Analyze IQ Lab
Version 3.0

Getting Started Guide

Table of Contents

1   Introduction

Analyze IQ Lab is a software package that uses state-of-the-art model-based techniques, drawn from chemometrics and data mining, for the rapid analysis of spectral data. The types of analysis that can be undertaken fall into two general categories:

1. Classification (also known as Qualitative Analysis or Discrimination): use models to predict whether a sample belongs to a specific category of materials; for example, predicting whether or not a sample of an unknown liquid contains a specific solvent.
2. Quantification (also known as Regression or Numerical Estimation): use models to predict a numeric value associated with a target substance; for example, predicting the concentration of a substance in a mixture.

Analyze IQ Lab also allows users to build their own models that can be deployed for the analysis of spectra. **Analyze IQ Lab** can be used for the following two core activities:

1. Application of models to the analysis of unknown spectral data.
2. The building of classification or quantification models.

These two core activities are carried on separate pages[1] of **Analyze IQ Lab**: the *Apply Model* page and the *Build Model* page. Spectral analysis can be carried out by using models built by the user or by applying pre-built models that have been included in **Analyze IQ Lab**. As part of the **Analyze IQ Lab** installation, sample models may be installed; if selected for the install, these models are ready for use when **Analyze IQ Lab** is first started.

This guide briefly outlines how **Analyze IQ Lab** can be used for the analysis of spectra. It describes how to apply one of the pre-built models to a spectrum. For more detail on the use of Analyze IQ Lab for the generation of models, see the ***Analyze IQ Lab User Manual*** (available from the *Help* menu in **Analyze IQ Lab** and downloadable from http://www.AnalyzeIQ.com).

---

[1] A *page* is a group of windows that function together for performing a task.

2   Installation

Analyze IQ Lab can be installed and run under all recent versions of the Windows desktop operating system, including Windows XP, Windows Vista, Windows 7 and Windows 8. It is 32-bit software and works fully on both 32-bit and 64-bit operating systems.

2.1   USB Key Installation

To install from USB key, insert the USB key into a USB slot and follow the instructions that appear after you open it.

If the installation screen does not appear automatically when the USB key is inserted, navigate to the top level of the drive and run the **StartHere.exe** program to start the Analyze IQ software installation.

During installation, the Setup program installs a Java Runtime Environment. If you already have the same one or a newer one installed, you can safely skip this step.

2.2   Website

If you wish to download **Analyze IQ Lab** from the Analyze IQ website, www.AnalyzeIQ.com, you must first register on it. To do so, go to the website 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, you can download the **Analyze IQ Lab** software package at the following address: http://www.AnalyzeIQ.com/Download.html. This page allows you to download the software setup file. After downloading the setup file, start the installation process by double-clicking on it.

2.3   Getting a License

At the end of the installation process, when you first run **Analyze IQ Lab**, you will be prompted to 'Get a License', which requires an internet connection. This final step must be carried out in order to be able to run **Analyze IQ Lab**.

You can decide to defer getting a license until a later time. Please see 2.5.5 for further details.

If you are installing an evaluation copy of the software, you will enter your registered username to get a license after you install the software. Otherwise, you will enter a Commercial License Code that is given to you by Analyze IQ Ltd, or your software supplier, when you purchase the software.

2.4   Upgrading Your Existing Installation

If you have a license for an older version of **Analyze IQ Lab**, you may be entitled to install new releases. If so, you are recommended to back up data on your computer before proceeding.

Depending on your specific computer configuration and operating system, if you have built your own models with an older version of **Analyze IQ Lab**, you may find that you cannot see them in the newer version of **Analyze IQ Lab** when you install it. The models are easily transferred into the newer version; please contact Technical Support for instructions specific to your computer's configuration.

Please note that you should also take care when upgrading to a new release of **Analyze IQ Spectra Manager** that you do not overwrite spectra that you have added to the database. Refer to the ***Spectra Manager User Manual*** or contact Technical Support for further information.

2.5   Help Menu

As shown in Figure 1, you can access details about your installed version of the program, access contact details for Technical Support, open the User Manual and Getting Started Guide in PDF format, and update your license.
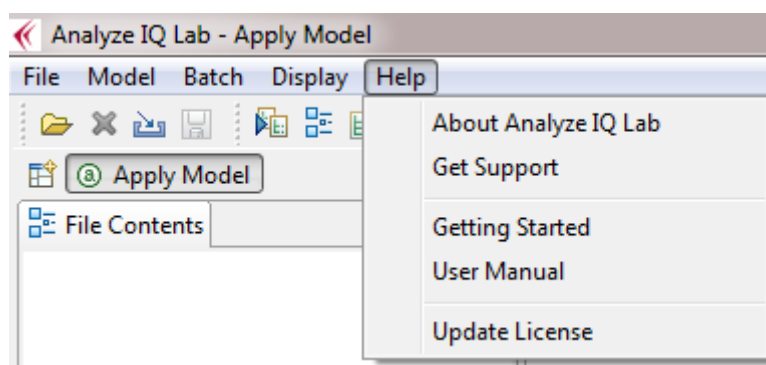

Figure 1: Help Menu
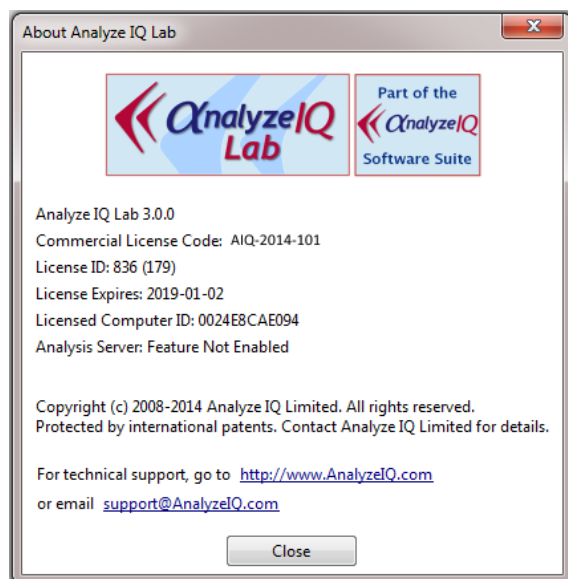
2.5.1 Help Menu - About Analyze IQ Lab

Figure 2: About Analyze IQ Lab

As shown above in Figure 2, the About **Analyze IQ Lab** menu shows you details regarding the version currently installed, including the software version number, your licence code, license ID, the license expiry date and the MAC address of the computer.

2.5.2 Help Menu - Get Support

In this menu, you can access contact details for Technical Support as can be seen in Figure 3.
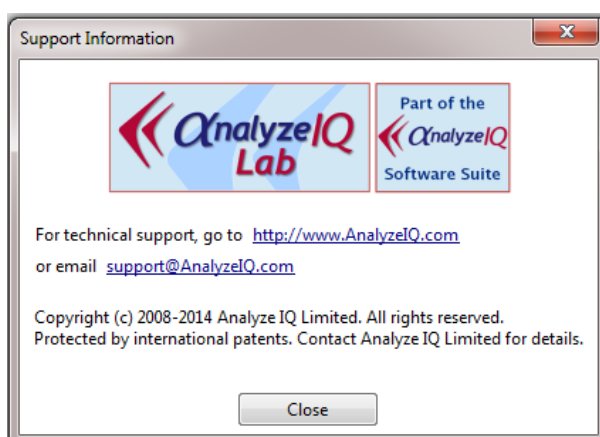

Figure 3: Get Support

2.5.3 Help Menu – Getting Started

From this menu, you can open the **Analyze IQ Lab** Getting Started Guide (this document) in PDF format.

2.5.4 Help Menu – User Manual

From this menu, you can open the **Analyze IQ Lab** User Manual in PDF format.

2.5.5 Help Menu – Update License

If you deferred getting a licence after first installing the software, or if you are extending an Evaluation Licence or upgrading to a Commercial Licence, you can update your licence from this menu. Enter either your user name for an Evaluation Licence or your Commercial License Code to acquire a license from our server (an internet connection is necessary). See Figure 4.
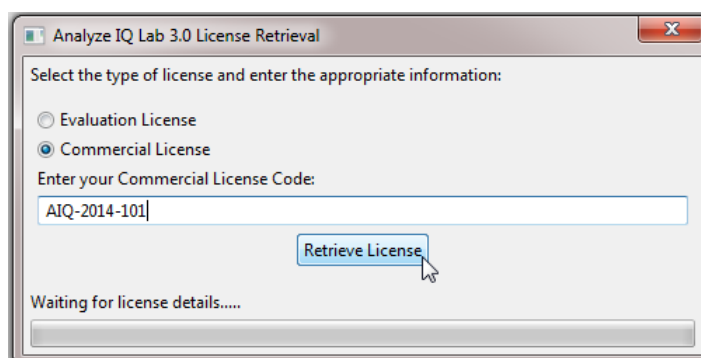

Figure 4: Update License

3   Getting Started with Analyze IQ Lab

3.1   Start Page

When the **Analyze IQ Lab** application is first started, you are presented with the *Apply Model* page as shown in Figure 5. (Note that this figure assumes that the sample models were selected in the installation of **Analyze IQ Lab**.) This figure highlights the five areas of this page, which are as follows:

1. ***Spectrum Details****:* shows details of the spectrum of the currently opened file, such as date recorded, instrument manufacturer etc.
2. ***View Spectrum****:* displays a plot of the spectrum of the currently opened file.
3. ***Models****:* shows the current set of models that are available for the analysis of the spectrum.
4. ***View Results****:* when a model has been applied to a spectrum, the results of the analysis are shown in this area.
5. ***Pre-processing****:* shows the pre-processing techniques that can be applied to the currently opened spectrum. It also shows a history of what pre-processing steps have already been applied.
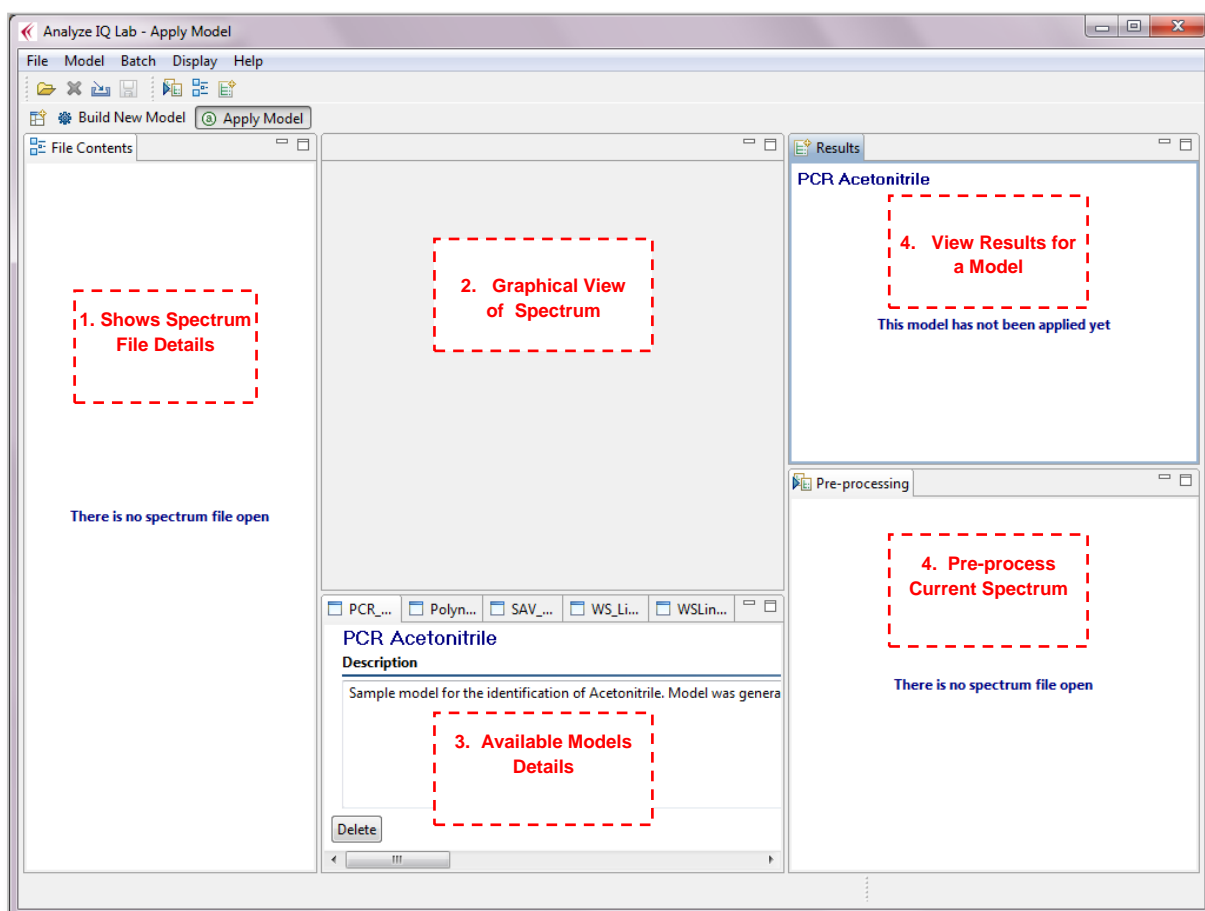

Figure 5: Starting page of Analyze IQ Lab

When **Analyze IQ Lab** is run for the first time, all areas of the *Apply Model* page are empty, unless pre-built models have been shipped with your **Analyze IQ Lab** package, in which case the *Available Models* area lists these models. In the example of Figure 5, three models are available:

1. PCR Acetonitrile
2. SAV Acetonitrile
3. WS Linear SVM Acetonitrile

All of these three sample models have been designed for the identification of acetonitrile; the difference between them is that each model has been generated using a different analysis technique; see the descriptions for each model.

3.2   *Using a Model for Analysis*

To perform an analysis of a spectrum with a model, such as the *PCR Acetonitrile* model shown in Figure 5, you must carry out the following steps:

1. Open a spectrum file (see Section 3.2.1), or acquire a spectrum from an instrument (see Section 3.2.3)
2. Select and apply a model (see Section 0).
3. View model results (see Section 3.2.6).

The following sections explain these steps.

3.2.1 Open a Spectrum File

A spectrum file can be opened either via the menu or the shortcut (see Figure 6). In either case, you are presented with an *Open File* window, in which you browse to the appropriate directory, select a spectrum file and click on *Open*, as shown in Figure 7. The spectrum file opened in Figure 7 happens to be in SPC format and stores the spectrum of a mixture made up of 10% acetonitrile, 70% methanol and 20% water. This spectrum file is one of the sample SPC files provided with **Analyze IQ Lab**. The sample spectrum files can be found in a sub-folder of the main **Analyze IQ Lab** installation folder.
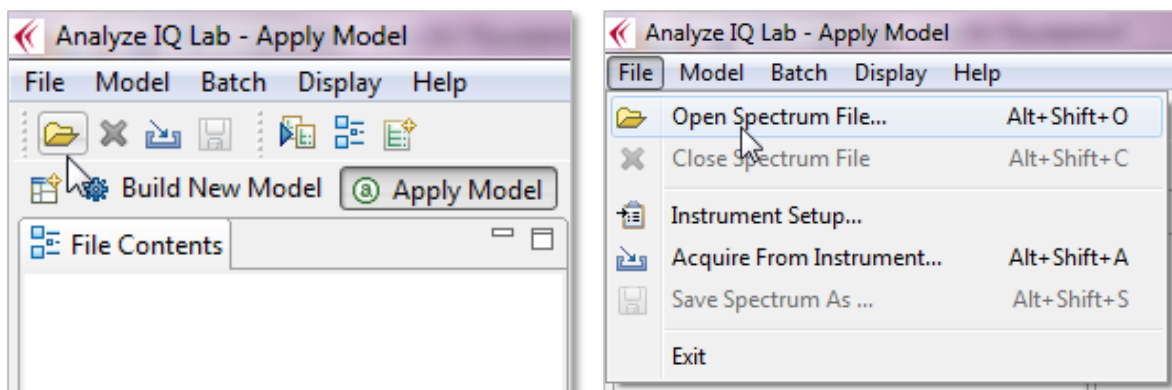
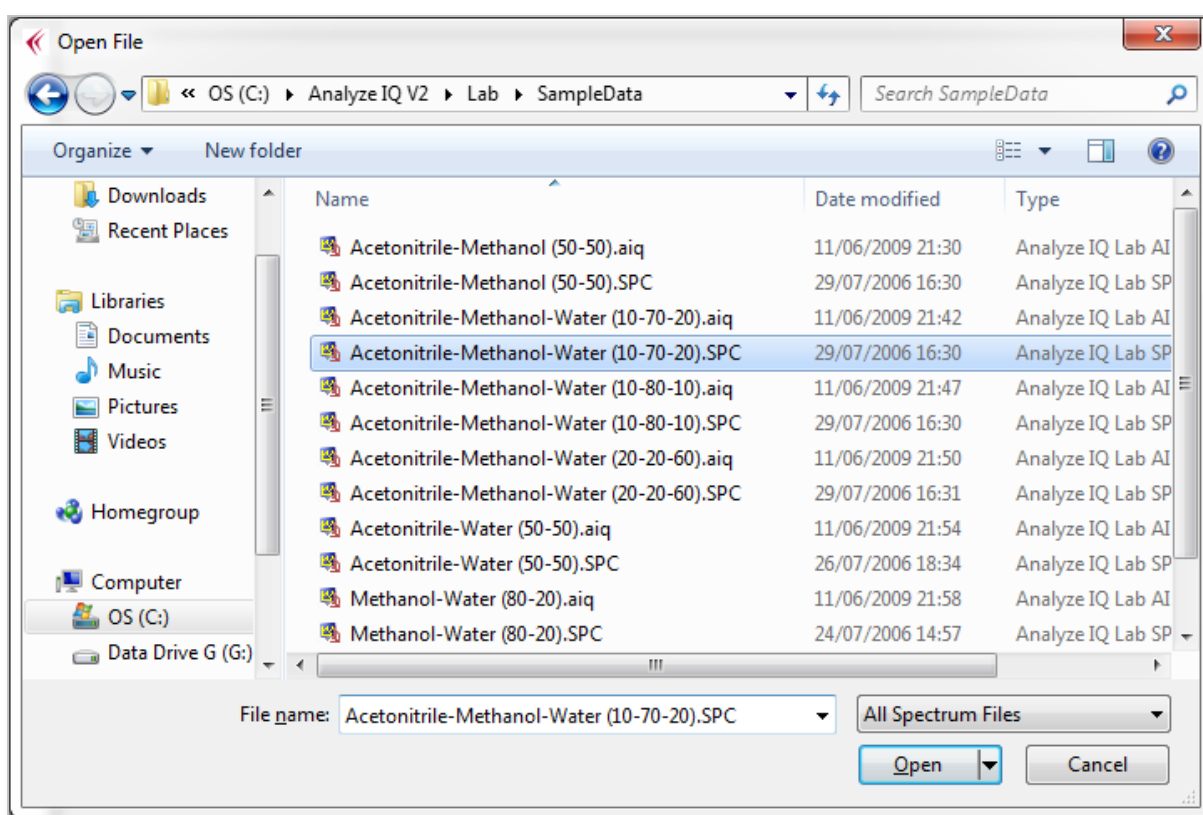**Figure 6: Open Spectrum file using: (left) the menu; (right) the shortcut**

Figure 7: Open Spectrum file window

3.2.2 File Formats

Analyze IQ Lab supports several popular file formats; see Figure 8:

1. **SPC:** Thermo-Fisher's 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. ***JCAMP-DX:*** IUPAC's popular JCAMP-DX file format. (Note that there are many variations of JCAMP-DX format; the Analyze IQ software supports most but may not support all. Contact Technical Support if you have problems.)
5. ***XY Text Files:*** These are simple files with either two rows or two columns of data, the first with X values and the second with Y values. See below for further details.
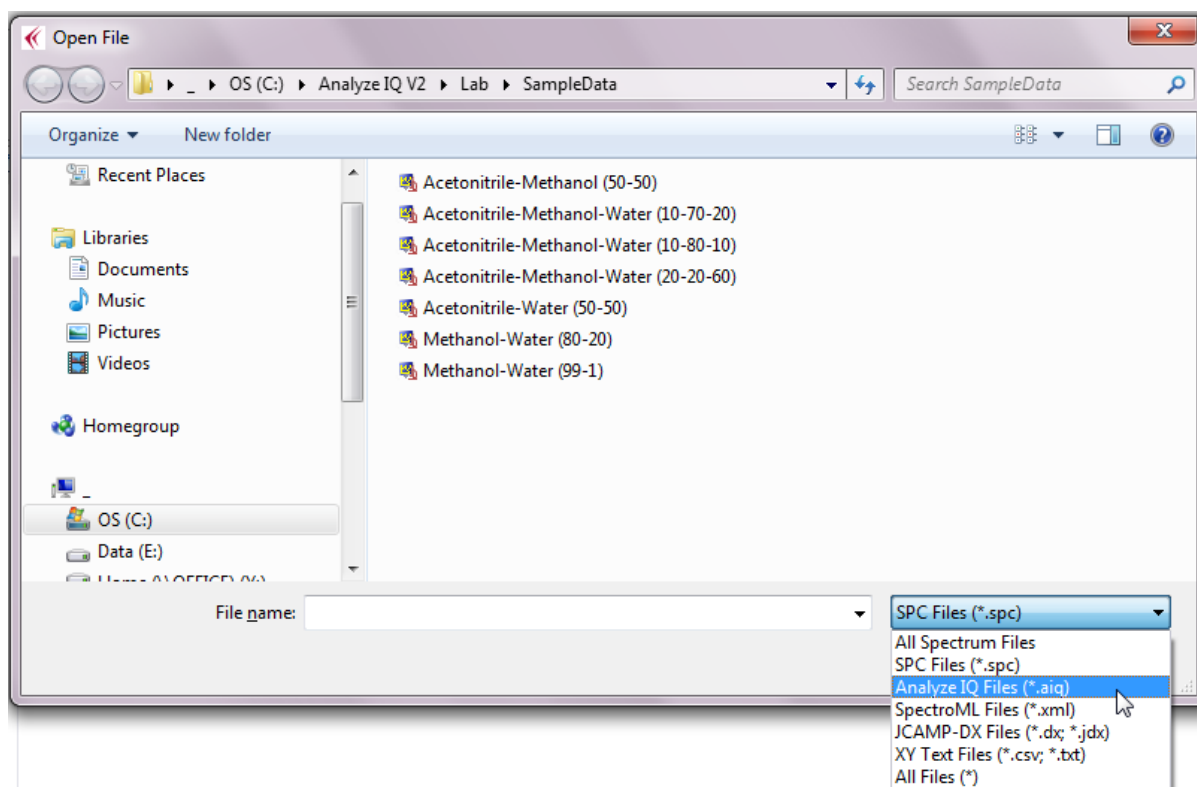

Figure 8: File Formats

As noted above, an *XY Text File* format simply consists of two rows or two columns of data, the first with X values and the second with Y values. Values may be separated by tabs or commas; the latter are known as Comma Separated Values (CSV) files. You may optionally include X and Y axis labels by putting them at the start of the two rows/columns.

The XY Text File format is particularly useful when you need to import data into Analyze IQ Lab from a software product that does not support any of our standard formats. You can easily generate files in this format with a spreadsheet program (such as Microsoft Excel or OpenOffice Calc) or a text editor.

An example of the start of an XY Text File is shown below; this one is in two rows and includes axis labels:

```
Wavenumber (cm-1)    250.0    252.0    254.0    256.0    ...
Intensity           2454.0   2439.0   2307.0   2202.0   ...
```

Figure 9: Example of the start of an XY Text File in row format with axis labels

When the spectrum file in any format is opened, details of the file contents are shown in the left-hand pane and a graph of the spectrum is shown in the middle of the *Apply Model* page (see Figure 10 below).

Note also that an *Apply* button is added to the *PCR Acetonitrile* pane; **Analyze IQ Lab** is now ready to apply this model (and any other models that are loaded) to the opened spectrum. For details on applying a model, see the next section.
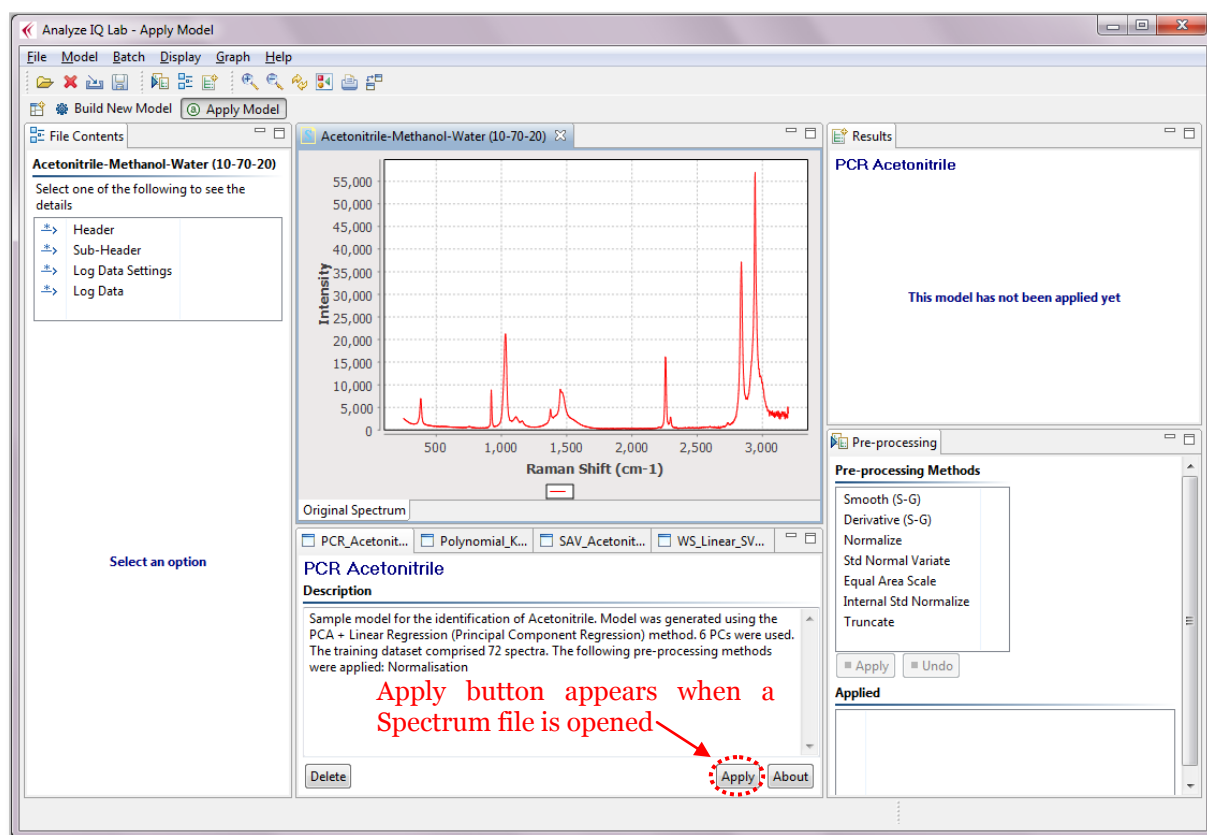

Figure 10: *Apply Model* page after Spectrum file is opened

3.2.3 Acquire from Instrument

With **Analyze IQ Lab**, you can acquire a spectrum directly from an attached spectrometer, provided that appropriate drivers have been supplied with your installation.

You can select which instrument to use by using the *Instrument Setup* menu option as shown in Figure 7 below. This opens an Instrument Setup dialog box (not shown) which shows the status of all installed instruments and allows you to select one.

After you have selected the instrument, you then can acquire a spectrum. To do this, select the *Acquire From Instrument...* option from the *File* menu, as shown in the figure below. An Instrument dialog box will appear, allowing you to specify settings appropriate to the specific instrument. (This dialog box is not shown, and its appearance varies from instrument to instrument.)
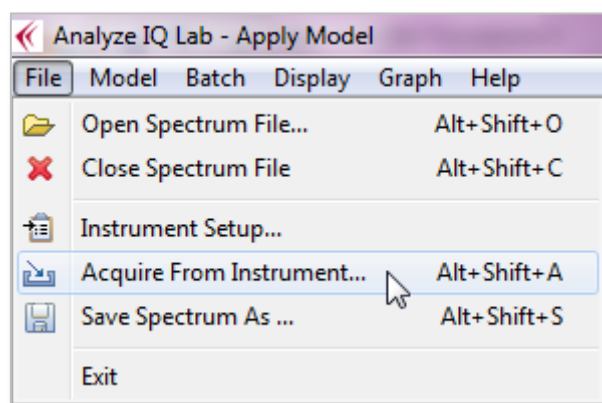

Figure 11: Menu options to select an instrument and acquire a spectrum directly from the attached instrument

Press the *Acquire* button on the Instrument dialog box to begin data acquisition. When data acquisition is finished, the Instrument dialog box will close and the data will be displayed, just as if you had opened a file.

If you are satisfied with the spectrum that you have acquired from the instrument, you will want to save it, as described next.

3.2.4 Save a Spectrum

The *File – Save Spectrum As...* menu function to save your data in either AIQ or SpectroML format. All ancillary information, as displayed on in the Contents view, is also saved.

Note that the spectrum data is saved in its 'raw' form, **without** any pre-processing you may have performed, such as normalisation or computing a derivative (see the ***Analyze IQ Lab User Manual*** for a description of pre-processing operations). This is to avoid problems subsequently arising with spectra being treated as 'raw' when they may have been pre-processed in a way that greatly changes their appearance, such as with a first derivative transform.

Note also that **Analyze IQ Lab** does not currently support saving SPC files; they are "read-only".

3.2.5 Apply Model

To analyze the current spectrum with a model, click on the *Apply* button of the model that you wish to apply (see Figure 12). In this example, clicking on the *Apply* button of the *PCR Acetonitrile* model will determine if the material, for which the current spectrum was recorded, contains acetonitrile or not (according to this particular model).
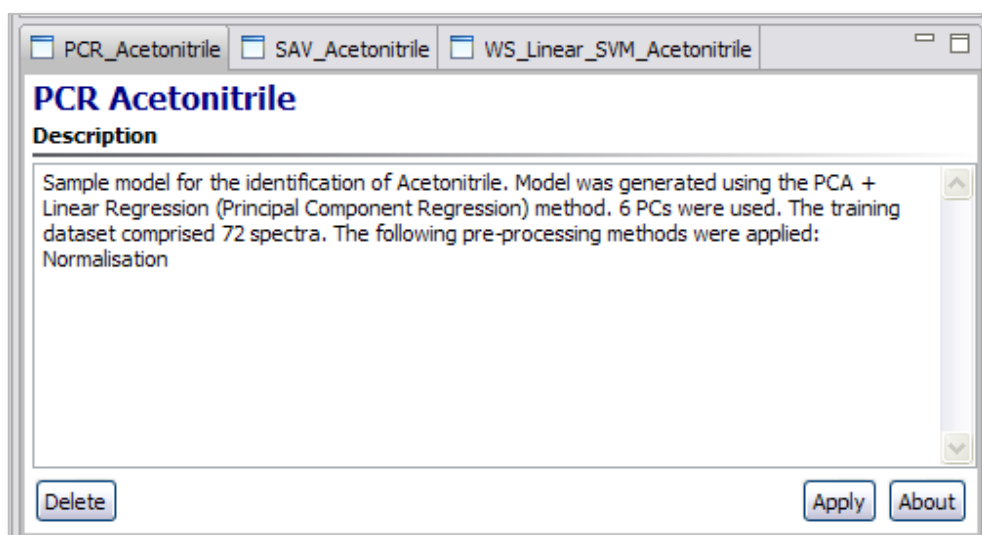

Figure 12: Applying the *PCR Acetonitrile* model

The next section describes how the results of applying a model are displayed.

3.2.6 View Model Results

When a model has been applied to a spectrum, the results are displayed in the top right-hand area of the *Apply Model* page. Figure 13 shows the results of applying the *PCR Acetonitrile* model on the spectrum opened in Figure 10. There are two parts to the displaying of results.

Firstly, the *Results* pane in the top right-hand area of the page lists the substances that the model has identified to be in the material associated with the test spectrum. In this example, the *PCR Acetonitrile* model has predicted the presence of acetonitrile in the material. This *Results* pane also lists details of any pre-processing steps that are applied by the model.

Secondly, a new spectrum is shown in the spectrum viewing area of the page; this illustrates the test spectrum after it has been pre-processed according to the requirements of the model (which can be determined by clicking on the *About* button for that model). Note that the pre-processing steps required for the model are automatically applied to the original test spectrum as it appears when the spectrum file is opened, i.e. any pre-processing steps that may have been applied in the bottom

right *Pre-processing* pane do not have any bearing on the application of a model. In this example, the *PCR Acetonitrile* model normalizes the sample spectrum, as can be seen in the *Results for PCR_Acetonitrile* graph in Figure 13 (i.e. all intensity values lie in the range 0 to 1).
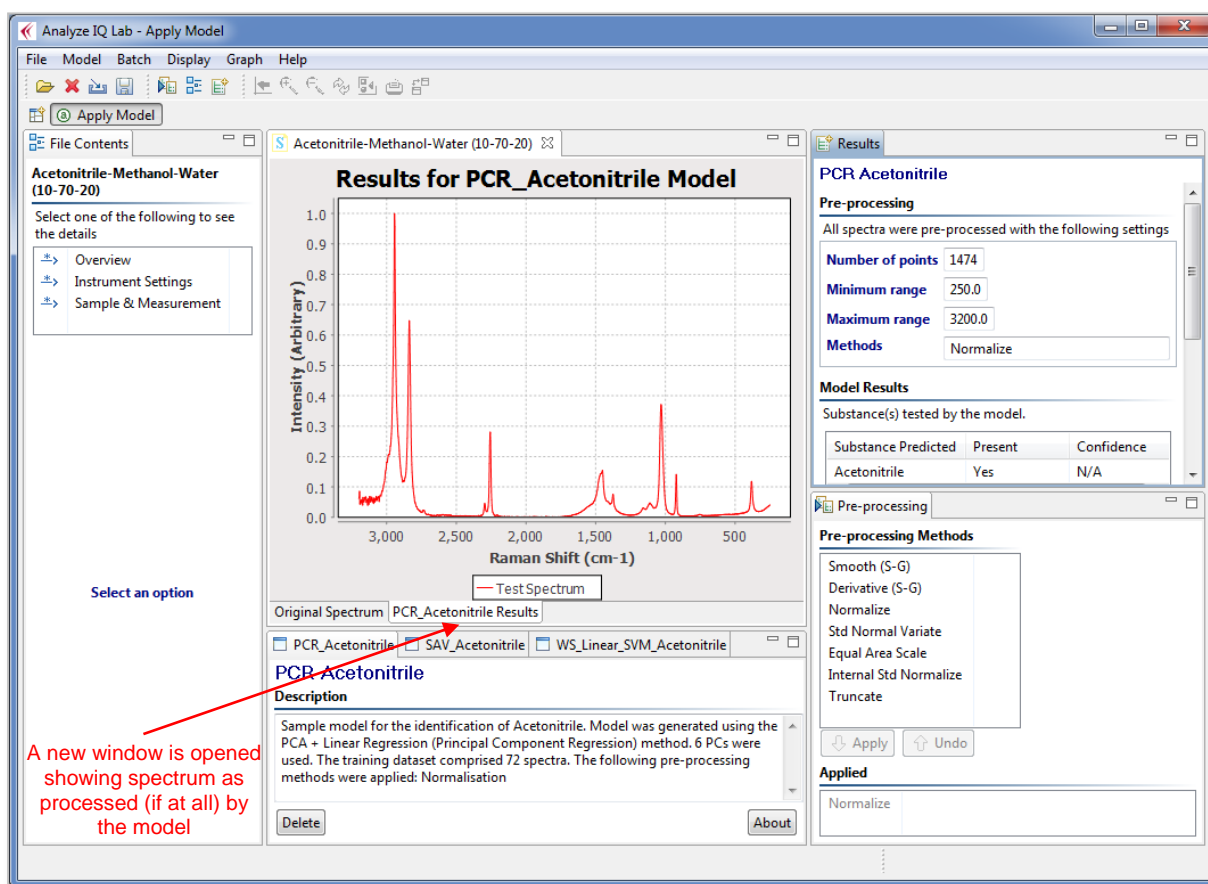

Figure 13: The results of applying the *PCR Acetonitrile* model

The *Results* pane of the *Apply Model* page (see Figure 14) also lists the target substances that the current model was designed to test for. One target substance, acetonitrile, is listed for the *PCR Acetonitrile* model.
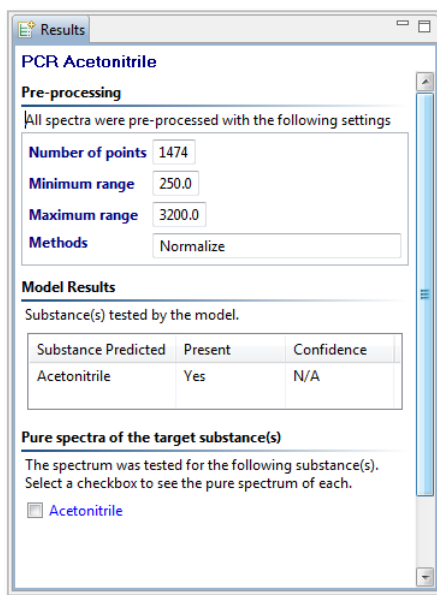
Figure 14: A closer view of the Results pane

Checking the box next to a listed target substance results in the spectrum of the target substance in its pure form being plotted in the same window containing the test spectrum (this pure target spectrum is also automatically pre-processed according to the requirements of the model). Figure 15 illustrates this feature, which is useful for visually comparing a test spectrum with the spectrum of a target substance of a model. A blue line is used for the plot of the pure target spectrum.
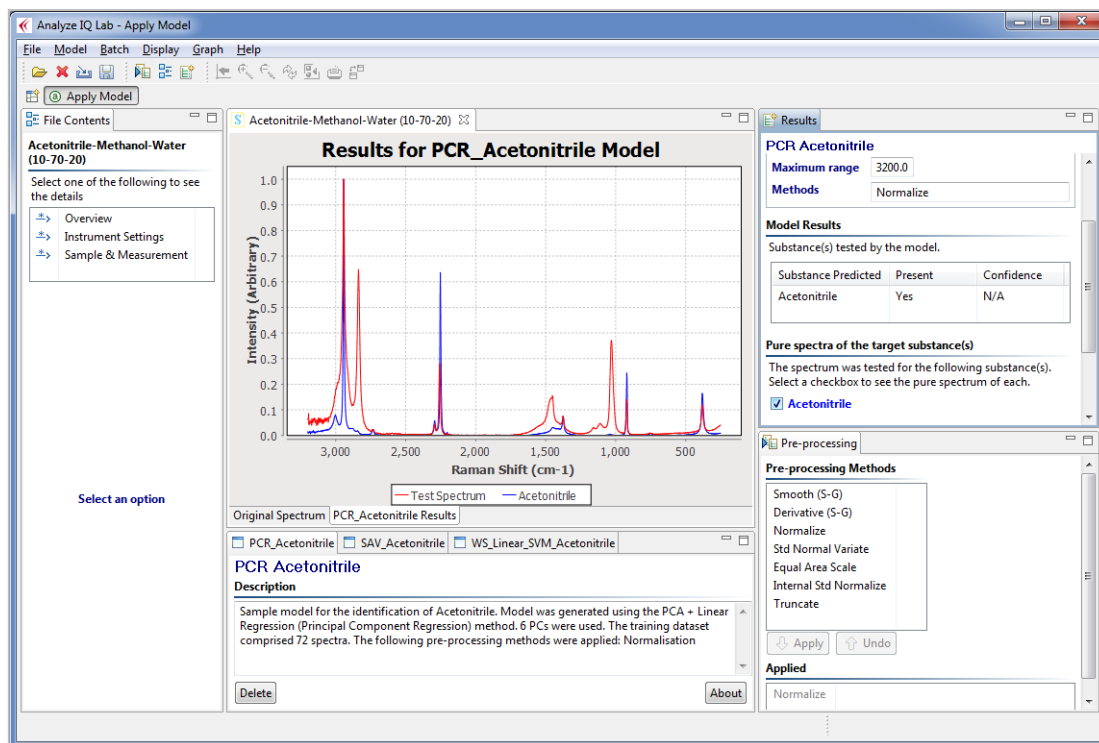

Figure 15: Displaying the spectrum of the pure target substance in the same graph that contains the spectrum of the test sample

The example of applying a model described above demonstrated a scenario in which the model returned a positive result, i.e. predicted the presence of the target substance. Figure 16 shows the result of applying the same *PCR Acetonitrile* model to another test spectrum, which is the spectrum of a mixture of methanol and water, i.e. not containing acetonitrile. The *Results* pane in this example states that the model's target substance (acetonitrile) has not been detected.
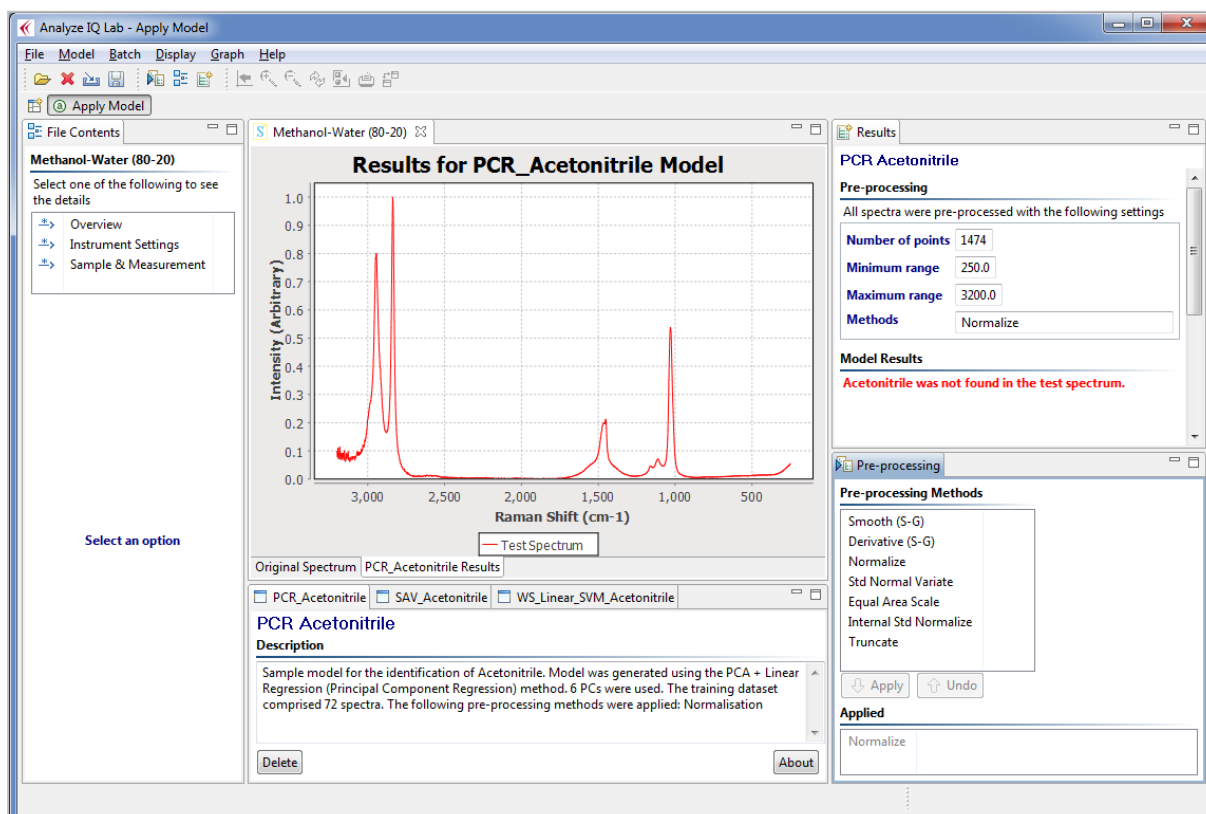

Figure 16: The PCR Acetonitrile model does not find its target substance in the test sample; this is correct since the test sample is a mixture of methanol and water

4 Next Steps with Analyze IQ Lab

After applying various models to different test spectra, the next step is to build your own models using the chemometric and innovative machine learning techniques provided in Analyze IQ.

The *Analyze IQ Lab User Manual* (which is installed with the **Analyze IQ Lab** software, and can be opened with the *Help – User Manual* menu command, and is also available for download at http://www.AnalyzeIQ.com) provides detailed instructions on how to do this and also provides more details on the analysis of spectra, such as how to view the detailed contents of a spectral data file and how to apply pre-processing methods to a sample spectrum.

5 Technical Support, Sales and Services

For assistance and technical support queries relating to **Analyze IQ Lab**, 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 **Analyze IQ Lab**, please contact our Sales Department by sending an email message to sales@AnalyzeIQ.com.

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

- Software training
- Data validation and analysis
- Chemometric model development
- Custom software development, including custom analysis solutions
- Integration of Analyze IQ chemometric models in third-party software
- Development of Instrument Interfaces
- OEM licensing

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