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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 KnowltAll 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 KnowltAll 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\Q C 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.	KnowltAll Informatics System 2020, Spectroscopy Edition File Edit View License Help Open Query Spectrum Ctrl+O Open Attachment(s) Settings Settings Digital Signature Administration Change Digital Signature Password Create PDF Report Exit Alt+F4
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.	Administrator Verification × Digital Signature: administrator Password: •••••••• OK Cancel



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5	In File > Settings , set the Organization to " Wiley Laboratories, Inc. " and add an address.	Settings General Reference/Validation Databases
		Organization: Wiley Laboratories, Inc.
		Address 1
		Folder for Reports: C:\Users\Public\Documents\W Browse
		Language for Reports: Same as QC Expert V
		OK Cancel Apply



Select Reference Database

	Action	Result
1	Action In the Reference/Validation Databases tab, click the Select by Browsing button. Navigate to C:\Users\Public\Documents\Wiley\KnowltAll\Samples folder. Select the Multi-Technique Sadtler Demo Database - Wiley [DEMO] database.	Settings General Reference/Validation Databases Technique: IR Database Settings Available for Searching: Refresh User ATR-IR - Sadtler Controlled & Pres DWX ATR-IR - Sadtler Controlled & Pres DWX <latest version=""> ATR-IR - Sadtler Controlled & Pres DWX <latest version=""> ATR-IR - Sadtler Controlled & Pres DWX <latest version=""> ATR-IR - Sadtler Controlled & Pres DWX <latest version=""> ATR-IR - Sadtler Controlled & Pres DWX <latest version=""> ATR-IR - Sadtler Controlled & Pres DWX <latest version=""> ATR-IR - Sadtler Controlled & Pres DWX <latest version=""> ATR-IR - Sadtler Controlled & Pres DWX <latest version=""> Attra - Resource Remove Remove Remove All</latest></latest></latest></latest></latest></latest></latest></latest>
		Selected for Searching: Name DB Code Multi-Technique Sadtler Dem DEMOX C\Users\hP\Downloads\KnowltAll 2020 Trai Select by Browsing OK Cancel
2	Click OK .	



3	Click on the Select Reference button at the lower right of the QC Expert window.	QC Expert Image: Sector Status Sample Spectrum Status Checklist Status Noise	. <mark> </mark>	u hat dat dat i t e	×
		QC Comparison Status	Selected Reference Spectrur	n Properties	Structure
					Attachments
		Create Report			Select Reference
4	At the prompt, login as administrator. The Add Reference Spectrum dialog box opens.	Add Reference Spectrum Iechnique: IR Filter: DEET		×	
	Type DEET in the Filter box to search for DEET.	Name C Lot Number CAS	Registry Num? Source of Sample ? Database Name ? 134-52-3 Sigma-Aldrich Multi-Technique Company LLC, Sattler Demo Source - Niew - Niew -		
	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.	Comparison Algorithm: Correlation (classic) Match Threshold: 95 + % Proximity Warning: 2 + %	<u>_</u> ~	OK Cancel	
				Cancer	



The Reference Spectrum Selection dialog box opens. 5 III Reference Spectrum Selection <u>F</u>ilter: Click on Add, and type epi in the Filter box. IR 7 CAS Registry Num7 Source of Sample 7 Database Name 134-62-3 Sigma-Aldrich Company LLC, Supelco Database - Wiley Name COTROL Proximity Wit Algorith 95 % DEET Select R-(-)-Epichlorohydrin and select the Correlation (classic) algorithm. Click OK. Add... <u>E</u>dit... <u>D</u>elete OK Cancel





Run QC Expert as a Non-administrator QC Analyst

	Action						Res	sult				
1	Click on the Select Reference button. Select the DEET spectrum by highlighting it. Click OK .		Reference Spectrum S	Selection								×
		r	Name	Lot Number	CAS Registry Nu	Source of Samp Sigma-Aldrich	Database Name Multi-Technique	Threshold	Proximity War	Algorithm	Attachments	\$
		t		LC07804V	134-62-3	Company LLC., Supelco	Sadtler Demo Database	95 %	2 %	Correlation (classic)	DEET.pdf	
		3	R-(-)-Epichlorohydrin		51594-55-9	Spectrochem Pvt. Ltd.	Multi-Technique Sadtler Demo Database	95 %	2 %	Correlation (classic)	R-(-)pdf	
		P.										
									Add	Edit Delete	ОК	Cancel



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EET safety datasheet and other associated information is displayed.			
MA-ALDRICH	sigma-aldrich.com		
	SAFETY DATA SHEET		

5	5 Double-click on the PDF attachment in the Attachment pane at the lower right.	Th	ne D	DEET safety da	ata	asheet and other associated information is displayed.	
			SIG	MA-ALDRIC	H	signa-aldrich.com SAFETY DATA SHEET Version 4.4 Revision Date 07/03/2014 Print Date 08/25/2015	
			1. PRO	DUCT AND COMPANY	IDEN	NTIFICATION	
			1.1	Product identifiers Product name	:	N,N-Diethyl-3-methylbenzamide	
				Product Number Brand Index-No.		: D100951 : Aldrich : 616-018-00-2	
				CAS-No.	:	: 134-62-3	
		1	1.2 Relevant identified uses of the substance or mixture and uses advised against				
				Identified uses	1	: Laboratory chemicals, Manufacture of substances	
		1.3	1.3	Details of the supplier of	of the	e safety data sheet	
				Company	:	: Sigma-Aldrich 3050 Spruce Street SAINT LOUIS MO 63103 USA	
				Telephone Fax	-	: +1 800-325-5832 : +1 800-325-5052	
			1.4	Emergency telephone n	umb	ber	
				Emergency Phone #	:	: (314) 776-6555	



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

	Action	Result			
1	Click on the Select Reference button.	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.			
	Select the R-(-)-Epichlorohydrin reference spectrum by highlighting it.	Reference Spectrum Selection Filter:			
	Click OK .	IR Name Lot Number CAS Registry NL* Source of Samp Database Name Threshold Proximity War Algorithm Attachments DEET LC07804V 134-62-3 Sigma-Aldrich Company LLC, Supelco Multi-Technique Sadtler Demo Database 95 % 2 % Correlation (classic) Image: Company LC, DEET, pdf R-(-)-Epichlorohydrin 51594-55-9 Spectrochem Pvt. Ltd. Sadtler Demo Database 95 % 2 % Correlation (classic) Image: Company LC, DEET, pdf			
		Add Edit Delete OK Cancel			
2	Click on New Comparison at the mid-left of the QC Expert window.	QC Comparison Status Sample File Name: Epichlorohydrin Sample Spectrum.irf Sample Title: Epichlorohydrin Sample Spectrum			
	Navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\QC Expert folder.	Uncertain at 95% Threshold with 2% Proximity Warning ① Match: 99.1%			
	Select Epichlorohydrin Sample Spectrum.irf.				
	Set Imported spectrum is to ATR-IR and ensure this option is checked.	Next Closest: S-(+)-Epichlorohydrin: 99.7%			
	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 ①.	ID Expert The sample spectrum meets the match threshold of the reference, but there are other spectra in the reference database shown as yellow bars that match even better or are within the proximity warning, and these spectra are not the same compound as the sample. OK
		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% .	Match % of All Reference Spectra 10 R-(-)-Epichlorohydrin: 99.1% 40 30 20 10 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% .	Match % of All Reference Spectra 10 10 10



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.	Add Sample Information and Digitally Sign Report × Digital Signature: administrator Password: ••••••• Sample Name: Epichlorohydrin Sample Spectrum		
		Lot / Batch Number:		
	Enter the password.	Manufacturer:		
	Fill out the sample information.	Handling Conditions: Storage Conditions: Packaging Materials: OK Cancel		
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		
		r age o – mormation about the reference spectrum		

