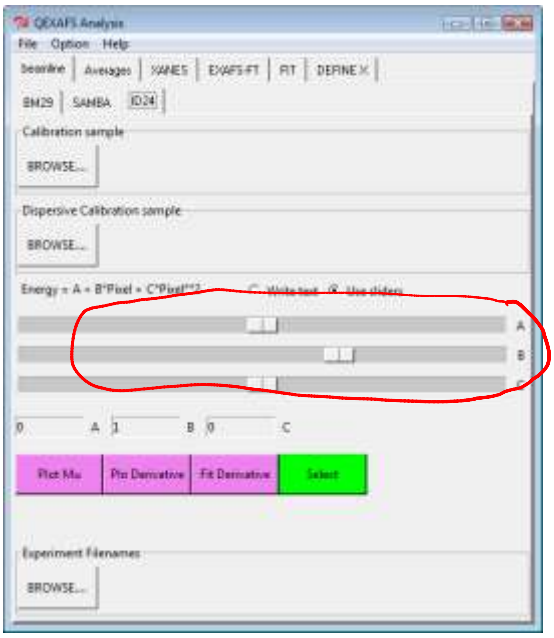
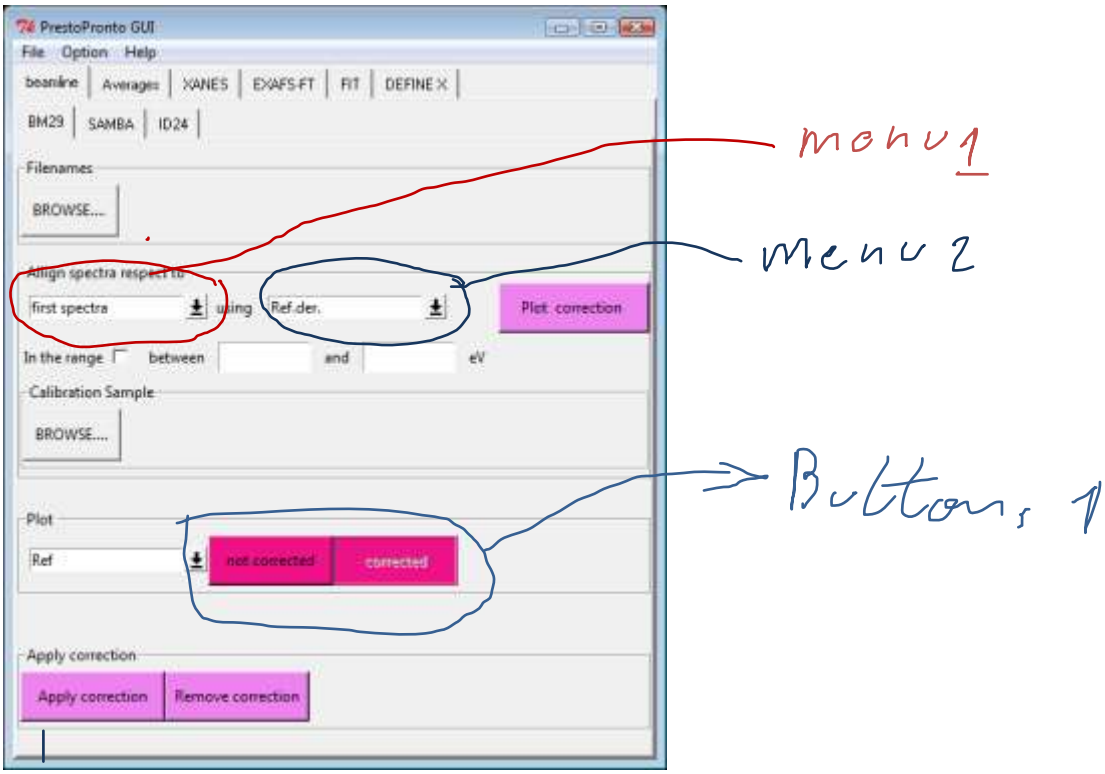
ID24



This page has as objective to select data files from ID24 and calibrate it. The calibration consists to substitute to the pixel index into Energy. The energy is calculated as a quadratic polynomial A+B*index +C*index^2, the factor ABC could be obtain by comparison between of the spectrum of a calibration sample collected on a double crystal monochromator (**Calibration sample**) and collected during the experiment (**Dispersive Calibration sample**). The user should plot the derivative of the spectra and using the three sliders try to superimpose the two spectra, the position of the three parameter could be fitted by pressing the button fit derivative. One time satisfied the choice of A BC have to be confirmed pressing Select. A B C could also introduced as a text but choice of A BC have to be confirmed pressing Select.

Browse Filename button serve to select the filename of the experiment.

BM29 Calibration



The BM29 calibration pannel have as a task to open BM29 files and allign them in order to remove the energy drifts induced by the heat loading.

There are several options that could be selected by pull-down menu1 or menu2

From menu 1 is possible set if the user want to allign respect the the first spectra of the series or an exsternal calibration energy

From menu 2 is possible set wich kind of method to use fopr the allignment. The option are using reference, or using derivative reference or I0, if the allignmet is done along the series. Otherwise the more commen choice is Calibration or derivative calibration. Importante to notice that it is possible also to use the the calibration reference or its derivative.

The allignment is done fitting the best energy shifht, for each spectra, in order to minimize the difference along the series.

Buttons 1 allow to appreciate the results of application of Correction on the different characteristic defined by the pull down menu

SAMBA Calibration

Correction for Samba files coming by moulinex routine. If the number of file is bigger than 350 is better use to open the option File in a directory.

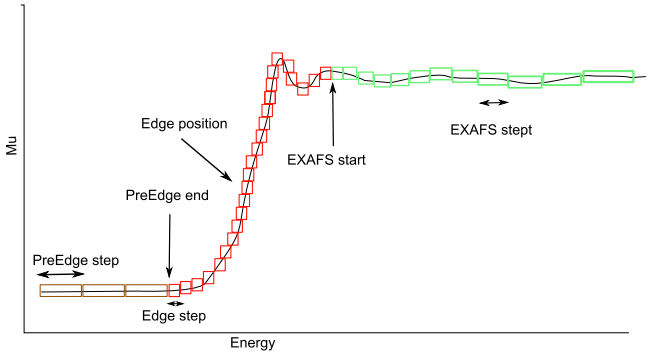
The slider and the fit could be used to align different runs using the reference spectra and a calibration

PAGE Average&Selection&Truncate

Select. In this set of entry is possible to select only a part of the set of spectra open previously. At this moment it is only possible remove spectra from the start or the end of experiment

Truncate In this set of entry is possible to select only a part of the of spectra open previously. At this moment is only possible the first part and/or the last part of the spectra.

Rebin. This set of parameter control the routine of rebinning. QEXAFS data are generally collected in constant energy step. With this kind of data collection at high k the sampling became over redundant and data files became big with too many experimental points. As a consequence software for data analysis became slow and unstable. The Rebin algorithm tries to avoid it re-sampling the data. More precisely the algorithm subdivide the spectra in a set of energy box and after calculate the spectra average for each box, the results will be the rebinned spectra. The wide of the box vary along the spectra: 1) wide constant energy box on the pre-edge; 2) narrow wide constant energy box on the edge; 2) constant wavevector box after the edge The parameters are necessary to define the wide of the box.

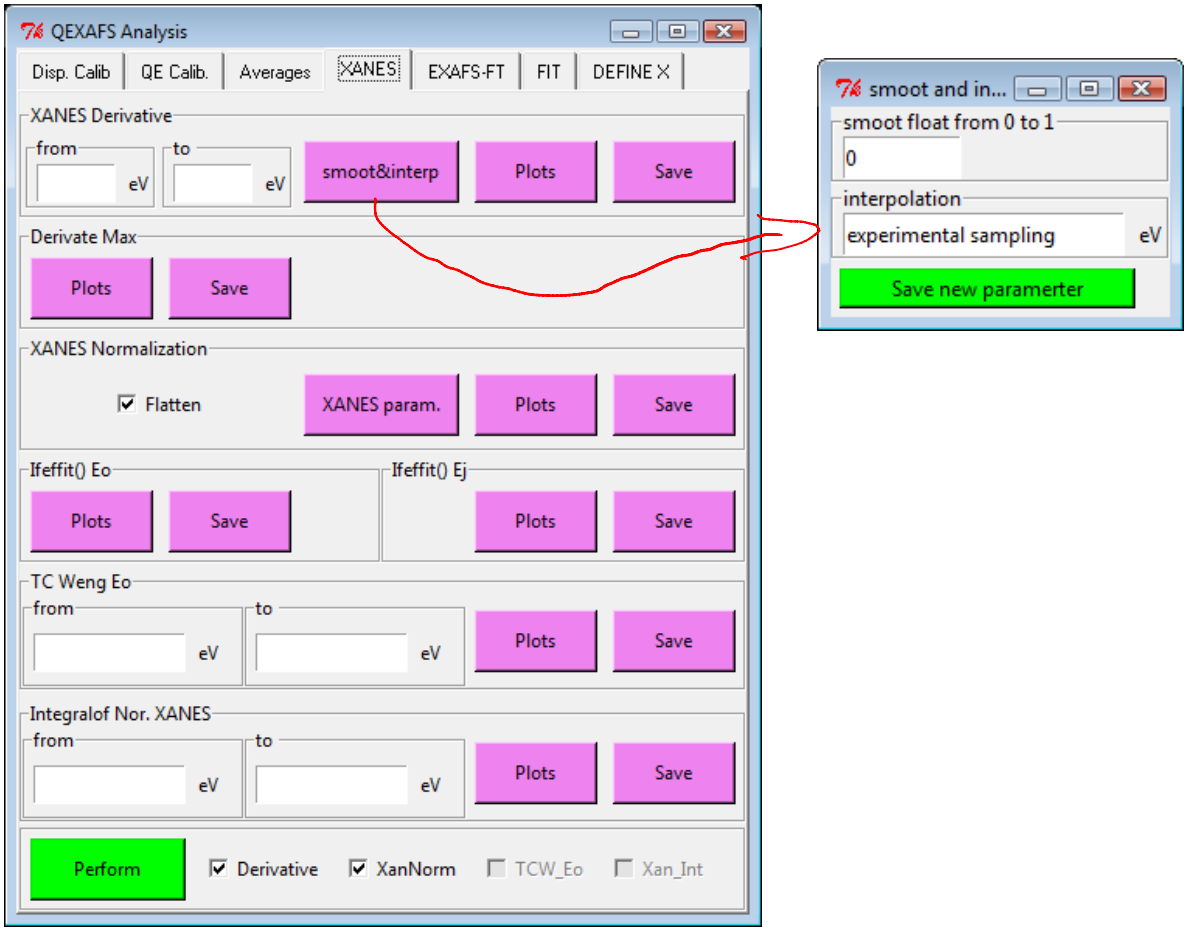


Average. In this page is also possible to partially average along the time a set of spectra. This is an important option, averaging each n file allow to saw modification clearly and with a minimum calculation time.

Plot button plot the original data as colored lines and rebinned and/or truncated and/or averaged data as scattered points.

The **save** is very useful for save all the corrected spectra in a single file format that could be open by the menu

PAGE XANES



Xanes Derivative it calculate the derivative of the spectra from… to….The derivative is calculated evaluating a set of cubic spine that pass from each point y of the spectra and successively the derivate is calculate analytically over the spine.

The parameter **interpolate** simply ask to calculate the derivative on the cubic spline along a different sampling.

The **smoot factor (s)** acts mainly during the evaluation of the spines. The amount of smoothness is determined by satisfying the conditions: sum((w * (y - g))**2,axis=0) <= s where g(x) is the smoothed interpolation of (x,y). The user can use s to control the tradeoff between closeness and smoothness of fit. Larger s means more smoothing while smaller values of s indicate less smoothing. Recommended values of s depend on the weights, w(Till now in Tscan1 the weigh is not evaluated). If the weights represent the inverse of the standard-deviation of y, then a good s value should be found in the range (m-sqrt(2*m),m+sqrt(2*m)) where m is the number of data points in x, y, and w. default : s=m-sqrt(2*m) if weights are supplied. s = 0.0 (interpolating) if no weights are supplied.

Further information on the documentation of function **`splrep and splrev`** in fortran routine **`fitpack`**

Xanes normalization performs XANES normalization using the routine pre_edge of ifeffit engine the various parameters of the routine are accessible by button XANES param. That allows to change the default parameters of Ifeffit:

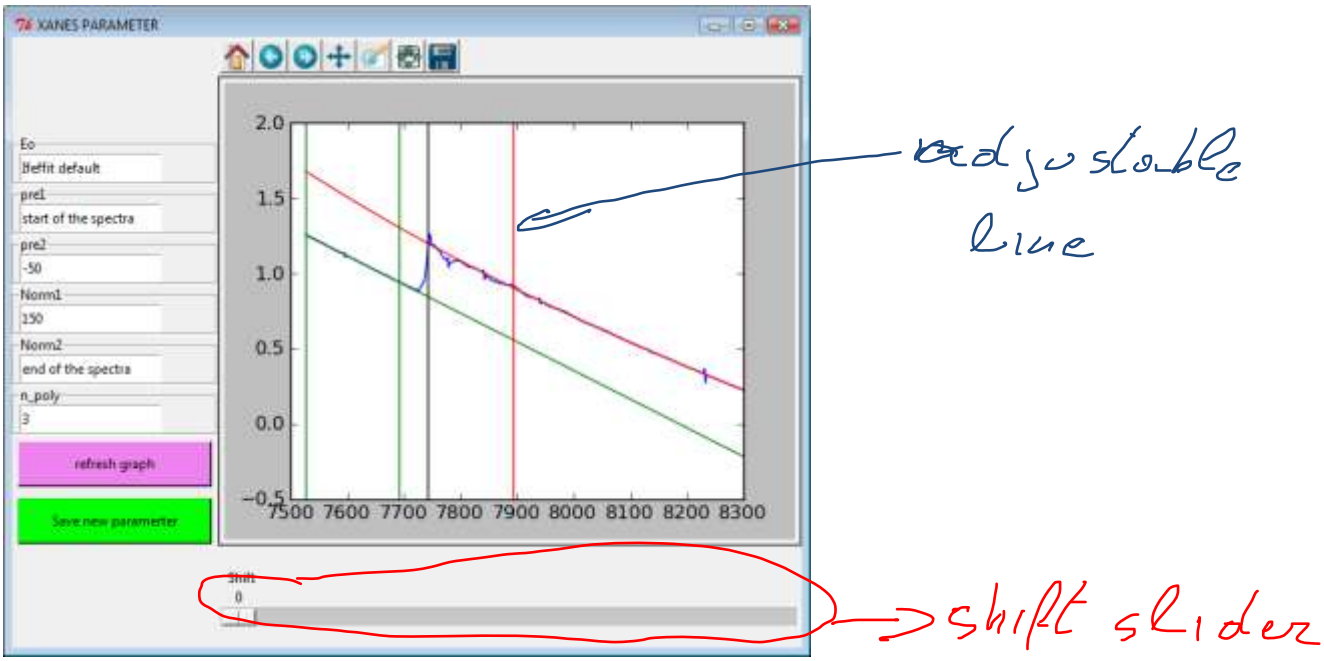
Eo =edge position parameter, if equal to "Ifeffit default" the program will take the first inflection point of the edge, if a numerical value if introduced, the Eo will be fixed for all the spectra range to this numerical value

Pre1 = first point to fit the preedge. Program default is the start of the spectrum, the user could modify inserting a different value. Pre1 is defined as the number of eV before the edge I.e. -200

Pre2 = last point to fit the preedge. Program default 50 eV from the edge, the user could modify inserting a different value. Pre1 is defined as the number of eV before the edge I.e. -20

Norm1 = first point to fit the postedge. Program default is 150 eV from the edge , the user could modify inserting a different value. Norm1 is defined as the number of eV before the edge I.e. 50

Norm2 = last point to fit the postedge. Program default the end of the spectra, the user could modify inserting a different value. Norm2 is defined as the number of eV before the edge I.e. 1200



This values could be evaluated pressing button **XANES param.** it the graph appearing the **shift slider** allow to see the effect of the parameter on the different spectrum while the **colored lines** could be shifted in order to evaluate the effect of different parameter on the same spectra.

Ifeffit Eo is the position of Fermi energy defined by pre_edge routine of ifeffit for extraction, generally is the first peak of edge derivative.

Ifeffit Ej is the estimation of edge jump done by pre_edge routine of ifeffit

TC Weng Eo is an alternative way to detect the Eo, developed by TC Weng (we use an another algorithm but the same philosophy). Eo is define as the position of a step function that have the same integral of the normalized mu(x). It could be applied only after the normalization.

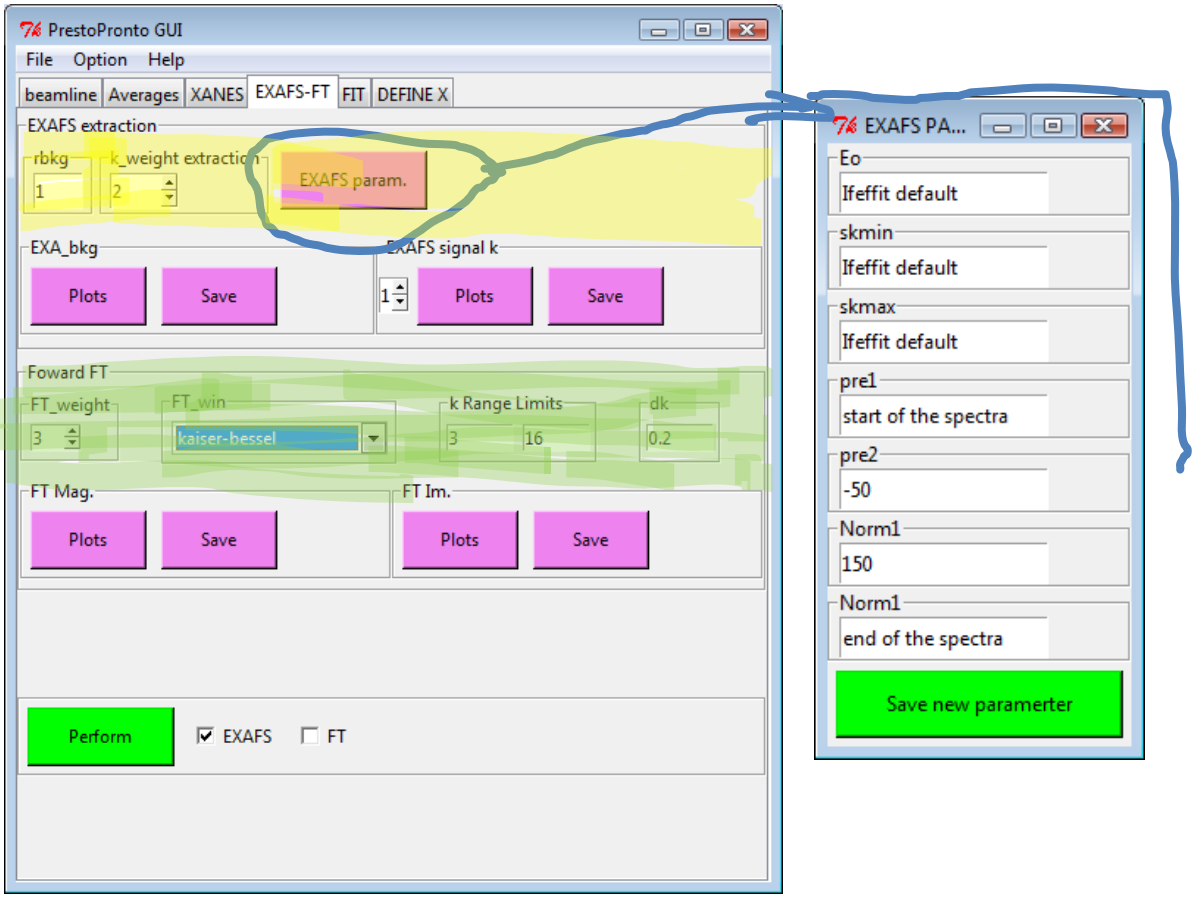
$$\int_{x_0}^{x_1} mu(x)dx = \int_{x_0}^{x_1} \delta(E_0)dx$$

Integral Nor XANES

Evaluate the integral of the a normalized XANES region for each spectra

PAGE EXAFS

In this page EXAFS extraction and Fourier calculation are done using the Ifeffit engine



the parameter for the extraction are underlined in yellow, while the parameters for Fourier transform are underline in green.

The parameter are the same of Ifeffit and its GUI (Athena, Sixpack). I suggest to choose the more appropriate parameter for extraction on a few selection of spectra using Athena and after apply on the large series with PrestoPronto.