Appendix 1. Aqualog Standard Operating Procedure (SOP) Walkthrough

Aqualog SOP v1.3
Aqualog software version: 3.6.7.21; Origin version 8.1090

Standard Operating Procedure

1. **Initial Preparations**
   a. Note: Always wear gloves when handling cuvettes or any samples for Aqualog
   b. Warm up instrument (at least 30 minutes)
   c. Log in samples to the OMRL Database
   d. Create standard reference material (1% SRM_{tea} in organic free water)
   e. Open Aqualog Version 3.6.7.21 on desktop

2. **Record lamp hours**
   a. Open application on desktop titled "USB Aqualog Config Tool." If you get an error message that the USB is not connected, close the error window, close Aqualog Version 3.6.7.21, reopen Aqualog Version 3.6.7.21, and try opening the application again.
   b. Select Light Sources tab
   c. Record lamp hours in Aqualog Record Book, close application

3. **Raman Scan (wrMMDDYY)**
   a. Prepare Aqualog cuvette
      i. Remove cuvette from HNO_3 container labeled *Aqualog* in Biology Lab fume hood
      ii. Rinse thoroughly with organic-free water (OFW), approximately 20 rinses
      iii. Fill cuvette with OFW, polish dry with lens paper ensuring it is free of spots, streaks, fingerprints, etc., and then place in sample chamber Position 1
      iv. Record water resistance from OFW system in log book, should be at least 18.0 meg-Ohm
   b. Click on Aqualog Main Experiment button
   c. Select Spectra, then Emission 2D, then Next
   d. Load wrexperiment1000.xml (Location: Libraries\Documents\Jobin Yvon\Data)
      i. Integration Time=10: Accumulation=1: Ex=350: Em=1.64: CCD Gain=Medium: Sample Only: Position 1
   e. Change data identifier to wrMMDDYY (e.g. wr011912)
   f. Select run
   g. When prompted, save the project.
      i. Hit browse (don't enter a project name in this window).
      ii. Navigate to the Desktop and open the folder [Local Aqualog Folder - Temp]. C:\Desktop\Local Aqualog Folder - Temp
      iii. Create a new folder within this folder using the naming convention **qYYYY-MM-DD** (e.g q2016-05-18). C:\Desktop\Local Aqualog Folder - Temp\qYYYY-MM-DD.
      iv. Double click on the folder to access it.
      v. Enter the project file name as **qYYYYMMDD** (e.g. q20160518).

  vi. The Project Name dialogue box will populate with this path and project file name. C:\Desktop\Local Aqualog Folder - Temp\qYYYY-MM-DD\ qYYYYMMDD.opj

  vii. Select ok.

 h. Saving and exporting the water Raman file

   1. The water Raman data file should be exported as a .dat file.

    a. Activate the worksheet entitled "**Emission Sample Data**"

    b. Select File from the drop-down menu, then Export, then ASCII.

    c. Rename the worksheet to "wrMMDDYY_Emission Sample Data" (e.g. wr051816_Emission Sample Data).

    d. Export to the Project folder that was created for this run date. C:\Desktop\Local Aqualog Folder - Temp\qYYYY-MM-DD\ wrMMDDYY_ Emission Sample Data.dat.

4. Baseline Scan (baMMDDYY)

 a. Use the same cuvette and OFW that was used for the Water Raman scan.

 b. Click on Aqualog Experiment button

 c. Select 3D, then EEM 3D CCD + Absorbance, then Next

 d. Load Baselinet100.xml

  i. Integration=1: Ex=600-240-3: Em=1.64: CCDGain=Medium: Position 1

 e. Under Data Description, change data identifier to baMMDDYY (e.g. ba051816)

 f. Under Blank/Sample Setup, select "Blank Only"

 g. Still under Blank/Sample Setup, select ellipsis next to blank only, and save as .blank file, baMMDDYY.blank (e.g. ba051816.blank) in same folder as the project file.

  i. C:\Desktop\Local Aqualog Folder - Temp\qYYYY-MM-DD\ baMMDDYY.blank

 h. Confirm Baseline cuvette position (positions are physically labeled on cuvette holder)

 i. Select run

 j. Saving and exporting the Baseline file

  i. The Baseline data file should be saved as a .xlsx file.

   1. In Origin select the worksheet entitled "**S1c/R1c**"

   2. Copy and paste the contents of "S1c/R1c" into an excel template. Select all using "ctrl A," Copy all using "ctrl C."

   3. Open AQUA Blank Template.xlsx. located here: \\IGSWCAWWAS9902\CAWSC Lab\LAB\LAB DATA\Aqualog - DOM\AQUA Blank Template.xlsx

    a. Template is an Excel file with column headers in Row 1 as emission wavelengths (nm) from 600 (Column B) through 240 (Column DR) in increments of 3.
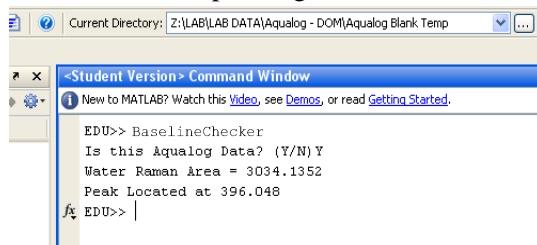
	A	B	C	D	E	F	G	H	I	J	K	L	M
1	Wavelength (nm)	600	597	594	591	588	585	582	579	576	573	570	567
2													
3													
4													

   4. In cell A2, use "ctrl V" to paste. Confirm there is data in cells A1:DR251.

5. Save the file as "baMMDDYY.xlsx" into the current project folder located here: C:\Desktop\Local Aqualog Folder - Temp\qYYYY-MM-DD\baMMDDYY.xlsx (e.g. ba051816.xlsx).

5. **Quality check the Baseline and water Raman Scans**
   a. Copy and paste the baseline file (baMMDDYY.xlsx) and corresponding water Raman file (wrMMDDYY_Emission Sample Data.dat) to the following location: \\IGSWCAWWAS9902\CAWSC Lab\LAB\LAB DATA\Aqualog - DOM\Aqualog Blank Temp
   b. Open MATLAB
      i. Run *BaselineChecker* code – This should generate water Raman info within MATLAB corresponding to the wr Area, and Peak Location shown below:

      ii. Record wrArea and Peak Location in the logbook.
      iii. MATLAB will also generate three EEMs images called *Todays Baseline*, *Baseline diff* and *3 x StDev* for visual determination of baseline quality.
      iv. Verify that the wrArea and Peak Location number is consistent with previous water Raman values (Area=[within 75% of the value obtained at the last lamp change], Peak=397 ± 1 nm) AND quality check the baseline by confirming the response is less than the long-term method detection limit (LT-MDL) in the region(s) of interest. If the wrArea value is not consistent or the EEMs images do not pass QA standards, then let the machine warm up for a little longer and repeat the water Raman and Baseline scans.

6. **Run a Blank (blMMDDYYa, blMMDDYYb, blMMDDYYc, etc.)**
   a. Prepare cuvette for running a blank
      i. Rinse cuvette 3x with OFW and fill just over half-way with OFW.
      ii. Polish cuvette sides with lens paper, ensuring it is free of spots, streaks, fingerprints, etc.
   b. Click on Aqualog Experiment button
   c. Select 3D, then EEM 3D CCD + Absorbance, then Next
   d. Load 240-600t100.xml
      i. Integration=1: Ex=600-240-3: Em=1.64: CCDGain=Medium: Position 1
   e. Under Data Description, change data identifier to blMMDDYYa (e.g. bl051816a)
   f. Under Blank/Sample Setup, select Blank from File. Use the ellipsis button to navigate to and select the Baseline.blank file saved in step 6g.
   g. Confirm Blank cuvette position (positions are physically labeled on cuvette holder)
   h. Click run
   i. Repeat two more times to run a total of three blanks before running a sample, see section 10 for batch sample running outline.

            i. Naming convention for multiple blanks is blMMDDYYa, blMMDDYYb, blMMDDYYc, etc.

7. **Analytical Set**
    a. Prepare cuvette for running a sample
        i. Rinse cuvette 3x with OFW
        ii. Shake the sample bottle to mix well
        iii. Condition cuvette once with sample water and fill just over half-way with the sample
        iv. Polish cuvette sides with lens paper, ensuring it is free of spots, streaks, fingerprints, etc.
    b. Choose Aqualog experiment menu button
    c. Choose 3D, then EEM 3D CCD + absorbance, then Next
    d. Load 240-600t100.xml
        i. Integration=1: Ex=600-240-3: Em=1.64: CCDGain=Medium: Postion 1
    e. Under Data Description, rename Data Identifier with OMRL unique lab identifier (e.g. gr12345)
    f. Under Blank/Sample Setup, select Blank from File. Use ellipsis button to navigate to and select the Baseline.blank file saved in step 6g
    g. Next sample
        i. Repeat Steps 7ai-7aiv
        ii. Click Previous Experiment Setup button
        iii. Change data identifier (e.g. from gr12345 to gr12346)
        iv. Click run
    h. Run up to 8 more samples (see step 8 for Batch Sample outline).
    i. Run SRM$_{Tea}$ standards.
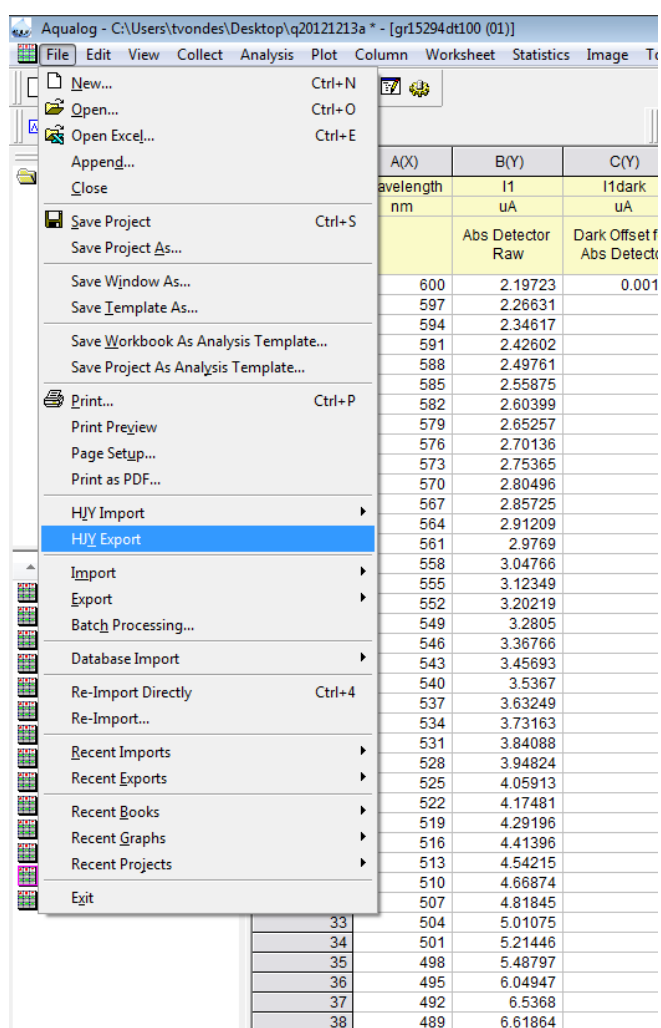   j. Run sample duplicate.

8. **Run Sample Outline**
    a. Please follow the QAQC Batch Sample outline in the table below:

Row	Scan Type
1	wrMMDDYY (water Raman)
2	blMMDDYY (baseline)
3	MMDDYYb1 (blank 1)
4	MMDDYYb2 (blank 2)
5	MMDDYYb3 (blank 3)
6	Sample 1
7	Sample 2
8	Sample 3
9	Sample 4
10	Sample 5
11	Sample 6
12	Sample 7
13	Sample 8
14	Sample 9
15	Sample 10

16	SRM 1 (SRM$_{tea}$ at 1% concentration; Run once per day)
17	SRM 2 (SRM$_{tea}$ at 1% concentration; Run once per day)
18	Sample 1d (duplicate)
19	MMDDYYb4 (blank 4)
20	MMDDYYb5 (blank 5); a minimum of 5 blanks should be run per day.
21	Continue with samples, repeating above sequence from rows 6-20, skipping rows 16 and 17. Always end the run with a duplicate followed by two blanks.

9. **Batch export Aqualog data**
    a. The following is a screen-by-screen guide to batch exporting data from the Aqualog software Version 3.6.7.21.
   b. Select File, then HJY Export.

c. Click on the Ellipsis ('…') button to the right of the blank window.

d. This is your exporting interface. The upper left window lists the samples run in the current project. The right side is the data selected to be exported. Simply highlight the project folder on the left and click the two arrows pointing right in the top middle to move it to the export side.
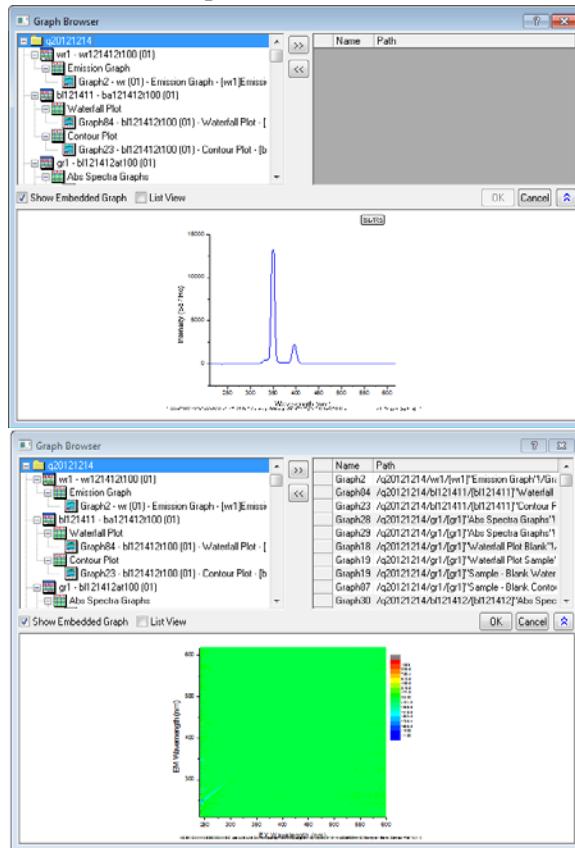
e. Select Ok.
f. The HJY: HJY_Export Dialog Box appears along with a smaller Script Window. Despite the seemingly random graph numbers displayed, this is accurate. Select Ok.
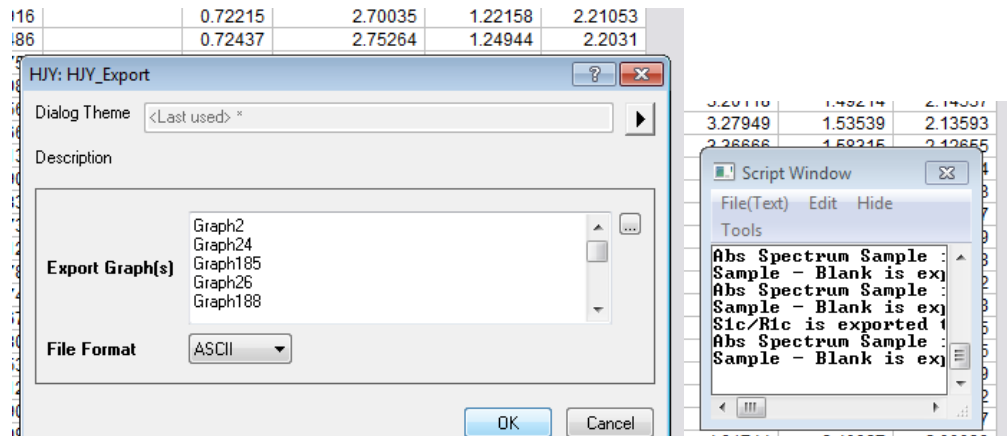
g. You will be prompted for a location to batch export. Export to the current rundate folder in the following location: C:\Desktop\Local Aqualog Folder - Temp\qYYYY-MM-DD.
    i. Select ok.
        1. Origin software is now batch exporting to your selected file location. A warning will appear for each sample that is exported. You will be prompted to 'Replace a File' for each Abs Spectra Graph.dat generated in your project file. This is because Origin stores two absorbance graphs as one filename. Select Yes each time to replace the file. The script window updates as the files are exported.
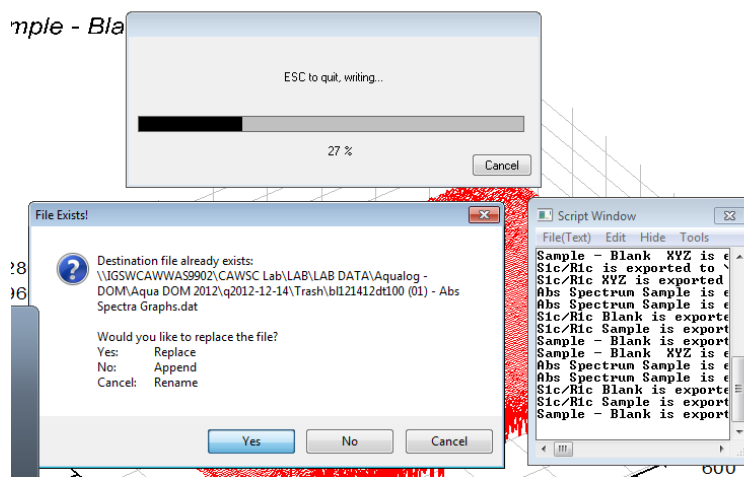
10. Transfer data to network
    a. Move today's project folder and all its contents to the network:
        i. From C:\Desktop\Local Aqualog Folder - Temp\qYYYY-MM-DD
        ii. To \\Igswcawwas9902\CAWSC Lab\LAB\LAB DATA\Aqualog - DOM\Aqua DOM 2016\qYYYY-MM-DD
11. Process the Data
    a. Open MATLAB, run processing routine *ProcessingInterface* (case sensitive). This takes approximately 2 minutes to complete.

     b. Note: Several files are exported for each sample during the HJY export process. MATLAB code version OM4.0 will sort through these during optical processing.

12. QAQC the processed data
     a. Access the lab QA templates located here:
          i. \\IGSWCAWWAS9902\CAWSC Lab\LAB\LAB QA\Analytical QA templates. There is a unique template for each instrument.
     b. Copy and paste data from Processed Data to Analytical QA template
     c. Evaluate QA summary. If it passes QAQC standards, save the file. If it fails QAQC, rerun samples.
     d. Save to appropriate location on network into the corresponding rundate for each analyte:
          i. Aqualog ABS: \\IGSWCAWWAS9902\CAWSC Lab\LAB\LAB DATA\Aqualog - DOM\Aqua DOM 2013\qYYYY-MM-DD\qaYYYY-MM-DD
          ii. Aqualog FLR: \\IGSWCAWWAS9902\CAWSC Lab\LAB\LAB DATA\Aqualog - DOM\Aqua DOM 2013\qYYYY-MM-DD\qfYYYY-MM-DD

13. Shutting down
     a. Thoroughly rinse cuvette with OFW and store in 10% by wt. HNO_3 acid bath in fume hood
     b. Close Aqualog program and save project when prompted
     c. Turn off Aqualog
     d. Log off computer

Instrument Performance: Aqualog Validation Tests

These validation tests are performed on a monthly basis to validate instrument performance. The validation tests (sections 2-5) below are referenced in the *Total Aqualog Manual*; see Chapter entitled *Validating System Performance* on page 4–3 for detailed information.

1. Initial Preparations
    a. Open the instrument software and let the instrument warm up for 30 minutes prior to use.
    b. Create a new project folder in the following location: C:\Desktop\Local Aqualog Folder - Temp\qYYYY-MM-DD
    c. Go to File – Save Project As- and save the project file as the following: qYYYYMMDD in the following location: C:\Desktop\Local Aqualog Folder - Temp\qYYYY-MM-DD
        i. Folder naming convention should use the same date as the project file.
2. Excitation Validation (Lamp Scan)
    a. Purpose: The purpose of this scan is to check lamp peak position and lamp performance.
    b. Procedure:
        i. Click on the Aqualog main experiment button
        ii. Select Spectra, then Absorbance
        iii. Hit Run. Leave all other parameters unchanged
        iv. Once scan has finished, highlight columns B and D, select Plot up on the main toolbar, select line, then line again
            i. Peak position should be 467 nm (±1nm).
3. Water Raman SNR and Emission Calibration (emission validation)
    a. Purpose: 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. The water sample used for this validation test should be research-quality triple-distilled or de-ionized water.
    b. Cells needed: Aqualog cuvette
    c. Procedure:
        i. Prepare a cuvette with OFW
        ii. Select Collect, Aqualog Validation Tests, and Water Raman SNR and Emission Calibration
        iii. Make sure to specify which sample position the cuvette is in
        iv. Hit Run
        v. A graph is generated. The Raman peak wavelength should be 397nm (±1nm). In the results column it should read PASS.
        vi. Select the Raman SNR Calculation Tab. In the B(Y) column below the comments section, there should be a number. This is the Lamp Intensity, and this value should be above 650,000 cps.
4. Absorbance Photometric Accuracy
    a. Purpose: This validation check examines the accuracy of the absorption function of the Aqualog. Use the absorption standard SRM 935a (Potassium Dichromate 60 mg/L) available from NIST.
    b. Cells needed: standard SRM 935a (Potassium Dichromate Blank, Potassium Dichromate 60mg/L)

c. Procedure:
    i. Select Collect, Aqualog Validation Tests, and Abs Photometric Accuracy SN 15740.
    ii. Make sure to specify which sample position the cuvette is in
        i. Position 1 is the Potassium Dichromate Blank; Position 2 is Potassium Dichromate (60mg/L)
        ii. Make sure when inserting the cells that the frosted sides are towards the front of the instrument and the clear sides are towards the left and right of the instrument.
    iii. Hit Run
    iv. On worksheet *Test Results*, the Pass/Fail column should display "P" for all four wavelengths measured.
5. Quinine Sulfate Unit
    a. Purpose: This function provides a standardized intensity for fluorescence measurements and EEMs.
    b. Cells needed: Quinine Sulfate standard kit (RM-QS00) (Quinine Sulfate blank; Quinine Sulfate standard at 1mg/L)
    c. Procedure:
        i. Select Collect, Aqualog Validation Tests, Quinine Sulfate Unit
        ii. Make sure that the Quinine Sulfate blank and the Quinine Sulfate standard cuvette are placed in the appropriate sample chamber position.
            i. Position 1 is the Quinine Sulfate Blank; Position 2 is the Quinine Sulfate Standard
        iii. Hit Run. This scan should only take a couple of seconds
        iv. Select the QSU Calculation Worksheet Tab. The absorbance value at 347.5nm should be 0.01384.
        v. Select the Emission Spectrum Graph Tab. Using the crosshairs icon locate the position of the peak. This value should be 450nm (±1nm).
6. Starna 6BF Reference Cells
    The set of Starna reference cells will be run the same way as live samples. However the reference cells will be run at an integration time of 0.05s rather than 1s to prevent oversaturation of the CCD.

    a. Record lamp hours
        i. Open application on desktop titled "USB Aqualog Config Tool." If you get an error message that the USB is not connected, close the error window, close Aqualog Version 3.6.7.21, reopen Aqualog Version 3.6.7.21, and try opening the application again.
        ii. Select Light Sources tab
        iii. Record lamp hours in Aqualog Record Book, close application
    b. Run Water Raman Test (wrMMDDYY)
        i. Prepare Aqualog cuvette
            i. Remove cuvette from HNO_3 container labeled Aqualog in Biology Lab fume hood

        ii. Rinse thoroughly with organic-free water (OFW), approximately 20 rinses

       iii. Fill cuvette with OFW and place in sample chamber, Position 1

       iv. Record water resistance from OFW system in log book, should be at least 18.0 mega-ohms

  ii. Click on Aqualog Main Experiment button   H₂O

  iii. Select Spectra, then Emission 2D, then Next

  iv. Load wrexperiment1000.xml (Location: Libraries\Documents\Jobin Yvon\Data)

       i. Experiment file loads: Integration Time=10: Accumulation=1: Ex=350: Em=1.64 (should match EEM set-up, so if that changes this needs to change too): CCD Gain=Medium: Sample Only: Position 1

  v. Change data identifier to wrMMDDYY (e.g. wr011912)

  vi. Select run

  vii. When prompted, save the project.

       i. Hit browse (don't enter a project name in this window).

       ii. Navigate to the Desktop and open the folder [Local Aqualog Folder - Temp]. C:\Desktop\Local Aqualog Folder - Temp

       iii. Create a new folder within this folder using the naming convention qYYYY-MM-DD
(e.g q2012-01-08). C:\Desktop\Local Aqualog Folder - Temp\qYYYY-MM-DD.

       iv. Double click on the folder to access it.

       v. Enter the project file name as qYYYYMMDD (e.g. q20130108).

       vi. The Project Name dialogue box will populate with this path and project file name. C:\Desktop\Local Aqualog Folder - Temp\qYYYY-MM-DD\qYYYYMMDD.opj

       vii. Select ok.

c. Run a Baseline (baMMDDYY)

  i. Use the same cuvette and OFW that was used for the Water Raman scan.

  ii. Click on Aqualog Experiment button

  iii. Select 3D, then EEM 3D CCD + Absorbance, then Next

  iv. Load Baselinet100.xml

       i. Integration=1: Ex=600-240-3: Em=1.64: CCDGain=Medium: Position 1

  v. Under Data Description, change data identifier to baMMDDYY (e.g. ba011912)

  vi. Under Blank/Sample Setup, check "Blank Only"

  vii. Still under Blank/Sample Setup, click ellipsis next to blank only, and save as .blank file, baMMDDYY.blank (e.g. ba091912.blank) in same folder as the project file: C:\Desktop\Local Aqualog Folder - Temp\qYYYY-MM-DD\baMMDDYY.blank

  viii. Confirm Baseline cuvette position (positions are physically labeled on cuvette holder)

  ix. Click run

  x. Saving and exporting the Baseline file

       i. The Baseline data file will need to be exported as an Excel .xlsx file.

- a. Activate the worksheet entitled "S1c/R1c"
- b. Copy and paste the contents of "S1c/R1c" into an excel template. Select all using "ctrl A," Copy all using "ctrl C."
- c. Open AQUA Blank Template.xlsx. located here: \\IGSWCAWWAS9902\CAWSC Lab\LAB\LAB DATA\Aqualog - DOM\Aqualog Blanks_stats\AQUA Blank Template.xlsx
- d. In cell A2, use "ctrl V" to paste. There should now be data in cells A1:DR251.
- e. Save the file as "baMMDDYY.xlsx" into the current project folder located here: C:\Desktop\Local Aqualog Folder - Temp\qYYYY-MM-DD\baMMDDYY.xlsx (e.g. ba091912.xlsx).

d. Quality check the Baseline
   - i. Copy and paste the baseline file (baMMDDYY.xlsx) and corresponding water Raman file (wrMMDDYY_Emission Sample Data.dat) to the following location: \\IGSWCAWWAS9902\CAWSC Lab\LAB\LAB DATA\Aqualog - DOM\Aqualog Blank Temp
   - ii. Open MATLAB at the Fluoromax-4 computer station (station #1107)
       - i. Run *BaselineChecker* routine – This should generate water Raman info within MATLAB corresponding to the wr Area, and Peak Location shown below:

       - ii. Record wrArea and Peak Location in the logbook.
       - iii. MATLAB will also generate three EEMs images called Todays Baseline, Baseline diff and 3 x StDev for visual determination of baseline quality.
       - iv. Verify that the wrArea and Peak Location number is consistent with previous water Raman values (Area=[within 75% of the value obtained since the last lamp change], Peak=397 nm $\pm$ 1 nm) AND quality check the baseline by confirming the response is less than the long-term method detection limit (LT-MDL) in the region(s) of interest. If the wrArea value is not consistent or the EEMs images do not pass QA standards, then let the machine warm up for a little longer and try again.

e. When the baseline has been quality-checked and the images have passed QA standards, immediately run a second water Raman and baseline scan, this time using the following parameters:
   - i. Water Raman Scan
       - i. Click on Aqualog Main Experiment button
       - ii. Select Spectra, then Emission 2D, then Next

      iii. Adjust the parameters to the following: (Integration time= 0.5s; Accumulation=1: Ex=350; Em=1.64: CCD Gain=Low; Sample Only; Position 1)

      iv. Change data identifier to wrMMDDYYt05 (e.g. wr011912t05)

      v. Select run

  ii. Baseline Scan

      i. Click on Aqualog Experiment button

      ii. Select 3D, then EEM 3D CCD + Absorbance, then Next

      iii. Adjust the parameters to the following: (Integration time= 0.05s; Ex=600-240-3; Em=1.64; CCD Gain=Low; Position 1)

      iv. Under Data Description, change data identifier to baMMDDYYt05 (e.g. ba011912t05) where t05 denotes an integration time of 0.05s.

      v. Under Blank/Sample Setup, check "Blank Only"

      vi. Still under Blank/Sample Setup, click ellipsis next to blank only, and save as .blank file, baMMDDYYt05.blank (e.g. ba091912t05.blank) in same folder as the project file: C:\Desktop\Local Aqualog Folder - Temp\qYYYY-MM-DD\ baMMDDYYt05.blank

      vii. Confirm Baseline cuvette position (positions are physically labeled on cuvette holder)

      viii. Click run

      ix. There is no MATLAB tool to quality check this water Raman or baseline. The previous scans above (steps b. and c.) act as a check instead.

      x. NOTE: Each subsequent scan will be named using the following format where t05 denotes an integration time of 0.05s (e.g. blMMDDYYt05, gr12345t05).

f. Run a Blank (blMMDDYYat05, blMMDDYYbt05, blMMDDYYct05, etc.)

  i. Prepare cuvette for running a blank

      i. Rinse cuvette 3x with OFW and fill just over half-way with OFW.

      ii. Dry cuvette with lens paper, ensuring it is free of spots, streaks, fingerprints, etc.

  ii. Click on Aqualog Experiment button

  iii. Select 3D, then EEM 3D CCD + Absorbance, then Next

  iv. Load 240-600t100.xml

      i. Integration time= 0.05s; Increment= 1.64nm (4 pixel); CCD Gain= Low; Position 1

  v. Under Data Description, change data identifier to blMMDDYYat05 (e.g. bl010812at05)

  vi. Under Blank/Sample Setup, select Blank from File. Use the ellipsis button to navigate to and select the Baseline.blank (baMMDDYYt05) file saved in step 6-e-ii-vi.

  vii. Confirm Blank cuvette position (positions are physically labeled on cuvette holder)

  viii. Click run

  ix. Repeat two more times to run a total of three blanks before running a sample, see section 10 for batch sample running outline.

    i. Naming convention for multiple blanks is blMMDDYYat05, blMMDDYYbt05, blMMDDYYct05, etc.

g. Run Samples (6 reference cells) (e.g. gr12345t05, gr12346t05, gr12347t05, etc.)

  i. Prepare cuvette for running a sample

    i. Ensure the Starna 6BF Reference Cells are free of spots, streaks, fingerprints, etc.

    ii. Lightly polish the cells with the Starna cloth and OFW if necessary. Do not use lens paper on the reference set.

    iii. Load the clean cell in sample chamber position 1.

  ii. Choose Aqualog experiment menu button

  iii. Choose 3D, then EEM 3D CCD + absorbance, then Next

  iv. Load 240-600t100.xml

    i. Integration time= 0.05s; Increment= 1.64nm (4 pixel); CCD Gain= Low; Position 1

  v. Under Data Description, rename Data Identifier, e.g. grRef1t05
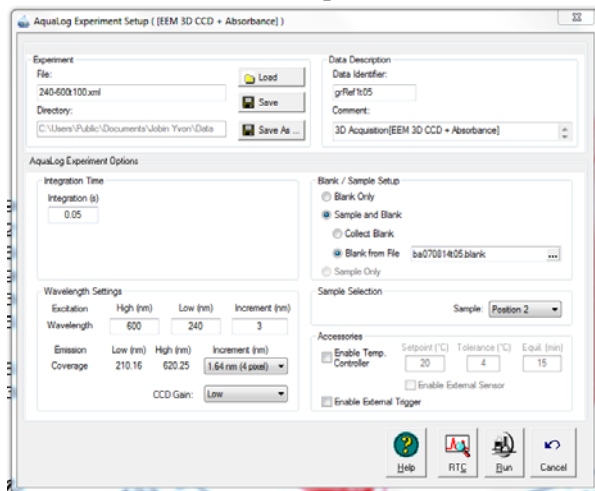
  vi. Under Blank/Sample Setup, select Blank from File. Use ellipsis button to navigate to and select the Baseline.blank file saved in step 10c.

  vii. Click run

  viii. Next sample

    i. Repeat Steps fi-fiii.

    ii. Click Previous Experiment Setup button

    iii. Change data identifier, e.g. grRef2t05

  ix. Run the remaining samples, duplicate, and blanks following the Run Sample Outline in section g.

h. Run Sample Outline

  i. Please follow the QAQC Batch Sample outline in the table below:

Row	Scan Type
1	wrMMDDYYt05 (water Raman)

2	baMMDDYYt05 (baseline)
3	blMMDDYYat05 (blank 1)
4	blMMDDYYbt05 (blank 2)
5	bkMMDDYYct05 (blank 3)
6	Sample gr12345t05 (Reference cell 1)
7	Sample gr12346t05 (Reference cell 2)
8	Sample gr12347t05 (Reference cell 3)
9	Sample gr12348t05 (Reference cell 4)
10	Sample gr12349t05 (Reference cell 5)
11	Sample gr12350t05 (Reference cell 6)
18	Sample gr12350t05d (Reference cell 6)
19	blMMDDYYdt05 (blank 4)
20	blMMDDYYet05 (blank 5); a minimum of 5 blanks should be run per day.

i. Instructions for *Batch export data*, *Transfer data*, *Process data*, *QAQC data*, and *Shutting Down* should be followed using Standard Operating Procedure section 9-13.

Instrument Performance: Evaluation of Lamp Performance and calibration of Emission Monochrometer

Perform this evaluation after the lamp has been replaced according to the instructions on Page 9–1, Section 1 entitled *Maintenance: Lamp Replacement* in the *Total AquaLog Manual* located on the laboratory server (CAWSC Lab (\\IGSWCAWWAS9902)\LAB\LAB DOCUMENTS\instrument eqpt manuals\Total AquaLog Manual.pdf).

Verify Lamp counts per second (CPS):

1. Optimize the lamp position following the instructions on Page 9–12, Section 11 entitled *Adjust the new xenon lamp* in the *Total AquaLog Manual* located on the laboratory server (CAWSC Lab (\\IGSWCAWWAS9902)\LAB\LAB DOCUMENTS\instrument eqpt manuals\Total AquaLog Manual.pdf).
2. A new replacement lamp target is >650,000 cps. To verify this:
    a. Run Validation Test Water Raman SNR and Emission Calibration.
    b. In Results Workbook, Select worksheet entitled Raman SNR Calculation.
    c. In column B Row 1 Record CPS value in Aqualog logbook (e.g. 1.20148 E6).
        i. Note: If CPS is <650,000 cps then repeat from Step 1 and optimize the lamp position following the instructions on Page 9–12, Section 11 entitled *Adjust the new xenon lamp* in the *Total AquaLog Manual* located on the laboratory server (CAWSC Lab (\\IGSWCAWWAS9902)\LAB\LAB DOCUMENTS\instrument eqpt manuals\Total AquaLog Manual.pdf).