OriginC Spectral Analysis

User Guide

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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.

Contents

1 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*.

2 Usage

1. Open the *Script Window*.

   (*Window* / *Script Window* or Shortcut *Alt* + *Shift* + *3*)
2. Type the name of a script (see Methods) 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.)

3 Extending

This package can easily be extended by other code modules.

See the Developer Guide and the *Example Plugin* code in the *src* directory.

4 Debugging

If you need to debug the runtime of any function from this library or your own, you can use the `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");
// output: "Transpose Sheet: 19 ms"
```


5 Methods

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

Helper methods are in the header files (`*.h`) in the corresponding subfolders. They can in principle also be called from the *Script Window*, however, in this case the function parameters must be passed immediately.

5.1 Data Handling

5.1.1 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*.

Parameters

Parameter	Description
`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

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

Data Type	Description
`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.

5.1.2 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.

Parameters (vary depending on the chosen method)

Parameter	Description
`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).

Methods (selected via checkboxes in initial dialog)

Method	Description
`Masked Data Removal`	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).

Method	Description
`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 Correction`	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*
`Jacobian 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*

Method	Description
`Normalisation`	Normalises all source datasets by dividing them by their respective maximum value. **Parameters:** *none*

5.1.3 analyze

Executes simple spectroscopic analytics on the current worksheet.

Parameters

Parameter	Description
`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*, values in the result sheet will be assigned *Y*, if set, values 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.

Methods

Method	Description
`Peak Position`	Finds the point with the highest *Y* value in the given range.
`Mass Centre`	Calculates the centroid in the given range.

Method	Description
`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 $Y \leq 0.5 \times Y\text{max}$ in both directions.

5.1.4 map

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

Parameters

Parameter	Description
`Method`	Dropdown field to select the data conversion method.

Methods

Method	Description
`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 map (e.g., from *NT-MDT* or *LabView*).

5.1.5 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.

Parameters

Parameter	Description
`New X-Axis`	The source column containing the new *X*-axis data.

5.1.6 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.

Parameters

Parameter	Description
`Name`	The dataset identifier used to name the result sheets.
`Target Column`	The source column from the *PeakProperties* sheet.

5.1.7 setLowerBound

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*).

Parameters

Parameter	Description
`lowerBound (0)`	This parameter must be passed when calling the method, there is no user dialog.

5.2 Miscellaneous

5.2.1 renameWbs

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

5.2.2 reduce

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

