Analyze IQ
Spectra Manager
Version 1.1

User Manual

Document Version: 1.1-2009-08-12

Table of Contents

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: http://www.AnalyzeIQ.com/User-Documentation.html; 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, www.AnalyzeIQ.com, you must first register on it. To do so, go to http://www.AnalyzeIQ.com 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: http://www.AnalyzeIQ.com/ Download.html. 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.

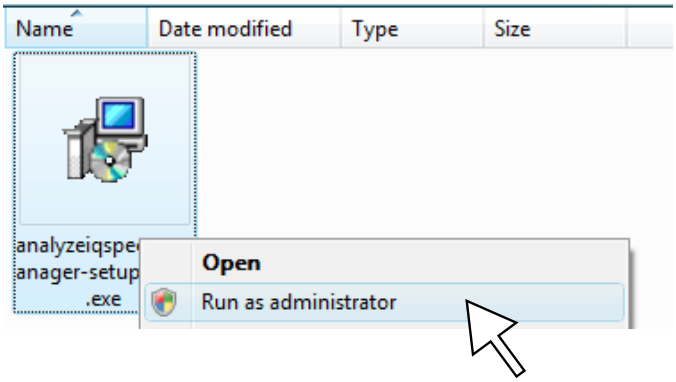

Figure 1: Under Windows Vista, the Setup program must be run as Administrator

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).

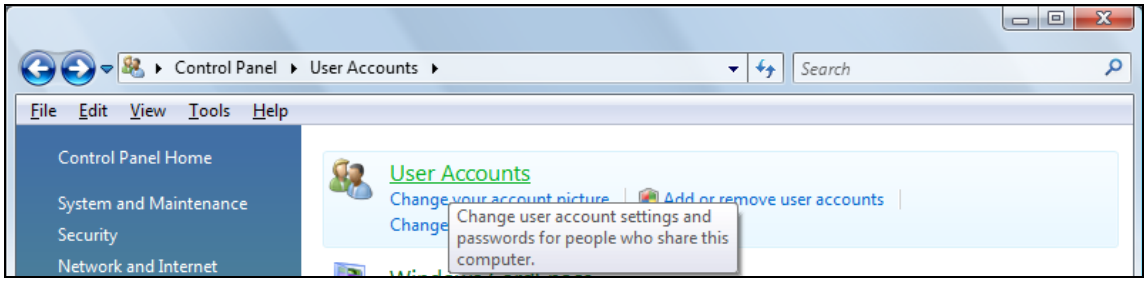

Figure 2: Under Windows Vista, selecting User Accounts in the Control Panel

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

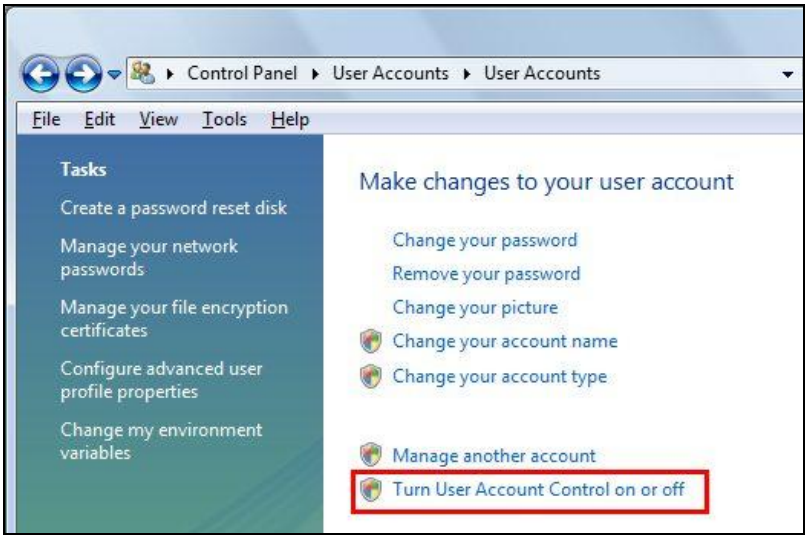

Figure 3: Under Windows Vista, turning off User Account Control

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 left-hand 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.

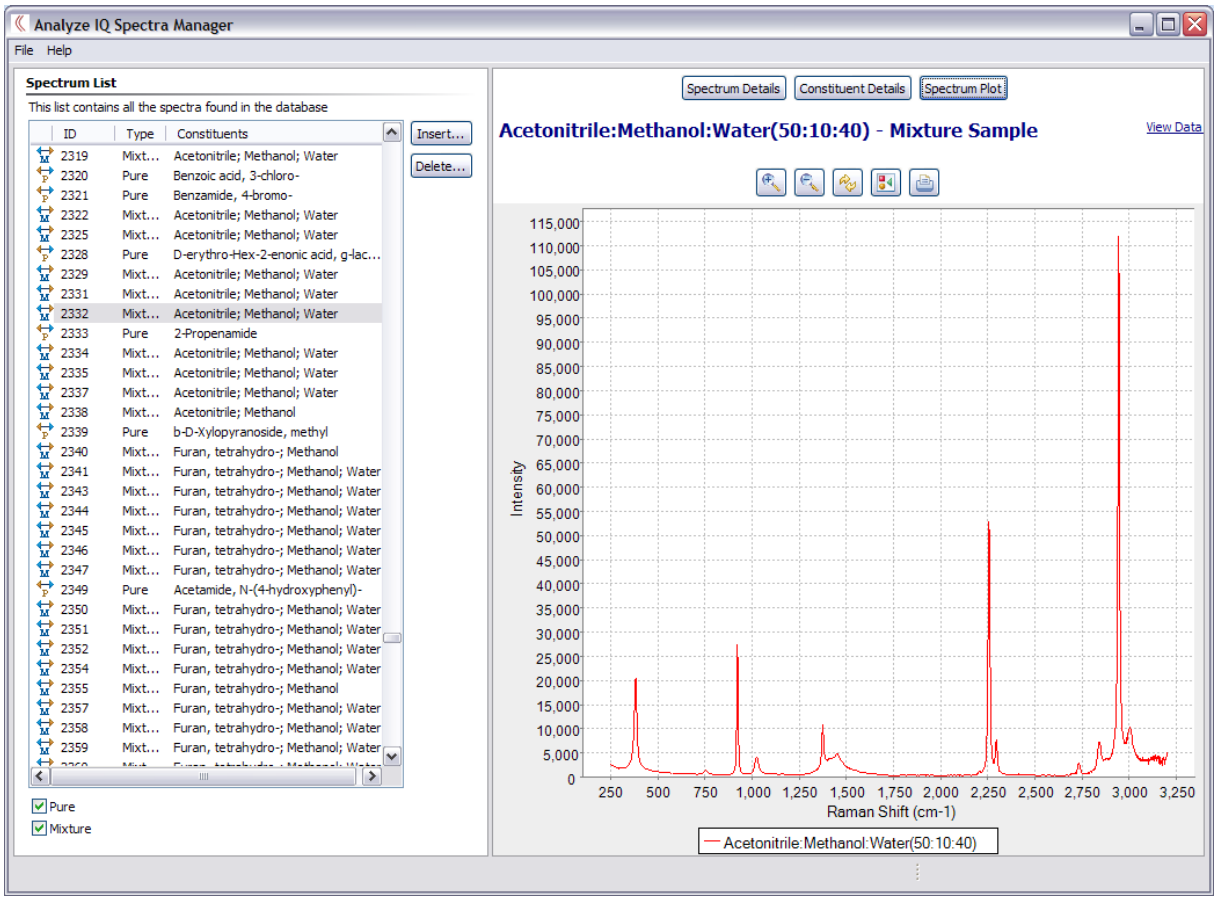

Figure 4: The Opening Screen of Spectra Manager

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.

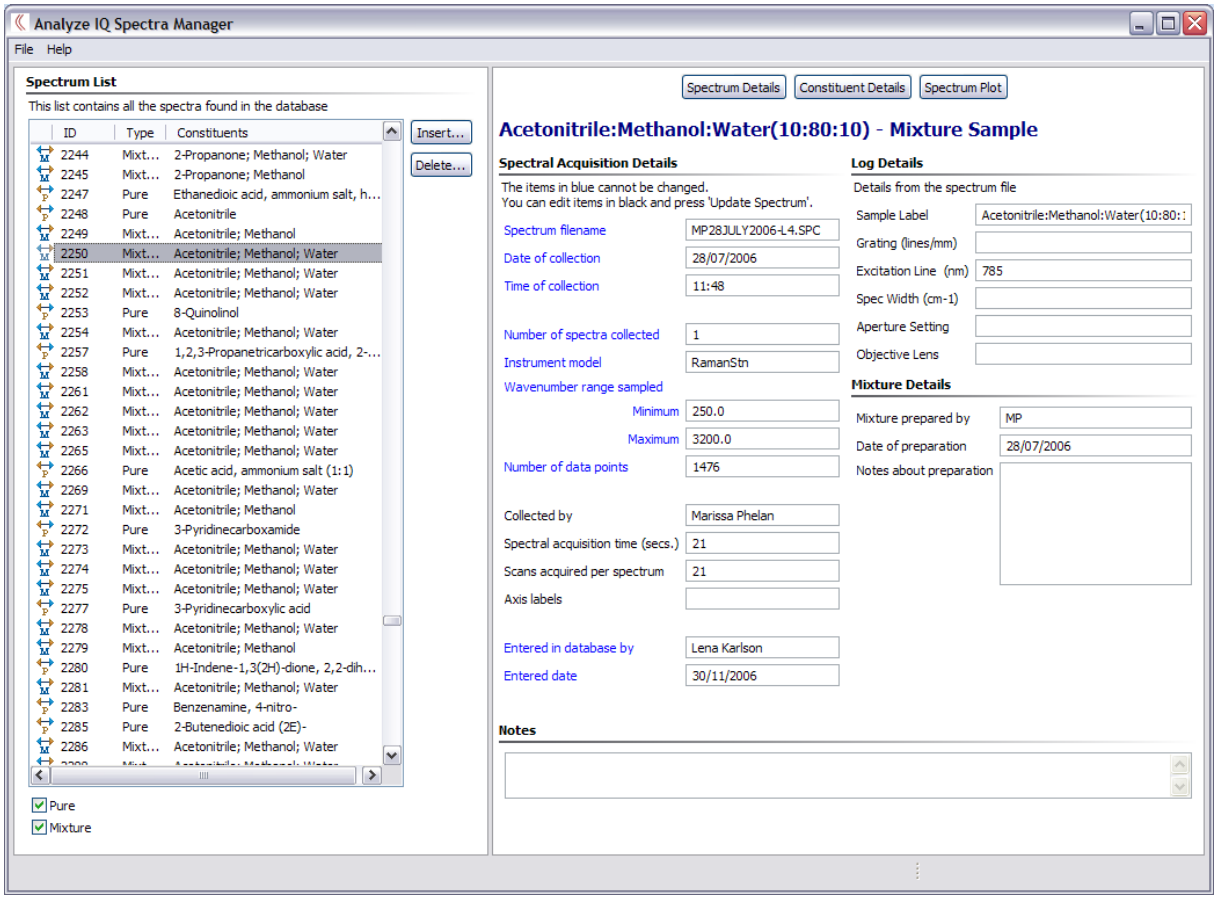

Figure 5: View Spectrum Details

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 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}.

- ***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.

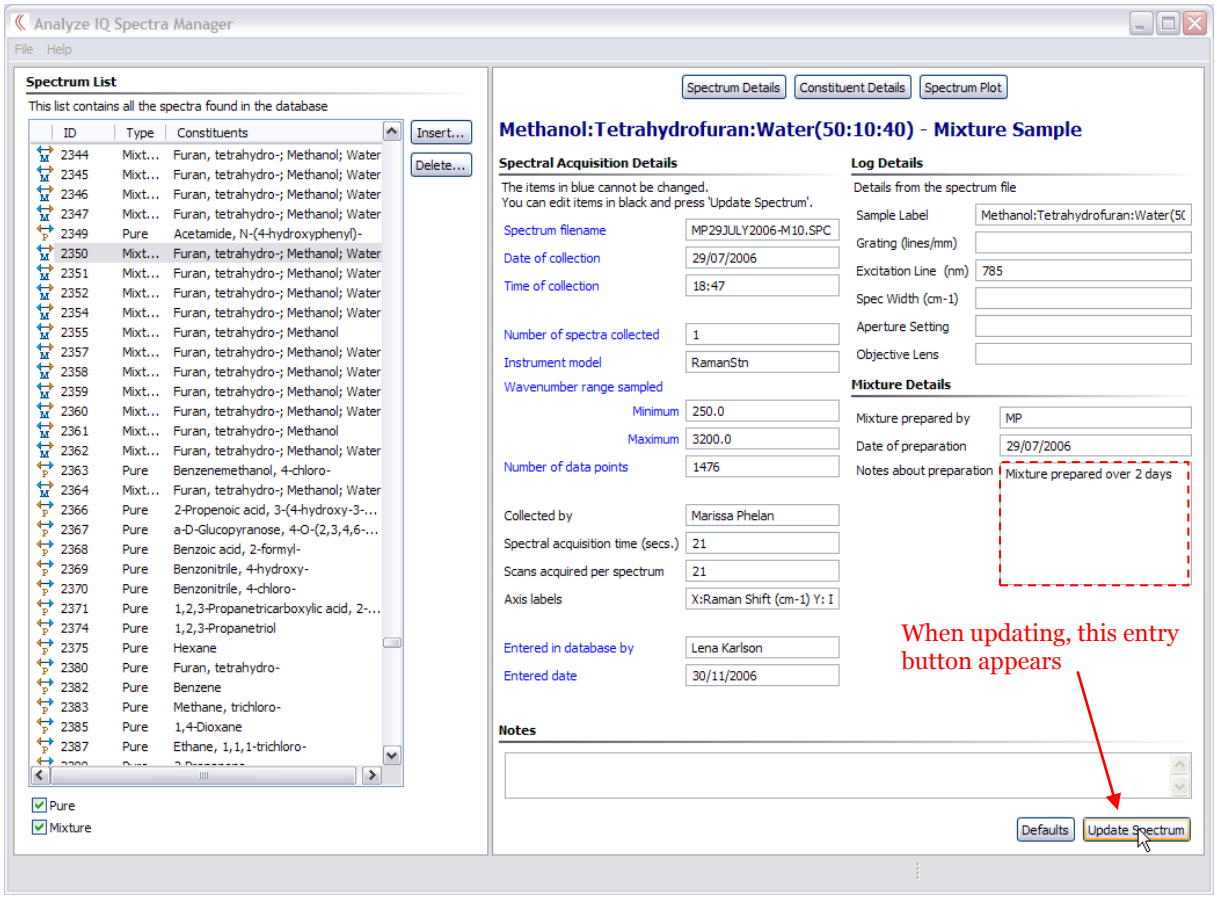

Figure 6: Edit Spectrum Details

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

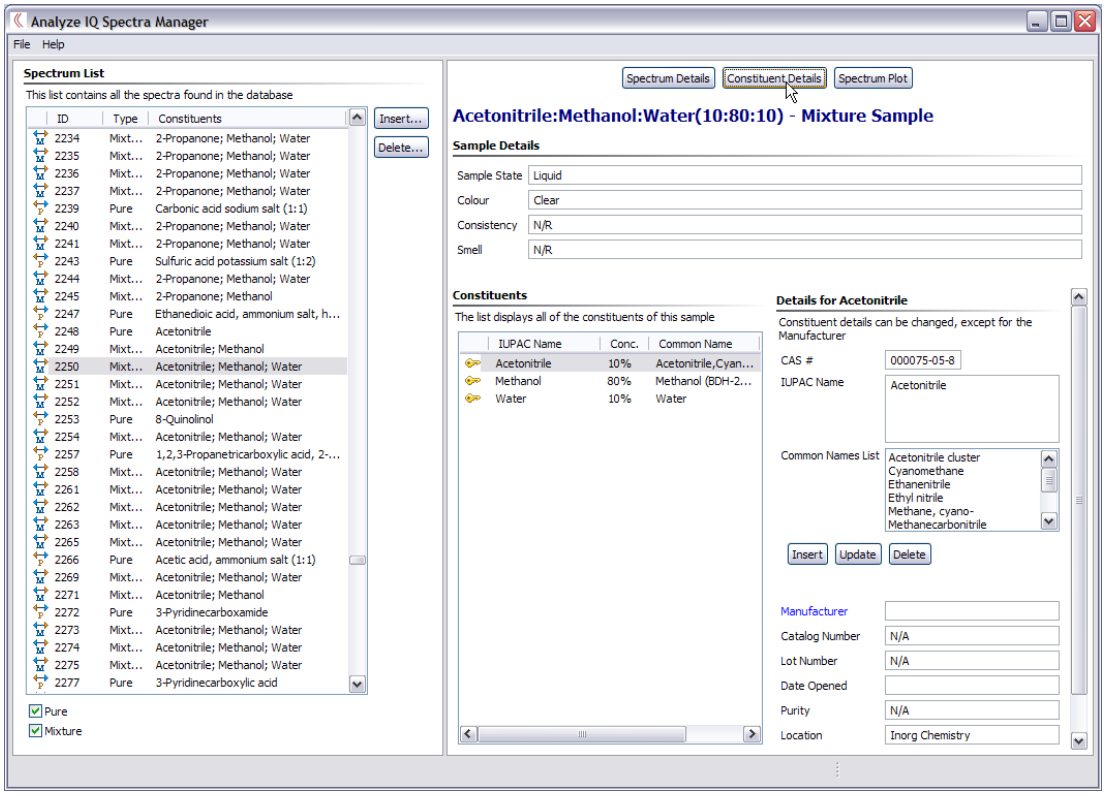

Figure 7: View Constituent Details

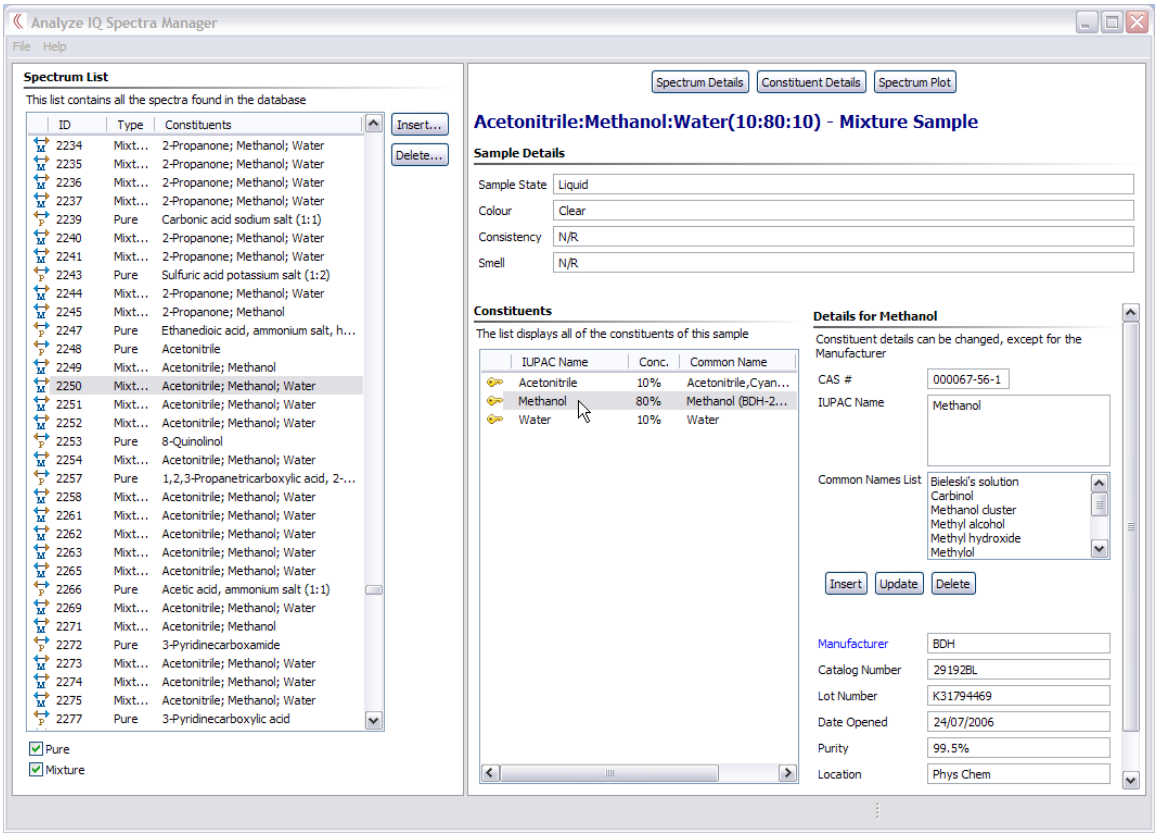

Figure 8: Selecting Constituent in Constituent Details

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.

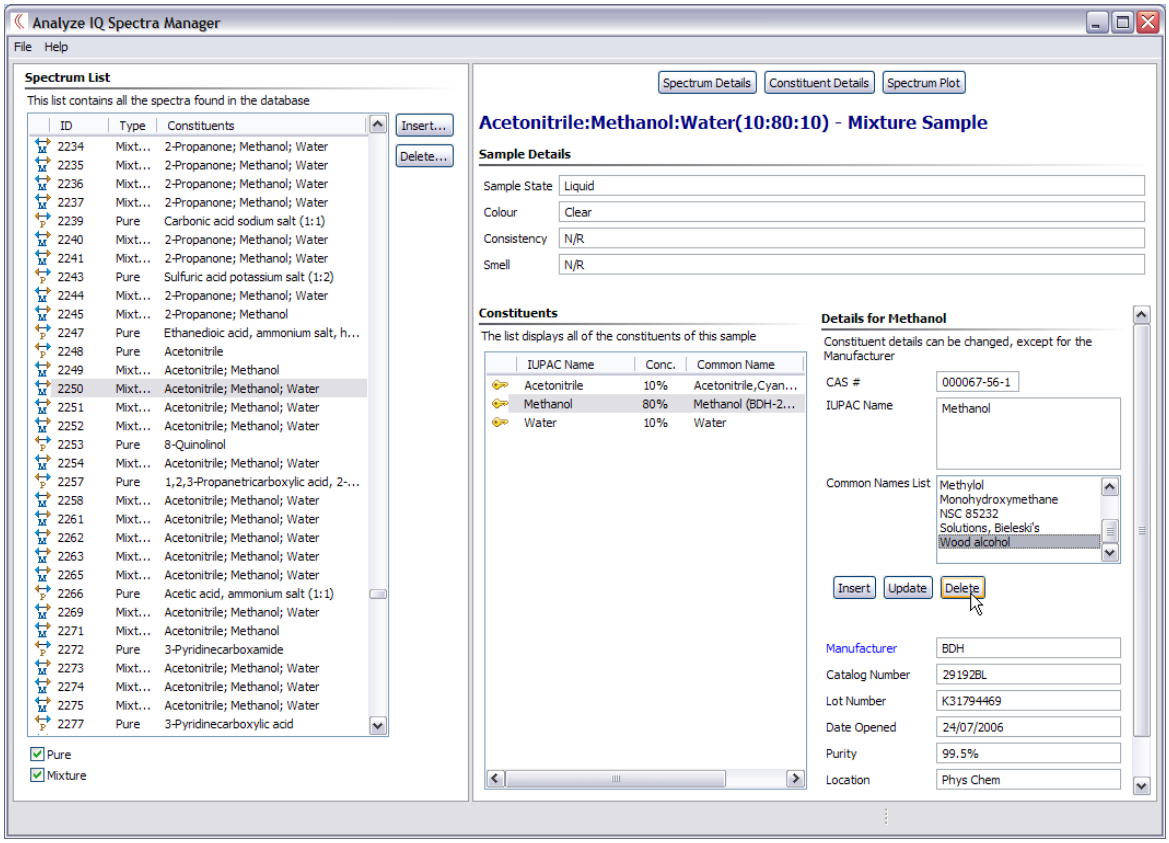

Figure 9: Delete Common Name–Step 1

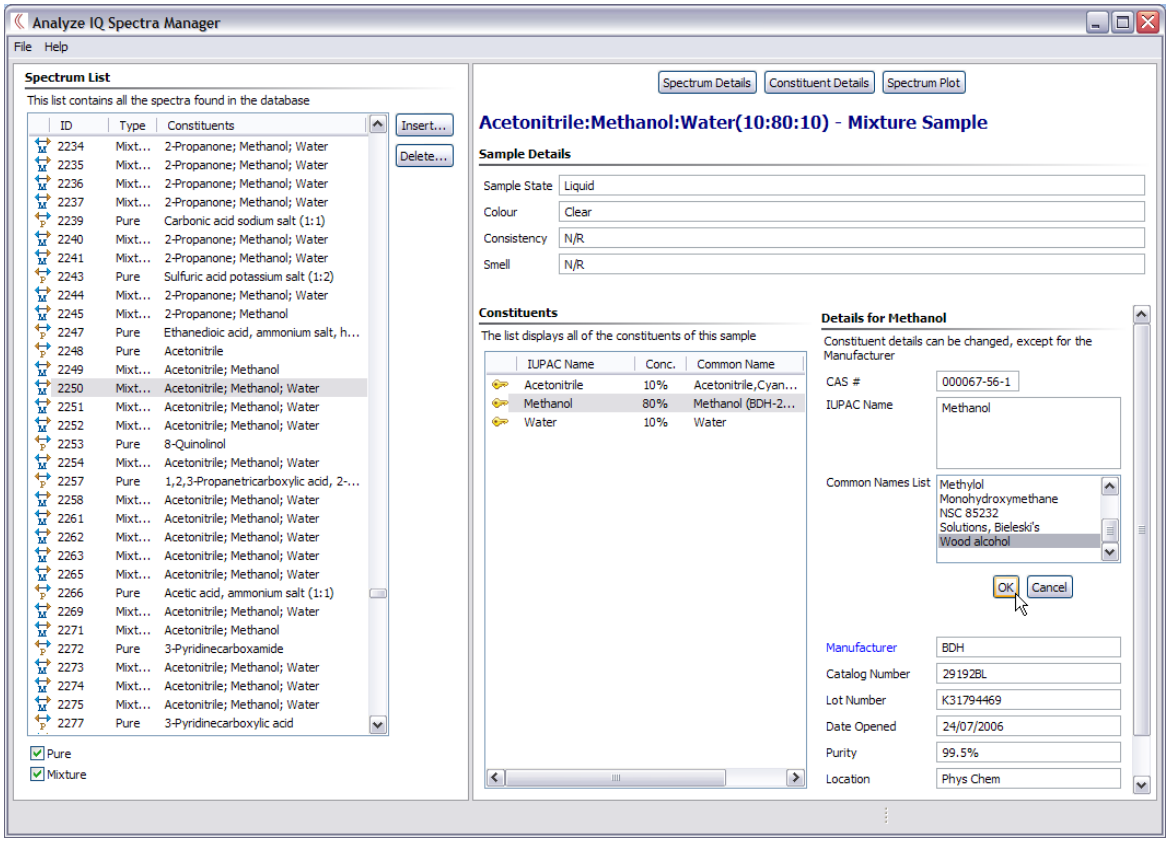

Figure 10: Delete Common Name—Step 2

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.

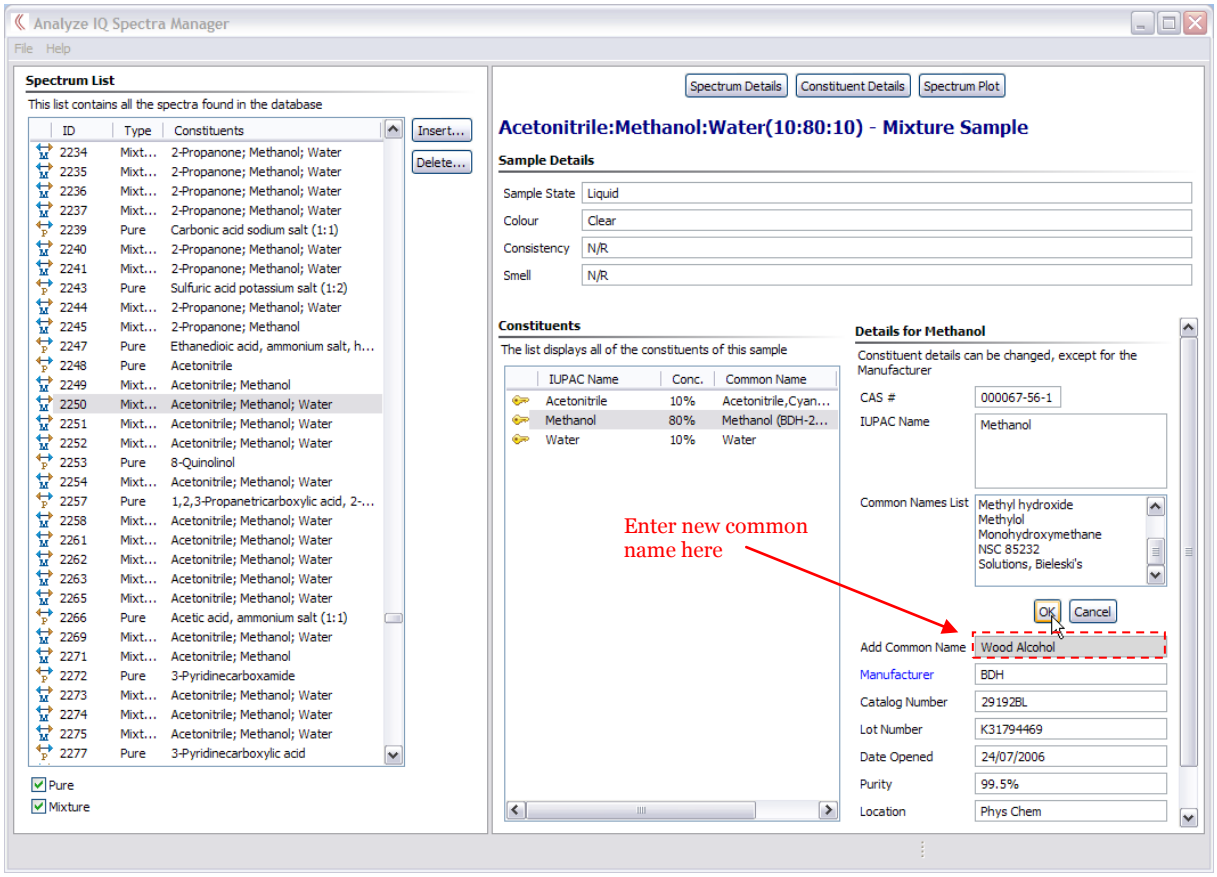

Figure 11: Add Common Name

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.

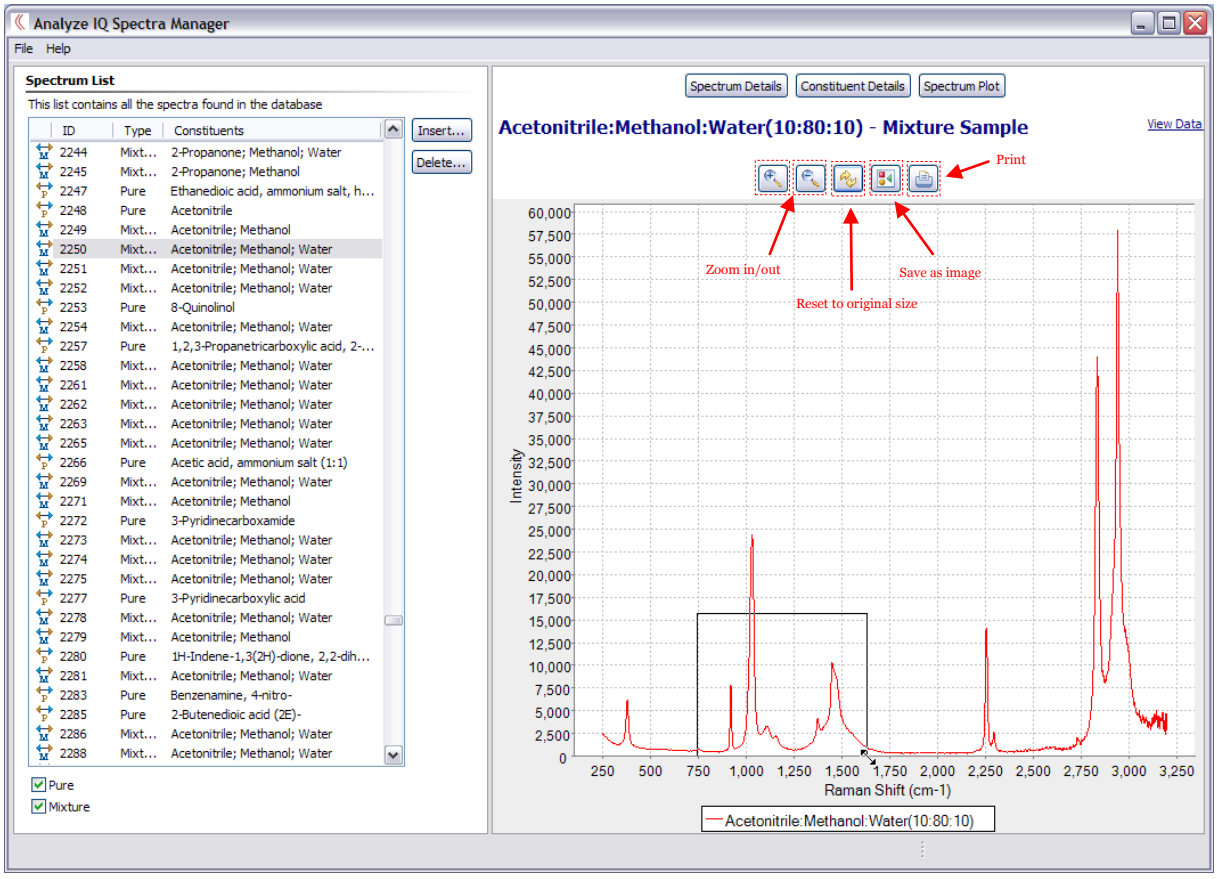

Figure 12: View Spectrum Plot

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.

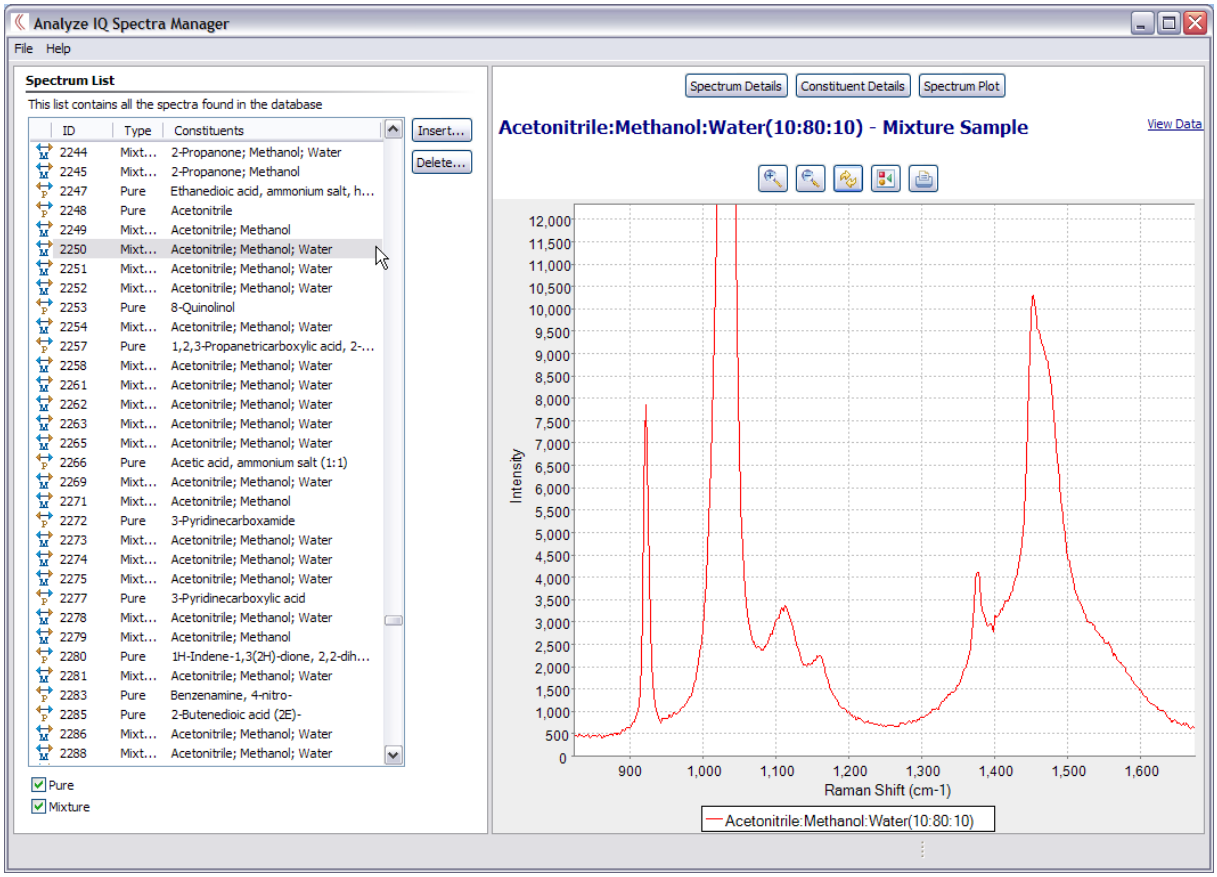

Figure 13: Zooming in on Spectrum Plot

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:

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

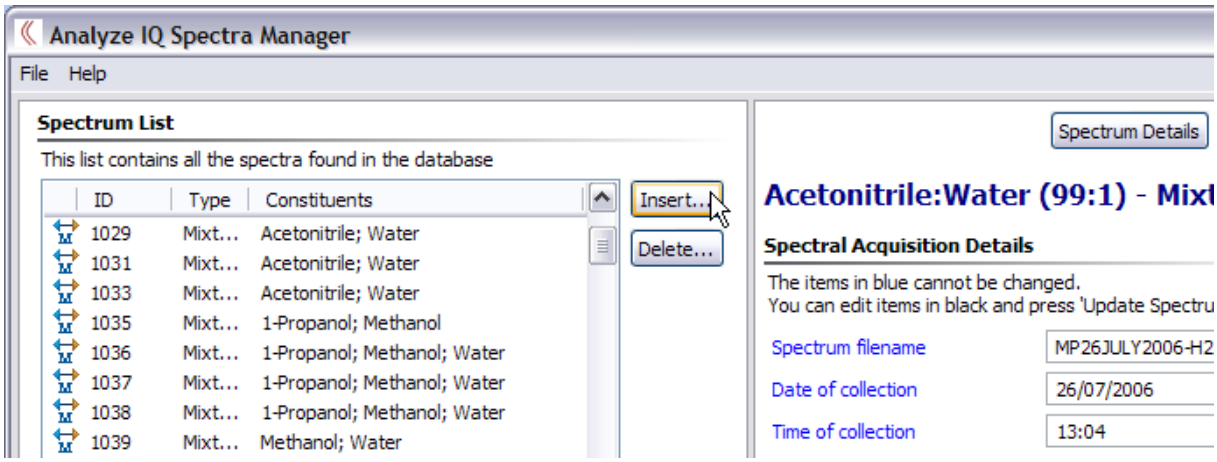

Figure 14: Adding a Spectrum—Step 1

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.

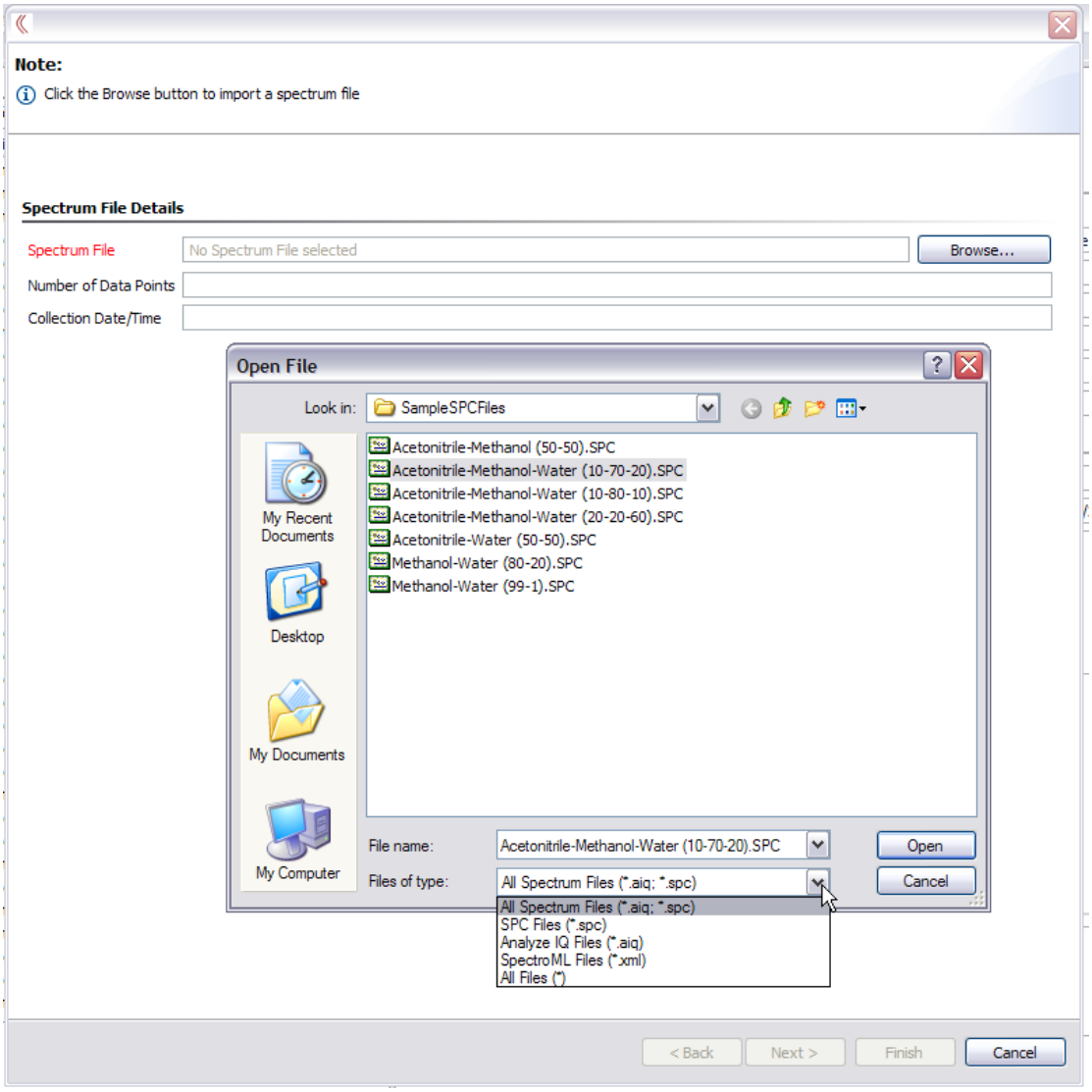

Figure 15: Adding a Spectrum—Step 2: Select Spectrum File

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.

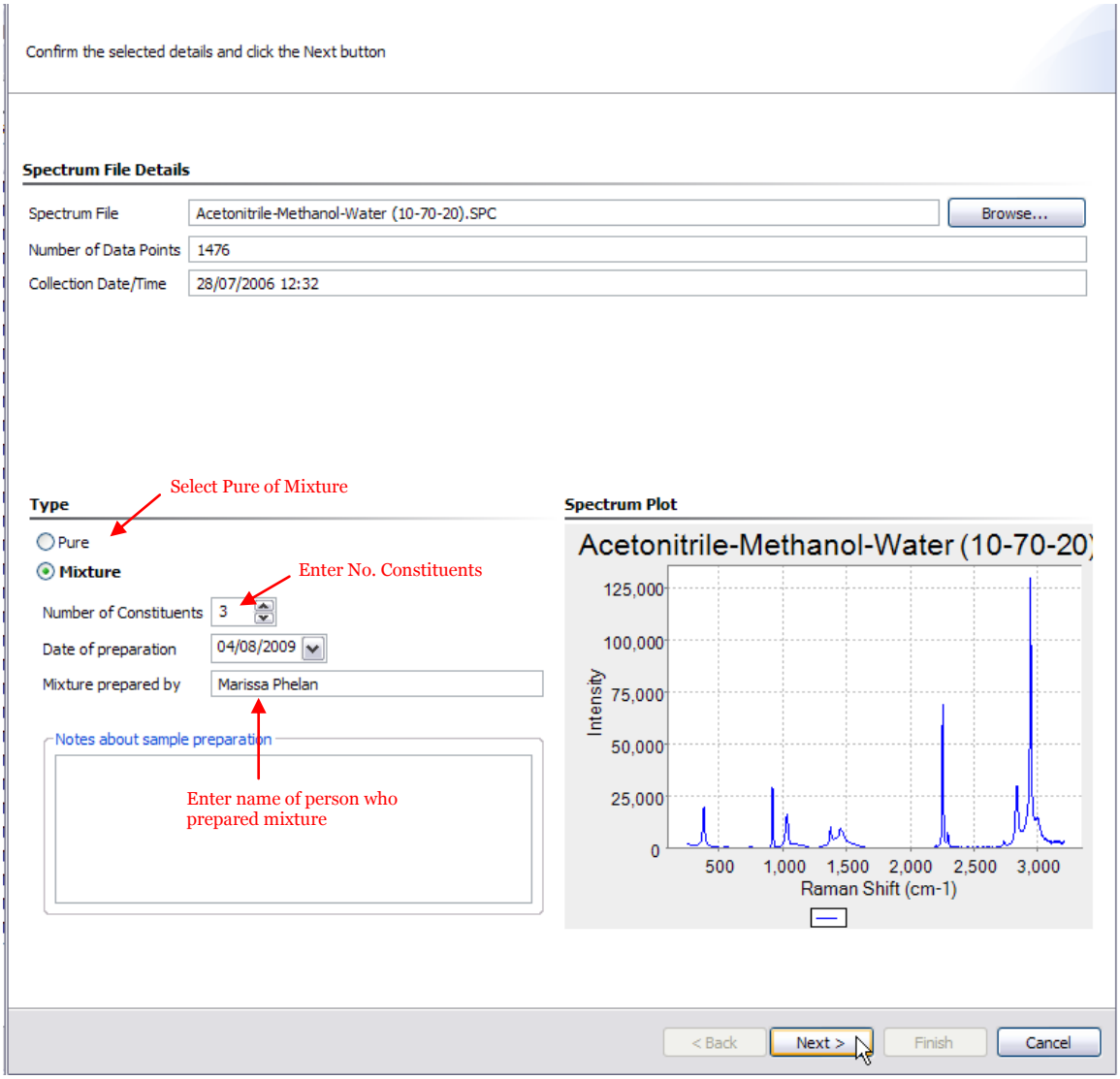

Figure 16: Adding a Spectrum—Step 3

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.

d. Enter the concentration for that constituent

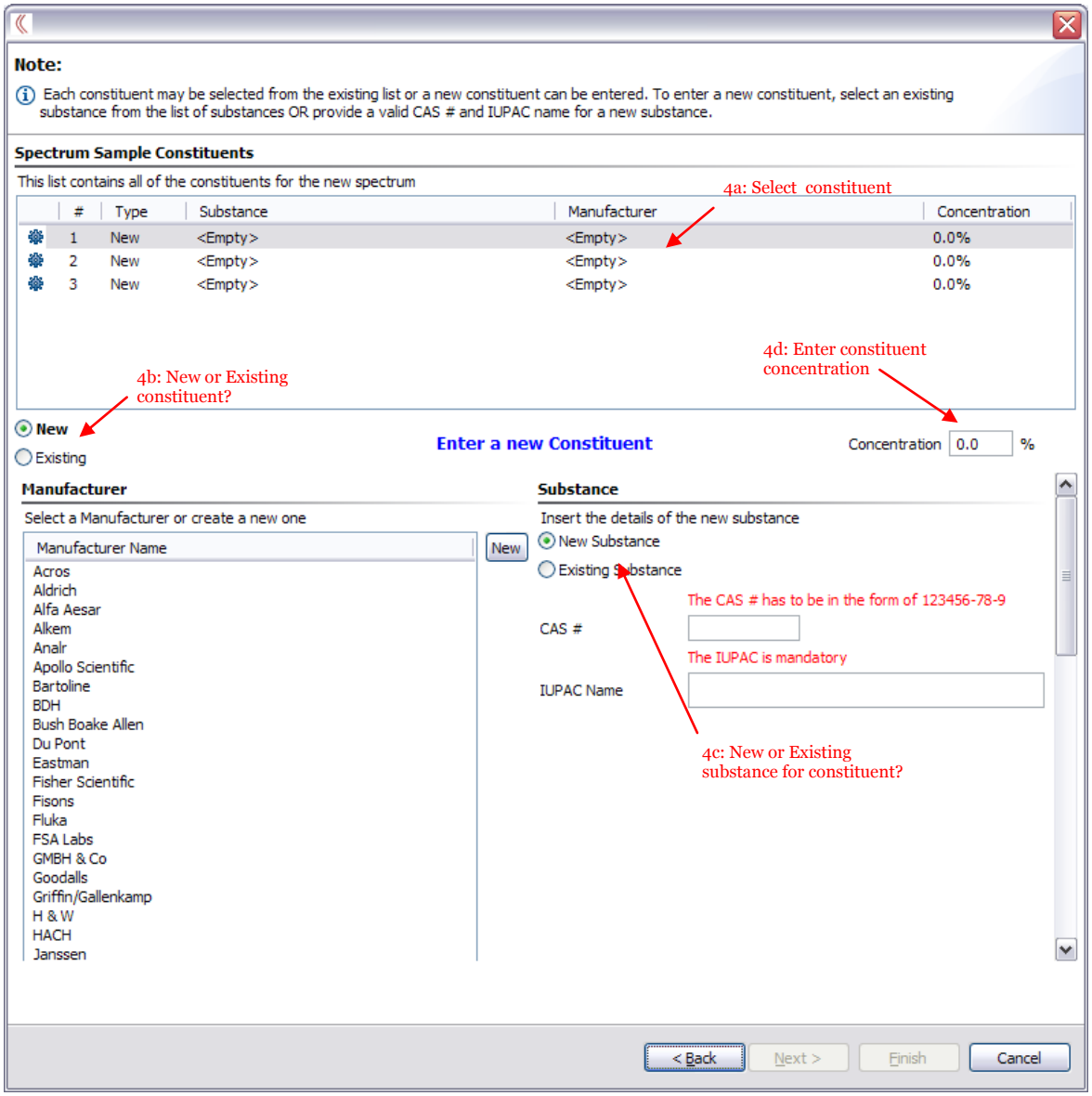

Figure 17: Adding a Spectrum—Step 4

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**

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.

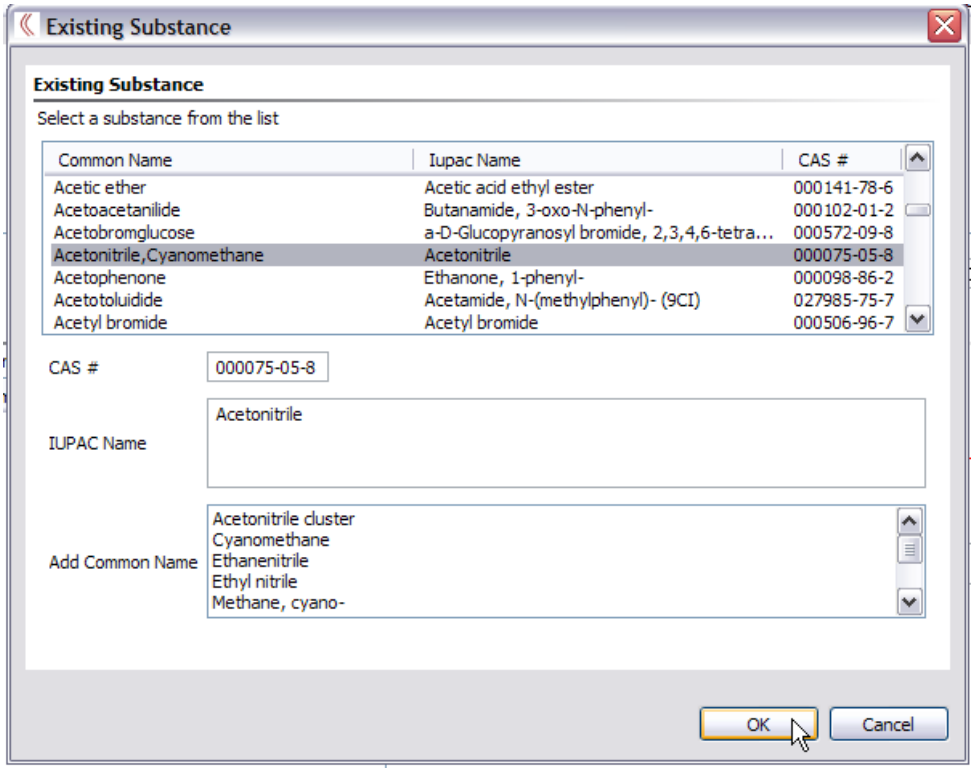

Figure 18: Adding a Spectrum—Step 5a: Selecting Acetonitrile from list of Existing Substances

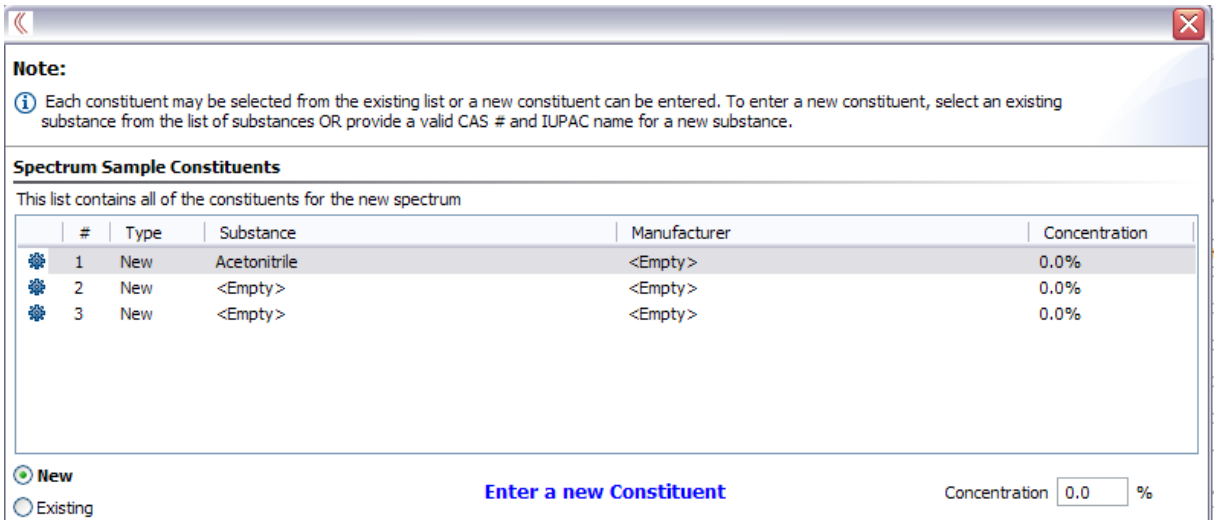

Figure 19: Adding a Spectrum—Step 5b: New Acetonitrile constituent

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.

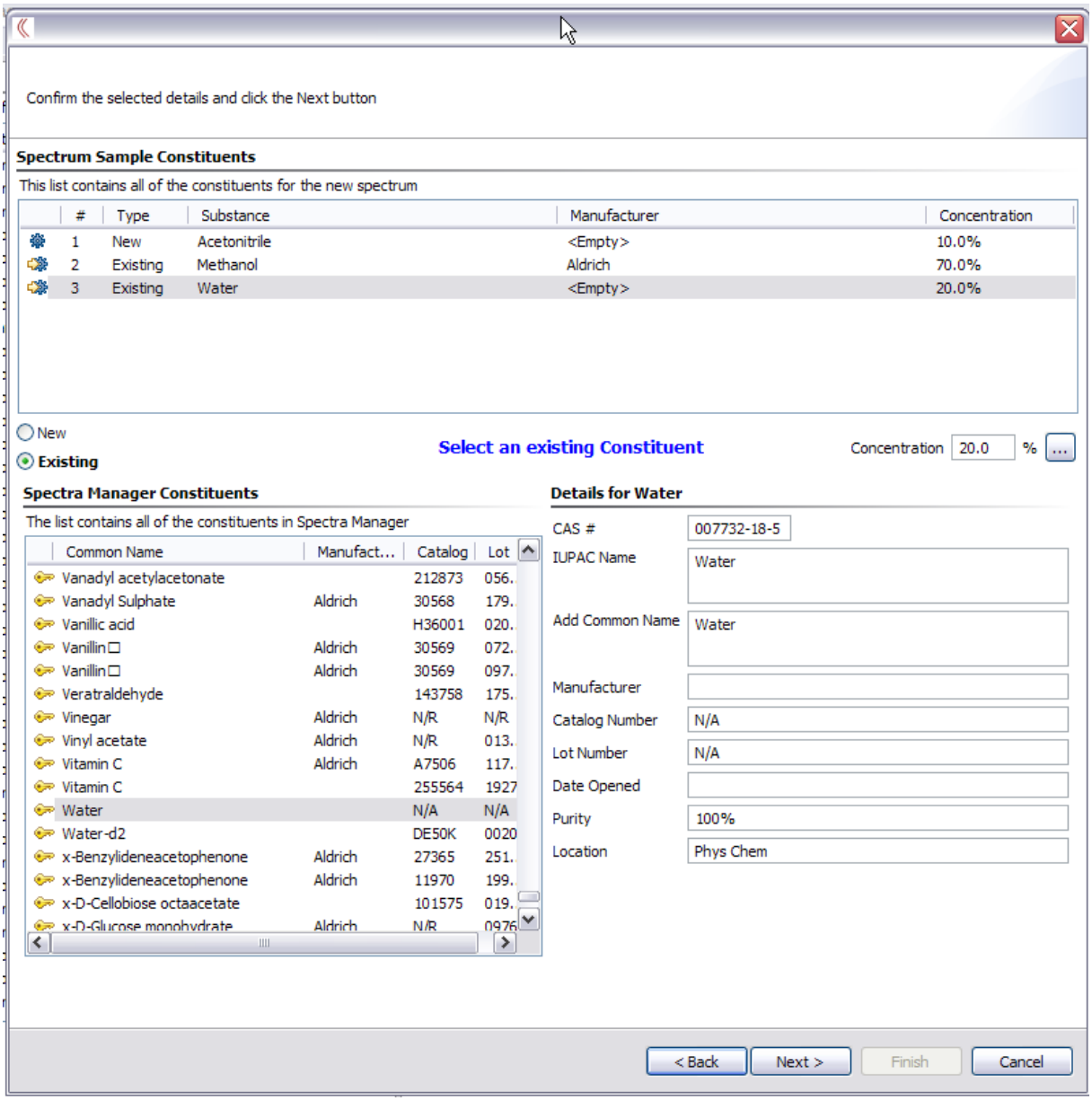

Figure 20: Adding a Spectrum—Step 6: Selecting remaining constituents (Methanol and Water) from the list of existing constituents in Spectra Manager

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.

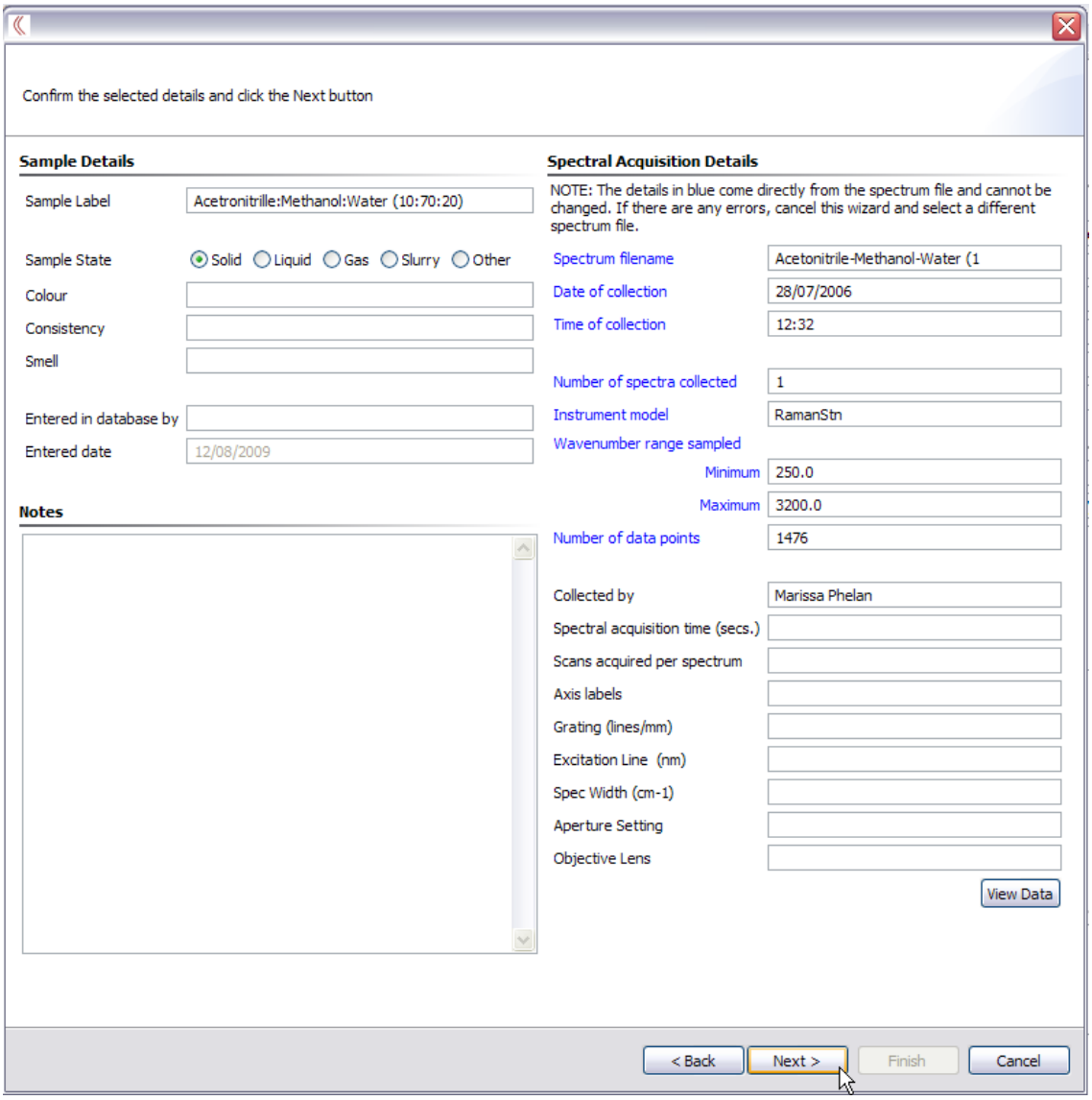

Figure 21: Adding a Spectrum—Step 7: Sample and Spectral Acquisition Details

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**.

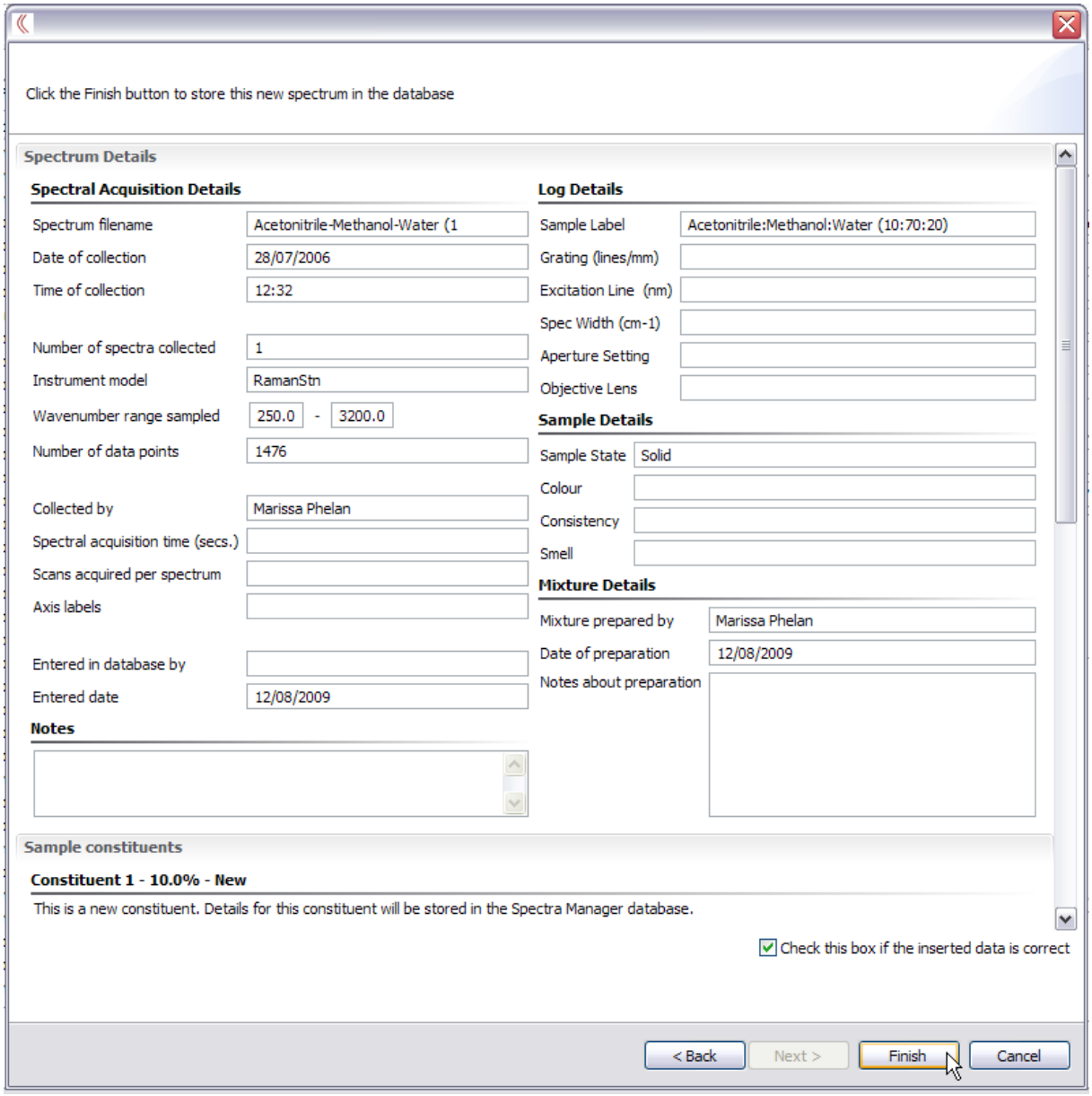

Figure 22: Adding a Spectrum—Step 8: Validation

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).

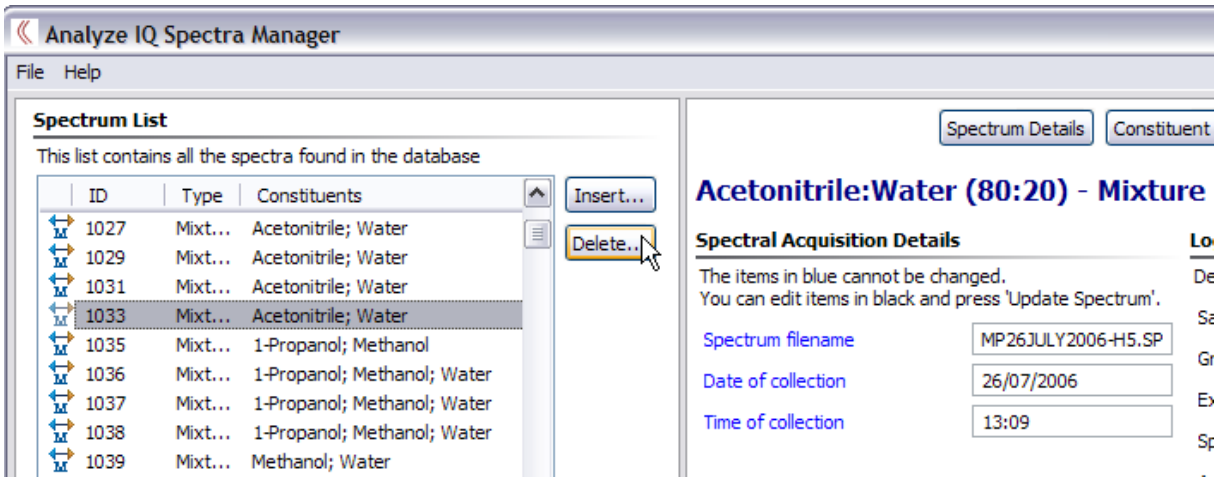

Figure 23: Deleting a Spectrum

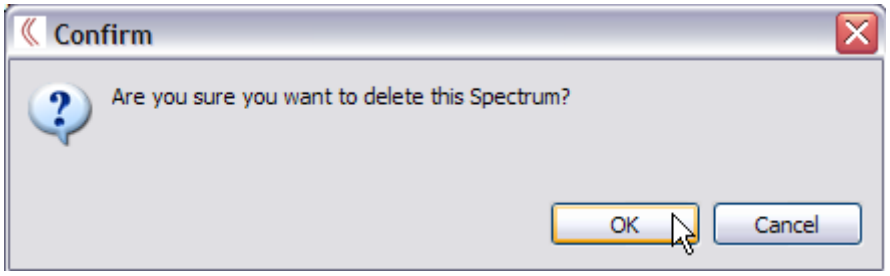

Figure 24: Deleting a Spectrum—Confirmation

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, http://www.AnalyzeIQ.com, or send an email message to support@AnalyzeIQ.com.

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 sales@AnalyzeIQ.com.

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 sales@AnalyzeIQ.com.

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