

# **KnowItAll Software**

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## Training Guide

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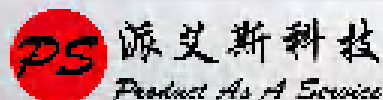


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# SOUNDPROOF

## YOUR LABORATORY

### WITH NOISE REDUCTION ENCLOSURES !

VACUUM PUMPS



WATER CHILLERS



ULTRASONIC BATHS



NITROGEN GENERATORS



# UP TO 80% DECREASE IN NOISE PERCEPTION



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## About this Training Guide

This training guide lead you through a series of exercises in the manner of a training course. Each lesson has a folder of example training files associated with it that can be downloaded here: [www.knowitall.com/training\\_files](http://www.knowitall.com/training_files)

Lesson	Description	Application Featured
<b>General Features</b>	<ul style="list-style-type: none"> <li>Explore the interface</li> <li>Learn to transfer data from one application to another</li> </ul>	KnowItAll "Interface"
<b>1 - Simple Spectral Search / Identification</b>	<ul style="list-style-type: none"> <li>Perform a "first pass" analysis of your spectrum against reference spectra</li> <li>Use patented optimized corrections technology to optimize search results</li> </ul>	KnowItAll ID Expert
<b>2 - Searching</b>	<ul style="list-style-type: none"> <li>Perform a basic, peak, structure, and multi-technique searches</li> <li>Create a search profile</li> <li>Limit search range / exclude search regions</li> <li>Perform a spectral subtraction</li> <li>"All" vs. "Pure Compound" search</li> </ul>	SearchIt
<b>3 - Mixture Analysis</b>	<ul style="list-style-type: none"> <li>Perform mixture analysis</li> <li>Interpret search results</li> </ul>	SearchIt
<b>4 - Create Databases</b>	<ul style="list-style-type: none"> <li>Create a database with spectra, structures, properties</li> <li>Batch import spectra, structures, properties, PubChem properties</li> <li>Create display profiles</li> </ul>	Minelt/Create Databases
<b>5 - Functional Group Analysis</b>	<ul style="list-style-type: none"> <li>Browse the knowledgebase of functional groups</li> <li>Correlate peaks from a structure</li> <li>Perform spectral analysis by functional group – IR, Raman. IR Polymers</li> <li>Create User Knowledgebases</li> </ul>	Analyzelt (IR, IR Polymer, Raman)
<b>6 - Drawing Structures &amp; Reactions</b>	<ul style="list-style-type: none"> <li>Use basic ChemWindow tools to create and edit a structure</li> <li>Create chemical reactions</li> </ul>	ChemWindow, ReportIt
<b>7 - Creating Reports</b>	<ul style="list-style-type: none"> <li>Use pre-defined report template</li> <li>Create customized templates</li> </ul>	ReportIt
<b>8 - Data Mining &amp; Analysis</b>	<ul style="list-style-type: none"> <li>Use patented Overlap Density Heatmaps for visual data mining</li> <li>Create an overlap consensus spectrum</li> </ul>	Minelt
<b>9 - Quality Control Analysis</b>	<ul style="list-style-type: none"> <li>Set up administrator account</li> <li>Select a standard and compare sample</li> </ul>	QC Expert

# **KnowItAll Software Training**

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## General Features

# General Features

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## Introduction to the Basic Applications in the KnowItAll Informatics System

### Purpose

This exercise demonstrates the features of the KnowItAll environment.

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### Objectives

This exercise will teach you:

- How to open individual KnowItAll applications;
  - How to access on-line help;
  - How to transfer information from one application to another.
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### Background

All KnowItAll solutions are designed using a unique architecture that allows the seamless transfer of information from one software tool to another without having to leave the main interface.

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

- Cholesterol.dsf

#### *KnowItAll Applications Used*

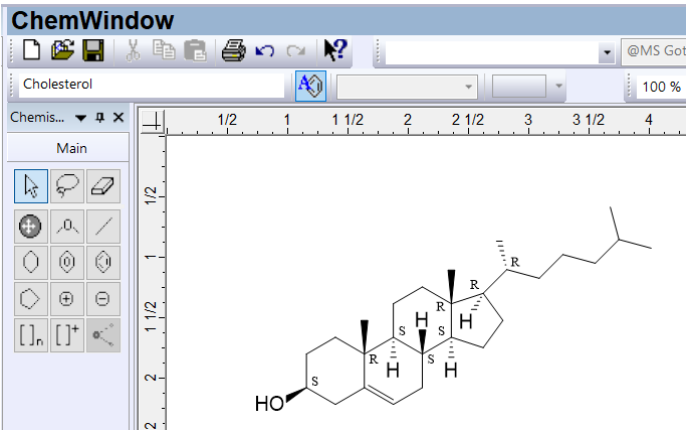
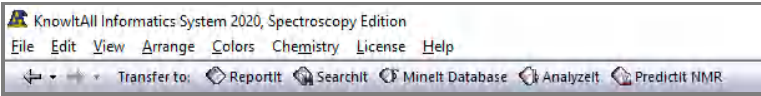
- Browselt™
- ChemWindow®
- SearchIt™
- ReportIt™

**The KnowItAll environment**

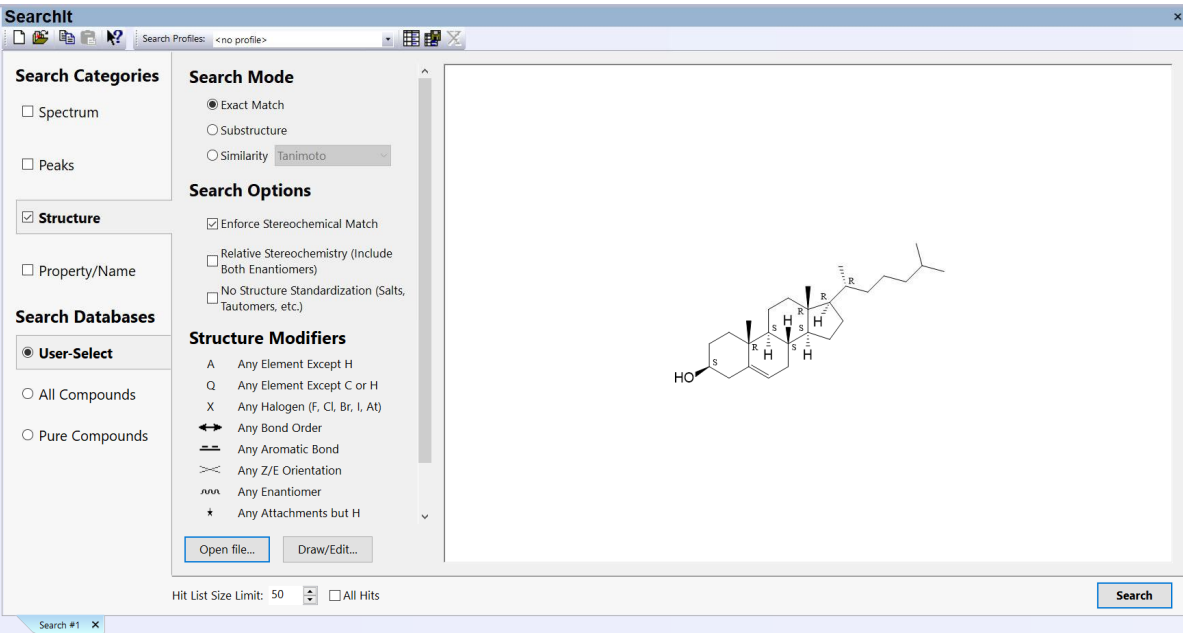
	Action	Result
1	Open the <b>KnowItAll Informatics System</b> by double-clicking its icon on the desktop.	<p>The KnowItAll Informatics System automatically opens to the <b>Browselt</b> application. This application offers access to a web community designed especially for KnowItAll users and access to training movies and other information.</p> <p>Notice the KnowItAll interface integrates a series of software applications within logically grouped toolboxes, so the user can move from one task to the next and transfer information from one application to another.</p> <p>As you move throughout the KnowItAll Informatics System, notice that certain screen elements are shared by all applications (e.g., Title and Menu bars; Back / Forward buttons; Transfer/Return to bar; and Application Toolboxes.)</p>
2	Explore the online <b>Help</b> .	Open the <b>Help</b> menu and choose <b>KnowItAll Help and Training</b> . This leads user to the online <b>Help</b> site.
3	Examine the contents of the <b>File</b> , <b>License</b> , and <b>Help</b> menus.	All KnowItAll Informatics System applications share the same Menu bar, located beneath the Title bar at the top of the application's window. The contents of the Menu bar change to reflect the current application as you move throughout the KnowItAll Informatics System. All applications include File, License, and Help menus. Other menus become available depending on the capabilities of each application.




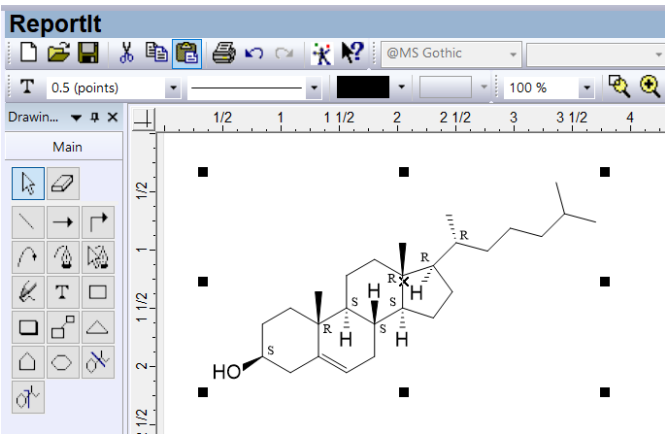
## The KnowItAll environment (continued)

	6	Result
4	Click each toolbox title in the Application Toolbox area on the left edge of the application window.	Depending on the edition(s) you have, this area can have <b>Basics</b> , <b>Data</b> , <b>Spectral Processing</b> and <b>Spectral Analysis</b> . Click a toolbox title to open it. Click icons within the toolboxes to open and explore different KnowItAll applications.
5	Navigate to the <b>Basics</b> toolbox, then open the <b>ChemWindow</b> application by clicking its icon.	The application opens to a blank drawing pane.
6	<ul style="list-style-type: none"> <li>Choose <b>File &gt; Open</b></li> <li>Navigate to <b>KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; General Features</b></li> <li>Open <b>Cholesterol.dsf</b>.</li> </ul> <p><b>Note:</b> The <b>Files of type</b> filter on the <b>Open</b> dialog box allows you to specify which file types are displayed.</p>	<p>The structure opens in the drawing area:</p>  <p>A tab with the structure's name is added. Multiple tabs can be open at the same time.</p>
7	Observe that the <b>Transfer to</b> bar (below the menu bar) now shows icons of the applications you can now transfer the structure to.	 <p>You can use the <b>Transfer to</b> bar to transfer information or objects from one application to another in KnowItAll. The bar displays all the applications that can accept selected information or objects from the application that is currently in use.</p>

## The KnowItAll environment (continued)

	Action	Result
8	Click <b>SearchIt</b> in the <b>Transfer to</b> bar.	<p>The structure is transferred to the <b>SearchIt</b> application:</p> 

## The KnowItAll environment (continued)

	Action	Result
9	Click the KnowItAll <b>Back</b> button  (located below the <b>File</b> menu).	<p>You are returned to the <b>ChemWindow</b> application. As you use different KnowItAll Informatics System applications, the KnowItAll <b>Back</b> and <b>Forward</b> buttons and corresponding drop-down lists become available.</p> <ul style="list-style-type: none"> <li>• Use the KnowItAll <b>Back</b> button to return to the most recently used application.</li> <li>• Use the KnowItAll <b>Back</b> button drop-down list to go back several steps.</li> </ul> <p>Once the KnowItAll <b>Back</b> button has been used, the KnowItAll <b>Forward</b> button and its drop-down list become available and can be used to move through KnowItAll applications in the opposite direction.</p>
10	Click <b>ReportIt</b> in the <b>Transfer to</b> bar.	<p>The structure opens in the <b>ReportIt</b> application, where you can create a standard report that includes this structure.</p> 

# **KnowItAll Software Training**

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## Simple Spectral Search / Identification with KnowItAll ID Expert

# Simple Spectral Search/Identification

## How to Use KnowItAll® ID Expert™ to Perform a Simple Spectral Search/Identification

### Purpose

These exercises demonstrate how to use KnowItAll® ID Expert™ to Identify IR, Raman and other spectra.

### Objectives

These exercises will teach you:

- Perform single component searches, multiple component searches, designer drug classification & functional group analyses simultaneously and view results on a single screen for complete view of all possibilities for the unknown spectrum
- De-convolute industrial material to organic and inorganic chemicals
- How KnowItAll ID Expert's patented optimized corrections technology can help you to find the optimal search results
- Generate PDF report with a single click

### Background

The KnowItAll ID Expert spectral identification software combined with the KnowItAll Spectral Libraries provides fast answers to scientists identifying unknown spectra.

It's easy to use. Simply open an unknown spectrum and KnowItAll ID Expert automatically performs single component searches, multiple component searches, possible designer drug classification and functional group analyses simultaneously and summarizes the results on a single screen to give a complete view of all possibilities for the unknown. It also can perform analysis using only pure organic and inorganic compound spectra, thus, breaks down industrial material into basic building blocks. If there are problems with the query spectrum, ID Expert has the spectral intelligence to identify issues and fix them using patented Optimized Corrections. Once the user has identified the unknown spectrum, a PDF report can be generated with a single click.

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

- 2 - ATR-IR of Unknown Sample 8675309.irf
- 4 - ATR-IR of Unknown Sample 1282013.irf
- Deformulation Example.irf
- Mint Candy.wdf

#### *KnowItAll Applications Used*

- KnowItAll ID Expert



## Optimized Corrections: A Breakthrough Technology for Spectral Searching

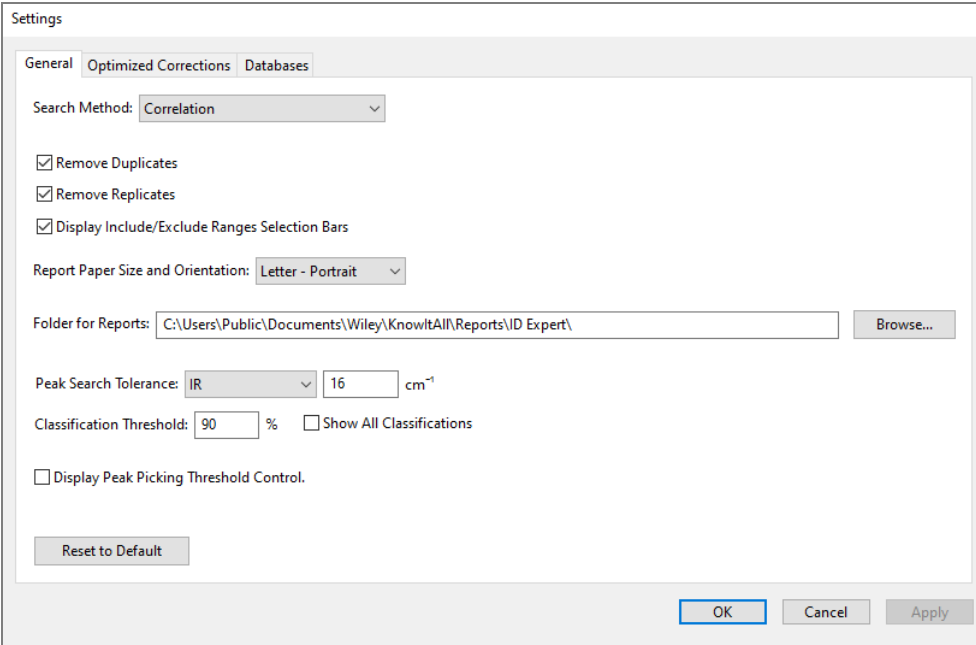
Spectral searching is one of the most important tools researchers use to classify or identify materials, yet it continues to be plagued by errors and imperfections. During a spectral search, a sample spectrum is compared to a database of reference spectra. To ensure that an optimal match is found in the database, spectra can be adjusted to compensate for differences between spectra caused by variability in instruments, accessories, environmental conditions, and other factors.

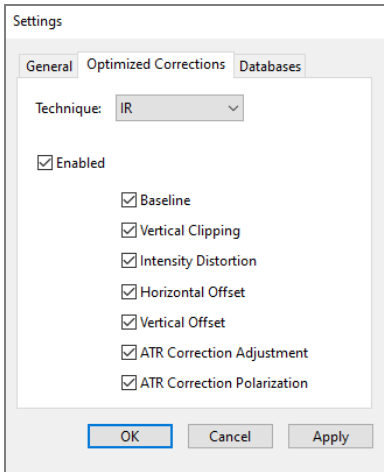
According to ASTM's guide on spectral searching<sup>1</sup>, various algorithms and manual methods exist to adjust spectra to get reasonable match scores when two compared spectra of the same compound differ for various reasons. While these methods may work in select cases, subtle discrepancies such as a shift of the X-axis are very hard to identify and correct manually. The inflexible mathematical algorithms typically employed do not compensate for these types of errors in spectra that are flawed.

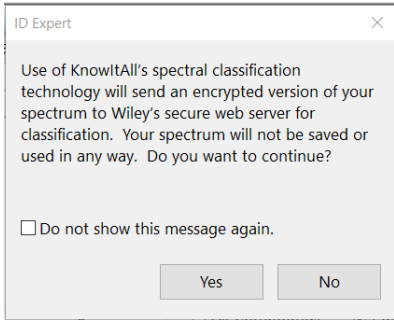
Manual corrections can be made by expert spectroscopists, but those less experienced in spectroscopy are often unaware of how to perform the necessary corrections on their sample spectrum to achieve the best search result. To address this growing concern, Wiley has introduced Optimized Corrections, a breakthrough patented technology that performs a computationally complex set of multiple corrections on all query and reference spectra in a search to find the optimal match between the query and each individual reference spectrum. We will demonstrate how the Optimized Corrections technology yields better matches between query and reference spectra than can be attained using rigid search algorithms alone or with manual methods to optimize spectra for searching.

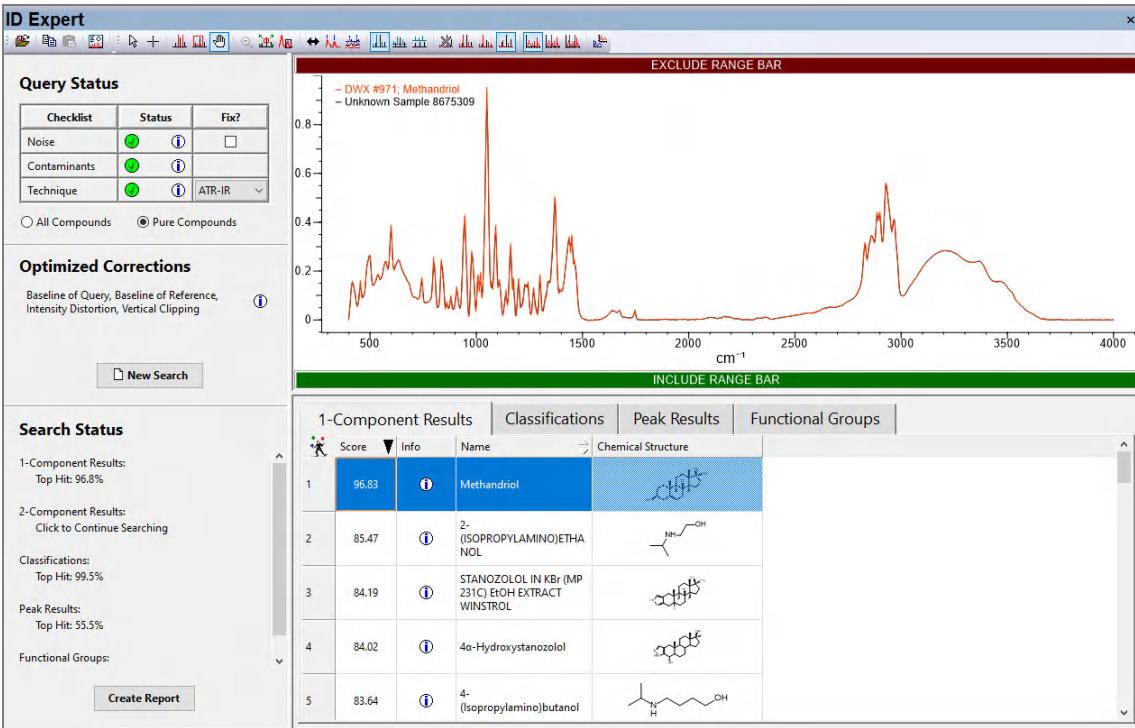
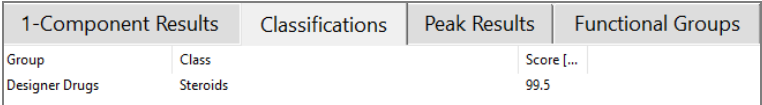
<sup>1</sup> E2310-04 - Standard Guide for Use of Spectral Searching by Curve Matching Algorithms with Data Recorded Using Mid-Infrared Spectroscopy, 2009. ASTM International Web Site. <http://www.astm.org/Standards/E2310.htm> (accessed March 4, 2015).

**Example 1: 2-ATR-IR of Unknown Sample 8675309.irf**

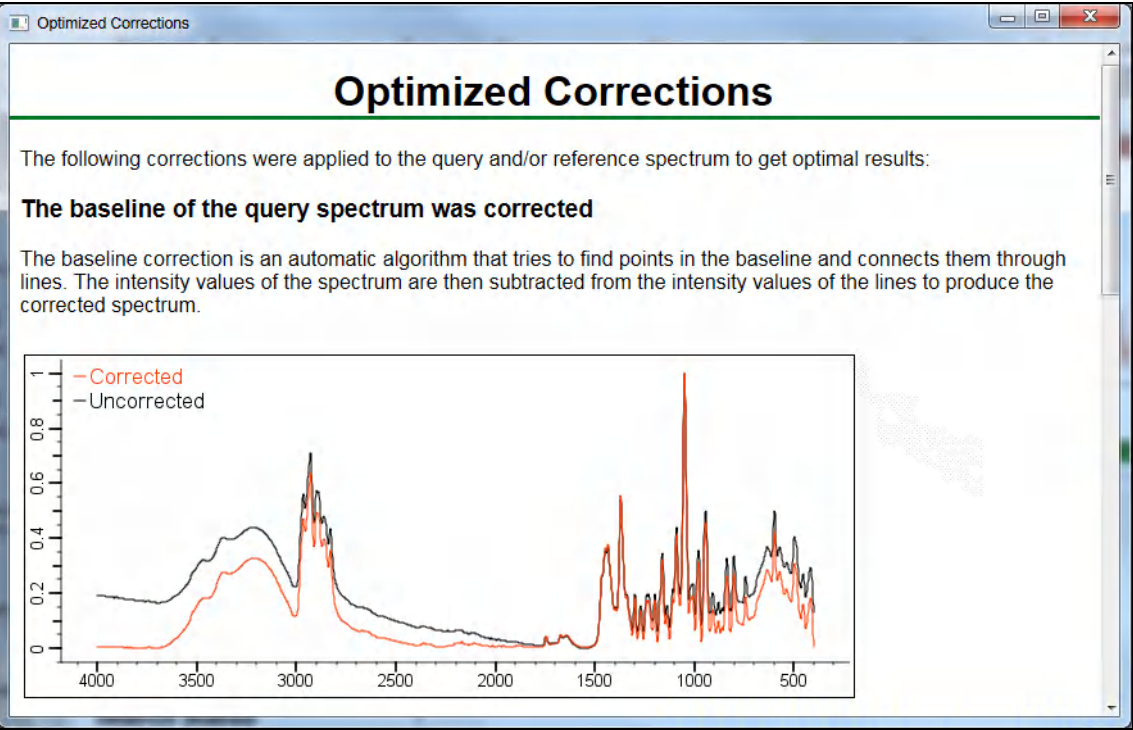
	Action	Result
1	Open the KnowItAll <b>ID Expert</b> application, either by double-clicking its icon on the desktop (standalone) mode or by clicking its icon in the KnowItAll application.	The application opens and a Windows <b>Open</b> dialog box pops-up.
2	Close the <b>Open</b> dialog box, then choose <b>File &gt; Settings</b> .	<p>The <b>Settings</b> form opens.</p> 

	Action	Result
3	Select the <b>Optimized Corrections</b> tab.	 <p>By default, <b>Optimized Corrections</b> is enabled for IR, Near IR, Raman, and NMR spectra. With the <b>Optimized Corrections</b> checkbox enabled, you can specify which corrections you wish to apply for each spectral technique.</p>
4	Check to see if <b>Optimized Corrections</b> for IR is enabled.  Click <b>OK</b> .	The <b>Settings</b> form closes. The word "None" shows under <b>Optimized Corrections</b> on the main KnowItAll ID Expert window.

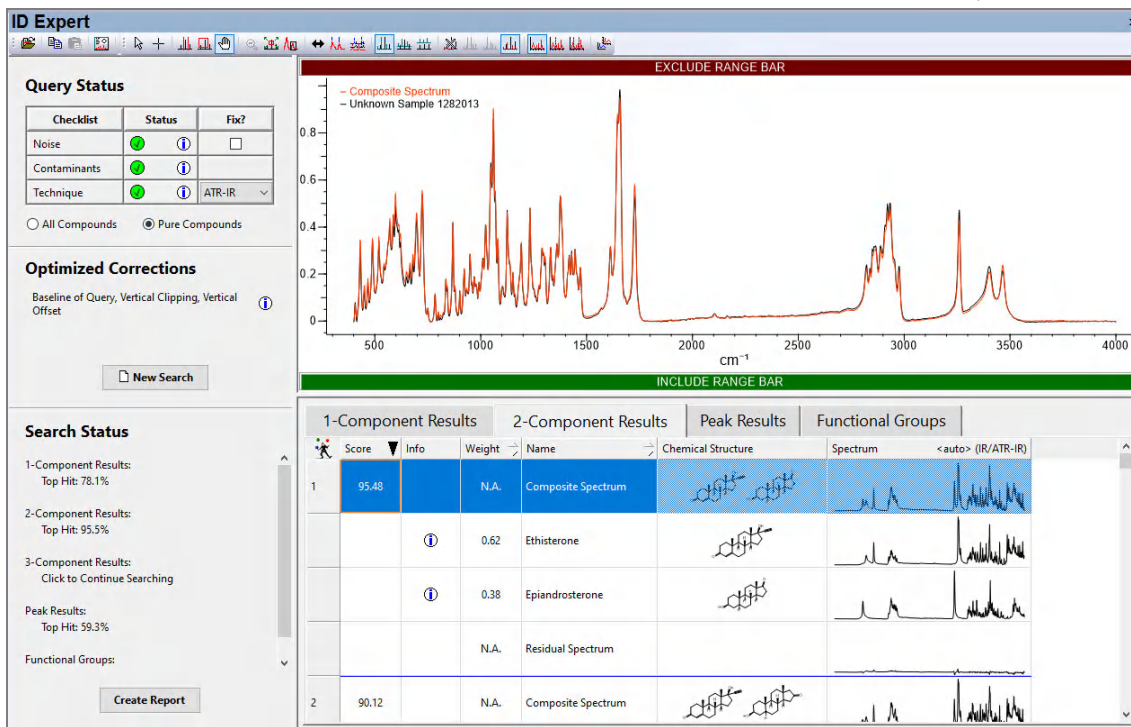
	Action	Result
5	<ul style="list-style-type: none"><li>Click <b>New Search</b> in the middle left of the window</li><li>Navigate to KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; Simple Spectrum Search &gt; ID Expert – IR</li><li>Select <b>2 - ATR-IR of Unknown Sample 8675309.irf</b>.</li><li>Check <b>Imported spectrum is ATR-IR</b></li><li>Click <b>Open</b>.</li></ul>	<p>User is prompted for a decision to send the spectrum to the secure Wiley web service for designer drug classification.</p> 

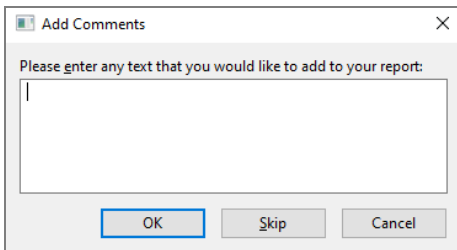
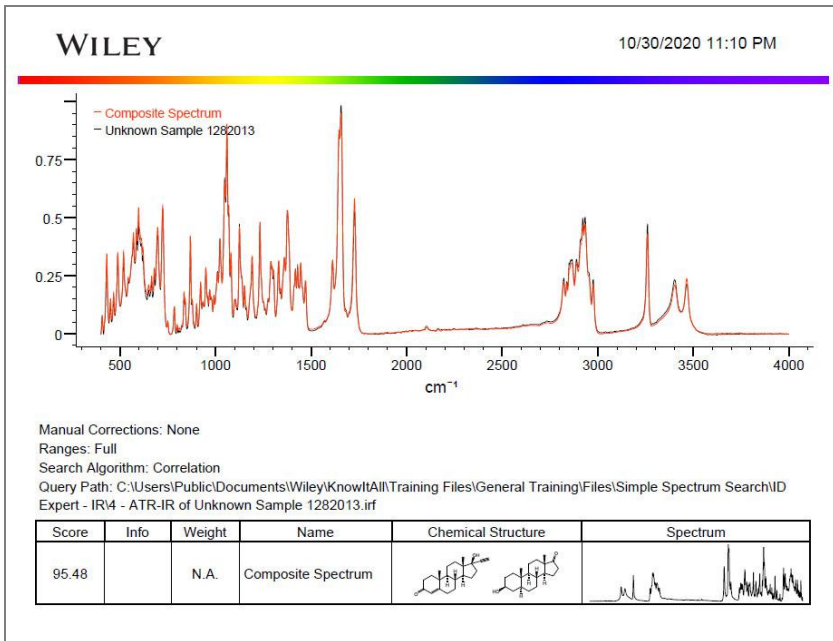
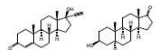

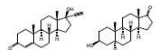

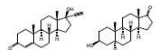

	Action	Result
6	Click either <b>Yes</b> or <b>No</b>	<p>The search proceeds automatically.</p>  <p>If user selected “Yes” in step 5, and the designer drug classification service return match score above <b>Classification Threshold</b> in step 2, then the <b>Classification</b> tab is displayed in result table, otherwise, you would not see it.</p> <p>The <b>Score</b> is the Hit Quality Index (<b>HQI</b>) in 100% unit – a comparison of reference spectrum to query spectrum.</p>
7	Click the <b>Classification</b> tab.	 <p>This spectrum is classified as a “Steroids” spectrum. This <b>score</b> measures probability for the classification.</p>



	Action	Result
8	Click the information icon ⓘ in the main window's <b>Optimized Corrections</b> section.	<p>The <b>Optimized Corrections</b> window opens.</p>  <p>Scroll down to view information about all of the optimized corrections that were applied.</p>

**Example 2: 4-ATR-IR of Unknown Sample 1282013.irf**

	Action	Result
1	Click <b>New Search</b> .	A Windows <b>Open</b> dialog box displays.
2	Open the spectral file <b>4-ATR-IR of Unknown Sample 1282013.irf</b> .  Click <b>No</b> at the prompt for submitting the spectrum to Wiley's secure classification server.	The search proceeds automatically: There is no excellent 1-Component match, and KnowItAll ID Expert automatically examines multiple component matches.
3	Allow the search to complete.	The <b>2-Component Results</b> tab under <b>Search Status</b> flashes, indicating that a good match has been found.
4	Click the <b>2-Component Results</b> tab.	The Composite Spectrum, individual component spectra, and Residual Spectrum are displayed: 

	Action	Result												
5	Click <b>Create Report</b> below the <b>Search Status</b> section.	<p>The <b>Add Comments</b> dialog box opens.</p> 												
6	Click <b>OK</b> .	<p>The report is created, and automatically opens in the Adobe Acrobat Reader:</p>  <table><tr><th>Score</th><th>Info</th><th>Weight</th><th>Name</th><th>Chemical Structure</th><th>Spectrum</th></tr><tr><td>95.48</td><td></td><td>N.A.</td><td>Composite Spectrum</td><td></td><td></td></tr></table>	Score	Info	Weight	Name	Chemical Structure	Spectrum	95.48		N.A.	Composite Spectrum		
Score	Info	Weight	Name	Chemical Structure	Spectrum									
95.48		N.A.	Composite Spectrum											

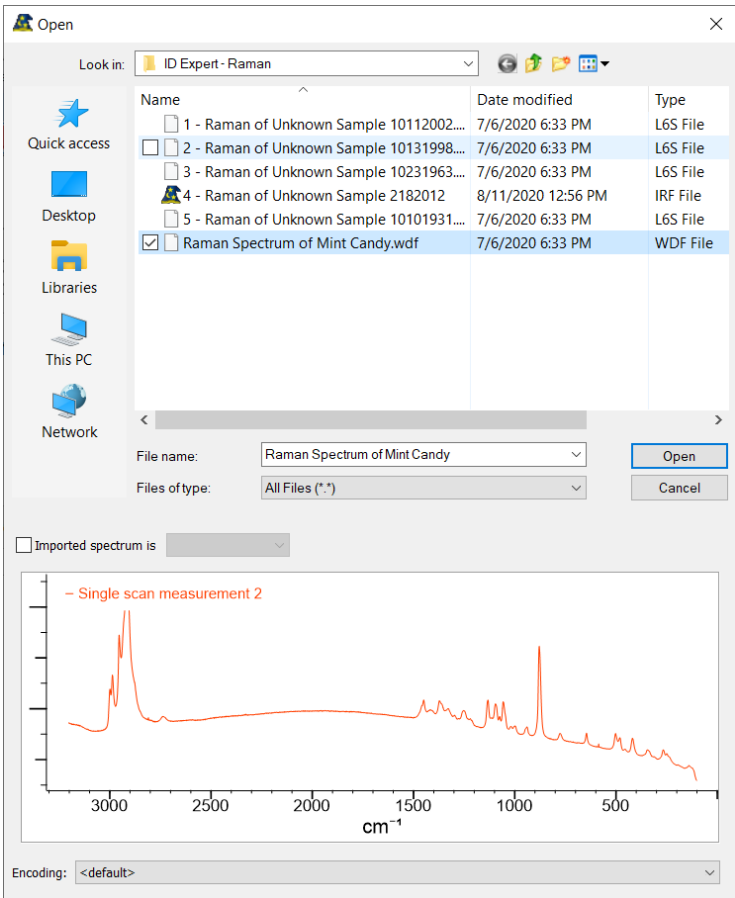
**Example 3: Deformulation Example.irf**

	Action	Result
1	Click <b>New Search</b> .	A Windows <b>Open</b> dialog box displays.
2	<ul style="list-style-type: none"><li>• Navigate to KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; Simple Spectrum Search &gt; Deformulation</li><li>• Select <b>Deformulation Example.irf</b></li><li>• Click <b>Open</b></li><li>• Click <b>No</b> at the prompt for submitting the spectrum to Wiley's secure classification server.</li></ul>	The search proceeds automatically: A perfect match is found – AKOLOUN S223-HM8. However, it is unclear what this material is made of.
3	Click the radio button <b>Pure Compounds</b>	ID Expert performs another search, but only on pure organic and inorganic chemical spectra.


	Action	Result
4	Click the <b>2-Component Results</b> tab.	<div>The Composite Spectrum, individual chemical component spectra, and Residual Spectrum are displayed. The sample is possibly made up of NYLON and Calcium salt:</div> <div><div><div><div><div><div>1</div><div>2</div><div>3</div><div>4</div><div>5</div><div>6</div><div>7</div><div>8</div><div>9</div><div>10</div><div>11</div><div>12</div><div>13</div><div>14</div><div>15</div><div>16</div><div>17</div><div>18</div><div>19</div><div>20</div><div>21</div><div>22</div><div>23</div><div>24</div><div>25</div><div>26</div><div>27</div><div>28</div><div>29</div><div>30</div><div>31</div><div>32</div><div>33</div><div>34</div><div>35</div><div>36</div><div>37</div><div>38</div><div>39</div><div>40</div><div>41</div><div>42</div><div>43</div><div>44</div><div>45</div><div>46</div><div>47</div><div>48</div><div>49</div><div>50</div><div>51</div><div>52</div><div>53</div><div>54</div><div>55</div><div>56</div><div>57</div><div>58</div><div>59</div><div>60</div><div>61</div><div>62</div><div>63</div><div>64</div><div>65</div><div>66</div><div>67</div><div>68</div><div>69</div><div>70</div><div>71</div><div>72</div><div>73</div><div>74</div><div>75</div><div>76</div><div>77</div><div>78</div><div>79</div><div>80</div><div>81</div><div>82</div><div>83</div><div>84</div><div>85</div><div>86</div><div>87</div><div>88</div><div>89</div><div>90</div><div>91</div><div>92</div><div>93</div><div>94</div><div>95</div><div>96</div><div>97</div><div>98</div><div>99</div><div>100</div><div>101</div><div>102</div><div>103</div><div>104</div><div>105</div><div>106</div><div>107</div><div>108</div><div>109</div><div>110</div><div>111</div><div>112</div><div>113</div><div>114</div><div>115</div><div>116</div><div>117</div><div>118</div><div>119</div><div>120</div><div>121</div><div>122</div><div>123</div><div>124</div><div>125</div><div>126</div><div>127</div><div>128</div><div>129</div><div>130</div><div>131</div><div>132</div><div>133</div><div>134</div><div>135</div><div>136</div><div>137</div><div>138</div><div>139</div><div>140</div><div>141</div><div>142</div><div>143</div><div>144</div><div>145</div><div>146</div><div>147</div><div>148</div><div>149</div><div>150</div><div>151</div><div>152</div><div>153</div><div>154</div><div>155</div><div>156</div><div>157</div><div>158</div><div>159</div><div>160</div><div>161</div><div>162</div><div>163</div><div>164</div><div>165</div><div>166</div><div>167</div><div>168</div><div>169</div><div>170</div><div>171</div><div>172</div><div>173</div><div>174</div><div>175</div><div>176</div><div>177</div><div>178</div><div>179</div><div>180</div><div>181</div><div>182</div><div>183</div><div>184</div><div>185</div><div>186</div><div>187</div><div>188</div><div>189</div><div>190</div><div>191</div><div>192</div><div>193</div><div>194</div><div>195</div><div>196</div><div>197</div><div>198</div><div>199</div><div>200</div><div>201</div><div>202</div><div>203</div><div>204</div><div>205</div><div>206</div><div>207</div><div>208</div><div>209</div><div>210</div><div>211</div><div>212</div><div>213</div><div>214</div><div>215</div><div>216</div><div>217</div><div>218</div><div>219</div><div>220</div><div>221</div><div>222</div><div>223</div><div>224</div><div>225</div><div>226</div><div>227</div><div>228</div><div>229</div><div>230</div><div>231</div><div>232</div><div>233</div><div>234</div><div>235</div><div>236</div><div>237</div><div>238</div><div>239</div><div>240</div><div>241</div><div>242</div><div>243</div><div>244</div><div>245</div><div>246</div><div>247</div><div>248</div><div>249</div><div>250</div><div>251</div><div>252</div><div>253</div><div>254</div><div>255</div><div>256</div><div>257</div><div>258</div><div>259</div><div>260</div><div>261</div><div>262</div><div>263</div><div>264</div><div>265</div><div>266</div><div>267</div><div>268</div><div>269</div><div>270</div><div>271</div><div>272</div><div>273</div><div>274</div><div>275</div><div>276</div><div>277</div><div>278</div><div>279</div><div>280</div><div>281</div><div>282</div><div>283</div><div>284</div><div>285</div><div>286</div><div>287</div><div>288</div><div>289</div><div>290</div><div>291</div><div>292</div><div>293</div><div>294</div><div>295</div><div>296</div><div>297</div><div>298</div><div>299</div><div>300</div><div>301</div><div>302</div><div>303</div><div>304</div><div>305</div><div>306</div><div>307</div><div>308</div><div>309</div><div>310</div><div>311</div><div>312</div><div>313</div><div>314</div><div>315</div><div>316</div><div>317</div><div>318</div><div>319</div><div>320</div><div>321</div><div>322</div><div>323</div><div>324</div><div>325</div><div>326</div><div>327</div><div>328</div><div>329</div><div>330</div><div>331</div><div>332</div><div>333</div><div>334</div><div>335</div><div>336</div><div>337</div><div>338</div><div>339</div><div>340</div><div>341</div><div>342</div><div>343</div><div>344</div><div>345</div><div>346</div><div>347</div><div>348</div><div>349</div><div>350</div><div>351</div><div>352</div><div>353</div><div>354</div><div>355</div><div>356</div><div>357</div><div>358</div><div>359</div><div>360</div><div>361</div><div>362</div><div>363</div><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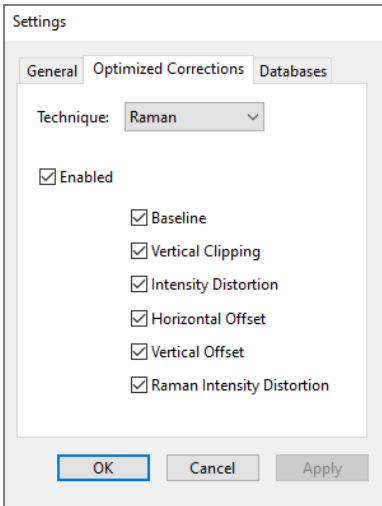


**Example 4: 5 - Raman of Mint Candy.wdf**

	Action	Result
1	Click <b>New Search</b> .	A Windows <b>Open</b> dialog box displays.
2	<ul style="list-style-type: none"> <li>Navigate to KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; Simple Spectrum Search &gt; ID Expert – Raman</li> <li>Select the spectral file <b>Raman Spectrum of Mint Candy.wdf</b></li> <li>Click <b>Open</b></li> </ul>	<p>From the preview, this is not a “good” spectrum.</p> 

Action	Result																																				
4 Allow the search to complete, then scroll through the <b>Search Status</b> area.	<div>We have a very good match:</div> <div><div><div><div><div>ID Expert</div><div><div><div><div><div>Query Status</div><div><table><tr><th>Checklist</th><th>Status</th><th>Fix?</th></tr><tr><td>Noise</td><td><div><div></div></div></td><td><div><div></div></div></td></tr></table></div><div><div>Optimized Corrections</div><div>Baseline of Query, Baseline of Reference, Intensity Distortion, Vertical Clipping, Horizontal Offset, Vertical Offset, Raman Intensity Distortion</div></div></div><div><div>New Search</div></div></div><div><div><div>Search Status</div><div><div>1-Component Results: Top Hit: 92.1%</div><div>2-Component Results: Click to Continue Searching</div><div>Classifications: No Hits Found</div><div>Peak Results: Top Hit: 78.2%</div><div>Functional Groups: 10 Functional Groups Found</div></div><div>Create Report</div></div></div><div><div><div><div>1-Component Results</div><div>Peak Results</div><div>Functional Groups</div></div><table><tr><th></th><th>Score</th><th>Info</th><th>Name</th><th>Chemical Structure</th></tr><tr><td>1</td><td>92.14</td><td><div><div></div></div></td><td>D-Sorbitol</td><td><div><div></div></div></td></tr><tr><td>2</td><td>74.10</td><td><div><div></div></div></td><td>Ethyl levulinate</td><td><div><div></div></div></td></tr><tr><td>3</td><td>73.67</td><td><div><div></div></div></td><td>Mucopolysaccharides</td><td></td></tr><tr><td>4</td><td>73.07</td><td><div><div></div></div></td><td>Calcium lactobionate monohydrate</td><td><div><div></div></div></td></tr><tr><td>5</td><td>72.97</td><td><div><div></div></div></td><td>p-(Vinyl alcohol)</td><td><div><div></div></div></td></tr></table></div><div><div><div><div><div>~ FFRX #439: D-Sorbitol</div><div>~ Single scan measurement 2</div></div><div><div>300000</div><div>250000</div><div>200000</div><div>150000</div><div>100000</div><div>50000</div><div>0</div></div><div><div>500</div><div>1000</div><div>1500</div><div>2000</div><div>2500</div><div>3000</div></div><div>cm<sup>-1</sup></div></div><div>EXCLUDE RANGE BAR</div><div>INCLUDE RANGE BAR</div></div></div></div></div></div></div></div></div></div>	Checklist	Status	Fix?	Noise	<div><div></div></div>	<div><div></div></div>		Score	Info	Name	Chemical Structure	1	92.14	<div><div></div></div>	D-Sorbitol	<div><div></div></div>	2	74.10	<div><div></div></div>	Ethyl levulinate	<div><div></div></div>	3	73.67	<div><div></div></div>	Mucopolysaccharides		4	73.07	<div><div></div></div>	Calcium lactobionate monohydrate	<div><div></div></div>	5	72.97	<div><div></div></div>	p-(Vinyl alcohol)	<div><div></div></div>
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	Action	Result
6	Click the  for <b>Optimized Corrections</b>	<div data-bbox="688 321 1816 922"><p><b>The Raman-specific intensity distortions were corrected by applying an adjustment factor of 60.4% to all regions above 2475.1 cm<sup>-1</sup></b></p><p>According to the ASTM E2911-13 Standard Guide for Relative Intensity Correction of Raman Spectrometers, "Generally, Raman spectra measured using grating-based dispersive or Fourier transform Raman spectrometers have not been corrected for the instrumental response (spectral responsivity of the detection system). Raman spectra obtained with different instruments may show significant variations in the measured relative peak intensities of a sample compound. This is mainly as a result of differences in their wavelength-dependent optical transmission and detector efficiencies. These variations can be particularly large when widely different laser excitation wavelengths are used, but can occur when the same laser excitation is used and spectra of the same compound are compared between instruments."</p><p>To compensate for these intensity variations when comparing Raman spectra that may not have been corrected for instrumental response, the following equation introduces an adjustment factor R and is applied to all spectral regions above the wavenumber value mentioned above:</p><math display="block">I_c = I \cdot (100\% - R)</math><p>where <math>I_c</math> is the corrected intensity, and <math>I</math> is the original intensity.</p><p><b>The top 5.8% of the reference spectrum was clipped</b></p><p>The industry standard practice of normalizing spectra for matching the spectrum curve of an unknown sample to the spectra of known reference compounds does not always produce optimal results. Smaller bands may be obfuscated by the search algorithm if the intensities of the largest peaks in the two spectra compared do not have identical Y-axis intensities. To overcome this problem, the top parts of the largest peaks have been clipped.</p></div> <p>We see that all kinds of spectrum correction have been done for the first hit. One unique to KnowItAll is the "Raman-specific intensity distortion.</p>

	Action	Result
7	Go to <b>File &gt; Settings, Optimize Correction</b> tab	<p>These are the corrections done for Raman sample and reference spectra:</p> 
8	As an exercise, one can check off <b>Enabled</b> and repeat the search to see a very different result.	

# **KnowItAll Software Training**

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## Searching

# Searching

## How to Perform a Basic Spectral Search

### Purpose

This exercise demonstrates how to perform a spectral search. In this exercise, we will perform a single spectral search, where we compare the IR spectrum of an unknown compound to IR spectra in a single database.

### Objectives

This exercise will teach you:

- How to select databases for searching;
- How to use search masks;
- How to configure and perform an IR spectral search.

### Background

Spectral searching against reference databases is frequently used in both the analysis of unknown compounds and compound verification.


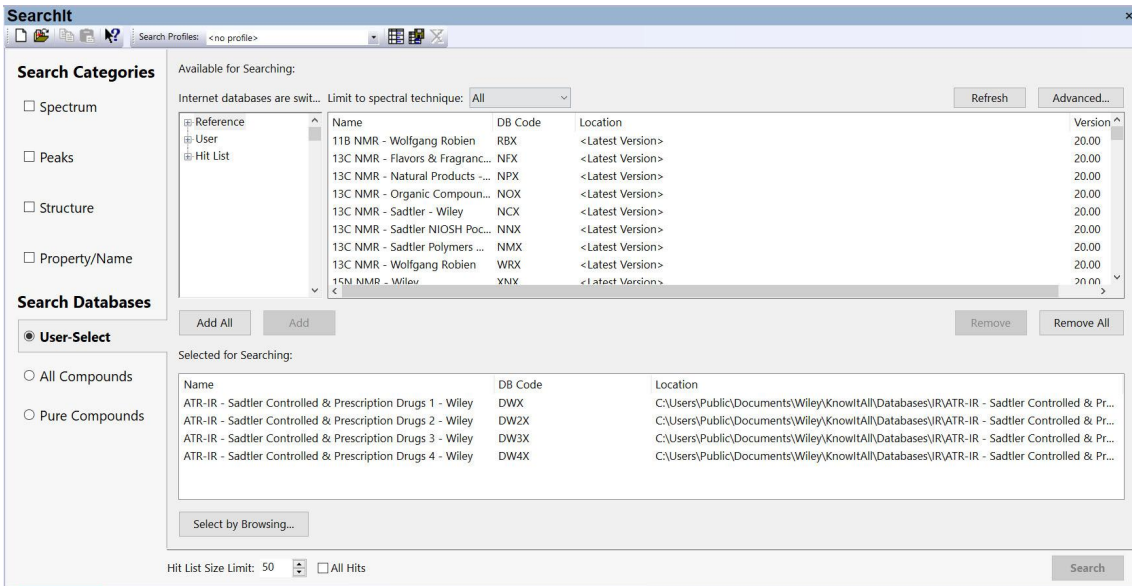
#### *Training Files Used In This Lesson*

- Acetic anhydride.dx
- Spectral Search Example.jdx.
- Multi-Technique Sadtler Demo Database – Wiley [DEMO].sdbx

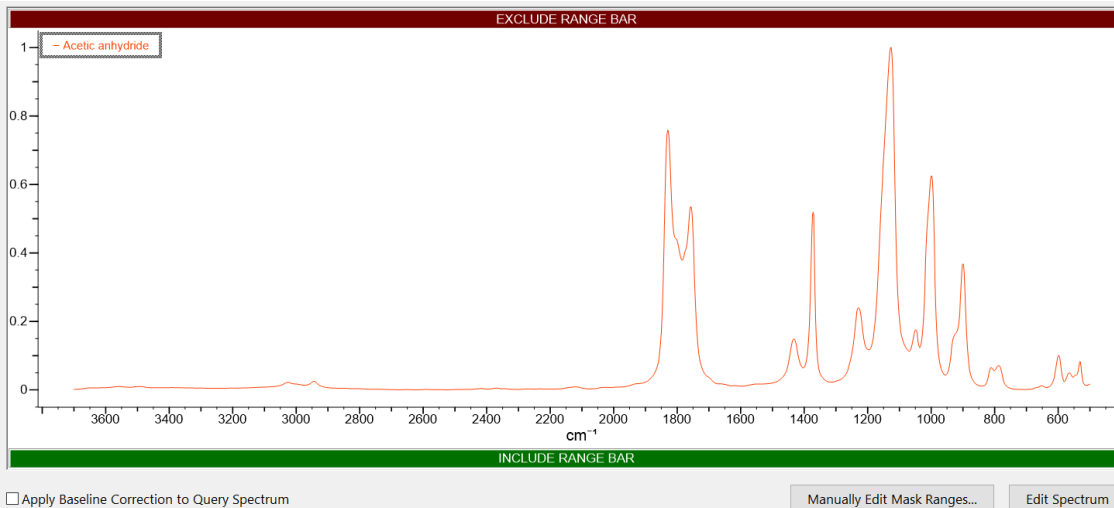
#### *KnowItAll Applications Used*

- SearchIt™
- MineIt™
- [optional] ProcessIt™

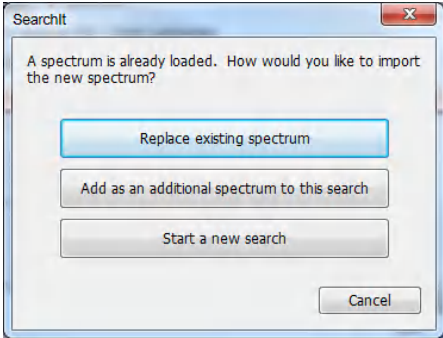

## Create a new search

	Action	Result																																																																	
1	<p>Do one of the following:</p> <ul style="list-style-type: none"><li>If the <b>SearchIt</b> application is not open, navigate to the <b>Data</b> toolbox and click its icon.</li><li>If the <b>SearchIt</b> application is already open, click the <b>Close</b> button  (located in the upper right corner) to close the current search.</li></ul>	<p>If <b>SearchIt</b> application's <b>User-Select</b> (under <b>Search Databases</b>) tab is selected, the <b>Selected for Searching</b> list displays the databases last used.</p>  <p><b>Search Categories</b></p> <p><input type="checkbox"/> Spectrum</p> <p><input type="checkbox"/> Peaks</p> <p><input type="checkbox"/> Structure</p> <p><input type="checkbox"/> Property/Name</p> <p><b>Search Databases</b></p> <p><input checked="" type="radio"/> <b>User-Select</b></p> <p><input type="radio"/> All Compounds</p> <p><input type="radio"/> Pure Compounds</p> <p><b>Available for Searching:</b></p> <p>Internet databases are swit... Limit to spectral technique: All</p> <table><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>11B NMR - Wolfgang Robien</td><td>RBX</td><td>&lt;Latest Version&gt;</td><td>20.00</td></tr><tr><td>Hit List</td><td>13C NMR - Flavors &amp; Fragranc...</td><td>NFX</td><td>&lt;Latest Version&gt;</td><td>20.00</td></tr><tr><td></td><td>13C NMR - Natural Products ...</td><td>NPX</td><td>&lt;Latest Version&gt;</td><td>20.00</td></tr><tr><td></td><td>13C NMR - Organic Compoun...</td><td>NOX</td><td>&lt;Latest Version&gt;</td><td>20.00</td></tr><tr><td></td><td>13C NMR - Sadtler - Wiley</td><td>NCX</td><td>&lt;Latest Version&gt;</td><td>20.00</td></tr><tr><td></td><td>13C NMR - Sadtler NIOSH Poc...</td><td>NNX</td><td>&lt;Latest Version&gt;</td><td>20.00</td></tr><tr><td></td><td>13C NMR - Sadtler Polymers ...</td><td>NMX</td><td>&lt;Latest Version&gt;</td><td>20.00</td></tr><tr><td></td><td>13C NMR - Wolfgang Robien</td><td>WRX</td><td>&lt;Latest Version&gt;</td><td>20.00</td></tr><tr><td></td><td>15N NMR - Wiley</td><td>YNY</td><td>&lt;Latest Version&gt;</td><td>20.00</td></tr></tbody></table> <p><b>Selected for Searching:</b></p> <table><thead><tr><th>Name</th><th>DB Code</th><th>Location</th></tr></thead><tbody><tr><td>ATR-IR - Sadtler Controlled &amp; Prescription Drugs 1 - Wiley</td><td>DWX</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\ATR-IR - Sadtler Controlled &amp; Pr...</td></tr><tr><td>ATR-IR - Sadtler Controlled &amp; Prescription Drugs 2 - Wiley</td><td>DW2X</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\ATR-IR - Sadtler Controlled &amp; Pr...</td></tr><tr><td>ATR-IR - Sadtler Controlled &amp; Prescription Drugs 3 - Wiley</td><td>DW3X</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\ATR-IR - Sadtler Controlled &amp; Pr...</td></tr><tr><td>ATR-IR - Sadtler Controlled &amp; Prescription Drugs 4 - Wiley</td><td>DW4X</td><td>C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\ATR-IR - Sadtler Controlled &amp; Pr...</td></tr></tbody></table> <p>Hit List Size Limit: 50 <input type="checkbox"/> All Hits</p>	Reference	Name	DB Code	Location	Version	User	11B NMR - Wolfgang Robien	RBX	<Latest Version>	20.00	Hit List	13C NMR - Flavors & Fragranc...	NFX	<Latest Version>	20.00		13C NMR - Natural Products ...	NPX	<Latest Version>	20.00		13C NMR - Organic Compoun...	NOX	<Latest Version>	20.00		13C NMR - Sadtler - Wiley	NCX	<Latest Version>	20.00		13C NMR - Sadtler NIOSH Poc...	NNX	<Latest Version>	20.00		13C NMR - Sadtler Polymers ...	NMX	<Latest Version>	20.00		13C NMR - Wolfgang Robien	WRX	<Latest Version>	20.00		15N NMR - Wiley	YNY	<Latest Version>	20.00	Name	DB Code	Location	ATR-IR - Sadtler Controlled & Prescription Drugs 1 - Wiley	DWX	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\ATR-IR - Sadtler Controlled & Pr...	ATR-IR - Sadtler Controlled & Prescription Drugs 2 - Wiley	DW2X	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\ATR-IR - Sadtler Controlled & Pr...	ATR-IR - Sadtler Controlled & Prescription Drugs 3 - Wiley	DW3X	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\ATR-IR - Sadtler Controlled & Pr...	ATR-IR - Sadtler Controlled & Prescription Drugs 4 - Wiley	DW4X	C:\Users\Public\Documents\Wiley\KnowItAll\Databases\IR\ATR-IR - Sadtler Controlled & Pr...
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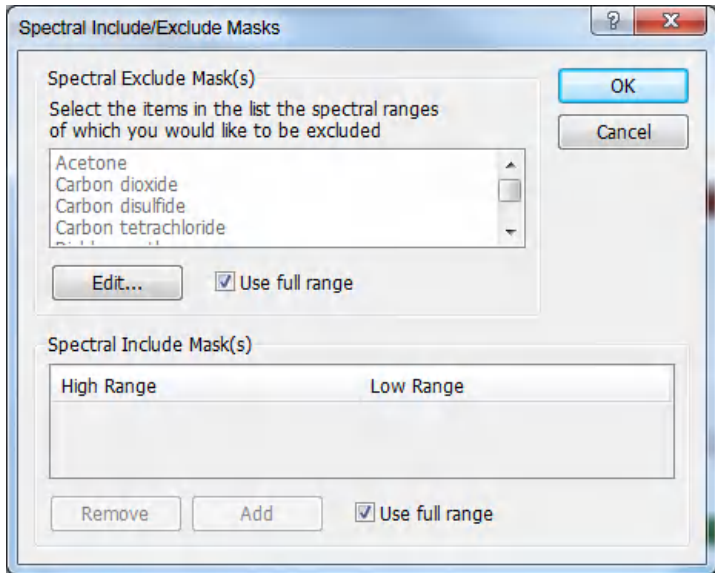
## Open the spectral file

	Action	Result
1	Click the <b>Spectrum</b> button under <b>Search Categories</b>	An <b>Open</b> dialog box appears.
2	<ul style="list-style-type: none"> <li>Navigate to <b>KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; Searching</b></li> <li>Select <b>Acetic anhydride.dx</b>.</li> </ul> <p>The lower part of the dialog box displays a preview of the selected spectrum.</p> <p>You can use the <b>Files of Type</b> filter to limit the display to specific types of files, such as JCAMP (*.dx, *.jdx), or to display all files (*.*)</p> <ul style="list-style-type: none"> <li>Click <b>Open</b>.</li> </ul>	<p>The spectrum is recognized as an IR spectrum and displayed in the spectral pane in the <b>Spectrum</b> tab.</p>  <p>The spectrum is displayed in the spectral pane. The x-axis represents wavenumber in cm⁻¹, ranging from 3600 to 600. The y-axis represents transmittance, ranging from 0 to 1. The spectrum shows several sharp peaks, with the most prominent ones at approximately 1780, 1720, 1270, 1100, and 720 cm⁻¹. The spectrum is labeled 'Acetic anhydride' in the top left corner. The plot area is bounded by a red 'EXCLUDE RANGE BAR' at the top and a green 'INCLUDE RANGE BAR' at the bottom. Below the plot, there is a checkbox labeled 'Apply Baseline Correction to Query Spectrum' and two buttons: 'Manually Edit Mask Ranges...' and 'Edit Spectrum'.</p> <p><b>NOTE:</b> You can use the checkbox at the bottom to apply baseline correction to the query spectrum, if desired. However, KnowItAll automatically corrects baseline.</p>
3	To select a different spectral file, press Ctrl+O.	An <b>Open</b> dialog box appears.

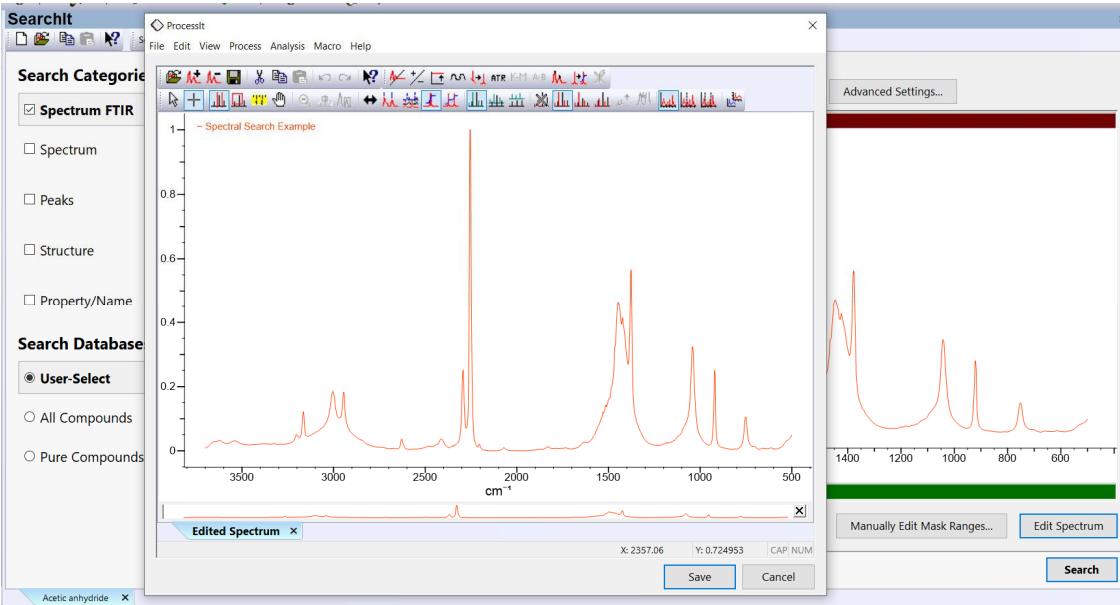


	Action	Result
4	Select <b>Spectral Search Example.jdx</b> from the training files' <b>Searching</b> folder. Click <b>Open</b> .	A message box appears and offers three choices 
5	Click <b>Replace existing spectrum</b> to close the message box and replace the previously displayed spectrum.	The new spectrum is displayed in the spectral pane. <b>Note:</b> You can also replace a search spectrum by clicking the SearchIt <b>Close</b> button  , then clicking the <b>Spectrum</b> button in the <b>Spectral</b> section of the <b>Search By</b> pane.

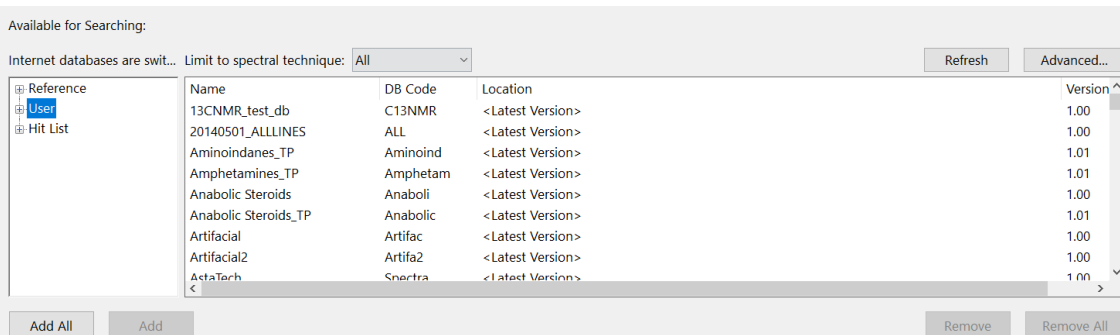
**Fine-tune before searching**

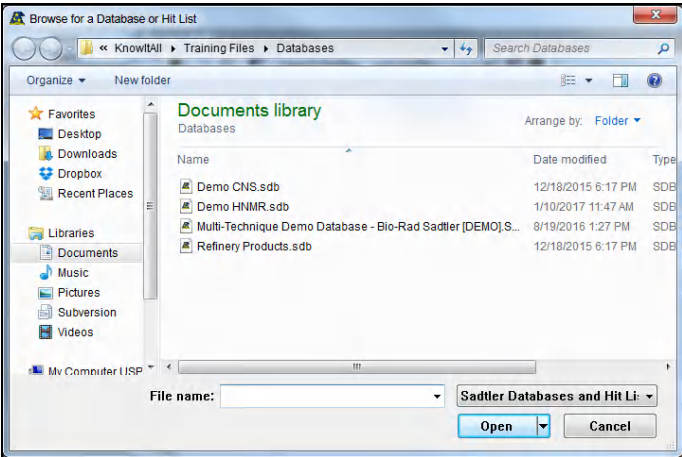
	Action	Result
1	Click <b>Manually Edit Mask Ranges</b> .	<p>The <b>Spectral Include/Exclude Masks</b> dialog box opens:</p>  <p><b>Note:</b> You can also click and drag in the <b>Spectral</b> pane's <b>Exclude Range Bar</b> and <b>Include Range Bar</b> after closing the <b>Spectral Include/Exclude Masks</b> window.</p>
2	Deselect the <b>Use full range</b> checkbox under the list of <b>Spectral Exclude Mask(s)</b> .	The list of pre-defined exclude masks becomes available. Select some to see how they work. The use of these masks will be demonstrated later in this lesson.

**Fine-tune before searching (continued)**

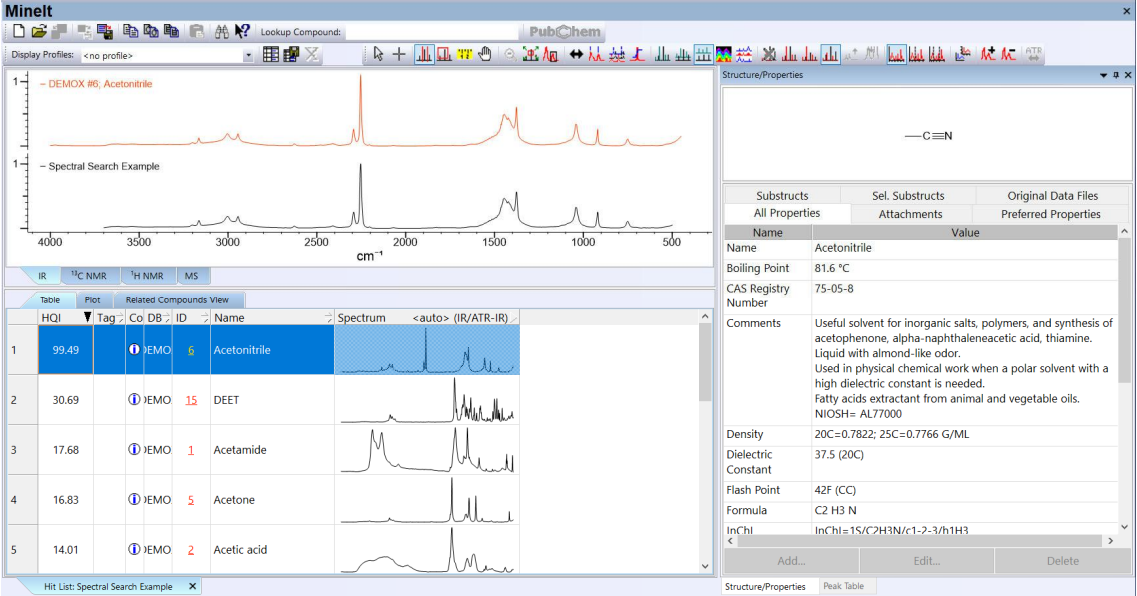
	Action	Result
3	Reselect the <b>Use full range</b> checkbox under the list of <b>Spectral Exclude Mask(s)</b> .	All Spectral Exclude Masks are removed from the spectrum.
4	Click <b>OK</b> to close the <b>Spectral Include/Exclude Masks</b> dialog box.	
5	Click <b>Edit Spectrum</b> at the bottom right of the spectral pane.	<p>The spectrum is transferred to the popped-up <b>ProcessIt</b> application, where you can correct potential searching problems and save the corrected spectrum into <b>SearchIt</b> spectrum pane.</p> 
6	Click <b>Cancel</b>	The spectrum is returned to the <b>SearchIt</b> application. Changes made in the <b>ProcessIt</b> IR application are not saved.

**Open the search database**


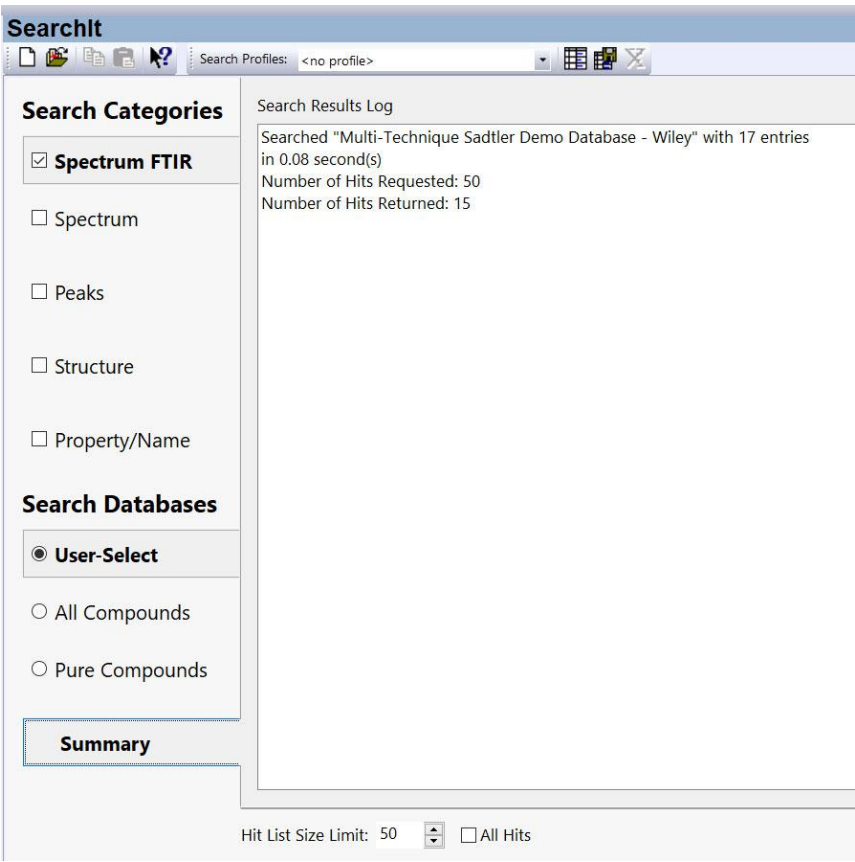

	Action	Result																																								
1	Click on <b>User-Select</b> under <b>Search Databases</b>	This option allows users to select the databases they want to search. Users can also include user-created databases in a search.																																								
2	If a list of databases already appears in the <b>Selected for Searching</b> pane at the bottom, click <b>Remove All</b> to clear this list.																																									
3	Expand each branch in the tree structure on the left of the window to display a particular database category - <b>Reference</b> , <b>User</b> , <b>Hit List</b> - and specify whether network, local, or all databases are displayed. The available databases are displayed at the right of the window.	<p>The <b>User</b> category is shown below:</p>  <p>Available for Searching:</p> <p>Internet databases are swit... Limit to spectral technique: All <span>Refresh</span> <span>Advanced...</span></p> <table><tr><th>Name</th><th>DB Code</th><th>Location</th><th>Version</th></tr><tr><td>13CNMR_test_db</td><td>C13NMR</td><td>&lt;Latest Version&gt;</td><td>1.00</td></tr><tr><td>20140501_ALLLINES</td><td>ALL</td><td>&lt;Latest Version&gt;</td><td>1.00</td></tr><tr><td>Aminoindanes_TP</td><td>Aminoind</td><td>&lt;Latest Version&gt;</td><td>1.01</td></tr><tr><td>Amphetamines_TP</td><td>Amphetam</td><td>&lt;Latest Version&gt;</td><td>1.01</td></tr><tr><td>Anabolic Steroids</td><td>Anaboli</td><td>&lt;Latest Version&gt;</td><td>1.00</td></tr><tr><td>Anabolic Steroids_TP</td><td>Anabolic</td><td>&lt;Latest Version&gt;</td><td>1.01</td></tr><tr><td>Artificial</td><td>Artifac</td><td>&lt;Latest Version&gt;</td><td>1.00</td></tr><tr><td>Artificial2</td><td>Artifa2</td><td>&lt;Latest Version&gt;</td><td>1.00</td></tr><tr><td>ArtifaTorch</td><td>Snertra</td><td>&lt;Latest Version&gt;</td><td>1.00</td></tr></table> <p><span>Add All</span> <span>Add</span> <span>Remove</span> <span>Remove All</span></p> <p><b>Note:</b> Your display may look different depending on whether or not you have access to databases available online. Click <b>Advanced</b> on the top right to open the <b>Advanced Options</b> dialog box, where you can control how you access online databases and add or remove local database locations. Click <b>Refresh</b> to update the display after settings are changed.</p>	Name	DB Code	Location	Version	13CNMR_test_db	C13NMR	<Latest Version>	1.00	20140501_ALLLINES	ALL	<Latest Version>	1.00	Aminoindanes_TP	Aminoind	<Latest Version>	1.01	Amphetamines_TP	Amphetam	<Latest Version>	1.01	Anabolic Steroids	Anaboli	<Latest Version>	1.00	Anabolic Steroids_TP	Anabolic	<Latest Version>	1.01	Artificial	Artifac	<Latest Version>	1.00	Artificial2	Artifa2	<Latest Version>	1.00	ArtifaTorch	Snertra	<Latest Version>	1.00
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ArtifaTorch	Snertra	<Latest Version>	1.00																																							

	Action	Result						
4	Click <b>Select by Browsing</b> button located at the lower left.	<p>The <b>Browse for a Database or Hit List</b> dialog box opens.</p> 						
5	Navigate to KnowItAll > Training Files > General Training > Databases and open <b>Multi-Technique Sadtler Demo Database – Wiley (DEMO)</b> .	<p>The database is displayed in the <b>Selected for Searching</b> list.</p> <p>Selected for Searching:</p> <table border="1" data-bbox="699 902 1902 1065"> <thead> <tr> <th>Name</th><th>DB Code</th><th>Location</th></tr> </thead> <tbody> <tr> <td>Multi-Technique Sadtler Demo Database - Wiley</td><td>DEMOX</td><td>C:\Users\ydsouza\OneDrive - Wiley\Desktop\KnowItAll Training Doc\2020 Training Doc\Kn...</td></tr> </tbody> </table> <p>Select by Browsing...</p>	Name	DB Code	Location	Multi-Technique Sadtler Demo Database - Wiley	DEMOX	C:\Users\ydsouza\OneDrive - Wiley\Desktop\KnowItAll Training Doc\2020 Training Doc\Kn...
Name	DB Code	Location						
Multi-Technique Sadtler Demo Database - Wiley	DEMOX	C:\Users\ydsouza\OneDrive - Wiley\Desktop\KnowItAll Training Doc\2020 Training Doc\Kn...						
6	<p>If necessary, clear the <b>All Hits</b> check box and set <b>Hit List Size Limit</b> to 50.</p> <p><b>Note:</b> When performing a spectral or peak search using more than two or three databases, it is better to limit the number of hits. Checking <b>All Hits</b> or using a larger value can drastically reduce search speed.</p>							

## Perform the search

	Action	Result
1	Click <b>Search</b> .	<p>The search results are automatically displayed in the <b>Minelt</b> application as a hit list, sorted by HQI. Both the unknown spectrum and the selected database spectrum are displayed.</p>  <p>The <b>HQI</b> (Hit Quality Index) value measures how close the reference spectrum is to that of query.</p>
	<b>TIPS</b>	<ul style="list-style-type: none"> <li>You can tag individual hits in the hit list as either "Accept", "Tentative", or "Reject" using the <b>Hit List &gt; Tag As</b> menu option, or by double clicking in the <b>Tag</b> column. You can then sort the hit list based on your tags.</li> <li>You can edit which columns in the hit list are displayed by right-clicking in the data table at the bottom left, selecting the <b>Edit Columns...</b> option, and selecting which columns you would like to display as well as the order in which they are displayed.</li> </ul>

## Perform the search (continued)

	Action	Result
2	Click the KnowItAll <b>Back</b> button  (located below the <b>File</b> menu).	<p>You are returned to the <b>SearchIt</b> application, where a <b>Summary</b> tab has been added to the main SearchIt window.</p> 
3	Click the KnowItAll <b>Forward</b> button  .	You are returned to <b>Minelt</b> and the hit list.

# Searching

---

## How to Create Search Profiles

### Purpose

This exercise demonstrates how to use search profiles.

---

### Objectives

This exercise will teach you:

- How to apply a search profile;
  - How to create a search profile.
- 

### Background

Search Profiles are pre-defined combinations of search parameters such as **Databases** and **Hit List Size Limit** that can be stored for later use. Using search profiles makes searching easier, especially when the same type of search is repeated.

#### *Training Files Used In This Lesson*


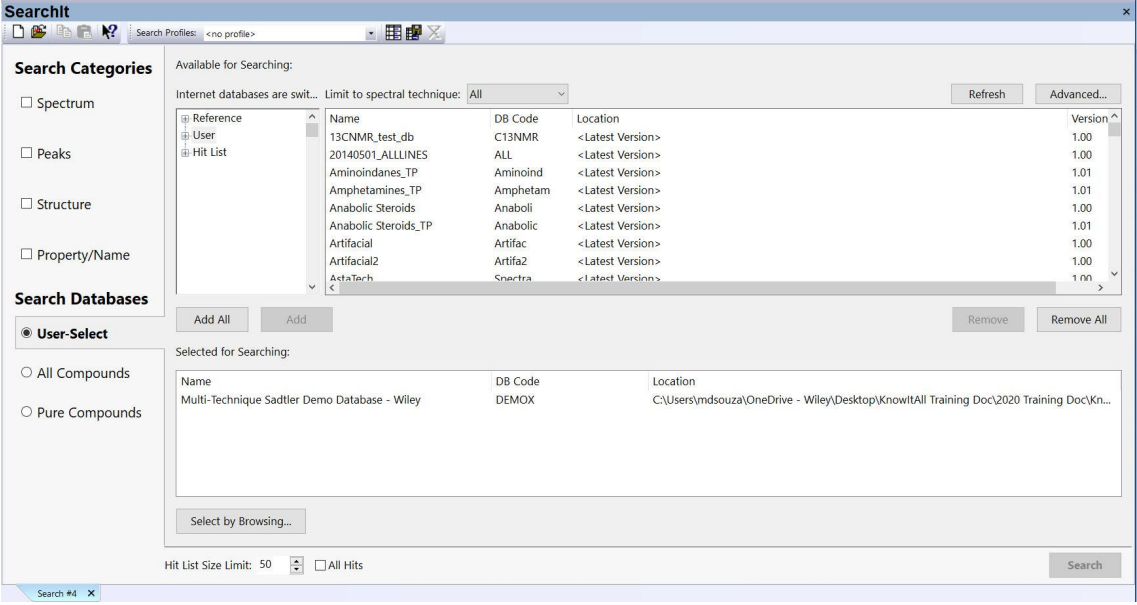

- none

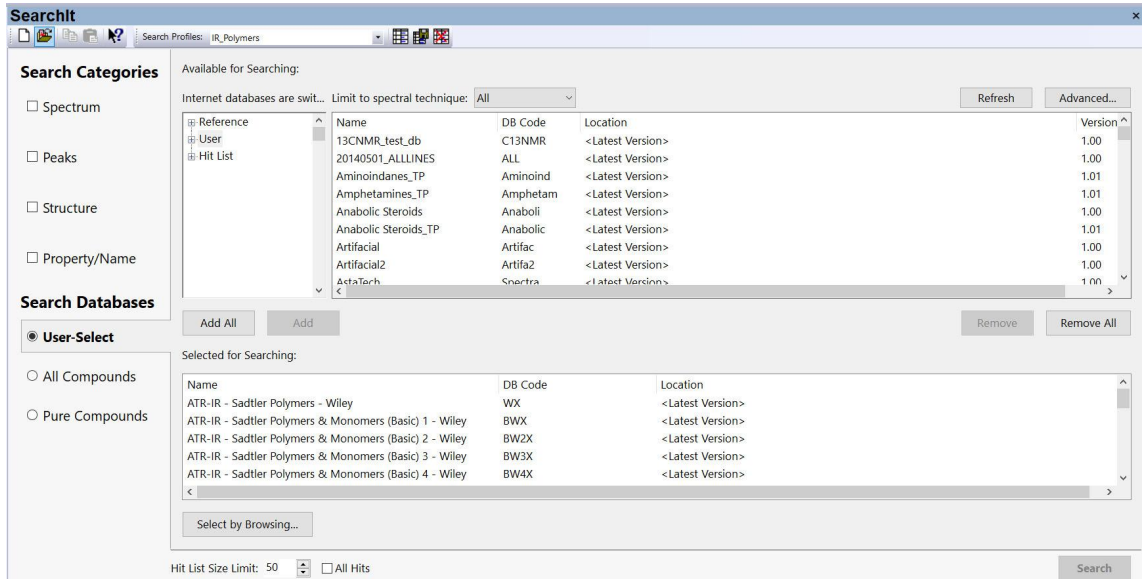
#### *KnowItAll Applications Used*

- SearchIt™



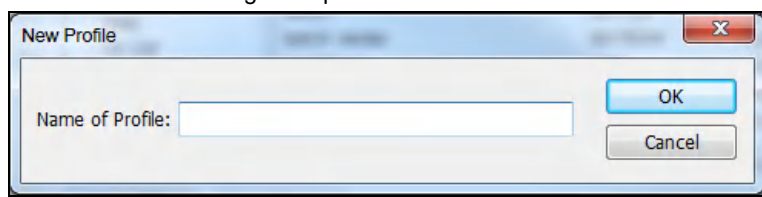



## Apply a pre-defined search profile

	Action	Result
1	Do one of the following: <ul style="list-style-type: none"> <li>If the <b>SearchIt</b> application is not open, navigate to the <b>Data</b> toolbox and click its icon.</li> <li>If the <b>SearchIt</b> application is already open, click the SearchIt Close button  to close the current search</li> </ul>	<p>The <b>SearchIt</b> application's <b>Databases</b> tab is displayed, and the <b>Selected for Searching</b> list displays the databases last used.</p> 
2	If databases are already selected for searching, click <b>Remove All</b> to clear the selections. You can also double-click individual entries to remove them from the list.	
3	If necessary, choose <b>View &gt; Profile Toolbar</b> to display Search Profiles tools.	

	Action	Result																																								
4	Select the <b>IR_Polymers</b> profile.	<p>Polymer databases are displayed in the <b>Selected for Searching</b> list.</p>  <p>The screenshot shows the SearchIt application window. On the left, under 'Search Categories', 'Spectrum' is selected. Under 'Search Databases', 'User-Select' is chosen. The 'Selected for Searching' list contains the following entries:</p> <table><tr><th>Name</th><th>DB Code</th><th>Location</th><th>Version</th></tr><tr><td>13CNMR_test_db</td><td>C13NMR</td><td>&lt;Latest Version&gt;</td><td>1.00</td></tr><tr><td>20140501_ALLLINES</td><td>ALL</td><td>&lt;Latest Version&gt;</td><td>1.00</td></tr><tr><td>Aminoindanes_TP</td><td>Aminoind</td><td>&lt;Latest Version&gt;</td><td>1.01</td></tr><tr><td>Amphetamines_TP</td><td>Amphetam</td><td>&lt;Latest Version&gt;</td><td>1.01</td></tr><tr><td>Anabolic Steroids</td><td>Anaboli</td><td>&lt;Latest Version&gt;</td><td>1.00</td></tr><tr><td>Anabolic Steroids_TP</td><td>Anabolic</td><td>&lt;Latest Version&gt;</td><td>1.01</td></tr><tr><td>Artifacial</td><td>Artifac</td><td>&lt;Latest Version&gt;</td><td>1.00</td></tr><tr><td>Artifacial2</td><td>Artifa2</td><td>&lt;Latest Version&gt;</td><td>1.00</td></tr><tr><td>ActaTech</td><td>Spectra</td><td>&lt;Latest Version&gt;</td><td>1.00</td></tr></table> <p>Below this list, the 'Selected for Searching' section shows a filtered list of ATR-IR databases from Sadtler Polymers &amp; Monomers (Basic) 1-4, all with DB Codes BWX, BW2X, BW3X, and BW4X, and all set to '&lt;Latest Version&gt;'. At the bottom, the 'Hit List Size Limit' is set to 50, and the 'All Hits' checkbox is unchecked.</p>	Name	DB Code	Location	Version	13CNMR_test_db	C13NMR	<Latest Version>	1.00	20140501_ALLLINES	ALL	<Latest Version>	1.00	Aminoindanes_TP	Aminoind	<Latest Version>	1.01	Amphetamines_TP	Amphetam	<Latest Version>	1.01	Anabolic Steroids	Anaboli	<Latest Version>	1.00	Anabolic Steroids_TP	Anabolic	<Latest Version>	1.01	Artifacial	Artifac	<Latest Version>	1.00	Artifacial2	Artifa2	<Latest Version>	1.00	ActaTech	Spectra	<Latest Version>	1.00
Name	DB Code	Location	Version																																							
13CNMR_test_db	C13NMR	<Latest Version>	1.00																																							
20140501_ALLLINES	ALL	<Latest Version>	1.00																																							
Aminoindanes_TP	Aminoind	<Latest Version>	1.01																																							
Amphetamines_TP	Amphetam	<Latest Version>	1.01																																							
Anabolic Steroids	Anaboli	<Latest Version>	1.00																																							
Anabolic Steroids_TP	Anabolic	<Latest Version>	1.01																																							
Artifacial	Artifac	<Latest Version>	1.00																																							
Artifacial2	Artifa2	<Latest Version>	1.00																																							
ActaTech	Spectra	<Latest Version>	1.00																																							

**Create a new search profile**

	Action	Result
1	Click the SearchIt <b>Close</b> button  , then click <b>Remove All</b> to clear the contents of the <b>Selected for Searching</b> list.	The <b>Databases</b> tab is displayed. The <b>Selected for Searching</b> list is empty.
2	Click the <b>Add a New Profile</b> button  on the <b>Profile</b> toolbar.	The <b>New Profile</b> dialog box opens: 
3	Type in the name of the new profile <b>[IR_Polymers_2]</b> , Click <b>OK</b> .	The new profile name is displayed in the <b>Search Profiles</b> text box.
4	Specify <b>IR</b> in the <b>Limit to spectral technique</b> drop-down list.	Only databases with IR spectra are displayed in the <b>Available for Searching</b> list. Note that <b>Multi-Technique Sadtler Demo Database – Wiley</b> is included in the list because it includes IR spectra.
5	In the <b>Available for Searching</b> list, click to select <b>IR – Polymers, Hummel – Wiley</b> (DB Code HUX) Click <b>Add</b> .	The IR – Polymers, Hummel – Wiley database is added to the <b>Selected for Searching</b> list.
6	In the <b>Available for Searching</b> list, double-click <b>IR – Polymers &amp; Monomers (Basic) 1 – Wiley</b> (DB Code BPX).	The IR – Polymers & Monomers (Basic) 1 – Wiley database is added to the <b>Selected for Searching</b> list.

	Action	Result
7	Continue adding databases BMX, CRX, DAX, FRX, and NEX.	
8	On the <b>Databases</b> tab, change the Hit List Size Limit to 10.	
9	Click the <b>Save Current Profile</b> button  on the Profile toolbar.	A message box asks if you wish to overwrite the current profile. Click <b>Yes</b> to save the new profile.
10	Close the current search, then select the newly-created <b>IR_Polymers_2</b> search profile.	The databases and search settings associated with this profile are displayed.

# Searching

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## How to Search a Database of Spectra or Chromatograms by Peak

### Purpose

This exercise demonstrates how to perform a peak search.

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### Objectives

This exercise will teach you:

- How to configure a peak search.
- 

### Background

The SearchIt application provides the capability of using peak information to perform a search of spectral or chromatographic data. This allows users to compare peak tables from databases to a peak table that you enter or extract from a spectrum.


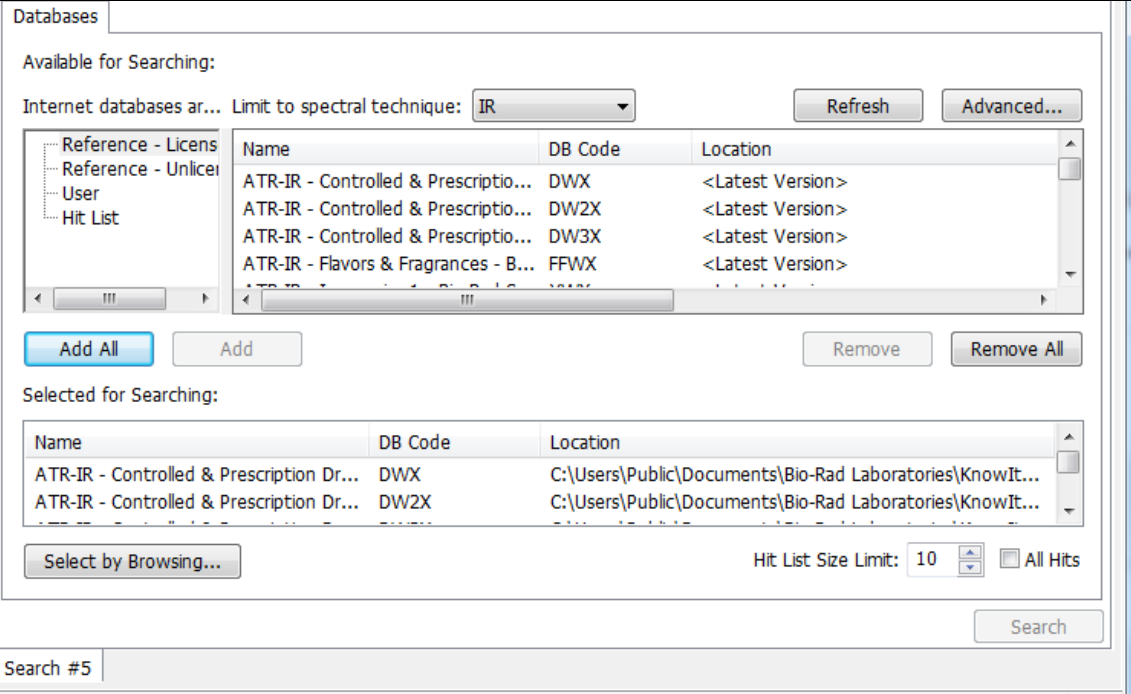
#### *Training Files Used in This Lesson*

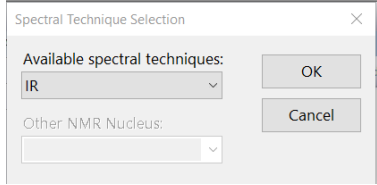
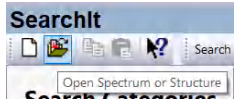
- Ethyl acrylate.dx

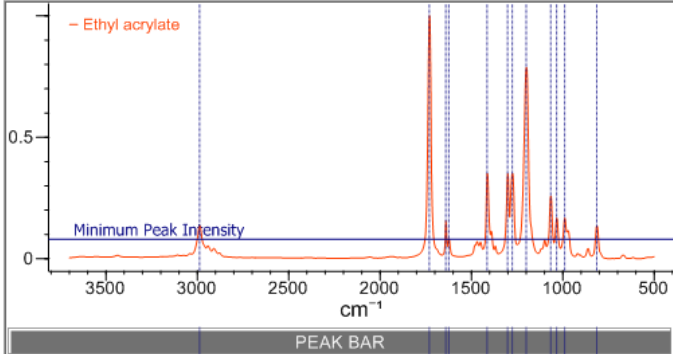
#### *KnowItAll Applications Used*

- SearchIt™
- Minelt™

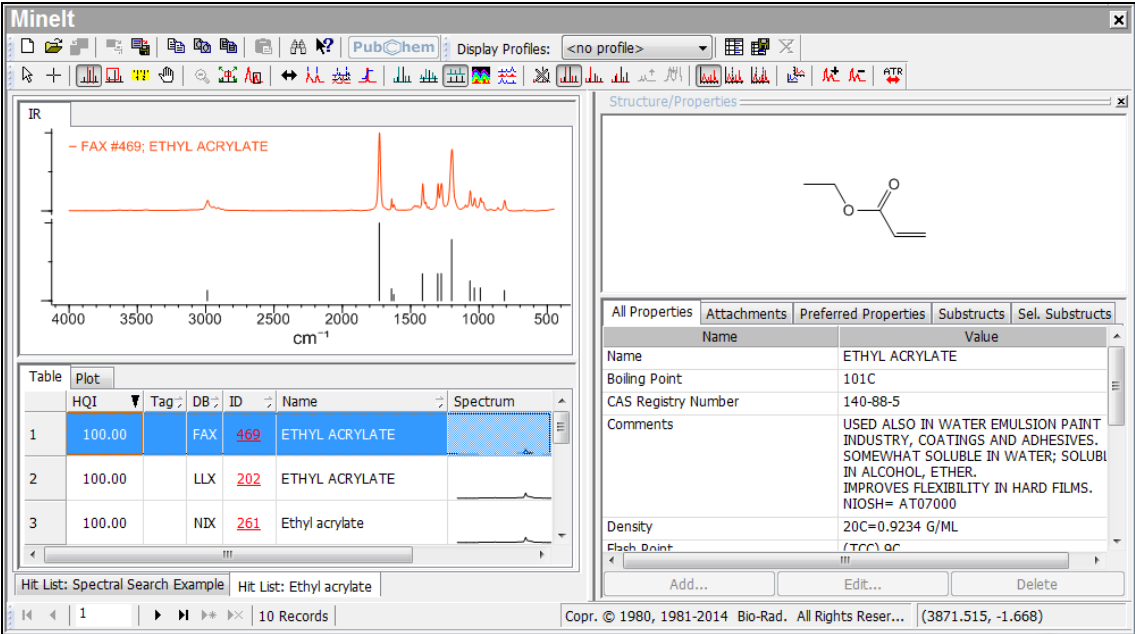
### Configure and perform a peak search

	Action	Result
1	Do one of the following: <ul style="list-style-type: none"> <li>If the SearchIt application is not open, navigate to the <b>Data</b> toolbox and click its icon.</li> <li>If the application is already open, click the <b>Close</b> button  to close the current search</li> </ul>	The SearchIt application's <b>Databases</b> tab is displayed, and the <b>Selected for Searching</b> list displays the databases last used.
2	<ul style="list-style-type: none"> <li>If databases are already selected for searching, click <b>Remove All</b> to clear the selections.</li> <li>Set <b>Limit to spectral technique</b> to IR.</li> <li>Click <b>Add All</b>.</li> </ul>	 <p>The screenshot shows the 'Databases' tab in the SearchIt application. It features two main sections: 'Available for Searching' and 'Selected for Searching'. In the 'Available for Searching' section, there is a dropdown menu for 'Limit to spectral technique' set to 'IR', and buttons for 'Refresh' and 'Advanced...'. Below this is a table with columns 'Name', 'DB Code', and 'Location'. The 'Selected for Searching' section also has a table with the same columns, showing two entries selected. At the bottom, there is a 'Search #5' field and a 'Search' button.</p>

	Action	Result
3	<ul style="list-style-type: none"> <li>Under <b>Search Categories</b> click <b>Peaks</b>.</li> <li>Choose <b>IR</b> in the pop-up dialog.</li> <li>Click <b>OK</b>.</li> </ul>	
4	Click <b>Open Spectrum or Structure</b>	
5	<ul style="list-style-type: none"> <li>Navigate to <b>KnowItAll &gt; Training Files &gt; General Training &gt; Databases</b></li> <li>Open <b>Ethyl acrylate.dx</b>.</li> </ul>	The spectrum is displayed.

	Action	Result																																																				
6	Click <b>Pick</b> .	<p>The peak table is created based on the current settings.</p> <div><div><div>DatabasesIR Peaks</div><div><p>— Ethyl acrylate</p><p>Minimum Peak Intensity</p><p>cm<sup>-1</sup></p><p>PEAK BAR</p><div><div>Peak Picking</div><div>Min. Intensity %: 8</div><div>Max. Noise %: 2</div><div>Pick</div><div><input type="checkbox"/> Peak Data is ATR</div><div>Peak Search Options...</div></div></div></div><div><div>Peaks to search:</div><table><thead><tr><th>Position (cm<sup>-1</sup>)</th><th>Height %</th><th>Tolerance (cm<sup>-1</sup>)</th><th>Required</th></tr></thead><tbody><tr><td>814</td><td>13.48</td><td>16</td><td>No</td></tr><tr><td>990</td><td>16.72</td><td>16</td><td>No</td></tr><tr><td>1034</td><td>16.70</td><td>16</td><td>No</td></tr><tr><td>1066</td><td>25.78</td><td>16</td><td>No</td></tr><tr><td>1200</td><td>78.72</td><td>16</td><td>No</td></tr><tr><td>1276</td><td>35.10</td><td>16</td><td>No</td></tr><tr><td>1302</td><td>34.99</td><td>16</td><td>No</td></tr><tr><td>1414</td><td>34.95</td><td>16</td><td>No</td></tr><tr><td>1624</td><td>8.14</td><td>16</td><td>No</td></tr><tr><td>1640</td><td>15.64</td><td>16</td><td>No</td></tr><tr><td>1730</td><td>100.00</td><td>16</td><td>No</td></tr><tr><td>2988</td><td>13.55</td><td>16</td><td>No</td></tr></tbody></table><div><div>Add...</div><div>Edit...</div><div>Delete</div></div><div>Search</div></div></div> <div>Ethyl acrylate</div>	Position (cm <sup>-1</sup> )	Height %	Tolerance (cm <sup>-1</sup> )	Required	814	13.48	16	No	990	16.72	16	No	1034	16.70	16	No	1066	25.78	16	No	1200	78.72	16	No	1276	35.10	16	No	1302	34.99	16	No	1414	34.95	16	No	1624	8.14	16	No	1640	15.64	16	No	1730	100.00	16	No	2988	13.55	16	No
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1640	15.64	16	No																																																			
1730	100.00	16	No																																																			
2988	13.55	16	No																																																			
TIP		<p>You can remove a peak from the peak table by selecting the peak and clicking the delete button or by double-clicking it in the peak bar. Similarly, you can also add or edit peaks using the corresponding buttons at the bottom of the table..</p>																																																				



	Action	Result																																										
7	Click <b>Search</b> .	<p>Search results are automatically displayed in the <b>Minelt</b> application.</p>  <p>The screenshot displays the Minelt application window. The top toolbar includes icons for file operations and a 'PubChem' link. The 'Display Profiles' dropdown is set to '&lt;no profile&gt;'. The main window is divided into three panes:</p> <ul style="list-style-type: none"><li><b>IR Spectrum:</b> Shows an IR spectrum for 'FAX #469; ETHYL ACRYLATE' with a wavenumber range from 4000 to 500 cm<sup>-1</sup>.</li><li><b>Table:</b> A table with columns: HQI, Tag, DB, ID, Name, and Spectrum. It lists three hits for Ethyl Acrylate.</li><li><b>Structure/Properties:</b> Displays the chemical structure of Ethyl Acrylate and a list of properties.</li></ul> <p><b>Table Data:</b></p> <table><tr><th></th><th>HQI</th><th>Tag</th><th>DB</th><th>ID</th><th>Name</th><th>Spectrum</th></tr><tr><td>1</td><td>100.00</td><td>FAX</td><td>469</td><td></td><td>ETHYL ACRYLATE</td><td></td></tr><tr><td>2</td><td>100.00</td><td>LLX</td><td>202</td><td></td><td>ETHYL ACRYLATE</td><td></td></tr><tr><td>3</td><td>100.00</td><td>NIX</td><td>261</td><td></td><td>Ethyl acrylate</td><td></td></tr></table> <p><b>Properties Panel:</b></p> <table><tr><th>Name</th><th>Value</th></tr><tr><td>Name</td><td>ETHYL ACRYLATE</td></tr><tr><td>Boiling Point</td><td>101C</td></tr><tr><td>CAS Registry Number</td><td>140-88-5</td></tr><tr><td>Comments</td><td>USED ALSO IN WATER EMULSION PAINT INDUSTRY, COATINGS AND ADHESIVES. SOMEWHAT SOLUBLE IN WATER; SOLUBI IN ALCOHOL, ETHER. IMPROVES FLEXIBILITY IN HARD FILMS. NIOSH= AT07000</td></tr><tr><td>Density</td><td>20C=0.9234 G/ML</td></tr><tr><td>Flash Point</td><td>(TCC) 9C</td></tr></table> <p>At the bottom, there is a 'Hit List: Spectral Search Example' and 'Hit List: Ethyl acrylate' section, and a status bar indicating '10 Records' and copyright information.</p>		HQI	Tag	DB	ID	Name	Spectrum	1	100.00	FAX	469		ETHYL ACRYLATE		2	100.00	LLX	202		ETHYL ACRYLATE		3	100.00	NIX	261		Ethyl acrylate		Name	Value	Name	ETHYL ACRYLATE	Boiling Point	101C	CAS Registry Number	140-88-5	Comments	USED ALSO IN WATER EMULSION PAINT INDUSTRY, COATINGS AND ADHESIVES. SOMEWHAT SOLUBLE IN WATER; SOLUBI IN ALCOHOL, ETHER. IMPROVES FLEXIBILITY IN HARD FILMS. NIOSH= AT07000	Density	20C=0.9234 G/ML	Flash Point	(TCC) 9C
	HQI	Tag	DB	ID	Name	Spectrum																																						
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Density	20C=0.9234 G/ML																																											
Flash Point	(TCC) 9C																																											

For each entry, the **Spectral** pane displays the hit list spectrum along with the peaks used to perform the search.

# Searching

## How to Search Spectral Databases Using a Limited Range in a Spectrum

### Purpose

This exercise demonstrates how to search spectral databases using a limited spectral range with the KnowItAll Informatics System's SearchIt™ application.

### Objectives

This exercise will teach you:

- How to use the **Include Range** bar when configuring a spectral search;
- How to use the **Search Masks** dialog box when configuring a spectral search.

### Background

Using a limited range spectral search is slightly faster because fewer points are needed for computation. Using a limited range also focuses a spectral search on feature-rich areas such as the fingerprint region in the IR below 1500 wavenumbers, and can be used in place of spectral subtraction by ignoring regions where impurities have peaks.


#### *Training Files Used In This Lesson*

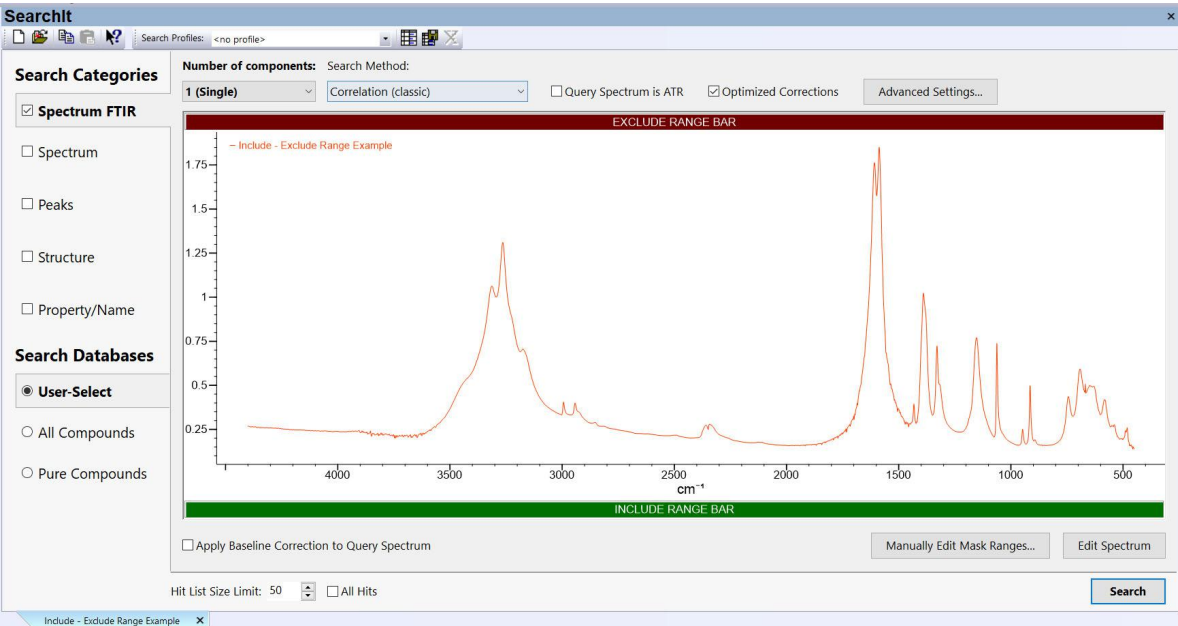
- Include – Exclude Range Example.jdx

#### *KnowItAll Applications Used*

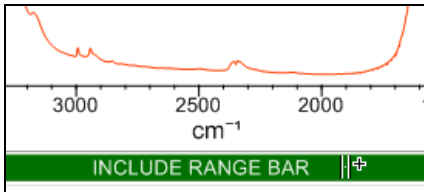
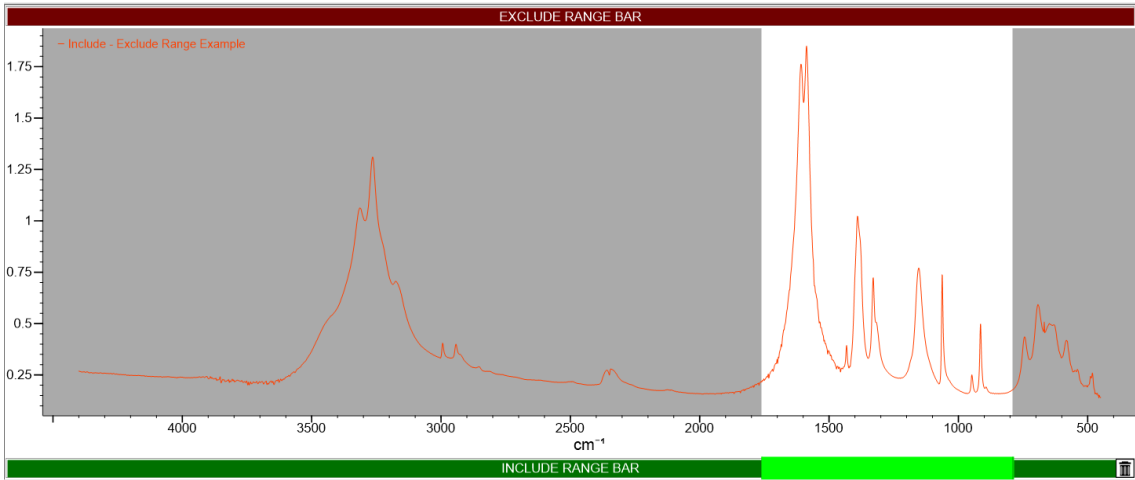
- SearchIt™
- Minelt™

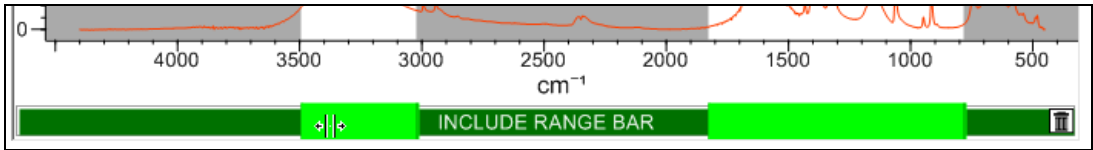

**Configure a spectral search**

	Action	Result
1	Do one of the following: <ul style="list-style-type: none"> <li>If the <b>SearchIt</b> application is not open, navigate to the <b>Data</b> toolbox and click its icon.</li> <li>If the <b>SearchIt</b> application is already open, click the SearchIt <b>Close</b> button  to close the current search</li> </ul>	The <b>SearchIt</b> application's <b>Databases</b> tab is displayed, and the <b>Selected for Searching</b> list displays the databases last used.
2	If databases are already selected for searching, click <b>Remove All</b> to clear the selections.	
3	Click <b>Reference – Licensed</b> in the tree control.	<b>Name</b> , <b>DB Code</b> , and <b>Location</b> are displayed for the available databases.  <b>Note:</b> Click <b>Advanced</b> to specify <b>Server Settings</b> , define local database paths, and find local databases. Expand the tree to view and select network and local database locations. You can also select user databases and hit lists for searching. Finally, you can locate a specific database by clicking <b>Select by Browsing</b> .
4	Click <b>Add All</b> .	Titles and locations are displayed in the <b>Selected for Searching</b> list.
5	Click <b>Spectrum</b> under <b>Search Categories</b>	An <b>Open</b> dialog box appears.

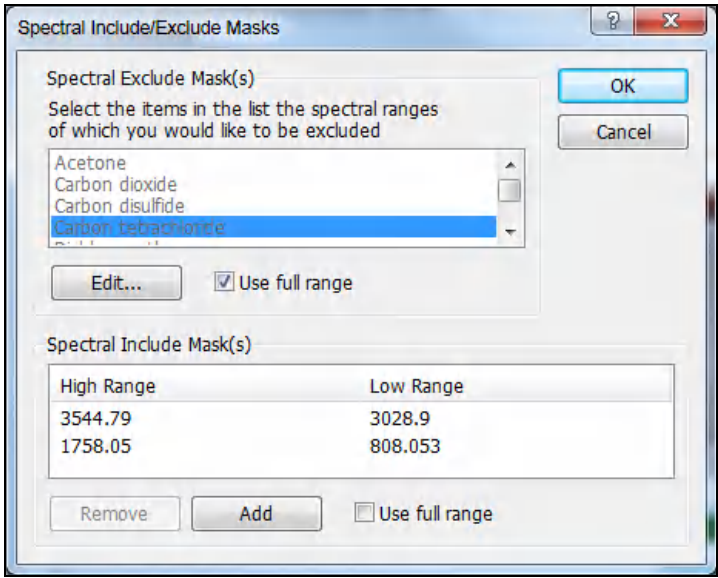
Action	Result
<ul style="list-style-type: none"><li>Navigate to <b>KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; Searching</b></li><li>Open <b>Include -Exclude Range Example.jdx</b>.</li></ul> <p><b>Note:</b> You can use the <b>Files of Type</b> filter to display JCAMP files (or all files).</p>	<p>The spectrum is displayed</p> 

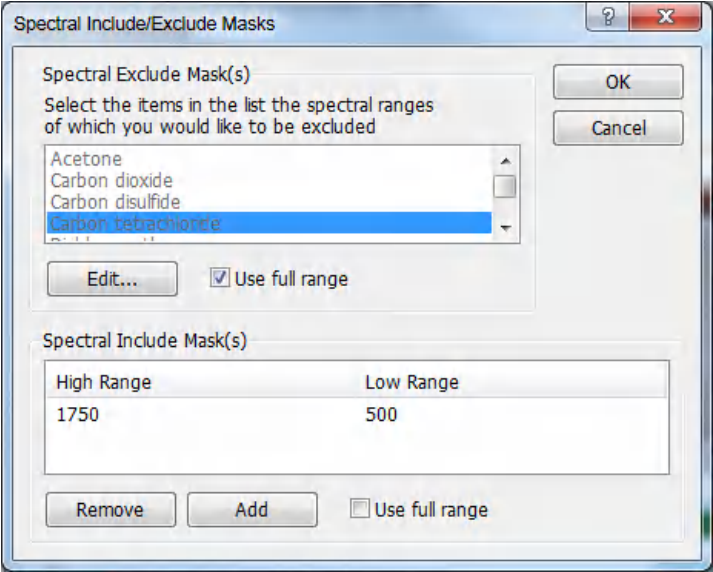
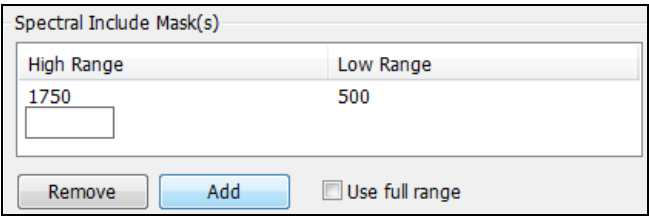
### Use the Include Range bar

	Action	Result
1	Move the cursor over the <b>Include Range Bar</b> beneath the spectrum.	<p>The cursor changes to a double pipe with a plus sign next to it:</p> 
2	Click, drag, and release within the <b>Include Range Bar</b> to define an <b>Include</b> region.	<p>The Include region is bright green in the <b>Include Range Bar</b>; the included spectral region has a white background. Spectral regions that will not be included in the search have a gray background.</p>  <p>Using the <b>Include Range</b> feature allows you to set one or more ranges to be included in a spectral search. This feature is primarily used on a per search basis. Although the ranges set using this method will be remembered until they are changed, the ranges are not permanently saved.</p>

	Action	Result
3	Click and drag to define a second Include region.	
4	To move a region, click within the region on the <b>Include Range Bar</b> and drag to a new location.	
	<b>TIP</b>	<p>To remove a single region, either click within the region on the <b>Include Range Bar</b> and drag to either side away from the spectral pane, or right-click within the region and choose <b>Yes</b> on the message box that opens.</p> <p>To remove all regions, click the garbage can icon at the right end of the <b>Include Range Bar</b>.</p>
5	To re-size a region, move the cursor into the <b>Include Range Bar</b> and position the cursor over an endpoint, then drag and release.	<p>The cursor changes to a cross with a double arrowhead:</p> 

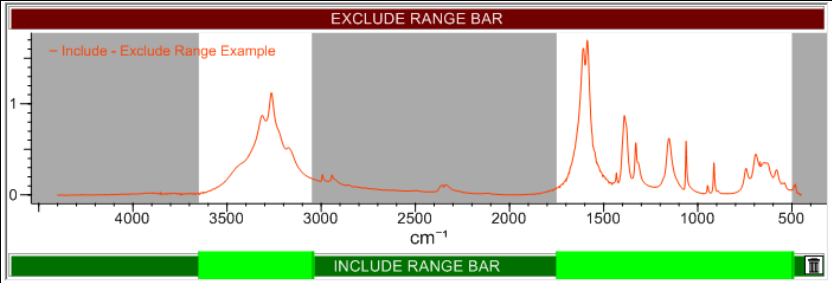
**Use the Search Masks dialog box**

	Action	Result
1	Click <b>Manually Edit Mask Ranges</b> .	<p>The <b>Spectral Include/Exclude Masks</b> dialog box opens:</p>  <p>Note that any <b>Include</b> regions defined using the <b>Include Range Bar</b> are displayed in the list of <b>Spectral Include Mask(s)</b>. However, if <b>Use full range</b> is checked, these regions will not be used.</p>
2	Click to select one of the include regions, then click <b>Remove</b> . <b>Note:</b> You can select either the high or low value to remove an Include region.	The region is removed from the list.
3	Click to select the <b>High Range</b> value in the remaining Include region and type in '1750.'	

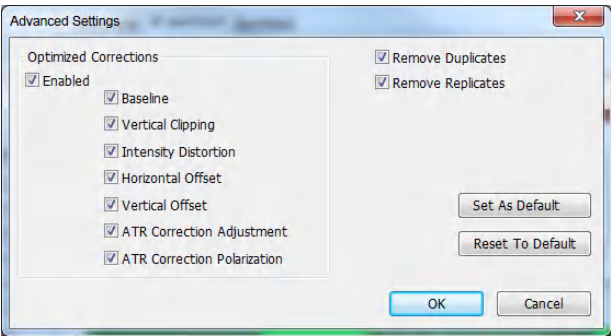
	Action	Result
4	Click to select the <b>Low Range</b> value in the remaining Include region and type in '500.'	
5	Click <b>Add</b> to create another Include region.	<p>A text box with cursor appears in the <b>High Range</b> column:</p> 
6	Type '3650' in the new <b>High Range</b> text box, then click in the <b>Low Range</b> column and type '3050.'	



## Use the Search Masks dialog box (continued)

	Action	Result
7	Click <b>OK</b> .	<p>The dialog box closes, and the search spectrum is displayed with the re-defined <b>Include</b> regions:</p> 
8	Click <b>Search</b> .	<p>The search is performed, and results are automatically displayed in the Minelt application as a hit list.</p>  <p>Clicking on the information icon  in the results table displays <b>Optimized Corrections</b> that have been performed.</p>

**Use the Search Masks dialog box (continued)**

	Action	Result
9	<p>Close the <b>Optimized Corrections</b> window, then use the KnowItAll <b>Back</b> button to return to the SearchIt application.</p> <p>Click <b>Advanced Settings</b> on the IR Spectrum tab.</p>	<p>The <b>Advanced Settings</b> dialog box opens.</p>  <p>Use this dialog box to enable and customize <b>Optimized Corrections</b>.</p>

# Searching

## How to Search Spectral Databases Using a Mask to Exclude Regions in Your Search

### Purpose

This exercise demonstrates how to create masks to exclude regions in a spectral search.

### Objectives

This exercise will teach you:

- How to create and use Exclude Masks when configuring a spectral search.

### Background

Exclude masks allow you to ignore regions during spectral searching, and can be defined for a variety of compounds such as solvents or impurities. Such masking allows for an easy method to remove these regions from consideration during a search.

Unlike Include regions, which are not permanent, exclude masks can be saved and re-used.


#### *Training Files Used In This Lesson*

- Include-Exclude Range Example.jdx

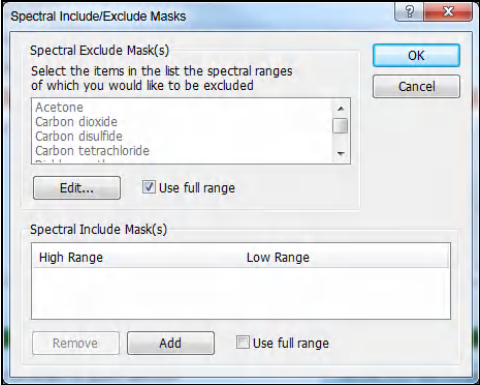
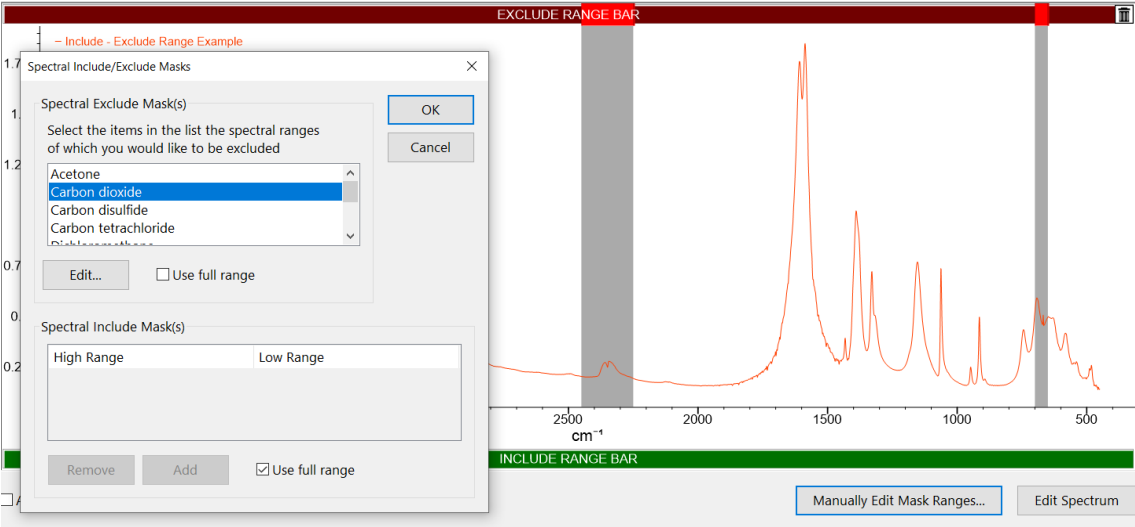
#### *KnowItAll Applications Used*

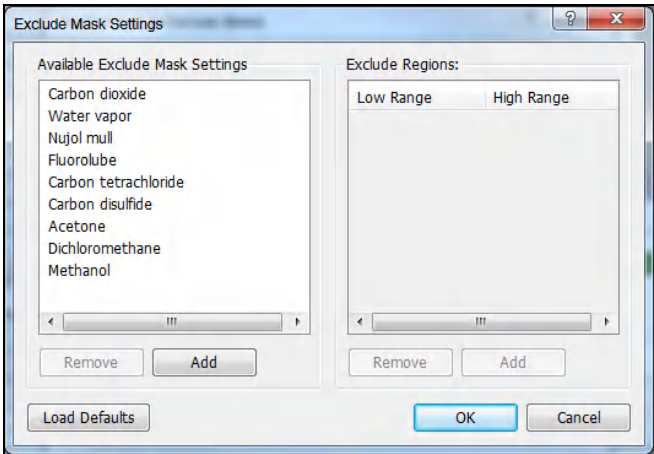
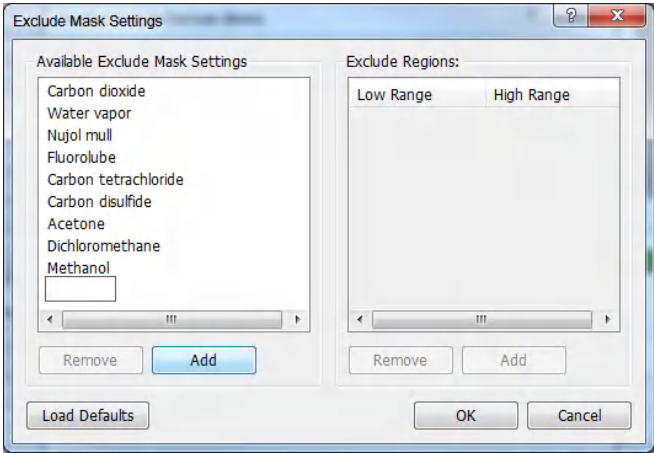
- SearchIt™
- MinIt™

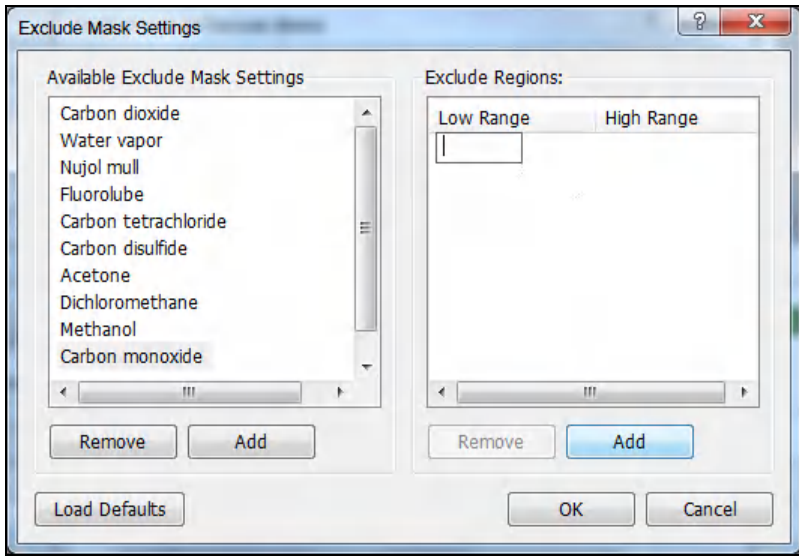
**Configure a spectral search**

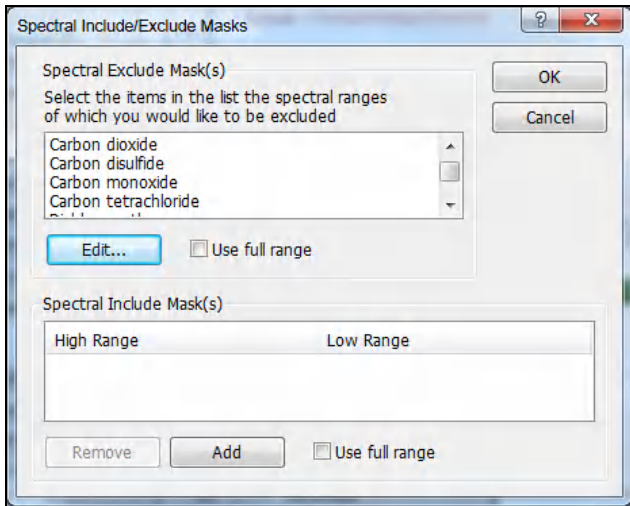
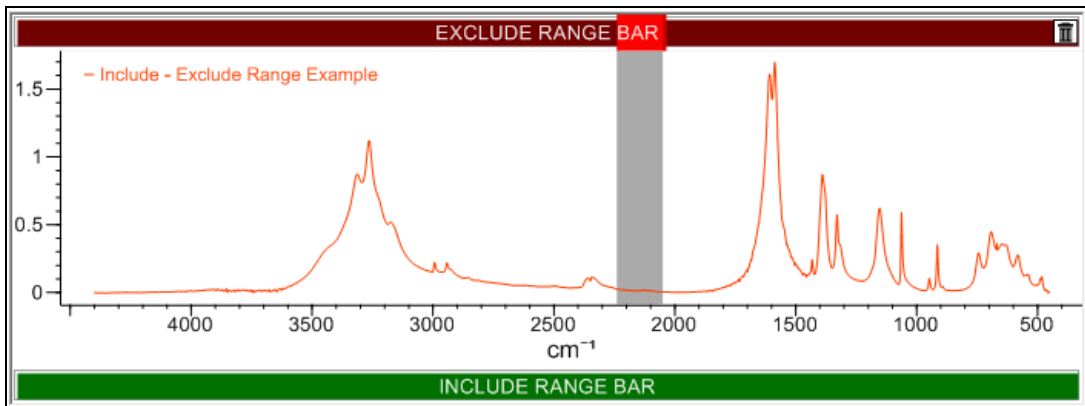
	Action	Result
1	Do one of the following: <ul style="list-style-type: none"> <li>If the <b>SearchIt</b> application is not open, navigate to the <b>Data</b> toolbox and click its icon.</li> <li>If the <b>SearchIt</b> application is already open, click the SearchIt Close button  to close the current search</li> </ul>	The SearchIt application's <b>Databases</b> tab is displayed, and the <b>Selected for Searching</b> list displays the databases last used.
2	If databases are already selected for searching, click <b>Remove All</b> to clear the selections.	
3	Click <b>Reference – Licensed</b> in the tree control.	<b>Name</b> , <b>DB Code</b> , and <b>Location</b> are displayed for the available databases. <b>Note:</b> Click <b>Advanced</b> to specify Server Settings, define local database paths, and find local databases. Expand the tree to view and select network and local database locations. You can also use user databases and hit lists for searching. Finally, you can locate a specific database by clicking <b>Select by Browsing</b> .
4	Select IR using the <b>Limit to spectral technique</b> control.	Only databases having IR spectra are displayed. <b>Note:</b> Many of the databases have only IR spectra, but others – such as the Multi-Technique Sadtler Demo Database – Wiley – include other types of spectra, and structures.
5	Click <b>Add All</b> .	Titles and locations are displayed in the <b>Selected for Searching</b> list.
6	Click <b>Spectrum</b> under <b>Search Categories</b>	An <b>Open</b> dialog box appears
7	<ul style="list-style-type: none"> <li>Navigate to <b>KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; Searching</b>.</li> <li>Open <b>Include-Exclude Range Example.jdx</b>.</li> </ul> <b>Note:</b> You can use the Files of type filter to display JCAMP files (or all files).	The spectrum is displayed in the IR Spectrum tab.

## Use the Search Masks dialog box

	Action	Result
1	Click <b>Manually Edit Mask Ranges</b> .	<p>The <b>Spectral Include/Exclude Masks</b> dialog box opens.</p> 
2	Uncheck <b>Use full range</b> under the list of <b>Spectral Exclude Mask(s)</b> , then click to select the <b>Carbon dioxide</b> exclude mask.	<p>Excluded regions are highlighted in bright red on the <b>Exclude Range Bar</b>, and in gray in the spectrum. The carbon dioxide exclude mask includes two regions.</p> 

	Action	Result
3	Click <b>Edit</b> on the <b>Spectral Include/Exclude Masks</b> dialog box.	<p>The <b>Exclude Mask Settings</b> dialog opens:</p> 
4	Click <b>Add</b> .	<p>A text box appears under <b>Available Exclude Mask Settings</b>.</p> 

	Action	Result
5	Type in <b>Carbon monoxide</b> , then click outside the text box.	
6	With <b>Carbon monoxide</b> selected in the list of <b>Available Exclude Mask Settings</b> , click <b>Add</b> under the list of <b>Exclude Regions</b> , or click under <b>Low Range</b> .	<p>A text box appears under <b>Exclude Regions</b>.</p> 
	<b>TIP</b>	Alternatively, you can also manually set exclude ranges using the <b>Exclude Range Bar</b> and clicking and dragging to select regions. See the section above on <a href="#">How to Search Spectral Databases Using a Limited Range in a Spectrum</a> . Manually setting the exclude range works in exactly the same way as manually setting the include range.

	Action	Result
7	Type in low and high range values (2050 and 2240), then click <b>OK</b> .	<p>The <b>Exclude Mask Settings</b> dialog box closes, and the new carbon monoxide mask is added to the list of exclude masks:</p> 
8	Select the new <b>Carbon monoxide</b> mask, then click <b>OK</b> to close the <b>Spectral Include/Exclude Masks</b> dialog box.	<p>The dialog box closes, and the search spectrum is displayed with the newly-defined exclude region:</p> 





# Searching

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## How to Subtract One Spectrum from Another

### Purpose

This exercise demonstrates how to use the spectral subtraction feature in the KnowItAll Informatics System.

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### Objectives

This exercise will teach you:

- How to use the spectral subtraction feature in KnowItAll.
- 

### Background

You can use the ProcessIt™ applications to perform a point-by-point subtraction of one spectrum from another. This capability is useful when analyzing mixtures or composite spectra.

#### *Training Files Used In This Lesson*

- Unknown Mixture 01011969.jdx

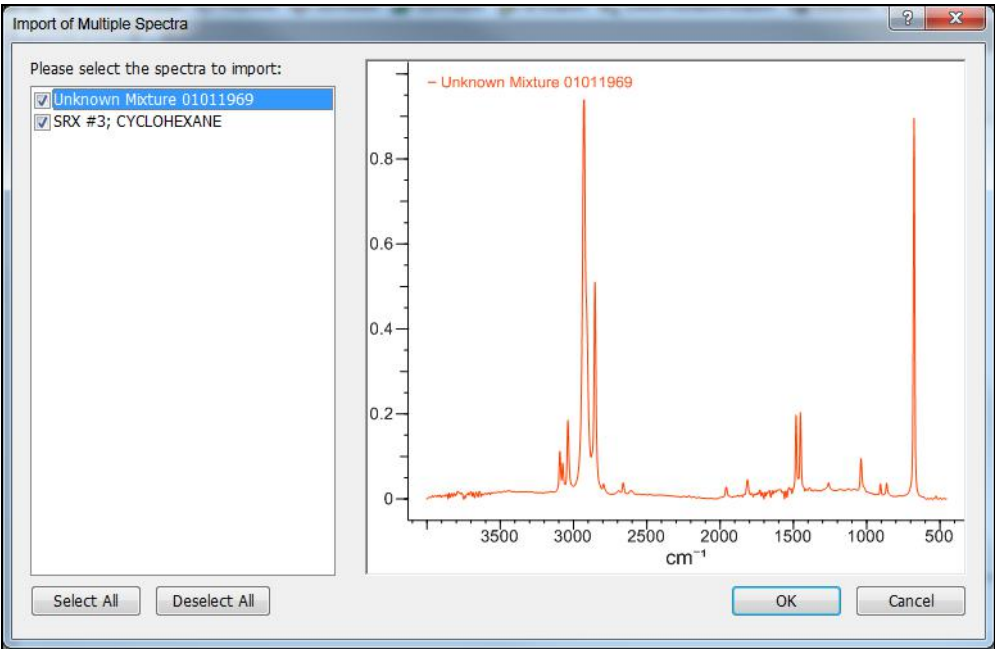
#### *KnowItAll Applications Used*

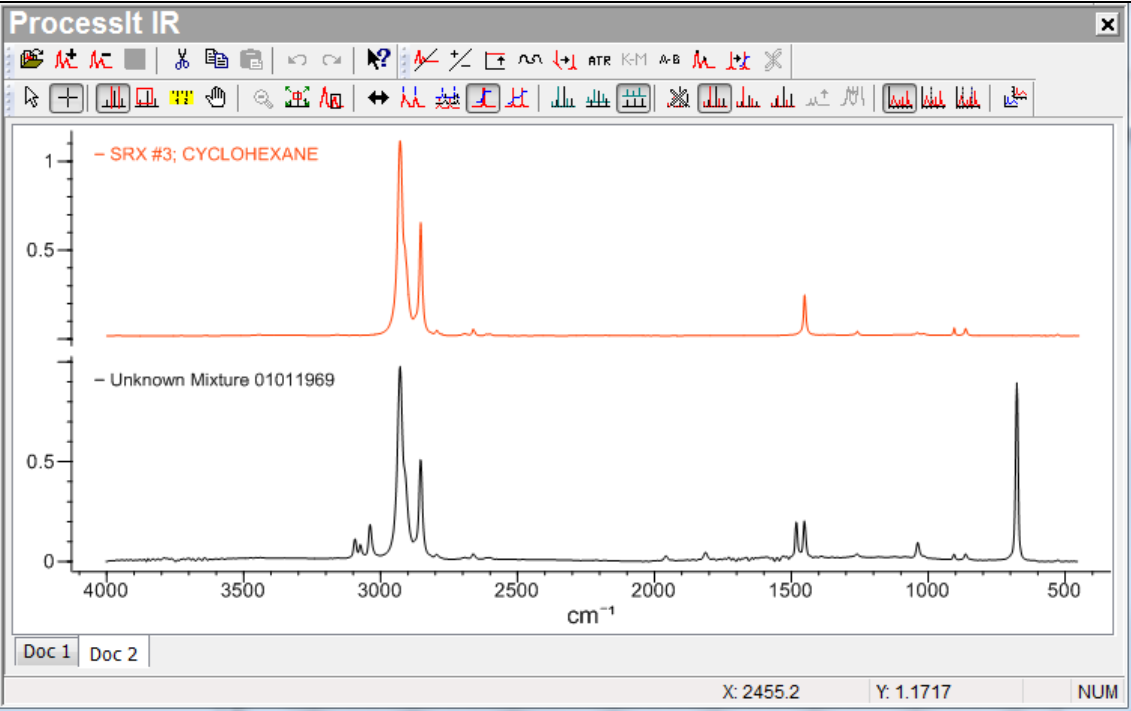
- SearchIt™
- MinIt™
- ProcessIt™ IR


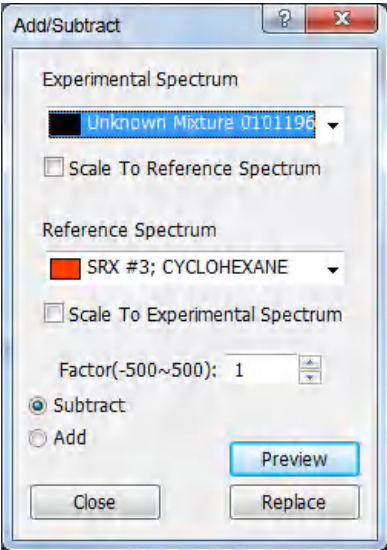
## Set up a spectral search against a mixture

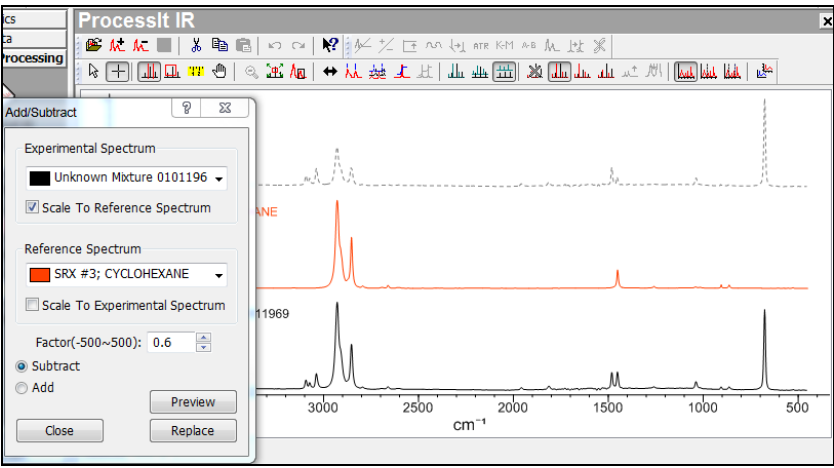
	Action	Result
1	<p>In the <b>SearchIt</b> application, set up and perform an IR spectral search using <b>Unknown Mixture 01011969.jdx</b> located in <b>KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; Searching</b> folder, and the <b>Multi-Technique Sadtler Demo Database – Wiley</b>.</p> <p><b>TIP</b> In the <b>SearchIt</b> application, click on the <b>DB Code</b> column to sort databases alphabetically by code in ascending or descending order.</p>	<p>Results are displayed in the <b>Minelt</b> application. The first hit is <b>cyclohexane</b>. Both spectra, the query and the first hit, are displayed in the spectral pane.</p> <div><div><div><div><div>1</div><div>– DEMOX #12, Cyclohexane</div></div><div><div>1</div><div>– Unknown Mixture 01011969</div></div></div><div></div><div><div>IR<sup>13</sup>C NMR<sup>1</sup>H NMR<sup>1</sup>MS</div><div><div>TablePlotRelated Compounds View</div><div><div>HQI▼Tag↗Col↗DB↗ID↗Name↗Spectrum&lt;auto&gt; (IR/ATR-IR)</div><div><div><div>1</div><div>77.29</div><div><div>1</div>DEMO</div><div>12</div><div>Cyclohexane</div><div></div></div><div><div>2</div><div>70.85</div><div><div>1</div>DEMO</div><div>8</div><div>Cyclohexene</div><div></div></div><div><div>3</div><div>50.48</div><div><div>1</div>DEMO</div><div>9</div><div>Hexane</div><div></div></div><div><div>4</div><div>32.49</div><div><div>1</div>DEMO</div><div>13</div><div>Benzene</div><div></div></div><div><div>5</div><div>28.36</div><div><div>1</div>DEMO</div><div>11</div><div>Poly(styrene)</div><div></div></div></div></div></div><div><div>Structure/Properties</div><div><div><div></div></div><div><div><div>Name</div><div>Cyclohexane</div></div><div><div>Boiling Point</div><div>80.7 °C</div></div><div><div>CAS Registry Number</div><div>110-82-7</div></div><div><div>Comments</div><div>HIGHLY FLAMMABLE LIQUID MISCIBLE WITH MOST ORGANIC SOLVENTS; SLIGHTLY SOLUBLE IN WATER. EXTRACTANT OF OILS AND USED ANALYTICALLY FOR MOLECULAR WEIGHT DETERMINATIONS. REAGENT USED IN SYNTHESIS OF NYLON 6 AND NYLON 66 AND OTHER ORGANIC COMPOUNDS. OCCURS IN SEDIMENTS. WIDELY USED ORGANIC SOLVENT ESPECIALLY FOR LACQUERS AND RESINS, PAINTS AND VARNISHES.</div></div></div></div></div></div></div></div>

**Create a difference spectrum**

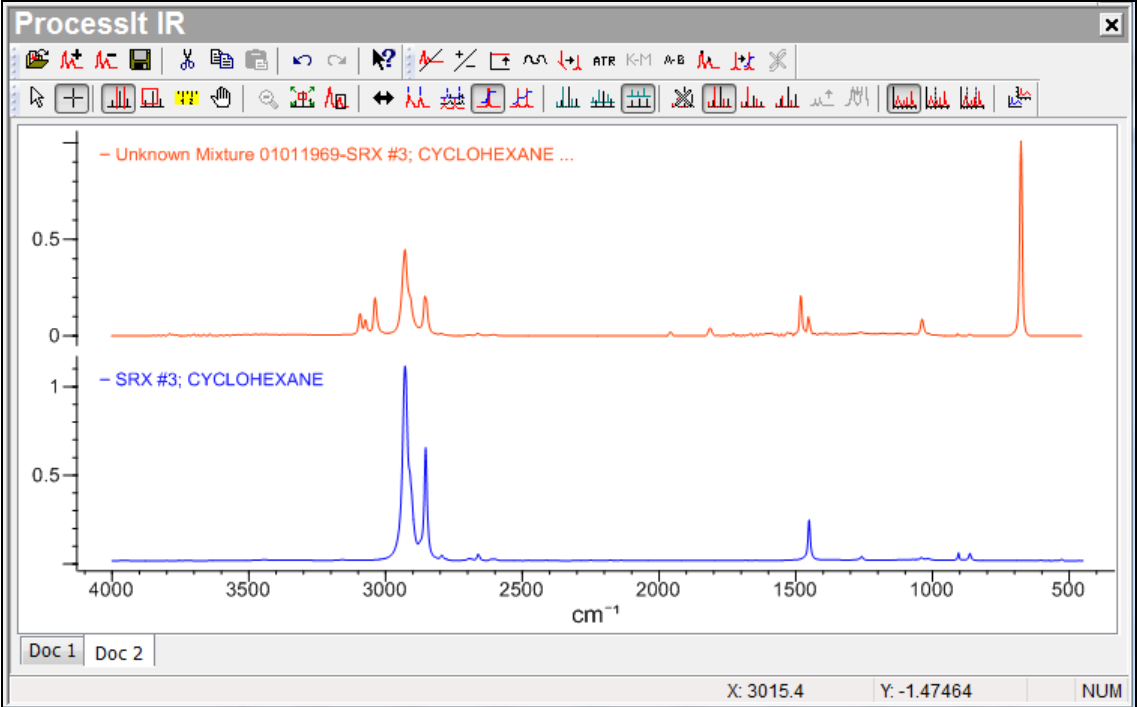
	Action	Result
1	With the hit list displayed in <b>Minelt</b> and the first record selected, click <b>ProcessIt</b> in the <b>Transfer to</b> bar.	<p>The <b>Import of Multiple Spectra</b> dialog box opens.</p>  <p>Both the query spectrum and the first hit are displayed.</p>

	Action	Result
2	Click <b>Select All</b> , then click <b>OK</b> on the <b>Import of Multiple Spectra</b> dialog box.	<p>Both spectra – the mixture and the first hit, cyclohexane - are transferred to the <b>ProcessIt IR</b> application.</p>  <p><b>Note:</b> Use spectrum toolbar buttons to adjust the display. The Stacked display is preferable to Offset or Overlay for spectral subtraction.</p>

	Action	Result
3	<p>Choose <b>Process &gt; Add/Subtract Spectrum</b>.</p> <p><b>Note:</b> You can also use the toolbar button . The command is not available unless two or more spectra are open.</p>	<p>The <b>Add/Subtract</b> dialog box opens.</p>  <p>The active spectrum is assumed to be the reference spectrum.</p>
4	<p>Make sure the mixture spectrum is the <b>Experimental Spectrum</b>, and cyclohexane is the <b>Reference Spectrum</b>. If needed, change these assignments using either of the drop-down lists.</p>	
5	<p>Check <b>Scale to Reference Spectrum</b>, set <b>Factor</b> to 1, and make sure the <b>Subtract</b> radio button is selected.</p>	

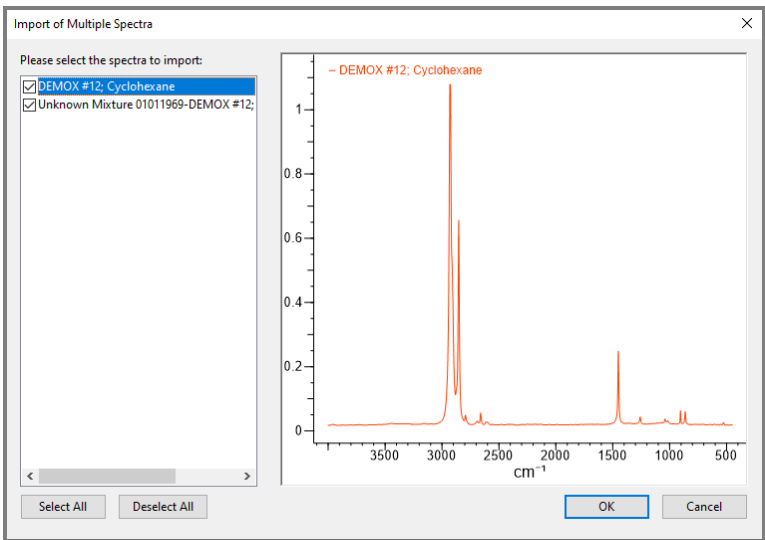
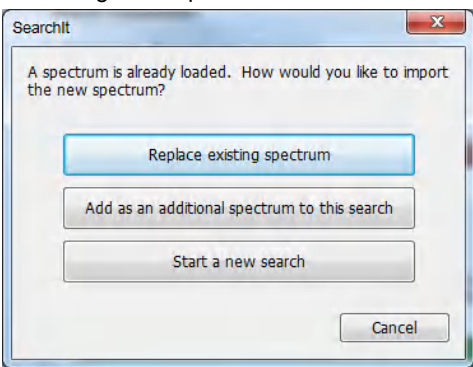
	Action	Result
6	Click <b>Preview</b> .	<p>The subtracted spectrum is displayed above the other two. Note the presence of negative peaks in the difference spectrum.</p> 
7	On the <b>Add/Subtract</b> dialog box, adjust <b>Factor</b> to 0.6.	<p>Negative peaks in the difference spectrum disappear.</p> 

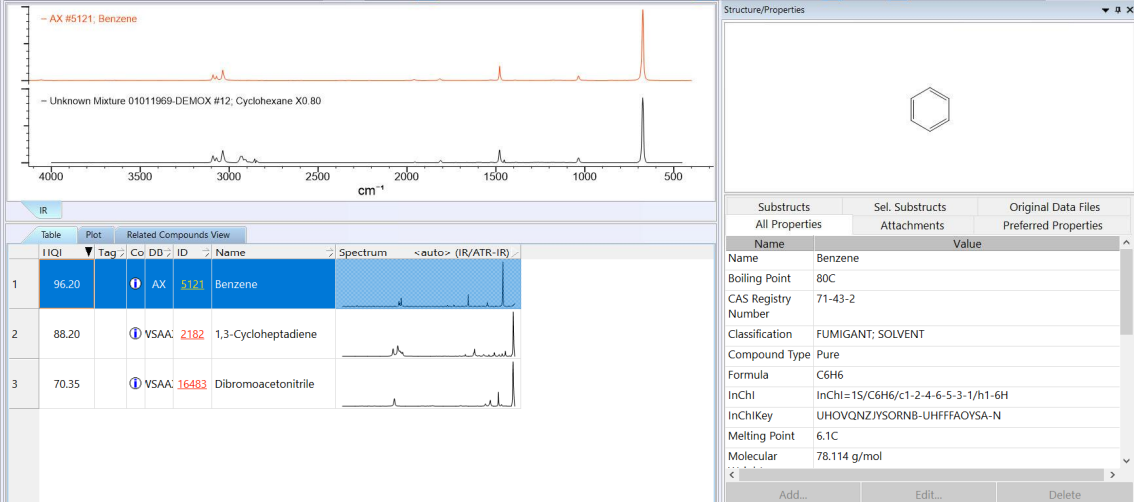
**Create a difference spectrum (continued)**

	Action	Result
8	Click <b>Replace</b> .	A message box opens, and asks whether negative values should be truncated to zero.
9	Click <b>Yes</b> .	The mixture spectrum is replaced by a difference spectrum, Unknown Mixture 01011969 - SRX #3, Cyclohexane. 



## Repeat the search using the difference spectrum

	Action	Result
1	Click <b>SearchIt</b> in the <b>Transfer to</b> bar.	<p>The <b>Import of Multiple Spectra</b> dialog box opens:</p> 
2	<p>De-select <b>DEMOX #12 Cyclohexane</b> so that only the difference spectrum is selected.</p> <p>Click <b>OK</b>.</p>	<p>A message box opens:</p> 
3	Click <b>Start a new search</b> .	The difference spectrum is loaded in <b>SearchIt</b> .

	Action	Result
4	<p>Click the <b>Databases</b> tab and make sure the <b>Multi-Technique Sadtler Demo Database – Wiley</b> is selected for searching</p> <p>Click <b>Search</b>.</p>	<p>Results are displayed in the <b>Minelt</b> application. The first hit is benzene, the other component of the mixture:</p> 

# Searching

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## How to Perform a Structure Search

### Purpose

This exercise demonstrates how to perform a structure search using the SearchIt™ application.

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### Objectives

This exercise will teach you:

- How to perform an exact match structure search;
  - How to perform a substructure search.
- 

### Background

In the SearchIt application, scientists can use a structure fragment as a search term to locate chemical structures containing that structural skeleton. This capability is useful for retrieving structure fragments because a substructure search always analyzes the entire molecular structure of a compound - not just the largest fragment.


#### *Training Files Used In This Lesson*

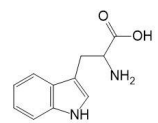
- tryptophan.dsf
- benzenethiol.dsf

#### *KnowItAll Applications Used*

- SearchIt™
- MinIt™
- ChemWindow®

**Configure an exact structure match search**

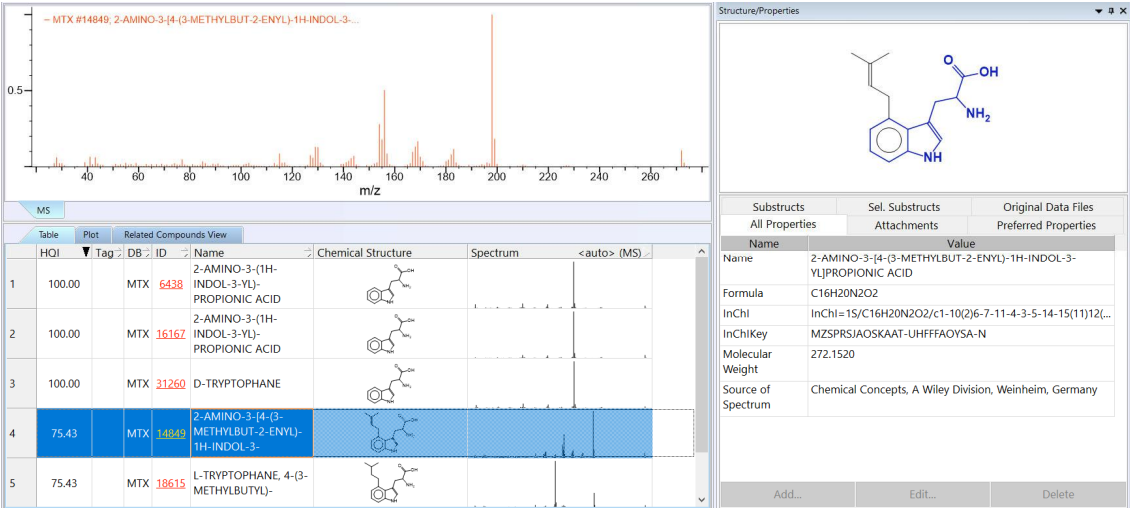
	Action	Result
1	Do one of the following: <ul style="list-style-type: none"><li>• If the <b>SearchIt</b> application is not open, navigate to the <b>Data</b> toolbox and click its icon.</li><li>• If the <b>SearchIt</b> application is already open, click the SearchIt <b>Close</b> button  to close the current search</li></ul>	The SearchIt application's <b>Databases</b> tab is displayed, and the <b>Selected for Searching</b> list displays the databases last used.
2	If databases are already selected for searching, click <b>Remove All</b> to clear the selections.	
3	Set <b>Limit to Spectral Technique</b> to <b>MS</b> .	Only databases with MS spectral data are displayed.
4	Select database <b>MTX</b> for searching.	
5	Click <b>Structure</b> under <b>Search Categories</b> .	

	Action	Result
6	<ul style="list-style-type: none"><li>Click <b>Open file</b> on the <b>Structure</b> tab.</li><li>Navigate to <b>KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; Searching</b>.</li><li>Open <b>Tryptophan.dsf</b>.</li></ul>	<p>The structure is displayed in the <b>Structure</b> tab.</p> <div><div><div><b>Search Categories</b></div><div><input type="checkbox"/> Spectrum</div><div><input type="checkbox"/> Peaks</div><div><input checked="" type="checkbox"/> <b>Structure</b></div><div><input type="checkbox"/> Property/Name</div><div><b>Search Databases</b></div><div><input checked="" type="radio"/> <b>User-Select</b></div><div><input type="radio"/> All Compounds</div><div><input type="radio"/> Pure Compounds</div></div><div><div><b>Search Mode</b></div><div><input checked="" type="radio"/> Exact Match</div><div><input type="radio"/> Substructure</div><div><input type="radio"/> Similarity <span>Tanimoto</span></div><div><b>Search Options</b></div><div><input checked="" type="checkbox"/> Enforce Stereochemical Match</div><div><input type="checkbox"/> Relative Stereochemistry (Include Both Enantiomers)</div><div><input type="checkbox"/> No Structure Standardization (Salts, tautomers, etc.)</div><div><b>Structure Modifiers</b></div><div>A Any Element Except H</div><div>Q Any Element Except C or H</div><div>X Any Halogen (F, Cl, Br, I, At)</div><div>↔ Any Bond Order</div><div>≡ Any Aromatic Bond</div><div>&gt;&lt; Any Z/E Orientation</div><div>↻ Any Enantiomer</div><div>* Any Attachments but H</div><div><span>Open file...</span> <span>Draw/Edit...</span></div></div></div> <div><chem>NC(Cc1c[nH]c2ccccc12)C(=O)O</chem></div>

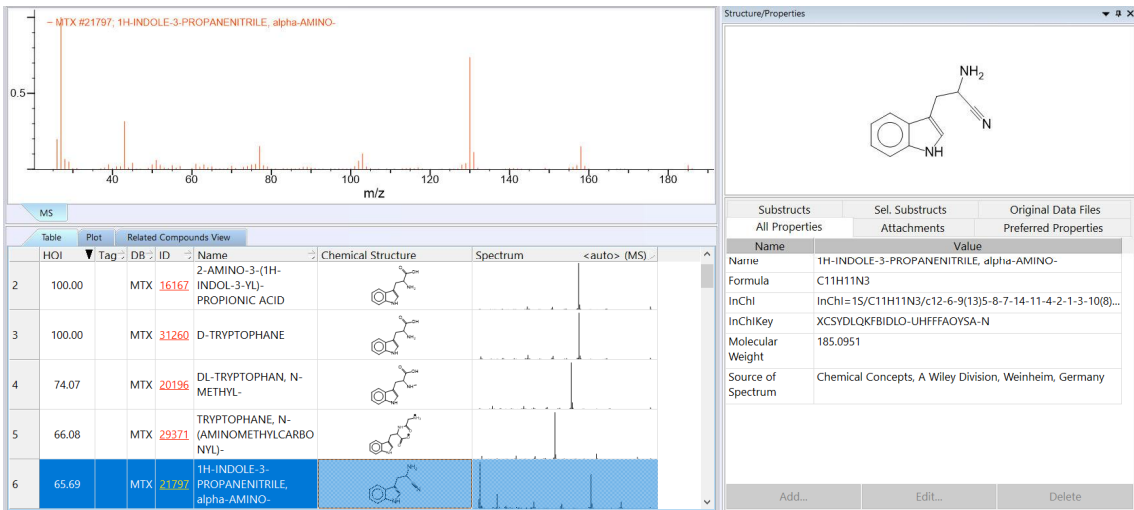
**Note:** You can also click **Draw/Edit** to create a structure using the **ChemWindow** application.



### Configure and perform a substructure search

	Action	Result
1	Click the KnowItAll <b>Back</b> button to return to <b>SearchIt</b> , then click to select the <b>Structure</b> tab.	
2	<p>Select <b>Substructure Search</b>, then click <b>Search</b>.</p> <p><b>Note:</b> Rather than finding only exact matches for the search structure, the substructure search returns records that contain the query structure as a part of the database structure.</p>	<p>The substructure search produces more hits than the exact match search. Note that the original hit list is still available, and can be accessed by clicking the appropriate tab (at the lower left corner).</p> 

### Configure and perform a similarity search

	Action	Result
1	Click the KnowItAll <b>Back</b> button to return to <b>SearchIt</b>	
2	Click the <b>Similarity Search</b> radio button. Accept the default scoring method, <b>Tanimoto</b> .	
3	Click <b>Search</b> .	<p>The results are displayed in the <b>Minelt</b> application:</p>  <p>The first hit is the exact structure. The second hit, toluene, is a similar structure.</p>



# Searching

## All Compounds and Pure Compounds Database Selections

### Purpose

This exercise demonstrates how to use the All Compounds and Pure Compounds Database Selections

### Objectives

This exercise will teach you:

- How to use All Compounds and Pure Compounds Database Selections.
- How to interpret the search result.

### Background

All Compounds and Pure Compounds database selections link data by structure, name, InChI, CAS Registry Number or synonym.


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

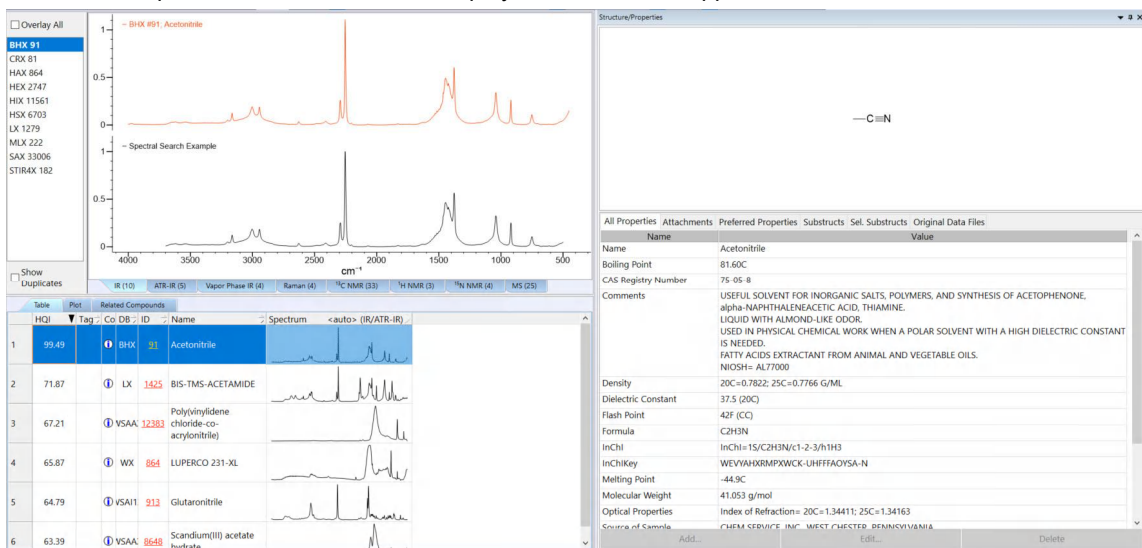
- Spectral Search Example

#### *KnowItAll Applications Used*

- SearchIt™
- MineIt™

**Configure and perform an All Compounds search**

	Action	Result
1	Do one of the following: <ul style="list-style-type: none"><li>• If the <b>SearchIt</b> application is not open, navigate to the <b>Data</b> toolbox and click its icon.</li><li>• If the <b>SearchIt</b> application is already open, click the SearchIt <b>Close</b> button  to close the current search.</li></ul>	The <b>SearchIt</b> application's <b>Databases</b> tab is displayed, and the <b>Selected for Searching</b> list displays the databases last used.
2	Select the <b>All Compounds</b> option under <b>Search Databases</b>	
3	<ul style="list-style-type: none"><li>• Click <b>Spectrum</b> under <b>Search Categories</b>.</li><li>• Open <b>Spectral Search Example.jdx</b></li></ul>	

	Action	Result
7	Click <b>Search</b> .	<p>The search is performed and results are displayed in the <b>Minelt</b> application.</p>  <p>Compared to the <b>User-Select</b> database search, you will see additional information related to the hit:</p> <ul style="list-style-type: none"> <li>Replicates are displayed in the upper-left panel. They do not participate in this search, and navigating through them does not change the value of HQI (Hit Quality Index). The bold ID signifies the hit spectrum.</li> <li>Other spectrum information related to the hit compound is displayed in tabs under the spectrum pane.</li> </ul>

- User-Select** - User selects which databases to search. This is where one can include user databases in a search.
- All Compounds** – All licensed reference databases. Records are linked by structure, name, InChI, CAS Registry Number or synonym.
- Pure Compounds** - All Compounds with the exclusion of commercial compounds.

# Searching

## How to Perform a Multi-Technique Spectral Search

### Purpose

This exercise demonstrates how to perform a multi-technique spectral search using the KnowItAll Informatics System.

### Objectives

This exercise will teach you:

- How to configure a multi-technique spectral search.
- How to analyze the results of a multi-technique search.

### Background

A multi-technique spectral search permits the optimization of chemical similarity based on several analytical techniques to maximize the chemical knowledge obtained on the unknown compound.


#### *Training Files Used In This Lesson*

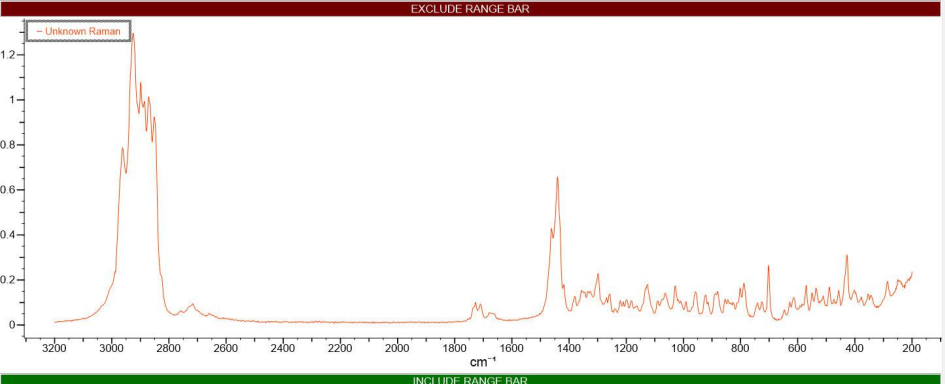
- Unknown IR.jdx
- Unknown Raman.jdx

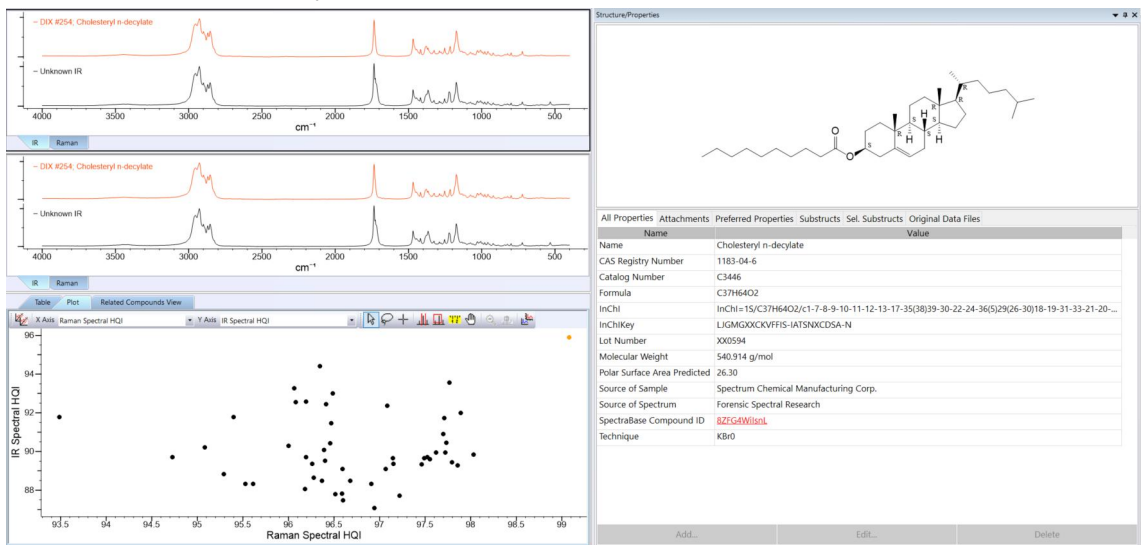
#### *KnowItAll Applications Used*

- SearchIt™
- MinIt™

**Configure and perform a multi-technique spectral search use User-Select Search Databases option**

	Action	Result
1	<p>Do one of the following:</p> <ul style="list-style-type: none"> <li>• If the <b>SearchIt</b> application is not open, navigate to the <b>Data</b> toolbox and click its icon.</li> <li>• If the <b>SearchIt</b> application is already open, click the SearchIt <b>Close</b> button  to close the current search.</li> </ul>	The <b>SearchIt</b> application's <b>Databases</b> tab is displayed, and the <b>Selected for Searching</b> list displays the databases last used.
2	Select <b>User-Select</b> under <b>Search Databases</b> option	
3	<ul style="list-style-type: none"> <li>• If databases are already selected for searching, click <b>Remove All</b> to clear the selections.</li> <li>• Add all <b>IR</b> and <b>Raman</b> databases to <b>Selected for Searching</b>.</li> </ul>	
4	<ul style="list-style-type: none"> <li>• Click <b>Spectrum</b> under <b>Search Categories</b>.</li> <li>• Navigate to <b>KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; Searching</b>.</li> <li>• Open <b>Unknown IR.jdx</b></li> </ul>	


	Action	Result
5	<ul style="list-style-type: none"><li>Click the new <b>Spectrum</b> under <b>Search Categories</b>.</li><li>Open <b>Unknown Raman.jdx</b>.</li></ul>	<div><div><div><b>Search Categories</b><ul style="list-style-type: none"><li><input checked="" type="checkbox"/> Spectrum FTIR</li><li><input checked="" type="checkbox"/> Spectrum Raman</li><li><input type="checkbox"/> Spectrum</li><li><input type="checkbox"/> Peaks</li><li><input type="checkbox"/> Structure</li><li><input type="checkbox"/> Property/Name</li></ul></div><div><b>Search Databases</b><ul style="list-style-type: none"><li><input checked="" type="radio"/> User-Select</li><li><input type="radio"/> All Compounds</li><li><input type="radio"/> Pure Compounds</li></ul></div></div><div><div>Number of components: 1 (Single) Search Method: Correlation (classic) <input checked="" type="checkbox"/> Optimized Corrections <a href="#">Advanced Settings...</a> <a href="#">Linking Options...</a></div><div></div><div><input type="checkbox"/> Apply Baseline Correction to Query Spectrum <a href="#">Manually Edit Mask Ranges...</a> <a href="#">Edit Spectrum</a></div><div>Hit List Size Limit: 50 <input checked="" type="checkbox"/> All Hits <a href="#">Search</a></div></div></div>

	Action	Result
6	Click <b>Search</b> .	<p>The search results are displayed in the <b>Minelt</b> application.</p>  <p>Because this was a multi-technique search, the <b>Database</b> pane's <b>Plot</b> tab automatically displays a scatter plot representing HQI values for the two spectral techniques. The point with the highest HQI values is selected at the upper right.</p>



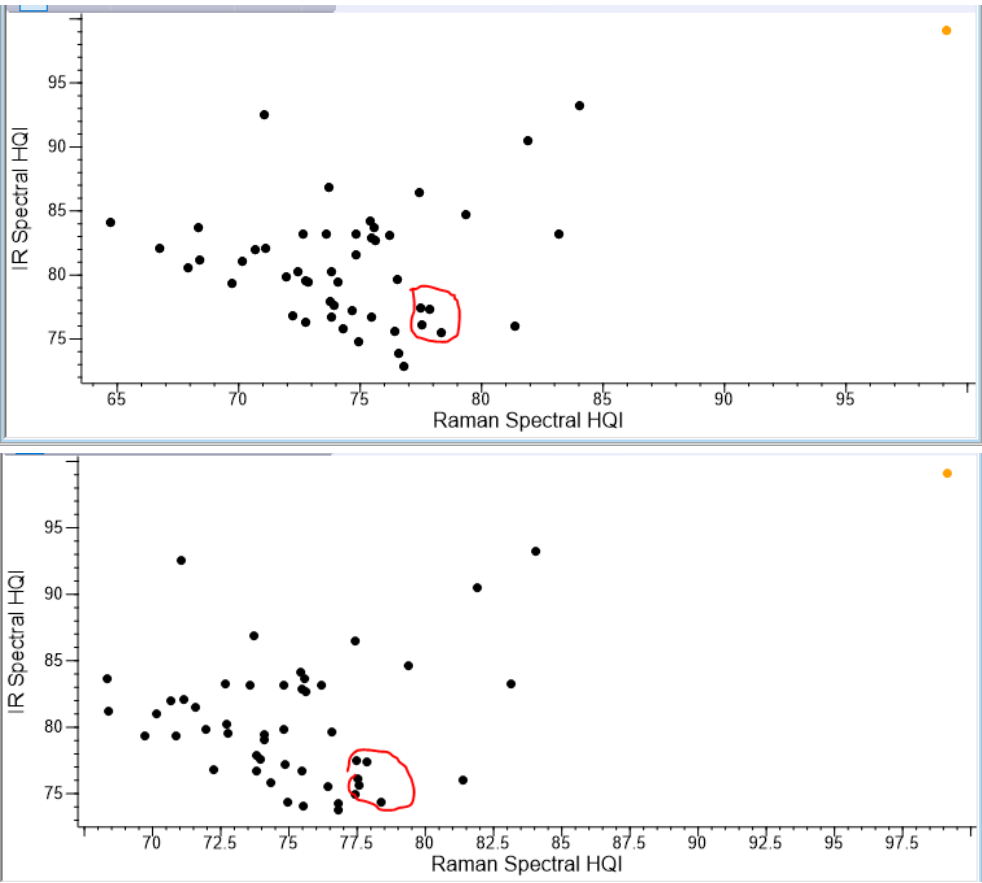


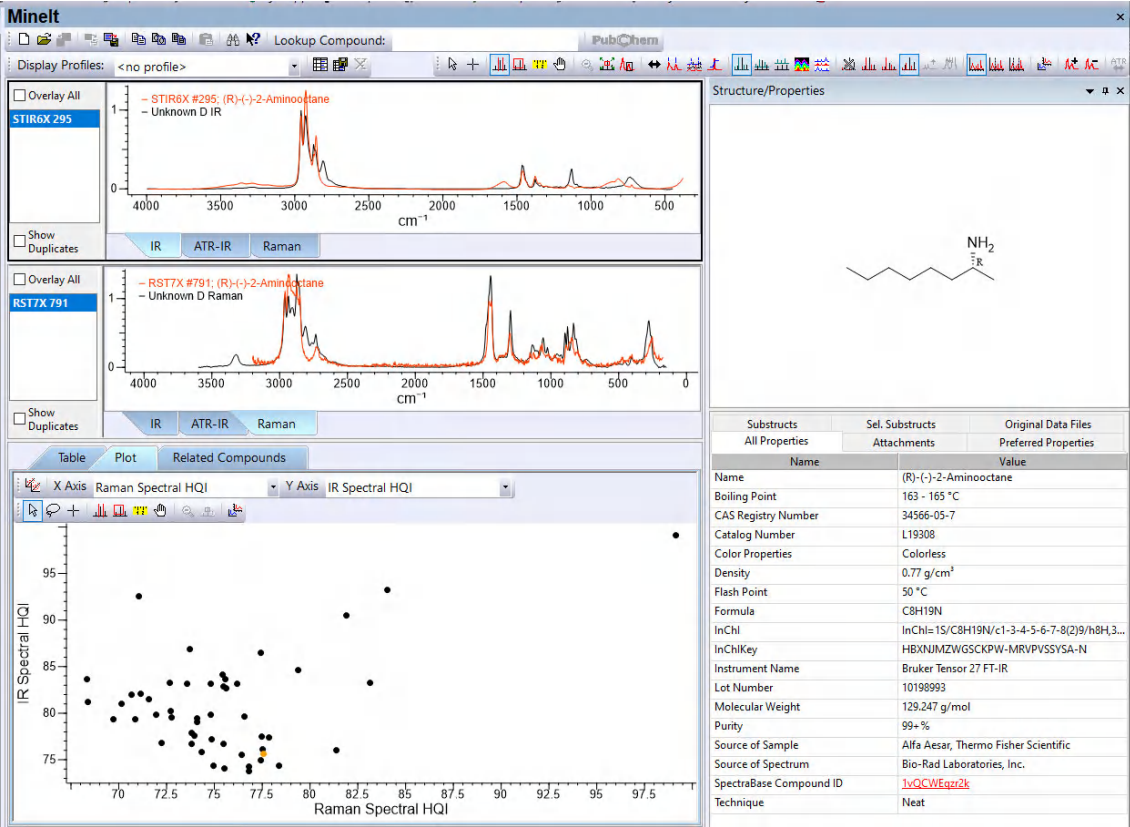
**Configure and perform a multi-technique spectral search with All Compounds Search Databases option**

	Action	Result
1	Do one of the following: <ul style="list-style-type: none"><li>• If the <b>SearchIt</b> application is not open, navigate to the <b>Data</b> toolbox and click its icon.</li><li>• If the <b>SearchIt</b> application is already open, click the SearchIt <b>Close</b> button  to close the current search.</li></ul>	The SearchIt application's <b>Databases</b> tab is displayed, and the <b>Selected for Searching</b> list displays the databases last used.
2	Check <b>All Compounds</b> under <b>Search Databases</b> option	
3	<ul style="list-style-type: none"><li>• Click <b>Spectrum</b> under <b>Search Categories</b>.</li><li>• Open <b>Unknown IR.jdx</b>.</li></ul>	



**Compare the search result with that from User-Select search**

	Action	Result
1		<p data-bbox="699 370 1869 397">Compare the scatter plot of the <b>User-Select</b> database search (top) and that of <b>All Compound</b> search (bottom)</p> <div data-bbox="699 402 1675 1279"><p>The figure consists of two vertically stacked scatter plots. Both plots have 'IR Spectral HQI' on the y-axis (ranging from 75 to 95) and 'Raman Spectral HQI' on the x-axis (ranging from 65 to 95). The top plot, labeled 'User-Select', shows a cluster of black data points with a red circle highlighting a specific region around (78, 78). The bottom plot, labeled 'All Compound', shows a similar cluster of black data points with a red circle highlighting a region around (78, 78). In both plots, there is a single orange outlier point at approximately (98, 98).</p></div> <p data-bbox="699 1287 1186 1315">We can see that more spots are in this region.</p>

Action	Result
Examine the extra spots	 <p>We can see that they are the stereoisomers whose IR and Raman spectral records are linked not by structure, but by other features in the record (name, InChI, CAS Registry Number or synonym).</p>

Action	Result																																																															
	<div><p><b>Minelt</b></p><p>Display Profiles: &lt;no profile&gt;</p><p>Lookup Compound: PubChem</p><p>Overlay All: <input type="checkbox"/> Show Duplicates: <input type="checkbox"/></p><p>STIR6X 137: - STIR6X #137: (S)-(+)-2-Aminooctane (ATR Corre... - Unknown D IR</p><p>RST7X 780: - RST7X #780: (S)-(+)-2-Aminooctane - Unknown D Raman</p><p>IR ATR-IR Raman</p><p>Table Plot Related Compounds</p><p>X Axis: Raman Spectral HQI Y Axis: IR Spectral HQI</p><p>IR Spectral HQI</p><p>Raman Spectral HQI</p><p>Structure/Properties</p><p><chem>CCCC[C@H](N)C</chem></p><table><thead><tr><th>Substructs</th><th>Sel. Substructs</th><th>Original Data Files</th></tr><tr><th>All Properties</th><th>Attachments</th><th>Preferred Properties</th></tr><tr><th>Name</th><th>Name</th><th>Value</th></tr></thead><tbody><tr><td>Name</td><td>(S)-(+)-2-Aminooctane</td><td></td></tr><tr><td>Boiling Point</td><td>163 - 165 °C</td><td></td></tr><tr><td>CAS Registry Number</td><td>34566-04-6</td><td></td></tr><tr><td>Catalog Number</td><td>L19309</td><td></td></tr><tr><td>Color Properties</td><td>Colorless</td><td></td></tr><tr><td>Density</td><td>0.77 g/cm<sup>3</sup></td><td></td></tr><tr><td>Flash Point</td><td>50 °C</td><td></td></tr><tr><td>Formula</td><td>C<sub>8</sub>H<sub>19</sub>N</td><td></td></tr><tr><td>InChI</td><td>InChI=1S/C<sub>8</sub>H<sub>19</sub>N/c1-3-4-5-6-7-8(2)/h8H,3...</td><td></td></tr><tr><td>InChIKey</td><td>HBXNIMZWGSKPW-QMMMGPBSA-N</td><td></td></tr><tr><td>Instrument Name</td><td>Bruker Tensor 27 FT-IR</td><td></td></tr><tr><td>Lot Number</td><td>10140654</td><td></td></tr><tr><td>Molecular Weight</td><td>129.247 g/mol</td><td></td></tr><tr><td>Purity</td><td>99+ %</td><td></td></tr><tr><td>Source of Sample</td><td>Alfa Aesar, Thermo Fisher Scientific</td><td></td></tr><tr><td>Source of Spectrum</td><td>Bio-Rad Laboratories, Inc.</td><td></td></tr><tr><td>SpectraBase Compound ID</td><td>60CJ6vTQzPa</td><td></td></tr><tr><td>Technique</td><td>Neat</td><td></td></tr></tbody></table></div> <p>The above is another stereo-isomer.</p>	Substructs	Sel. Substructs	Original Data Files	All Properties	Attachments	Preferred Properties	Name	Name	Value	Name	(S)-(+)-2-Aminooctane		Boiling Point	163 - 165 °C		CAS Registry Number	34566-04-6		Catalog Number	L19309		Color Properties	Colorless		Density	0.77 g/cm <sup>3</sup>		Flash Point	50 °C		Formula	C <sub>8</sub> H <sub>19</sub> N		InChI	InChI=1S/C <sub>8</sub> H <sub>19</sub> N/c1-3-4-5-6-7-8(2)/h8H,3...		InChIKey	HBXNIMZWGSKPW-QMMMGPBSA-N		Instrument Name	Bruker Tensor 27 FT-IR		Lot Number	10140654		Molecular Weight	129.247 g/mol		Purity	99+ %		Source of Sample	Alfa Aesar, Thermo Fisher Scientific		Source of Spectrum	Bio-Rad Laboratories, Inc.		SpectraBase Compound ID	60CJ6vTQzPa		Technique	Neat	
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# **KnowItAll Software Training**

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## Mixture Analysis



# Mixture Analysis

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## How to Analyze Mixture Spectra

### Purpose

This exercise demonstrates how to perform a mixture analysis using the KnowItAll Informatics System's SearchIt application.

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### Objectives

This exercise will teach you:

- How to configure a mixture analysis;
  - How to interpret the results of a mixture analysis.
- 

### Background

The spectral analysis of mixtures in experimental data is a challenging task. Manual separation of spectral components, even when they are known in advance, is a tedious job. Attempting to do this analysis in an automated fashion creates a whole new level of challenges.

This chapter introduces how to use SearchIt application to perform Mixture Analysis.

#### *Training Files Used In This Lesson*

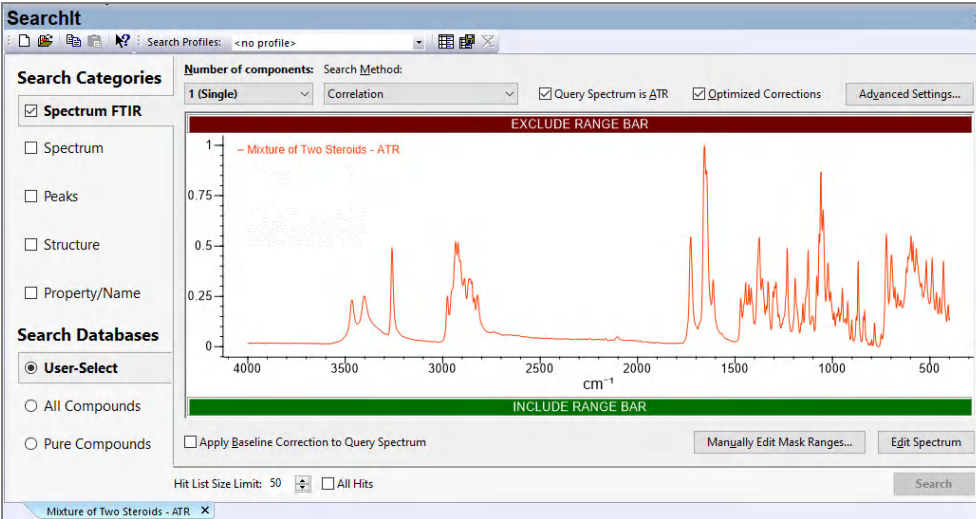
- Mixture of Two Steroids – ATR-IR.irf

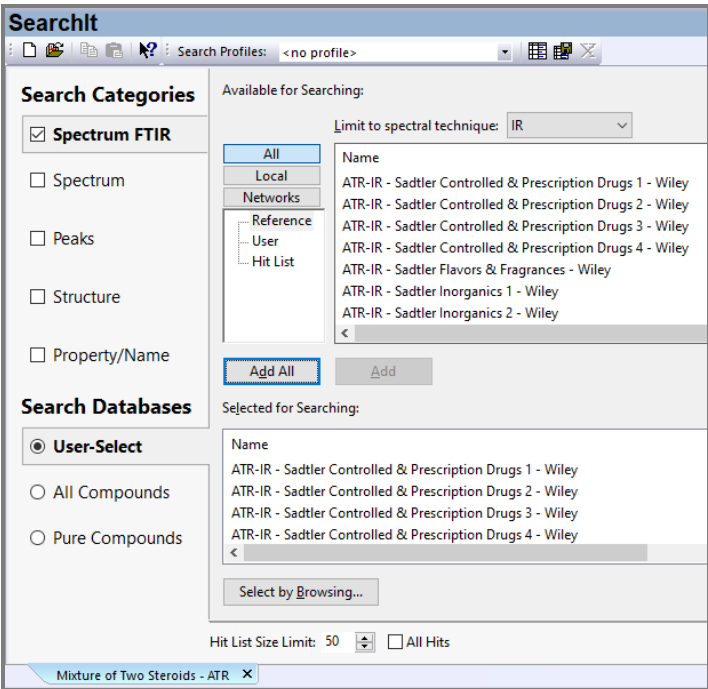
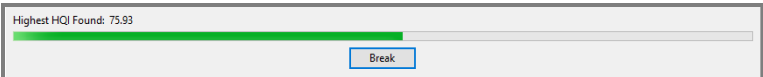
#### *KnowItAll Applications Used*

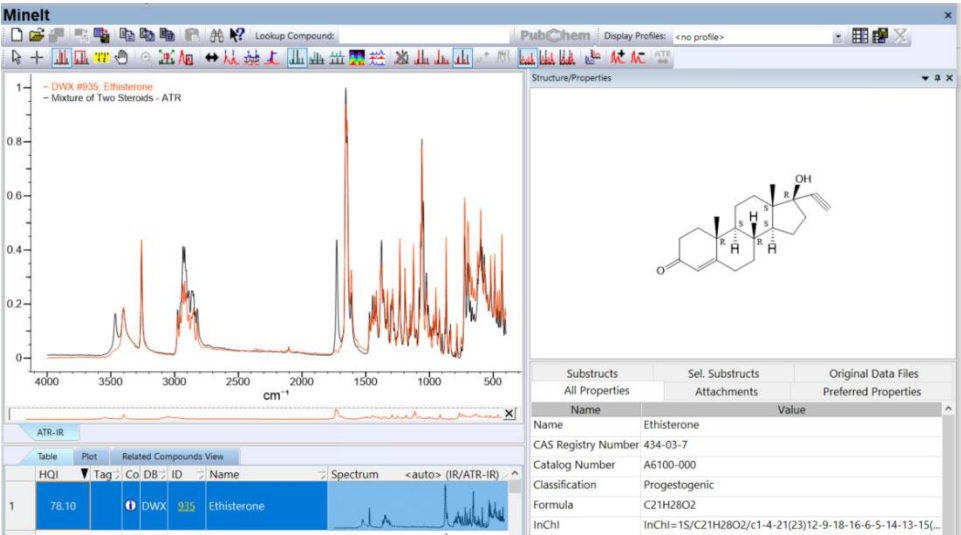
- SearchIt™
- Minelt™

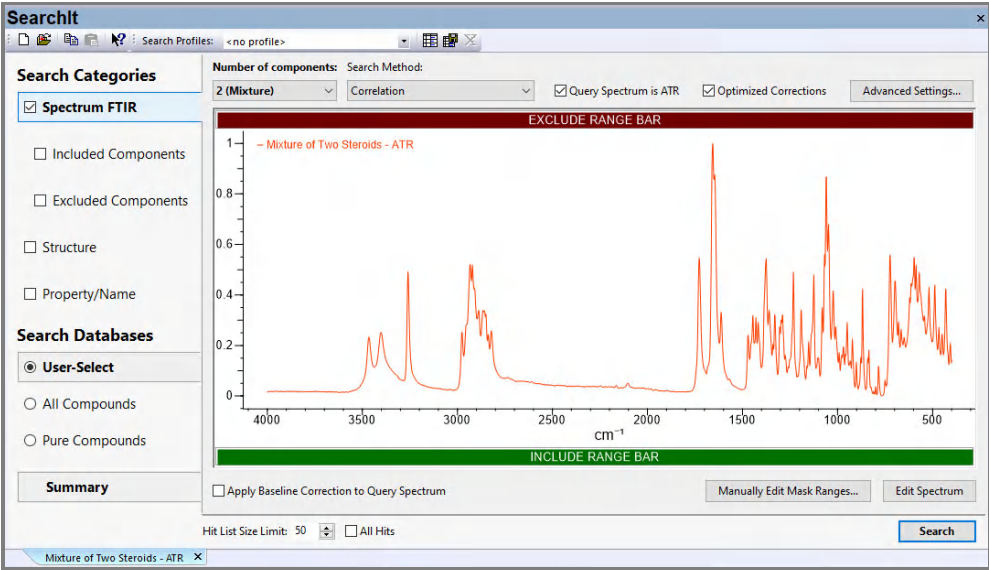
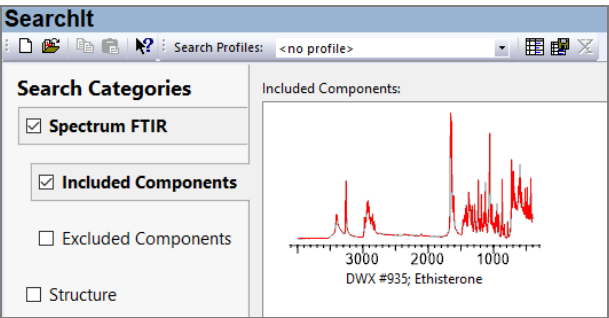


## A typical mixture analysis work flow

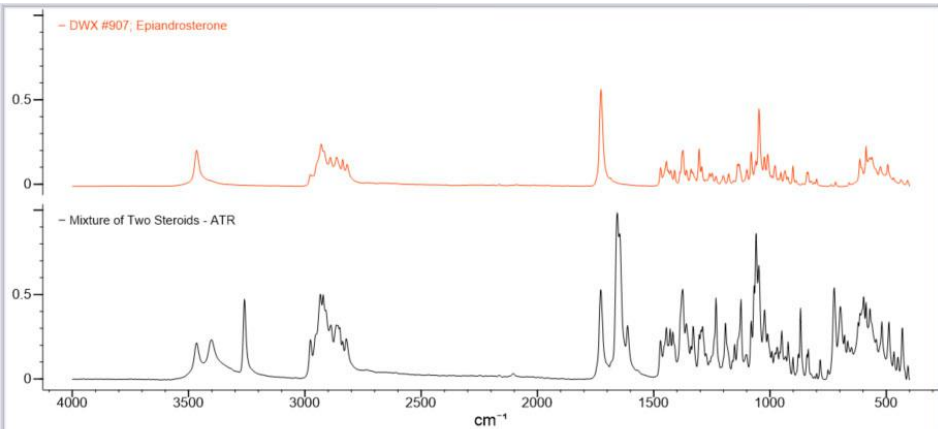







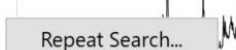







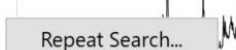







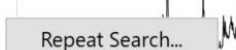
	Action	Result
1	<p>Navigate to the <b>Data</b> toolbox and open the <b>SearchIt</b> application</p> <p>Check <b>Spectrum</b>, and in the resulting <b>Open</b> dialog box navigate to KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; Mixture Analysis and open <b>Mixture of Two Steroids - ATR-IR</b>.</p> <ul style="list-style-type: none"> <li>• Set <b>Search Method</b> to <b>Correlation</b></li> <li>• Click on <b>User-Select</b> under <b>Search Databases</b></li> <li>• Set <b>Limit</b> to spectral technique to <b>IR</b></li> <li>• Click <b>Add All</b> at the bottom of <b>Available for searching</b> menu</li> </ul>	 <p>The screenshot displays the SearchIt application window. On the left, the 'Search Categories' panel has 'Spectrum FTIR' checked. Below it, 'Search Databases' shows 'User-Select' as the active option. The main area features a plot of the ATR-IR spectrum for 'Mixture of Two Steroids'. The x-axis represents wavenumber in cm<sup>-1</sup>, ranging from 4000 to 500. The y-axis represents intensity, ranging from 0 to 1. A red line shows the spectrum, with several prominent peaks. Above the plot is an 'EXCLUDE RANGE BAR' and below it is an 'INCLUDE RANGE BAR'. The title bar of the window reads 'SearchIt'.</p>













	Action	Result
1	<p>Do the following:</p> <ul style="list-style-type: none"> <li>• Set <b>Search Method</b> to <b>Correlation</b></li> <li>• Click on <b>User-Select</b> under <b>Search Databases</b></li> <li>• Set <b>Limit to spectral technique</b> to <b>IR</b></li> <li>• Click <b>Add All</b> at the bottom of <b>Available for searching</b> menu</li> </ul>	 <p>The screenshot shows the SearchIt application window. On the left, under 'Search Categories', 'Spectrum FTIR' is checked. Under 'Search Databases', 'User-Select' is selected. On the right, 'Available for Searching' lists several databases with 'Limit to spectral technique' set to 'IR'. The 'Add All' button is highlighted. Below it, 'Selected for Searching' shows the same list of databases. At the bottom, 'Hit List Size Limit' is set to 50 and 'All Hits' is unchecked. The window title bar shows 'Mixture of Two Steroids - ATR'.</p>
2	Click <b>Search</b> .	<p>Wait for the search to complete.</p>  <p>The screenshot shows a progress bar with the text 'Highest HQI Found: 75.93' and a 'Break' button.</p>

	Action	Result
		<p>One component search result returns to <b>Minelt</b> application.</p>  <p>Obviously, the sample is a mixture.</p>
3	<p>Highlight the 1st hit. <b>Edit &gt; Copy Active Spectrum</b></p>	

	Action	Result
4	<p>Go back to <b>SearchIt</b>, Click the <b>Spectrum FTIR</b> button to bring up the query spectrum. Update the <b>Number of components</b> to <b>2 (Mixture)</b>.</p>	 <p>The <b>Included Components</b> and <b>Excluded Components</b> checkboxes show up now.</p>
5	<p>Check the <b>Included Components</b> Paste the copied spectrum.</p>	

	Action	Result																																																						
6	<p>Click the <b>Spectrum FTIR</b> button to bring up the query spectrum.</p> <p>Click <b>Search</b>.</p>	<div><div><div>Minelt</div><div><div>Lookup Compound: PubChem</div><div>Display Profiles: &lt;no profile&gt;</div></div><div><div><div><div><div>Composite Spectrum</div><div>Mixture of Two Steroids - ATR</div></div><div></div></div></div><div><div>ATR-IR</div><table><thead><tr><th colspan="2">Table</th><th>Plot</th><th colspan="2">Related Compounds View</th><th colspan="2"></th><th></th><th></th></tr><tr><th>HQI</th><th>Weight</th><th>Exclude</th><th>Co DB</th><th>ID</th><th>Name</th><th>Chemical Structure</th><th>Spectrum</th><th>&lt;auto&gt; (IR/ATR-IR)</th></tr></thead><tbody><tr><td>1</td><td>95.48</td><td>N.A.</td><td></td><td></td><td>Composite Spectrum</td><td></td><td></td><td></td></tr><tr><td></td><td>0.62</td><td></td><td></td><td></td><td>DWX #935; Ethisterone</td><td></td><td></td><td></td></tr><tr><td></td><td>0.38</td><td></td><td></td><td></td><td>Eplandrosterone</td><td></td><td></td><td></td></tr><tr><td></td><td>N.A.</td><td></td><td></td><td></td><td>Residual Spectrum</td><td></td><td></td><td></td></tr></tbody></table></div></div></div><p>Now we have a good two-component match.</p><p><b>Note:</b> Each composite spectrum (row 1) is accompanied by the individual component spectra (middle rows) that comprise the composite, as well as the residual spectrum (last row) – the difference between the query spectrum and the composite. The composite spectra are ranked by how closely they resemble the query spectrum. A relatively flat residual spectrum indicates that the software has correctly identified the individual components of the mixture. The <b>Weight</b> value for each component spectrum indicates how much it contributes to the composite spectrum.</p></div>	Table		Plot	Related Compounds View						HQI	Weight	Exclude	Co DB	ID	Name	Chemical Structure	Spectrum	<auto> (IR/ATR-IR)	1	95.48	N.A.			Composite Spectrum					0.62				DWX #935; Ethisterone					0.38				Eplandrosterone					N.A.				Residual Spectrum			
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	N.A.				Residual Spectrum																																																			

Action		Result																																																												
7	<p>The circle in <b>Exclude</b> column can be checked to exclude a component from consideration.</p> <p>Check to exclude <b>DWX 907</b>. <b>Repeat Search</b> button shows up for user to repeat Mixture Analysis without considering DWX 907</p>	<div><p>ATR-IR</p></div> <div><p>Table Plot Related Compounds View</p><table><tr><th>HQI</th><th>Weight</th><th>Exclude</th><th>Co</th><th>DB</th><th>ID</th><th>Name</th><th>Chemical Structure</th><th>Spectrum</th><th>&lt;auto&gt; (IR/ATR-IR)</th></tr><tr><td>1</td><td>95.48</td><td>N.A.</td><td></td><td></td><td></td><td>Composite Spectrum</td><td></td><td></td><td></td></tr><tr><td></td><td>0.62</td><td></td><td></td><td></td><td></td><td>DWX #935; Ethisterone</td><td></td><td></td><td></td></tr><tr><td></td><td>0.38</td><td><input checked="" type="checkbox"/></td><td></td><td></td><td>DWX 907</td><td>Epiandrosterone</td><td></td><td></td><td></td></tr><tr><td></td><td>N.A.</td><td></td><td></td><td></td><td></td><td>Residual Spectrum</td><td></td><td></td><td></td></tr><tr><td>2</td><td>95.48</td><td>N.A.</td><td></td><td></td><td></td><td>Composite Spectrum</td><td></td><td></td><td></td></tr></table><div>Repeat Search...</div></div>	HQI	Weight	Exclude	Co	DB	ID	Name	Chemical Structure	Spectrum	<auto> (IR/ATR-IR)	1	95.48	N.A.				Composite Spectrum					0.62					DWX #935; Ethisterone					0.38	<input checked="" type="checkbox"/>			DWX 907	Epiandrosterone					N.A.					Residual Spectrum				2	95.48	N.A.				Composite Spectrum			
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	Action	Result																																																										
8	Click <b>Repeat Search</b> .	<p>The new result does not contain excluded DWX 907:</p> <div><p>- Composite Spectrum</p><p>- Mixture of Two Steroids - ATR</p></div> <p>ATR-IR</p> <table><tr><th>Table</th><th>Plot</th><th colspan="5">Related Compounds View</th><th></th></tr><tr><th></th><th>HQI</th><th>▼ Weight</th><th>Exclude</th><th>Co</th><th>DB</th><th>ID</th><th>Name</th><th>Chemical Structure</th><th>Spectrum &lt;auto&gt; (IR/ATR-IR)</th></tr><tr><td>1</td><td>95.33</td><td>N.A.</td><td></td><td></td><td></td><td></td><td>Composite Spectrum</td><td></td><td></td></tr><tr><td></td><td></td><td>0.64</td><td></td><td></td><td></td><td></td><td>DWX #935; Ethisterone</td><td></td><td></td></tr><tr><td></td><td></td><td>0.36</td><td></td><td></td><td>VSA</td><td>5052</td><td>Epiandrosterone</td><td></td><td></td></tr><tr><td></td><td></td><td>N.A.</td><td></td><td></td><td></td><td></td><td>Residual Spectrum</td><td></td><td></td></tr></table>	Table	Plot	Related Compounds View							HQI	▼ Weight	Exclude	Co	DB	ID	Name	Chemical Structure	Spectrum <auto> (IR/ATR-IR)	1	95.33	N.A.					Composite Spectrum					0.64					DWX #935; Ethisterone					0.36			VSA	5052	Epiandrosterone					N.A.					Residual Spectrum		
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**Notes:**

- You do not have to specify **Included** or **Excluded** components to perform a mixture analysis. You can simply open a spectrum in **SearchIt** and specify **Number of components** to a value larger than 1.

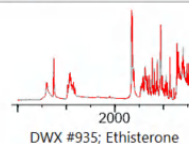
**Number of components:**

3 (Mixture)
1 (Single)
2 (Mixture)
3 (Mixture)
4 (Mixture)
5 (Mixture)

- You can add **Included** or **Excluded** components from files by clicking the **Add** button.

**Search Categories**

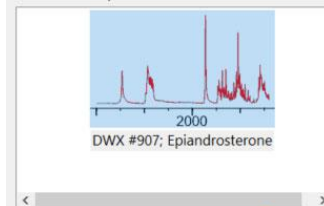
- ☒ Spectrum FTIR
- ☒ Included Components
- ☒ Excluded Components

**Included Components:**

Add...

Delete

- You can exclude spectrally similar records.

**Excluded Components:**

Add...

Delete

☐ Apply Bas

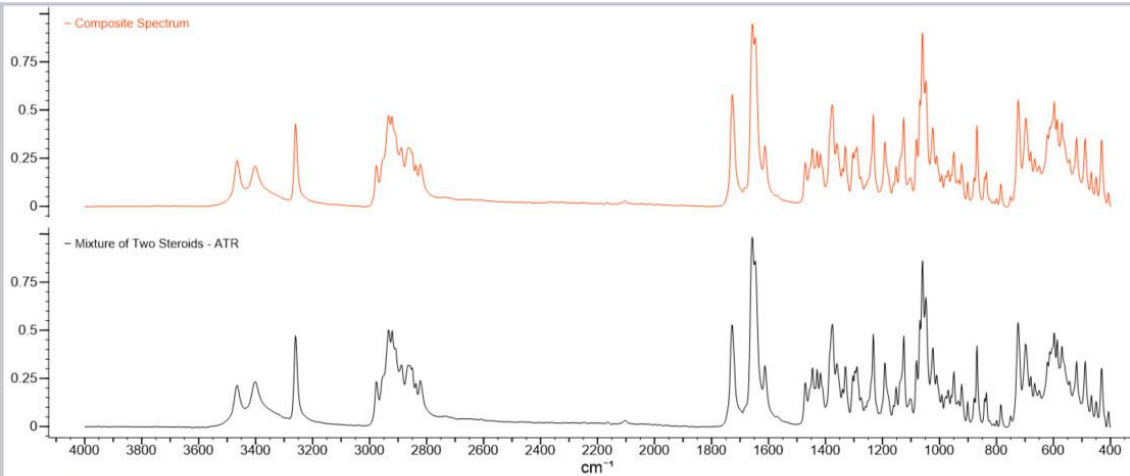






























Image Size:

☒ Spectrum☒ Exclude compounds that are similar within a limit of: 95



**Add all components together**

	Action	Result
1	<ul style="list-style-type: none"><li>• In the <b>Data</b> toolbox, open the <b>SearchIt</b> application</li><li>• Check <b>Spectrum</b></li><li>• In the resulting <b>Open</b> dialog box, navigate to <b>KnowItAll &gt; Samples &gt; Mixture Analysis &gt; IR Examples</b></li><li>• Open <b>Mixture of Two Steroids - ATR-IR</b>.</li><li>• Set <b>Search Method</b> to <b>Correlation</b>.</li><li>• Set <b>Number of components</b> to <b>2 (Mixture)</b>:</li></ul>	
2	<p>Check <b>Included Components</b></p> <p>Add following files from <b>KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; Mixture Analysis &gt; Components</b> folder:</p> <ul style="list-style-type: none"><li>• <b>Epiandrosterone ATR-IR</b></li><li>• <b>Ethisterone ATR-IR</b></li></ul> <p><b>Note:</b> use ctrl key to select multiple files in the <b>Open</b> dialog box.</p>	

Action	Result																																																												
<div>3</div> <div>Click <b>Search</b>.</div> <div><b>Note:</b> toggle between different spectra display modes by selecting available options from <b>View &gt; Display Mode</b>.</div>	<div></div> <div><div>ATR-IR</div><div><div>Table</div><div>Plot</div><div>Related Compounds View</div></div><table><thead><tr><th></th><th>HQI</th><th>Weight</th><th>Exclude</th><th>Co</th><th>DB</th><th>ID</th><th>Name</th><th>Spectrum</th><th>&lt;auto&gt; (IR/ATR-IR)</th></tr></thead><tbody><tr><td>1</td><td>95.48</td><td>N.A.</td><td></td><td></td><td></td><td></td><td>Composite Spectrum</td><td></td><td></td></tr><tr><td></td><td></td><td>0.62</td><td></td><td></td><td></td><td></td><td>Ethisterone ATR</td><td></td><td></td></tr><tr><td></td><td></td><td>0.38</td><td></td><td></td><td></td><td></td><td>Epiandrosterone ATR</td><td></td><td></td></tr><tr><td></td><td></td><td>N.A.</td><td></td><td></td><td></td><td></td><td>Residual Spectrum</td><td></td><td></td></tr><tr><td>2</td><td>78.10</td><td>1.00</td><td></td><td></td><td></td><td></td><td>Ethisterone ATR</td><td></td><td></td></tr></tbody></table></div> <div>In this case, KnowItAll simply returns possible combinations of two provided components, without going through a database search.</div>		HQI	Weight	Exclude	Co	DB	ID	Name	Spectrum	<auto> (IR/ATR-IR)	1	95.48	N.A.					Composite Spectrum					0.62					Ethisterone ATR					0.38					Epiandrosterone ATR					N.A.					Residual Spectrum			2	78.10	1.00					Ethisterone ATR		
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# **KnowItAll Software Training**

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## Create Databases

# Create Databases

## How to Build Your Own User Databases of Multiple Analytical Techniques

### Purpose

This exercise demonstrates how to use KnowItAll's Minelt™ Database Building feature to create searchable user databases that include multiple analytical techniques. You can also customize properties displayed, create user properties and display profiles.

### Objectives

This exercise will teach you:

- How to create a user database;
- How to add spectra to a user database;
- How to add structures to a user database;
- How to add user properties;
- How to perform above tasks in batch; and
- How to create and use a Minelt display profile.

### Background

Generating user databases protects intellectual property and promotes sharing of information within an organization. Ultimately, researchers can improve their analyses.

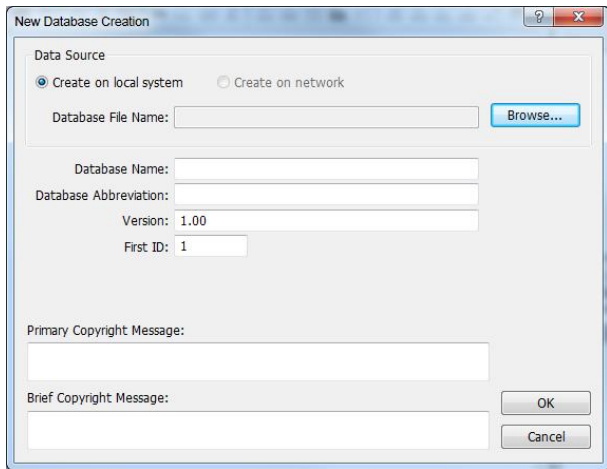
#### *Training Files Used in This Lesson*

- IR/Ethyl acetate.dx
- Raman/Ethyl acetate.irf
- BatchImportProperties.csv
- Spectral files from the Batch Import Spectra folder
- MSDS Web Link.txt
- Ethyl acetate MSDS.pdf
- Spectral files from the PubChem/Raman folder

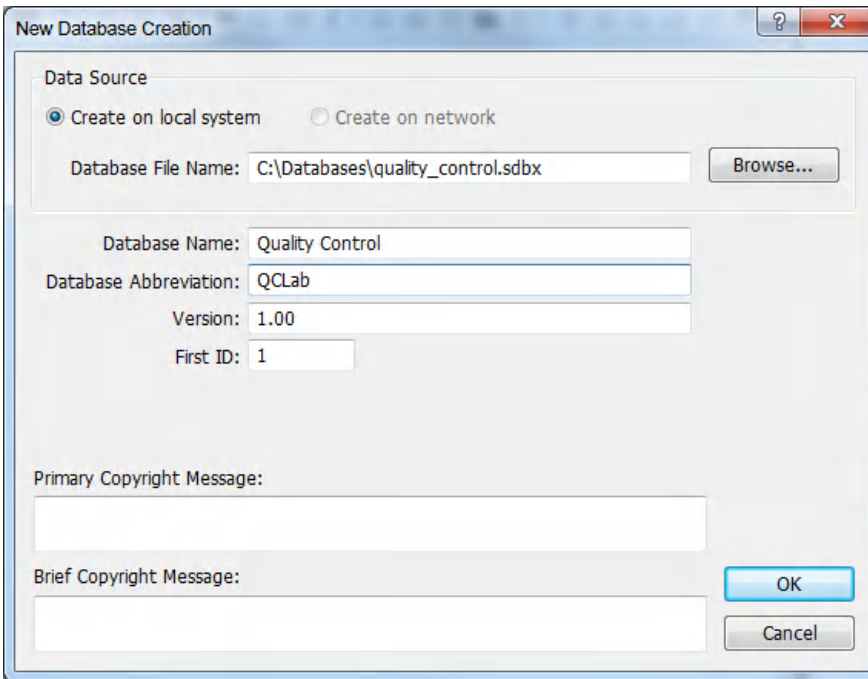
#### *KnowItAll Applications Used*

- Minelt™
- ChemWindow®
- Browselt™

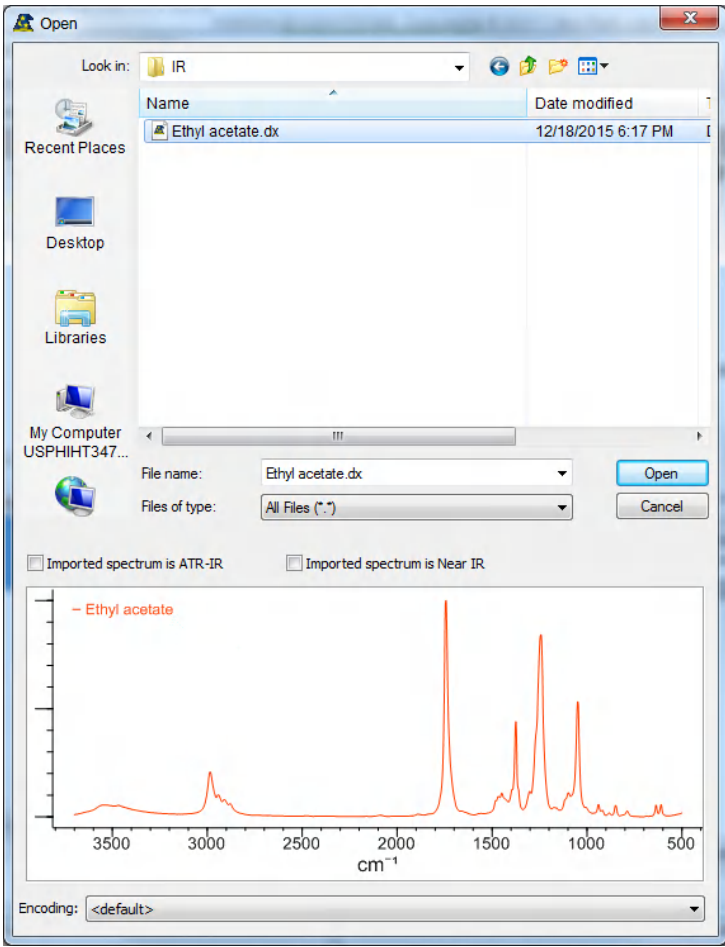
**Create a user database**

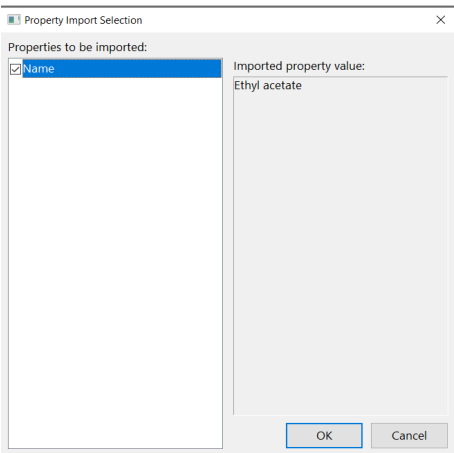
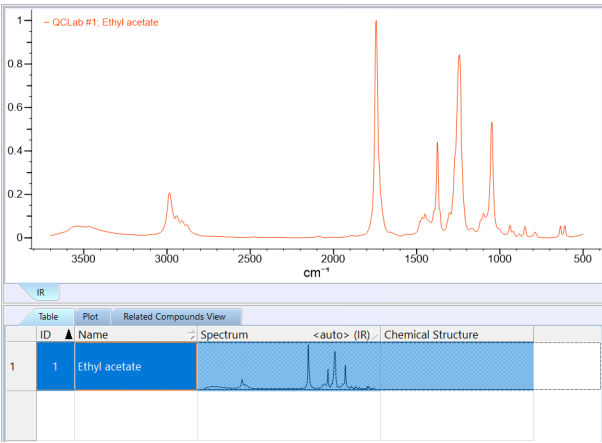
	Action	Result
1	Navigate to the <b>Data</b> toolbox and open the Minelt application by clicking the <b>Minelt/Create Database</b> icon.	The Minelt application opens.
2	Choose <b>Database &gt; New</b> .	<p>The <b>New Database Creation</b> dialog box opens.</p> 
3	Select <b>Create on local system</b> .	The new database is saved locally.
4	<ul style="list-style-type: none"> <li>Click <b>Browse</b>.</li> <li>Create a folder named <b>Databases</b> on a local drive</li> <li>Open the folder, then type in the file name <b>quality_control</b></li> <li>Click <b>Save</b>.</li> </ul>	<p>The *.sdbx extension is added automatically.</p> <p><b>Note:</b> The SDBX database format allows spectra to be stored without conforming to a fixed range and resolution. This allows reference spectra to be offered at higher resolution, and allows users to store original spectra as produced.</p>
5	<p>Type <b>Quality Control</b> in the <b>Database Name</b> text box.</p> <p><b>Note:</b> The file name is used if no other name is specified.</p>	

**Create a user database (continued)**

	Action	Result
6	Type <b>QCLab</b> in the <b>Database Abbreviation</b> text box.  <b>Note:</b> The abbreviation must be 3-7 characters long.	
7	Enter <b>Version</b> number and the <b>First (starting) ID</b> , and type in copyright messages.  <b>Note:</b> You can use the Windows Character Map (Programs > Accessories > System Tools in Windows 7) to copy and paste in the copyright symbol.	
8	Click <b>OK</b> .	The new database has been created to receive your data. The Database Abbreviation 'QCLab' appears on the database tab below the database pane (lower left), and copyright information appears in the status area (lower edge of the main window).


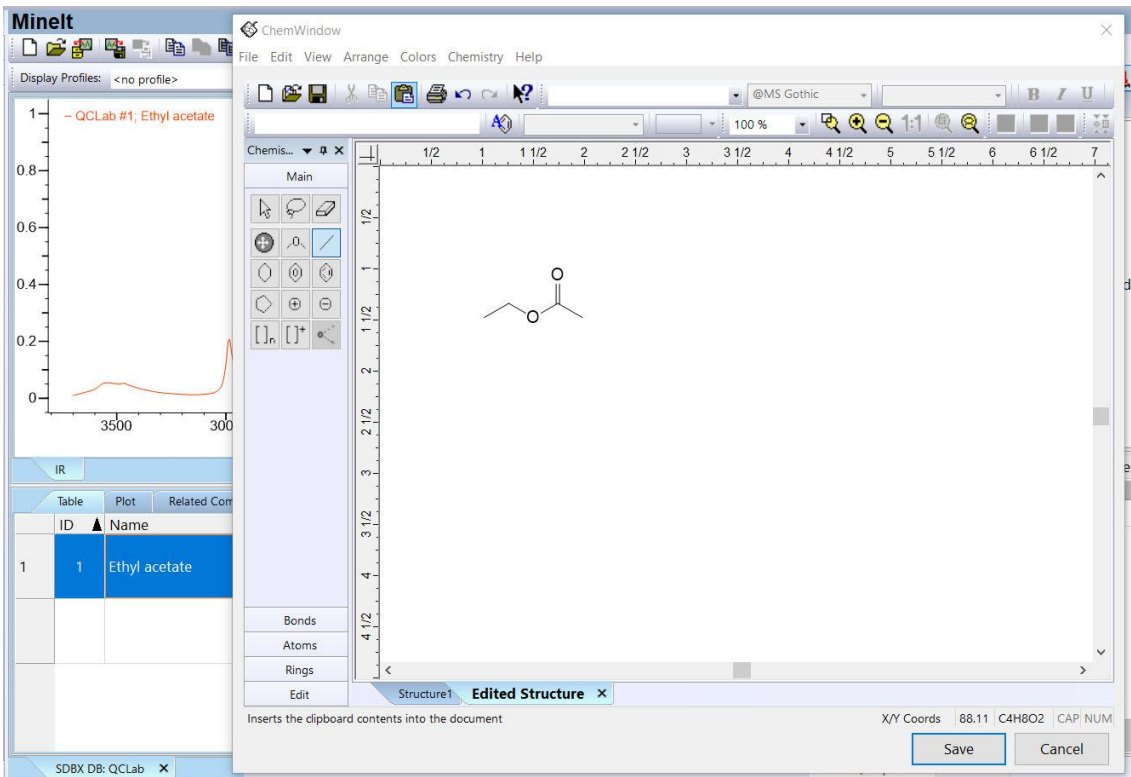
**Add the first record to the user database**

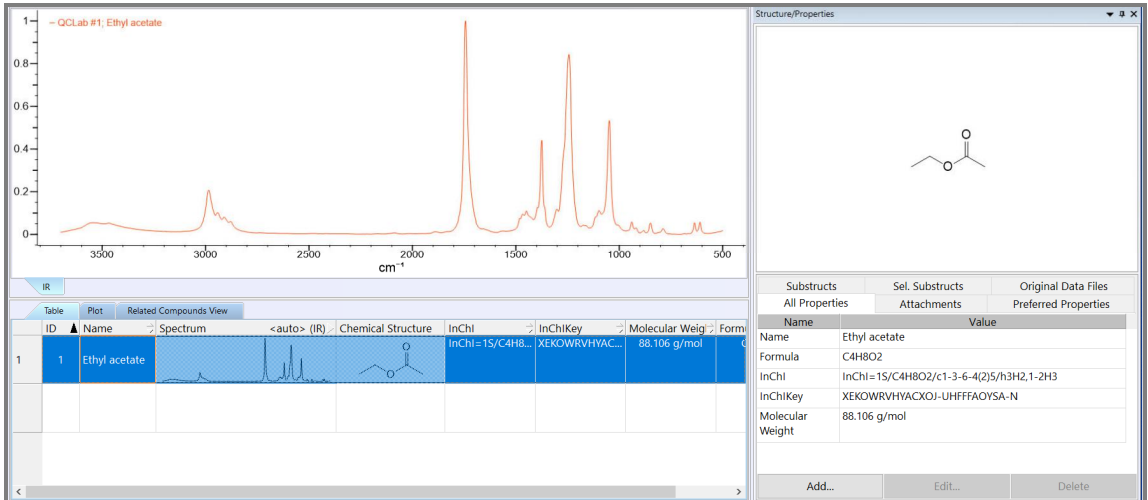
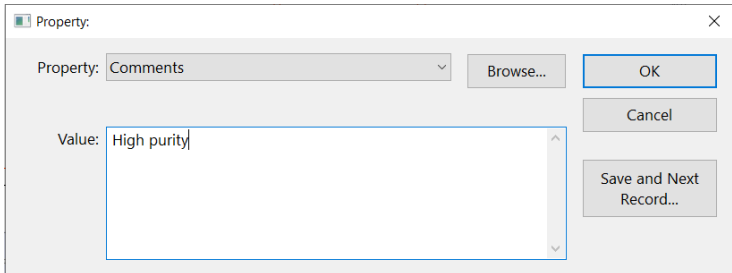
	Action	Result
1	<p>Create the first database record by importing a spectrum:</p> <ul style="list-style-type: none"><li>Choose <b>File &gt; Import</b> or press Ctrl+I.</li><li>Navigate to <b>KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; Creating Databases &gt; IR</b></li><li>Open <b>Ethyl acetate.dx</b></li></ul> <p><b>Note:</b> Use the <b>Files of type</b> filter to locate IRF, JCAMP, and many other specific spectral files.</p>	<p>A Windows <b>Open</b> dialog box appears.</p>  <p>The screenshot shows a Windows 'Open' dialog box. The 'Look in:' dropdown is set to 'IR'. The file list contains one entry: 'Ethyl acetate.dx' with a date modified of '12/18/2015 6:17 PM'. The 'File name:' field contains 'Ethyl acetate.dx'. The 'Files of type:' dropdown is set to 'All Files (*.*)'. At the bottom, there is a checkbox for 'Imported spectrum is ATR-IR' and a checkbox for 'Imported spectrum is Near IR'. Below these is a plot of the IR spectrum for 'Ethyl acetate', showing transmittance versus wavenumber (cm<sup>-1</sup>) from 3500 to 500. The spectrum shows several characteristic peaks, including a sharp peak around 1735 cm<sup>-1</sup> and a broad peak around 3000 cm<sup>-1</sup>.</p>

	Action	Result
2	Click <b>Open</b> .	<p>The <b>Property Import Selection</b> dialog box opens:</p>  <p>This dialog box appears when you transfer information into a user database. All available properties are shown. Select each property in turn; then use the checkboxes to define the action for each property.</p>
3	Click <b>OK</b> .	<p>The dialog box closes. The spectrum has been added to the user database as the first record:</p> 



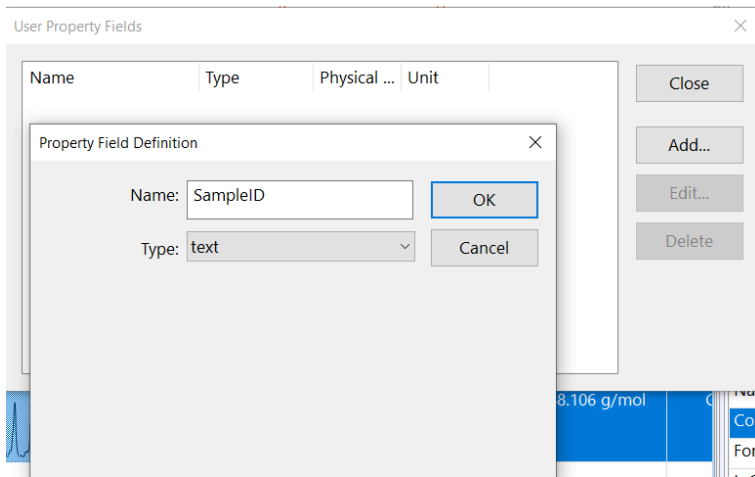
**Add a chemical structure and properties to the first database record**

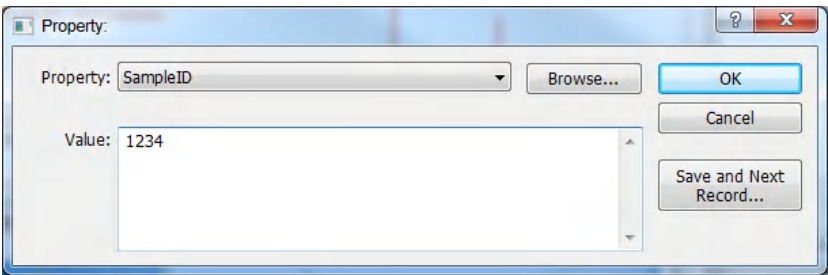
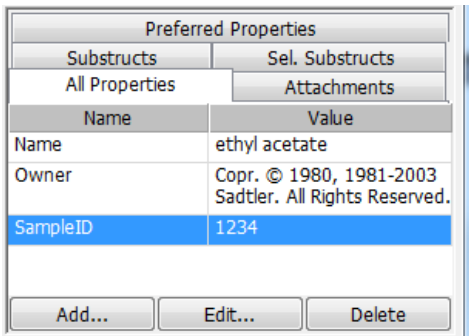
	Action	Result
1	With the first record selected, double-click the Structure/Properties pane at the top right of the window ( <b>Double-click to edit structure in ChemWindow</b> ).	The ChemWindow application pops up. Alternatively, one can use <b>Transfer to:</b> to go to the ChemWindow application. 
2	Use the drawing tools to create this structure	

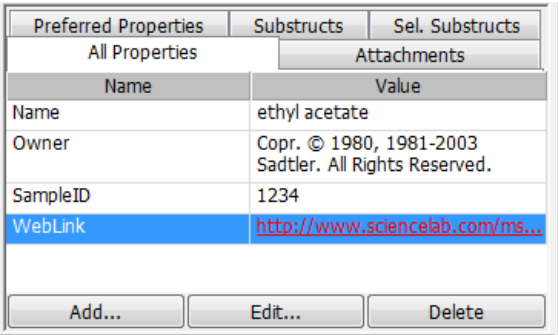
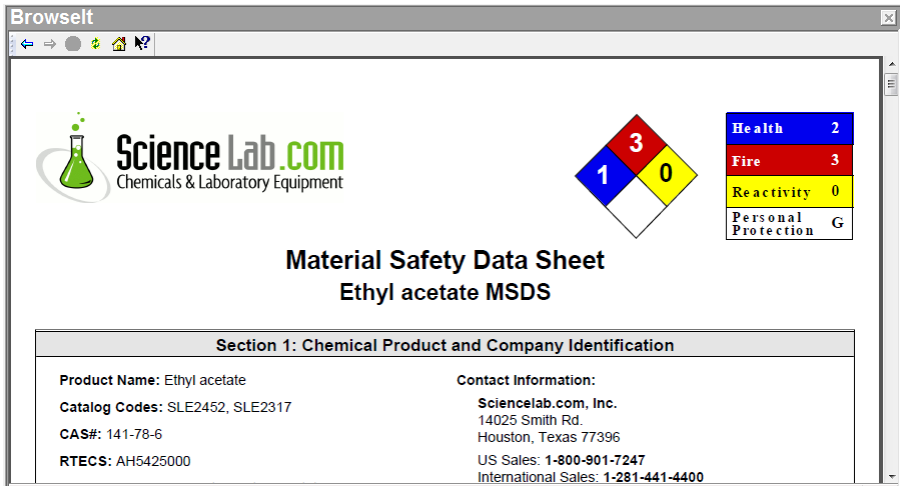
	Action	Result
3	Click <b>Save</b> .	<p>The structure is added to the first record, and is displayed both in the <b>Chemical Structure</b> column in the <b>Database</b> pane and the <b>Structure/Properties</b> pane.</p>  <p>NOTE: Some chemical properties such as InChI, InChIKey, Molecular Weight, etc., can be set to be automatically calculated when a structure is saved in a record.</p>
4	Click <b>Add</b> at the bottom of the Structure/Properties pane.	The <b>Property</b> dialog box appears.
5	Use the drop-down list to select the property you wish to add – <b>Comments</b> .	

	Action	Result																											
6	Click <b>OK</b> .	<p>The <b>Property</b> dialog box closes, and the name and value of the added property appear in the <b>Structure/Properties</b> pane.</p> <table border="1"> <tr> <td>Substructs</td><td>Sel. Substructs</td><td>Original Data Files</td></tr> <tr> <td>All Properties</td><td>Attachments</td><td>Preferred Properties</td></tr> <tr> <th>Name</th><th colspan="2">Value</th></tr> <tr> <td>Name</td><td colspan="2">Ethyl acetate</td></tr> <tr> <td>Comments</td><td colspan="2">High purity</td></tr> <tr> <td>Formula</td><td colspan="2">C4H8O2</td></tr> <tr> <td>InChI</td><td colspan="2">InChI=1S/C4H8O2/c1-3-6-4(2)5/h3H2,1-2H3</td></tr> <tr> <td>InChIKey</td><td colspan="2">XEKOWRVHYACXOJ-UHFFFAOYSA-N</td></tr> <tr> <td>Molecular Weight</td><td colspan="2">88.106 g/mol</td></tr> </table>	Substructs	Sel. Substructs	Original Data Files	All Properties	Attachments	Preferred Properties	Name	Value		Name	Ethyl acetate		Comments	High purity		Formula	C4H8O2		InChI	InChI=1S/C4H8O2/c1-3-6-4(2)5/h3H2,1-2H3		InChIKey	XEKOWRVHYACXOJ-UHFFFAOYSA-N		Molecular Weight	88.106 g/mol	
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Name	Ethyl acetate																												
Comments	High purity																												
Formula	C4H8O2																												
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	<b>TIP</b>	You can select multiple database records and use the <b>Add</b> or <b>Edit</b> button at the bottom of the <b>Structure/Properties</b> pane to input the same value for a field.																											

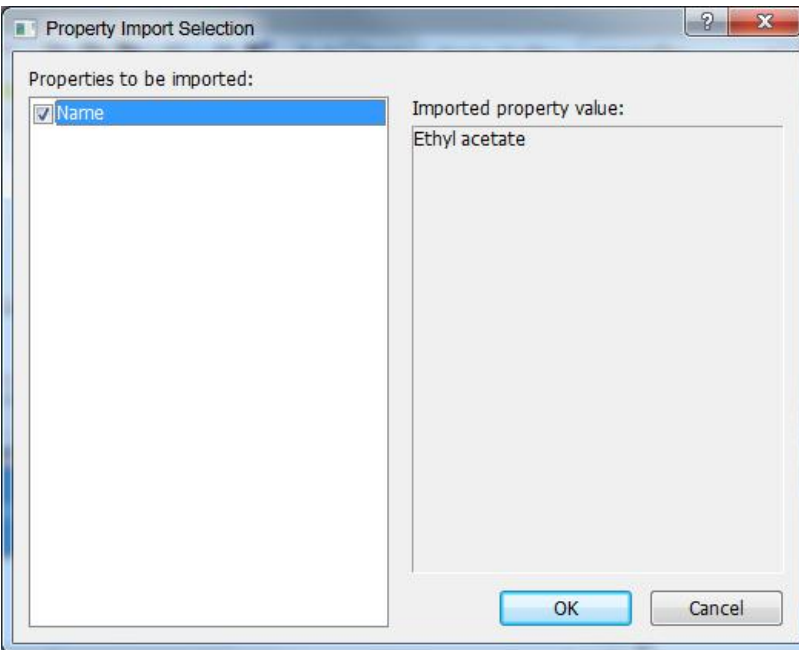
**Add user properties**

	Action	Result
1	Choose <b>Database &gt; Define User Property Fields</b>	The <b>User Property Fields</b> dialog box opens.
2	Click <b>Add</b> . Use the drop-down list to set <b>Type</b> to text.	<p>The <b>Property Field Definition</b> dialog box opens.</p>  <p><b>Note:</b> Which controls are available depends on which type of field is specified: numeric, text, or enumeration.</p>
3	Click <b>OK</b> , then <b>Close</b>	
4	Click <b>Add</b> in the <b>Structure/Properties</b> pane.	<p>The <b>Property</b> dialog box opens.</p> <p><b>Note:</b> Choose <b>View &gt; Windows/Tables &gt; Structure/Properties Table</b> or press Alt+3 if the pane is not visible.</p>
5	Click the down arrow to display all available properties.	Both pre-defined and user-defined properties are displayed. User-defined properties are at the beginning of the list.
6	Select <b>SampleID</b> .	<p>The Value text box is added to the dialog.</p> <p><b>Note:</b> Which text boxes are added depends on whether the property is numeric, text, or enumeration.</p>

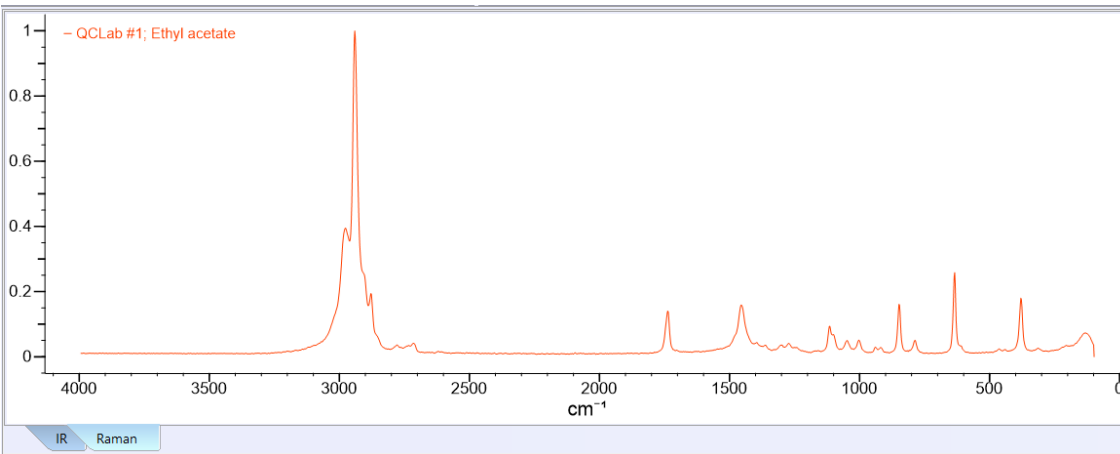
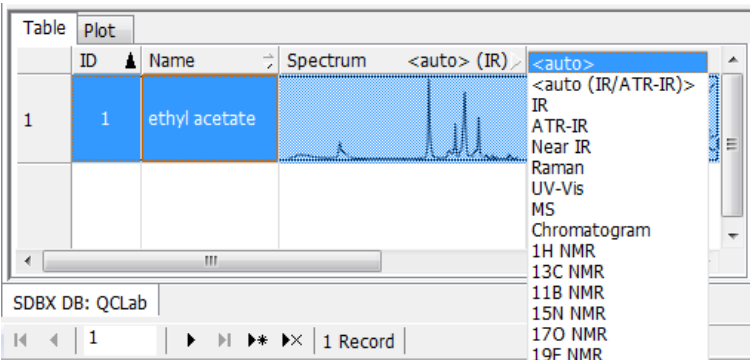
7	Type '1234' in the <b>Value</b> text box.	
8	Click <b>OK</b> .	<p>The dialog box closes. The property <b>SampleID</b> with value 1234 is added to the <b>Structure/Properties</b> pane for the first record.</p> 

	Action	Result
9	<p>Repeat steps 1-10 to create the user property WebLink and display it in the <b>Structure/Properties</b> pane.</p> <p>Type 'https://pubchem.ncbi.nlm.nih.gov/compound/ethyl-acetate' in the <b>Property</b> dialog box's <b>Value</b> field.</p> <p><b>Note:</b> You can copy the text string from MSDS Web link.txt in the KnowItAll Training files.</p>	<p>The property <b>WebLink</b> with a web address is added to the <b>Structure/Properties</b> pane for the first record.</p> 
10	Click the web address in the <b>Structure/Properties</b> pane.	<p>The web page opens in the <b>Browselt</b> application.</p> 
11	Click the KnowItAll <b>Back</b> button to return to the <b>Minelt</b> application.	

**Add another spectrum (Raman) to the first database record**

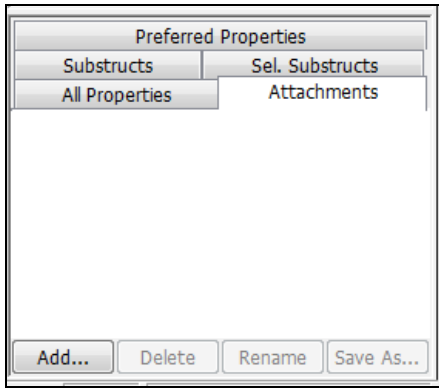
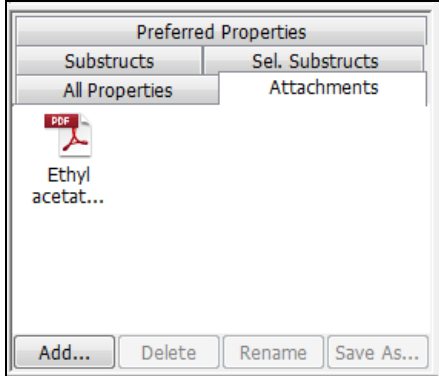
	Action	Result
1	Make sure the first database record is selected, then choose <b>File &gt; Import</b> .	The <b>Open</b> dialog box with preview pane appears.
2	Navigate to <b>KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; Creating Databases &gt; Raman</b> Open <b>Ethyl acetate.irf</b> .	<p>The <b>Property Import Selection</b> dialog box opens.</p>  <p>This dialog box appears when you transfer information into a user database. All available properties are shown.</p>

**Add another spectrum (Raman) to the first database record (continued)**

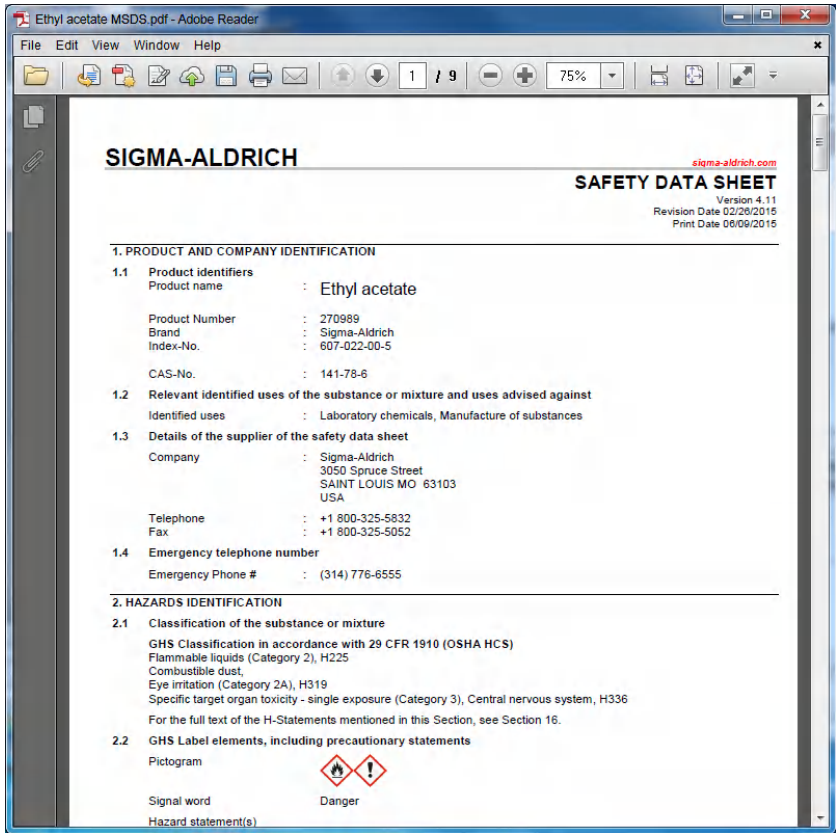
	Action	Result
3	Click <b>OK</b> .	<p>A new <b>Raman</b> tab is added to the <b>Spectral</b> pane for the display of the Raman spectrum.</p> 
4	Switch between spectra by using the tabs at the bottom left of the spectral pane.	
5	You can also switch between spectra by clicking the arrow in the <b>Database</b> pane's <b>Spectrum</b> column.	




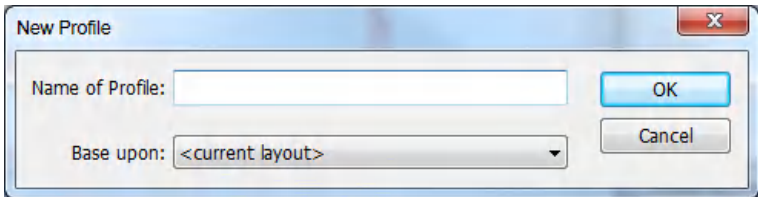
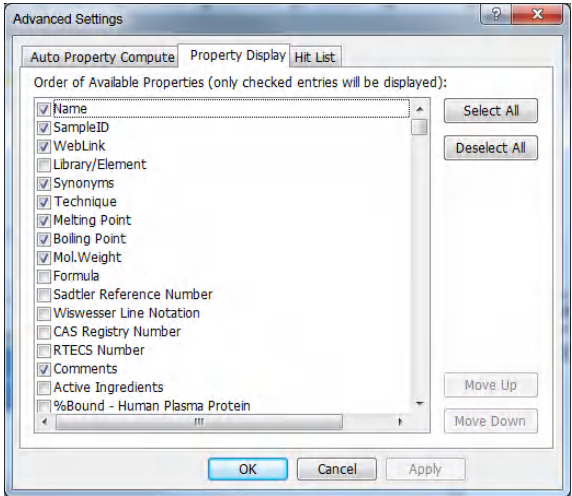
**Add an attachment to the first database record**

	Action	Result
1	With the first database record selected, click the <b>Attachments</b> tab in the <b>Structure/Properties</b> pane.	<p>The <b>Attachments</b> tab is empty:</p> 
2	Choose <b>File &gt; Import Attachment(s)...</b>	A Windows <b>Open</b> dialog box is displayed.
3	Navigate to KnowItAll > Training Files > General Training > Files > Creating Databases and select Ethyl acetate MSDS.pdf, then click <b>Open</b> .	<p>An icon is added to the <b>Attachments</b> tab:</p> 

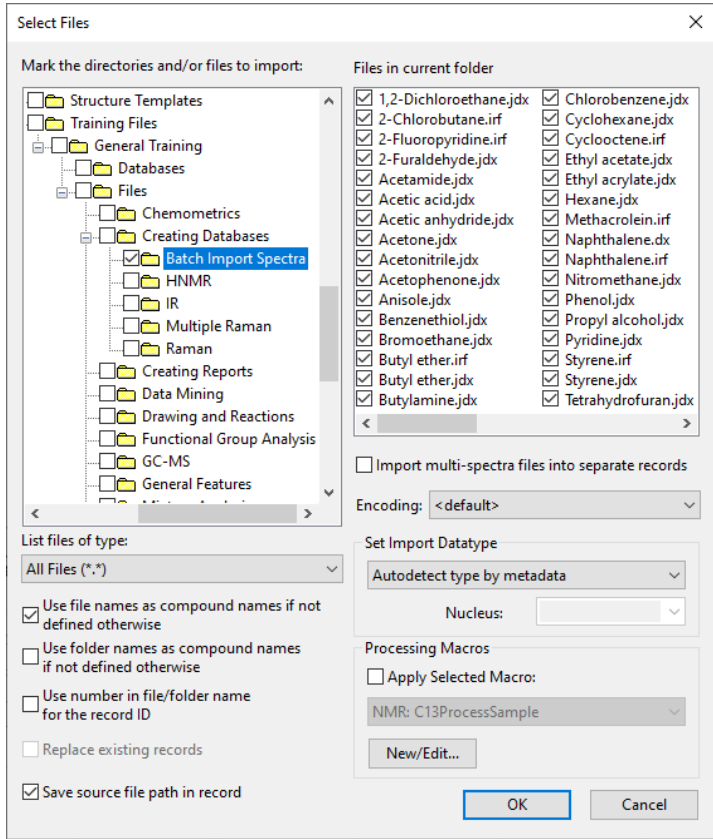
**Add an attachment to the first database record (continued)**

	Action	Result
4	Double click the icon in the <b>Attachments</b> tab.	<p>The document opens in its native application – in this case, Adobe Acrobat.</p>  <p><b>Note:</b> Any type of file can be added to a record in a user database using the <b>Attachments</b> tab. In addition, you can export an attached file by choosing <b>File &gt; Export &gt; Attachments</b>.</p>

**Create a new Minelt display profile**

	Action	Result
1	Click the <b>Add a New Profile</b> button  in the <b>Profile</b> toolbar.	<p>The <b>New Profile</b> dialog box opens:</p> 
2	Type in the profile name <b>QC Lab</b> and click <b>OK</b> .	<p>This layout is now available to apply to any database or hit list display in the <b>Minelt</b> application.</p>
	<i>TIP</i>	<p>When creating a database and to ensure individual users in your laboratory consistently enter all pertinent information into databases, you should set up preferred properties.</p> <p>To do so, go to File &gt; Preferences. In the Preferences dialog, select the <b>Property Display</b> tab. Click on <b>Deselect All</b> to clear the properties; then select the properties that you want entered and the order of those properties.</p>  <p>Then the user will enter the information required for that profile. If there is no information for a particular property, it will not appear under All Properties.</p>

**Batch Import: many spectra, many records, import properties from a spreadsheet**

	Action	Result
1	Create a new empty database as in the above example.	
2	<p>Choose <b>File &gt; Batch Import</b>, to open the <b>Select Files</b> dialog box.</p> <p>Navigate to KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; Creating Databases &gt; Batch Import Spectra, select all spectral files in the folder and click <b>OK</b>.</p> <p><b>Note:</b> Check the box next to a folder name to select all files in the folder.</p>	 <p>A record is created in the new database for each spectral file.</p>

- 3
- Choose **File > Import**
  - Navigate to **KnowItAll > Training Files > General Training > Files > Creating Databases**
  - Select **BatchImportProperties.csv** to map properties to the spectrum files using a spreadsheet
  - Make sure to check **File Contains Header Line**
  - Click **Next**

The **Spreadsheet File Import** wizard opens:

Spreadsheet File Import

Step 1: Analyzing File

☐ File is a Spectrum

Rows to import

☒ All ☐ Rows:

Layout

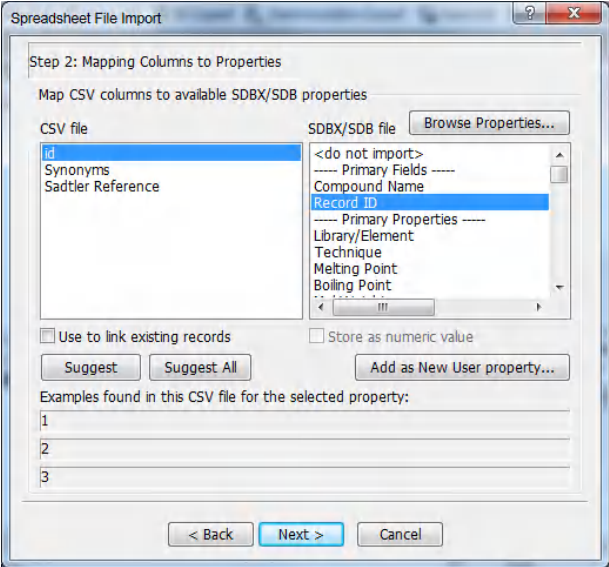
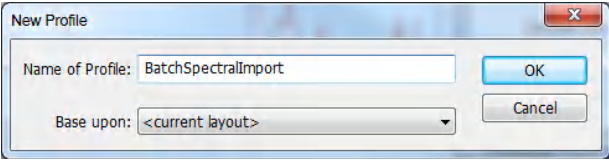
☒ File Contains Header Line:

Delimiting Character:  Encoding:

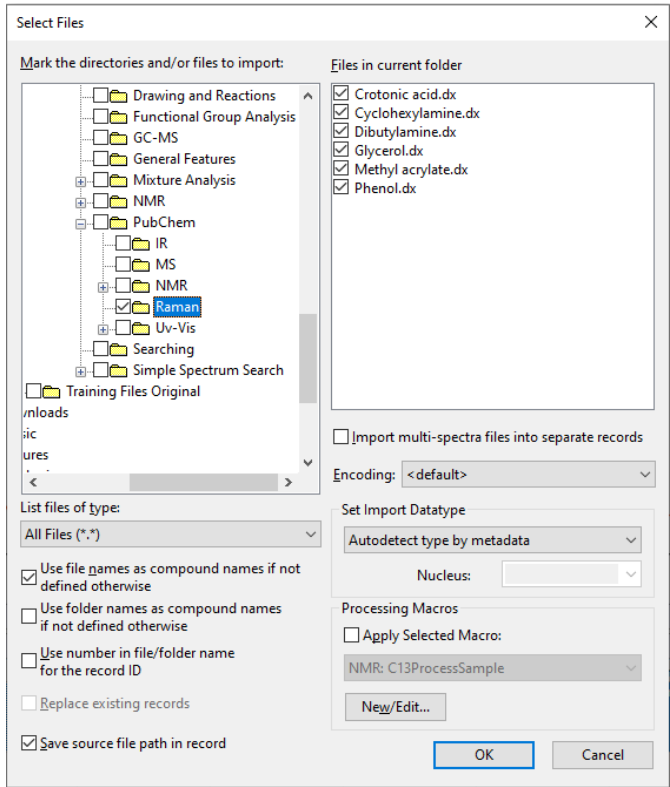
id	Synonyms	Sadtler Refe...
1	1, 2-Dichlor...	1001
2	2-Furaldehy...	1002
3	Acetamide	1003
4	Acetic acid	1004
5	Acetic anhy...	1005
6	Acetone	1006
7	Acetonitrile	1007
8	Acetopheno...	1008

The file was analyzed successfully (35 rows read).

**Batch Import: many spectra, many records, import properties from a spreadsheet (continued)**

	Action	Result
4	<p>Match</p> <ul style="list-style-type: none"> <li>• <b>CSV file 'id' to SDBX/SDB file 'Record ID';</b></li> <li>• <b>CSV file 'Synonyms' to SDBX/SDB file "Synonyms";</b></li> <li>• <b>CSV file 'Sadtler Reference' to SDBX/SDB file 'Sadtler Reference Number'.</b></li> </ul> <p>Alternatively, you can click <b>Suggest All</b>, then review the automatic field matches.</p> <p>Click <b>Next</b>.</p>	
5	<p>Click <b>Finish</b>.</p> <p>You do not have to <b>Compact database now</b> at the prompt.</p>	<p>The database now has fields <b>Synonyms</b> and <b>Sadtler Reference</b> populated by the CSV file.</p>
	<p><b>TIP</b></p>	<p>You can rearrange the spreadsheet portion of this database (for example, to get rid of empty structure columns, right-click and choose <b>Delete Columns</b>). When edits are completed, you can save this column arrangement as a Minelt profile. Click <b>Save Current Profile</b> on the <b>Profile</b> toolbar, then type in a name for the new profile:</p>  <p>This profile will be linked with this database. It can also be selected for use with other databases.</p>

**Batch Import: many spectra, many records, import properties from PubChem**

	Action	Result
1	Create a new empty database as in the above example.	
2	<ul style="list-style-type: none"> <li>Choose <b>File &gt; Batch Import</b></li> <li>Navigate to <b>KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; PubChem &gt; Raman</b></li> <li>Select all spectral files in the folder</li> <li>Click <b>OK</b>.</li> </ul>	 <p>A record is created in the new database for each spectral file.</p>

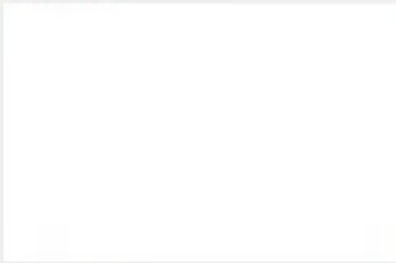
- 3 Select the first record, then click the **PubChem** toolbar button.

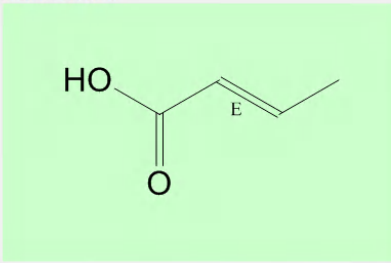


**PubChem** records are searched. If information is located, the **PubChem Data Selection** dialog box opens:

The dialog box displays a table of data for Crotonic acid, comparing current values with values from PubChem. The 'PubChem Structure' panel shows the chemical structure of Crotonic acid, which is (E)-but-2-enoic acid.

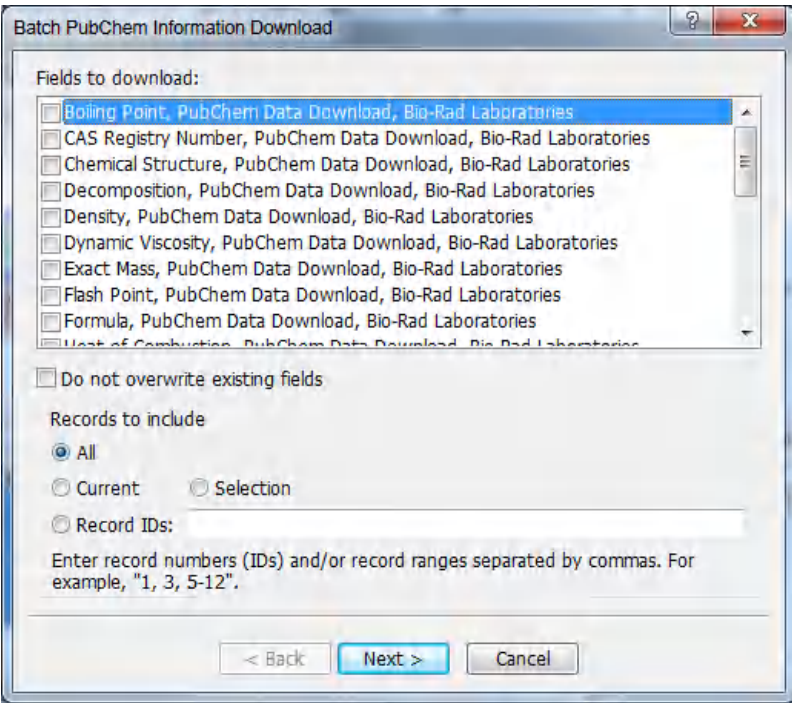
Imported Data		PubChem Record
Checked items will be imported		
Name	<input checked="" type="checkbox"/> Crotonic acid	<input type="checkbox"/> Crotonic acid
IUPAC Name	<input type="checkbox"/>	<input checked="" type="checkbox"/> (E)-but-2-enoic acid
Mol.Weight	<input type="checkbox"/>	<input checked="" type="checkbox"/> 86.09 g/mol
Exact Mass	<input type="checkbox"/>	<input checked="" type="checkbox"/> 86.037 u
Formula	<input type="checkbox"/>	<input checked="" type="checkbox"/> C4H6O2
		<input type="checkbox"/> CH3-CH=CH-COOH
CAS Registry Number	<input type="checkbox"/>	<input checked="" type="checkbox"/> 107-93-7
		<input type="checkbox"/> 3724-65-0
InChI	<input type="checkbox"/>	<input checked="" type="checkbox"/> InChI=1S/C4H6O2/c1-2-3-4(5)6/h2-3H,1H3,(H,5,6)/b3-2+
InChI Key	<input type="checkbox"/>	<input checked="" type="checkbox"/> LDHQCZJRKDOVOX-NSCUHMMNSA-N
PubChem Compound ID	<input type="checkbox"/>	<input checked="" type="checkbox"/> 637090

Current Structure: 

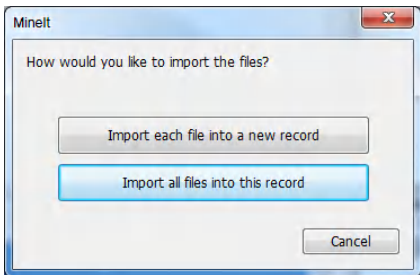
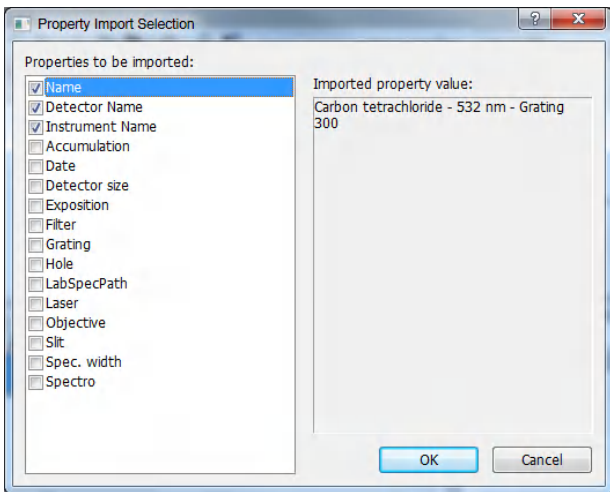
PubChem Structure: 

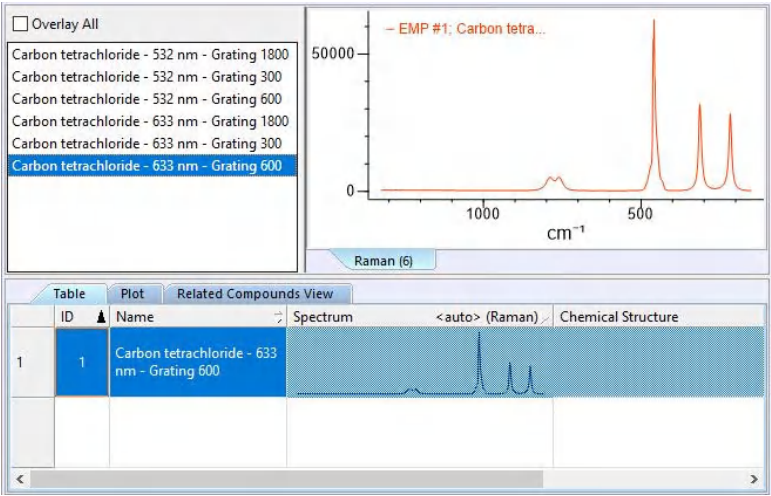
Structure Style: <default> OK Cancel

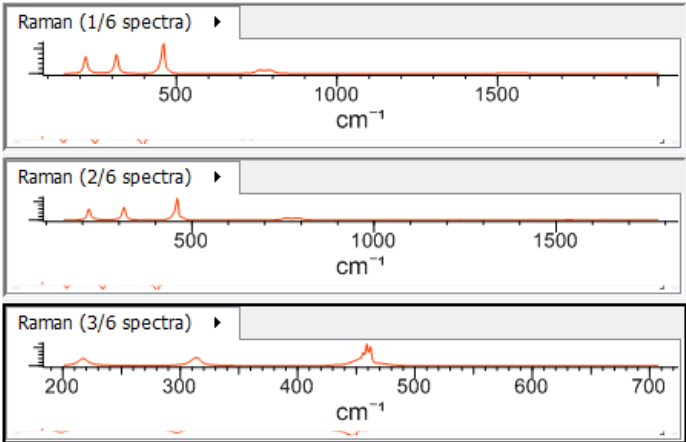


	Action	Result
4	Click <b>OK</b> .	New properties from <b>PubChem</b> are added to the first database record.
5	Select the remaining database records by holding the Shift key, then choose <b>Database &gt; Batch PubChem Information Download</b> .	<p>The <b>Batch PubChem Information Download</b> dialog box opens:</p> 
6	Check the property fields you wish to add to the database records, then click <b>Next</b> .	New properties from PubChem are added to the remaining database records.

**Batch Import: many spectra, one record**

	Action	Result
1	Create a new empty database as in the above example.	
2	<ul style="list-style-type: none"> <li>Choose <b>File &gt; Import</b></li> <li>Navigate to <b>KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; Creating Databases &gt; Multiple Raman</b></li> <li>Select all files in the folder</li> <li>Click <b>Open</b></li> </ul>	<p>A dialog box opens and asks how you want to import the files:</p> 
3	Click <b>Import all files into this record</b> .	<p>The <b>Property Import Selection</b> dialog opens:</p>  <p>Check the properties you wish to import.</p>

	Action	Result
4	Click <b>OK</b> each time the dialog appears.	The dialog box appears once for each spectrum in the record.
5	With the first record selected, observe the <b>Spectrum</b> pane.	<p>The tab shows that there are 6 Raman spectra associated with the first record:</p> 
6	Click the name of a spectrum in the left pane to display it.	

	Action	Result
7	Choose <b>Window &gt; Split Threefold</b> .	<p>The <b>Spectral</b> pane is split into 3 panes, displaying 3 of the 6 spectra:</p> 

# Creating Databases (optional section)

## How to Create a Database with Structures

### Purpose

This exercise demonstrates how to use the KnowItAll's Minelt™ Database Building feature to create searchable user databases that include structures.

### Objectives

This exercise will teach you:

- How to create a user database;
- How to add structures to a user database;
- How to display stereochemical properties; and
- How to add user properties.

### Background

Generating user databases protects intellectual property and promotes sharing of information within an organization. Ultimately, researchers can improve their analyses.

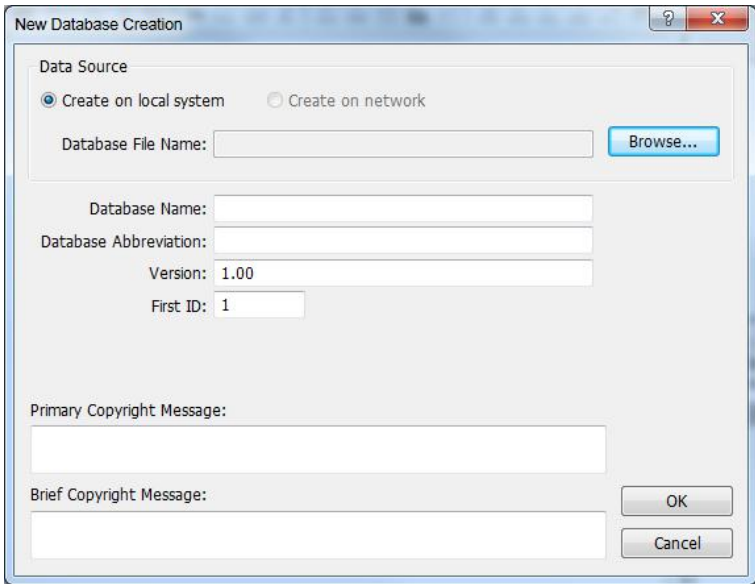
#### *Training Files Used In This Lesson*

- benzylpenicillin.dsf

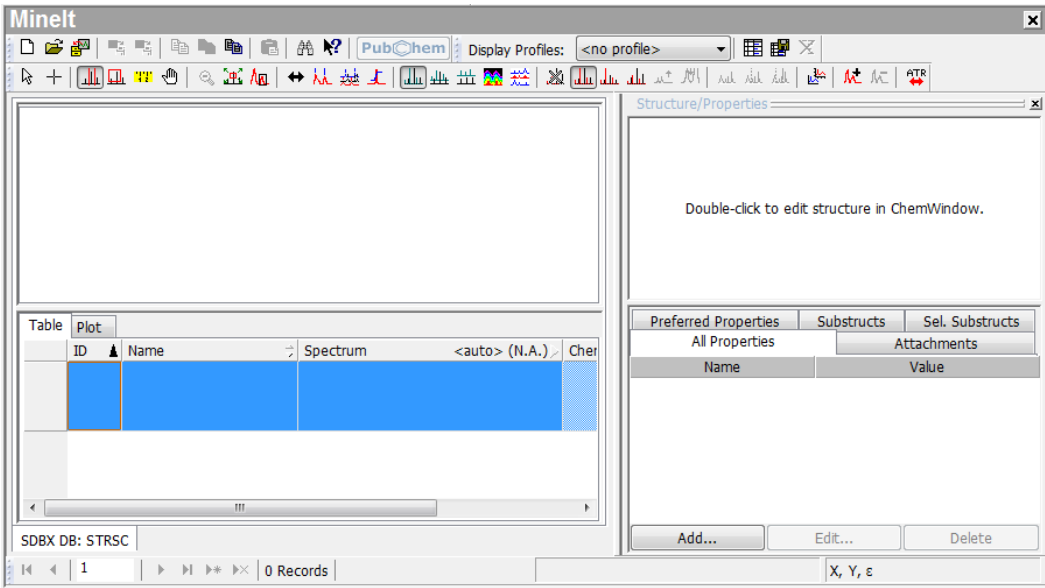
#### *KnowItAll Applications Used*


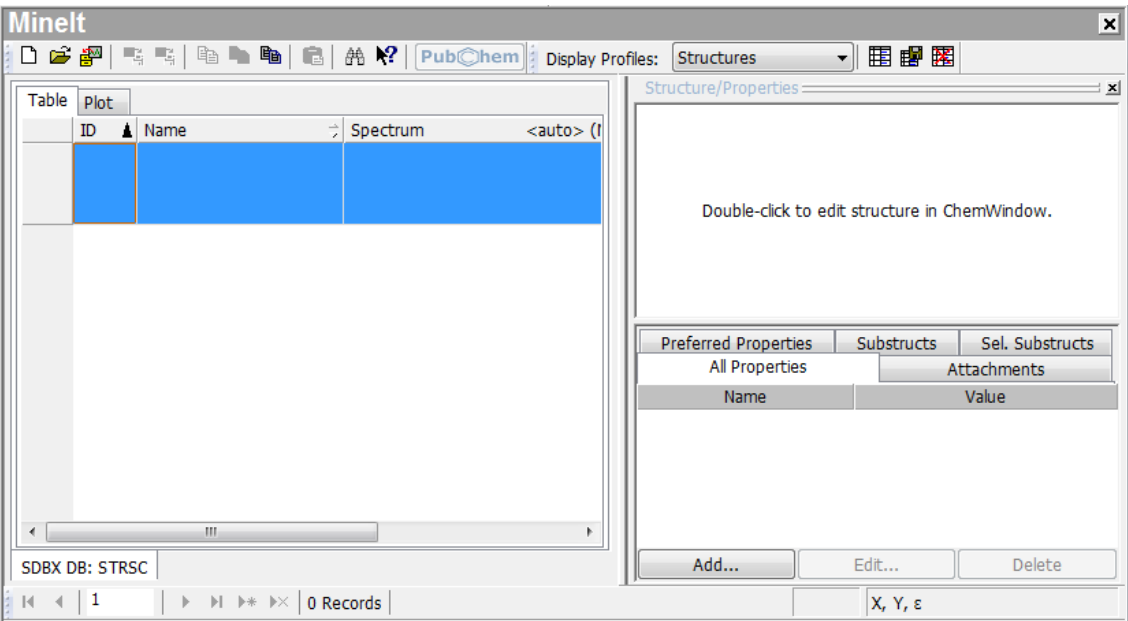
- Minelt™
- ChemWindow®

**Create a user database**

	Action	Result
1	In the Minelt application, choose <b>Database &gt; New</b> .	<p>The <b>New Database Creation</b> dialog box opens.</p> 
3	Select <b>Create on local system</b> .	The new database is saved locally.
4	<ul style="list-style-type: none"> <li>Click <b>Browse</b></li> <li>Navigate to the <b>Databases</b> folder you created earlier,</li> <li>Type <b>structures-sc</b> in the <b>Database File Name</b></li> <li>Click <b>Save</b>.</li> </ul>	<p>The *.sdbx extension is added automatically.</p> <p><b>Note:</b> The SDBX database format allows spectra to be stored without conforming to a fixed range and resolution. This allows reference spectra to be offered at higher resolution, and allows users to store original spectra as produced.</p>
5	<p>Type <b>Structures</b> in the <b>Database Name</b> text box.</p> <p><b>Note:</b> The file name is used if no other name is specified.</p>	

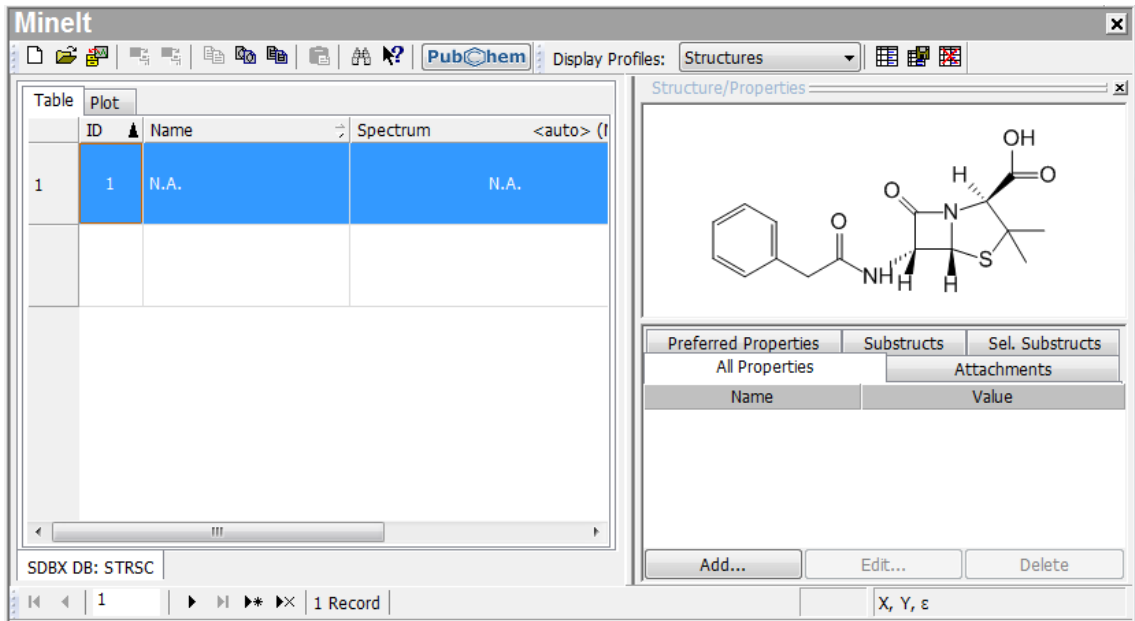
**Create a user database (continued)**

	Action	Result
6	Type 'STRSC' in the <b>Database Abbreviation</b> text box. <b>Note:</b> The abbreviation must be 3-7 characters long.	
7	Click <b>OK</b> .	<p>The new database has been created to receive your data. The Database Abbreviation appears on the database tab.</p>  <p>The screenshot shows the Minelt application window. At the bottom, a tab labeled 'SDBX DB: STRSC' is active. The main area displays a table with columns: ID, Name, Spectrum, and Chemical Structure (represented by a small structure icon). The 'Spectrum' column is highlighted in blue. To the right of the table is a 'Structure/Properties' panel with tabs for 'Preferred Properties', 'Substructs', and 'Sel. Substructs'. Below these are 'All Properties' and 'Attachments' sections, each with 'Name' and 'Value' columns. At the bottom of the panel are 'Add...', 'Edit...', and 'Delete' buttons. The status bar at the very bottom indicates '1' record and '0 Records'.</p>
8	Choose <b>View &gt; Windows/Tables &gt; Spectrum Pane</b> to remove the spectral display from the layout. <b>Note:</b> This command (and others like it) toggle the display of different panes in the main window.	

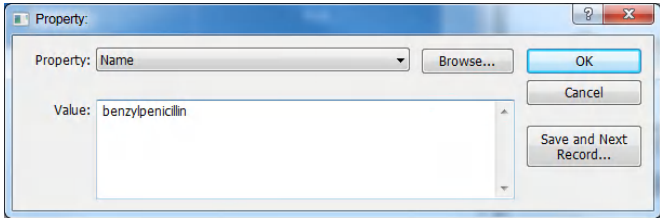
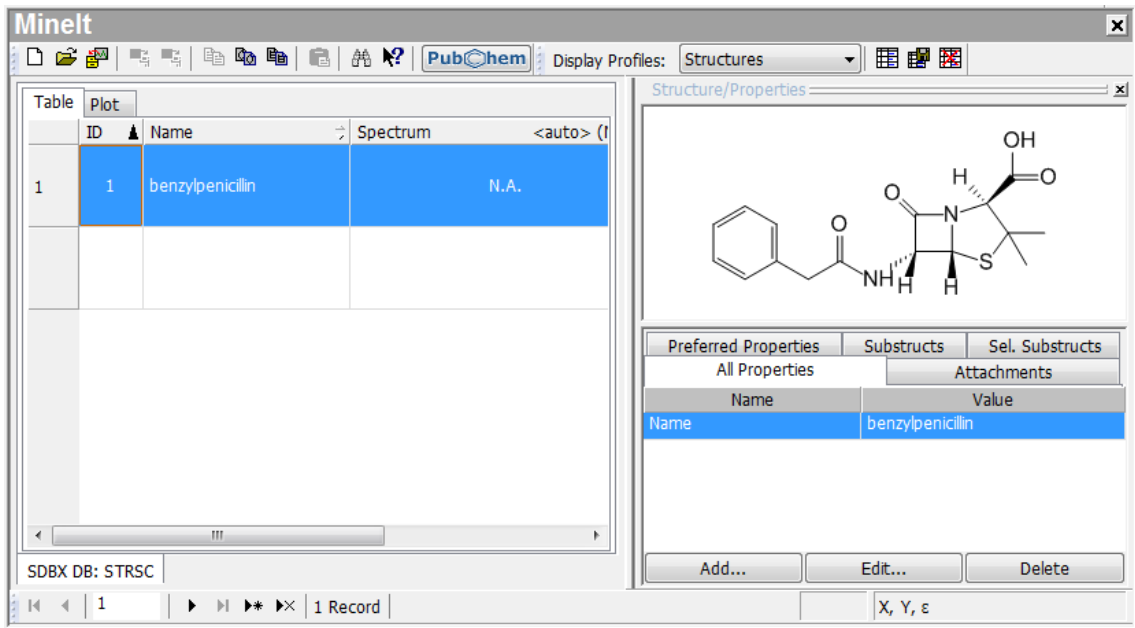
	Action	Result
9	Click the <b>Add a New Profile</b> toolbar button  , type the name 'Structures' in the <b>New Profile</b> dialog box, then click <b>OK</b> .	 <p>The screenshot shows the Minelt software interface. The title bar reads 'Minelt'. The menu bar includes 'File', 'Edit', 'View', 'Tools', 'Database', 'Help', and 'PubChem'. The 'Display Profiles' dropdown is set to 'Structures'. The main window is divided into two panes. The left pane, titled 'Table', shows a table with columns 'ID', 'Name', and 'Spectrum'. The 'Name' column is highlighted in blue. The right pane, titled 'Structure/Properties', contains the text 'Double-click to edit structure in ChemWindow.' Below this text are tabs for 'Preferred Properties', 'Substructs', and 'Sel. Substructs'. Under 'Preferred Properties' are 'All Properties' and 'Attachments'. Under 'Sel. Substructs' is 'Value'. At the bottom of the right pane are buttons for 'Add...', 'Edit...', and 'Delete'. The status bar at the bottom shows 'SDBX DB: STRSC', a page number '1', and '0 Records'.</p>



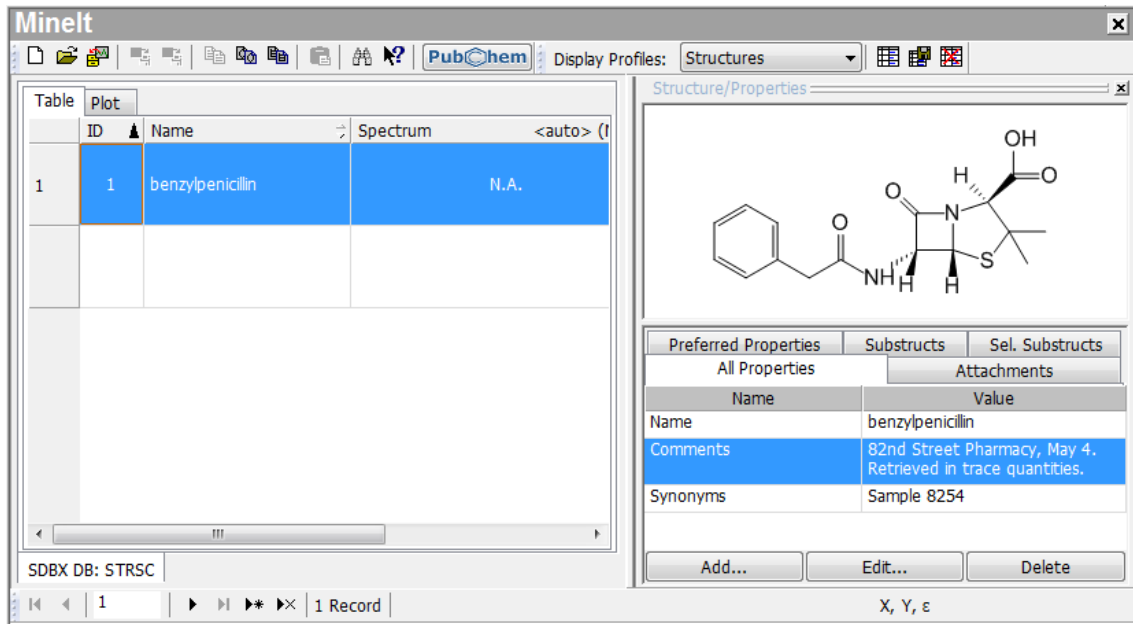
## Add a structure to the first database record

	Action	Result
1	<ul style="list-style-type: none"> <li>Choose <b>File &gt; Import</b></li> <li>Navigate to <b>KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; Creating Databases</b></li> <li>Open the structure file <b>Benzylpenicillin.dsf</b>.</li> </ul>	<p>The structure is displayed in the <b>Structure/Properties</b> pane:</p>  <p>The screenshot shows the Minelt software interface. On the left, there is a table with columns ID, Name, and Spectrum. The first row has ID 1, Name N.A., and Spectrum N.A. Below the table, it says 'SDBX DB: STRSC' and '1 Record'. On the right, the 'Structure/Properties' pane displays the chemical structure of Benzylpenicillin. The structure is a penicillin derivative with a benzyl group. Below the structure, there are tabs for 'Preferred Properties', 'Substructs', and 'Sel. Substructs'. Under 'Preferred Properties', there are 'All Properties' and 'Attachments' tabs. Below these, there is a table with columns 'Name' and 'Value'. At the bottom of the structure pane, there are buttons for 'Add...', 'Edit...', and 'Delete'. The status bar at the bottom shows 'X, Y, ε'.</p>
2	Open the <b>View</b> menu and check <b>Stereochemistry</b> if it is not already checked.	Stereochemical descriptors are shown on the structure when <b>Stereochemistry</b> is enabled on the <b>View</b> menu.

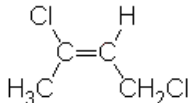
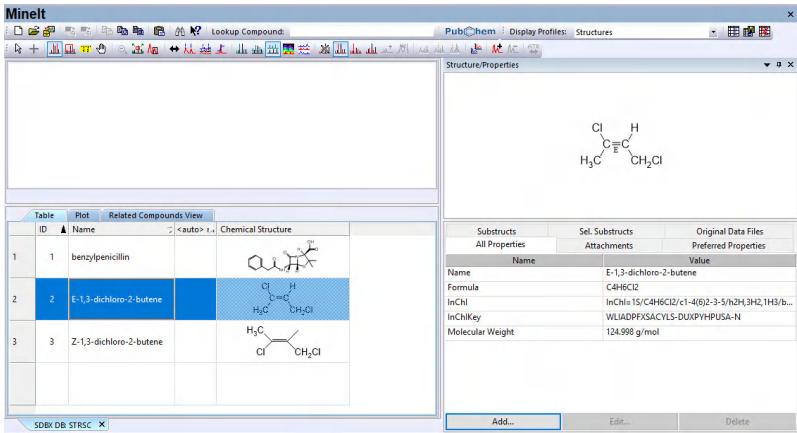
**Add properties to the first database record**

	Action	Result
1	Click <b>Add</b> in the <b>Structure/Properties</b> pane.	The <b>Property</b> dialog box opens.
2	Select the property <b>Name</b> , then type 'benzylpenicillin' in the <b>Value</b> text box.	
3	Click <b>OK</b> .	The <b>Property</b> dialog box closes, and the added property <b>Name</b> appears in the <b>Structure/Properties</b> pane. 

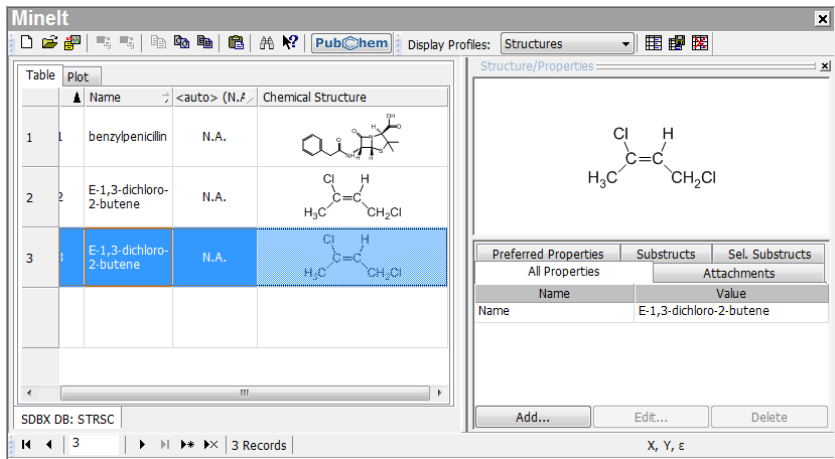
**Add properties to the first database record (continued)**

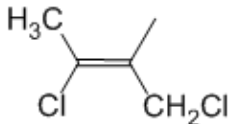
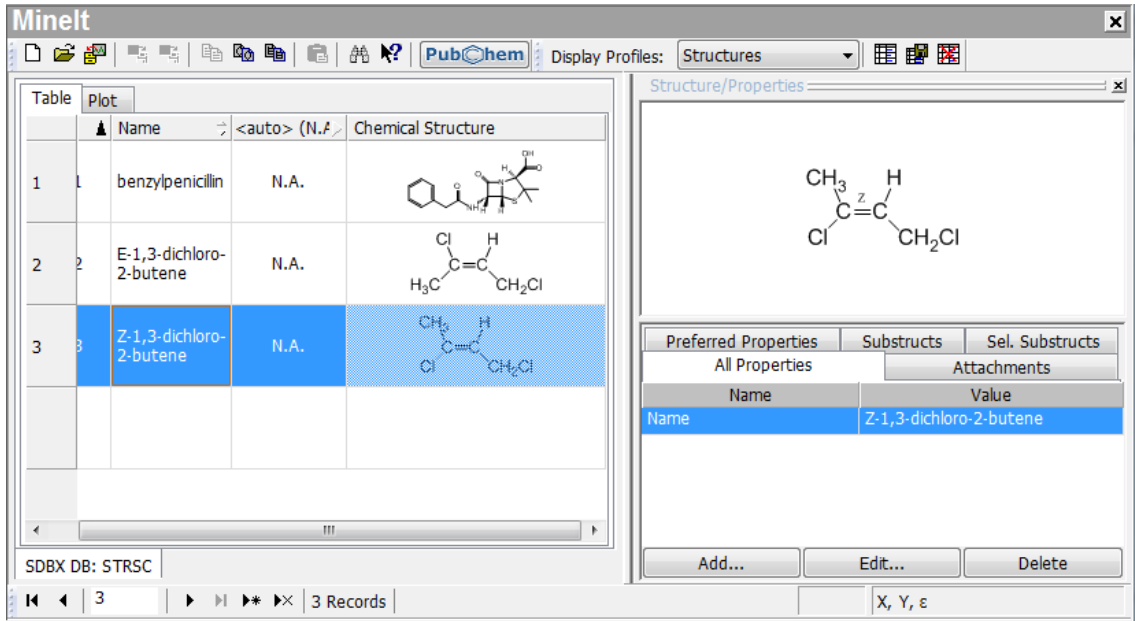
	Action	Result												
4	Repeat to add the property <b>Synonyms</b> with the value 'Sample 8254.'													
5	Repeat to add the property <b>Comments</b> with the value '82 <sup>nd</sup> Street Pharmacy, May 4. Retrieved in trace quantities.'	 <p>The screenshot shows the Minelt software interface. On the left, a table lists database records. The first record is selected, showing ID 1, Name benzylpenicillin, and Spectrum N.A. On the right, the 'Structure/Properties' window is open. It displays the chemical structure of benzylpenicillin. Below the structure, there is a table of properties:</p> <table><tr><th colspan="2">Preferred Properties</th></tr><tr><th colspan="2">All Properties</th></tr><tr><th>Name</th><th>Value</th></tr><tr><td>Name</td><td>benzylpenicillin</td></tr><tr><td>Comments</td><td>82<sup>nd</sup> Street Pharmacy, May 4. Retrieved in trace quantities.</td></tr><tr><td>Synonyms</td><td>Sample 8254</td></tr></table> <p>Buttons for 'Add...', 'Edit...', and 'Delete' are visible at the bottom of the properties window. The status bar at the bottom indicates '1 Record'.</p>	Preferred Properties		All Properties		Name	Value	Name	benzylpenicillin	Comments	82 <sup>nd</sup> Street Pharmacy, May 4. Retrieved in trace quantities.	Synonyms	Sample 8254
Preferred Properties														
All Properties														
Name	Value													
Name	benzylpenicillin													
Comments	82 <sup>nd</sup> Street Pharmacy, May 4. Retrieved in trace quantities.													
Synonyms	Sample 8254													

## Add a second database record

	Action	Result
1	Navigate to the <b>Basics</b> toolbox, then open the ChemWindow application by clicking its icon. <b>Note:</b> Do not use the <b>Transfer to</b> bar in this case.	
2	Draw this structure: 	
3	Use the <b>Selection</b> tool to select the structure, then choose <b>Edit &gt; Copy</b> .	
4	Use the KnowItAll <b>Back</b> button to return to the Minelt application.	
5	With the second database entry selected, choose <b>Edit &gt; Paste</b> . A message box asks "Would you like to append the new data as a new record?" Click <b>OK</b> .	The structure is added to the second record: 
6	Add the property <b>Name</b> with the value 'E-1,3-dichloro-2-butene.'	

**Add a third database record**

	Action	Result
1	With the second database record still selected, choose <b>Edit &gt; Copy Structure</b> .	
2	<p>Select the third database record and choose <b>Edit &gt; Paste</b>.</p> <p>A message box asks "Would you like to append the new data as a new record?" Click <b>OK</b>.</p>	<p>The structure and properties are added to the third database record.</p>  <p>The screenshot shows the Minelt software window. On the left, a table lists three records. The third record, 'E-1,3-dichloro-2-butene', is highlighted. The 'Structure/Properties' pane on the right displays the chemical structure of E-1,3-dichloro-2-butene (H<sub>3</sub>C-CH=CH-CH<sub>2</sub>Cl) and a table of its properties, including Name, Value, and Attachments.</p>
3	With the third database record selected, double click in the <b>Structure/Properties</b> pane to open the structure in <b>ChemWindow</b> .	

	Action	Result
4	Edit the structure as shown, then click <b>Return to Minelt Database and Save.</b> 	The structure is added to the third database record.
5	Edit the property <b>Name</b> to 'Z-1,3-dichloro-2-butene.'	

# **KnowItAll Software Training**

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## Functional Group Analysis

# Functional Group Analysis

## How to Use the Knowledgebases to Identify or Differentiate Classes of Compounds by Structure or Functional Group

### Purpose

This exercise demonstrates how to use the Analyzelt™ IR, Analyzelt Raman, and Analyzelt Polymer IR Knowledgebases to identify or differentiate chemical compounds, and to correlate peaks by structure.

### Objectives

This exercise will teach you:

- How to specify the Knowledgebase;
- How to browse by functional group; and
- How to correlate a structure.

### Background

The IR and Raman Knowledgebases include group frequencies with over 600 band assignments, corresponding to over 200 functional groups, subdivided into general chemical classes.

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


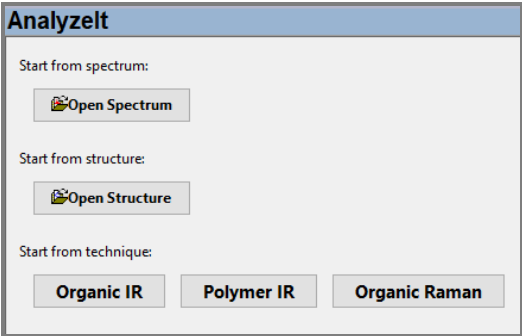
- Test Structure.dsf

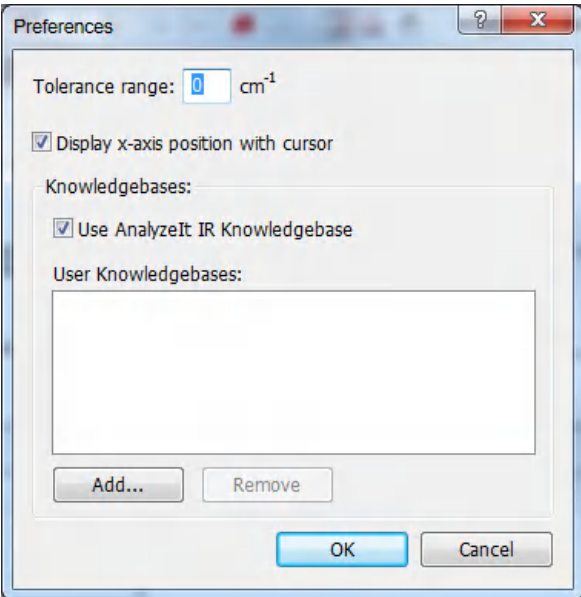
#### *KnowItAll Applications Used*

- Analyzelt™

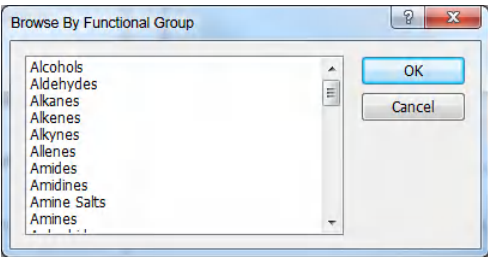
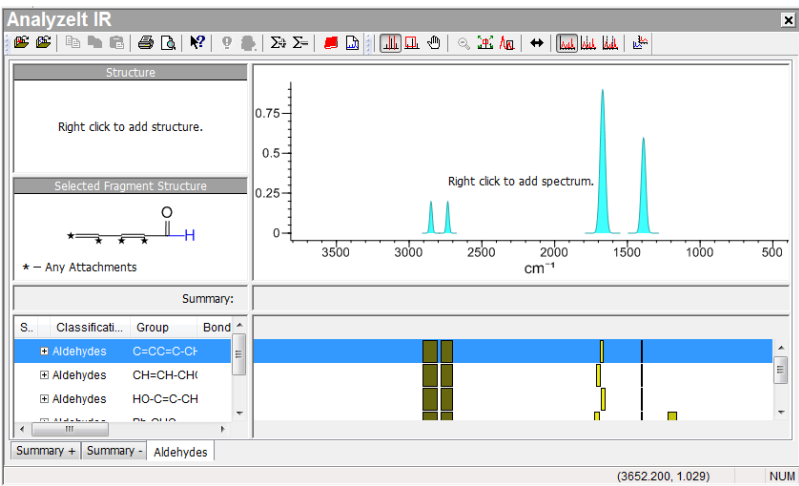


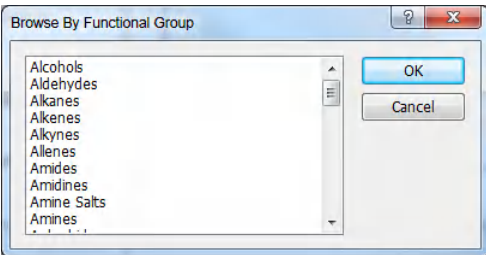
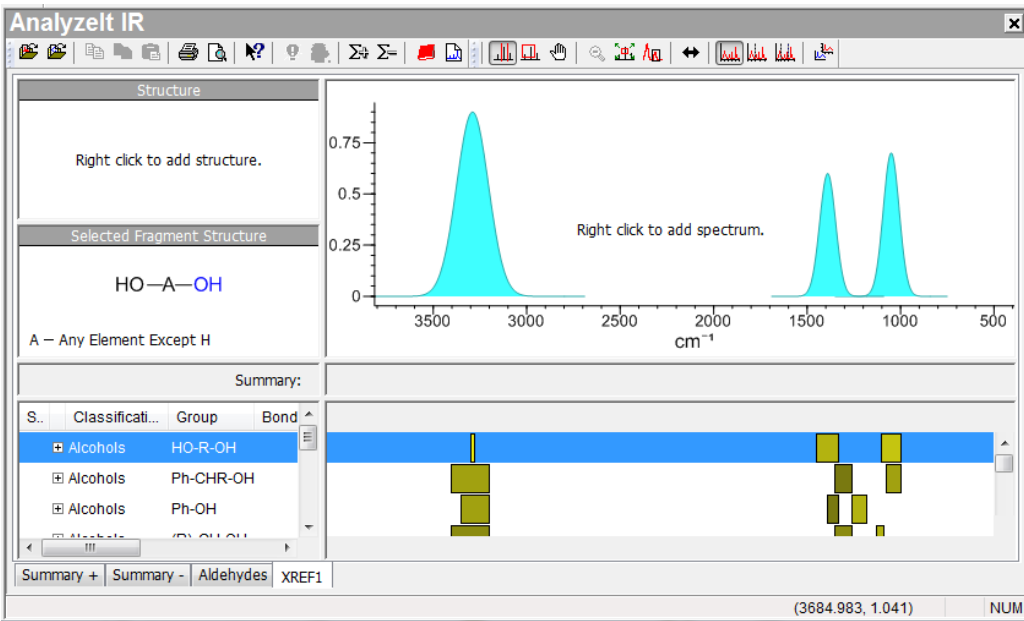
## Specify the Knowledgebase

	Action	Result
1	<p>Navigate to the <b>Spectral Analysis</b> toolbox</p> <p>Click <b>Analyzelt</b></p>	  <p><b>Open Spectrum</b> - starts with any spectrum file. Upon selecting an IR spectrum, <b>KnowItAll</b> asks user if it should be put into <b>Organic IR</b> or <b>Polymer IR</b> application.</p> <p><b>Open Structure</b> - starts with any structure file. Upon selecting a structure file, <b>KnowItAll</b> asks user if it should be put into <b>Organic IR</b> or <b>Organic Raman</b> application.</p> <p>By the same token,</p> <ul style="list-style-type: none"> <li>• <b>IR Organic</b> - starts a blank <b>Analyzelt IR</b> application</li> <li>• <b>Polymer IR</b>- starts a blank <b>Analyzelt Polymer IR</b> application</li> <li>• <b>Raman Organic</b> - starts a blank <b>Analyzelt Raman</b> application</li> </ul>

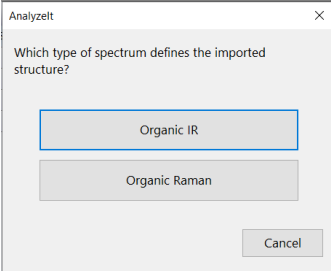
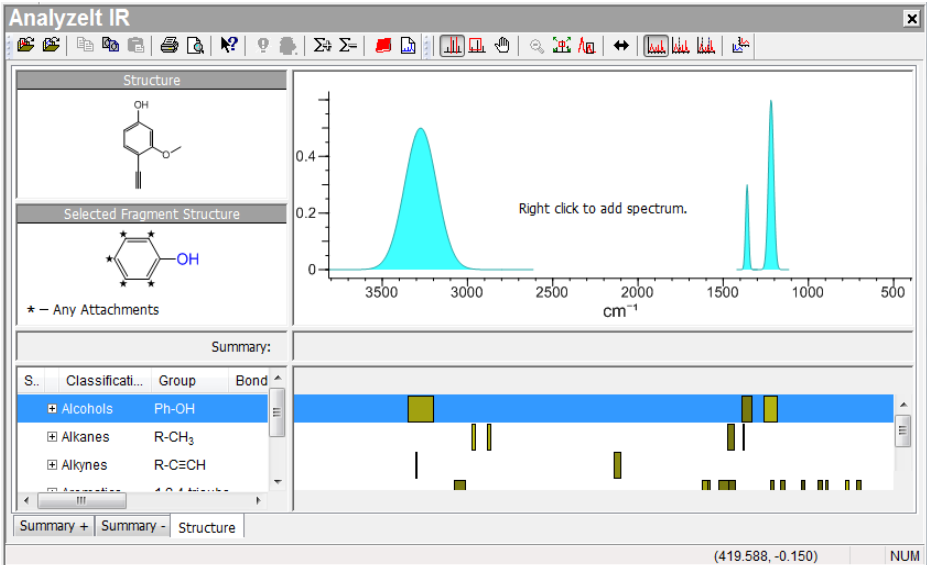
2	<p>Let's start from technique: <b>Organic IR</b></p> <p>Click <b>Organic IR</b> and then choose <b>File &gt; Preferences</b>.</p>	<p>The <b>Preferences</b> dialog box opens:</p>  <p>Setting the <b>Tolerance range</b> allows you to determine how precise the matches are between your spectrum peak and the database. You can also choose to display a wavenumber (x-axis position) marker with the cursor as it moves around the <b>Spectrum</b> pane. Finally, use the check boxes to select the knowledgebase you wish to use.</p>
3	<p>Make sure <b>AnalyzeIt IR Knowledgebase</b> is selected</p> <p>Click <b>OK</b></p>	

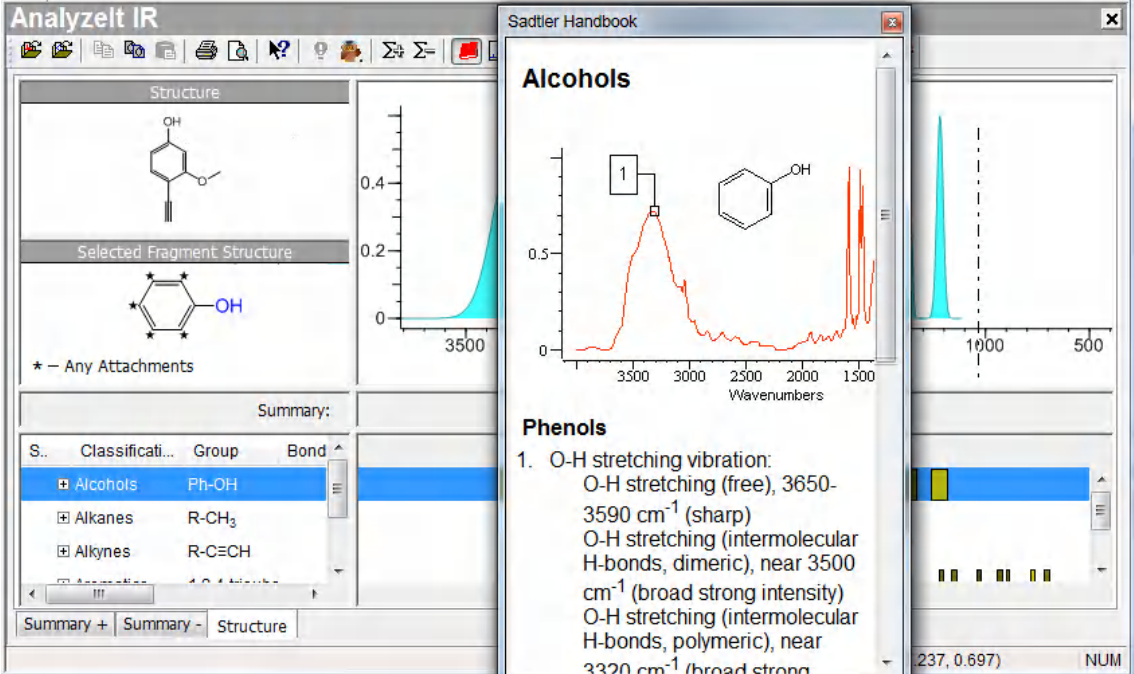
**Browse by functional group**

	Action	Result
1	Choose <b>Analyze &gt; Browse a Functional Group</b> .	<p>The <b>Browse By Functional Group</b> dialog box opens:</p> 
2	Select <b>Aldehydes</b> and click <b>OK</b> .	<p>The <b>Aldehydes</b> tab is added to the Analyze IR display:</p>  <p>Each functional group in the aldehydes group is listed separately in the <b>Functional Group Data</b> pane at the lower left, and each entry includes classification, group, bond, range, intensity, mode, and notes.</p> <p>Colored bars in the <b>Bar Chart</b> pane at the lower right represent the peaks associated with each functional group class selected in the <b>Functional Group Data</b> pane. The bars are intensity coded; lighter color means greater intensity. Corresponding peaks appear in the <b>Spectrum</b> pane.</p>

	Action	Result
3	Choose <b>Analyze &gt; Browse a Functional Group</b> again.	<p>The <b>Browse By Functional Group</b> dialog box opens:</p> 
4	<p>Select both <b>Alcohols</b> and <b>Anhydrides</b>, then click <b>OK</b>.</p> <p><b>Note:</b> Select the first class, then hold down the ctrl key and click to select a second class.</p>	<p>The XREF1 tab is added to the Analyzelt IR display:</p>  <p>The tab is labeled XREF1 because it is the first tab containing a combination of classes.</p>

## Correlate peaks from a structure

	Action	Result
1	<ul style="list-style-type: none"> <li>Choose <b>File &gt; Close</b> to clear the previous example display</li> <li>Click <b>Open Structure</b> button</li> <li>Navigate to <b>KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; Functional Group Analysis</b></li> <li>Open <b>Test Structure.dsf</b></li> </ul>	<p>A dialog box prompts user to choose between IR or Raman</p> 
2	Click <b>Organic IR</b>	<p>After the knowledge base is analyzed, the results are displayed in a <b>Structure</b> tab. The <b>Functional Group Data</b> pane includes an entry for each group found in the structure.</p> 

	Action	Result
3	Choose <b>View &gt; Sadtler Handbook</b> to display the handbook information related to a particular functional group.	<p>The <b>Sadtler Handbook</b> pane displays information from the Sadtler Handbook of Reference Spectra - IR for the specific functional group selected in the <b>Functional Group Data Pane</b>.</p>  <p>Double clicking the <b>Sadtler Handbook</b> pane's title bar allows you to dock and un-dock the pane with reference to the main display.</p>
4	Choose <b>File &gt; Close</b> .	The display is cleared.

# Functional Group Analysis

## How to Perform a Basic Spectral Analysis Using Software-Assisted Functional Group Analysis

### Purpose

This exercise demonstrates how to use the Analyzelt™ application to perform a basic spectral analysis.

### Objectives

This exercise will teach you:

- How to select peaks for correlation; and
- How to use the Summary+ and Summary- tabs.

### Background

The Analyzelt application can be used to help interpret spectra through the use of its knowledge bases of over 200 functional groups. They can be used to obtain functional group information from a spectrum or a structure, or by browsing the chemical classes included in the knowledge bases.

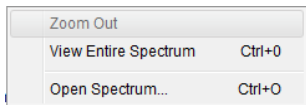
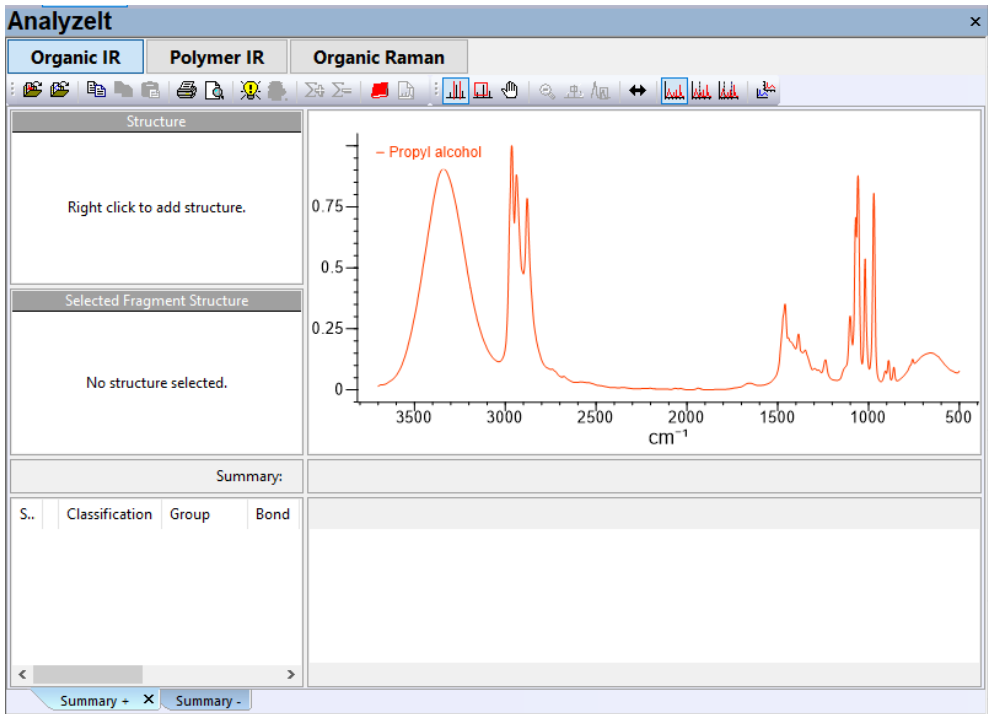
#### *Training Files Used in This Lesson*

- Peak Interpretation Example.dx (IR)

#### *KnowItAll Applications Used*


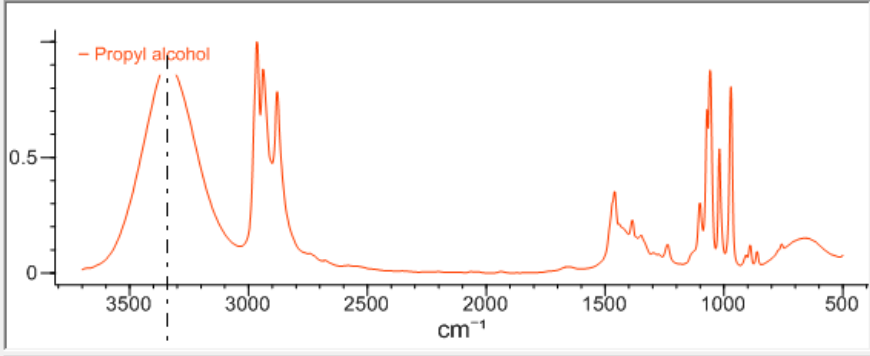
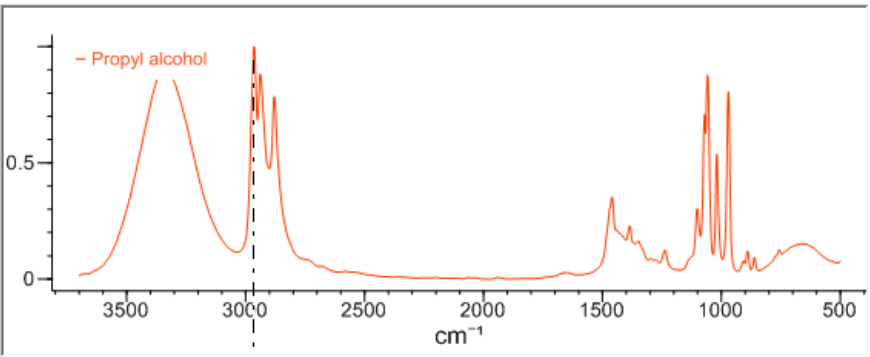
- Analyzelt™


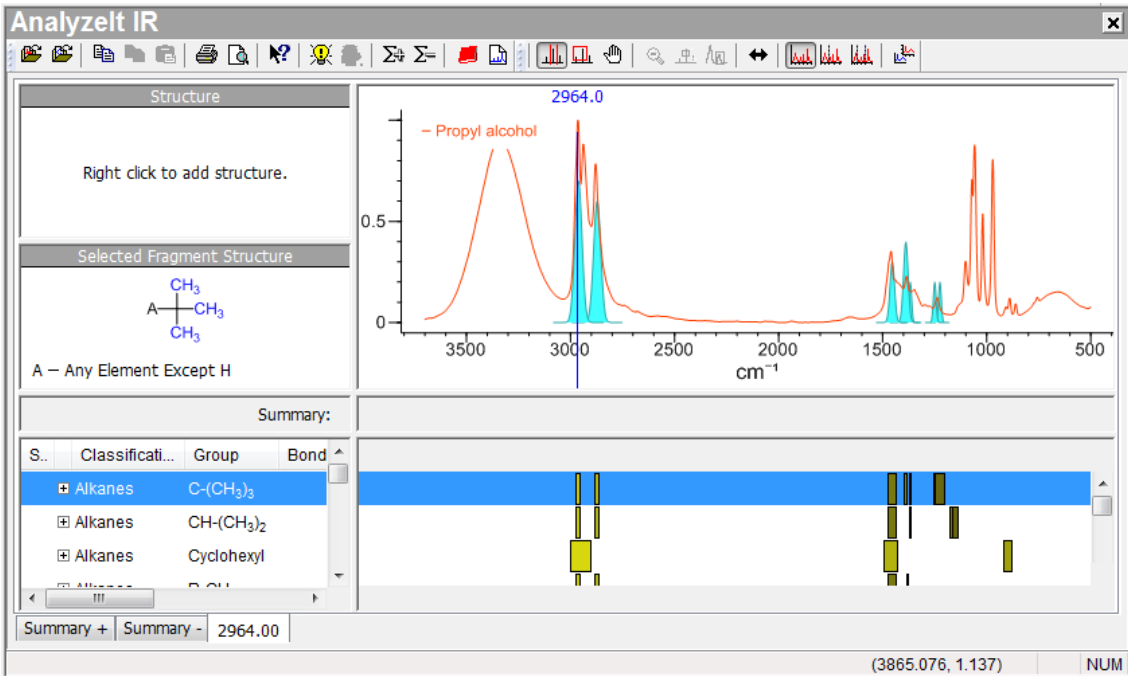
## Open a spectrum

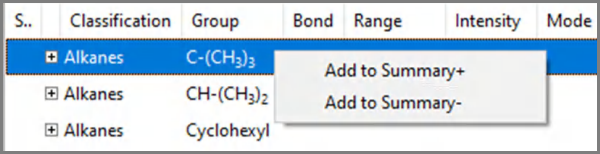
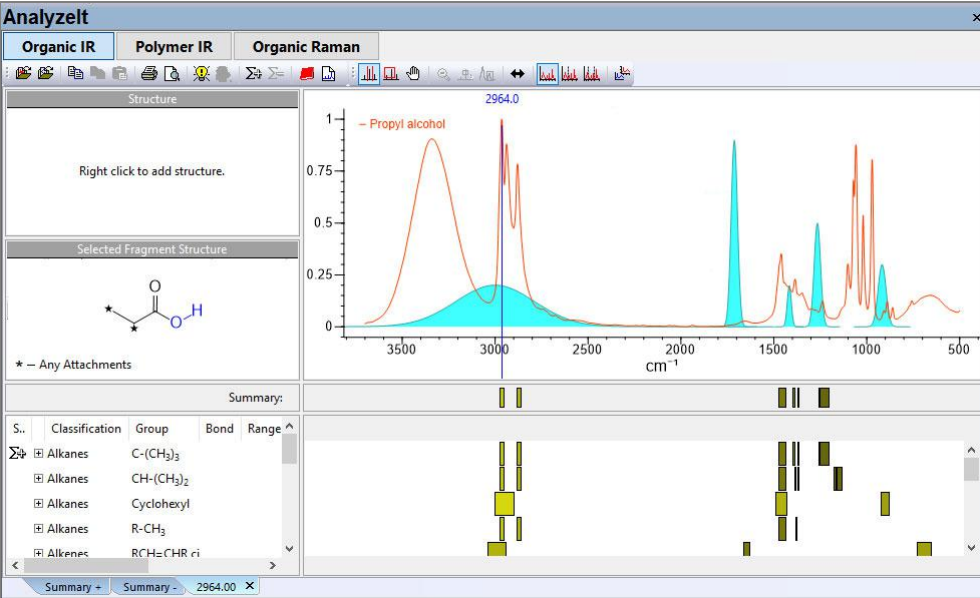
	Action	Result
1	Navigate to the <b>Spectral Analysis</b> toolbox, and click <b>Analyzelt</b> followed by <b>Organic IR</b> .	
2	Right-click in the <b>Spectral Pane</b> .	A pop-up menu opens: 
3	<ul style="list-style-type: none"> <li>Click <b>Open Spectrum</b></li> <li>Navigate to <b>KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; Functional Group Analysis</b></li> <li>Open <b>Peak Interpretation Example.dx</b>.</li> <li>Since this particular spectrum does not have the X-axis unit defined, KnowItAll warns the user with a pop-up saying <b>The information stored as "Propyl alcohol" does not have X axis unit defined for the spectral trace. KnowItAll will attempt to read the data as cm<sup>-1</sup>.</b></li> <li>Click <b>OK</b>.</li> </ul>	<p>The spectrum is displayed:</p> 

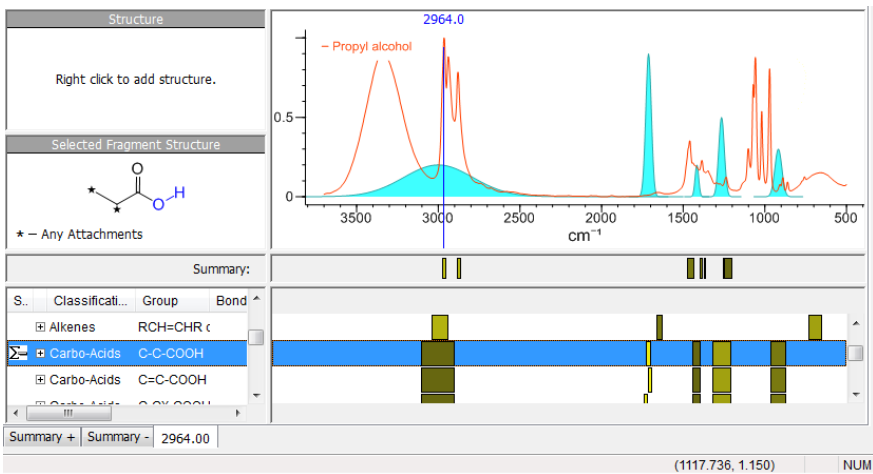
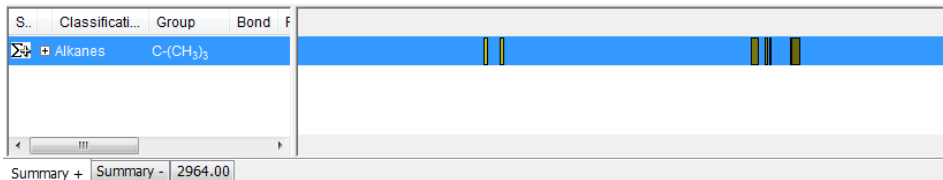
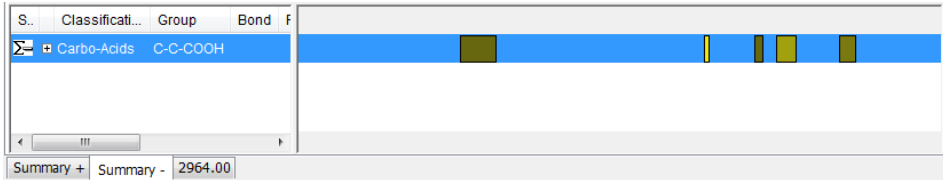


## Analyze the spectrum

	Action	Result
1	Click the <b>Suggest</b> toolbar button  .	<p>The application selects a peak to analyze:</p>  <p>In general, it is best to begin a correlation with a peak above 1500 wavenumbers that is unique and strong. The <b>AnalyzeIt</b> application uses a set of rules to select a good starting point.</p>
2	Click the <b>Suggest</b> toolbar button again. <b>Note:</b> You can also select peaks by clicking in the spectral pane.	<p>Another peak is suggested:</p>  <p>As you click the <b>Suggest a Peak</b> toolbar button repeatedly, the application cycles through the suggested starting points.</p>

	Action	Result
3	<p>Click <b>Suggest</b> until the second peak (at 2964) is selected and then click the <b>Correlate</b> button .</p>	<p>After the knowledge base is analyzed, the results are displayed in a tab labeled with the wavenumber.</p> 

	Action	Result
4	<ul style="list-style-type: none"> <li>Select the alkanes entry C-(CH<sub>3</sub>)<sub>3</sub> in the <b>Functional Group Data</b> pane</li> <li>Right-click to open the <b>Summary</b> pop-up menu.</li> </ul> <p><b>Note:</b> The <b>Summary+</b> and <b>Summary-</b> tabs are created automatically, and are provided to allow you to keep track of functional groups that are consistent with or inconsistent with the measured spectrum.</p>	
5	<p>Because the methyl group correlates well with the spectrum, click <b>Add to Summary+</b>.</p>	<p>The peaks are added to the <b>Summary+</b> tab and the <b>Summary Bar Chart</b> pane (between the spectral display and the <b>Bar Chart</b> pane), and a summary plus symbol appears in the <b>Functional Group Data</b> pane next to this group.</p> 

	Action	Result
6	Select the first carboxylic acid entry (C-COOH) in the <b>Functional Group Data Pane</b> , then right-click to open the <b>Summary</b> pop-up menu.	
7	Because the results indicate that there should also be a strong band near the 1740 region, move this group to the <b>Summary-</b> tab.	 <p>The screenshot displays the software's IR analysis results. On the left, the 'Structure' pane shows a chemical structure with a carboxylic acid group. The 'Selected Fragment Structure' pane shows a carboxylic acid group. The 'Summary:' pane shows a list of functional groups with 'Carbo-Acids C-C-COOH' selected. The IR spectrum on the right shows a peak at 2964.0 cm⁻¹. The 'Summary+' tab is active, showing the selected group.</p>
8	Click the <b>Summary+</b> tab to display any groups added to this tab.	 <p>The screenshot shows the 'Summary+' tab selected in the Functional Group Data Pane. The list of functional groups includes 'Alkanes C-(CH₃)₃', which is highlighted. The IR spectrum is not visible in this view.</p>
9	Click the <b>Summary-</b> tab to display any groups added to this tab.	 <p>The screenshot shows the 'Summary-' tab selected in the Functional Group Data Pane. The list of functional groups includes 'Carbo-Acids C-C-COOH', which is highlighted. The IR spectrum is not visible in this view.</p>
10	Choose <b>File &gt; Close</b> .	The display is cleared.

# Functional Group Analysis

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## How to Perform a Basic Spectral Analysis Using Analyzelt™ for Polymer

### Purpose

This exercise demonstrates how to use the Analyzelt application to perform a basic spectral analysis of polymer

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### Objectives

This exercise will teach you:

- How to analyze spectra from polymer samples.
- 

### Background

The Analyzelt Polymer IR Knowledge Base can provide clear and rapid verification and identification of functional groups in the mid-infrared. It features over 100 functional groups and hundreds of interpretation frequencies.

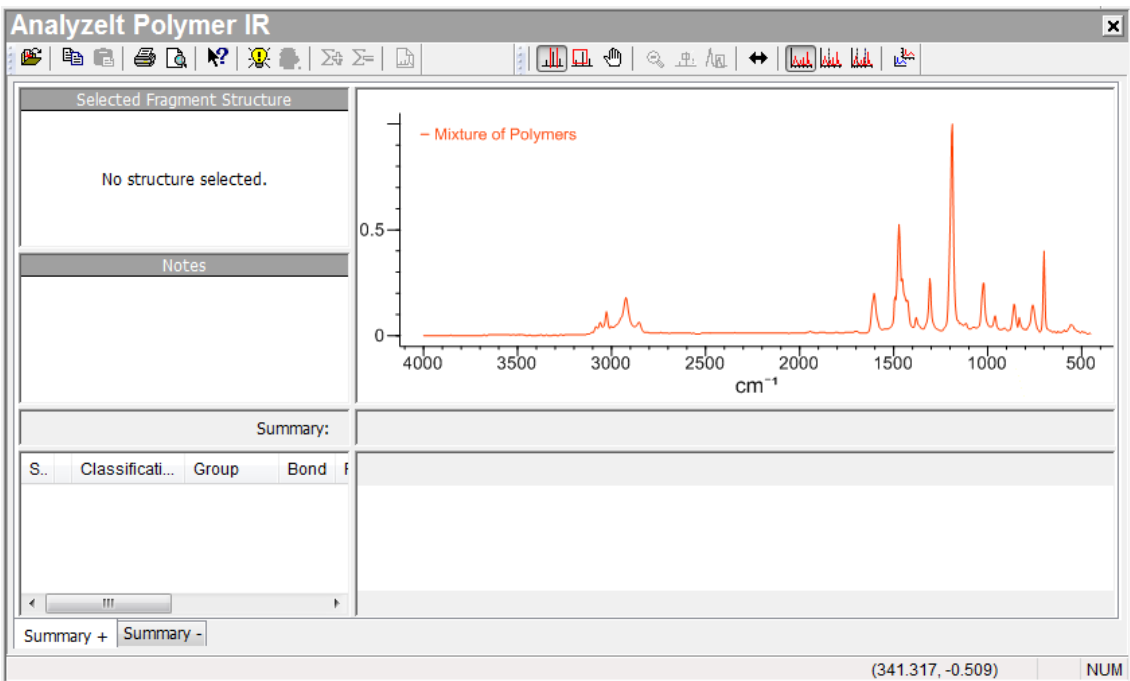
#### *Training Files Used in This Lesson*


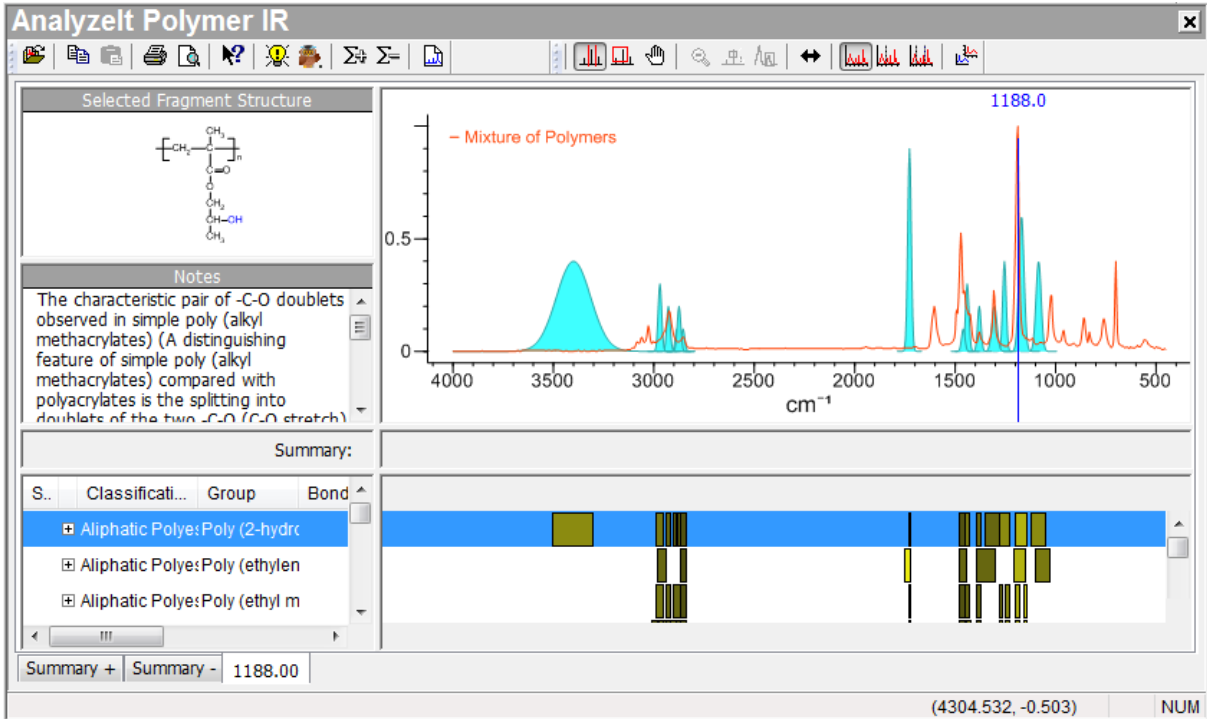
- Mixture of Polymers.irf
- Polystyrene.irf

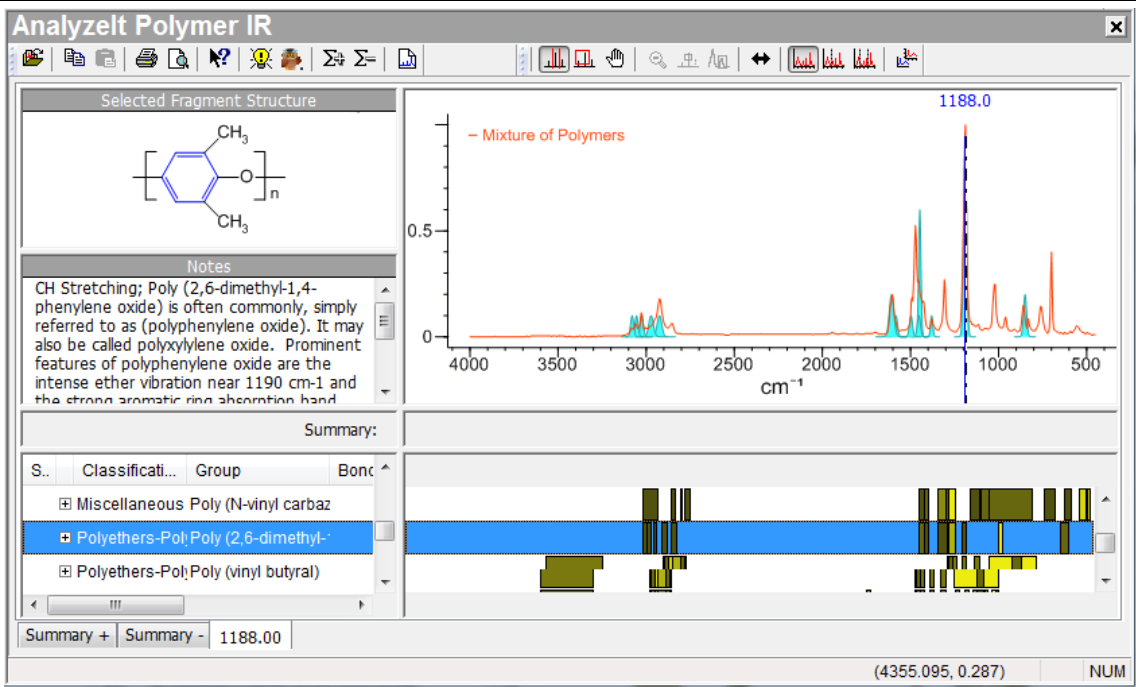
#### *KnowItAll Applications Used*

- Analyzelt™


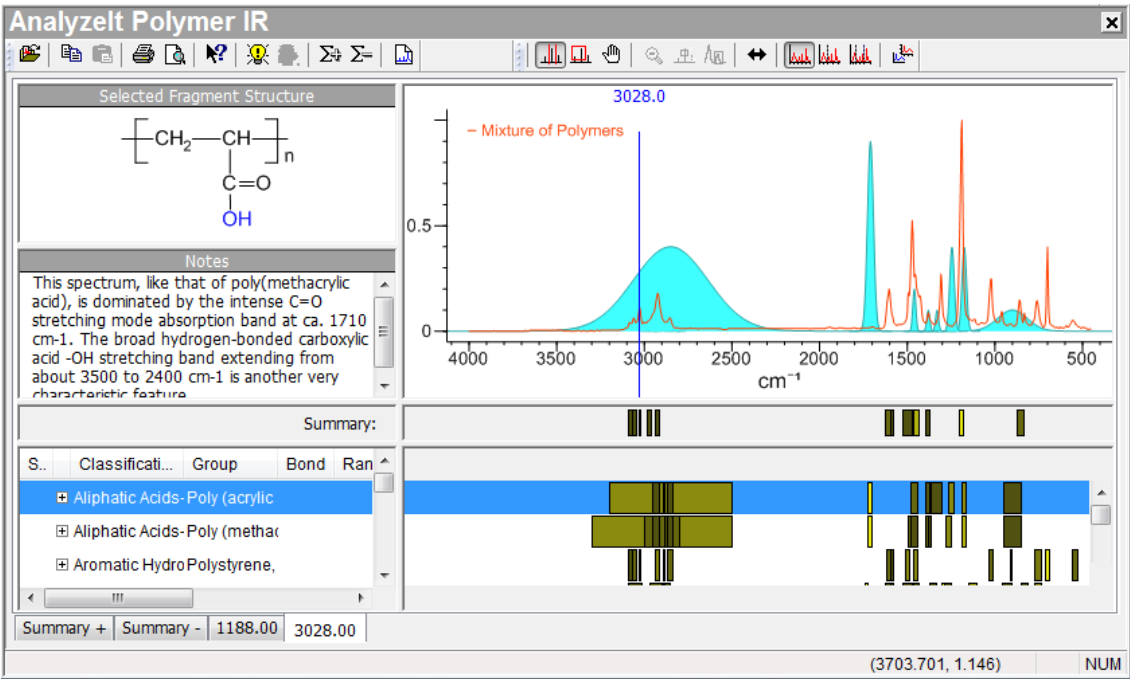
### Open and analyze a mixture spectrum

	Action	Result
1	Navigate to the <b>Spectral Analysis</b> toolbox, click on <b>Open Spectrum</b>	
2	<ul style="list-style-type: none"> <li>Navigate to <b>KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; Functional Group Analysis</b></li> <li>Open <b>Mixture of Polymers.irf</b>.</li> <li>Click on <b>Polymer IR</b> button in the pop-up dialog.</li> </ul> <p><b>Note:</b> Use the <b>Files of type</b> filter to locate IRF, JCAMP, and many other specific spectral files. You can also select <b>All files (*.*)</b>.</p>	<p>The spectrum opens:</p> 

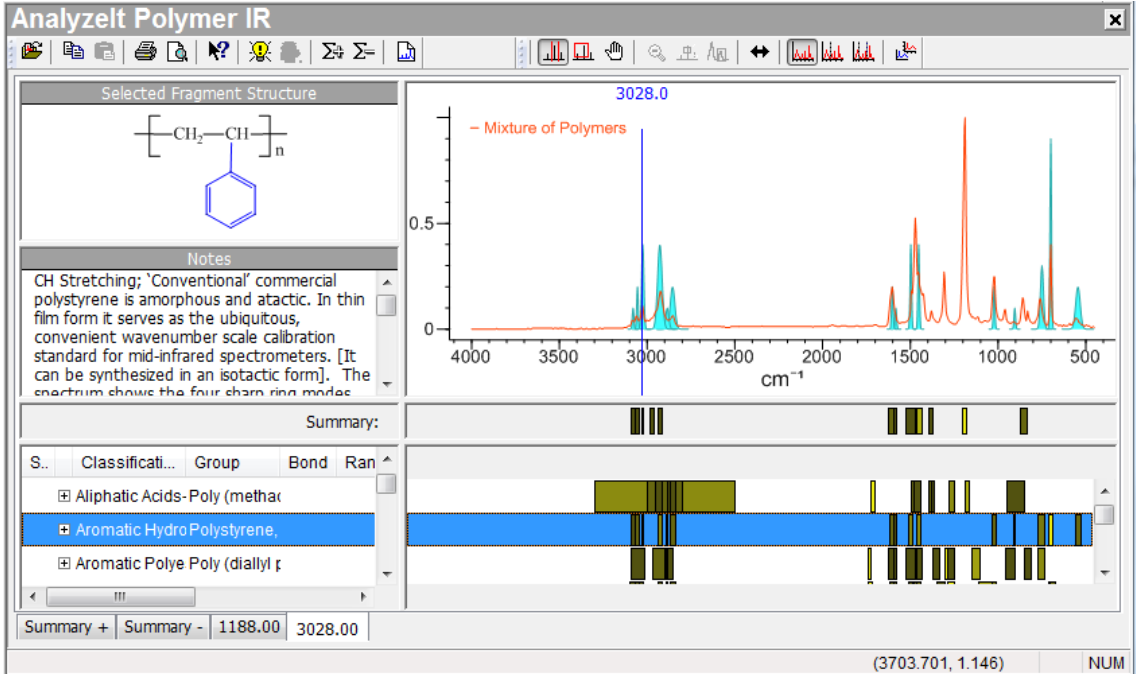
	Action	Result
3	<p>Use the <b>Suggest</b> button to select the tallest peak (at 1188), then click the <b>Correlate</b> button .</p> <p>Alternatively, you can double-click a peak to both select it and initiate searching the knowledgebase(s) for functional group matches.</p>	<p>After the knowledgebase is analyzed, the results are displayed in a tab labeled with the wavenumber (1188).</p> 

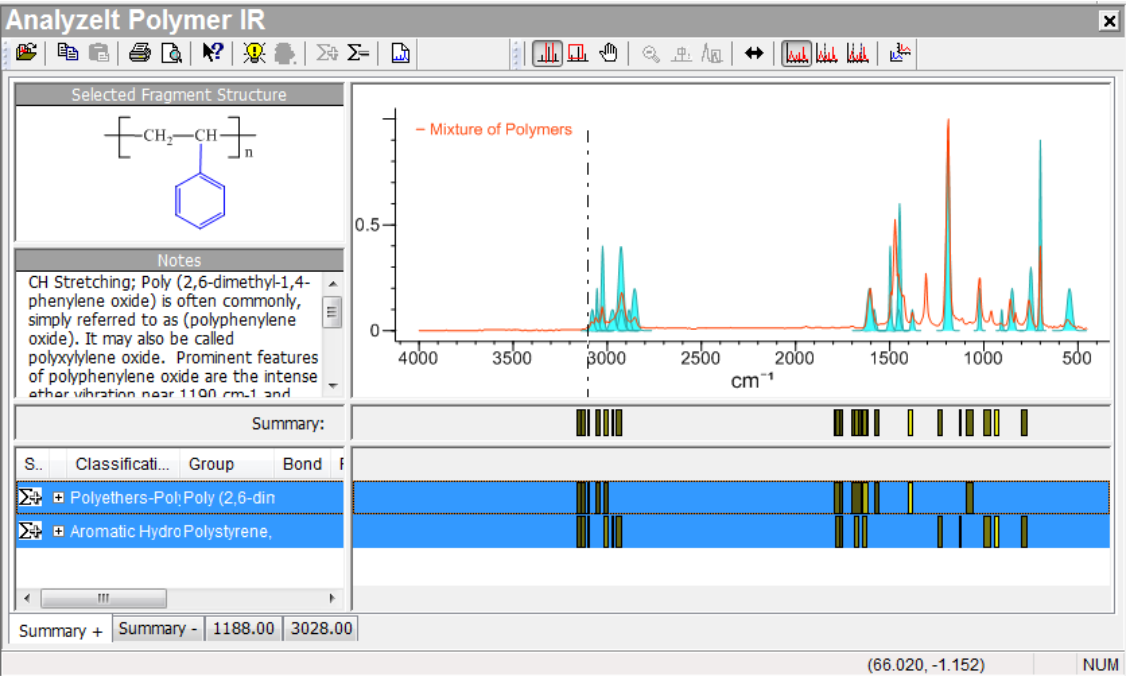
	Action	Result
4	<p>Select each entry in the <b>Functional Group Data</b> pane in turn.</p> <p>Note that the first Polyether-Polymer IR entry (Poly (2,6-dimethyl-1,4-phenylene oxide)) is a good match.</p>	
5	<p>Right-click the entry, then select <b>Add to Summary+</b>.</p>	<p>The entry is added to the <b>Summary+</b> tab.</p>



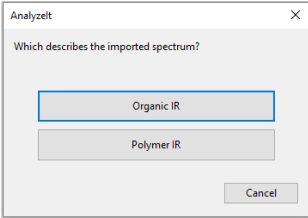
	Action	Result
6	<p>Click the <b>Suggest</b> button to select the peak at 3028, then click the <b>Correlate</b> button .</p>	<p>After the knowledge base is analyzed, the results are displayed in a tab labeled with the wavenumber.</p>  <p>Note the detailed notes available with many <b>Functional Group</b> entries.</p>

## Open and analyze a mixture spectrum (continued)

	Action	Result
7	<p>Select each entry in the <b>Functional Group Data</b> pane in turn.</p> <p>Note that the Aromatic Hydrocarbon (Polystyrene) entry is a good match.</p>	
8	<p>With the Aromatic Hydrocarbon (Polystyrene) entry selected, right-click then select <b>Add to Summary+</b>.</p>	<p>The entry is added to the <b>Summary+</b> tab.</p>

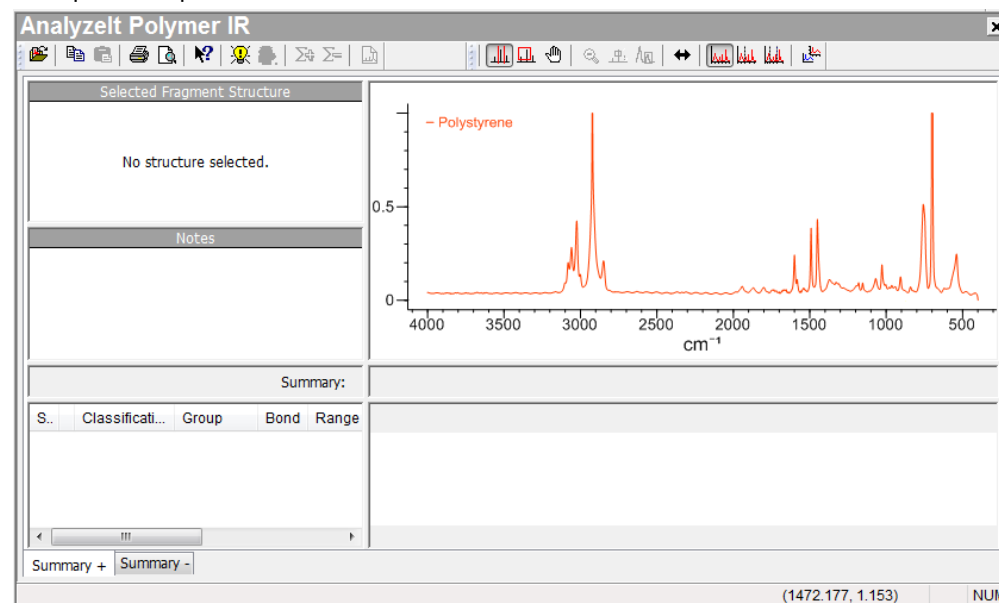
	Action	Result
9	<p>Open the <b>Summary+</b> tab and select both entries.</p> <p><b>Note:</b> Select the first entry, then hold down the ctrl key and click to select the second entry.</p>	<p>We see that these functional groups account for most of the peaks in the mixture spectrum.</p> 

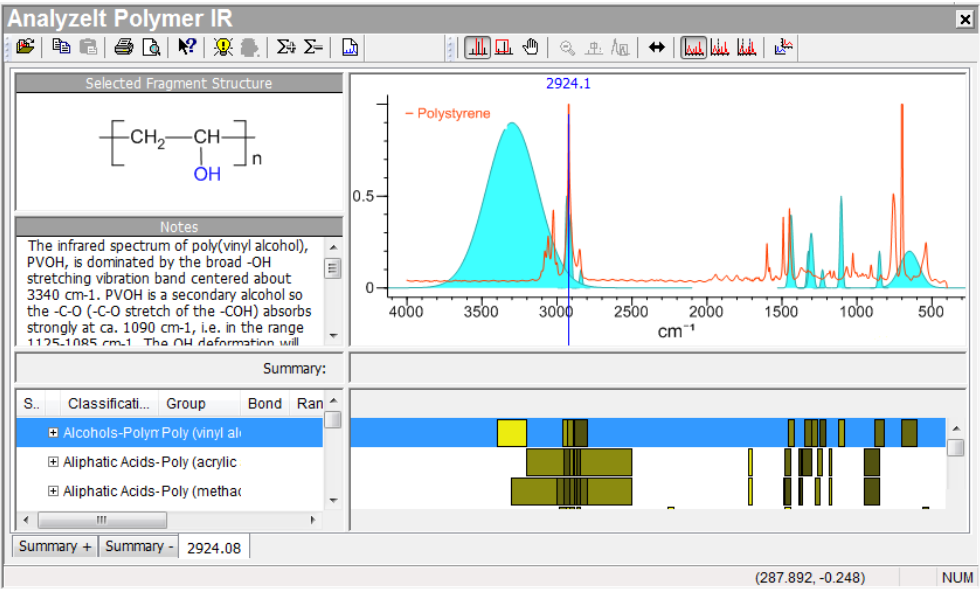
**Open and analyze a single component spectrum**

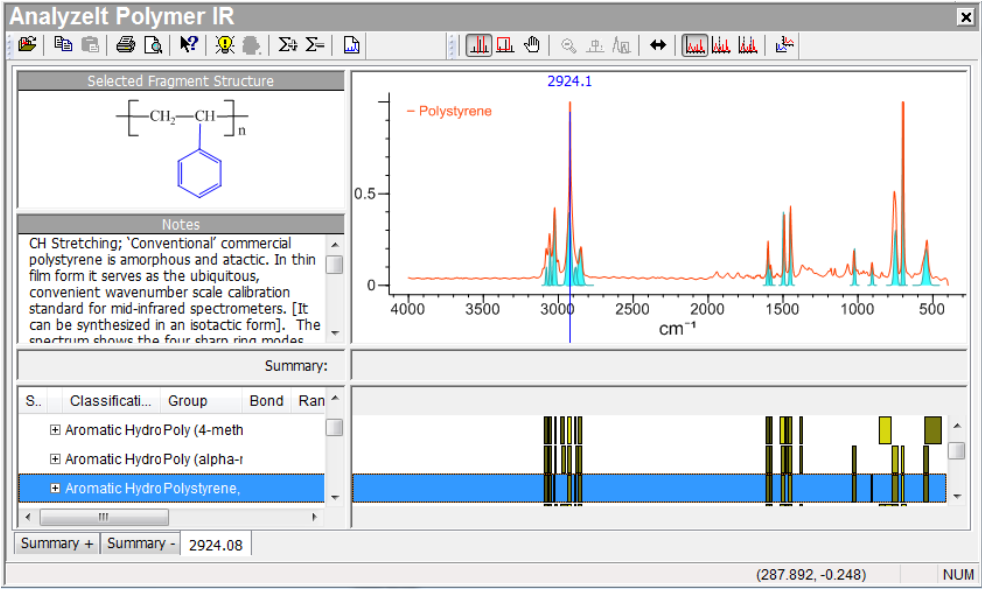
	Action	Result
1	Close the previous analysis by clicking the close button in the upper right-hand corner.	
2	<ul style="list-style-type: none"> <li>Choose <b>File &gt; Open Spectrum</b>,</li> <li>Navigate to <b>KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; Functional Group Analysis</b></li> <li>Open <b>Polystyrene.irf</b>.</li> </ul> <p><b>Note:</b> Use the <b>Files of type</b> filter to locate IRF, JCAMP, and many other specific spectral files. You can also select <b>All files (*.*)</b>.</p>	<p>A pop-up dialog displays two options;</p> 

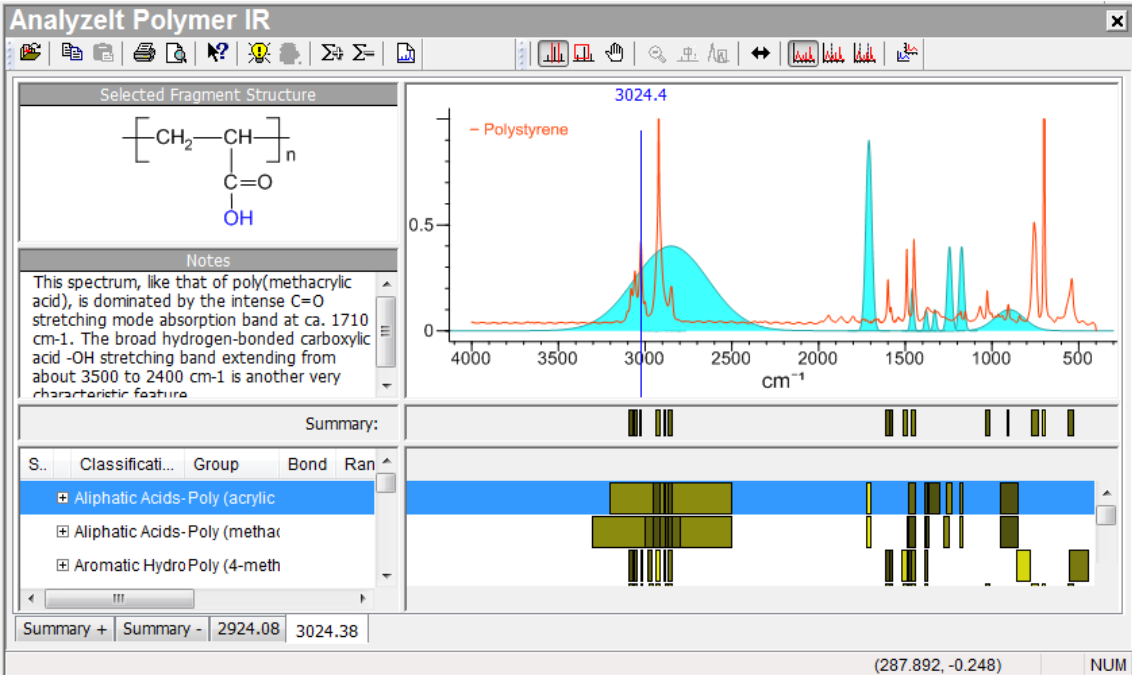
3 Click on **Polymer IR**.

The spectrum opens:

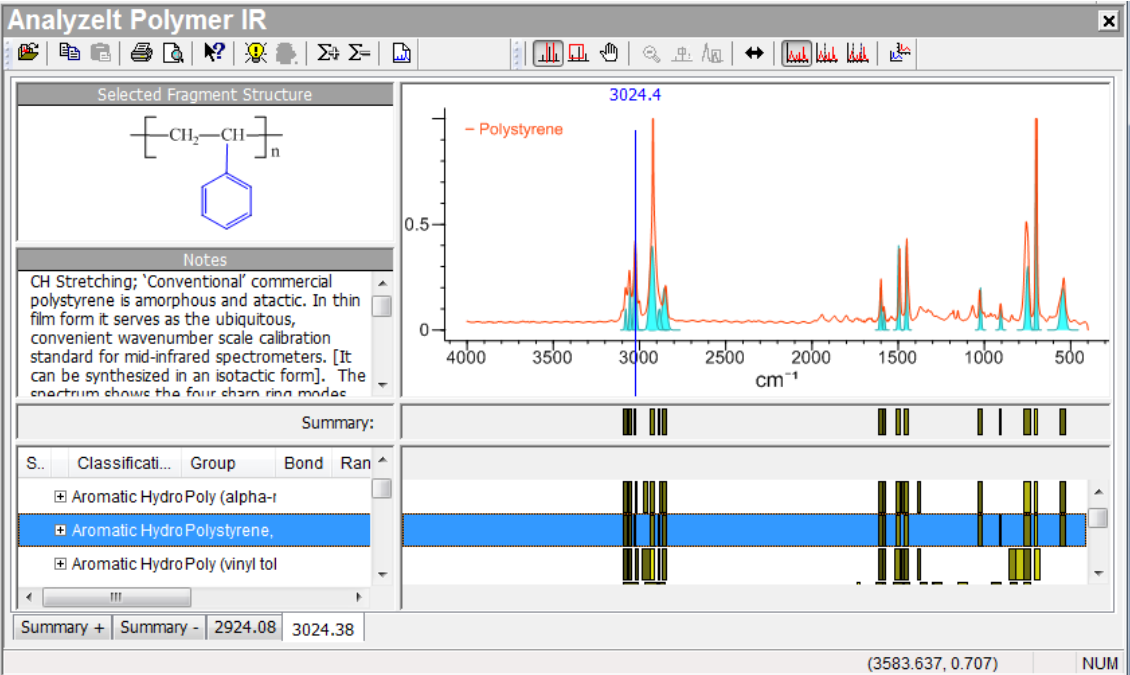


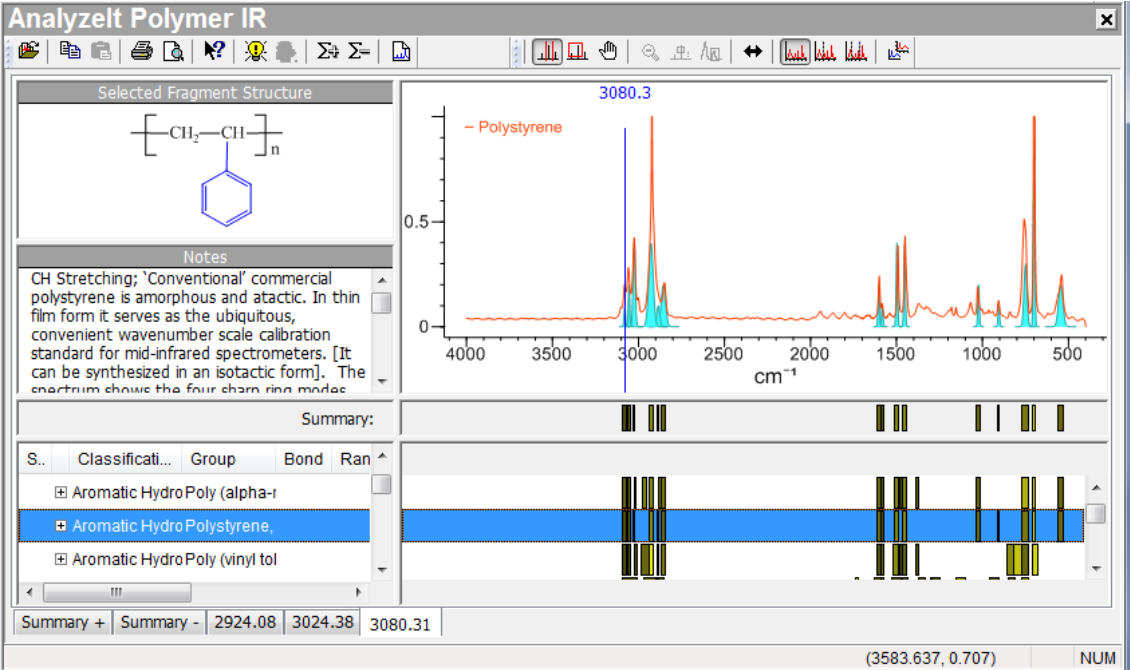
	Action	Result
3	Click the <b>Suggest</b> button to select the peak at 2924.1, then click the <b>Correlate</b> button.	<p>After the knowledge base is analyzed, the results are displayed in a tab labeled with the wavenumber (2924.08).</p> 

	Action	Result
4	Select each entry in the <b>Functional Group Data</b> pane in turn.	<p>Note that Aromatic Hydrocarbon (Polystyrene) is a good fit:</p> 
5	With the Aromatic Hydrocarbon (Polystyrene) entry selected, right-click, then select <b>Add to Summary+</b> .	The functional group is added to the <b>Summary+</b> tab.

	Action	Result
6	Click the <b>Suggest a Peak</b> toolbar button again, then click the <b>Correlate</b> toolbar button.	<p>After the knowledge base is analyzed, the results are displayed in a tab labeled with the wavenumber (3024.38).</p> 



	Action	Result
7	Select each entry in the <b>Functional Group Data</b> pane in turn.	<p>Note that the Aromatic Hydrocarbon (Polystyrene) is, once again, a good fit:</p> 

	Action	Result
8	Repeat the process to analyze the third suggested peak (3080.3), then select each entry in the <b>Functional Group Data</b> pane in turn.	<p>Aromatic Hydrocarbon (Polystyrene) is a good fit:</p> 

# Functional Group Analysis

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## How to Create a User Knowledgebase

### Purpose

This exercise demonstrates how to create and use user Knowledgebases in the Analyzelt™ applications.

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### Objectives

This exercise will teach you:

- How to create a user Knowledgebase;
  - How to browse by functional group; and
  - How to correlate a structure.
- 

### Background

Users can build their own knowledgebases with functional groups and bands from their own data. The knowledgebases can be used in conjunction with KnowItAll's knowledgebases to determine the functional groups in a spectrum.

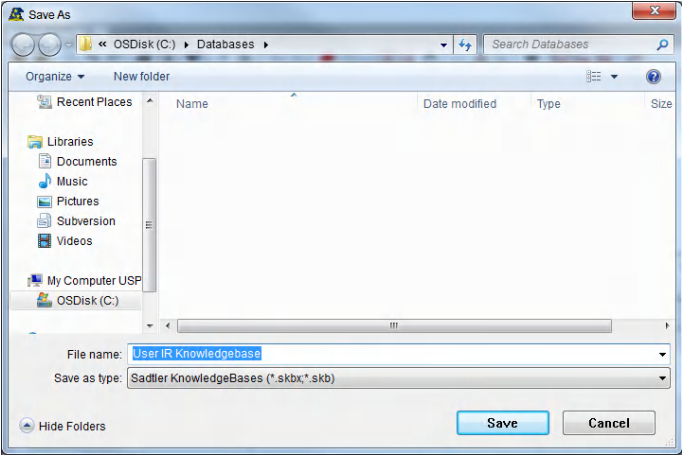
#### *Training Files Used in This Lesson*

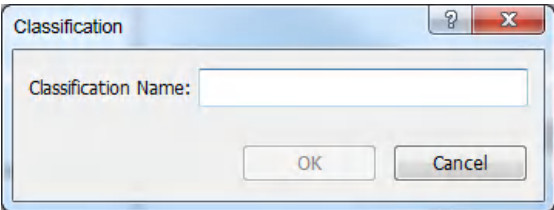
- Test Structure.dsf
- Butylamine.jdx

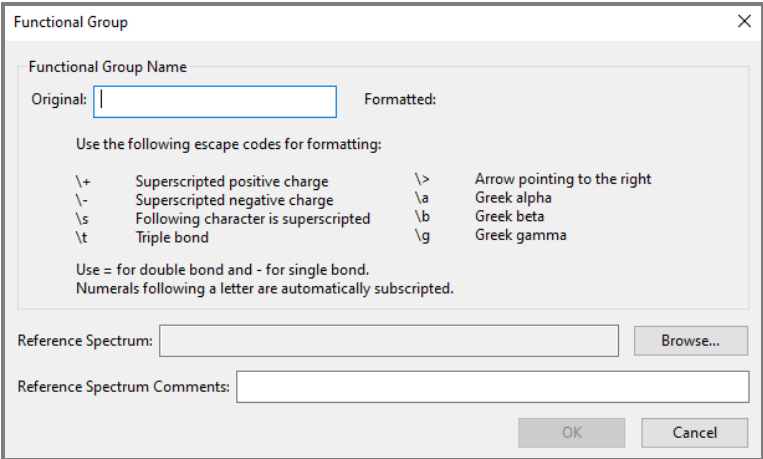
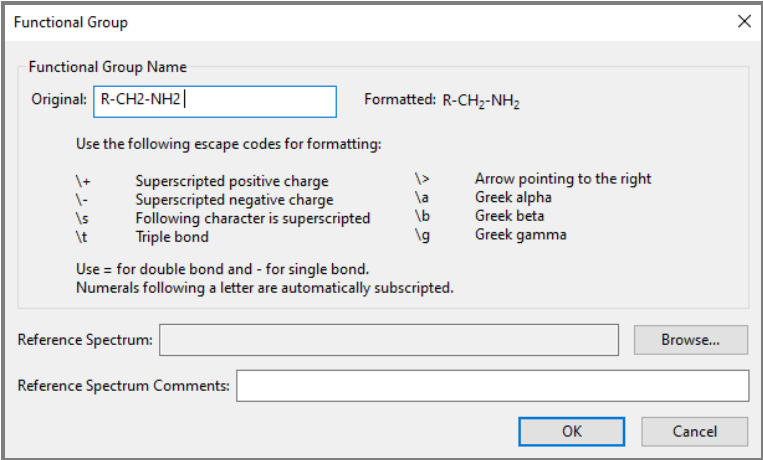
#### *KnowItAll Applications Used*

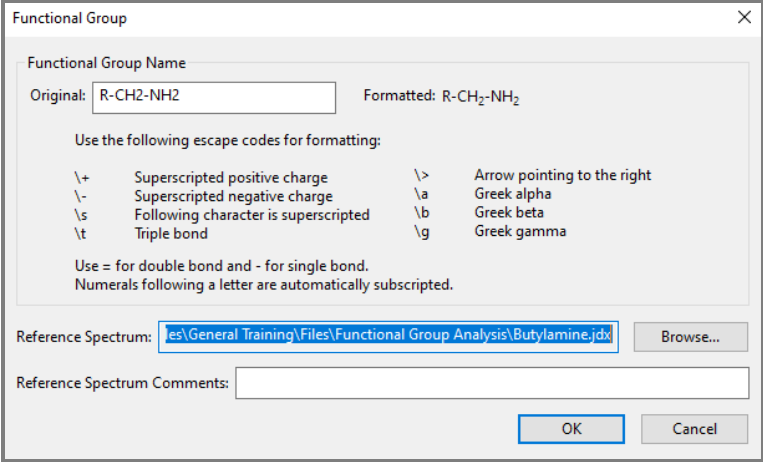
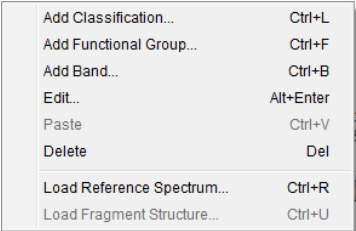
- Analyzelt™

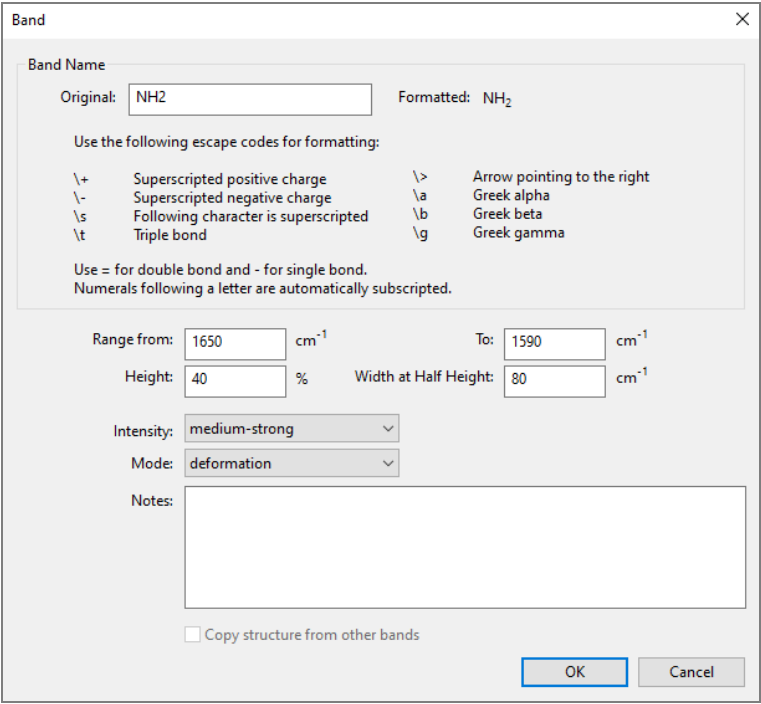
**Create a user knowledgebase**

	Action	Result
1	Navigate to the <b>Spectral Analysis</b> toolbox and open the <b>Analyzelt</b> application by clicking its icon. Click <b>Organic IR</b> button.	
2	Choose <b>Knowledgebase &gt; New</b> .	A <b>Save As</b> dialog box opens.
3	Type in a name for the user knowledgebase (such as <b>User IR Knowledgebase</b> ) and save it to a location on your hard drive.	 <p>The file type - Sadtler Knowledgebase, *.skbx or *.skb – cannot be changed.</p>

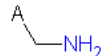
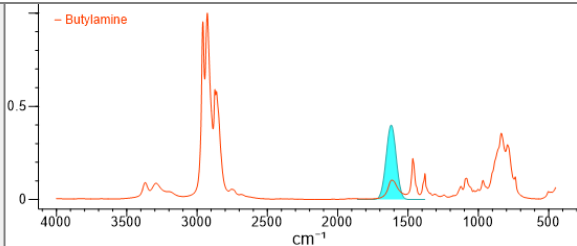



4	Right-click in the <b>Functional Group Tree</b> pane (on the left), then select <b>Add Classification</b> .	<p>The <b>Classification</b> dialog box opens:</p>  <p>Type in AmineA and click <b>OK</b>.</p> <p><b>Note:</b> Use a descriptive identifier to make sure the classification appears in the correct order when browsing for a functional group. Add a unique identifier to the end of the classification name to identify the knowledgebase where the entry appears. Changes can be made easily if necessary.</p>
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	Action	Result
5	Right-click on the new classification name AmineA, then select <b>Add Functional Group</b> .	<p>The <b>Functional Group</b> dialog box opens:</p> 
6	Type R-CH <sub>2</sub> -NH <sub>2</sub> in the upper text box.	<p>The text is automatically formatted:</p> 

	Action	Result
7	<ul style="list-style-type: none"> <li>Click <b>Browse</b></li> <li>Navigate to <b>KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; Functional Group Analysis</b></li> <li>Select <b>Butylamine.jdx</b></li> <li>The path and file name is displayed in the <b>Reference Spectrum</b> text box.</li> </ul>	
8	<p>Click <b>OK</b> to close the dialog box.</p> <p>Right-click on R-CH<sub>2</sub>-NH<sub>2</sub> in the <b>Functional Group Tree</b>.</p>	<p>A pop-up menu opens:</p> 

	Action	Result
9	<ul style="list-style-type: none"> <li>Click <b>Add Band</b>.</li> <li>Type in NH<sub>2</sub>, then add other information as follows:</li> <li><b>Range from</b> 1650 to 1590 <b>Height:</b> 40 <b>Width at Half Height:</b> 80 <b>Intensity:</b> medium-strong <b>Mode:</b> deformation</li> <li>Click <b>OK</b>.</li> </ul>	<p>The <b>Band</b> dialog box opens:</p> 
10		



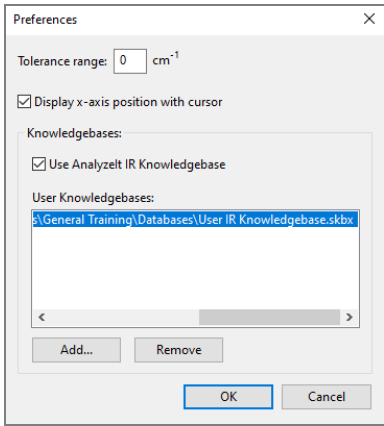
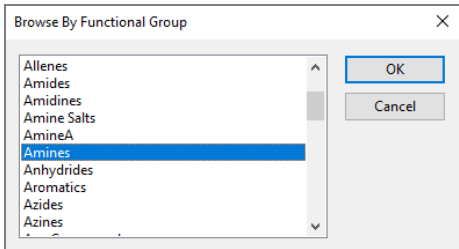
	Action	Result																				
11	Double-click in the <b>Fragment Structure</b> pane to open <b>ChemWindow</b> , then draw this structure: 																					
12	Click <b>Save</b> .	<p>The structure is added to the display:</p> <div><div><div><div>AmineA</div><div>R-CH<sub>2</sub>-NH<sub>2</sub></div><div>NH<sub>2</sub> (1650-1590 cm<sup>-1</sup>)</div></div><div></div></div><table><thead><tr><th>Fragment Structure</th><th>Field</th><th>Value</th></tr></thead><tbody><tr><td rowspan="8"></td><td>Bond</td><td>NH<sub>2</sub></td></tr><tr><td>Range From</td><td>1650 cm<sup>-1</sup></td></tr><tr><td>Range To</td><td>1590 cm<sup>-1</sup></td></tr><tr><td>Height</td><td>40 %</td></tr><tr><td>Width at Half Height</td><td>80 cm<sup>-1</sup></td></tr><tr><td>Intensity</td><td>medium-strong</td></tr><tr><td>Mode</td><td>deformation</td></tr><tr><td>Notes</td><td></td></tr></tbody></table></div>	Fragment Structure	Field	Value		Bond	NH <sub>2</sub>	Range From	1650 cm <sup>-1</sup>	Range To	1590 cm <sup>-1</sup>	Height	40 %	Width at Half Height	80 cm <sup>-1</sup>	Intensity	medium-strong	Mode	deformation	Notes	
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	Mode	deformation																				
	Notes																					

**AmineA**

**R-CH<sub>2</sub>-NH<sub>2</sub>**

- CN (1090-1068 cm<sup>-1</sup>)
- NH<sub>2</sub> (1650-1590 cm<sup>-1</sup>)
- NH (3400-3320 cm<sup>-1</sup>)
- NH (3328-3250 cm<sup>-1</sup>)
- NH (850-750 cm<sup>-1</sup>)

**Specify the user knowledgebase**

	Action	Result
1	Navigate to the <b>Spectral Analysis</b> toolbox and open the <b>Analyzelt IR</b> application by clicking its icon.	
2	Choose <b>File &gt; Preferences</b> .	The <b>Preferences</b> dialog box opens.
3	Click <b>Add</b> , then browse to and select the newly created user knowledgebase.	<p>The user knowledgebase is displayed in the <b>Preferences</b> dialog box:</p> 
4	Click <b>OK</b> to close the <b>Preferences</b> dialog box.	
5	Choose <b>Analyze &gt; Browse a Functional Group</b> .	<p>The contents of the user knowledgebase have been added to the list of functional groups:</p> 

# **KnowItAll Software Training**

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## Drawing and Reactions

# Optional: Drawing and Reactions

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## How to Draw Chemical Structures

### Purpose

The ChemWindow® application is a full-featured 2-dimensional structure drawing program. You can use the ChemWindow application to create chemical structures that can be used throughout the KnowItAll Informatics System for searching, prediction, and reporting chemical composition.

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### Objectives

This exercise will teach you:

- How to use basic ChemWindow tools to create and edit a structure drawing;
  - How to save a structure for further use.
- 


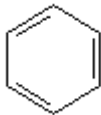


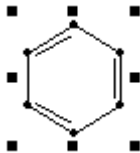
### Background

Chemical structures can be used throughout the KnowItAll Informatics System for searching, prediction, and reporting chemical composition.



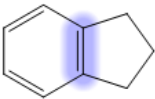

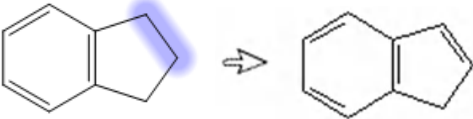

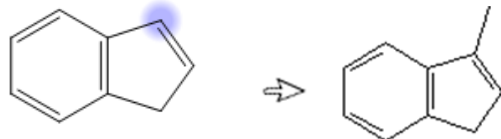
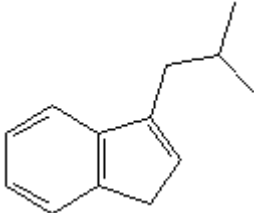
#### *KnowItAll Applications Used*

- ChemWindow®

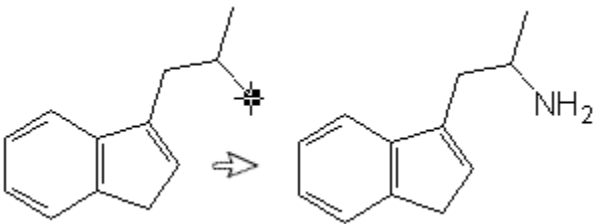
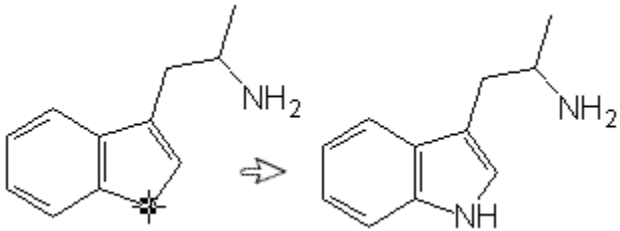
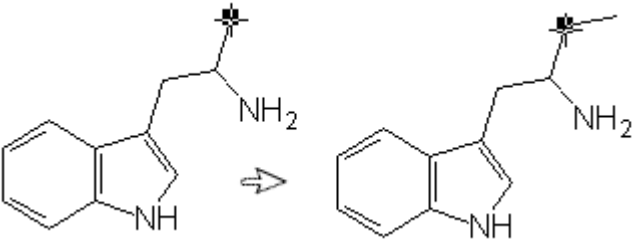
**Begin a new structure drawing**

	Action	Result
1	Click the <b>ChemWindow</b> icon in the <b>Basics</b> toolbox.	The <b>ChemWindow</b> application opens to a blank drawing pane.
2	Select the <b>Benzene Ring</b> tool  in the <b>Main</b> section of the <b>Chemistry Toolbar</b> .	
3	Move the cursor into the drawing area, then click to draw a benzene ring.	The benzene ring structure is placed in the drawing area: 
4	If desired, use tools on the zoom toolbar to change the magnification. <b>Note:</b> Choose <b>View &gt; Zoom Toolbar</b> to toggle the toolbar display.   The <b>ctrl + scroll</b> function can also be used to zoom in and out quickly.	
5	Use the <b>Selection</b> tool  to select the structure and move it within the workspace.	Graphic handles appear when the structure is selected: 

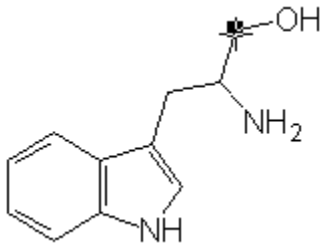
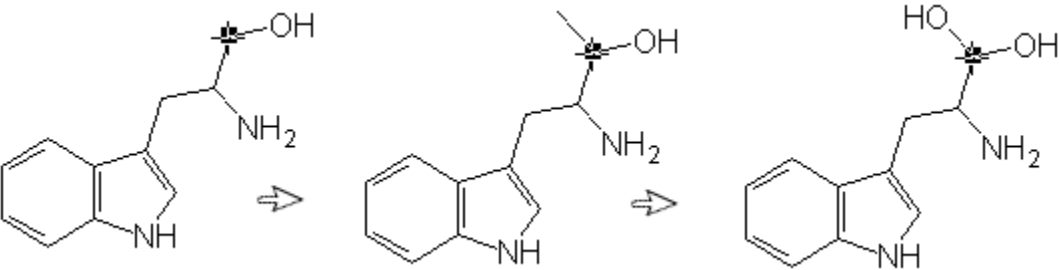
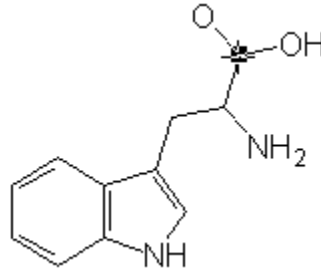
## Add features to the structure

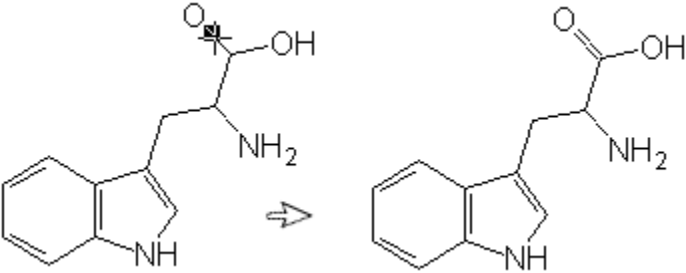
	Action	Result
1	Select the <b>Cyclopentane</b> tool  , then move the cursor to the highlighted bond on the benzene ring.	
2	Click to join a cyclopentane ring to the benzene ring.	
3	Open the <b>Bonds</b> group in the <b>Drawing Toolbar</b> , select the <b>Inside Double Bond</b> tool  , then use it to add a double bond to the structure.	
4	Select the <b>Single Bond</b> tool  , then move the cursor over the atom's hit box as shown. Click to create a single bond.	 <b>Note:</b> If you don't release the cursor, you can control the bond direction by dragging.
5	Continue adding single bonds by clicking on hit boxes on atoms.	

**Use hot keys to add nitrogen and oxygen atoms**

	Action	Result
1	Move the cursor over the terminal carbon, then press n on your keyboard.	<p><b>NH<sub>2</sub></b> appears at the end of the bond:</p>  <p><b>Note:</b> Numbers are automatically displayed as subscripts when using hot keys, which are shortcut keys you can use to quickly label atoms.</p> <p>You can also use the atom label tool to add atoms to a drawing. However, unlike atoms added while using a bond tool, atoms in atom labels are not actually part of the structure, and will not be included when calculating the mass or chemical formula.</p>
2	Repeat to replace a carbon atom with <b>NH</b> .	
3	With the single bond tool still selected, place your cursor over the terminal carbon atom and click to add another single bond.	




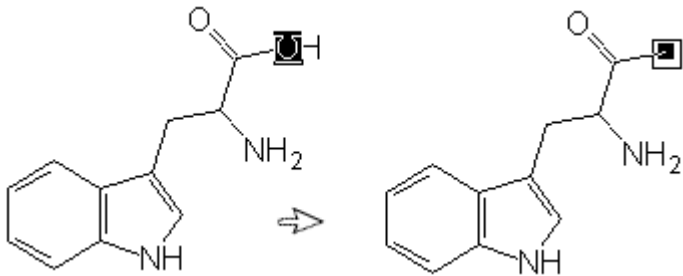
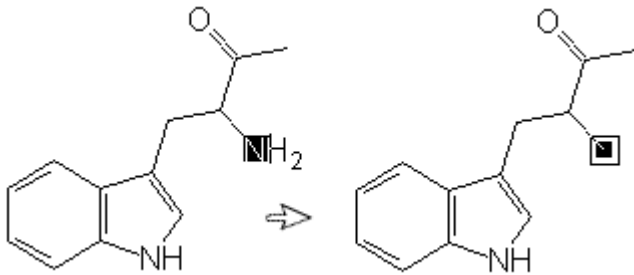

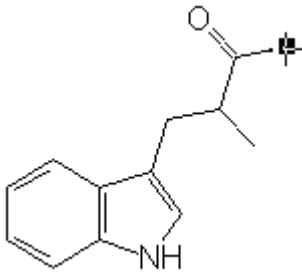
	Action	Result
4	Without moving the cursor, press o on your keyboard.	 The diagram shows the chemical structure of L-tryptophan, consisting of an indole ring system attached to a side chain. The side chain is a two-carbon chain where the alpha-carbon is bonded to an amino group (NH <sub>2</sub> ) and a hydroxyl group (OH). A cursor, represented by a small black square with a cross, is positioned on the alpha-carbon atom.
5	Click to sprout another single bond, then press o on the keyboard to add a hydroxyl group.	 This row illustrates the step-by-step addition of a second hydroxyl group to the alpha-carbon. It is shown in three stages separated by right-pointing arrows. In the first stage, the structure is the same as in row 4, with the cursor on the alpha-carbon. In the second stage, a single bond has been 'sprouted' from the alpha-carbon, and the cursor is now on this new bond. In the third stage, a hydroxyl group (OH) has been added to the alpha-carbon, resulting in a geminal diol (a carbon atom bonded to two hydroxyl groups).
6	Press o again to remove the hydrogen. <b>Note:</b> When using a hot key, you can change the number of hydrogens attached to the atom by pressing the hot key repeatedly.	 The diagram shows the final chemical structure of L-tryptophan, where the alpha-carbon is now part of a carboxylic acid group. The alpha-carbon is bonded to the indole ring, the amino group (NH <sub>2</sub> ), and a carboxyl group (COOH). The carboxyl group consists of a carbon atom double-bonded to an oxygen atom and single-bonded to a hydroxyl group (OH). The cursor is still positioned on the alpha-carbon atom.

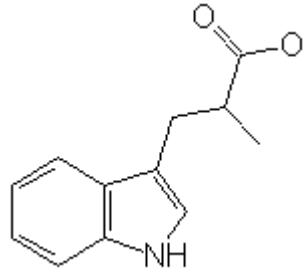


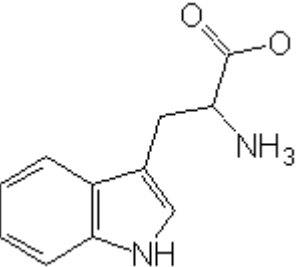

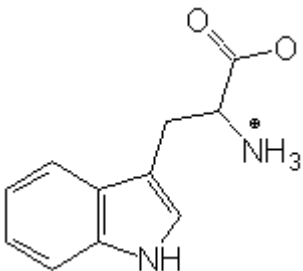
	Action	Result
7	Move the cursor to the hit box on the bond, then click to create a double bond.	 <p>The diagram illustrates a chemical transformation. On the left, a molecule consists of an indole ring system attached to a side chain. The side chain has a chiral center bonded to an amino group (NH<sub>2</sub>) and a carboxylic acid group (COOH). A small square hit box is positioned on the C-C single bond between the chiral center and the carbonyl carbon. An arrow points to the right, where the resulting molecule is shown. In this molecule, the C-C bond has been converted to a double bond, and the carboxylic acid group is now a carboxylic acid derivative (COOH).</p>


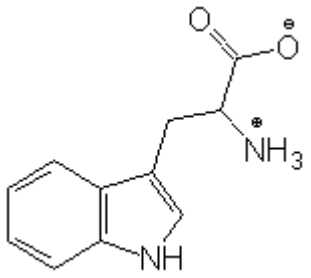
**Save the structure**

	Action	Result
1	Choose <b>File &gt; Save</b> . <b>Note:</b> You can also click the <b>Save</b> button on the toolbar, or press Ctrl+S.	The <b>Save As</b> dialog box opens. The default file type (ChemWindow structure file, *.dsf) is already selected, and will be used for this structure. Other file types include ChemWindow Structure Template & Style (*.dst) and MDL Mol file (*.mol).
2	Navigate to the folder where you wish to save the structure file, then type in the file name "tryptophan."	
3	Click <b>Save</b> .	The structure is saved, and the file name is displayed on the drawing tab.

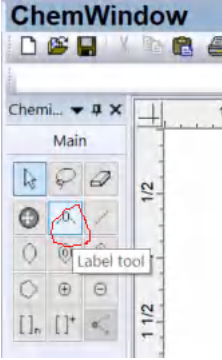
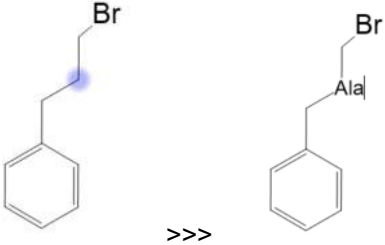
## Edit the structure and use atom labels and atom tags

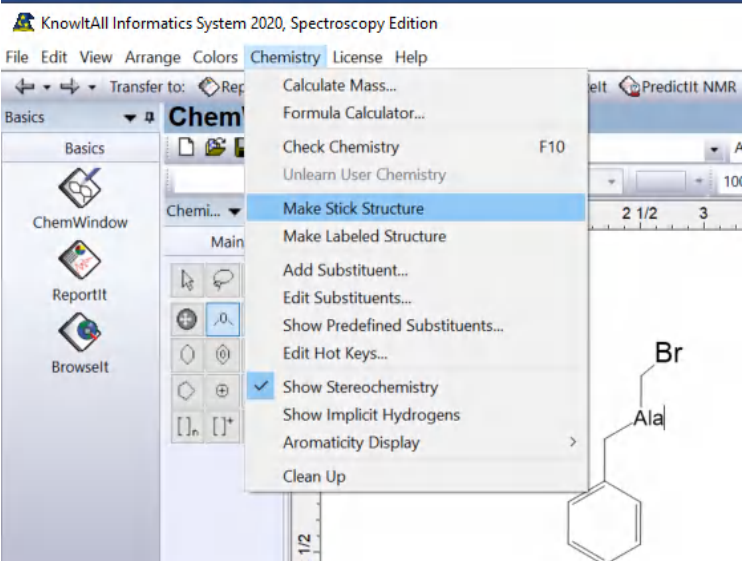
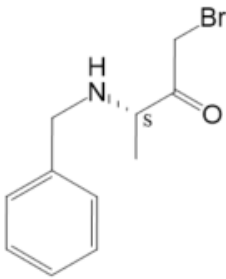
	Action	Result
1	Select the <b>Eraser</b> tool  , then click to remove the hydroxyl...	
2	...and amino groups.	
3	Open the <b>Main</b> group on the <b>Drawing Toolbar</b> , select the <b>Atom Label</b> tool  , then click where the hydroxyl group was located.	

	Action	Result
4	Type uppercase O. <b>Note:</b> Atom labels are case-sensitive.	
5	Move to the other atom and type uppercase NH3. <b>Note:</b> Numbers are automatically displayed as subscripts if the <b>Text</b>  is selected. <b>Style</b> toolbar's <b>Formula</b> tool  is selected.	
6	Select the <b>Positive Charge Atom Tag</b> tool  to add a positive charge to the atom.	
	<i>TIP</i>	Clicking and dragging a charge allows you more control over the placement of the charge. You can also use the <b>Lasso</b> tool to move the charge.

	Action	Result
7	Repeat with the <b>Negative Charge Atom Tag</b> tool  to add a negative charge to the oxygen atom.	
8	Choose <b>File &gt; Save As</b> to save the structure with file name <b>tryptophan2.dsf</b> .	

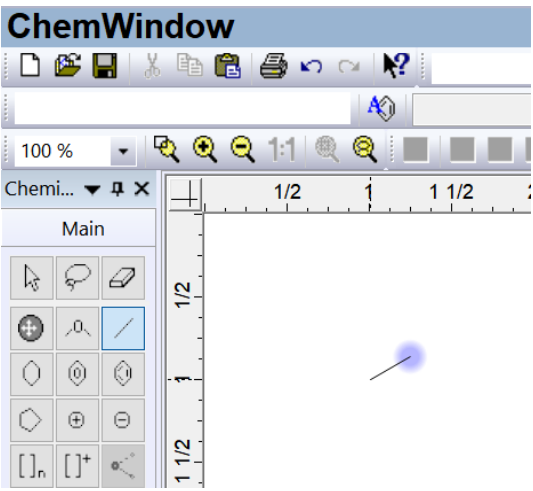
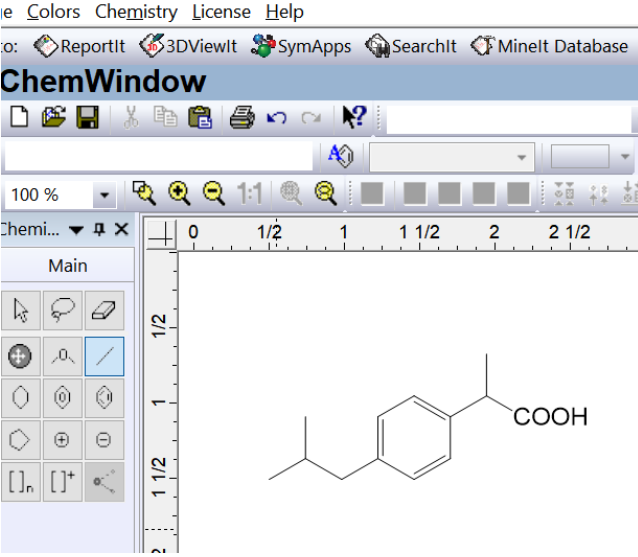
## Use pre-defined substituents

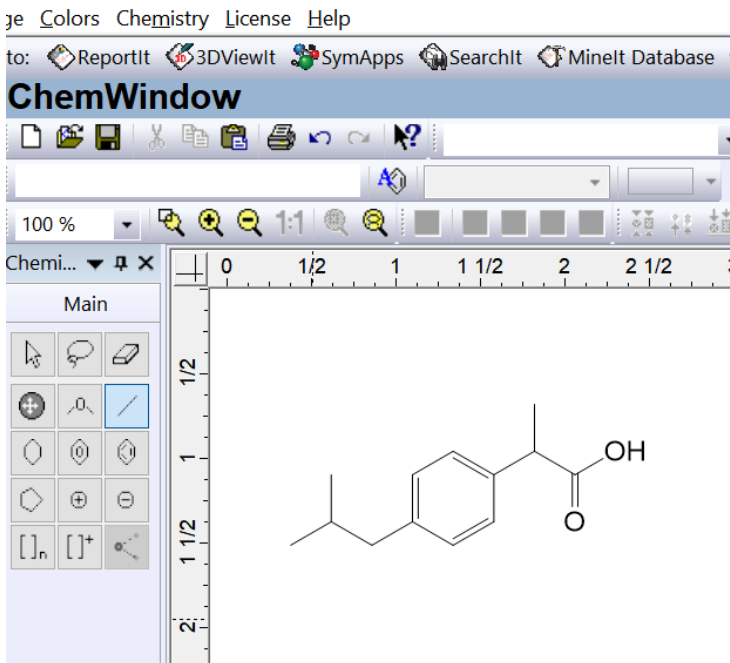
	Action	Result
1	Click on the <b>Label</b> tool	
2	Select an atom and click to type <b>Ala</b> (a pre-defined substituent)	

	Action	Result
3	Click <b>Chemistry &gt; Make Stick Structure</b>	
4		 <p data-bbox="699 1230 1129 1255">The above is the expanded structure</p>



## Use Hotkeys

	Action	Result
1	<ul style="list-style-type: none"><li>In the Main toolbox, select the <b>Standard bond</b> tool.</li><li>Click the structure pane to insert the single bond. The end of the bond will be highlighted automatically.</li></ul>	
2	Type the following characters on your keyboard: 9, 1, 3, 9, 0 (Capital O)	

	Action	Result
3	Click <b>Chemistry &gt; Make Stick Structure</b>	 <p>The above is the expanded structure</p>

# Drawing and Reactions

## How to Draw Chemical Reactions

### Purpose

The ReportIt™ application is a full-featured chemical publishing program. Use the ReportIt application to import objects such as structures and spectra, arrange them on the page, and add text, annotations, reaction arrows, polygons, or orbitals.

The ease with which information can be passed from one KnowItAll Informatics System application to another is especially evident in the way the ReportIt and ChemWindow® applications work together. Use ChemWindow to create structures and transfer them to ReportIt for incorporation in a report. Transfer structures from ReportIt to ChemWindow for editing.

### Objectives

This exercise will teach you:

- How to transfer objects between the ChemWindow and ReportIt applications;
- How to use ReportIt tools to create a report that includes chemical reactions.

### Background

Scientists can use the KnowItAll ChemWindow and ReportIt applications to add reaction schemes to reports. This capability is useful to anyone communicating the results of laboratory procedures.

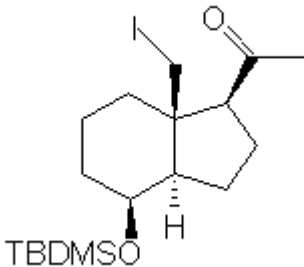
#### *Training Files Used in This Lesson*

- Structure 1.dsf
- Structure 2.dsf


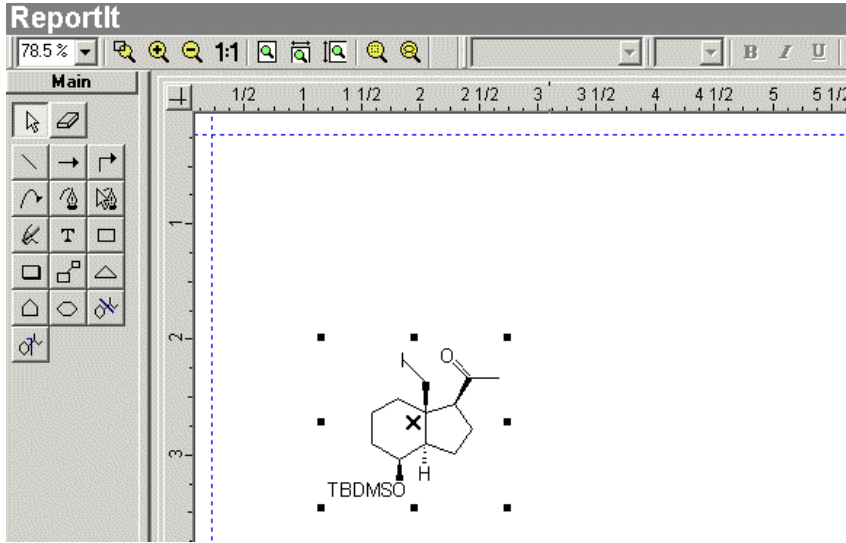
#### *KnowItAll Applications Used*

- ChemWindow®
- ReportIt™


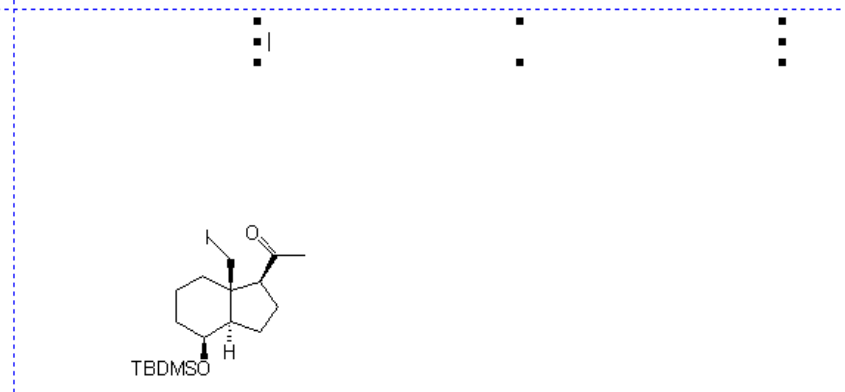

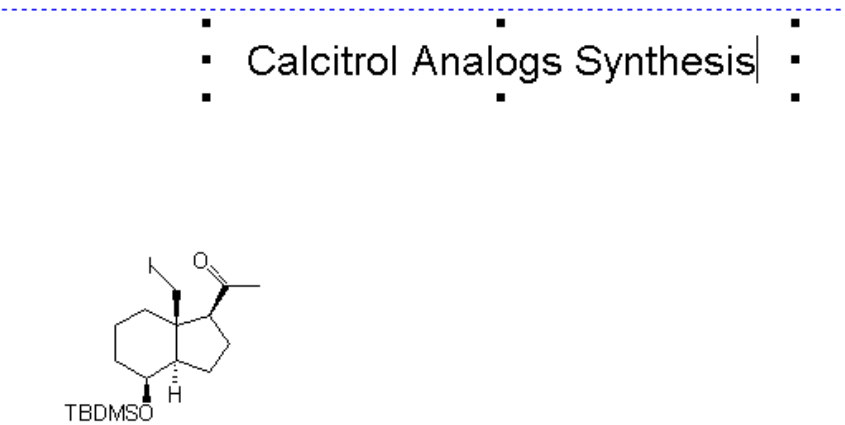
**Open a structure in the ChemWindow application**

	Action	Result
1	Click the <b>ChemWindow</b> icon in the <b>Basics</b> toolbox.	The <b>ChemWindow</b> application opens to a blank drawing.
2	<ul style="list-style-type: none"><li>• Navigate to <b>File &gt; Open</b>, then navigate to KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; Drawing and Reactions</li><li>• Select <b>Structure 1.dsf</b>.</li><li>• Click <b>Open</b></li></ul>	<p>The file opens in the workspace:</p> 
3	Click <b>ReportIt</b> in the <b>Transfer to</b> bar.	The structure opens in the <b>ReportIt</b> application. It is already selected and can be moved, re-sized, etc.




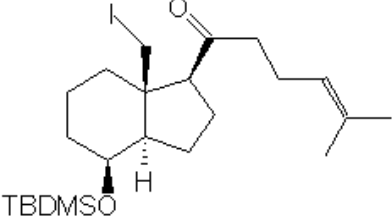
## Set up the report

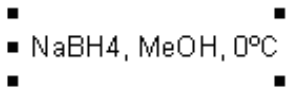


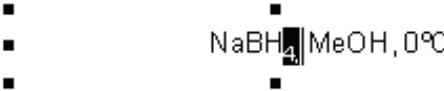
	Action	Result
1	Click the <b>Fit to Page Width</b> tool  on the <b>Zoom</b> toolbar.	The display adjusts so the entire page width is visible.
2	<p>Move the image so it is about 1" in from the left edge, and about 2" below the top of the page.</p> <p><b>Note:</b> Choose <b>View &gt; Rulers</b> to display rulers in the drawing area.</p> <p>Choose <b>File &gt; Preferences</b> and select the <b>Templates/Units</b> tab to specify default measurement units on the drawing area rulers.</p>	

## Use Text tools

	Action	Result
1	Select the <b>Text</b> tool  on the <b>Drawing</b> toolbar's <b>Main</b> group, then click and drag at the top of the page to create a text box.	When you release the mouse button, the text box is bounded by hit boxes and the cursor is inside, ready for typing. Text tools become available. 
2	If necessary, display the <b>Text Style</b> toolbar ( <b>View</b> menu), then adjust the font size to 24.	
3	Type <b>Calcitriol Analogs Synthesis</b> then click the <b>Center Alignment</b> tool  to center the text in the text box.	


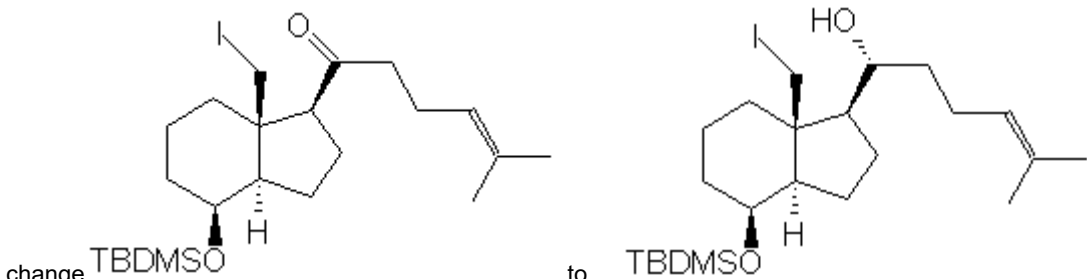
## Create reaction arrows, and add a second structure


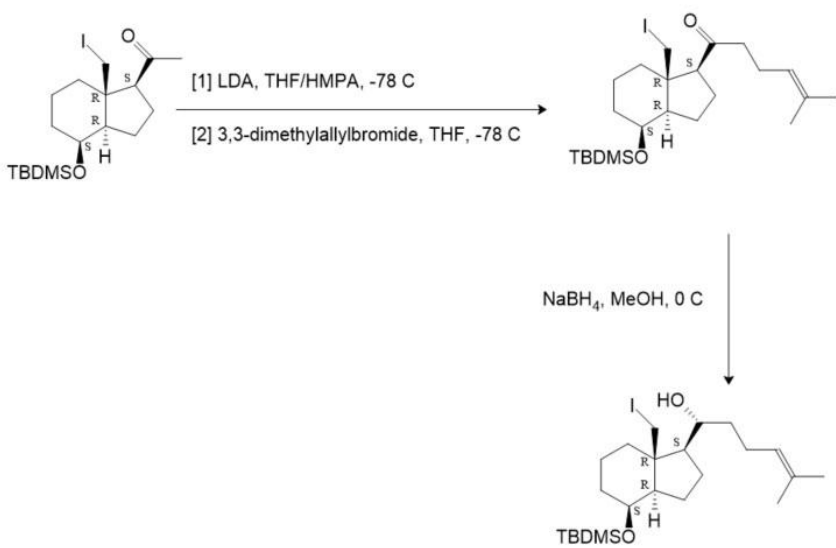
	Action	Result
1	Select the <b>Reaction Arrow</b> tool  in the <b>Drawing</b> toolbar's <b>Main</b> group, then click and drag to draw an arrow to the right of the structure.	When you release the mouse button, the arrow is selected and ready to be moved or re-sized:  Once the arrow has been drawn, you can resize it, reposition it, and change the direction and style of the arrowhead, if desired. Refer to <b>ChemWindow</b> online help or the KnowItAll User Guide for more information.
2	Draw a text box above the arrow and type in the text shown at right. Repeat below the arrow.  <b>Note:</b> You can type in the degree symbol by opening the <b>Windows Character map</b> (Start Menu > Programs > Accessories > System Tools in Windows 10), selecting and copying the symbol, then pasting it in the text box.	[1] LDA, THF/HMPA, -78°C   [2] 3,3-dimethylallylbromide, THF, -78°C
3	<ul style="list-style-type: none"> <li>Use the KnowItAll <b>Back</b> button to return to the <b>ChemWindow</b> application</li> <li>Navigate to <b>File &gt; Open</b>, then navigate to <b>KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; Drawing and Reactions</b></li> <li>Open <b>Structure 2.dsf</b>.</li> </ul>	
4	Click <b>ReportIt</b> in the <b>Transfer to</b> bar.	The drawing is copied into the ReportIt document.
5	Use the <b>Selection</b> tool to move the newly-copied structure to the right of the reaction arrow.	
6	Draw another reaction arrow pointing downwards from the newly-copied structure.	

	Action	Result
7	Add a text box to the left of the arrow and type in the text shown at right.	
8	Click the <b>Right Align</b> tool  ...	
9	...then select '4' in NaBH4 and click the <b>Subscript</b> tool  .	



## Use ReportIt tools to create a third structure

	Action	Result
1	Click the <b>Selection</b> tool, then select the second structure, copy it, and paste the copy below the reaction arrow. <b>Note:</b> There are many ways to access the copy and paste commands. Right-clicking is one of the easiest.	
2	Double click the newly-pasted structure.	<p>The <b>Structure</b> toolbar appears at the right edge of the drawing area.</p>  <p>The <b>Structure</b> toolbar can be moved anywhere on the desktop, but remains only as long as the structure is selected.</p>
3	Use the <b>Structure</b> toolbar's drawing tools to edit the structure. <b>Note:</b> Use the <b>Atom Label</b> and <b>Hashed Wedge Bond</b> tools to make the changes.	 <p>change TBDMSO to TBDMSO</p>

	Action	Result
4	Click outside the structure to close the <b>Structure</b> toolbar, then click the <b>Fit to Page</b> button  to view the entire page.	<p style="text-align: center;">Calcitrol Analogs Synthesis</p>  <p>The reaction scheme illustrates the synthesis of Calcitrol Analogs. It begins with a bicyclic ketone derivative featuring a TBDMSO group and an iodine atom. This starting material undergoes two sequential steps: (1) treatment with LDA in THF/HMPA at -78 °C, followed by (2) reaction with 3,3-dimethylallylbromide in THF at -78 °C, to yield an enone intermediate. Subsequently, the enone is reduced using NaBH<sub>4</sub> in MeOH at 0 °C to produce the final alcohol product.</p>
5	Choose <b>File &gt; Save</b> .	

# **KnowItAll Software Training**

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## Create Reports

# Create Reports

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## How to Create Customized Report Templates

### Purpose

KnowItAll users can use report templates to easily generate high-quality documents including structures, spectra, tables, clip art, and more. Reports can be exported using a variety of formats, making it easier to share results with others.

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### Objectives

This exercise will teach you:

- How to open and use pre-defined KnowItAll report templates;
  - How to create and use customized report templates.
- 

### Background

In addition to serving as the basis for reports, templates are used when objects and information are transferred to the ReportIt application from other KnowItAll applications. A template must be selected before any transfer can occur. A default template can be selected for each application, or a template can be chosen every time information is transferred to the ReportIt application.

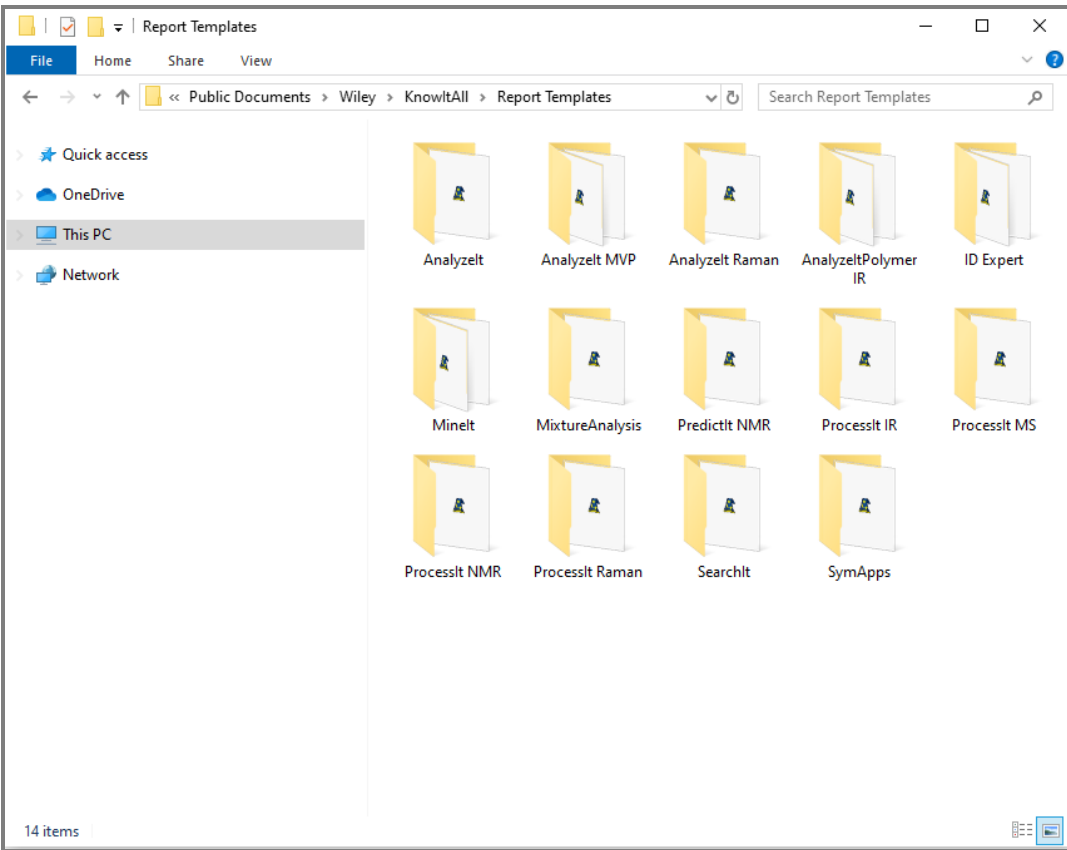
#### ***Training Files Used in This Lesson***

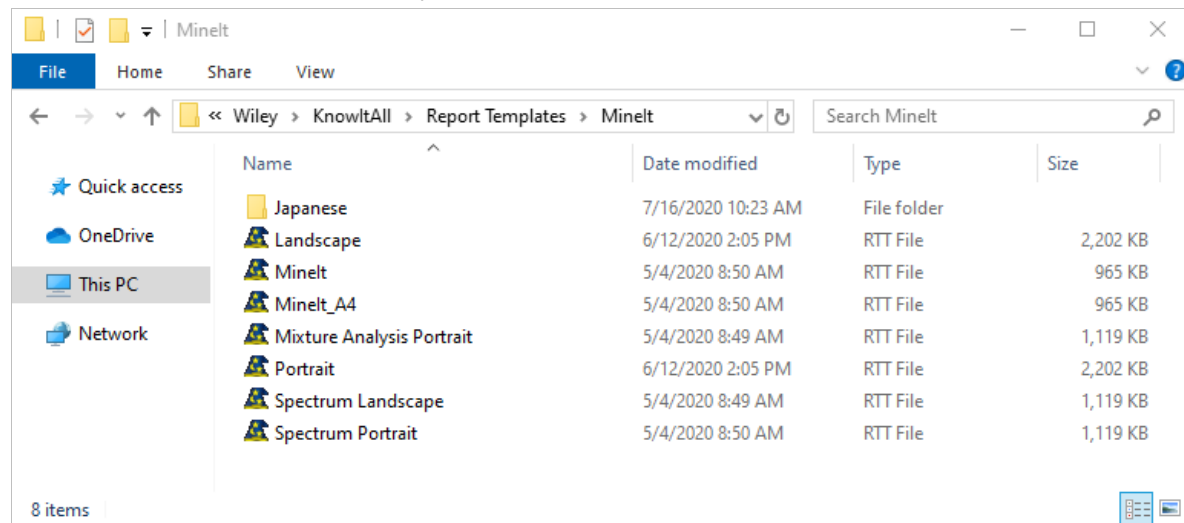
- Wiley.GIF
- Landscape.rtt

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

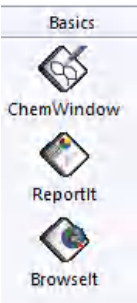
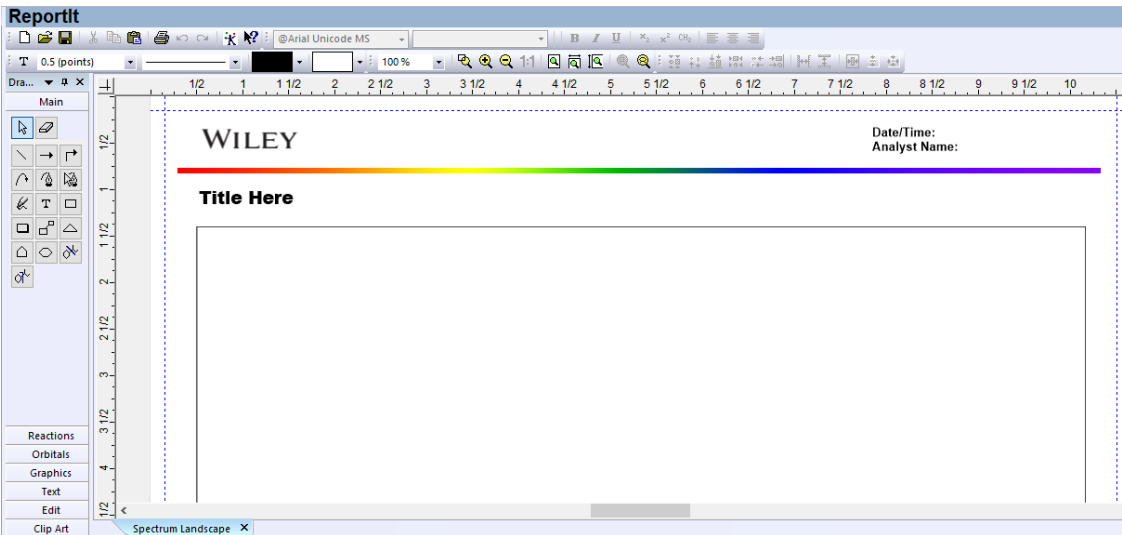
- ReportIt™
- MinelIt™

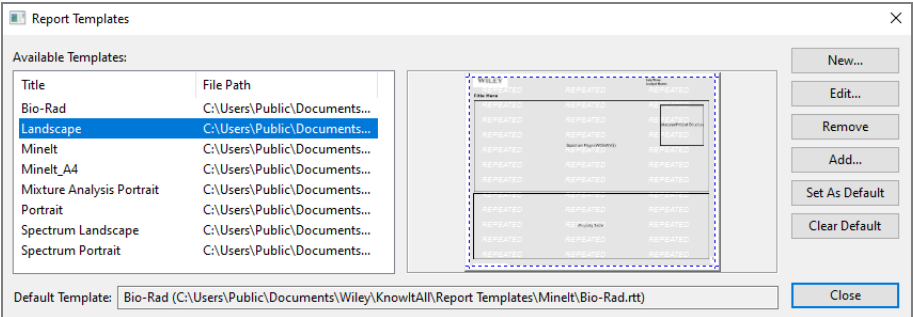
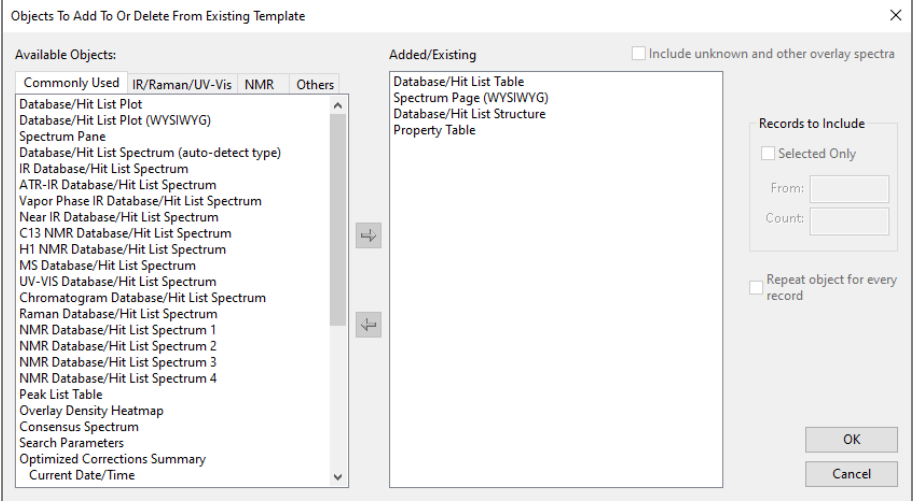
**Examine predefined KnowItAll templates**

	Action	Result
1	<p>Open Windows Explorer, then navigate to <b>Documents &gt; Wiley &gt; KnowItAll &gt; Report Templates</b> (Windows 10)</p> <p><b>Note:</b> If you cannot find it in your version of Windows, use the Explorer search to locate it.</p>	<p>Each KnowItAll application has its own report templates folder:</p> 

	Action	Result																																				
2	Open the <b>Minelt</b> folder.	<p>The <b>Minelt</b> report templates are displayed:</p>  <p>The screenshot shows a Windows Explorer window titled 'Minelt'. The address bar shows the path: &lt;&lt; Wiley &gt; KnowItAll &gt; Report Templates &gt; Minelt. The left sidebar shows 'This PC' selected. The main pane displays a list of 8 items:</p> <table><thead><tr><th>Name</th><th>Date modified</th><th>Type</th><th>Size</th></tr></thead><tbody><tr><td>Japanese</td><td>7/16/2020 10:23 AM</td><td>File folder</td><td></td></tr><tr><td>Landscape</td><td>6/12/2020 2:05 PM</td><td>RTT File</td><td>2,202 KB</td></tr><tr><td>Minelt</td><td>5/4/2020 8:50 AM</td><td>RTT File</td><td>965 KB</td></tr><tr><td>Minelt_A4</td><td>5/4/2020 8:50 AM</td><td>RTT File</td><td>965 KB</td></tr><tr><td>Mixture Analysis Portrait</td><td>5/4/2020 8:49 AM</td><td>RTT File</td><td>1,119 KB</td></tr><tr><td>Portrait</td><td>6/12/2020 2:05 PM</td><td>RTT File</td><td>2,202 KB</td></tr><tr><td>Spectrum Landscape</td><td>5/4/2020 8:49 AM</td><td>RTT File</td><td>1,119 KB</td></tr><tr><td>Spectrum Portrait</td><td>5/4/2020 8:50 AM</td><td>RTT File</td><td>1,119 KB</td></tr></tbody></table> <p>8 items</p>	Name	Date modified	Type	Size	Japanese	7/16/2020 10:23 AM	File folder		Landscape	6/12/2020 2:05 PM	RTT File	2,202 KB	Minelt	5/4/2020 8:50 AM	RTT File	965 KB	Minelt_A4	5/4/2020 8:50 AM	RTT File	965 KB	Mixture Analysis Portrait	5/4/2020 8:49 AM	RTT File	1,119 KB	Portrait	6/12/2020 2:05 PM	RTT File	2,202 KB	Spectrum Landscape	5/4/2020 8:49 AM	RTT File	1,119 KB	Spectrum Portrait	5/4/2020 8:50 AM	RTT File	1,119 KB
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Spectrum Portrait	5/4/2020 8:50 AM	RTT File	1,119 KB																																			
3	Close Windows Explorer.																																					

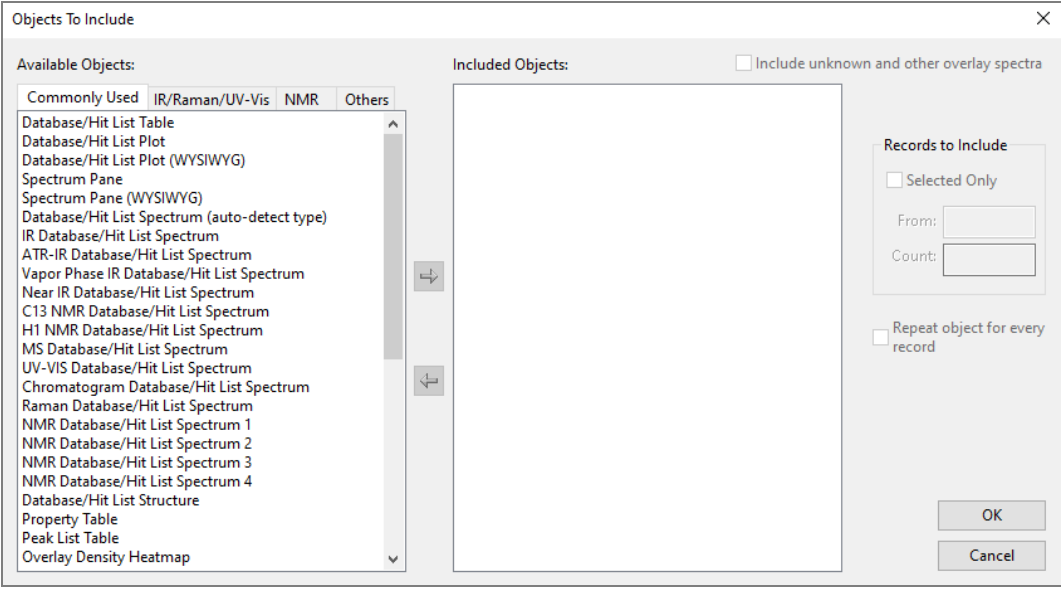
**Open a predefined template in the ReportIt and Minelt applications**

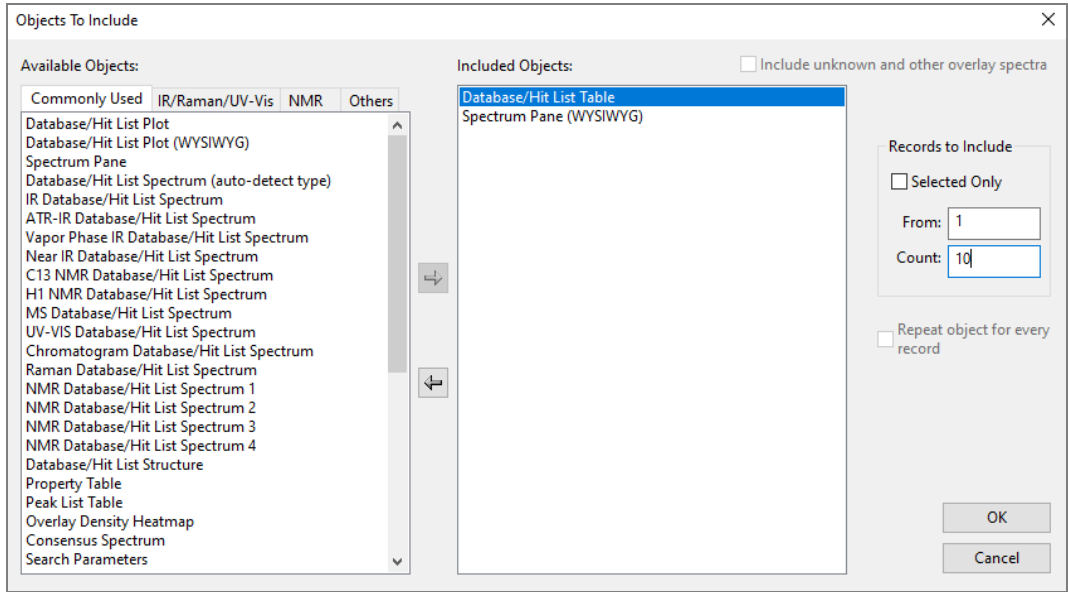
	Action	Result
1	Navigate to the <b>Basics</b> toolbox, open the <b>ReportIt</b> application by clicking its icon, then choose <b>File &gt; Open</b> .	 <p>An <b>Open</b> dialog box appears.</p>
2	<ul style="list-style-type: none"><li>Set the <b>Files of type</b> filter to ReportIt Template Document Files (*.rtt),</li><li>Navigate to <b>KnowItAll &gt; Report Templates &gt; Minelt</b></li><li>Open <b>Spectrum Landscape.rtt</b> in the folder we examined earlier.</li></ul>	<p>The template opens:</p> 

	Action	Result
3	<ul style="list-style-type: none"> <li>Navigate to the <b>Data</b> toolbox</li> <li>Open the <b>Minelt</b> application by clicking its icon</li> <li>Choose <b>File &gt; Edit Report Templates</b></li> <li>Select the <b>Landscape</b> template.</li> </ul>	<p>The <b>Report Templates</b> dialog box opens.</p> 
4	Click <b>Edit</b> .	<p>The <b>Objects to Add to Or Delete from Existing Template</b> dialog box opens.</p>  <p>Use this dialog box to see which objects are included with the template. You can also use this dialog to add or remove objects.</p>
5	Click <b>Cancel</b> ; then click <b>Close</b> on the <b>Report Templates</b> dialog box.	No changes were made to the template.



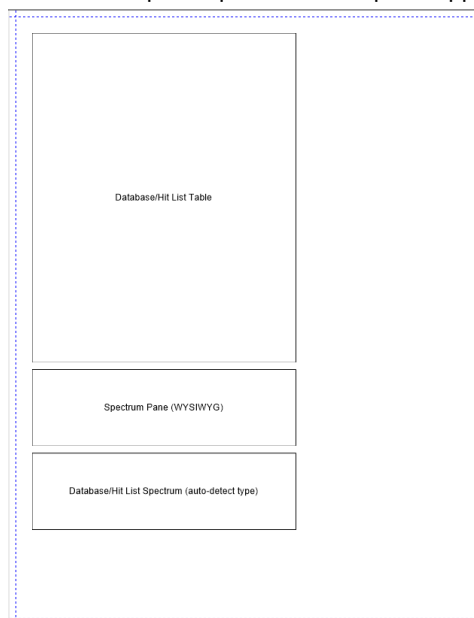
### Create a new MineIt template

	Action	Result
1	<p>The easiest method to create a new <b>MineIt</b> template is to start with an existing template.</p> <p>With the <b>MineIt</b> application open, choose <b>File &gt; Edit Report Templates</b>; then click <b>New</b> on the <b>Report Templates</b> dialog box.</p>	<p>The <b>Objects to Include</b> dialog box opens:</p> 
2	<p>Move <b>Spectrum Pane (WYSIWYG)</b> from the list of <b>Available Objects</b> to the list of <b>Included Objects</b> by selecting it in the list on the left and clicking the right arrow available between the two lists.</p>	
3	<p>Move <b>Database/Hit List Table</b> from the list of <b>Available Objects</b> to the list of <b>Included Objects</b>.</p>	

4	With <b>Database/Hit List Table</b> selected in the list of <b>Included Objects</b> , uncheck <b>Selected Only</b> , then type 1 in the <b>From</b> box and 10 in the <b>Count</b> box.	<p>The first ten hits will be included on the template.</p> 
5	Move <b>Database/Hit List Spectrum (auto-detect type)</b> from the list of <b>Available Objects</b> to the list of <b>Included Objects</b> , uncheck <b>Repeat object...</b> and <b>Selected Only</b> ; then type 1 in the <b>Count</b> box.	The structure will be included only for the first item in the hit list.
6	Move <b>Property Table</b> from the list of <b>Available Objects</b> to the list of <b>Included Objects</b> , uncheck <b>Repeat object...</b> and <b>Selected Only</b> ; then type 1 in the <b>Count</b> box.	The property table will be included only for the first item in the hit list.
7	Move <b>Current Date/Time</b> from the list of <b>Available Objects</b> to the list of <b>Included Objects</b> .	A date/time field is added to the template.

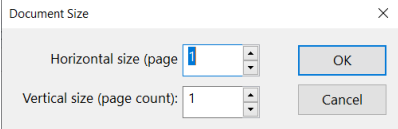
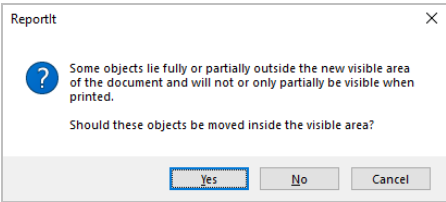
8 Click **OK**.


The new template opens in the ReportIt application.



We see object placeholders corresponding to the choices we made on the **Objects to Include** dialog box. You may have to scroll down the report template to see them all. We can now use **ReportIt** tools to arrange the placeholders and add other objects, such as images and text boxes.

**Edit the template in ReportIt**




	Action	Result
1	Choose <b>File &gt; Document Size</b> .	<p>The <b>Document Size</b> dialog box opens:</p> 
2	Change <b>Horizontal size</b> to 2 and <b>Vertical size</b> to 1; then click <b>OK</b> .	<p>A message box appears to tell you that some objects may no longer be completely visible.</p> 

3	<p>Click <b>Yes</b>.</p> <p>Move the database structure and property table to the second page, and re-size them as desired.</p>	
4	<ul style="list-style-type: none"><li>• Navigate to <b>KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; Creating Reports</b></li><li>• Open <b>Wiley.gif</b> using any image editor (example MS Paint)</li><li>• Select and copy the image.</li></ul>	

- 5 Return to the **ReportIt** application and choose **Edit > Paste**.

The image is added to the template:



	Action	Result
6	Using the <b>Text box</b> tool  , draw a text box, then type 'Operator:'.	
7	Choose the <b>Selection</b> tool, then hold down the shift key and select both the Date/Time field and the text box.	
8	Choose <b>Arrange &gt; Group</b> .	The two objects can now be moved, re-sized, etc., in exactly the same way.
9	Double click within the WYSIWYG Spectrum Page.	A spectrum toolbar opens. These tools can be used to adjust the spectral display in the template.
10	On the <b>Transfer to</b> bar, click <b>Minelt Database and Save</b> .	 A <b>Save As</b> dialog box opens.
11	Type in the new template's name (WILEY) and click <b>Save</b> .	The dialog box closes, revealing that the new template has been added to Minelt's <b>Report Templates</b> dialog box.
12	Select the new template and click <b>Set as Default</b> , then click <b>Close</b> .	Because we have set the new template as the default template, it will be used automatically whenever information is transferred from <b>Minelt</b> to <b>ReportIt</b> . Setting a default template is useful when you want to use a single template most of the time. However, you can also choose not to have a default template, and select from the list of available templates each time you transfer information to ReportIt.

# **KnowItAll Software Training**

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## Data Mining & Analysis



# Data Mining & Analysis

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## Overlap Density Heatmap Technology: A New Technology to Analyze Spectral, Chromatographic, and Other Graphical Data

### Purpose

This exercise demonstrates how to use Overlap Density Heatmap technology for data mining and visualization.

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### Objectives

This exercise will teach you:

- How to view and manipulate an Overlap Density Heatmap.
- 

### Background

Wiley's patented Overlap Density Heatmap technology is useful for visual data mining and analysis to assess the similarities and dissimilarities in large amounts of spectral, chromatographic, and other graphical data.

This technology allows the visualization of common features of overlapped objects, such as spectra or chromatograms, by color-coding the areas from highest to lowest overlap.


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

- Hexane.jdx

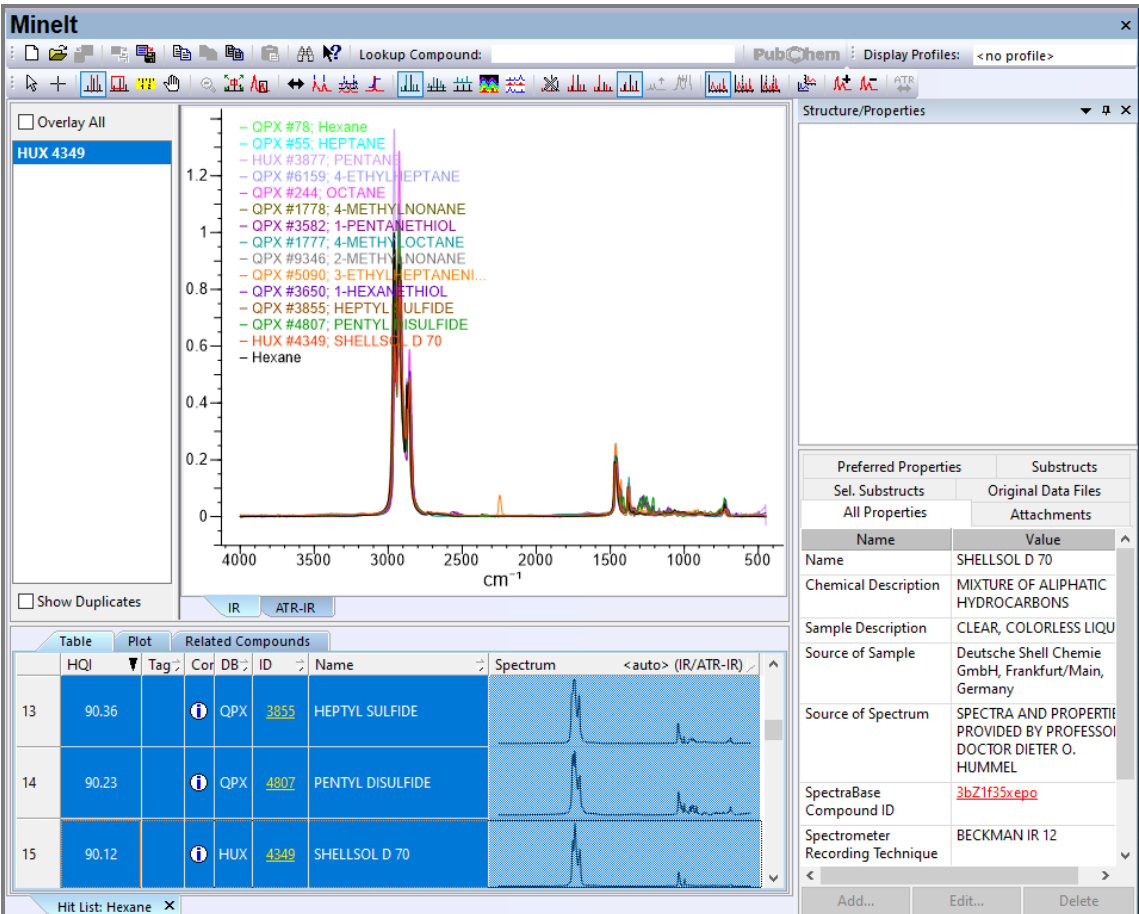
#### *KnowItAll Applications Used*

- Minelt™


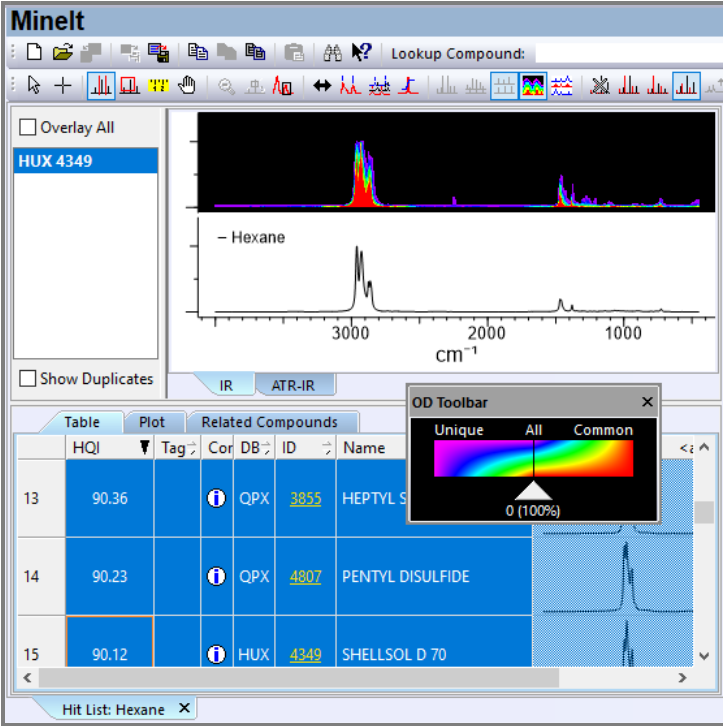
**Open a spectral hit list in the Minelt application**

	Action	Result
1	<p>In the <b>SearchIt</b> application, click <b>User-Select</b> under <b>Search Databases</b>.</p> <p>If databases are present in the <b>Selected for Searching</b> pane, click <b>Remove All</b>.</p> <p>Add the <b>IR – Sadtler Standards (Selected Subset) – Wiley</b> (DB Code SLX) to the <b>Selected for Searching</b> pane.</p>	
2	<p>Click <b>Spectrum</b> in the <b>Search Categories</b> pane</p> <p>Navigate to <b>KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; Data Mining</b></p> <p>Open <b>Hexane.jdx</b>.</p>	

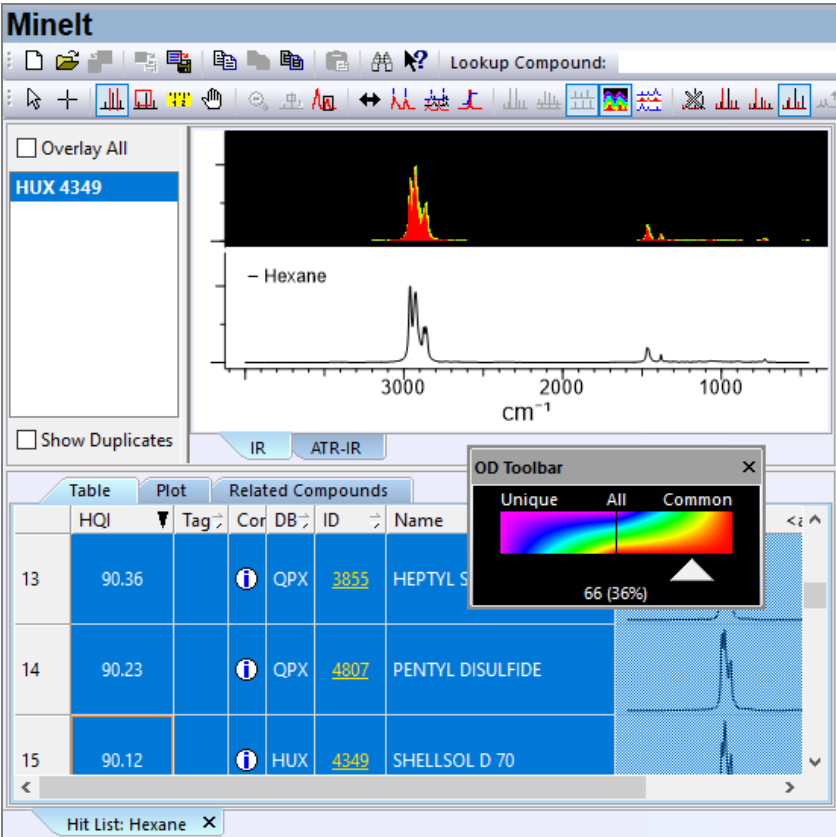
Action	Result
3 Click <b>Search</b> .	<p>The results are displayed in the Minelt application:</p>

	Action	Result																																													
4	<p>Select the first 15 entries in the hit list.</p> <p><b>Note:</b> Select the first record, hold down the shift key, then scroll to and select the 15<sup>th</sup> entry.</p>	<p>All the selected hits are displayed in the spectral pane.</p>  <p>The screenshot shows the Minelt software interface. The top panel displays an IR spectrum plot with the x-axis labeled "cm<sup>-1</sup>" ranging from 4000 to 500. The y-axis represents intensity from 0 to 1.2. Multiple spectral traces are overlaid, corresponding to the compounds listed in the hit list below. The hit list table at the bottom shows the first 15 entries, with columns for HQI, Tag, Cor, DB, ID, Name, and Spectrum. The selected entries are highlighted in blue.</p> <table><tr><th></th><th>HQI</th><th>Tag</th><th>Cor</th><th>DB</th><th>ID</th><th>Name</th><th>Spectrum</th></tr><tr><td>13</td><td>90.36</td><td></td><td>QPX</td><td>3855</td><td>HEPTYL SULFIDE</td><td>[Spectrum]</td></tr><tr><td>14</td><td>90.23</td><td></td><td>QPX</td><td>4807</td><td>PENTYL DISULFIDE</td><td>[Spectrum]</td></tr><tr><td>15</td><td>90.12</td><td></td><td>HUX</td><td>4349</td><td>SHELLSOL D 70</td><td>[Spectrum]</td></tr></table> <p>The right panel shows the "Structure/Properties" section with a table of properties for SHELLSOL D 70:</p> <table><tr><th>Name</th><th>Value</th></tr><tr><td>Name</td><td>SHELLSOL D 70</td></tr><tr><td>Chemical Description</td><td>MIXTURE OF ALIPHATIC HYDROCARBONS</td></tr><tr><td>Sample Description</td><td>CLEAR, COLORLESS LIQUID</td></tr><tr><td>Source of Sample</td><td>Deutsche Shell Chemie GmbH, Frankfurt/Main, Germany</td></tr><tr><td>Source of Spectrum</td><td>SPECTRA AND PROPERTIES PROVIDED BY PROFESSOR DOCTOR DIETER O. HUMMEL</td></tr><tr><td>SpectraBase Compound ID</td><td>3bZ1f35xepo</td></tr><tr><td>Spectrometer Recording Technique</td><td>BECKMAN IR 12</td></tr></table>		HQI	Tag	Cor	DB	ID	Name	Spectrum	13	90.36		QPX	3855	HEPTYL SULFIDE	[Spectrum]	14	90.23		QPX	4807	PENTYL DISULFIDE	[Spectrum]	15	90.12		HUX	4349	SHELLSOL D 70	[Spectrum]	Name	Value	Name	SHELLSOL D 70	Chemical Description	MIXTURE OF ALIPHATIC HYDROCARBONS	Sample Description	CLEAR, COLORLESS LIQUID	Source of Sample	Deutsche Shell Chemie GmbH, Frankfurt/Main, Germany	Source of Spectrum	SPECTRA AND PROPERTIES PROVIDED BY PROFESSOR DOCTOR DIETER O. HUMMEL	SpectraBase Compound ID	3bZ1f35xepo	Spectrometer Recording Technique	BECKMAN IR 12
	HQI	Tag	Cor	DB	ID	Name	Spectrum																																								
13	90.36		QPX	3855	HEPTYL SULFIDE	[Spectrum]																																									
14	90.23		QPX	4807	PENTYL DISULFIDE	[Spectrum]																																									
15	90.12		HUX	4349	SHELLSOL D 70	[Spectrum]																																									
Name	Value																																														
Name	SHELLSOL D 70																																														
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Sample Description	CLEAR, COLORLESS LIQUID																																														
Source of Sample	Deutsche Shell Chemie GmbH, Frankfurt/Main, Germany																																														
Source of Spectrum	SPECTRA AND PROPERTIES PROVIDED BY PROFESSOR DOCTOR DIETER O. HUMMEL																																														
SpectraBase Compound ID	3bZ1f35xepo																																														
Spectrometer Recording Technique	BECKMAN IR 12																																														

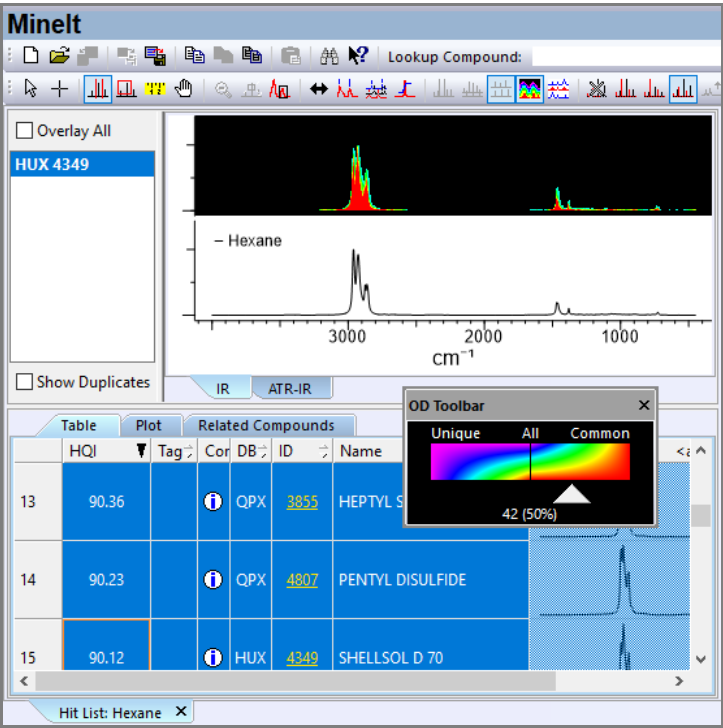
### Change the spectral display to Overlap Density Heatmap

	Action	Result
1	Click the <b>Overlap Density (OD) Heatmap</b> tool  in the <b>Spectral</b> toolbar.	<p>The spectral display changes, and the <b>Overlap Density (OD) Toolbar</b> is added to the display.</p>  <p>The default Overlap Density Heatmap display shows all overlap levels. High levels of overlap are displayed in red; low levels are displayed in violet. The <b>OD Toolbar</b> allows you to control the amount of overlap displayed using the slider. In the default Overlap Density Heatmap, the slider is set at OD level = 0, where all colors – representing all overlap density levels – are shown.</p>

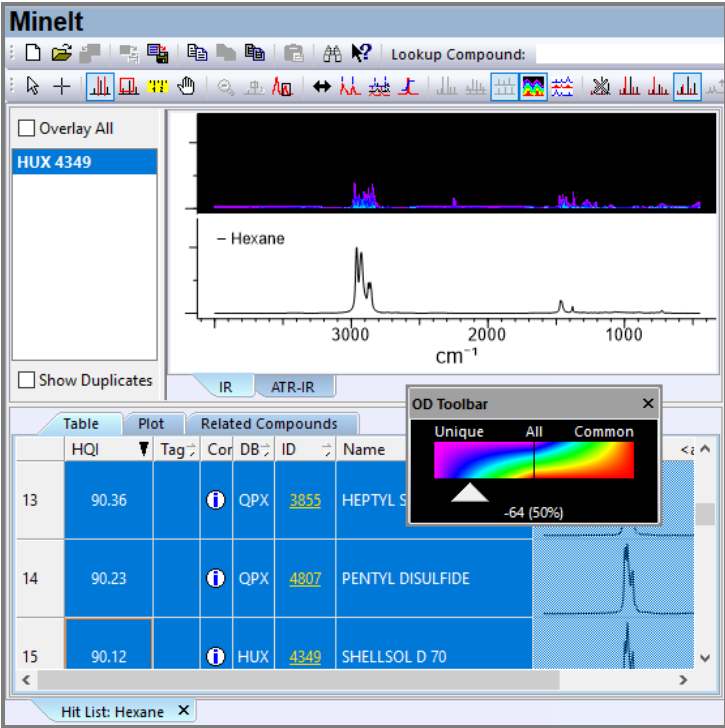


### Manipulate the Overlap Density Heatmap

	Action	Result															
1	Move the slider on the <b>OD Toolbar</b> to the right.	<p>As the slider moves to the right, the areas of common overlap are shown. Only the areas of most common overlap are shown as the OD Level approaches 100.</p>  <p>The screenshot shows the Minelt software interface. The main window displays a list of compounds with their HQI values and IR spectra. The OD Toolbar is a small window with a color gradient bar and a slider. The main window shows a list of compounds with their HQI values and IR spectra. The OD Toolbar is currently set to 66 (36%).</p> <table border="1"> <thead> <tr> <th>Table</th> <th>Plot</th> <th>Related Compounds</th> </tr> <tr> <th>HQI</th> <th>Tag</th> <th>Cor DB ID Name</th> </tr> </thead> <tbody> <tr> <td>13</td> <td>90.36</td> <td>QPX 3855 HEPTYL S</td> </tr> <tr> <td>14</td> <td>90.23</td> <td>QPX 4807 PENTYL DISULFIDE</td> </tr> <tr> <td>15</td> <td>90.12</td> <td>HUX 4349 SHELLSOL D 70</td> </tr> </tbody> </table> <p>Hit List: Hexane</p>	Table	Plot	Related Compounds	HQI	Tag	Cor DB ID Name	13	90.36	QPX 3855 HEPTYL S	14	90.23	QPX 4807 PENTYL DISULFIDE	15	90.12	HUX 4349 SHELLSOL D 70
Table	Plot	Related Compounds															
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14	90.23	QPX 4807 PENTYL DISULFIDE															
15	90.12	HUX 4349 SHELLSOL D 70															

	Action	Result																												
2	Move the slider to the left.	<p>As the OD Level approaches -100, only the areas of lowest overlap – the unique areas – are shown.</p> <p>The screenshot shows the Minelt software interface. At the top, there's a toolbar with various icons and a "Lookup Compound:" field. Below this, there's a section for "HUX 4349" with a checkbox for "Overlay All". To the right, an IR spectrum plot is displayed with a peak labeled "- Hexane" at approximately 2900 cm<sup>-1</sup>. Below the plot, there's a checkbox for "Show Duplicates" and tabs for "IR" and "ATR-IR". At the bottom, there's a "Table" tab with columns: HQI, Tag, Cor, DB, ID, Name. The table contains three rows of data:</p> <table><thead><tr><th></th><th>HQI</th><th>Tag</th><th>Cor</th><th>DB</th><th>ID</th><th>Name</th></tr></thead><tbody><tr><td>13</td><td>90.36</td><td></td><td>i</td><td>QPX</td><td>3855</td><td>HEPTYL S</td></tr><tr><td>14</td><td>90.23</td><td></td><td>i</td><td>QPX</td><td>4807</td><td>PENTYL DISULFIDE</td></tr><tr><td>15</td><td>90.12</td><td></td><td>i</td><td>HUX</td><td>4349</td><td>SHELLSOL D 70</td></tr></tbody></table> <p>An "OD Toolbar" is overlaid on the table, showing a heatmap with "Unique", "All", and "Common" regions. A slider is positioned at -83 (40%). Below the table, there's a "Hit List: Hexane" button.</p> <p>As you move the slider to change the OD Level, a second value is shown in parentheses. This value is the percent area under the curve, or %AUC, relative to the value at OD Level = 0. In this case, %AUC = 40%. We can use the OD Level and %AUC to quantify the OD Heatmap.</p>		HQI	Tag	Cor	DB	ID	Name	13	90.36		i	QPX	3855	HEPTYL S	14	90.23		i	QPX	4807	PENTYL DISULFIDE	15	90.12		i	HUX	4349	SHELLSOL D 70
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	Action	Result
3	Move the slider to the point where %AUC equals approximately 50%.	<p>The OD Level on the common side – or ODC – required to show 50% of the area that is most in common, is 42.</p>  <p>Another way to express this is to say that <math>ODC_{50} = 42</math>. An alternative is to say that <math>\%AUC_{42} = 50</math>.</p>



	Action	Result
4	Next, move the slider to the left to where %AUC equals approximately 50%.	<p>The OD Level on the unique side – or ODU – required to show 50% of the area that is most unique is -57.</p>  <p>Another way to express this is to say that <math>ODU_{50} = -64</math>. An alternative is to say that <math>\%AUC_{-64} = 50</math>.</p>
	<b>TIP</b>	<p>Use the <b>Horizontal Zoom</b> tool  to examine different regions. To do this, select the Horizontal Zoom tool, and then click and drag over an area on the spectrum to zoom in. Use the <b>View Entire Spectrum</b> tool  to zoom out.</p>

# Data Mining & Analysis

## How to Create and use Overlap Density Consensus Spectra

### Purpose

This exercise demonstrates how to create and use Overlap Density Consensus Spectra in the KnowItAll Informatics System.

### Objectives

This exercise will teach you:

- How to view and manipulate an Overlap Density Consensus spectrum;
- How to use an Overlap Density Consensus spectrum in a search.

### Background

Wiley's patented Overlap Density Heatmap technology is useful for visual data mining and analysis to assess the similarities and dissimilarities in large amounts of spectral, chromatographic, and other graphical data.

By tracing the outline of the highest level of overlap at a given OD Level, it is possible to mathematically construct a composite spectrum by using the maximum spectral y-values at each spectral x-value in the OD Heatmap. This Overlap Density Consensus Spectrum can be used in a spectral search to find similar spectra, or can be stored in a database for future use.


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

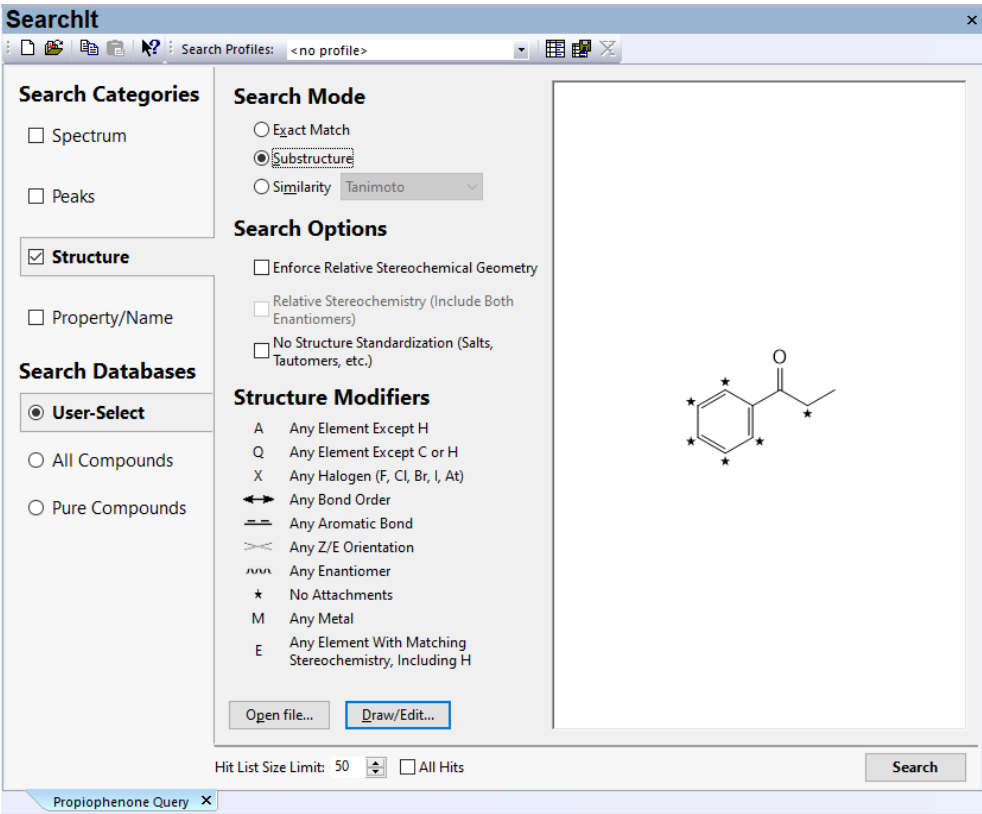
- Propiophenone Query.dsf

#### *KnowItAll Applications Used*

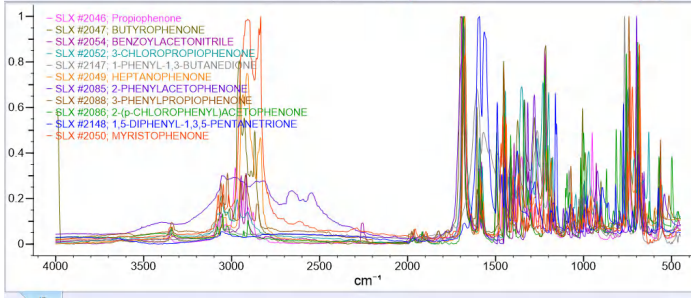



















- SearchIt™
- Minelt™


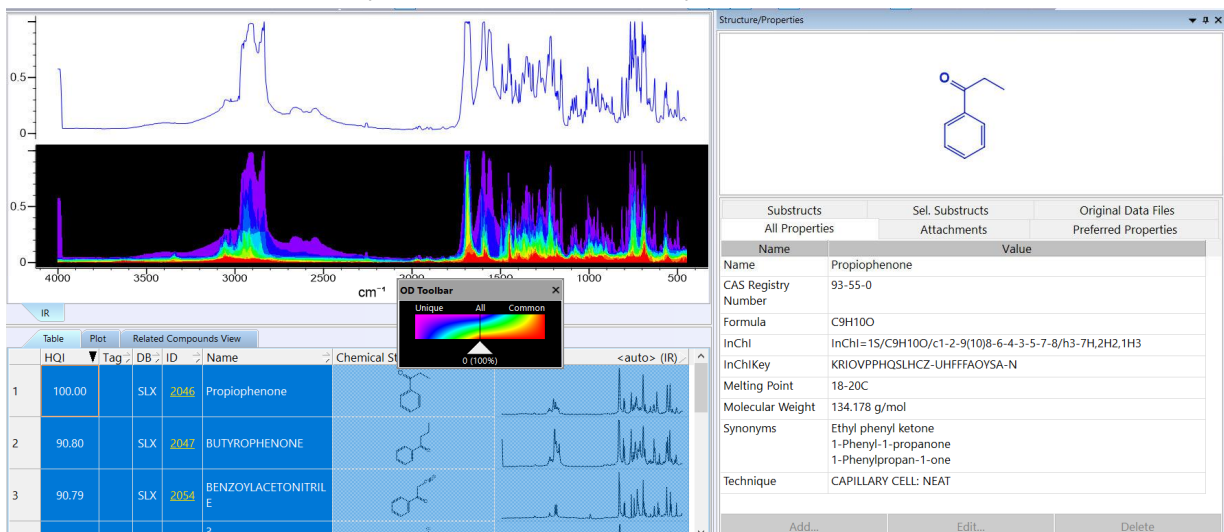
**Perform a substructure search**

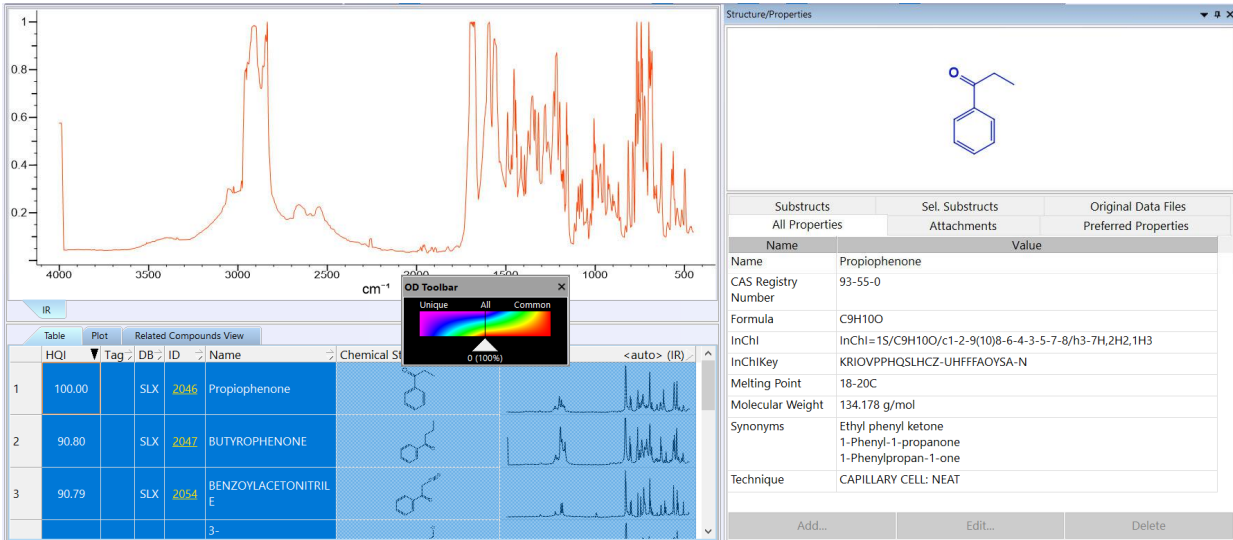
	Action	Result
1	<ul style="list-style-type: none"><li>In the <b>SearchIt</b> application, click <b>User-select</b> under <b>Search Databases</b>.</li><li>Under <b>Available for Searching</b>, select <b>IR – Sadtler Standards (Selected Subset) – Wiley</b> (DB Code SLX)</li><li>Click <b>Add</b></li></ul>	
2	<ul style="list-style-type: none"><li>Click <b>Structure</b> button</li><li>Click <b>Open Spectrum or Structure</b> icon</li></ul>	

	Action	Result
3	<p>Navigate to <b>KnowItAll &gt; Training Files &gt; General Training &gt; Files &gt; Data Mining</b></p> <p>Open <b>Propiophenone Query.dsf</b>.</p>	<p>The structure is displayed in the <b>Structure</b> tab.</p> 
4	<p>Make sure <b>Search Mode</b> is set to <b>Substructure</b>.</p> <p>Click <b>Search</b>.</p>	<p>Results are displayed in the <b>Minelt</b> application.</p>

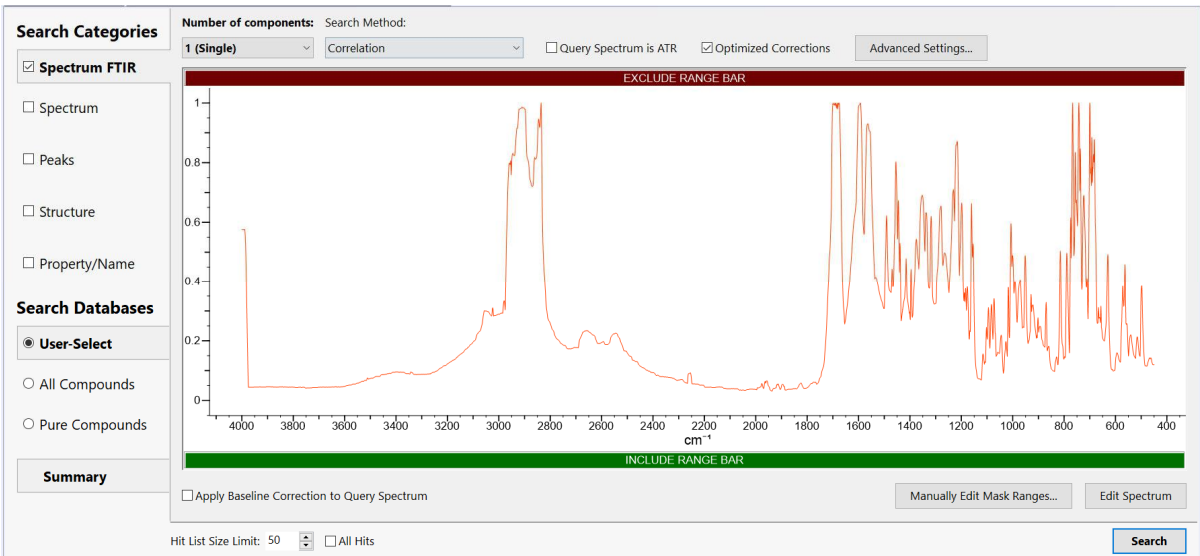
## Examine the results in Minelt

	Action	Result																																																																																					
1	<p>Select all eleven records in the hit list.</p> <p><b>Note:</b> Select the first record, hold down the shift key, then scroll to and select the last record.</p>	<p>All spectra are displayed in the spectral pane:</p> <div></div> <div><p>IR</p><table><thead><tr><th>Table</th><th>Plot</th><th colspan="4">Related Compounds View</th></tr><tr><th>HQI</th><th>Tag</th><th>DB</th><th>ID</th><th>Name</th><th>Chemical Structure</th><th>Spectrum</th></tr></thead><tbody><tr><td>1</td><td>100.00</td><td>SLX</td><td>2046</td><td>Propiophenone</td><td></td><td></td></tr><tr><td>2</td><td>90.80</td><td>SLX</td><td>2047</td><td>BUTYRPHENONE</td><td></td><td></td></tr><tr><td>3</td><td>90.79</td><td>SLX</td><td>2054</td><td>BENZOYLACETONITRILE</td><td></td><td></td></tr></tbody></table></div> <div><p>Structure/Properties</p><div></div><table><thead><tr><th colspan="2">Substructs</th><th>Sel. Substructs</th><th>Original Data Files</th></tr><tr><th colspan="2">All Properties</th><th>Attachments</th><th>Preferred Properties</th></tr><tr><th>Name</th><th colspan="3">Value</th></tr></thead><tbody><tr><td>Name</td><td colspan="3">Propiophenone</td></tr><tr><td>CAS Registry Number</td><td colspan="3">93-55-0</td></tr><tr><td>Formula</td><td colspan="3">C9H10O</td></tr><tr><td>InChI</td><td colspan="3">InChI=1S/C9H10O/c1-2-9(10)8-6-4-3-5-7-8/h3-7H,2H2,1H3</td></tr><tr><td>InChIKey</td><td colspan="3">KRIOVPPHQSLLHCZ-UHFFFAOYSA-N</td></tr><tr><td>Melting Point</td><td colspan="3">18-20C</td></tr><tr><td>Molecular Weight</td><td colspan="3">134.178 g/mol</td></tr><tr><td>Synonyms</td><td colspan="3">Ethyl phenyl ketone 1-Phenyl-1-propanone 1-Phenylpropan-1-one</td></tr><tr><td>Technique</td><td colspan="3">CAPILLARY CELL: NEAT</td></tr></tbody></table></div> <tr><td>2</td><td>Click the <b>OD Heatmap</b> toolbar button...</td><td></td></tr>	Table	Plot	Related Compounds View				HQI	Tag	DB	ID	Name	Chemical Structure	Spectrum	1	100.00	SLX	2046	Propiophenone			2	90.80	SLX	2047	BUTYRPHENONE			3	90.79	SLX	2054	BENZOYLACETONITRILE			Substructs		Sel. Substructs	Original Data Files	All Properties		Attachments	Preferred Properties	Name	Value			Name	Propiophenone			CAS Registry Number	93-55-0			Formula	C9H10O			InChI	InChI=1S/C9H10O/c1-2-9(10)8-6-4-3-5-7-8/h3-7H,2H2,1H3			InChIKey	KRIOVPPHQSLLHCZ-UHFFFAOYSA-N			Melting Point	18-20C			Molecular Weight	134.178 g/mol			Synonyms	Ethyl phenyl ketone 1-Phenyl-1-propanone 1-Phenylpropan-1-one			Technique	CAPILLARY CELL: NEAT			2	Click the <b>OD Heatmap</b> toolbar button...	
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	Action	Result
3	<p>...then click the <b>OD Consensus</b></p> <p><b>Spectrum</b> toolbar button .</p>	<p>The consensus spectrum is displayed above the Overlap Density Heatmap:</p> 

	Action	Result																																																
4	Click the <b>OD Heatmap</b> toolbar button again to turn off this display.	<div>The consensus spectrum remains in the display.</div> <div><p>The screenshot displays the software interface with the following components:</p><ul style="list-style-type: none"><li><b>IR Spectrum Plot:</b> A plot showing transmittance (0 to 1) versus wavenumber (4000 to 500 cm<sup>-1</sup>). A red line represents the consensus spectrum.</li><li><b>Table:</b> A table with columns: HQI, Tag, DB, ID, Name, Chemical Structure, and Spectrum. It lists three compounds:</li></ul><table><thead><tr><th>HQI</th><th>Tag</th><th>DB</th><th>ID</th><th>Name</th><th>Chemical Structure</th><th>Spectrum</th></tr></thead><tbody><tr><td>1</td><td>100.00</td><td>SLX</td><td>2046</td><td>Propiophenone</td><td><chem>CCC(=O)c1ccccc1</chem></td><td>[Spectrum]</td></tr><tr><td>2</td><td>90.80</td><td>SLX</td><td>2047</td><td>BUTYROPHENONE</td><td><chem>CCCC(=O)c1ccccc1</chem></td><td>[Spectrum]</td></tr><tr><td>3</td><td>90.79</td><td>SLX</td><td>2054</td><td>BENZOYLACETONITRILE</td><td><chem>CCC#Nc1ccccc1</chem></td><td>[Spectrum]</td></tr></tbody></table><ul style="list-style-type: none"><li><b>Chemical Structure Window:</b> Displays the structure of Propiophenone (<chem>CCC(=O)c1ccccc1</chem>).</li><li><b>Properties Panel:</b> A table with columns: Substructures, Sel. Substructures, and Original Data Files. It lists various properties for Propiophenone:</li></ul><table><thead><tr><th>Name</th><th>Value</th></tr></thead><tbody><tr><td>Name</td><td>Propiophenone</td></tr><tr><td>CAS Registry Number</td><td>93-55-0</td></tr><tr><td>Formula</td><td>C<sub>9</sub>H<sub>10</sub>O</td></tr><tr><td>InChI</td><td>InChI=1S/C<sub>9</sub>H<sub>10</sub>O/c1-2-9(10)8-6-4-3-5-7-8/h3-7H,2H2,1H3</td></tr><tr><td>InChIKey</td><td>KRIQVPPHQLHCZ-UHFFFAOYSA-N</td></tr><tr><td>Melting Point</td><td>18-20C</td></tr><tr><td>Molecular Weight</td><td>134.178 g/mol</td></tr><tr><td>Synonyms</td><td>Ethyl phenyl ketone 1-Phenyl-1-propanone 1-Phenylpropan-1-one</td></tr><tr><td>Technique</td><td>CAPILLARY CELL: NEAT</td></tr></tbody></table></div>	HQI	Tag	DB	ID	Name	Chemical Structure	Spectrum	1	100.00	SLX	2046	Propiophenone	<chem>CCC(=O)c1ccccc1</chem>	[Spectrum]	2	90.80	SLX	2047	BUTYROPHENONE	<chem>CCCC(=O)c1ccccc1</chem>	[Spectrum]	3	90.79	SLX	2054	BENZOYLACETONITRILE	<chem>CCC#Nc1ccccc1</chem>	[Spectrum]	Name	Value	Name	Propiophenone	CAS Registry Number	93-55-0	Formula	C <sub>9</sub> H <sub>10</sub> O	InChI	InChI=1S/C <sub>9</sub> H <sub>10</sub> O/c1-2-9(10)8-6-4-3-5-7-8/h3-7H,2H2,1H3	InChIKey	KRIQVPPHQLHCZ-UHFFFAOYSA-N	Melting Point	18-20C	Molecular Weight	134.178 g/mol	Synonyms	Ethyl phenyl ketone 1-Phenyl-1-propanone 1-Phenylpropan-1-one	Technique	CAPILLARY CELL: NEAT
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## Use the consensus spectrum to perform a search

	Action	Result
1	Click <b>SearchIt</b> in the <b>Transfer to</b> bar.	<p>The consensus spectrum is displayed on the <b>IR Spectrum</b> search tab.</p> 
2	Click the <b>Search</b> button. <b>Note:</b> The IR – Sadtler Standards (Selected Subset) – Wiley database remains in the spectrum pane.	<p>The results are displayed in the <b>Minelt</b> application on a new tab:</p> <p>As you can see from this example, the Overlap Density Consensus Spectrum created from a hit list of spectra containing the propiophenone substructure produces a spectrum that is very similar to propiophenone itself. The use of Overlap Density Consensus Spectra, therefore, has clear applicability in structure elucidation and unknown identification.</p>



# **KnowItAll Informatics Training**

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## Quality Control Analysis with QC Expert

# QC Expert

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## Perform a Quality Control Comparison of a Sample Spectrum Against a Reference Spectrum

### Objectives

This exercise will teach you:

- How to set up an account
- How to select a standard
- How to compare to a selected standard
- How to generate a report

---

### Background

Wiley's KnowItAll QC Expert software performs a rapid quality check of a sample IR or Raman spectrum against a "gold standard" user spectrum to verify that a material meets control specifications.

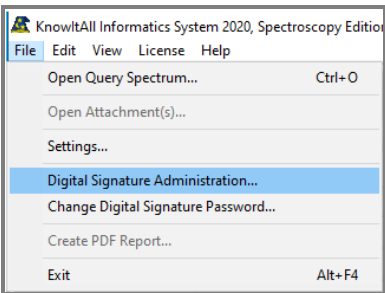
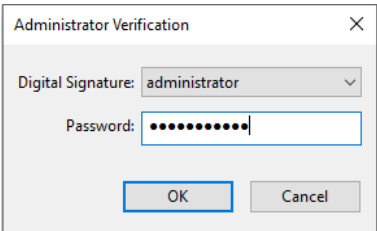
#### *Training Files Used in This Lesson*

- DEET.SPA
- Epichlorohydrin Sample Spectrum.irf

#### *KnowItAll Applications Used*

- QC Expert

**Set Up Administrator Account and Address**

	Action	Result
1	Navigate to the <b>Data</b> toolbox and open the <b>QC Expert</b> application.	
2	To create an administrative account, go to <b>File &gt; Digital Signature Administration...</b>	
3	<ul style="list-style-type: none"> <li>Enter your preferred user ID in the <b>Digital Signature</b> field</li> <li>Enter preferred password in the <b>Password</b> and <b>Confirm Password</b> fields</li> <li>Click <b>OK</b></li> </ul>	
4	In the <b>Administrator Verification</b> pop-up that appears, enter your user name and password.	

- 5 In **File > Settings**, set the Organization to **“Wiley Laboratories, Inc.”** and add address.

The screenshot shows the 'Settings' dialog box with the 'Reference/Validation Databases' tab selected. The 'Organization' field is filled with 'Wiley Laboratories, Inc.'. The 'Address' field is empty. The 'Folder for Reports' field shows 'C:\Users\Public\Documents\W' with a 'Browse...' button next to it. The 'Language for Reports' dropdown is set to 'Same as QC Expert'. At the bottom are 'OK', 'Cancel', and 'Apply' buttons.

Settings

General Reference/Validation Databases

Organization: Wiley Laboratories, Inc.

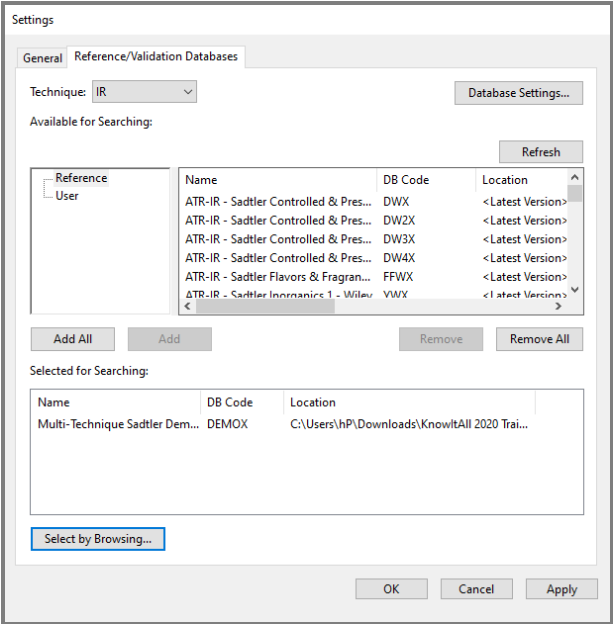
Address:

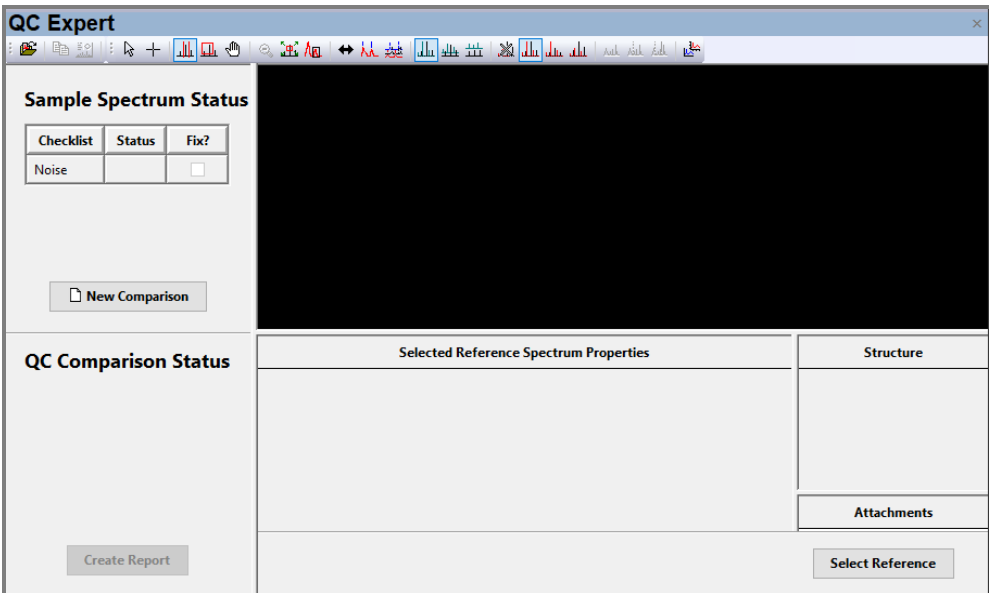
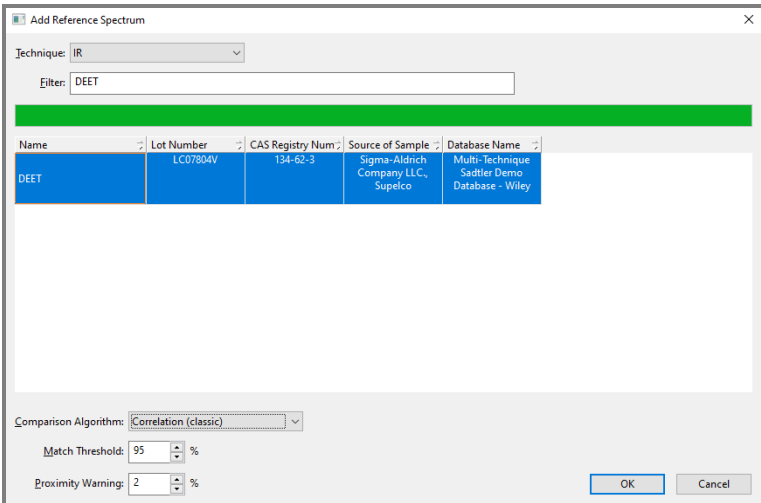
Folder for Reports: C:\Users\Public\Documents\W Browse...

Language for Reports: Same as QC Expert

OK Cancel Apply

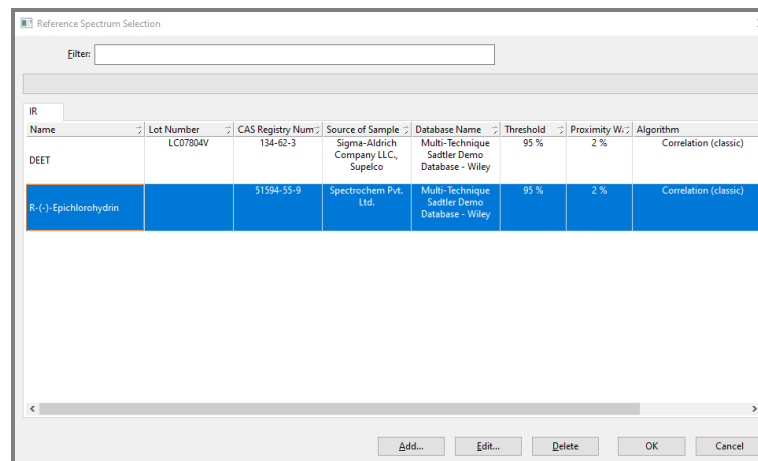
**Select Reference Database**

	Action	Result
1	<ul style="list-style-type: none"> <li>In the <b>Reference/Validation Databases</b> tab, click the <b>Select by Browsing</b> button</li> <li>Navigate to <b>KnowItAll &gt; Training Files &gt; General Training &gt; Databases &gt; Samples</b> folder</li> <li>Select the <b>Multi-Technique Sadtler Demo Database - Wiley [DEMO]</b> database.</li> </ul>	
2	Click <b>OK</b> .	

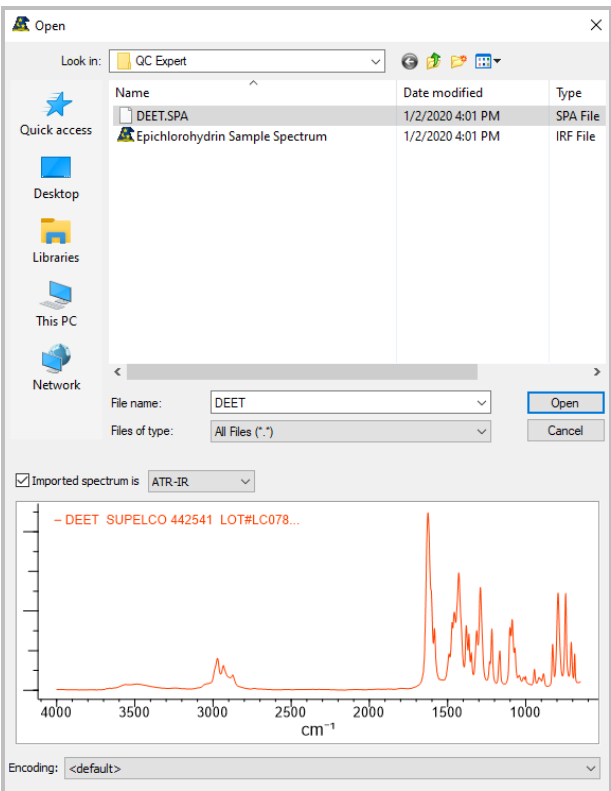
<p>3</p> <p>Click on the <b>Select Reference</b> button at the lower right of the <b>QC Expert</b> window.</p>	
<p>4</p> <ul style="list-style-type: none"> <li>At the prompt, login as administrator. The <b>Add Reference Spectrum</b> dialog box opens.</li> <li>Type <b>deet</b> in the <b>Filter</b> box to search for DEET.</li> <li>Point out the <b>Comparison Algorithm</b>, <b>Match Threshold</b>, and <b>Proximity Warning</b> parameters in the lower left.</li> <li>Select the <b>Correlation (Classic)</b> algorithm for the demo.</li> <li>Click <b>OK</b> to add the spectrum.</li> </ul>	

5

- The **Reference Spectrum Selection** dialog box opens.
- Click on **Add**, and type **epi** in the **Filter** box.
- Select **R-(-)-Epichlorohydrin** and select the **Correlation (classic)** algorithm.
- Click **OK**.



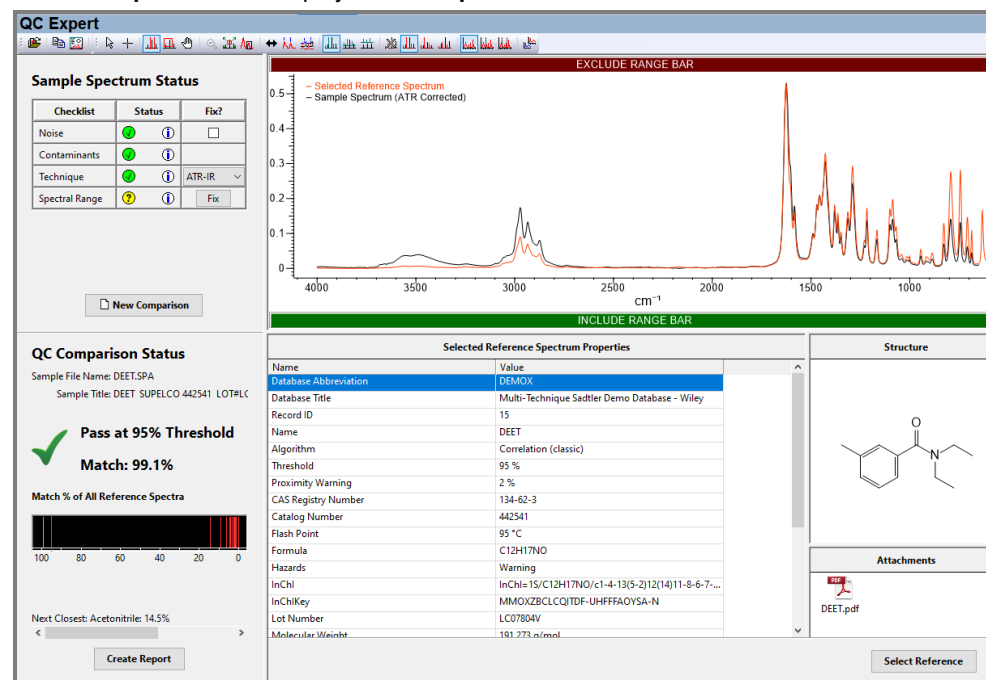
**Run QC Expert as a Non-administrator QC Analyst**

	Action	Result
1	<ul style="list-style-type: none"> <li>Navigate to the <b>Data</b> toolbox and open the <b>QC Expert</b> application.</li> <li>Click on the <b>Select Reference</b> button. Select the <b>DEET</b> spectrum</li> <li>Click <b>OK</b>.</li> </ul>	
2	<ul style="list-style-type: none"> <li>Click on <b>New Comparison</b> at the mid-left of the QC Expert window.</li> <li>Navigate to KnowItAll &gt; Samples &gt; QC Expert folder and select <b>DEET.SPA</b>.</li> <li>Set <b>Imported spectrum is</b> to <b>ATR-IR</b> and ensure this option is checked.</li> <li>Click <b>Open</b>.</li> </ul>	



3

The QC Expert window displays the **Comparison Status**.

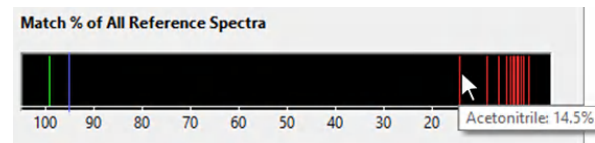


We get an excellent match of 99.1% and a green check mark indicating that the quality control comparison passes.

4

Mouse over the green and red bars in the **Match % of All Reference Spectra** chart.


**Note:** When you mouse over the various bars in the Match% Chart, you see the corresponding display in the **Spectrum Pane** at the top.

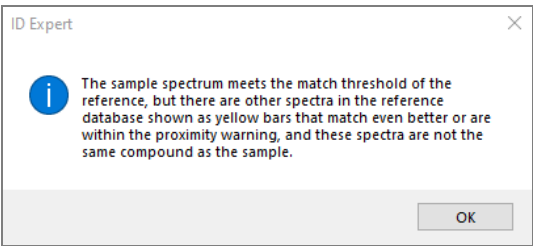
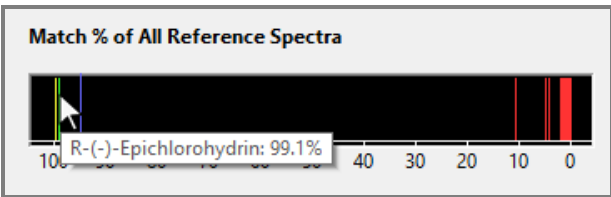
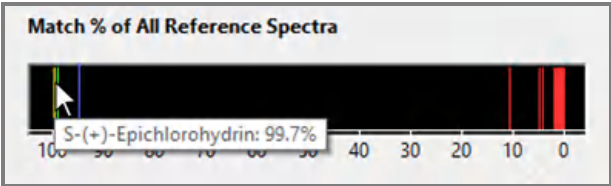


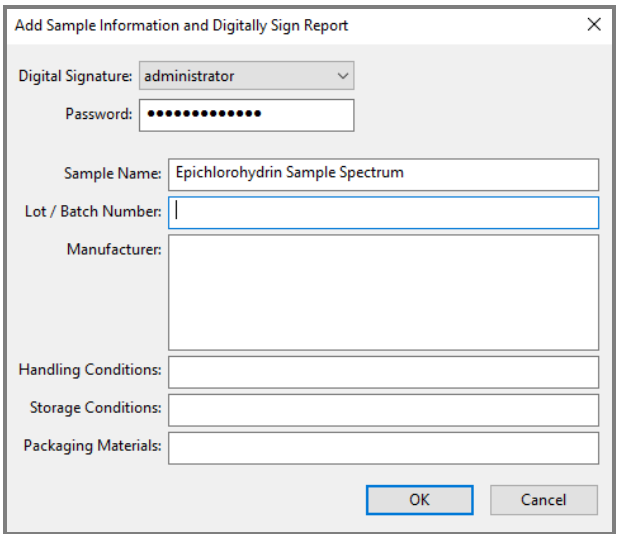
The **Match % of All Reference Spectra** chart shows the comparison of the sample spectrum to spectra from the entire reference database. The **green bars** are for the comparison of the sample spectrum against the selected reference spectrum as well as all other reference spectra for different lots of the same compound. The **blue line** is the quality control threshold, and the **red lines** are the match % values for the comparison of the sample spectrum against all the other spectra in the database.

5	Double-click on the PDF attachment in the <b>Attachment</b> pane at the lower right.	<p>The DEET safety datasheet and other associated information is displayed.</p> <div><p><b>SIGMA-ALDRICH</b> <small>sigma-aldrich.com</small></p><p><b>SAFETY DATA SHEET</b></p><p>Version 4.4 Revision Date 07/03/2014 Print Date 08/25/2015</p><p><b>1. PRODUCT AND COMPANY IDENTIFICATION</b></p><p><b>1.1 Product identifiers</b></p><p>Product name : <i>N,N</i>-Diethyl-3-methylbenzamide</p><p>Product Number : D100951 Brand : Aldrich Index-No. : 616-018-00-2</p><p>CAS-No. : 134-62-3</p><p><b>1.2 Relevant identified uses of the substance or mixture and uses advised against</b></p><p>Identified uses : Laboratory chemicals, Manufacture of substances</p><p><b>1.3 Details of the supplier of the safety data sheet</b></p><p>Company : Sigma-Aldrich 3050 Spruce Street SAINT LOUIS MO 63103 USA</p><p>Telephone : +1 800-325-5832 Fax : +1 800-325-5052</p><p><b>1.4 Emergency telephone number</b></p><p>Emergency Phone # : (314) 776-6555</p></div>
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**Demo Protocol - QC Analyst Comparison of R-(-)-Epichlorohydrin Sample Spectrum to Reference**

	Action	Result
1	<ul style="list-style-type: none"> <li>Navigate to the <b>Data</b> toolbox and open the <b>QC Expert</b> application.</li> <li>Click on the <b>Select Reference</b> button.</li> <li>Select the <b>R-(-)-Epichlorohydrin</b> reference spectrum.</li> <li>Click <b>OK</b>.</li> </ul>	This is to open a spectrum of a sample of <b>R-(-)-Epichlorohydrin</b> and perform a quality control comparison to make sure that the sample actually is what it is supposed to be.
2	<ul style="list-style-type: none"> <li>Click on <b>New Comparison</b> at the mid-left of the QC Expert window.</li> <li>Navigate to <b>KnowItAll &gt; Samples &gt; QC Expert</b> folder.</li> <li>Select <b>Epichlorohydrin Sample Spectrum.irf</b>.</li> <li>Set <b>Imported spectrum is</b> to <b>ATR-IR</b> and ensure this option is checked.</li> <li>Click <b>Open</b>.</li> </ul>	<p><b>QC Comparison Status</b></p> <p>Sample File Name: Epichlorohydrin Sample Spectrum.irf Sample Title: Epichlorohydrin Sample Spectrum</p> <p><b>? Uncertain at 95% Threshold with 2% Proximity Warning ⓘ</b> <b>Match: 99.1%</b></p> <p>Match % of All Reference Spectra</p>  <p>Next Closest: S-(+)-Epichlorohydrin: 99.7%</p> <p>The Match% between the selected reference spectrum and sample spectrum is excellent at 99.1%, but the QC comparison is <b>Uncertain</b>.</p>

3	Click on the information button ⓘ.	 <p>An <b>ID Expert</b> pop-up says that the sample spectrum meets the match threshold, but there are other spectra that match even better or are within the proximity warning.</p>
4	Click <b>OK</b> to close the dialog box.	
5	On the Match% chart, mouse over the bars near 100% and look at the corresponding spectra in the spectrum pane above.	There are two lines above the blue threshold line indicating two hits, one in green and one in yellow.
6	Mouse over the green bar in the Match % Chart. The hover-over text says <b>R-(-)-Epichlorohydrin: 99.1%</b> .	 <p>The green bar in the Match % chart indicates the comparison of the sample spectrum to the reference spectrum. The match percent is 99.1%</p>
7	Mouse over the yellow bar in the Match % Chart. The hover-over text says <b>S-(+)- Epichlorohydrin: 99.7%</b> .	 <p>The yellow bar is for <b>S-(+)- Epichlorohydrin</b>, which is the enantiomer of the R-(-) isomer. The R and S forms of Epichlorohydrin are stereoisomers that are indistinguishable by IR.</p>

8	<p>Click on <b>Create Report</b> button below the Match% chart to create a digitally signed report.</p> <ul style="list-style-type: none"><li>• Select your user name from the <b>Digital Signatures</b> drop-down.</li><li>• Enter the password</li><li>• Fill out the sample information..</li></ul>	
9	<p>Click <b>OK</b> to view the report.</p>	<p>The digitally signed PDF contains the following information:</p> <p>Page 1 – Information about the test</p> <p>Page 2 – Information about the spectral comparison</p> <p>Page 3 – Information about the reference spectrum</p>



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