Handling Data with OriginC

# Functionality

**Last Update:** 12.11.2020

This is a medium-size *OriginC* library providing several scripts for importing, handling, and evaluating spectroscopic data.

No warranty is given for functionality or correctness, so please verify all results generated with this script manually. 😊

All methods have been tested with *OriginPro 2018-2021*; older program versions should be updated anyways.

# Installation

1. Copy the folder *OriginC* (currently at "[\\...\2\_Allgemein Lehrstuhl\Skripte\](\\\\fs-4.uni-due.de\\wet-daten\\2_Allgemein Lehrstuhl\\Skripte\\)" to a permanent location on your computer.
2. Run *OriginPro* and open the *Code Builder*.

(*View* → *Code Builder* or Shortcut *Alt + 4*)

1. Rightclick the folder *User [AutoLoad]* in the *Workspace* and choose *Add files ...*.
2. Navigate to your local copy of the *OriginC* folder and select the *main.c* file.
3. Click *Rebuild All* from the toolbar (or Shortcut *Alt+ F8*).
4. If the output window on the bottom left displays an error, please consult the suggestion box at Fr. Merker.
5. Rightclick the *Origin C Workspace* in the *Workspace* tree and disable the *Build on Startup* option.
6. All scripts will now be available after each start of *OriginPro*. The *Code Builder* can now be closed.

# Usage

1. Open the *Script Window*.

(*Window* → *Script Window* or Shortcut *Alt + Shift + 3*)

1. Type the name of a script (see *D*) into the window and confirm with *Enter*.

(Each *Enter* inside the *Script Window* will be interpreted as a command call. If the current row does not contain a valid script name, an error will be printed.)

# Functions

All callable functions can be looked up in the file *main.c* and do not require any parameters to <<be passed when calling them.

Subfunctions are in the header files (*\*.h*) in the corresponding subfolders. These functions can in principle also be called from the *Script Window*, however, in this case the function parameters must be passed immediately.

## import

Automates data import from a variety of sources.

### Parameters

*Target Workbook*: Name of the workbook to append the imported data to. If not set, will create a new workbook.

*Target Worksheet*: Name of the worksheet to append the imported data to. If not set, will create a new worksheet.

*Data Type*: The source type of the data (see *b*).

*Delimiter*: The column value delimiter of the source file (usually *Tab*, sometimes *Whitespace*).

*Dec. Separator*: The decimal separator of the source file.

*Constant X-Axes*: If checked, removes the *X*-Columns of all imported files except the first.

*Create Sparklines?*: If checked, creates sparklines for all imported data columns. (Use with caution! Creates heavy CPU load!)

### Datatypes

*Spectra Files*: E.g., spectra from *LabSpec* or *UVProbe*. Imported file names will be written to the column comments.

*3D-Maps*: E.g., time traces from *LabSpec* or peak maps from *NT-MDT*. The file structure must be *XY-I*… File names are used as worksheet names. *XY*-coordinates are written to the user parameters.

*4D-Maps*: E.g., raw map data from *NT-MDT* (*XY-λ-I*…). File names are used as worksheet names. *XY*-coordinates are written to the user parameters. Note that *NT-MDT* data must be exported from *Image Analysis* as a *MATLAB* file (*\*.m*)!

*Tracks*: XML-Files generated via the *ImageJ TrackMate* analysis containing particle tracking information. The map metadata (e.g., *time axis* and *XY*-coordinates) are written to the user parameters.

## correct

Manipulates all datasets in a selectable worksheet of the active workbook. For each selected method, the results are stored in a new worksheet, which is then used as the data source worksheet for the subsequent correction method.

### Parameters (vary depending on the chosen method)

*Data Source*: Dropdown field to select the source data worksheet.

*Worksheet*: Dropdown field to select the reference data worksheet (only in selected methods).

*Parameter*: Dropdown field to select the user parameter row containing the reference data (in the current worksheet) or connecting the data and reference worksheets (only in selected methods).

### Methods (selected via checkboxes in initial dialog)

*Clean Masked Data*: Clears all cells of the source worksheet that have been *masked* (e.g., in a graph window) and fills them with mean values (averaging window: 10 data points).

*Background Subtraction*: Subtracts reference data from all datasets.

The *Reference* modeuses reference spectra connected via a selectable user parameter.

Parameters: *Worksheet*, *Parameter*

The *Average* mode uses the mean value of the user defined spectral subregion.

Parameters: *Start*, *Stop*

*Spike Removal*: Automatically removes spikes from the work­sheet. This method is based on the Whitaker-Hayer algorithm, see [Chemolab 2018](https://dx.doi.org/10.1016/j.chemolab.2018.06.009).

Parameters: *Z-Threshold*, *Averaging Width*

*Setup Correction*: Applies a setup calibration curve to the source data by division. Currently, only the first two columns of the reference worksheet are used as a single *XY* dataset.

Parameters: *Worksheet*

*Filter Correction*: Corrects the source data with a set of neutral density filter transmission curves by division. The transmission data of the filters must be absolute values.

Parameters: *Worksheet*, *Parameter*

*Integration Time*: Divides all datasets by the integration time provided in a user parameter of the source worksheet. The selected user label must only contain numerical data!

Parameters: *Parameter*

*Energy Transformation*: Performs a Jacobian Transformation to the energy space on all source datasets (Caution! Not to be used for PLE or absorption data.).

Parameters: *none*

*Data Normalisation*: Normalises all source datasets by dividing them by their respective maximum value.

Parameters: *none*

## analyse

Executes simple spectroscopic analytics on the current worksheet or workbook.

### Parameters

*Method*: Dropdown field to select the evaluation method.

*Source Type*: Dropdown field to select the data source type.

### Methods

*Spectra*: Basic spectral analysis of all *XY*-datasets in the worksheet or workbook (e.g., *Peak Position*, *Area*, *FWHM*, …).

*4D-Linescan*: Extracts a line scan along one axis from an imported *XY-λ-I m*ap (e.g., *NT-MDT*). Note that the parameter *width* is not implemented yet.

## convert

Transforms the datasets in the currently active worksheet to a different representation (e.g., generate *3D-Map* from *XYZ* columns).

### Parameters

*Method*: Dropdown field to select the data conversion method.

### Methods

*XYZ-Data to Matrix*: Transforms a *Z* dataset into an *XYZ*-Map. *XY* data can be extracted from the column designations or from user input.

## alignText

Aligns a selectable text field in the currently active graph layer. The active window must be a graph window!

### Parameters

*Text Object*: Dropdown field to select the text element that is to be aligned (e.g., *XB* = X-Bottom, *YL* = Y-Left, …)

*Alignment*: Dropdown field to select the desired text field alignment.

## renameWbs

Renames the *Short Name* field of all workbooks in the current folder based on their *Long Names* (to enable sorting, e.g.).

## setLowerBound (*threshold* = 0)

Replaces all values in the active worksheet smaller than *threshold* with *0*. *threshold* default to *0* if omitted (all negative data are set to *0*).

Note that the *threshold* parameter must be passed when calling the method.

## reduce

Reduces the project’s CPU load by deleting (!) all sparklines in the project and hiding all windows.