# Analyze IQ Spectra Manager Version 1.1

Analyze IQ

# **User Manual**

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# 1 Introduction

**Analyze IQ Spectra Manager** is a spectral database and data management package that allows users to manage a library of spectra. **Spectra Manager** includes the following features:

- 1. The user can retrieve and list spectra by IUPAC (International Union of Pure and Applied Chemistry) and common name.
- 2. For mixtures, the user can store all the relevant data, such as concentration and manufacturer of each constituent. Mixtures can also be tracked by material lot numbers.
- 3. The user can store CAS (Chemical Abstracts Service) and registry numbers and QA details.

Once installed, **Spectra Manager** links seamlessly with **Analyze IQ Lab**, allowing users to select data from their database for the development of Analyze IQ models. See *Analyze IQ User Manual* (available for download at the following address: <u>http://www.AnalyzeIQ.com/User-Documentation.html</u>; you must register to access this page) for instructions on how to use **Analyze IQ Lab** in conjunction with **Spectra Manager**.

This guide contains instructions on the use of **Spectra Manager** for managing your collection of spectral data.

**Section 2** describes the **Spectra Manager** installation process, including how to install Spectra Manager on Windows 2000, XP or Vista.

Section 3 briefly describes the data stored in **Spectra Manager** and explains key terms used.

**Section 4** describes the information that is stored in **Spectra Manager** for each spectral sample. It also describes how to modify certain details stored for a spectrum.

**Section 5** details how to add new spectra to **Spectra Manager** and how to enter information about new substances or constituents of a sample. It also describes how to delete existing spectra from **Spectra Manager**.

**Section 6** contains some information about the collection process for the spectral samples that are provided with **Spectra Manager**.

Section 7 contains some information on technical support and sales.



# 2 Installation

As part of installing the **Spectra Manager** package, the following components are installed:

- Microsoft SQL Server 2005, *Express Edition*: used by Spectra Manager as the underlying database software.
- Microsoft .NET Framework 2.0: required for installation of Microsoft SQL Server 2005, *Express Edition*.
- Windows Installer: required for installation of Microsoft .NET framework.

If the same components, or later versions of them, are already installed on your system, they will not be re-installed or you may manually cancel their installation. You may see warnings/errors. Most such errors can be safely ignored, but please do not hesitate to contact Technical Support with any concerns, or if you require assistance with installation of the software. Please refer to Section 7 for contact information.

The instructions below apply to installation under Windows XP and Windows 2000. Please see Section 1.4 for additional information on installing and running Analyze IQ under Windows Vista.

### 2.1 CD or USB Key Installation

To install from CD, insert the Analyze IQ software installation CD into the drive. Follow the instructions presented for the installation of **Spectra Manager**.

Likewise, to install from USB Key, insert it into a USB port and follow the instructions.

If the CD or USB key does not automatically run after being inserted, navigate to the top level of the drive and run **StartHere.exe** file to start the installation.

### 2.2 Website

If you wish to download **Spectra Manager** from the Analyze IQ website, <u>www.AnalyzeIQ.com</u>, you must first register on it. To do so, go to <u>http://www.AnalyzeIQ.com</u> and click on *Register* under the login form. A confirmation email is sent to the address that you entered into the registration form. This confirmation email includes a link for activating your new Analyze IQ account.

After you have registered as a user, the **Spectra Manager** setup file can be downloaded at the following address: <u>http://www.AnalyzeIQ.com/ Download.html</u>. Note that you must log in with your registered username before being given access to the download area. After downloading the setup file, start the installation process by double-clicking on the file.



### 2.3 Get License Key

At the end of the installation process, you will have the option to 'Get **Spectra Manager** License', which requires an internet connection. This final step must be carried out in order to be able to run **Spectra Manager**. You can decide to defer the retrieval of a license key until a later time. If you defer, you will need to retrieve a license key subsequently by running the *Get Spectra Manager License* program, found under the **Analyze IQ Spectra Manager** program group: click on *Start->All Programs->Analyze IQ->Spectra Manager*.

If you are installing an evaluation copy of the software, you will use your registered username to retrieve a license key after you install the software. Otherwise, you will use a Purchase Order code that is given to you by Analyze IQ Ltd. after purchasing the software.

## 2.4 Installing Under Windows Vista

Under Windows Vista, **Spectra Manager** needs to be installed in Administrator mode.

### 2.4.1 Installing Under Vista

When installing **Spectra Manager** under Windows Vista, right-click on the setup file (either that you have downloaded from the website, or on the installation CD or USB key) and select **Run as administrator** (see Figure 1). You can then proceed to run the installer program as usual.



Figure 1: Under Windows Vista, the Setup program must be run as Administrator

### 2.4.2 User Account Control

Depending on the configuration of your Windows Vista system, it may be necessary to turn **User Account Control** off for the duration of the installation. It may be



turned back on afterwards; it does not need to be off when running **Spectra Manager**.

Step 1: Go to Control Panel: Select User Accounts (see Figure 2).



Figure 2: Under Windows Vista, selecting User Accounts in the Control Panel

Step 2: In User Accounts: *Turn User Account Control off* (see Figure 3).



Figure 3: Under Windows Vista, turning off User Account Control

After installation is finished, you can go through the same sequence of steps to turn User Account Control back on.

# 3 Data stored in Spectra Manager Database

**Spectra Manager** stores a list of spectra, where each spectrum is assigned a unique ID within the database. In addition to storing the frequency and spectral intensity for each data point in the spectrum, **Spectra Manager** maintains information related to the sample for which the spectrum was recorded:

- It stores a list of *substances*, where a substance is a compound that is defined by a CAS number and an IUPAC name.
- It stores a list of *constituents*, where a constituent refers to a particular specimen of a substance and is described by the following properties: *Substance, Manufacturer, Lot Number, Catalog Number, Purity, Location* and *Date Opened*. Note that apart from substance, the other properties of a constituent may be unspecified. For example, a substance with IUPAC name Acetonitrile and CAS Number 000075-05-8 is stored in the **Spectra Manager** list of substances. A sample of Acetonitrile manufactured by Aldrich with 99% purity and Lot Number 3725 is an example of one constituent. For each substance recorded in **Spectra Manager**, one or more constituents are also recorded.
- A spectrum represents either a *pure* sample, which comprises a single constituent at 100% concentration, or a *mixture* of two or more constituents, where the sum of the constituent concentrations is equal to 100%.

**Spectra Manager** is shipped with spectral data, comprising a set of spectra, constituents and substances. Users may insert new spectra into the **Spectra Manager** database. To insert a new spectrum, details of the sample constituents and their corresponding substances must be provided. In providing these details, a user may be choose from the existing list of constituents and substances stored in **Spectra Manager** or enter information for a new constituent or substance. See Section 5.1 for detailed instructions on how to add a spectrum to **Spectra Manager**.

If you purchase the **Analyze IQ Raman Library**, all of its spectra and associated information are included in **Spectra Manager** when you install it. Whether or not you purchase this library, you can always add your own collection of additional spectra (from Raman or any other form of spectroscopy) to **Spectra Manager**.



# **4** Viewing Data Stored in Spectra Manager

### 4.1 Launching Spectra Manager

When **Spectra Manager** is launched, the current list of spectra is shown in the lefthand pane, as in the example of Figure 4. This list shows the ID (each spectrum in the database is assigned a unique ID), whether it is a mixture or pure sample and lists the constituents of the sample (or a single constituent if a pure sample) that the spectrum was recorded for. By selecting the checkboxes under the spectrum list, it can be filtered to show only pure samples, mixtures or all samples.



Figure 4: The Opening Screen of Spectra Manager



### 4.2 File Formats

Analyze IQ Spectra Manager supports three file formats.

- 1. SPC: Thermo-Electron GRAMS SPC file format.
- 2. *SpectroML:* NIST's XML-based format for spectroscopy and chromatography data.
- 3. *AIQ:* The .AIQ file format is used to store data in a suitable format for Analyze IQ. It is also used in Instrument Interfaces. AIQ files use an XML format that is almost a subset of the NIST SpectroML format, **except** that it has an added property, instrumentSetting.excitationLine, that does not occur in SpectroML.

### 4.3 Spectrum Details

Select a spectrum in the list to view its details. Figure 5 shows the details of the spectrum of a mixture.

🔇 Ana	lyze IQ !	Spectra	Manager					_ 🗆 🖂
File He	elp							
Spec	trum List							
This li	ist contains	all the s	pectra found in the database			Spectrum Details Constit	spectrum	Plot
	10	Time		Trees	Acotonitrile	nol·Wator(10:80)	10) - Mixturo G	Sample
	10	Type	2 Deserves Methodels Weter	Insert	Acetonicinemetha	101. Water (10.00.	iu) mixture :	ampie
₩	2244	Mixt	2-Propanone; Methanol; Water	Delete	Spectral Acquisition Details		Log Details	
₩.	2245	Plixt	Ethapedioic acid, ammonium salt, h		The items in blue cannot be changed.		Details from the spect	trum file
l 🐳	2248	Pure	Acetonitrile		You can edit items in black and p	ress 'Update Spectrum'.	Sample Label	Acetonitrile:Methanol:Water(10:80:1
l 🕁	2249	Mixt	Acetonitrile; Methanol		Spectrum filename	MP28JULY2006-L4.SPC		
	2250	Mixt	Acetonitrile; Methanol; Water		Date of collection	28/07/2006	Grating (lines/mm)	
<b>☆</b>	2251	Mixt	Acetonitrile; Methanol; Water			2010112000	Excitation Line (nm)	785
	2252	Mixt	Acetonitrile; Methanol; Water		Time of collection	11:48	Spec Width (cm-1)	
	2253	Pure	8-Quinolinol				Annah un Cattina	
	2254	Mixt	Acetonitrile; Methanol; Water		Number of spectra collected	1	Aperture Setting	
	2257	Pure	1,2,3-Propanetricarboxylic acid, 2		Instrument model	RamanStn	Objective Lens	
II  ¥	2258	Mixt	Acetonitrile; Methanol; Water		Wavenumber range sampled		Mixture Details	
II   ₩	2261	MIXt	Acetonitrile; Methanol; Water		Main m	250.0	1	
₩	2202	Mixt	Acetonitrile; Methanol; Water		Minimum	250.0	Mixture prepared by	MP
₩	2205	Mixt	Acetonitrile: Methanol: Water		Maximum	3200.0	Date of preparation	28/07/2006
H 🕂	2265	Pure	Acetic acid, ammonium salt (1:1)		Number of data points	1476	Notes about preparat	tion
l 🔶	2269	Mixt	Acetonitrile; Methanol; Water					
↔	2271	Mixt	Acetonitrile; Methanol		Collected by	Maricea Phelan	1	
	2272	Pure	3-Pyridinecarboxamide		Collected by	Pidrissa Priciali	]	
III 1 ₩	2273	Mixt	Acetonitrile; Methanol; Water		Spectral acquisition time (secs.)	21		
	2274	Mixt	Acetonitrile; Methanol; Water		Scans acquired per spectrum	21	]	
	2275	Mixt	Acetonitrile; Methanol; Water		Δvis labels		1	
	2277	Pure	3-Pyridinecarboxylic acid					
	2278	Mixt	Acetonitrile; Methanol; Water	′			1	
X	2279	Mixt	Acetonitrile; Methanol		Entered in database by	Lena Karlson		
	2280	Pure	1H-Indene-1,3(2H)-dione, 2,2-dih		Entered date	30/11/2006	]	
l ¥	2281	MIXt	Acetonitrile; Methanol; Water					
	2203	Dure	2-Butenedioic acid (2E)-					
l l ↔	2286	Mixt	Acetonitrile: Methanol: Water		Notes			
	2200	8.40.14						~
<								~
PI	ure							
М 🗹 м	ixture							

**Figure 5: View Spectrum Details** 

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The Spectrum Details view has four main sections, as listed below.

#### **1.** Spectral Acquisition Details

This includes data that was automatically entered into the database from the Spectrum file (this cannot be edited) and information recorded during the entry of the spectral sample into **Spectra Manager**:

- **Spectrum filename:** The spectrum file name from which the spectrum was imported.
- *Date of collection:* The date the spectrum was recorded.
- *Time of collection:* The time the spectrum was recorded.
- Number of spectra collected: The number of spectra collected.
- *Instrument:* Name assigned to the instrument used to record the spectrum.
- *Wavenumber range sampled:* The minimum and maximum wavenumber over which the spectrum was recorded.
- *Number of data points:* Number of data points in the spectrum.
- *Collected by:* Name of person who recorded the spectrum.
- **Spectral acquisition time (secs):** Duration of spectral acquisition in seconds.
- **Scans acquired per spectrum:** Number of scans acquired for this spectrum.
- Axis Labels: X and Y axis labels.
- *Entered in database by:* Name of person who entered this spectrum into **Spectra Manager**.
- *Entered date:* Date of entry of this spectrum into **Spectra Manager**.

#### 2. Log Details

This data is extracted from the *Log* section of the spectrum file from which the spectrum was imported:

- *Sample Label:* Name given to this sample.
- *Grating:* For dispersive spectrometers, the choice of diffraction
- Grating used during analysis, expressed in lines/millimetre, e.g. 50 lines/mm and 1800 lines/mm.
- *Excitation Line:* The wavelength, in nanometres, of the spectrometer, e.g. 785.
- **Spec. Width:** For dispersive spectrometers, the width of the slit that the dispersed scattered signal is passed through. This determines the frequency resolution of the spectrum. For example, a spectrum recorded at an interval of  $350-2000 \text{ cm}^{-1}$  (1650 channels) with a confocal aperture setting of 200 micrometres, using a 950 lines per mm grating, gives a spectral resolution of ~1 cm<sup>-1</sup>.

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- *Aperture Setting:* The confocal aperture setting, expressed in micrometres.
- *Objective Lens:* The choice of objective lens used to magnify and illuminate the sample with laser light, e.g. 10x, 40x, 50x or 100x.

#### 3. Mixture Details

This section only applies to the spectra of mixtures:

- *Mixture prepared by:* Name of person who prepared this mixture.
- **Date of preparation:** Date on which the sample was prepared.
- *Notes about preparation:* Additional notes about the mixture preparation.

#### 4. Notes

This section is used to record additional information that may be of benefit to an analyst. An example entry is "The material had a yellow colour that might indicate decomposition of the material."

#### **4.3.1 Edit Spectrum Details**

When viewing spectrum details as shown in the screenshot of Figure 6, the details with black labels can be changed by the user, whereas those with blue labels cannot be changed after the spectrum has been initially inserted. For example, to change the *Notes about preparation* entry, select the textbox beside this label. As soon as a textbox is edited, an *Update Spectrum* button appears at the bottom right-hand corner of the window, as shown in Figure 6. After you have finished editing a textbox, click on the *Update Spectrum* button to apply the change.



					Spectrum Details Constitu	uent Details Spectrum	n Plot
is list contai	ns all the s	pectra found in the database					
ID	Туре	Constituents	Insert	Methanol:Tetrahyd	rofuran:Water(50	):10:40) - Mixt	ure Sample
2344	Mixt	Furan, tetrahydro-; Methanol; Water	Delete	Spectral Acquisition Details		Log Details	
2345	Mixt	Furan, tetrahydro-; Methanol; Water	Delete	The items is blue second by shoe		Details from the second	hum film
2346	Mixt	Furan, tetrahydro-; Methanol; Water		You can edit items in black and p	geo. ress 'Update Spectrum'.	Details from the speci	dum nie
2347	Mixt	Furan, tetrahydro-; Methanol; Water				Sample Label	Methanol:Tetrahydrofuran:Water
2349	Pure	Acetamide, N-(4-hydroxyphenyl)-		Spectrum filename	MP29JULY2006-M10.SPC	Grating (lines/mm)	
2350	Mixt	Furan, tetrahydro-; Methanol; Water		Date of collection	29/07/2006	ordang (incorning	
2351	Mixt	Furan, tetrahydro-; Methanol; Water				Excitation Line (nm)	785
2352	Mixt	Furan, tetrahydro-; Methanol; Water		Time of collection	18:47	Spec Width (cm-1)	
2354	Mixt	Furan, tetrahydro-; Methanol; Water					
2355	Mixt	Furan, tetrahydro-; Methanol		Number of spectra collected	1	Aperture Setting	
2357	Mixt	Furan, tetrahydro-; Methanol; Water				Objective Lens	
2358	Mixt	Furan, tetrahydro-; Methanol; Water		Instrument model	Ramanstn		
2359	Mixt	Furan, tetrahydro-; Methanol; Water		Wavenumber range sampled		Mixture Details	
2360	Mixt	Furan, tetrahydro-; Methanol; Water		Minimum	250.0	Mixture propered by	MD
2361	Mixt	Furan, tetrahydro-; Methanol			2200.0	Mixture prepared by	414
2362	Mixt	Furan, tetrahydro-; Methanol; Water		Maximum	3200.0	Date of preparation	29/07/2006
2363	Pure	Benzenemethanol, 4-chloro-		Number of data points	1476	Notes about prepara	tion Mixture prepared over 2 day
2364	Mixt	Furan, tetrahydro-; Methanol; Water					mixture prepared over 2 day
2366	Pure	2-Propenoic acid, 3-(4-hvdroxy-3		Collected by	Maxima Dhalan		
2367	Pure	a-D-Glucopyranose, 4-Q-(2,3,4,6		Collected by	Marissa Phelan		
2368	Pure	Benzoic acid. 2-formyl-		Spectral acquisition time (secs.)	21		
2369	Pure	Benzonitrile 4-hydroxy-		Scape acquired per exectrum	21		
2370	Dure	Benzonitrile, 4-chloro-		Scans acquired per spectrum	21		L
2370	Dure	1.2.3-Propagetricarboxylic acid 2-		Axis labels	X:Raman Shift (cm-1) Y: I		
> 2371	Duro	1,2,3 Propanetrial				7.17]	1.
2074	Pure	1,2,3-Propanetrio		Entered in database by	Lees Karlees	When	updating, this entr
23/3	Pure	Furan tatrahudra		Lintered in database by	Lena Adrison	button	appears
2380	Pure	Furan, tetranyoro-		Entered date	30/11/2006	button	appears 1
p' 2382	Pure	Benzene					1
p 2383	Pure	Methane, trichloro-					1
2385	Pure	1,4-Dioxane		Notes			
2387	Pure	Ethane, 1, 1, 1-trichloro-					
2200	D						1
			1				
Pure							

**Figure 6: Edit Spectrum Details** 



## 4.4 Constituent Details

After launching **Spectra Manager**, when a spectrum is selected in the list, the Spectrum Details are displayed by default. To view the details of the constituents of the sample associated with a particular spectrum, select the spectrum and click on the *Constituent Details* button, as shown in Figure 7. Figure 7 shows the constituent details for a mixture of Acetonitrile, Methanol and Water. The *Sample Details* sections lists information about the sample as a whole: the sample state (liquid, gas or solid), colour, consistency and smell. The notation "N/R" entered for consistency and smell in Figure 7 indicates "Not Recorded". The *Constituents* section lists each constituent in a mixture and the *Details for...* section on the right shows the details for the currently selected constituent. In Figure 7, the Acetonitrile constituent has been selected. The following details for a constituent are displayed:

- CAS Number
- IUPAC Name
- Common Names List: this list can be edited by the user; See Section 4.4.1
- Manufacturer of the constituent material
- Catalog number
- Lot Number
- Date Opened
- Purity
- Location

Spectrum list         Spectrum list         The list contains all the spectra found in the database         ID       Type Constituents         Determine the database         Sample Details         Sample Details         Sample Details         Sample Details for Accounties         Constituents         Details for Accounties         Constituents         Constituents         Constituents         Constituents         Constituents         Constituents         Constituents         Constituents <th col<="" th=""><th>《 Analyze IQ</th><th>Spectra</th><th>a Manager</th><th></th><th></th><th></th><th></th><th></th><th></th><th></th><th>_</th><th></th></th>	<th>《 Analyze IQ</th> <th>Spectra</th> <th>a Manager</th> <th></th> <th></th> <th></th> <th></th> <th></th> <th></th> <th></th> <th>_</th> <th></th>	《 Analyze IQ	Spectra	a Manager								_		
Spectrum List         This list contains all the spectra found in the database         Matter contains all the spectra found in the database         Matter contains all the spectra found in the database         Matter contains all the spectra found in the database         Matter contains all the spectra found in the database         Matter contains all the spectra found in the database         Matter contains all the spectra found in the database         Matter contains all the spectra found in the database         Matter contains all the spectra found in the database         Matter contains all the spectra found in the database         Matter contains all the spectra found in the database         Matter contains all the spectra found in the database         Matter contains all the spectra found in the database         Matter contains all the spectra found in the database         Matter contains all the spectra found in the database         Spectrum Details       Constituent Contains and the spectra found in the database         Matter contains all the spectra found in the database         Matter contains all the spectra found in the database         Matter contains all the spectra found in the database <th co<="" td=""><td>File Help</td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></th>	<td>File Help</td> <td></td>	File Help												
Interfactor during the database         Interfactor during the database <t< td=""><td>Spectrum Lis</td><td>+</td><td></td><td></td><td>1</td><td></td><td></td><td>-</td><td></td><td></td><td></td><td></td></t<>	Spectrum Lis	+			1			-						
ID       Type       Constituents       Inserturi	This list contain	ns all the s	spectra found in the database					Spe	ctrum Details Constit	uent Details Spectrun	Plot			
Display     Display     Display     Display       2234     Mich		Tune	Canadity canta	A Tasart	An	Acotonitrilo:Mothanol:Water(10:90:10) - Mixture Sample								
W Lizzasi       Programore, Nethanoj, Water         W Lizzasi       Actonitrile, Methanoj, Water         W Lizzasi       Mit	↔ 2224	Mixt	2 Dreppeners Methapple Water	Insert	1	ctonic	. inclusion	ununon	uutei(10.00.1	oj mixture o	umpic			
<sup>1</sup> / <sub>2</sub> 223 <sup>1</sup> / <sub>2</sub> Mixt <sup>2</sup> / <sub>2</sub> Proparance; Methanol; Water <sup>1</sup> / <sub>2</sub> 223 <sup>1</sup> / <sub>2</sub> Mixt <sup>2</sup> / <sub>2</sub> Proparance; Methanol; Water <sup>1</sup> / <sub>2</sub> 2240 <sup>1</sup> / <sub>2</sub> Mixt <sup>2</sup> / <sub>2</sub> Proparance; Methanol; Water <sup>1</sup> / <sub>2</sub> 2240 <sup>1</sup> / <sub>2</sub> Mixt <sup>2</sup> / <sub>2</sub> Proparance; Methanol; Water <sup>1</sup> / <sub>2</sub> 2240 <sup>1</sup> / <sub>2</sub> Mixt <sup>2</sup> / <sub>2</sub> Proparance; Methanol; Water <sup>1</sup> / <sub>2</sub> 2247 <sup>1</sup> / <sub>2</sub> Pire <sup>1</sup> / <sub>2</sub> Ethanol; Methanol; Water <sup>1</sup> / <sub>2</sub> 2247 <sup>1</sup> / <sub>2</sub> Pire <sup>1</sup> / <sub>2</sub> Actonitrile; Methanol; Water <sup>1</sup> / <sub>2</sub> 2247 <sup>1</sup> / <sub>2</sub> Pire <sup>1</sup> / <sub>2</sub> Actonitrile; Methanol; Water <sup>1</sup> / <sub>2</sub> Constituents <sup>1</sup> / <sub>2</sub> 2250 <sup>1</sup> / <sub>Mixt</sub> Actonitrile; Methanol; Water <sup>1</sup> / <sub>2</sub> Mixt         Actonitrile; Methanol; Water <sup>1</sup> / <sub>2</sub> 2250 <sup>1</sup> / <sub>Mixt</sub> Actonitrile; Methanol; Water <sup>1</sup> / <sub>2</sub> Mixt         Actonitrile; Methanol; Water <sup>1</sup> / <sub>2</sub> 2250 <sup>1</sup> / <sub>Mixt</sub> Actonitrile; Methanol; Water <sup>1</sup> / <sub>2</sub> Mixt         Actonitrile; Methanol; Water <sup>1</sup> / <sub>2</sub> 2257 <sup>1</sup> / <sub>Mixt</sub> Actonitrile; Methanol; Water <sup>1</sup> / <sub>2</sub> Mixt         Actonitrile; Methanol; Water      <	₩ 2234	Mixt	2-Propanone: Methanol: Water	Delete	Sam	ple Deta	ails							
	2236	Mixt	2-Propanone: Methanol: Water		San	nle State	Liquid							
<sup>†</sup> 2239        Pure        Carbonic add sodum salt (1:1) <sup>†</sup> Constituents <sup>†</sup> 2249         Mixt	2237	Mixt	2-Propanone; Methanol; Water			pie o to te	angara -					=		
	Sec. 2239	Pure	Carbonic acid sodium salt (1:1)		Cold	bur	Clear							
<sup>1</sup> 2241 <ul> <li>Mixt 2-Propanne; Methanol; Water</li> <li>2:43 Pure Sufficie add potassium salt (1:2)</li> <li>2:44 Mixt 2-Propanne; Methanol</li> <li>2:44 Mixt 2-Propanne; Methanol</li> <li>2:45 Mixt 2-Propanne; Methanol</li> <li>2:45 Mixt 2-Propanne; Methanol</li> <li>2:44 Mixt 2-Propanne; Methanol</li> <li>2:45 Mixt Acetonitie; Methanol; Water</li> <li>2:42 Mixt Acetonitie; Methanol; Water</li> <li>2:2:5 Mixt Acetonitie; Methanol; Water</li> <li>2:2:2: Mixt Acetonit</li></ul>	2240	Mixt	2-Propanone; Methanol; Water		Con	isistency	N/R							
<sup>1</sup> 2243        Pure         Sufficic acid potassium selt (1:2) <sup>1</sup> 2244         Mixt <sup>2</sup> 24ropanone; Methanol        Water <sup>1</sup> 2244         Mixt <sup>1</sup> Accontrile; Methanol        Constituents of this sample <sup>1</sup> 2249         Mixt         Accontrile; Methanol        Manufacturer <sup>1</sup> 2249         Mixt         Accontrile; Methanol        Mathanol <sup>1</sup> 2250         Mixt         Accontrile; Methanol         Water <sup>1</sup> 2046 <sup>1</sup> 2252         Mixt         Accontrile; Methanol; Water <sup>1</sup> Methanol <sup>1</sup> 80% <sup>1</sup> 2253         Mixt         Accontrile; Methanol; Water <sup>1</sup> Methanol <sup>1</sup> 80% <sup>1</sup> 2253         Mixt         Accontrile; Methanol; Water <sup>1</sup> Methanol <sup>1</sup> 80% <sup>1</sup> 2253         Mixt         Accontrile; Methanol; Water <sup>1</sup> Methanol <sup>1</sup> 80% <sup>1</sup> 2255         Mixt         Accontrile; Methanol; Water <sup>1</sup> Methanol <sup>1</sup> 80% <sup>1</sup> 2255         Mixt         Accontrile; Methanol; Water <sup>1</sup> 10% <sup>1</sup> 2255         Mixt         Accontrile; Methanol; Water <sup>2</sup> 2271         Mix	2241	Mixt	2-Propanone; Methanol; Water		Smr	-	N/R							
	2243	Pure	Sulfuric acid potassium salt (1:2)											
	2244	Mixt	2-Propanone; Methanol; Water									_		
• 2247         Pure         Ethanedicic codd, ammonium salt, h           Constituent details can be changed, except for the         Markaturer         Constituent details can be changed, except for the         Markaturer         Castomitrile; Methanol;         Water         V 2250         Mixt Acetonitrile; Methanol; Water         V 2252         Mixt Acetonitrile; Methanol; Water         V 2253         Mixt Acetonitrile; Methanol; Water         V 2254         Mixt Acetonitrile; Methanol; Water         V 2255         Mixt Acetonitrile; Methanol; Water         V 2257         Pure         1,2,3-Propaneticarboxylic add, 2         V Water         10%         Water         10%         Vater         10%         Vater         Common Names         Castomitrile         Common Names         CAs =         000075-05-0         LIPAC Name         Common Names         CAs =         000075-05-0         LIPAC Name         Acetonitrile         Vater         Vater         Vater         Vater         Vater         Vater         Vater         Vater         Vater         Common Names         Common Names         Castomitrile         Common Names         CAs =         Common Names         CAstonitrile         Vater         Vater         Vater         Vater         Vater         Vater         Common Names         Common Names         LIPAC Name         Vanoethanee         Vanoethanee         Common Names         LipAc Name         Lip	2245	Mixt	2-Propanone; Methanol		Con	stituent	s			Details for Aceton	trile	^		
Pure       Acetonitrie; Methanol         V 2248       Mixt Acetonitrie; Methanol; Water         V 2250       Mixt Acetonitrie; Methanol; Water         V 2251       Mixt Acetonitrie; Methanol; Water         V 2253       Pure       8-Quinolinol         V 2254       Mixt Acetonitrie; Methanol; Water	*p 2247	Pure	Ethanedioic acid, ammonium salt, h		The	list displa	ys all of the	constituents	of this sample	Constituent details ca	an be changed, except for the			
x 2249       Mixt       Acetonitrile, Methanoly Water         x 2251       Mixt       Acetonitrile, Methanoly Water         x 2252       Mixt       Acetonitrile, Methanoly Water         x 2252       Mixt       Acetonitrile, Methanoly Water         x 2253       Mixt       Acetonitrile, Methanoly Water         x 2254       Mixt       Acetonitrile, Methanoly Water         x 2255       Mixt       Acetonitrile, Methanoly Water         x 2256       Mixt       Acetonitrile, Methanoly Water         x 2255       Mixt       Acetonitrile, Methanoly Water         x 2256       Mixt       Acetonitrile, Methanoly Water         x 2257       Pure       Acetonitrile, Methanoly Water         x 2258       Mixt       Acetonitri	*p* 2248	Pure	Acetonitrile			IUPA	C Name	Conc.	Common Name	Manufacturer				
R 2200       MALL. Actionitie; Methanol; Water         V 2251       Mixt Actionitie; Methanol; Water         V 2253       Pure       8-Quinlinol         V 2254       Mixt Actionitie; Methanol; Water         V 2257       Pure       1,2,3-Propanetricarboxylic add, 2         V 2258       Mixt Actionitie; Methanol; Water         V 2257       Pure       1,2,3-Propanetricarboxylic add, 2         V 2258       Mixt Actionitie; Methanol; Water         V 2251       Mixt Actionitie; Methanol; Water         V 2255       Mixt Actionitie; Methanol; Water         V 2256       Mixt Actionitie; Methanol; Water         V 2257       Mixt Actionitie; Methanol; Water         V 2272       Pure       Actionitie; Methanol; Water         V 2272       Mixt Actionitie; Methanol; Water         V 2272       Mixt Actionitie; Methanol; Water         V 2272       Mixt Actionitie; Methanol; Water         V 2277       Pure         V Pure       Puridinecarboxylic add	₩ 2249	Mixt	Acetonitrile; Methanol: Water		6	Aceto	nitrile	10%	Acetonitrile.Cvan	CAS #	000075-05-8			
Witter       Weter       10%       Water         Water       10%       Water	₩ 2250	Mixt	Acetonitrile: Methanol: Water			<ul> <li>Metha</li> </ul>	anol	80%	Methanol (BDH-2	IUPAC Name	Acetonitrile			
<sup>2</sup> 2233        Pure <sup>8</sup> 4Quinolind <sup>2</sup> 2234 <sup>1</sup> Mixt         Acetonitrile; Methanol; Water <sup>2</sup> 2237 <sup>1</sup> Pure <sup>2</sup> 2235 <sup>1</sup> Mixt         Acetonitrile; Methanol; Water <sup>2</sup> 2238 <sup>2</sup> 2235 <sup>1</sup> Mixt         Acetonitrile; Methanol; Water <sup>2</sup> 2237 <sup>1</sup> Mixt         Acetonitrile; Methanol; Water <sup>2</sup> 2235 <sup>1</sup> Mixt         Acetonitrile; Methanol; Water <sup>2</sup> 2235 <sup>1</sup> Mixt         Acetonitrile; Methanol; Water <sup>2</sup> 2255 <sup>1</sup> Mixt         Acetonitrile; Methanol; Water <sup>1</sup> Mixt         Acetonitrile; Methanol; Water <sup>2</sup> 2256 <sup>1</sup> Mixt         Acetonitrile; Methanol; Water <sup>1</sup> Methane, cyano- <sup>2</sup> 2255 <sup>1</sup> Mixt         Acetonitrile; Methanol; Water <sup>1</sup> Methane, Water <sup>2</sup> 2259 <sup>1</sup> Mixt         Acetonitrile; Methanol; Water <sup>1</sup> Mixt         Acetonitrile; Methanol; Water <sup>2</sup> 2273 <sup>1</sup> Mixt         Acetonitrile; Methanol; Water <sup>1</sup> Mixt         Acetonitrile; Methanol; Water <sup>2</sup> 2273 <sup>2</sup> Mixt         Acetonitrile; Methanol; Water <sup>1</sup> Mixt         Acetonitrile; Methanol; Water	2252	Mixt	Acetonitrile: Methanol: Water			<ul> <li>Wate</li> </ul>	r	10%	Water		Acetonialie			
<sup>1</sup> 2254 <sup>1</sup> Mixt Actonitrile; Methanol; Water <sup>1</sup> 1,2,3-Propanetricarboxylic add, 2 <sup>1</sup> 2257 <sup>1</sup> Pure <sup>1</sup> 1,2,3-Propanetricarboxylic add, 2 <sup>1</sup> 2257 <sup>1</sup> Mixt Actonitrile; Methanol; Water <sup>1</sup> 2258 <sup>1</sup> Mixt Actonitrile; Methanol; Water <sup>1</sup> 2255 <sup>1</sup> Mixt Actonitrile; Methanol; Water <sup>1</sup> 2256 <sup>1</sup> Mixt Actonitrile; Methanol; Water <sup>1</sup> 2256 <sup>1</sup> 2257 <sup>1</sup> Mixt Actonitrile; Methanol; Water <sup>1</sup> 2257 <sup>1</sup> Mixt Actonitrile; Methanol; Water <sup>1</sup> 2257 <sup>1</sup> Mixt Actonitrile; Methanol; Water <sup>1</sup> 2257 <sup>1</sup> 2258 <sup>1</sup> Mixt Actonitrile; Methanol; Water <sup>1</sup> 2227 <sup>1</sup> Mixt Actonitrile; Methanol; Water <sup>1</sup> 2277 <sup>1</sup> Mixt Actonitrile; Methanol; Wa	2253	Pure	8-Ouinolinol											
<sup>†</sup> 2257 <sup>†</sup> Pure <sup>†</sup> Common Names List <sup>†</sup> Actionitifie; Methanol; Water <sup>†</sup> Pure <sup>†</sup> Common Names List <sup>†</sup> Actionitifie; Methanol; Water <sup>†</sup> Pure <sup>†</sup> Common Names List <sup>†</sup> Actionitifie; Methanol; Water <sup>†</sup> Pure <sup>†</sup> Common Names List <sup>†</sup> Actionitifie; Methanol; Water <sup>†</sup> <sup>†</sup> 2256 <sup>†</sup> Pure <sup>†</sup> Pure <sup>†</sup> Common Names List <sup>†</sup> <sup>†</sup> Actionitifie; Methanol; Water <sup>†</sup>	2254	Mixt	Acetonitrile; Methanol; Water											
<sup>1</sup> 2258        Mixt Acetonitrile; Methanol; Water <sup>1</sup> Cyanomethane <sup>1</sup> Cyazon	2257	Pure	1,2,3-Propanetricarboxylic acid, 2							Common Names List	Acetonitrile cluster	ā 🛛		
<sup>1</sup> 2251 <sup>1</sup> Mixt Acetonitrile; Methanol; Water <sup>1</sup> 2252 <sup>1</sup> Mixt Acetonitrile; Methanol; Water <sup>1</sup> 2255 <sup>1</sup> Mixt Acetonitrile; Methanol; Water <sup>1</sup> 2256 <sup>1</sup> Mixt Acetonitrile; Methanol; Water <sup>1</sup> 2256 <sup>1</sup> Mixt Acetonitrile; Methanol; Water <sup>1</sup> 2256 <sup>1</sup> Mixt Acetonitrile; Methanol; Water <sup>1</sup> 2257 <sup>1</sup> Mixt Acetonitrile; Methanol; Water <sup>1</sup> 2257 <sup>1</sup> Mixt Acetonitrile; Methanol; Water <sup>1</sup> 2227 <sup>1</sup> Mixt Acetonitrile; Methanol; Water <sup>1</sup> 2277 <sup>1</sup> Pure <sup>2</sup> Pure <sup>2</sup> - <sup>2</sup> - <sup>2</sup> - <sup>2</sup> - <sup></sup>	2258	Mixt	Acetonitrile; Methanol; Water								Cyanomethane	-		
Image: See 2822       Mixt Acetonitrie; Wethano; Water         Image: See 2825       Mixt Acetonitrie; Wethano; Water         Image: See 2827       Mixt Acetonitrie; Wethano; Water	2261	Mixt	Acetonitrile; Methanol; Water								Ethanenitrile	1		
<sup>1</sup> 2263 <sup>1</sup> Witt Acetonitrik: Methanol; Water <sup>1</sup> 2265 <sup>1</sup> Pure Acete: acid, ammonium salt (1:1) <sup>1</sup> 2266 <sup>1</sup> Pure Acete: acid, ammonium salt (1:1) <sup>1</sup> 2227 <sup>1</sup> Witt Acetonitrik: Methanol; Water <sup>1</sup> 2277 <sup>1</sup> Vitt Acetonitrik: Methanol; Mater <sup>1</sup> 2277 <sup>1</sup> Vitt Acetonitrik: Methanol; Mater <sup>1</sup> 2277 <sup>1</sup> Vitt Acetonintrik: Methanol; Mater <sup>1</sup> 2277 <sup>1</sup> V	2262	Mixt	Acetonitrile; Methanol; Water								Methane, cyano-	_		
W 2265       Mixt Actionitrie; Wethanol; Water         Y 2266       Pure Acetic add, amonumus salt (1:1)         Y 2269       Mixt Actionitrie; Methanol; Water         Y 2271       Mixt Actionitrie; Methanol; Water         Y 2273       Mixt Actionitrie; Methanol; Water         Y 2273       Mixt Actionitrie; Methanol; Water         Y 2277       Pure 3-Pyridinecarboxylic acid         Y 2277       Pure 3-Pyridinecarboxylic acid         Y Pure	2263	Mixt	Acetonitrile; Methanol; Water								Methanecarbonitrile			
<sup>™</sup> 2266        Pure <sup>™</sup> Acetonitrile; Methanol; Water <sup>™</sup> 2273 <sup>™</sup> Mixt Acetonitrile; Methanol; Water <sup>™</sup> 2273 <sup>™</sup> Mixt Acetonitrile; Methanol; Water <sup>™</sup> 2275 <sup>™</sup> Mixt Acetonitrile; Methanol; Water <sup>™</sup> 2277 <sup>™</sup> Mixt Acetonitrile; Methanol; Water <sup>™</sup> 2275 <sup>™</sup> 10	2265	Mixt	Acetonitrile; Methanol; Water							Incert Lindate	Delete			
W 2209       Mixt Acetonitrie; Wethanol; Water         W 2271       Mixt Acetonitrie; Wethanol; Water         W 2273       Mixt Acetonitrie; Wethanol; Water         W 2274       Mixt Acetonitrie; Wethanol; Water         W 2277       Mixt Acetonitrie; Methanol; Water         W 2277       Mixt Acetonitrie; Methanol; Water         W 2277       Pure         W Pure       Date Opened         Purity       N/A         Mixture       Location	P 2266	Pure	Acetic acid, ammonium salt (1:1)							unsert	Delete			
X 22/1     PIXC     Accounting: wethanoi       Y 22/2     Pure 3-Pyridinecarboxnide     Manufacturer       Y 22/2     Mixt     Accontrile; Wethanoi; Water       Y 22/2     Pure 3-Pyridinecarboxylic add     Image: Control (Control (Contro) (Control (Control (Control (Contro	2269	Mixt	Acetonitrile; Methanol; Water											
Pure     >Pure     >Pure     >Pure     >Pure     >Pure     >       ✓     Mixture     ▲cetonitrile; Methanol; Water     ✓      Catalog Number     N/A       ✓     Pure     >Pure     >Pure     >Pure     >     >	₩ 22/1	MIXt	Acetonitrile; Methanol							Manufacturar		- I I		
Image: Section Recentration Recentratio Recentration Recentration Recentration Recentration Recentration	22/2	Mixt	Acetopitrile: Methanol: Water							Handracturer		-		
Image: Second	2274	Mixt.	Acetonitrile: Methanol: Water							Catalog Number	N/A			
Image: product of the system     Image: product of the system     Date Opened       Image: product of the system     Purity     N/A       Image: product of the system     Image: product of the system     Image: product of the system	2275	Mixt	Acetonitrile: Methanol: Water							Lot Number	N/A			
Image: Control of the second secon	2277	Pure	3-Pyridinecarboxylic acid	~						Date Opened		<b>F</b>		
V Pure     Purity     NA       V Mixture     Inorg Chemistry     V			, , , , , , , , , , , , , , , , , , , ,							bate opened		= -		
V Mixture Location Inorg Chemistry	✓ Pure									Purity	N/A			
	Mixture 🖌				<				>	Location	Inorg Chemistry	~		
					1									

**Figure 7: View Constituent Details** 



Analyze IC Help	) Spectra	Manager										
ipectrum Li	st						Spe	ectrum Details Const	tituent Details Spectrum	n Plot		
This list conta	ins all the s	pectra found in the database										
ID	Type	Constituents	Insert	Ace	Acetonitrile:Methanol:Water(10:80:10) - Mixture Sample							
2234	Mixt	2-Propanone; Methanol; Water		6.000	la Data	ile						
2235	Mixt	2-Propanone; Methanol; Water	Delete	Samp	ie Deta	lis						
2236	Mixt	2-Propanone; Methanol; Water		Samp	le State	Liquid						
2237	Mixt	2-Propanone; Methanol; Water		Colou		Clear						
2239	Pure	Carbonic acid sodium salt (1:1)				Cicui						
2240	Mixt	2-Propanone; Methanol; Water		Consi	stency	N/R						
2241	Mixt	2-Propanone; Methanol; Water		Smell		N/R						
2243	Pure	Sulfuric acid potassium salt (1:2)										
2244	Mixt	2-Propanone; Methanol; Water										
2245	Mixt	2-Propanone; Methanol		Const	ituents	•			Details for Methar	ol		
2247	Pure	Ethanedioic acid, ammonium salt, h		The lis	t display	s all of the	constituents	of this sample	Constituent details c	an be changed, except for the		
2248	Pure	Acetonitrile			TURA	Name	Conc	Common Name	Manufacturer			
2249	Mixt	Acetonitrile; Methanol			101 20	e riterite	100/	Asstanitile Gues	CAS #	000067-56-1		
2250	Mixt	Acetonitrile; Methanol; Water			Aceto	nitrile	10%	Acetonitrie, Cyan		000007-00-1		
2251	Mixt	Acetonitrile; Methanol; Water			Water		109/	Water	IUPAC Name	Methanol		
2252	Mixt	Acetonitrile; Methanol; Water			water		10.76	water				
p 2253	Pure	8-Quinolinol										
<u>₩</u> 2254	Mixt	Acetonitrile; Methanol; Water										
*p* 2257	Pure	1,2,3-Propanetricarboxylic acid, 2							Common Names List	Bieleski's solution		
₩ 2258	MIXE	Acetonitrile; Methanol; Water								Methanol duster		
M 2201	MIXt	Acetonitrile; Methanol; Water								Methyl alcohol		
₩ 2202	Mixt	Acetonitrile; Methanol; Water								Methyl hydroxide		
M 2200 ↔ 2005	Mint	Acetonitrile; Methanol; Water								Methyloi		
M 2200 ↔ 2266	Dure	Acetic acid, ammonium calt (1:1)							Insert Update	Delete		
₽ 2200	Mist	Acetopitrile: Methapoli Water										
₩ 2209	Mixt	Acetonitrile: Methanol										
2272	Pure	3-Pyridipecarboxamide							Manufacturer	BDH		
2273	Mixt	Acetonitrile: Methanol: Water										
2273	Mixt	Acetonitrile: Methanol: Water							Catalog Number	29192BL		
2275	Mixt.	Acetonitrile: Methanol: Water							Lot Number	K31794469		
2277	Pure	3-Pvridinecarboxylic acid							Data Oppond	24/07/2006		
P 22/1	, arc	o r ynameeurooxyne deu							Date Opened	24/07/2000		
Pure									Purity	99.5%		
Mixture 🗸				<			Ш	>	Location	Phys Chem		

Figure 8: Selecting Constituent in Constituent Details

To view the details of a different constituent in a mixture, select that constituent in the *Constituents* section, as shown in Figure 8, where the Methanol constituent has been selected.

### 4.4.1 Edit Common Names List

The list of common names associated with a constituent can be modified, either by deleting a common name or by inserting a new common name. To delete a common name from the list, select the name and click on the *Delete* button, as shown in Figure 9. After clicking the *Delete* button, *OK* and *Cancel* buttons appear, as shown in Figure 10. Click on the *OK* button to complete the deletion of the common name.



🔇 Analyze IQ	) Spectra	Manager									_			
File Help														
Spectrum Lis	st						Sp	ectrum Details	Constit	uent Details Spectrun	1 Plot			
This list contai	ns all the s	pectra found in the database												
ID	Type	Constituents	Insert	A	cetonit	rile:Me	ethanol	Water(10	):80:1	0) - Mixture S	ample			
2234	Mixt	2-Propanone; Methanol; Water		6-	male Det	sile								
2235	Mixt	2-Propanone; Methanol; Water	Delete	2	inple Dec	1115								
2236	Mixt	2-Propanone; Methanol; Water		s	ample State	Liquid								
2237	Mixt	2-Propanone; Methanol; Water			alaur	Clear								
2239	Pure	Carbonic acid sodium salt (1:1)		۲,	.01001	Ciedi								
2240	Mixt	2-Propanone; Methanol; Water		C	onsistency	N/R								
2241	Mixt	2-Propanone; Methanol; Water		s	mell	N/R								
2243	Pure	Sulfuric acid potassium salt (1:2)												
2244	Mixt	2-Propanone; Methanol; Water										_		
2245	Mixt	2-Propanone; Methanol			onstituent	5				Details for Methan	ol	^		
2247	Pure	Ethanedioic acid, ammonium salt, h		Tł	ne list displa	ys all of the	constituent	s of this sample		Constituent details c	an be changed, except for the			
2248	Pure	Acetonitrile		Lп	TUDA	C Name	Conc	Common Na	me	Manufacturer	5 / 1			
2249	Mixt	Acetonitrile; Methanol		LE		e indirie	100/	Asstasibile	iie i	CAS #	000067-56-1			
2250	Mixt	Acetonitrile; Methanol; Water			Aceto	nitrie	10%	Acetonitrie,	yan		000007 00 1	-		
2251	Mixt	Acetonitrile; Methanol; Water			Methoda		109/	Methanol (bu	/=-2	IUPAC Name	Methanol			
2252	Mixt	Acetonitrile; Methanol; Water			wate		10 %	water						
P 2253	Pure	8-Quinolinol												
<u>₩</u> 2254	Mixt	Acetonitrile; Methanol; Water												
1°p' 2257	Pure	1,2,3-Propanetricarboxylic acid, 2								Common Names List	Methylol	•		
2258	MIXt	Acetonitrile; Methanol; Water									NSC 85232			
<u>₩</u> 2261	MIXE	Acetonitrile; Methanol; Water									Solutions, Bieleski's			
₩ 2262	MIXE	Acetonitrile; Methanol; Water									Wood alcohol			
₩ 2203	Mixt	Acetonitrile; Methanol; Water		11								-		
₩ 2203	Pure	Acetic acid ammonium salt (1:1)		11						Insert Update	Delete			
2269	Mixt.	Acetonitrile: Methanol: Water		11							<u> </u>			
2271	Mixt.	Acetonitrile: Methanol		11							•			
2272	Pure	3-Pyridinecarboxamide		H.						Manufacturer	BDH	٦ 🗌		
2273	Mixt	Acetonitrile: Methanol: Water		H.								4 🗌		
2274	Mixt	Acetonitrile: Methanol: Water		H.						Catalog Number	29192BL			
2275	Mixt	Acetonitrile: Methanol: Water								Lot Number	K31794469			
2277	Pure	3-Pyridinecarboxylic acid	•							Date Opened	24/07/2006	ן ר		
✓ Pure			-							Purity	99.5%	Ī		
Mixture					<		ш		>	Location	Phys Chem	~		
										:				

#### Figure 9: Delete Common Name–Step 1



Figure 10: Delete Common Name–Step 2



To add a new common name to the existing list, click on the *Insert* button, which makes a new textbox appear, as shown in Figure 11. After entering the new common name, click on the *OK* button to add it to the existing list.

Analyze IC	) Spectra Manager							-					
e nep	et .												
This list contai	ins all the spectra found in the databa	ase			St	Dectrum Details Constitu	uent Details Spectrun	n Plot					
ID	Type Constituents	^	Insert	Acetonit	Acetonitrile:Methanol:Water(10:80:10) - Mixture Sample								
2234	Mixt 2-Propanone; Methanol;	Water		Cample Det-	ile			-					
2235	Mixt 2-Propanone; Methanol;	Water	Delete	Sample Deta									
2236	Mixt 2-Propanone; Methanol;	Water		Sample State	Liquid								
2237	Mixt 2-Propanone; Methanol;	Water		Colour	Clear								
2239	Pure Carbonic acid sodium salt	t (1:1)		Colodi	Cicu								
2240	Mixt 2-Propanone; Methanol;	Water		Consistency	N/R								
2241	Mixt 2-Propanone; Methanol;	Water		Smell	N/R								
2243	Pure Sulfuric acid potassium sa	alt (1:2)											
2244	Mixt 2-Propanone; Methanol;	Water											
2245	Mixt 2-Propanone; Methanol			Constituents	i		Details for Methan	ol					
p 2247	Pure Ethanedioic acid, ammoni	ium salt, h		The list display	s all of the constituen	ts of this sample	Constituent details c	an be changed, except for the					
p 2248	Pure Acetonitrile			TIPA	C Name Conc	Common Name	Manufacturer						
2249	Mixt Acetonitrile; Methanol			Acata	oitrilo 10%	Acotonitrilo Cvan	CAS #	000067-56-1					
<u>₩</u> 2250	Mixt Acetonitrile; Methanol; W	Vater		Metha	nol 80%	Methanol (BDH-2	TUDAC Name						
2251	Mixt Acetonitrile; Methanol; W	vater		water	10%	Water	IUPAC Name	Methanol					
<u>₩</u> 2252	Mixt Acetonitrile; Methanol; V	vater		- Water	1070	Water							
'p' 2253	Pure 8-Quinolinol	la bas											
₩ 2254	Mixt Acetonitrile; Methanol; W	vater											
p 2257	Nixt Asstantitile: Mathaneli M	lic dolu, 2			-		Common Names List	Methyl hydroxide Methylol	^				
₩ 2200	Mixt Acetonitrile; Methanol; W	Valer			Enter ne	ew common		Monohydroxymethane					
M 2201 ↔ 2262	Mixt Acetonitrile; Methanol; W	Valer			name he	ere 🥆		NSC 85232	≡				
₩ 2202 ↔ 2262	Mixt. Acetopitrile: Methapoli W	valer Vater						Solutions, Bieleski's	$\overline{\mathbf{v}}$				
M 2200 ↔ 2200	Mixt. Acetonitrile, Methanely M	vater Vater											
M 2200 ↔ 2266	Pure Acetic acid ammonium ca	vater						OK Cancel					
p 2200 t 2260	Mixt Acetopitrile: Methapol: W	later	,					,%	1				
2271	Mixt Acetonitrile: Methanol						Add Common Name	Wood Alcohol					
2272	Pure 3-Pvridinecarboxamide						Manufacturer	BDH	1				
2273	Mixt Acetonitrile: Methanol: W	/ater											
2274	Mixt Acetonitrile; Methanol: W	/ater					Catalog Number	29192BL					
2275	Mixt Acetonitrile; Methanol: W	Vater					Lot Number	K31794469					
2277	Pure 3-Pyridinecarboxylic acid	~	1				Date Opened	24/07/2006					
U.C.	, .,		2				Durity	00 5%					
✓ Pure							Fully	55.370					
Mixture Mixture				<	1111	>	Location	Phys Chem					

Figure 11: Add Common Name

In addition to deleting or adding common names, an existing common name can be updated by selecting the common name in the list and clicking on the *Update* button. A textbox with this common name then appears and can be edited; clicking on the *OK* button commits this change of the common name.



# 4.5 Spectrum Plot

To view a spectrum plot, select the spectrum in the list and click on the *Spectrum Plot* button, as shown in Figure 12.



Figure 12: View Spectrum Plot

The spectral plot can be magnified or made smaller by clicking on the Zoom In and Zoom Out buttons indicated in Figure 12. To zoom in on a specific area (e.g. a peak) of the plot, click on the plot area and draw a rectangle around the section of interest. For example, selecting the area shown in Figure 12 results in the plot displayed Figure 13. Click on the Reset button indicated in Figure 12 to bring the plot back to its original settings. As shown in Figure 12, there are also buttons to allow the user to save the spectrum as an image or print it.





Figure 13: Zooming in on Spectrum Plot



# 5 Modifying Data Stored in Spectra Manager

## 5.1 Adding a New Spectrum

**Spectra Manager** supports the addition of a new spectrum through the import of an spectrum file for the spectrum. (Future versions of **Spectra Manager** will support other file formats.) To add a new spectrum to **Spectra Manager**, carry out the following steps:

K Analyz	e IQ Spectra	a Manager			
Spectrur This list co	<b>1 List</b> ntains all the s	pectra found in the database			Spectrum Details
ID	Type Mixt	Constituents Acetonitrile; Water	Insert	Acetonitrile:Wa	ter (99:1) - Mixt etails
103 ₩ 103 ₩ 103	1 Mixt 3 Mixt 5 Mixt	Acetonitrile; Water Acetonitrile; Water 1-Propanol; Methanol		The items in blue cannot b You can edit items in black	e changed. and press 'Update Spectru
103 ₩ 103	5 Mixt 7 Mixt	1-Propanol; Methanol; Water 1-Propanol; Methanol; Water		Spectrum filename Date of collection	MP26JULY2006-H2 26/07/2006
₩ 103 ₩ 103	9 Mixt	1-Propanol; Methanol; Water Methanol; Water		Time of collection	13:04

1. Click on the *Insert* button – see Figure 14.

Figure 14: Adding a Spectrum–Step 1

2. In the new window that is opened, click on the *Browse* button and select the spectrum for the spectrum to be inserted – see Figure 15.



<ul> <li><b>Note:</b></li> <li>(i) Click the Browse butt</li> </ul>	on to import a spectrum file	
Spectrum File Details		
Spectrum File	No Spectrum File selected Browse.	
Number of Data Points		
Collection Date/Time		
	Open File	=
	Look in: 🔁 SampleSPCFiles 🔍 🕝 🎓 😁 🖽 -	=
	Windowski       Mathematical Science         My Recent Documents       Acetonitrile-Methanol-Water (10-70-20).SPC         Macetonitrile-Methanol-Water (10-80-10).SPC         Macetonitrile-Methanol-Water (20-20-60).SPC         Macetonitrile-Methanol-Water (20-20-60).SPC         Methanol-Water (80-20).SPC         Methanol-Water (80-20).SPC         Methanol-Water (99-1).SPC         Methanol-Water (99-1).SPC	
	File name:     Acetonitrile-Methanol-Water (10-70-20).SPC     Open       My Computer     Files of type:     All Spectrum Files (* sig: * spec)     Cancel	
	All Spectrum Files ("aiq: "spc) SPC Files ("siq) SPC Files ("aiq) SpectroML Files ("xml) All Files (")	
	< Back Next > Finish Ca	ancel

Figure 15: Adding a Spectrum–Step 2: Select Spectrum File

3. After the previous step, a plot of the spectrum is shown at the bottom of the window and the two fields, *Number of Data Points* and *Collection Date/Time*, are filled in with information read from the selected spectrum file. Indicate whether this is the spectrum of a pure sample or a mixture, enter the number of constituents and the name of person who prepared the mixture; see Figure 16.



Confirm the selected de	tails and click the Next button	
Spectrum File Details		
Spectrum File	Acetonitrile-Methanol-Water (10-70-20).SPC	Browse
Number of Data Points	1476	
Sa	lost Duro of Minturo	
Туре		Spectrum Plot
Pure     Mixture	Enter No. Constituents	Acetonitrile-Methanol-Water (10-70-20)
Number of Constituer	its 3	125,000
Date of preparation	04/08/2009	100,000
Mixture prepared by	Marissa Phelan	2 75,000
Notes about sample	preparation	Ĕ 50,000
	Enter name of person who prepared mixture	25,000 0 500 1,000 1,500 2,000 2,500 3,000 Raman Shift (cm-1)
		< Back Next > N Finish Cancel
		Concer

Figure 16: Adding a Spectrum–Step 3

- 4. After clicking on the *Next* button of the window shown in Figure 16, a new window (Figure 17) is opened in which you must enter details for every constituent of the sample mixture (or for a single constituent if it is a pure sample). In this example, there are three constituents. For each constituent, the following steps (highlighted in Figure 17) are carried out:
  - a. Select constituent in the *Spectrum Constituents* list.
  - b. Choose whether this constituent of the mixture already exists in **Spectra Manager** or not.
  - c. If the constituent does not already exist in **Spectra Manager** then add a new constituent by choosing the substance and optionally entering other details, such as the manufacturer. The substance of a new constituent may be selected from an existing list of substances in **Spectra Manager** or a new substance may be used, in which case the CAS number and IUPAC name must be specified.

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<b>«</b>								
Note	: ach coi bstand	nstituent ma ce from the li	y be selected from the existing list o st of substances OR provide a valid	or a new consti CAS # and IU	tuent can be entered. To en PAC name for a new substan	iter a new constituent	t, select an existing	
Spect	trum	Sample Co	nstituents					
This li	st con	tains all of th	e constituents for the new spectrum	n		4a: Select cor	stituent	
	#	Туре	Substance		Manufacturer	/	Concentration	1
*	1	New	<empty></empty>		<empty></empty>		0.0%	
靀	2	New	<empty></empty>		<empty></empty>		0.0%	
*	3	New	<empty></empty>		<empty></empty>		0.0%	
• Ne	w	4b: N const	ew or Existing ituent?			4d: Ente concentr	r constituent ation	
OExi	sting			Enter a	new Constituent		Concentration 0.0 %	6
Man	ufact	urer			Substance			^
Selec Ma Acr Ald Aff Alka Ana Apo Bar BDH Bus Du Eas Fish Fish Fish GM Goorf H 8 HA(A Jan	tt a Mä nufact os rich a Aesa an alr bllo Sci toline a Aesa an h Boal Pont ttman ner Sci ons ca L Labs BH & C bdalls CH cssen	anufacturer o turer Name or entific ke Allen entific Co llenkamp	or create a new one	54   	Insert the details of the Insert the details of the Existing Substance CAS #	e new substance The CAS # has to be i The IUPAC is mandate 4c: New or Exist: substance for cor	in the form of 123456-78-9 pry ing nstituent?	
					< <u>E</u>	Back Next >	Einish Cano	el

Figure 17: Adding a Spectrum–Step 4

- 5. In this example, the mixture is composed of three constituents using the following substances: Acetonitrile, Methanol and Water. These three constituents correspond to substances already stored in the **Spectra Manager** list of substances. In this example, the Acetonitrile constituent is entered as a new constituent, but the Acetonitrile substance is selected from the existing substance list stored in **Spectra Manager**. The two remaining constituents, Methanol and Water, will be selected from **Spectra Manager**'s existing list of constituents. The new Acetonitrile constituent is recorded as follows:
  - a. Select the *Existing Substance* option and click on the *Existing* button. Then select Acetonitrile from the current list of **Spectra Manager**

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substances and click on OK – see Figure 18. The CAS number and IUPAC name are automatically retrieved for an existing substance. For new substances, this information must be provided by the user.

- b. Enter the concentration amount, which is automatically updated in the *Spectrum Constituents* table see Figure 19.
- c. You can optionally enter in the manufacturer of the constituent and other details: Catalog Number, Lot Number, Date Opened, Purity and Location.

Common Name		Iupac Name	CAS #
Acetic ether		Acetic acid ethyl ester	000141-78-6
Acetoacetanilide		Butanamide, 3-oxo-N-phenyl-	000102-01-2 🗆
Acetobromglucose		a-D-Glucopyranosyl bromide, 2,3,4,6-tetra	000572-09-8
Acetonitrile,Cyanor	nethane	Acetonitrile	000075-05-8
Acetophenone		Ethanone, 1-phenyl-	000098-86-2
Acetotoluidide		Acetamide, N-(methylphenyl)- (9CI)	027985-75-7
Acetyl bromide		Acetyl bromide	000506-96-7
CAS #	000075-05-8		
TUDAC Name	Acetonitrile		
IOFAC Name			
	Acetonitrile cluster		^
	Cyanomethane		
Add Common Name	Ethanenitrile		
	Ethyl nitrile		
	Methane, cyano-		×

Figure 18: Adding a Spectrum—Step 5a: Selecting Acetonitrile from list of Existing Substances

«						
Note	e:					
SU	ubs	tance	e from the	e list of substances OR provid	de a valid CAS # and IUPAC name for a new substance.	int, select an existing
Spec	tru	um S	ample (	constituents	i opertrum	
		#	Type	Substance	Manufacturer	Concentration
*		1	New	Acetonitrile	<empty></empty>	0.0%
靀	- 1	2	New	<empty></empty>	<empty></empty>	0.0%
*	:	3	New	<empty></empty>	<empty></empty>	0.0%
⊙ Ne ○ Ex	ew cisti	ng			Enter a new Constituent	Concentration 0.0 %

Figure 19: Adding a Spectrum–Step 5b: New Acetonitrile constituent



6. The second and third constituents (Methanol and Water) are selected from the existing list of constituents in **Spectra Manager**. For example to specify the Methanol constituent, select *Existing* option under the *Spectrum Constituents* table and scroll the list of constituents and select one. Note that many different constituents of the same substance may be present (each typically having a different manufacturer, catolog or lot number). After selecting the constituent, enter the concentration. In this example, the Water constituent is also selected from the existing constituents list. Figure 20 shows the three constituents entered and note that the concentration amounts must add up to 100% for the entire mixture. After entering all of the constituent details, click on the *Next* button to move onto the next step.



			N	
<b>«</b>			4	X
Confirm the selected details and click the Next but	tton			
Spectrum Sample Constituents				
This list contains all of the constituents for the new	spectrum			
# Type Substance			Manufacturer	Concentration
🏶 1 New Acetonitrile			<empty></empty>	10.0%
🍄 2 Existing Methanol			Aldrich	70.0%
🎲 3 Existing Water			<empty></empty>	20.0%
○ New ⓒ Existing	Selec	ct an ex	isting Constitue	nt Concentration 20.0 %
Spectra Manager Constituents			Details for Water	
The list contains all of the constituents in Spectra	Manager		CAS #	007732-18-5
Common Name Manu	fact   Catalog   212873	Lot 🔨	IUPAC Name	Water
Vanadyl Sulphate Aldrich	h 30568	179.		
🐖 Vanillic acid	H36001	020.	Add Common Name	Water
🐖 Vanillin 🗆 🛛 🗛 Aldrich	h 30569	072.		
🐖 Vanillin 🗆 🛛 🗛 Aldrich	h 30569	097.	Mapufacturer	
Veratraldehyde	143758	175. N/D		
<ul> <li>Vinegar</li> <li>Aldrid</li> <li>Vinyl acetate</li> <li>Aldrid</li> </ul>	h N/R	013	Catalog Number	N/A
Vitamin C Aldrick	h A7506	117.	Lot Number	N/A
🐖 Vitamin C	255564	1927	Date Opened	
🖙 Water	N/A	N/A	Purity	100%
🖙 Water-d2	DE50K	0020		Dhua Chara
x-Benzylideneacetophenone Aldrich	h 27365	251.	Location	Phys Chem
x-Benzylideneacetophenone Aldrich Addrich Addrich	n 11970	199.		
x-D-Cellobiose occaacetate           Image: Second s	101375 b N/R	0976		
<		>		
			<	Back Next > Finish Cancel

Figure 20: Adding a Spectrum–Step 6: Selecting remaining constituents (Methanol and Water) from the list of existing constituents in Spectra Manager

7. The next step in the addition of a new spectrum entry is to enter the *Sample Details, Spectral Acquisition Details* and the optional *Notes* section, as demonstrated in Figure 21. After completing these details, click on the *Next* button.



<b>«</b>			$\overline{\mathbf{X}}$
Confirm the selected det	ails and click the Next button		
Sample Details		Spectral Acquisition Details	
Sample Label	Acetronitrille:Methanol:Water (10:70:20)	NOTE: The details in blue come d changed. If there are any errors spectrum file.	irectly from the spectrum file and cannot be , cancel this wizard and select a different
Sample State	⊙ Solid ◯ Liquid ◯ Gas ◯ Slurry ◯ Other	Spectrum filename	Acetonitrile-Methanol-Water (1
Colour		Date of collection	28/07/2006
Consistency		Time of collection	12:32
Smell			
		Number of spectra collected	1
Entered in database by		Instrument model	RamanStn
Entered date	12/08/2009	wavenumber range sampled Minimum	250.0
		Maximum	3200.0
Notes		Number of data points	1476
		Collected by	Marissa Phelan
		Spectral acquisition time (secs.)	
		Scans acquired per spectrum	
		Axis labels	
		Grating (lines/mm)	
		Excitation Line (nm)	
		Spec Width (cm-1)	
		Aperture Setting	
		Objective Lens	
			View Data
	*		
		1	
		< Back	Next > Finish Cancel

Figure 21: Adding a Spectrum—Step 7: Sample and Spectral Acquisition Details

8. The final step is to validate all of the data that has been entered for the new spectrum. When you are satisfied that all of the information is correct, tick the checkbox at the bottom of the window and click on the *Finish* button (Figure 22). Note that you may have to scroll down to see all of the information. Click *Yes* on the confirmation window that appears to finalise the entry of this new spectrum into **Spectra Manager**.



Skitcher Finsh button to store this new spectrum in the database         Spectrum Details       Iog Details         Spectrum Acquisition Details       Iog Details         Spectrum Infename       Acetonitrile-Methanol-Water (1       Sample Label       Acetonitrile:Methanol-Water (10: 70: 20)       Details         Date of colection       28/07/2006       Grating (ines/mm)	<b>«</b>					X
Spectrum Details   Spectral Acquisition Details   Spectrum filename   Acctonitrie-Methanol-Water (1)   Sample Label   Colcection   12:32   Excitation Line (m)   Inser of spectra collection   12:32   Excitation Line (m)   Instrument model   RamanSin   Object Line   Wavenumber range sampled   25:0.0   Sample Details   Number of data points   1476   Sample Details   Number of data points   1476   Colcected by   Marissa Phelan   Colcustion   Sanaquired per spectrum   Axis labels   Nuture prepared by   Marissa Phelan   Colcected by   Marissa Phelan   Colcected by   Marissa Phelan   Colcected by   Marissa Phelan   Colcected by   Marissa Phelan   Date of preparation   Notes about preparati	Click the Finish button to store th	is new spectrum in the database				
Spectral Acquisition Details       Log Details         Spectrum filename       Accionitrile-Methandi-Water (1       Sample Label       Accionitrile-Methandi-Water (10:70:20)         Date of collection       28/07/2006       Graing (Inesymm)       Inesymmetric       Inesymmetric         Time of collection       12:32       Excitation Line (m)       Inesymmetric       Spec: Width (cm-1)       Spec: Width (cm-1) <t< th=""><th>Spectrum Details</th><th></th><th></th><th></th><th></th><th></th></t<>	Spectrum Details					
Spectrum filename Acetonitrile-Methanol-Water (1) Sample Label Acetonitrile:Methanol:Water (10:70:20)   Date of collection 28/07/2006 Graing (ines/mm)	Spectral Acquisition Details		Log Details			
Date of collection 28/07/2006   Grating (lines/mm)	Spectrum filename	Acetonitrile-Methanol-Water (1	Sample Label	A	cetonitrile:Methanol:Water (1	0:70:20)
Time of collection 12:32 Excitation Line (nm)   Number of spectra collected 1 Aperture Setting   Instrument model RamanStn Objective Lens   Wavenumber range sampled 250.0 - 3200.0 Sample Octails   Number of data points 1476 Sample State   Collected by Marissa Phelan Colour   Collected by Marissa Phelan Colour   Sectral acquisiton time (secs.) Smell   Scans acquired per spectrum Mixture Prepared by   Axis labels Mixture prepared by   Entered in database by 12/08/2009   Notes Notes about preparation   Stample constituents 12/08/2009   Sample constituents for this constituent will be stored in the Spectra Manager database.	Date of collection	28/07/2006	Grating (lines/	(mm)		
Spect Width (cm-1)   Instrument model   RamanStn   Objective Lens   Wavenumber range sampled   250.0   250.0   3200.0   Sample Details   Number of data points   1476   Sample State   Collected by   Marissa Phelan   Colour   Collected by   Marissa Phelan   Colour   Spectral acquisiton time (secs.)   Sample State   Solid   Sanse acquired per spectrum   Axis labels   Mixture prepared by   Marissa Phelan   Date of preparation   12/08/2009   Notes about preparation   12/08/2009   Sample constituents   Constituent 1 - 10.0% - New   This is a new constituent will be stored in the Spectra Manager database.   Image: Constituent Details for this constituent will be stored in the Spectra Manager database.	Time of collection	12:32	Excitation Line	e (nm)		
Number of spectra collected 1   Aperture Setting			Spec Width (c	m-1)		
Instrument model       RamanStn       Objective Lens         Wavenumber range sampled       250.0 - 3200.0       Sample Details         Number of data points       1476       Sample Details         Number of data points       1476       Sample State       Solid         Collected by       Marissa Phelan       Colour       Colour       Colour       Colour         Spectral acquisition time (secs.)       Smell       Consistency       Smell       Colour       Consistency       Smell       Colour	Number of spectra collected	1	Aperture Sett	ing		≡
Wavenumber range sampled 250.0 - 3200.0 Sample Details   Number of data points 1476 Sample State Solid   Collected by Marissa Phelan Colour Colour   Spectral acquisition time (secs.) Smell Smell   Scans acquired per spectrum Mixture prepared by Marissa Phelan   Axis labels Mixture prepared by Marissa Phelan   Entered in database by Date of preparation 12/08/2009   Notes Notes about preparation 12/08/2009   Sample constituents  Constituent 1 - 10.0% - New  This is a new constituent. Details for this constituent will be stored in the Spectra Manager database.	Instrument model	RamanStn	Objective Len	s		
Number of data points 1476     Sample State Solid     Collected by Marissa Phelan     Spectral acquisition time (secs.)   Scans acquired per spectrum   Axis labels     Entered in database by   Entered in database by   Entered date   12/08/2009   Notes about preparation      Sample constituents     Constituent 1 - 10.0% - New   This is a new constituent. Details for this constituent will be stored in the Spectra Manager database.      If the inserted data is correct	Wavenumber range sampled	250.0 - 3200.0	Sample Deta	ails		
Collected by Marissa Phelan   Spectral acquisition time (secs.) Consistency   Scans acquired per spectrum Smell   Axis labels Mixture Details   Axis labels Mixture prepared by   Marissa Phelan Date of preparation   12/08/2009 Notes about preparation   Pattered date 12/08/2009   Sample constituents    Somple constituents   Constituent 1 - 10.0% - New   This is a new constituent. Details for this constituent will be stored in the Spectra Manager database.    Image: Constituent of the inserted data is correct	Number of data points	1476	Sample State	Solid		
Collected by Marissa Phelan Consistency			Colour			
Spectral acquisition time (secs.)     Scans acquired per spectrum     Axis labels     Entered in database by   Entered date   12/08/2009     Notes     Notes     Sample constituents        Constituent 1 - 10.0% - New   This is a new constituent. Details for this constituent will be stored in the Spectra Manager database.   Image: Check this box if the inserted data is correct	Collected by	Marissa Phelan	Consistency			
Scans acquired per spectrum     Axis labels     Axis labels     Entered in database by   Entered date   12/08/2009     Notes about preparation     Notes     Sample constituents     Constituent 1 - 10.0% - New   This is a new constituent. Details for this constituent will be stored in the Spectra Manager database.   Image: Check this box if the inserted data is correct	Spectral acquisition time (secs.)		Smell			
Axis labels Mixture prepared by Marissa Phelan Date of preparation 12/08/2009 Entered date 12/08/2009 Notes about preparation Notes about preparation Sample constituents Constituents This is a new constituent. Details for this constituent will be stored in the Spectra Manager database. Constituent 1 - 10.0% - New This is a new constituent. Details for this constituent will be stored in the Spectra Manager database. Constituent 1 - 10.0% - New This is a new constituent. Details for this constituent will be stored in the Spectra Manager database. Constituent 1 - 10.0% - New	Scans acquired per spectrum		Mixture Det	ails		
Entered in database by Date of preparation 12/08/2009 Entered date 12/08/2009 Notes about preparation Notes about preparation Notes Notes	Axis labels		Mixture prepa	red by	Marissa Phelan	
Entered date 12/08/2009 Notes about preparation Notes about preparation Sample constituents Constituent 1 - 10.0% - New This is a new constituent. Details for this constituent will be stored in the Spectra Manager database. Check this box if the inserted data is correct	Entered in database by		Date of prepa	ration	12/08/2009	
Notes         Sample constituents         Constituent 1 - 10.0% - New         This is a new constituent. Details for this constituent will be stored in the Spectra Manager database.         Image: Check this box if the inserted data is correct	Entered date	12/08/2009	Notes about p	preparation	n	
Sample constituents Constituent 1 - 10.0% - New This is a new constituent. Details for this constituent will be stored in the Spectra Manager database. Check this box if the inserted data is correct	Notes					
Sample constituents Constituent 1 - 10.0% - New This is a new constituent. Details for this constituent will be stored in the Spectra Manager database.  Constituent Details for this constituent will be stored in the Spectra Manager database.  Constituent of the Inserted data is correct		~				
Sample constituents Constituent 1 - 10.0% - New This is a new constituent. Details for this constituent will be stored in the Spectra Manager database. Check this box if the inserted data is correct						
Sample constituents Constituent 1 - 10.0% - New This is a new constituent. Details for this constituent will be stored in the Spectra Manager database. Constituent of the inserted data is correct Constituent of the inserted data is correct						
Constituent 1 - 10.0% - New This is a new constituent. Details for this constituent will be stored in the Spectra Manager database.  Check this box if the inserted data is correct	Sample constituents					
Check this box if the inserted data is correct	Constituent 1 - 10.0% - New	l a far this canatity ant will be stared in the Co	a stra Managar	databasa		
Check this box if the inserted data is correct	This is a new constituent. Detail	s for this constituent will be stored in the sp	ectra Manager (	JalaDase.	_	~
					Check this box if	the inserted data is correct
< Back Next > Finish Cancel				< Ba	ack Next >	Finish Cancel

Figure 22: Adding a Spectrum–Step 8: Validation



## 5.2 Deleting a Spectrum

To delete a spectrum, select it in the *Spectrum List* on the left, click on the *Delete* button, as shown in Figure 23, and finally click on the *OK* button in the confirmation window (see Figure 24).

Help					
ipectrum Li	st				Spectrum Details Const
This list conta	ins all the s	pectra found in the database			
ID	Type	Constituents	Insert	Acetonitrile:Wa	ter (80:20) - Mixt
1027	Mixt	Acetonitrile; Water		Spectral Acquisition De	tails
1029	Mixt	Acetonitrile; Water	Deleten	Spectral Acquisition De	cons
1031	Mixt	Acetonitrile; Water		The items in blue cannot be You can edit items in black	e changed. and press 'Lindate Spectrum'
1033	Mixt	Acetonitrile; Water		Tou can eur tems in black	and press opuate spectrum.
1035	Mixt	1-Propanol; Methanol		Spectrum filename	MP26JULY2006-H5.SP
1036	Mixt	1-Propanol; Methanol; Water		Date of collection	26/07/2006
1027	Mixt	1-Propanol; Methanol; Water			
W 1037	Misch	1-Propagol: Methagol: Water		Time of collection	13:09
₩ 1037 ₩ 1038	PIXL	I reparely rectanoly water			

Figure 23: Deleting a Spectrum



Figure 24: Deleting a Spectrum–Confirmation



# 6 Spectra Manager Pre-Loaded Spectral Data

**Spectra Manager** is shipped with a set of spectral data. The size and composition of this dataset will depend on what was purchased. The spectral data shipped with **Spectra Manager** were collected in the School of Chemistry, National University of Ireland Galway on an Avalon Instruments Raman station spectrometer using 785 nm excitation. Where possible the spectra were cross-checked against publically available Raman spectral databases.

The CAS numbers, IUPAC, and common names were cross checked using a variety of electronic databases including SciFinder Scholar.

#### Disclaimer

Analyze IQ Ltd. have undertaken to compile a high quality database with a large amount of supporting information. While every effort has been made to validate all the information contained in the database, Analyze IQ Ltd. shall not be liable for any problems that may result from errors in the database.



# 7 Technical Support, Sales and Services

For assistance and technical support queries relating to **Spectra Manager**, please go to the **User Area** of the Analyze IQ website, <u>http://www.AnalyzeIQ.com</u>, or send an email message to <u>support@AnalyzeIQ.com</u>.

For information on extending an evaluation license or purchasing a full license for **Spectra Manager**, please contact our Sales Department by sending an email message to <u>sales@AnalyzeIQ.com</u>.

In addition to software sales and technical support, Analyze IQ Ltd. provides the following services for customers:

- Software training
- Data validation and analysis
- Bespoke model development

For information on these services, please contact our Sales Department by sending an email message to <u>sales@AnalyzeIQ.com</u>.

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