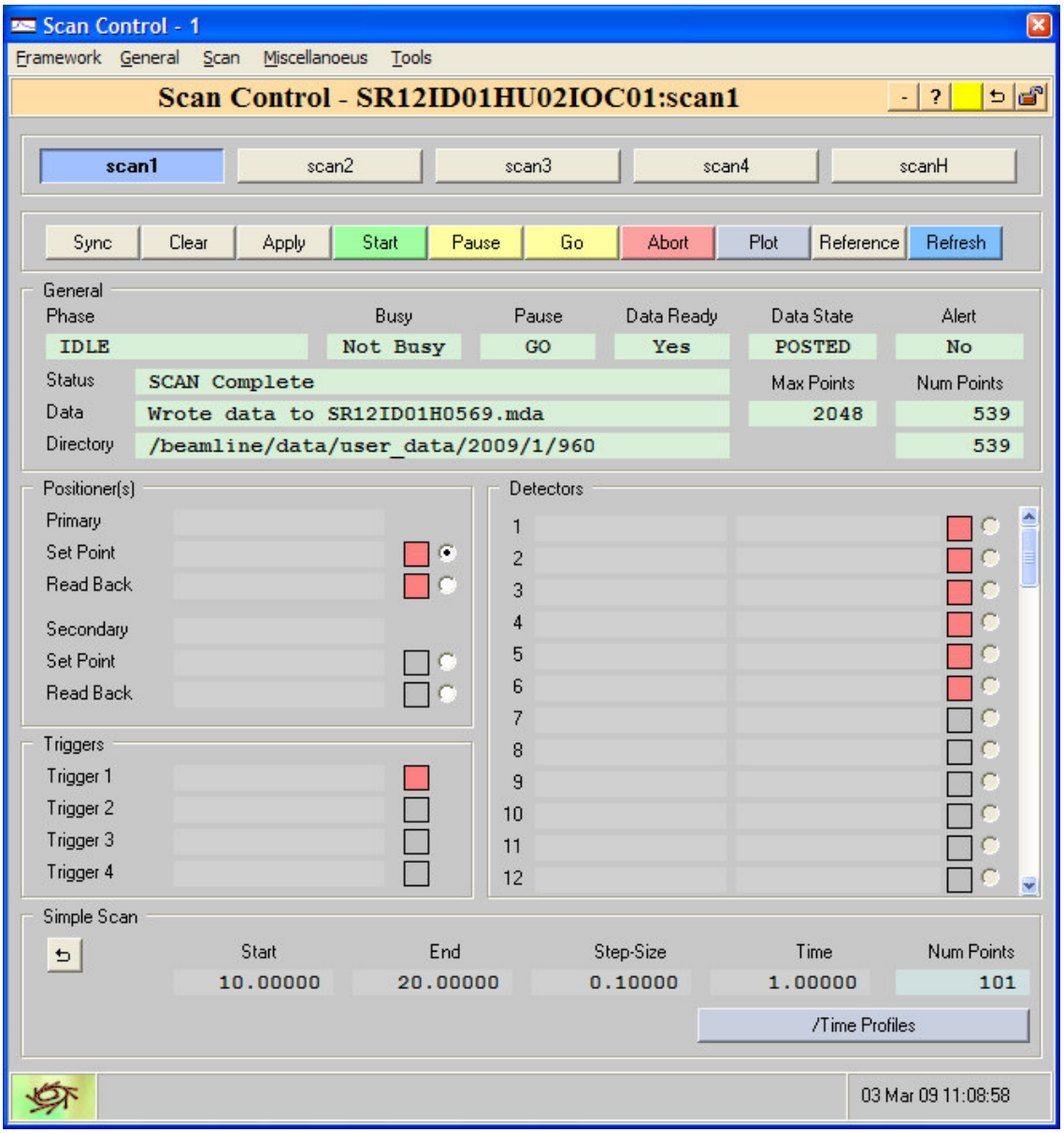
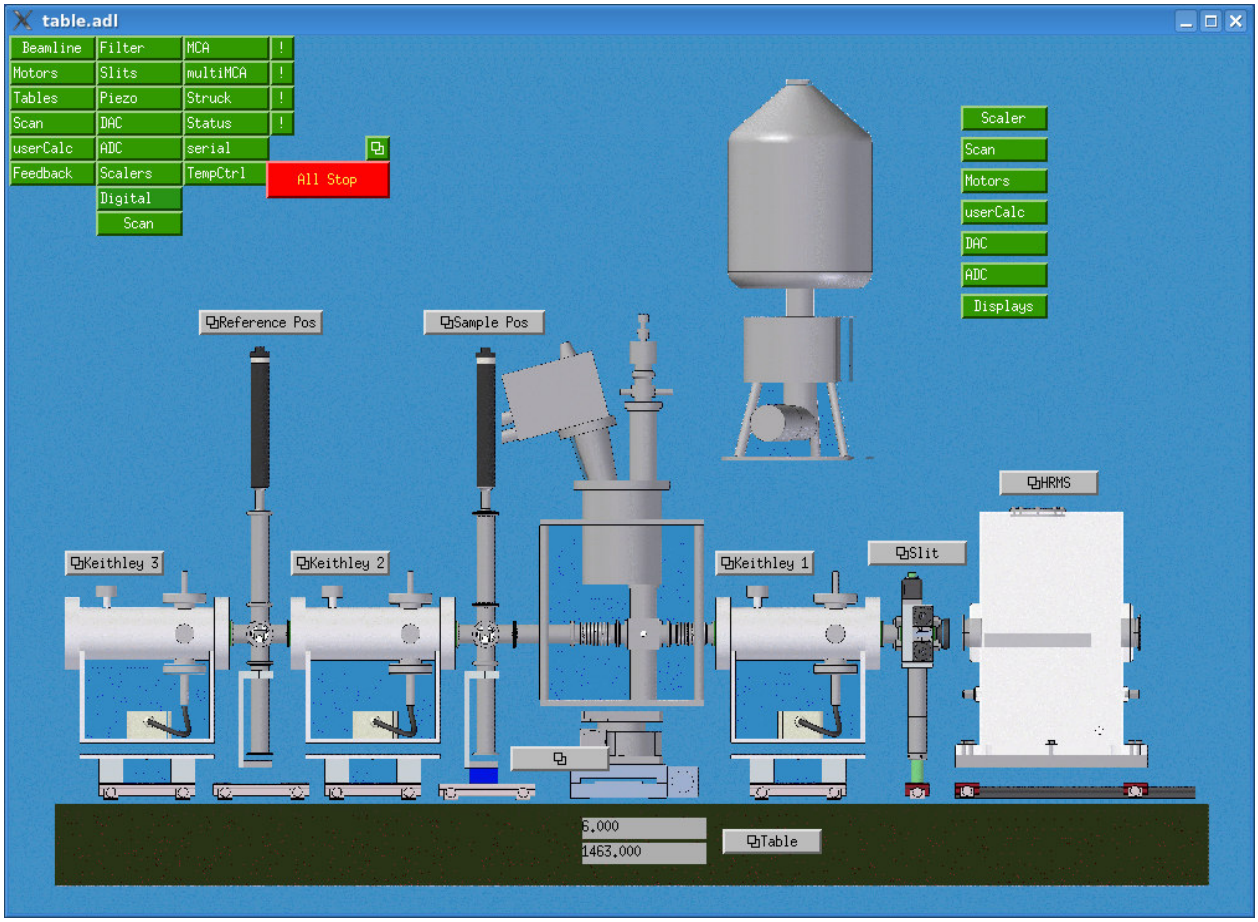
XAS software

To run a XAFS spectrum you need to use the scan control program. See below:



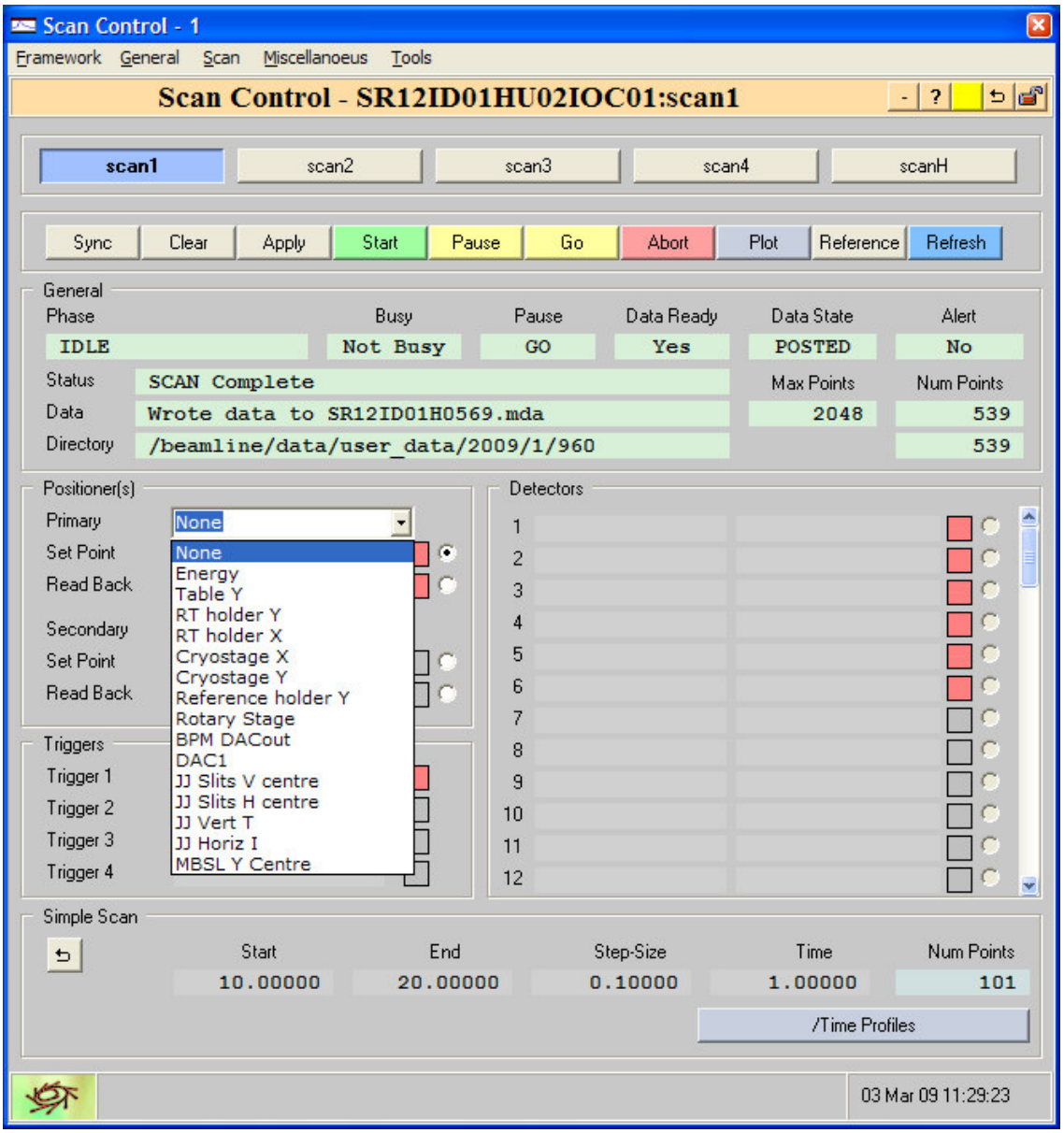
You will also need the XAFS endstation GUI to do basic operations before running the spectrum: centre the sample, upload the right positions for the sample holder and adjust the gains of the keithleys.



You can find these interfaces, already opened, in the pc, labelled PC1.

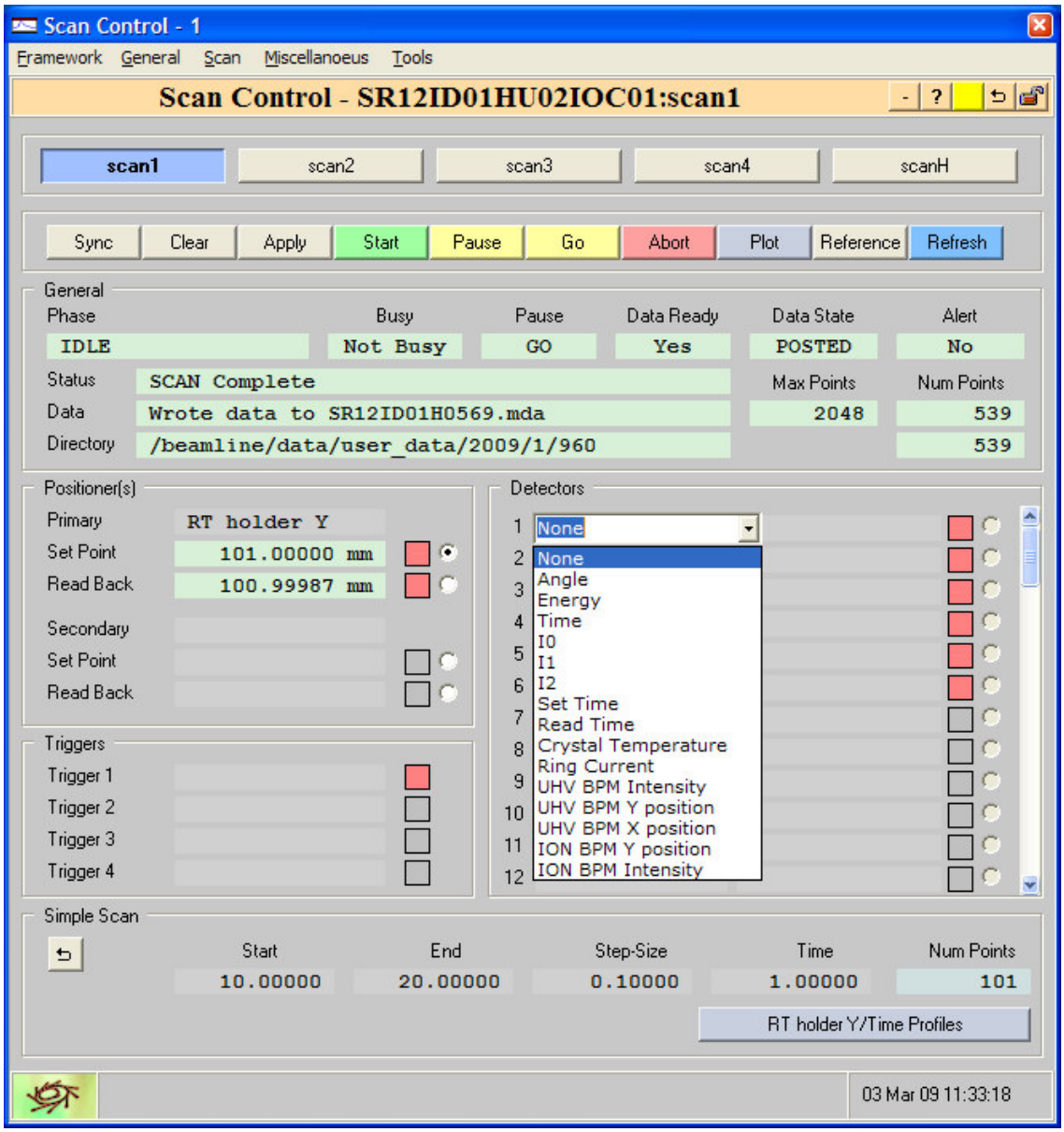
To acquire correctly the spectrum you need to follow these steps:

- **Centre your sample**
    - Go to the scan control program.
    - Left-click on ‘positioner(s) – Primary’



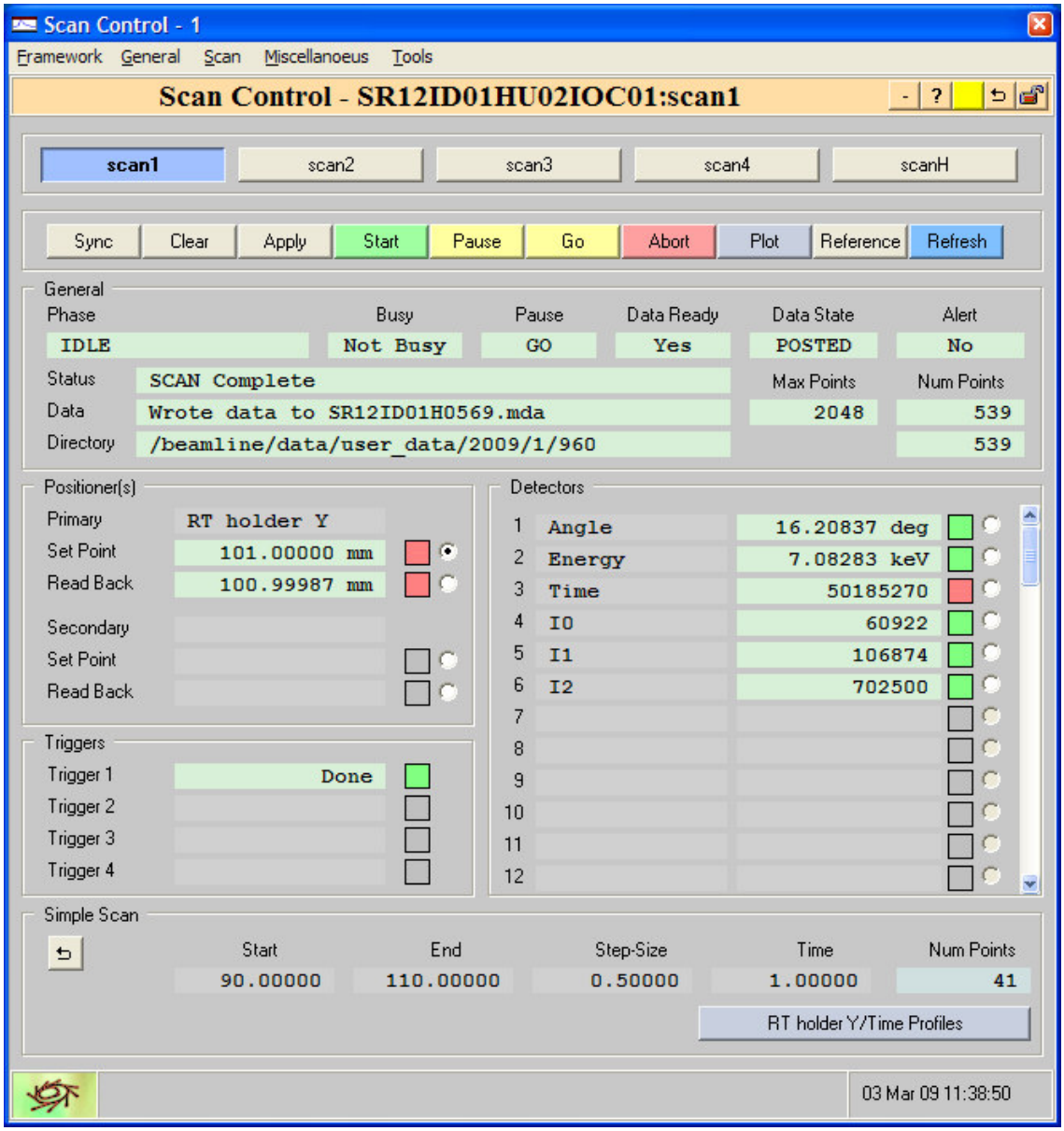
Select: RT holder (x and y) if you are performing measurements at room temperature; Cryostage (x and y) if you are measuring at cryotemperature.

- Left click on Detectors.

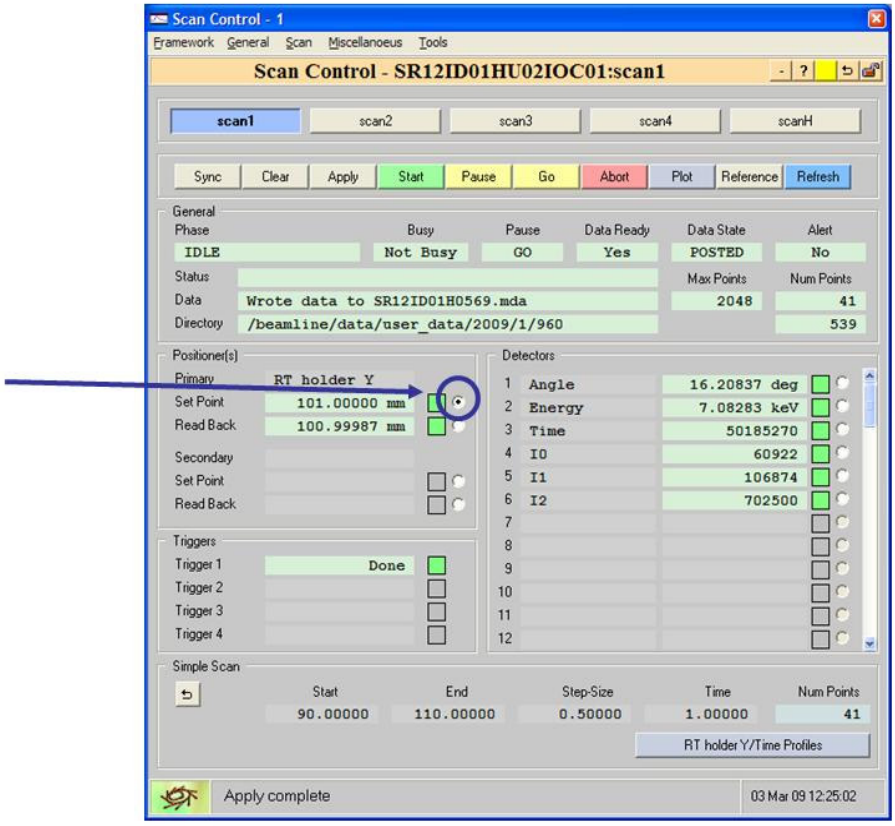


For scanning the positions you need I0, I1, I2, which are related to the incoming beam, the flux after the sample, and the flux after the reference, respectively.

- Enter the min and max values and the steps into the ‘simple scan’ region at the bottom of the window.



- **Apply** the scan parameters and start the scan. Please notice that your values must be **applied** before starting the scan**.** The plot window should pop up automatically. If it does not, press the plot button. To visualise the plot correctly you **must** select on the scan control program the variable that you want as the x variable (In this case the position of the sample holder).



You have also to select in the plot window which variable you want to see as the y variable.

- Once you have identified the x and y centre for your samples (and your references) you have to upload these values. To do that select ‘Sample pos’ and ‘reference pos’ from the endstation GUI.

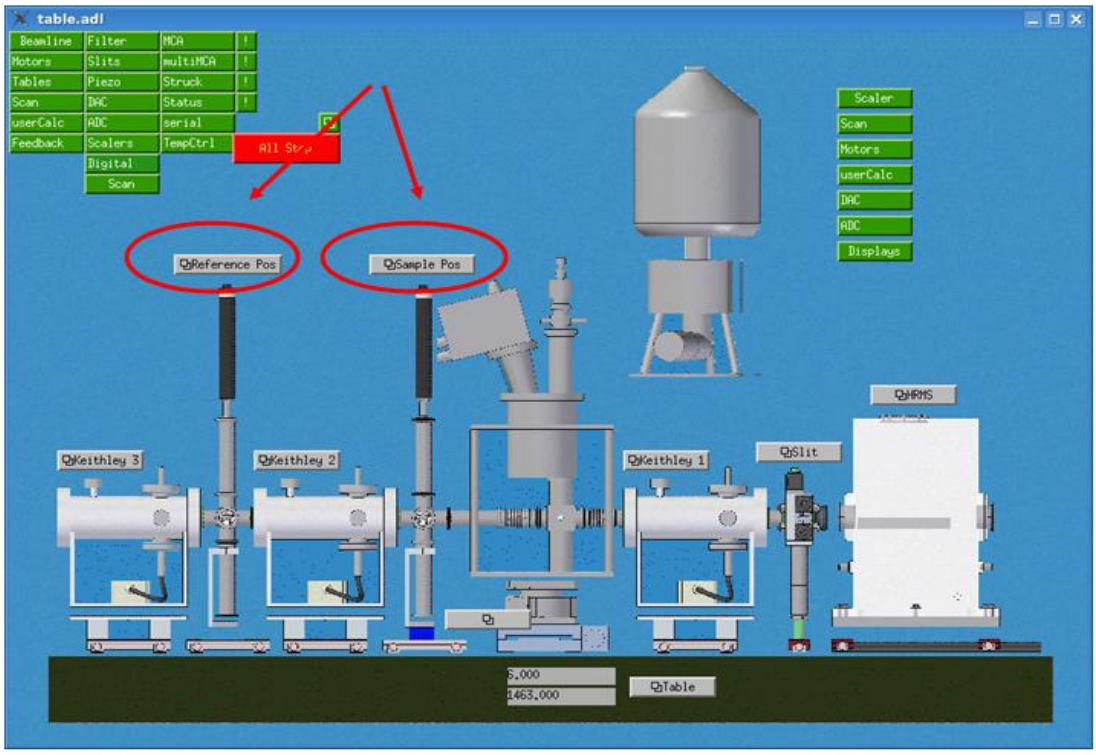
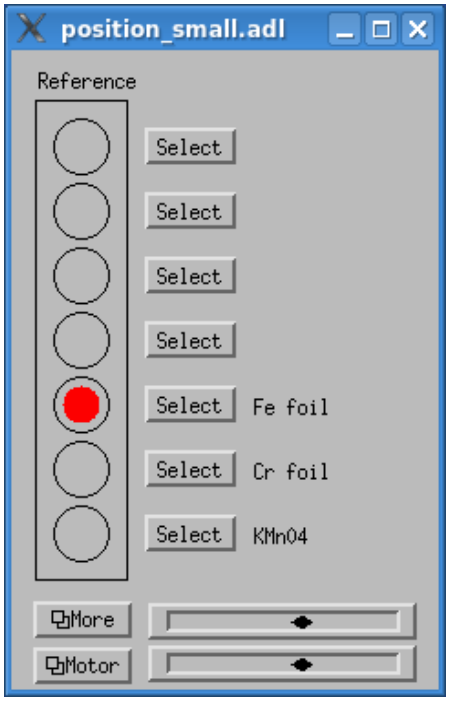
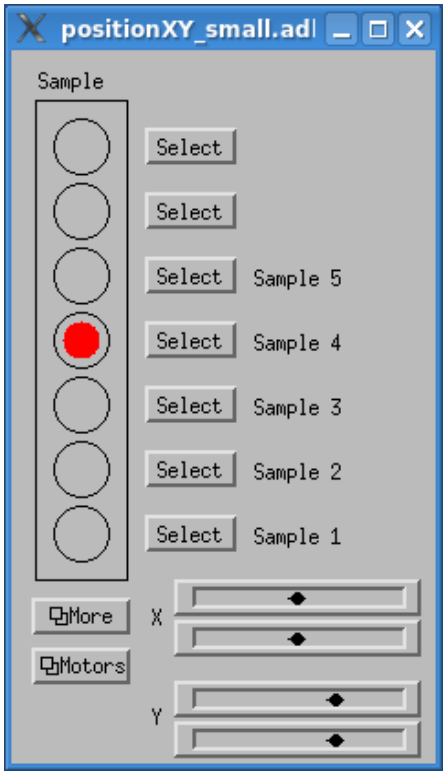
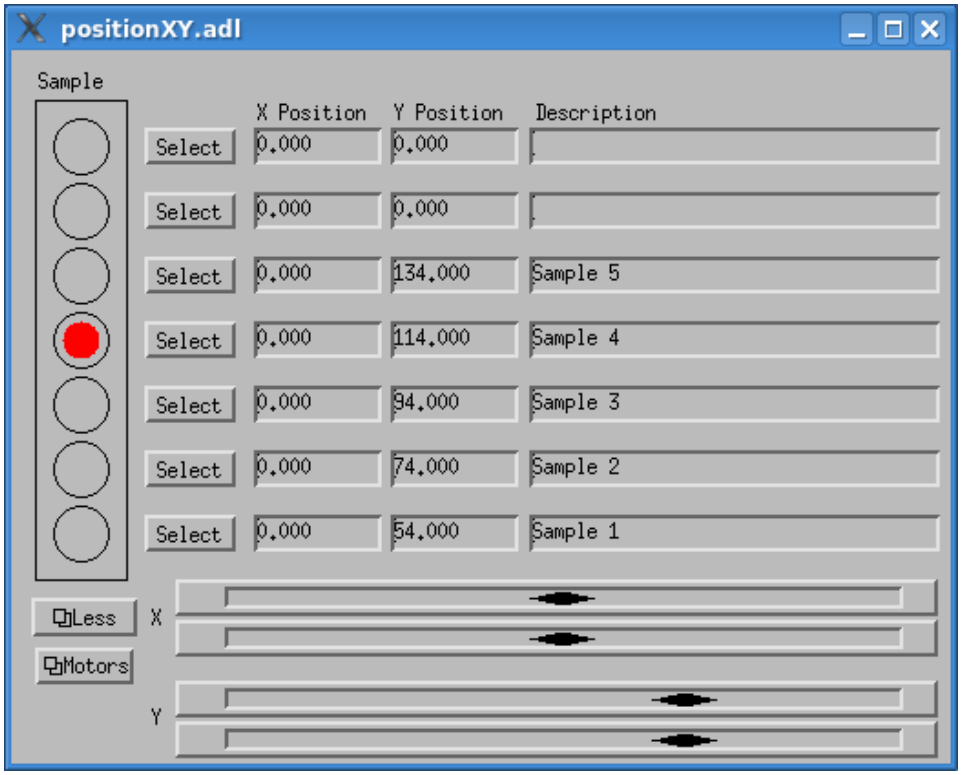


table.adl
Beamline
Filter
MCA
Motors
Slits
multiMCA
Tables
Piezo
Struck
Scan
DAC
Status
userCalc
ADC
serial
Feedback
Scalers
TempCtrl
Digital
Scan
Reference Pos
Sample Pos
Scaler
Scan
Motors
userCalc
DAC
ADC
Displays
HRMS
Keithley 3
Keithley 2
Keithley 1
Slit
Table


position_small.adl
Reference
Select
Select
Select
Select
Select
Fe foil
Select
Cr foil
Select
KMnO4
More
Motor


positionXY_small.adl
Sample
Select
Select
Select
Sample 5
Select
Sample 4
Select
Sample 3
Select
Sample 2
Select
Sample 1
More
Motors
X
Y

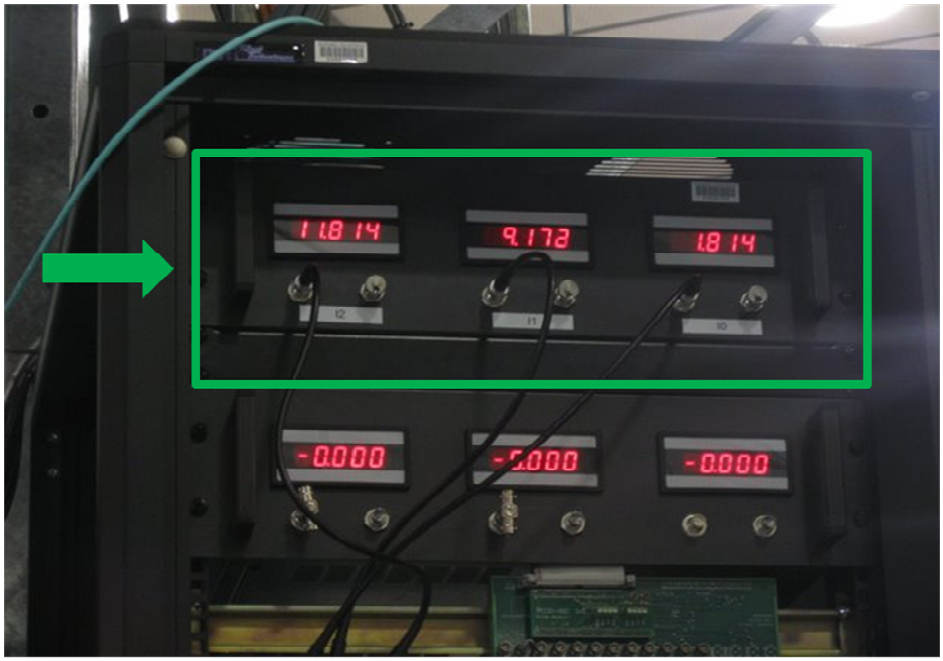
- Click on ‘more’:



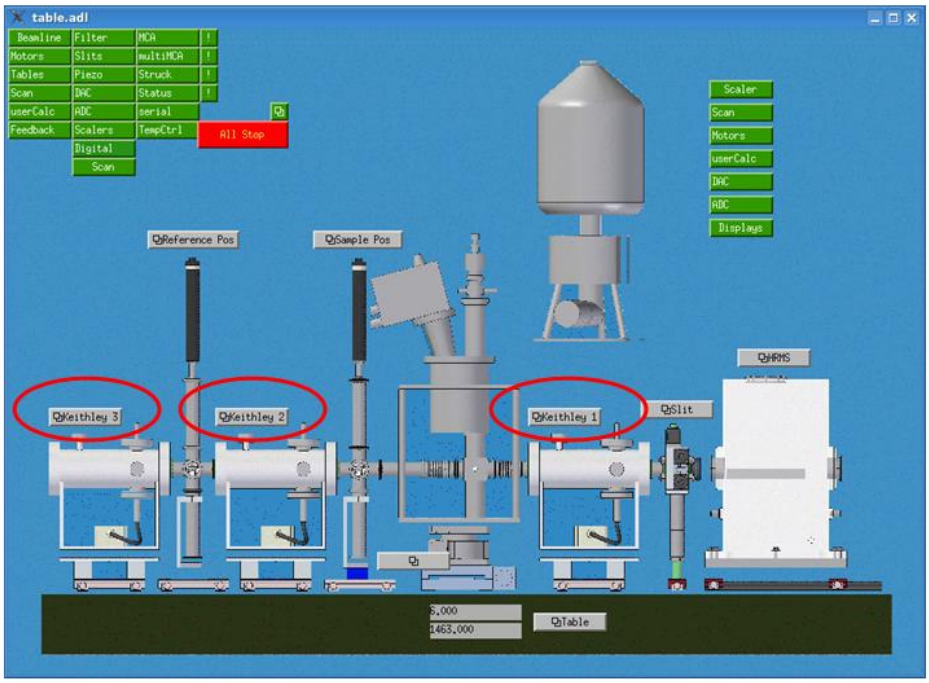
- Enter the correct values for the x and y of the different samples. To centre each sample it is now sufficient to click on the respective ‘select’ button.

- **Verify that the gains of the keithleys are set correctly.**

To do that you need first to check that the signals for I0, I1 and I2 are within 1 and 10. These values are displayed in the upper side of the electronic rack near Hutch B. They are labelled as I0, I1 and I2.



You should adjust the keithley (Keithley1, Keithley2 and Keithley3 for I0,I1 and I2, respectively) gains in order for these values to be in the right range. Click on the keithley button in the endstation GUI

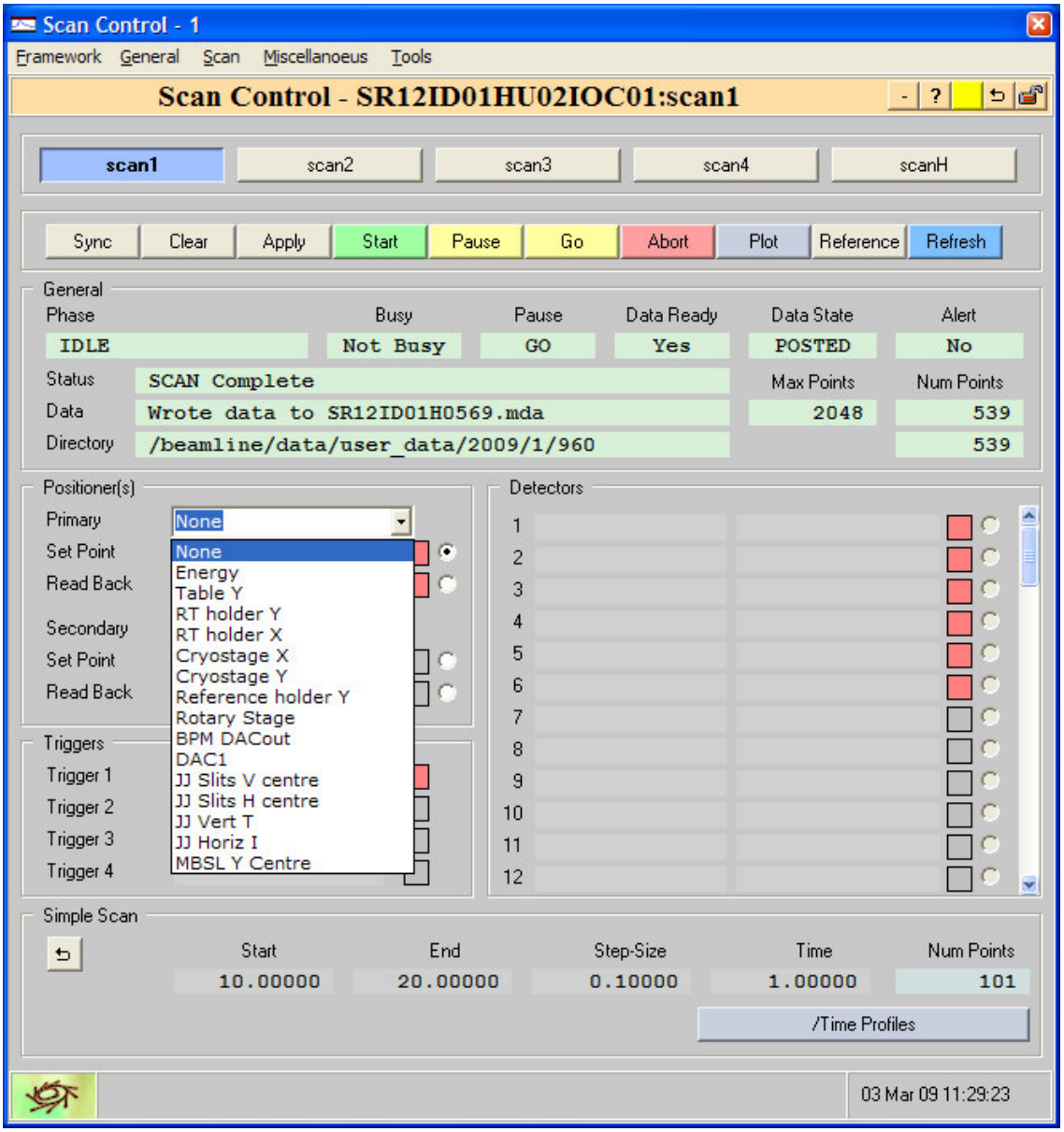


The following window will pop up:

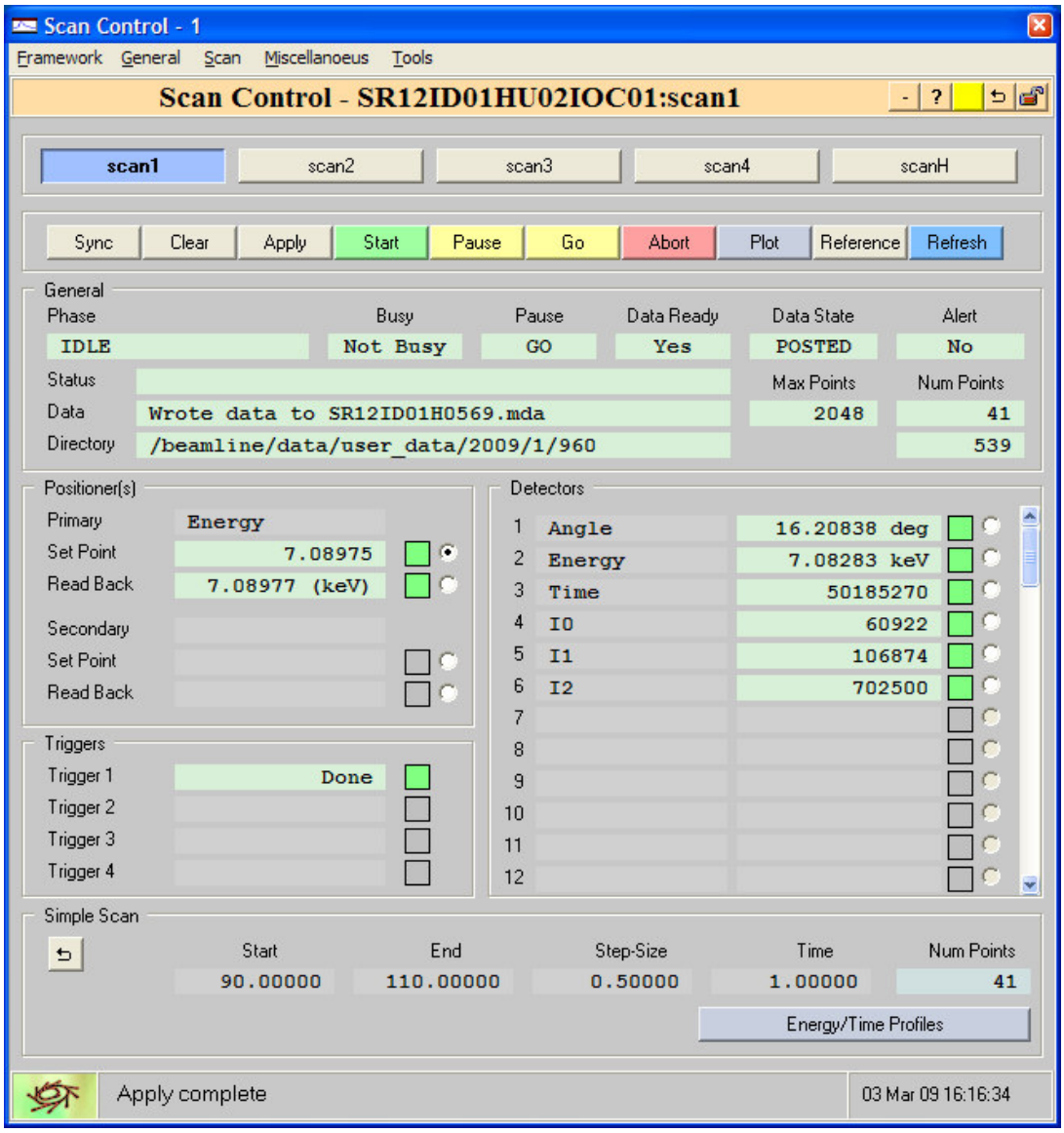
Select the right value from the gain button.

- **Run the EXAFS scan**

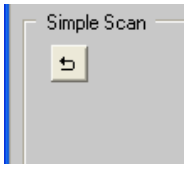
    - Go to the scan control program.
    - Left-click on ‘positioner(s) – Primary’



    - Select Energy
    - Left click on Detectors.
    - Select: Angle, Energy, Time, I0, I1, I2

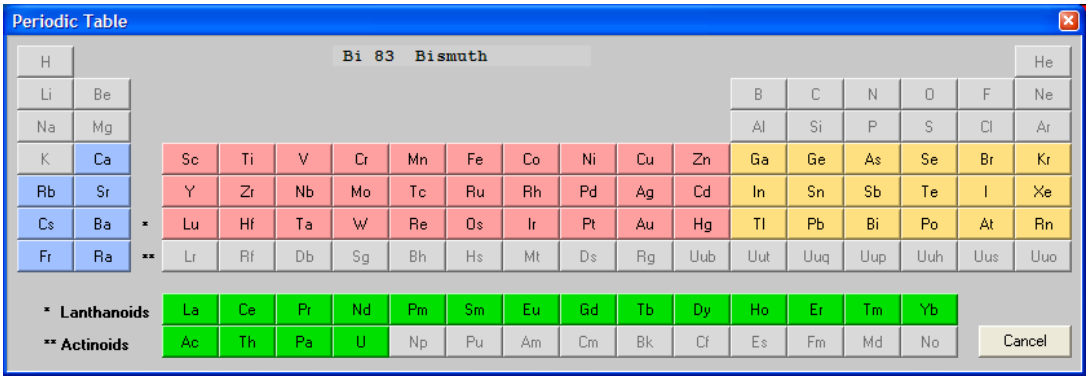


- To set the EXAFS scan parameters go to ‘EXAFS Scan’ section by clicking on the arrow on the left bottom of the window.



This button allows switch between ‘simple scan’ and ‘EXAFS scan mode’.

- Select the element and the edge (K or L3) that you want to measure by clicking on the 'Element(K)' or 'Element(L3)' button. A periodic table window will pop up. Click on the desired element.



This upload the values suited for the selected edge: the edge energy, the energy intervals, the energy steps and the integration time. The number of points in each interval (Num Points) and the number of points in total (Total Points) are calculated on the basis on the given parameters. If you are not satisfied with the given parameters you can change them by inserting a new value. In the pre-edge and edge ranges (phase 1 and 2) the step-size is given in eV (energy space) whereas in phase 3 is given in $Å^{-1}$ (K space). Usually you may want to increase the energy resolution in the edge region. Minimum resolution values vary with energy and monochromator crystals. Typical values are around 0.25 eV. For the integration time you have the possibility to choose between two 'time modes': square and linear. This will simply change the function through which the integration time is increasing.

You have to press the 'apply' button in order to upload the scan record. When the selected values are actually uploaded the colour of the squares should change from red to green.

- Press start to begin the scan. The plot window should pop up automatically. If it does not, press the plot button.

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