

KnowItAll Informatics Training

Quality Control Analysis with QC Expert

QC Expert

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

Purpose

These exercises demonstrate how to perform quality control comparisons using KnowItAll QC Expert software.

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, Raman, or GC spectrum against a "gold standard" user spectrum to verify that a material meets control specifications.

Training Files Used in This Lesson

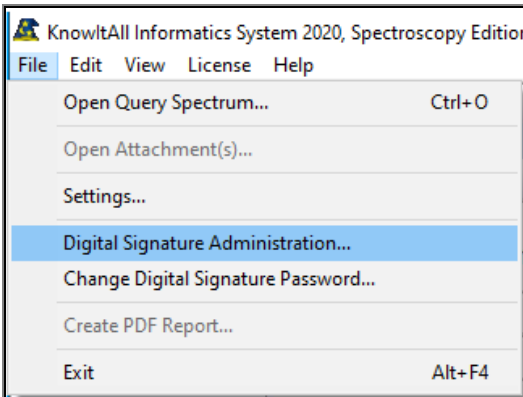
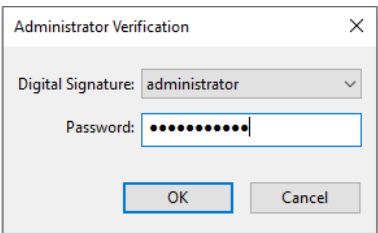
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\QC Expert

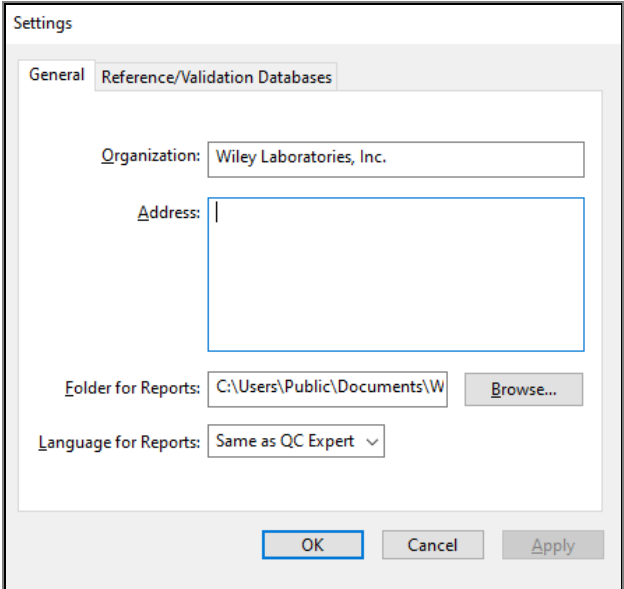
- DEET.SPA
- Epichlorohydrin Sample Spectrum.irf

KnowItAll Applications Used

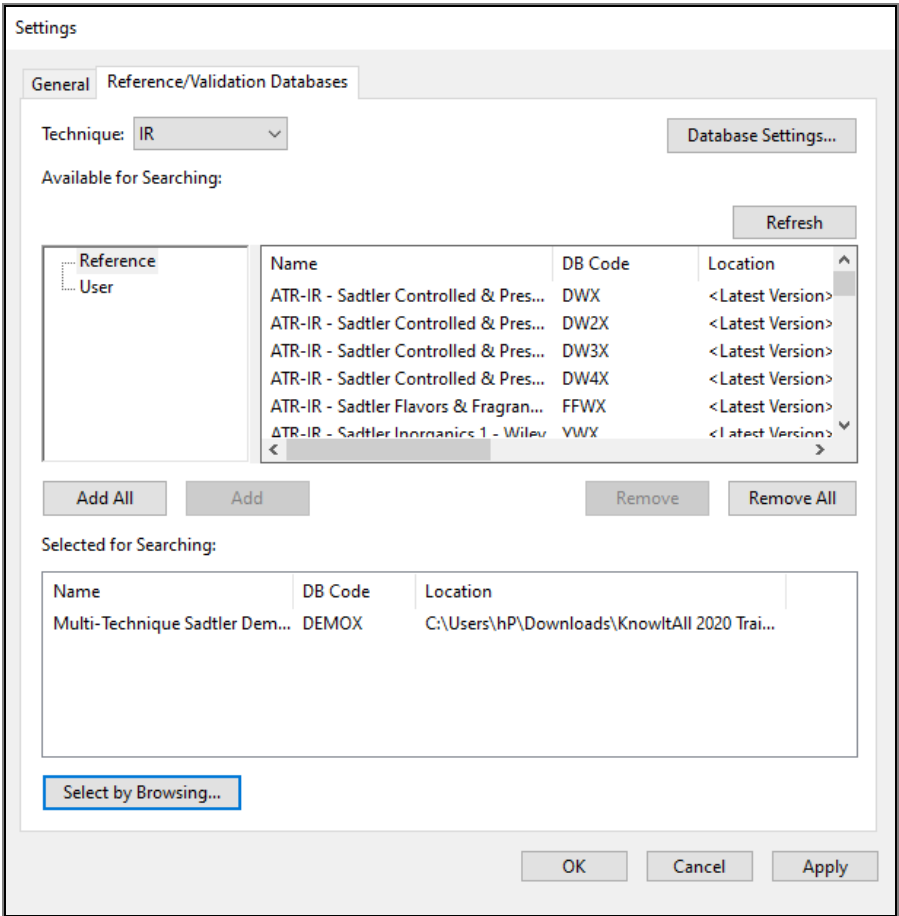
- QC Expert

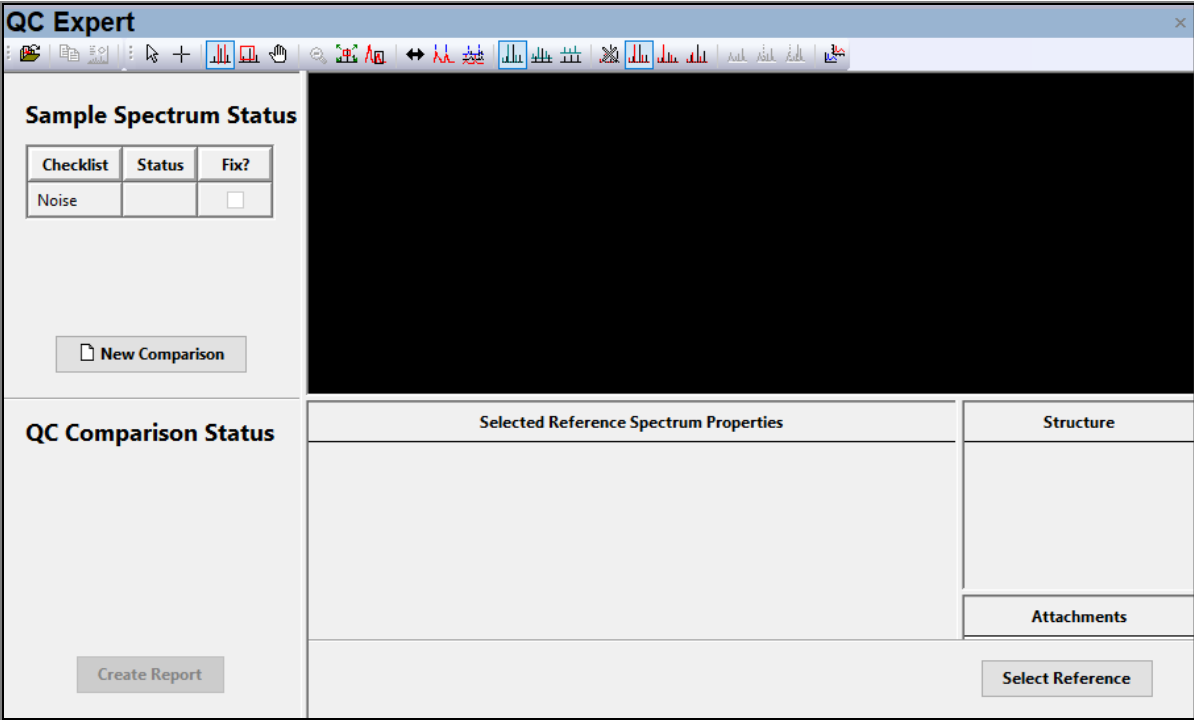
Set Up Administrator Account and Address

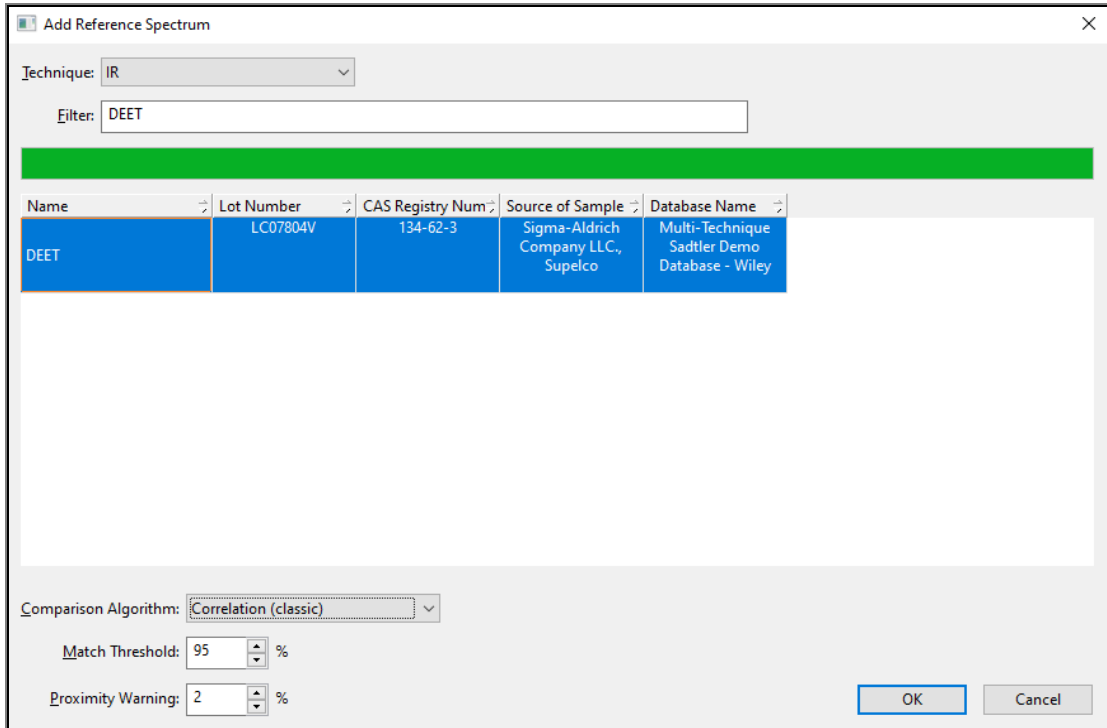
	Action	Result
1	Navigate to the Data toolbox and open the QC Expert application.	
2	To create an administrative account, go to File > Digital Signature Administration .	
3	<p>Enter your preferred user ID in the Digital Signature field.</p> <p>Enter preferred password in the Password and Confirm Password fields.</p> <p>Click OK.</p>	
4	In the Administrator Verification pop-up that appears, enter your username and password.	

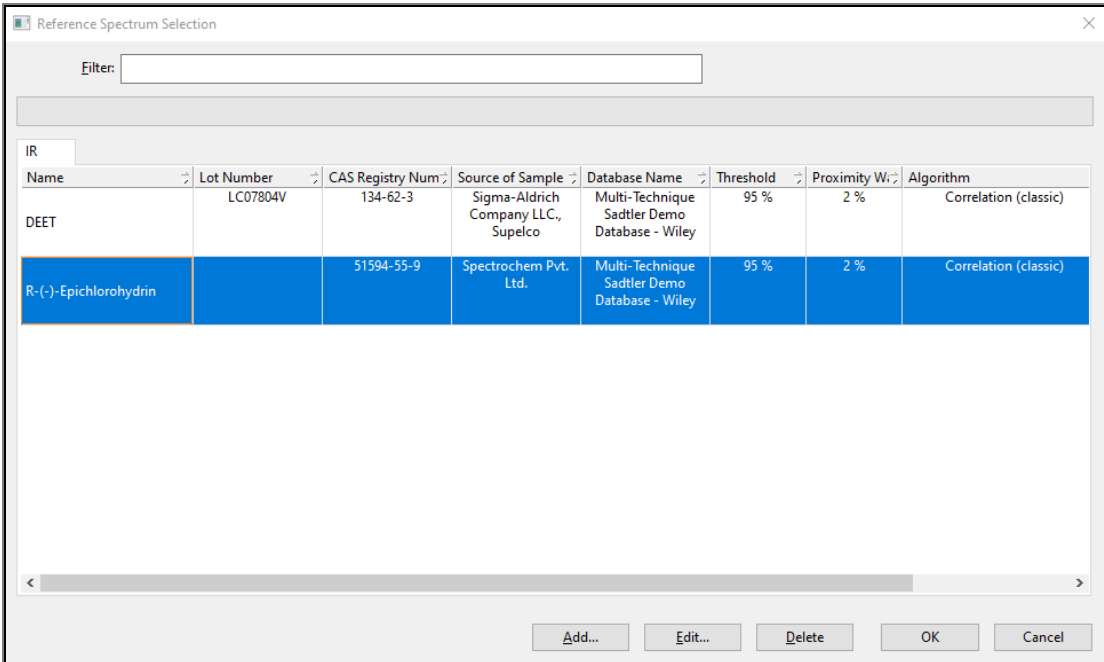
	Action	Result
5	<p>In File > Settings, set the Organization to "Wiley Laboratories, Inc." and add an address.</p> <p>Do not immediately click OK.</p>	 <p>The screenshot shows the 'Settings' dialog box with the 'Reference/Validation Databases' tab selected. The 'Organization' field contains 'Wiley Laboratories, Inc.' and the 'Address' field is empty. The 'Folder for Reports' is 'C:\Users\Public\Documents\W' with a 'Browse...' button. The 'Language for Reports' is 'Same as QC Expert'. The 'OK' button is highlighted.</p>

Select Reference Database

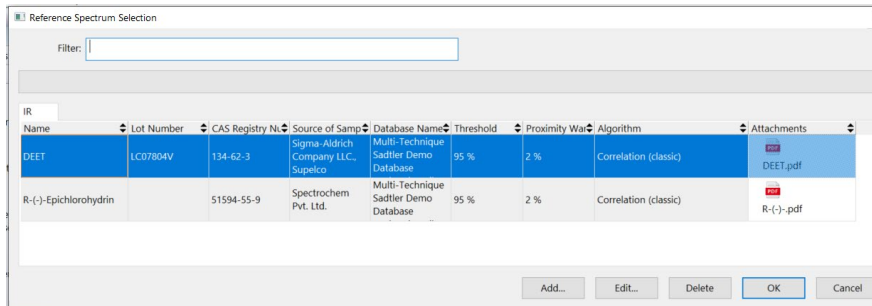
	Action	Result
1	<p>Click on the Reference/Validation Databases tab, click the Select by Browsing button.</p> <p>Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples folder.</p> <p>Select the Multi-Technique Sadtler Demo Database - Wiley [DEMO] database.</p>	 <p>The screenshot shows the 'Settings' dialog box with the 'Reference/Validation Databases' tab selected. The 'Technique' is set to 'IR'. The 'Available for Searching' list contains several databases, including 'Multi-Technique Sadtler Demo Database - Wiley [DEMO]'. The 'Selected for Searching' list also contains this database. The 'Select by Browsing...' button is highlighted.</p>
2	Click OK .	

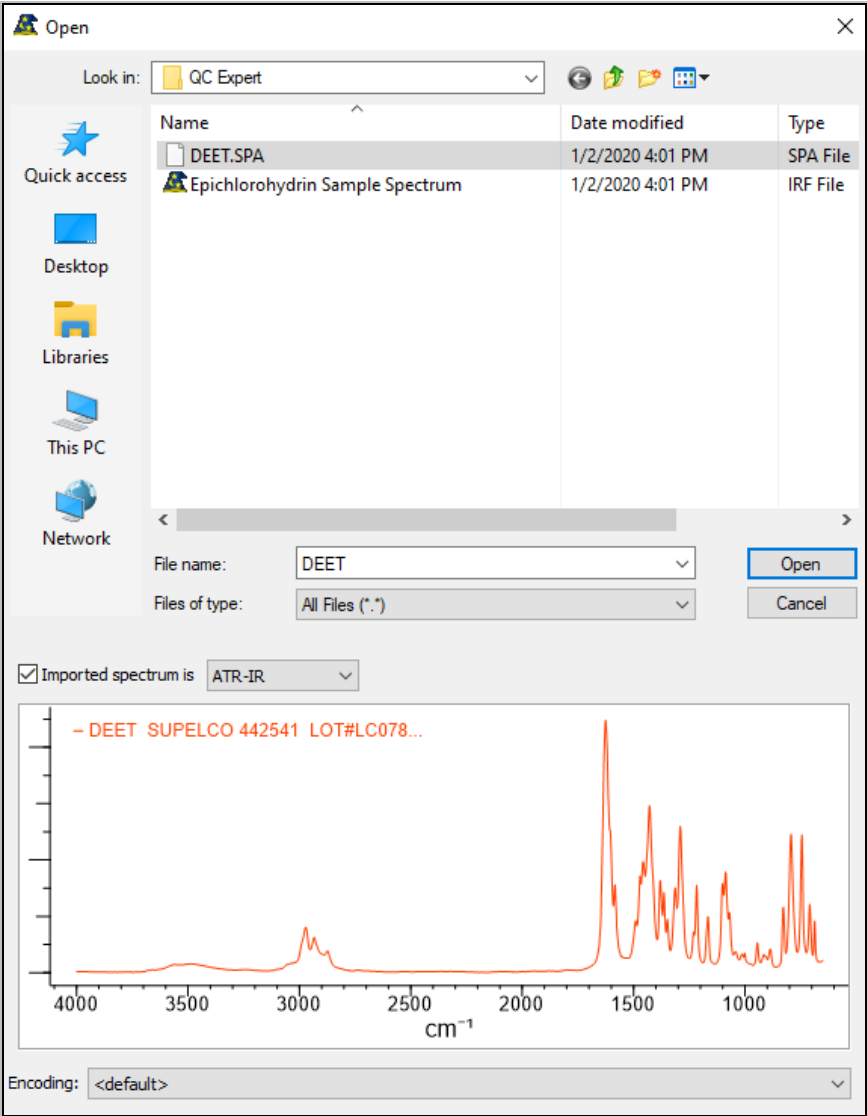
	Action	Result
3	Click on the Select Reference button at the lower right of the QC Expert window.	 <p>The screenshot shows the QC Expert software interface. At the top is a title bar labeled "QC Expert" with a standard window control bar. Below the title bar is a toolbar with various icons for file operations, zooming, and analysis. The main workspace is divided into several panels. On the left, there's a "Sample Spectrum Status" panel containing a table with columns "Checklist", "Status", and "Fix?". The "Fix?" column has a checkbox. Below this table is a "New Comparison" button. To the right of the "Sample Spectrum Status" panel is a large black rectangular area. Below the "Sample Spectrum Status" panel is a "QC Comparison Status" panel with a "Create Report" button. To the right of the black area are two panels: "Selected Reference Spectrum Properties" and "Structure". Below the "Structure" panel is an "Attachments" panel. At the bottom right of the interface is a "Select Reference" button.</p>

	Action	Result										
4	<p>At the prompt, login as administrator. The Add Reference Spectrum dialog box opens.</p> <p>Type DEET in the Filter box to search for DEET.</p> <p>Select the Correlation (Classic) algorithm for the demo.</p> <p>Note the Comparison Algorithm, Match Threshold and Proximity Warning parameters in the lower left.</p> <p>Click OK to add the spectrum.</p>	 <p>Add Reference Spectrum</p> <p>Technique: IR</p> <p>Filter: DEET</p> <table><tr><th>Name</th><th>Lot Number</th><th>CAS Registry Num</th><th>Source of Sample</th><th>Database Name</th></tr><tr><td>DEET</td><td>LC07804V</td><td>134-62-3</td><td>Sigma-Aldrich Company LLC, Supelco</td><td>Multi-Technique Sadtler Demo Database - Wiley</td></tr></table> <p>Comparison Algorithm: Correlation (classic)</p> <p>Match Threshold: 95 %</p> <p>Proximity Warning: 2 %</p> <p>OK Cancel</p>	Name	Lot Number	CAS Registry Num	Source of Sample	Database Name	DEET	LC07804V	134-62-3	Sigma-Aldrich Company LLC, Supelco	Multi-Technique Sadtler Demo Database - Wiley
Name	Lot Number	CAS Registry Num	Source of Sample	Database Name								
DEET	LC07804V	134-62-3	Sigma-Aldrich Company LLC, Supelco	Multi-Technique Sadtler Demo Database - Wiley								

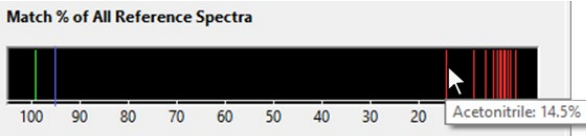

	Action	Result
5	<p>The Reference Spectrum Selection dialog box opens.</p> <p>Click on Add, and type epi in the Filter box.</p> <p>Select R-(-)-Epichlorohydrin and select the Correlation (classic) algorithm.</p> <p>Click OK.</p>	

Run QC Expert as a Non-administrator QC Analyst

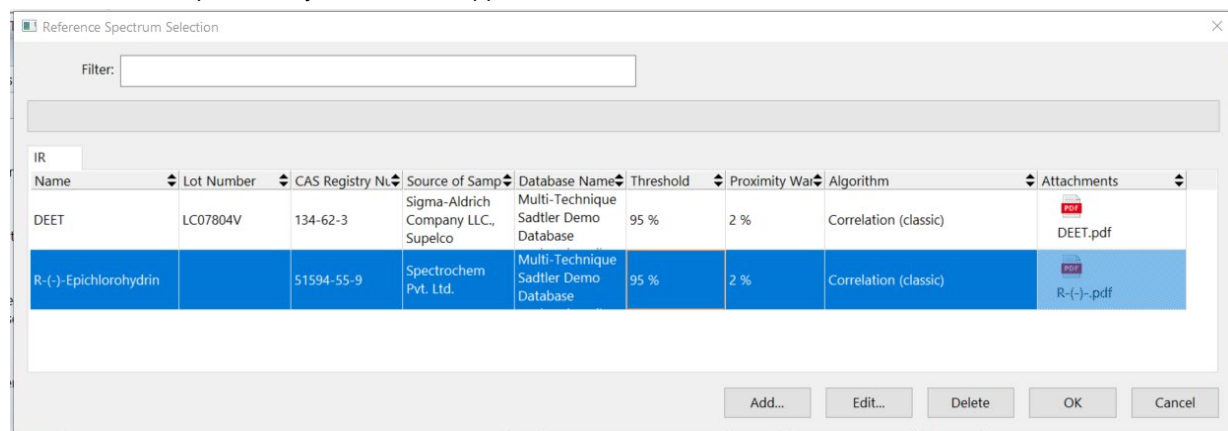

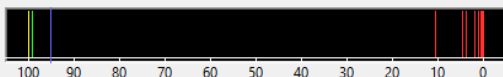
	Action	Result
1	Select the DEET spectrum by highlighting it. Click OK .	

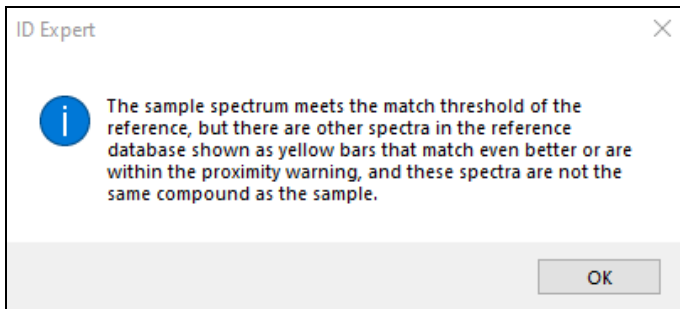
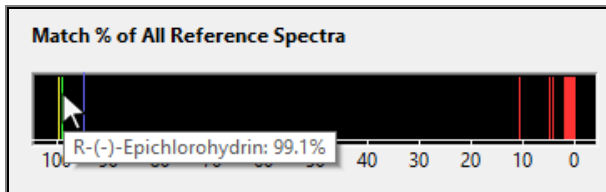
	Action	Result
2	<p>Click on New Comparison at the mid-left of the QC Expert window.</p> <p>Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\QC Expert folder and select DEET.SPA.</p> <p>Click on the 'Imported spectrum is' check box. Select ATR-IR from the drop down.</p> <p>Click Open.</p>	

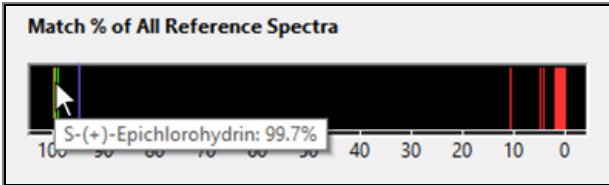
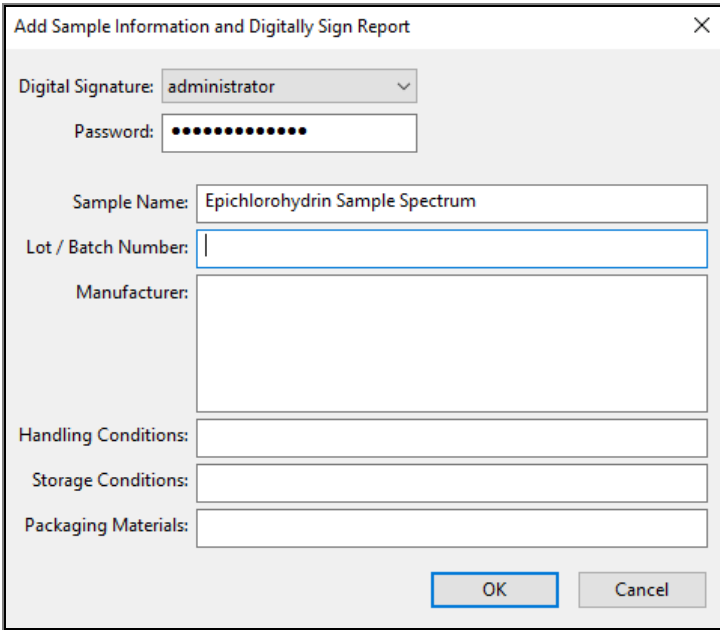
Action	Result															
3	<p>The QC Expert window displays the Comparison Status.</p> <div><div><div><h3>QC Expert</h3><div><div><div><div>Sample Spectrum Status</div><table><thead><tr><th>Checklist</th><th>Status</th><th>Fix?</th></tr></thead><tbody><tr><td>Noise</td><td>● ⓘ</td><td><input type="checkbox"/></td></tr><tr><td>Contaminants</td><td>● ⓘ</td><td></td></tr><tr><td>Technique</td><td>● ⓘ</td><td>ATR-IR ▼</td></tr><tr><td>Spectral Range</td><td>? ⓘ</td><td><input type="button" value="Fix"/></td></tr></tbody></table><div><input type="button" value="New Comparison"/></div></div><div><div><div>QC Comparison Status</div><div>Sample File Name: DEET.SPA Sample Title: DEET SUPELCO 442541 LOT#LC</div><div><div>✔</div><div>Pass at 95% Threshold Match: 99.1%</div></div><div>Match % of All Reference Spectra</div><div><div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div>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Noise	● ⓘ	<input type="checkbox"/>	Contaminants	● ⓘ		Technique	● ⓘ	ATR-IR ▼	Spectral Range	? ⓘ	<input type="button" value="Fix"/>
Checklist	Status	Fix?														
Noise	● ⓘ	<input type="checkbox"/>														
Contaminants	● ⓘ															
Technique	● ⓘ	ATR-IR ▼														
Spectral Range	? ⓘ	<input type="button" value="Fix"/>														

	Action	Result
4	<p>Mouse over the green and red bars in the Match % of All Reference Spectra chart.</p> <p>Note: When you mouse over the various bars in the Match % Chart, you see the corresponding display in the Spectrum pane at the top.</p>	 <p>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.</p>
5	<p>Double-click on the PDF attachment in the Attachment pane at the lower right.</p>	<p>The DEET safety datasheet and other associated information is displayed.</p>  <p>SIGMA-ALDRICH sigma-aldrich.com</p> <p style="text-align: right;">SAFETY DATA SHEET Version 4.4 Revision Date 07/03/2014 Print Date 08/25/2015</p> <p>1. PRODUCT AND COMPANY IDENTIFICATION</p> <p>1.1 Product identifiers</p> <p>Product name : <i>N,N</i>-Diethyl-3-methylbenzamide</p> <p>Product Number : D100951</p> <p>Brand : Aldrich</p> <p>Index-No. : 616-018-00-2</p> <p>CAS-No. : 134-62-3</p> <p>1.2 Relevant identified uses of the substance or mixture and uses advised against</p> <p>Identified uses : Laboratory chemicals, Manufacture of substances</p> <p>1.3 Details of the supplier of the safety data sheet</p> <p>Company : Sigma-Aldrich 3050 Spruce Street SAINT LOUIS MO 63103 USA</p> <p>Telephone : +1 800-325-5832</p> <p>Fax : +1 800-325-5052</p> <p>1.4 Emergency telephone number</p> <p>Emergency Phone # : (314) 776-6555</p>

QC Analyst Comparison of R-(-)-Epichlorohydrin Sample Spectrum to Reference

	Action	Result
1	<p>Click on the Select Reference button.</p> <p>Select the R-(-)-Epichlorohydrin reference spectrum by highlighting it.</p> <p>Click OK.</p>	<p>This is to open a spectrum of a sample of R-(-)-Epichlorohydrin and perform a quality control comparison to make sure that the sample actually is what it is supposed to be.</p> 
2	<p>Click on New Comparison at the mid-left of the QC Expert window.</p> <p>Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\QC Expert folder.</p> <p>Select Epichlorohydrin Sample Spectrum.irf.</p> <p>Set Imported spectrum is to ATR-IR and ensure this option is checked.</p> <p>Click Open.</p>	<div><p>QC Comparison Status</p><p>Sample File Name: Epichlorohydrin Sample Spectrum.irf Sample Title: Epichlorohydrin Sample Spectrum</p><p> Uncertain at 95% Threshold with 2% Proximity Warning ⓘ</p><p>Match: 99.1%</p><p>Match % of All Reference Spectra</p><p>Next Closest: S-(+)-Epichlorohydrin: 99.7%</p></div> <p>The Match % between the selected reference spectrum and sample spectrum is excellent at 99.1%, but the QC comparison is Uncertain.</p>

	Action	Result
3	Click on the information button ⓘ.	 <p>An ID Expert 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 OK 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 R-(-)-Epichlorohydrin: 99.1% .	 <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>

	Action	Result
7	Mouse over the yellow bar in the Match % Chart. The hover-over text says S-(+)- Epichlorohydrin: 99.7% .	 <p>The yellow bar is for S-(+)- Epichlorohydrin, 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 Create Report button below the Match % chart to create a digitally signed report.</p> <p>Select your username from the Digital Signatures drop-down menu.</p> <p>Enter the password.</p> <p>Fill out the sample information.</p>	
9	Click OK to view the report.	<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>