# MaxQuant.Live Documentation

*Release latest*

**May 30, 2022**

# Overview

Welcome to the user documentation of MaxQuant.Live, a software framework for real-time monitoring of mass spectrometric data and controlling of the data acquisition. MaxQuant.Live can be downloaded on http://maxquant.live

**Publication: MaxQuant.Live enables global targeting of more than 25,000 peptides**
*Christoph Wichmann, Florian Meier, Sebastian Virreira Winter, Andreas-David Brunner, Juergen Cox, Matthias Mann* doi: 10.1074/mcp.TIR118.001131

# User Interface

The main window of MaxQuant.Live consists of three sections, which you can open by clicking on the symbols in the main menu.

## 1.1 Instrument

The instrument type can be selected here connected using the "connect instrument" button. In this version, only Thermo Fisher Scientific Q Exactive HF-X mass spectrometers are supported (Tune Versions 2.9, 2.11).

## 1.2 Main Module

This part of the software is the link between the instrument and the scan protocol Library. It consists of a log message window and the configuration of the log directory. It is recommended to always load the log directory before

connecting the instrument. The files written to this directory contain all log messages that were also shown in the graphical user interface. There are two types of log file written out by MaxQuant.Live Global log file: MaxQuant.Live will create global log files on every day. The filename is the date itself. These files contain all the log messages that were thrown when no scan protocol was running. Specific log files: During the execution of a scan protocol, the log messages are written to scan proto-col specific log file. The file name starts with the four-digit identification number, followed by the date and the time of execution. When the scan protocol ended, the log messages are again written into the global log file.

## 1.3 Scan Protocol Library



Scan protocols implement various the acquisition strategies supported by our software. Every scan proto-col has a certain type (BoxCar, EasiTag. . . ), a unique four-digit identification number and a short experiment description. All scan protocols are stored in a library. In the scan protocol section of the software you can manage the library.
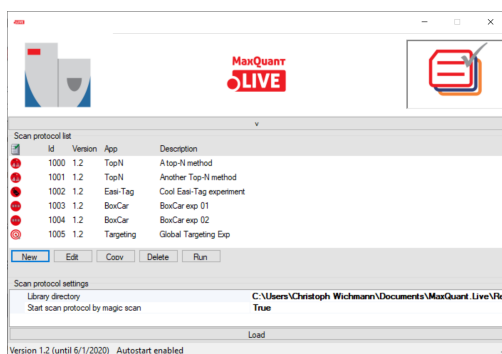
## Operation Modes

The logo in the middle of the symbol bar of MaxQuant.Live displays the current operation mode of the software. There are three operation modes:

## 2.1 Setup Mode



This is the initial operation mode after software startup. In this modus, three parts of MaxQuant.Live (Sec. 4) can be configured. After loading the log-directory, the scan protocol library and connecting the instru-ment, MaxQuant.Live switches to the Listening Mode.

## 2.2 Listening Mode



In this mode, the software receives all the spectra acquired by the instrument but does not send any commands to the mass spectrometer. MaxQuant.Live is therefore not affecting the data acquisition of the mass spectrometer. Scan protocols can be started in the software is in this operation mode. After the startup of a scan protocol, MaxQuant.Live switches to the Running Mode.

## 2.3 Running Mode



This operation mode is active during the execution of a scan protocol. Afterwards, the software automati-cally switches back to the listening mode.

Installation

## 3.1 Check requirements

- Microsoft .NET Framework 4.7.2

- Q-Exactive Tune 2.9 or higher

**Note:** Q Exactive classic/plus instruments were not tested and are not officially supported.

## 3.2 Download and unpack

The latest version 1.2 can be downloaded from http://maxquant.live and is valid until 6/1/2020. Unpack the zip file in a new folder on the local hard drive of the acquisition computer.

📁 lib
📁 log
📁 scanProtocols
🔴 MqLive.exe
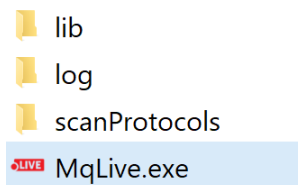
If necessary, create empty 'log' and 'scanProtocols' folders manually. To set up MaxQuant.Live, continue reading here.

Create and edit Scan Protocols

## 4.1 New scan protocol



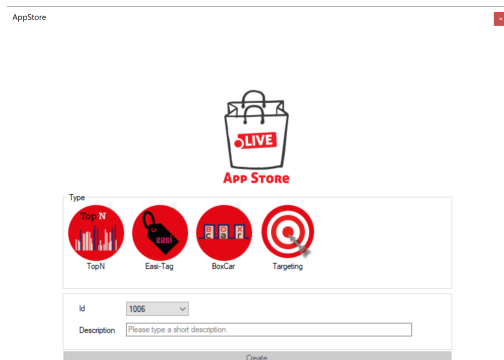When you click on the "New" button, the app store opens. First, select the acquisition method that should be used in the new scan protocol. Click on the big symbol to open the settings for the selected app. A green checkmark indicates which app has been selected. Next, select a unique identification number for your scan protocol. The list in the drop-down menu excludes id numbers that are already present in the library. Finally fill in a short description of the experiment and click create. The scan protocol will be saved as file in the scan protocol folder and appear in the scan protocol library.

## 4.2 Edit scan protocols
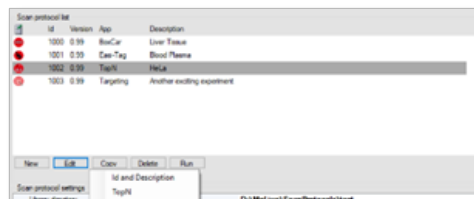


Scan protocols in the library can be edited later by clicking the "Edit" button. It is possible to change the global properties like the ID number and the short description of the scan protocol. Furthermore, it is possible to edit the specific parameters of an acquisition strategy using the respective app.

## 4.3 Copy and Delete

Existing scan protocols can be easily copied by clicking the "Copy" button. The copy gets automatically an ID number assigned, is added to the library and can be edited afterwards by the user. Existing Scan Protocols can also be deleted by the user by clicking the "Delete" button.

## 4.4 Storage

Scan protocols are saved as files (".mqlive") local library, which serves as scan protocol library. The path has to be set at when the software is started but can be changed after-wards during runtime. Therefore is it possible to use several scan protocol libraries for different experi-ments or users.

## 4.5 Compatibility

Please note that every scan protocol has a version number, which is the version of the MaxQuant.Live that has been used to create or edit it the last time. Compatibility is not guaranteed if the scan protocols and the MaxQuant.Live version differ. Possibly incompatible scan protocols are highlighted in red and their settings should be checked carefully and saved with the new version before running.

**Note:** MaxQuant.Live versions 0.99 and 1.2 are not fully compatible! Check your old scan protocols before running them.

## 4.6 Run scan protocol

Continue reading here

# Run Scan protocols

When MaxQuant.Live is in Listening Mode scan protocols can be started either manually or in an automated manner.

## 5.1 Manual startup

To be able to start a scan protocol manually, the instrument has to be in Running Mode. Therefore, is has to run idle or an Xcalibur method. Check, by using the control software Tune, if the instrument is constantly performing scans. Only in this instrument modus can MaxQuant.Live start scan protocols. To start up a scan protocol, navigate to the library, select the desired scan protocol and click the "run" button. MaxQuant.Live switches into the Running Mode. While a scan protocol is running, you can see its Id number in the symbol bar right of the GUI. MaxQuant.Live is now directing the data acquisition according to the logic implemented in the scan protocol. If you switch to Tune, then you should see incoming log messages indicating that MaxQuant.Live took over the control of the mass spectrometer. Switching back to MaxQuant.Live, the execution of the scan protocol can be terminated by clicking the "Stop scan protocol" button. MaxQuant.Live then switches back into Listening Mode.

## 5.2 Automated startup

The startup of a scan protocol can be triggered by an incoming so-called "magic scan". If MaxQuant.Live is in Listening Mode and receives Ms1 scans with the scan range m/z 909 to XXXX, then the scan protocol with Id number XXXX is loaded from the library and started immediately. This feature enables a seamless integration of MaxQuant.Live into the standard LC-MS controlled by Xcalibur, because the magic scans can be easily defined as Xcalibur method. Doing this, MaxQuant.Live switches into Running Mode and takes over the control directly after a 'magic' Xcalibur method starts.

### 5.2.1 Xcalibur method setup
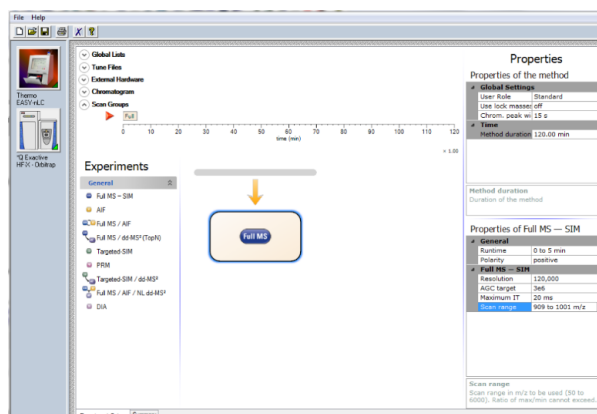


1. Create a new Xcalibur method via the standard method editor. Enter LC settings, Tune files, etc. as you would normally do. Please refer to the Xcalibur user manual for help. Caution: Make sure that the MS method duration is equal to your LC run time.

2. In the MS method, create one Full MS – SIM scan with the scan range m/z 909 to MaxQuant.Live Id, for example m/z 909 to 1001 for the MaxQuant.Live scan protocol with the unique identifier 1001 created above. Set the scan runtime to an arbitrary value >1 min, but less than the method duration. The scan resolution should be equal to the Full Scan resolution set in the MaxQuant.Live scan protocol.

3. Add a second Full MS – SIM scan as in Step 2, but now set the scan range from m/z 908 to "1000 + LC run time", for example m/z 908 to 1100 for a 100 min LC-MS experiment. This step is required! If you forget it your instrument can switch to mode in which MaxQuant.Live won't start anymore. In this case the instrument has to be restarted.

4. Review all settings and save the method.

### 5.2.2 Data acquisition

1. Make sure that MaxQuant.Live is in Listening mode.

2. Check if your scan protocol library is loaded and the scan protocol with ID number defined before (1001) is present in the list. The setting "Start scan protocol by magic scan" has to be true (default).

3. Open the Xcalibur software and set up a new acquisition sequence. Select the Xcalibur method generated above as the instrument method for your BoxCar runs. Note that different MaxQuant.Live protocols require different Xcalibur methods.

4. Start the acquisition sequence. MaxQuant.Live will take over control as soon as the trigger signal (full MS scan with a scan range starting at m/z 909, 'magic scan') is identified. The home view will indicate that the software is now in Running Mode (Sec. 5.3). Acquisition will stop automatically at the end of the LC-MS run and the Xcalibur sequence will continue with the next run (if applicable). Stop scan protocol stops any running protocol immediately.

|   | Sample Type | Position | Inj Vol | File Name | Path | Inst Meth |
|---|---|---|---|---|---|---|
| 1 | Unknown | A1 | 1.0 | Raw_file_name | D:\ | C:\Xcalibur\methods\ ... 100min_id1001 |
| * |  |  | 0.0 |  |  |  |

5. Disconnect the instrument and close MaxQuant.Live once all experiments are finished.
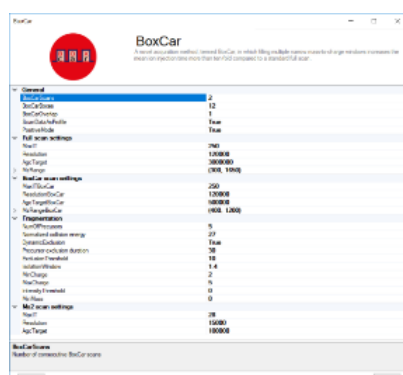
# BoxCar



**BoxCar acquisition method enables single-shot proteomics at a depth of 10,000 proteins in 100 minutes** *Florian Meier, Philipp E. Geyer, Sebastian Virreira Winter, Juergen Cox & Matthias Mann* doi: 10.1038/s41592-018-0003-5

The BoxCar acquisition method for high resolution mass spectrometry-based proteomic builds on the combined acquisition of narrow m/z windows to enhance the mean ion filling time as compared to stand-ard full scans.

## 6.1 Acquisition

All MS parameters are defined and saved in MaxQuant.Live scan protocols. The pop-up window allows you to set all instrument parameters required for BoxCar runs. The acquisition cycle comprises one Full Scan, N BoxCar scans and Z data-dependent MS2 scans. Precursors for MS2 are se-lected from the Full Scan. Note that the mass resolution in the full scan must equal the mass resolution setting in the BoxCar scans for MaxQuant data analysis. For BoxCar scans, each box will be assigned a maximum ion injection time of 1/N th of the total, for example 10 ms for each of 10 boxes per scan with a total max. ion injection time of 100 ms. The same applies to the AGC target value. The BoxCar window placement will be automatically scaled to the expected m/z distribution of tryptic peptides.

> **Warning:** Choosing a too high AGC target for BoxCar scans may cause space-charge effects by overloading the Orbitrap.

> **Warning:** Currently, only profile scans are recognized by MaxQuant.

| Method parameter | Description |
|---|---|
| **General** | |
| ScanDataAsProfile | Profile (true) or centroid (false) spectra |
| Positive mode | Electrospray polarity |
| **Full Scan settings** | |
| MaxIT | Maximum ion injection time (ms) |
| Resolution | MS resolving power at m/z 200 |
| AGCtarget | AGC target value (charges) |
| MzRange | Scan range (m/z) |
| **BoxCar settings** | |
| BoxCar Scans | Number of BoxCar scans per acquisition cycle |
| BoxCar Boxes | Number of boxes per BoxCar scan |
| BoxCar overlap | M/z overlap of neighboring boxes (Th) |
| PdfMu | Mu value of log-normal ion distribution function |
| PdfSigma | Mu value of log-normal ion distribution function |
| MaxBoxRatio | Max. allowed ratio of box sizes. Box sizes are adjusted automatically to fulfill this constraint. |
| MaxIT | Maximum total ion injection time (ms) for BoxCar scans. Each box is assigned 1/N th of this value. |
| Resolution | MS resolving power at m/z 200 |
| AgcTarget | Total AGC target value for each BoxCar scan (charges). Each box is assigned 1/N th of this value. |
| MzRange | Scan range (m/z) |
| **Fragmentation** | |
| NumOfPrecursors | Number of precursor ions per acquisition cycle |
| Normalized collision energy | Normalized collision energy (NCE) |
| DynamicExclusion | Switch for dynamic exclusion |
| Precursor exclusion duration | Dynamic exclusion time of precursors after first spectrum (s) |
| Exclusion threshold | Intensity threshold for dynamic exclusion [ppm] |
| Isolation window | Width of the precursor isolation window (Th) |
| MinCharge | Minimum charge state of the precursor |
| MaxCharge | Maximum charge state of the precursor |
| Intensity threshold | Precursor intensity threshold (cps) |
| MinMass | Minimum mass threshold for precursor ions (Da) |
| **Ms2 scan settings** | |
| MaxIT | Maximum ion injection time (ms) |
| Resolution | MS resolving power at m/z 200 |
| AgcTarget | AGC target value (charges) |
| LowerMzBound | Lower Mz boundary for MS2 spectra |

## 6.2 Optimization of ion distribution

The box sizes are calculated from the expected ion distribution which is described by a log-normal distribution function. The shape of the function is defined by the two parameters mu and sigma. Their default values were derived from HeLa LC-MS runs and lead to box sizes comparable to the ones in the BoxCar publication. If another ion distribution

is expected, these parameters should be changed to guarantee an optimal description through the log-normal function and the perfectly suitable box sizes.

## 6.3 Analysis

MaxQuant is a software package for quantitative high resolution mass-spectrometry based proteomics (Cox and Mann, Nature Biotechnology 2008 (26), 1367-1372, doi: 10.1038/nbt.1511) and can be downloaded from http://www.maxquant.org. We have recently published a detailed and up-to-date description of the MaxQuant computational platform (Tyanova et al., Nature Protocols 2016 (11), 2301–2319, doi: 10.1038/nprot.2016.136). Please refer to this publication for information about different processing workflows and a detailed description of the parameters. Here, we provide a step-by-step protocol to analyze raw files acquired with the BoxCar method. Default parameters were used unless indicated.

1. Open a new MaxQuant (v1.6.1.0 or later) session and load or 'drag and drop' Thermo .raw files into the MaxQuant window.

2. Set experiment name for each raw file (or load experimental design template if applicable).

3. Set parameter groups for each raw file. BoxCar and shotgun experiments need to be in separate parameter groups. Fractions (if applicable) should not be specified when matching from a fractionated peptide library into single runs is intended.

4. Set group specific parameters. Select "Type / Standard" for each experiment group containing regular shotgun experiments and "Type / BoxCar" for each group containing BoxCar experiments, respectively.
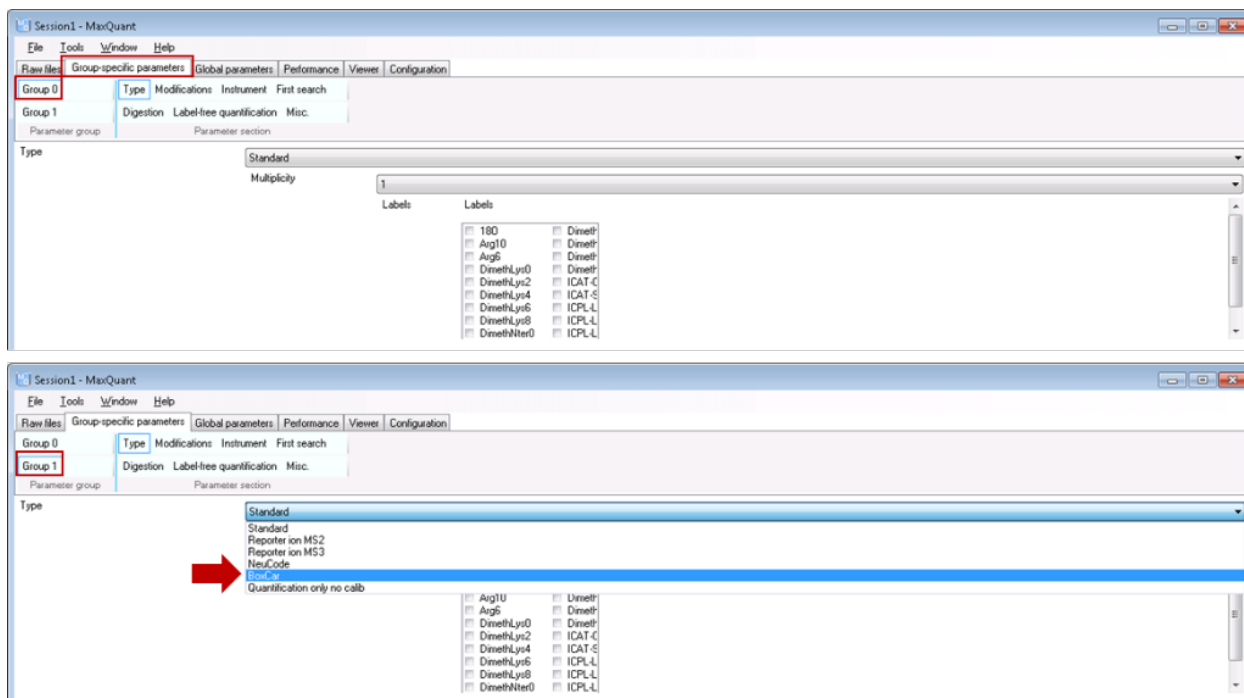




5. Set global parameters:

- Add the corresponding FASTA file(s) for the species under investigation.

- To transfer MS/MS identifications between runs, check "Match between runs" in the "Adv. identification" tab. It is recommended to adjust matching time tolerances according to your chromatography setup.

6. Start the automated processing workflow. MaxQuant output files will be written in the 'combinedtxt' folder when finished.

# Easitag and TopN
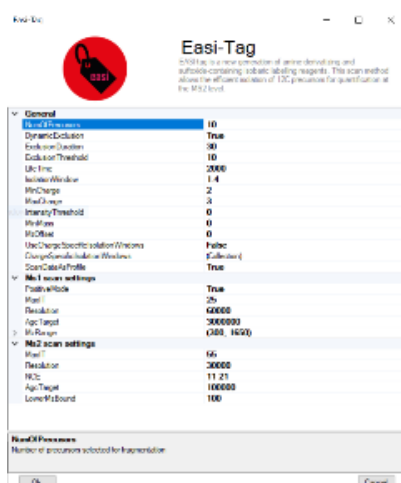


**EASI-tag enables accurate multiplexed and interference-free MS2-based proteome quantification** *Sebastian Virreira Winter, Florian Meier, Christoph Wichmann, Juergen Cox, Matthias Mann & Felix Meissner* doi: 10.1101/225649

The EasiTag strategy is based on the standard topN strategy but has some modifications and extensions. In EasiTag, the precursor selection is more stringent and only select monoisotopic peaks for fragmentation. Furthermore, the isolation windows are shifted by a global offset and their size chosen to be charge state dependent.

| Method parameter | Description |
| --- | --- |
| **General** | |
| NumOfPrecursors | Number of precursor ions per acquisition cycle |
| DynamicExclusion | Switch for dynamic exclusion |
| ExclusionDuration | Dynamic exclusion time of precursors after first spectrum (s) |
| ExclusionThreshold | Mass tolerance for dynamic exclusion (ppm) |
| LifeTime | Max time a MS2 scan stays in the queue (ms) |
| Isolation window | Width of the precursor isolation window (Th) |
| MinCharge | Minimum charge state of the precursor |
| MaxCharge | Maximum charge state of the precursor |
| Intensity threshold | Precursor intensity threshold (cps) |
| MinMass | Minimum mass threshold for precursor ions (Da) |
| MzOffset | Offset that is added to the peak mz-value (Th) |
| UseChargeSpecificIsolationWindows | Switch to enable charge specific isolation windows |
| ChargeSpecificIsolationWindows | Define isolation windows widths for every allowed charge state |
| ScanDataAsProfile | Profile (true) or centroid (false) spectra |
| **MS1 Scan settings** | |
| PositiveMode | Ion polarity |
| MaxIT | Maximum ion injection time (ms) |
| Resolution | MS resolving power at m/z 200 |
| AGCtarget | AGC target value (charges) |
| MzRange | Scan range (m/z) |
| **Ms2 scan settings** | |
| MaxIT | Maximum ion injection time (ms) |
| Resolution | MS resolving power at m/z 200 |
| NCE | Normalized collision energies (whitespace separated - only EasiTag) |
| AgcTarget | AGC target value (charges) |
| LowerMzBound | Lower Mz boundary for Ms2 spectra |
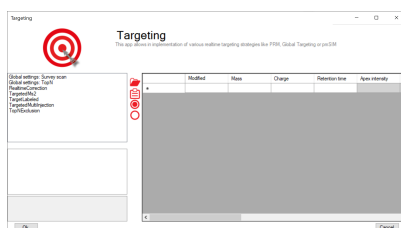
# Targeting



**MaxQuant.Live enables global targeting of more than 25,000 peptides** *Christoph Wichmann, Florian Meier, Sebastian Virreira Winter, Andreas-David Brunner, Juergen Cox, Mat-thias Mann*

The Targeting app allows the realization of various targeting strategies within on user interface. First, the list of targeting peptides has to be populated and afterward the targeting strategy has to be defined and the parameters have to be set.

## 8.1 Steps to setup a targeting run

1. Populate the peptide list

2. Set global parameters

3. Set up targeting action

## 8.2 Peptide ions list

The targeting should comprise a set of peptides of interest and a set of high abundant peptides used for the real-time corrections of mass-to-charge values, expected retention times and peptide intensities.

| Column | Description | |
|---|---|---|
| Modified sequence | String containing the modified sequence | optional; Needed if isotopic labeling is used |
| Mass | Ion mass | mandatory |
| Charge | Ion charge state | mandatory |
| Retention time | Expected retention time (min) | mandatory |
| Apex Intensity | Expected Apex intensity | optional |
| Fragments mz | mz values of expected fragment ions | optional; needed for ms2 based corrections |
| MaxIt | Maximum injection time for triggered scans | optional; if empty the global MaxIt is used |
| NCE factors | Scaling factors for stepped CE (white space separated: 1.2 2.3) | optional; |
| Collision Energies | Collision energies for fragmentation (white space separated: 11 21) | optional; if empty the global NCE is used |
| RealtimeCorrection | Use this ion to calibrate the realtime correction | |
| TargetedMs2 | Trigger Ms2 scan(s) if ion detected (see TargetedMs2 ) | |
| TargetLabeled | Use labeled counterpart of this ion as trigger ion (see TargetLabeled) | |
| TgtMultiInjection | Trigger multi injection scans for this ion and the labeled counterparts | |
| TopNExclusion | Exclude this ion from the stochastic Top-N method | |

### 8.2.1 Mandatory information

Mandatory columns have a white background and columns containing optional information/settings have a gray background. The required information of every peptide ion is the mass, the expected retention time and its charge state.

Additionally the modified sequence should be provided to be able to identify the peptide later in the MaxQuant.Live log file. If the selected targeting strategy comprises the usage of heavy labels, the modified is used by MaxQuant.Live to calculate the mass differences between the light and heavy channel.

The Apex Intensity is optional. If not set, the ion counts as detected if the number of set isotopic if present in a survey scan. If set, the ion counts as detected if the ratio of the intensity of the most intense isotopic peak present in the survey scan and expected Apex intensity is higher than the IntensityPeakRatioThreshold.

The other columns contain checkboxes to enable actions called when the peptide is detected. These actions are also contained in the left list in the targeting app window.

### 8.2.2 Automatic population of the targeting table

The peptide table can either be filled out manually, or populated automatically by either pasting a table from the clipboard, or by using tab separated text files.

When pasting from the clipboard, a tabular calculation program like Microsoft Excel can be used to set up the peptide list. Select the rows of peptides in Excel, copy to the clipboard and click on the paste icon in MaxQuant.Live to paste into the peptide list. Make sure that the header row is also copied and that it contains the same labels as the MaxQuant.Live peptide list. A dialog window helps you to map the column headers of the copied content to the MaxQuant.Live table.

The option to populate the table by using tab separated files is the easiest one. First, the evidence files - which is part of the MaxQuant analysis output - is selected. The column headers mapping is detected automatically, but can

be changed by the user. Please note, that the evidence table should be inspected beforehand and peptides without intensities sorted out. Of course, the selected file doesn't need to be an evidence file but can be any tab separated text file containing the required information and the corresponding column headers.

To add the values of the Apex intensity and the fragment ions, which are not present in the evidence table, the msms table - also part of the MaxQuant analysis output - can be read in to complete the targeting list. As before, the column mapping can be checked by the user, before the files are parsed by the software and the MaxQuant.Live targeting list is populated accordingly.

## 8.3 Global settings

The left list consists of global settings as well as the settings of the various scan actions which can be activated for every peptide ion in the list by settings the corresponding checkboxes. Whe a list entry is selected the settings are shown in the box below.

### 8.3.1 Setup of targeting actions

There are three ways to select targeting actions for peptides in the list 1. Click on the checkbox for every peptide manually 2. Select one or more peptides in the list, then select an action from the list of actions in the left panel and click on the check mark symbol in the middle. 3. Add a column with the name of the action to your peptide list in Excel and will it with the Boolean values `TRUE` or `FALSE`. When pasting the peptide in MaxQuant.Live, the software will set the checkboxes automatically.

### 8.3.2 Global settings: SurveyScan

The survey scans for the peptide recognition can be either MS1 scan or BoxCar scan. The parameters are described in the BoxCar section.

### 8.3.3 Global settings: TopN

The TopN strategy is applied on top of the targeting scans. Note, that peptides can also be excluded from being selected as precursors by using the "ExcludeFromTopN" feature.

### 8.3.4 RealtimeCorrection

The adaptive real-time correction adjusts the expected retention times based on the deviations of the peptide observed before. We refer to our MaxQuant.Live paper for more information about the real-time correction algorithm.

| Parameter | Description | Default value |
|---|---|---|
| MzToler-ances | Lower and upper bounds for the peptide mz tolerance [ppm] | (4.5,10) |
| Retention-TimeToler-ances | Lower and upper bounds for the retention time tolerance[min] | (1,10) |
| SigmaS-caleFac-torRt | Scaling factor for retention time window adjustment | 3 |
| PeptideHis-toryLength | Time span considered to calculate the corrections [min] | 2 |
| MinUsed-Correction-Peptides | Minimum number of peptides used to calculate the corrections | 50 |
| IntPeakRa-tioThresh-old | The ratio of the current peak intensity to the apex value has to be higher than this threshold | 1.00E-05 |
| PepdideDe-tectionIso-Peaks | Number of isotopic peaks that need to be found | 2 |
| IsotopeTol-erance | Isotopic peaks distance tolerance [ppm] | 9 |
| Ms2DetectionNeeded | Used only peptide those peptides for the realtime correction whose fragment ion have been already detected. Make sure that the targetedMs2 is activated and the Fragments mz column populated for these peptide ions. | False |
| Ms2ExcludeDetectedPeps | Disable refragmentation of Ms2-detected peptides | False |
| Ms2NormIntensity | Minimal valid intensity normalized to the max. Ms2 peak | 0.1 |
| Ms2MzTolerance | Mz tolerance for fragment ion detection in Ms2 scans [ppm] | 20 |

### 8.3.5 TargetedMs2

| Parameter | Description | Default value |
|---|---|---|
| BatMode | Fragment ion in every cycle within the retention time, even if not detected | FALSE |
| AutoPriority | Prioritize MS2 scan, if the peptide was not fragmented before | TRUE |
| MaxNumOfScans | Upper limit for the number of fragmentations per peptide. 0=no limit | 0 |
| MzOffset | Shift the isolation window by this mz value [th] | 0 |
| LowerMzBound | Lower mz boundary for Ms2 scans | 100 |
| CollisionEnergy | Collision energy for fragmentation | 27 |
| LifeTime | Max time span before a scheduled MS2 scan get deleted [ms] | 2000 |
| MaxIT | Maximum ion injection time (ms) | 28 |
| Resolution | MS resolving power at m/z 200 | 15000 |
| AgcTarget | AGC target value (charges) | 100000 |
| PositiveMode | Ion polarity | TRUE |

### 8.3.6 TargetLabeled

This action adds the SILAC label masses to the peptides masses in the list. The "Modified is used to calculate the number Arg and Lys amino acids. The masses of SILAC labels can be freely defined here.

### 8.3.7 TargetedMultiInjection

With this action, scans are triggered in which the heavy and the light channel are both selected by the quadrupole and analyzed together. If fragmentation is switched on, this resembles a PRM experiment. If fragmentation is turned off, it corresponds to an SIM experiment. The pmSIM acquisition strategy described in the paper can be implemented with this action turning on the BatMode switch.

| Parameter | Description | Default value |
|---|---|---|
| Window-Size | Size of the isolation windows [th] | 1.4 |
| Window-Offset | Shift the isolation window centers by this offset [th] | 0 |
| BatMode | Fragment ion in every cycle within the retention time tolerance window, even if not detected | FALSE |
| NceLight / Heavy | Normalized collision energy for the light/heavy channel | 0 |
| ItBox-Size | Maximum injection time per light or heavy mass range. If smaller than MaxIt, the MaxIt is spread over multiple injections, each fulfilling the max. injection time per box condition. | 100 |
| Isotopic label | Masses of SILAC labels | |
| Positive-Mode | Ion polarity | TRUE |
| Collision-Energy | Collision energy for fragmentation | 0 |
| Lower-MzBound | Lower mz boundary for Ms2 scans | 100 |
| LifeTime | Max time span before a scheduled MS2 scan get deleted [ms] | 1000 |
| Resolution | MS resolving power at m/z 200 | 30000 |
| AutoPriority | Prioritize MS2 scan, if the peptide was not fragmented before | TRUE |
| MaxNumOfScans | Upper limit for the number of fragmentations per peptide. 0=no limit | 0 |
| MaxIT | Maximum ion injection time (ms) [not used] | 50 |
| MaxItLight /Heavy | Maximum ion injection time for light/heavy channel (ms) | 100 |
| AgcTarget | AGC target value (charges) | 100000 |
| InjectTargetL/H | AGC target value for light/heavy peptide (charges) | 50000 |

## 8.3.8 ExcludeFromTopN

| Parameter | Description | Default value |
|---|---|---|
| BatMode | Exclude ion from TopN within the retention time tolerance window , even if not detected | FALSE |
| StaticExclusion-Time | Time span the peptide is excluded from TopN (30) | 30 |
| AdaptiveExclusion-Time | Automatic exclusion of the peptide from TopN | TRUE |