Integrate Spectra

Integrate spectra in various ways.

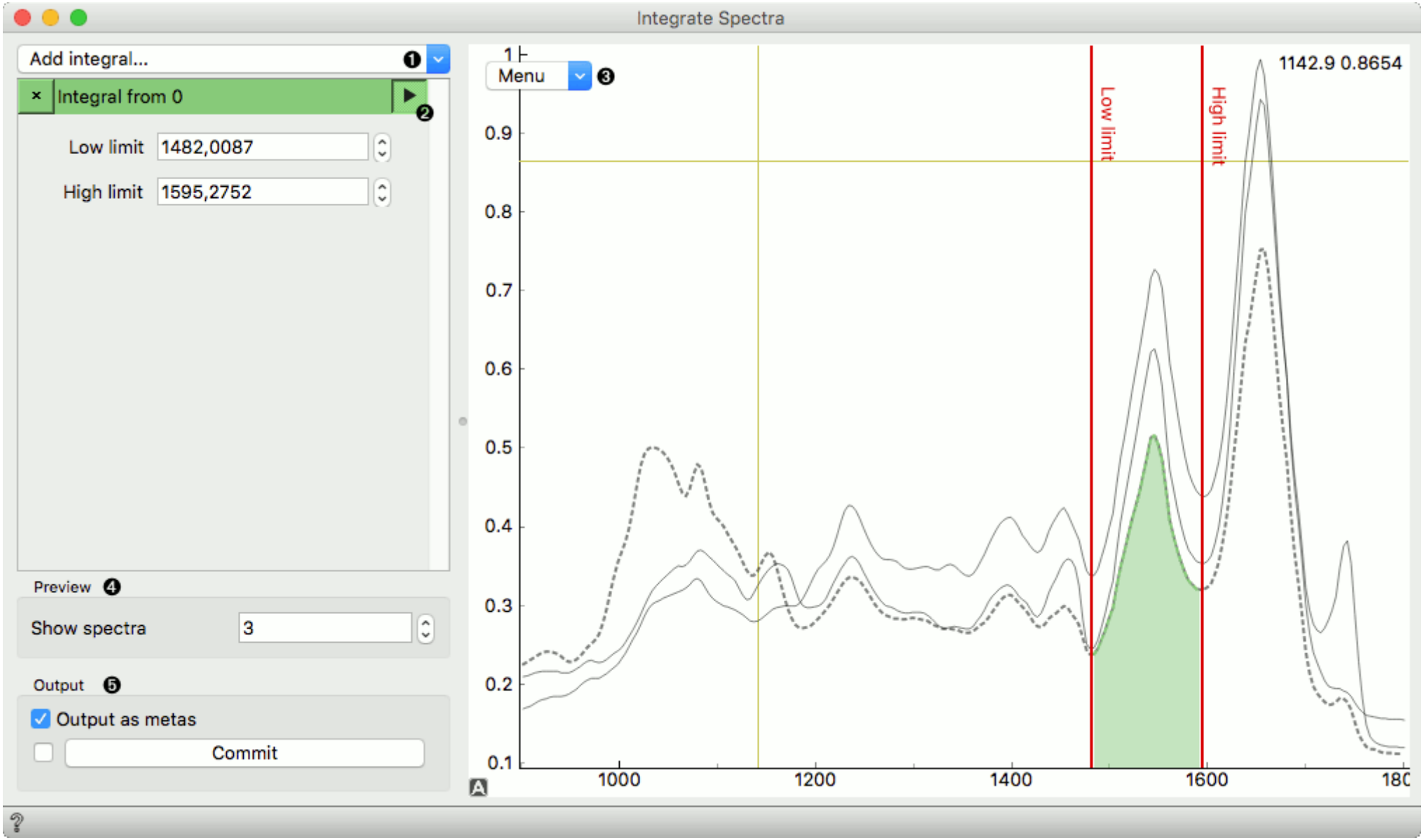
Inputs

- Data: input dataset

Outputs

- Integrated Data: data with integrals appended
- Preprocessor: preprocessing method

The **Integrate Spectra** widget allows you to add integrals to your data by selecting regions of interest and integrating them with several methods.



1. Add integral:
    - Integral from 0:
    - Integral from baseline:
    - Peak from 0:
    - Peak from baseline:
    - Closest value:

    - X-value of maximum from 0:
    - X-value of maximum from baseline
2. Toggle preview.
3. Preview plot with its editor menu like in the Spectra widget.
4. Show a subsample of the spectra (implemented for performance).
5. Output integrals as meta attributes. Otherwise only integrals will be output. Commit to send the changes to the output.

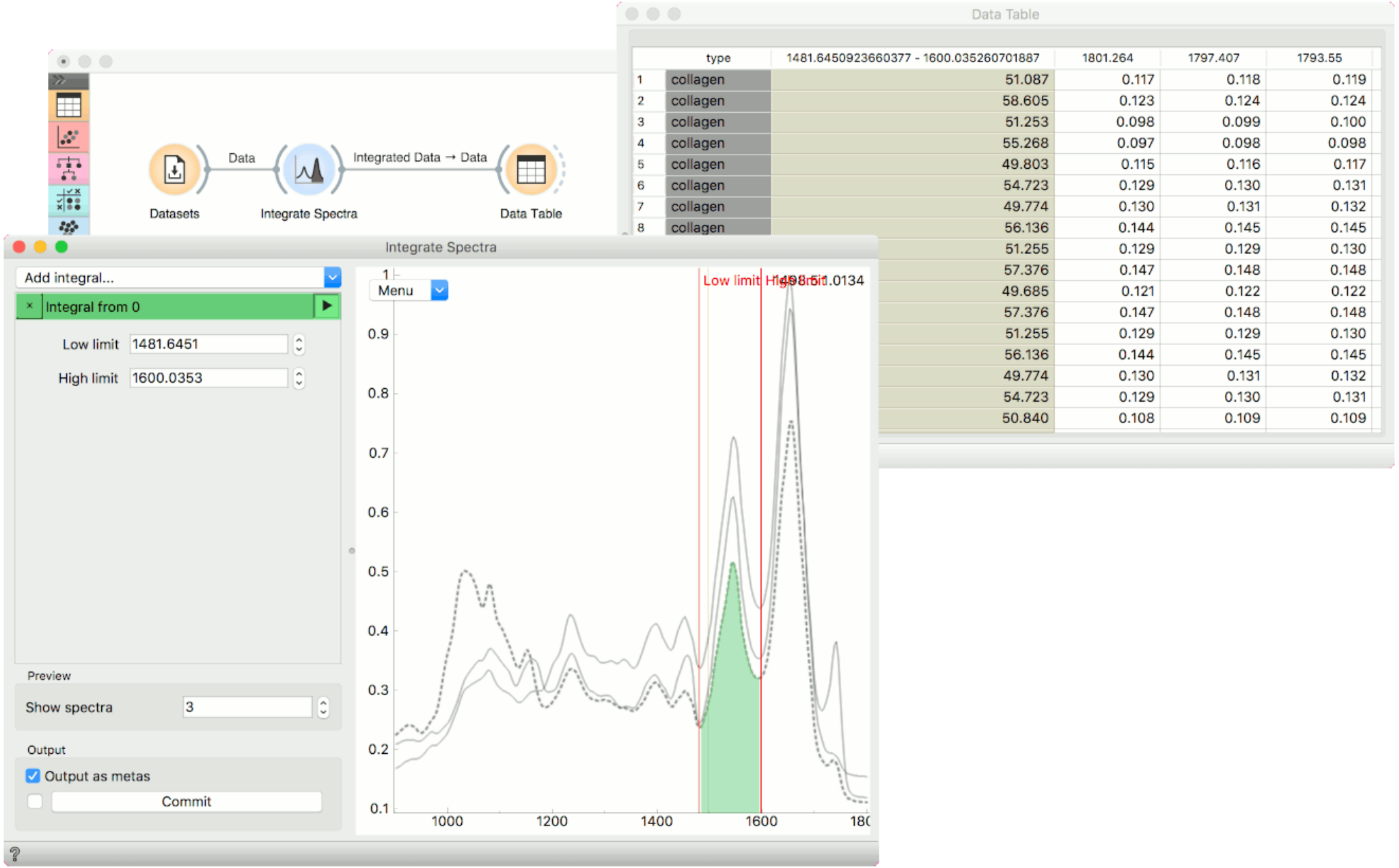
Example

This is a simple example on how to use the **Integrate Spectra** widget. The widget provides many options for integrating spectral areas and the results are appended as additional columns to the data.

We are using the *liver spectroscopy* data set from the **Datasets** widget. In **Integrate Spectra** we have selected *integral from 0* and set the lower and upper limit with the red lines. We could also do it by setting the *Low limit* and *High limit* values on the left.

To observe the integrated area, we need to press the triangular play button next to the method. To output the data, we need to press *Commit*.

Finally, we can observe the additional column with the integral values of the area in a **Data Table**.


Data
Integrated Data → Data
Datasets
Integrate Spectra
Data Table
Integrate Spectra
Add integral...
Integral from 0
Low limit 1481.6451
High limit 1600.0353
Preview
Show spectra 3
Output
Output as metas
Commit
Menu
Low limit
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
1000
1200
1400
1600
Data Table
type
1481.6450923660377 - 1600.035260701887
1801.264
1797.407
1793.55
1 collagen 51.087 0.117 0.118 0.119
2 collagen 58.605 0.123 0.124 0.124
3 collagen 51.253 0.098 0.099 0.100
4 collagen 55.268 0.097 0.098 0.098
5 collagen 49.803 0.115 0.116 0.117
6 collagen 54.723 0.129 0.130 0.131
7 collagen 49.774 0.130 0.131 0.132
8 collagen 56.136 0.144 0.145 0.145
51.255 0.129 0.129 0.130
57.376 0.147 0.148 0.148
49.685 0.121 0.122 0.122
57.376 0.147 0.148 0.148
51.255 0.129 0.129 0.130
56.136 0.144 0.145 0.145
49.774 0.130 0.131 0.132
54.723 0.129 0.130 0.131
50.840 0.108 0.109 0.109