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.

🔇 An	alyze IQ	Spectra	Manager					🛛 🔀
File H	lelp							
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₩	2244	Mixt Mixt	2-Propanone; Methanol; Water 2-Propanone; Methanol	Delete	Spectral Acquisition Details		Log Details	
	2243	Pure	Ethanedioic acid, ammonium salt, h		The items in blue cannot be char		Details from the spect	rum file
🐳	2248	Pure	Acetonitrile		You can edit items in black and p	ress 'Update Spectrum'.	Sample Label	Acetonitrile:Methanol:Water(10:80:1
l 🕁		Mixt	Acetonitrile; Methanol		Spectrum filename	MP28JULY2006-L4.SPC		
	2250	Mixt	Acetonitrile; Methanol; Water		Date of collection	28/07/2006	Grating (lines/mm)	
III 1 ₩	2251	Mixt	Acetonitrile; Methanol; Water				Excitation Line (nm)	785
₩	2252	Mixt	Acetonitrile; Methanol; Water		Time of collection	11:48	Spec Width (cm-1)	
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	
	2258 2261	Mixt	Acetonitrile; Methanol; Water		Wavenumber range sampled		Mixture Details	
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	2262	Mixt	Acetonitrile; Methanol; Water		Minimum		Mixture prepared by	MP
	2265	Mixt	Acetonitrile; Methanol; Water		Maximum	3200.0	Date of preparation	28/07/2006
	2266	Pure	Acetic acid, ammonium salt (1:1)		Number of data points	1476	Notes about preparat	ion
l 🕁	2269	Mixt	Acetonitrile; Methanol; Water					
H 🔂	2271	Mixt	Acetonitrile; Methanol		Collected by	Marissa Phelan	1	
Ģ	2272	Pure	3-Pyridinecarboxamide		-]	
III ☆	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		Axis labels		1	
		Pure	3-Pyridinecarboxylic acid]	
	2278	Mixt	Acetonitrile; Methanol; Water	′			1	
	2279	Mixt	Acetonitrile; Methanol		Entered in database by	Lena Karlson		
	2280 2281	Pure	1H-Indene-1,3(2H)-dione, 2,2-dih		Entered date	30/11/2006		
l 🐺	2281	Mixt Pure	Acetonitrile; Methanol; Water Benzenamine, 4-nitro-					
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	lixture							

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⁻¹.

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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.



This lat contains all the spectra found in the database ID Type Constituents Insert 2344 Mixt Furan, tetrahydro-; Methanol; Water Delete Delete 2345 Mixt Furan, tetrahydro-; Methanol; Water Delete Delete 2345 Mixt Furan, tetrahydro-; Methanol; Water Delete Delete 2350 Mixt Furan, tetrahydro-; Methanol; Water Date of collection 29/07/2006 2351 Mixt Furan, tetrahydro-; Methanol; Water Date of collection 29/07/2006 2352 Mixt Furan, tetrahydro-; Methanol; Water Date of collection 29/07/2006 2352 Mixt Furan, tetrahydro-; Methanol; Water Date of collection 29/07/2006 2353 Mixt Furan, tetrahydro-; Methanol; Water Mixture preamethanol; Water Mixture preamethanol; Water 2354 Mixt Furan, tetrahydro-; Methanol; Water Mixture preamethanol; Water Mixture preamethanol; Water 2355 Mixt Furan, tetrahydro-; Methanol; Water Mixture preamethanol; Water Mixture preamethanol; Water 2356 Mixt Furan, tetrahydro-; Methanol	pectrum Lis	st				Spectrum Details Constitu	uent Details Spectrum	1 Plot
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2354 Mixt Furan, tetrahydro-; Methanol; Water 2355 Mixt Furan, tetrahydro-; Methanol; Water 2358 Mixt Furan, tetrahydro-; Methanol; Water 2359 Mixt Furan, tetrahydro-; Methanol; Water 2359 Mixt Furan, tetrahydro-; Methanol; Water 2350 Mixt Furan, tetrahydro-; Methanol; Water 2351 Mixt Furan, tetrahydro-; Methanol; Water 2360 Mixt Furan, tetrahydro-; Methanol; Water 2361 Mixt Furan, tetrahydro-; Methanol; Water 2362 Mixt Furan, tetrahydro-; Methanol; Water 2363 Pure Benzenemethanol, 4-chloro- 2364 Mixt Furan, tetrahydro-; Methanol; Water 2367 Pure Benzonitrile, 4-dhoro-; 2367 Pure Benzonitrile, 4-dhoro-; 2370 Pure Benzonitrile, 4-dhoro-; 2371 Pure I,2,3-Propanetiol 2380 Pure Benzonitrile, 4-dhoro-; 2380 Pure Benzonitrile, 4-dhoro-; 2380 Pure Fure Hexane; 23		Mixt	Furan, tetrahydro-; Methanol; Water		Time of collection	18:47	Spec Width (cm-1)	
X 235 Mixt Furan, tetrahydro-; Methanol; Water X 2357 Mixt Furan, tetrahydro-; Methanol; Water X 2359 Mixt Furan, tetrahydro-; Methanol; Water X 2350 Mixt Furan, tetrahydro-; Methanol; Water X 2350 Mixt Furan, tetrahydro-; Methanol; Water X 2361 Mixt Furan, tetrahydro-; Methanol; Water X 2362 Mixt Furan, tetrahydro-; Methanol; Water X 2362 Mixt Furan, tetrahydro-; Methanol; Water X 2364 Mixt Furan, tetrahydro-; Methanol; Water X 2365 Pure Benzenemethanol, 4-chloro- X 2367 Pure Benzonitale, 4-thloro- X 2370 Pure Benzonitale, 4-thloro- X 2371 Pure 1,2,3-Propaneticadoxy- X 2370 Pure Benzonitale, 4-thloro- X 2371 Pure 1,2,3-Propaneticadoxy- X 2372 Pure Harane Instrument model X 2380 Pure Furan, tetrahydro- Entered in database by Lena Karlson X 2380 Pure Benzene 30/11/2006 When updating, </td <td></td> <td>Mixt</td> <td>Furan, tetrahydro-; Methanol; Water</td> <td></td> <td></td> <td></td> <td></td> <td></td>		Mixt	Furan, tetrahydro-; Methanol; Water					
2358 Mixt Furan, tetrahydro-; Methanol; Water Mixture prepared by Mixture prepared by Mixture prepared by Mp 2361 Mixt Furan, tetrahydro-; Methanol; Water Mixture prepared by Mixture prepared by Mp 2361 Mixt Furan, tetrahydro-; Methanol; Water Mixture prepared by Mp 2362 Mixt Furan, tetrahydro-; Methanol; Water Mixture prepared by Mp 2363 Mixt Furan, tetrahydro-; Methanol; Water Mixture prepared by Mp 2364 Mixt Furan, tetrahydro-; Methanol; Water Number of data points 11476 Notes about preparation 29/07/2006 2367 Pure Benzonitrale, 4-thioro- Spectral acquisition time (secs.) 21 Scans acquired per spectrum 21 2370 Pure Benzonitrale, 4-thioro- Spectral acquisition time (secs.) 21 Scans acquired per spectrum 21 2375 Pure Hazane Entered in database by Lena Karlson When updating, button appears 2380 Pure Furan, trahydro- Entered date 30/11/2006 When appears 2385 Pure <td>2355</td> <td>Mixt</td> <td>Furan, tetrahydro-; Methanol</td> <td></td> <td>Number of spectra collected</td> <td>1</td> <td>Aperture Setting</td> <td></td>	2355	Mixt	Furan, tetrahydro-; Methanol		Number of spectra collected	1	Aperture Setting	
2358 Mixt Furan, tetrahydro-; Methanoi; Water 2359 Mixt Furan, tetrahydro-; Methanoi; Water 2359 Mixt Furan, tetrahydro-; Methanoi; Water 2351 Mixt Furan, tetrahydro-; Methanoi; Water 2352 Mixt Furan, tetrahydro-; Methanoi; Water 2354 Mixt Furan, tetrahydro-; Methanoi; Water 2364 Mixt Furan, tetrahydro-; Methanoi; Water 2364 Pure Benzontemethanol, 4-chloro- 2365 Pure a-D-Glucopyranose, 4-O-(2,3,4,6) 2369 Pure Benzonitrile, 4-tylorxy 2370 Pure Benzonitrile, 4-tylorxy- 2371 Pure 1,2,3-Propanetricarboxylic acid, 2, 2372 Pure Benzonitrile, 4-tyloro- 2380 Pure Benzonitrile, 4-tyloro- 2380 Pure Furan, tetrahydro- 2380 Pure Furah, triahydro- <td></td> <td>Mixt</td> <td>Furan, tetrahydro-; Methanol; Water</td> <td></td> <td></td> <td></td> <td>Objective Lens</td> <td></td>		Mixt	Furan, tetrahydro-; Methanol; Water				Objective Lens	
2359 Mixt Furan, tetrahydro-; Methanol; Water 2360 Mixt Furan, tetrahydro-; Methanol; Water 2361 Mixt Furan, tetrahydro-; Methanol; Water 2362 Mixt Furan, tetrahydro-; Methanol; Water 2363 Pure Benzenemethanol, 4-chloro- 2364 Mixt Furan, tetrahydro-; Methanol; Water 2365 Pure 254-Mixt 2366 Pure 254-Mixt 2367 Pure a-0-Glucopyranose, 4-0-(2,3,4,6) 2368 Pure Benzonithie, 4-thloro- 2370 Pure Benzonithie, 4-thloro- 2371 Pure 1,2,3-Propanetricarboxylic acid, 2-cn 2372 Pure 1,2,3-Propanetriol 2380 Pure Furan, tetrahydro-; 2380 Pure Furan, tetrahydro- 2381 Pure Benzene 2382 Pur	2358	Mixt	Furan, tetrahydro-; Methanol; Water			RamanStr		
2361 Mixt Furan, tetrahydro-; Methanol; Water 2362 Mixt Furan, tetrahydro-; Methanol; Water 2363 Pure Benzenemthanol, 4-chloro- 2364 Mixt Furan, tetrahydro-; Methanol; Water 2365 Pure 2-Propenoic add, 3-(4+hydroxy-3) 2366 Pure 2-Propenoic add, 3-(4-hydroxy-3) 2367 Pure a-0-Glucopyranose, 4-O-(2,3,4,6) 2368 Pure Benzonitrile, 4+dydroxy- 2369 Pure Benzonitrile, 4+dydroxy- 2370 Pure Benzonitrile, 4+dydroxy- 2371 Pure 1,2,3-Propanetricarboxylic adid, 2 2372 Pure Hexane 2380 Pure Hexane <td>2359</td> <td>Mixt</td> <td>Furan, tetrahydro-; Methanol; Water</td> <td></td> <td>Wavenumber range sampled</td> <td></td> <td>Mixture Details</td> <td></td>	2359	Mixt	Furan, tetrahydro-; Methanol; Water		Wavenumber range sampled		Mixture Details	
2361 Mixt Furan, tetrahydro-; Methanol Maximum 3200.0 Date of preparation 29/07/2006 2362 Mixt Furan, tetrahydro-; Methanol; Water Maximum 3200.0 Date of preparation 29/07/2006 2363 Pure Benzenemethanol, 4-chloro- Maximum 3200.0 Date of preparation 29/07/2006 2364 Mixt Furan, tetrahydro-; Methanol; Water 1476 Number of data points 1476 Notes about preparation Maximum 29/07/2006 2364 Pure a-0-Glucopyranose, 4-0-(2,3,4,6) 29/07/2006 Number of data points 1476 Notes about preparation Maximum Maximum Maximum 20/07/2006 2369 Pure Benzonitrile, 4+dydroxy- 21 Spectral acquisition time (secs.) 21 Spectral acquisition time (secs.) 21 Axis labels X:Raman Shift (cm-1) Y: I When updating, button appears 2380 Pure Herahydro- Benzene 30/11/2006 When updating, button appears Spectral acquisition time (secs.) 21 Spectral acquisition time (secs.) 21 Spectral acquisition time (secs.) 21 Spectral acquisition time	2360	Mixt	Furan, tetrahydro-; Methanol; Water		Minimum	250.0	Mixture propered by	MD
2362 Mixt Furan, tetrahydro-; Methanol; Water 2363 Pure Benzenemethanol, 4-chioro- 2364 Mixt Furan, tetrahydro-; Methanol; Water 2366 Pure 2-Propenoic acid, 3-(4-hydroxy-3) 2367 Pure a-D-Glucopyranose, 4-O-(2,3,4,6) 2368 Pure Benzoitadid, 2-formyl- 2369 Pure Benzoitadid, 2-formyl- 2370 Pure Benzoithile, 4+doloro- 2371 Pure 1,2,3-Propanetricarboxylic acid, 2 2372 Pure 1,2,3-Propanetriol 2374 Pure Furan, tetrahydro- 2380 Pure Furan, tetrahydro- 2371 Pure 1,2,3-Propanetriol 2372 Pure Entered in database by Lena Karlson 2380 Pure Furan, tetrahydro- 2380 Pure Benzene 2381 Pure Benzene 2382 Pure Benzene 2383 Pure Methane, trichloro- 2384 Pure Methane, trichloro- 2385 Pure <	2361	Mixt	Furan, tetrahydro-; Methanol			2222.0	Mixture prepared by	1 THE
2363 Pure Benzenemethanol, 4-chloro- 2364 Mixt Furan, tetrahydro-; Methanol; Water 2365 Pure 2.200 2367 Pure a-0-Glucopyranose, 4-0-(2,3,4,6,) 2368 Pure Benzonitrile, 4-thydroxy3 2369 Pure Benzonitrile, 4-thydroxy3 2369 Pure Benzonitrile, 4-thydroxy 2370 Pure Benzonitrile, 4-thydroxy- 2371 Pure 1,2,3-Propanetricarboxylic aid, 2 2372 Pure 1,2,3-Propanetriol 2380 Pure Furan, tetrahydro- 2380 Pure Furan, tetrahydro- 2380 Pure Furan, tetrahydro- 2380 Pure Benzene 2380 Pure Benzene 2380 Pure Benzene 2380 Pure Benzene 2380 Pure Methane, trichloro- 2380 Pure Methane, trichloro- 2380 Pure Methane, trichloro- 2380 Pure Methane, trichloro- 2380 <td></td> <td>Mixt</td> <td>Furan, tetrahydro-; Methanol; Water</td> <td></td> <td>Maximum</td> <td>3200.0</td> <td>Date of preparation</td> <td>29/07/2006</td>		Mixt	Furan, tetrahydro-; Methanol; Water		Maximum	3200.0	Date of preparation	29/07/2006
2364 Mixt Furan, tetrahydro-; Methanol; Water 2366 Pure 2-Propenoic add, 3-(4-hydroxy-3) 2367 Pure a-D-Glucopyranose, 4-O-(2,3,4,6) 2368 Pure Benzoitalid, 2-formyl- 2369 Pure Benzoitalid, 4-hydroxy- 2369 Pure Benzoitalid, 2-formyl- 2370 Pure Benzoitalid, 2-formyl- 2371 Pure 1,2,3-Propanetriad 2375 Pure 1,2,3-Propanetriad 2376 Pure Hexane 2380 Pure Furan, tetrahydro- 2380 Pure Furan, tetrahydro- 2380 Pure Benzene 2381 Pure Hothane, trichloro- 2385 Pure Itrinintrahydro- <	2363	Pure	Benzenemethanol, 4-chloro-		Number of data points	1476	Notes about prepara	tion Mixture prepared over 2 day
2366 Pure 2-Propenoic acid, 3-(4-hydroxy-3) 2367 Pure a-D-Glucopyranose, 4-O-(2,3,4,6) 2368 Pure Benzoic acid, 2-formyl- 2369 Pure Benzoic acid, 2-formyl- 2369 Pure Benzoic acid, 2-formyl- 2370 Pure Benzointile, 4+doloro- 2371 Pure 1,2,3-Propanetricarboxylic acid, 2 2374 Pure 1,2,3-Propanetriol 2375 Pure K:Raman Shift (cm-1) Y: I 2370 Pure Furan, tetrahydro- 2371 Pure Furan, tetrahydro- 2382 Pure Benzene 2382 Pure Benzene 2382 Pure Methane, trichloro- 2383 Pure Methane, trichloro- 2384 Pure Methane, trichloro- 2385 Pure Methane, trichloro- 2385 Pure Methane, trichloro- 2385 Pure Methane, trichloro-		Mixt	Furan, tetrahydro-: Methanol: Water					Mixture prepared over 2 da
2367 Pure a-D-Glucopyranose, 4-O-(2,3,4,6) 2368 Pure Benzoit add, 2-formyl- 2369 Pure Benzonitrile, 4-th/droxy- 2370 Pure Benzonitrile, 4-th/droxy- 2371 Pure 1,2,3-Propanetricarboxylic add, 2 2372 Pure 1,2,3-Propanetricarboxylic add, 2 2380 Pure Furan, tetrahydro- 2380 Pure Furan, tetrahydro- 2380 Pure Benzene 2380 Pure Hethane, trichloro- 2380 Pure Hethane, trichloro- 2380 Pure Hethane, trichloro- 2380 Pure Methane, trichloro-		Pure	2-Propenoic acid, 3-(4-hvdroxy-3		Collected by	Maxima Dhalan		
2368 Pure Benzoic acid, 2-formyl- 2369 Pure Benzonitrile, 4-hydroxy- 2370 Pure Benzonitrile, 4-hydroxy- 2371 Pure 1,2,3-Propanetricarboxylic acid, 2 2374 Pure 1,2,3-Propanetricarboxylic acid, 2 2375 Pure Hexane 2380 Pure Furan, tetrahydro- 2382 Pure Benzene 2383 Pure Methane, trichloro- 2385 Pure 1,4/10xxane		Pure			Collected by	Marissa Phelan		
2369 Pure Benzonitrile, 4-hydroxy- 2370 Pure Benzonitrile, 4-hydroxy- 2371 Pure 1,2,3-Propanetriol 2374 Pure 1,2,3-Propanetriol 2375 Pure Hexane 2380 Pure Furan, tetrahydro- 2382 Pure Benzene 2383 Pure Intered date 2385 Pure 1,4/10xoane					Spectral acquisition time (secs.)	21		
2370 Pure Benzonitrile, 4-chloro- 2371 Pure 1,2,3-Propanetricarboxylic acid, 2 2374 Pure 1,2,3-Propanetricarboxylic acid, 2 2375 Pure 1,2,3-Propanetricarboxylic acid, 2 2376 Pure 1,2,3-Propanetricarboxylic acid, 2 2375 Pure Hexane 2380 Pure Furan, tetrahydro- 2382 Pure Benzene 2383 Pure Methane, trichloro- 2385 Pure 1,4-Dioxane Notes					Scape acquired per exectrum	21		
2371 Pure 1,2,3-Propanetricarboxylic add, 2 2374 Pure 1,2,3-Propanetricarboxylic add, 2 2375 Pure 1,2,3-Propanetricarboxylic add, 2 2372 Pure Hexane 2380 Pure Furan, tetrahydro- 2380 Pure Benzene 2383 Pure Methane, trichloro- 2384 Pure 1,4-Dioxane					Scans acquired per spectrum	21		L
2374 Pure 1,2,3-Propanetriol 2375 Pure Hexane 2380 Pure Furan, tetrahydro- 2382 Pure Benzene 2383 Pure Motes					Axis labels	X:Raman Shift (cm-1) Y: I		
2375 Pure Hexane Interest in database by Lena Karlson Filtered in database by 2380 Pure Furan, tetrahydro- Entered in database by Lena Karlson button appears 2382 Pure Benzene 30/11/2006 button appears 2383 Pure Methane, trichloro- Notes							7.47	
2380 Pure Furan, tetrahydro- 2382 Pure Benzene 2383 Pure Methane, trichloro- 2383 Pure Motes)	Entered in database by	Long Karlson	When	updating, this enti
2382 Pure Methane, trichloro- 2385 Pure 1,4-Dioxane Notes							button	appears
2383 Pure Methane, trichloro- 2385 Pure 1,4-Dioxane Notes					Entered date	30/11/2006	Sacton	···· /
2385 Pure 1,4-Dioxane Notes								
					Notes			
2337 Pure Ethane, 1, 1, 1-trichloro-			V	1				\
								\
	1-							
Pure Defaulte								

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

🔇 Analyze IQ	Spectra	a Manager								_					
File Help															
Spectrum Lis	+						-								
·		pectra found in the database			Spectrum Details Constituent Details Spectrum Plot										
ID	Type		∧ Insert	Ac	Acetonitrile:Methanol:Water(10:80:10) - Mixture Sample										
2234	Mixt	2-Propanone; Methanol; Water	▲ Insert	1 not	ctonic	. inclusion	ununon	uutei(10.00.1	oj mixture o	umpic					
2235	Mixt		Delete	Sam	ple Deta	ails									
2236	Mixt			Sam	ple State	Liquid					—				
2237	Mixt	2-Propanone; Methanol; Water				-									
5 2239	Pure	Carbonic acid sodium salt (1:1)		Colo	bur	Clear									
2240	Mixt	2-Propanone; Methanol; Water		Con	sistency	N/R									
2241	Mixt	2-Propanone; Methanol; Water		Sme		N/R					_				
2243	Pure	Sulfuric acid potassium salt (1:2)									— I				
2244	Mixt														
2245		2-Propanone; Methanol			stituent	-			Details for Aceton	itrile	^				
♦ 2247 ♦ 2248	Pure	Ethanedioic acid, ammonium salt, h		The	list displa	ys all of the	constituents	of this sample		an be changed, except for the					
★ 2248 ★ 2249	Pure	Acetonitrile Acetonitrile: Methanol			IUPA	C Name	Conc.	Common Name	Manufacturer						
2249		Acetonitrile; Methanol: Water			Aceto	nitrile	10%	Acetonitrile,Cyan	CAS #	000075-05-8					
2250	Mixt				Metha	anol	80%	Methanol (BDH-2	IUPAC Name	Acetonitrile	- I I				
2251		Acetonitrile; Methanol; Water			Wate	r	10%	Water		Acetoniulie					
2253	Pure	8-Quinolinol													
2254	Mixt	Acetonitrile; Methanol; Water													
2257	Pure	1,2,3-Propanetricarboxylic acid, 2							Common Names List	Acetonitrile cluster	a III				
2258	Mixt	Acetonitrile; Methanol; Water								Cyanomethane					
2261	Mixt	Acetonitrile; Methanol; Water								Ethanenitrile Ethyl nitrile	1				
2262	Mixt	Acetonitrile; Methanol; Water								Methane, cyano-	_				
2263	Mixt									Methanecarbonitrile	1				
2265		Acetonitrile; Methanol; Water							Insert Update	Delete					
2266	Pure	Acetic acid, ammonium salt (1:1)							unsert	Delete					
2269	Mixt														
2271	Mixt	Acetonitrile; Methanol							Manufacturer		-				
2272	Pure Mixt	3-Pyridinecarboxamide Acetonitrile; Methanol; Water									- 1				
2273	Mixt								Catalog Number	N/A					
2275		Acetonitrile; Methanol; Water							Lot Number	N/A					
2277	Pure		~						Date Opened		F I I				
L.5.		,							1 C C C C C C C C C C C C C C C C C C C						
Pure									Purity	N/A					
Mixture				<	[11	11	>	Location	Inorg Chemistry					
][

Figure 7: View Constituent Details



Help									
ipectrum Li	st					Spe	ctrum Details Constitu	ent Details Spectrum	Plot
This list conta	ins all the s	spectra found in the database				<u> </u>			
ID	Туре	Constituents	Insert	Acetoni	trile:Metha	nol:	Water(10:80:1	D) - Mixture Sa	ample
2234	Mixt	2-Propanone; Methanol; Water	Delete	Sample Det	ails				
2235	Mixt	2-Propanone; Methanol; Water	Deletern						
2236	Mixt	2-Propanone; Methanol; Water		Sample State	e Liquid				
2237	Mixt	2-Propanone; Methanol; Water		Colour	Clear				
🔂 2239	Pure	Carbonic acid sodium salt (1:1)		Coloci					
2240	Mixt	2-Propanone; Methanol; Water		Consistency	N/R				
2241	Mixt	2-Propanone; Methanol; Water		Smell	N/R				
5 2243	Pure	Sulfuric acid potassium salt (1:2)							
2244	Mixt	2-Propanone; Methanol; Water							
2245	Mixt	2-Propanone; Methanol		Constituen	s			Details for Methan	ol
🔂 2247	Pure	Ethanedioic acid, ammonium salt, h		The list displa	avs all of the const	ituents	of this sample	Constituent details of	n be changed, except for the
5 2248	Pure	Acetonitrile						Manufacturer	in be changed, exception the
2249	Mixt	Acetonitrile; Methanol		IUP	AC Name	Conc.	Common Name		
2250	Mixt	Acetonitrile; Methanol; Water		🔛 🔶 Acet	onitrile	10%	Acetonitrile,Cyan	CAS #	000067-56-1
2251	Mixt	Acetonitrile; Methanol; Water		🤛 Meth		30%	Methanol (BDH-2	IUPAC Name	Methanol
2252	Mixt	Acetonitrile; Methanol; Water		📄 🐖 Wat	er Vd	10%	Water		
🔂 2253	Pure	8-Quinolinol							
2254	Mixt	Acetonitrile; Methanol; Water							
2257	Pure	1,2,3-Propanetricarboxylic acid, 2						Common Names List	Bieleski's solution
2258	Mixt	Acetonitrile; Methanol; Water							Carbinol
2261	Mixt	Acetonitrile; Methanol; Water							
2262	Mixt	Acetonitrile; Methanol; Water							Methyl alcohol Methyl hydroxide
2263	Mixt	Acetonitrile; Methanol; Water							Methylol
2265	Mixt	Acetonitrile; Methanol; Water						\square	
2266	Pure	Acetic acid, ammonium salt (1:1)						Insert Update	Delete
2269	Mixt								
2271	Mixt								
2272	Pure	3-Pyridinecarboxamide						Manufacturer	BDH
2273	Mixt	Acetonitrile; Methanol; Water						Catalog Number	29192BL
2274	Mixt	Acetonitrile; Methanol; Water						catalog Number	271720L
2275	Mixt	Acetonitrile; Methanol; Water						Lot Number	K31794469
2277	Pure	3-Pyridinecarboxylic acid						Date Opened	24/07/2006
Pure								Purity	99.5%
Mixture				<	1111		>	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.



Help		-									_	
ectrum Li	st							Spe	ctrum Details Constitu	uent Details Spectrum	Plot	_
								(-+				
ID	Type	Constituents	~	Insert	Ace	tonit	rile:Me	thanol:\	Water(10:80:1	0) - Mixture S	ample	
2234	Mixt	2-Propanone: Methanol: Water										
	Mixt	2-Propanone; Methanol; Water		Delete	Samp	le Deta	lls					
2236	Mixt	2-Propanone; Methanol; Water			Sampl	e State	Liquid					
2237	Mixt	2-Propanone; Methanol; Water					Clear					
2239	Pure	Carbonic acid sodium salt (1:1)			Colour		Clear					
2240	Mixt	2-Propanone; Methanol; Water			Consis	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 Methan	ol	
2247	Pure	Ethanedioic acid, ammonium salt, h			The lis	t displa	s all of the	constituents	of this sample	Constituent details ca	an be changed, except for the	
2248	Pure	Acetonitrile				TUDA	C Name	Conc.	Common Name	Manufacturer	in be changed, exception the	
2249	Mixt	Acetonitrile; Methanol								CAS #	000067-56-1	
2250	Mixt	,				Aceto		10%	Acetonitrile,Cyan			
2251	Mixt					Metha		80%	Methanol (BDH-2	IUPAC Name	Methanol	
2252	Mixt					Water		10%	Water			
2253	Pure	8-Quinolinol										
2254	Mixt	Acetonitrile; Methanol; Water										
2257	Pure	1,2,3-Propanetricarboxylic acid, 2								Common Names List		~
2258	Mixt	Acetonitrile; Methanol; Water									Monohydroxymethane NSC 85232	
2261	Mixt	Acetonitrile; Methanol; Water										
2262	Mixt										Wood alcohol	_
2263	Mixt	Acetonitrile; Methanol; Water										
2265	Mixt	Acetonitrile; Methanol; Water								Insert Update	Delete	
	Pure	Acetic acid, ammonium salt (1:1)								Choose Copublic		
2269	Mixt	the second s									. 8	
2271	Mixt Pure	Acetonitrile; Methanol 3-Pvridinecarboxamide								Manufacturer	BDH	
2272	Mixt	Acetonitrile; Methanol; Water								Manufacturer	BDH	_
2273	Mixt	Acetonitrile; Methanol; Water								Catalog Number	29192BL	
2275	Mixt									Lot Number	K31794469	
2273	Pure		~							Data Oracad	24/07/2006	4
8 2211	Fulc	Stri yn ain feldir Dox ylle actu	¥							Date Opened	24/07/2006	
Pure										Purity	99.5%	
Mixture					<				>	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.

Help											
pectrum Li	st							Spe	ctrum Details Constitu	uent Details Spectrum	Plot
This list contai	ins all the s	pectra found in the database									
ID	Type	Constituents	^	Insert	Acet	tonit	rile:Me	ethanol:	Water(10:80:1	0) - Mixture S	ample
2234	Mixt	2-Propanone; Methanol; Water		Delete	Samp	e Deta	ils				
2235	Mixt	2-Propanone; Methanol; Water			<u> </u>						
2236	Mixt	2-Propanone; Methanol; Water			Sample	e State	Liquid				
2237	Mixt	2-Propanone; Methanol; Water			Colour		Clear				
2239	Pure	Carbonic acid sodium salt (1:1)									
2240	Mixt	2-Propanone; Methanol; Water			Consis	tency	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				tuents				Details for Methan	ol
2247	Pure	Ethanedioic acid, ammonium salt, h			The list	t display	s all of the	constituents	of this sample		an be changed, except for the
2248	Pure	Acetonitrile				TUPAC	Name	Conc.	Common Name	Manufacturer	
2249	Mixt	Acetonitrile; Methanol			-	Acetor		10%	Acetonitrile,Cyan	CAS #	000067-56-1
2250	Mixt	Acetonitrile; Methanol; Water				Metha		80%	Methanol (BDH-2	IUPAC Name	
2251	Mixt	Acetonitrile; Methanol; Water				Water		10%	Water	IOPAC Name	Methanol
	Mixt	Acetonitrile; Methanol; Water			. · · ·	water		10 /0	Water		
😴 2253 🕁 2254	Pure Mixt	8-Quinolinol Acetonitrile; Methanol; Water									
2254	Pure	1.2.3-Propanetricarboxylic acid, 2									
2257	Mixt	Acetonitrile; Methanol; Water					_			Common Names List	Methyl hydroxide
2250	Mixt	Acetonitrile; Methanol; Water							v common		Monohydroxymethane
2261		Acetonitrile; Methanol; Water					n	ame her	e 🥆		NSC 85232
2262	Mixt	Acetonitrile; Methanol; Water									Solutions, Bieleski's
2265	Mixt	Acetonitrile; Methanol; Water									
2265	Pure	Acetic acid, ammonium salt (1:1)									OK Cancel
2260	Mixt	Acetonitrile; Methanol; Water								· · · · · · · · · · · · · · · · · · ·	
2209	Mixt	Acetonitrile; Methanol								Add Common Name	Wood Alcohol
2272	Pure	3-Pyridinecarboxamide								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		~							Date Opened	24/07/2006
Pure										Purity	99.5%
✓ Mixture										· ·	
- mixture					<				>	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:

e Help						
5pectrum Li	st					Spectrum Details
This list conta	ins all the sp	pectra found in the database				
ID	Туре	Constituents	^	Insert	Acetonitrile:Wa	ter (99:1) - Mix
1029	Mixt	Acetonitrile; Water		Delete	Spectral Acquisition De	stails
1031 🔛	Mixt	Acetonitrile; Water		Delete	<u> </u>	
1033 🔛	Mixt	Acetonitrile; Water			The items in blue cannot b You can edit items in black	
1035 🔛	Mixt	1-Propanol; Methanol			Tou can earchems in black	and press opuate spect
1036	Mixt	1-Propanol; Methanol; Water			Spectrum filename	MP26JULY2006-H
1037	Mixt	1-Propanol; Methanol; Water			Date of collection	26/07/2006
1038	Mixt	1-Propanol; Methanol; Water				
1039	Mixt	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.



 Note: (i) Click the Browse butt 	ion to import a spectrum file	
Spectrum File Details	5	-
Spectrum File	No Spectrum File selected Browse.	
Number of Data Points		
Collection Date/Time		
	Open File	-
	Look in: 🔁 Sample SPC Files 🔽 🕥 🎓 📅 -	-
	My Recent Documents Macetonitrile-Methanol-Water (10-70-20).SPC My Recent Documents Acetonitrile-Methanol-Water (10-80-10).SPC Methanol-Water (20-20-60).SPC Methanol-Water (50-50).SPC Methanol-Water (80-20).SPC Methanol-Water (99-1).SPC My Documents	
	File name: Acetonitrile-Methanol-Water (10-70-20).SPC Open	
	My Computer Files of type: All Spectrum Files (*.aiq; *.spc) Cancel	
	All Spectrum Files (".aiq; ".spc) SPC Files (".spc) Analyze IQ Files (".aiq) SpectroML Files (".xml) All Files (")	
	< Back Next > Finish C	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 Collection Date/Time	1476 28/07/2006 12:32	
Sa	lect Pure of Mixture	
Туре		Spectrum Plot
Pure Mixture	, Enter No. Constituents	Acetonitrile-Methanol-Water (10-70-20)
Number of Constituer		125,000
Date of preparation	04/08/2009	100,000
Mixture prepared by	Marissa Phelan	₹
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 > 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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u. Enter the concentration for that constituen	d.	Enter the concentration f	for that constituent
--	----	---------------------------	----------------------

«								
	ach co		y be selected from the existing list o st of substances OR provide a valid				, 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 con	stituent	
	#	Туре	Substance		Manufacturer	/	Concentration	n
*	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 🔺		lew or Existing ituent?			4d: Enter concentra		
OExi	- E			Enter a	new Constituent		Concentration 0.0	%
Man	ufact	urer			Substance			<u>^</u>
Ma Acr Alda Alfa Alaa Apo Ban BD Bus Du Eas Fish Fish Fish Fish GMI Goo Grif H & HAO	nufact os rich a Aesa em alr lollo Scici toline H h Boal Pont ttman ner Sci uns ca A Labs BH & C BH & C BH & C Shalls	turer Name ir entific ke Allen entific	or create a new one		CAS #		ng	
					Eac	k <u>N</u> ext >	<u>Finish</u> Can	cel

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.

	om the list		
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	
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		
IUPAC Name	Acetonitrile		
	Acetonitrile cluster		^
Add Common Name	Cyanomethane Ethanenitrile		=
Add Common Name	Ethyl nitrile		
	Methane, cyano-		~

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

				ing list or a new constituent can be entered. To enter a new consti e a valid CAS # and IUPAC name for a new substance.	tuent, select an existing
_		-	onstituents		
his li	st con	Type	the constituents for the new : Substance	Manufacturer	Concentration
*	1	New	Acetonitrile	<empty></empty>	0.0%
\$	2	New	<empty></empty>	<empty></empty>	0.0%
*	3	New	<empty></empty>	<empty></empty>	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	
K		\searrow	X
Confirm the selected details and dick the Next but	ton		
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	Select an	existing Constitue	nt Concentration 20.0 %
Spectra Manager Constituents		Details for Water	
The list contains all of the constituents in Spectra N	Manager	CAS #	007732-18-5
Common Name Manut	fact Catalog Lot 212873 056.	IUPAC Name	Water
 Vanadyl Sulphate Aldrich 			
🖙 Vanillic acid	H36001 020.	Add Common Name	Water
🖙 Vanillin 🗆 🛛 Aldrich	30569 072.		
🐖 Vanillin 🗆 🛛 🗛 Aldrich		Manufacturer	
🐖 Veratraldehyde	143758 175.		
 Vinegar Aldrich Vinvl acetate Aldrich 		Catalog Number	N/A
Viryi acetate Addref Addref Addref Addref Addref		Lot Number	N/A
🔛 Vitamin C	255564 1927	Date Opened	
😔 Water	N/A N/A	Purity	100%
🖙 Water-d2	DE50K 0020	1	
🖙 x-Benzylideneacetophenone Aldrich		Location	Phys Chem
x-Benzylideneacetophenone Aldrich			
 x-D-Cellobiose octaacetate x-D-Glucose monohydrate Aldrich 	101575 019. N/R 0976	~	
ADDONE MODORVOIALE ADDON			
		_<	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.



«			$\overline{\mathbf{X}}$
Confirm the selected det	ails and click the Next button		
Sample Details		Spectral Acquisition Details	
Sample Label	Acetronitrille:Methanol:Water (10:70:20)		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**.



«						
Click the Finish button to store th	is new spectrum in the database					
Spectrum Details						^
Spectral Acquisition Details		Log Details				
Spectrum filename	Acetonitrile-Methanol-Water (1	Sample Label	Ac	cetonitrile:Methanol:Wa	ater (10:70:20)	
Date of collection	28/07/2006	Grating (lines/	mm)			
Time of collection	12:32	Excitation Line	e (nm)			
		Spec Width (o	m-1)			
Number of spectra collected	1	Aperture Sett	ing			
Instrument model	RamanStn	Objective Len	s			
Wavenumber range sampled	250.0 - 3200.0	Sample Deta	ails			
Number of data points	1476	Sample State	Solid			
		Colour				
Collected by	Marissa Phelan	Consistency				
Spectral acquisition time (secs.)		Smell				
Scans acquired per spectrum		Mixture Det	ails			
Axis labels		Mixture prepa	red by	Marissa Phelan		
Entered in database by		Date of prepa	ration	12/08/2009		
Entered date	12/08/2009	Notes about p	reparation	1		
Notes	12/00/2003					
	~					
	×					
Sample constituents						
Constituent 1 - 10.0% - New						
This is a new constituent. Details	s for this constituent will be stored in the Sp	ectra Manager (latabase.			~
				Check this	box if the inserted data i	s correct
			< Ba	k Next >	Finish Ca	incel

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).

e Help					
ipectrum Li	st				Spectrum Details Consti
This list conta	ins all the s	pectra found in the database			
ID	Туре	Constituents	Insert	Acetonitrile:Wa	ter (80:20) - Mixti
1027	Mixt	Acetonitrile; Water	DeleteN	Spectral Acquisition De	tails
1029	Mixt	Acetonitrile; Water	Delete.	· · · · · · · · · · · · · · · · · · ·	
1031	Mixt	Acetonitrile; Water		The items in blue cannot b	e changed. and press 'Update Spectrum'.
1033	Mixt	Acetonitrile; Water		Tou can eur nems 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
1037	Mixt	1-Propanol; Methanol; Water			
1038	Mixt	1-Propanol; Methanol; Water		Time of collection	13:09
1039	Mixt	Methanol; 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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