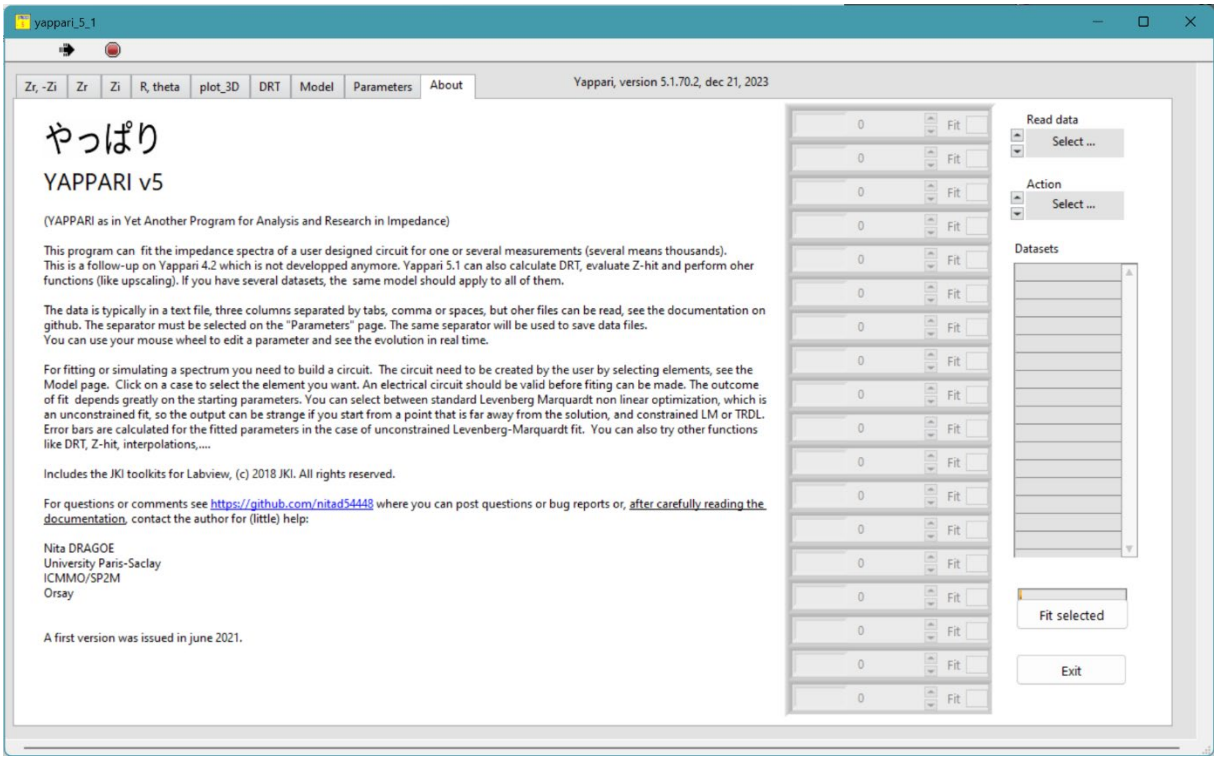
# Yappari 5.1

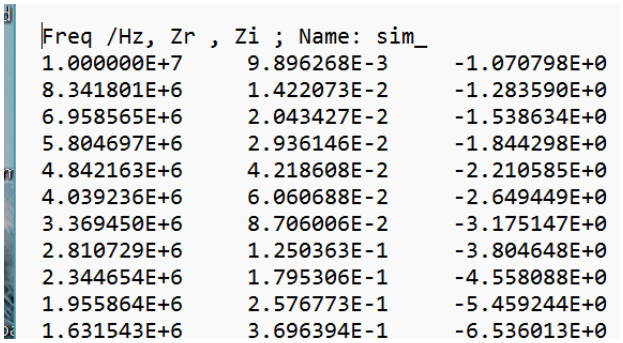
## Another tutorial

version January 24, 2024.

When starting the program you should see in the center of your main screen this image: it is a brief introduction to the program.



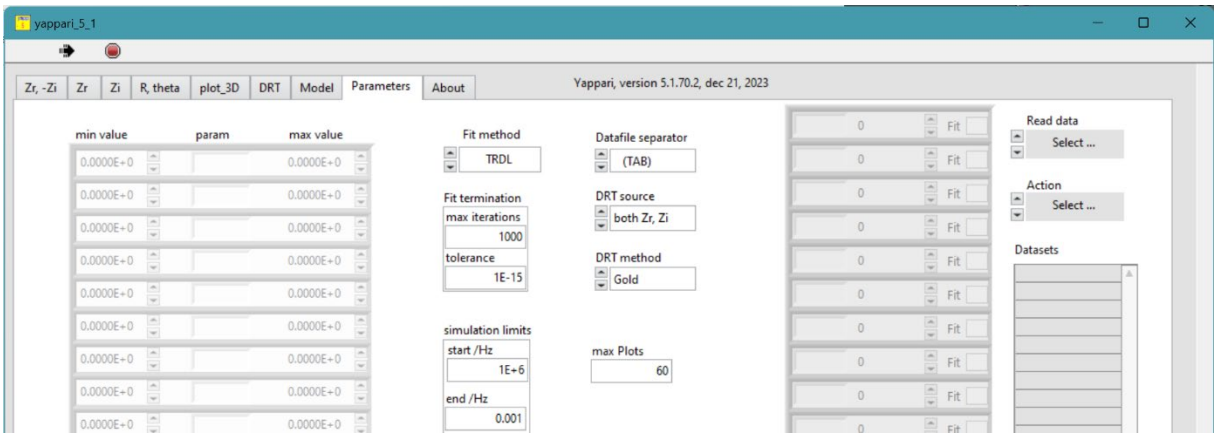

The first thing to do is to select the ”separator” in the datafile: you need to check your datafile, most of the time it is a TAB. If we look at the data file we can see it is a TAB for this case.



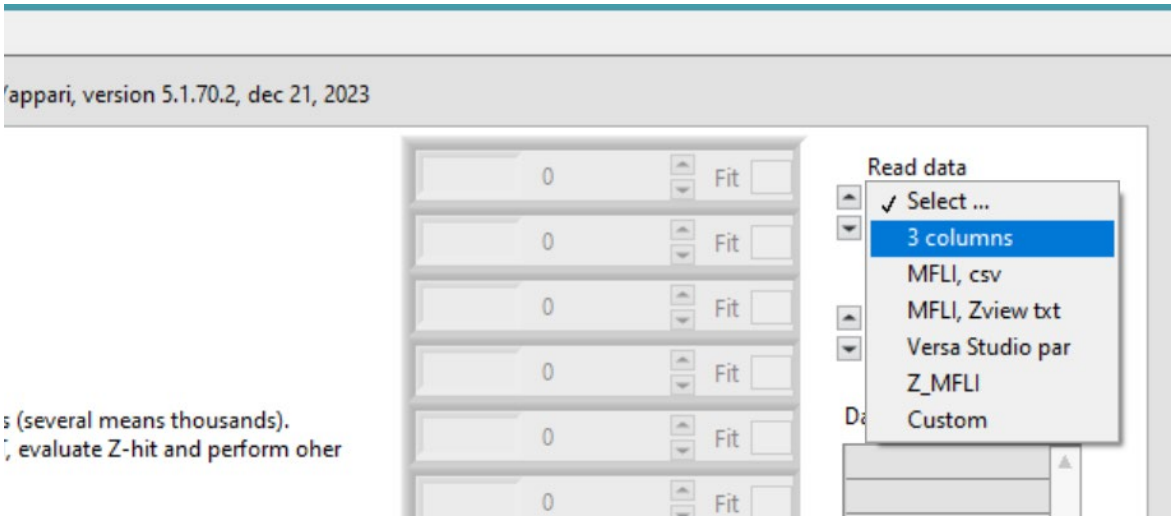
```
Freq /Hz, Zr , Zi ; Name: sim_
1.000000E+7     9.896268E-3     -1.070798E+0
8.341801E+6     1.422073E-2     -1.283590E+0
6.958565E+6     2.043427E-2     -1.538634E+0
5.804697E+6     2.936146E-2     -1.844298E+0
4.842163E+6     4.218608E-2     -2.210585E+0
4.039236E+6     6.060688E-2     -2.649449E+0
3.369450E+6     8.706006E-2     -3.175147E+0
2.810729E+6     1.250363E-1     -3.804648E+0
2.344654E+6     1.795306E-1     -4.558088E+0
1.955864E+6     2.576773E-1     -5.459244E+0
1.631543E+6     3.696394E-1     -6.536013E+0
```

The first line is a comment: it is not required, it can be used if there are no numbers in this line. The data should be as frequency in Hz, Z_real and Z_im.

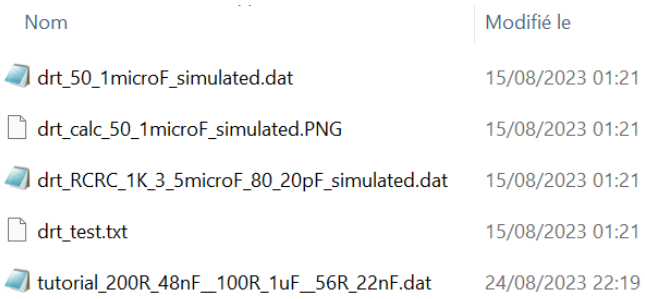
Go to "*Parameters*" panel and select the "Datafile separator" value as TAB




We'll open this 3 columns file by selecting *Read data/3 columns*:

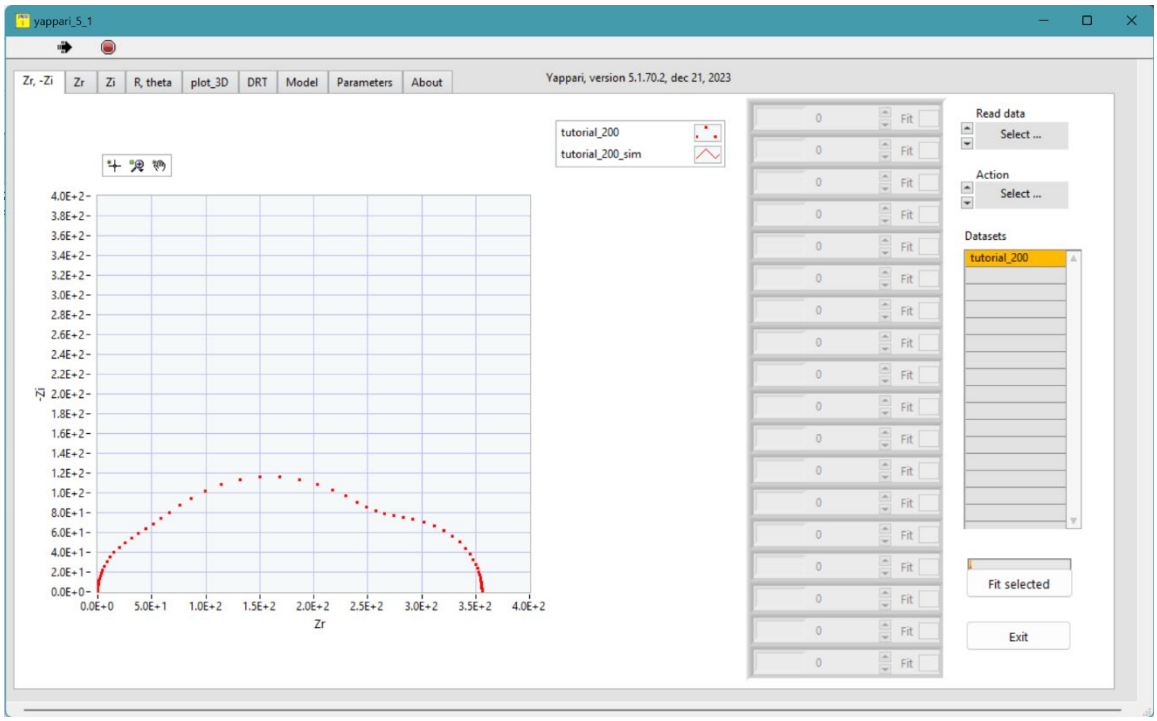



The file **tutorial_200R_48nF…** is located in **yappari/drt** folder



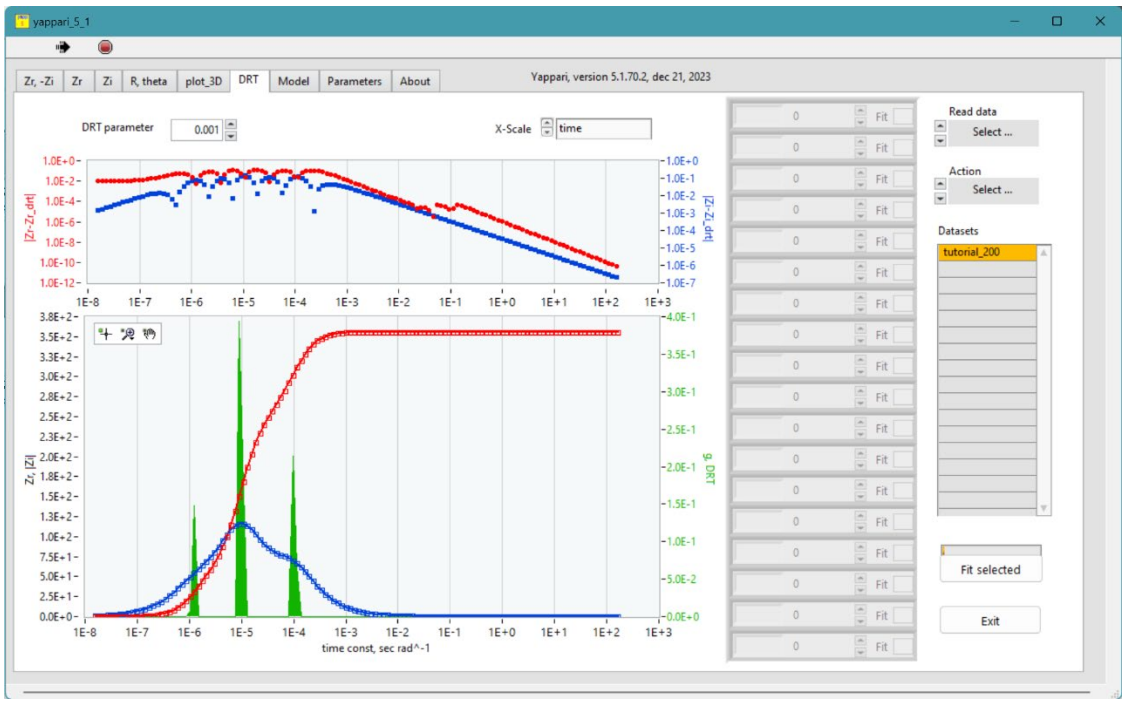

This is a simulated data (with this program) with a circuit of 3 RC elements in series, with the values given in the name of the file.

Once read, the program lists the name of the datasets found in the file, for this case only one dataset is listed. We'll see later on in this document how to deal with a multiple datasets file. By changing the panel one can visualize the plots of the data file. Some points can be removed, if there are obvious outliers (see *Action* menu).

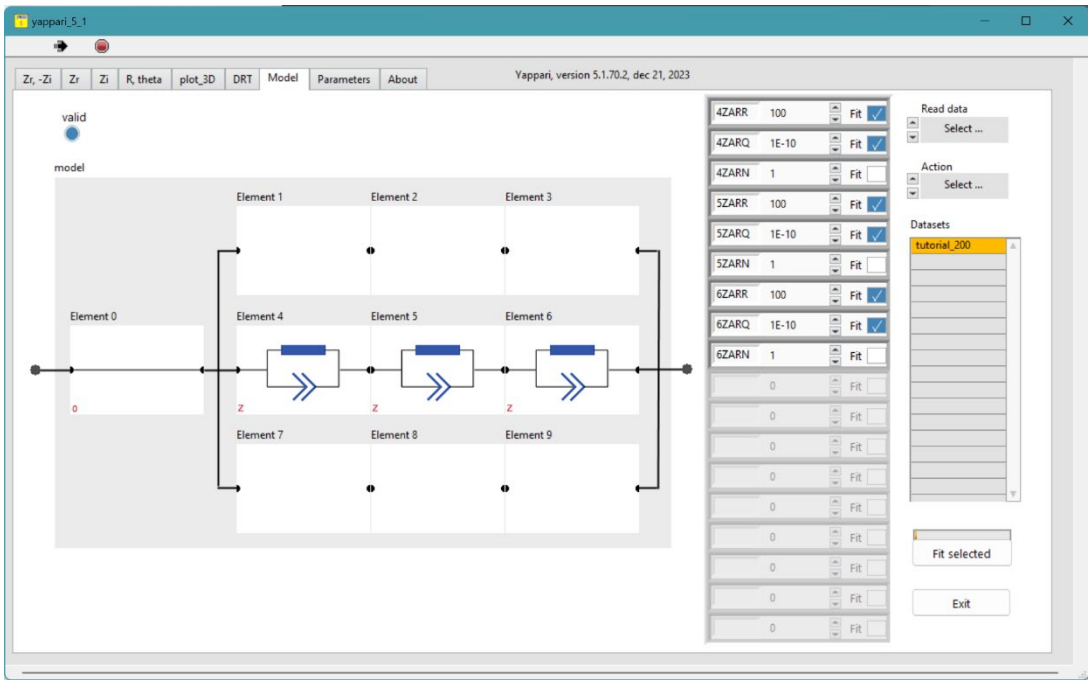



For simple cases like this (simple RC circuits) one can use DRT to verify how many relaxations are present. This works fine if the data is “clean” and if there are at least 10 or 12 points per decade, ideally in log scale.

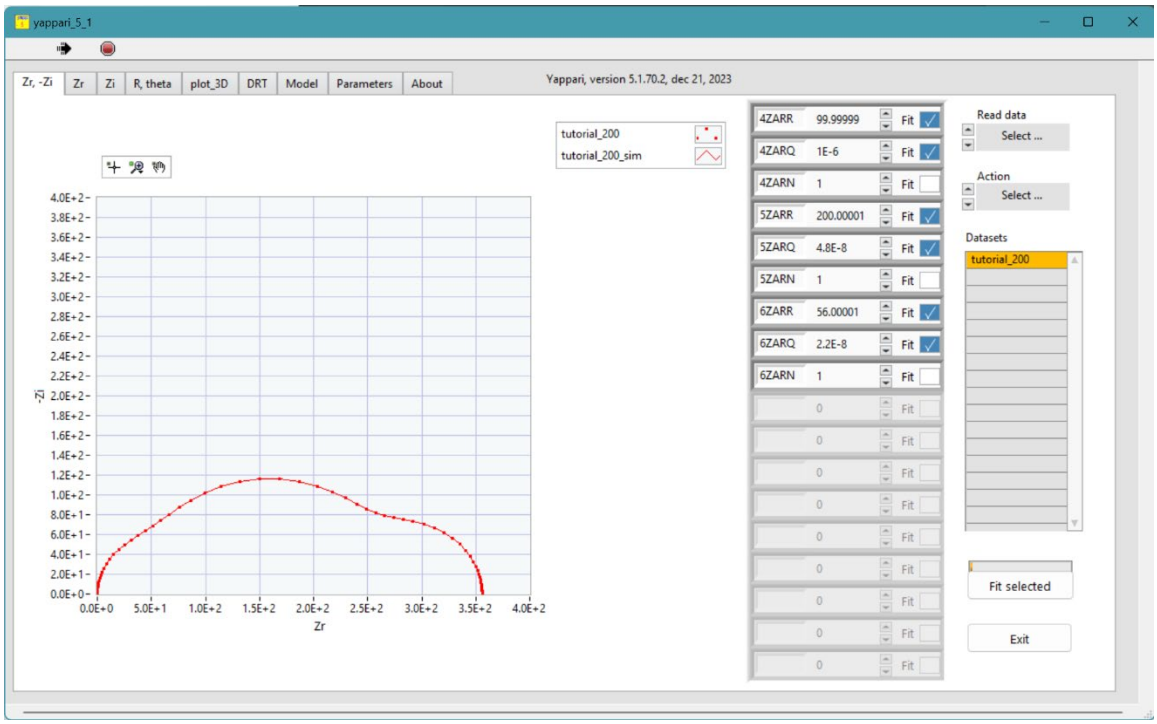
By clicking on the DRT parameters we can obtain a distribution of the relaxation times. For the case shown below, I used the Tikhonov algorithm (two others are available and can be selected in the *Parameters* page). The DRT shows clearly three relaxation and their times. One can directly calculate from the relaxation times the RC product (the program will show these calculations if you hover with the mouse on the DRT image).



Because we can assume there are three relaxations (which we can also see in the Nyquist plot), we may build a circuit in the *Model* panel. It should look like this :




On the parameters column we can see some labels : *4ZARR*, *4ZARQ*... and values. This indicates the element number (4 in this case) and we can see in the element 4 of the circuit a resistor and a pseudo-capacitor. The values are generated by default, when the circuit is built.

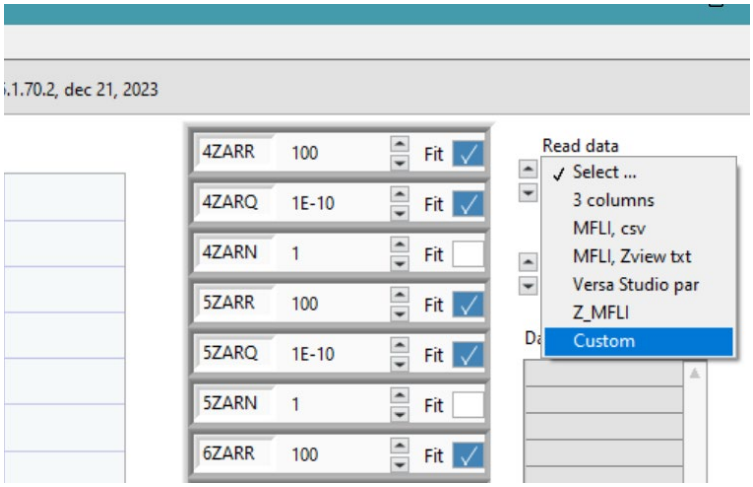



One should adapt the starting parameters for the fit, but for this case it is not required. The fitting method is the one selected in the *Parameters* panel. Note that standard deviation values are given only for the unconstrained fitting method. The range of constrained parameters can also be changed in the *Parameters* panel.

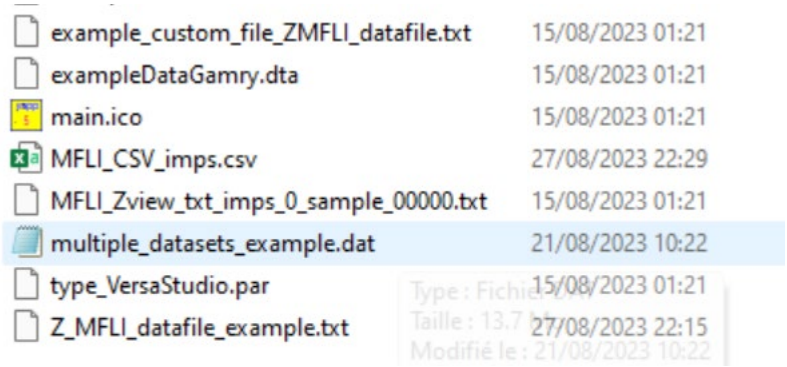
The obtained parameters are very close to the expected ones, this is no surprise since the simulated data is easy to fit (unlike real world data!). We can save the parameters and write a report after a fit.

Let's look at a more complex case: fitting multiple data sets. Some custom datafiles are in the **yappari/files** directory. One of them is **multiple_datasets_example.dat**

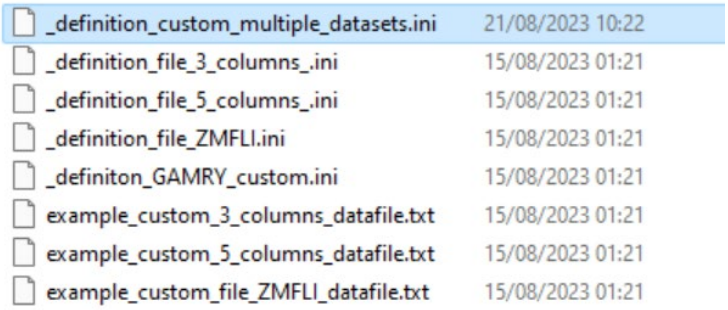
Select *Read data/Custom*




Then select the **multiple_datasets_example.dat** file

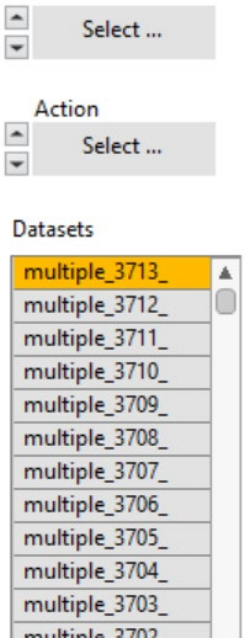



Since this is a custom datafile, a definition of its format is required. For this case the definition file is also provided and needs to be selected after reading the first datafile:

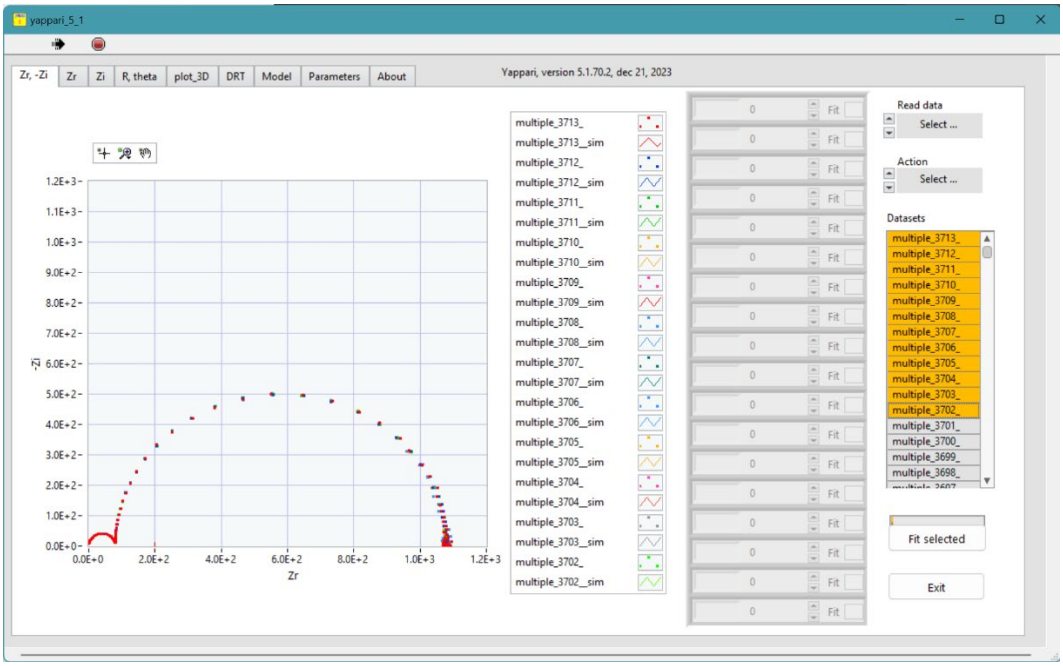



After a few seconds, you'll see the *Datasets* list adding the names of experiments that were in the multisets datafile. The names are the first 12 characters found in the file followed by a number, which

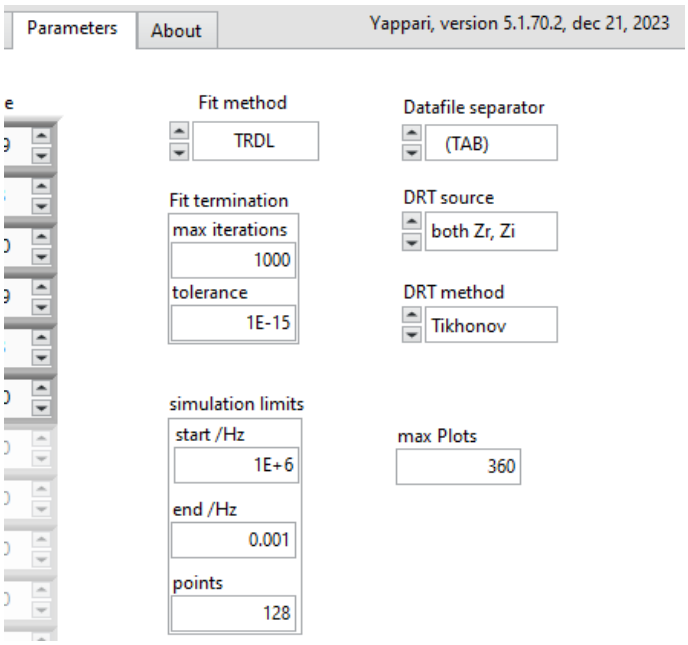
is the order in which these datasets are listed in the file. In the file used here there are 3714 spectra (these spectra are simulated with this same program, with some random noise added)



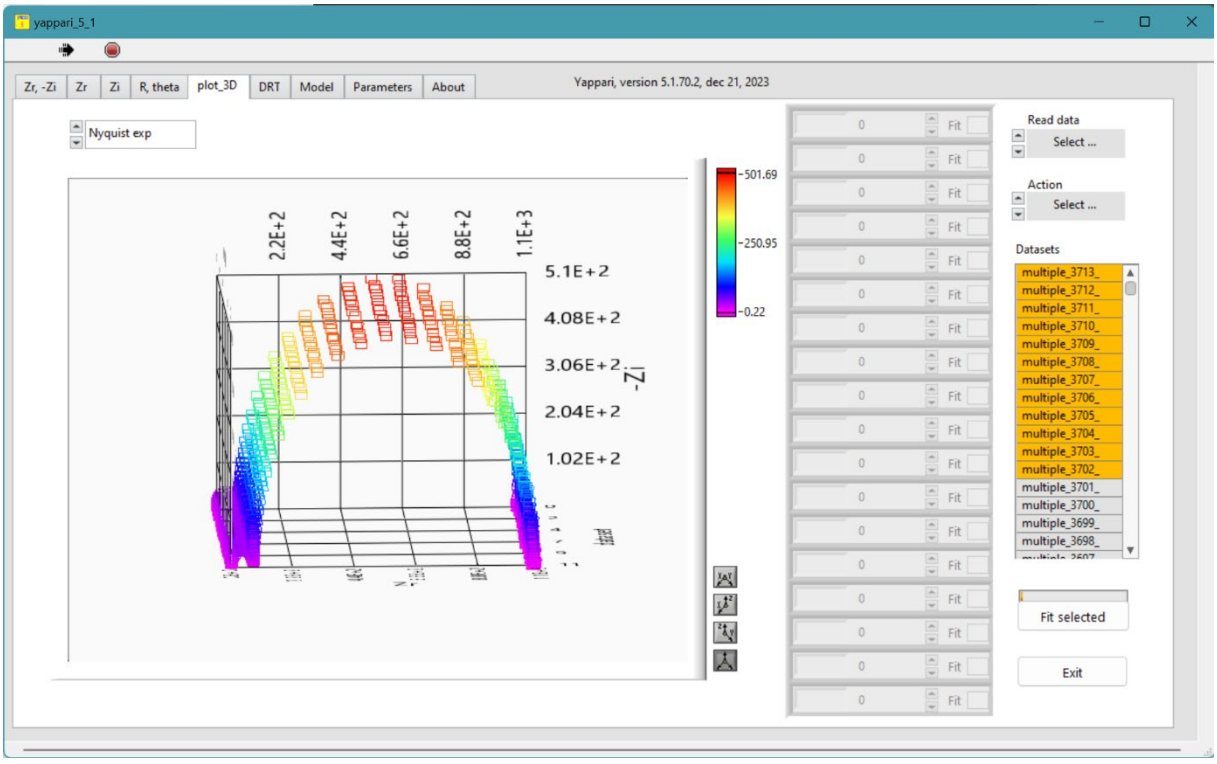

The last spectrum listed here is multiple_0, which is the first spectrum found in the file.



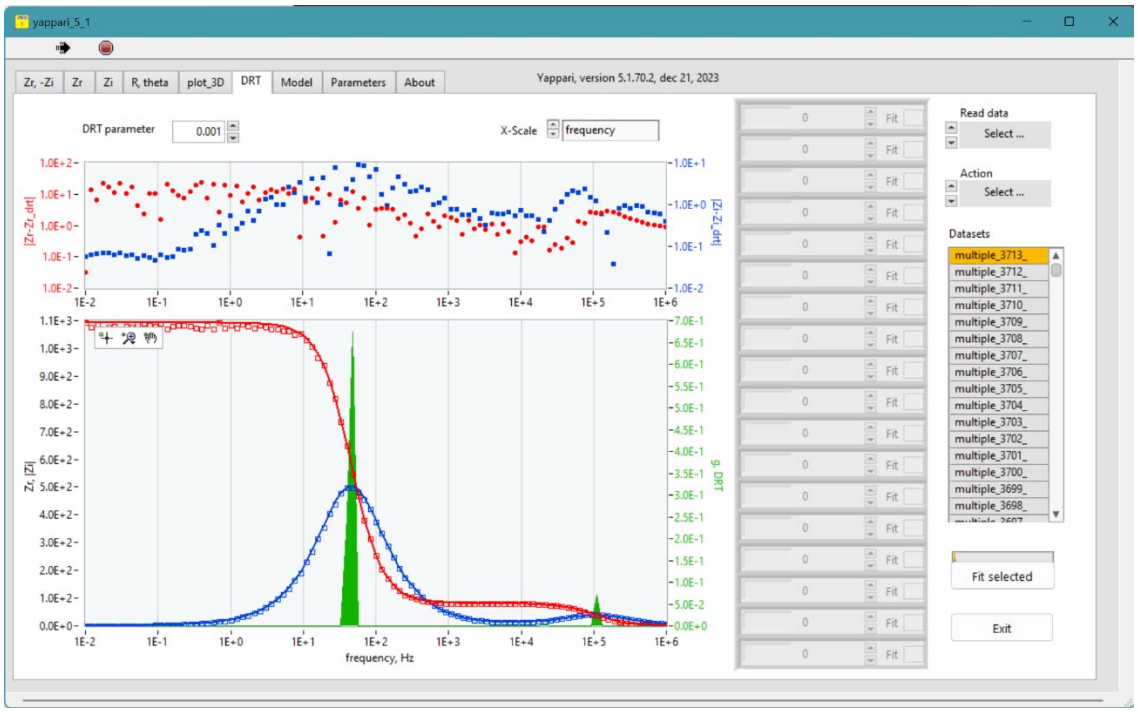

By selecting several datasets, they will be plotted together (the max number of plots can be defined in *Parameters* panel in *max Plots* control).



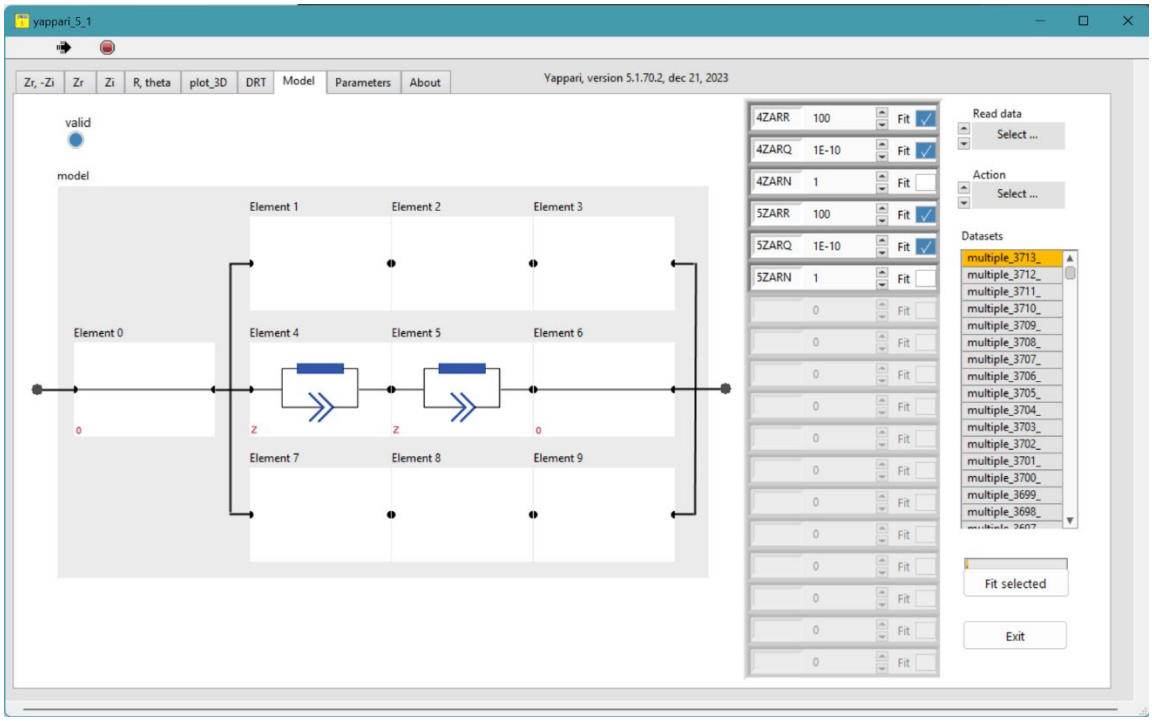

This also applies to the 3D graphics functions.



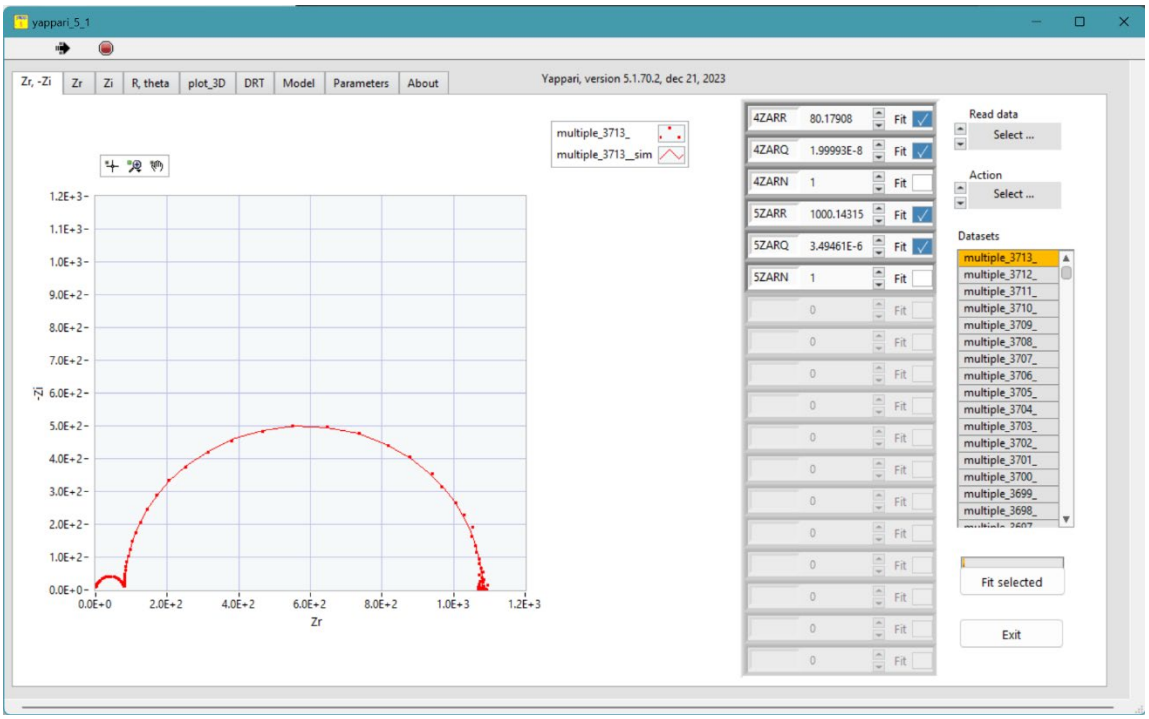

Here again we can take a look at the DRT, we can see two relaxations (again, these are simulated spectra so it is easy).



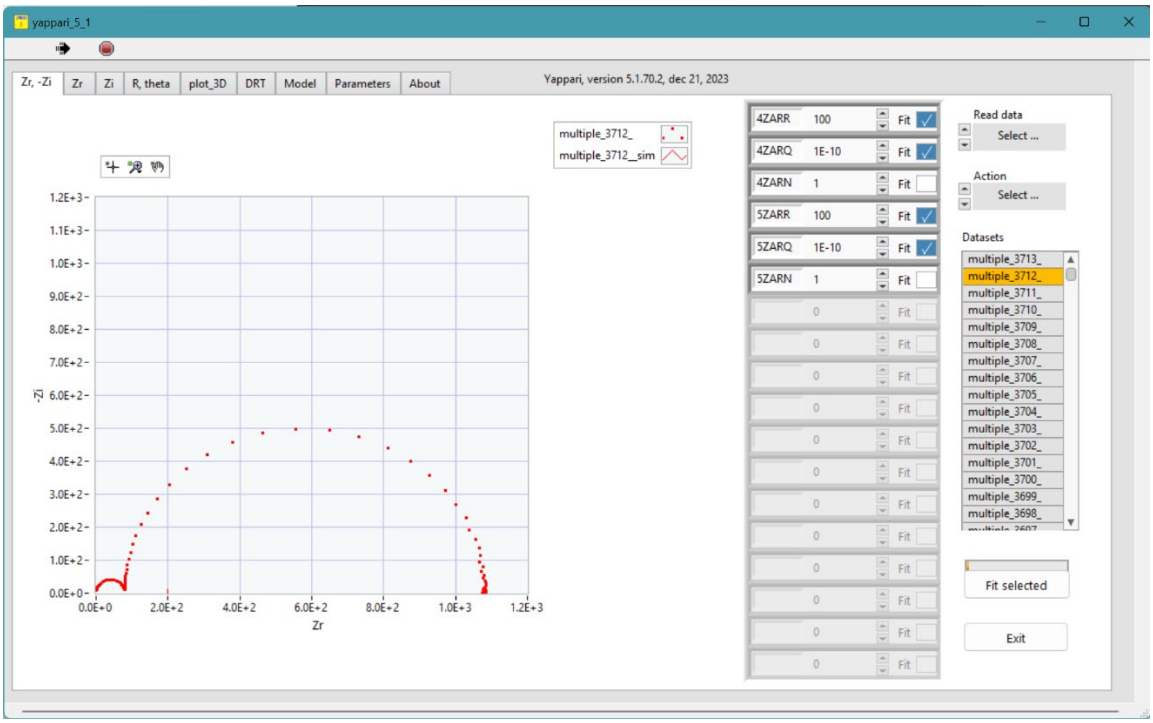

Let’s build a simple circuit with two RQs elements:



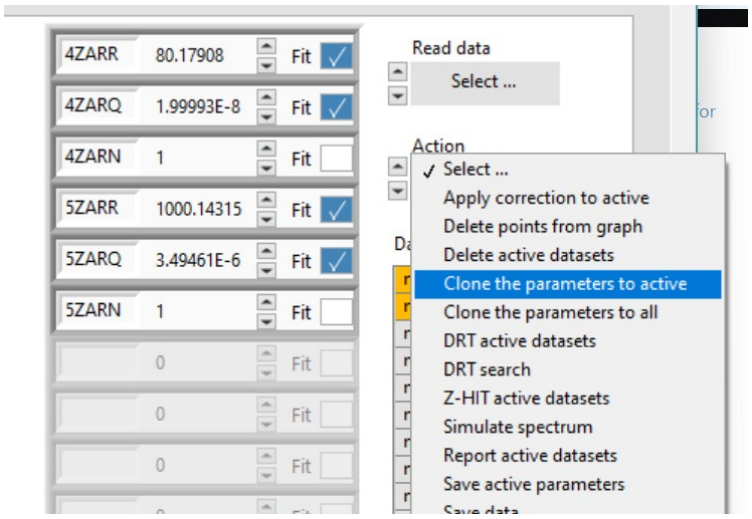

We can fit directly this circuit with the default parameters and we’ll get something like this with experimental and calculated data together with the best fitting parameters:



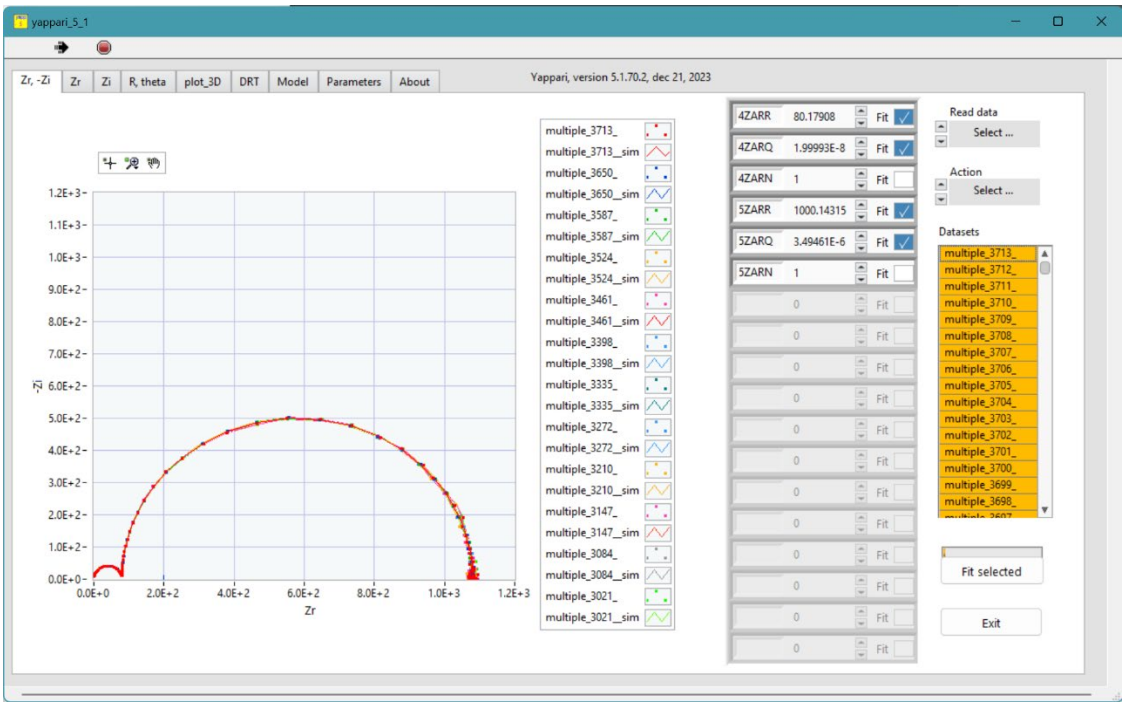

Note that only the selected spectrum (in yellow here in image) is fitted. If we select the second spectrum in the list, one can observe that the parameters are the default ones and that there is no calculated spectrum.




To fit the other spectra we can select the ones of interest and apply "*Fit selected*". This possible but is not recommended as the starting parameters are, in general, far from the ideal values. A better approach is to copy the fitted parameters ("*Clone*") to the other spectra

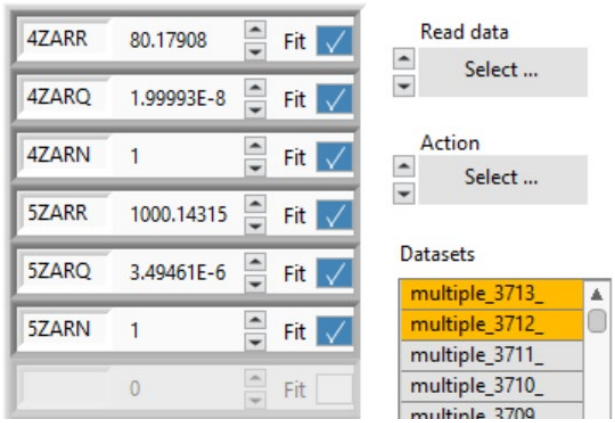



This will ensure similar starting values for the fit of all these spectra. We can select all spectra we want to fit (Ctrl+A to select all the list, 3714 spectra for this case) then *Fit selected*.

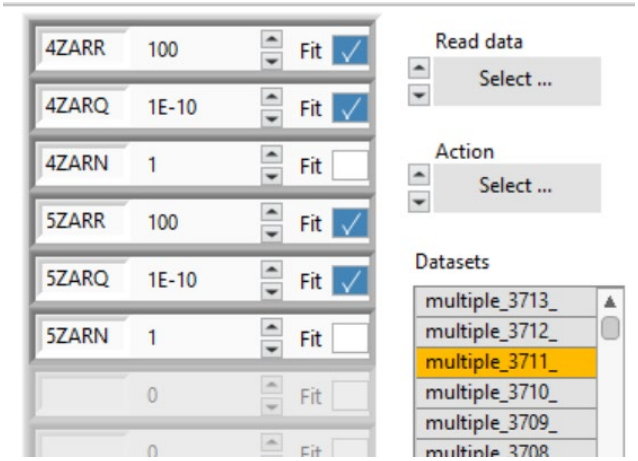



It will take several minutes to fit all these, an indication of the progress is shown at the top of the *Fit selected* button.

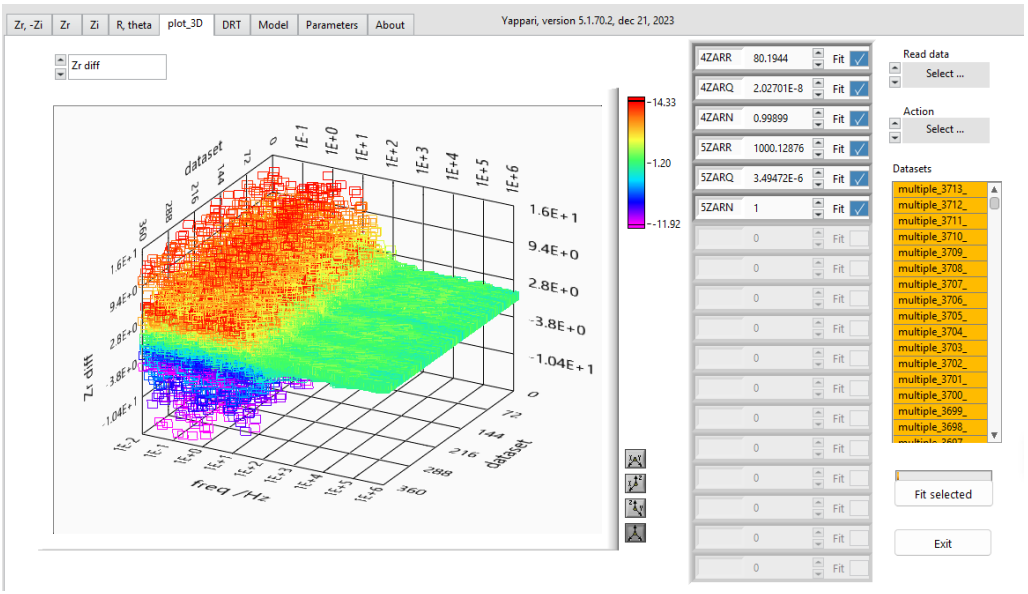
You need to be careful of the manual change of the parameters values : this will propagate to all selected spectra. For example, if you select the first two spectra and impose the fitting of N1 and N2, this will apply for both selected datasets:



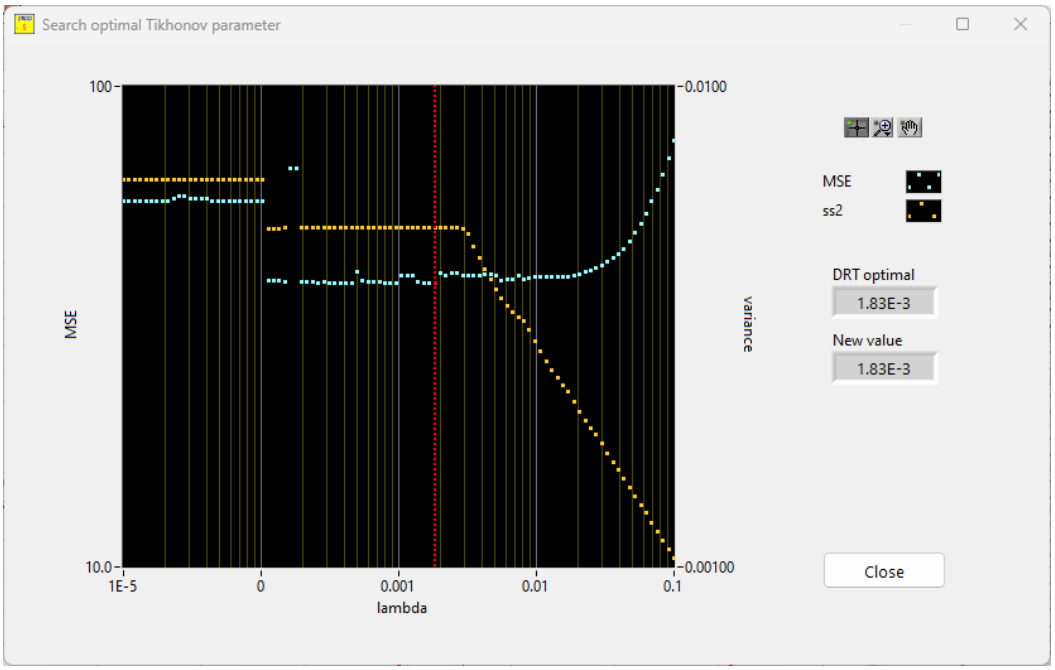

But the third dataset (which was not selected) retains its old values :




Several other functions are available, I recommend to read the instructions carefully. For instance, one can plot differences between the calculated and experimental values for many datasets:




Another function is to calculate and plot the optimal value for Tikhonov regularization, such in the following




In addition you can simulate various spectra, average spectra, add random noise, interpolate, smooth, calculate Z-Hit transform, apply geometrical correction factors, etc. All these functions are described in the help file available on Github. If something is missing or it is not clear, feel free to contact the author or better yet, write tutorials.

Orsay, january 24th 2024