Spectral Analysis with OriginC

A Functionality

Last Update: 13.09.2021 (v1.2.0)

This is an *OriginC* library providing several scripts for importing, handling, and evaluating spectroscopic data. No warranty is given for functionality or correctness, please verify all results generated with this script manually.

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

For extending the packages functionality, see the *Developer Guide* and the *Example Plugin* code in the *src* directory.

B Installation

1. Copy the file *build/Spectral Analysis.opx* to a location on your computer.
2. Run *OriginPro*.
3. Drag and drop *Spectral Analysis.opx* into *OriginPro*. The installation process will start automatically and add all required files to the *User Folder Workspace*.
   If any errors occur, the script will show a prompt. Please contact the script provider with the displayed error code.
4. All scripts will now be available after each start of *OriginPro*.

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 Debugging

If you need to debug the runtime of any function from this library or your own, you can use the new *timer(*string *label)* method.

1. Skipping the *label* parameter resets the timer without output:
   timer(); (no output)
2. To generate output, pass a descriptor to the *label* parameter:
   timer("Transpose Sheet"*)*; (Transpose Sheet: 19 ms)

E 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. The import functions for spectra, 3D-maps and XY-λ-I data support pushing header lines to the OriginPro worksheet user parameters with the pseudo-syntax *ParamName:{TAB}Value*.

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 *ImageJ TrackMate* containing particle tracking information. 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 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 *Median* mode uses the median value of the user defined spectral subregion.
Parameters: *Start*, *Stop*
The *Constant* mode uses a fixed value.
Parameters: *Value*

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. If no reference user label is selected, this method defaults to the first two columns of the reference worksheet.
Parameters: *Worksheet, Parameter*

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. analyze

Executes simple spectroscopic analytics on the current worksheet.

a) Parameters

Dataset Name: The name that will appear in the long name of the result column in the evaluation sheet.

Method: The mathematical evaluation method to apply to the data.

Skip Abscissae? If checked, does not generate new abscissa in the result sheet, e.g., if they have already been generated with the last run of the method.

X-Abscissa: The name of the user label that holds the data representing the new *X* values of the evaluation result.

Y-Abscissa: See *X-Abscissa*. If set to *none*, ordinates in the result sheet will be assigned *Y*, if set to other values, ordinates will be assigned *Z* (e.g., for map analysis).

X Start Value: The lower bound of *X* values to evaluate; if *0*, will default to the first data row.

X Stop Value: The upper bound of *X* values to evaluate; if *0*, will default to the last data row.

b) Methods

Peak Position: Finds the point with the highest *Y* value in the given range.

Mass Centre: Calculates the centroid in the given range.

Peak Intensity: Returns the highest *Y* value in the given range.

Peak Area: Summarizes all *Y* values in the given range (pseudo-area)

Peak FWHM: Calculates the *full width at half maximum* by finding the *Peak Position* Y_{max} in the given range and iterating to higher and lower *X* values until *Y* is $\leq 0.5 \cdot Y_{max}$ in both directions.

4. map

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.

4D-Linescan: Extracts a line scan along one axis from an imported *XY-λ-I m*ap (e.g., *NT-MDT*).

5. interpolate

Interpolates all *XY*-datasets in the currently active worksheet onto a new *X*-axis. The new axis must be included in the same worksheet.

a) Parameters

New X-Axis: The source column containing the new *X*-axis data.

6. 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.

7. 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.

8. renameWbs

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

9. 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.

10. reduce

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