Handling Data with OriginC

A Functionality

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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.

B Installation

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

C Usage

1. Open the *Script Window*.
   (*Window* → *Script Window* or Shortcut *Alt* + *Shift* + *3*)
2. 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.)

D 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.

1. import

Automates data import from a variety of sources.

a) 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!)

b) 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*, peak maps from *NT-MDT* or Raman images generated with the *Raman Tool Set 2.0*. The file structure must be *XY-I*... File names are used as worksheet names. *XY*-coordinates and other axes 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.

2. 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.

a) 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).

b) 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* mode uses 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.
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*

3. analyse

Executes simple spectroscopic analytics on the current worksheet or workbook.

a) Parameters
Method: Dropdown field to select the evaluation method.
Source Type: Dropdown field to select the data source type.

b) 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.

4. convert

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

a) Parameters
Method: Dropdown field to select the data conversion method.

b) 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.

5. peaks

Convenience method for peak fitting that collects a selected column from all *PeakProperties** worksheets in the currently active workbook. The data are collected in a new sheet, transposed and some basic statistics (mean and standard deviation) are calculated. All results are auto-updated such that adjustments to individual fittings will directly be reflected.

a) Parameters
Name: The dataset identifier used to name the result sheets.
Target Column: The source column from the *PeakProperties* sheet.

6. alignText

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

a) 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.

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

8. **setLowerBound (*lowerBound* = 0)**
   Replaces all values in the active worksheet smaller than *lowerBound* with *0*. *lowerBound* defaults to *0* if omitted (all negative data are set to *0*).

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

9. **reduce**
   Reduces the project's CPU load by deleting (!) all sparklines in the project and hiding all windows.