# *SPECTR-O-MATIC APP*
# USER GUIDE

This user guide applies to the Spectr-O-Matic for MATLAB® and Spectr-O-Matic for Windows™ apps.

Version 2.0
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# INTRODUCTION

## What is the Spectr-O-Matic App?

The Spectr-O-Matic App is an interactive program for working with *spectra*:

- Import/Export spectra using different file formats (MATLAB, text, CSV, Microsoft Excel)
- Graphical and table view of spectra
- Calculator with 20 functions, including:
    - Arithmetic – add, subtract, power, etc.
    - Extract minimum, maximum, area
    - Calculate sum and average of spectra
    - Normalize and smooth spectra
- Search and organize
    - Find spectra by properties and keywords
    - Organize in groups and objects for quick operations

## Glossary

| | |
|---|---|
| *Spectrum* | A set of two related *data* arrays, X and Y, plus some *metadata* that describe it |
| *Magnitude* | The Y value of the spectrum at a given spectral position (X) |
| *Metadata* | Information about the spectrum, such as name (*ID*), date of the measurement (*DateTime*), data type (*XType*, *YType*), etc. |
| *Object* | A container storing spectra or other data |
| *Group* | A named subgroup of spectra within one object, used for quick selections and operations per group. |

## App vs Toolbox

The Spectr-O-Matic App comes in two flavors – as a MATLAB® app or as a stand-alone Windows™ application. They have the same interface and functionality except for copying data directly to the MATLAB workspace.

The Spectr-O-Matic App is a graphical shell (interface) for selected commonly used functions of the command-based Spectr-O-Matic Toolbox for MATLAB®. The app provides fast and simple point-and-click actions, whereas the script-based toolbox allows greater functionality and flexibility and takes advantage of an arsenal of MATLAB commands and tools. Switching and exchanging data between the app and the command-based environment is straightforward.

### Feature comparison

| | Spectr-O-Matic App | Spectr-O-Matic Toolbox |
|---|---|---|
| **Interface** | Graphical user interface | Command-based |
| **Operations are performed by** | Point-and-click | Commands and scripts |
| **Can work without MATLAB®** | Yes | No |
| **Ease of use** | Easier | More difficult |
| **Set up analysis** | Faster | Slower |
| **Function set** | Limited | Infinite<br>*(use all available MATLAB programming tools)* |
| **Edit / recall command history** | No<br>(*though you can recall intermediate results)* | Yes<br>*(any script can be altered at will and run with different sets of data)* |
| **Output publication-ready figures** | No | Yes |
| **Batch operations on spectra** | Yes | Yes |
| **Operations per group (split-apply-combine)** | Yes<br>*(using logical grouping)* | Yes<br>*(logical and categorical grouping)* |
| **Exchange data with MATLAB®** | Yes | Yes |
| **Exchange data with other applications (Excel, etc.)** | Yes | Yes |

## System requirements

### Spectr-O-Matic for MATLAB®

- MATLAB release 2017a
- The Spectr-O-Matic Toolbox (download it from the MATLAB File Exchange) or the Spectr-O-Matic App package

### Spectr-O-Matic for Windows™

- 64-bit Microsoft Windows 7 or later
- Up to 1 GB of hard disk space (to install the MCR runtime)

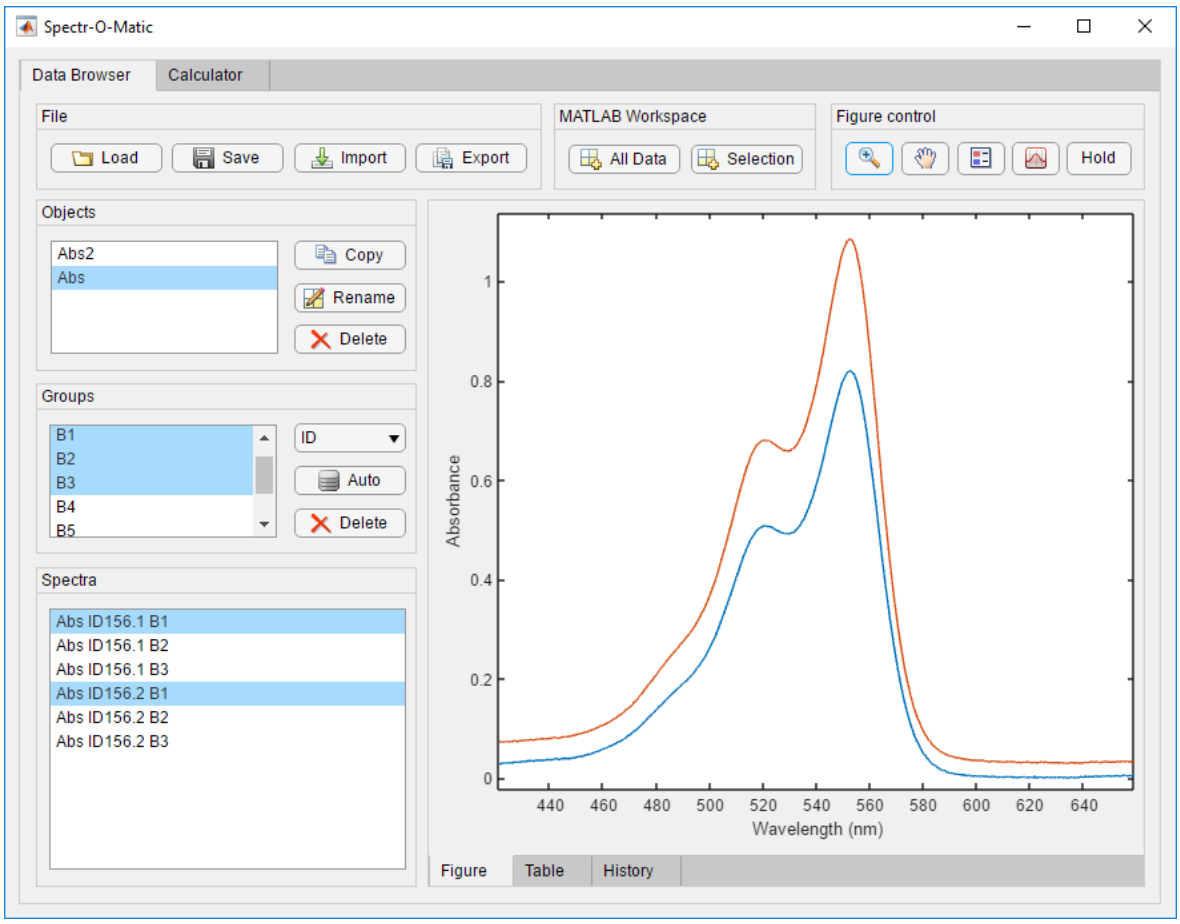
## Install and run the app

### Spectr-O-Matic for MATLAB®

- Option 1 – download and install the Spectr-O-Matic Toolbox from the MATLAB File Exchange. The app is included in the toolbox. To run the app, type *spectromatic* at the MATLAB command window.
- Option 2 – download and install the Spectr-O-Matic App package. To run the app, click on its icon in the Apps section of the MATLAB ribbon.

### Spectr-O-Matic for Windows™

- Run the Spectr-O-Matic for Windows™ web installer. If the MATLAB runtime (MCR 2017a) is not found on your computer, the installer will download it from the Internet (about 1 GB).
- Run the Spectr-O-Matic App from the start menu or desktop shortcut.




The Spectr-O-Matic App interface

# USING THE APP

## App layout

The app is organized in two tab panels – *Data Browser* and *Calculator*.

### Data Browser

The Data Browser serves to load, save and visualize data. It has three control areas:

1. Top – buttons for import and export of data and graph options
2. Left – lists and selects objects, groups and spectra
3. Right – a graphical or tabular view of the selected spectra

### Calculator

Data manipulation is done in the calculator panel. There are two working areas on the page:

1. **SEL** (left side) – controls for selecting objects and spectra
2. **CAL** (right side) – calculator operations

## Exploring Data

### Load and save data

There are two different ways to load data in the Spectr-O-Matic App – **Load** and **Import**.

The native file format of the Spectr-O-Matic App is **.mat**. To load a .mat file, click Load in the Data Browser and select a .mat file. If the file has been previously created with the app, all data and groups will be restored. Otherwise, the app will load only those objects from the file that contain spectra. Click Save to save all objects and groups in a new .mat file.

To load data from other file formats, click the Import button. You can select more than one file. The contents of all selected files will be aggregated in a single object *data*. Presently, the following file types are recognized:

- Microsoft Excel spreadsheets (.xls, .xlsx)
- Tab- or space-delimited delimited text files with text column headers
- Comma-separated values (*.csv)
- Text files in PRODATA format (generated by Jasco)
- Text files or .csv files generated by Chirascan (Applied Photophysics)
- Files exported from SpectraSuite (OceanOptics).

*Note:* If an object named *data* already exists in the memory, the newly imported data will be in *data1*, etc.

When loading files containing multiple columns of data, the first column is interpreted as X and all subsequent columns as Y values (different spectra with the same X axis). The Export button will export a similar table if multiple spectra sharing a common X axis are selected in the app. Exported file formats are

- MATLAB file (*.mat)
- Tab-delimited text (.txt)
- Comma-delimited (.csv)
- Microsoft Excel (.xls, .xlsx)

*Note:* Exported text or Excel files contain only the selected spectra in the *spectra* list box, and only if they have the same X axes. In contrast, exported MATLAB files (.mat) will contain all data in the selected objects, regardless of their type.

### Copy data to other applications (via Clipboard)

You can copy spectra as well as numeric data to the clipboard so that they can be pasted in other applications (e.g. Excel). To copy spectra, first select the object that contains them from *Objects*, then select one or more spectra (see below how to make selections), then press Copy from the top row of buttons. To copy numerical data, simply select the object and press Copy.

### Copy data to MATLAB

(This function does not work in Spectr-O-Matic for Windows®)

To copy all objects and groups to the MATLAB environment, click the All data button in the Data Browser. This will create two struct variables in the MATLAB base workspace – *Data* and *Groups* – with fields for each object in the app. To copy only a selected object (or objects), click Selection. A specdata variable with the same object name will be created in the MATLAB base workspace. If the object contains any groups, they will be copied into another struct variable with the *ix* prefix.

### View spectra as graphs

To view a spectrum, first select the object that contains it from the *Objects* list box in the Data Browser. The spectra contained in the object are listed in the *Spectra* list box. You can narrow down the listed spectra by selecting a group from the *Groups* list box (if listed). Click on the name of a spectrum in the *Spectra* list box to view it in the figure panel on the right.

*Note:* Depending on the speed of your machine, there may be a considerable delay the first time you select a spectrum to plot, until the graphics system is initialized.

To select several spectra simultaneously, press and hold the CTRL key on the keyboard. To select a range of spectra, select the first one, press and hold the SHIFT key and then select the last one. You can also select several objects and groups simultaneously. The list of spectra will show the contents of all selected objects and groups.

### Graph options

The **Figure Control** panel contains five buttons: Zoom  , Pan  , Legend  , Peaks  and Hold:

- Press the Zoom  button to activate zoom mode. Click inside the graph to zoom in, hold Shift and click to zoom out.
- Press the Pan  button to activate pan mode. Click and drag inside the graph to pan.
- Press the Legend  button to show or hide the legend box.
- Press the Peaks  button to show peak labels on the graph. Peak labels (x,y) mark the position and magnitude of detected peaks in the displayed spectra.
- Press Hold to activate overlay mode. With overlay mode on, when you select new spectra to plot, they are overlaid onto the current graph.

### Tabular view of data

Click the *Table* subpanel to view the selected spectra as a table. Click the *Figure* subpanel to switch back to the graphical view.

*Note:* The Table view displays not only spectra but also the contents of other data types. The graphical view only shows spectra. For example, if the selected object is a simple numerical array, the *Spectra* list box will be empty, but the Table view will still show its contents.

### Copy, rename and delete objects

To make a copy of an existing object under a different name, select the object and click Duplicate in the Data Browser and type a new name in the input box. There may be a delay before the input box appears.

To rename an object without changing its contents, click Rename. To combine several objects as one, select them by holding the CTRL key and click Duplicate. The new object will contain the spectra and groups of all selected objects.

*Note:* If the new name is the same as the name of an existing object, that object will be erased from memory.

Press Delete next to the *Objects* list box to remove the selected objects and their contents from memory.

### Create an automatic keyword index

Press the Auto button in the Data Browser to automatically create groups for every keyword found in the IDs (or ExpID, Xtype, YType) of the selected object. If autoindex generates any unwanted or irrelevant groups, select them in the Groups list box, holding CTRL or SHIFT, and click the Delete button next to the *Groups* list box.

## Selecting and Organizing Data

All operations on data are done in the Calculator tab panel. Before you perform any operations, you must first select the spectra you want to operate with.

### Select spectra for operation

Pick an object from the *Object* drop-down box in the Calculator panel. The spectra in that object will be listed in the data table along with their main properties (metadata). Pick a group from the *Group* box to narrow down the spectra listed in the table.

The first column in the table, Sel, contains checkboxes that mark which spectra are selected for operation. Click on the checkbox next to each spectrum you want to include it in the operation.

Click the button All to include all listed spectra. Click None to clear the selection.

### Select spectra by searching in properties

To make a quick selection (filter) among the listed spectra based on their properties (metadata), use the *Find* panel. First, pick a property to search in. Then type a value (keyword) to search for, or select from the drop-down list. You can filter by ID, ExpID, DateTime, XType, YType, or Group. Finally, press one of the three buttons below:

- Select – add the spectra that match the filter to the current selection
- Refine – select only those spectra matching the filter among the currently selected spectra
- Unselect – remove the spectra that match the filter from the current selection

### Create new objects or groups from the selection

To create a new object from the selected spectra, make sure the switch in the *Save selection* panel points to *SEL*, then click the New object button.

To create a new group without actually copying any data, click the New group button.

*Note:* Groups can also be created and deleted in the Data Browser. In fact, the quickest way to organize your data is usually by using the Autoindex button in the Data Browser.

## Perform calculations

### Function buttons

To perform any calculation, first make a selection of spectra in the Calculator tab panel. Then press a function button from the *Functions* panel. The selected spectra will be the operand to this function. To execute the operation, click the = button in the *Operation* panel. If the operation is successful, the

indicator lamp turns green. The result is stored in the calculator memory (*CAL*) for further use and also copied as object *CALR*.

When data are entered in the calculator memory (*CAL*), the operation text area displays the object name and any selected functions or operators and the indicator lamp turns yellow. The *CAL memory* status box at the bottom of the window shows the type of data in memory.

### Specify function parameters

Some functions can take additional scalar parameters. For example, the max and min functions can search for local extrema in a specified spectral (X) region. Use the *Range* input boxes to give additional parameters. First enter the desired value(s) and only then click the respective function button (e.g. max). Observe that the correct parameter values are displayed in the operation text area.

### Stacking functions

By pressing function buttons in order you can create a pipeline of operations with the selected data. The result of each function will be the operand to the next one. It is not necessary to press = after each operation. The stack of operations is displayed in the operations text box. For example, to find the maximum of the absolute value of A in the spectral range from 600 to 700, enter this sequence:

1. Select the object (A) and spectra
2. Press abs
3. Enter 600-700 in *Range*
4. Press max

The operations text box should display an expression like this:

```
abs(A(:)).max([600 700])
```

Press **=** to evaluate it.

### Binary functions

Arithmetic operations (+, -, *, /, ^) require two operands. After choosing the function, select new data to use as a second operand and then click = to execute the operation.

If you want to change the data in the *CAL* memory, make a new selection and then click the **CAL** button at the top right corner of the app window.

If you want to use a scalar value (number) as an operand, instead of spectra, enter the number in the *Scalar value* panel at the bottom of the window and click the **CAL** button.

### Order of operations

Operations are executed in the order they are entered. However, unary operations (all except +, -, *, /, ^) have precedence over binary (arithmetic) operations. That is, you can stack unary operations to both operands of a binary operation and they will be evaluated before the binary operation. Here is an example expression with two objects a and b:

```
A(:) – A(:).Yx(500) / B(:).max
```

This expression shifts the spectra in A to 0 at X = 500 and then normalizes them to the maximum of B. It contains four operations entered in the sequence -, Y(X), /, max. However, Yx and max have precedence over - and /, so they are evaluated first. The order of evaluation is then:

1. Calculate A.Yx(500)
2. Subtract A.Yx(500) from A
3. Calculate B.max
4. Divide A – A.Yx(500) by B.max

Note that division has no precedence over subtraction. They are evaluated in the order of entry.

### View calculation results

To view the result of the last calculation, go to the Data Browser and select the CALR object.

If you want to just copy the calculation result without leaving the Calculator tab panel, make sure the switch in the *Save selection* panel points to *CAL*, then enter a name and click the New object button.

### Correct errors / clear memory

To clear the last operand entered or cancel the last operation before it is executed, click the CE button in the *Operation* panel.

To cancel all undergoing operations and clear the *CAL* memory, click the C button.

### Performing operations per group

Spectr-O-Matic can split data into groups and perform a chosen operation with each group automatically. To perform operation by groups, the groups must be defined first (see the previous section). The quickest way to define groups is using the Autoindex button in the Data Browser.

Once you have defined the relevant groups, pick the object that contains them, and select all or some spectra. Chose a function or stack several functions using the function buttons. Then press the GRP button in the *Operations* panel. The pressed state of the GRP button indicates that the operation will be done separately on each group. Press = to execute the operation.

It is important to carefully consider what groups will be defined in the object before executing operations by groups. Groups can be defined based on IDs or other properties (see Selecting and Organizing Data). If you do not wish to use all defined groups to split the data, delete the irrelevant groups from the Data Browser.

*Example:*

The object *data* contains spectra of two experimental groups – “control group” and “test group”. The spectra IDs indicate the group with the keywords “ctrl” and “test”, respectively. To average the spectra based on experimental group, follow this sequence:

1. Create groups “ctrl” and “test” in *data* based on ID, using the Autoindex button, or using filters.
2. If you used Autoindex, delete any other irrelevant groups it may have created (if it found other keywords).
3. In the Calculator, select *data*, *<all groups>*, and click All to mark all spectra.
4. Click mean
5. Click GRP. Make sure the button is in a pressed state.
6. Click =.

The result of the operation will contain two spectra – averages for the control and test group.

### Recalling the operations log

All newly created objects contain a log of operations that can be used to trace back their origin. To recall the operations log, select an object in the Data Browser and open the **History** panel.

# LIST OF FUNCTIONS

| Function name | Data type | Description |
|---|---|---|
| **+, -, *, /, ^** | Spectra and scalar | Arithmetic operations (add, subtract, multiply, divide, power) |
| **+/-** | Spectra and scalar | Negate (unary minus) |
| **abs** | Spectra and scalar | Absolute value |
| **area** | Spectra | Area under the curve in a spectral range |
| **diff** | Spectra | 1st Derivative. Repeat function for higher-order derivatives. |
| **ln, log10** | Spectra and scalar | Natural and decimal logarithm |
| **max** | Spectra | Maximal value / maximal magnitude (Y) in a spectral (X) range. |
| **mean** | Spectra and scalar | Average |
| **merge** | Spectra | Join spectra with different spectral (X) axes |
| **min, max** | Spectra | Minimal value / minimal magnitude (Y) in a spectral range. |
| **norm** | Spectra | Normalize spectra (divide by maximal magnitude or by the magnitude at a given spectral position/range) |
| **smooth** | Spectra | Smooth spectra (moving average of N points). Specify N using the Range box |
| **sum** | Spectra and scalar | Sum |
| **Xlim** | Spectra | Trim spectra to specified spectral range |
| **Y(x)** | Spectra | Magnitude (Y) at a given spectral position (X) |

# EXAMPLES

## Load / Import Data

### Load .mat file

| Operation sequence | Command equivalent |
|---|---|
| 1. Click Load in the Data Browser<br>2. Navigate to and select file<br>3. Click OK | `load data.mat` |

### Import data from text files

*Import text or CSV files (automatic delimiter and header recognition)*

| Operation sequence | Command equivalent |
|---|---|
| 1. Click Import in the Data Browser<br>2. Choose file type (e.g. 'Delimited Text Files')<br>3. Navigate to and select files<br>4. Click OK | `data = specdata.load('*.txt')` |

*Import text files (ignore headers and non-numeric data)*

| Operation sequence | Command equivalent |
|---|---|
| 5. Click Import in the Data Browser<br>6. Choose file type (e.g. 'Generic Text Files - ignore header')<br>7. Navigate to and select files<br>8. Click OK | `data = specdata.load('*.txt', ...`<br>`'FileType','ASCII')` |

# Perform calculations

## Extract magnitudes

Extract the magnitudes (Y) of all spectra in *data* at X = 675

| Operation sequence | Command equivalent |
|---|---|
| 1. Pick *data* object in the Calculator<br>2. Click All<br>3. Enter 675 in the first *Range* box<br>4. Click Y(X)<br>5. Click = | `result = data.Yx(675);` |

## Linear transformation of spectra

Transform all spectra in *data* so that Y' = 2*Y + 10 at every X position
(scale up 2-fold and then shift up by 10 units)

| Operation sequence | Command equivalent |
|---|---|
| 1. Pick *data* object in the Calculator<br>2. Click All<br>3. Click *<br>4. Enter 2 in the *Scalar* box and click CAL<br>5. Click +<br>6. Enter 10 in the *Scalar box* and click CAL<br>7. Click = | `result = 2*data + 10;` |

## Calculate difference spectra

Calculate difference spectra of the spectra in objects *A* and *B*, i.e. $A_1$ - $B_1$, $A_2$ - $B_2$, $A_3$ - $B_3$, …

| Operation sequence | Command equivalent |
|---|---|
| 1. Pick *A* object (or group) in the Calculator<br>2. Click All or select spectra<br>3. Click -<br>4. Pick *B* object / group<br>5. Click All or select group or spectra<br>6. Click = | `result = A - B;`<br>or<br>`result = data(A) – data(B);` |

The operation is successful if the number of selected spectra in *A* and *B* is equal, or *B* contains only one spectrum. To perform operations with different numbers of spectra, see Performing operations per group.

## Normalize spectra

### *Normalize to own maximum*

Normalize spectra to their maximum in a spectral range from 600 to 800.

| Operation sequence | Command equivalent |
|---|---|
| 1. Pick *A* object / group<br>2. Click [All] or select spectra<br>3. Click [norm]<br>4. Enter 600 and 800 in the *Range* boxes<br>5. Click [=] | `result = A.norm([600 800]);` |

### *Normalize to other spectra*

Normalize the spectra in *A* to the maximum of the spectra in *B* in the spectral range 600-800.

*B* must have the same number of spectra as *A*

| Operation sequence | Command equivalent |
|---|---|
| 1. Pick *A* object / group<br>2. Click [All] or select spectra<br>3. Click [/]<br>4. Pick *B* object / group<br>5. Click [All] or select spectra<br>6. Enter 600 and 800 in the *Range* boxes<br>7. Click [max]<br>8. Click [=] | `result = A / B.max([600 800]);` |

## Grouped operations

### *Subtract baseline by type*

Object A has spectra of different type (YType). Some of the spectra are baseline spectra, one baseline for each YType.

| Operation sequence |
|---|
| 1. Select *A* object in Data Browser<br>2. In the Groups panel, select [YType] and click [Auto] to define type groups<br>3. Pick *A* object in Calculator<br>4. Click [All]<br>5. Unselect baseline spectra with the finder<br>6. Click [-]<br>7. Select baseline spectra<br>8. Press [GRP]<br>9. Click [=] |

### *Average spectra per group*

| Operation sequence (option 1) |
|---|
| 1. Select *A* object in Data Browser<br>2. Click [Auto] to automatically define experimental groups<br>3. Select all groups to be averaged together* |

4. Click Delete in the Groups panel
5. Pick *A* object in Calculator
6. Click All
7. Click mean
8. Press GRP
9. Click =

* Keep those groups of spectra that have meaningful differences between them. Delete those groups that specify differences you do not want to take into account. For example the data may contain groups SampleA, SampleB, Trial1, Trial2. Delete the groups Trial1 and Trial2 if you want to average spectra across trials but keep them separated by sample.