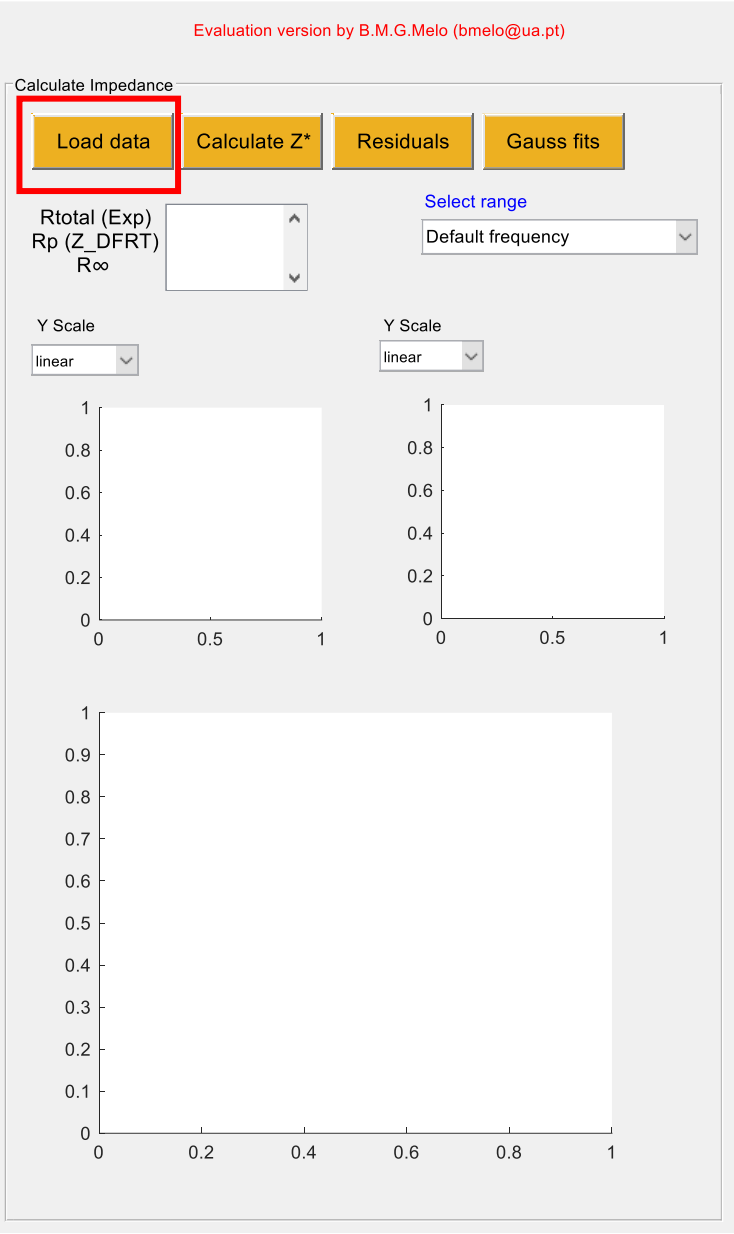
DFRTtoEIS user manual

1. Prepare the text file to the DFRTtoEIS software. Please see the example below.

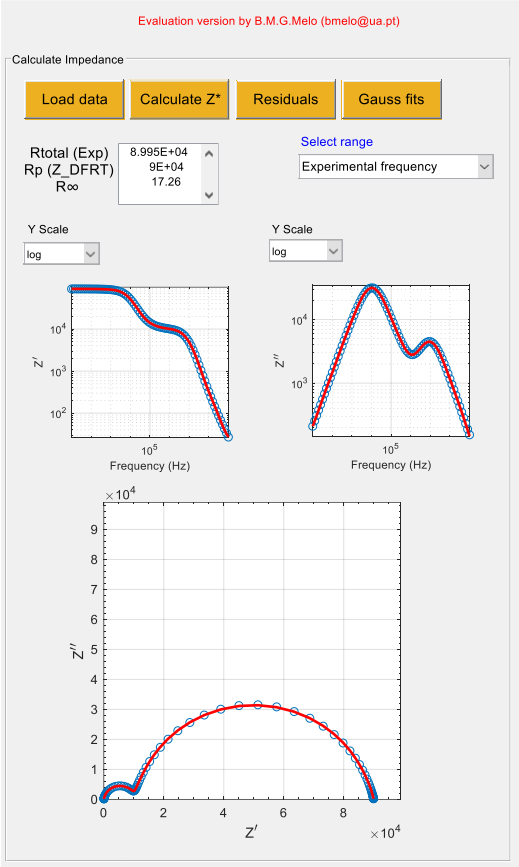
    a. In the first line should be the R_∞ value. If you do not have the R_∞ value obtained by the DFRT fitting, you can leave this value as zero and the program will assume R_∞ as the resistance value at highest frequency. In this example is 114.603 Ω;
    b. From second line onwards, first row (column A in the excel example) should be the time constant (τ) values of the DFRT, second column should be the DFRT values [Rp.G(τ)], third column the experimental frequency, fourth column the Z' values, and fifth column the -Z'' data;
    c. User should save the data as a text file (tab delimited)

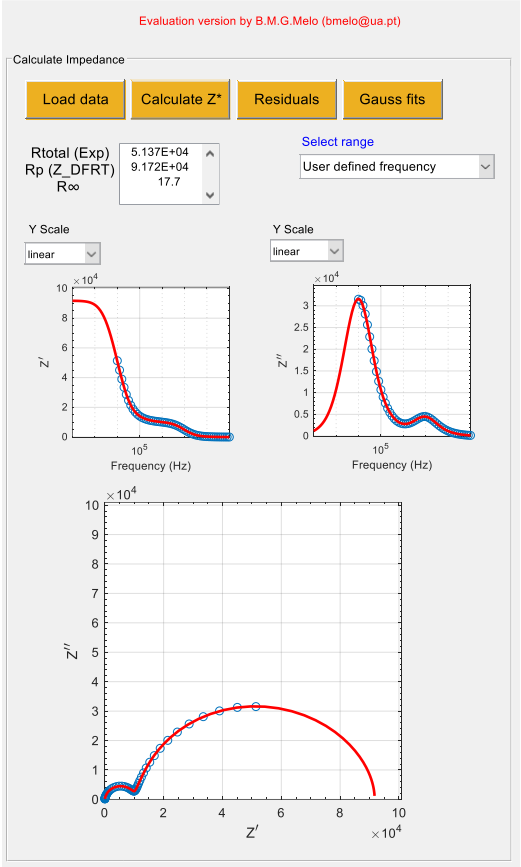
	A	B	C	D	E
1	0				
2	1.00E-07	2.69E-01	1000000	114.603	-324.081
3	1.02E-07	2.99E-01	891251	123.578	-361.046
4	1.03E-07	3.31E-01	794328	133.738	-401.726
5	1.05E-07	3.67E-01	707946	145.435	-446.292
6	1.07E-07	4.07E-01	630957	158.83	-495.277
7	1.09E-07	4.51E-01	562341	174.264	-549.068
8	1.11E-07	4.99E-01	501187	192.074	-608.114
9	1.13E-07	5.51E-01	446684	212.619	-672.935
10	1.15E-07	6.09E-01	398107	236.408	-743.909
11	1.17E-07	6.72E-01	354813	264.027	-821.589
12	1.19E-07	7.41E-01	316228	295.935	-906.493
13	1.21E-07	8.17E-01	281838	332.955	-999.048
14	1.23E-07	8.99E-01	251189	375.856	-1099.77
15	1.25E-07	9.89E-01	223872	425.544	-1209.06
16	1.27E-07	1.09E+00	199526	482.889	-1327.33
17	1.29E-07	1.19E+00	177828	549.523	-1454.79
18	1.31E-07	1.31E+00	158489	626.075	-1591.79
19	1.34E-07	1.44E+00	141254	714.33	-1738.25
20	1.36E-07	1.58E+00	125893	815.678	-1894.15
21	1.38E-07	1.73E+00	112202	931.449	-2059.34
22	1.41E-07	1.89E+00	100000	1063.74	-2232.97
23	1.43E-07	2.07E+00	89125.1	1213.96	-2414.41
24	1.46E-07	2.26E+00	79432.8	1383.85	-2602.3
25	1.48E-07	2.46E+00	70794.6	1575.19	-2795.12
26	1.51E-07	2.69E+00	63095.7	1789.31	-2991.59
27	1.53E-07	2.93E+00	56234.1	2027.86	-3187.88
28	1.56E-07	3.19E+00	50118.7	2291.68	-3382.13
29	1.59E-07	3.47E+00	44668.4	2581.03	-3571.17
30	1.61E-07	3.78E+00	39810.7	2896.11	-3750.79

2. Load the data in the DFRTtoEIS software. Press ***Load data*** and select the text file to import.

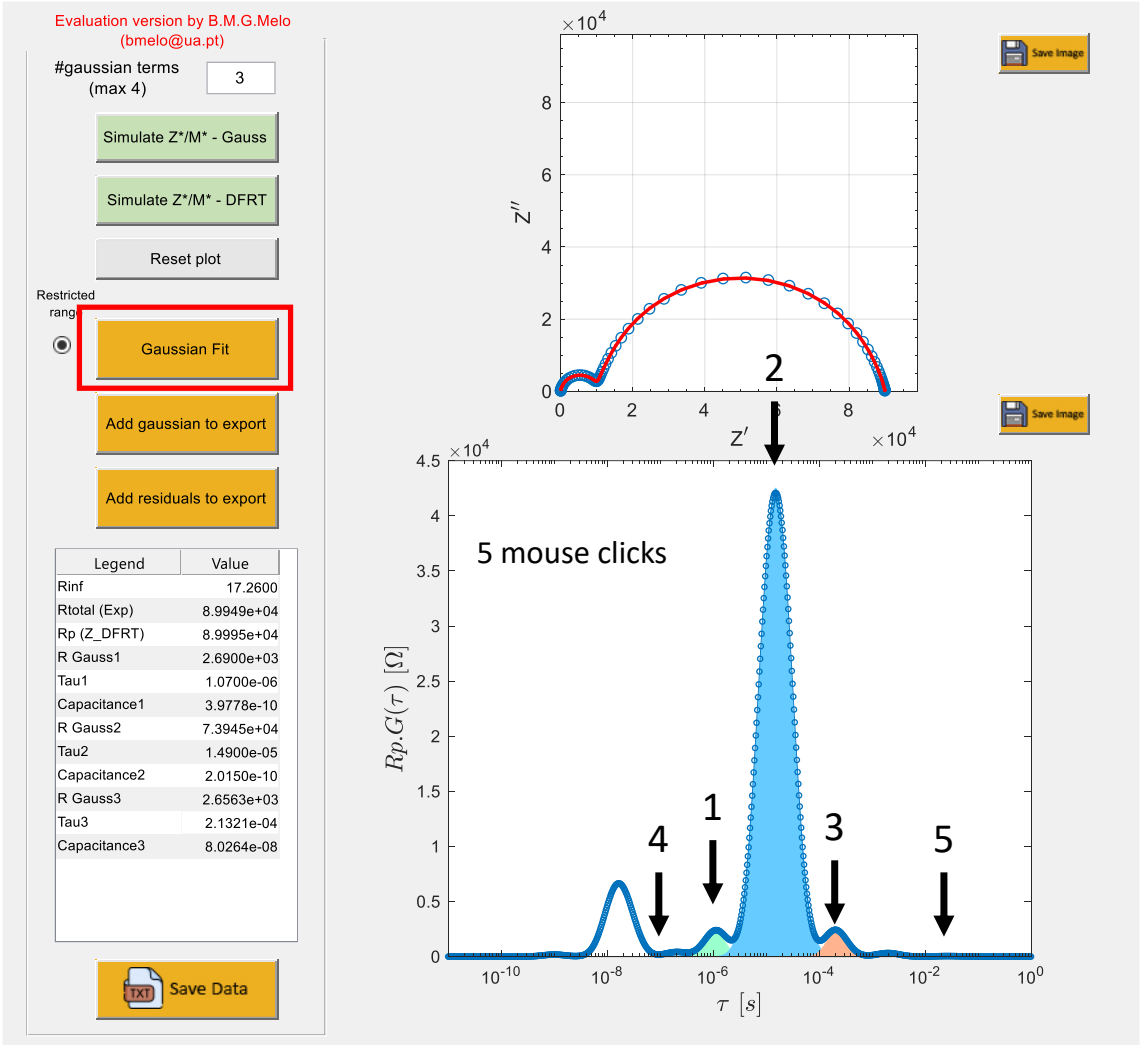


3. Select the desired frequency range from the ***Select range*** menu and press the calculate Z* button. The software will calculate the reconstructed impedance from the imported DFRT and the user can compare it to the experimental impedance.
    a. By default, the option selected is ***default frequency***. This means that the software will calculate the reconstructed impedance based on the frequency range defined as $f = \frac{1}{2\pi\tau}$;
    b. One can calculate the reconstructed impedance to a user-defined frequency range. This option can be useful to extrapolate the impedance data beyond the experimental data;
    c. The user can calculate the reconstructed impedance to the same frequency values as the experimental data loaded in the text file. This option allows to calculate the residuals plot and to evaluate the accuracy of the of the DFRT imported.

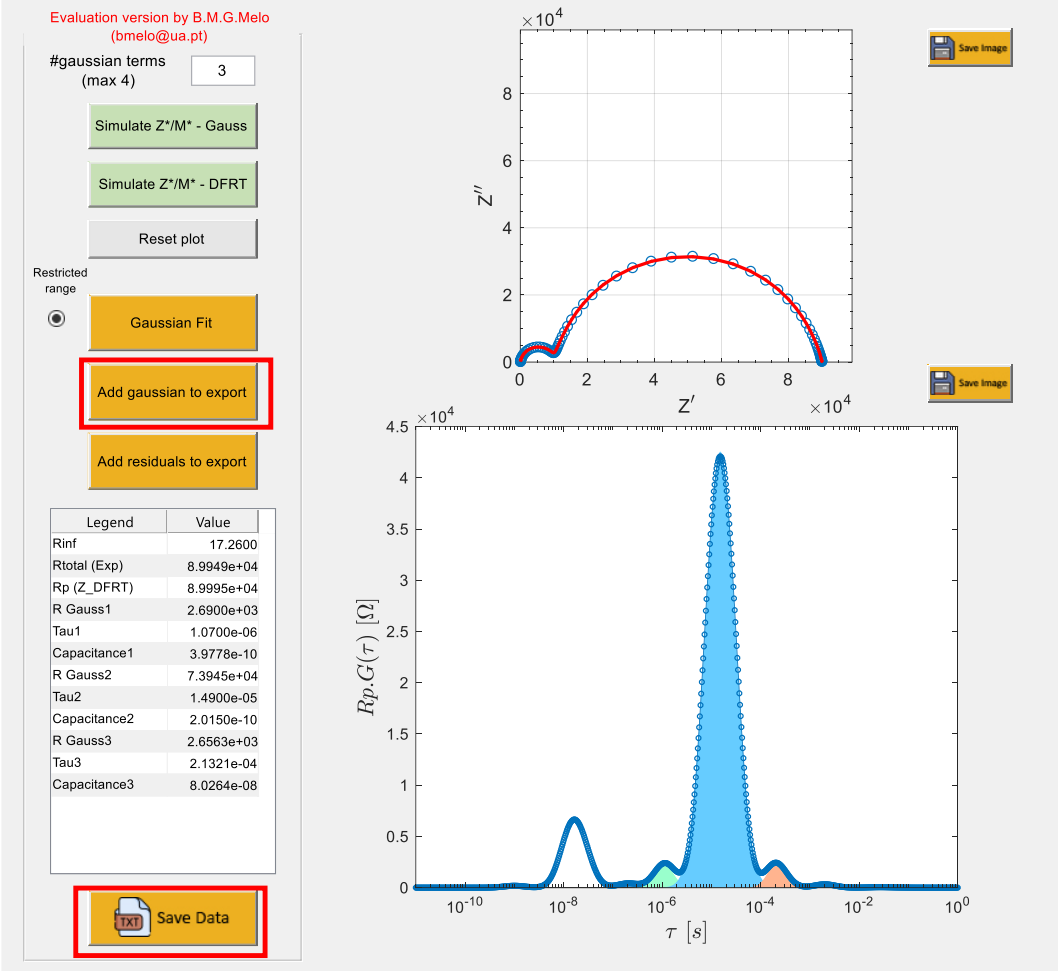




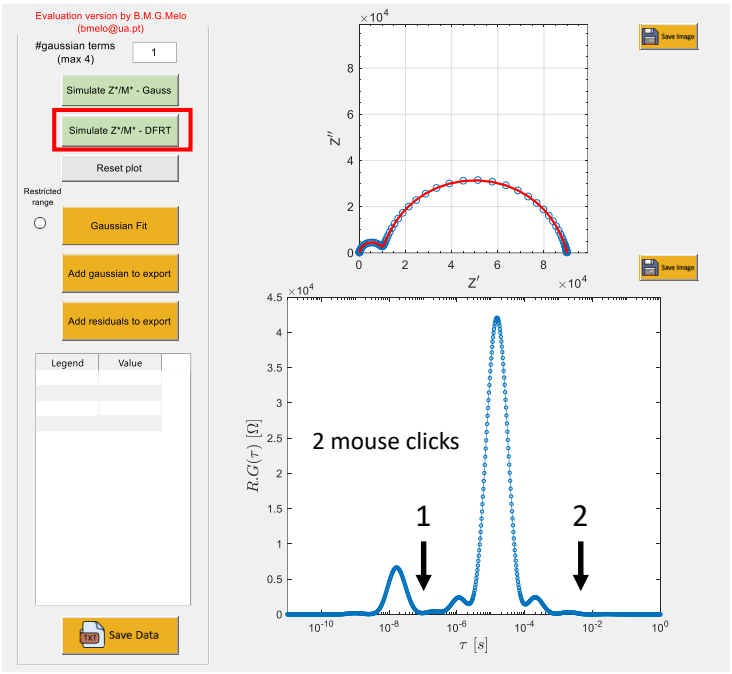
4. The ***Gauss fits*** button opens a new window where the user can adjust the DFRT using Gaussian functions and estimate the values of resistance, capacitance, and time constant of each electrochemical process.
5. Insert the number of ***Gaussian terms*** to adjust and press the ***Gaussian Fit*** button.
    a. If ***Restricted Range*** button is off, the software will request a mouse click to indicate the position of the center of each Gaussian. For 1 ***Gaussian terms***, the user should give 1 mouse click, for 2 ***Gaussian terms***, 2 mouse clicks, and so on. In this fitting mode the software adjusts the Gaussian functions to the entire τ region.
    b. If ***Restricted Range*** button is on, the software requests 1 mouse click for the center of the Gaussian band, plus 2 mouse clicks indicating the τ region which should be considered to the fit. If the user wishes to fit 2 ***Gaussian terms***, then, one should first give the position of each peak (mouse click for first peak, followed by mouse click for the second peak), and then 2 mouse clicks indicating the τ region to fit. In this fitting mode the software adjusts the Gaussian functions to a user defined region which allows to analyze a region of interest.

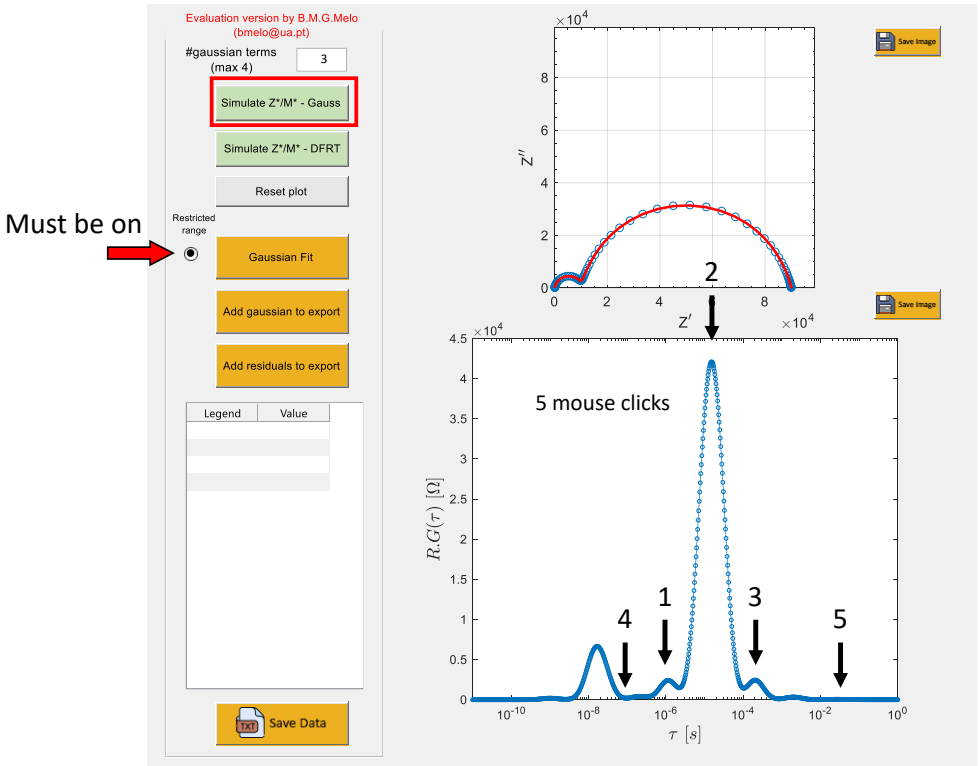


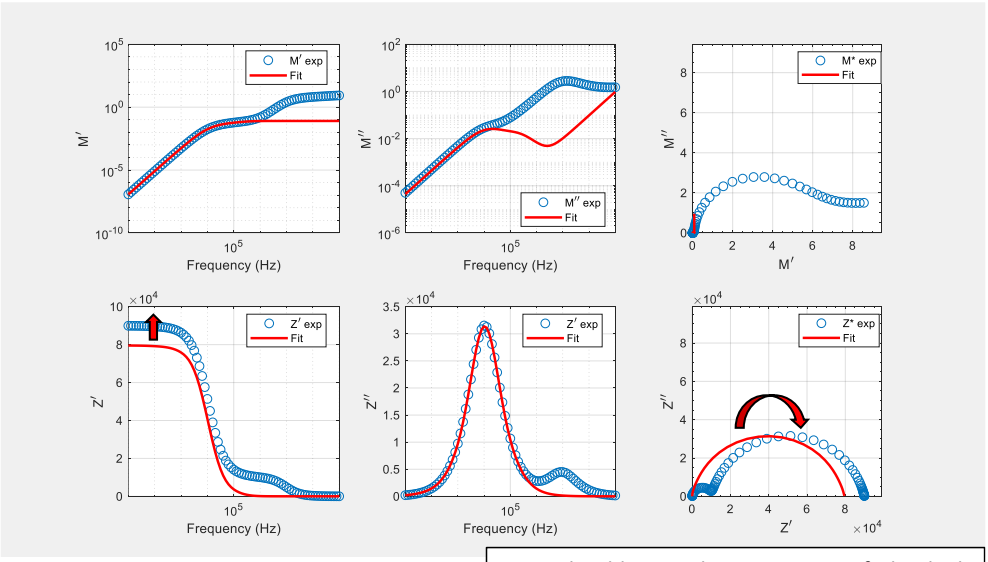
6. When the user is satisfied with a given fit, press the ***Add gaussian to export*** button for each fit. The software allows to add multiple fits to the same output and ***Save Data*** as text file in the end. The software will save the DFRT, the fitted Gaussian functions and the resistance, capacitance, and time constant for each process. A popup menu appears when saving the data explaining the saved data.



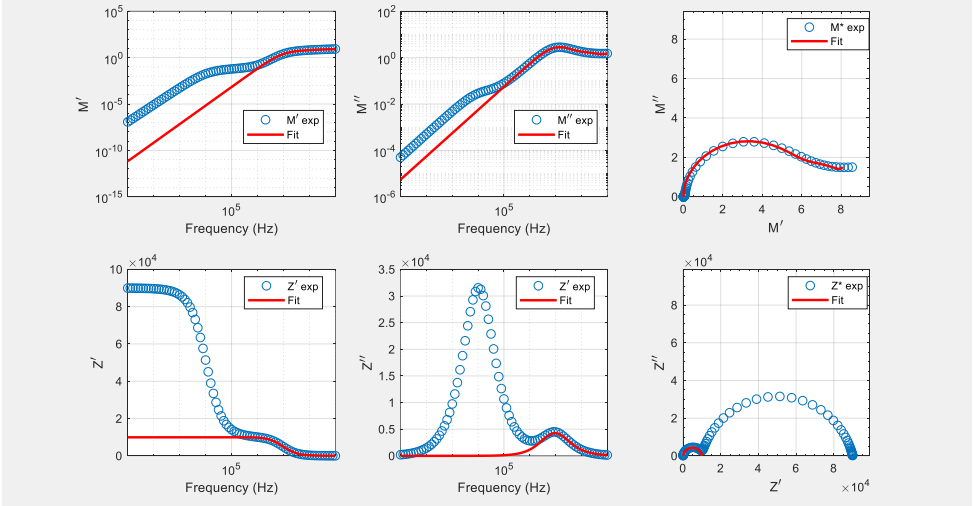
7. The DFRTtoEIS software allows to examine the reconstructed impedance from the entire DFRT or to simulate/reconstruct the complex impedance and the complex dielectric modulus of each individual electrochemical process. The results are given as an output graphic and can be saved to a text file. This option can be helpful to estimate the impedance response of overlapped processes in the frequency domain. One can use the ***Simulate Z*/M* - Gauss*** mode which fits the DFRT to Gaussian functions (same procedure as the ***Gaussian Fit*** option) or the ***Simulate Z*/M* - DFRT*** mode which asks the user to choose the DFRT region to reconstruct.

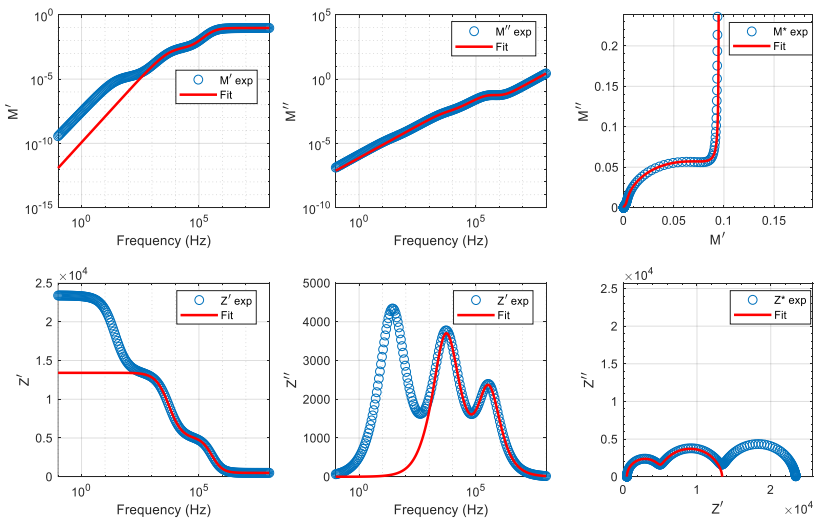






User should sum the resistance of the high frequency process to the Z′ data





The software can calculate the reconstructed Z* and M* data of several processes.