Aqualog® Software

User's Guide for version 3.6

http://www.HORIBA.com/Scientific

JOBIN YVON Technology

HORIBA Scientific

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revision B

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0: Introduction

About Aqualog® software

Aqualog® software is an easy data-acquisition software ever created by HORIBA Scientific. Spectrofluorometer control is available with only a few mouse-clicks or keystrokes, with a minimum of overlapping screens and windows. Data can be previewed while they are being recorded, and then immediately used with Origin® presentation and graphical analysis. Aqualog® software runs using Windows® 2000 or higher.

Note: *Keep this and the other reference manuals near the system.*

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- Following all precautions
- Referring to additional safety documentation, such as Material Safety Data Sheets (MSDS), when advised

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Symbols used in this manual

Certain symbols are used throughout the text for special conditions when operating the instruments:

Note:

General information is given concerning operation of the equipment.

1: Aqualog® Software Installation

Requirements

To successfully install Aqualog® software, your host computer needs the following:

Software

Windows® 2000, Windows® XP Pro, Windows® 7 (in compatibility mode), or Windows® Vista (in compatibility mode)

Hardware

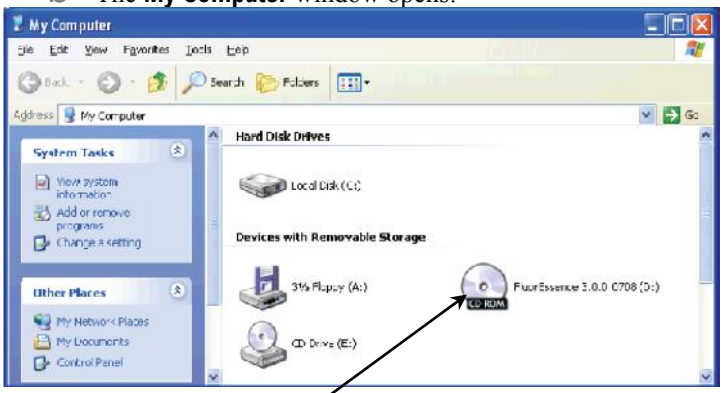
- Supports Windows® 2000, Windows® XP Pro, Windows® 7 (in compatibility mode), or Windows® Vista (in compatibility mode)
- 1 GB RAM
- 1 GB hard-disk space
- One DVD-ROM drive
- One available USB port
- Video resolution of at least 1024 × 768

Installation instructions

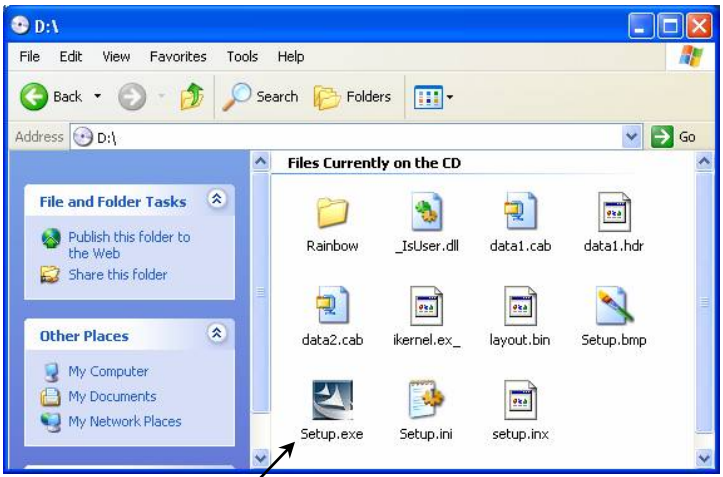
1. Remove any HORIBA USB software key (if inserted) from the host computer before starting the installation.
2. Insert the Aqualog® DVD in the host computer's DVD drive.
3. Open the DVD:

   a. On the desktop, open the My Computer icon.

   b. The **My Computer** window opens:



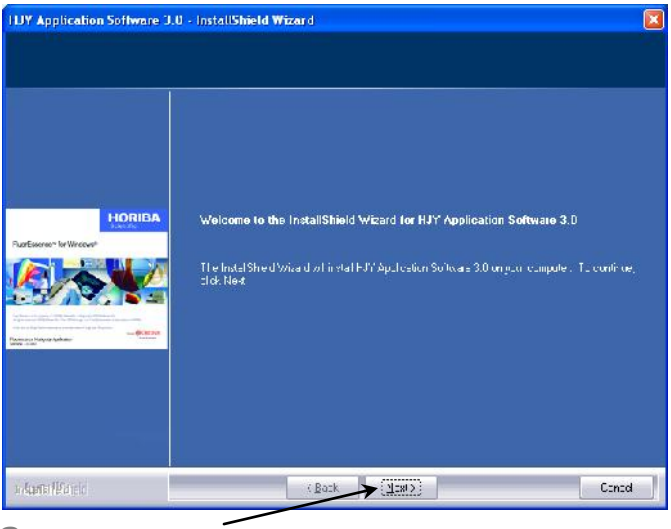
   c. Double-click on the DVD drive to open the Aqualog® DVD:



   d. Click the Setup.exe icon.

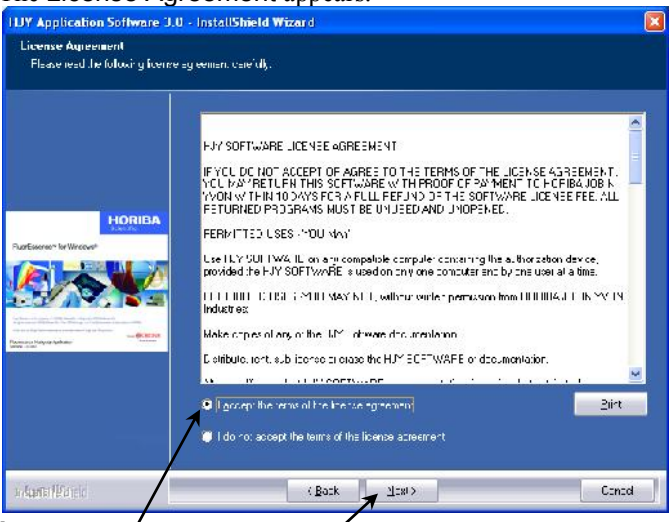
4 Install the Aqualog® software:

The InstallShield® Wizard starts.



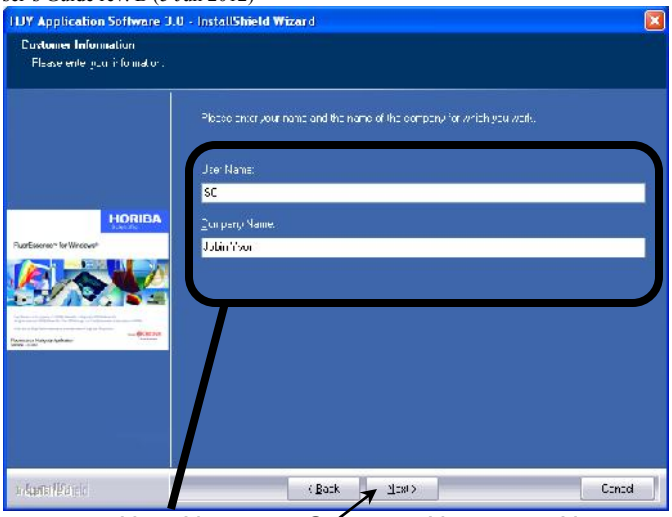
a Click the Next > button.

The License Agreement appears.



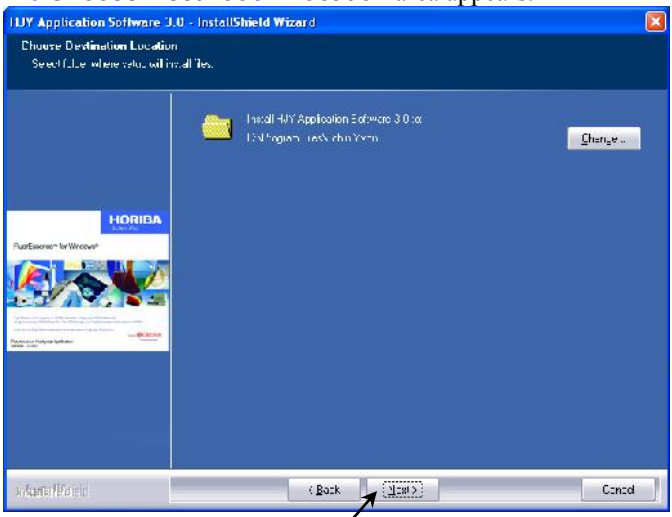
b Click I accept the terms of the license agreement radio button, then the Next > button.

The Customer Information area appears.



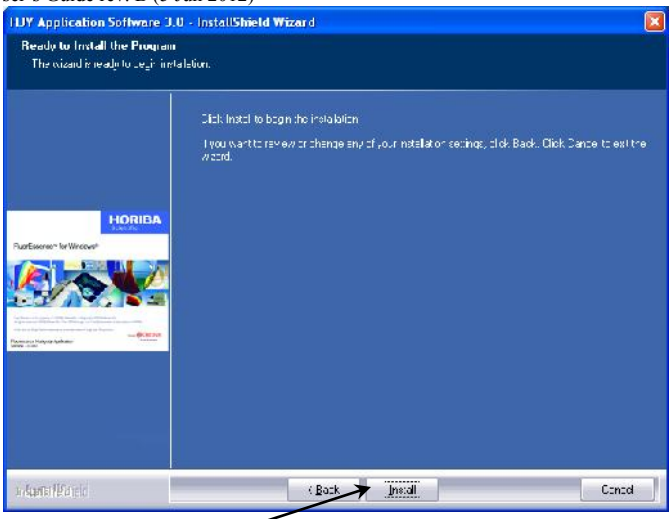
Enter your User Name and Company Name. The Next > button activates.

c Click the Next > button.
The Choose Destination Location area appears.



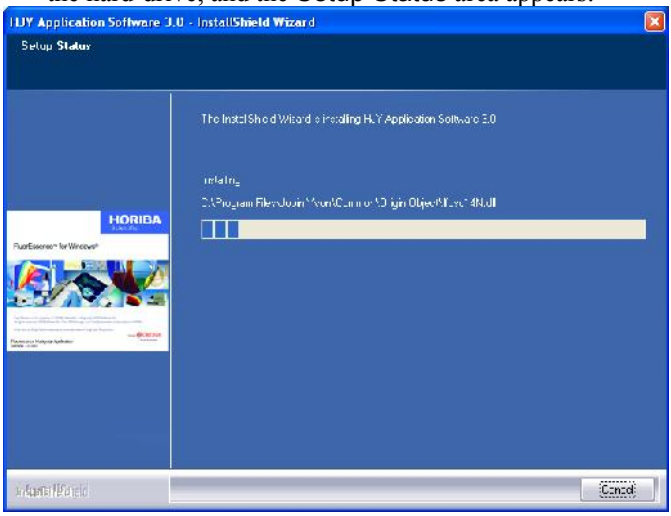
d Choose the location where Aqualog® is to be installed. Most people prefer the default location. Click the Change button to find a different location.

e Click the Next > button.
The Ready to Install the Program area appears:



f Click the Install button.

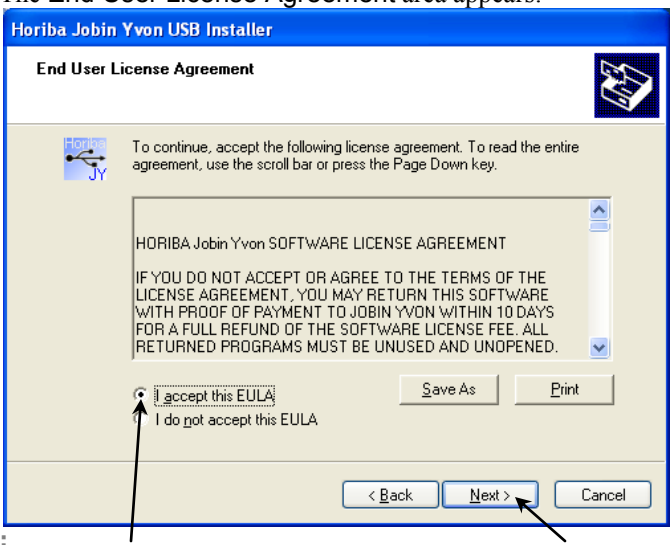
g The computer starts copying the files from the DVD to the hard-drive, and the Setup Status area appears:



Eventually the **Horiba Jobin Yvon USB Installer** window appears:

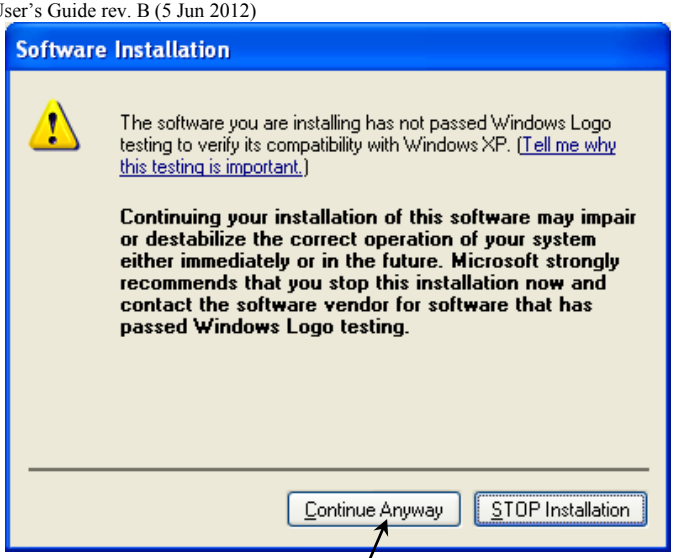
h Click the Next > button.

The End User License Agreement area appears:



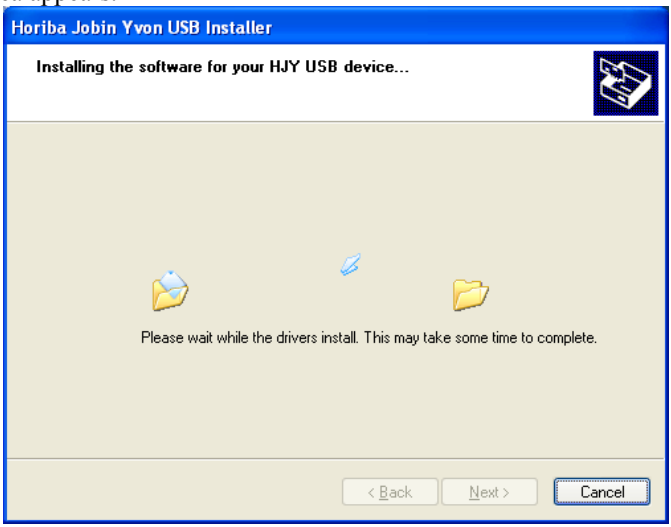
i Click the I accept this EULA radio button, then click the Next > button.

j A **Software Installation** warning window may appear:



k Click the Continue Anyway button.

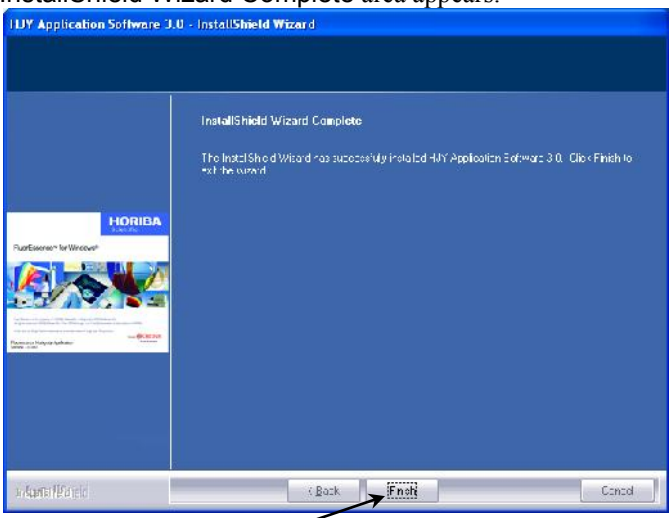
The Installing the software for your HJY USB device... area appears.



When complete, the Congratulations! You are finished installing your HJY USB device. area appears:

l Click the Finish button.

The **Horiba Jobin Yvon USB Installer** window closes. The InstallShield Wizard Complete area appears.



m Click the Finish button.

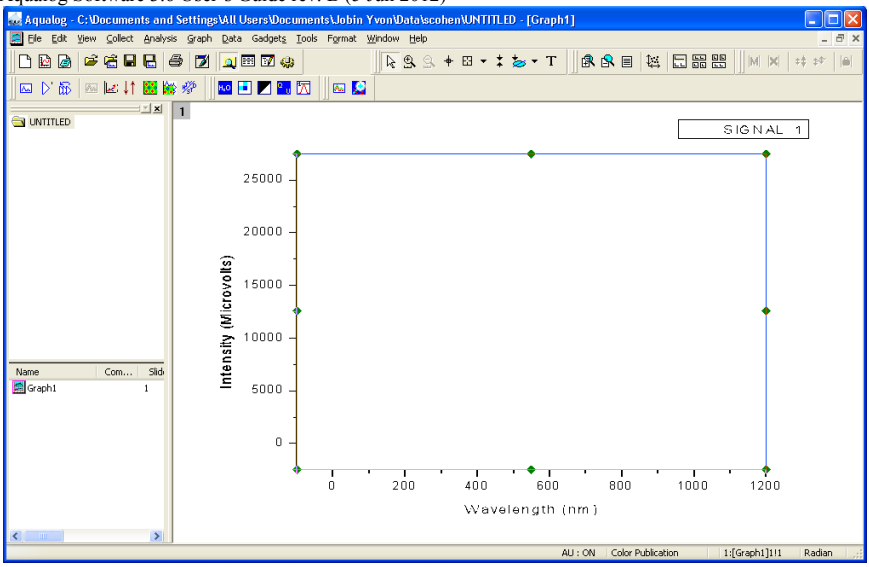
Installation of Aqualog® software is complete.

n Plug in all HORIBA software keys. Remove the Aqualog® DVD from the host computer.

5 Start Aqualog® software.

a On the desktop, double-click the Aqualog V3.6 icon.

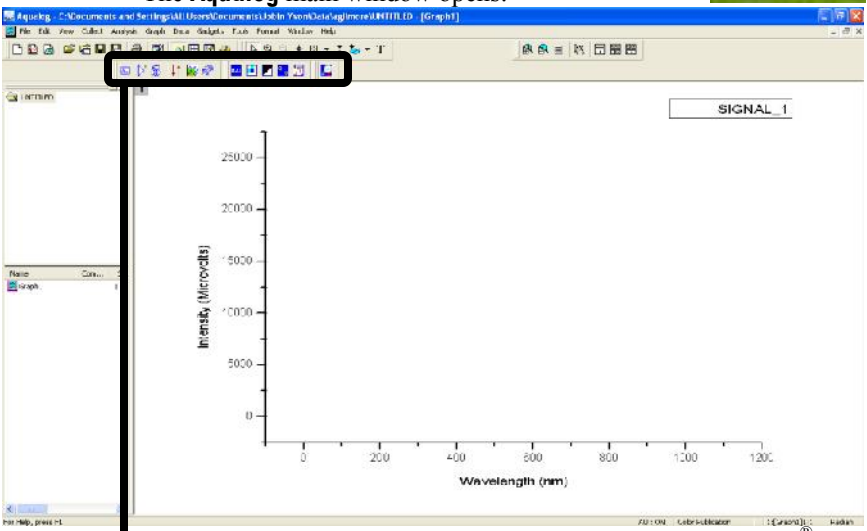
The **Aqualog** window appears:


Aqualog - C:\Documents and Settings\All Users\Documents\Jobin Yvon\Data\scohen\UNTITLED - [Graph1]
File Edit View Collect Analysis Graph Data Gadgets Tools Format Window Help
UNTITLED
Name Com... Slid
Graph1 1
SIGNAL 1
Intensity (Microvolts)
25000
20000
15000
10000
5000
0
0 200 400 600 800 1000 1200
Wavelength (nm)
AU : ON Color Publication 1:[Graph1]1!1 Radian

2: Quick Guide to Running a Scan

1. Turn on the host computer, the Aqualog® instrument, and all accessories, as explained in their respective instruction manuals.
2. Click on the Aqualog short-cut to start Aqualog® software.

The **Aqualog** main window opens.



There are special buttons for running experiments in Aqualog® software:

Previous Experiment button		Modify slightly a previously set-up experiment, and run it.
Auto Run Previous Experiment button		Run a previously set-up experiment without modification.

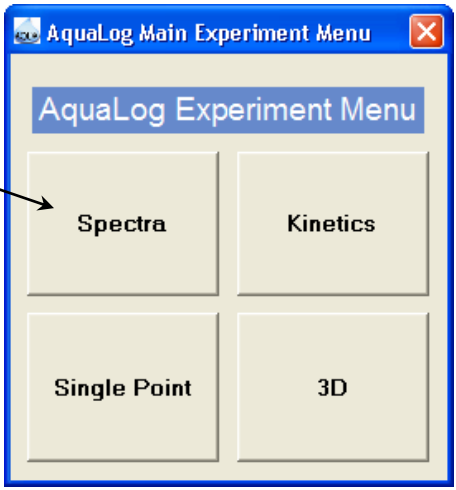
Run JY Batch Experiments button		Run an automated series of experiments, including adjustable repeats and delays between experiments.
Rescale Y button		Rescale the *y*-axis on an open graph to fit the data on-scale.
Profile Tool button		Provide a user-specified two-dimensional profile of an excitation-emission matrix. The active file must be such a data matrix.
Switch menu between HJY Software Application and Origin Std. button		Switch the menus at the top of the **Aqualog** main window between Aqualog® software and Origin® functions.
Experiment Menu button		Choose an overall type of experiment to run, such as general Spectra, Kinetics, 3D, or Single Point.
Aqualog IFE button		Remove artifacts pertaining to the inner-filter effect from the data.
Rayleigh Masking button		Mask Rayleigh scattering lines that appear in the data.
Quinine Sulfate Units button		Provide a standardized intensity for fluorescence measurements and EEMs.
Normalize button		Automatically normalize the active data to intensities between 0 and 1.
3D Zoom button		Change the *x*-*y*-*z* axes in a three-dimensional waterfall plot.

3 Click the Experiment Menu button  .

The **Aqualog Main Experiment Menu** appears:

4 Click an available scan-type button, say, Spectra.

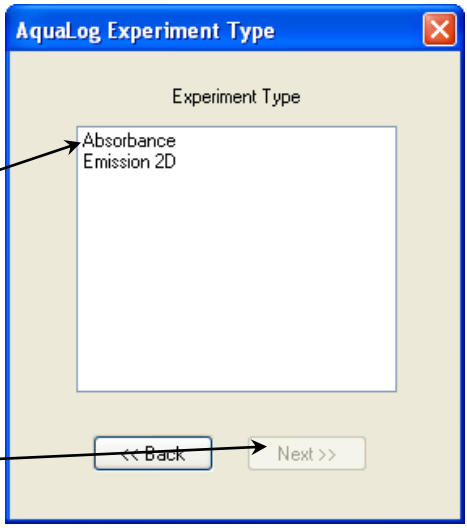
If there is a subtype of that experiment, the **Experiment Type** window appears.



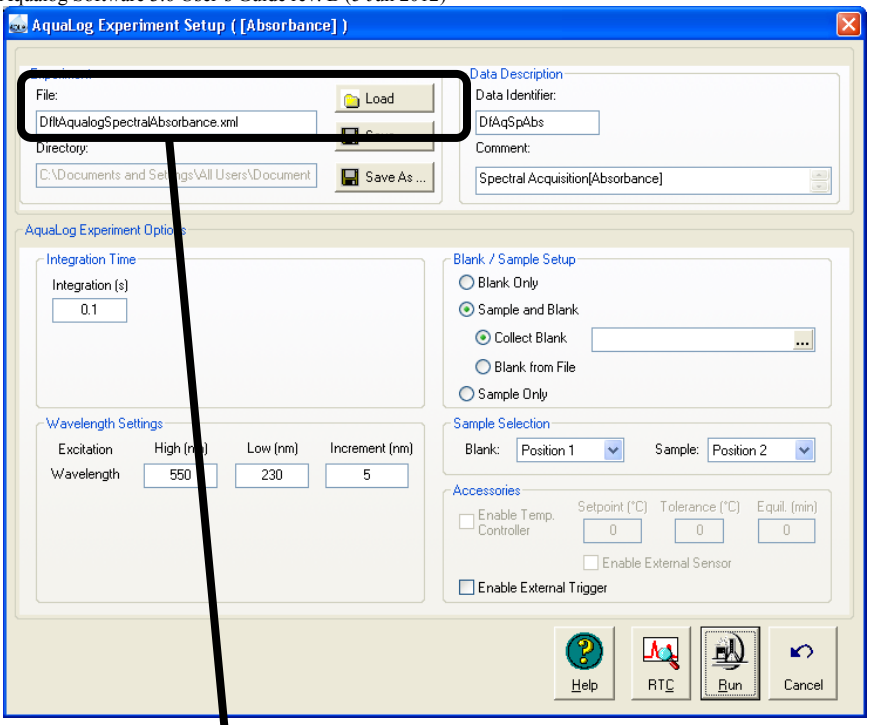
5 Choose an Experiment Type from the menu, say, Absorbance.

The parameters required for an absorbance scan are loaded into the **Experiment Setup** window, which appears.

6 Click the Next >> button.



The **Experiment Setup** window opens:



7 Click the File field, and enter a new file name, or select a previously saved file with the Load button.

8 Verify that the experimental parameters are correct.

9 Insert the sample(s) into the sample compartment, and close the sample compartment's lid.

10 Click the Run button 

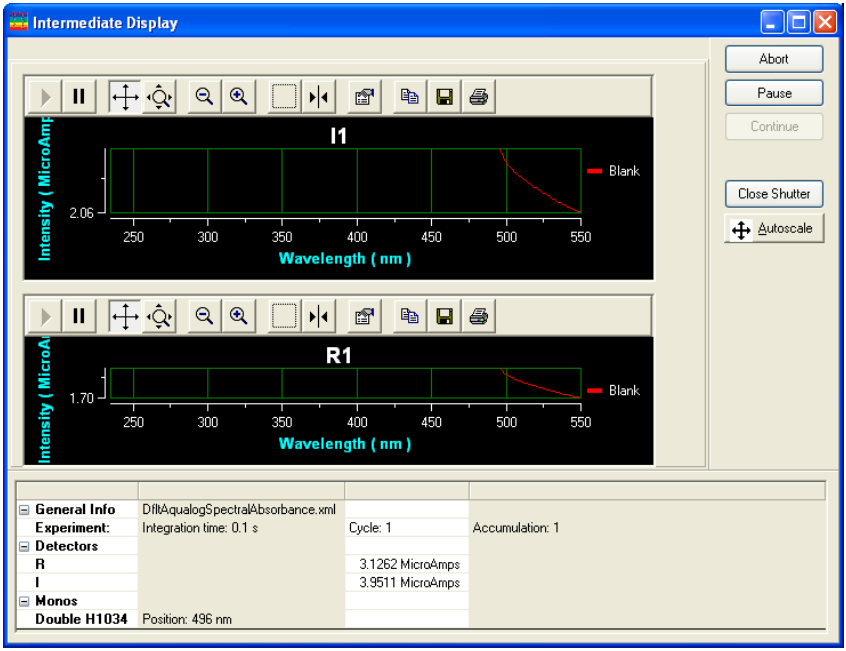
.

If you do not have an automatic sample-changer, a prompt appears to insert the blank or sample.

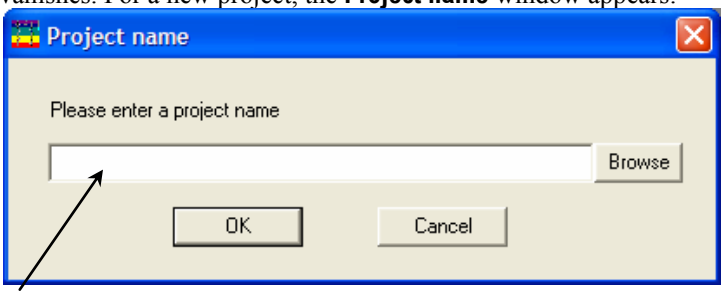
11 Click the OK button when you have inserted the blank or sample and closed the cover.

Note: *If the scan is extremely fast, the* ***Intermediate Display*** *may be only incompletely or rapidly displayed before the* ***Origin*** *window appears.*

The collected spectrum is displayed on the **Intermediate Display** screen:

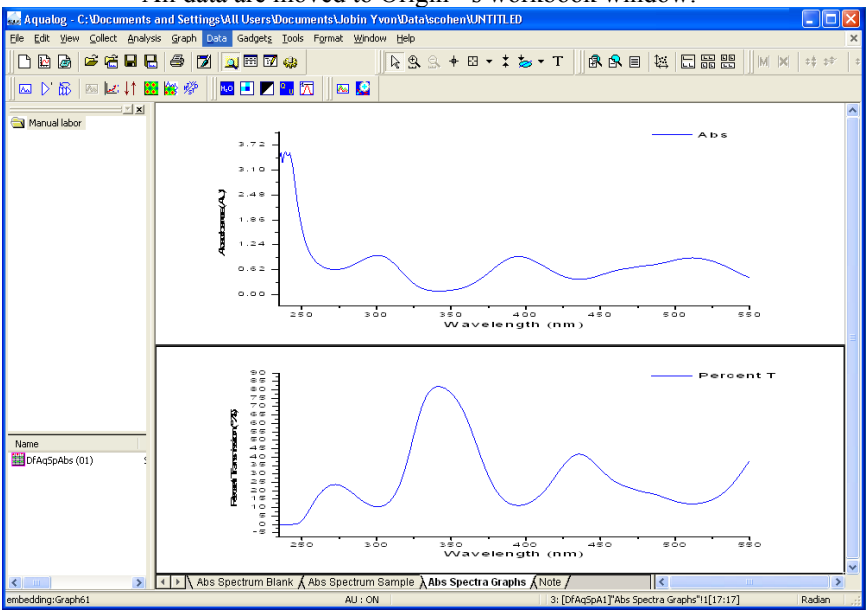


You can watch the incoming data in real time, along with how the positions of accessories vary. The scan may be paused, continued, or aborted. After all data are recorded, the **Intermediate Display** vanishes. For a new project, the **Project name** window appears:



12 Enter a name for the entire project, or browse for an existing project name with the Browse button, then click the OK button.

All data are moved to Origin®'s workbook window:



13 Double-click on the spectrum to see it better in a separate window for editing.

14 Do post-processing as needed, using the Aqualog IFE button  , Rayleigh Masking button  , and Normalization button  .

3: Aqualog® Software Tips & Tricks

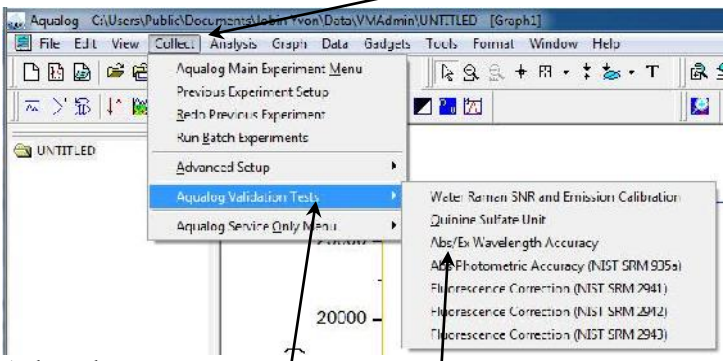
Validating the calibration of your instrument

Absorbance/excitation wavelength accuracy validation

This validation check examines the accuracy of the wavelengths scanned using the xenon lamp and absorbance detector, using the Starna RM sample.

1 Start the Aqualog® software.

2 In the **Aqualog** main window, choose Collect.



A drop-down menu appears.

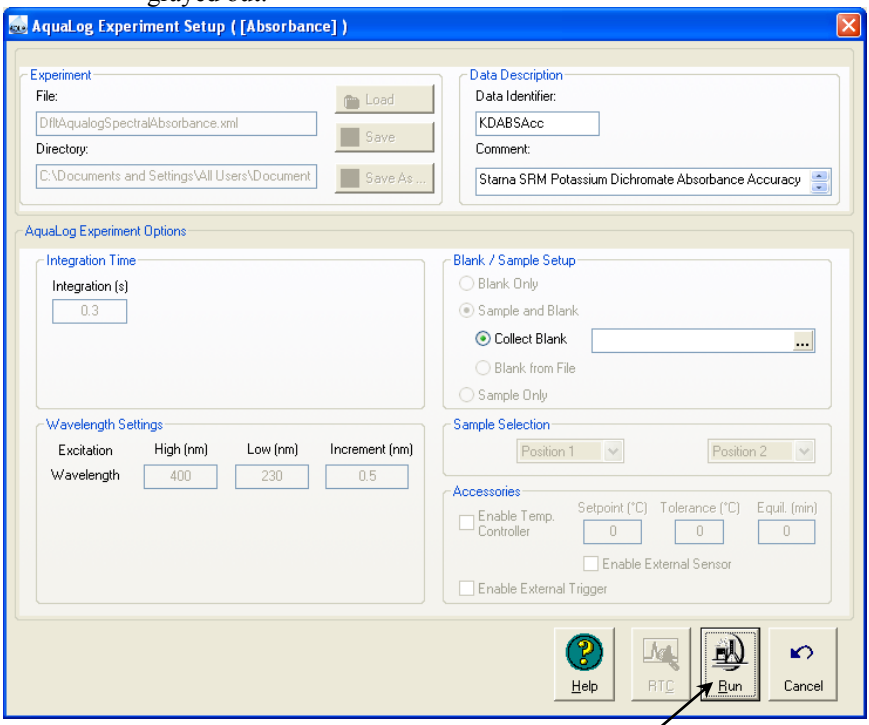
3 Choose Aqualog Validation Tests.

Another drop-down menu appears.

4 Choose Abs/Ex Wavelength Accuracy.

Note: *The Quinine Sulfate standard kit, RM-06HLKI-R, is available from Starna Cells, Inc., 5950 Traffic Way, Atascadero, CA 93422; phone: 800-228-4482; 805-466-8855; website is www.starnacells.com*

If the instrument has not initialized, initialization occurs. The validation experiment automatically loads with some of the fields grayed out:

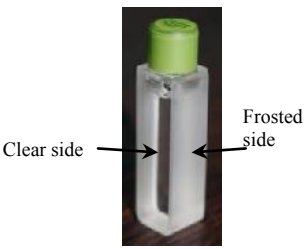


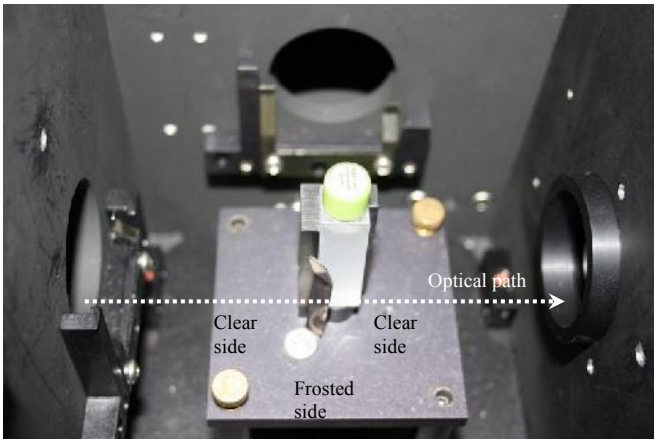
5 Click the Run button .

A message telling you to insert the blank appears:

6 Insert the $K_2Cr_2O_7$ blank with the frosted side toward the front of the instrument, and the clear sides toward the left and right of the instrument.

This allows a clear optical path.





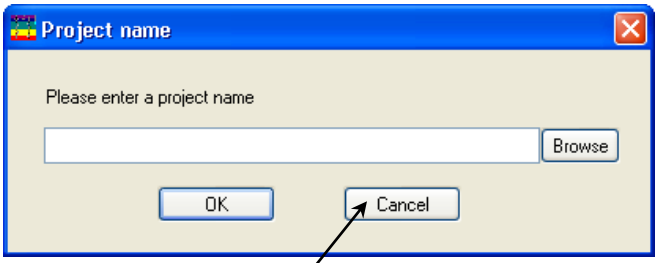
7 Close the sample-compartment lid, and click the OK button.

The **Experiment Status** window opens. The validation scan runs.
A message telling you to insert the blank appears.

8 Insert the holmium sample with the frosted side toward the front of the instrument, and the clear sides toward the left and right of the instrument.

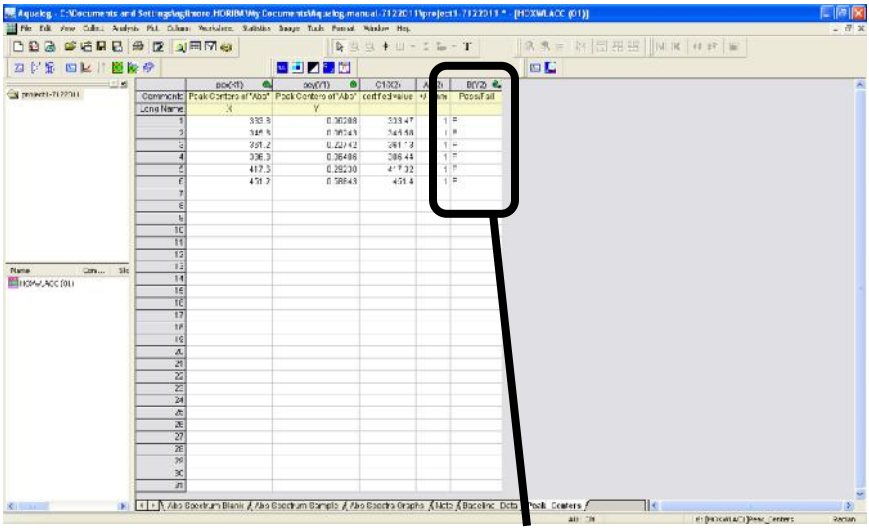
9 Close the sample-compartment lid, and click the OK button.

The **Project name** window appears:



10 Click the Cancel button.

A table of the validation test appears. In the B(Y2) column, there should be all P's (passes).



11 If the test shows all "Pass" values, continue to the next test.

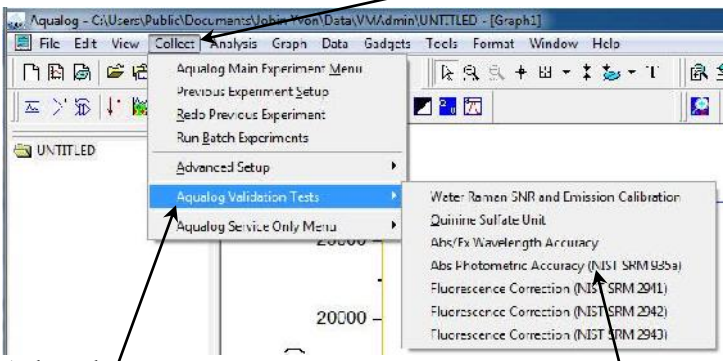
If there are failures, please call the HORIBA Scientific Service Department.

Absorption-accuracy validation

This validation check examines the accuracy of the absorption function of the Aqualog®. Use the absorption standard SRM 935a available from NIST.

Note: *The absorbance calibration standard kit, RM-06HLKI-R, is available from Starna Cells, Inc., 5950 Traffic Way, Atascadero, CA 93422; phone: 800-228-4482; 805-466-8855; website is www.starnacells.com*

1 In the **Aqualog** main window, choose Collect.



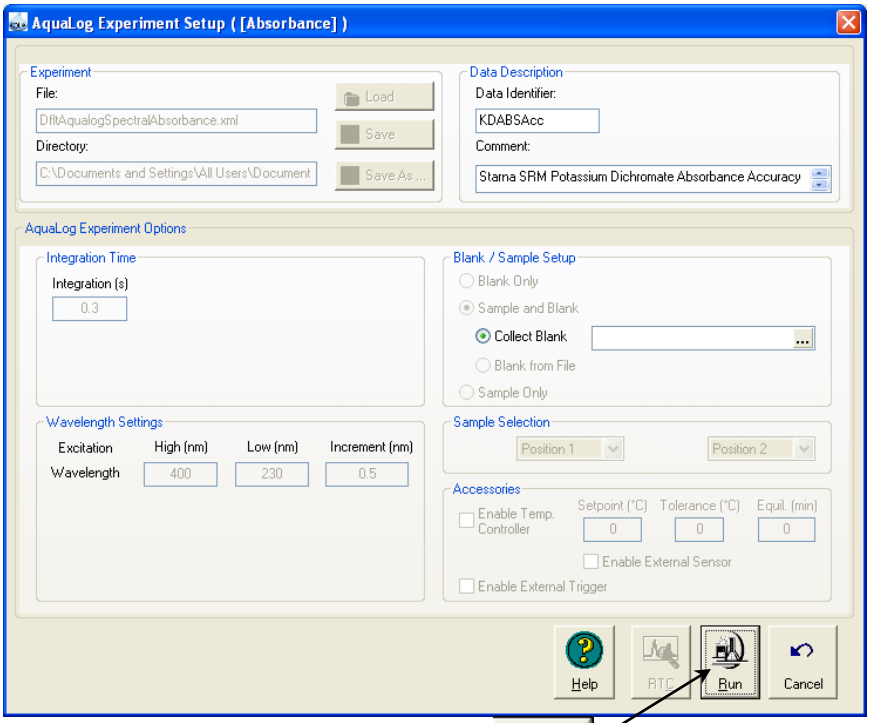
A drop-down menu appears.

2 Choose Aqualog Validation Tests.

Another drop-down menu appears.

3 Choose Abs Photometric Accuracy (NIST SRM 935a).

The validation experiment automatically loads with some of the fields grayed out:

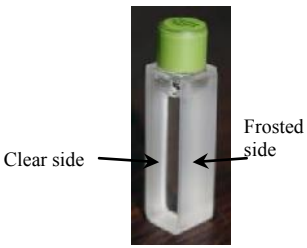


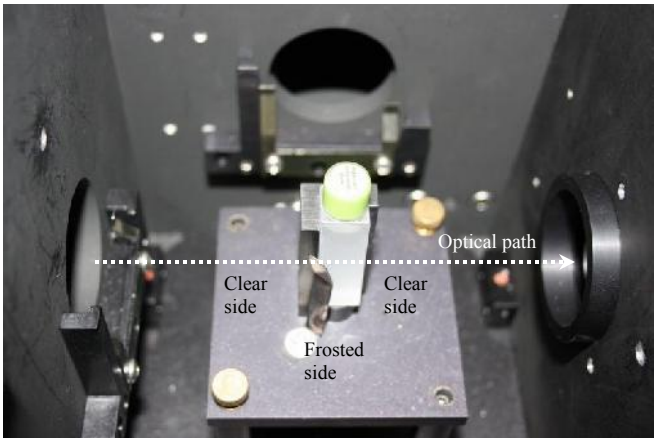
4 Click the Run button .

A message telling you to insert the blank appears:

5 Insert the $K_2Cr_2O_7$ blank with the frosted side toward the front of the instrument, and the clear sides toward the left and right of the instrument.

This allows a clear optical path.





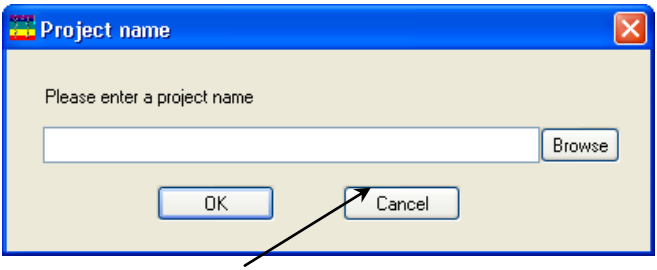
6 Close the sample-compartment lid, and click the OK button.

The **Experiment Status** window opens. The validation scan runs. A message telling you to insert the sample appears.

7 Insert the potassium dichromate (60 mg L^{-1}) sample with the frosted side toward the front of the instrument, and the clear sides toward the left and right of the instrument.

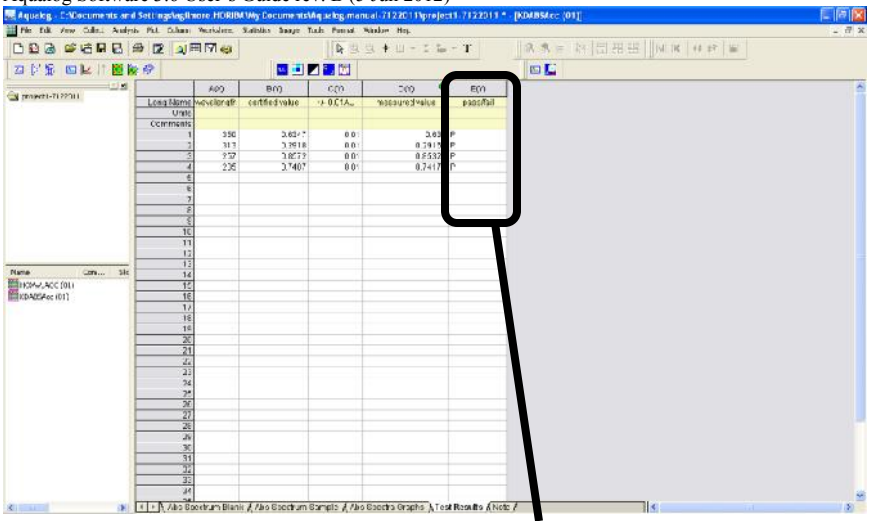
8 Close the sample-compartment lid, and click the OK button.

The **Project name** window appears:



9 Click the Cancel button.

A table of the validation test appears. In the E(Y) column, there should be all P's (passes).



10 If the test shows all "Pass" values, continue to the next test.

If there are failures, please call the HORIBA Scientific Service Department.

Water-Raman-peak signal-to-noise and emission calibration validation

This validation check examines the wavelength calibration of the CCD detector. It is an emission scan of the Raman-scatter band of water performed in right-angle mode.

Note: *Avoid glass or acrylic cuvettes: they may exhibit UV fluorescence or filtering effects.*

The water sample should be research-quality, triple-distilled or de-ionized water. HPLC-grade (18-MΩ spec.) or equivalent water is suggested for the Raman scan. HORIBA Scientific recommends the Starna sealed water-Raman sample. Impure samples of water will cause elevated background levels as well as distorted spectra with (perhaps) some unwelcome peaks. Use a 4-mL quartz cuvette.

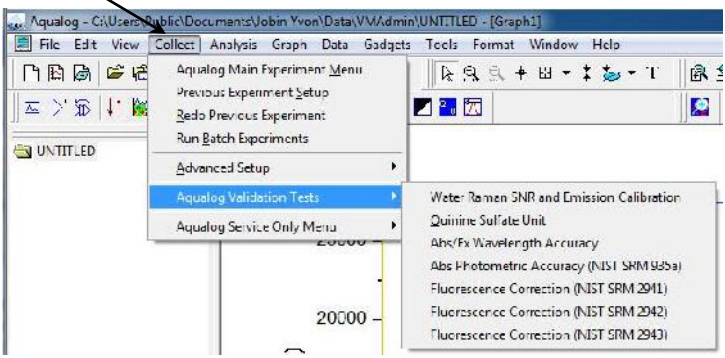
Note: *The water Raman sample is available from Starna Cells, Inc., 5950 Traffic Way, Atascadero, CA 93422; phone: 800-228-4482; 805-466-8855; website is www.starnacells.com*

1. Insert the water sample into the sample compartment.

   With an automated sample changer, note the position number in which the sample cell is placed.

2. Close the lid of the sample chamber.

3. In the **Aqualog** main window, choose Collect.



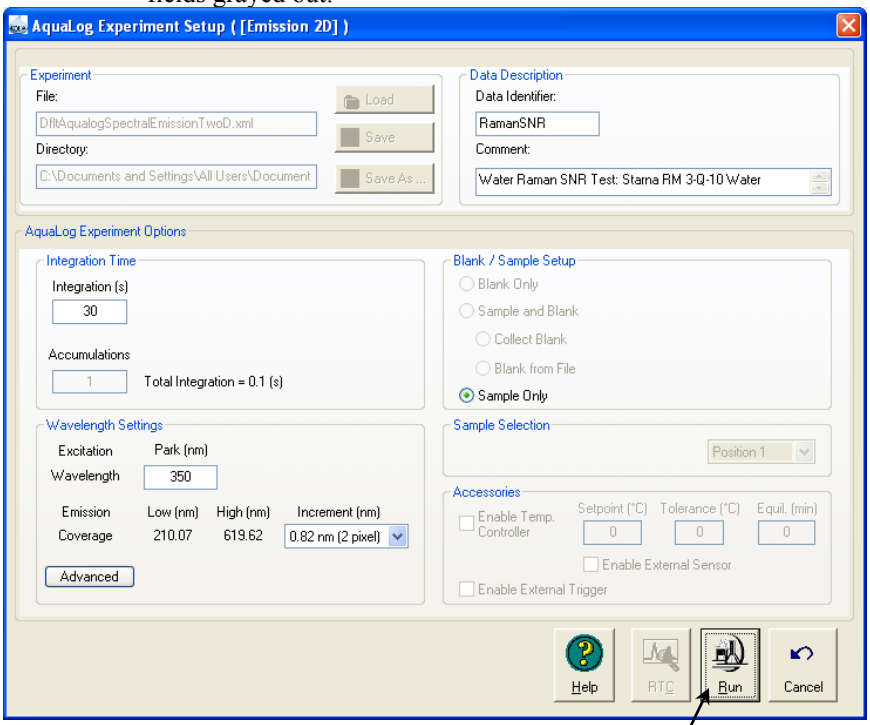
A drop-down menu appears.

4 Choose Aqualog Validation Tests.

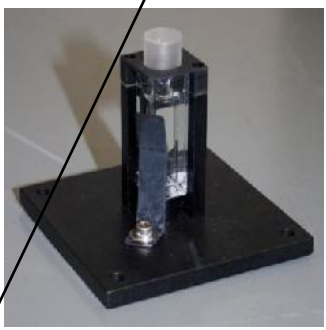
Another drop-down menu appears.

5 Choose Water Raman SNR and Emission Calibration.

The validation experiment automatically loads with some of the fields grayed out:



6 Place the Starna water sample in the special sample holder, and mount the sample holder in the sample compartment. Close the sample-compartment lid.



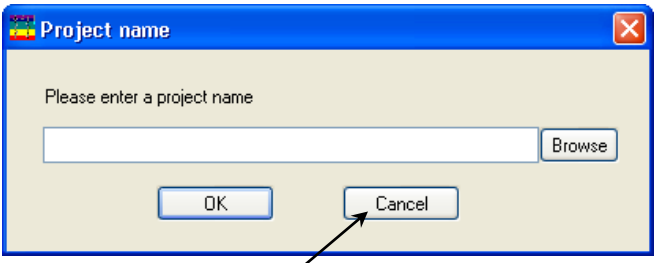
7 Click the Run button 

.

A message telling you to insert the sample appears.

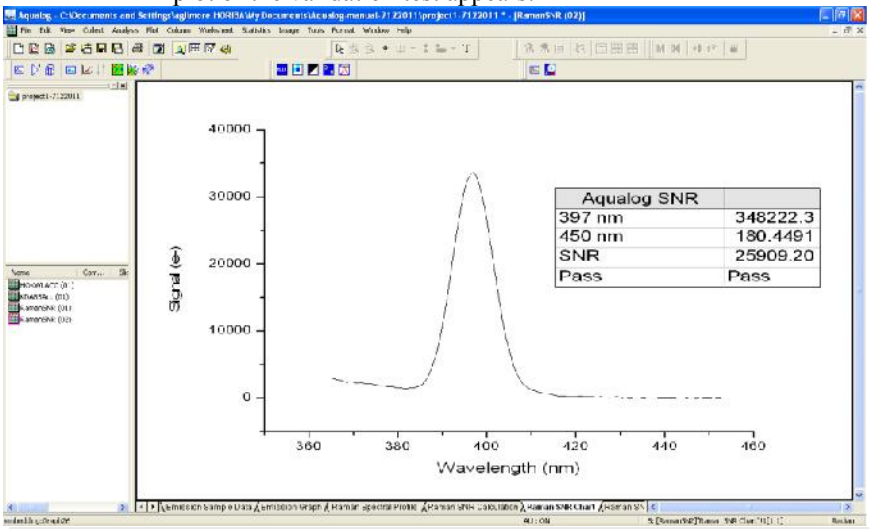
8 Click the OK button.

The **Experiment Status** window opens.
The validation scan runs. The **Project name** window appears:



9 Click the Cancel button.

A plot of the validation test appears:



Note: *Observed throughput (and hence peak intensity) is affected by lamp age and alignment, slit settings, and sample purity. As the xenon lamp ages, the throughput of the system will decline slowly. Therefore, low water-Raman peak intensity may indicate a need to replace the xenon lamp.*

10 If the test shows a "Pass" value, continue to the next test.

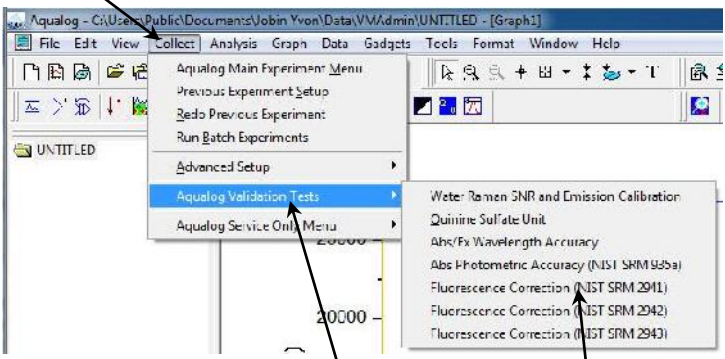
If the plot displays "fail", please call the HORIBA Scientific Service Department.

Fluorescence correction validation with NIST SRM 2941 sample

This validation check examines the accuracy of the fluorescence correction file of the Aqualog®. Use the fluorescence standards (SRM 2941, SRM 2942, and SRM 2943) available from NIST.

Note: *Fluorescence standards (SRM 2941, SRM 2942, and SRM 2943) are available from National Institute for Standards and Technology (NIST), phone: 301-975-2200; website is www.nist.gov*

1 In the **Aqualog** main window, choose Collect.



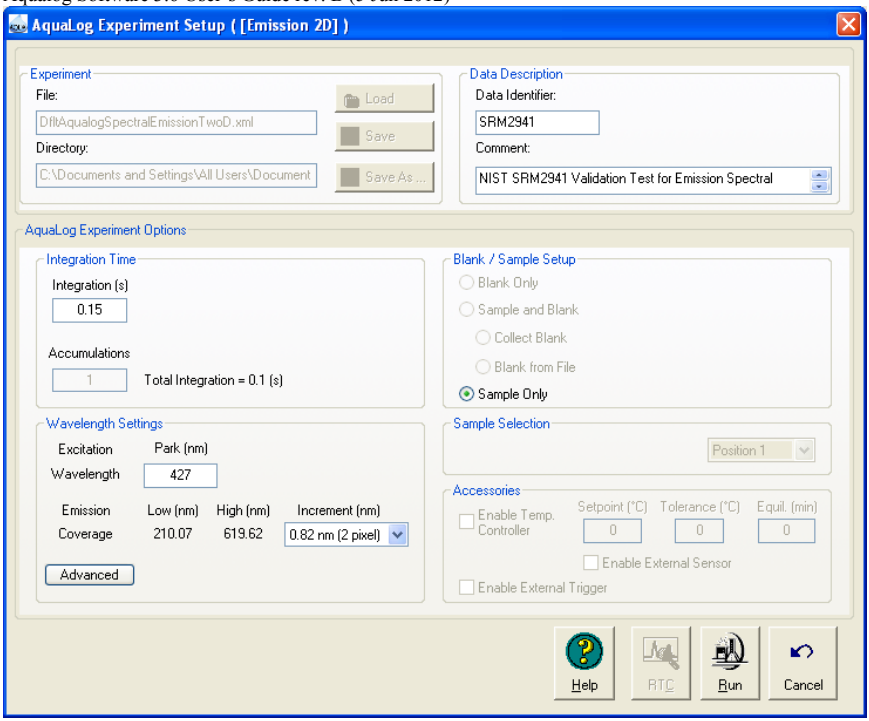
A drop-down menu appears.

2 Choose Aqualog Validation Tests.

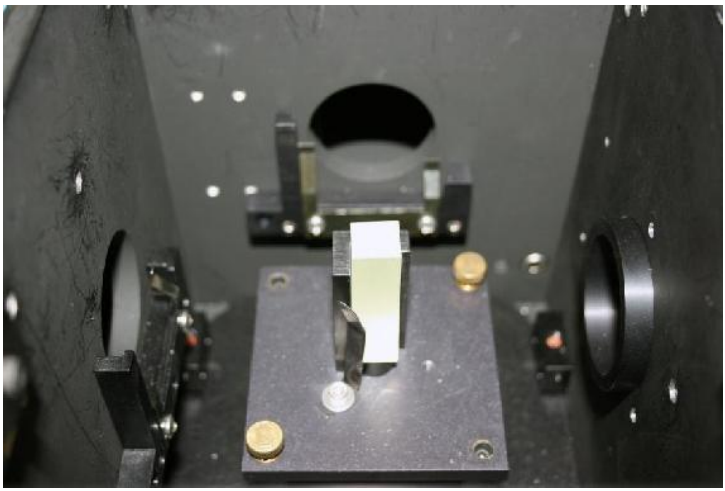
Another drop-down menu appears.

3 Choose Fluorescence Correction (NIST SRM 2941).

The validation experiment automatically loads with some of the fields grayed out:



4 Insert the 2941 standard with the frosted side toward the front of the instrument (for fluorescence), and the clear sides toward the left and right of the instrument. Close the sample-compartment lid.



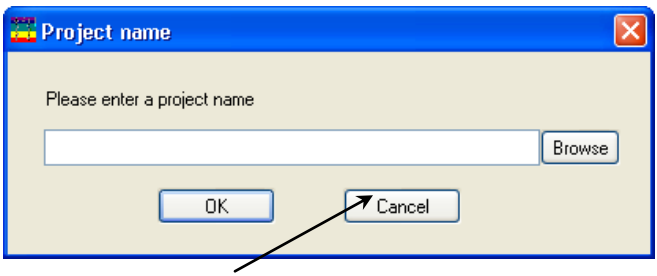
5 Click the Run button 

.

A message telling you to insert the blank appears.

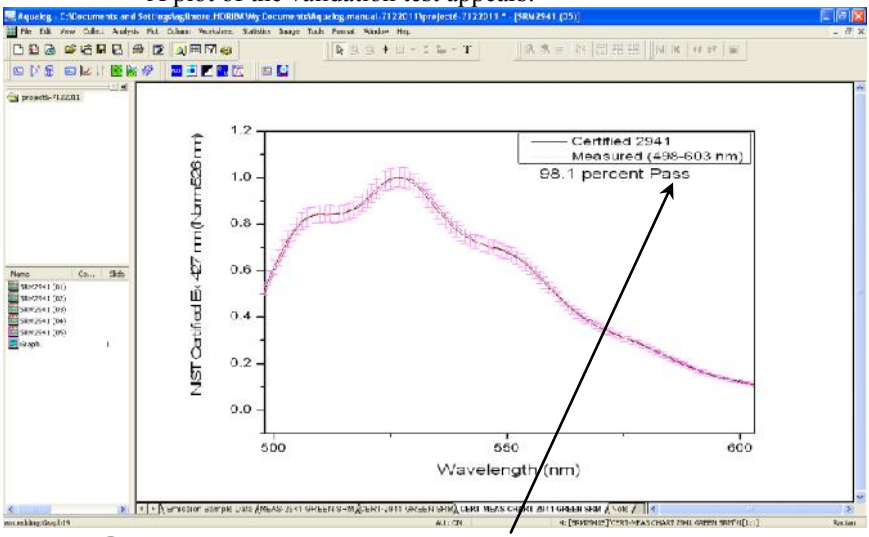
6 Click the OK button.

The **Experiment Status** window opens.
The validation scan runs. The **Project name** window appears:



7 Click the Cancel button.

A plot of the validation test appears:



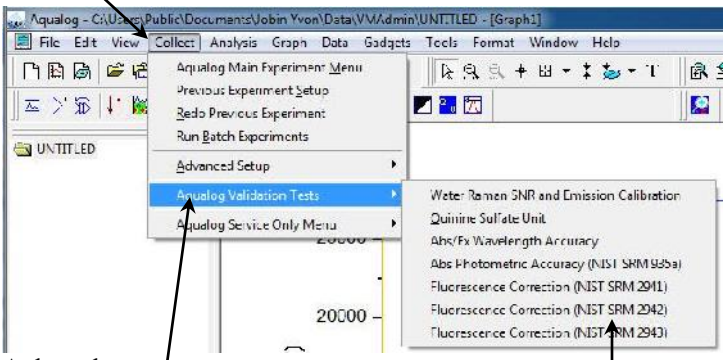
8 If the test shows a "Pass" value, continue to the next test.

If the plot displays "fail", please call the HORIBA Scientific Service Department.

Fluorescence correction validation with NIST SRM 2942 sample

This validation check examines the accuracy of the fluorescence correction file of the Aqualog®.

1 In the **Aqualog** main window, choose Collect.



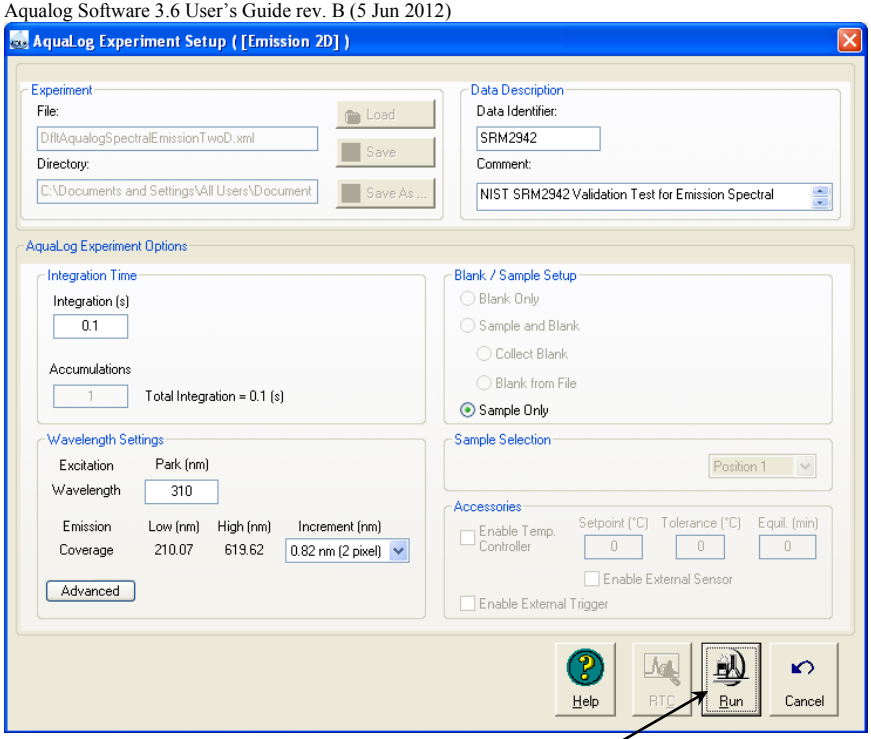
A drop-down menu appears.

2 Choose Aqualog Validation Tests.

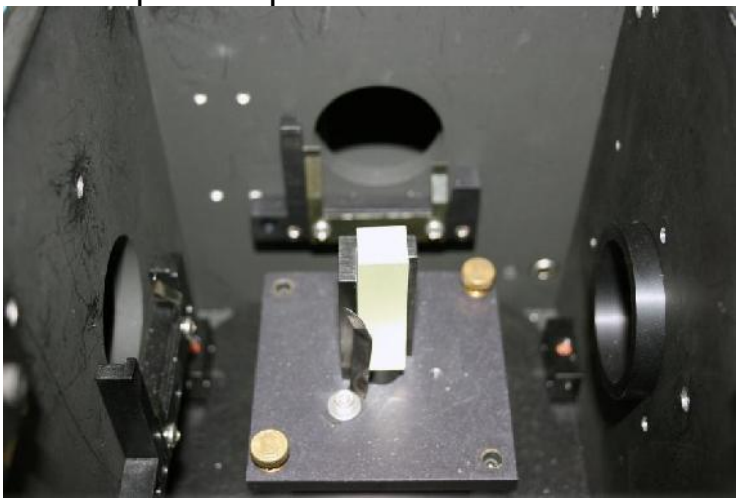
Another drop-down menu appears.

3 Choose Fluorescence Correction (NIST SRM 2942).

The validation experiment automatically loads with some of the fields grayed out:



4 Insert the 2942 standard with the frosted side toward the front of the instrument (for fluorescence), and the clear sides toward the left and right of the instrument. Close the sample-compartment lid.



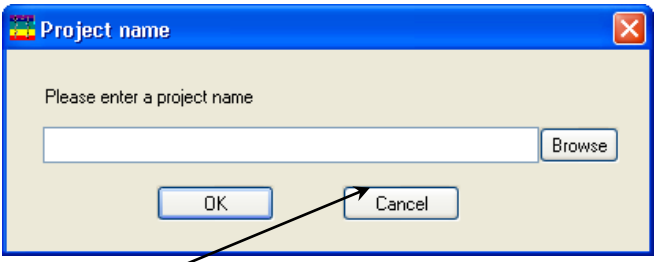
5 Click the Run button 

.

A message telling you to insert the blank appears.

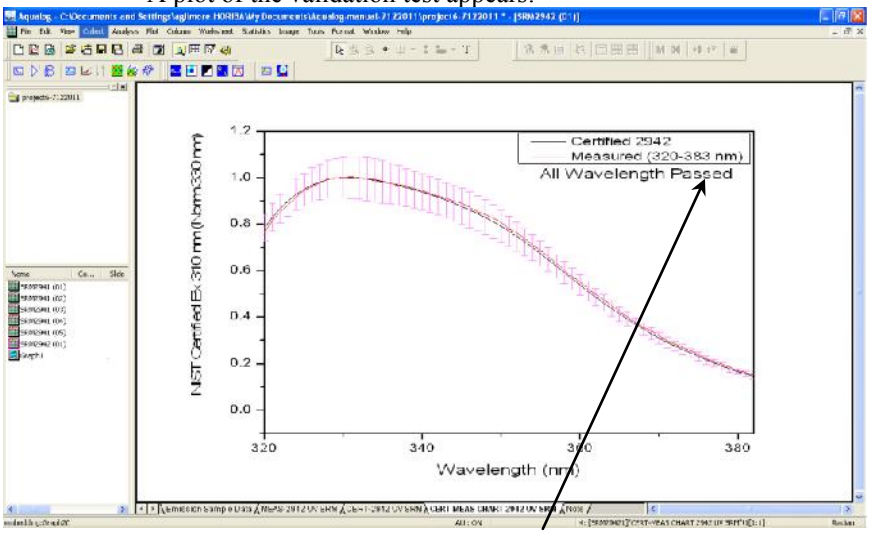
6 Click the OK button.

The **Experiment Status** window opens.
The validation scan runs. The **Project name** window appears:



7 Click the Cancel button.

A plot of the validation test appears:



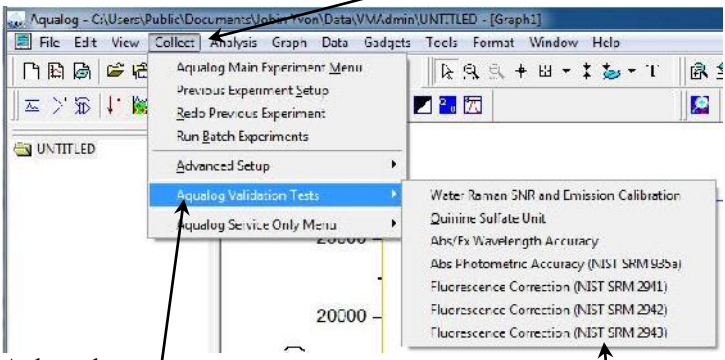
8 If the test shows a "Passed" value, continue to the next test.

If the plot displays "fail", please call the HORIBA Scientific Service Department.

Fluorescence correction validation with NIST SRM 2943 sample

This validation check examines the accuracy of the fluorescence correction file of the Aqualog®.

1 In the **Aqualog** main window, choose Collect.



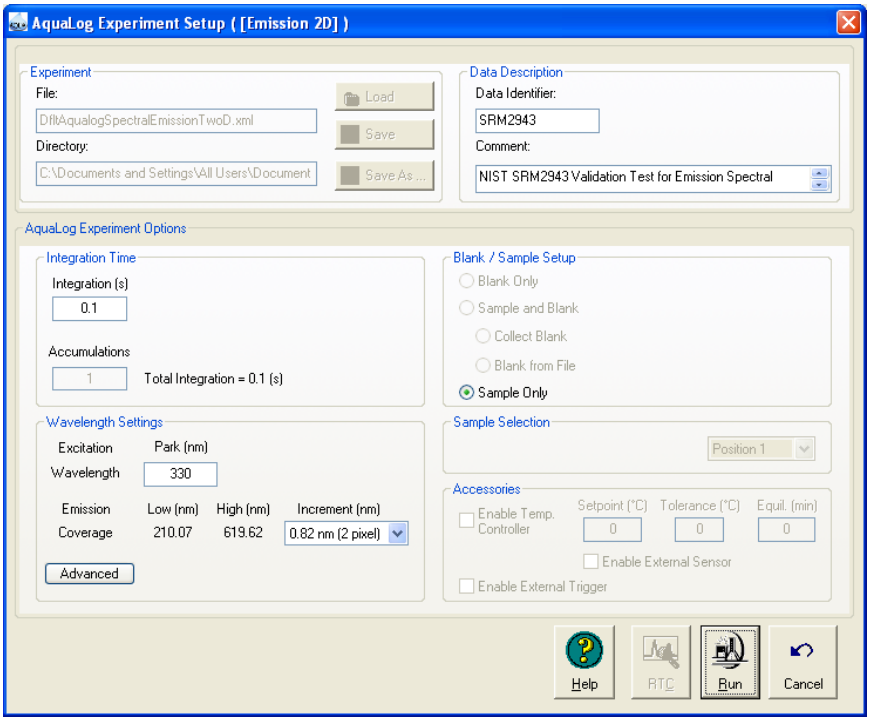
A drop-down menu appears.

2 Choose Aqualog Validation Tests.

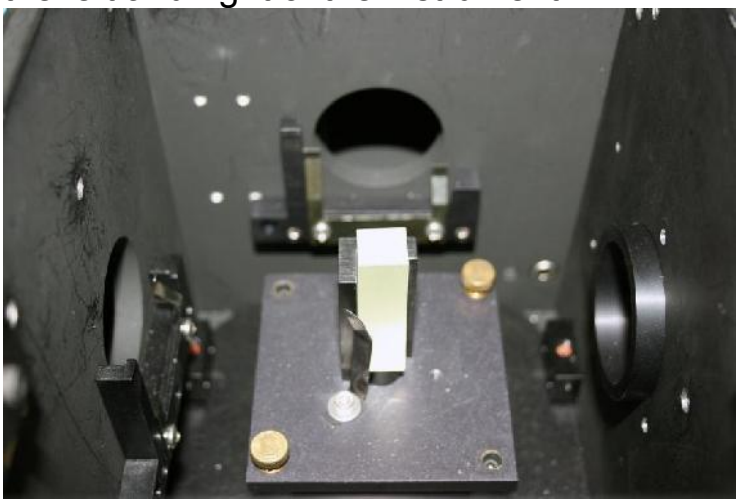
Another drop-down menu appears.

3 Choose Fluorescence Correction (NIST SRM 2943).

The validation experiment automatically loads with some of the fields grayed out:



4 Insert the 2943 standard with the frosted side toward the front of the instrument (for fluorescence), and the clear sides toward the left and right of the instrument.



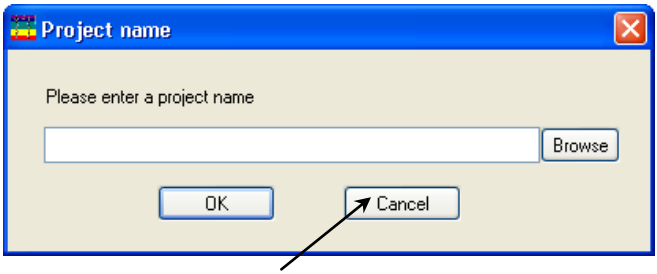
5 Click the Run button 

.

A message telling you to insert the blank appears.

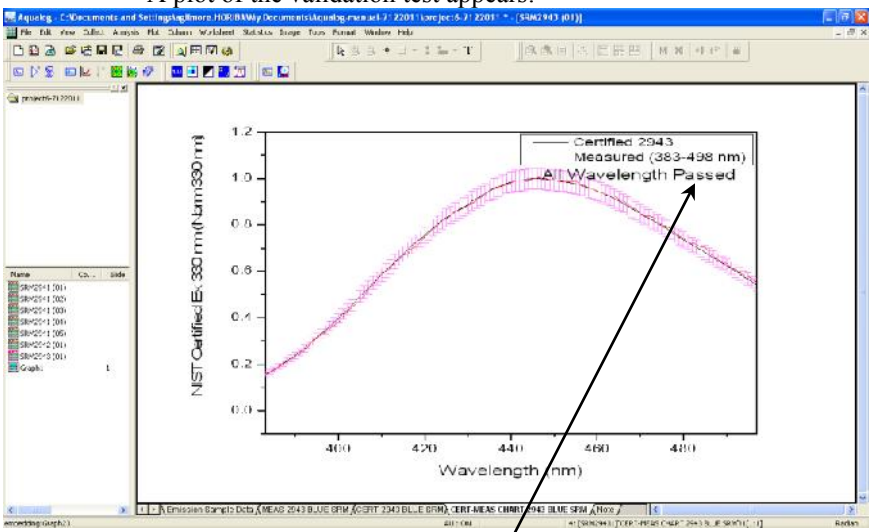
6 Close the sample-compartment lid, and click the OK button.

The **Experiment Status** window opens.
The validation scan runs. The **Project name** window appears:



7 Click the Cancel button.

A plot of the validation test appears:



8 If the test shows a "Passed" value, the Aqualog® is calibrated properly.

If the plot displays "fail", please call the HORIBA Scientific Service Department.

Corrected signals

Note: *All dark-offset, $X_{correct}$, $M_{correct}$, I_c/R_c, and S_c/R_c corrections (see below for definitions) are automatically done in Aqualog® software. Inner-filter effects, Rayleigh-masking, and normalizations are user-activated.*

Introduction to EEMs for CDOM

Given the complex multitude of CDOM components in many bodies of water, a rapid method for qualitative and quantitative determinations has obvious value to the water-quality research and analysis community. The most conventional method of analyzing CDOM using fluorescence is the excitation-emission map (EEM). EEMs are recorded by scanning the excitation spectrum (or absorbance) of the fluorescent sample's components at the same time as the fluorescence-emission spectrum is recorded, for each excitation wavelength. This results in a "three-dimensional" intensity map of the sample's fluorescence, showing both the emission and absorbance spectra of all fluorescent components in the measured wavelength region. The EEM, however, does not contain the absorbance spectral information of non-fluorescent components in the sample. Moreover, the EEM spectral information can be distorted by inner-filter effects associated with absorbance of the excitation beam and fluorescence. So it follows that ideally the EEM should be measured *along with* the absorbance spectrum of the sample to ease inner-filter effect correction and monitoring bleaching of the sample, as well as to provide information about non-fluorescent compounds absorbing light in the sample.

Spectral correction: Wavelength-dependent detector response

Because most CDOM studies rely on comparison to traceable spectral and concentration standard samples, the spectral-correction of the EEM is of prime concern. A typical EEM scans the sample across the excitation wavelengths from about 240–500 nm, and across the emission wavelengths from 250–600 nm. Bandpass and resolution are typically (and fixed in the Aqualog® to) 5 nm. To account for variations in the excitation beam's intensity, a reference detector, *R*, collects a small fraction of the excitation beam, and the emission detector's output, *S*, is ratioed to the reference detector signal (*S*/*R*).

However, the instrument's optical responsivity is not ideal throughout the wavelength-range of the experiment, so a series of instrumental spectral correction-factors must be used to obtain reproducible ideal spectra that are traceable to established, calibrated spectral standard samples, detectors, and light sources.

- Dark-current signals must be subtracted, respectively, from both the *S* and *R* detector signals.
- The *S* and *R* detectors' signals must also be respectively multiplied by the excitation ($X_{correct}$) and emission ($M_{correct}$) spectral correction factors.

It follows that the final signal plotted as a function of wavelength in an EEM involves both the corrected reference signal, R_c,

$$R_c = (R - \text{dark}) \cdot X_{\text{correct}}$$

and the corrected emission-detector signal, S_c,

$$S_c = (S - \text{dark}) \cdot M_{\text{correct}}$$

The final fluorescence signal recorded is thus S_c/R_c for both the sample to be evaluated and for a representative reference or blank sample as discussed below.

Simultaneous to the EEM, the sample's spectral transmittance and absorbance properties can be recorded with the Aqualog®. From the Beer-Lambert law, absorbance de-fined as $Abs = \varepsilon cl$, where ε is the extinction coefficient, c is the concentration and l is the pathlength of the sample cell. Within the Aqualog®, the transmission detector signal, $A_c = A$ – dark signal, is used to calculate the *Abs* and transmittance (*T*) values. The transmission detector's signal, A_c, is also corrected for the excitation-source intensity measured using the reference detector signal (R_c) formulated above as $A_c/R_c = I_0$ from a representative blank or reference sample and $I = A_c/R_c$ from the sample to be evaluated as per below. For CDOM measurements, the blank or reference sample is usually highly purified water, with resistance ≥ 18.2 MΩ and total organic carbon < 2 ppb. The transmission, percent transmission and absorbance values Abs_λ at a given wavelength λ are calculated as follows:

$$T_\lambda = \left(\frac{I}{I_0}\right)$$

$$\%T_\lambda = 100 \times \left(\frac{I}{I_0}\right)$$

$$Abs = -\log(T)$$

EEM spectral correction: blank-subtraction, Rayleigh-masking and Raman scattering

The current practice for EEMs involves measuring the excitation and emission scan-ranges, which includes their overlap regions. These overlap regions manifest in intense signals from the scattered photons from the monochromatic excitation source in the emission detector's response. These lines are caused by both the first- (and second-) order Rayleigh-scattering features consistent with the well-known grating equation. Additionally another spectral feature, associated water samples, is the water Raman scattering line. The Raman scattering line is related to the Rayleigh scattering line by a constant energy shift of 3382 cm^{-1}. Most CDOM component libraries contain spectra for which the artifactual Rayleigh and water-Raman spectral features have been removed, and hence EEM data is usually processed to remove both the Rayleigh and Raman scattering features systematically. The Aqualog® software package can remove both artifacts. Subtraction of the blank EEM from the sample EEM effectively removes the Raman scatter line. Applying a Rayleigh-masking algorithm based on the excitation and emission spectral bandwith nullifies the signal intensities for both the first- and second-order Rayleigh lines.

EEM spectral correction: primary and secondary inner-filter effects

Common, recommended practice is to correct the EEM data for inner-filter effects (IFE) using the parallel absorbance measurements from the sample and blank as mentioned above. One obvious criterion for accurate IFE is the requirement for the concentration of the sample to fall within the linear Beer-Lambert region for the absorbance spectral region associated with the EEM. The IFE algorithms used in Aqualog® involve measuring the absorbance spectrum of the sample for the overlapping range of both the excitation and emission spectra to correct for both the primary and secondary IFEs. The basic IFE algorithm employed in the Aqualog® software requires use of conventional 1 × 1 cm path-length cuvettes. The equation below is applied to each excitation-emission wavelength coordinate of the EEM:

$$F_{ideal} = F_{obs}^{10^{\frac{Abs_{Ex}+Abs_{Em}}{2}}}$$

where F_{ideal} is the ideal fluorescence-signal spectrum expected in the absence of IFE, F_{obs} is the observed fluorescence signal, and Abs_{Ex} and Abs_{Em} are the measured absorbance values at the respective excitation and emission wavelength-coordinates.

A number of advanced algorithms described in the literature can also account for variations of the optical geometrical parameters of the cuvette path-length, beam- or slit-width, and positioning or shifting of the cuvette relative to the excitation and emission beam paths. However, the fixed optical geometry of the Aqualog® lends itself to the simple solution above because neither the slit-widths that determine the beam geometry, nor the pathlengths or overlap volume of the absorbance and emission paths are user-adjustable. Moreover, IFE corrections are generally only important when the absorbance values exceed 0.05 in a 1 cm path-length, so there is generally little information to be gained in the EEM from either an extended or shortened path-length cell. The fixed geometry of the Aqualog® further lends the use of the instrument to support valid intra- and inter-laboratory comparisons by eliminating variances in the chief parameters of absorbance and emission pathlength. The fixed optical geometry also makes accurate and reproducible spectral correction easy as well as easy validation of such with standard traceable samples.

EEM spectral correction: intensity standardization to quinine-sulfate-unit equivalents and water-Raman scattering intensity

Whereas the absorbance spectral response of the Aqualog® with respect to sample concentration is generally invariant over the lifetime of the instrument, the fluorescence-detection path is subject to changes in the excitation source's intensity and detector response that should be routinely monitored with standard samples and experimental conditions. Moreover, to ease comparison with other instruments and studies, such standardization is conventional and recommended practice. Most commonly the throughput response of a fluorometer including the Aqualog® is measured by evaluating the water-Raman scattering intensity under standard conditions of 350 nm excitation and 397 nm emission at 5 nm bandpass for a fixed time interval. Likewise, many CDOM studies calibrate the instrument's throughput and CDOM concentration relative to a quinine-sulfate-unit equivalent (QSU), based on the excitation at 347.5 nm of 1 ppm of QSU dissolved in 0.1 mol of perchloric acid, and the instrument measuring the emission intensity at 450 nm. The Aqualog® contains a built-in tool for calculating and applying both the water-Raman and QSU standardization and normalization.

EEM spectral correction: nonlinear least-squares and multivariate spectral analyses

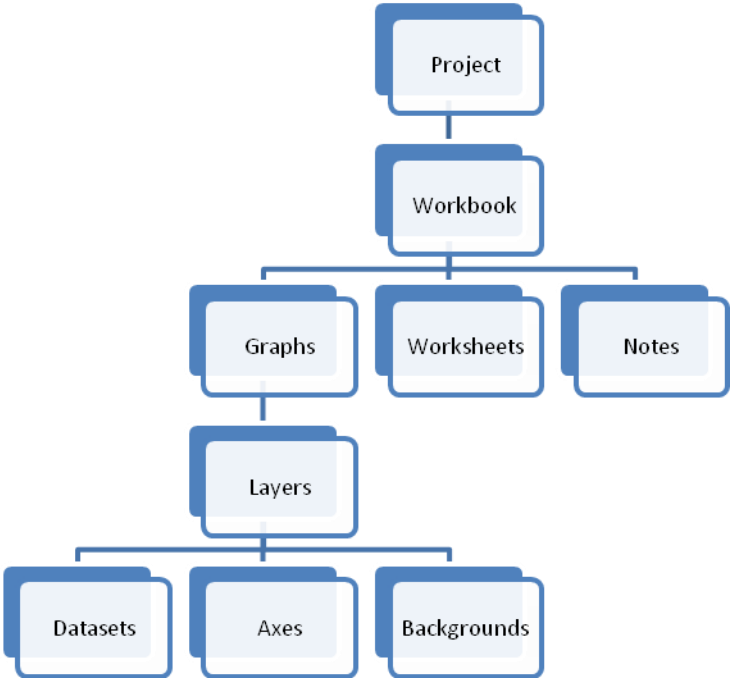
As required by the CDOM research community, the concerted application of the instrumental spectral corrections, Rayleigh-line masking, water-Raman subtraction, Raman or QSU normalization and IFE correction are readily enabled by the EEM-processing tools in our Aqualog® software. As mentioned above, the purpose of the spectral corrections and EEM-processing is to make the identification and quantification easier of the CDOM components that are usually based on a reference-component library or model. Here we focus attention on a popular and promising library-based multivariate technique for CDOM analysis, namely, PARAFAC, which has been do-cumented extensively by researchers including many using HORIBA's fluorescence instruments. Importantly, the Aqualog® software offers direct access to a MatLab® console for purposes of processing data using the PARAFAC tools in N-way Toolbox, a public-domain package especially developed for CDOM analysis. The modeling advantages of PARAFAC center on its ability to simultaneously evaluate the EEM data as a matrix, and to envelop multiple (often hundreds) of EEMs simultaneously for increased statistical significance. PARAFAC has been successful at identifying a wide range of CDOM components including humic and fulvic acids, tryptophan- and tyrosine-like substances, quinones, several polycyclic aromatic hydrocarbons, and distinguishing microbial, marine and terrestrial CDOM sources. More importantly, PARAFAC has been used to diagnose trends in CDOM components as a function of several key chemical and physical parameters, including water-recycling-plant treatment stages, sewage dispersion, stream flow, and ocean and estuarial currents, among many others. Indeed, the application of PARAFAC has been proposed as a standard modeling technique for a variety of water-quality applications.

Projects and files

What is a project?

A project is a collection of workbooks of data, which hold:

- Graphs (visual diagrams of the data)
- Worksheets (tables of data)
- Notes (comments about the data)



Graphs themselves may contain multiple kinds of information, including separate layers describing the data, the axes, the background colors, etc.

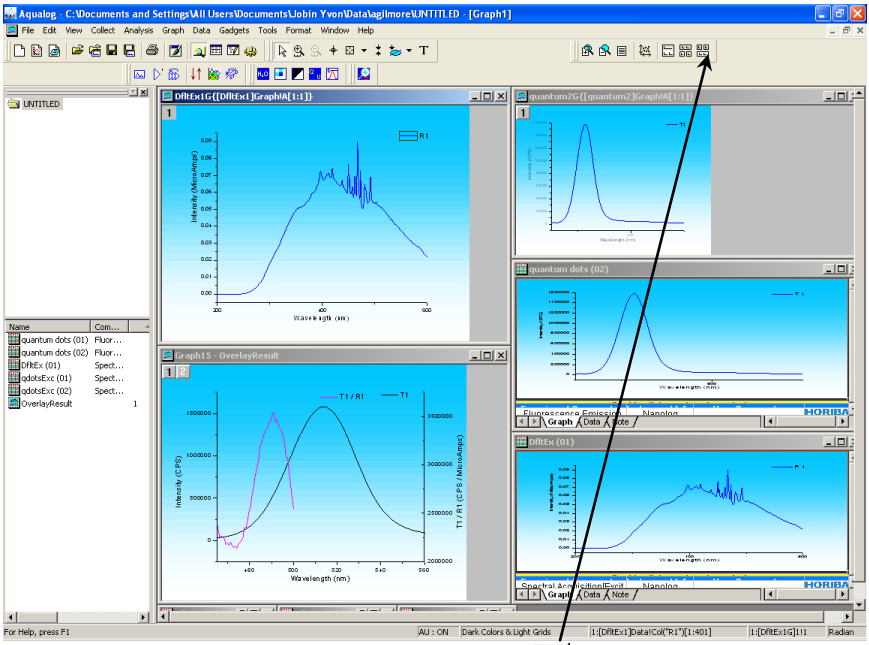
Concerning worksheets, a dataset must contain at least two columns, corresponding to *x*-*y* data pairs. Multiple *y* columns may correspond to a single *x* column.

Note: *For greater detail about projects, graphs, layers, and how to merge, combine, and separate them, see the Origin® on-line help files.*

Merging two or more graph windows

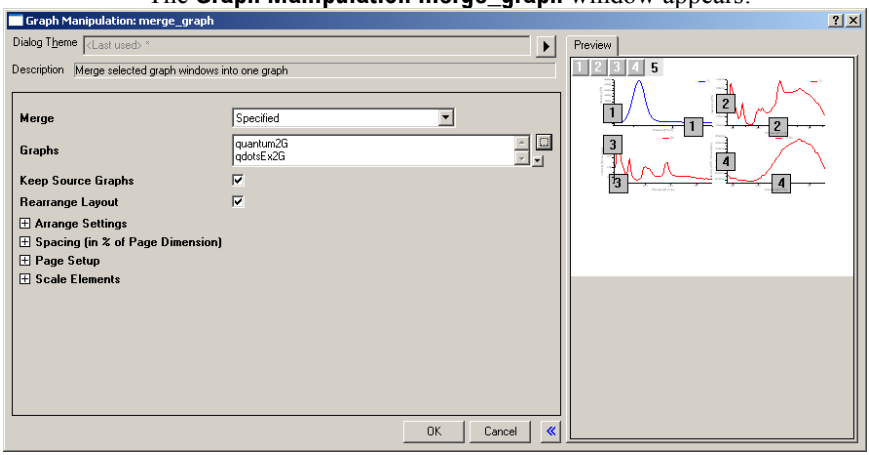
This puts all the open layers on one single page.

1 Close all graph windows you don't want to merge.



2 Click the Merge button  .

The **Graph Manipulation merge_graph** window appears:



3 Click the Browse button ... to browse for the files to merge.

4 Activate the listview checkbox.

5 Select the desired graphs to merge.

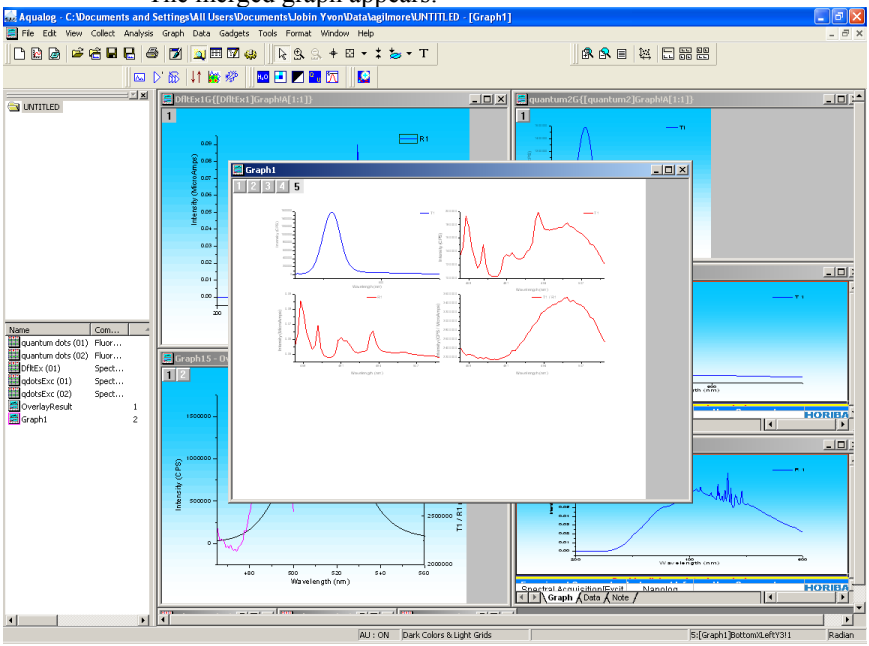
6 Click the >> button to add the desired graphs to the combining list.

7 Click the OK button.

The window closes, and the Preview updates with both graphs together.

8 Click the OK button.

The merged graph appears:

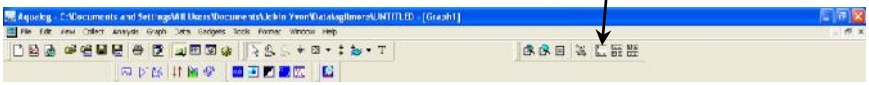


Splitting two graphs by extraction

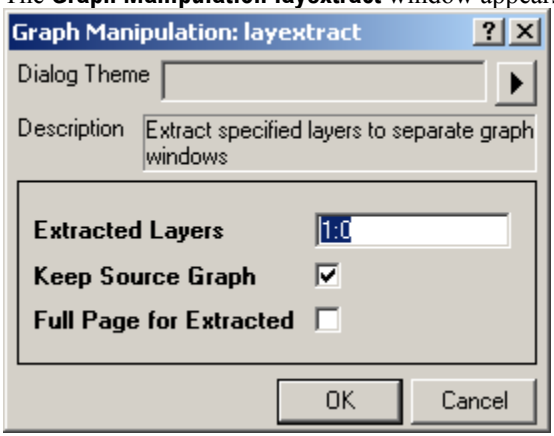
This extracts each plot to a separate layer in the graph.

1 Click on the desired plot to activate it.

2 In the toolbar, choose the Extract to Layers button  .



The **Graph Manipulation layextract** window appears:



3 Click the OK button.

The new graphs appear.

Note: *Other buttons available using the Customize Toolbar command are the button for splitting each layer into a separate graph window, and the button for merging all open graph windows into one graph. See the Origin® on-line help for more information.*

Saving and recalling a file

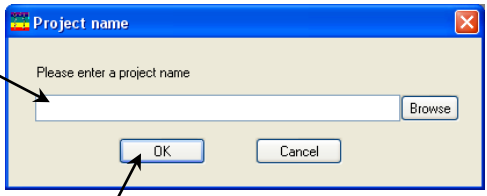
To save a project, when in a new, untitled project

Note: *To determine if you are in an untitled, new experiment, examine the path shown at the top of the main* ***Aqualog*** *window. It should show the word "UNTITLED" at the end of the path.*

1 Run an experiment.

When the experiment is complete, the **Intermediate Display** disappears. The **Project Name** window appears.

2 Enter a new name for the project, or browse for an existing one.



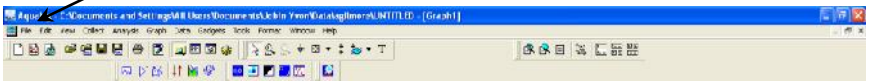
Note: *If you are using an existing project name, the software will allow you to overwrite existing data, or append the new data to the project.*

3 Click the OK button.

The path of the project appears at the top of the main **AquaLog** window. The data are now saved.

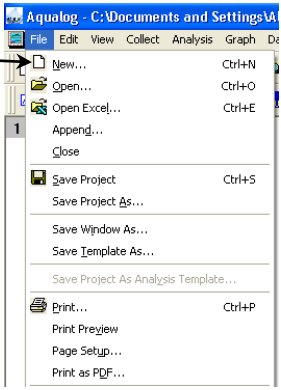
To save data into a new project when another project is already open

1 Choose File.

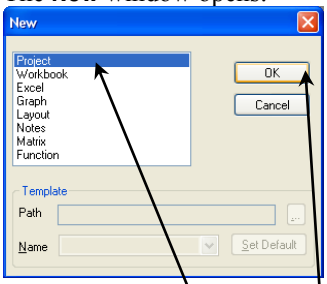


The File menu opens:

2 Choose New....



The **New** window opens:



3 Choose Project from the list of objects to create, then click the OK button.

Note: *Only a Graph or a Matrix lets you pick a new Path and Name.*

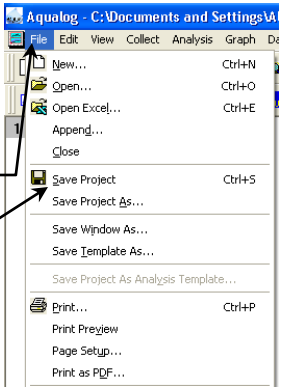
4 Run the experiment.

The data are now in an untitled project. Next you must create the name for the file.

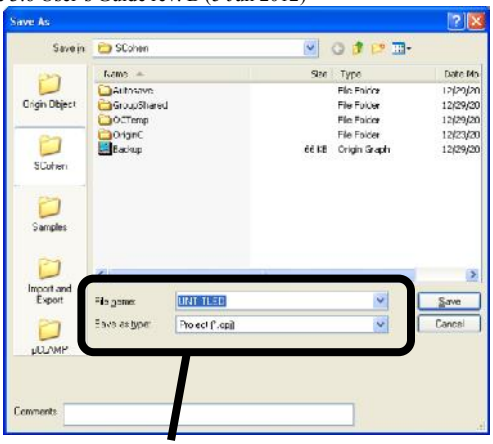
5 Choose File again.

The File menu opens.

6 Choose Save Project As....



The **Save As** window appears:



7 In the File name field, enter a name. In the Save as type field, choose Project (*.opj) from the list.

8 Click the Save button.

Now the project has a new name.

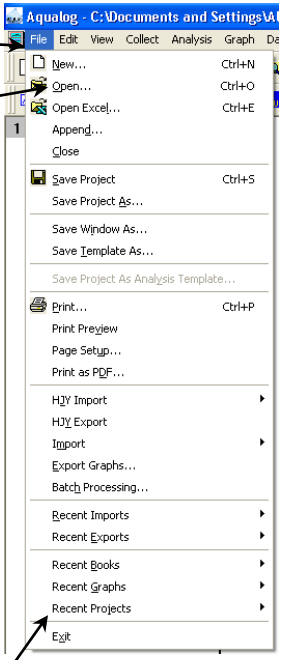
To recall and open an existing project

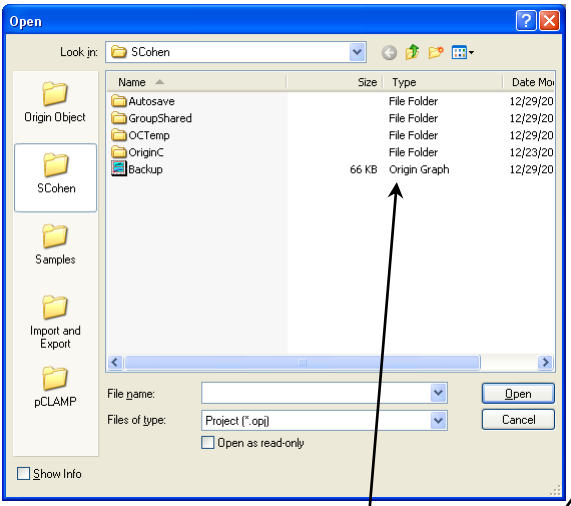
1 Click File.

The File menu opens.

2 Choose Open....

The **Open** window appears:





3 Browse for the desired project, or examine the Recent Projects list.

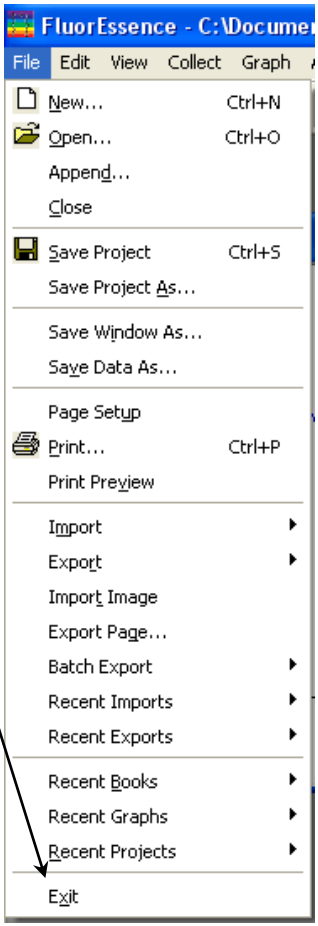
4 Click the Open button.

The project opens.

4: Shutting Down Aqualog® Software

1. Save experiment files (and data files, if created).
2. In the **Aqualog Experiment Setup** window, click the Close button or the Cancel button 

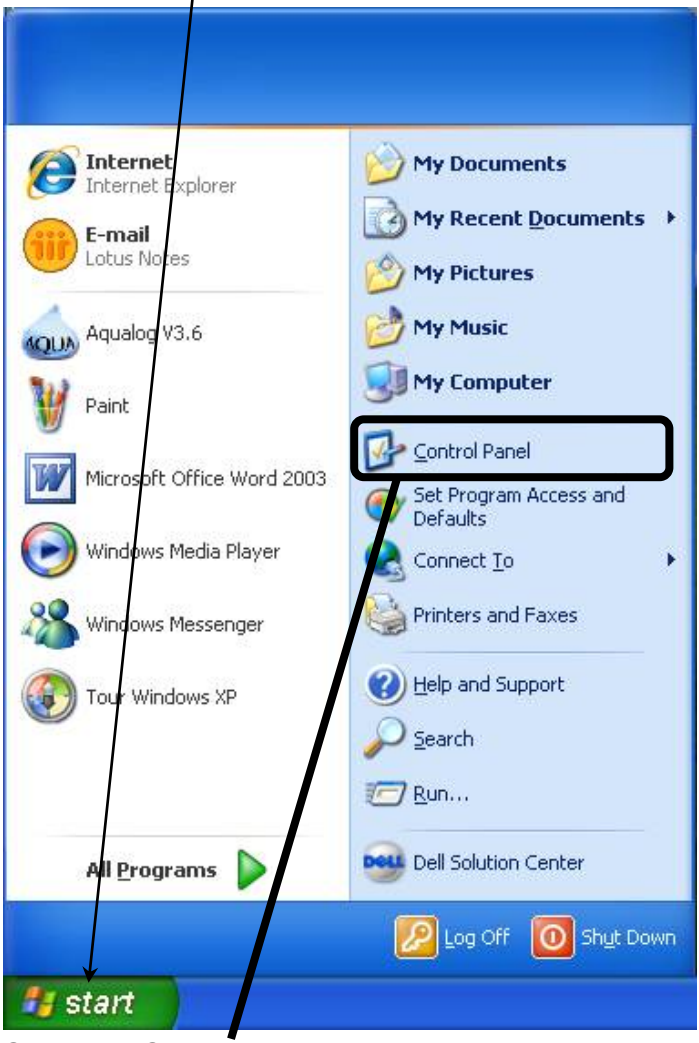
.
3. Close the **Aqualog** main window, using either the Close button , or, in the File drop-down menu, Exit.



5: Un-Installation

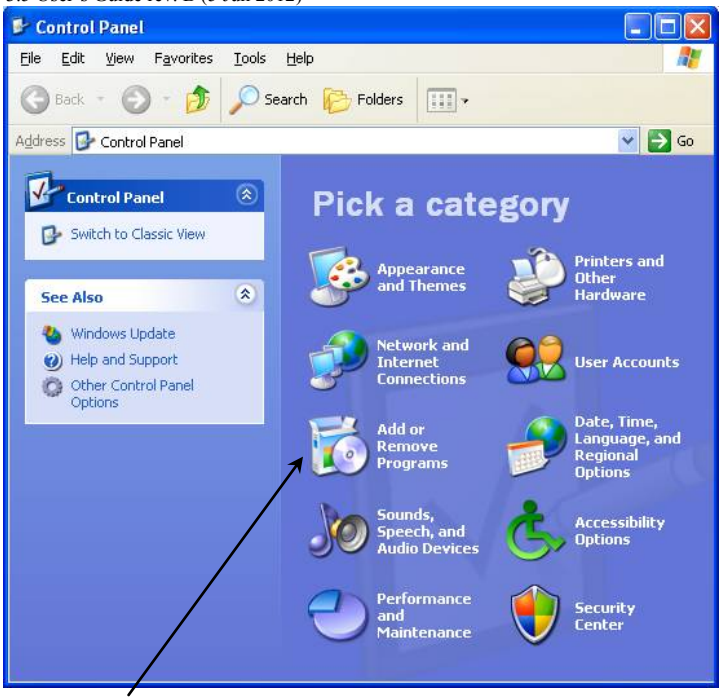
1 Close Aqualog® software.

2 Click the Start button to open the Start menu.



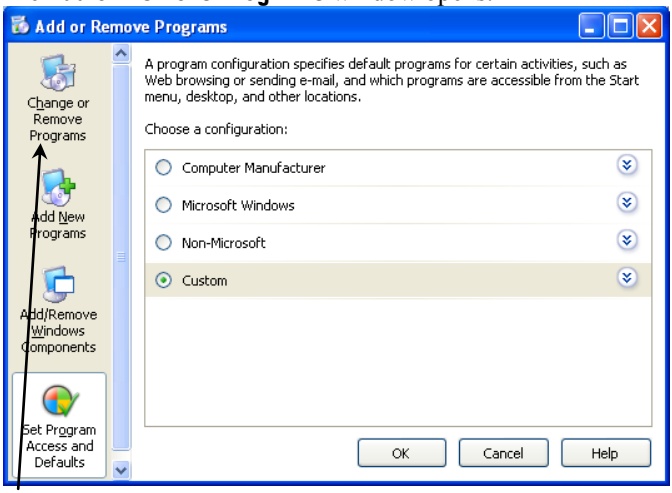
3 Choose Control Panel.

The **Control Panel** opens:



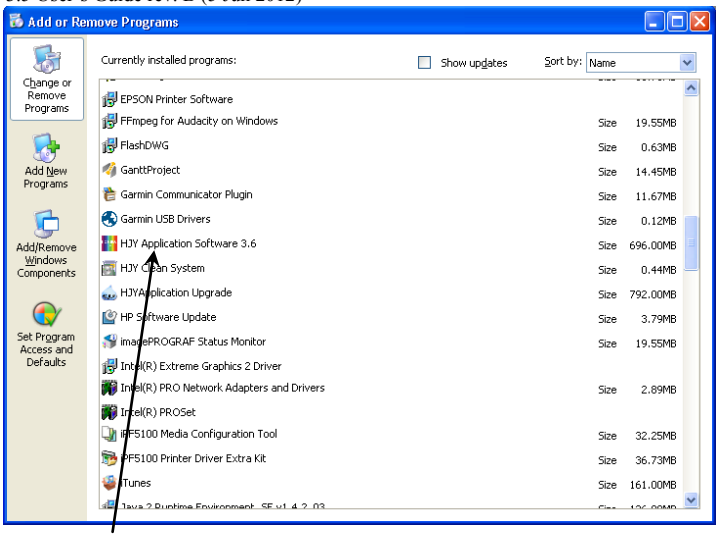
4 Click Add or Remove Programs.

The **Add or Remove Programs** window opens.

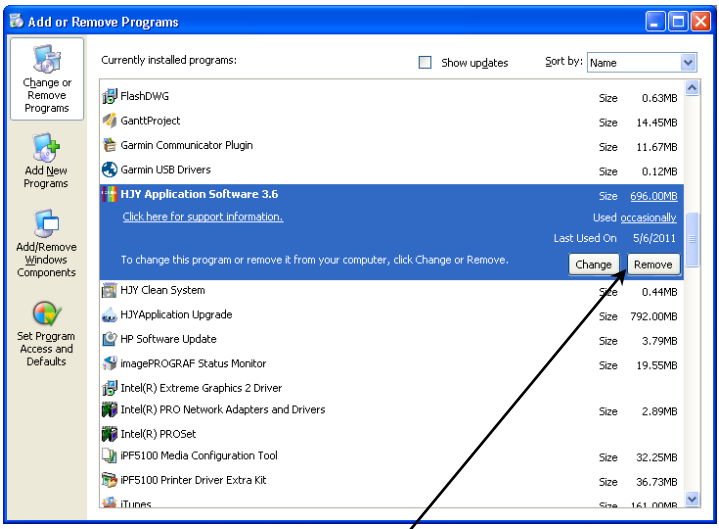


5 Click the Change or Remove Programs icon.

A list of currently installed programs on the host computer appears:



6 Click HJY Application Software 3.6, which becomes active:



7 Click the Remove button.

8 Follow the instructions to remove Aqualog® software.

9 You may need to reboot the host computer.

Aqualog® software is removed from the host computer.

10 Remove the USB key from the USB port.

6: Aqualog® Software Troubleshooting & Technical Support

Troubleshooting

If the special buttons are gray,

1. Exit and restart the Aqualog® software.

   The special buttons should become active again.

2. If step 1 doesn't fix the problem,

   a. Exit the software.

   b. Shut down the Aqualog® instrument.

   c. Restart the instrument and Aqualog® software.

On-line help files

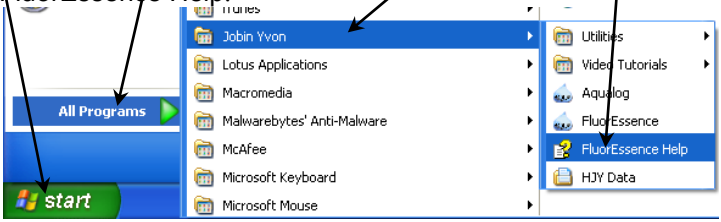
Access from the Windows® Start menu:

1 Click the Windows® Start button.

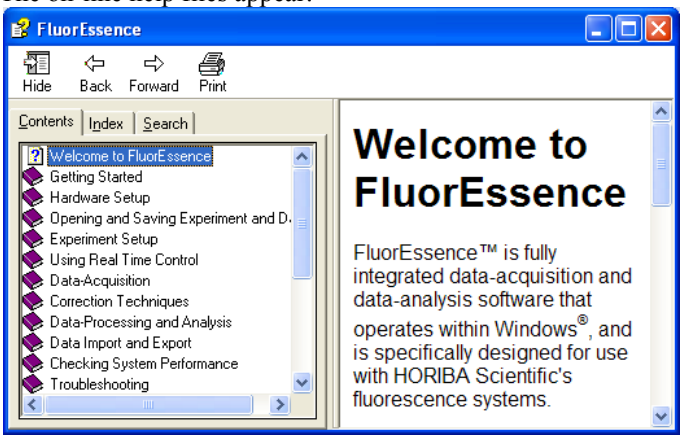
A drop-down menu appears.

2 Choose All Programs.

From the drop-down list, select the Jobin Yvon group, then FluorEssence Help.



The on-line help files appear:



Resize the window to your liking.

Access from the **Experiment Setup** or **Real Time Control** window:

1 Click the Help button 

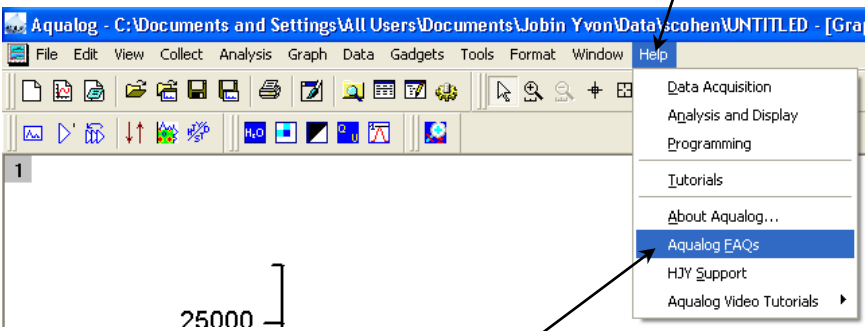
or the `F1` key.

Context-sensitive on-line help files appear. Resize the window to your liking.

Frequently-asked questions about Aqualog® software

Many frequently-asked questions (FAQs) about Aqualog® software may be found on the HORIBA Scientific website.

1 In the **Aqualog** toolbar, choose Help.



A drop-down menu appears.

2 Choose Aqualog FAQs.

If your computer is connected to the internet, your web browser automatically opens in the Aqualog® software webpage:

Video tutorials

For some common procedures, video tutorials are available to guide you. The videos are `.avi` files, which can be played by software such as RealPlayer®, Windows Media Player, etc.

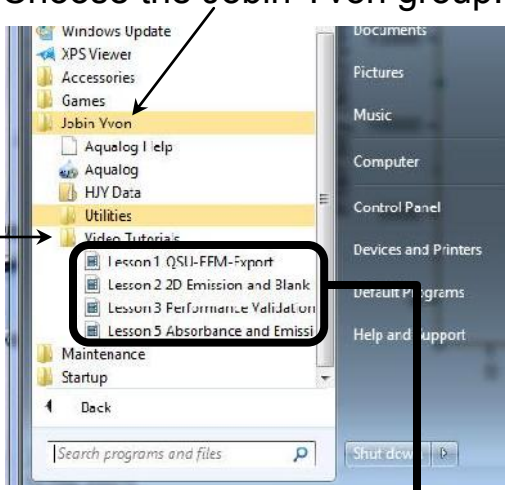
Access to video tutorials

1 Click the Windows® Start button.

The Start menu appears.

2 Choose All Programs.

3 Choose the Jobin Yvon group.



4 Choose the Video Tutorials subgroup.

5 Click on the desired tutorial.

The tutorial opens in your chosen video-playing software.

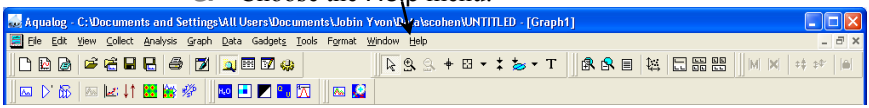
If you have a technical problem,

1. Please consult the Aqualog® software help files and this User's Guide, as well as all other manuals supplied with the system.

If you are unable to solve the problem,

2. Note the problem and any accompanying error messages.
3. Determine Aqualog® software's version number.

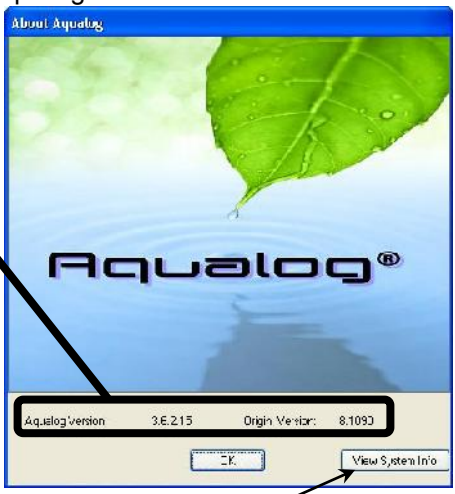
a. Choose the Help menu.



A drop-down menu appears.

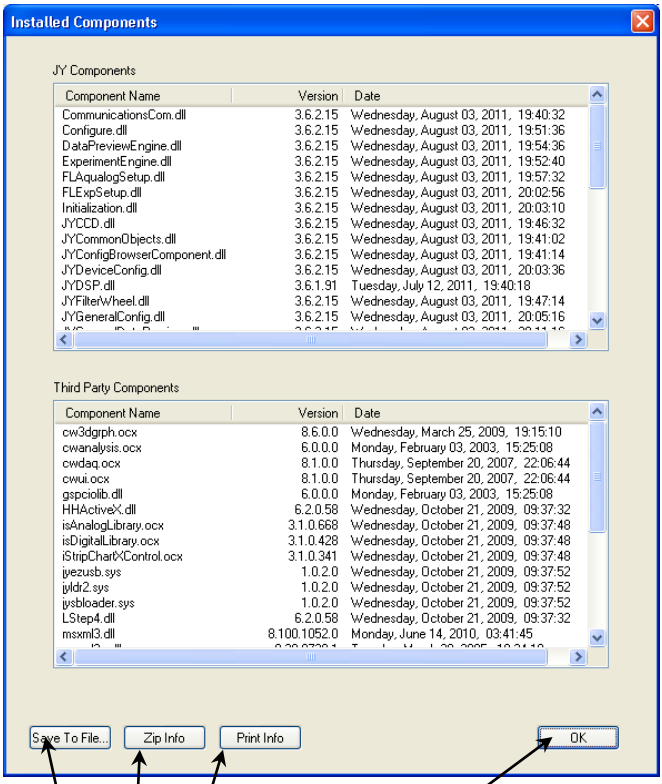
b. Choose About Aqualog....

The **About Aqualog** window opens. Near the bottom are the Aqualog® software and Origin® version numbers.



c. Click the View System Info button.

The **Installed Components** window appears, displaying all the software required for Aqualog® software.



d Record the information by clicking the:

- Save To File... button, which saves the information to a file;
- Zip Info button, which compresses the information while saving it;
- Print Info button, which prints out the software information.

e Click the OK button to close the **Installed Components** window.

f Click the OK button to close the **About Aqualog** window.

4 Write down the software's version numbers, along with the purchase dates, model numbers, system configuration, and serial numbers of the instrument and its accessories.

5 Please contact a HORIBA Scientific Service Department listed below.

Be prepared to describe the malfunction and the attempts, if any, to correct it. Note any error messages observed, and have any relevant spectra (sample, validation tests, etc.) and system information ready for us to assist you.

Contact information

Via the internet:

World-Wide Web	www.horiba.com/scientific
E-mail	info.sci@horiba.com

In North America:

Telephone	1-732-494-8660
Fax	1-732-549-5125

In France:

Telephone	+33 (0) 1 64 54 13 00
Fax	+33 (0) 1 69 09 93 19

Worldwide:

China	+86 (0) 10 6849 2216
Germany	+49 (0) 89 462317-15
Italy	+39 (0) 2 57603050
Japan	+81 (0) 3 58230141
UK	+44 (0) 20 8204 8142

7: Index

Key to the entries:

Times Roman font	subject or keyword
Arial font	command, menu choice, or data-entry field
Arial Condensed Bold font	window
`Courier New` font	file name or expression

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