/></td><td>359</td><td>4.53967</td></tr><tr><td><input type="checkbox"/></td><td>360</td><td>4.54917</td></tr><tr><td><input type="checkbox"/></td><td>361</td><td>4.55883</td></tr><tr><td><input type="checkbox"/></td><td>362</td><td>4.56917</td></tr><tr><td><input type="checkbox"/></td><td>363</td><td>4.579</td></tr><tr><td><input type="checkbox"/></td><td>364</td><td>4.58833</td></tr><tr><td><input type="checkbox"/></td><td>365</td><td>4.59817</td></tr><tr><td><input checked="" type="checkbox"/></td><td>366</td><td>4.60767</td></tr><tr><td><input type="checkbox"/></td><td>367</td><td>4.61733</td></tr><tr><td><input type="checkbox"/></td><td>368</td><td>4.62767</td></tr><tr><td><input type="checkbox"/></td><td>369</td><td>4.63733</td></tr><tr><td><input type="checkbox"/></td><td>370</td><td>4.64683</td></tr><tr><td><input type="checkbox"/></td><td>371</td><td>4.6565</td></tr><tr><td><input type="checkbox"/></td><td>372</td><td>4.666</td></tr><tr><td><input type="checkbox"/></td><td>373</td><td>4.67633</td></tr></tbody></table> <p>Select All Deselect All</p> <p>Time of current scan: 2.37783 min</p> <p>Spectrum import mode</p> <p><input checked="" type="checkbox"/> Import MS spectrum/spectra</p> <p><input type="checkbox"/> Import chromatogram</p> <p>OK Cancel</p> 	<input type="checkbox"/>	354	4.49167	<input type="checkbox"/>	355	4.50133	<input type="checkbox"/>	356	4.51083	<input type="checkbox"/>	357	4.5205	<input type="checkbox"/>	358	4.53	<input type="checkbox"/>	359	4.53967	<input type="checkbox"/>	360	4.54917	<input type="checkbox"/>	361	4.55883	<input type="checkbox"/>	362	4.56917	<input type="checkbox"/>	363	4.579	<input type="checkbox"/>	364	4.58833	<input type="checkbox"/>	365	4.59817	<input checked="" type="checkbox"/>	366	4.60767	<input type="checkbox"/>	367	4.61733	<input type="checkbox"/>	368	4.62767	<input type="checkbox"/>	369	4.63733	<input type="checkbox"/>	370	4.64683	<input type="checkbox"/>	371	4.6565	<input type="checkbox"/>	372	4.666	<input type="checkbox"/>	373	4.67633
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	Action	Result
3	<p>Multiple search tabs are created.</p>	
4	<p>One can either search these MS spectra one by one by clicking the Search button in each tab.</p> <p>Or use Batch Search button and reply Yes when prompted.</p> <div data-bbox="241 1120 625 1177"> Batch Search Search </div>	

Action	Result
5 Analyze the search results in Minelt:	<div><div><div><div>Minelt</div><div><div>Lookup Compound:</div><div>PubChem</div><div>Display Profiles: <no profile></div></div><div><div><div><div><div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div>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Other Tools for Mass Spectrometry

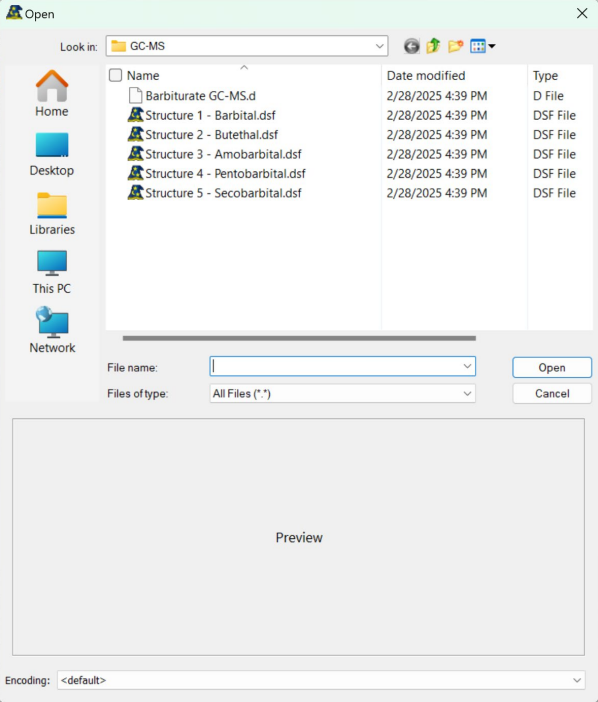
Elemental Composition

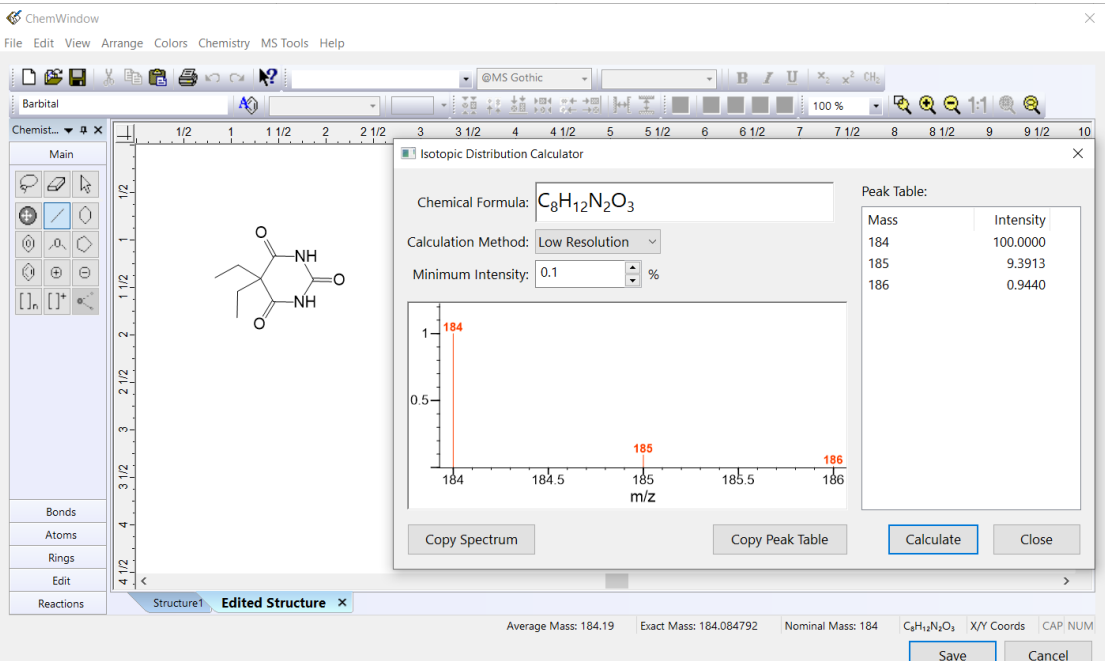
	Action	Result
1	Begin in Minelt . From the Menu , navigate to MS Tools > Calculate Elemental Composition .	<div><div>Elemental Composition Calculator</div><div><div>Target Mass: 388 ± 0.5 u</div><div><div><div>Element:</div><div>Mass:</div><div>Min. Count:</div><div>Max. Count:</div><div>Charge:</div></div><div><div>C</div><div>12</div><div>1</div><div>20</div><div><input type="radio"/> -1 <input checked="" type="radio"/> 0 <input type="radio"/> +1</div></div><div><div>H</div><div>1.0078250322</div><div>1</div><div>36</div><div></div></div><div><div>O</div><div>15.994914619</div><div>1</div><div>2</div><div></div></div><div><div>I</div><div>126.90447</div><div>0</div><div>1</div><div></div></div><div><div></div><div></div><div></div><div></div><div></div></div><div><div></div><div></div><div></div><div></div><div></div></div></div><div><div>Reset</div><div>Calculate</div><div>Close</div></div></div></div> <div>You can fill in this dialog with target mass and elemental information.</div>

	Action	Result																																																								
2	Click Calculate .	<div><div>Elemental Composition Results</div><div>Target Mass: 388 ± 0.5 u Charge: 0 Result Count: 6</div><table><tr><th>C</th><th>H</th><th>O</th><th>I</th><th>m</th><th>Δm [u]</th><th>Δm [ppm]</th><th>RDB</th></tr><tr><td>18</td><td>13</td><td>2</td><td>1</td><td>387.9960</td><td>-0.0040</td><td>-10.2457</td><td>12</td></tr><tr><td>19</td><td>17</td><td>1</td><td>1</td><td>388.0324</td><td>0.0324</td><td>83.5314</td><td>11</td></tr><tr><td>20</td><td>5</td><td>1</td><td>1</td><td>387.9385</td><td>-0.0615</td><td>-158.4799</td><td>18</td></tr><tr><td>17</td><td>25</td><td>2</td><td>1</td><td>388.0899</td><td>0.0899</td><td>231.7656</td><td>5</td></tr><tr><td>19</td><td>1</td><td>2</td><td>1</td><td>387.9021</td><td>-0.0979</td><td>-252.2570</td><td>19</td></tr><tr><td>18</td><td>29</td><td>1</td><td>1</td><td>388.1263</td><td>0.1263</td><td>325.5427</td><td>4</td></tr></table><div><input type="checkbox"/> Show only integral RDB Results Copy To Clipboard Close</div></div>	C	H	O	I	m	Δm [u]	Δm [ppm]	RDB	18	13	2	1	387.9960	-0.0040	-10.2457	12	19	17	1	1	388.0324	0.0324	83.5314	11	20	5	1	1	387.9385	-0.0615	-158.4799	18	17	25	2	1	388.0899	0.0899	231.7656	5	19	1	2	1	387.9021	-0.0979	-252.2570	19	18	29	1	1	388.1263	0.1263	325.5427	4
C	H	O	I	m	Δm [u]	Δm [ppm]	RDB																																																			
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17	25	2	1	388.0899	0.0899	231.7656	5																																																			
19	1	2	1	387.9021	-0.0979	-252.2570	19																																																			
18	29	1	1	388.1263	0.1263	325.5427	4																																																			

KnowItAll provides combinations of these elements.

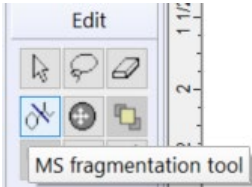
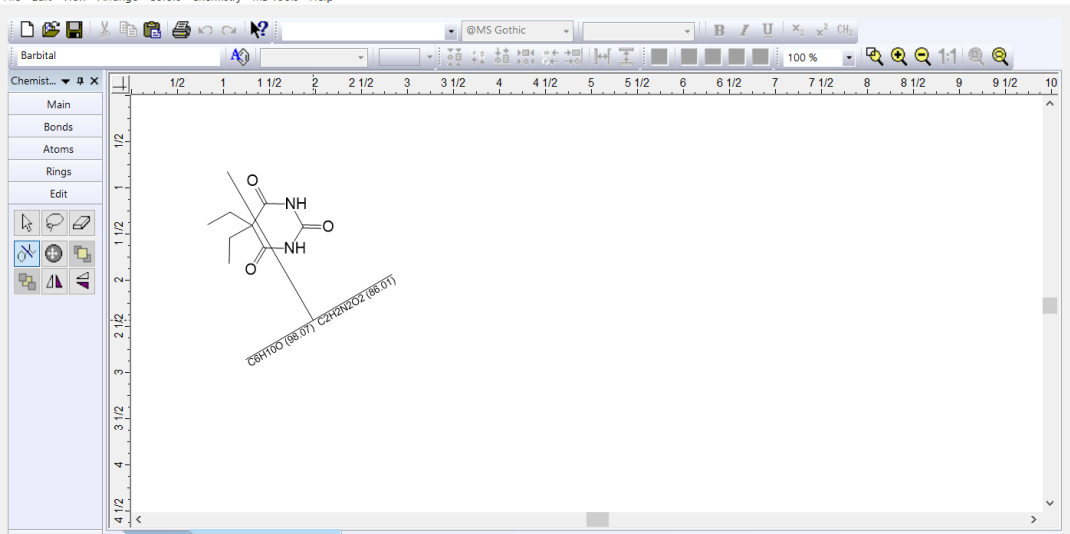
Isotopic Distribution

	Action	Result
1	<p>Go to ChemWindow.</p> <p>Click File > Open.</p> <p>Select a structure from the Samples > GC-MS folder.</p>	

	Action	Result								
2	<p>Navigate to MS Tools > Calculate Isotopic Distribution.</p> <p>Click Calculate.</p>	 <p>ChemWindow</p> <p>File Edit View Arrange Colors Chemistry MS Tools Help</p> <p>Barbitol</p> <p>Chemist... ▾</p> <p>Main</p> <p>Bonds</p> <p>Atoms</p> <p>Rings</p> <p>Edit</p> <p>Reactions</p> <p>Structure1 Edited Structure</p> <p>Average Mass: 184.19 Exact Mass: 184.084792 Nominal Mass: 184 C₈H₁₂N₂O₃ X/Y Coords CAP NUM</p> <p>Isotopic Distribution Calculator</p> <p>Chemical Formula: C₈H₁₂N₂O₃</p> <p>Calculation Method: Low Resolution</p> <p>Minimum Intensity: 0.1 %</p> <p>Copy Spectrum</p> <p>Copy Peak Table</p> <p>Calculate</p> <p>Close</p> <p>Peak Table:</p> <table border="1"><thead><tr><th>Mass</th><th>Intensity</th></tr></thead><tbody><tr><td>184</td><td>100.0000</td></tr><tr><td>185</td><td>9.3913</td></tr><tr><td>186</td><td>0.9440</td></tr></tbody></table>	Mass	Intensity	184	100.0000	185	9.3913	186	0.9440
Mass	Intensity									
184	100.0000									
185	9.3913									
186	0.9440									

Molecular Fragmentation

In ChemWindow, you can use the MS fragmentation tools to view possible fragments and corresponding masses.

	Action	Result
1	<p>Begin in ChemWindow. In the Edit toolbar on the left, click on the MS fragmentation tool.</p>  <p>Point to a position, then drag a line—this is the fragmentation line.</p>	 <p>The screenshot shows the ChemWindow interface with the chemical structure of Barbituric acid (C₂H₂N₂O₂, 86.07) displayed. A fragmentation line is drawn across the structure, indicating a potential cleavage point. The x-axis represents mass-to-charge ratio (m/z) from 1 to 10, and the y-axis represents relative intensity from 1 to 4 1/2. The structure is labeled 'Barbital' and 'C₂H₂N₂O₂ (86.07)'.</p>

Solid Triangle Marks Nominal Mass

- In the spectrum display, KnowItAll marks the nominal mass of the structure that corresponds to the spectrum. This mass is shown as a black triangle.
- When importing a spectrum from a data file, a number of import formats define fields for molecular m/z (also called precursor m/z or base peak m/z in some cases) and the charge of the molecular ion. To convert from molecular m/z to exact mass, the following formulae are used:
 - For positive charges:
 - $M_{\text{exact}} = (Mz - M(\text{H}) + M(\text{e})) * \text{charge}$, where $M(\text{H})$ is the mass of a hydrogen atom, and $M(\text{e})$ is the mass of an electron.
 - For negative charges:
 - $M_{\text{exact}} = (Mz - M(\text{e})) * (-\text{charge})$.
 - If no charge is defined, a default charge of +1 is assumed.
- If a data file does not have the molecular m/z field defined, the exact mass is calculated from the formula field, if available.