

SPECTR-O-MATIC APP

App Interface Tutorial

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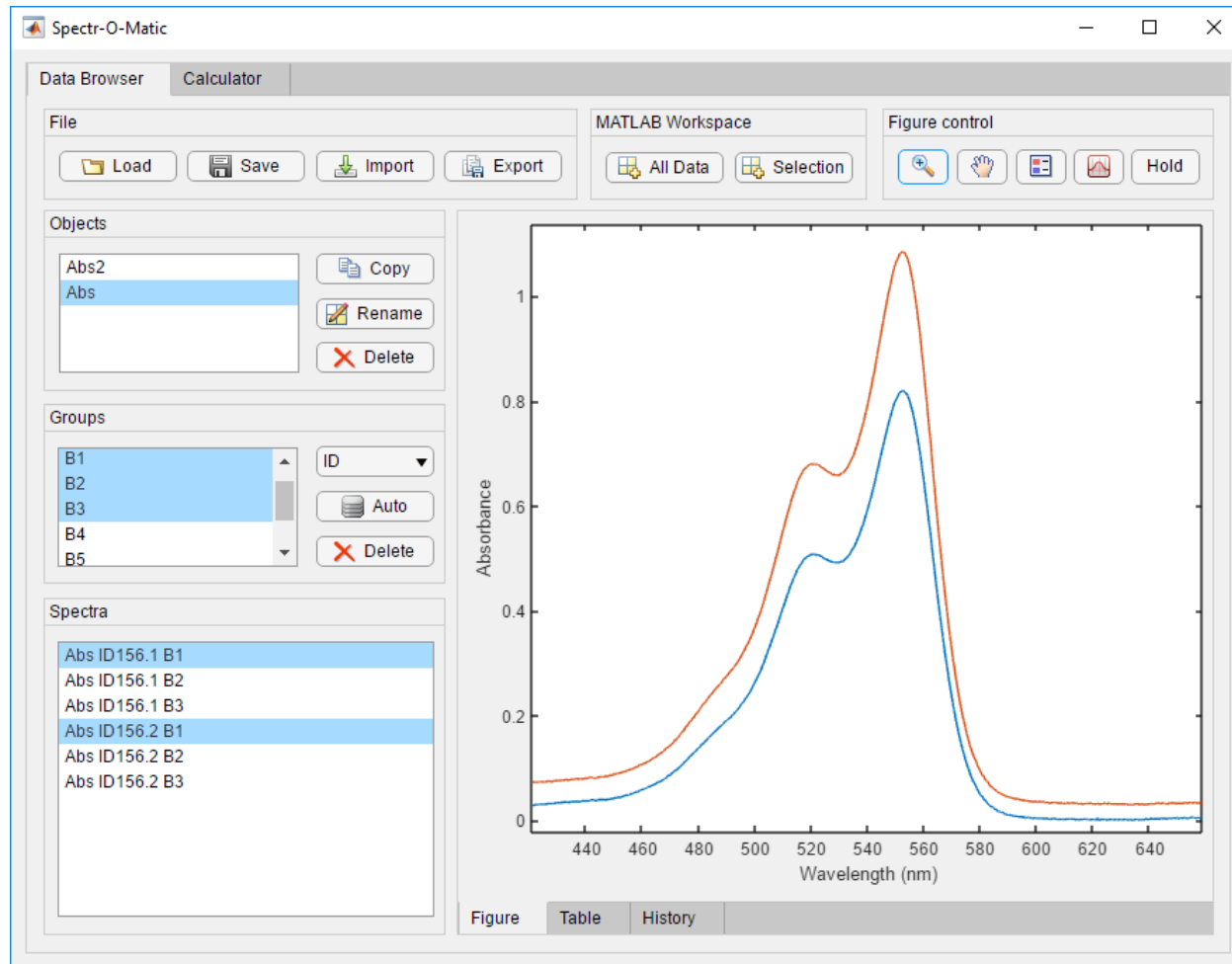
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I. The Data Browser

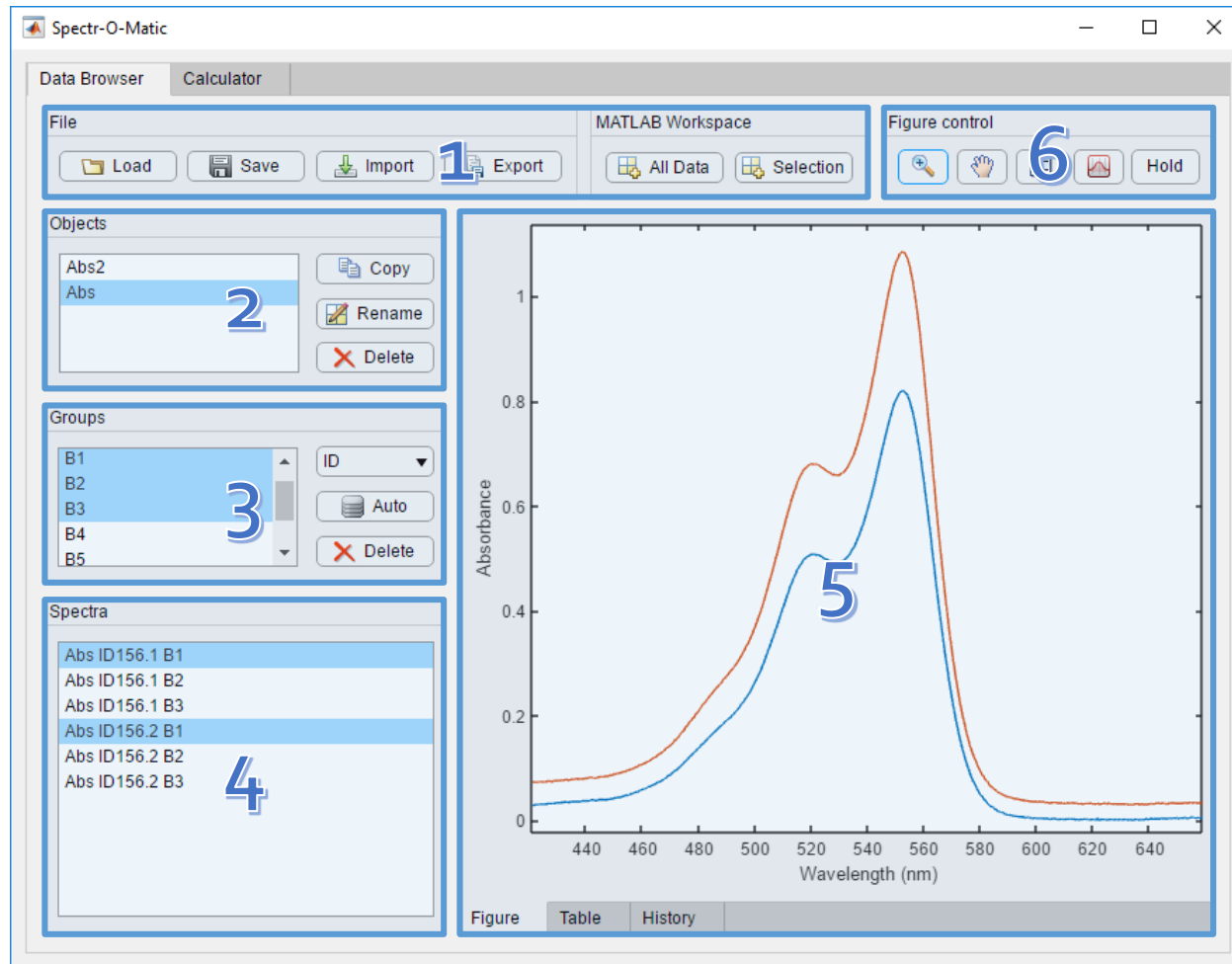


The Data Browser is what you see when you start the app.

The Data Browser lets you

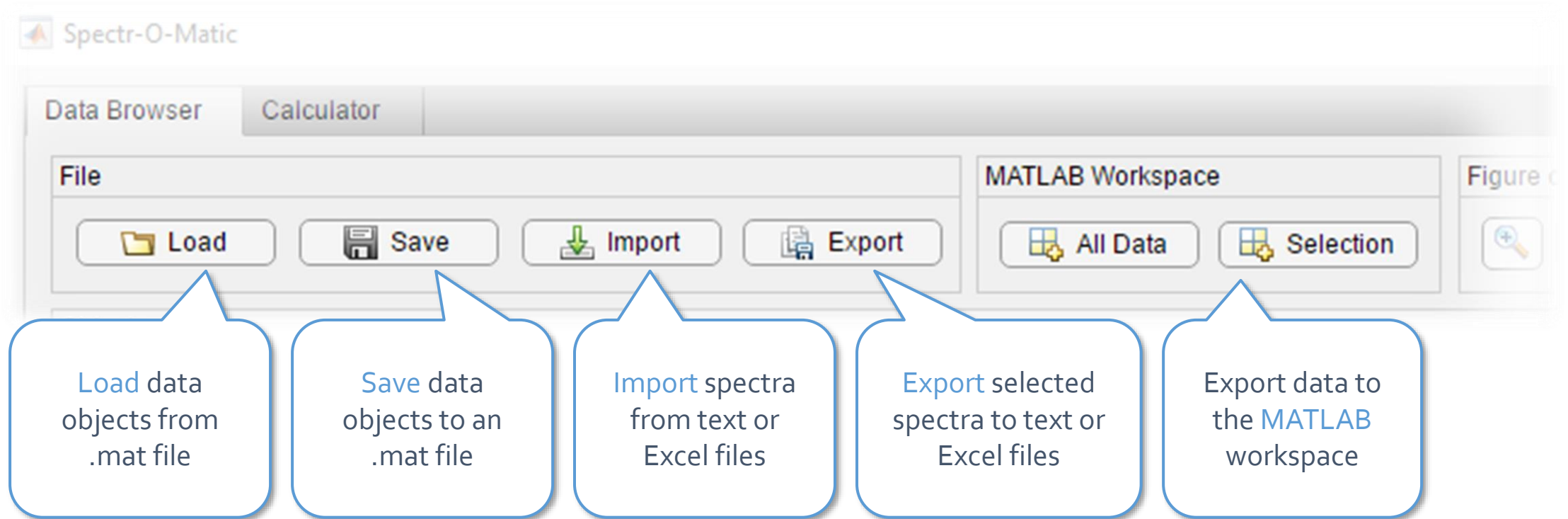
- load/save spectra
- copy, rename, delete data objects
- visualize spectra

Data Browser Components



1. Import / export data
2. Select and manage data objects
3. Select and manage named groups
4. Select spectra for visualization
5. Graph/table view of spectra
6. Figure (graph) controls

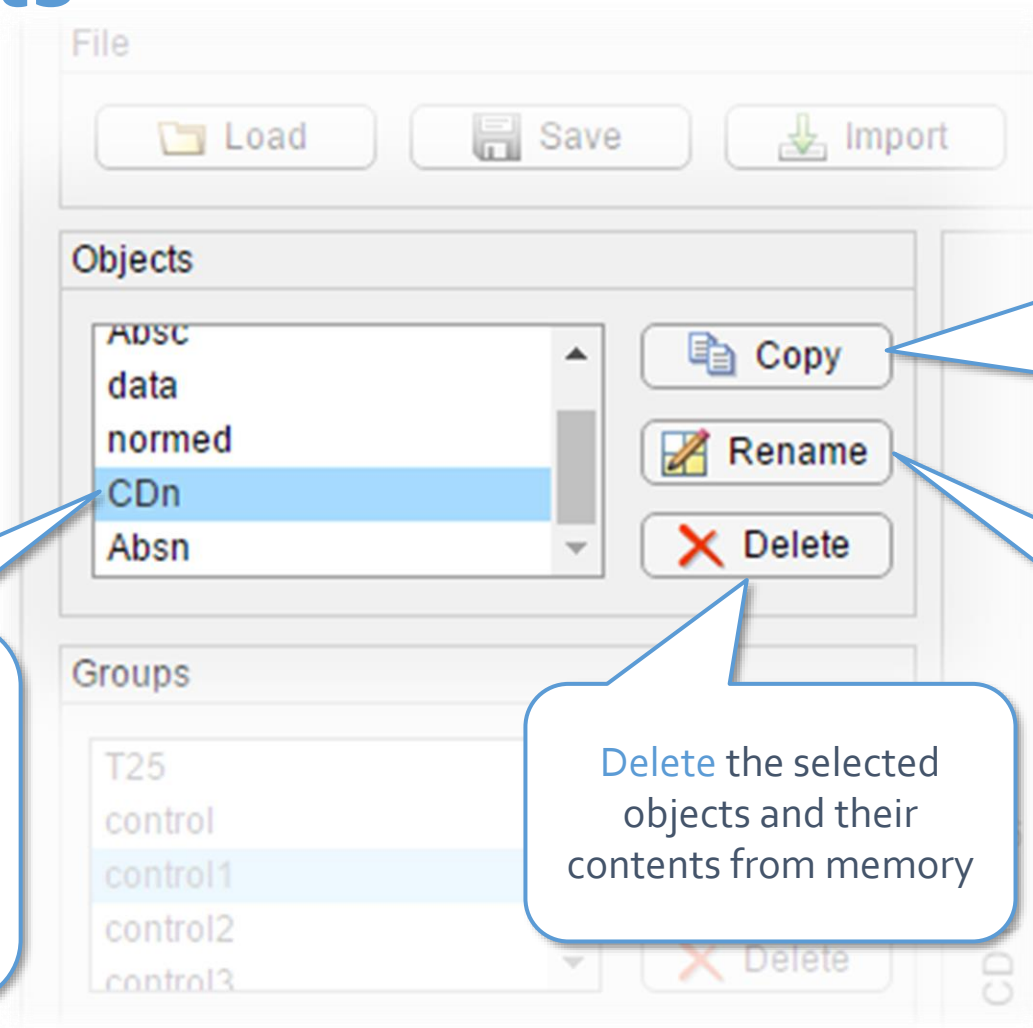
Import / export data



Data objects

Objects are named containers for spectra and other types of data

Click to **select an object**.
Hold control or shift to
select multiple objects



Copy an object and its contents
(If multiple objects of the same type are selected, their contents are combined.)

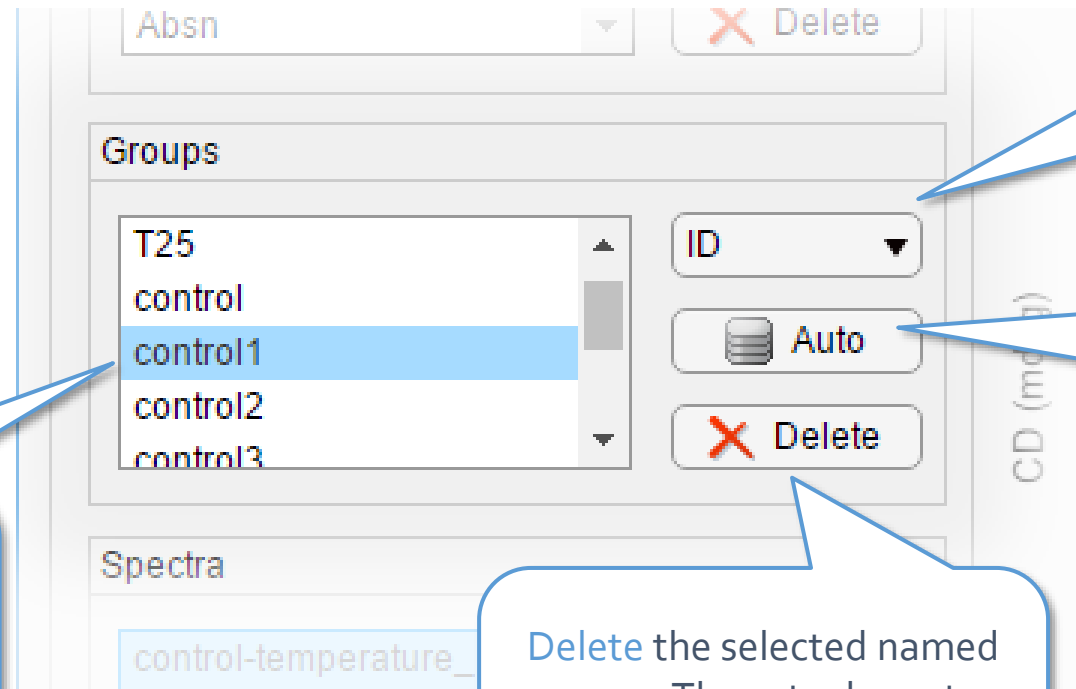
Rename an object
(or the combined contents of multiple objects)

Delete the selected objects and their contents from memory

Groups

Groups are named collections of spectra in an object. (Spectra can belong to more than one group)

List of groups in the selected object(s). Click to **select a group**. Hold control/shift for multiple selections



Select a **property** to use for automatic grouping (ID, type, etc.).

Automatically create groups based on the selected property.

Delete the selected named groups. The actual spectra are **not** deleted, only their group designation.

Spectra

Lists the spectra in the selected object(s) and group(s).

The selected spectra will be visualized in the figure on the right.

Click to select spectra.
Hold control/shift for
multiple selections

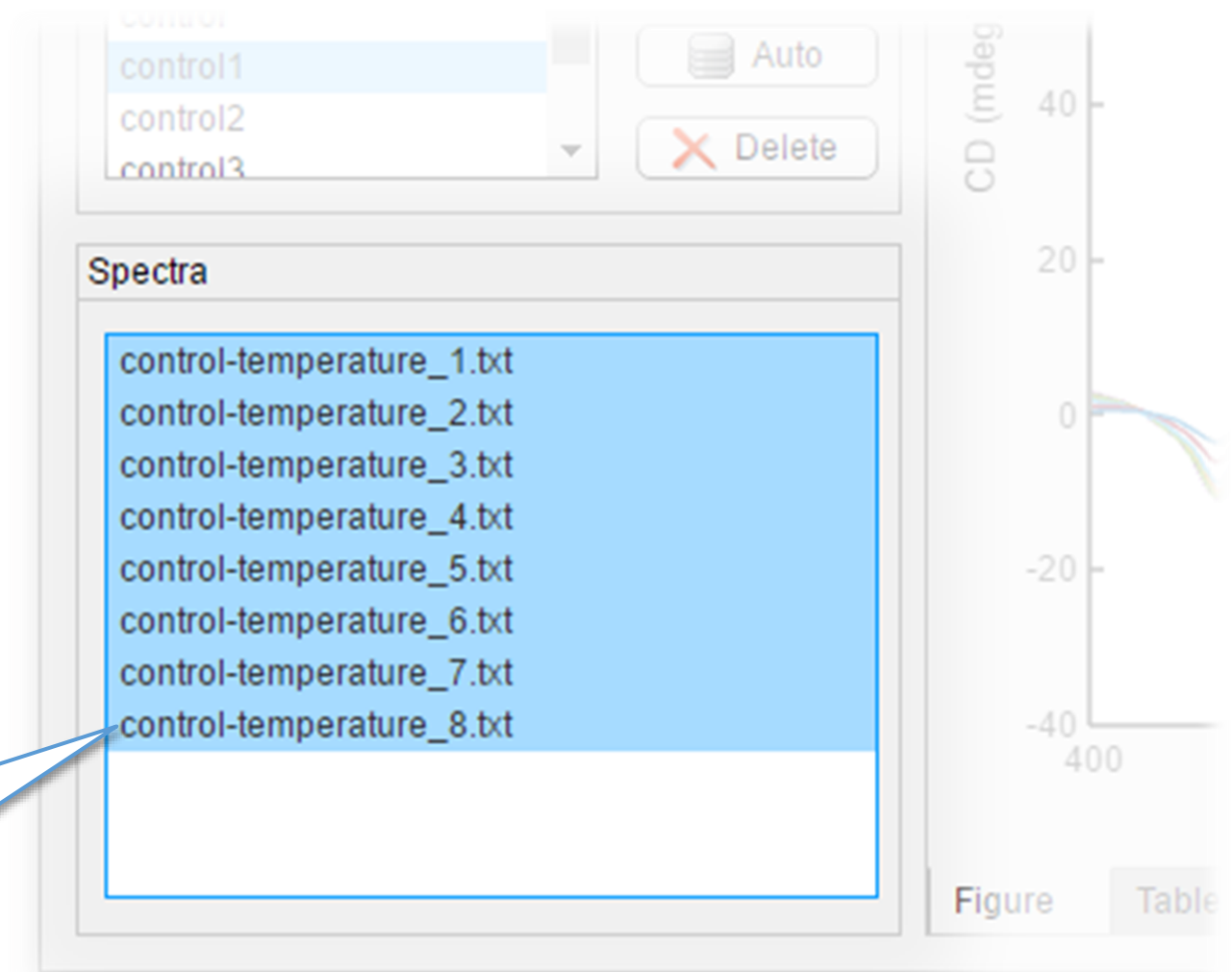


Figure / Table view

These are the selected spectra in the selected object(s). They can be visualized as a graph or viewed as a table.

Switch between graphical view, tabular view, or see the history of operations

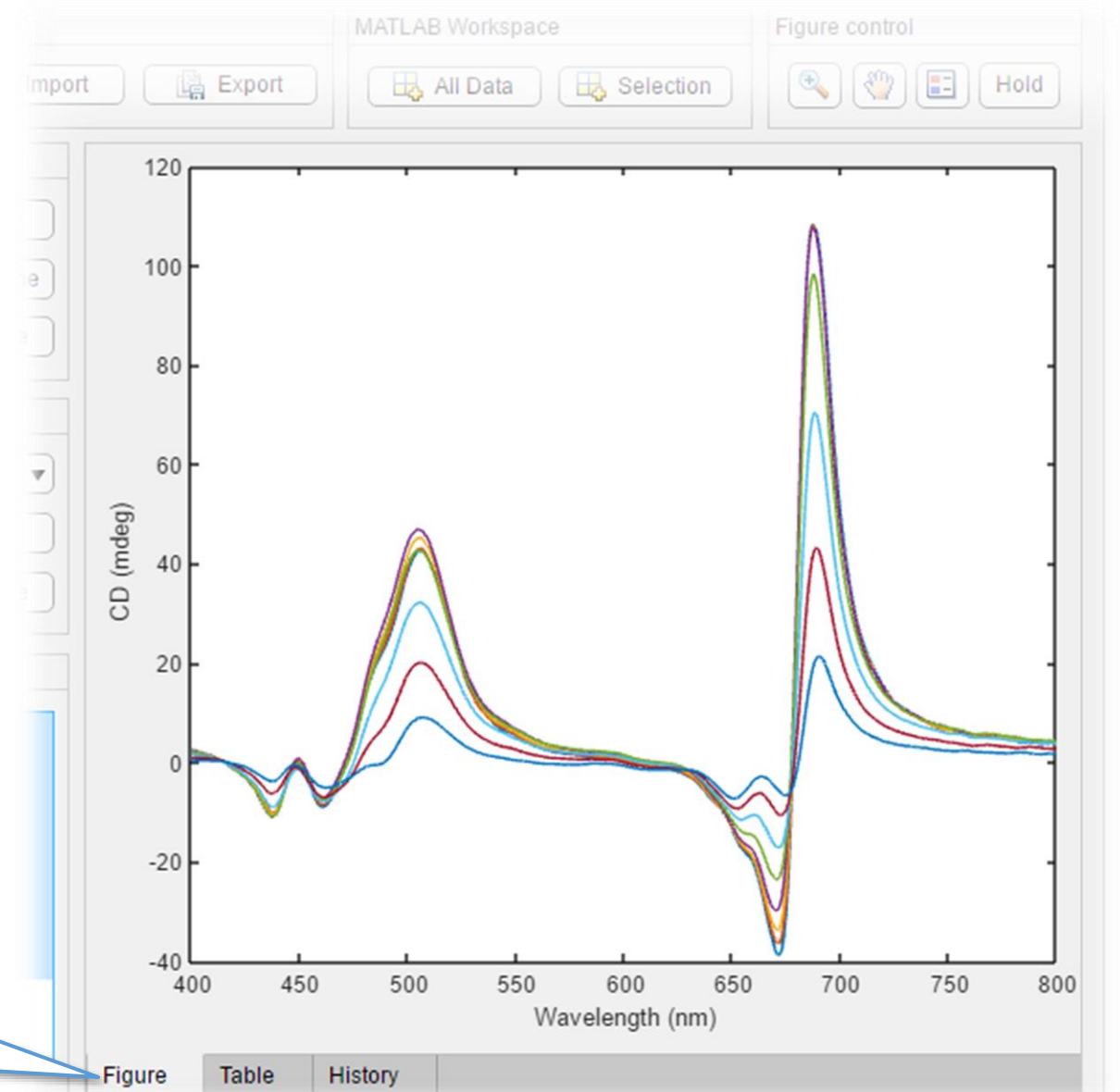


Figure controls

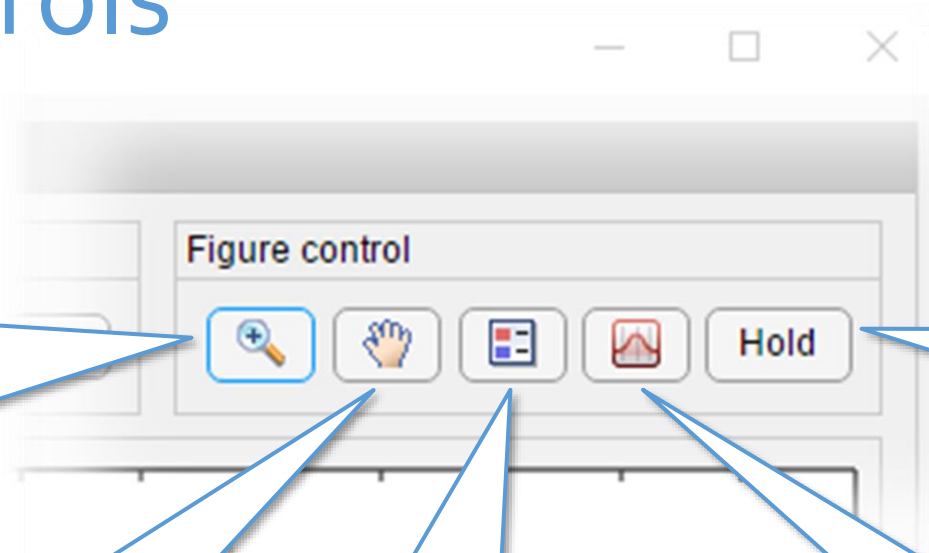
Zoom mode on/off.
When active, click in the figure to zoom in, Shift + click to zoom out.

Pan mode on/off.
When active, click and drag in the figure to move the graph around.

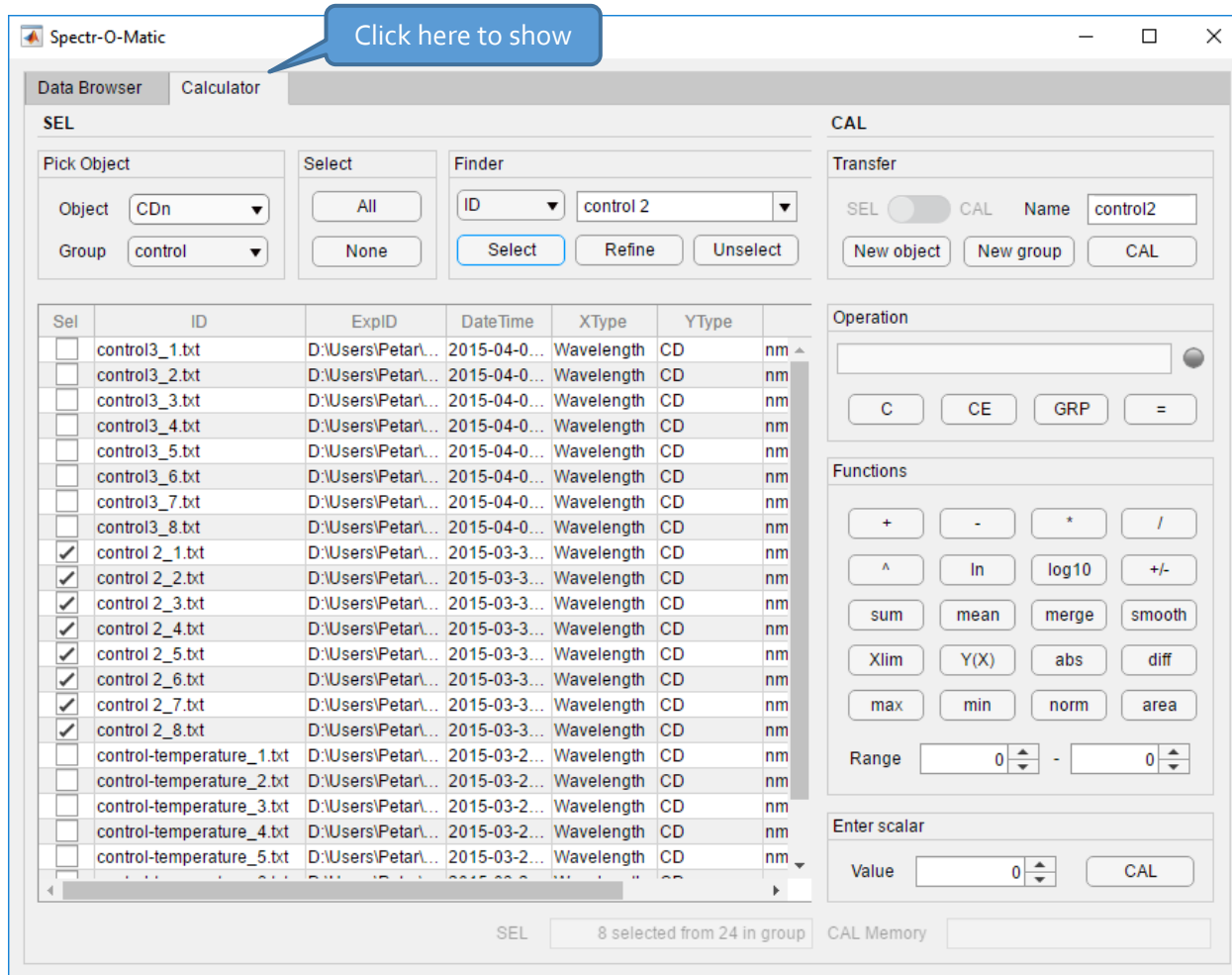
Show/hide legend

Show peak labels

Hold on/off.
When active, newly selected spectra will be overlaid onto the current graph.



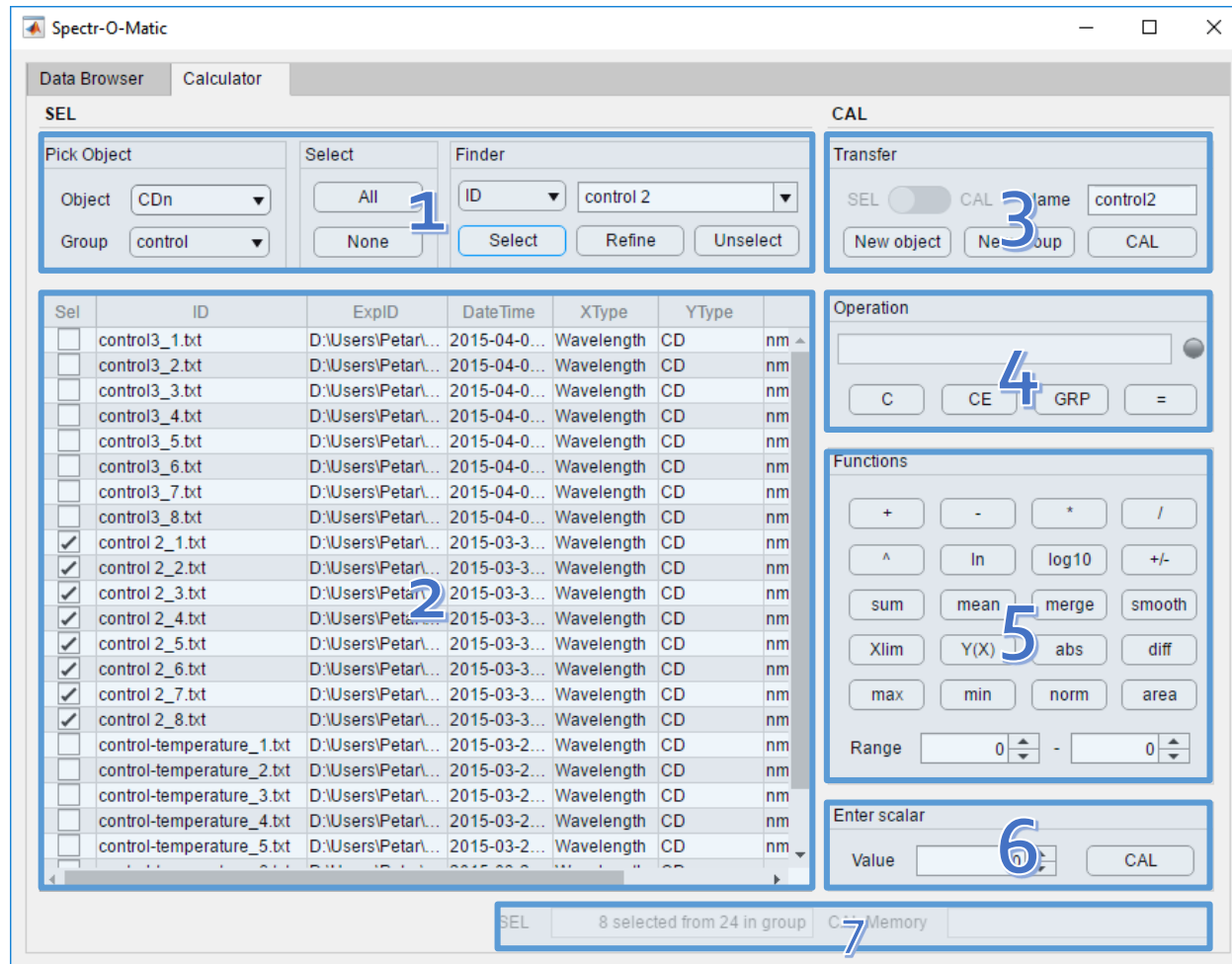
II. The Calculator



The Calculator is used to:

- find and select specific spectra
- create new groups and objects based on selections
- perform calculations with the selected spectra

Calculator Components



1. Object picker, finder
2. Data table
3. Transfer data
4. Operations
5. Functions
6. Scalar input
7. Memory status indicators

Object picker, finder

The interface is titled "SEL" and contains three main sections: "Pick Object", "Select", and "Finder".

- Pick Object:** Contains two dropdown menus. The "Object" dropdown is set to "CDn" and the "Group" dropdown is set to "control".
- Select:** Contains two buttons: "All" and "None".
- Finder:** Contains a dropdown menu set to "ID", a text input field containing "control 2", and three buttons: "Select", "Refine", and "Unselect".

Callouts explaining the functions:

- Pick object and group to work with:** Points to the "Object" and "Group" dropdowns.
- Select or unselect all spectra in the group:** Points to the "All" and "None" buttons.
- Select spectra whose property (e.g. ID) contains the search text:** Points to the "Select" button.
- Refine selection – only search among those spectra that are already selected:** Points to the "Refine" button.
- Unselect the spectra that match the search:** Points to the "Unselect" button.
- Find spectra by searching in their properties:** Points to the "Finder" section.
- Type text to search for:** Points to the text input field in the "Finder" section.

Data table

The screenshot shows a software interface with a data table. At the top, there are filters: 'Object' set to 'CDn', 'Group' set to 'control', and a 'Select' button. The table has columns: 'Sel' (checkboxes), 'ID', 'ExpID', 'DateTime', 'XType', 'YType', and a partially visible 'nm' column. The first 8 rows (control3_1.txt to control3_8.txt) have unchecked 'Sel' boxes. The next 8 rows (control 2_1.txt to control 2_8.txt) have checked 'Sel' boxes. A callout 'Property Columns' points to the 'ExpID' header. A callout on the left explains that the first 8 rows are not selected. A callout on the right explains that double-clicking a cell will edit the property for all selected rows.

Sel	ID	ExpID	DateTime	XType	YType	nm
<input type="checkbox"/>	control3_1.txt	D:\Users\Petar\...	2015-04-0...	Wavelength	CD	nm
<input type="checkbox"/>	control3_2.txt	D:\Users\Petar\...	2015-04-0...	Wavelength	CD	nm
<input type="checkbox"/>	control3_3.txt	D:\Users\Petar\...	2015-04-0...	Wavelength	CD	nm
<input type="checkbox"/>	control3_4.txt	D:\Users\Petar\...	2015-04-0...	Wavelength	CD	nm
<input type="checkbox"/>	control3_5.txt	D:\Users\Petar\...	2015-04-0...	Wavelength	CD	nm
<input type="checkbox"/>	control3_6.txt	D:\Users\Petar\...	2015-04-0...	Wavelength	CD	nm
<input type="checkbox"/>	control3_7.txt	D:\Users\Petar\...	2015-04-0...	Wavelength	CD	nm
<input type="checkbox"/>	control3_8.txt	D:\Users\Petar\...	2015-04-0...	Wavelength	CD	nm
<input checked="" type="checkbox"/>	control 2_1.txt	D:\Users\Petar\...	2015-03-3...	Wavelength	CD	nm
<input checked="" type="checkbox"/>	control 2_2.txt	D:\Users\Petar\...	2015-03-3...	Wavelength	CD	nm
<input checked="" type="checkbox"/>	control 2_3.txt	D:\Users\Petar\...	2015-03-3...	Wavelength	CD	nm
<input checked="" type="checkbox"/>	control 2_4.txt	D:\Users\Petar\...	2015-03-3...	Wavelength	CD	nm
<input checked="" type="checkbox"/>	control 2_5.txt	D:\Users\Petar\...	2015-03-3...	Wavelength	CD	nm
<input checked="" type="checkbox"/>	control 2_6.txt	D:\Users\Petar\...	2015-03-3...	Wavelength	CD	nm
<input checked="" type="checkbox"/>	control 2_7.txt	D:\Users\Petar\...	2015-03-3...	Wavelength	CD	nm
<input checked="" type="checkbox"/>	control 2_8.txt	D:\Users\Petar\...	2015-03-3...	Wavelength	CD	nm

Property Columns

These spectra are not selected. Click the boxes to select.

These spectra are selected

Double click the cell to edit the property. The change will affect all selected spectra.

Transfer data

The image shows a software interface window titled "CAL". Inside, there is a "Transfer" section with a toggle switch labeled "SEL" (currently off) and a label "CAL". To the right of the toggle is a text input field labeled "Name" containing the text "NewName". Below these are three buttons: "New object", "New group", and "CAL". Below the buttons is an "Operation" section with a text input field containing ".norm" and a green circular button. Five callout boxes provide explanations for the interface elements:

- Transfer data from the data table (SEL) or from the calculator memory (CAL)
- Name for the new object/group
- Copy selected spectra (SEL) or calculator memory (CAL) as a new object
- Assign the selected spectra to a new named group
- Transfer the selection to the calculator memory

Operations

Execute or cancel calculations
and check their status

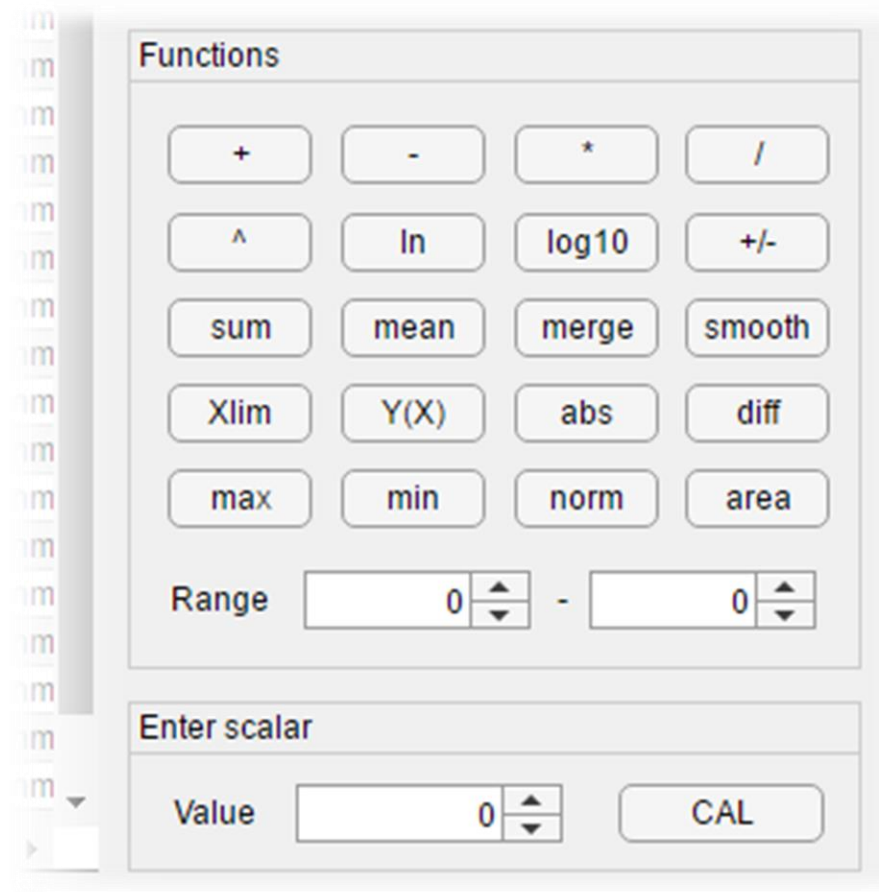
The image shows a calculator interface with several callouts explaining its functions:

- Calculation expression:** Points to the input field containing the expression `CD(n=3).norm`.
- CAL status:** A legend box explaining the status indicator:
 - memory clear
 - pending calculation
 - result in memoryThe status indicator in the image is a green dot, indicating the result is in memory.
- Cancel all pending calculations and clear CAL memory:** Points to the **C** button.
- Clear the last input:** Points to the **CE** button.
- Grouped operation on/off:** Points to the **GRP** button.
- Execute / evaluate:** Points to the **=** button.

Calculator functions

To perform calculations with spectra:

- Select the spectra in the data table
- Press a function button
- If necessary, make a new selection (second operand)
- Press " = " in the operations box to execute the calculation OR
- Press another function button to define a sequence of operations



Calculator functions (cont.)

+ - * /	Add, subtract, divide, multiply spectra (require two operands – spectra or scalar)
^	Power (two operands, spectra or scalar)
ln, log10	Natural, decimal logarithm
+/-	Invert sign (negate)
sum	Sum of spectra or scalars
mean	Average spectra or scalars
merge	Join spectra into one (connect different X range)
smooth	Smooth spectra (moving average) – optionally specify number of points in the left Range box

The image shows a software calculator interface. At the top, there are four buttons: 'C', 'CE', 'GRP', and '='. Below these is a section titled 'Functions' containing a grid of buttons: '+', '-', '*', '/', '^', 'ln', 'log10', '+/-' in the first row; 'sum', 'mean', 'merge', 'smooth' in the second row; 'Xlim', 'Y(X)', 'abs', 'diff' in the third row; and 'max', 'min', 'norm', 'area' in the fourth row. Below the function grid is a 'Range' section with two input boxes, each containing '0' and a vertical scroll bar, separated by a minus sign. At the bottom is an 'Enter scalar' section with a 'Value' input box containing '0' and a 'CAL' button.

Calculator functions (cont.)

Xlim	Truncate spectral range - specify minimum and maximum X values in the Range boxes (enter range values before hitting the function button)
abs	Modulus (absolute value)
diff	Differentiate (1 st derivative)
max	Maximal magnitude (Y value) in a specified spectral range (use the Range boxes)
min	Minimal magnitude (Y value) in a spectral range
norm	Normalize spectra to: - their maximum or to the value at a certain X position (use left Range box to specify) or to the maximum in a spectral range (use the two Range boxes)
area	Integral (area under the spectrum)

The image shows a software calculator interface. At the top, there are four buttons: 'sum', 'mean', 'merge', and 'smooth'. Below these are four more buttons: 'Xlim', 'Y(X)', 'abs', and 'diff'. The next row contains 'max', 'min', 'norm', and 'area'. Below the buttons is a 'Range' section with two input boxes, each containing the number '0', separated by a minus sign. At the bottom, there is a section titled 'Enter scalar' which includes a 'Value' input box (also containing '0') and a 'CAL' button. A blue callout bubble points to the 'CAL' button.

To input scalar (number) as an operand, enter the number and press CAL