

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
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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.

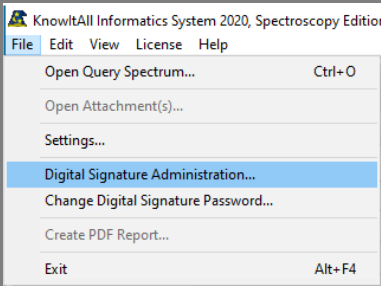
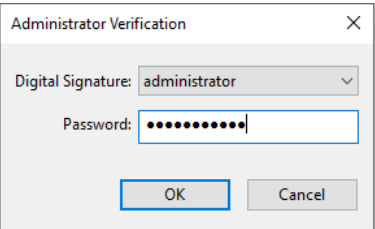
Training Files Used in This Lesson

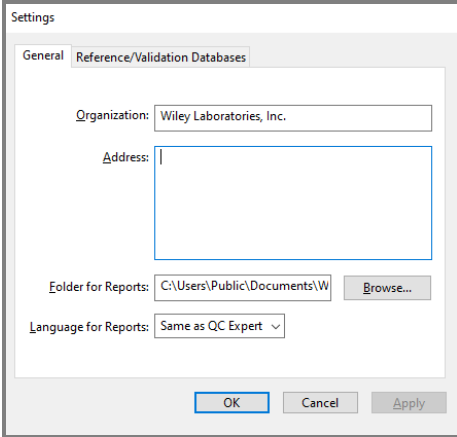
- DEET.SPA
- Epichlorohydrin Sample Spectrum.irf

KnowItAll Applications Used

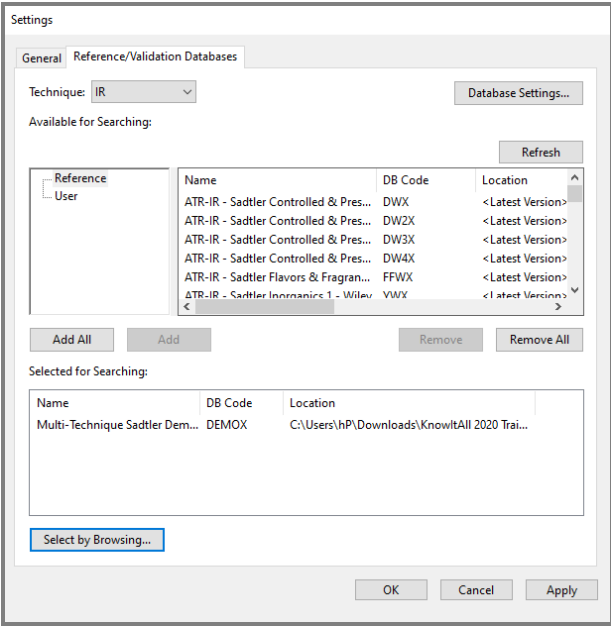
- QC Expert

Set Up Administrator Account and Address

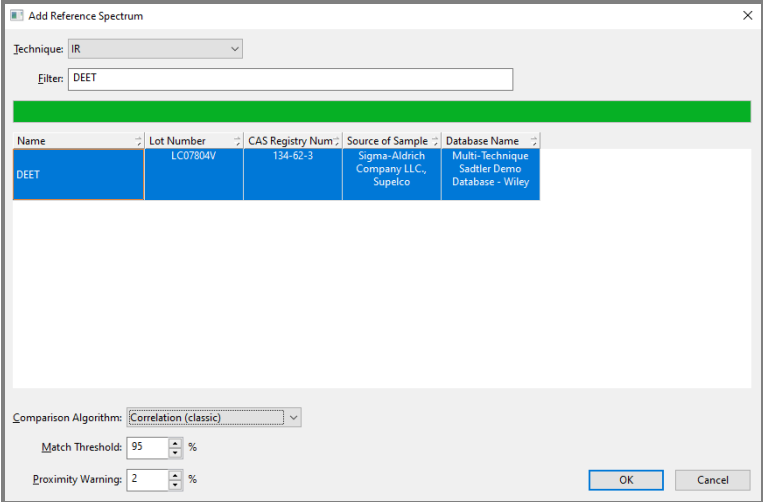
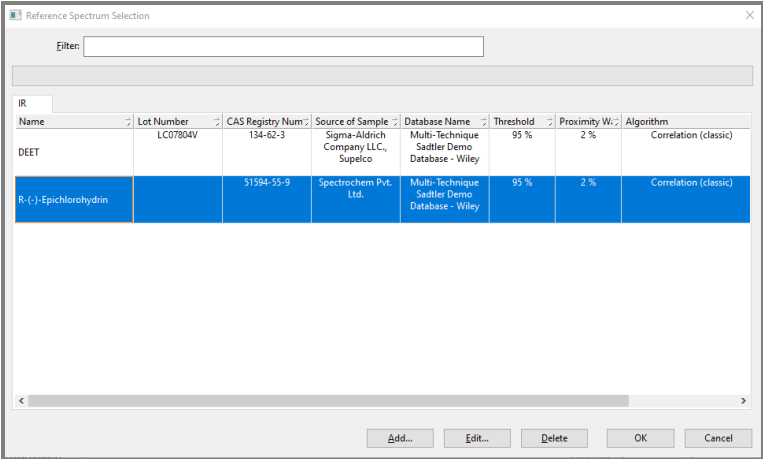
	Action	Result
1	Navigate to the Data toolbox and open the QC Expert application.	
2	To create an administrative account, go to File > Digital Signature Administration .	
3	<p>Enter your preferred user ID in the Digital Signature field.</p> <p>Enter preferred password in the Password and Confirm Password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

<p>5 In File > Settings, set the Organization to “Wiley Laboratories, Inc.” and add an address.</p>	 <p>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. The 'Folder for Reports' is 'C:\Users\Public\Documents\W' with a 'Browse...' button. The 'Language for Reports' is 'Same as QC Expert'. At the bottom are 'OK', 'Cancel', and 'Apply' buttons.</p>
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Select Reference Database

	Action	Result
1	<p>In the Reference/Validation Databases tab, click the Select by Browsing button.</p> <p>Navigate to KnowItAll Training Files > Databases.</p> <p>Select the Multi-Technique Sadtler Demo Database - Wiley [DEMO] database.</p>	
2	Click OK .	

<p>3 Click on the Select Reference button at the lower right of the QC Expert window.</p>	
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<p>4</p> <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>Point out the Comparison Algorithm, Match Threshold and Proximity Warning parameters in the lower left.</p> <p>Select the Correlation (Classic) algorithm for the demo.</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</p> <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>	 <p>Reference Spectrum Selection</p> <p>Filter: epi</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>51994-55-9</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		51994-55-9	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

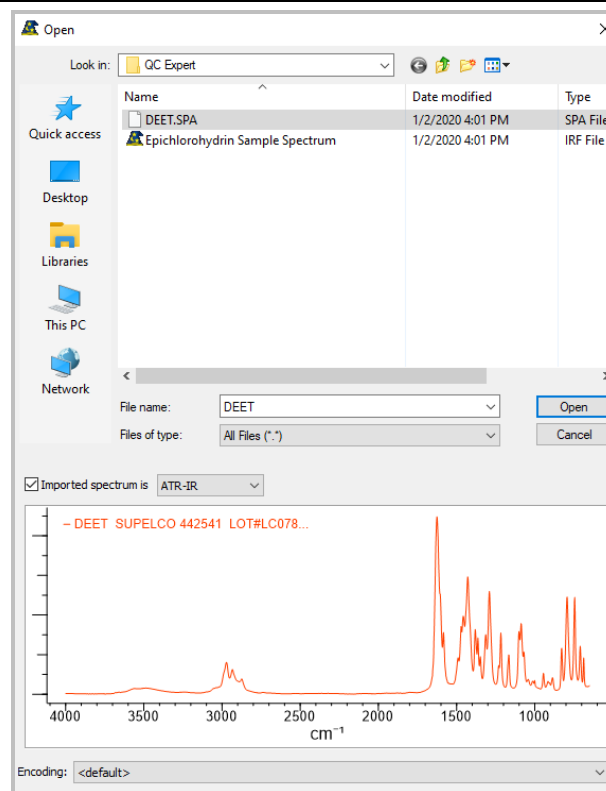
	Action	Result
1	<p>Navigate to the Data toolbox and open the QC Expert application.</p> <p>Click on the Select Reference button. Select the DEET spectrum.</p> <p>Click OK.</p>	

2 Click on **New Comparison** at the mid-left of the **QC Expert** window.

Navigate to KnowItAll > Samples > QC Expert folder and select **DEET.SPA**.

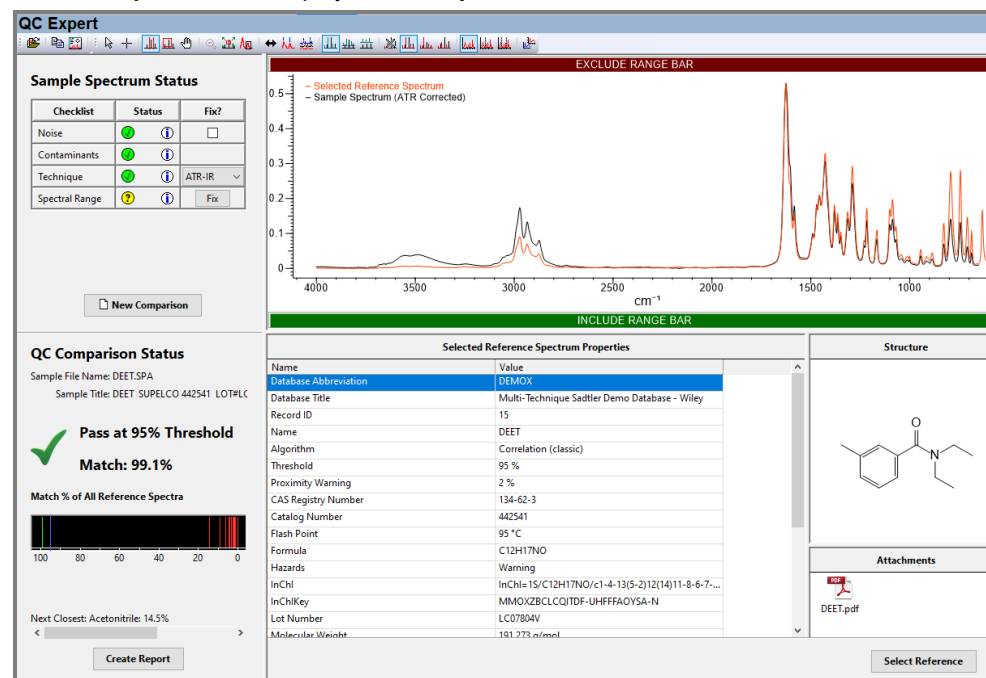
Set **Imported spectrum is** to **ATR-IR** and ensure this option is checked.

Click **Open**.



3

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

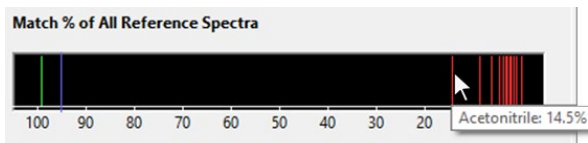


We get an excellent match of 99.1% and a green check mark indicating that the quality control comparison passes.

4

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

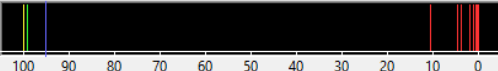
Note: When you mouse over the various bars in the Match % Chart, you see the corresponding display in the **Spectrum Pane** at the top.

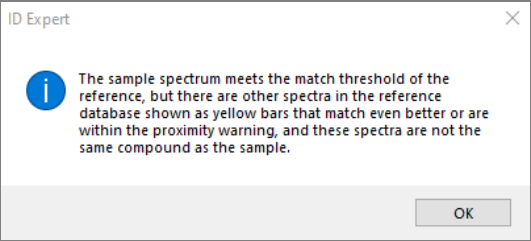
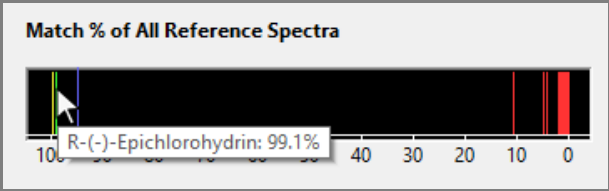
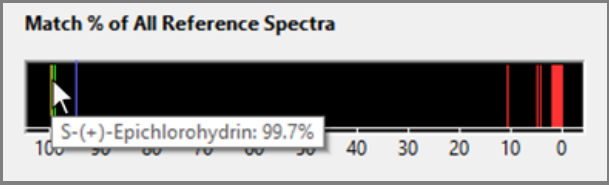


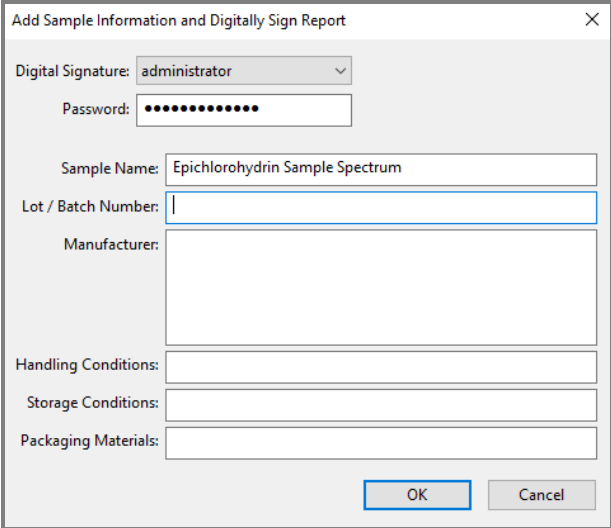
The **Match % of All Reference Spectra** chart shows the comparison of the sample spectrum to spectra from the entire reference database. The **green bars** are for the comparison of the sample spectrum against the selected reference spectrum as well as all other reference spectra for different lots 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 Attachment pane at the lower right.	<p>The DEET safety datasheet and other associated information is displayed.</p> <div data-bbox="699 313 1455 816"><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 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 Identified uses : Laboratory chemicals, Manufacture of substances</p><p>1.3 Details of the supplier of the safety data sheet 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 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>Navigate to the Data toolbox and open the QC Expert application.</p> <p>Click on the Select Reference button.</p> <p>Select the R-(-)-Epichlorohydrin reference spectrum.</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 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="699 756 1228 1198" style="border: 1px solid black; padding: 5px;"> <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: Page 1 – Information about the test Page 2 – Information about the spectral comparison Page 3 – Information about the reference spectrum</p>