

Using MaxQuant.Live Methods

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www.LCMSmethods.org

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Short description of the software: The MaxQuant.Live software interacts with the instrument acquisition control software of Thermo Fisher Q Exactive series mass spectrometers via the Instrument Application Programming Interface (IAP), and is hereby capable of reading and processing scan data as well as mass spectrometry system information during its runtime. Furthermore, the software can place customized scans into the acquisition queue of the mass spectrometer, which may or may not use the information above to adapt scan parameters in real-time. The software executes 'scan protocols' that may or may not extend the functionalities of standard mass spectrometry acquisition methods. Software tools to generate such scan protocols are provided as an integrated part of the MaxQuant.Live software.

The following components of the software are provided in compiled form and executable on the instrument's acquisition computer:

- a) The MaxQuant.Live core program that communicates with the acquisition control software and executes the acquisition methods.
- b) Software applications to generate acquisition method files ('scan protocols') with pre-defined templates.

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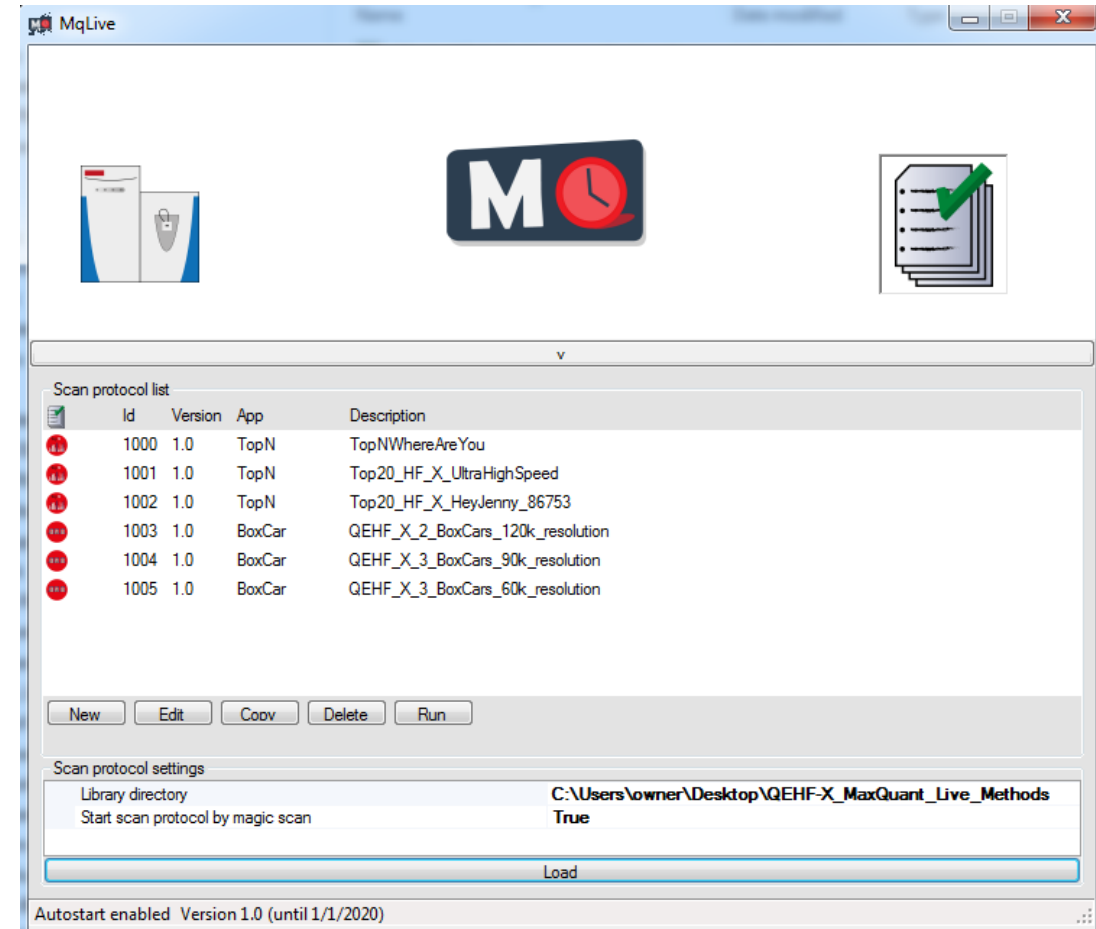
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Instructions for using MaxQuant.Live are at MaxQuant.Live

- These slides are for how to use the PreMade methods in the ASMS 2019 release of www.LCMSMethods.org
- To use MaxQuant.Live methods you will need these 4 things:
 - Your normal Xcalibur software
 - A “dummy” Xcalibur method that triggers MaxQuant.Live to start
 - MaxQuant.Live
 - Your MaxQuant.Live method

Load the MaxQuant.Live methods

- Find where the LCMSthree.org folder went
- I've included a dummy file called "TopNWhereAreYou" if you need to use the Windows search bar to find it
- Use the Load button to find that folder and get these methods. It should look something like that →
- Please note there are 2 separate folders for QE HF and HF-X. Only the Xcalibur methods and names differ in case compatibility with Xcalibur is an issue
- It is probably best to delete the folder that your instrument does not need.



Add your chromatography into your Xcalibur method and save it

- Please note that the default for all methods here is 120min
- I have my first MS1 scan as shown, triggering my 1004 MaxQuant.Live 3 BoxCar method (1004) and I have the scan ending 1 min before the end of the 120 min chromatography gradient
- Scan 2 should be adjusted to match your gradient as well.
- For example: If you are using a 90 min gradient, the end mass in scan two should be 1090 (1000+gradient time)

The screenshot displays the Xcalibur software interface for configuring a method. The top section shows a timeline from 0 to 120 minutes. Below this, the 'Experiments' panel lists various acquisition methods, including 'Full MS - SIM', 'AIF', 'Full MS / AIF', 'Full MS / dd-MS² (TopN)', 'Targeted-SIM', 'PRM', 'Targeted-SIM / dd-MS²', 'Full MS / AIF / NL dd-MS²', 'DIA', and 'TMT'. The main area shows two 'Full MS' acquisition blocks, each triggered by a yellow arrow. The right panel displays the 'Properties' of the method and the specific scans.

Global Lists

- ▼ Tune Files
- ▼ External Hardware
- ▼ Chromatogram
- ▲ Scan Groups

Full MS - SIM

Full MS - SIM

time (min)

0 10 20 30 40 50 60 70 80 90 100 110 120

Experiments

General

- Full MS - SIM
- AIF
- Full MS / AIF
- Full MS / dd-MS² (TopN)
- Targeted-SIM
- PRM
- Targeted-SIM / dd-MS²
- Full MS / AIF / NL dd-MS²
- DIA
- TMT

Experiment Setup Summary

Properties

Properties of the method

Use lock mass: best

Chrom. peak width: 15 s

Time

Method duration: 120.00 min

Method duration

Duration of the method

Properties of Full MS - SIM

General

Runtime: 0 to 119 min

Polarity: positive

Full MS - SIM

Resolution: 120,000

AGC target: 3e6

Maximum IT: 200 ms

Scan range: 909 to 1004 m/z

Scan 1

Properties of Full MS - SIM

General

Runtime: 0 to 119 min

Polarity: positive

Full MS - SIM

Resolution: 120,000

AGC target: 3e6

Maximum IT: 200 ms

Scan range: 908 to 1120 m/z

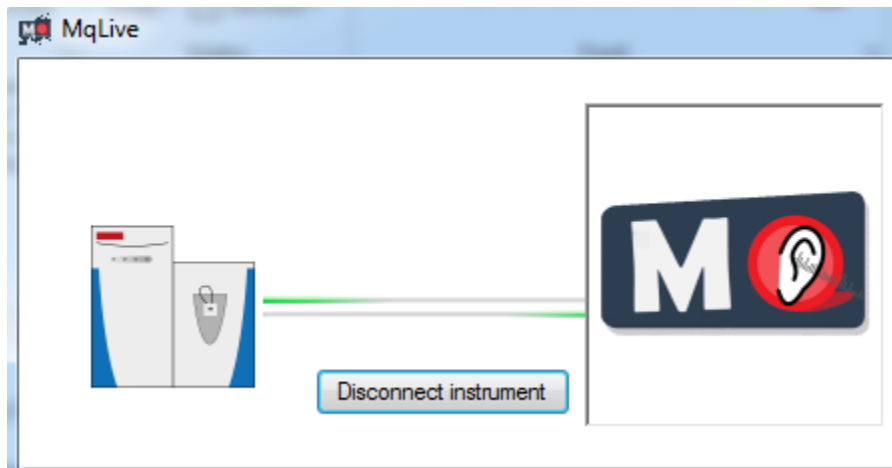
Scan 2

Runtime

Data acquisition start time and end time for selected MS experiment [min] (0.00 ...

Start MaxQuant.Live

- MaxQuant.Live should be listening for Xcalibur
- Click on the Q Exactive cartoon
- Click the big LOAD button at the bottom
- The Icon should change to listening as shown
- Start your Xcalibur method normally



Control Bar				
File Name	Path	Inst Meth	Position	Inj Vol
QEHF-X_3BoxCars_Anthraxis_test	C:\Xcalibur\Data	QEHF-X_MaxQuant_Live_Methods\120min_QEHF-X_3_BoxCars_90k_res	F4	1.00

Enjoy your new superpowers!

