KnowItAll Informatics Training

Quality Control Analysis with QC Expert

WILEY

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

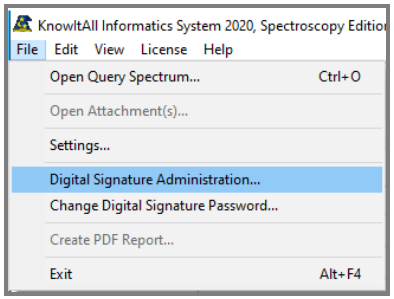
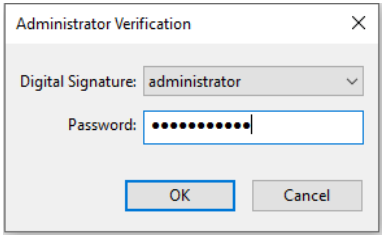
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\QC Expert

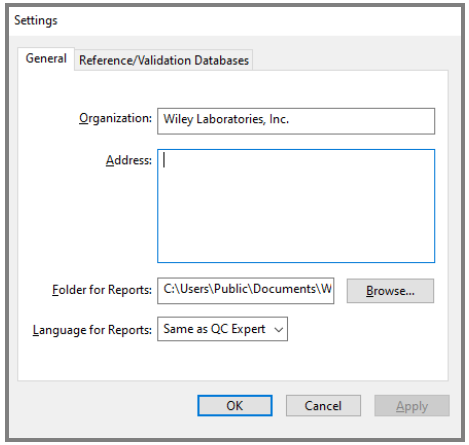
- DEET.SPA
- Epichlorohydrin Sample Spectrum.irf

KnowItAll Applications Used

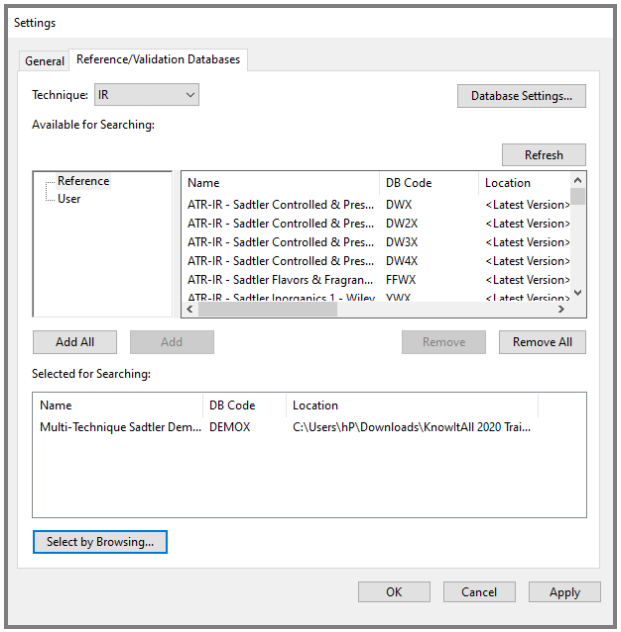
- QC Expert

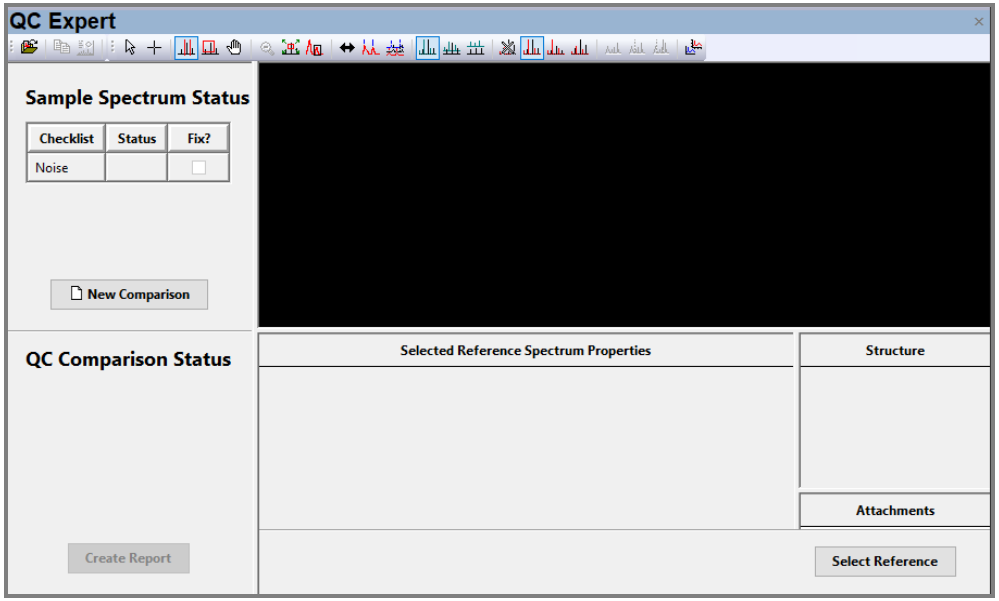
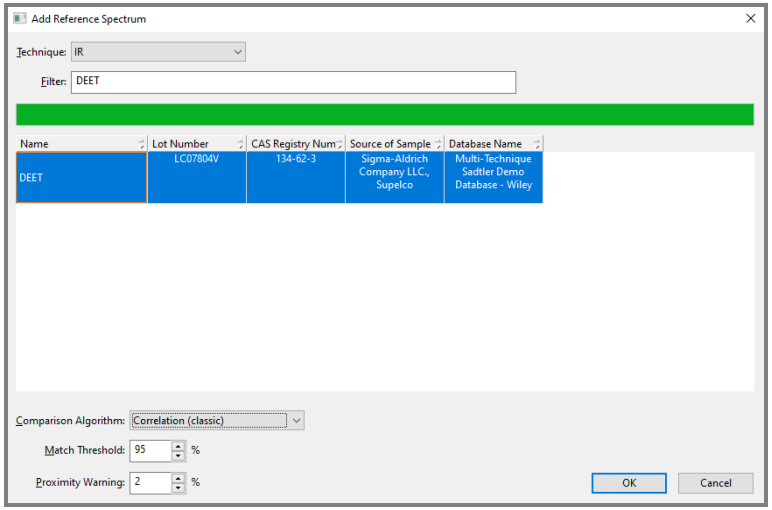
Set Up Administrator Account and Address

	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	Enter your preferred user ID in the **Digital Signature** field. Enter preferred password in the **Password** and **Confirm Password** fields. Click **OK**.	
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.	

Select Reference Database

	Action	Result
1	In the **Reference/Validation Databases** tab, click the **Select by Browsing** button. Navigate to **C:\Users\Public\Documents\Wiley\KnowItAll\Samples** folder. Select the **Multi-Technique Sadtler Demo Database - Wiley [DEMO]** database.	
2	Click **OK**.	

3	Click on the **Select Reference** button at the lower right of the **QC Expert** window.	
4	At the prompt, login as administrator. The **Add Reference Spectrum** dialog box opens. Type **DEET** in the **Filter** box to search for DEET. Point out the **Comparison Algorithm**, **Match Threshold** and **Proximity Warning** parameters in the lower left. Select the **Correlation (Classic)** algorithm for the demo. Click **OK** to add the spectrum.	

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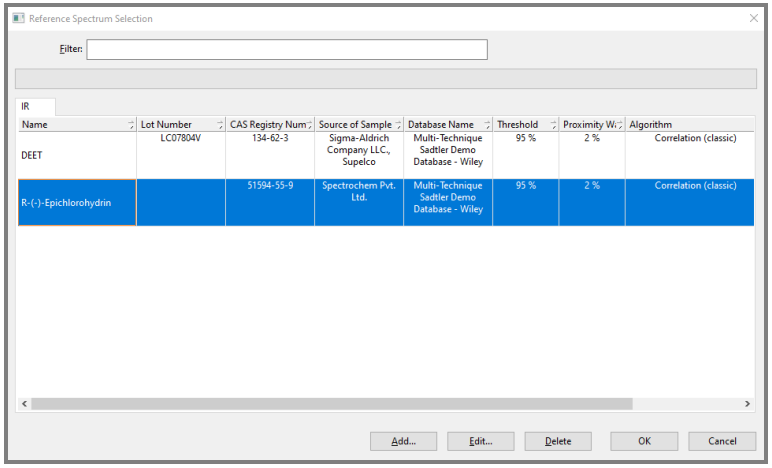
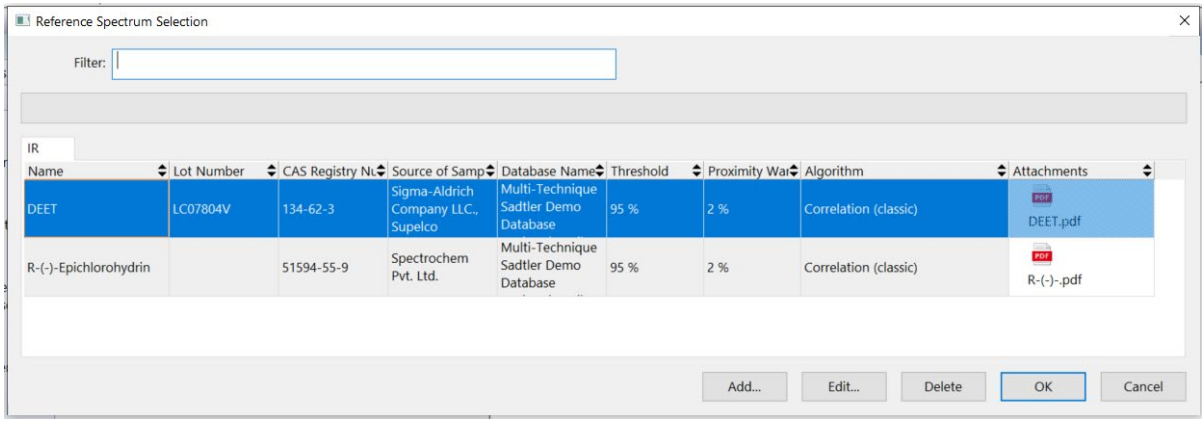
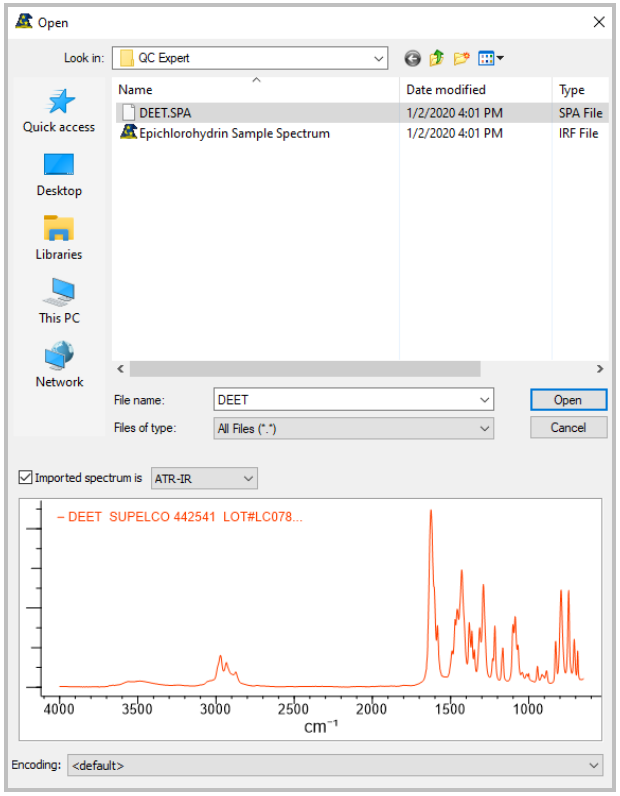
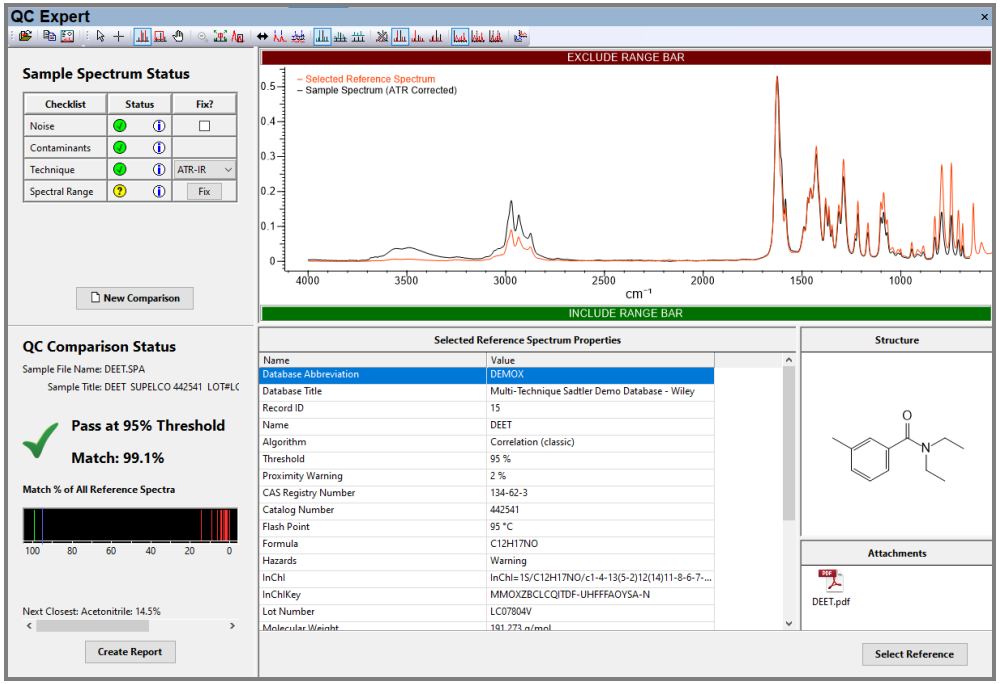
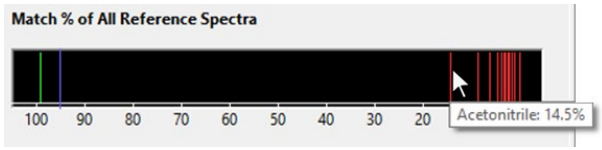
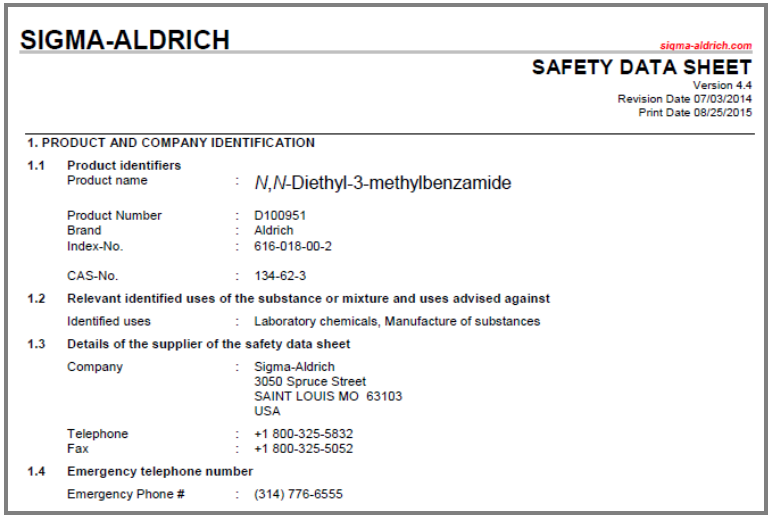
5	The **Reference Spectrum Selection** dialog box opens. Click on **Add**, and type **epi** in the **Filter** box. Select **R-(-)-Epichlorohydrin** and select the **Correlation (classic)** algorithm. Click **OK**.	

Run QC Expert as a Non-administrator QC Analyst

	Action	Result
1	Click on the **Select Reference** button. Select the **DEET** spectrum by highlighting it. Click **OK**.	

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**. 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.	The DEET safety datasheet and other associated information is displayed. 

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SAFETY DATA SHEET
Version 4.4
Revision Date 07/03/2014
Print Date 08/25/2015

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : *N,N*-Diethyl-3-methylbenzamide

Product Number : D100951
Brand : Aldrich
Index-No. : 616-018-00-2

CAS-No. : 134-62-3

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

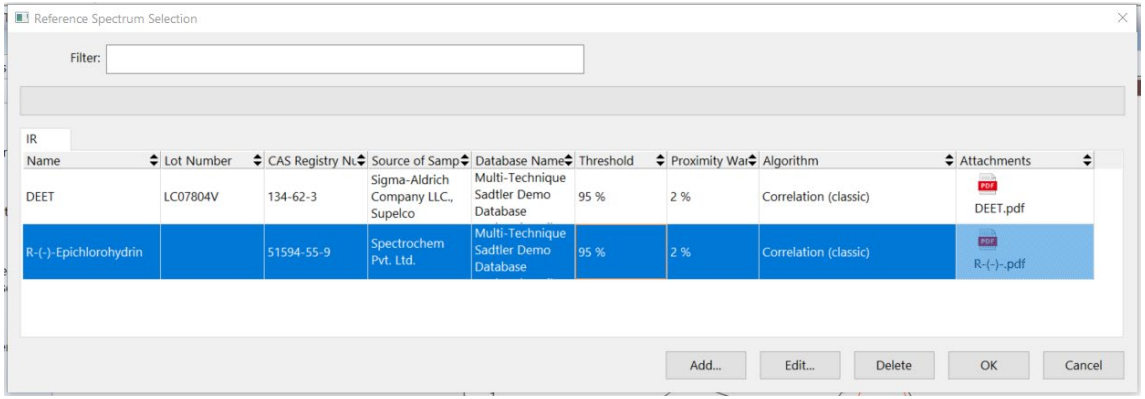
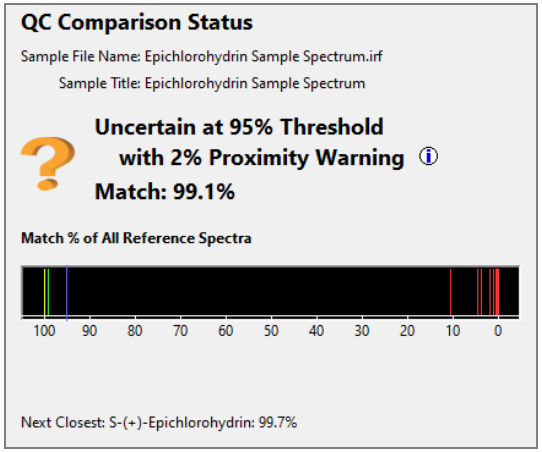
Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

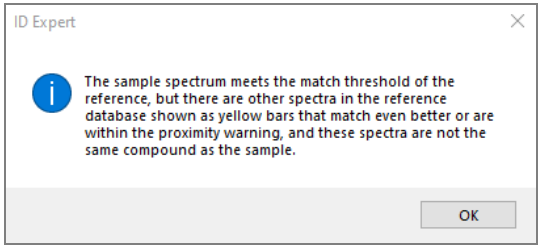
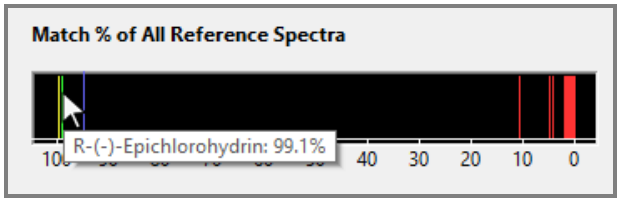
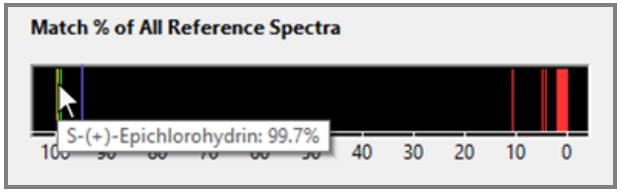
Telephone : +1 800-325-5832
Fax : +1 800-325-5052

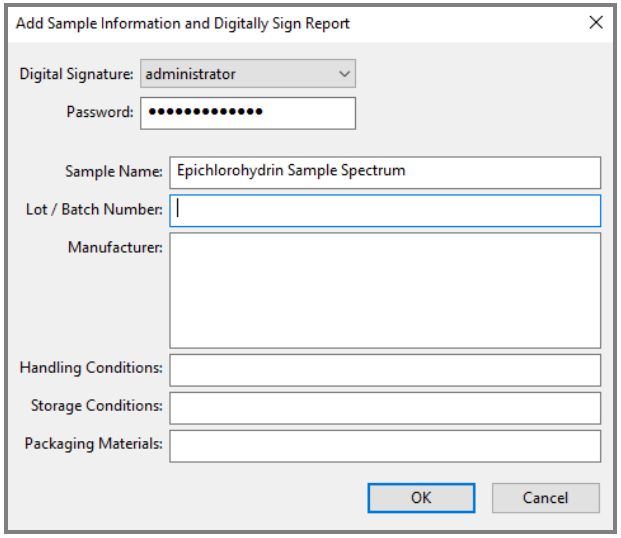
1.4 Emergency telephone number

Emergency Phone # : (314) 776-6555

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

	Action	Result
1	Click on the **Select Reference** button. Select the **R-(-)-Epichlorohydrin** reference spectrum by highlighting it. Click **OK**.	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. 
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**.** Select **Epichlorohydrin Sample Spectrum.irf**. Set **Imported spectrum is** to **ATR-IR** and ensure this option is checked. Click **Open**.	 The Match % between the selected reference spectrum and sample spectrum is excellent at 99.1%, but the QC comparison is **Uncertain**.

3	Click on the information button ⓘ.	 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.
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%**.	 The green bar in the Match % chart indicates the comparison of the sample spectrum to the reference spectrum. The match percent is 99.1%.
7	Mouse over the yellow bar in the Match % Chart. The hover-over text says **S-(+)- Epichlorohydrin: 99.7%**.	 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.

8	Click on **Create Report** button below the Match % chart to create a digitally signed report. Select your username from the **Digital Signatures** drop-down menu. Enter the password. Fill out the sample information.	
9	Click **OK** to view the report.	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

