Setting up experiment series with SetupSeries

User Manual

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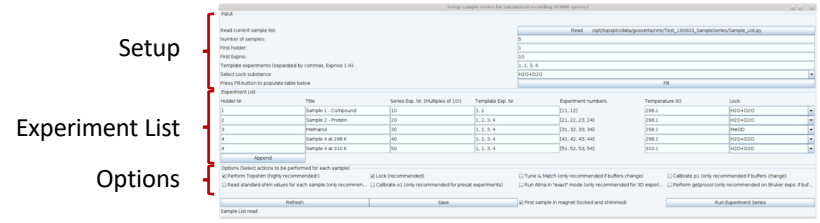
Setting up an experiment series

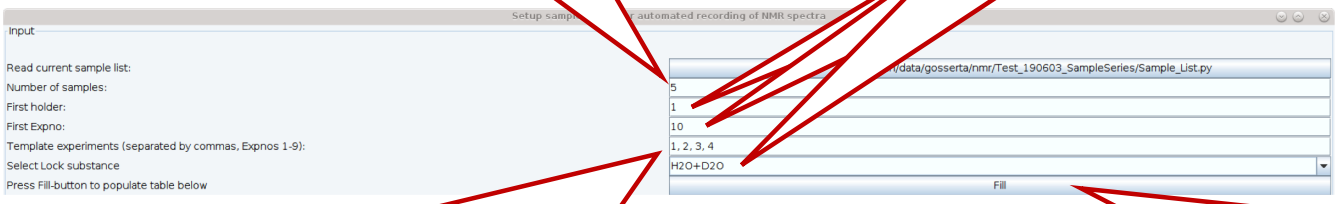
1. **Prepare a new dataset** and copy all required types of experiments as “templates” into Exp. Nr. 1–9. Perform the necessary pulse calibrations and set the desired acquisition parameters.

2. **Type** “**SetupSeries**” into Topspin command line. The following window will appear. It has three areas – Setup, Experiment List and Options – that are described in greater detail below.

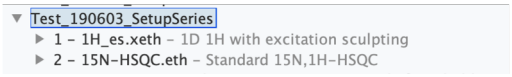


3. Set the number of samples.
This will determine the number of input fields in the experiment list below.

4. Select number of first holder, first experiment (≥10) and lock substance.
These will be used for populating the input fields below.

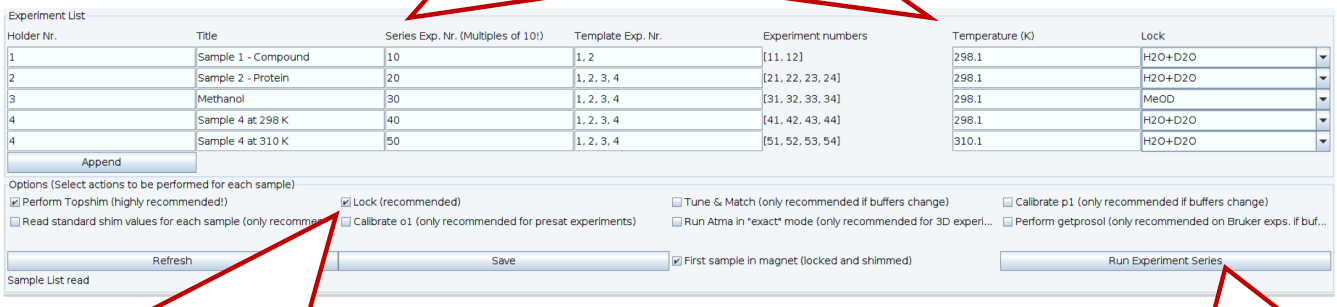


5. Set the numbers of the template experiments.
Template experiments with adapted parameters must be copied beforehand to experiment numbers 1–9 in the current dataset.



6. Press ‘Fill’ Button to populate the table below.
Attention, this function overwrites the entries in the table below.

7. Manually edit fields, if needed.
Press the ‘refresh’ button at the bottom after editing.



8. Choose calibrations to be performed for each sample.
Calibrations are typically only needed if the buffer or the temperature changes compared to the template experiments. Calibrations will be performed in the Series Exp. Nr. and results are stored there (wobble curve, shim map etc.).

9. Start measurements.

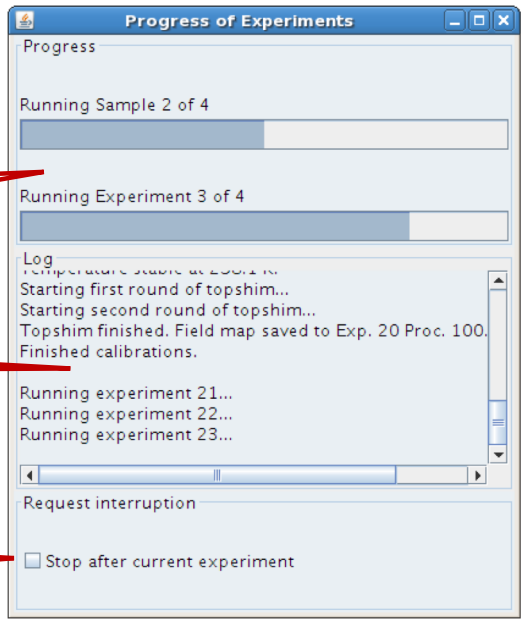
Running an experiment series

After pressing the 'Run' button, the dialog below will open and the experiments are started:

Bars inform about the current progress Samples are shown in the first bar, in the second bar the experiments per sample are shown, where the calibrations count as experiment '0'

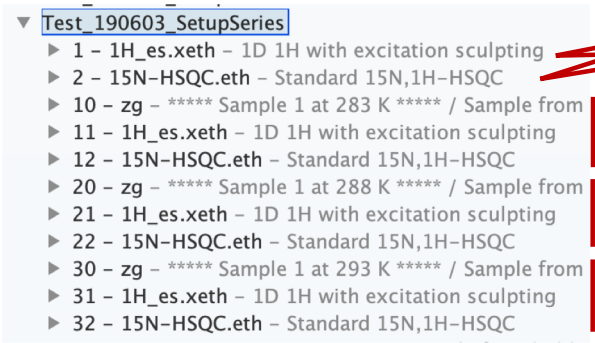
The Log window shows the current steps

In case a series should be stopped, activate this check box. Experiments will be stopped at the next safe moment (i.e. after completing an experiment or after calibrations.)



Structure of experiment folders generated in TopSpin

After pressing the 'Run' button the script will progressively generate new experiments using the following structure:

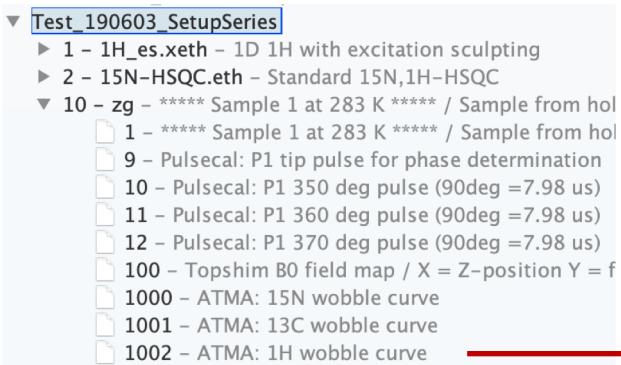


Experiments 1–9 are the template experiments previously setup by the user.

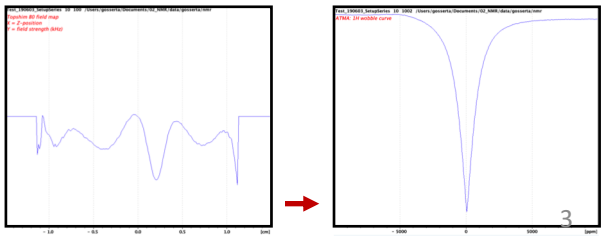
For each sample (or each line in the SetupSeries window) experiment folders will be generated.

- Experiment …0 (10, 20, 30 …) will contain the title and the calibration experiments (see also below).
- Experiments ..1, ..2, etc. will contain the actual experiments as defined by the template experiments above (here 1 and 2).

Details on calibration experiments:



Depending on the options chosen, data from the calibration experiments will be written to subprocesses in experiment number …0

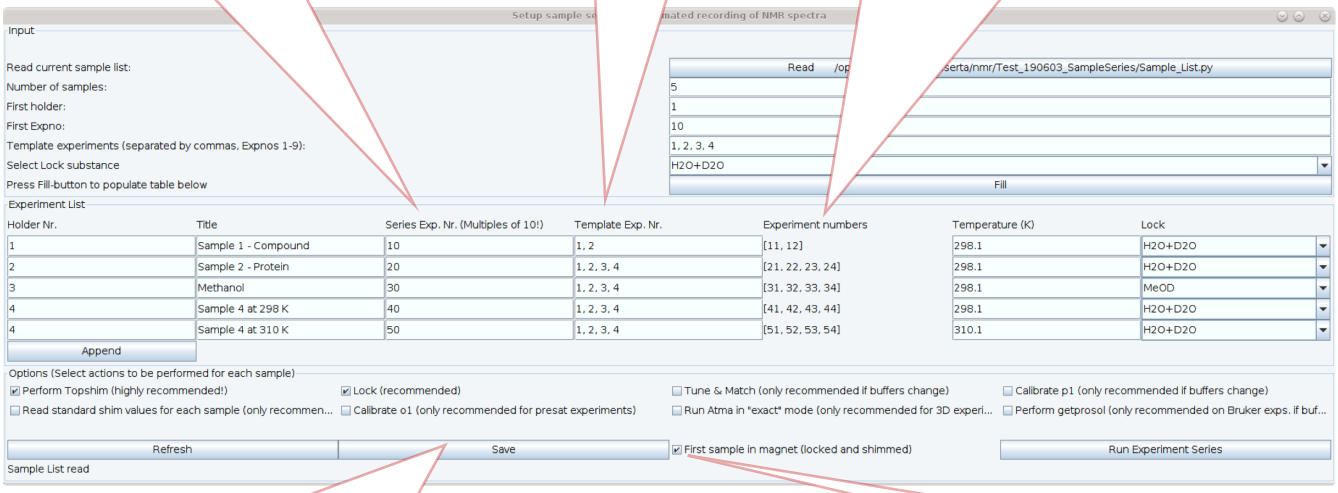


Further options and explanations

This field determines the first experiment number in a series. Typically multiples of 10 are used.

Determine which of the template experiments should be recorded in each series.

The actual experiment numbers are automatically calculated (= Series Exp. Nr. + Template Exp. Nr.) and displayed here (press ‘Refresh’ button at bottom left to force a refresh)



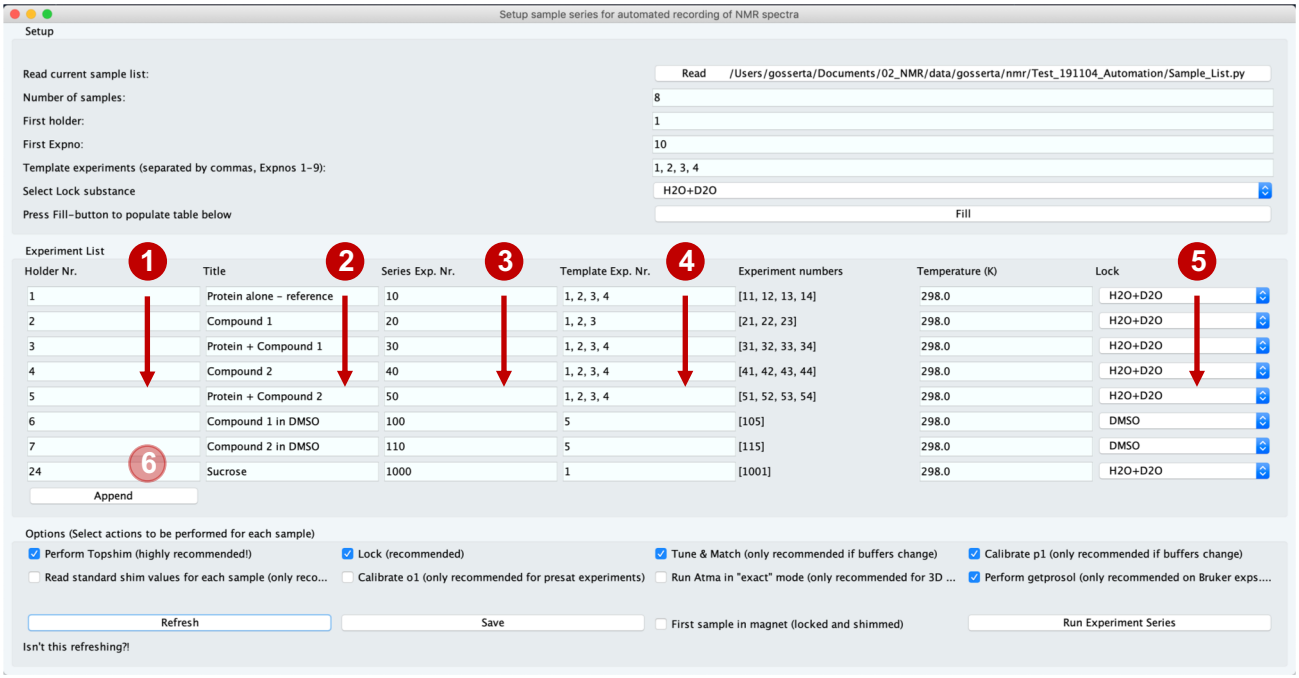
Save current list to Sample_List.py. The settings can be loaded again later with the ‘Read’ button at the top right.

Set, if first sample is already locked and shimmed. This will omit shimming and tuning for first sample.

Examples

Multiple samples with multiple experiments

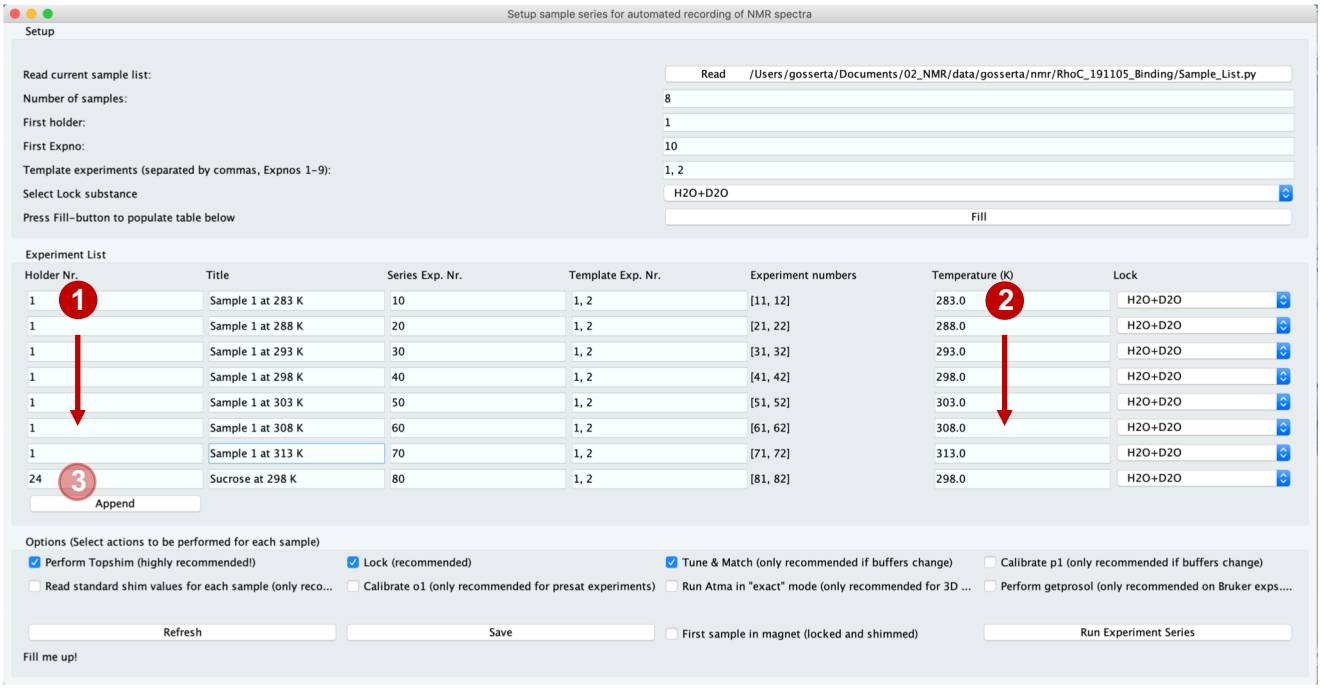
In this example, most features of the script are used. The scenario is that compounds are being tested for binding against a protein. For the protein, 4 experiments are being recorded: a 1D ^{1}H experiment (template experiment 1), two 1D ^{1}H-T1rho experiments with two different spin lock durations (2 and 3) and a 2D [^{15}N,^{1}H]-HSQC (4). All experiments were previously set up in experiment numbers 1–4 as template experiments. For the compounds in holders 2 and 4, the HSQC is not recorded, that's why only experiments 1–3 will be recorded.
Additionally, the stock solutions of the compounds in DMSO-d6 shall be recorded, for which a different lock substance is needed (holders 6 and 7)
In the "Options" section in a addition to shimming, and locking, automated tuning and matching, pulse calibration and getprosol is chosen, in order to account for the change in solvent.



1. Identify holder position in the sample changer for each sample. (They don't need to be in sequence)
2. Set meaningful titles to identify experiments later.
3. Set preferred starting numbers for experiments series
   (use multiples of 10 and don't repeat numbers, but otherwise you're free)
4. Choose, which of the template experiments should be run on each sample.
   (As soon as you press the refresh button on the bottom left, the column next to it will be updated)
5. Set individual lock substances.
6. Put in the sucrose sample at the end of the measurement series.

Temperature series on a single sample

In this example a temperature series is measured on one sample (which is in holder 1 of the sample changer). For each temperature a 1D ^{1}H experiment and a 2D [^{15}N,^{1}H]-HSQC are recorded (previously set up in experiment numbers 1 and 2 as template experiments). For each temperature a single row needs to be filled in the “Experiment list”.
In the “Options” section the user chose to run topshim, to lock, and to run automated tuning and matching for each temperature step.



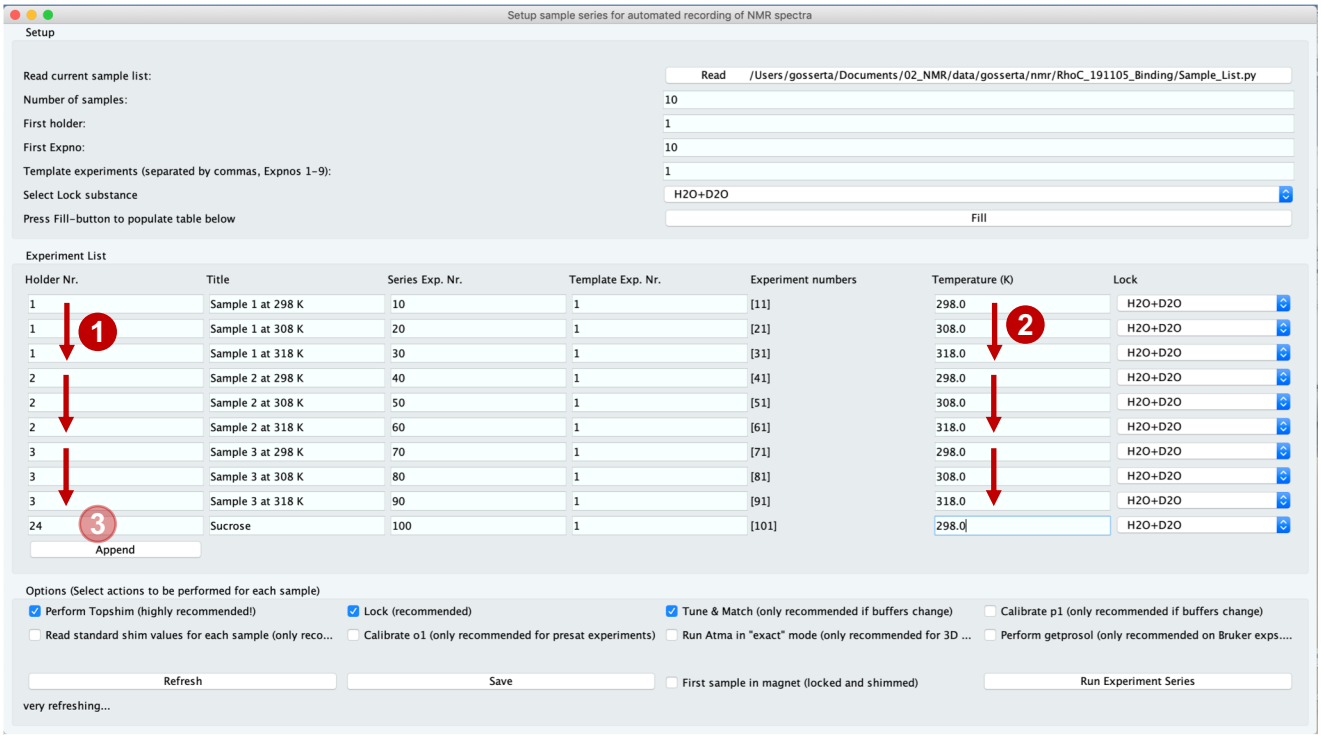
1. Holder stays constantly on number 1
   (no sample is being exchanged; however, topshim and other selected options are being performed.)

2. Temperatures are set here.

3. Put in the sucrose sample at the end of the measurement series.

Temperature series on multiple samples

In this example 3 samples are measured (which are in holders 1, 2 and 3 of the sample changer). For each temperature a 1D ^{1}H experiment is recorded (previously set up in experiment number 1 as a template experiments). For each sample, therefore, 3 rows are filled in the “Experiment list” for each respective temperature.
In the “Options” section the user chose to run topshim, to lock, and to run automated tuning and matching for each temperature step.



1. On each holder three different temperatures are measured.
2. Temperatures are set here.
3. Put in the sucrose sample at the end of the measurement series.

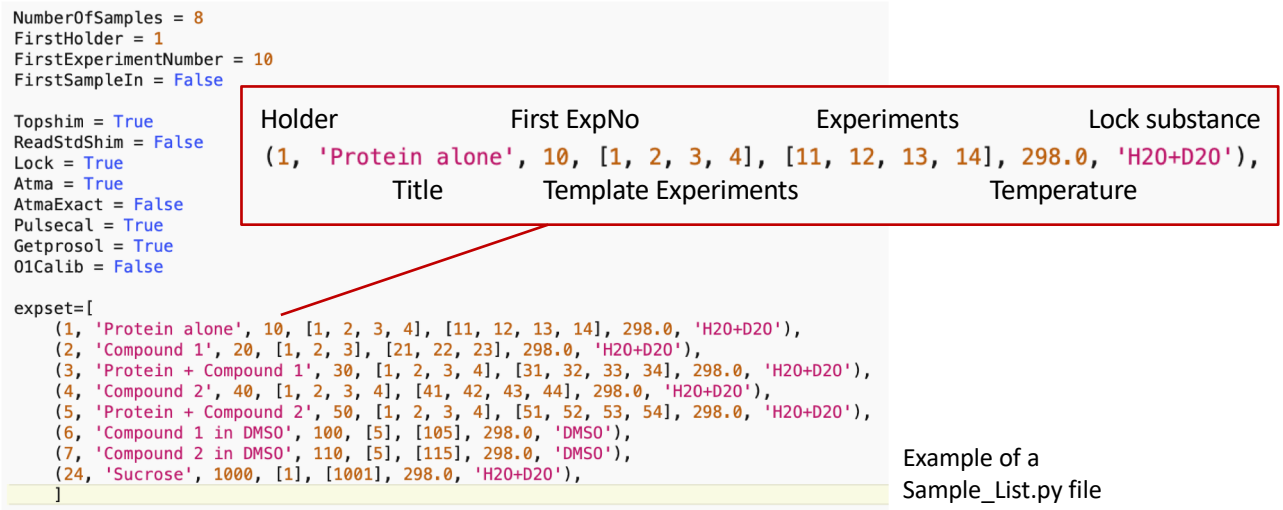
Appendix

Behind the scenes

The SetupSeries tool actually consists of two python scripts: SetupSeries.py and RunSeries.py.

SetupSeries.py provides the graphical user interface for filling in all the values and options needed for setting up an experiment series. RunSeries.py will then perform the actual experiments.

In the SetupSeries.py window, the user fills in all the required values. When the “Save” button is pressed, a text file in python format is written that contains all the information about the experiment series. This file is named “Sample_List.py” and is saved in the data folder where the experiment series is run. It can be read in by pressing the button ”Read /opt/topspin/…../SampleList.py” on the upper right of the SetupSeries window. (Here the full path to the Sample_List.py file is shown). This file can in principle be edited manually, but this is not recommended.



Example of a Sample_List.py file

For starting the actual experiments, the user presses the “Run Experiment Series” button. At this point the Sample_List.py file will be written again and the RunSeries.py script will be called.

The RunSeries.py script will load the Sample_List.py file and start running the experiments according to the entries in that list. The user is informed about the progress in a simple information window. The user information shown here is also written to a log file called “automation.log”, which is saved in the experiment data folder.

Credits

The SetupSeries tool is based on code by Yaroslav Nikolayev, Simon Rüdisser and Alvar Gossert.