SPECTR-O-MATIC APP

App Interface Tutorial

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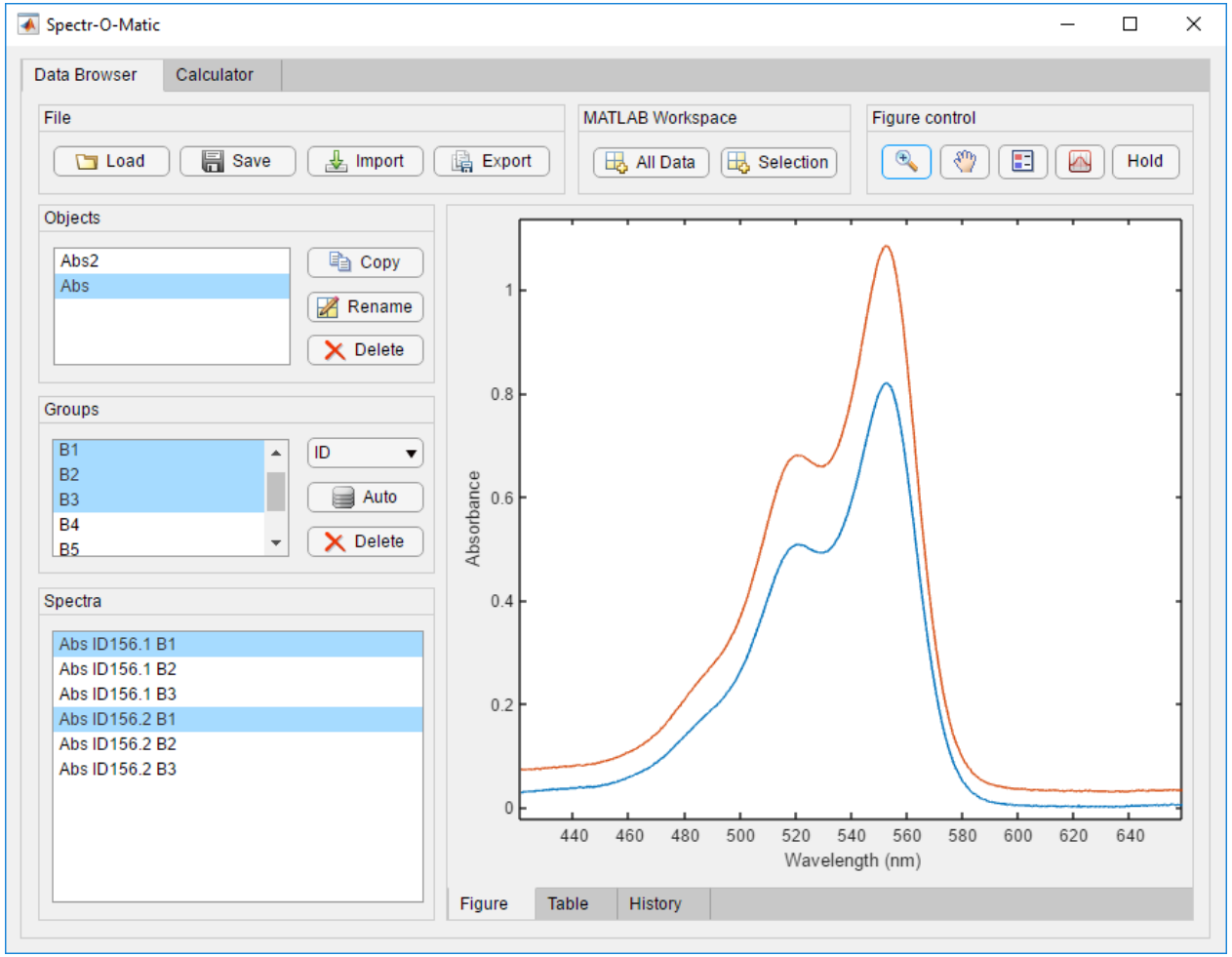
Press Ctrl-L to view in full screen

I. The Data Browser

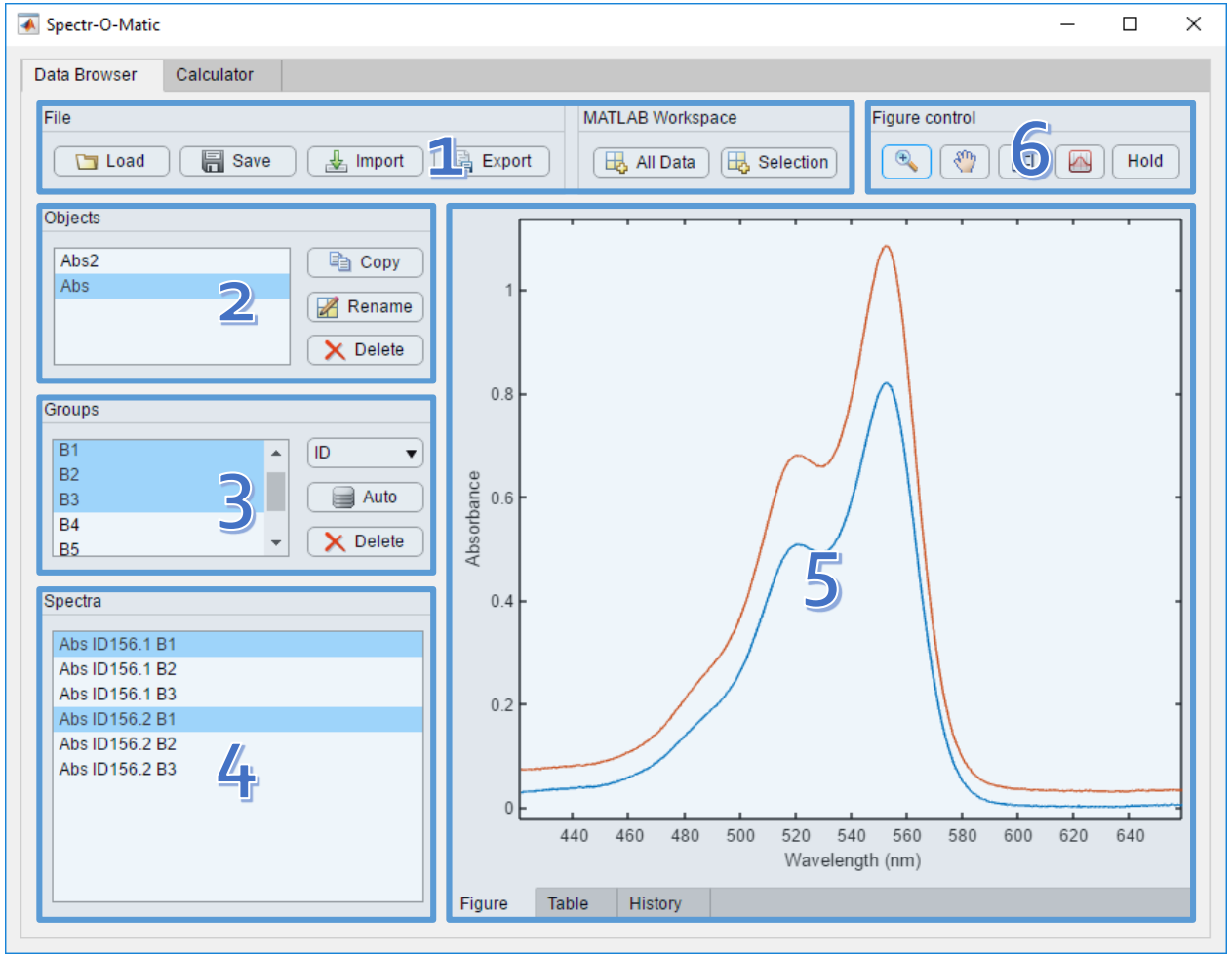


The Data Browser is what you see when you start the app.

The Data Browser lets you

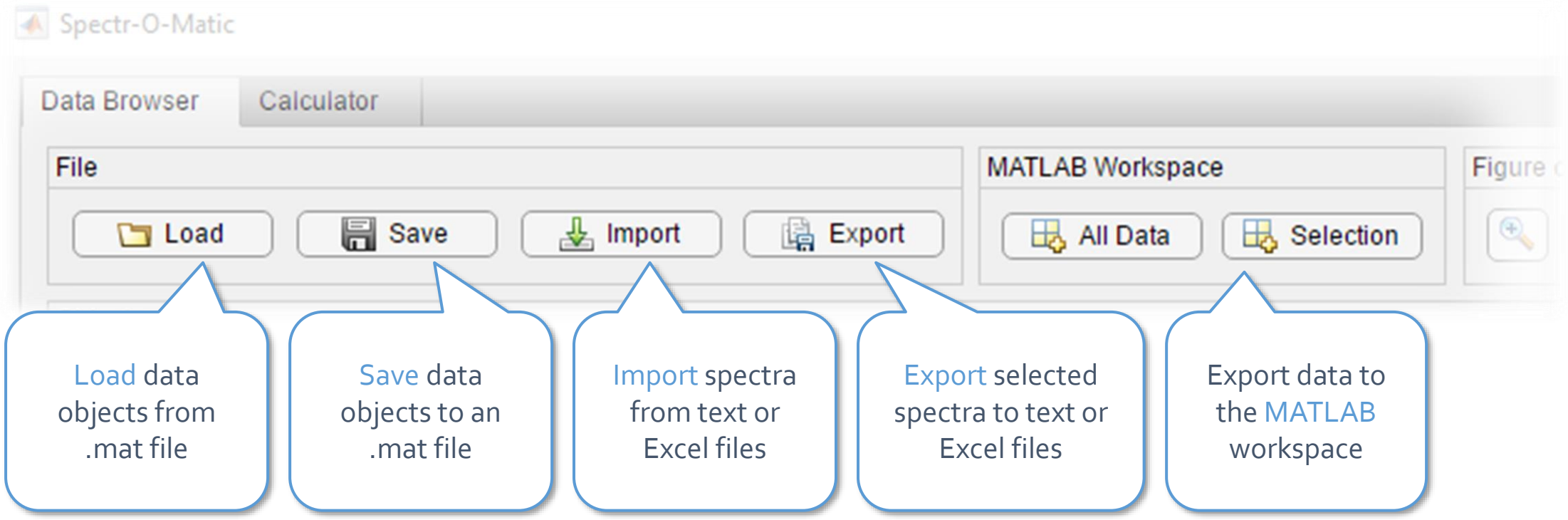
- load/save spectra
- copy, rename, delete data objects
- visualize spectra

Data Browser Components



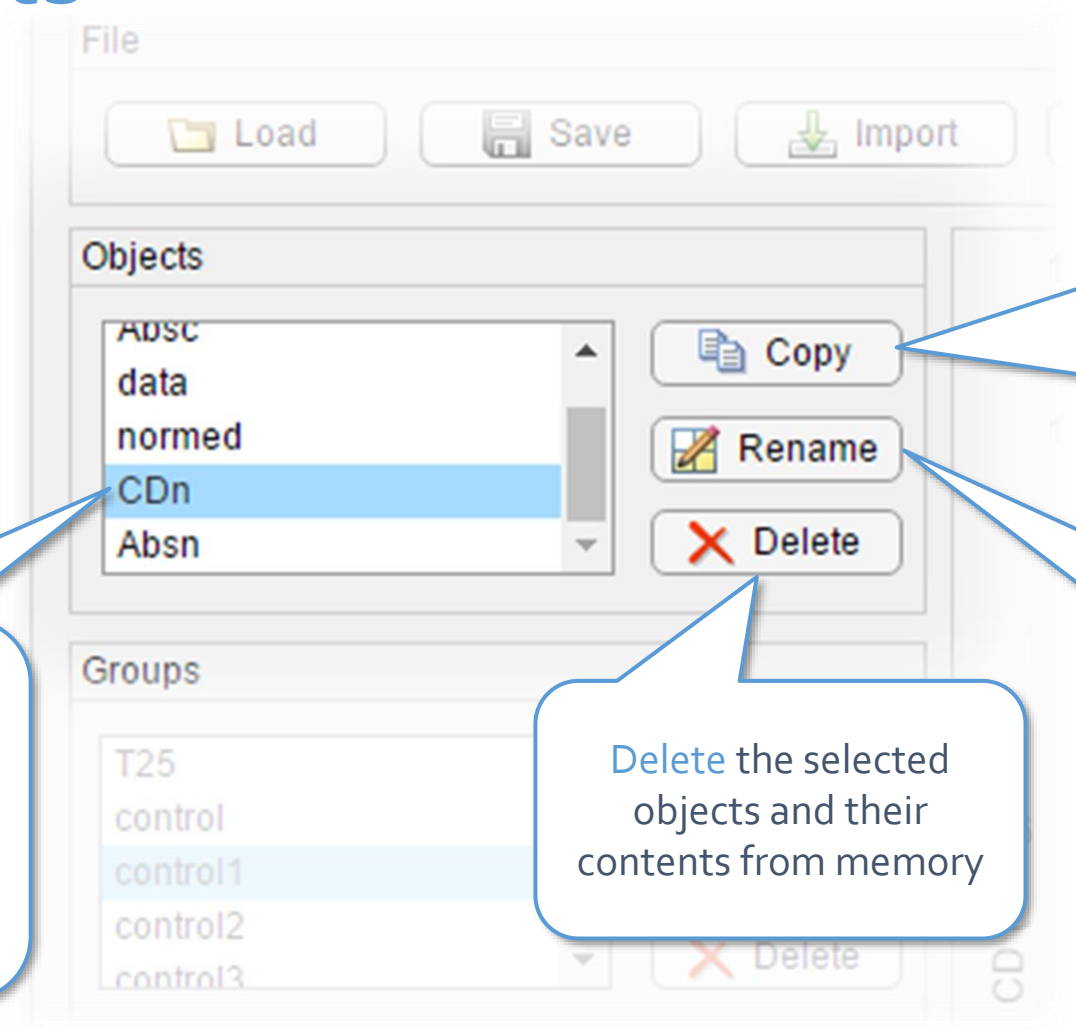
1. Import / export data
2. Select and manage data objects
3. Select and manage named groups
4. Select spectra for visualization
5. Graph/table view of spectra
6. Figure (graph) controls

Import / export data



Data objects

Objects are named containers for spectra and other types of data



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

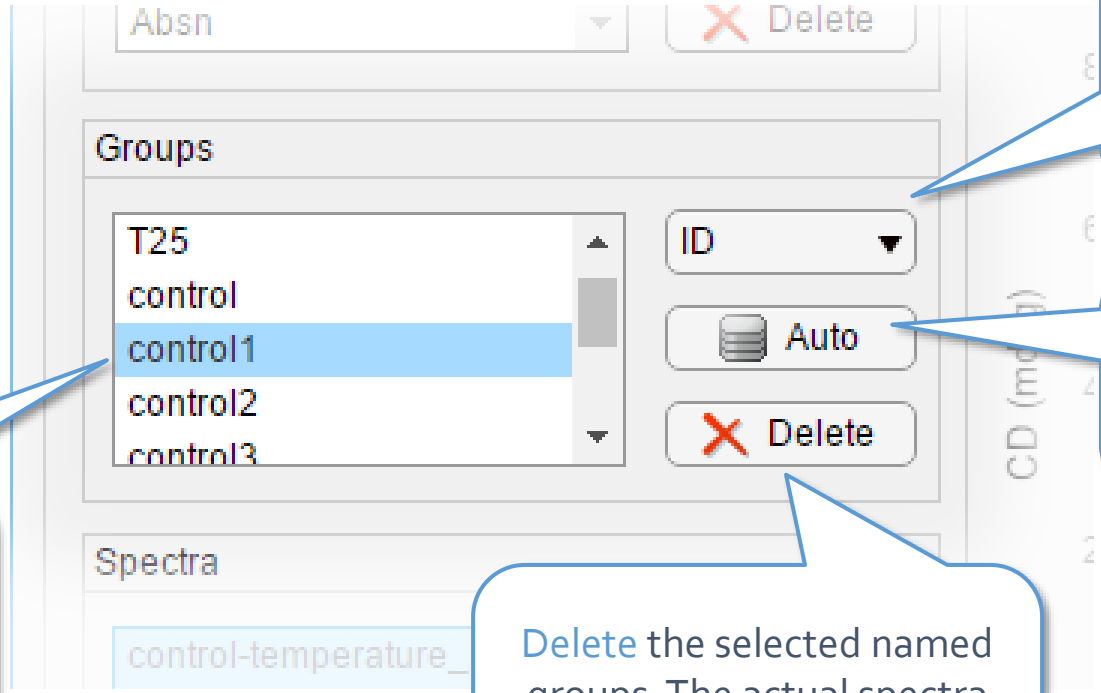
Rename an object
(or the combined contents of multiple objects)

Click to select an object. Hold control or shift to select 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)



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

Automatically create groups based on the selected property.

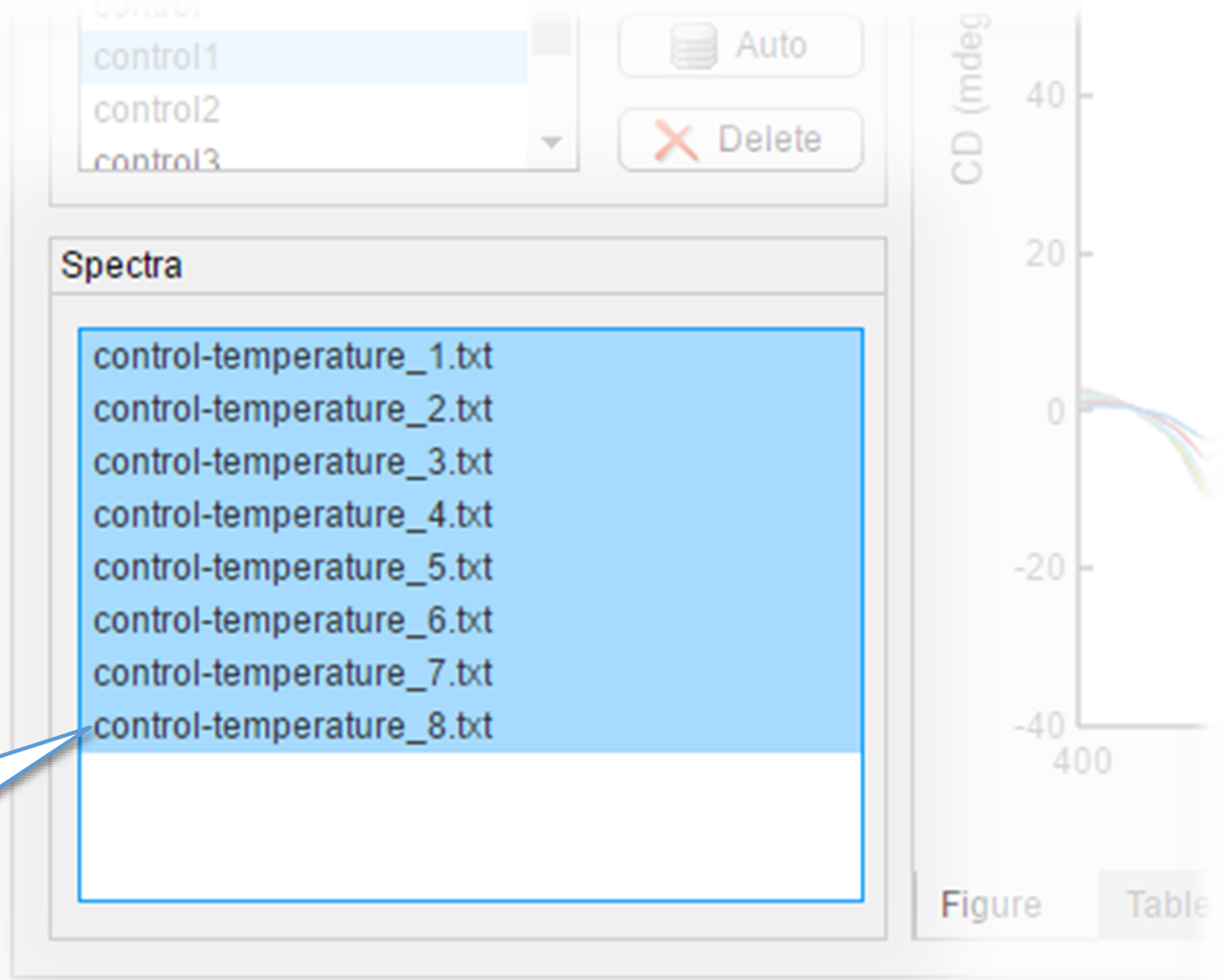
List of groups in the selected object(s). Click to select a group. Hold control/shift for multiple selections

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).

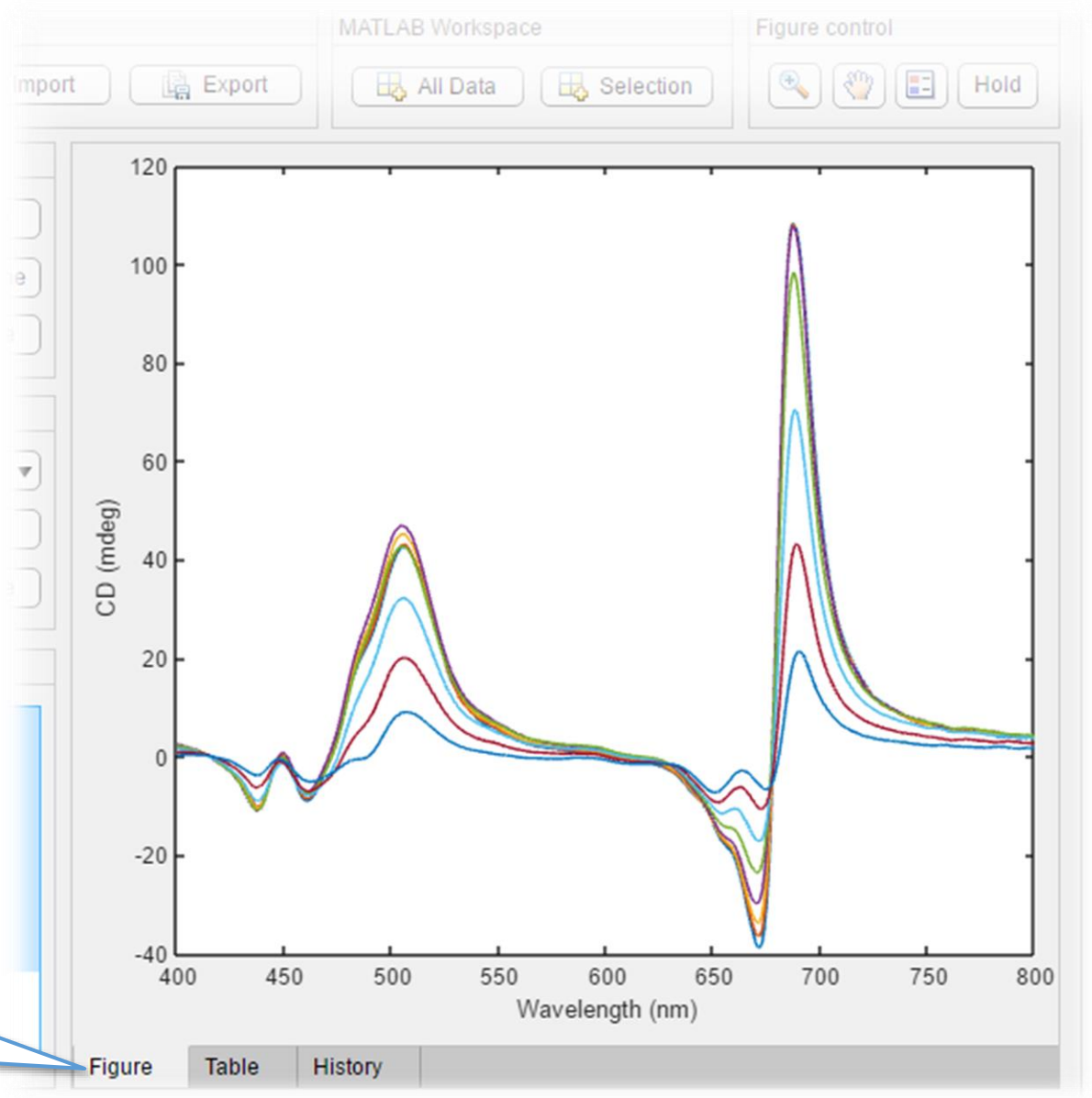
The selected spectra will be visualized in the figure on the right.



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

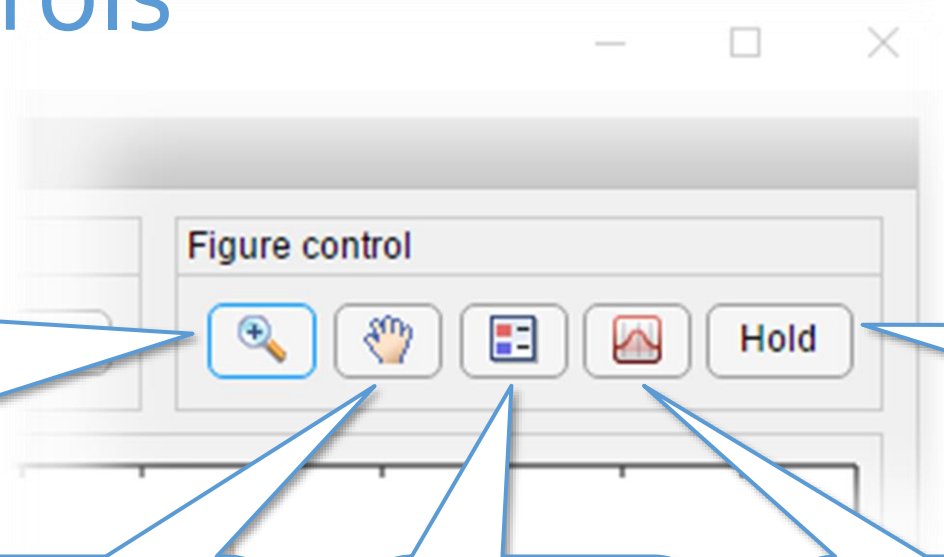
Figure / Table view

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.

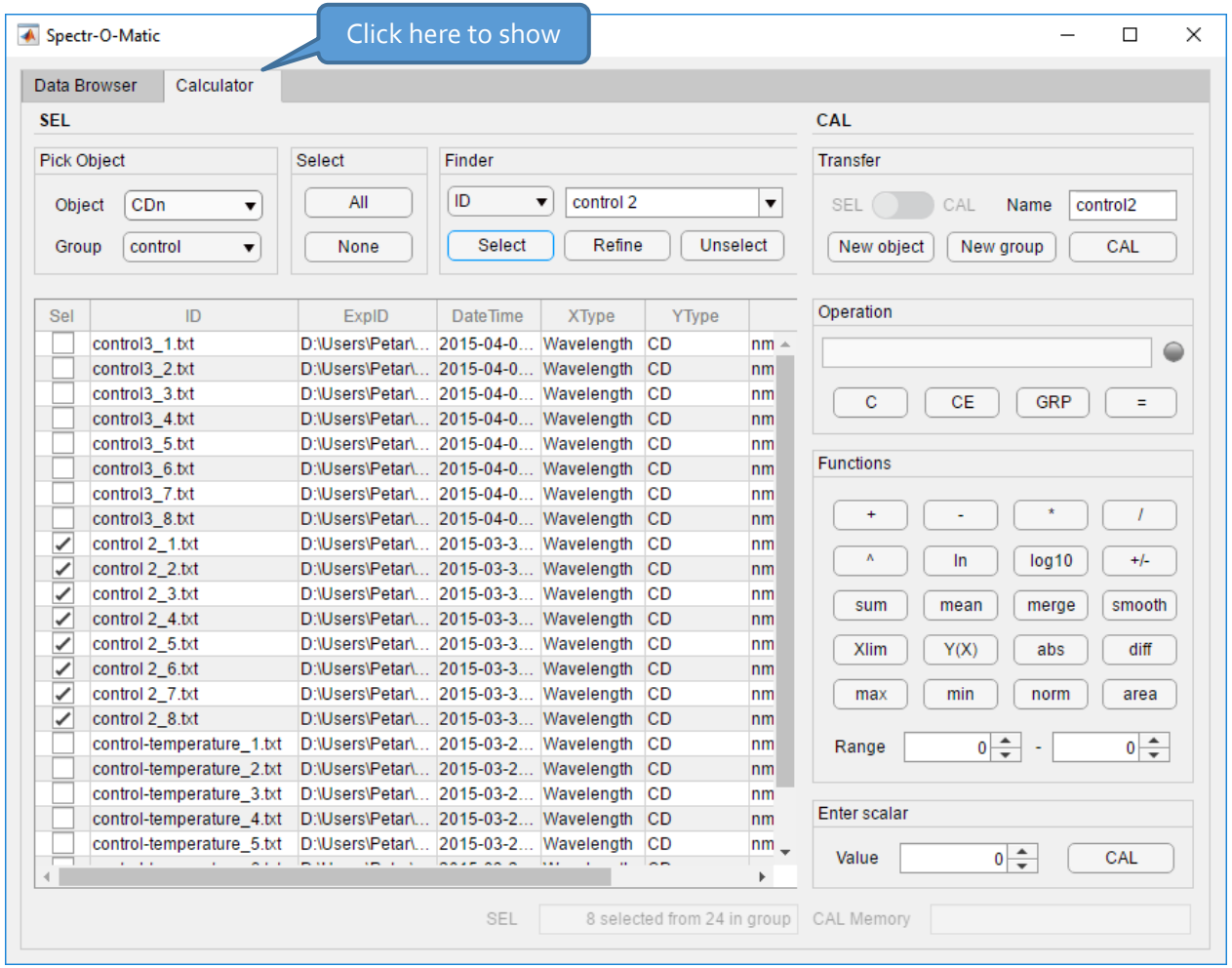
Hold on/off.
When active, newly selected spectra will be overlaid onto the current graph.

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

Show/hide legend

Show peak labels

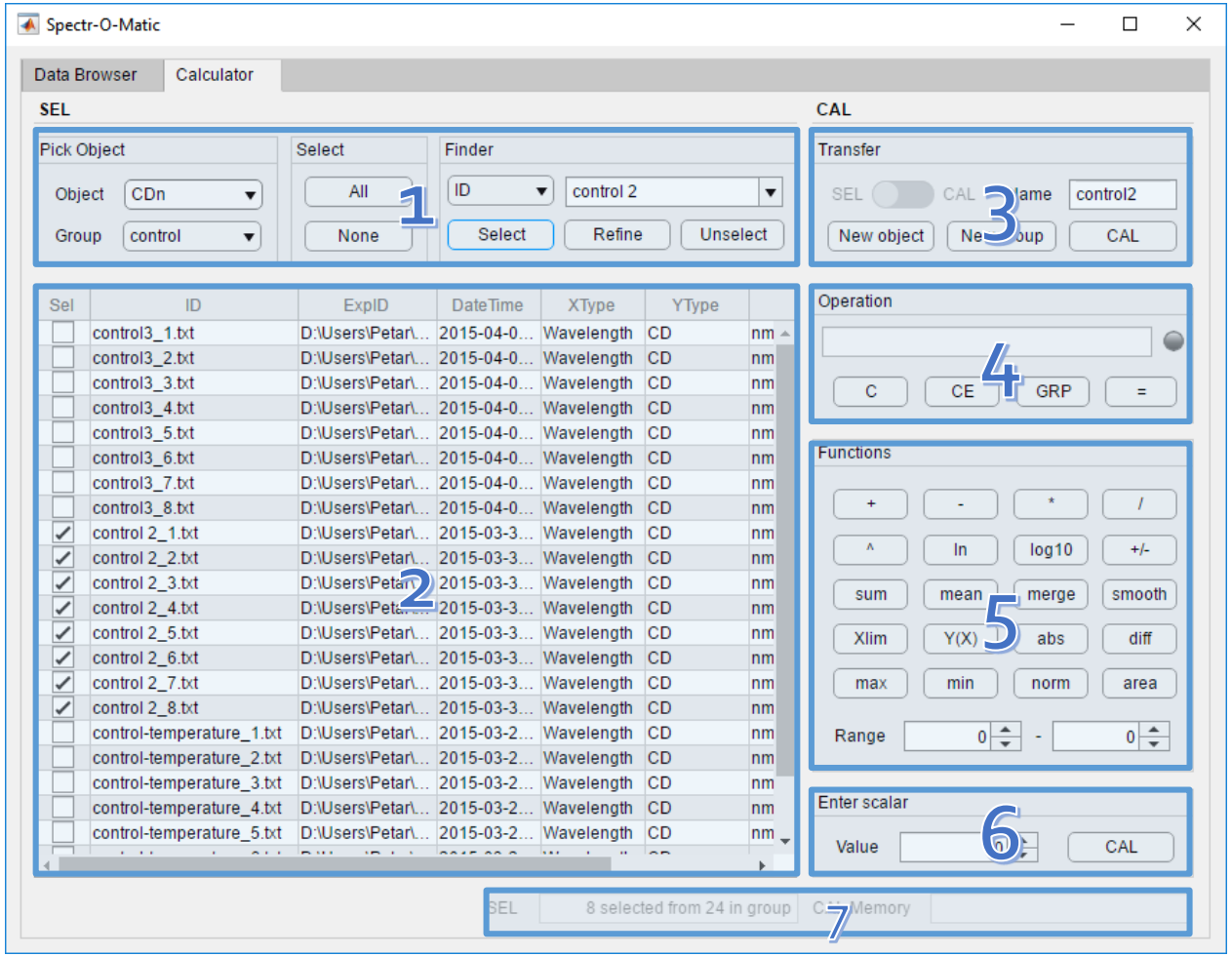
II. The Calculator



The Calculator is used to:

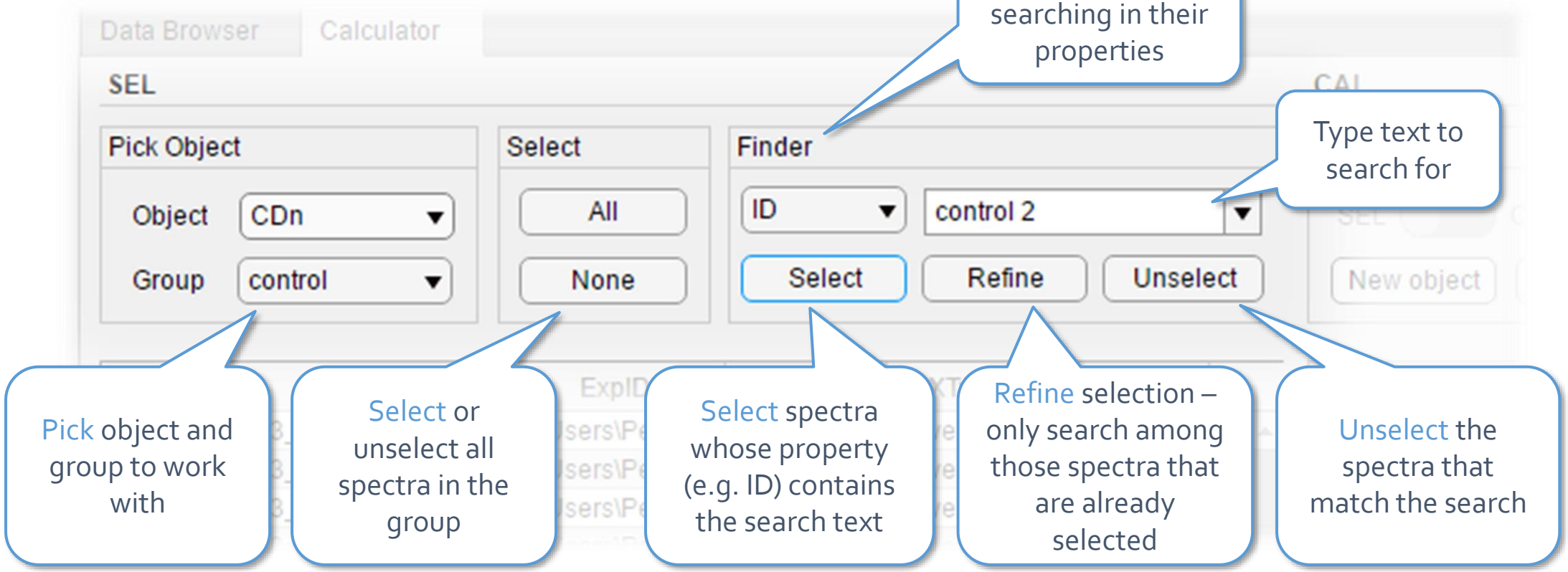
- find and select specific spectra
- create new groups and objects based on selections
- perform calculations with the selected spectra

Calculator Components

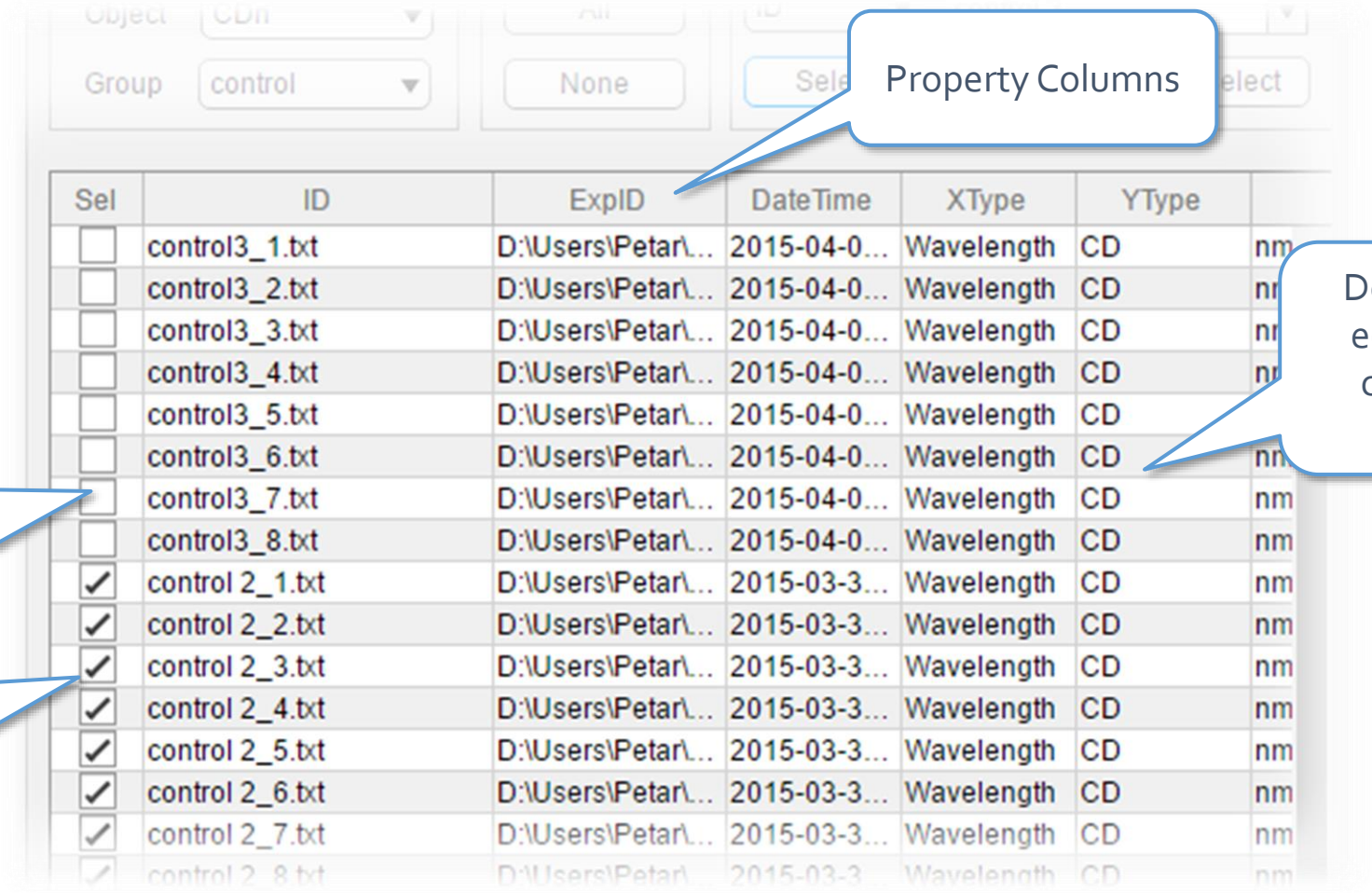


1. Object picker, finder
2. Data table
3. Transfer data
4. Operations
5. Functions
6. Scalar input
7. Memory status indicators

Object picker, finder



Data table

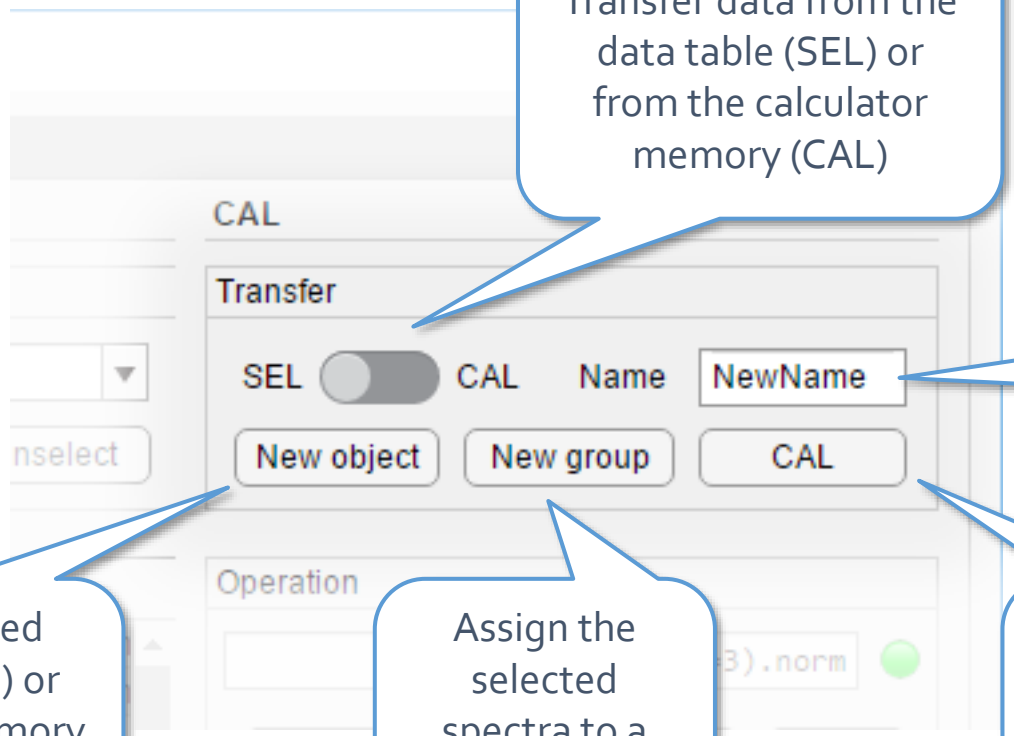


These spectra are not selected. Click the boxes to select.

These spectra are selected

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

Transfer data



Transfer data from the data table (SEL) or from the calculator memory (CAL)

Name for the new object/group

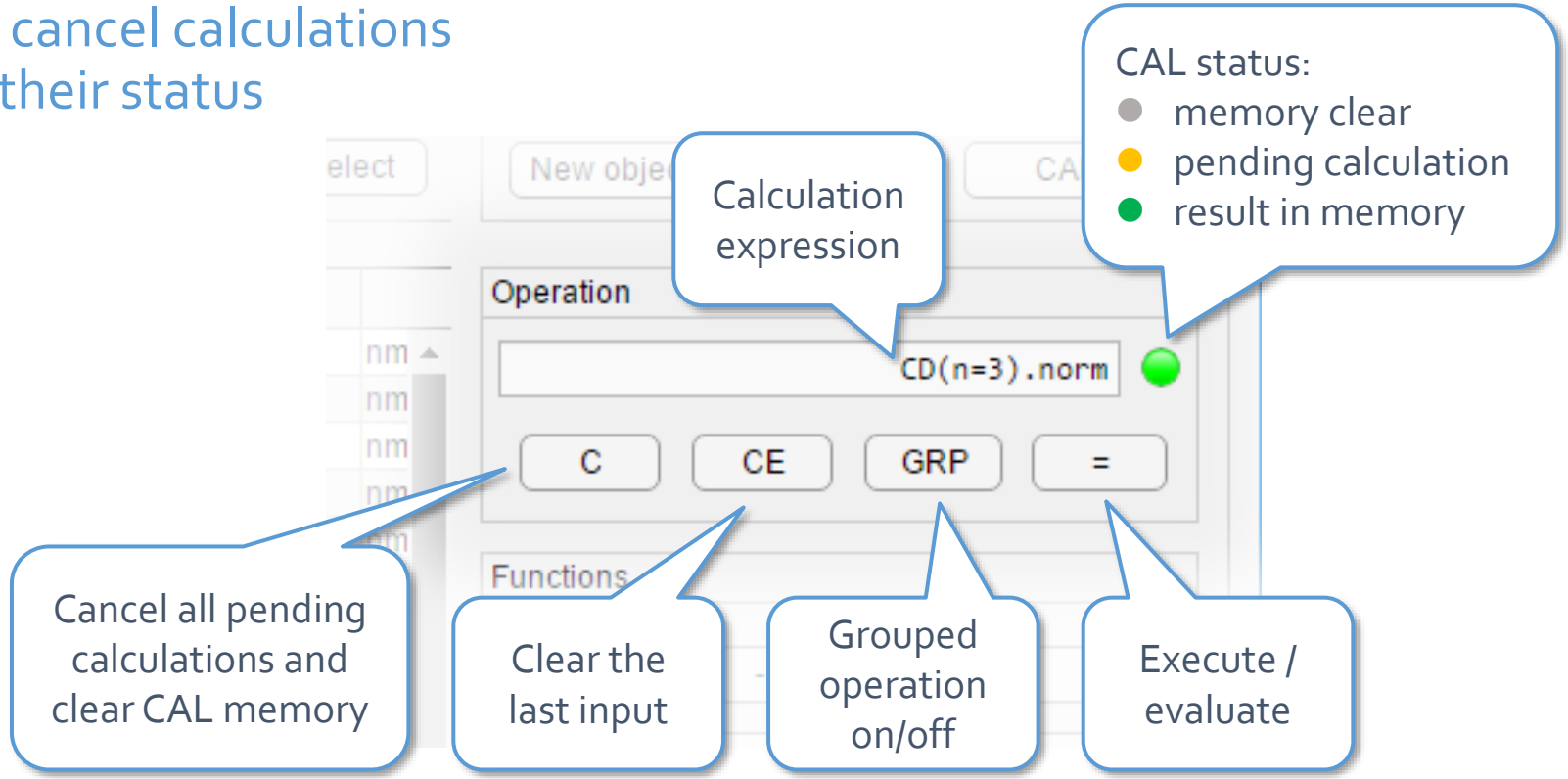
Copy selected spectra (SEL) or calculator memory (CAL) as a new object

Assign the selected spectra to a new named group

Transfer the selection to the calculator memory

Operations

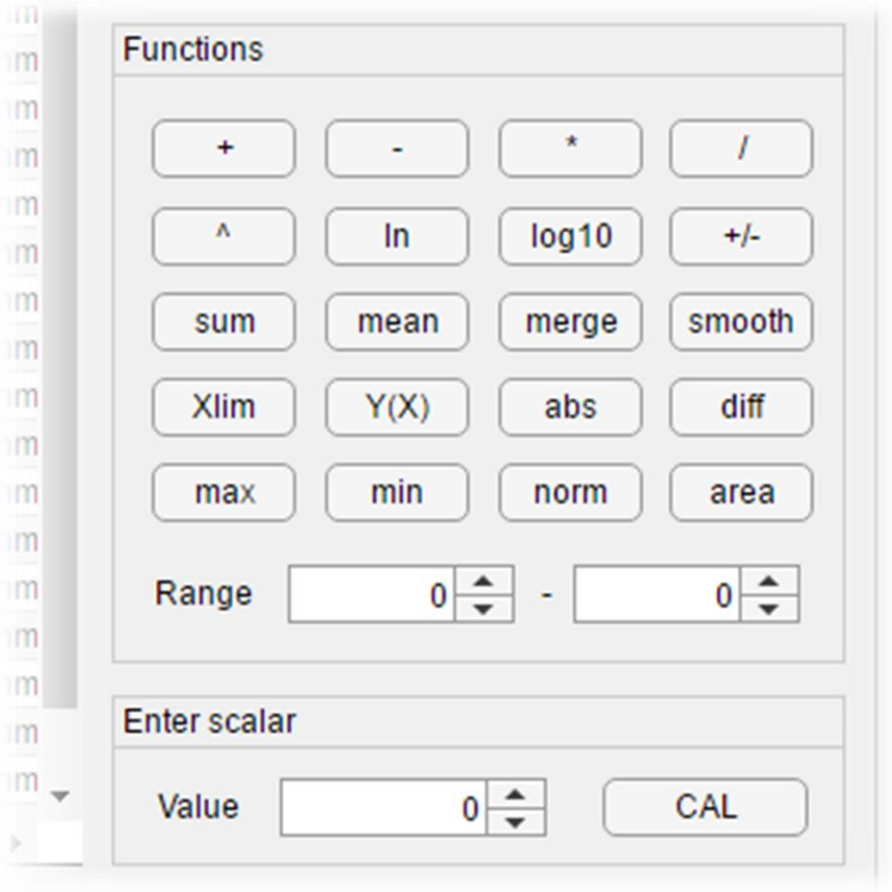
Execute or cancel calculations and check their status



Calculator functions

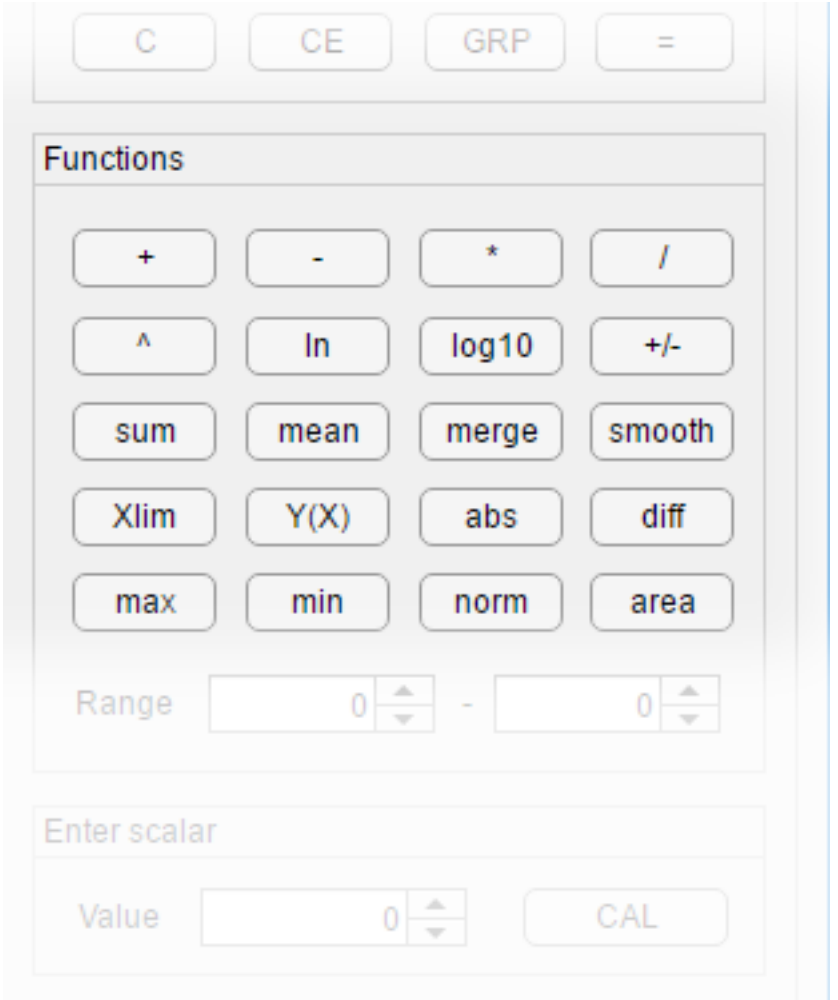
To perform calculations with spectra:

- 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



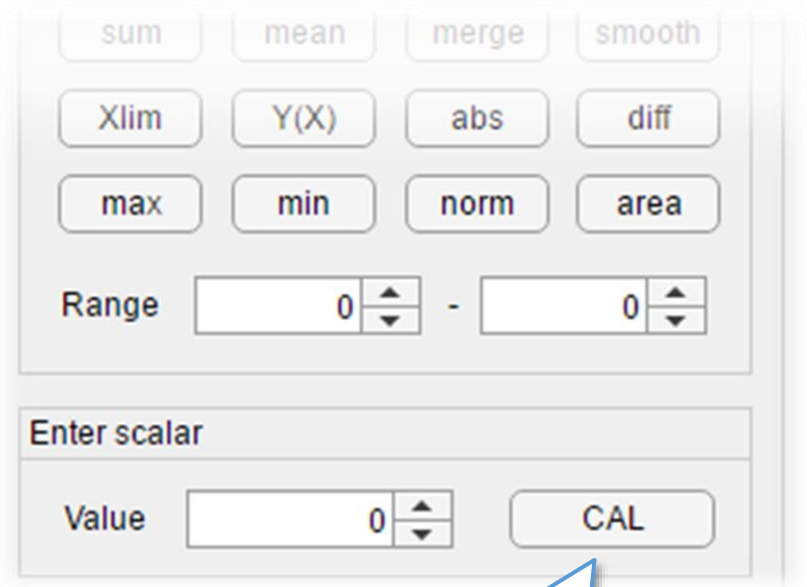
Calculator functions (cont.)

+ - * /	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



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 (1st 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)



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