

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

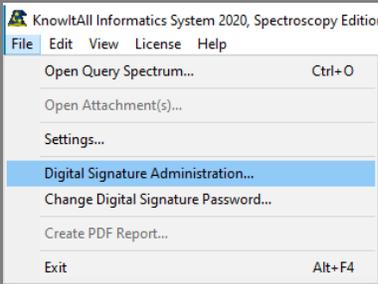
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\QC Expert

- DEET.SPA
- Epichlorohydrin Sample Spectrum.irf

KnowItAll Applications Used

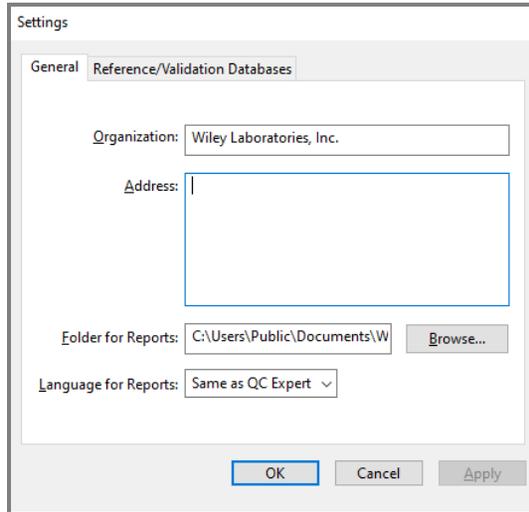
- QC Expert

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.	

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

Do not immediately click **OK**.



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

Settings

General Reference/Validation Databases

Organization: Wiley Laboratories, Inc.

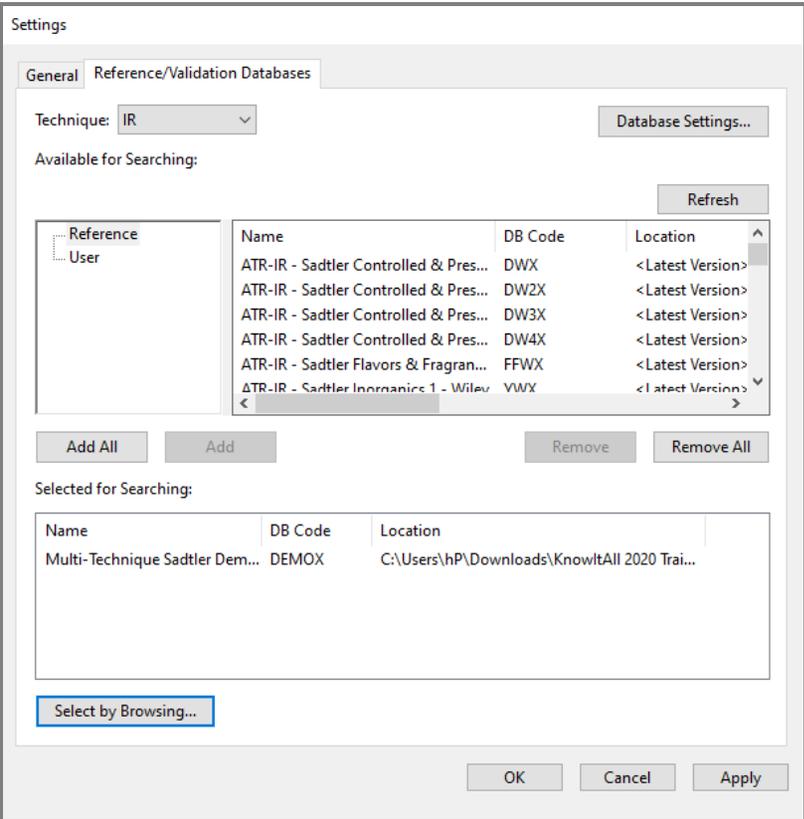
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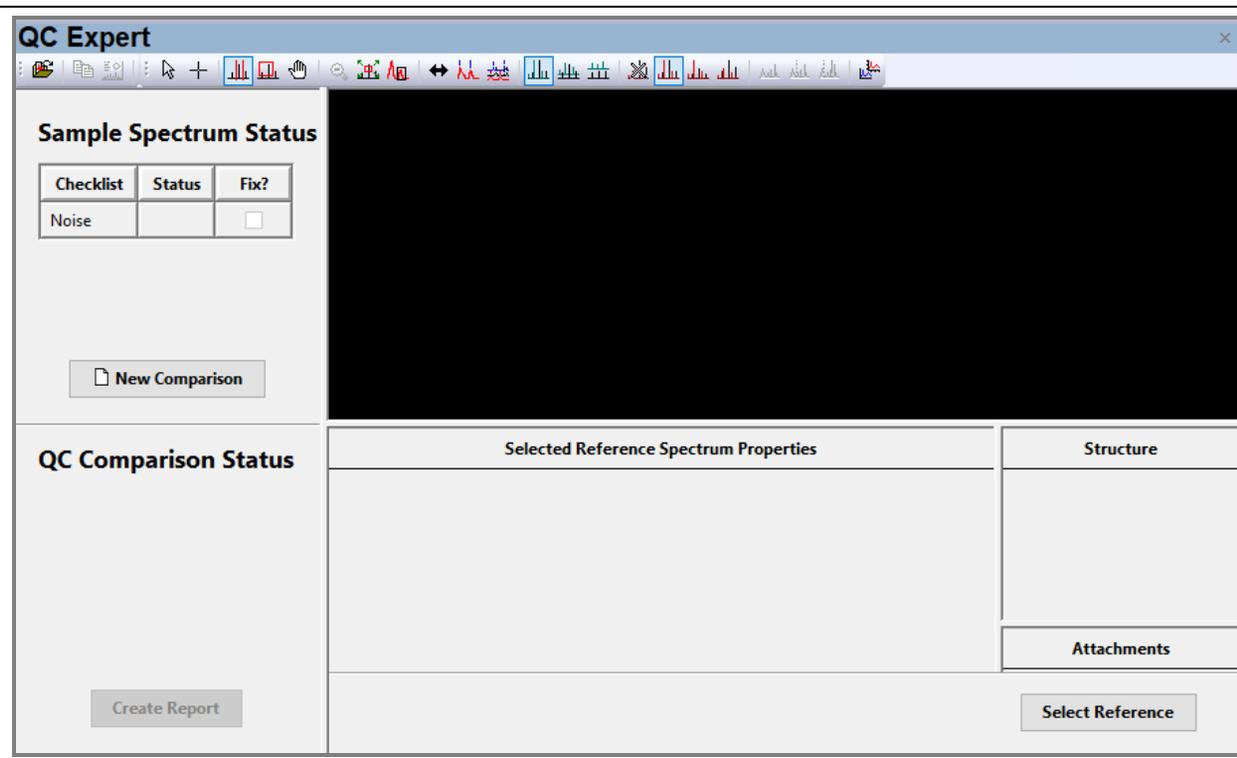
Language for Reports: Same as QC Expert ▾

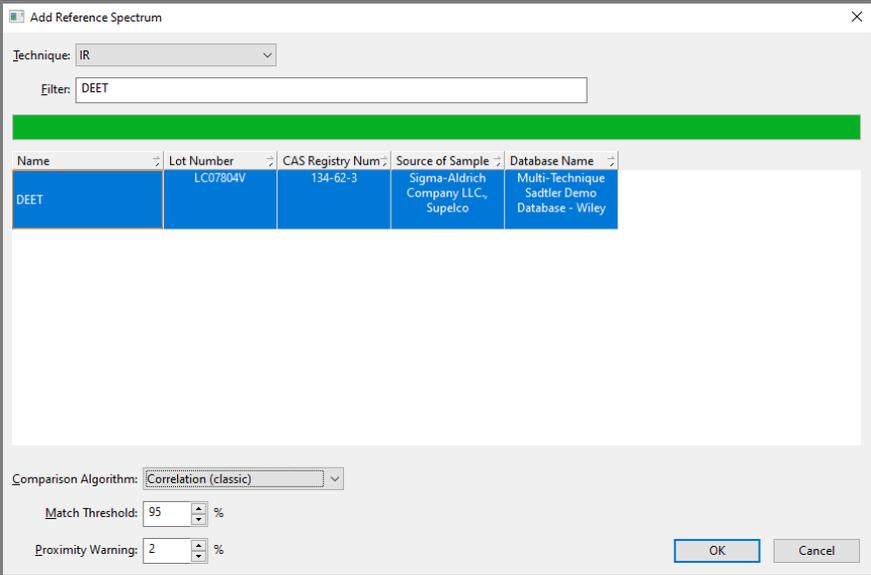
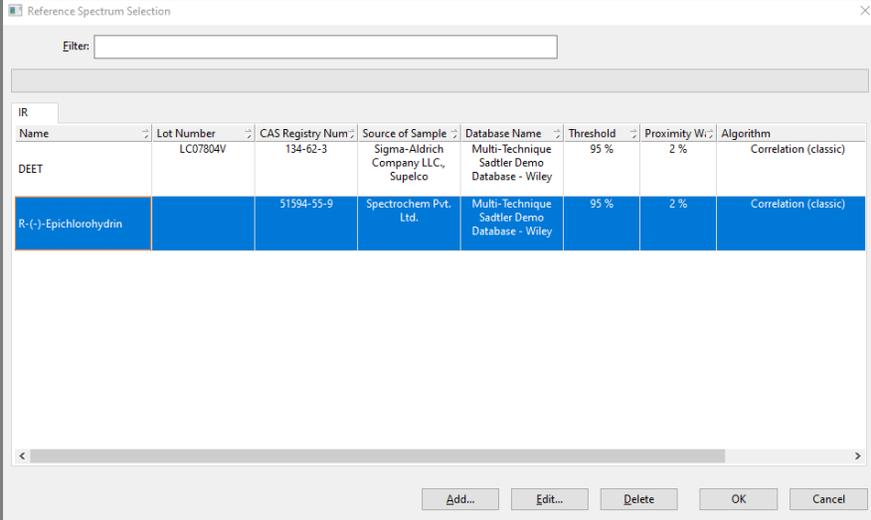
OK Cancel Apply

Select Reference Database

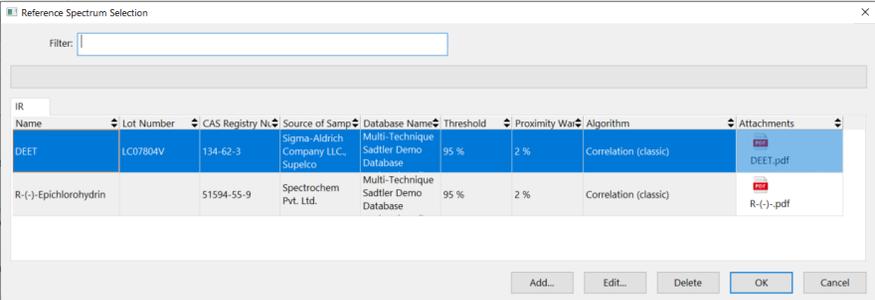
	Action	Result
1	<p>Click on the Reference/Validation Databases tab, click the Select by Browsing button.</p> <p>Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples folder.</p> <p>Select the Multi-Technique Sadtler Demo Database - Wiley [DEMO] database.</p>	 <p>The screenshot shows the 'Settings' dialog box with the 'Reference/Validation Databases' tab selected. The 'Technique' dropdown is set to 'IR'. Below it, a list of available databases is shown with columns for Name, DB Code, and Location. The 'Multi-Technique Sadtler Demo Database' is highlighted. Below the list, there are buttons for 'Add All', 'Add', 'Remove', and 'Remove All'. The 'Selected for Searching' section shows the selected database and its location path. At the bottom, there is a 'Select by Browsing...' button and 'OK', 'Cancel', and 'Apply' buttons.</p>
2	Click OK .	

3 Click on the **Select Reference** button at the lower right of the **QC Expert** window.



<p>4 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 border="1"> <thead> <tr> <th>Name</th> <th>Lot Number</th> <th>CAS Registry Num</th> <th>Source of Sample</th> <th>Database Name</th> </tr> </thead> <tbody> <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> </tbody> </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														
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<p>5 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>	 <p>Reference Spectrum Selection</p> <p>Filter:</p> <p>IR</p> <table border="1"> <thead> <tr> <th>Name</th> <th>Lot Number</th> <th>CAS Registry Num</th> <th>Source of Sample</th> <th>Database Name</th> <th>Threshold</th> <th>Proximity W:</th> <th>Algorithm</th> </tr> </thead> <tbody> <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> <td>95 %</td> <td>2 %</td> <td>Correlation (classic)</td> </tr> <tr> <td>R-(-)-Epichlorohydrin</td> <td></td> <td>51594-55-9</td> <td>Spectrochem Pvt. Ltd.</td> <td>Multi-Technique Sadtler Demo Database - Wiley</td> <td>95 %</td> <td>2 %</td> <td>Correlation (classic)</td> </tr> </tbody> </table> <p>Add... Edit... Delete OK Cancel</p>	Name	Lot Number	CAS Registry Num	Source of Sample	Database Name	Threshold	Proximity W:	Algorithm	DEET	LC07804V	134-62-3	Sigma-Aldrich Company LLC., Supelco	Multi-Technique Sadtler Demo Database - Wiley	95 %	2 %	Correlation (classic)	R-(-)-Epichlorohydrin		51594-55-9	Spectrochem Pvt. Ltd.	Multi-Technique Sadtler Demo Database - Wiley	95 %	2 %	Correlation (classic)
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Run QC Expert as a Non-administrator QC Analyst

	Action	Result																											
1	Select the DEET spectrum by highlighting it. Click OK .	 <p>The screenshot shows a 'Reference Spectrum Selection' dialog box. At the top, there is a 'Filter:' text box. Below it is a table with the following data:</p> <table border="1"> <thead> <tr> <th>Name</th> <th>Lot Number</th> <th>CAS Registry No.</th> <th>Source of Sample</th> <th>Database Name</th> <th>Threshold</th> <th>Proximity Weight</th> <th>Algorithm</th> <th>Attachments</th> </tr> </thead> <tbody> <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</td> <td>95 %</td> <td>2 %</td> <td>Correlation (classic)</td> <td>DEET.pdf</td> </tr> <tr> <td>R-(-)-Epichlorohydrin</td> <td></td> <td>51594-55-9</td> <td>Spectrochem Pvt. Ltd.</td> <td>Multi-Technique Sadtler Demo Database</td> <td>95 %</td> <td>2 %</td> <td>Correlation (classic)</td> <td>R-(-)-.pdf</td> </tr> </tbody> </table> <p>The 'DEET' row is highlighted in blue. At the bottom of the dialog, there are buttons for 'Add...', 'Edit...', 'Delete', 'OK', and 'Cancel'.</p>	Name	Lot Number	CAS Registry No.	Source of Sample	Database Name	Threshold	Proximity Weight	Algorithm	Attachments	DEET	LC07804V	134-62-3	Sigma-Aldrich Company LLC, Supelco	Multi-Technique Sadtler Demo Database	95 %	2 %	Correlation (classic)	DEET.pdf	R-(-)-Epichlorohydrin		51594-55-9	Spectrochem Pvt. Ltd.	Multi-Technique Sadtler Demo Database	95 %	2 %	Correlation (classic)	R-(-)-.pdf
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2 Click on **New Comparison** at the mid-left of the **QC Expert** window.

Navigate to **C:\Users\Public\Documents\Wiley\KnowItAll\Samples\QC Expert** folder and select **DEET.SPA**.

Click on the **'Imported spectrum is'** check box. Select **ATR-IR** from the drop down.

Click **Open**.

Open

Look in: QC Expert

Name	Date modified	Type
DEET.SPA	1/2/2020 4:01 PM	SPA File
Epiclorohydrin Sample Spectrum	1/2/2020 4:01 PM	IRF File

File name: DEET

Files of type: All Files (*.*)

Imported spectrum is ATR-IR

- DEET SUPELCO 442541 LOT#LC078...

cm⁻¹

Encoding: <default>

3

The QC Expert window displays the Comparison Status.

Checklist	Status	Fix?
Noise	Pass	<input type="checkbox"/>
Contaminants	Pass	<input type="checkbox"/>
Technique	Pass	ATR-IR
Spectral Range	Fail	<input type="button" value="Fix"/>

Name	Value
Database Abbreviation	DEMOX
Database Title	Multi-Technique Sadtler Demo Database - Wiley
Record ID	15
Name	DEET
Algorithm	Correlation (classic)
Threshold	95 %
Proximity Warning	2 %
CAS Registry Number	134-62-3
Catalog Number	442541
Flash Point	95 °C
Formula	C12H17NO
Hazards	Warning
InChI	InChI=1S/C12H17NO/c1-4-13(5-2)12(14)11-8-6-7...
InChIKey	MMOXZBCLCQIDF-UHFFFAOYSA-N
Lot Number	LC07804V
Molecular Weight	181.273 g/mol

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

4

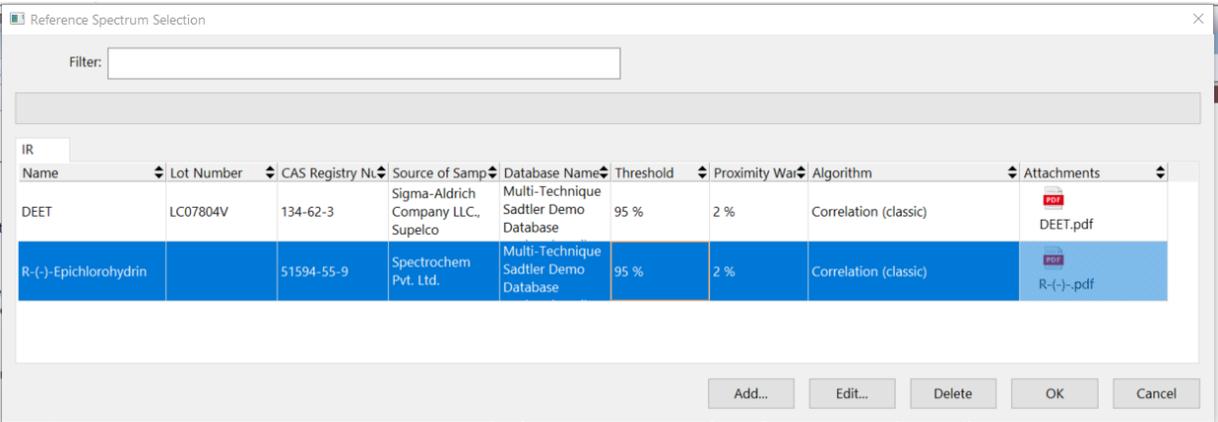
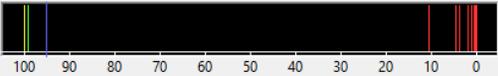
Mouse over the green and red bars in the Match % of All Reference Spectra chart.

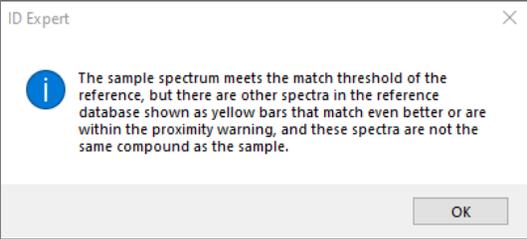
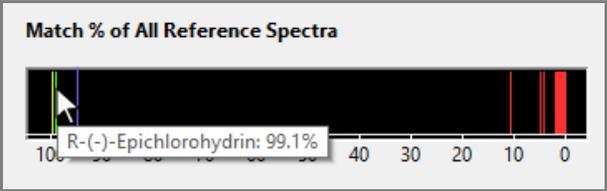
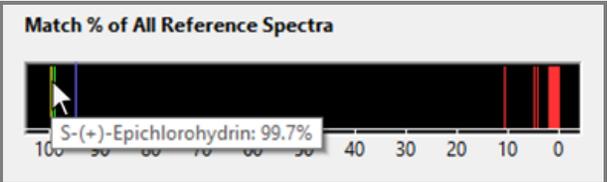
Note: When you mouse over the various bars in the Match % Chart, you see the corresponding display in the Spectrum pane at the top.

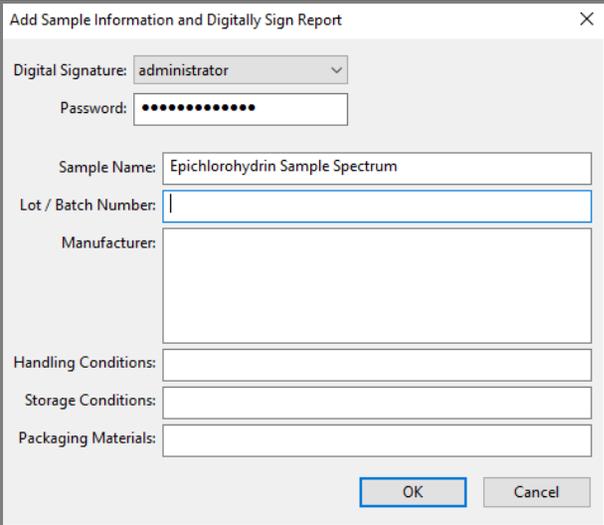
The Match % of All Reference Spectra chart shows the comparison of the sample spectrum to spectra from the entire reference database. The **green bars** are for the comparison of the sample spectrum against the selected reference spectrum as well as all other reference spectra for different lots of the 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 Attachment pane at the lower right.	<p>The DEET safety datasheet and other associated information is displayed.</p> <div data-bbox="695 310 1753 1019" style="border: 1px solid black; padding: 10px;"><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><hr/><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 Brand : Aldrich Index-No. : 616-018-00-2 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 Fax : +1 800-325-5052</p><p>1.4 Emergency telephone number</p><p>Emergency Phone # : (314) 776-6555</p></div>
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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>  <table border="1" data-bbox="695 592 1913 755"> <thead> <tr> <th>Name</th> <th>Lot Number</th> <th>CAS Registry No.</th> <th>Source of Sample</th> <th>Database Name</th> <th>Threshold</th> <th>Proximity Warning</th> <th>Algorithm</th> <th>Attachments</th> </tr> </thead> <tbody> <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</td> <td>95 %</td> <td>2 %</td> <td>Correlation (classic)</td> <td>DEET.pdf</td> </tr> <tr style="background-color: #0070C0; color: white;"> <td>R-(-)-Epichlorohydrin</td> <td></td> <td>51594-55-9</td> <td>Spectrochem Pvt. Ltd.</td> <td>Multi-Technique Sadtler Demo Database</td> <td>95 %</td> <td>2 %</td> <td>Correlation (classic)</td> <td>R-(-)-.pdf</td> </tr> </tbody> </table>	Name	Lot Number	CAS Registry No.	Source of Sample	Database Name	Threshold	Proximity Warning	Algorithm	Attachments	DEET	LC07804V	134-62-3	Sigma-Aldrich Company LLC, Supelco	Multi-Technique Sadtler Demo Database	95 %	2 %	Correlation (classic)	DEET.pdf	R-(-)-Epichlorohydrin		51594-55-9	Spectrochem Pvt. Ltd.	Multi-Technique Sadtler Demo Database	95 %	2 %	Correlation (classic)	R-(-)-.pdf
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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 data-bbox="695 894 1222 1336"> <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>																											

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>
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>

<p>8</p>	<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>	
<p>9</p>	<p>Click OK to view the report.</p>	<p>The digitally signed PDF contains the following information:</p> <ul style="list-style-type: none"> Page 1 – Information about the test Page 2 – Information about the spectral comparison Page 3 – Information about the reference spectrum