

Supplementary File 3 (S3)

A step-by-step guideline to estimate bulk resistance (R_b) using exclusive EIS software

Introduction

These step-by-step guidelines are to estimate bulk resistance (R_b) of solid polymer electrolyte (SPE) using the exclusive electrochemical impedance spectroscopy (EIS) software named NOVA software (version 2.1.4). We note here, this software may be served as a “black box” for beginners if data analysis or equivalent circuit fitting is done without much appreciation of the models used. Again, a good fit to the experimental impedance data is not sufficient to validate a model adopted from the EIS software. Most EIS software have the capability to analyze the impedance data using its intuitive and effective graphical interface/representation. This NOVA software is frequently used by many researchers and students to estimate electrical properties of the measured impedance using EIS [*e.g.* bulk resistance (R_b), capacitance (C) *etc.*]. However, it is advisable for the beginners to comprehend the fundamental of electrochemical impedance before employing this software for data extraction and later on for data interpretation.

This software has the ability to estimate the R_b value of measured impedance quantity using EIS by employing data fitting based on the empirical equivalent circuit model. Equivalent circuit model can be used to distinguish the existence of possible circuit element in the measured quantity such as resistance, capacitance, double layer capacitance *etc.* Two examples of Nyquist plots for SPEs *i.e.* poly(ethylene oxide) (PEO) added with low and high content of lithium perchlorate (LiClO_4), Case I and Case II, respectively, will be used for the extraction of R_b using EIS software. Similar approach can be applied for both cases as long as the equivalent circuits are to be defined in order to obtain a good fitting for estimation of R_b values.

Estimation of R_b from Nyquist plot for Case I and Case II

1. The first step is to import the impedance data file using the “import data” or “new procedure” functions.

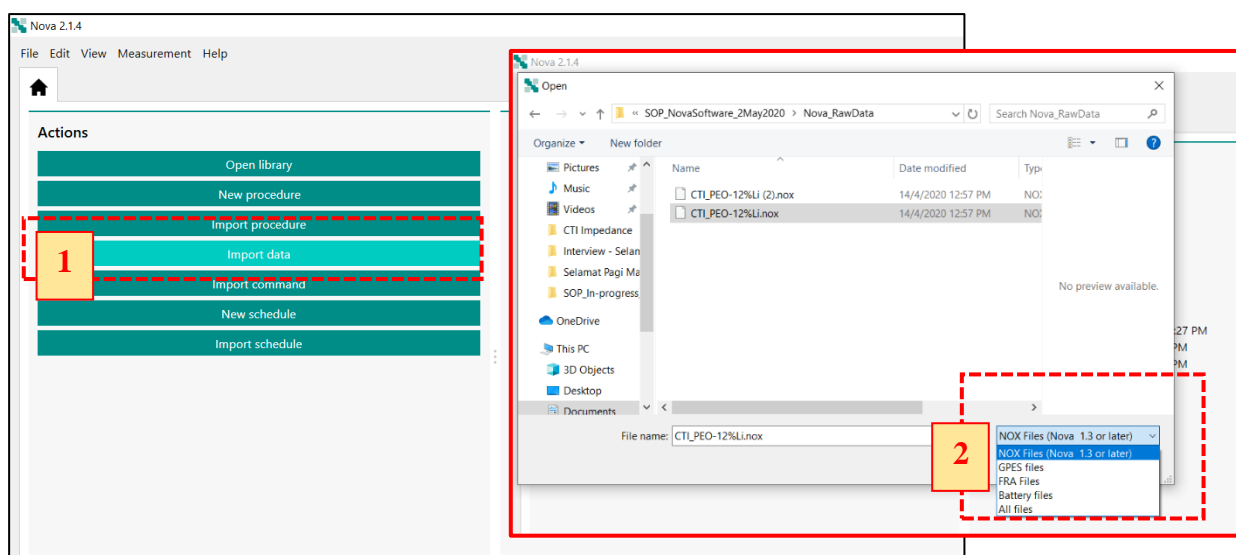


Figure S3.1. Main page of NOVA software

2. Ensure the input commands of the imported data are correctly inserted. You may update accordingly based on the imported files. Then, click “more” to check if the columns are arranged and named accordingly.

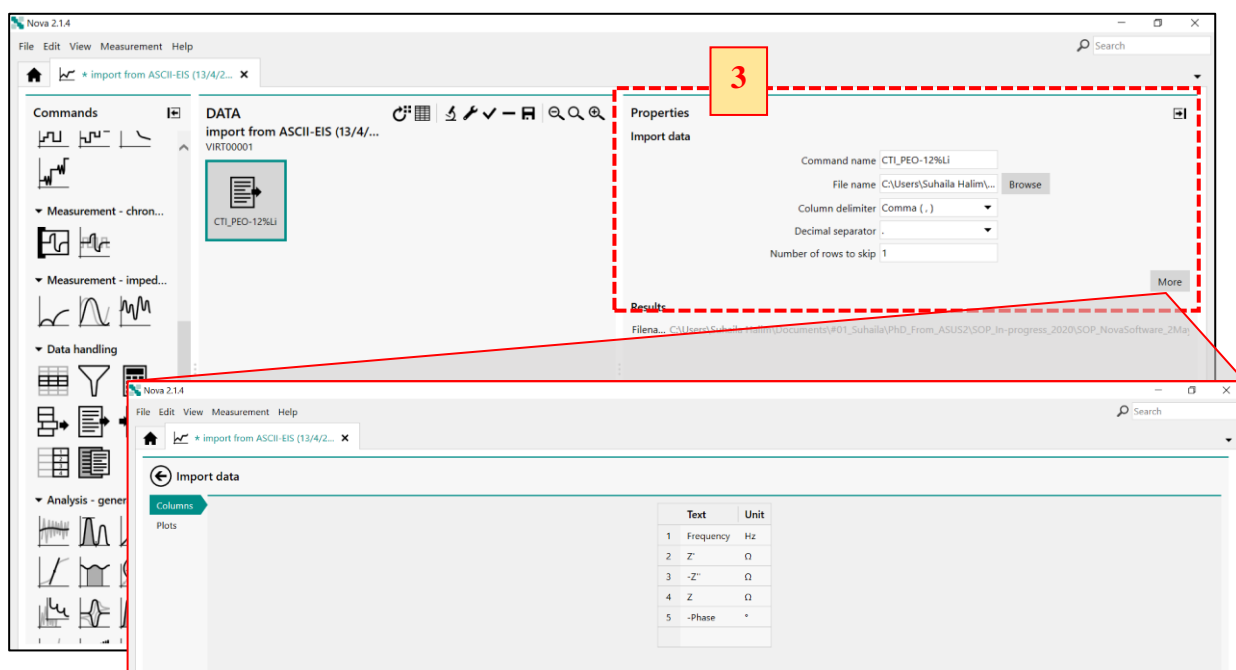
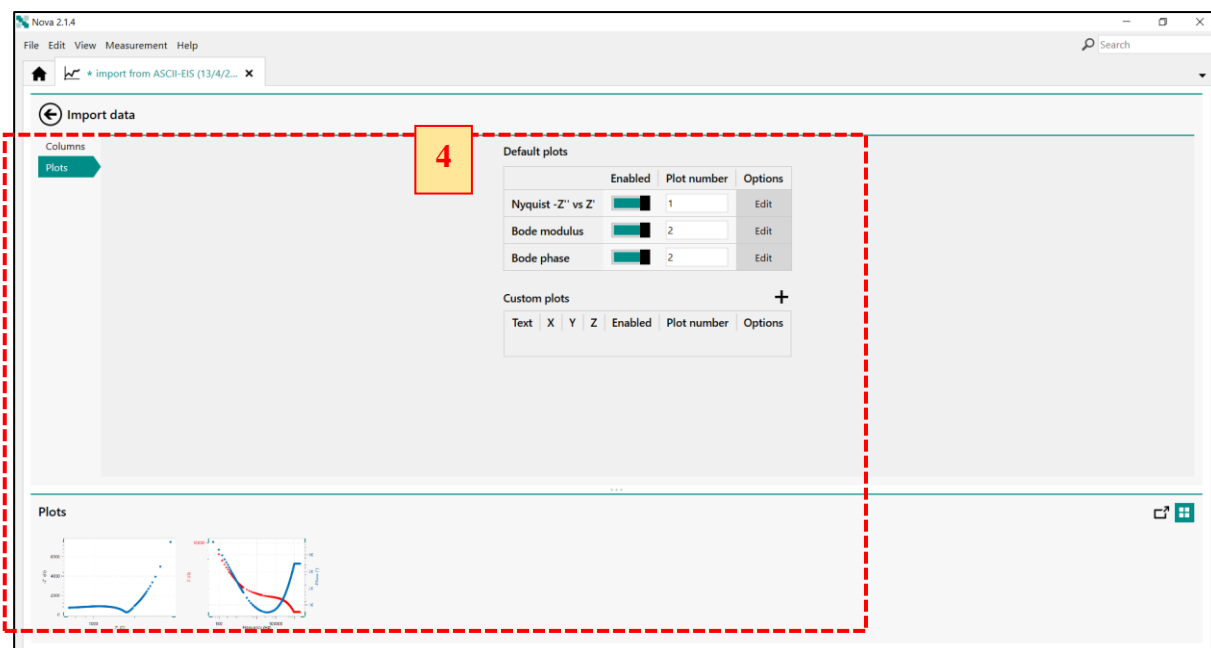


Figure S3.2. Importing impedance data into NOVA software

3. The software has the option to display various types of plots and customize plots based on the preference of the user. In this SOP, we will fit the Nyquist plot using the built-in interface to estimate the R_b of the measured quantity.



FigureS3.3. Optional plots available in the NOVA software

4. Next, fit the impedance data of the Nyquist plot using the built-in functional interface named “Fit and simulation” in order to extract the electrical properties (*e.g.* R_b of the electrolyte) of the measured impedance. Click the “Fit and simulation” interface to proceed the next step.

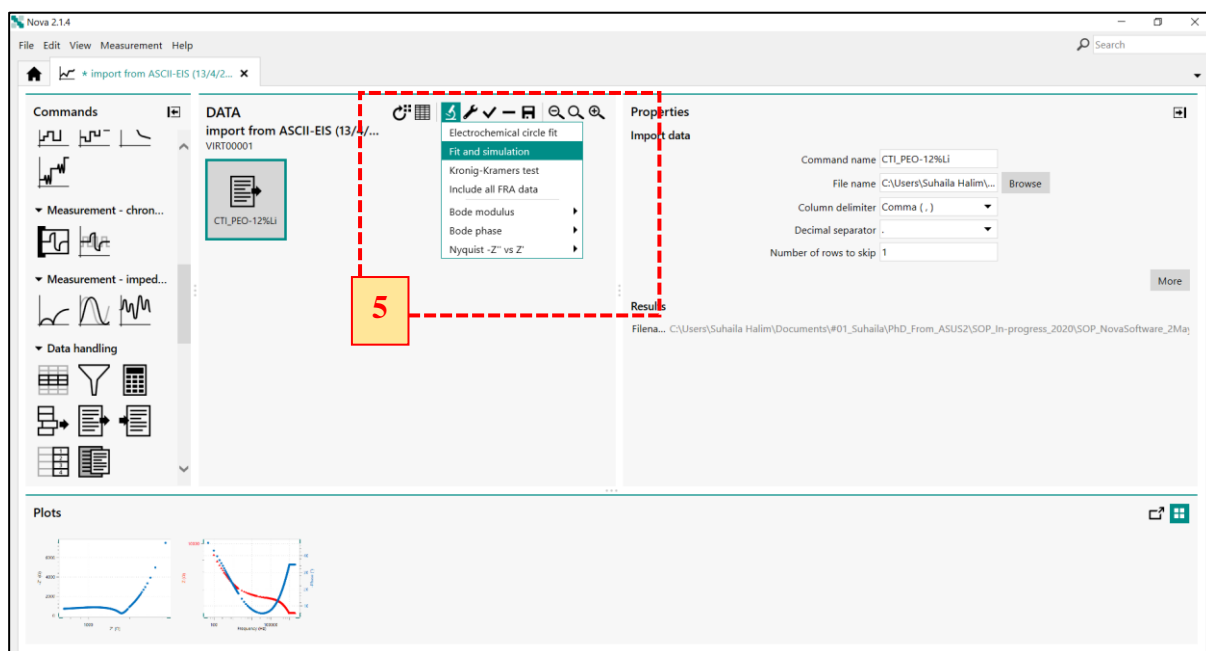


Figure S3.4. In-built fitting and simulation regression function in the NOVA software

- The exclamation mark on right-corner of the data box indicates the data fitting and simulation cannot be performed correctly unless the correct equivalent circuit is demonstrated carefully. The equivalent circuit can be inserted in the “window” as shown in **Figure S3.5** below. The proposed or pre-defined equivalent circuit can be edited by right-click and select the “add element” to add the possible elements that may fit-well for the measured impedance. The default initial values of the circuit elements will be displayed in blue (refer to **Figure S3.6**) and the values will be calculated against the pre-defined equivalent circuit illustrated in the editor window of “Fit and simulation” function (refer to **Figure S3.8**). *Special attention:* It is of prime importance for user to be able to propose an equivalent circuit which *may represent* the measured impedance before performing any fitting and simulation for meaningful data extraction subsequently. A good fit of the measured impedance using one equivalent circuit does not “validate” the model used, since a given impedance data set can be fitted with more than one unique equivalent circuits.

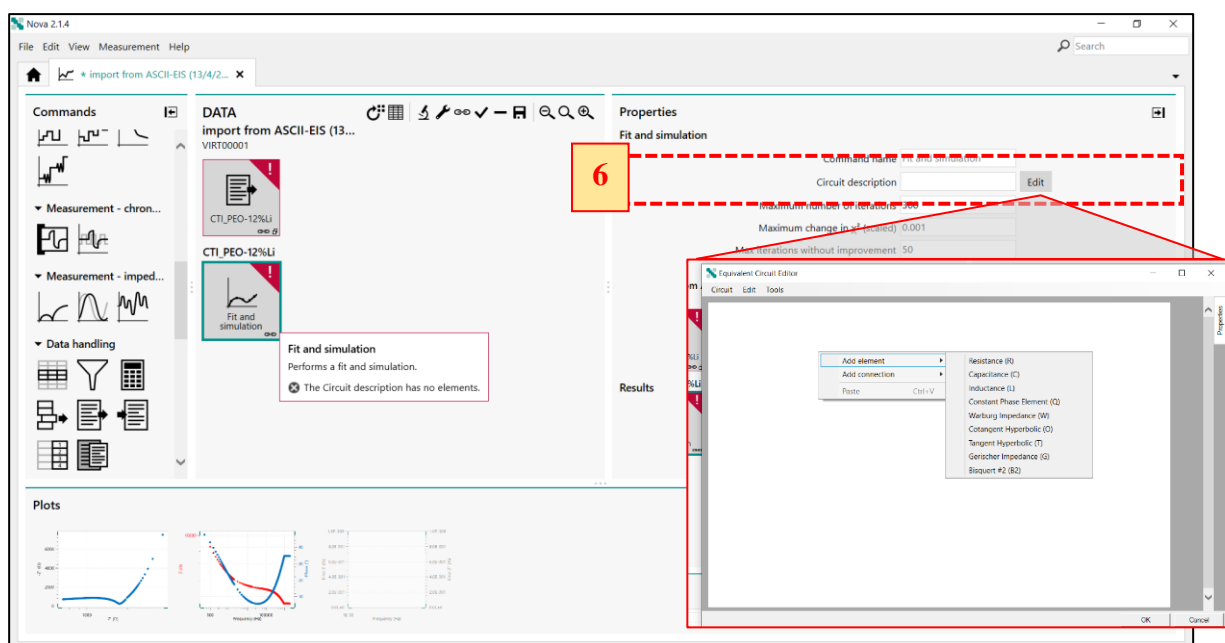


Figure S3.5. The execution of fit and simulation function in NOVA software

- One pre-defined equivalent circuit for Case II that may represent the binary PEO-LiClO₄ SPE at 25 °C. The Nyquist plot will be fitted with the pre-defined equivalent circuit for estimation R_b value.

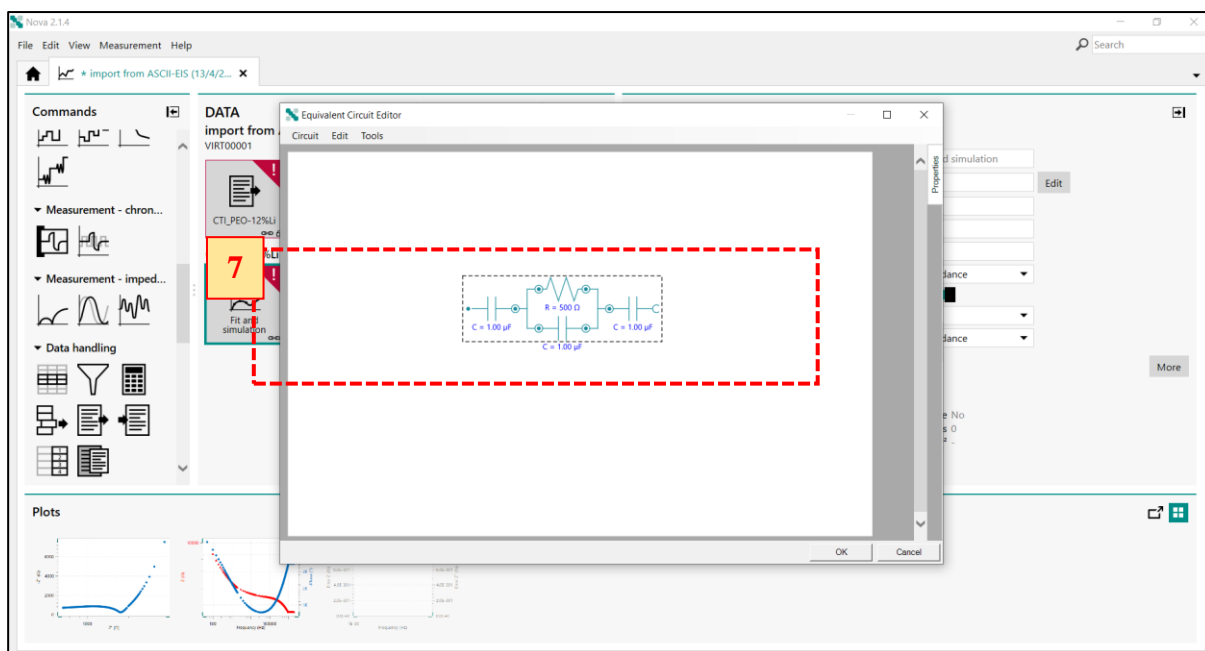


Figure S3.6. The equivalent circuit proposed for PEO added with 11 wt.% of LiClO_4 solid polymer electrolyte at 25 °C

7. After inserting the proposed equivalent circuit, the exclamation mark on the data box disappears and the impedance data points will be fitted as shown by the solid blue curve, indicating the completion of fitting and calculation. Then, click on the Nyquist plot to enlarge the plot.

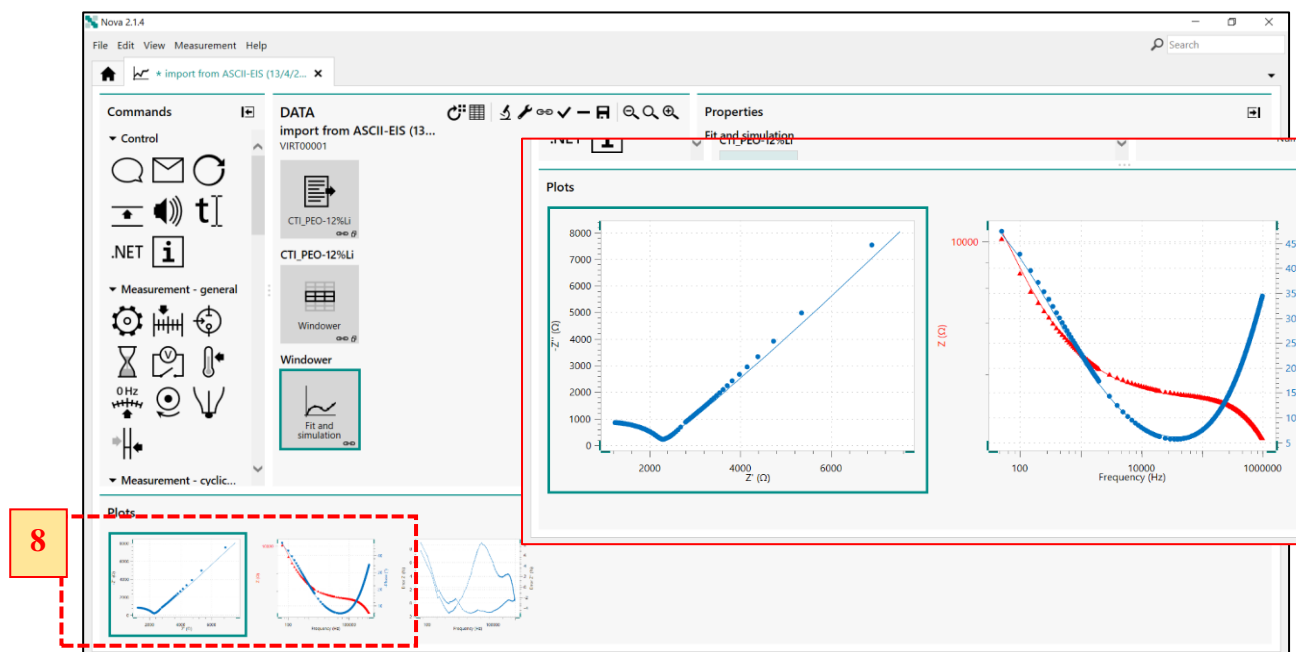


Figure S3.7. The fitting of the experimental data with the proposed equivalent circuit for PEO added with 11 wt.% of LiClO_4 SPE at 25 °C

8. After enlargement of the Nyquist plot, the R_b value of the measured impedance calculated using the equivalent circuit model can be extracted from the “equivalent circuit editor window” located at the properties. For instance, the R_b value of the measured impedance of PEO added with 11 wt.% of LiClO_4 is equal to $2.49 \times 10^3 \Omega$ (c.f. **Figure S3.8**).

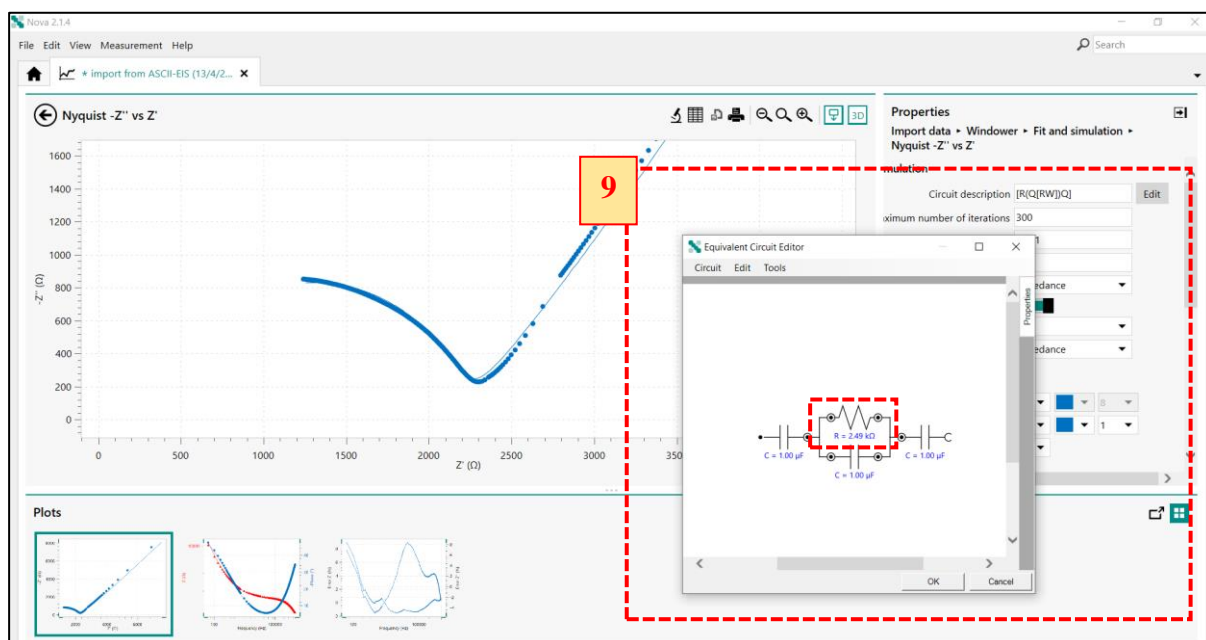


Figure S3.8. The estimation of R_b value for PEO added with 11 wt.% of LiClO_4 SPE at 25 °C

9. Then, the same steps of number 5 to number 9 from the Section 1 can be applied to estimate R_b value of the measured impedance with an equivalent circuit using the “Fit and simulation” function. The R_b value of the measured impedance can be extracted from the “equivalent circuit editor window” located at the properties. For instance, the R_b value of the measured impedance PEO added with 0.5 wt.% of LiClO_4 (Case I) is equal to $2.82 \times 10^6 \Omega$ (c.f. **Figure S3.8**).

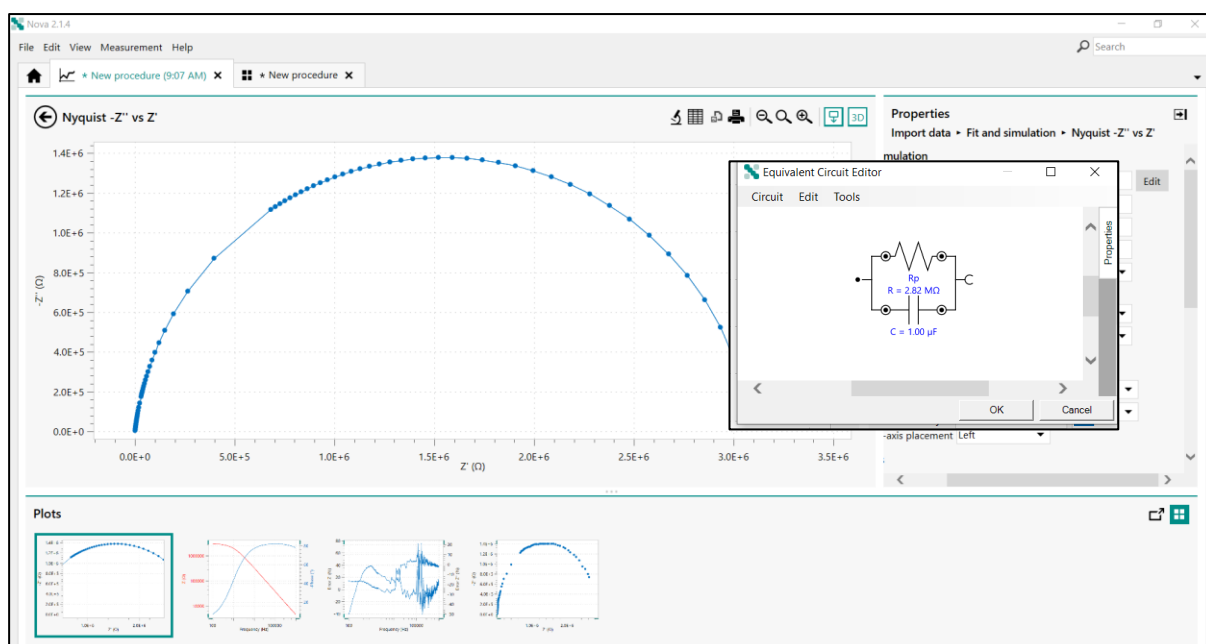


Figure S3.9. The proposed equivalent circuit for PEO added with 0.5 wt.% of LiClO_4 SPE at 25 °C.