

Canadian Light Source Inc.

User's Manual VESPERS

Guide to using the user interface.

Revised: April 26th, 2018

This document contains a basic guide on how to use the user interface on the VESPERS beamline.

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Opening The VESPERS User Interface

- 1) Open the User Interface by clicking the “User Interface” icon.
- 2) A window will appear prompting you to select a data output folder. Enter your proposal number (i.e. ##-####), which can be found on the front page of your permit displayed on the VESPERS – Beamline Health and Safety Information Centre. Once entered, a message will appear in green saying “Valid proposal number!”. After entering in your proposal number, click “Enter”. Alternatively, you can create your own pathway name. Once entered, a message will appear in black saying “New experiment!”.
- 3) The User Interface will open to the Endstation screen (See the Endstation Screen section on page 3 for more information).
- 4) A screen will appear asking if you would like to reset the sample stage positions (either H,V,N or X,Y,Z). Clicking “OK” will reset all stage positions to 0. Clicking “Later” will load the previously used stage positions. More information on the sample stage positions can be found “Persistent View” section on page 5.
- 5) Welcome screen: The Welcome screen will ask you to select your current run. Runs are used to organize your data for each visit to the facility. The default run for the VESPERS beamline is “VESPERS”. If you would like to organize your data in a different run, click “Add New Run”. You will be asked to select a facility (i.e. CLS VESPERS Beamline”) and “New Run Name”. After entering the run name, click “Enter”.

Important Note: After entering in your permit number (or pathway name), two “User Data” folders will be created: One on the local drive (i.e. the computer running the user interface) and one on a server. The User Interface will sync both folders every time you open it. DO NOT manually modify either folder (i.e. add or delete files from the “User Data” folder). If you have modified these folders, the message “both sides (network and local) have been modified” will appear and the user interface will not open.

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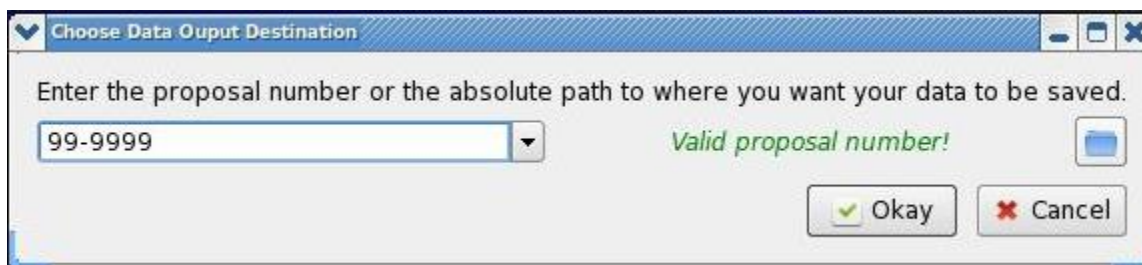


Fig. 1. Screen shot of the VESPERS user interface loading screen

Endstation Screen

1) The Endstation screen contains a cartoon with all of the pertinent detectors (i.e. 1 element Vortex detector, 4-element Vortex detector, and Pilatus area detector) and accessories (i.e. microscope, microscope light, and laser) pointing at the sample with a box that controls a motor to the right of the cartoon. There are buttons along the line of sight from the detectors and microscope to the sample that show the feedback position of that particular motor. If the button is clicked, the motor screen is updated to use the appropriate motor. Note that this means you can only move one detector at a time, and some of the motors will become inaccessible if other detectors are considered in a collision hazard (i.e. the Pilatus area detector and microscope). If this is the case the button will turn orange and if clicked will inform you of the collision hazard. Once the collision hazard is no longer possible, the button will return to a light gray color and once again be accessible. If the motor becomes inaccessible while trying to use it, the motor control box will turn gray and look disabled.

2) The button for the laser is slightly different where clicking it controls the power of the laser. When the laser is off, the laser symbol will be black and read OFF, and when it is on the laser symbol will be red and the feedback value should update as a green number. If the laser sensor value is invalid then the value will be -FFFFFF in red.

3) The microscope light is controlled by a combination of the button with a light bulb as the icon and the slider on the left of the cartoon. The slider controls the light intensity and the light bulb button turns the light bulb on and off. The slider position is saved when the light is turned off; turning the light back on will return the intensity to its previous intensity.

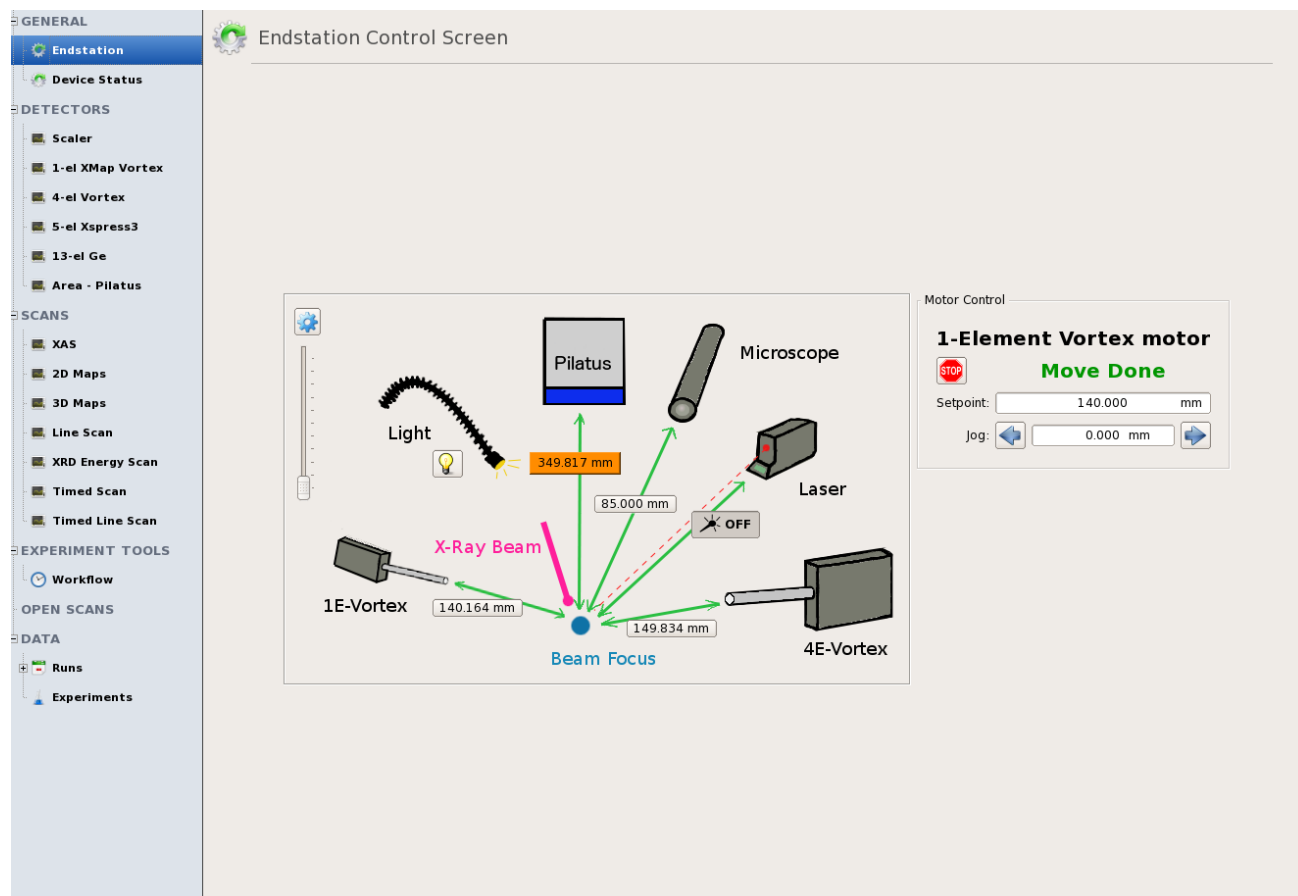


Fig. 2: Screen shot of the Endstation screen.

Persistent View (panel on the right side)

The persistent view is always visible and shows important aspects of the beamline that should always be visible and accessible. All of the pieces will be described from top to bottom.

1) The Disk Space Used bar is purely for informational purposes. Once the used disk space is greater than 80 %, the bar will appear red. Contact the beamline staff when the bar appears red.

2) The primary photon shutters for the beamline. These include two safety shutters and two photon shutters. There is beamline control over the last three shutters. As long as the hutches are locked, these shutters can be controlled by these buttons. The shutter is open when the button is green and closed when the button is red. Alternatively, you can use the Beam On and Beam Off buttons and they will do all the necessary work if they are able.

3) You can switch between the different beams by clicking on the appropriate button. The available choices are Pink, 10%, 1.6%, and Si. These are the $\Delta E/E$ of the different beams from the monochromator. The Si beam has a $\Delta E/E$ of 10^{-4} . The pink beam is the only exception to this because the beam contains all the available wavelengths the beamline has to offer simultaneously and does not use a monochromator.

4) When using the 10%, 1.6%, or Si beam, the energy selection becomes visible.

5) The intermediate slits are provided because they need to be adjusted when changing beams. When using the pink beam the slits should be $H = 0.100$ mm and $V = 0.100$ mm and if using any of the monochromated beams use $H = 0.800$ mm and $V = 0.800$ mm.

6) The sample stage allows you to move around your sample in the plane of the beam. You can move the stage by setting a jog size and use the arrow buttons to jog in the direction of choice. The left, right, up, and down arrows move in those directions on your sample (and the arrows moving in and out control the normal position of the sample). Moving the sample in the normal direction is how you get your sample into the focus of the beam. There is a status light on the top left that is on while the motor is moving and also the arrow buttons are disabled while the motor is moving. Alternatively, you can put in exact coordinates, if you know them. To manually enter the coordinates, click on the text box next to the coordinate you wish to set. This will prompt a pop-up window to appear. Enter in the coordinate number and select “Enter”. The motor will move in the desired direction. There is a status light next to each motor. When a particular motor is moving, the status light will appear red. When the motor is not moving, the status light will be green. There are many different sample stages to choose from in the drop down menu, but the two primary stages are “Sample Stage – H, V, N” and “Sample Stage – X, Z, Y”. Selecting “Big Beam

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–X, Z” will allow you to move the sample stage located upstream on the endstation. This sample stage can be used for big beam measurements. Whenever you switch between sample stages, you will be prompted to reset the sample stage. It is highly encouraged that you reset the stage; otherwise the result of the first move will be unexpected.

Note that the sample stage stops moving after you hit a hard motor limit. When you hit a hard limit, the “PID–Sample Stage Repair” button will appear and flash red. Press the repair button and you will be able to move the sample stage motor again. The repair button will also disappear after you press it. **After repairing the motor, remember to move the sample stage in the opposite direction of the one that triggered the repair button to appear.** Otherwise, you will continue to hit the hard motor limit and will have to repair the sample stage motor again.

7) The “Experiment Ready Status” light indicates whether all of the necessary components to setting up the beamline are setup correctly. If the light is green then everything is good to go.

8) The endstation section has a fast shutter that can be used to stop the beam as well as aluminum filters that can be used to attenuate the incoming beam. The filters can be placed with the overall thickness of the filters being anywhere between 0 μm to 800 μm in 50 μm steps.

9) Some general beamline status lights. From left to right, the status lights indicate the status of temperature, pressure, water, and whether all the valves are open or not. If any of these are red, contact the beamline staff.

10) There are four ion chambers located on the endstation: Split (Isplit), Pre-KB (Iprekb), Mini (Imini), and Post (Ipost). The Split ion chamber is located upstream on the endstation, in front of the filters and fast shutter. Pre-KB ion chamber is located behind the fast shutter and in front of the KB mirror box. The Mini ion chamber is located in front of the sample and behind the KB mirror box. A Post ion chamber is located behind the sample. For information on the ion chamber calibration, check out the Calibrating Ion Chambers section (see page 9).

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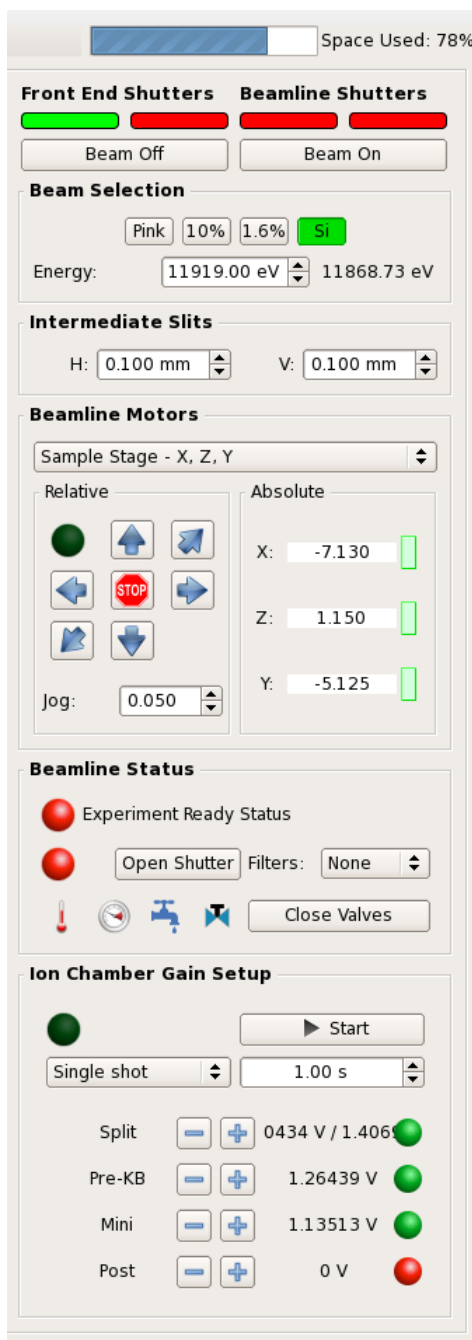


Fig. 3: Screen shot of the Persistent View panel.

Mounting And Focusing Your Sample

Step 1. Before mounting your sample, make sure all detectors are far away from your sample. This is to reduce the possibility of accidentally puncturing the windows at the front of the detectors.

Step 2. Mount your sample. Take care not to touch the detectors, camera, or microscope.

Step 3. Using the normal motor (on the persistent side view), get the laser sensor value to match the provided reference focus value. You should ensure that the sample is focused on the microscope.

Calibrate The Ion Chambers

Step 1 Open all shutters by clicking “Beam On” in the persistent view.

Step 2 Make sure the ion chambers are continuously collecting. Note that after a scan finishes, the scalers will not update (i.e. the scalers will be in “single shot” mode) To continuously update the scales, change “single shot” to “continuous”. You can also adjust the time that the scalers update by adjusting the dwell time. Note that you cannot change the dwell time when the scaler is in continuous mode. You must change the dwell time in single shot mode before switching to continuous mode. Alternatively, you can switch scaler modes by clicking on the scaler tab.

Step 3 Changing the gain: You can change the gain by using either the +/- buttons or using the drop down menus to set the gain explicitly.

Step 4 Proper calibration: The ion chamber is properly calibrated when the output is between 1.0 V and 4.5 V or the status light is green.

Notes about calibrating the ion chambers

There are many different views and ways to calibrate the ion chambers. They are meant to accommodate the various types of users and their familiarity with equipment of this type. The default view is simplified by having only the +/- buttons and the voltage displayed.

When using the +/- buttons and using the voltage view, use the + button when the voltage is less than 1.0 V and use the - button when the voltage is more 4.5 V.

When using the drop down menus and using either the status view or voltage view, change the value and units (order of magnitude selection) drop down menus until voltage is between 1.0 V and 4.5 V.

To switch between any of the views, right click on the split ion chamber value and select “Show sensitivity buttons”. To switch from voltage view to counts view, right click on the split ion chamber value and select “Show counts”. It is not recommended to use the counts view for calibration purposes.

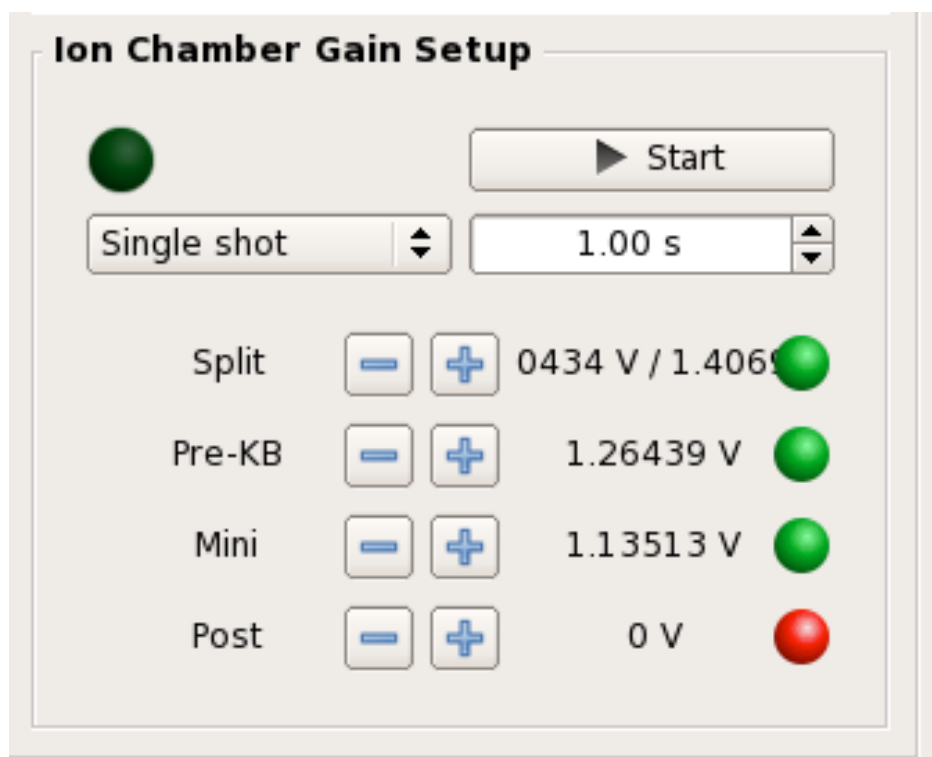


Fig. 4: Screen shot of the ion chamber calibration.

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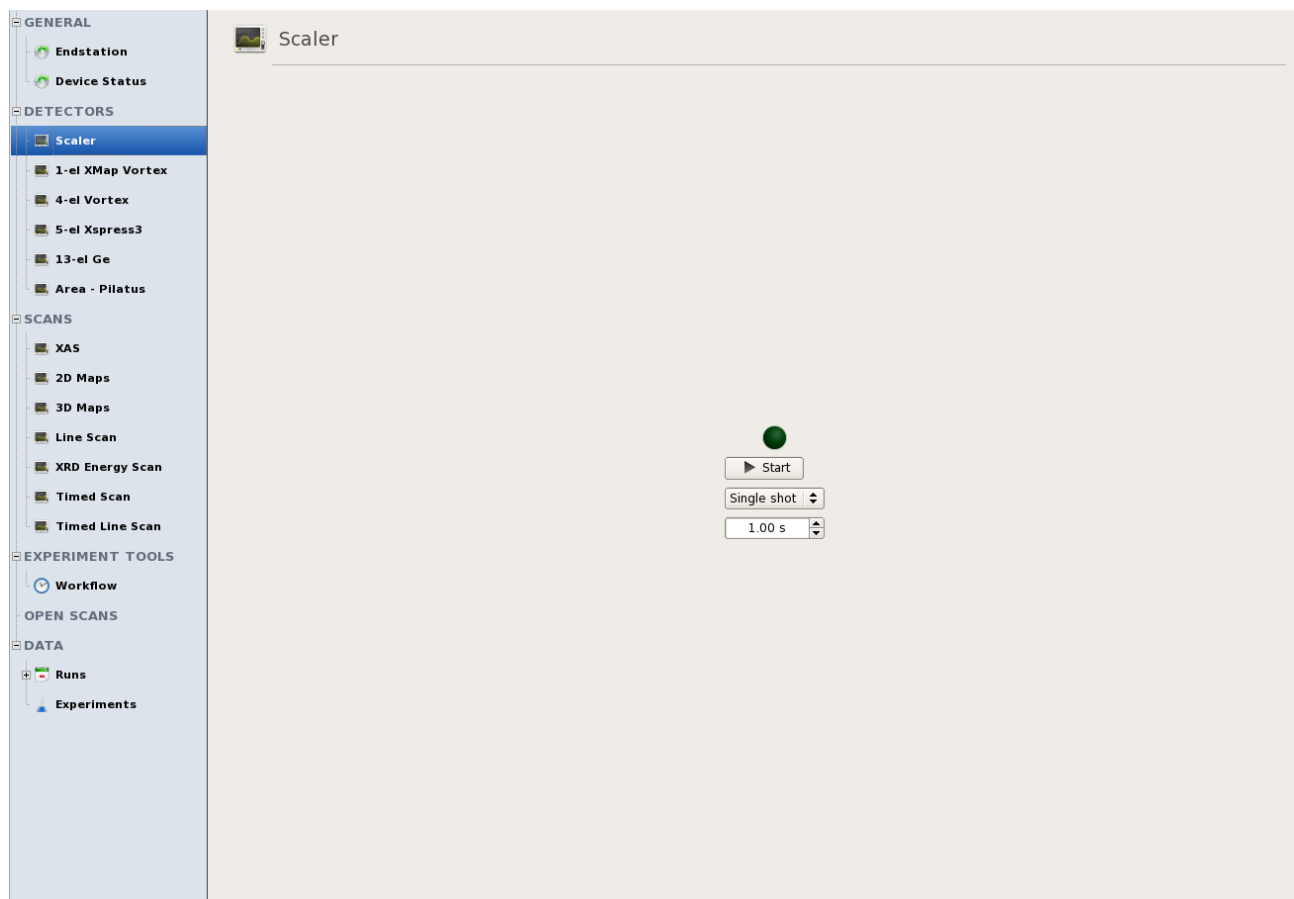


Fig. 5. Screen shot of the scaler set-up window

Setting Up The Fluorescence Detectors

Step 1. There are four fluorescence detectors available at VESPERS: 1-element XMAP Vortex (new 1-el XMAP Vortex screen), 4-element XMAP Vortex (4-el Vortex screen), 5-element Vortex (5-el Xspress3) and 13-element Germanium (13-el Ge). Consult with the beamline staff to know which detector to use for your experiment. Note that the 13-element germanium detector is only available for large beam experiments.

Step 2. Click “Beam On” to open all shutters.

Step 3. Collect a spectrum by clicking the “Acquire” button located to the left of the large window. The “Time” box located below the Acquire” button allows you to set the time you would like the detectors to accumulate counts. The default setting is 1 s.

Step 4. Make sure the Dead Time is under 30%. If the dead time is close to 0% or over 30%, move the detector closer or farther away (from the Endstation screen) and/or change the filter thickness (from the Persistent View screen).

Step 5. Add all the regions of interest (ROI). This is done by clicking on an element in the periodic table and then clicking on the check box beside each emission line that you want to add. For every emission line added, there is a semi-transparent green rectangle that shows up on the spectra plot that represents the width of the region.

Step 6. If the default widths are not quite accurate enough, you can edit them by clicking on the "Edit ROIs" button. This pops up a window that lets you customize the low and high value for each ROI.

Notes about using the Fluorescence detector screens

The plot that shows the spectra has a couple features that are worth noting. First, it is possible to zoom into the plot using either the mouse wheel and by clicking and dragging a box around the section of the plot you wish to zoom into. You can undo the zoom by right clicking the mouse anywhere on the plot. If you have performed multiple zoom actions, keep right clicking until the full spectrum can be viewed easily. Second, for each ROI you've added to the plot, there will be a corresponding semi-transparent green column over the data. If an element is currently selected in the periodic table (discussed later) and has a selected ROI, the green box turns purple. This provides quick identification of the ROIs that have been set for a particular element when many ROIs have already been set. Third, there are colored vertical lines that show the locations of every

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measurable emission line for the currently selected element in the periodic table. This provides a quick reference of which elements are being measured in the current spectrum very easily.

The periodic table has some features that should be mentioned as well. Many were alluded to in the previous section, such as semi-transparent green markers visually showing regions of interest after they have been added and showing all the current measurable emission lines for the current element. To be specific, the periodic table works off a "current element". Every time an element is clicked everything about the element is shown; whether it is in the element view to the right of the periodic table having boxes checked off for chosen ROIs, updating green plot markers to purple, or showing all of the measurable emission lines. Clicking on the element again will remove the measurable emissions lines from the spectrum. If you have multiple elements selected, you can remove all measurable emission lines by clicking the "Clear Emission Lines" button. If an element has an ROI selected, the button will change color from gray to either green for K-lines, yellow for L-lines, and teal for M-lines. This is to provide quick and easy at-a-glance information configured ROIs and what type of line it is. Any element buttons that are disabled cannot be measured on VESPERS. Although an individual element can be added or removed by using the check boxes, if you wish to just remove all ROIs and start over, click the "Clear Regions of Interest" button. Similar to the spectra plot, the element view to the right of the periodic table only lists emission lines that can be measured.

Here is some generic information about the detector information to the right of the spectra plot. The acquiring light is bright green when the detector is acquiring, otherwise it looks dark. The current elapsed and dead time is shown. The colored box (or four boxes if using the four element detector) changes color based on the dead time. If the dead time is under 30% then the box is green, between 30% and 50% it is yellow, and above 50% it is red. For the four element detector, clicking on a box will deactivate that particular channel. When deactivated, the coloured box will appear grey. When doing an experiment, the dead time should always be under 30%. Click on the log button to look at the spectra logarithmically. Click it again to return to a linear plot. Clicking on the Spectrum drop down menu shows any specific spectrum and the Show Multiple Spectra button will show every spectrum that is selected. The "Save Spectra" button saves the current state of the detector to a text file after choosing the name and location of the file.

The settings button shows two parameters that are customizable for advanced users. The two parameters are the peaking time and maximum energy. There is also a minimum energy, but this only changes the periodic table and does not affect any of the detector parameters. The "Show Pile Up Peaks" check box adds extra lines based on the current element and shows where pile up peaks would appear (a circumstance when the detector has a high dead time). The standard look shows where the typical pile up peaks would be for the current element, but you can also combine the current element with another element to see where combined pile up peaks might show up in the spectra. To choose the extra element, click on the "Combination Pile Up Peak" button and click on the element button. It will pop up a window with a periodic table on it, click on the

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element you wish to see combined with the current element and then extra pile up lines will be shown in the plot.

The "Edit ROIs" button pops up a window where every ROI can be customized if the default width of the region is not sufficient for your purposes. As you change the width, the associated green box in the plot will update automatically for easy reference.

Note that the 5-element Xspress3 detector is actually the 4-element and 1-element Vortex detectors using the Xspress3 detector electronics rather than the Xmap detector electronics. The top four colour boxes corresponds to the four detector channels of the 4-element Vortex detector and the bottom single colour box corresponds to the single detector channel of the 1-element Vortex detector. Users have the option to use only the channels associated with either detector when setting up a scan. When using the 5-element Xspress3 detector, you have to first activate the detector by clicking the "Initialize" button. Clicking the "Disarm" button will deactivate the detector. Once activated, you can collect XRF spectra the same way as with the other fluorescence detectors. Note that with the 5-element Xspress3 detector you do need to set the number of frames (i.e. spectra). The detector will disarm once the number of frames have been exceeded.

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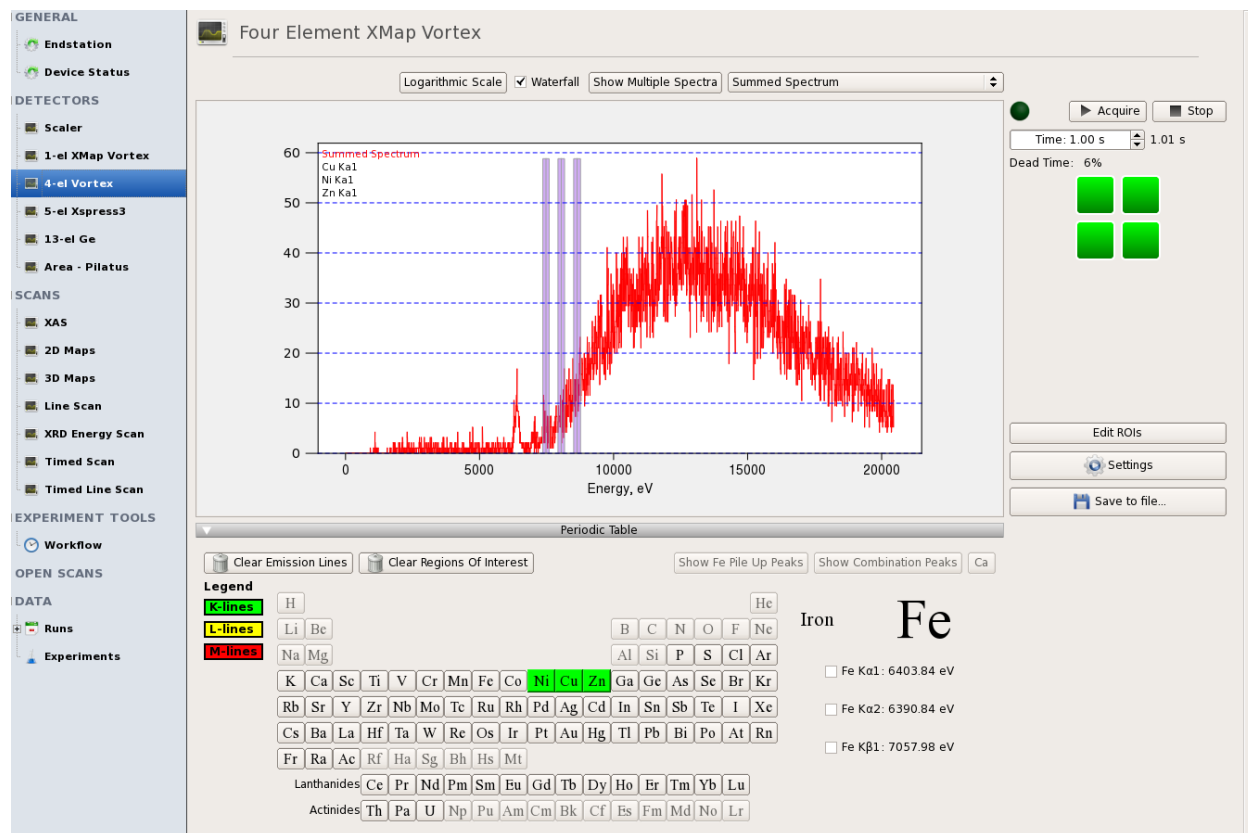


Fig. 6: Screen shot of the fluorescence detector configuration

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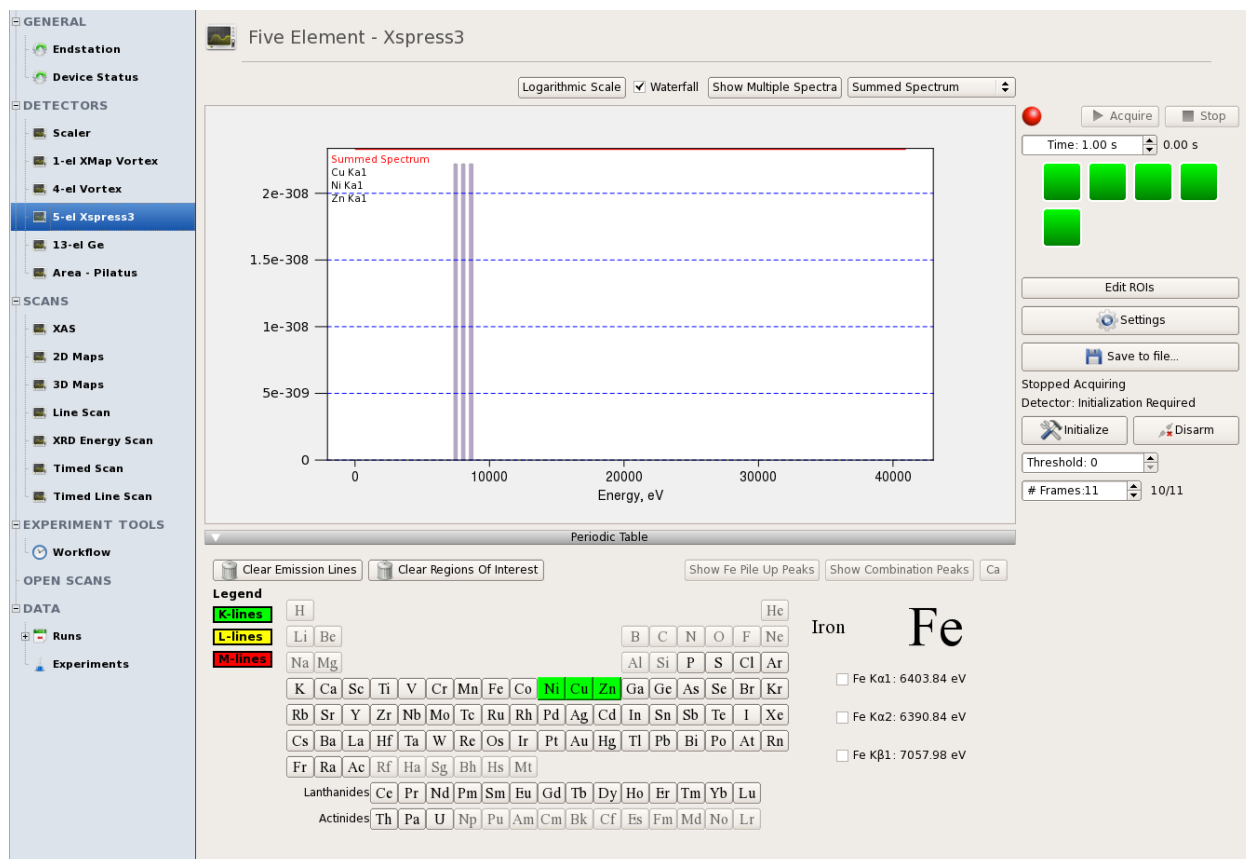


Fig. 7: Screen shot of the 5-element Xspress3 fluorescence detector configuration

Setting Up The Pilatus Pixel Array Area Detector

The control screen for the Pilatus detector is very simple. There are three primary areas of interest: one is the aurora file system, one controls the acquisition of a single image, and the last controls the path, file name, and file number for the images.

- 1) The aurora file system box is meant purely for information purposes.
- 2) The acquisition box is very straight forward. The top row contains the start and stop acquisition buttons and the acquisition status. The bottom row contains the box to change desired integration time as well as the elapsed time label. If the new file name conflicts with an existing image, then a warning message box will pop up asking if you wish to overwrite the name. If you want to change the name, click cancel and then update the file name or number from the boxes in the image file options box.
- 3) The image file options box contains the path, name, and number. The path is auto-set for you during the start-up of the user interface and the name and number are auto-set for you during the initialization of 2D maps, line scans, and energy scans. If you are taking single images, then you will need to manually change the name and number yourself.

Important: The path should always be of the form “/ramdisk/##-####/” where ##-#### is your proposal number. DO NOT ALTER THE PATHWAY.

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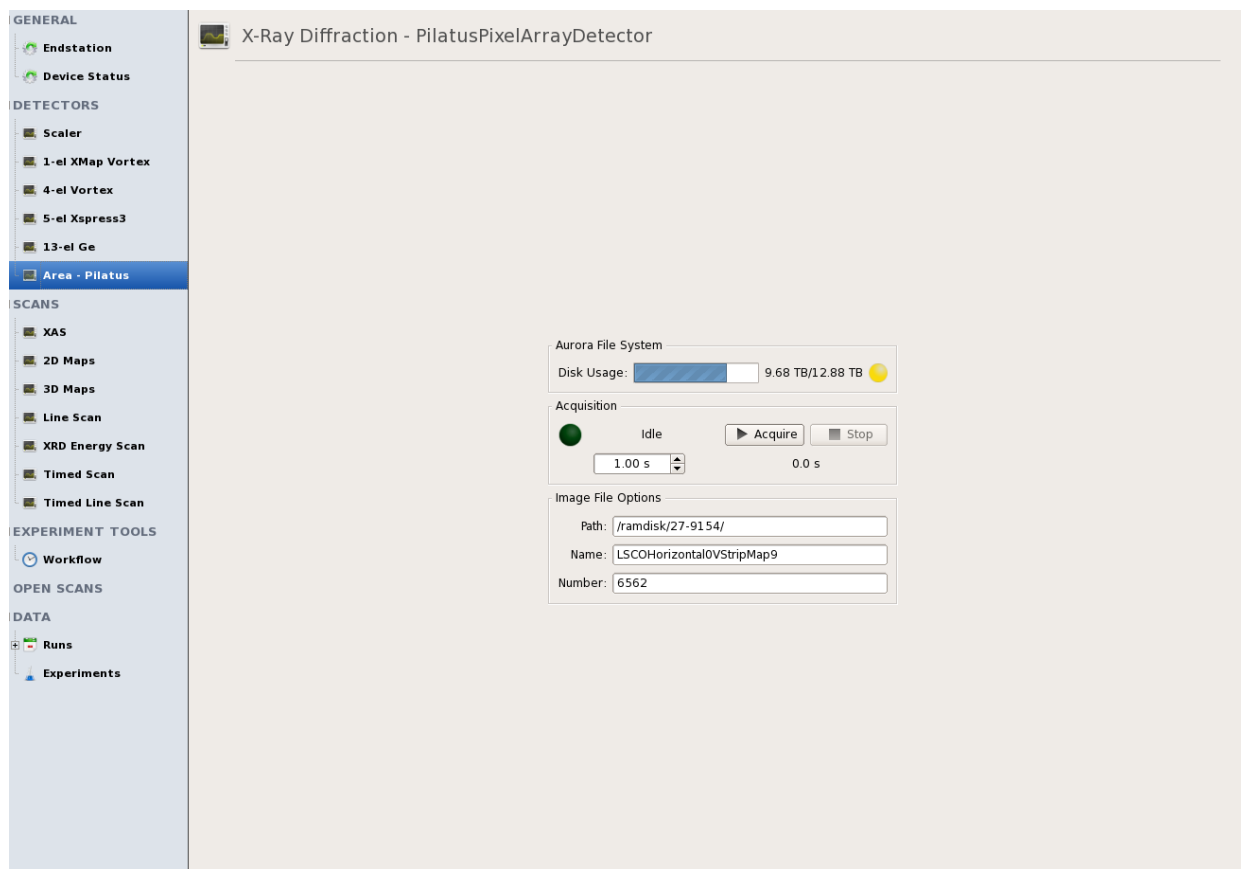


Fig. 8: The Pilatus pixel array area detector control screen

Setting up A XAS Scan

Step 1. Mount your sample and get it in focus (see page 9).

Step 2. Set up the fluorescence detector(s) (see page 12).

Step 3. Calibrate the ion chambers (persistent view panel) (see page 9).

Step 4 Set up the dimensions of the scan (XAS screen, under Scans):

a) Choosing the edge: Click on the button with the element symbol and choose which element you wish to scan. Then choose the edge you wish to scan from the drop down menu.

b) Setting the regions: Choose the start, end, step size, and time per point. These values are relative to the energy of the edge being scanned. If you wish to start from a standard XANES or EXAFS configuration, click on the "Default XANES" or "Default EXAFS" button. When modifying regions in k-space you need to make sure that the region you've added is a k-space region.

c) Choosing a fluorescence detector: Select the detector(s) you configured in Step 2.

d) Choosing I0: Select which ion chamber you would like to use as the default normalization ion chamber (I0). Imini is closest to the sample and is generally recommended for I0. However, if Imini is fluctuating too much or there are not sufficient counts, it is recommended to use Iprekb.

e) Choosing It: Select which ion chamber you would like to use as the transmission ion chamber (It). This will always be further downstream from whichever ion chamber was chosen for I0. If you change I0 after you choose It and It becomes invalid, the program will automatically move it to the closest valid ion chamber to avoid potential errors.

f) Choose a scan name: Name your scan whatever you wish. All exported data will begin with this name before any auto-indexing.

g) Having a predefined starting position: Enable "Update motor position automatically" to collect the XAS scan from the current motor position. If you want to manually set the motor position, ensure that "Update motor position automatically" is unchecked. Note that constantly updating the motor position automatically is the default option.

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h) Export options: In the “Export Option” box, check the “Export Spectra” box to export ASCII files of the XAS scan and the fluorescence spectra obtained from the fluorescence detector at each energy point. Selecting “Export data as columns instead of rows” will list the fluorescence spectra as columns.

i) After scan: After your scan has finished, you have the option to close the end station shutter and/or clean up the scales in the “After Scan” box. It is recommended to close the shutter to limit the risk of X-ray beam-induced damage.

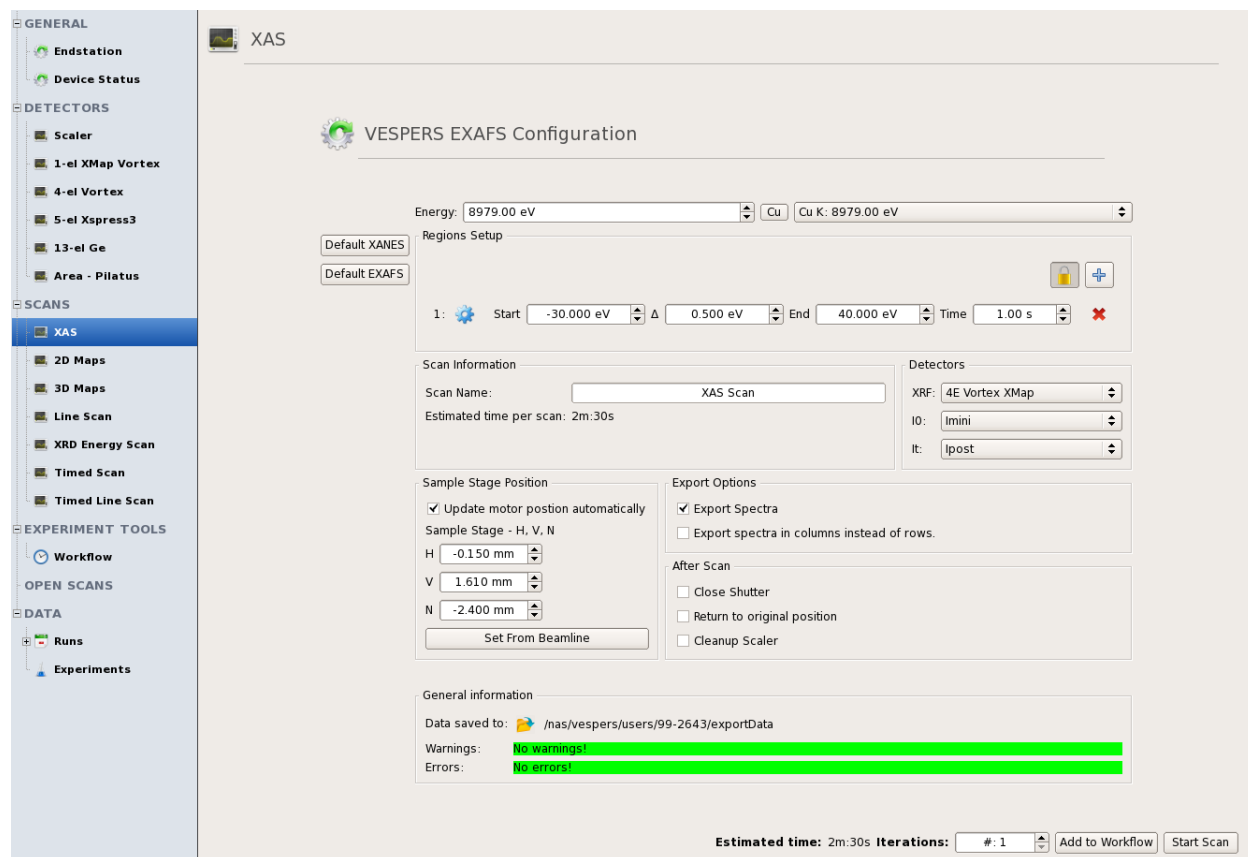
j) Choose the number of scans: If you wish to do a set of scans, set that number in the “Iterations” box. The default setting is 1. The estimated time will update based on the number of repeat scans you wish to do.

k) Starting the scan: If you wish to set up more than one scan, click “Add to Workflow” and then follow steps a) through j) again. More information on the Workflow can be found on page 31. If you wish to start your scan immediately, click “Start Scan”.

Step 5. See page 33 for notes on actions you can take while the scan is running.

Step 6. See page 38 for notes on actions to take after your scan has finished.

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The screenshot shows the 'VESPERs EXAFS Configuration' window. The left sidebar contains a tree view with categories: GENERAL (Endstation, Device Status), DETECTORS (Scaler, 1-el XMap Vortex, 4-el Vortex, 5-el Xspress3, 13-el Ge, Area - Pilatus), SCANS (XAS, 2D Maps, 3D Maps, Line Scan, XRD Energy Scan, Timed Scan, Timed Line Scan), EXPERIMENT TOOLS (Workflow), OPEN SCANS, and DATA (Runs, Experiments). The 'XAS' option is selected.

The main configuration area is titled 'VESPERs EXAFS Configuration'. It includes the following sections:

- Energy:** 8979.00 eV (Cu K: 8979.00 eV)
- Regions Setup:**
 - 1: Start: -30.000 eV, Δ: 0.500 eV, End: 40.000 eV, Time: 1.00 s
- Scan Information:**
 - Scan Name: XAS Scan
 - Estimated time per scan: 2m:30s
- Sample Stage Position:**
 - ☒ Update motor position automatically
 - Sample Stage - H, V, N
 - H: -0.150 mm
 - V: 1.610 mm
 - N: -2.400 mm
 - Set From Beamline
- Export Options:**
 - ☒ Export Spectra
 - ☐ Export spectra in columns instead of rows.
- After Scan:**
 - ☐ Close Shutter
 - ☐ Return to original position
 - ☐ Cleanup Scaler
- Detectors:**
 - XRF: 4E Vortex XMap
 - ID: Imini
 - It: Ipost
- General information:**
 - Data saved to: /nas/vespers/users/99-2643/exportData
 - Warnings: No warnings!
 - Errors: No errors!

At the bottom, the status bar shows: Estimated time: 2m:30s Iterations: # 1 Add to Workflow Start Scan

Fig. 9: Screen shot of the XAS scan configuration

Setting Up A 2D Map Scan

Step 1. Mount your sample and get it in focus (see page 9).

Step 2. Set up the fluorescence detector(s) (see page 12).

Step 3 Calibrate the ion chambers (right panel) (see page 9).

Step 4. Set up the dimensions of the scan (2D Maps screen, under Scans)

a) Setting the start position: The start position is the bottom left corner of the map. Move to the location you want to start the map by using the sample stage control on the persistent view panel. Once you have reached the correct location, click on the "Use Current" button. This will take the current motor coordinates and place them correctly into the boxes.

b) Setting the end position: The end position is the top right corner of the map. Like the start position, move to the location like in step a) that you want to end you map on and click "Use Current" button.

c) Setting the step size: Choose the step size for both horizontal and vertical dimensions. Once you've chosen your step size, the map size in micrometers and points will be displayed to give you an idea of the size of the map you've chosen.

d) Setting the dwell time: In the "Dwell Time" box, put the desired time you would like the detectors to accumulate per point. Combined with the map size, the "Estimated time per scan" will update to properly tell you how long the map you have set up will take to finish.

e) Optional: If doing X-Ray diffraction simultaneously with X-Ray fluorescence, make sure that "Pilatus" is chosen in the XRD selection menu. Make sure you have set up the Pilatus detector before starting (see Page 17).

f) Choosing a sample stage: Make sure that the selected sample stage matches the sample stage name in the persistent view panel on the right.

g) Choosing a fluorescence detector: Select the detector(s) you configured in Step 2.

h) Choosing I0: Select which ion chamber you would like to use as the default normalization ion chamber. Imini is closest to the sample and is generally recommended for I0. However, if Imini is fluctuating too much or there are not sufficient counts, it is recommended to use Iprekb.

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i) Choose a scan name: Name your scan whatever you wish. All exported data will begin with this name before any auto-indexing. If using the Pilatus detector, the name **CANNOT** contain spaces.

j) Export options: In the “Export Options” box, check the “ASCII” or “SMAK” boxes to export the 2D maps and X-ray fluorescence spectra. Note that the SMAK file format is only compatible with the SMAK software program. If you select the ASCII format, you have the additional option to export the X-ray fluorescence spectra files in columns rather than rows by checking the “Export data as columns instead of rows” box.

k) After scan: After your scan has finished, you have the option to close the end station shutter, clean up the scales, and/or go back to the start position in the “After Scan” box. It is recommended to close the shutter if you limit the risk of X-ray beam-induced damage.

l) Starting the scan: If you wish to set up more than one scan, click "Add to Workflow" and then follow steps a) through k) again. More information on the Workflow can be found on page 31. If you wish to start your scan immediately, click "Start Scan".

Step 5. See page 33 for notes on actions you can take while the scan is running.

Step 6. See page 38 for notes on actions to take after your scan has finished.

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GENERAL

Endstation

Device Status

DETECTORS

Scaler

1-el XMap Vortex

4-el Vortex

5-el Xpress3

13-el Ge

Area - Pilatus

SCANS

XAS

2D Maps

3D Maps

Line Scan

XRD Energy Scan

Timed Scan

Timed Line Scan

EXPERIMENT TOOLS

Workflow

OPEN SCANS

DATA

Runs

Experiments

2D Maps

VESPERS 2D Map Configuration

Positions

Start:

H: 0.000 mm

V: 0.000 mm

Use Current

End:

H: 1.000 mm

V: 1.000 mm

Use Current

Step Size:

H: 5.0 μ m

V: 5.0 μ m

Focus Position:

N: -2.400 mm

Set Normal

Map Size: 1000.0 μ m x 1000.0 μ m

Points: 201 x 201

Time

Dwell Time: 1.0 s

Scan Information

Scan Name: 2D Map

Estimated time per scan: 15h:42m:50s

Detectors

XRF: 4E Vortex XMap

XRD: None

I0: Imini

Stage: H & V

Export Options

☒ Ascii
 ☐ SMAK

☒ Export Spectra
 ☐ Export spectra in columns instead of rows.

After Scan

☒ Close Shutter
 ☐ Return to original position
 ☐ Cleanup Scaler

General information

Data saved to: /nas/vespers/users/99-2643/exportData

Warnings: No warnings!

Errors: No errors!

Add to Workflow

Start Scan

Fig. 10: Screen shot of the 2D map configuration

Setting Up A Spatial Line Scan

Step 1. Mount your sample and get it in focus (see page 9).

Step 2. Set up the fluorescence detector(s) (see page 12).

Step 3. Calibrate the ion chambers (right panel) (see page 9).

Step 4. Set up the dimensions of the scan (Line Scan screen, under Scans)

a) Setting the start position: The start position should be either the bottom or left point of the scan. Move to the location you want to start the line scan by using the sample stage control on the persistent panel. Once you have reached the correct location, click on the "Use Current" button. This will take the appropriate current motor coordinate and place it correctly into the configuration.

b) Setting the end position: The end position should be either the top or right point of the scan. Like the start position, move to the location that you want to end the scan on and click "Use Current" button.

c) Setting the step size: Choose the step size. Once you've chosen your step size, the scan size in micrometers and number of points will be displayed to give you an idea of the size of the scan you've setup.

d) Setting the dwell time: In the "Dwell Time" box, put the desired time you would like the detectors to accumulate per point. Combined with the scan size, the "Estimated time per scan" will update to properly tell you how long the scan you've set up will take to finish.

e) Optional: If doing X-Ray diffraction simultaneously with X-Ray fluorescence make sure that the Pilatus is chosen in the XRD selection menu. Make sure you have set up the Pilatus detector before starting (see Page 17).

f) Choosing a motor: Make sure that the selected motor matches the sample stage name in the persistent panel on the right.

g) Choosing a fluorescence detector: Select the detector(s) you configured in Step 2.

h) Choosing I0: Select which ion chamber you would like to use as the default normalization ion chamber. Imini is closest to the sample and is generally recommended for I0.

However, if Imini is fluctuating too much or there are not sufficient counts, it is recommended to use Iprekb.

i) Choosing It: Select which ion chamber you would like to use as the transmission ion chamber. The program prevents you from selecting a transmission ion chamber that is upstream from I0.

j) Choose a scan name: Name your scan whatever you wish. All exported data will begin with this name before any auto-indexing. If using the Pilatus, the name **CANNOT** contain spaces.

k) Export options: In the “Export Options” box, check “Export spectra” to export the line scan and X-ray fluorescence spectra. Checking “Export data as columns instead of rows” will export the spectra as columns.

l) After scan: After your scan has finished, you have the option to close the end station shutter, clean up the scales, and/or go back to the start position in the “After Scan” box. It is recommended to close the shutter if you limit the risk of X-ray beam-induced damage.

m) Starting the scan: If you wish to set up more than one scan, click "Add to Workflow" and then follow steps a) through i) again. More information on the Workflow can be found on page 31. If you wish to start your scan immediately, click "Start Scan".

Step 5. See page 33 for notes on actions you can take while the scan is running.

Step 6. See page 38 for notes on actions to take after your scan has finished.

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Line Scan

VESPERS Line Scan Configuration

Positions Start: 0.000 mm [Use Current] End: 1.000 mm [Use Current] Step Size: 5.0 μ m Vertical motor, V: 1.610 mm Focus Position: N: -2.400 mm [Set Normal] Scan Size: 1000.0 μ m Points: 201	Detectors XRF: 4E Vortex XMap XRD: None IO: lmini It: lpost Stage: H
Time Dwell Time: 1.0 s	Export Options <input checked="" type="checkbox"/> Export Spectra <input type="checkbox"/> Export spectra in columns instead of rows.
Scan Information Scan Name: Line Scan Estimated time per scan: 4m:50s	After Scan <input checked="" type="checkbox"/> Close Shutter <input type="checkbox"/> Return to original position <input type="checkbox"/> Cleanup Scaler
General information Data saved to: /nas/vespers/users/99-2643/exportData Warnings: No warnings! Errors: No errors!	

Add to Workflow Start Scan

Fig. 11: Screen shot of the line scan configuration

Setting Up An Energy Scan

Step 1. Mount your sample and get it in focus (see page 9).

Step 2. Set up the Pilatus detector (see page 17)

Step 3. Set up the dimensions of the scan (Energy Scan screen, under Scans)

a) Setting the regions: choose the start, end, step size, and time per point. These values are in absolute energy units.

b) Choosing a XRD detector: Very easy since the only option is the Pilatus.

c) Choose a scan name: Name your scan whatever you wish. All exported data will begin with this name before any auto-indexing. If using the Pilatus, the name **CANNOT** contain spaces.

d) Having a predefined starting position: Enable "Update motor position automatically" to collect the XAS scan from the current motor position. If you want to manually set the motor position, ensure that "Update motor position automatically" is unchecked. Note that constantly updating the motor position automatically is the default option.

e) Starting the scan: If you wish to set up more than one scan, click "Add to Workflow" and then follow steps a) through d) again. More information on the Workflow can be found on page 31. If you wish to start your scan immediately, click "Start Scan".

Step 5. See page 33 for notes on actions you can take while the scan is running.

Step 6. See page 38 for notes on actions to take after your scan has finished.

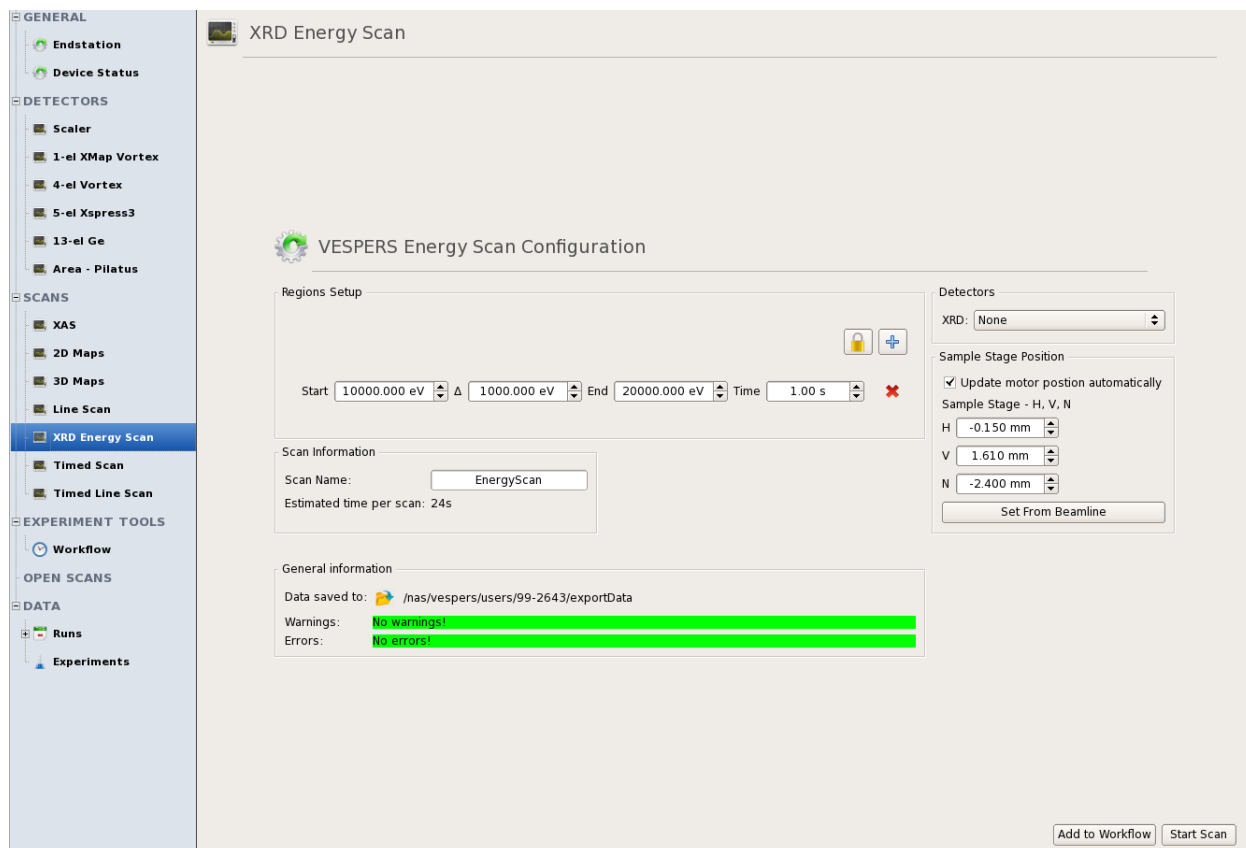


Fig. 12: Screen shot of the energy scan configuration

Additional Scans

Additional scans (Timed Scan, Timed Line Scan, 3D map) are available at VESPERS. Consult with the beamline staff if you would like to know more about these features.

The Workflow and Bottom Bar

Workflow

The workflow is a system where multiple scans and other actions may be setup in advance to perform many tasks in sequence. Whether this is having a couple small maps consecutively or setting up many XAS scans on different edges on a sample, this is where they are configured and executed from. There are three primary components to the workflow: completed actions, the current action, and upcoming actions.

1) The completed actions section shows a list of all actions you have ever done on the beamline. For every action that was performed, it shows the name and a short description, the status of the action, when it finished, and how long it took to run. The status will be either a green check mark, an orange x, or red exclamation point. Each is associated with the final state the action ended in. The green check mark denotes that the action completed successfully, the orange x denotes that the action was cancelled, and the red exclamation point denotes that the action failed. To anchor your eye, the entire row is colored with the same color for quick reference. Finally, every action that is in the completed action list can be added to the upcoming action list by right-clicking on the action you wish to re-run and choose "Re-run this action". This will add an exact copy of the action to the end of the current list.

2) The current action section provides information on the action currently being run. It shows the name and a short description of the action. It shows the current progress as well as some buttons that can change the state of the action. Every action can be cancelled, and some actions may be paused or skipped. Cancelling the action stops as soon as it is able and also stops the workflow from proceeding. If actions can be paused, then it will stop and wait as soon as it can after you click the pause button. It will remain paused until you click the resume button. Skipping an action is analogous to something being "good enough". If you are doing a scan and it is sufficient and you just want to move onto the next scan, clicking skip will stop the scan (there may be different options for skipping based on the action) as requested and do any standard clean up that is typical of that action and then the workflow will proceed with the next action. This is an important distinction for scans because the successful scans automatically export their data and cancelled scans do not. Therefore, by clicking skip, you are artificially telling the scan that it has completed successfully and it will automatically export the data as expected.

3) The upcoming actions section holds a list of actions that have been prepared to run in the workflow. These actions can be rearranged by dragging and dropping and can be customized up until they are started in the current action piece. You can also copy or delete any actions you've already added to the list. Clicking the big blue button that says "Click to start" starts the workflow.

It then changes to a green color says "Click to stop". If you choose to stop the workflow, the next action will not be loaded into the current action section once the current action finishes. You can customize any action that is in the upcoming actions section by double clicking on the action.

4) Clicking "Add Action" in the top right corner of the Workflow screen will bring up a number of actions that you can add to the workflow. Select the desired action and click the "Add to Workflow" button. The action can also be added to the workflow by double clicking on the desired action. Actions that can be added to the workflow are:

a) Loop: Repeats a set of sub-actions. When added to the workflow, drop and drag actions inside it. Select the number of repeats by double clicking on the Loop action.

b) Sequential List: Runs a list of sub-actions. When added to the workflow, drop and drag actions inside it.

c) Control Move: Moves a motor control to an absolute or relative position. When added to the workflow, double click on the control move to select the control you wish to move (i.e. sample stage, energy, etc.). Enter in control move value. If you would like to make a move that is relative to the current position, make sure "Relative Move" is selected.

d) Parallel List: Run a number of actions in parallel to each other. When added to the workflow, drop and drag actions inside it.

Bottom Bar

The bottom bar provides a simplified view of the current action section of the workflow. The advantage being that the bottom bar is visible regardless of what you are doing in the user interface. You will always have knowledge of what is currently running and have the ability to pause, skip, or cancel the action. It also provides a progress bar for quick reference as well. Note that if your current action is a XAS scan, you can change the number of repeat scans you are collecting from the bottom bar.

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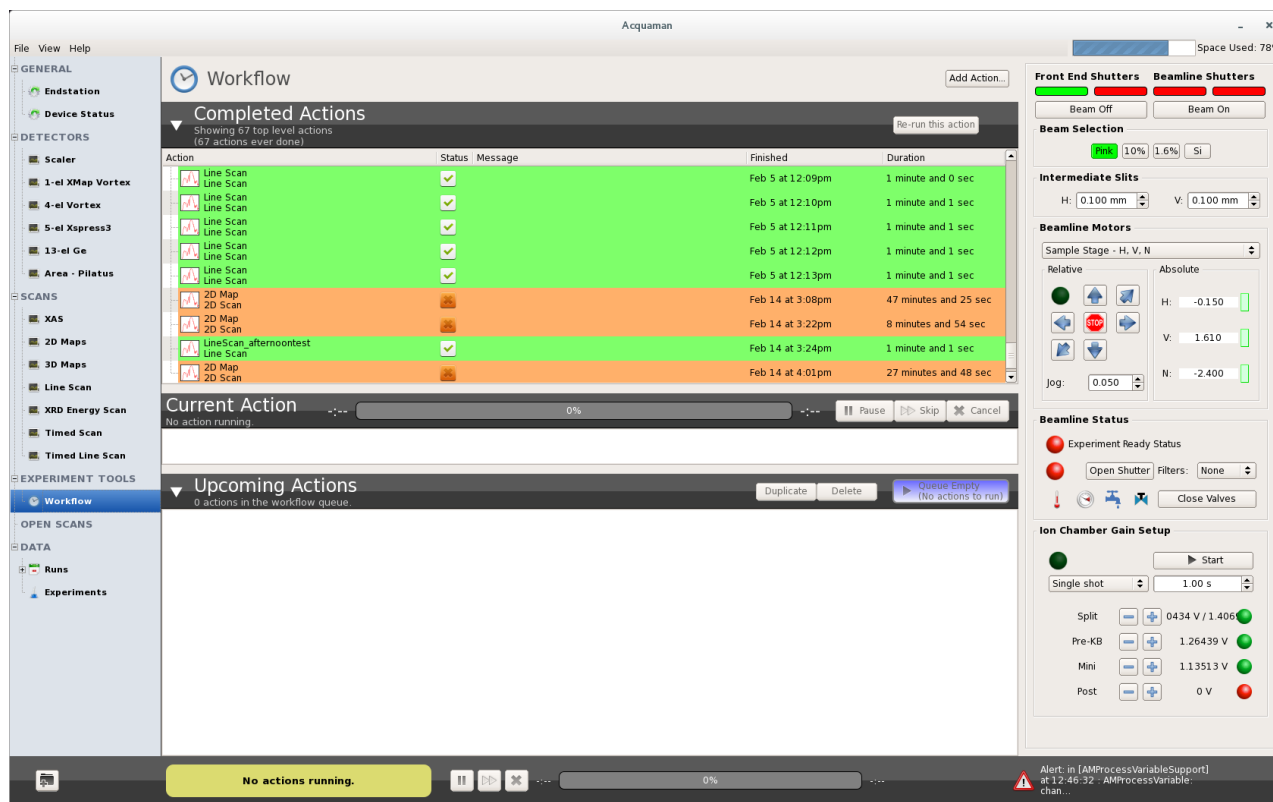


Fig. 13: Screen shot of the workflow and the bottom bar.

While A Scan is Running

Viewing your scan (XAS, Line scans, Energy scans):

When the scan starts you will be brought to a new screen that has a large window in the center where the data from the scan will appear. There will be many curves that will be in your scan which you can change by clicking the buttons immediately under the plot that have names like "CuKα1" or "norm_CuKα1". This lets you quickly look at different curves. Alternatively, the different curves are accessible in the "Data Set" box located to the left of the large window. Clicking the "Add Analysis Tool" box allows you to add additional curves (i.e. derivative curves, 2D summing) to the data set.

There are four different viewing modes (accessible by clicking one of the four icons at the bottom left of the plot): exclusive mode (the default), show multiple data sources mode, show multiple data sources for each open scan mode, and show similar data sources from different scans together. The last two require more than one scan open in the editor to be useful, but there is no negative impact if you choose one of those modes when looking at only one scan.

There are some viewing options that can be played with such as "Show at same scale" (enable/disable normalization) and setting up a waterfall plot.

The four icons at the top left of the plot allows you to select the plot you want to display (Plot Selector), display the energy for a specific data point (Data Selector), drag and zoom a region of the plot (Drag Zoomer), and use the mouse wheel to zoom in and out of the plot (Wheel Zoomer). If you click on the "Show Spectra" button, another window will pop up. If you click on a specific point on the plot using the data position button, the corresponding spectrum for that energy position will be displayed in the window. If you click on any of the non-grayed out element buttons, the available emission lines will be displayed on the plot as well. This will help to guide your eye as to what peaks are associated with what element.

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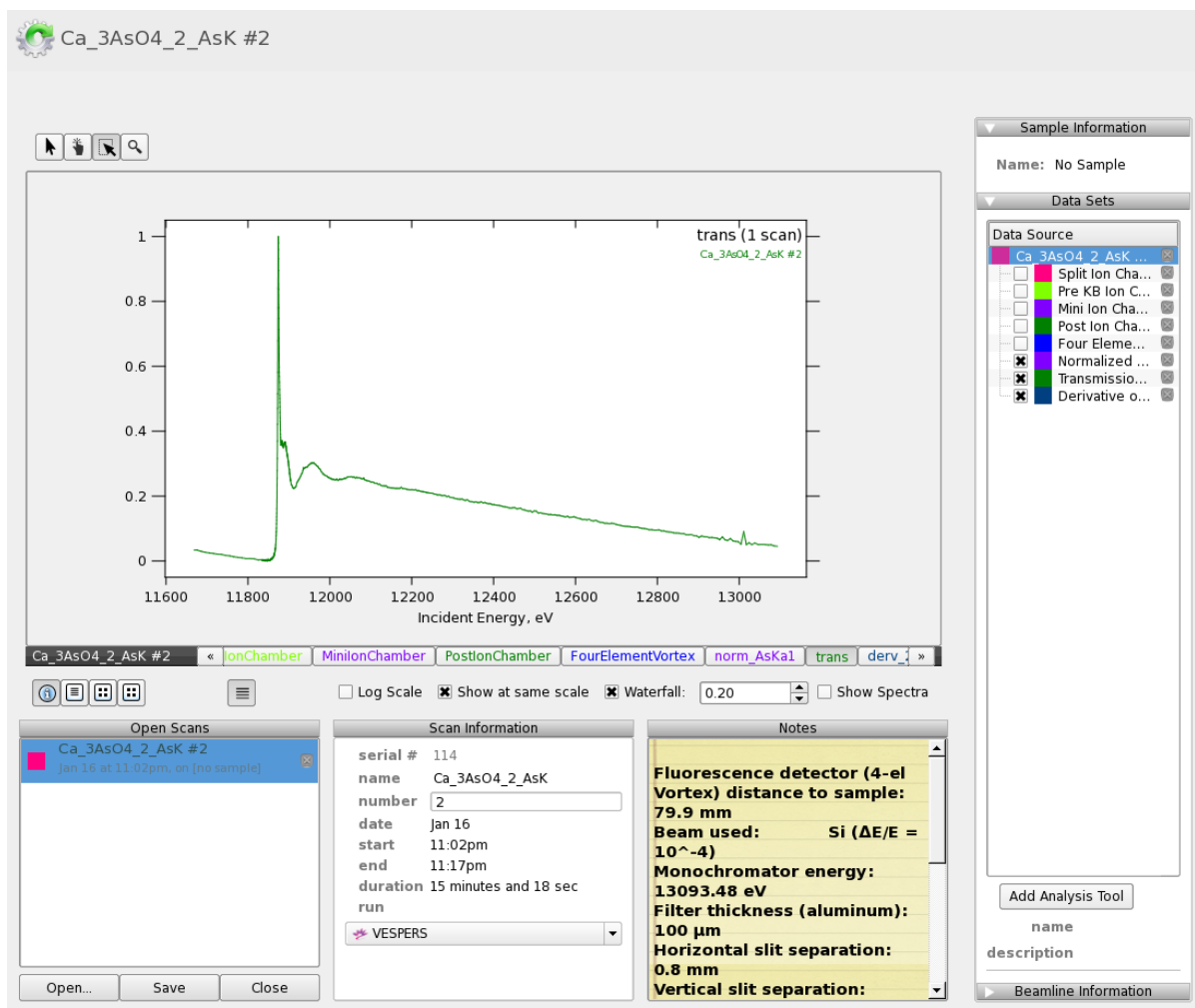


Fig. 14: Screen shot of an open XAS scan.

Viewing your scan (2D maps):

When the scan starts you will be brought to a new screen that has a large image in the center and another popup screen with many small images inside. The big image is an enlarged version of a particular map. You can change the image by clicking on the buttons immediately under the image that will have names like "ZnK α 1". This allows you to easily look at any individual map. Alternatively, the different images are accessible in the "Data Set" box located to the left of large window. Additional 2D maps can be created by clicking on the "Add Analysis Tool" button. You can create a normalized 2D map using a different Io than the one used when configuring the 2D map scan (2D map normalization) or create a 2D map using a new ROI (3D Binning) Note that the coloured scale bar (located to the left of the image) will update automatically and corresponds to the minimum (blue) and maximum (red) signal of your map. Double clicking on the scale bar also you to manually adjust the minimum and maximum the scale of the selected map.

The other window shows you all of the regions of interest at a glance. They are all labeled with the name of the region of interest emission line (e.g.: "ZnK α 1") for easy identification. You can increase or decrease the number of images shown simultaneously by clicking on a name at the bottom of that window. All the buttons that look "Pressed" are already selected and are currently being shown.

If you click on a particular pixel on the big image, the coordinates and intensity value are displayed for that pixel. You can highlight a specific region of the map by clicking and dragging the cursor over the area. There is an option to collect a 2d map scan within the highlighted region by right-clicking on the plot and selecting ("2D Map Scan").

If you click on the "Show Spectra" button, another window will pop up. If you click on any pixel, the corresponding spectrum for that pixel will be displayed in the window. If you click and drag a box around a particular area of the image, the spectrum with sum together the spectra of all pixels in the highlighted region. The list of available spectra is shown is shown on the right side of the window. This list will include the summed dead time corrected XRF spectrum and the raw XRF spectra of each detector channel. For every box you check off there will be an extra spectrum shown simultaneously. Note that the more spectra that are shown simultaneously, the slower the updates might be. If you click on any of the non-grayed out element buttons, the available emission lines will be displayed on the plot as well. This will help to guide your eye as to what peaks are associated with what element. There is an option to select pile-up peaks for different combinations of elements. Greyed out element buttons become available by adjusting the minimum and maximum energies in the bottom right side of the window.

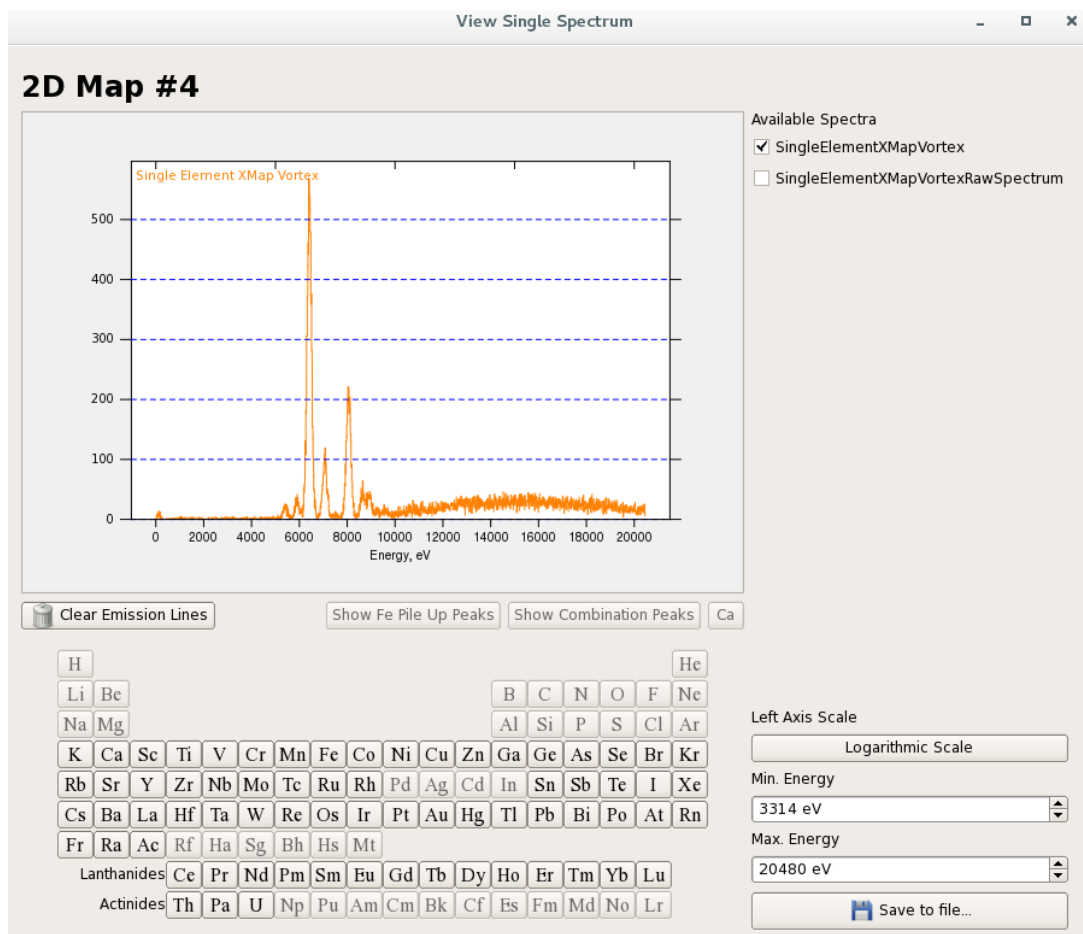


Fig. 15: Screen shot of the pop-up XRF spectrum window.

Pausing/Stopping

You can pause or stop your scan from either the workflow or the buttons in the bottom bar. The button with an "x" is the cancel button, and the button with two vertical lines is the pause button. If paused, the icon on the button will turn into an arrow and becomes a resume button. In the event of a beam dump, the scan will automatically pause.

Cancelling the scan does not cause your data to be exported and also stops the workflow from proceeding. See below for more information on this topic.

You can stop your scan where it is (if a 2D map, you can also stop at the end of the line) if you feel your scan is good enough as it is by clicking on the double arrowed button and choosing "Stop now" (or if 2D, "Stop at the end of line" is also an option).

Important notes about stopping your scans: Your data is automatically exported from the program whenever a scan **successfully** finishes. This is either when the scan finishes as configured or you click the double arrow button. If you cancel your scan, your scan is stopped and not exported. The data still exists and can be exported manually from the "Runs" screen at any time.

Runs screen:

This screen gives you an "at a glance" view of all the scans you have collected at the beamline. You can change the view of the scans in the run screen (i.e. thumbnail, detailed list, etc.) by clicking on one of the three boxes found in the top right corner. You may look at any old scans you have collected by double clicking on the icon or by selecting a scan and then clicking on the "Edit" button (bottom left corner). The scan will appear under the "Open Scans" tab. You can also export scans from the run screen by clicking on the "Export" button (See "After A Scan Has Finished" on page 37 for more details). The search for specific scans by clicking on the "Search" button located in the top left corner.

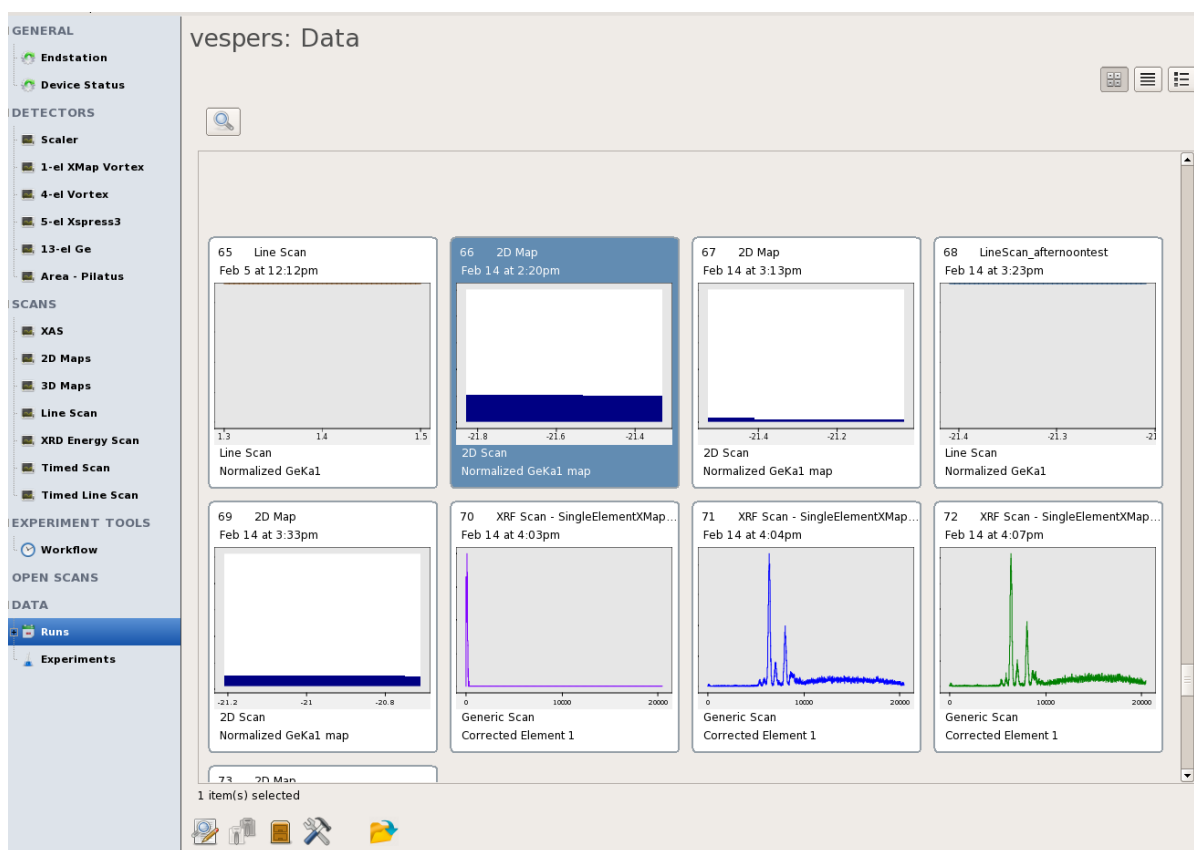


Fig 16. Screen shot of the Run screen

After A Scan Has Finished Exporting Data

Once the scan finishes, it will automatically export the data if you selected the export option when setting up your scan. If you have cancelled a scan or wish to export the data in a different file format, you can manually export the data from the “Runs” screen. Highlight the scan(s) you would like to export and click on the “Export” button near the bottom of the screen. Alternatively, right-click on the scan and select “Export”

A window will pop up prompting you to select export file location and format. File formats include XDI Specifications (XAS ASCII text file), Athena Style (XAS), VESPERS 2D Map Style, VESPERS SMAK 2D Map, and VESPERS Line Scan Style. Once you select the desired format, click “Next”. Users have the option to alter the file format template. For example, users can alter the header, the number of data sets included in the exported file, the layout, and file name. It is recommended that you use a standard template when exporting a file. Once you have selected the format, click “Next”.

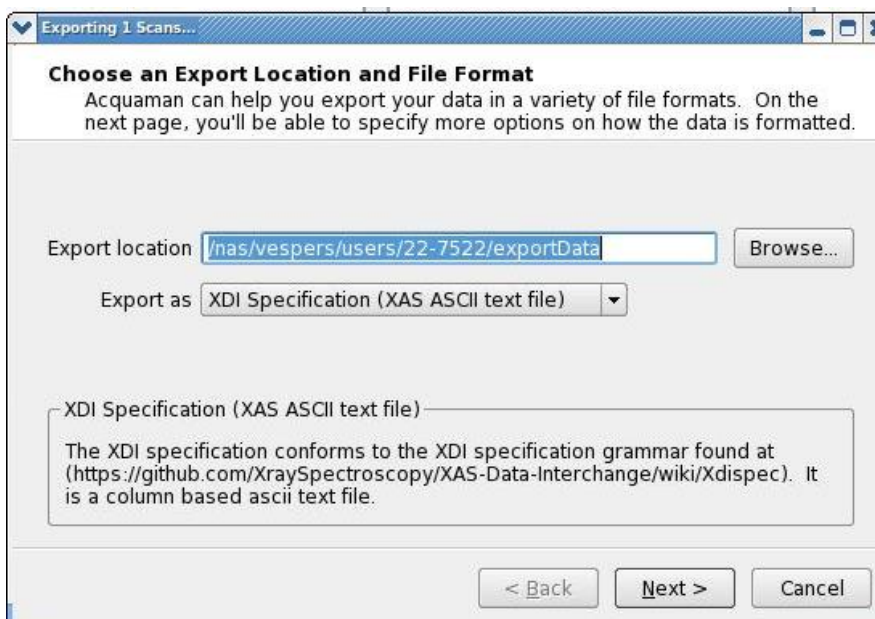


Fig. 17. Screen shot of the Export Data screen

2D Map scans ONLY

On the big image view, if you click on a pixel to see the current position and value. After you've done this, you can right-click anywhere on image and a popup menu will give you the following options:

a) Setup XANES scan: Does about 80% of the setup for a standard XANES scan. Chooses the edge, selects the appropriate fluorescence detector and uses some default region positions for XANES.

b) Setup EXAFS scan: Does about 80% of the setup for a standard EXAFS scan. Chooses the edge, selects the appropriate fluorescence detector and uses some default regions for EXAFS.

c) Setup Energy scan: Does most of the setup for an Energy scan.

d) Go To Immediately: Immediately moves the sample stage to that location.

e) On the big image view, you can click and drag a box over any area of the map. After you've done this, right click on the image and another option becomes available, "Setup 2D map". This takes the coordinates from the box and sets the start position, end position, and time. The defaults the step size to 5.0 μm in both directions. It also transfers over which detector(s) you were using, the choice for IO, and the name. If you did XRD simultaneously, this is also transferred over.