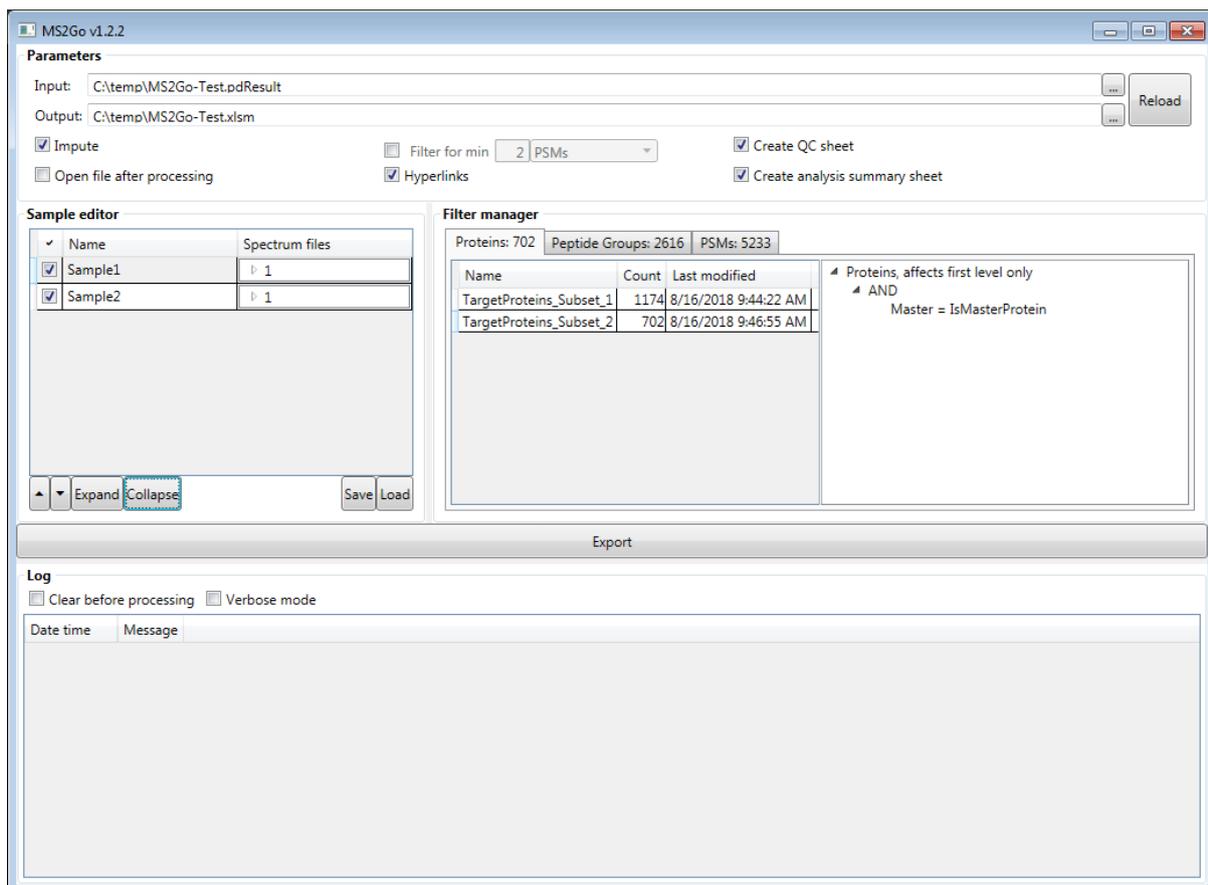


MS2Go User manual

Overview

The basic user interface of MS2Go is divided into various segments looks like this:



Parameters section

This section administrates the basic parameters required for exporting.

Parameters

Input:

Output:

Impute Filter for min Create QC sheet

Open file after processing Hyperlinks Create analysis summary sheet

The following parameters can be set:

| Name | Description |
|-------------------------------|---|
| Input | The path to the *.pdResult file. Can be also set via the corresponding '...' -button, in this case the output file path is set with the same file name, but different extension. IMPORTANT: A *.pdResultView file with the same name has to be in the same folder. |
| Output | The path to the *.xlsm file. Can be also set via the corresponding '...' -button |
| Impute | Turns area value imputation on/off. Requires <i>NormalisationPlus</i> in the PD workflow, otherwise this option has no effect. |
| Open file after processing | Opens the exported file in Excel after processing is finished. |
| Filter for min ... | Filters the proteins based on a minimum number of PSMs/peptides/unique peptides. |
| Hyperlinks | Turns hyperlinking between sheets on/off. (Huge result files tend to exceed Excel's maximum number of hyperlinks per sheet.) |
| Create QC sheet | Determines whether sheet <i>Quality control</i> is created, or not. |
| Create Analysis summary sheet | Determines whether sheet <i>Analysis summary</i> is created, or not. |

Sample editor

Sample editor

| ✓ | Name | Spectrum files |
|-------------------------------------|---------|--|
| <input checked="" type="checkbox"/> | Sample1 | ▲ 1 20180207_QexHF1_RSLC1_DC_Hela25ng_1501_01.raw |
| <input checked="" type="checkbox"/> | Sample2 | ▶ 1 |

▲ ▼ Expand Collapse Save Load

Here the samples can be manipulated in multiple ways:

- Rename
- Move position
- Exclude

The changes made can be saved/load by file. To reset the sample settings, simply press the 'Reload' button in 'Parameters' section.

Filter manager

Filter manager

Proteins: 702 Peptide Groups: 2616 PSMs: 5233

| Name | Count | Last modified |
|-------------------------|-------|----------------------|
| TargetProteins_Subset_1 | 1174 | 8/16/2018 9:44:22 AM |
| TargetProteins_Subset_2 | 702 | 8/16/2018 9:46:55 AM |

▲ Proteins, affects first level only
 ▲ AND
 Master = IsMasterProtein

In this section the filter applied to the result can be chosen (per default the latest filters are selected).

The left segments groups the filters by item type, including the item count.

The right segment displays the filter properties in a tree view.

Log panel

The Log panel tracks all messages which occur during processing (for a more detailed logging, enable the option **Verbose mode**).

Note: The messages are also logged to file (see Folder *logs* in the MS2Go application directory).

Log

Clear before processing Verbose mode

| Date time | Message |
|-----------|-------------------------------------|
| 12:16:41 | Loading entities... |
| 12:16:41 | Reading 'PeptideSpectrumMatch'. |
| 12:16:42 | Reading 'Peptide'. |
| 12:16:42 | Reading 'Protein'. |
| 12:16:42 | Reading 'Modification'. |
| 12:16:42 | Could not load entity 'QuanResult'. |
| 12:16:42 | Connecting entities... |
| 12:16:43 | Processing proteins... |
| 12:16:44 | Processing peptides... |
| 12:16:44 | Processing PSMs... |