

# **KnowItAll Software Training**

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## GC-MS Analysis Using KnowItAll MS Expert And SearchIt

# GC-MS Analysis By Automatic Deconvolution

## How to Perform GC-MS Analysis by Automatic Deconvolution

### Purpose

These exercises demonstrate how to use KnowItAll MS Expert to automatically deconvolute/analyze GC-MS.

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### Objectives

These exercises will teach you:

- How to use KnowItAll MS Expert to auto-deconvolute GC-MS data into chemical component MS spectra which are automatically searched against millions of references.
  - How to generate reports.
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### Background

GC-MS data are information rich. Analysis can be time consuming, especially when examining complex analytes. We present a computer system that combines fast, flexible automated deconvolution, automatic database search to identify knowns and unknowns. Novel compounds can be identified, and structural characteristics deduced from applying the MS Adaptive search that uses fragmentation and structural data to propose likely structural details of the unknown.

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

- C:\Users\Public\Documents\Wiley\KnowItAll\Samples\MS Expert folder files

#### *KnowItAll Applications Used*

- KnowItAll MS Expert

## GC-MS Deconvolution Algorithms

Our system follows individual  $m/z$  values across multiple spectra and extracts a pure spectrum from the data for each individual component while trying to separate components with overlapping  $m/z$  value peaks. If accurate  $m/z$  value data are available and the user selects this data to use it instead of unit  $m/z$  values, the chosen instrument accuracy (automatic, ppm, or fixed value) is used to determine the correct accurate  $m/z$  values throughout the entire GC-MS analysis. The  $m/z$  values in the raw data are converted into correct accurate values based on the closest value found by taking the instrument resolution into account. The corrected  $m/z$  values form the basis of the following deconvolution.

During the deconvolution step, individual  $m/z$  values are traced across multiple raw spectra, and a component spectrum is extracted while trying to separate components with overlapping  $m/z$  value peaks. The details of the algorithm are summarized to a large extent by the papers listed below<sup>1-4</sup>.

Additional steps are added to automatically detect components with low intensity Reconstructed Total Ion Current (RTIC) chromatographic peaks as long as they can well be separated from neighboring components.

Although the algorithm is very complex, the details of the algorithm are summarized to a large extent by the following papers:

1. S. E. Stein. An Integrated Method for Spectrum Extraction and Compound Identification from Gas Chromatography/Mass Spectrometry Data. *J Am Soc Mass Spectrom* 1999, **10**, 770–781.
2. R. G. Dromey, M. J. Stefik, T. C. Rindfleisch, A. M. Duffield. Extraction of Mass Spectra Free of Background and Neighboring Component Contributions from Gas Chromatography Mass Spectrometry Data. *Analytical Chemistry*, 1976, **48(9)**, 1368-1375.
3. J. E. Biller, K. Biemann. Reconstructed Mass Spectra, A Novel Approach For The Utilization Of Gas Chromatography-Mass Spectrometer Data. *Analytical Letters* 1974, **7**, 515-28.
4. B. N. Colby. Spectral Deconvolution for Overlapping GC/MS Components. *J Am Soc Mass Spectrom* 1992, **3**, 558-562.

## MS Spectral Comparison Algorithms

### Research article

Journal of  
MASS  
SPECTROMETRY

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## Evaluation of mass spectral library search algorithms implemented in commercial software

Andrey Samokhin,<sup>a\*</sup> Ksenia Sotnezova,<sup>a</sup> Vitaly Lashin<sup>b</sup> and Igor Revelsky<sup>a</sup>

MS SEARCH

Composite algorithm

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

Spectrum search type – identity (normal)

Presearch – default

Included Libs – MainLib

Apply limits – unchecked

Use constraints – unchecked

Dot-product algorithm<sup>2</sup>

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

Spectrum search type – similarity (simple)

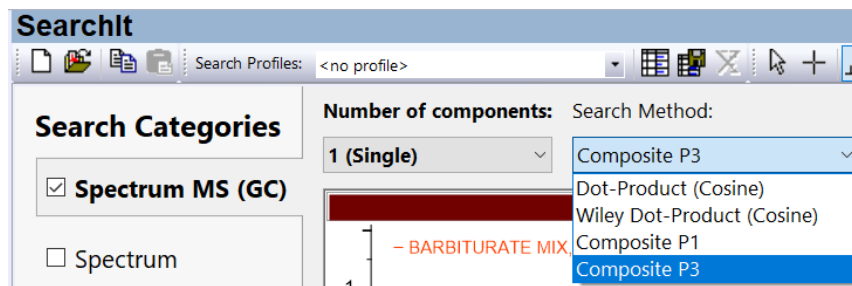
Presearch – default

Included Libs – MainLib

Apply limits – unchecked

Use constraints – unchecked

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



KnowItAll has 4 different algorithms:

Where

- Dot-Product (Cosine) – second equation in above image
- Wiley Dot-Product (Cosine) (old KnowItAll algorithm) - the old 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 image
- Composite P3 – first equation in above image  
P1 and P3 are different by the power applied to the weighted intensity of peak.

## Example 1: GC-MS of Unit m/z Values

### *GUI explanation*

The image below shows the deconvoluted GC-MS data of unit m/z values, and the search results for each component within the massive Wiley GC-MS database.

A – GC panel, showing the deconvoluted component peaks. One can use the checkboxes on right side of the GC panel to turn on/off chromatogram(s) display.

When the box corresponding to the selected component peak of the chromatogram is selected, the box has a darker color;

B – Component Profile panel, highlights selected ions or components of the chromatogram(s);

C – Component Models panel, identifies the reference ion(s) used to model a component;

D – Database Match panel, shows the extracted spectrum (top) vs reference spectrum (bottom);

E – Components panel, where the Score is the combined spectrum search and reverse search Hit Quality Index (HQI) and, each component's GC area under curve (AUC) value;

G – Panel where parameters can be adjusted in algorithm.

**MS Expert**

Analysis Method: Deconvolutic Analysis Profiles: <no profile>

**GC**

**Component Profile**

**Raw Spectrum**

**Database Match**

**Components**

RT [min]	#	Match	Score	HQI	R.H...
3.5817	1	Octanol	98.71	98.70	98.84
3.9367	1	Phenol, 2,6-dimethyl-	99.10	99.09	99.23
4.2085	1	Undecane	99.08	99.08	99.08
4.6773	1	Aniline <2,6-dimethyl->	97.64	97.62	97.87
5.0278	1	Hexanoic acid, 2-ethyl-	93.19	93.19	93.19
5.2090	1	Hexanoic acid, 2-ethyl-	92.50	92.47	92.74
6.7302	1	DECAANOIC ACID, METHYL ESTER	98.38	98.38	98.38
	2	Methylcaprate	96.85	96.85	96.85
	3	Methylcaprate	93.59	93.31	96.15
	4	Methylcaprate	92.40	92.35	92.83
	5	Decanoic acid, methyl ester	90.75	89.77	99.57
	6	Methyl 8-methyl-nonanoate	90.68	90.68	90.68
	7	Decanoic acid, 2-methyl-	88.61	88.20	92.27
	8	Undecanoic acid, 2-methyl-	86.87	86.15	93.40
	9	Methyl nonylate	86.37	85.78	91.72
	10	Hexanoic acid methyl ester	85.21	83.84	97.52
7.6824	1	Cyclohexanamine, N-cyclohexyl-	98.20	98.20	98.20
7.7894	1	Undecanoic acid, methyl ester	98.38	98.32	98.93
8.9421	1	Dodecanoic acid, methyl ester	98.37	98.37	98.37

**Component Models**

Reference Ion(s): 74

Parameters:

Contributing Ions: 74  
 Energy: 1.4159  
 Area: 209385504.8  
 Base Peak Vertex: 8562039.9

Resolution %: 50  Automatic

Sensitivity %: 50

Peak Shape Requirements %: 50

**MASS CHROMATOGRAM m/z RANGES**

## Features of MS Expert

The Component Table (E) contains useful information:

- It shows each Components' estimated area.
- One can add **Notes** to a match. This can be done by clicking on the space below **Notes**, in the row of the matched component of interest.
- Right mouse-click brings up actions that the user can take. Among many, **Edit Component Columns** allows one to rearrange the display.

Components										
RT [min]	#	Match	Score	HQI	R.H...	Notes	Area %	Area	CAS Registry Number	
15.9260	1	Bicyclo[4.3.1]decan-8-one, 1-bromo-	92.34	91.88	96.52	Interesting	1.40	1675158	56-23-5	
16.5463	1	Ethane, 2-bromo-1,1-dichloro-	80.98	79.86	91.07		1.41	1685546	75-27-4	
17.4897	1		67.37	65.48	84.40		0.41	491611	563-80-4	
17.9705	1	Propanoic acid, 2,2-dichloro-	31.89	31.28	37.37		2.14	2558302	78-87-5	
18.2397	1	1,3-Propanedithiol	35.82	34.32	49.30		1.69	2020873	10061-01-5	
18.7663	1	3-(Chloromethyl)thiophene	30.20	28.74	43.33		1.95	2323999	79-01-6	
19.2624	1	(3E)-1,3,7-Octatrien-5-yne	37.90	35.83	56.47		2.92	3490076	329-71-5	
19.5835	1	1,4-Bis(ethenyl)benzene	51.34	50.52	58.70		2.91	3475740	124-48-1	
19.6127	1	4-Chloroaniline						3621261	124-48-1	
19.6533	1	(Trimethylsilyl)acetylene						2365877	79-00-5	
20.7145	1	Propanoic acid, 2,2-dichloro-						2490372	110-75-8	
21.0187	1	Myristic acid, methyl ester						252045	623-42-7	
21.9853	1	3-Pentenoic acid, 4-methyl-						2344254	540-36-3	
22.5330		No match found						1333680		
22.8777	1	9H-Fluoren-9-one						1703804	108-10-1	
23.7254	1	2-Octanol, acetate						127023	2051-50-5	
24.5232	1	Acetone-oxime						1652274		
24.8421		No match found						3787639		
24.8642		No match found						3078006		
24.9644	1	Dichloromethyl ethyl sulfone						1572112		

Component Models	
	Hide



A hidden feature is the **Lookup** of a displayed property by using the **Control + F** action. For example, one can use **Lookup** to find a match to CAS Numbers such as CAS Number 329-7105.

Components									
RT [min]	#	Match	Score	HQI	R.H...	Notes	Area %	Area	CAS Registry Number
15.9260	1	Bicyclo[4.3.1]decan-8-one, 1-bromo-	92.34	91.88	96.52	Interesting	1.40	1675158	56-23-5
16.5463	1	Ethane, 2-bromo-1,1-dichloro-	80.98	79.86	91.07		1.41	1685546	75-27-4
17.4897	1		67.37	65.48	84.40		0.41	491611	563-80-4
17.9705	1	Propanoic acid, 2,2-dichloro-	31.89	31.28	37.37		2.14	2558302	78-87-5
18.2397	1	1,3-Propanedithiol	35.82	34.32	49.30		1.69	2020873	10061-01-5
18.7663	1	3-(Chloromethyl)thiophene	30.20	28.74	43.33		1.95	2323999	79-01-6
19.2624	1	(3E)-1,3,7-Octatrien-5-yne	37.90	35.83	56.47		2.92	3490076	329-71-5
19.5835	1	1,4-Bis(ethenyl)benzene	51.34	50.52	58.70		2.91	3475740	124-48-1
19.6127	1	4-Chloroaniline	35.77	34.29	49.11		3.03	3621261	124-48-1
19.6533	1	(Trimethylsilyl)acetylene	40.12	37.81	60.96		1.98	2365877	79-00-5
20.7145	1	Propanoic acid, 2,2-dichloro-	43.45	43.17	46.02		2.09	2490372	110-75-8
21.0187	1						0.21	252045	623-42-7
21.9853	1						1.96	2344254	540-36-3
22.5330							1.12	1333680	
22.8777	1						1.43	1703804	108-10-1
23.7254	1						0.11	127023	2051-50-5
24.5232	1						1.38	1652274	
24.8421							3.17	3787639	
24.8642							2.58	3078006	
24.9644	1	Dichloromethyl ethyl sulfone	70.57	67.65	94.71		1.32	1572112	

Find

Find what: 329-71-5

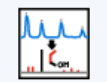
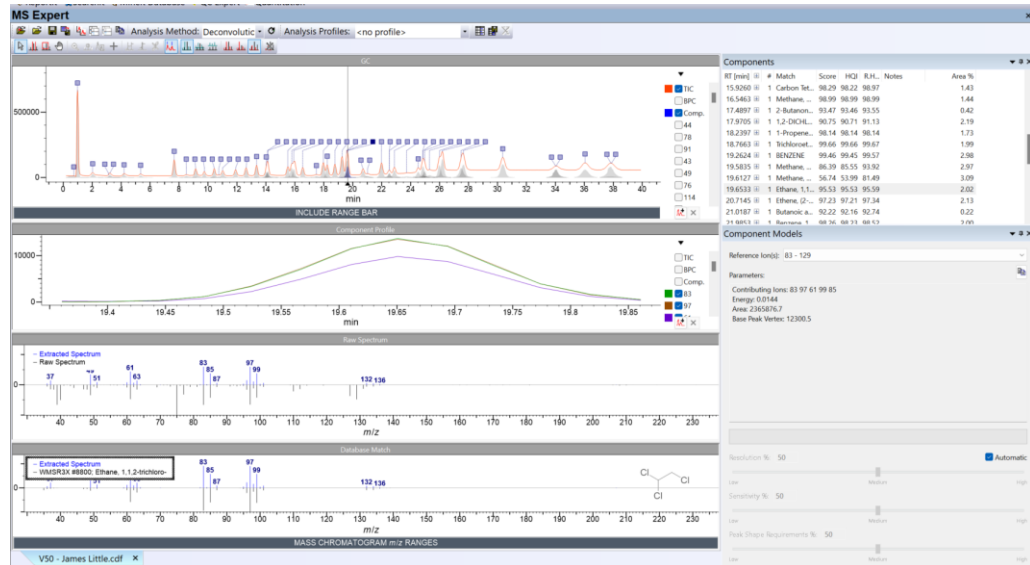
Direction:  Up  Down

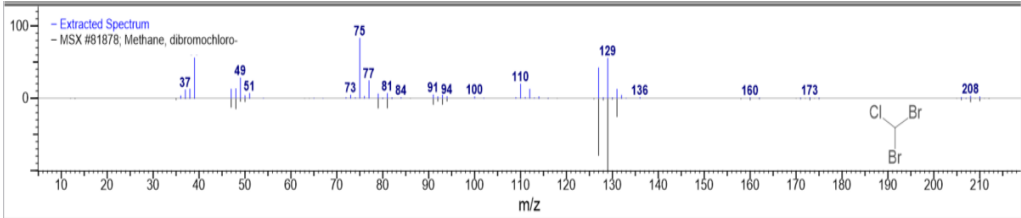
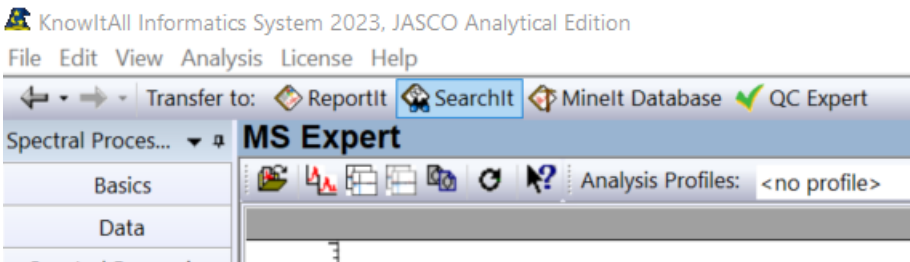
Match case

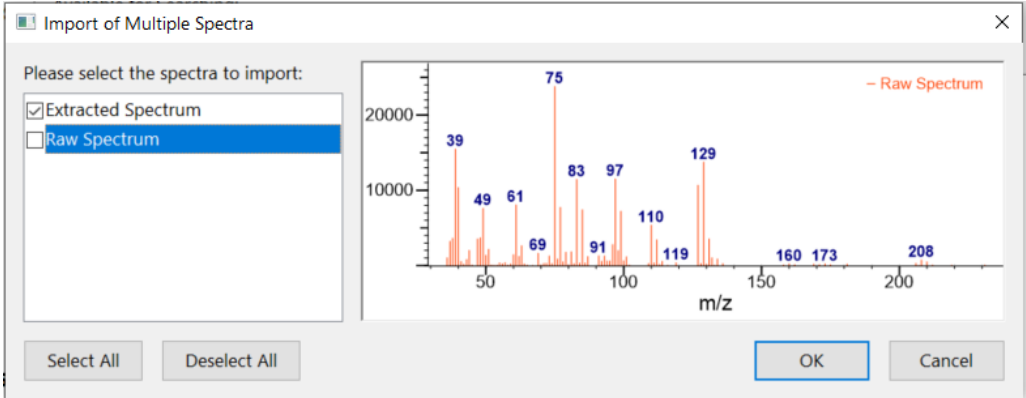
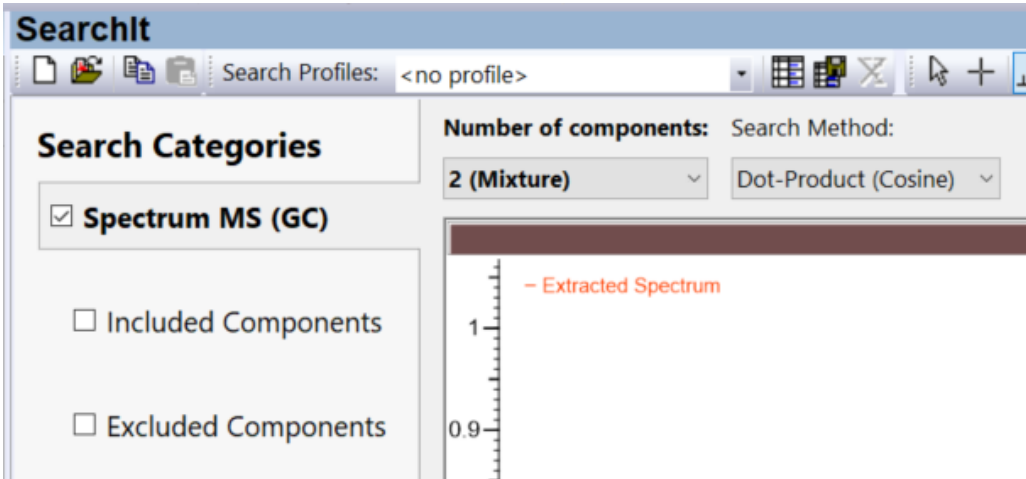
Find Next

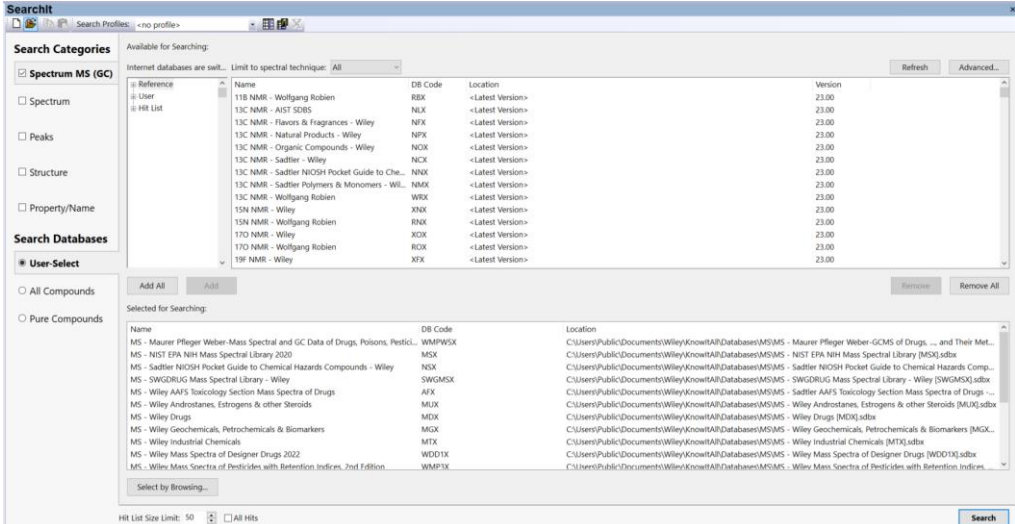
Cancel

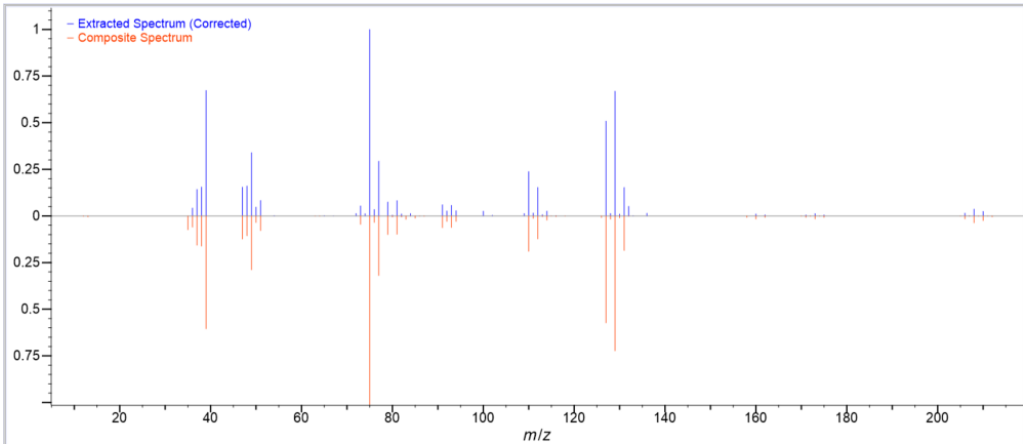
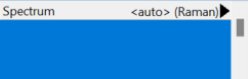
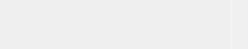

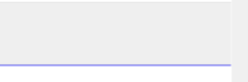
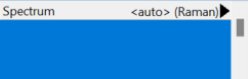
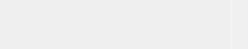

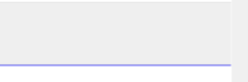
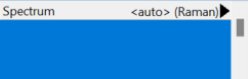
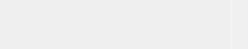

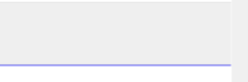
Now, we will go through a complete process.

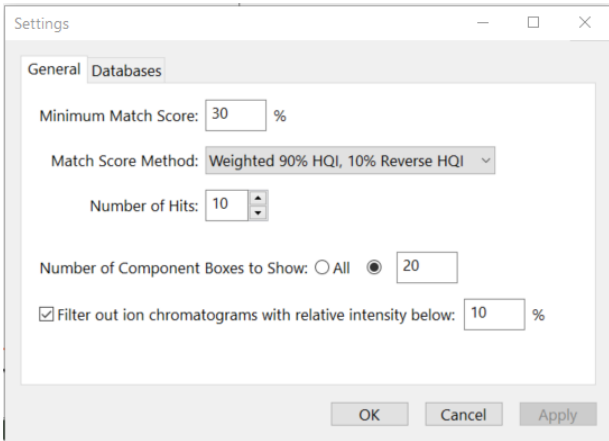
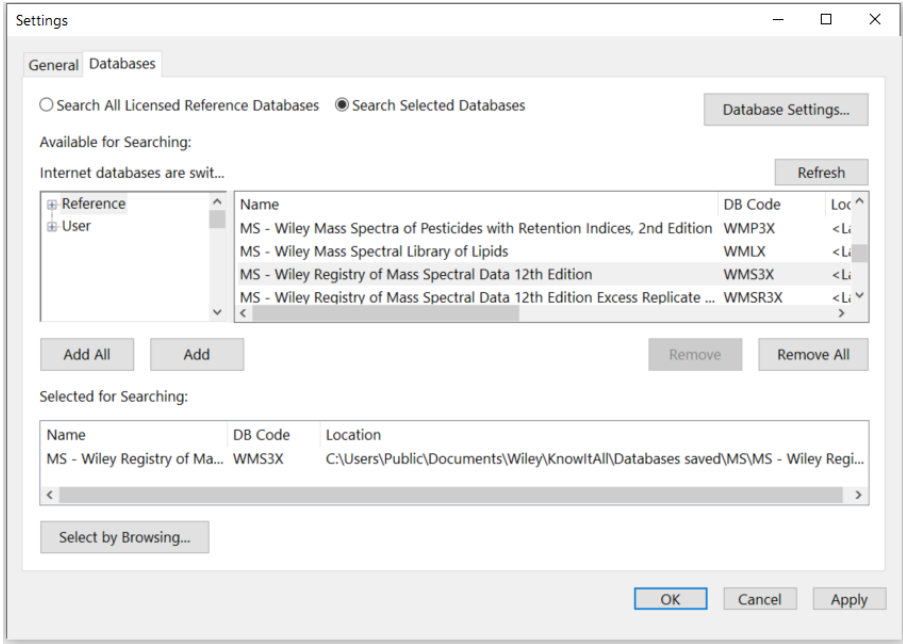
	Action	Result																																																																																																		
1	<p>Go to the <b>MS Expert</b> application under <b>Spectral Process</b> toolbar</p>  <p>Click <b>Open Raw GC-MS Data File</b> button</p> <p>Navigate to folder  <b>C:\Users\Public\Documents\Wiley\KnowItAll\Samples\MS Expert\V50 - James Little.cdf</b> file</p> <p>Go to Component at 19.6533 min</p>	<p><b>MS Expert</b> automatically performs</p> <ol style="list-style-type: none"> <li>GC deconvolution to component extracted MS</li> <li>Search extracted MS again reference databases</li> <li>Report top hits</li> </ol>  <p>The screenshot displays the MS Expert interface with the following components table:</p> <table border="1"> <thead> <tr> <th>RT [min]</th> <th># Match</th> <th>Score</th> <th>HQI</th> <th>R.H.</th> <th>Notes</th> <th>Area %</th> </tr> </thead> <tbody> <tr><td>15.9260</td><td>1</td><td>Carbon Tet.</td><td>98.29</td><td>98.22</td><td>98.97</td><td>1.43</td></tr> <tr><td>16.5483</td><td>1</td><td>Methane...</td><td>98.99</td><td>98.99</td><td>98.99</td><td>1.44</td></tr> <tr><td>17.4897</td><td>1</td><td>2-Butanol...</td><td>93.47</td><td>93.46</td><td>93.55</td><td>0.42</td></tr> <tr><td>17.9705</td><td>1</td><td>1,2-DICHL...</td><td>90.75</td><td>90.71</td><td>91.13</td><td>2.19</td></tr> <tr><td>18.2397</td><td>1</td><td>1-Propene...</td><td>98.14</td><td>98.14</td><td>98.14</td><td>1.73</td></tr> <tr><td>18.7663</td><td>1</td><td>Nitrobenz...</td><td>99.66</td><td>99.66</td><td>99.67</td><td>1.99</td></tr> <tr><td>19.2624</td><td>1</td><td>BENZENE</td><td>99.46</td><td>99.45</td><td>99.57</td><td>2.98</td></tr> <tr><td>19.5835</td><td>1</td><td>Methane...</td><td>86.39</td><td>85.55</td><td>93.92</td><td>2.97</td></tr> <tr><td>19.6127</td><td>1</td><td>Methane...</td><td>56.74</td><td>53.99</td><td>81.69</td><td>3.09</td></tr> <tr><td>19.6533</td><td>1</td><td>Ethane, 1,1,2-trichloro...</td><td>95.33</td><td>95.53</td><td>95.99</td><td>2.62</td></tr> <tr><td>20.7145</td><td>1</td><td>Ethane (2-...</td><td>97.23</td><td>97.21</td><td>97.34</td><td>2.13</td></tr> <tr><td>21.0187</td><td>1</td><td>Butane a...</td><td>92.22</td><td>92.16</td><td>92.74</td><td>0.22</td></tr> <tr><td>21.9913</td><td>1</td><td>Nonane 1...</td><td>89.76</td><td>89.73</td><td>89.73</td><td>7.92</td></tr> </tbody> </table> <p>The database match for Ethane, 1,1,2-trichloro- is shown with a chemical structure: <chem>CC1(Cl)C(Cl)C1</chem>.</p>	RT [min]	# Match	Score	HQI	R.H.	Notes	Area %	15.9260	1	Carbon Tet.	98.29	98.22	98.97	1.43	16.5483	1	Methane...	98.99	98.99	98.99	1.44	17.4897	1	2-Butanol...	93.47	93.46	93.55	0.42	17.9705	1	1,2-DICHL...	90.75	90.71	91.13	2.19	18.2397	1	1-Propene...	98.14	98.14	98.14	1.73	18.7663	1	Nitrobenz...	99.66	99.66	99.67	1.99	19.2624	1	BENZENE	99.46	99.45	99.57	2.98	19.5835	1	Methane...	86.39	85.55	93.92	2.97	19.6127	1	Methane...	56.74	53.99	81.69	3.09	19.6533	1	Ethane, 1,1,2-trichloro...	95.33	95.53	95.99	2.62	20.7145	1	Ethane (2-...	97.23	97.21	97.34	2.13	21.0187	1	Butane a...	92.22	92.16	92.74	0.22	21.9913	1	Nonane 1...	89.76	89.73	89.73	7.92
RT [min]	# Match	Score	HQI	R.H.	Notes	Area %																																																																																														
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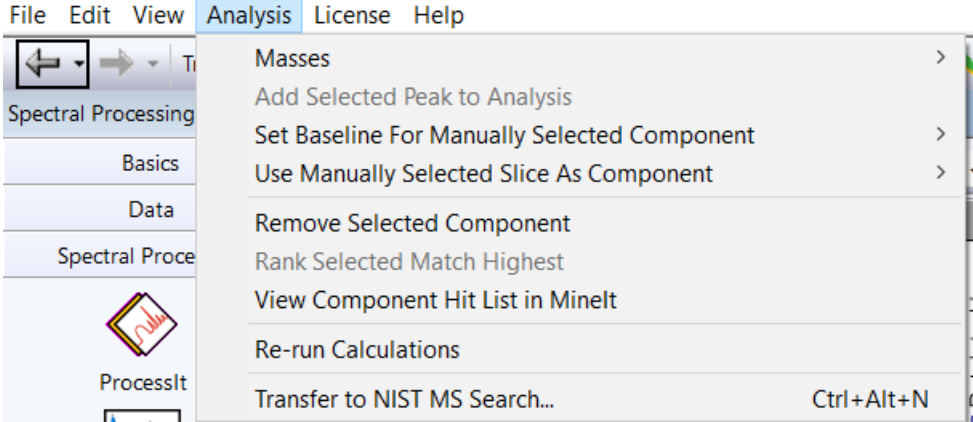
	Action	Result
2	<p>Examine the hit lists for each deconvoluted components in the <b>Components</b> table</p> <p>Go to <b>RT (MIN)</b> 19.6127, notice the <b>Score</b> for this hit is very low, 56.74.</p>	 <p>V50 - James Little.cdf x</p> <p>From the comparison of <b>Extracted Spectrum</b> (top) and reference spectrum of methane, dibromochloro- in the bottom pane, we can see that the <b>Extract Spectrum</b> contains methane, dibromochloro- as well as other components.</p>
3	Transfer the <b>Extracted Spectrum</b> to <b>SearchIt</b>	 <p>KnowItAll Informatics System 2023, JASCO Analytical Edition</p> <p>File Edit View Analysis License Help</p> <p>Transfer to: ReportIt SearchIt Minelt Database QC Expert</p> <p>Spectral Proces... MS Expert</p> <p>Basics</p> <p>Data</p> <p>Analysis Profiles: &lt;no profile&gt;</p>

	Action	Result
4	Only check the <b>Extracted Spectrum</b> at prompt  Click <b>OK</b>	
5	In <b>SearchIt</b> , set to search for <b>2 (Mixture)</b>	

	Action	Result																																																																																																															
6	Click the <b>User-Select</b> tab to add all licensed MS databases  <b>Search</b>	 <p>The screenshot shows the SearchIt application window. On the left, the 'Search Databases' section has 'User-Select' selected. The main area is divided into 'Available for Searching' and 'Selected for Searching'.</p> <p><b>Available for Searching:</b></p> <table border="1"> <thead> <tr> <th>Reference</th> <th>Name</th> <th>DB Code</th> <th>Location</th> <th>Version</th> </tr> </thead> <tbody> <tr><td>   User</td><td>118 NMR - Wolfgang Robien</td><td>REX</td><td>&lt;Latest Version&gt;</td><td>23.00</td></tr> <tr><td>   HR List</td><td>13C NMR - NIST SDBS</td><td>NEX</td><td>&lt;Latest Version&gt;</td><td>23.00</td></tr> <tr><td></td><td>13C NMR - Flavors &amp; Fragrances - Wiley</td><td>NFX</td><td>&lt;Latest Version&gt;</td><td>23.00</td></tr> <tr><td></td><td>13C NMR - Natural Products - Wiley</td><td>NPX</td><td>&lt;Latest Version&gt;</td><td>23.00</td></tr> <tr><td></td><td>13C NMR - Organic Compounds - Wiley</td><td>NOX</td><td>&lt;Latest Version&gt;</td><td>23.00</td></tr> <tr><td></td><td>13C NMR - Sadler - Wiley</td><td>NEC</td><td>&lt;Latest Version&gt;</td><td>23.00</td></tr> <tr><td></td><td>13C NMR - Sadler NIOSH Pocket Guide to Chem...</td><td>NOX</td><td>&lt;Latest Version&gt;</td><td>23.00</td></tr> <tr><td></td><td>13C NMR - Sadler Polymers &amp; Monomers - Wil...</td><td>NMX</td><td>&lt;Latest Version&gt;</td><td>23.00</td></tr> <tr><td></td><td>13C NMR - Wolfgang Robien</td><td>WEX</td><td>&lt;Latest Version&gt;</td><td>23.00</td></tr> <tr><td></td><td>15N NMR - Wiley</td><td>XNX</td><td>&lt;Latest Version&gt;</td><td>23.00</td></tr> <tr><td></td><td>15N NMR - Wolfgang Robien</td><td>RNX</td><td>&lt;Latest Version&gt;</td><td>23.00</td></tr> <tr><td></td><td>17O NMR - Wiley</td><td>XOX</td><td>&lt;Latest Version&gt;</td><td>23.00</td></tr> <tr><td></td><td>17O NMR - Wolfgang Robien</td><td>BOX</td><td>&lt;Latest Version&gt;</td><td>23.00</td></tr> <tr><td></td><td>19F NMR - Wiley</td><td>XFX</td><td>&lt;Latest Version&gt;</td><td>23.00</td></tr> </tbody> </table> <p><b>Selected for Searching:</b></p> <table border="1"> <thead> <tr> <th>Name</th> <th>DB Code</th> <th>Location</th> </tr> </thead> <tbody> <tr><td>MS - Maurer Pfleger Weber-Mass Spectral and GC Data of Drugs, Poisons, Pestic...</td><td>WMPWSX</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\MSMS - Maurer Pfleger Weber-GCMS of Drugs, ... and Their Met...</td></tr> <tr><td>MS - NIST EPA NIH Mass Spectral Library 2020</td><td>MSX</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\MSMS - NIST EPA NIH Mass Spectral Library [MSQ].sdbx</td></tr> <tr><td>MS - Sadler NIOSH Pocket Guide to Chemical Hazards Compounds - Wiley</td><td>NEX</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\MSMS - Sadler NIOSH Pocket Guide to Chemical Hazards Comp...</td></tr> <tr><td>MS - SWGDRUG Mass Spectral Library - Wiley</td><td>SWGMSX</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\MSMS - SWGDRUG Mass Spectral Library - Wiley [SWGMSX].sdbx</td></tr> <tr><td>MS - Wiley AAFS Toxicology Section Mass Spectra of Drugs</td><td>AFX</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\MSMS - Sadler AAFS Toxicology Section Mass Spectra of Drugs ...</td></tr> <tr><td>MS - Wiley Androstanes, Estrogens &amp; other Steroids</td><td>MUX</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\MSMS - Wiley Androstanes, Estrogens &amp; other Steroids [MUX].sdbx</td></tr> <tr><td>MS - Wiley Drugs</td><td>MDX</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\MSMS - Wiley Drugs [MDX].sdbx</td></tr> <tr><td>MS - Wiley Geochemicals, Petrochemicals &amp; Biomarkers</td><td>MGX</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\MSMS - Wiley Geochemicals, Petrochemicals &amp; Biomarkers [MGX...</td></tr> <tr><td>MS - Wiley Industrial Chemicals</td><td>MTX</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\MSMS - Wiley Industrial Chemicals [MTX].sdbx</td></tr> <tr><td>MS - Wiley Mass Spectra of Designer Drugs 2022</td><td>WDD1X</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\MSMS - Wiley Mass Spectra of Designer Drugs [WDD1X].sdbx</td></tr> <tr><td>MS - Wiley Mass Spectra of Pesticides with Retention Indices, 2nd Edition</td><td>WMP1X</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\MSMS - Wiley Mass Spectra of Pesticides with Retention Indices...</td></tr> </tbody> </table>	Reference	Name	DB Code	Location	Version	User	118 NMR - Wolfgang Robien	REX	<Latest Version>	23.00	HR List	13C NMR - NIST SDBS	NEX	<Latest Version>	23.00		13C NMR - Flavors & Fragrances - Wiley	NFX	<Latest Version>	23.00		13C NMR - Natural Products - Wiley	NPX	<Latest Version>	23.00		13C NMR - Organic Compounds - Wiley	NOX	<Latest Version>	23.00		13C NMR - Sadler - Wiley	NEC	<Latest Version>	23.00		13C NMR - Sadler NIOSH Pocket Guide to Chem...	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Action	Result																																																
7	<p>Mixture analysis returns a very good <b>Composite Spectrum</b> match top of the hit list:</p>  <p>Raman MS (GC) NMR</p> <table border="1" data-bbox="905 828 1921 1144"> <thead> <tr> <th colspan="8">Table Plot Related Compounds View</th> </tr> <tr> <th>HQI</th> <th>Ratio</th> <th>Exclude</th> <th>Cor. DB</th> <th>ID</th> <th>Name</th> <th>Chemical Structure</th> <th>Spectrum</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>94.09</td> <td>N.A.</td> <td></td> <td></td> <td>Composite Spectrum</td> <td><chem>ClC=CClC(Br)Br</chem></td> <td></td> </tr> <tr> <td></td> <td>0.59</td> <td><input type="radio"/></td> <td>WMSR3X</td> <td>4571</td> <td>1-Propene, 1,3-dichloro-, (Z)-</td> <td><chem>ClC=CCl</chem></td> <td></td> </tr> <tr> <td></td> <td>0.41</td> <td><input type="radio"/></td> <td>MSRX</td> <td>27959</td> <td>Methane, dibromochloro-</td> <td><chem>ClC(Br)Br</chem></td> <td></td> </tr> <tr> <td></td> <td>N.A.</td> <td><input type="radio"/></td> <td></td> <td></td> <td>Residual Spectrum</td> <td></td> <td></td> </tr> </tbody> </table> <p>The <b>Composite Spectrum</b> in the first row is a mix of two components: 1-propene, 1,3-dichloro- (new component) and methane, dibromochloro-. The <b>Residual Spectrum</b> in the last row, the difference between <b>Extracted Spectrum</b> and <b>Composite Spectrum</b> is negligible, indicating no more components remain undetected.</p>	Table Plot Related Compounds View								HQI	Ratio	Exclude	Cor. DB	ID	Name	Chemical Structure	Spectrum	1	94.09	N.A.			Composite Spectrum	<chem>ClC=CClC(Br)Br</chem>			0.59	<input type="radio"/>	WMSR3X	4571	1-Propene, 1,3-dichloro-, (Z)-	<chem>ClC=CCl</chem>			0.41	<input type="radio"/>	MSRX	27959	Methane, dibromochloro-	<chem>ClC(Br)Br</chem>			N.A.	<input type="radio"/>			Residual Spectrum		
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	Action	Result
8	<p>Go back to <b>MS Expert</b>,                      One can go to <b>File &gt; Settings</b> menu to adjust component hit list parameters</p>	<p>Hits evaluation parameters:</p>  <p>Reference database choices</p> 

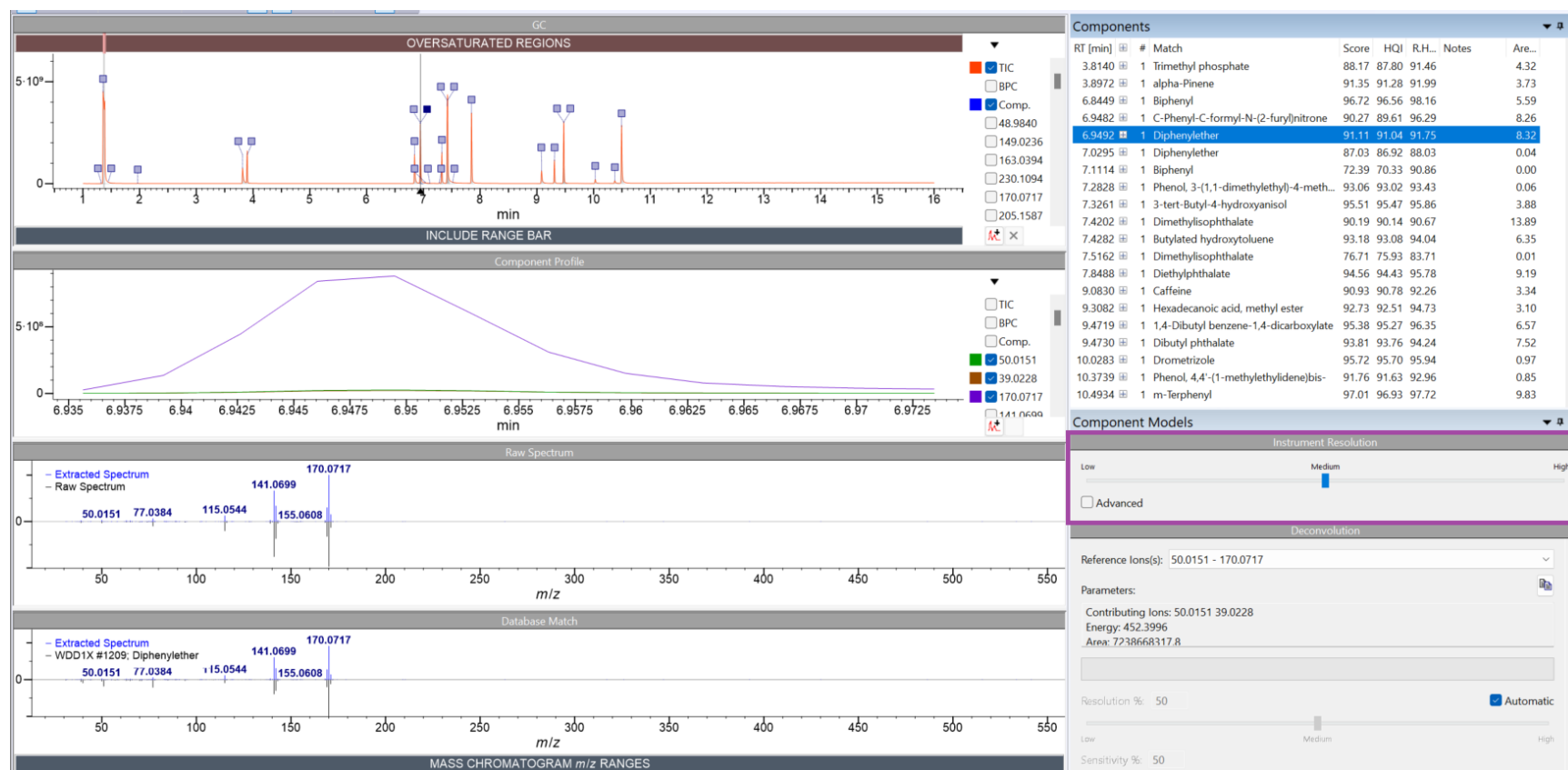
	Action	Result
9	<p>One can click the TIC pane to add peaks manually, then select <b>Analysis &gt; Add Selected Peak To Analysis</b> to perform a new analysis</p> <p>One can select <b>View Component Hit List in Minelt</b> to see Component table contents in <b>Minelt</b></p>	 <p>The screenshot shows the 'Analysis' menu with the following options: Masses, Add Selected Peak to Analysis, Set Baseline For Manually Selected Component, Use Manually Selected Slice As Component, Remove Selected Component, Rank Selected Match Highest, View Component Hit List in Minelt, Re-run Calculations, and Transfer to NIST MS Search... (Ctrl+Alt+N). The 'View Component Hit List in Minelt' option is highlighted.</p>



## Example 2: High-Resolution GC-MS

### GUI explanation

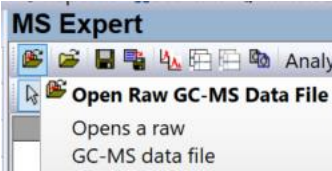
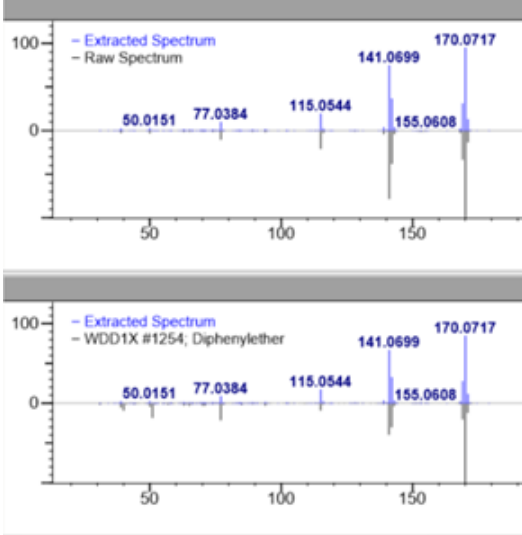
The instrument resolving power is required for the algorithm to automatically calculate the accurate  $m/z$  value of the data. Therefore, we use what our research considers a reasonable value by default that has a constant value and a variable value depending on mass (ppm). Empirically, this works in most cases. Increasing the  $m/z$  value accuracy too much incurs the danger of splitting an individual  $m/z$  value into individual mass spectral peaks that should be considered as just one. Decreasing the  $m/z$  value accuracy too much may cause individual mass spectral peaks to merge, resulting in incorrectly reported accurate  $m/z$  values.

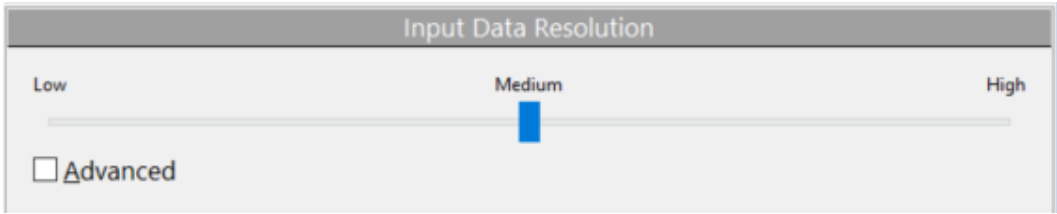
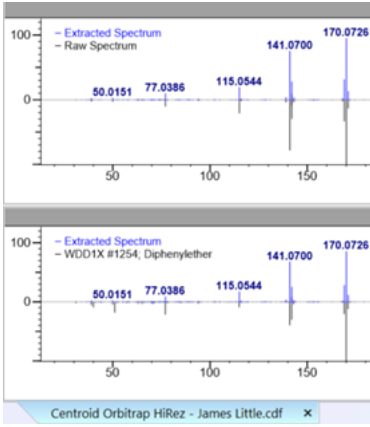


If a user knows the instrument's resolving power, that value should be entered in the **Instrument Resolution** panel, highlighted by the purple box, in above figure by clicking on 'Advanced' and manually entering the value.

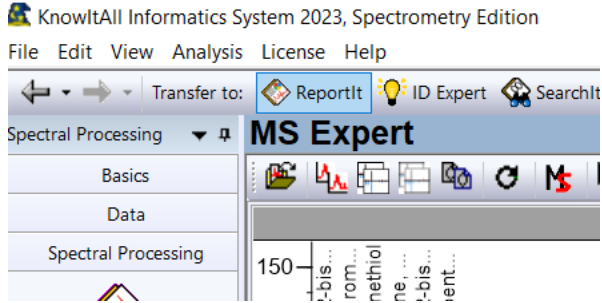
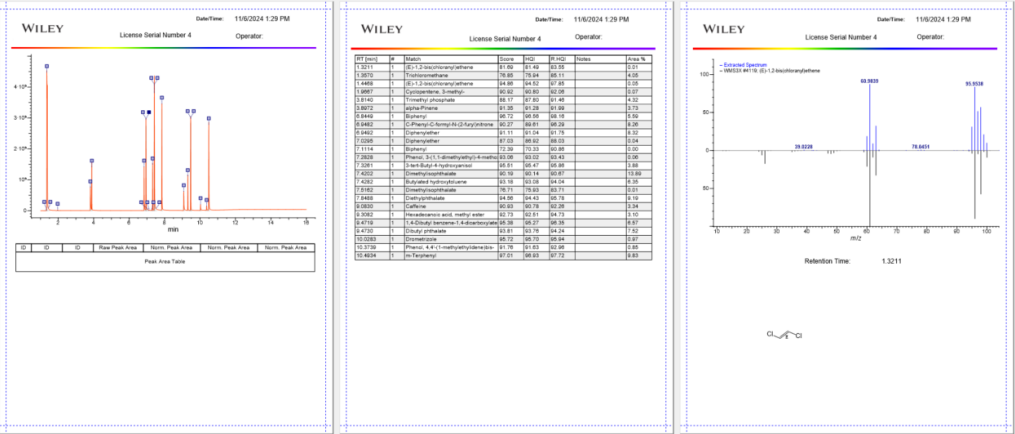
It is possible to save the instrument's resolving power as part of a profile, which can then be selected depending on the type of instrument. A user can create several profiles with different resolution settings for different types of data (and instruments).

## Hi-Resolution GC-MS Analysis using MS Expert – Exercise 1

	Action	Result
1	<p>Note: If you have changed your <b>File &gt; Settings</b> in previous exercise, you should go back to <b>File &gt; Settings</b> to reset for this exercise.</p> <p>Start a new analysis by clicking on the <b>Open Raw GC-MS Data File</b> button.</p>  <p>Navigate to the folder: <b>C:\Users\Public\Documents\Wiley\KnowItAll\Samples\MS Expert</b></p> <p>Select the file: <b>Centroid Orbitrap HiRez - James Little.cdf</b></p> <p><i>Note: A pop-up window will appear. Click 'OK' to ignore the warning.</i></p> <p>Using the <b>Components</b> panel, find the <b>RT (MIN)</b> 6.9482 and click on that component.</p>	 <p>The m/z value of 170.0717 is slightly off for this compound.</p>

	Action	Result
2	Check <b>Advanced</b> in the <b>Instrument Resolution</b> panel. Set the instrument resolution at 3 ppm, click <b>OK</b> .	<p><b>MS Expert</b> recognizes this is a high-resolution data file and uniquely allows user to fill in resolution information or adjust resolution:</p> 
3		<p>The m/z value is corrected to 170.0726. This is the correct value. This instrument resolution set-up is persistent.</p>  <p>Centroid Orbitrap HiRez - James Little.cdf x</p>

	Action	Result																																																																																																																																																																								
4	<p>To expand the component hits of a selected match, click on the (⊕) to the left of the component name.</p> <p>For example, find the component with RT 7.4282. Click the (⊕) icon.</p>	<div data-bbox="909 329 1663 354">Components <span style="float: right;">▼ ⊕ ×</span></div> <table border="1"> <thead> <tr> <th>RT [min]</th> <th>#</th> <th>Match</th> <th>Score</th> <th>HQI</th> <th>R.H...</th> <th>Notes</th> <th>Are...</th> </tr> </thead> <tbody> <tr><td>3.8952</td><td>⊕ 1</td><td>alpha-Pinene</td><td>91.32</td><td>91.26</td><td>91.84</td><td></td><td>3.33</td></tr> <tr><td>6.8448</td><td>⊕ 1</td><td>Biphenyl</td><td>96.92</td><td>96.76</td><td>98.35</td><td></td><td>4.93</td></tr> <tr><td>6.9475</td><td>⊕ 1</td><td>C-Phenyl-C-formyl-N-(2-furyl)nitro...</td><td>90.05</td><td>89.37</td><td>96.14</td><td></td><td>13.03</td></tr> <tr><td>6.9482</td><td>⊕ 1</td><td>2-Phenyl-phenol</td><td>88.53</td><td>88.33</td><td>90.34</td><td></td><td>7.32</td></tr> <tr><td>7.0295</td><td>⊕ 1</td><td>Diphenylether</td><td>76.46</td><td>75.56</td><td>84.53</td><td></td><td>0.04</td></tr> <tr><td>7.0370</td><td>⊕ 1</td><td>3,1,2-Azaazonaboratin, 5-cyano-2,2-...</td><td>69.55</td><td>69.25</td><td>72.26</td><td></td><td>0.03</td></tr> <tr><td>7.1106</td><td>⊕ 1</td><td>1,5-Dinaphthalen-1-yl-4-oxidanyl-pe...</td><td>62.70</td><td>60.99</td><td>78.08</td><td></td><td>0.01</td></tr> <tr><td>7.2828</td><td>⊕ 1</td><td>Phenol, 3-(1,1-dimethylethyl)-4-meth...</td><td>93.04</td><td>92.99</td><td>93.56</td><td></td><td>0.06</td></tr> <tr><td>7.3261</td><td>⊕ 1</td><td>3-tert-Butyl-4-hydroxyanisol</td><td>95.80</td><td>95.76</td><td>96.16</td><td></td><td>3.76</td></tr> <tr><td>7.4200</td><td>⊕ 1</td><td>Dimethylisophthalate</td><td>90.14</td><td>90.07</td><td>90.76</td><td></td><td>13.55</td></tr> <tr style="background-color: #e0e0e0;"><td>7.4282</td><td>⊕ 1</td><td>Butylated hydroxytoluene</td><td>93.41</td><td>93.31</td><td>94.27</td><td></td><td>6.08</td></tr> <tr><td></td><td>2</td><td>Butylated Hydroxytoluene</td><td>92.49</td><td>92.42</td><td>93.13</td><td></td><td></td></tr> <tr><td></td><td>3</td><td>Butylated hydroxytoluene</td><td>91.82</td><td>91.74</td><td>92.49</td><td></td><td></td></tr> <tr><td></td><td>4</td><td>Butylated hydroxytoluene</td><td>91.59</td><td>91.53</td><td>92.16</td><td></td><td></td></tr> <tr><td></td><td>5</td><td>Phenol, 2,6-bis(1,1-dimethylethyl)-4-...</td><td>90.19</td><td>90.11</td><td>90.96</td><td></td><td></td></tr> <tr><td></td><td>6</td><td>Phenol, 2,6-bis(1,1-dimethylethyl)-4-...</td><td>90.16</td><td>90.05</td><td>91.09</td><td></td><td></td></tr> <tr><td></td><td>7</td><td>Phenol, 2,4,6-tris(1-methylethyl)-</td><td>88.77</td><td>88.65</td><td>89.83</td><td></td><td></td></tr> <tr><td></td><td>8</td><td>Butylated hydroxy toluene</td><td>87.80</td><td>87.29</td><td>92.46</td><td></td><td></td></tr> <tr><td></td><td>9</td><td>Phenol, 2,4-bis(1,1-dimethylethyl)-6-...</td><td>86.76</td><td>86.68</td><td>87.44</td><td></td><td></td></tr> <tr><td></td><td>10</td><td>(5S,6S)-6-(cyclohepta-2,4,6-trien-1-yl...</td><td>86.29</td><td>85.83</td><td>90.48</td><td></td><td></td></tr> </tbody> </table>	RT [min]	#	Match	Score	HQI	R.H...	Notes	Are...	3.8952	⊕ 1	alpha-Pinene	91.32	91.26	91.84		3.33	6.8448	⊕ 1	Biphenyl	96.92	96.76	98.35		4.93	6.9475	⊕ 1	C-Phenyl-C-formyl-N-(2-furyl)nitro...	90.05	89.37	96.14		13.03	6.9482	⊕ 1	2-Phenyl-phenol	88.53	88.33	90.34		7.32	7.0295	⊕ 1	Diphenylether	76.46	75.56	84.53		0.04	7.0370	⊕ 1	3,1,2-Azaazonaboratin, 5-cyano-2,2-...	69.55	69.25	72.26		0.03	7.1106	⊕ 1	1,5-Dinaphthalen-1-yl-4-oxidanyl-pe...	62.70	60.99	78.08		0.01	7.2828	⊕ 1	Phenol, 3-(1,1-dimethylethyl)-4-meth...	93.04	92.99	93.56		0.06	7.3261	⊕ 1	3-tert-Butyl-4-hydroxyanisol	95.80	95.76	96.16		3.76	7.4200	⊕ 1	Dimethylisophthalate	90.14	90.07	90.76		13.55	7.4282	⊕ 1	Butylated hydroxytoluene	93.41	93.31	94.27		6.08		2	Butylated Hydroxytoluene	92.49	92.42	93.13				3	Butylated hydroxytoluene	91.82	91.74	92.49				4	Butylated hydroxytoluene	91.59	91.53	92.16				5	Phenol, 2,6-bis(1,1-dimethylethyl)-4-...	90.19	90.11	90.96				6	Phenol, 2,6-bis(1,1-dimethylethyl)-4-...	90.16	90.05	91.09				7	Phenol, 2,4,6-tris(1-methylethyl)-	88.77	88.65	89.83				8	Butylated hydroxy toluene	87.80	87.29	92.46				9	Phenol, 2,4-bis(1,1-dimethylethyl)-6-...	86.76	86.68	87.44				10	(5S,6S)-6-(cyclohepta-2,4,6-trien-1-yl...	86.29	85.83	90.48		
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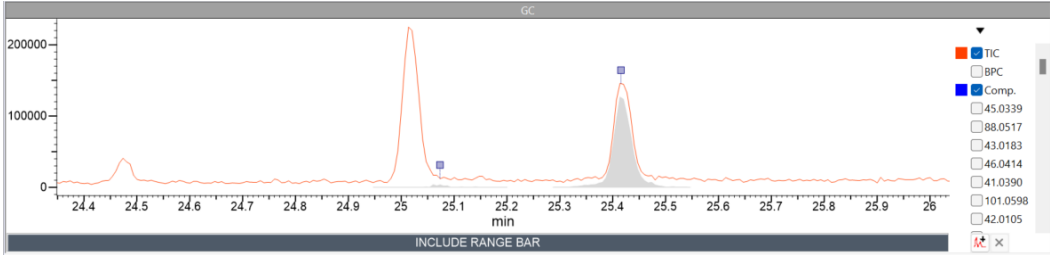
	Action	Result
<p>5 To export results to <b>ReportIt</b>, use the <b>Transfer to:</b> toolbar. Click on <b>ReportIt</b>.</p> <p>A window will pop-up. Select the preferred report template. Click OK.</p>  <p>Select the <b>MS_Expert_Portrait</b> template</p>	<p><b>Result</b></p>  <p>Note: if this is the first time using the MS Expert reporting feature, templates will need to be added ahead of this step. The following steps should be performed using <b>MS Expert</b>.</p> <ul style="list-style-type: none"> <li>• File &gt; Edit Report Templates</li> <li>• Choose <b>Add</b> button in the pop-up window.</li> <li>• Select the files, MS_Expert Landscape and MS_Expert Portrait.</li> <li>• Click <b>Open</b>.</li> <li>• Click <b>Close</b> in the Report Templates pop-up window.</li> </ul>	

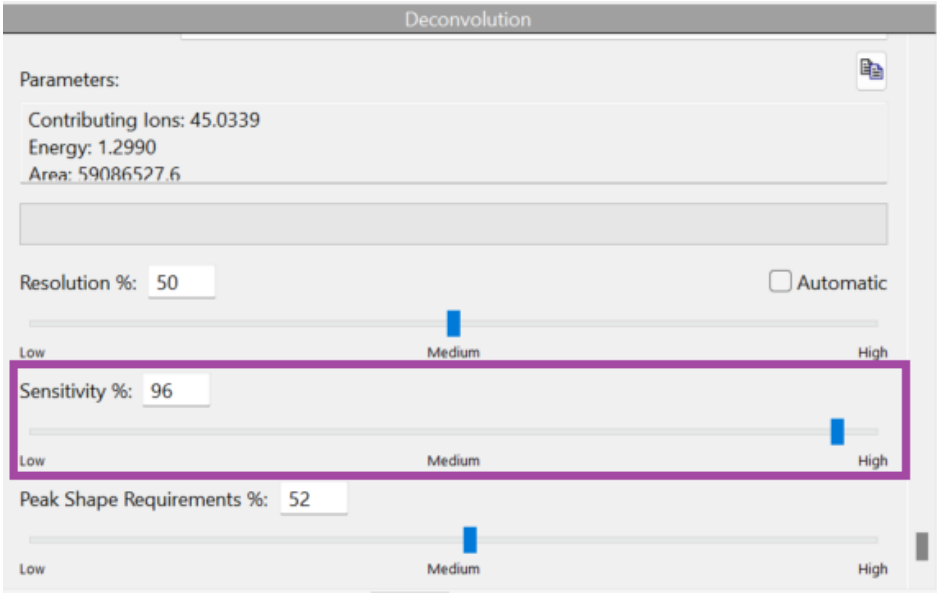
Action		Result								
6	Go back to <b>MS Expert</b> .									
	Expand a few components' reference hits, and add some comments									
	Right-mouse click the <b>Components</b> table and select <b>Copy All Component Information</b> . One can then paste this information to Excel or Word, etc.									
		1	RT [min]	#	Match	Score	HQI	R.HQI	Notes	Area %
		2	1.3211		1 (E)-1,2-bis	81.69	81.49	83.55		0.01
		3	1.357		1 Trichlorom	76.85	75.94	85.11		4.05
		4	1.4468		1 (E)-1,2-bis	94.86	94.52	97.85		0.05
		5	1.9667		1 Cyclopent	90.92	90.8	92.06		0.07
		6	3.814		1 Trimethyl p	88.17	87.8	91.46		4.32
		7	3.8972		1 alpha-Pine	91.35	91.28	91.99		3.73
		8	6.8449		1 Biphenyl	96.72	96.56	98.16		5.59
		9	6.9482		1 C-Phenyl-C	90.27	89.61	96.29		8.26
		10	6.9492		1 Diphenylet	91.11	91.04	91.75		8.32
		11	7.0295		1 Diphenylet	87.03	86.92	88.03	This is righ	0.04
		12			2 DIPHENYL	85.7	84.87	93.22		
		13			3 C-Phenyl-C	84.56	83.32	95.75		
		14			4 2-Phenyl-p	84.5	84.18	87.39		
		15			5 Biphenylol	82.6	82.52	83.33		
		16			6 8-Methyl-1	81.62	80.31	93.42		
		17			7 5-Methyl-1	81.57	80.26	93.36		
		18			8 1,2-Dihydr	80.56	79.27	92.21		
		19			9 1H,3H-Naj	80.43	80.31	81.46		
		20			10 1-Naphtha	80.15	78.86	91.74		
		21	7.1114		1 Biphenyl	72.39	70.33	90.86		0
		22	7.2828		1 Phenol, 3-	93.06	93.02	93.43		0.06
		23	7.3261		1 3-tert-Buty	95.51	95.47	95.86		3.88
		24	7.4202		1 Dimethylis	90.19	90.14	90.67		13.89
		25	7.4282		1 Butylated l	93.18	93.08	94.04		6.35
		26	7.5162		1 Dimethylis	76.71	75.93	83.71		0.01
		27	7.8488		1 Diethylpht	94.56	94.43	95.78		9.19
		28	9.083		1 Caffeine	90.93	90.78	92.26		3.34
		29	9.3082		1 Hexadecar	92.73	92.51	94.73		3.1
		30	9.4719		1 1,4-Dibuty	95.38	95.27	96.35		6.57
		31	9.473		1 Dibutyl pht	93.81	93.76	94.24		7.52
	32	10.0283		1 Drometriz	95.72	95.7	95.94		0.97	
	33	10.3739		1 Phenol, 4,	91.76	91.63	92.96		0.85	
	34	10.4934		1 m-Terpher	97.01	96.93	97.72		9.83	


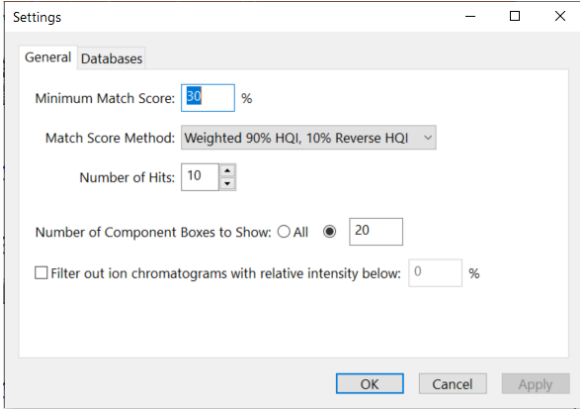
**Hi-Resolution GC-MS Analysis using MS Expert – Exercise 2**

	Action	Result
1	<p>Open another high-resolution GC-MS file from the same folder.</p> <p>Navigate to the folder: <b>C:\Users\Public\Documents\Wiley\KnowItAll\Samples\MS Expert</b></p> <p>Select the file: <b>OBAN 14 JEOL HiRez - James Little.cdf</b></p> <p>Right-mouse-click the <b>GC</b> panel.</p> <p>Choose Horizontal Zoom or Box Zoom mode.</p>	



	Action	Result
2	<p>Zoom into region 24 – 26 min (3 tiny peaks).</p> <p>Using Horizontal Zoom;</p> <ul style="list-style-type: none"><li>Using the mouse cursor, click on region of 24 min and drag the cursor to region 26 min.</li></ul> <p>Using Box Zoom mode.</p> <ul style="list-style-type: none"><li>Using the mouse cursor, click on region 24 toward the top of the GC panel. Drag the cursor to the right and down to include region 26min.</li><li>This creates a box around the region of interest.</li></ul>	

	Action	Result
3	<p>We can increase the algorithm's Sensitivity to resolve the second issue.</p> <p>In the <b>Deconvolution</b> panel, uncheck the box for <b>Automatic</b> deconvolution. Move the <b>Sensitivity</b> bar to <b>High</b>.</p>	 <p>The screenshot displays the 'Deconvolution' panel with the following settings:</p> <ul style="list-style-type: none"><li>Parameters: Contributing Ions: 45.0339, Energy: 1.2990, Area: 59086527.6</li><li>Resolution %: 50 (slider positioned at Medium)</li><li><input type="checkbox"/> Automatic (unchecked)</li><li>Sensitivity %: 96 (slider positioned at High, highlighted with a purple box)</li><li>Peak Shape Requirements %: 52 (slider positioned at Medium)</li></ul>

	Action	Result																																																																																																																																																
4		<p>Now the second component is correctly identified as the missing hexadecanoic acid.</p>  <p>The screenshot displays the GC-MS analysis interface. At the top, a Total Ion Chromatogram (TIC) shows two distinct peaks. The first peak is at 25.01 minutes and the second is at 25.04 minutes. Below the TIC, the 'Component Profile' shows the deconvolution of these peaks. The 'New Spectrum' section shows the extracted mass spectra for both peaks, with the base peak at m/z 277.8458. The 'Library Match' section shows a list of potential compounds, with Hexadecanoic acid (WFCX 82831) being the top match with a score of 89.44.</p> <table border="1" data-bbox="1612 354 1959 584"> <thead> <tr> <th>RT [min]</th> <th>#</th> <th>Match</th> <th>Score</th> <th>HQI</th> <th>RtL</th> <th>Notes</th> <th>Ass...</th> </tr> </thead> <tbody> <tr><td>15.5692</td><td>1</td><td>Hexane, 2,3-dimethyl-</td><td>76.68</td><td>75.04</td><td>91.44</td><td></td><td>0.03</td></tr> <tr><td>16.7976</td><td>1</td><td>Tetradecanol &lt;-&gt;</td><td>97.64</td><td>97.52</td><td>98.66</td><td></td><td>1.12</td></tr> <tr><td>17.8803</td><td>1</td><td>Palmitate &lt;-&gt;</td><td>95.33</td><td>95.09</td><td>97.44</td><td></td><td>0.47</td></tr> <tr><td>17.8821</td><td>1</td><td>Cyclopentanol, nitrate</td><td>75.33</td><td>74.60</td><td>83.90</td><td></td><td>0.06</td></tr> <tr><td>18.0233</td><td>1</td><td>1,2-Decanediol</td><td>49.60</td><td>48.94</td><td>55.53</td><td></td><td>0.48</td></tr> <tr><td>18.0328</td><td>1</td><td>n-Decanoic acid</td><td>97.35</td><td>97.34</td><td>97.48</td><td></td><td>3.88</td></tr> <tr><td>18.1300</td><td>1</td><td>EtHyl 9-hexadecanoate</td><td>87.84</td><td>87.70</td><td>88.11</td><td></td><td>0.90</td></tr> <tr><td>19.2240</td><td>1</td><td>Hexadecanol &lt;-&gt;</td><td>97.12</td><td>97.11</td><td>97.20</td><td></td><td>0.50</td></tr> <tr><td>19.2284</td><td>1</td><td>Cyclotetradecane</td><td>95.29</td><td>95.21</td><td>95.96</td><td></td><td>0.52</td></tr> <tr><td>20.8995</td><td>1</td><td>Dodecanoic acid</td><td>94.91</td><td>94.89</td><td>95.07</td><td></td><td>4.03</td></tr> <tr><td>22.8895</td><td>1</td><td>MYRISTIC ACID</td><td>92.39</td><td>92.27</td><td>93.51</td><td></td><td>0.42</td></tr> <tr><td>25.0187</td><td>1</td><td>Hexadecanoic acid &lt;-&gt;</td><td>89.44</td><td>89.21</td><td>91.48</td><td></td><td>0.34</td></tr> <tr><td>25.4155</td><td>1</td><td>Methanamine, N-(phenylmethyl)-</td><td>74.86</td><td>73.92</td><td>83.34</td><td></td><td>0.09</td></tr> <tr><td>34.2401</td><td>1</td><td>Cyclotetradecane, octamethyl-</td><td>95.89</td><td>95.68</td><td>97.84</td><td></td><td>0.39</td></tr> <tr><td>34.2515</td><td>1</td><td>2,2,4,4,6,6,8-heptamethyl-1,3,5,7,2,4...</td><td>64.40</td><td>62.92</td><td>77.70</td><td></td><td>0.31</td></tr> <tr><td>34.2659</td><td>1</td><td>Cyclotetradecane, octamethyl-</td><td>95.19</td><td>94.81</td><td>98.60</td><td></td><td>0.65</td></tr> <tr><td>34.2919</td><td>1</td><td>3-Thiophenecarbonitrile, 2-amino-5-(...</td><td>67.72</td><td>65.33</td><td>89.17</td><td></td><td>0.35</td></tr> </tbody> </table>	RT [min]	#	Match	Score	HQI	RtL	Notes	Ass...	15.5692	1	Hexane, 2,3-dimethyl-	76.68	75.04	91.44		0.03	16.7976	1	Tetradecanol <->	97.64	97.52	98.66		1.12	17.8803	1	Palmitate <->	95.33	95.09	97.44		0.47	17.8821	1	Cyclopentanol, nitrate	75.33	74.60	83.90		0.06	18.0233	1	1,2-Decanediol	49.60	48.94	55.53		0.48	18.0328	1	n-Decanoic acid	97.35	97.34	97.48		3.88	18.1300	1	EtHyl 9-hexadecanoate	87.84	87.70	88.11		0.90	19.2240	1	Hexadecanol <->	97.12	97.11	97.20		0.50	19.2284	1	Cyclotetradecane	95.29	95.21	95.96		0.52	20.8995	1	Dodecanoic acid	94.91	94.89	95.07		4.03	22.8895	1	MYRISTIC ACID	92.39	92.27	93.51		0.42	25.0187	1	Hexadecanoic acid <->	89.44	89.21	91.48		0.34	25.4155	1	Methanamine, N-(phenylmethyl)-	74.86	73.92	83.34		0.09	34.2401	1	Cyclotetradecane, octamethyl-	95.89	95.68	97.84		0.39	34.2515	1	2,2,4,4,6,6,8-heptamethyl-1,3,5,7,2,4...	64.40	62.92	77.70		0.31	34.2659	1	Cyclotetradecane, octamethyl-	95.19	94.81	98.60		0.65	34.2919	1	3-Thiophenecarbonitrile, 2-amino-5-(...	67.72	65.33	89.17		0.35
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15.5692	1	Hexane, 2,3-dimethyl-	76.68	75.04	91.44		0.03																																																																																																																																											
16.7976	1	Tetradecanol <->	97.64	97.52	98.66		1.12																																																																																																																																											
17.8803	1	Palmitate <->	95.33	95.09	97.44		0.47																																																																																																																																											
17.8821	1	Cyclopentanol, nitrate	75.33	74.60	83.90		0.06																																																																																																																																											
18.0233	1	1,2-Decanediol	49.60	48.94	55.53		0.48																																																																																																																																											
18.0328	1	n-Decanoic acid	97.35	97.34	97.48		3.88																																																																																																																																											
18.1300	1	EtHyl 9-hexadecanoate	87.84	87.70	88.11		0.90																																																																																																																																											
19.2240	1	Hexadecanol <->	97.12	97.11	97.20		0.50																																																																																																																																											
19.2284	1	Cyclotetradecane	95.29	95.21	95.96		0.52																																																																																																																																											
20.8995	1	Dodecanoic acid	94.91	94.89	95.07		4.03																																																																																																																																											
22.8895	1	MYRISTIC ACID	92.39	92.27	93.51		0.42																																																																																																																																											
25.0187	1	Hexadecanoic acid <->	89.44	89.21	91.48		0.34																																																																																																																																											
25.4155	1	Methanamine, N-(phenylmethyl)-	74.86	73.92	83.34		0.09																																																																																																																																											
34.2401	1	Cyclotetradecane, octamethyl-	95.89	95.68	97.84		0.39																																																																																																																																											
34.2515	1	2,2,4,4,6,6,8-heptamethyl-1,3,5,7,2,4...	64.40	62.92	77.70		0.31																																																																																																																																											
34.2659	1	Cyclotetradecane, octamethyl-	95.19	94.81	98.60		0.65																																																																																																																																											
34.2919	1	3-Thiophenecarbonitrile, 2-amino-5-(...	67.72	65.33	89.17		0.35																																																																																																																																											
5	<p>Sometimes, there are too many GC peaks crowding the GC panel. To adjust the display to reduce crowding, click <b>File &gt; Settings</b> to set preferences:</p>	 <p>The screenshot shows the 'Settings' dialog box with the 'General' tab selected. The following parameters are visible:</p> <ul style="list-style-type: none"> <li>Minimum Match Score: 50 %</li> <li>Match Score Method: Weighted 90% HQI, 10% Reverse HQI</li> <li>Number of Hits: 10</li> <li>Number of Component Boxes to Show: 20</li> <li>Filter out ion chromatograms with relative intensity below: 0 %</li> </ul>																																																																																																																																																

## How to Perform GC-MS Analysis by Peak Picking

### Purpose

These exercises demonstrate how to use KnowItAll MS Expert to analyze GC-MS data by peak picking.

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### Objectives

These exercises will teach you:

- How to use KnowItAll MS Expert to analyze GC-MS using peak picking.
  - How to generate reports.
- 

### Background

GC-MS data can be analyzed by peak picking without going through deconvolution. Novel compounds can be identified, and structural characteristics deduced from applying the MS Adaptive search that uses fragmentation and structural data to propose likely structural details of the unknown.

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

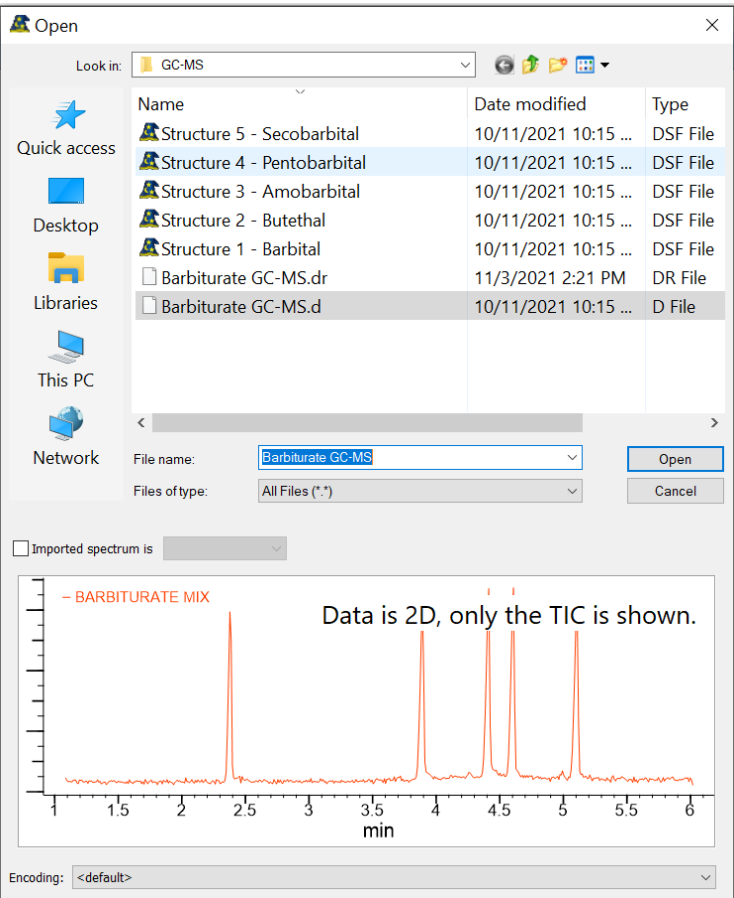
- C:\Users\Public\Documents\Wiley\KnowItAll\Samples\GC-MS\Barbiturate GC-MS.d

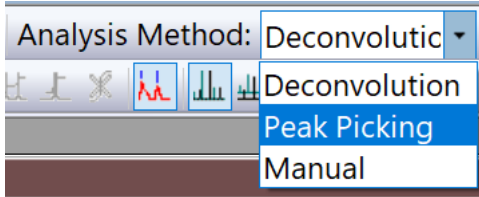
#### *KnowItAll Applications Used*

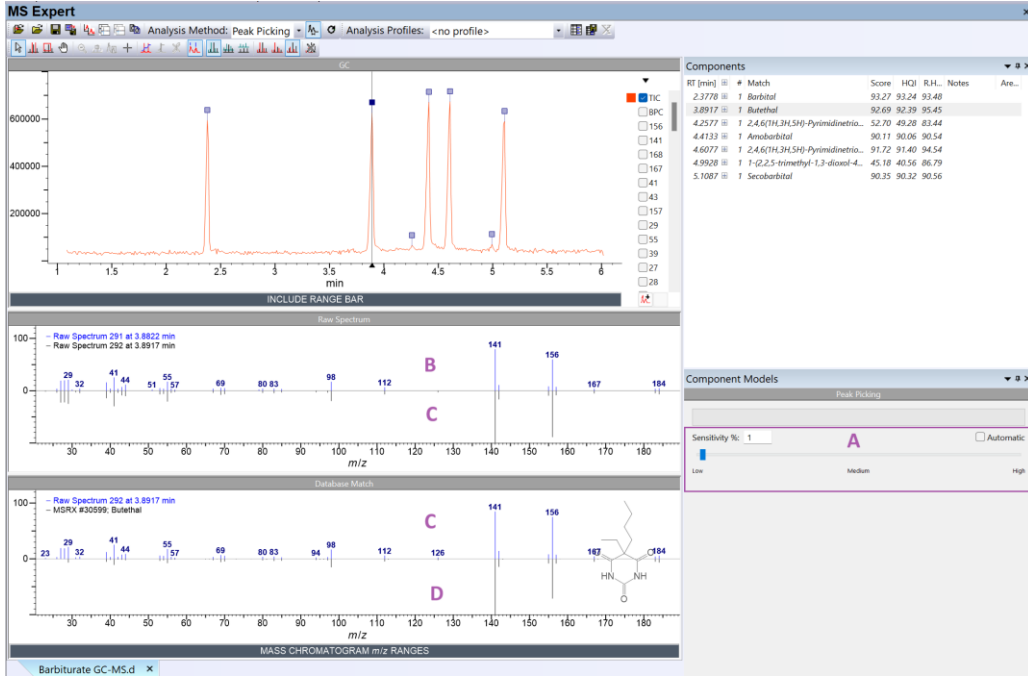
- KnowItAll MS Expert

KnowItAll MS Expert defaults to perform deconvolution, however one can just use the **Peak Picking** option to analyze GC-MS data, especially if the GC separates components well enough.

### Example: Peak Picking

	Action	Result
1	<p>Click <b>Open Raw GC-MS Data File</b> button.</p> <p>Navigate to “C:\Users\Public\Documents\Wiley\KnowItAll\Samples\GC-MS”</p> <p>Select the file: <b>Barbiturate GC-MS.d</b></p>	 <p>The screenshot shows a file explorer window titled 'Open' with the 'Look in' path set to 'GC-MS'. A list of files is displayed with columns for Name, Date modified, and Type. The file 'Barbiturate GC-MS.d' is selected. Below the file list, the 'File name' field contains 'Barbiturate GC-MS' and the 'Files of type' is set to 'All Files (*.*)'. An 'Open' button is visible. Below the file list, there is a section for 'Imported spectrum is' and a chromatogram plot. The plot shows a Total Ion Chromatogram (TIC) with several peaks. The x-axis is labeled 'min' and ranges from 1 to 6. The y-axis represents intensity. The plot is titled 'BARBITURATE MIX' and includes the text 'Data is 2D, only the TIC is shown.' The encoding is set to '&lt;default&gt;'.</p>

	Action	Result
2	Switch <b>Analysis Method</b> to <b>Peak Picking</b> .	

	Action	Result
3	<p>Reduce the <b>Sensitivity</b> to <b>Low</b> so that only main peaks are picked (A).</p> <p>Select the peak at 3.8917 min.</p> <p>Hold the mouse cursor over the solid square denoting the selected peak in the <b>GC</b> panel.</p> <ul style="list-style-type: none"> <li>In the <b>Raw Spectrum</b> panel, <b>B</b> displays the MS spectrum the of the selected peak</li> <li><b>C</b>, in both the <b>GC</b> and the <b>Database Match</b> panels, displays selected peak's MS spectrum;</li> <li>In the <b>Database Match</b> panel, <b>D</b> indicates the reference spectrum match to the selected spectrum indicated by <b>C</b>.</li> </ul>	 <p>The screenshot displays the MS Expert software interface. The top panel shows a GC chromatogram with several peaks. A peak at 3.8917 min is selected. The Raw Spectrum panel shows the MS spectrum of the selected peak. The Database Match panel shows the reference spectrum match to the selected spectrum. The Components panel shows a list of identified compounds, including Barbitital, Bulethial, and Amobarbital. The Sensitivity % is set to 1 (Low).</p>

# Manually Analyze GC-MS

## How to manually analyze GC-MS

### Purpose

These exercises demonstrate how to use KnowItAll MS Expert to manually analyze GC-MS.

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### Objectives

These exercises will teach you:

- How to use KnowItAll MS Expert to manually analyze GC-MS.
- 

### Background

The KnowItAll MS Expert allows one to examine GC-MS data and, perform spectral subtraction. Matches to the subtracted spectrum are searched for against the reference data.

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

- C:\Users\Public\Documents\Wiley\KnowItAll\Samples\GC-MS\Barbiturate GC-MS.d

#### *KnowItAll Applications Used*

- KnowItAll MS Expert



Average MS (green bar in GC pane), defined by clicking the mouse on the bar, drag and drop

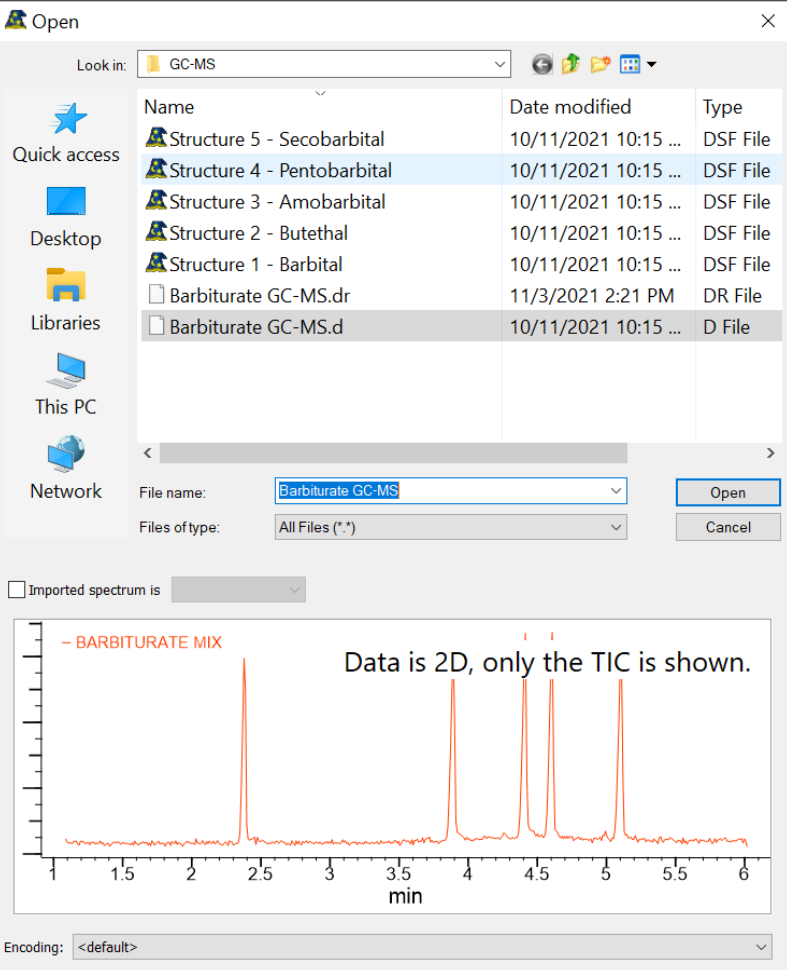
- Average MS (green bar) - background (red bar)

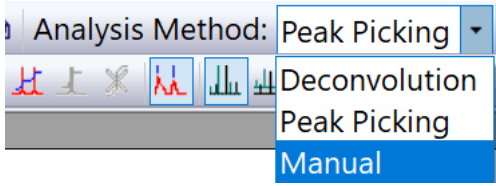
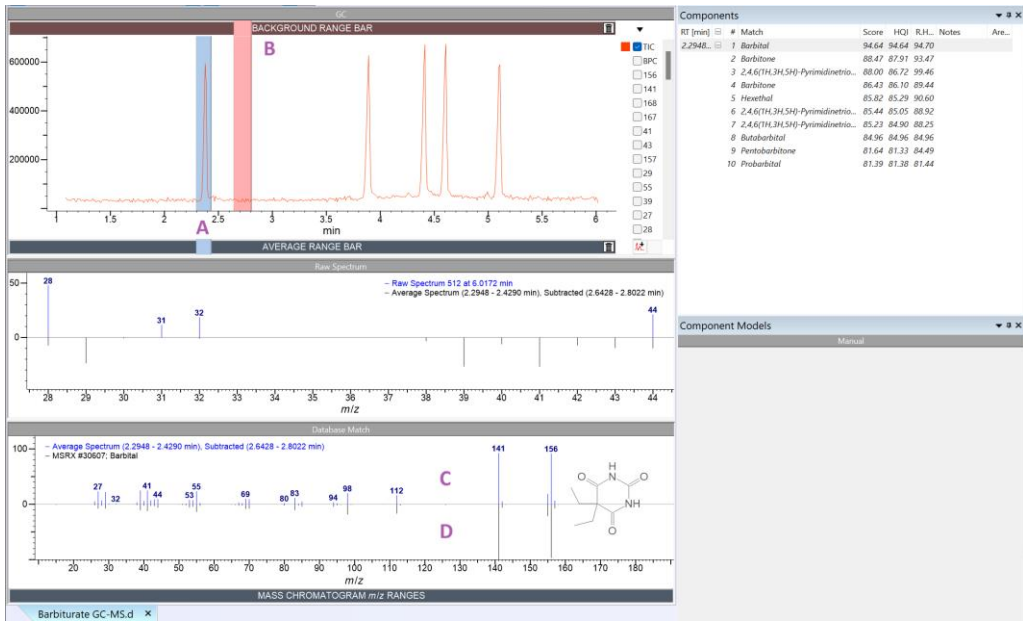
The **Matches** table are database search hit list for the selected MS.

The selected MS can be transferred to **SearchIt** application for spectrum search.

The area under curve (AUC) and peak height values for the ion chromatogram can be calculated by using the **Analysis > Peak Area/Integration** menu-item.

## Example: Manual Analysis

	Action	Result																								
1	<p>In <b>MS Expert</b>, click on the <b>Open Raw GC-MS Data File</b> button.</p> <p>Navigate to: "C:\Users\Public\Documents\Wiley\KnowItAll\Samples\GC-MS"</p> <p>Select the file: <b>Barbiturate GC-MS.d</b></p>	 <p>The screenshot shows a Windows File Explorer window titled "Open" with the "Look in:" path set to "GC-MS". The file list contains the following items:</p> <table border="1"><thead><tr><th>Name</th><th>Date modified</th><th>Type</th></tr></thead><tbody><tr><td>Structure 5 - Secobarbital</td><td>10/11/2021 10:15 ...</td><td>DSF File</td></tr><tr><td>Structure 4 - Pentobarbital</td><td>10/11/2021 10:15 ...</td><td>DSF File</td></tr><tr><td>Structure 3 - Amobarbital</td><td>10/11/2021 10:15 ...</td><td>DSF File</td></tr><tr><td>Structure 2 - Butethal</td><td>10/11/2021 10:15 ...</td><td>DSF File</td></tr><tr><td>Structure 1 - Barbital</td><td>10/11/2021 10:15 ...</td><td>DSF File</td></tr><tr><td>Barbiturate GC-MS.dr</td><td>11/3/2021 2:21 PM</td><td>DR File</td></tr><tr><td>Barbiturate GC-MS.d</td><td>10/11/2021 10:15 ...</td><td>D File</td></tr></tbody></table> <p>The "File name:" field contains "Barbiturate GC-MS" and the "Files of type:" dropdown is set to "All Files (*.*)".</p> <p>Below the dialog, a chromatogram plot is displayed with the title "BARBITURATE MIX". The x-axis is labeled "min" and ranges from 1 to 6. The y-axis is unlabeled. The plot shows several peaks. The text "Data is 2D, only the TIC is shown." is overlaid on the plot. The "Encoding:" dropdown is set to "&lt;default&gt;".</p>	Name	Date modified	Type	Structure 5 - Secobarbital	10/11/2021 10:15 ...	DSF File	Structure 4 - Pentobarbital	10/11/2021 10:15 ...	DSF File	Structure 3 - Amobarbital	10/11/2021 10:15 ...	DSF File	Structure 2 - Butethal	10/11/2021 10:15 ...	DSF File	Structure 1 - Barbital	10/11/2021 10:15 ...	DSF File	Barbiturate GC-MS.dr	11/3/2021 2:21 PM	DR File	Barbiturate GC-MS.d	10/11/2021 10:15 ...	D File
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	Action	Result																																																																													
2	Switch <b>Analysis Method</b> to <b>Manual</b> .																																																																														
3	<p>Use the <b>Average Range Bar</b> (A) to define a selected region of the MS chromatogram.</p> <ul style="list-style-type: none"> <li>Click and drag the mouse cursor along the <b>Average Range Bar</b>.</li> <li>You select many ranges.</li> </ul> <p>Use the <b>Background Range Bar</b> (B) to define the selected background region of the chromatogram.</p> <ul style="list-style-type: none"> <li>Click and drag the mouse cursor along the <b>Background Range Bar</b>.</li> <li>You select many ranges.</li> </ul>	<p>The MS spectrum with the subtracted background (C) and the corresponding matched reference MS spectrum (D) is displayed in the bottom panel.</p>  <p>The chromatogram shows a Total Ion Chromatogram (TIC) with several peaks. The Average Range Bar (A) is positioned over a peak at approximately 2.948 minutes, and the Background Range Bar (B) is positioned over a region from approximately 2.6428 to 2.8022 minutes. The mass spectra panels show the raw spectrum (C) and the subtracted background spectrum (D) for the peak at 2.948 minutes. The reference spectrum (D) is identified as barbiturate, with a chemical structure shown next to it.</p> <table border="1"> <caption>Components</caption> <thead> <tr> <th>RT [min]</th> <th># Match</th> <th>Score</th> <th>HQI</th> <th>R.H.L.</th> <th>Notes</th> <th>Are...</th> </tr> </thead> <tbody> <tr> <td>2.2948</td> <td>1</td> <td>94.64</td> <td>94.64</td> <td>94.70</td> <td></td> <td></td> </tr> <tr> <td></td> <td>2</td> <td>88.47</td> <td>87.91</td> <td>93.47</td> <td></td> <td></td> </tr> <tr> <td></td> <td>3</td> <td>88.00</td> <td>86.72</td> <td>99.46</td> <td></td> <td></td> </tr> <tr> <td></td> <td>4</td> <td>86.43</td> <td>86.10</td> <td>89.44</td> <td></td> <td></td> </tr> <tr> <td></td> <td>5</td> <td>85.82</td> <td>85.29</td> <td>90.60</td> <td></td> <td></td> </tr> <tr> <td></td> <td>6</td> <td>85.44</td> <td>85.05</td> <td>88.92</td> <td></td> <td></td> </tr> <tr> <td></td> <td>7</td> <td>85.23</td> <td>84.90</td> <td>88.25</td> <td></td> <td></td> </tr> <tr> <td></td> <td>8</td> <td>84.96</td> <td>84.96</td> <td>84.96</td> <td></td> <td></td> </tr> <tr> <td></td> <td>9</td> <td>81.64</td> <td>81.33</td> <td>84.49</td> <td></td> <td></td> </tr> <tr> <td></td> <td>10</td> <td>81.39</td> <td>81.38</td> <td>81.44</td> <td></td> <td></td> </tr> </tbody> </table>	RT [min]	# Match	Score	HQI	R.H.L.	Notes	Are...	2.2948	1	94.64	94.64	94.70				2	88.47	87.91	93.47				3	88.00	86.72	99.46				4	86.43	86.10	89.44				5	85.82	85.29	90.60				6	85.44	85.05	88.92				7	85.23	84.90	88.25				8	84.96	84.96	84.96				9	81.64	81.33	84.49				10	81.39	81.38	81.44		
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