Yappari tutorial : Simulate a spectrum and introduction to DRT

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Data from paper

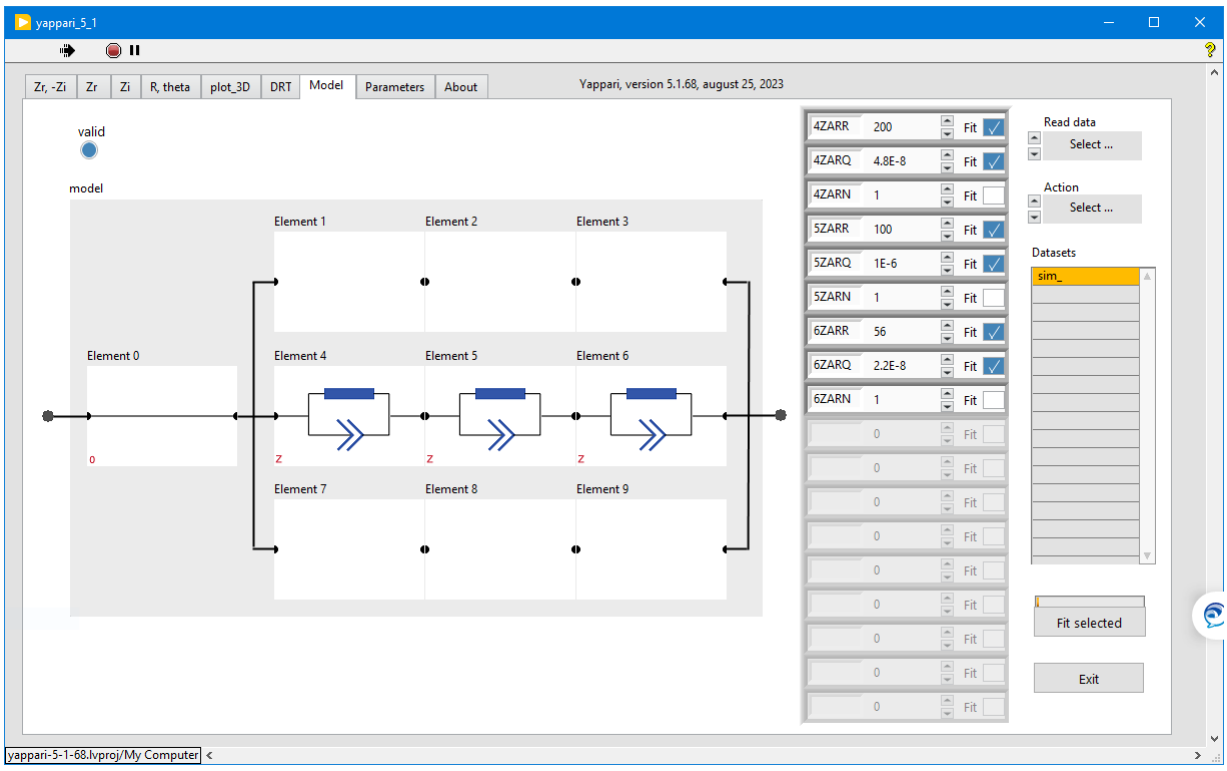
Analysis of Impedance Spectroscopy Measurements of Biological Tissue using the Distribution of Relaxation Times Method, January 2017; DOI: 10.5220/0006253902240228

The simulated circuit discussed in this paper is

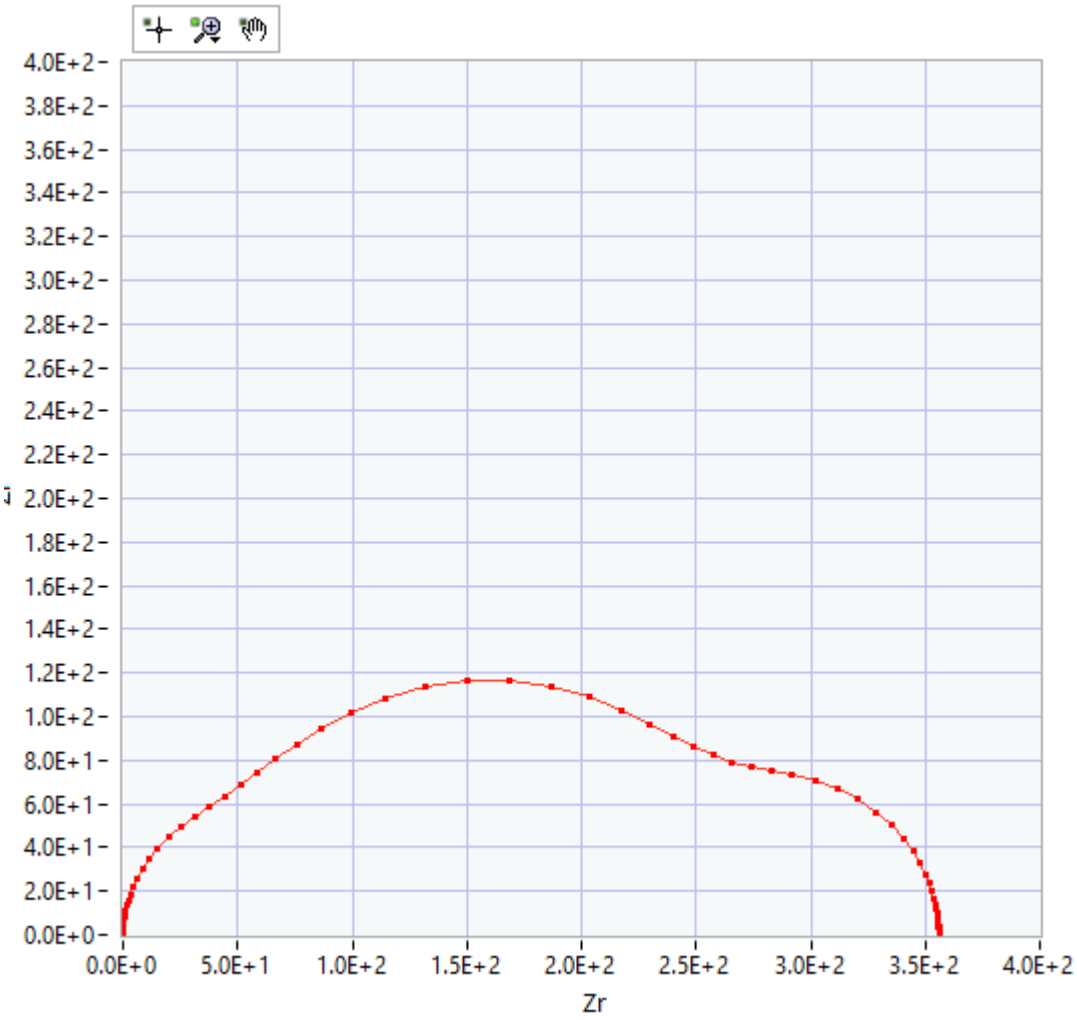
Table 1: Data for simulated RC circuits.

Circuit	R (Ω)	C (nF)	τ (µs)	f_0 (kHz)
RC_1	200.0	48.0	9.6	17.0
RC_2	100.0	1000.0	100.0	1.6
RC_3	56.0	22.0	1.2	130.0

Let's make a model ; fix n=1 so as to have a capacitor instead of Q. Fill the values as in this example then *Action*/*Simulate spectrum*

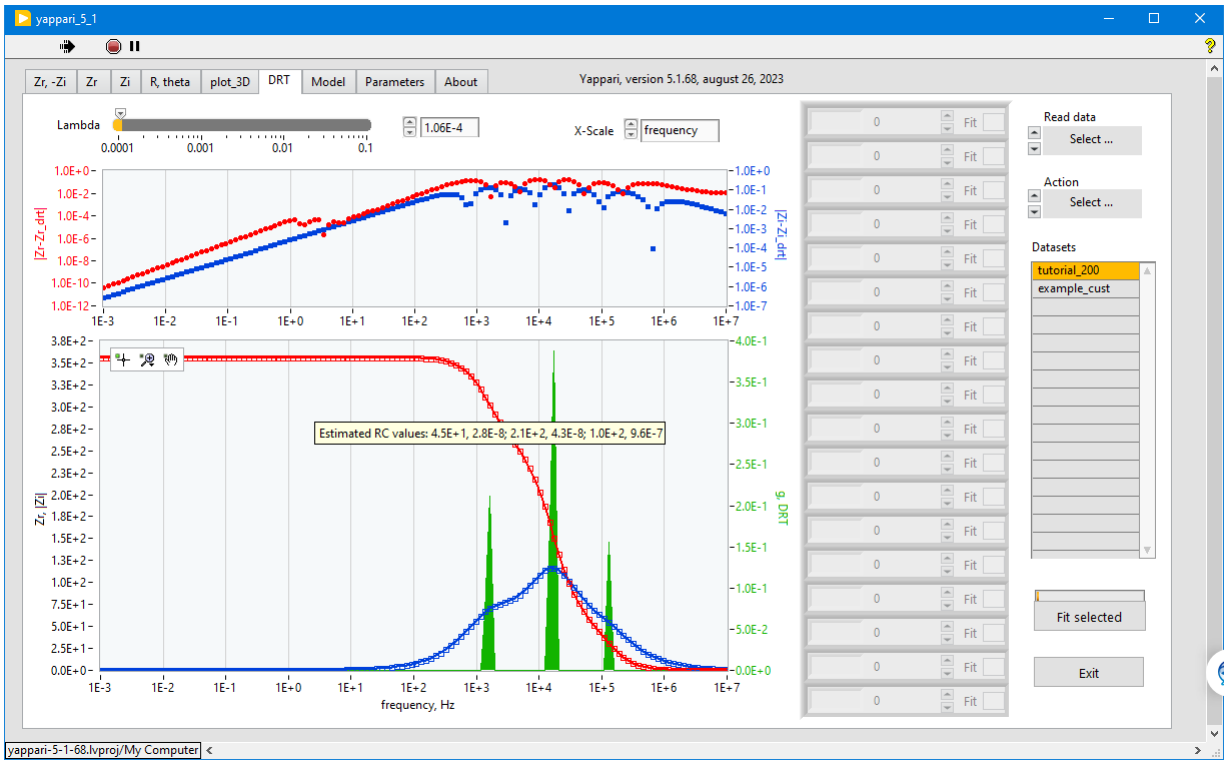


We can see then the Nyquist plot (we can see there are at least three contributions)



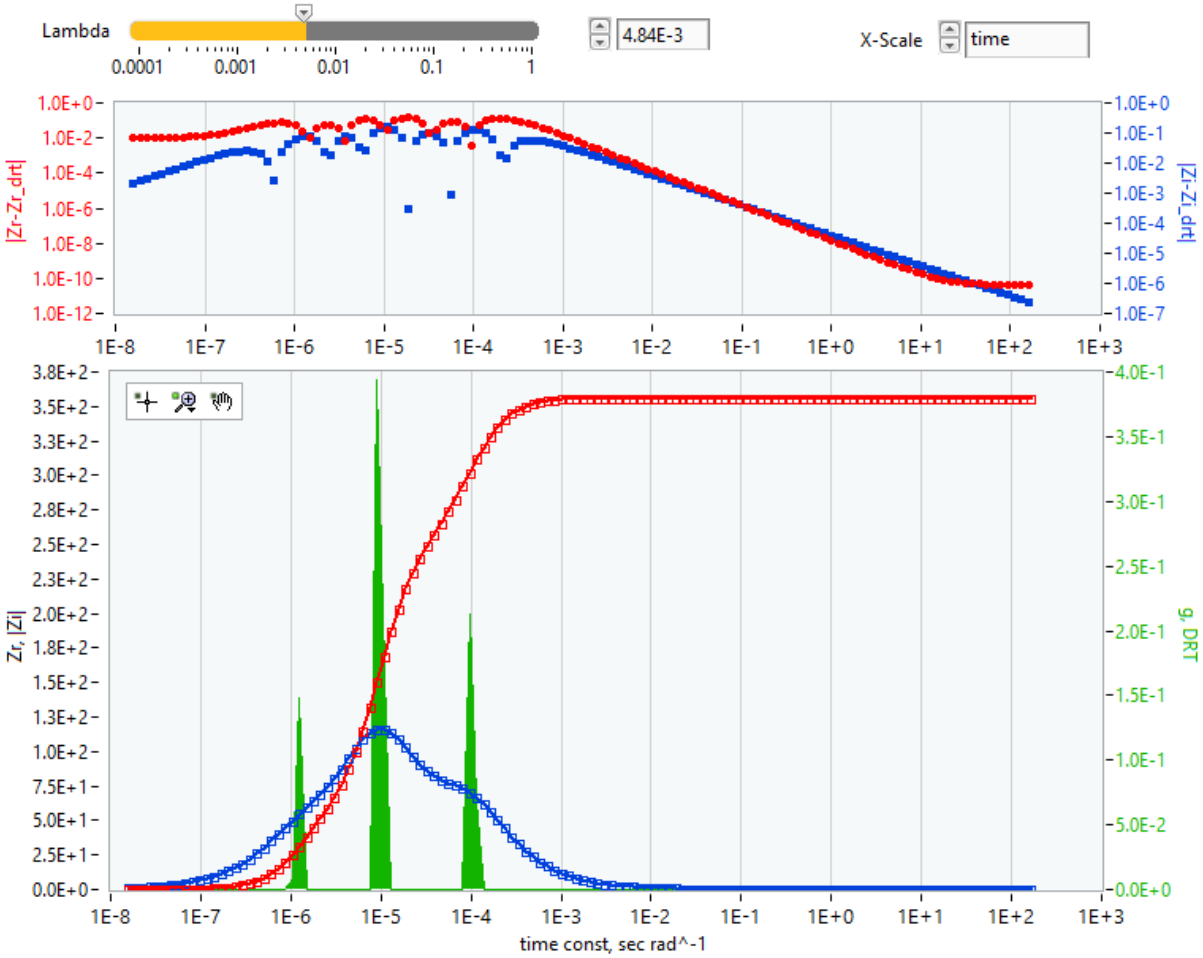
We can perform a simple DRT calculation, with default parameters : *Action*/*DRT active datasets*

Then we can see this nice result :



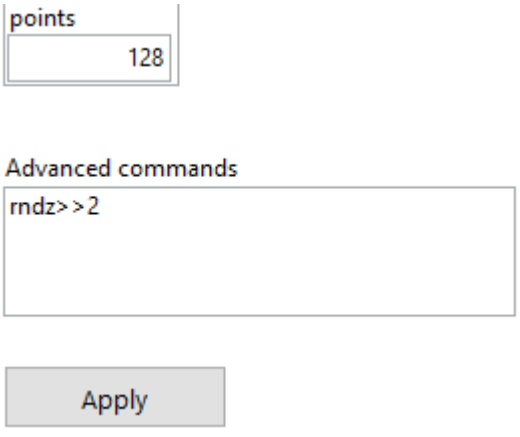
Three contributions, the time constants are in agreement with simulation. The “Tip” of the graph indicates the values of RCs, if the peak are not convoluted. We can see the values calculated from DRT as 45 Ohm, 28nF; 210 Ohm and 43 nF, 100 Ohm and 0.96 microF. These are quite close to the simulated values and can be used as starting point for a fit.

Let’s try to improve this, if possible, by searching an optimal Tikhonov parameter : do *Action*/*Search Lambda*

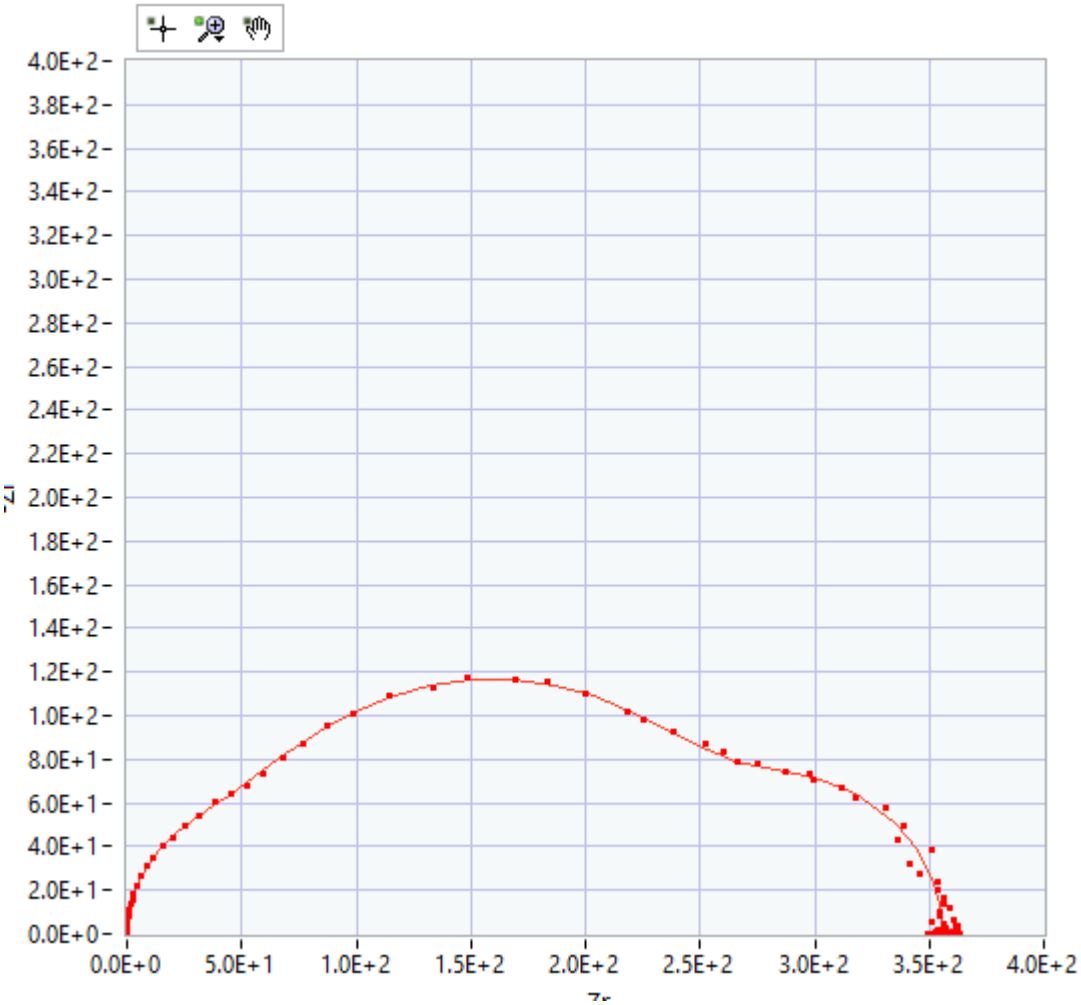


The error is a little bit smaller but not essential.

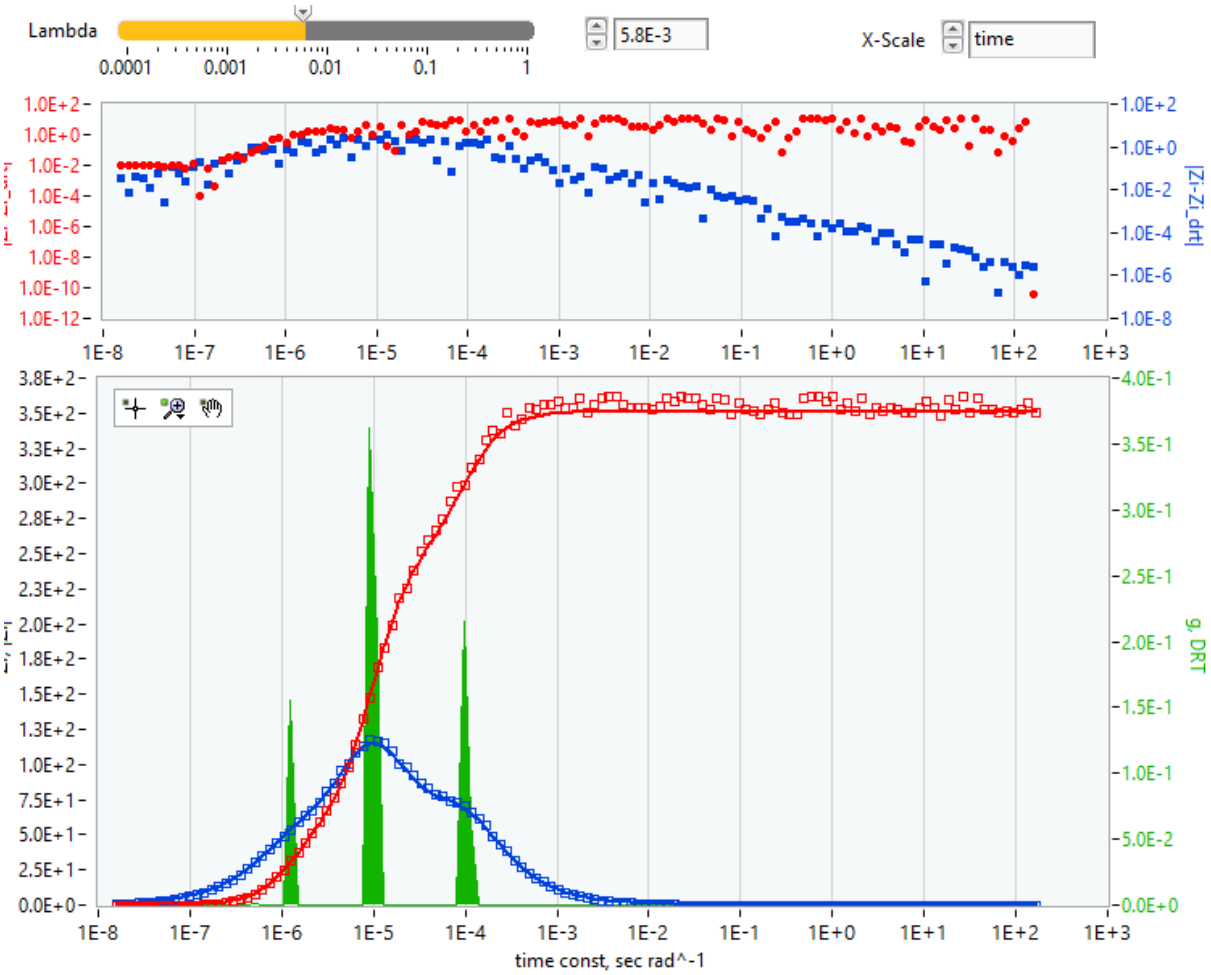
Of course, on simulated data is easy. Let's add some with noise, up to + or - 2% of value of Z. The command to do this is rndz>>2. See Parameters panel, Advanced commands.



If we look at the Nyquist spectrum it is a bit noisy, particularly at low frequency. This looks more like experimental data than the nice simulated spectrum before.

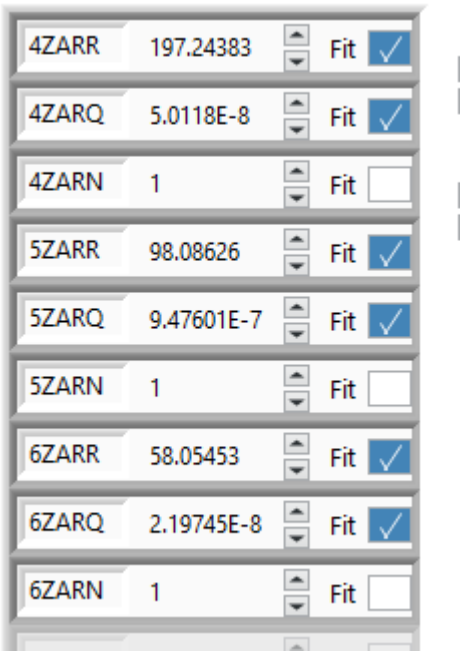


Performing DRT on this data we obtain :



Errors are much larger, it is to be expected, yet we see three contributions at the relaxation times we should.

Let’s perform a classical fit with 3 zarcs, the fit is very good, and the Parameters panel shows the results (close to the simulated values).



And if you want also the error bars use *Report* or *Save parameters*.

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All parameters :
4ZARR: 1.97244E+2, 4ZARQ: 5.01180E-8, 4ZARN: 1.00000E+0, 5ZARR: 9.80863E+1, 5ZARQ:
9.47601E-7, 5ZARN: 1.00000E+0, 6ZARR: 5.80545E+1, 6ZARQ: 2.19745E-8, 6ZARN:
1.00000E+0,
Dataset name : sim_
Fitted parameters and calculated standard error :
4ZARR 1.972E+2 +/- 5.91E+0
4ZARQ 5.012E-8 +/- 3.59E-9
5ZARR 9.809E+1 +/- 0.00E+0
5ZARQ 9.476E-7 +/- 5.13E+0
6ZARR 5.805E+1 +/- 1.12E-7
6ZARQ 2.197E-8 +/- 0.00E+0

R square: 9.984960E-1
Chi square: 1.541100E-1
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