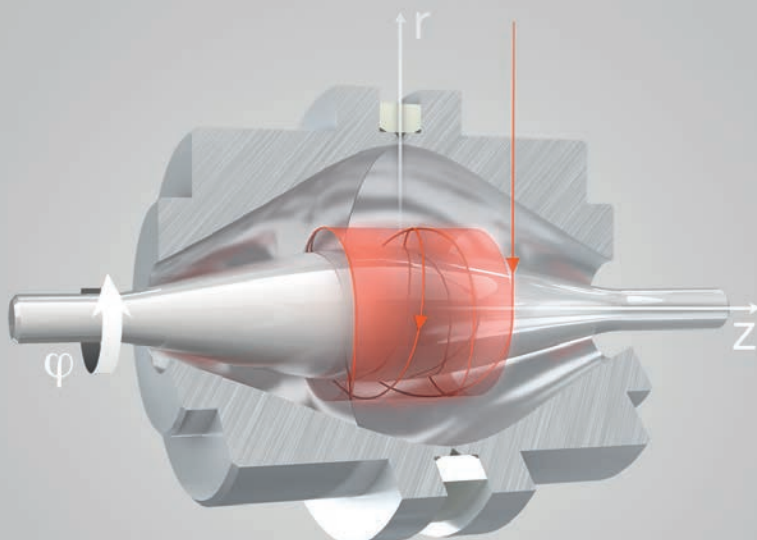




Q Exactive UHMR

Software Manual

Exactive Series 2.12

BRE0015812 Revision C March 2021

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Software Manual

Exactive Series 2.12

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Revision C released in March 2021.

Software Version: Exactive Series 2.12

For Research Use Only. Not for use in diagnostic procedures.

Read this First

Welcome to the Thermo Scientific Q Exactive UHMR system! Q Exactive™ UHMR is a member of the Thermo Scientific™ family of mass spectrometer (MS) detectors that are powered by Orbitrap™ technology.

About this Guide

This *Q Exactive UHMR Software Manual* provides reference information about the parameters in the Instrument Configuration window, the Instrument Setup window, and the Q Exactive UHMR Tune window. For information about the operating procedures for the Q Exactive UHMR mass spectrometer, we recommend that you read the *Exactive Series Operating Manual* in its entirety.

Who Uses this Guide

This *Q Exactive UHMR Software Manual* is intended for all personnel that need to perform measurements with the Q Exactive UHMR mass spectrometer, especially the key operator. This manual should be kept near the instrument to be available for quick reference.

Scope of this Guide

The *Q Exactive UHMR Software Manual* includes these chapters:

- [Chapter 1, “Instrument Configuration Window”](#) describes the Instrument Configuration window, which displays configuration information.
- [Chapter 2, “Q Exactive UHMR Readback Status Page for the Information View”](#) describes the page that allows controlling the instrument from the Roadmap view of the Xcalibur™ Home Page window.
- [Chapter 3, “Instrument Setup”](#) describes Instrument Setup, which is used to specify instrument settings.
- [Chapter 4, “Explore Q Exactive UHMR Tune”](#) provides information about Q Exactive UHMR Tune, its views, functions, and features.

- [Chapter 5, “Procedures in Q Exactive UHMR Tune”](#) provides information about procedures in Q Exactive UHMR Tune.
- [Chapter 6, “Reference Information”](#) provides information about various file types and other supplemental information.

Related Documentation

In addition to this manual, Thermo Fisher Scientific provides these documents for the Q Exactive UHMR mass spectrometer:

- *Exactive Series Pre-Installation Requirements Guide*
- *Exactive Series Operating Manual*
- *Q Exactive UHMR QuickStart Guide*
- Manuals for the delivered ion sources and other software.

You can access PDF files of the documents listed above and of this guide from the data system computer. The software also provides Help.

❖ To view product manuals

Go to **Start > Programs > Thermo Exactive Series > Manuals**.

❖ To open Help

- From the Q Exactive UHMR Tune window, choose **Help > Help Content**.
- If available for a specific window or dialog box, click **Help** or press **F1** for information about setting parameters.

For more information, including upcoming application notes, visit www.thermofisher.com.

Contacting Us

There are several ways to contact Thermo Fisher Scientific. You can use your smartphone to scan a QR Code, which opens your email application or browser.

Contact	Link / Remarks	QR Code
Brochures and Ordering Information	www.thermofisher.com/orbitrap	
Planet Orbitrap	PlanetOrbitrap.com is a scientific and community-based microsite that features detailed application workflows along with a searchable scientific library with links to peer-reviewed articles, product literature, and online presentations. This site also features technology, products, news, events, and community content.	
Patent Information	www.thermofisher.com/ms-patents	
Service Contact	www.unitylabservices.com	
Technical Documentation SharePoint	❖ To get user manuals for your product 1. With the serial number (S/N) of your instrument,* request access on our customer SharePoint as a customer at www.thermoscientific.com/Technicaldocumentation 2. For the first login, you have to create an account. Follow the instructions given on screen. Accept the invitation within six days and log in with your created Microsoft™ password. 3. Download current revisions of user manuals and other customer-oriented documents for your product. Translations into other languages may be available there as well. * You can find the serial number of your instrument on the name plate. Refer to the <i>Exactive Series Operating Manual</i> for the location.	

Contact	Link / Remarks	QR Code
Customer Feedback	❖ To suggest changes to this manual You are encouraged to report errors or omissions in the text or index. Send an email message to the Technical Editor at documentation.bremen@thermofisher.com. The PDF versions of our manuals allow adding comments with Adobe Acrobat Reader or other freely available PDF reader programs.	

Typographical Conventions

This section describes typographical conventions that have been established for Thermo Fisher Scientific manuals.

Signal Words

Make sure that you follow the precautionary statements presented in this manual. The special notices appear different from the main flow of text:

NOTICE

Points out possible material damage, data loss, impaired data quality and other important information in connection with the instrument.

Tip Highlights helpful information that can make a task easier.

Data Input

Throughout this manual, these conventions indicate data input and output via the computer:

- Messages displayed on the screen are represented by capitalizing the initial letter of each word and by italicizing each word.
- Input that you enter by keyboard is identified by quotation marks: single quotes for single characters, double quotes for strings.
- For brevity, expressions such as “choose **File > Directories**” are used rather than “pull down the File menu and choose Directories.”
- Any command enclosed in angle brackets < > represents a single keystroke. For example, “press <**F1**>” means press the key labeled *F1*.
- Any command that requires pressing two or more keys simultaneously is shown with a plus sign connecting the keys. For example, “press <**Shift**> + <**F1**>” means press and hold the <Shift> key and then press the <F1> key.
- Any button that you click on the screen is represented in bold face letters. For example, “click **Close**.”

Topic Headings

These headings are used to show the organization of topics within a chapter:

Chapter Name

Second Level Topics

Third Level Topics

Fourth Level Topics

Contents

Chapter 1	Instrument Configuration Window	1-1
Chapter 2	Q Exactive UHMR Readback Status Page for the Information View	2-1
Chapter 3	Instrument Setup.....	3-1
	Instrument Setup Window.....	3-2
	File Menu for the Instrument Setup Window	3-3
	Help Menu for the Instrument Setup Window	3-4
	Instrument Setup Window Toolbar	3-5
	Method Editor	3-6
	Experiment Setup Page	3-7
	Global Settings Pane	3-8
	Experiment Pane.....	3-20
	Graph Pane	3-22
	Properties Pane	3-23
	Summary Page	3-43
	Dialog Boxes of the Experiment Setup Page.....	3-44
	Lock Masses Dialog Box	3-44
	Inclusion List Dialog Box.....	3-47
	Exclusion List Dialog Box	3-52
	Mass Calculator	3-57
Chapter 4	Explore Q Exactive UHMR Tune	4-1
	Q Exactive UHMR Tune Overview	4-2
	Q Exactive UHMR Tune Menus.....	4-5
	File Menu	4-5
	Windows Menu	4-6
	Reports Menu	4-7
	Help Menu	4-8
	Toolbar	4-9
	Tasks Panel	4-12
	Instrument Control Window	4-12
	Mass Traces Window	4-23
	Calibrate Window.....	4-25
	Evaluate Window.....	4-27
	Vacuum / Bakeout Window.....	4-29
	Display Panel	4-32
	Spectrum Window	4-33
	Instrument Status Window	4-36
	Messages Window.....	4-41

Analysis Graphs Window	4-42
Debug Messages Window	4-43
Dialog Boxes	4-46
About Dialog Box	4-47
Autoselect Ion Source Values Dialog Box.....	4-47
Isolation Range Dialog Box.....	4-48
License Dialog Box	4-49
Mass Calculator	4-50
Syringe Pump Settings Dialog Box.....	4-52
Scan Parameters History Dialog Box.....	4-53
Scan Range Dialog Box.....	4-54
Fragmentation Dialog Box	4-55
Collection Modification Dialog Box	4-57
Lock Masses Dialog Box	4-57
Lock Mass Removal Dialog Box.....	4-60
Lock Mass Replacement Dialog Box	4-61
New Lock Mass Collection Dialog Box.....	4-62
Delete Lock Mass Collection Dialog Box.....	4-62
Name Change Dialog Box	4-63
Display Options Dialog Box	4-64
 Chapter 5 Procedures in Q Exactive UHMR Tune	5-1
Adding a License	5-2
Using Lock Masses and Lock Mass Collections	5-3
Adding a Lock Mass.....	5-3
Deleting Lock Masses.....	5-4
Exporting and Importing Lock Masses.....	5-4
Creating a new Lock Mass Collection	5-10
Renaming a Lock Mass Collection	5-10
Adding a Lock Mass to a Lock Mass Collection	5-11
Removing a Lock Mass from a Lock Mass Collection	5-11
Deleting a Lock Mass Collection.....	5-11
Performing a System Bakeout.....	5-12
Changing Default Settings of Q Exactive UHMR Tune	5-14
Displaying the High Vacuum Readback.....	5-14
Entering Parameters for the Syringe Pump.....	5-15
Changing the Settings for the Performance Status Check	5-16
Changing the Sweep Gas Flow in Standby Mode.....	5-17
Using Specific Settings in Q Exactive UHMR Tune	5-19
Averaging Spectra.....	5-19
Displaying the Mass Calibration List for UHMR Mode	5-20
Setting the HCD Trapping Gas Pressure	5-20
Switching the Detector Mode	5-21

Chapter 6	Reference Information	6-1
	Log Files	6-2
	Tune Files and Calibration Files.....	6-3
	API Source Settings for Various LC Flow Rates	6-4
	Default Parameters and Ranges for HESI-2	6-5
	One-Letter Abbreviations for Amino Acids	6-6
	Glossary.....	G-1
	Index	I-1

Instrument Configuration Window

Tip Do not change the settings in this window except during the installation of the instrument. Any changes in this window affect the data acquisition or the functionality of your instrument. A later change will rarely solve problems users have to face.

The Instrument Configuration window displays Q Exactive UHMR configuration information.

Thermo Exactive Series at 192.168.153.200 is connected

Note:
Any changes here affect the data acquisition or the functionality of your instrument. **Never change anything except during installation of the instrument.** A later change will rarely solve problems users have to face.

Path to instrument files: C:\Xcalibur\system\Exactive\Instrument

Path to log files: C:\Xcalibur\system\Exactive\Log

Base port: 6018

Network address: 00-0C-29-6F-F9-7A

IP address: 192.168.153.200

Public Name: Exactive Series slot #1

Max. audit record length: 0

Instrument type: Q Exactive UHMR

IP address range: 169.254.158.200 - 169.254.158.209, 192.168.32.200 - ...

Instrument Thermo Exactive Series is connected to the service.

Apply Reset changes Help

Figure 1-1. Instrument Configuration window

The Instrument Configuration window has these parameters:

Parameter	Description
Path to instrument files	Displays the location of the instrument files. To change the path, click the folder button on the right side of the text box. A dialog box appears where you can select another location.
Path to log files	Displays the location of the log files. For information about the content of the log files, see “Log Files” on page 6-2. To change the path, click the folder button on the right side of the text box. A dialog box appears where you can select another location
Base port	Displays the first TCP/UDP port in use for this particular instrument. Leave the field empty for an automatic assignment.
Network address	Displays the hardware address of the network card installed in the instrument. Leave the field empty for an automatic assignment.
IP address	Displays the IP address. Leave the field empty for an automatic assignment.
Public Name	Displays the name that is shown in the About dialog box of Q Exactive UHMR Tune.
Max. audit record length	Use this list box to select the maximum audit record length. These options are available: • 0 disables auditing • 50 is common for an Access audit database initialized by Platform’s Database Configuration • 255 is common for an Oracle audit database initialized by Platform’s Database Configuration • 1000 is common if auditing is done by Chromeleon. It is a compromise between size and readability
Instrument type	Displays the configured instrument type, that is Q Exactive UHMR.
IP address range	Displays the IP address or IP address range which should be assigned to the instrument during its starting phase. Use the numeric form, for example “172.16.2.1-172.16.2.15.” Tip Change only when advised by your network administrator.
Message box	Displays information about the instrument and connection status.
Buttons	
Apply	Saves your changes in this window.
Reset changes	Discards your changes in this window.
Help	Displays the Help for this window.

❖ To display this window

1. Choose **Programs > Thermo Foundation 3.1 > Instrument Configuration**.

2. From the Instrument Configuration window, click Q Exactive UHMR - Orbitrap MS in the Configured Devices area.
3. Click **Configure**.

Q Exactive UHMR Readback Status Page for the Information View

The readback status of each Xcalibur-configured instrument appears on the Status page of the Information view. When you click an instrument, Xcalibur™ displays current readings for the instrument on a page below the Run Manager pane.

Right-click any of the instruments to display a shortcut menu where you can switch your instrument to On, Off, or Standby mode.

Tip This view is normally displayed on the left side of the Home Page window. If this view is not displayed, the view has been turned off.

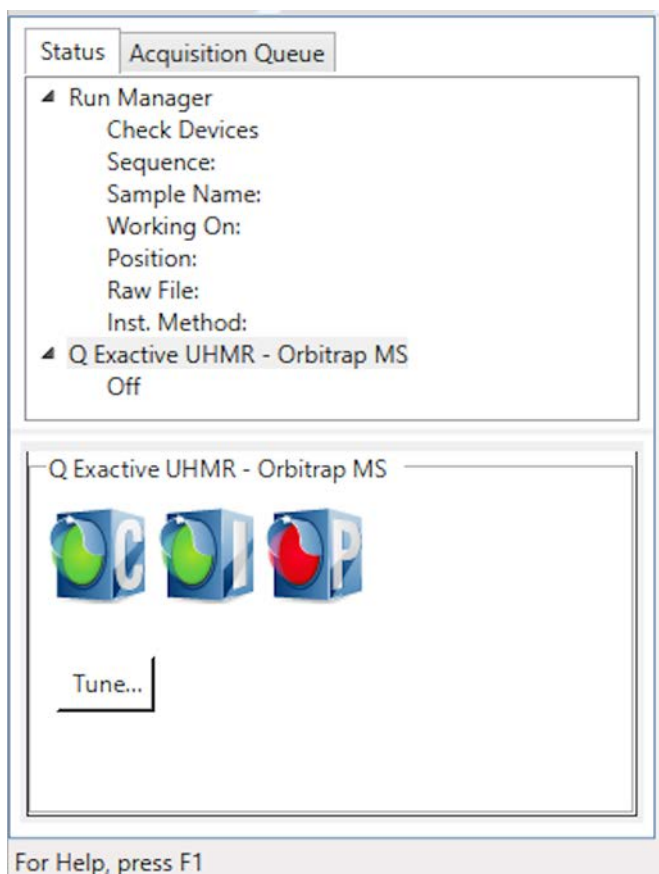


Figure 2-1. Q Exactive UHMR Readback Status Page for the Information View

These functions are available:

Button	Description	
	Communication Status	Shows the actual communication status of the system: • Green: communication with instrument is OK. • Yellow: only service is accessible (no instrument). • Red: communication is broken (no instrument, no service).
	Instrument Status	Shows the actual hardware status of the system (top instrument tree state): • Green: all readbacks are in specifications (green hooks). • Red: one or more readbacks are out of range.
	Performance Status	Shows the actual performance status of the system: • Green: the last evaluation/calibration was successful. • Yellow: last evaluation/calibration was successful, but is out of date. • Red: the evaluation/calibration was not successful.
Tune	Opens the Q Exactive UHMR Tune window.	

❖ **To open this page**

1. From the Home Page window, choose **View > Info View** to display the Information view.
2. Click the **Status** tab.
3. Click **Q Exactive UHMR - Orbitrap MS**.

Instrument Setup

After you have selected in the Instrument Configuration program which instruments you want Xcalibur to control, use Instrument Setup to specify your instrument settings.

Contents

- [Instrument Setup Window](#)
- [Experiment Setup Page](#)
- [Summary Page](#)
- [Dialog Boxes of the Experiment Setup Page](#)

Instrument Setup Window

The Instrument Setup window displays the icons of the instruments that you have selected using the Instrument Configuration window. (See the View bar on the left side of the window.) If you have configured more instruments than can be displayed on your screen, a vertical scroll bar appears in the View bar. So, you can access all of the instruments.

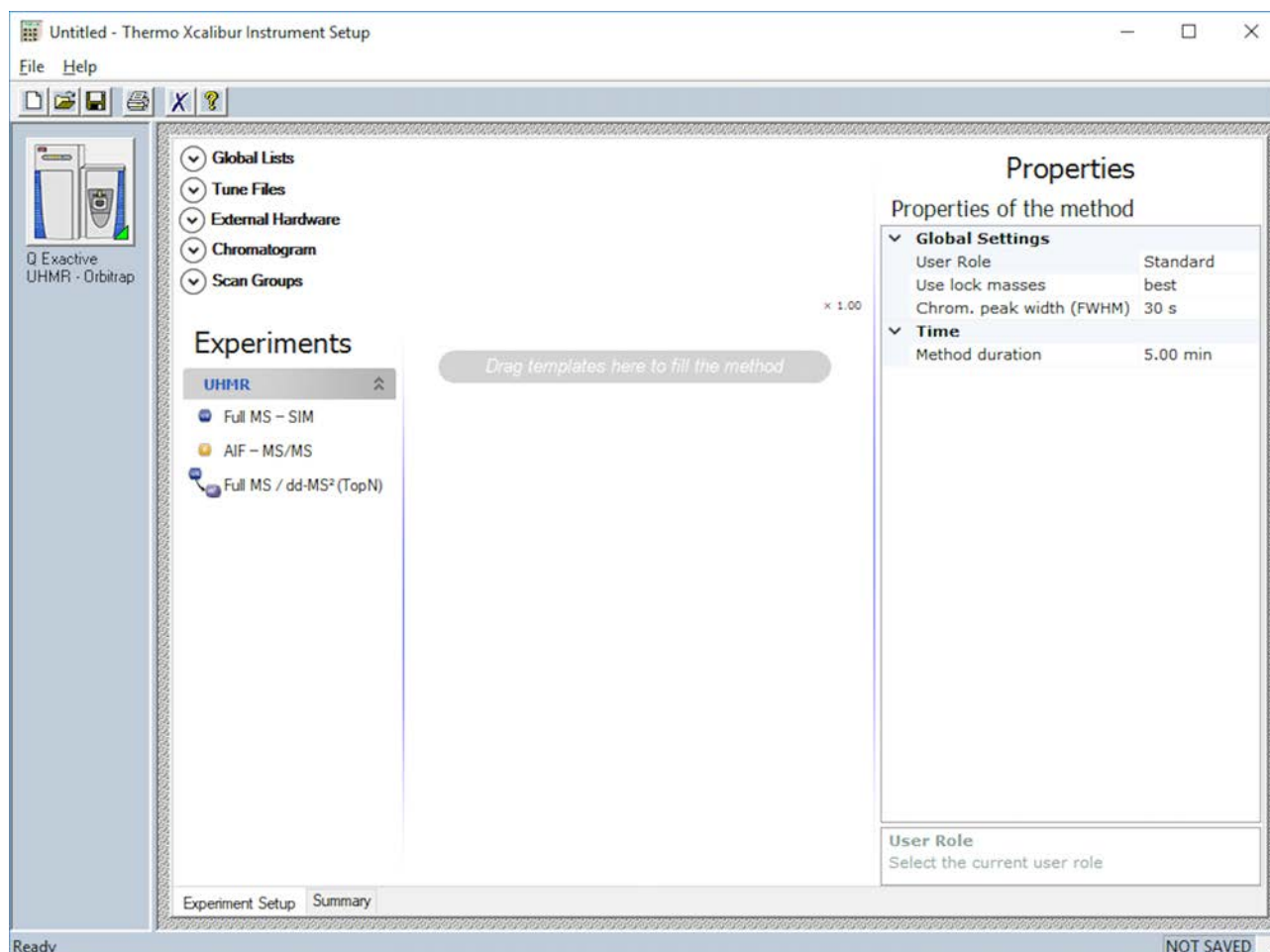


Figure 3-1. Instrument Setup window

To enter the setup parameters for a particular instrument, click the icon for that instrument. Xcalibur displays one or more pages of parameters to be set for the one you selected.

Tip Before you use the Instrument Setup window, select the instruments that you wish to use for your experiment in the Instrument Configuration program.

Use Instrument Setup to specify settings for your instruments after you have selected with the Instrument Configuration program the instruments that you want Xcalibur to control. The Instrument Setup window displays the setup parameters required for each instrument that you select on the View bar. These might include your autosampler,

LC pump, mass spectrometer, divert valves, syringe pump, contact closure timing sequence, and/or all other Xcalibur supported instruments that you have configured.

You can create new methods, modify existing methods, and save method files.

❖ **To display this window**

- Click the Instrument Setup icon  (toolbar) or  (Roadmap View) of the Home Page window.
- Or, choose **GoTo > Instrument Setup**.

View Bar

The View bar is a vertical bar on the left of the Instrument Setup window. It contains buttons for each of the instruments that you have selected by using the Instrument Configuration program.

Menus

Instrument Setup contains these menus:

- [File Menu for the Instrument Setup Window](#)
- [Help Menu for the Instrument Setup Window](#)

Toolbar

Instrument Setup Window Toolbar

File Menu for the Instrument Setup Window

The File menu provides commands for file and program operations. It has these commands:

Button	Command	Description
	New	Create a new method file having the appropriate extension.
	Open	Find and open a file that already exists.
	Save	Save the active method. Changes will be recorded in Audit Trail after the method is saved.

Button	Command	Description
	Save As	Edit user and description information, and view header information about the active file. Xcalibur opens the Save As dialog box. Changes will be recorded in Audit Trail after the method is saved.
	Summary Information	Edit user and description information, and view header information about the active file.
	Change Study Name	Select a dataset from a predefined list of names. The text of this menu item might be different if the administrator chose to use another name for a dataset. For example, this menu item might be Change Job Name.
	Audit Trail	View all auditable events and changes made to data files in the current application.
	Print	Print the parameters in your instrument method.
	Print Preview	View your page setup so that you can see what it looks like before printing it.
	Print Setup	Select these printing options: printer, form, orientation, and one-sided or two-sided printing.
	Most Recently Used Files	View the paths and names of the last four files used. These are located above the Exit command. Both open and closed files are displayed. Click a displayed file to load it. If the selected file was closed, it will be opened.
	Exit	Close the active window. If you exit before clicking OK from an active dialog box, Xcalibur asks if you want to save your changes.

Help Menu for the Instrument Setup Window

The Help menu lists these commands:

Command	Description
Q Exactive UHMR - Orbitrap MS Help	Open the Configuration and Setup Help for the instrument.
Instrument Setup Help	Open Xcalibur Help and display Help for the Instrument Setup window.
Help On Current Item	View Help for the Instrument Setup page that is currently displayed.
Q Exactive UHMR - Orbitrap MS Contents and Index	View the Contents, Index, and Find Help pages for the selected instrument.
Xcalibur Help	Open Xcalibur Help.
Glossary	Open the Xcalibur glossary.

Command	Description
How to use Online Help	Open Help that describes how to use the Help viewer.
About Instrument Setup	View the version number of the Instrument Setup program and the Thermo Fisher Scientific copyright notice.

Instrument Setup Window Toolbar

The toolbar provides symbol shortcuts for frequently used commands. These commands are available:

Button	Description
 New	Create a new instrument method.
 Open	Find and open an existing file.
 Save	If your method has not been saved before, clicking Save opens the Save As dialog box. Select the name and location for your instrument method. When you click Save , the File Summary Information Dialog Box opens. Enter header information for your instrument method. The file is saved when you click OK .
 Print	Print the parameters in your instrument method.
 Home Page	View the Home Page window—Roadmap view.
 Help	View Help for the Instrument Setup page that is currently displayed.

Method Editor

Use the Method Editor to specify the type of mass spectrometer experiment you plan to perform.

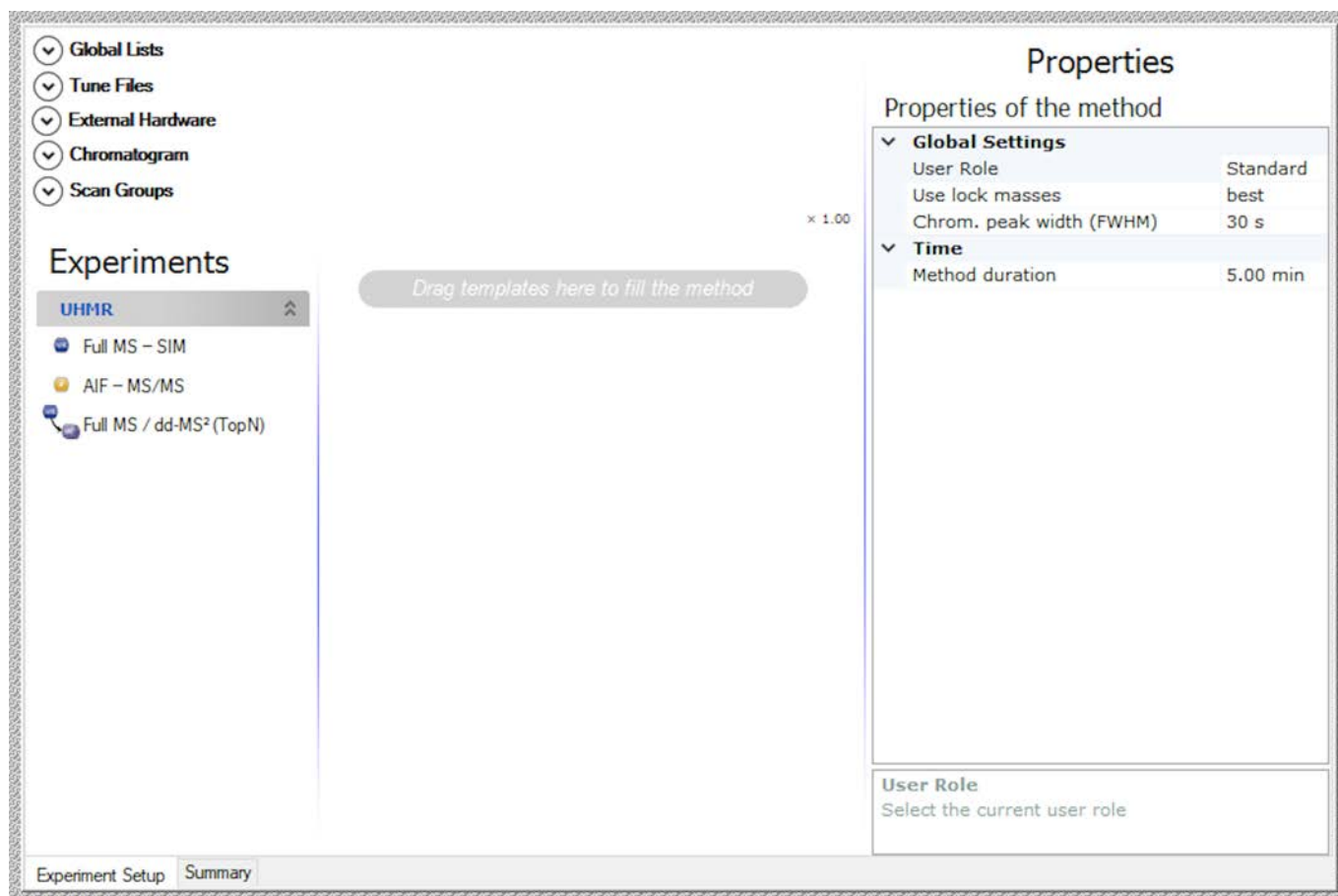


Figure 3-2. Method Editor (Xcalibur)

The Method Editor comprises these pages:

- Experiment Setup Page
- Summary Page

❖ **To display this view**

Click **Instrument Setup** from the Roadmap View of the Home Page window or choose **GoTo > Instrument Setup**.

Experiment Setup Page

Use the Experiment Setup page to set up Q Exactive UHMR mass spectrometer experiments. You use this page to specify values for the Q Exactive UHMR parameters and save the parameters in an instrument method.

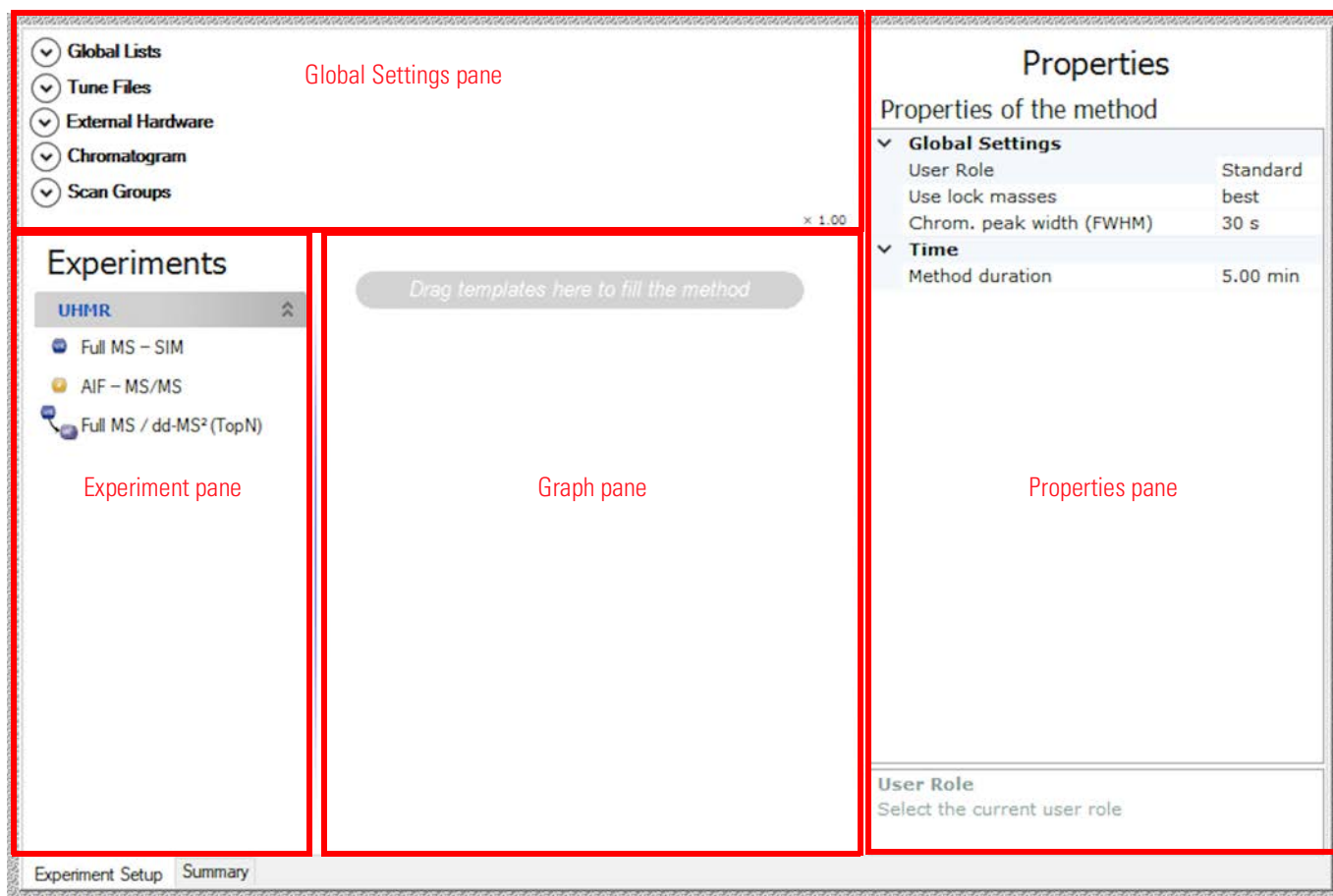


Figure 3-3. Method Editor—Experiment Setup page

The Experiment Setup page comprises four major windows:

- [Global Settings Pane](#)
- [Experiment Pane](#)
- [Graph Pane](#)
- [Properties Pane](#)

Global Settings Pane

The Global Settings pane is located on the top left side of the Experiment Setup page. It gives access to global lists, tune files, external hardware, chromatogram, and scan groups.

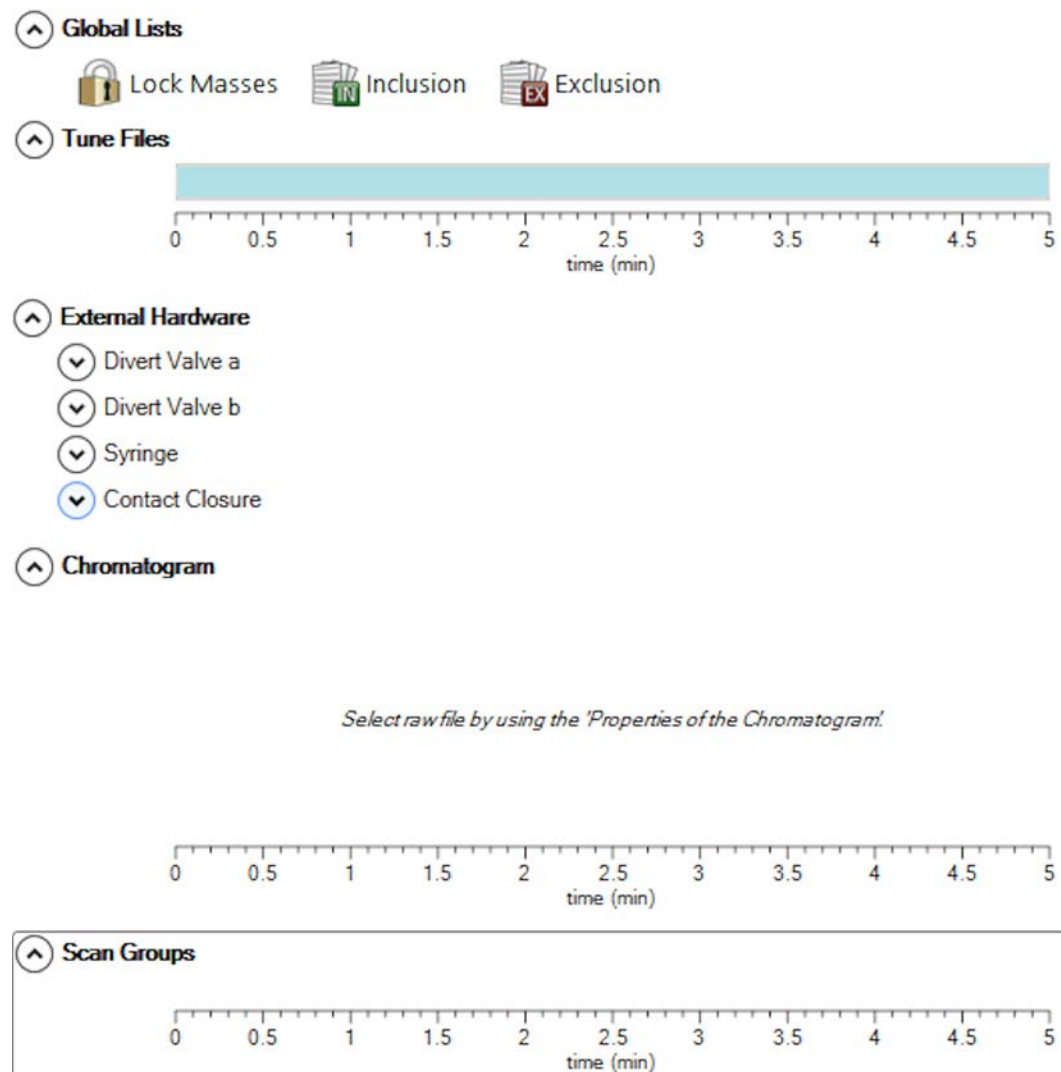


Figure 3-4. Method Editor—Global Settings pane

The Global Settings pane contains these panes:

- [Global Lists](#)
- [Tune Files](#)
- [External Hardware](#)
- [Chromatogram](#)
- [Scan Groups](#)

Click the title bar of an individual pane to display it. Click again to hide it.

Global Lists

Use the Global Lists pane of the Experiment Setup page to perform intelligent automated MS/MS and SIM type experiments by efficiently utilizing the mass spectrometer to characterize precursor ions independent of the “current segment” model. Use the Global Lists pane to specify precursor, reject, and/or non-data dependent MS/MS and SIM masses with customizable and independent time windows. Scan events that reference the mass lists that you create here run only if there is a corresponding mass/time window at that particular retention time.



Figure 3-5. Method Editor—Global Lists pane

These dialog boxes are available:

- [Lock Masses Dialog Box](#)
- [Inclusion List Dialog Box](#)
- [Exclusion List Dialog Box](#)

To display a dialog box, click the respective icon.

Tune Files

The Tune Files pane shows a graphical representation of the tune files usage during the various phases of the experiment. In addition to the base tune file, you can specify up to 50 other tune files.

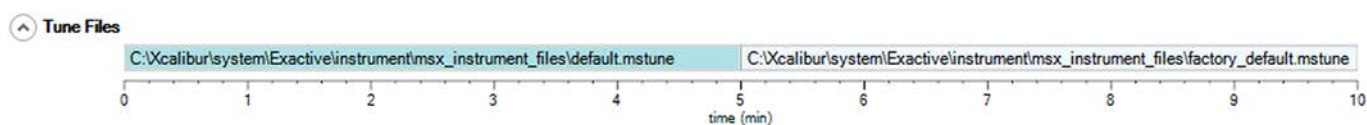


Figure 3-6. Method Editor—Tune Files

❖ To assign tune files

1. Do one of the following:
 - Point to a position on the time bar and right-click. Choose **Change to another tune file at <time at pointer position>** in the shortcut menu.

- Change the value of the Switch Count parameter in the Properties of Tunefiles pane.
2. In the Properties of Tunefiles pane, click the button next to the respective box of the Base Tunefile or New Tunefile parameter and browse for the new tune method file. Select the tune files and assign them to the experiment phases.

Properties of Tunefiles

General	
Switch Count	2
Base Tunefile	C:\Xcalibur\system\Exactive\instrument\msx_instrument_files\de
Element 1	
At	5.00
New Tunefile	C:\Xcalibur\system\Exactive\instrument\msx_instrument_files\fa
Element 2	
At	7.50
New Tunefile	

Figure 3-7. Properties of Tunefiles

The name and path way of the tune files will be shown on the respective time bar on the Tune Files pane.

❖ To change the starting time for tune files

- Position the cursor between adjacent tune files and drag the scan event along the time bar.
- In the Properties of Tunefiles pane, enter the time in the box of the At parameter of the respective Element.

❖ To remove a tune file

1. Position the cursor between adjacent tune files
2. Right-click to display the shortcut menu and choose **Remove change to tune file at <time at pointer position>**. The tune file to the right is removed.

❖ To zoom on the Tune Files pane

- Position the mouse pointer within the time axis area and drag the mouse across the time area of interest.
- To zoom in, position the mouse pointer within the pane and roll the mouse wheel forward.
- To zoom out, roll the wheel backward.
- To increase the zooming factor by two, keep the **<Shift>** key pressed while using the mouse wheel.

❖ **To unzoom the Tune Files pane**

Right-click in the pane to display the shortcut menu. Choose **Unzoom**.

❖ **To display this view**

On the External Hardware pane, expand the Tune Files item.

External Hardware

Use the External Hardware pane to configure and control optional hardware.

Divert Valve a / Divert Valve b

The Divert Valve items show graphic representations of the activities of the optional switching valves during the active acquisition. The normal LC flow through the switching valve (Position 1-2) is to the mass spectrometer. When the switching valve is activated (Position 1-6), LC flow is diverted to waste.

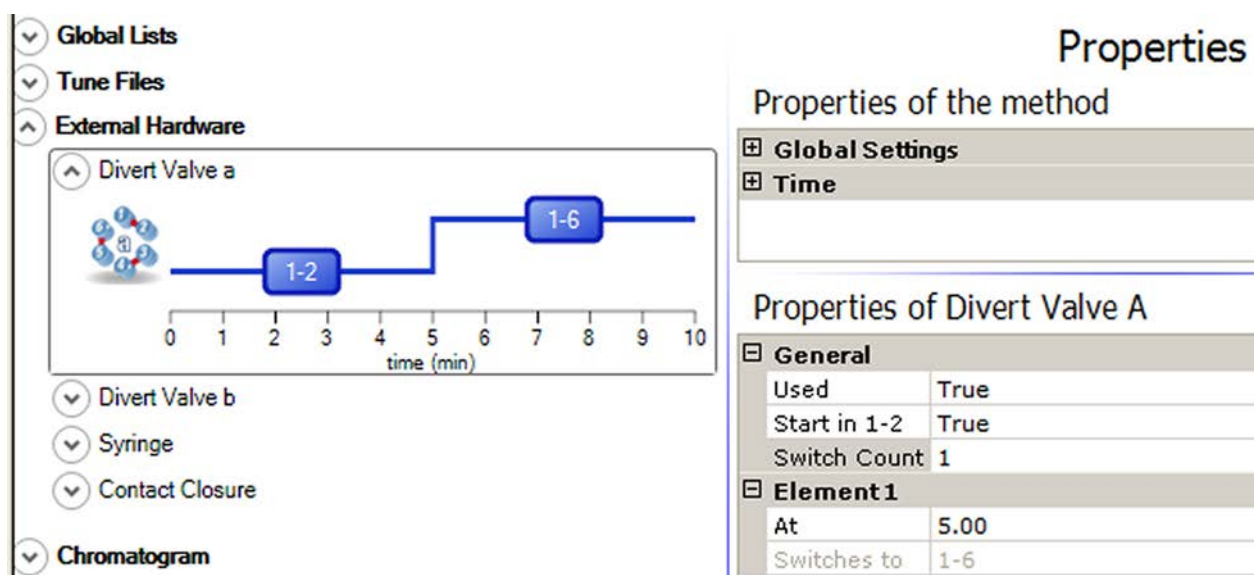


Figure 3-8. Properties of a switching valve that is used

❖ **To display this view**

On the External Hardware pane, expand the Divert Valve a or Divert Valve b item.

Use the shortcut menu of a Divert Valve item and the parameters of its Properties pane to control its activities:

❖ **To activate a switching valve**

- Right-click in the pane to display the shortcut menu. Choose **Activate**. The gray color  changes to the blue color . See [Figure 3-8](#).
- Click the valve symbol to select it. Set the Used parameter on the Properties pane to **True**.

❖ **To deactivate a switching valve**

- Right-click in the pane to display the shortcut menu. Choose **Deactivate**. The blue color changes to a gray color . See [Figure 3-9](#).
- Click the valve symbol to select it. Set the Used parameter on the Properties pane to **False**.

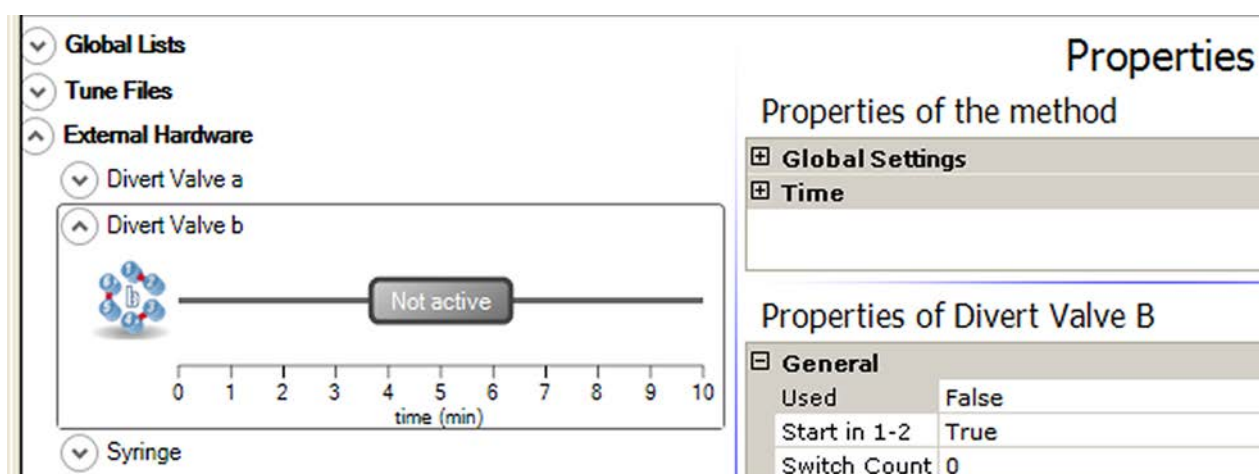


Figure 3-9. Properties of a switching valve that is not used

❖ **To change the start position of a switching valve**

- Right-click in the pane to display the shortcut menu. Depending on the active start position, choose **Start in 1-6** or **Start in 1-2**. The valve changes its start position.
- Click the valve symbol to select it. Depending on the active start position, set the Start in 1-2 parameter on the Properties pane to **True** or **False**.

❖ **To add a switch position for a switching valve**

1. Activate the switching valve as described above.

2. Do one of the following:
 - Use the mouse:
 - a. Move the mouse pointer to the position on the time line where you want to establish a switch position (5 minutes, for example).
 - b. Right-click in the pane to display the shortcut menu. Choose **Add switch at 5.00**.
 - Use the Properties pane:
 - a. Click the valve symbol to select it.
 - b. Set the Switch count parameter on the Properties pane to **1**.

A step in the line of the graphic representation indicates the new switch point. See [Figure 3-8](#).

3. To change the time of the switch position, do one of the following:
 - Drag the step that indicates the switch position to the new time.
 - On the Properties pane, set the At parameter of the respective Element to the new time.

❖ **To delete a switch position**

1. Move the mouse pointer to the switch position on the time line (at 5 minutes, for example).
2. Right-click in the pane to display the shortcut menu. Choose **Remove switch at 5.00**.

Syringe

The Syringe item shows a graphic representation of the activities of the optional syringe pump during the active acquisition.

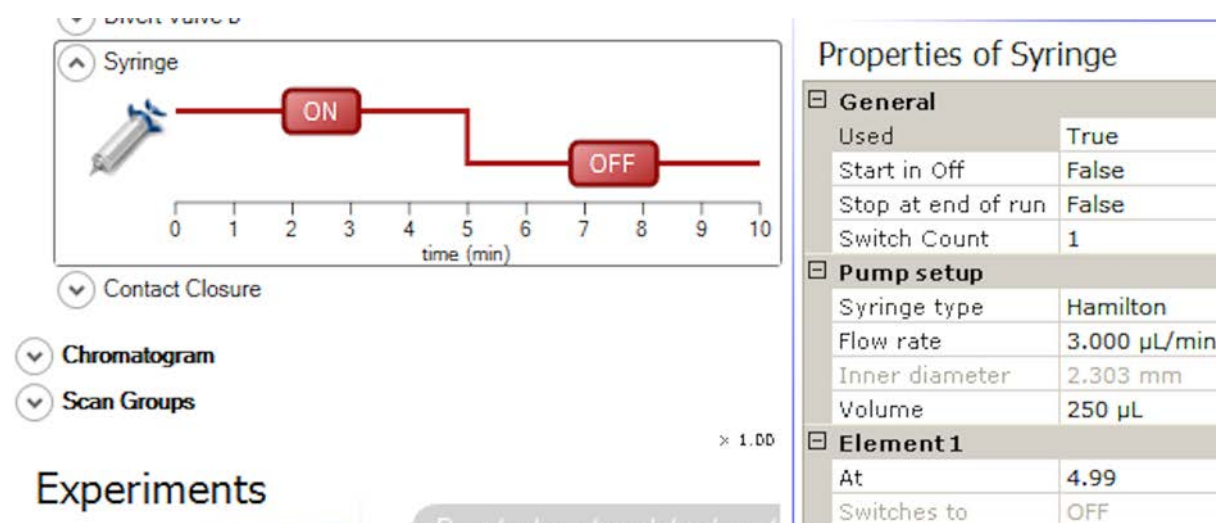


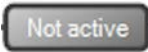
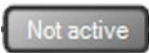
Figure 3-10. Syringe Pump pane

❖ To display this view

On the External Hardware pane, expand the Syringe Pump item.

Use the shortcut menu of the Syringe Pump item and the parameters of its Properties pane to control the activity of the syringe pump:

❖ To activate the syringe pump

- Right-click in the pane to display the shortcut menu. Choose **Activate**. The gray color  changes to the red color . See [Figure 3-10](#).
 - Click the valve symbol to select it. Set the Used parameter on the Properties pane to **True**.
- ### ❖ To deactivate the syringe pump
- Right-click in the pane to display the shortcut menu. Choose **Deactivate**. The red color changes to a gray color .
 - Click the valve symbol to select it. Set the Used parameter on the Properties pane to **False**.

❖ **To change the start position of the syringe pump**

- Right-click in the pane to display the shortcut menu. Depending on the active start position, choose **Start in ON** or **Start in OFF**. The pump changes its start position.
- Click the syringe symbol to select it. Depending on the active start position, set the Start in Off parameter on the Properties pane to **True** or **False**.

❖ **To add a switch position for the syringe pump**

1. Activate the syringe pump as described above.
2. Do one of the following:
 - Use the mouse:
 - a. Move the mouse pointer to the position on the time line where you want to establish a switch position (5 minutes, for example).
 - b. Right-click in the pane to display the shortcut menu. Choose **Add switch at 5.00**.
 - Use the Properties pane:
 - a. Click the syringe symbol to select it.
 - b. Set the Switch count parameter on the Properties pane to **1**.

A step in the line of the graphic representation indicates the new switch point. See [Figure 3-10](#).

3. To change the time of the switch position, do one of the following:
 - Drag the step that indicates the switch position to the new time.
 - On the Properties pane, set the At parameter of the respective Element to the new time.

❖ **To delete a switch position**

1. Move the mouse pointer to the switch position on the time line (at 5 minutes, for example).
2. Right-click in the pane to display the shortcut menu. Choose **Remove switch at 5.00**.

Contact Closure

The Contact Closure item shows a graphic representation of the contact closure activities during the active acquisition.

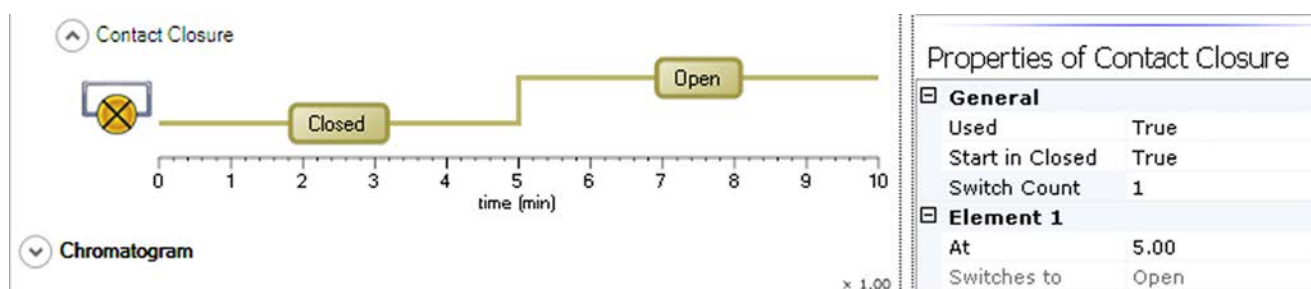


Figure 3-11. Contact closure

The settings of the Contact Closure item control the signals that the mass spectrometer transmits via the port labeled *Start Out* at its peripheral control output connection.

❖ To display this view

On the External Hardware pane, expand the Contact Closure item.

Use the shortcut menu of the Contact Closure item and the parameters of its Properties pane to control the contact closure activities:

❖ To activate the contact closure

- Right-click in the pane to display the shortcut menu. Choose **Activate**. The gray color  changes to the green color . See [Figure 3-11](#).
- Click the contact closure symbol to select it. Set the Used parameter on the Properties pane to **True**.

❖ To deactivate the contact closure

- Right-click in the pane to display the shortcut menu. Choose **Deactivate**. The green color changes to a gray color .
- Click the contact closure symbol to select it. Set the Used parameter on the Properties pane to **False**.

❖ To change the start position of the contact closure

- Right-click in the pane to display the shortcut menu. Depending on the active start position, choose **Start in Open** or **Start in Closed**. The contact closure changes its start position.

- Click the contact closure symbol to select it. Depending on the active start position, set the Start in Closed parameter on the Properties pane to **True** or **False**.

❖ **To add a switch position for the contact closure**

1. Activate the contact closure as described above.
2. Do one of the following:
 - Use the mouse:
 - a. Move the mouse pointer to the position on the time line where you want to establish a switch position (5 minutes, for example).
 - b. Right-click in the pane to display the shortcut menu. Choose **Add switch at 5.00**.
 - Use the Properties pane:
 - a. Click the contact closure symbol to select it.
 - b. Set the Switch count parameter on the Properties pane to **1**.

A step in the line of the graphic representation indicates the new switch point. See [Figure 3-10](#).

3. To change the time of the switch position, do one of the following:
 - Drag the step that indicates the switch position to the new time.
 - On the Properties pane, set the At parameter of the respective Element to the new time.

❖ **To delete a switch position**

1. Move the mouse pointer to the switch position on the time line (at 5 minutes, for example).
2. Right-click in the pane to display the shortcut menu. Choose **Remove switch at 5.00**.

Chromatogram

The chromatogram display shows the chromatogram for the selected raw file. If you have previously obtained a raw file (*.raw) of the chromatographic component separation, you can open this file.

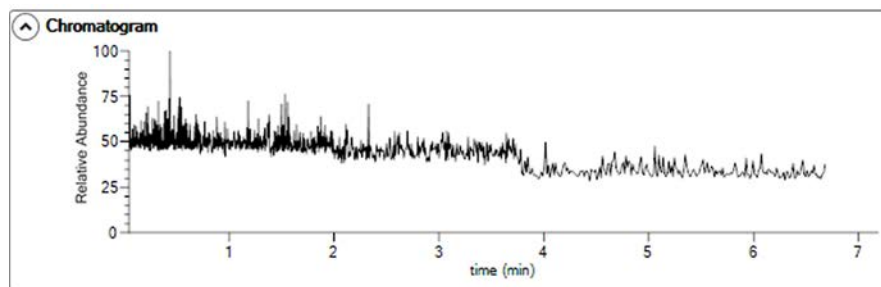


Figure 3-12. Chromatogram Display

❖ To display a chromatogram

1. In the Properties of Chromatogram pane, click into the empty field of the Rawfile parameter to display the  button.

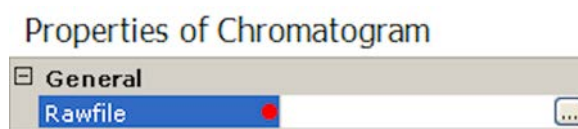


Figure 3-13. Selecting a raw file

2. Click the  button to open a dialog box where you can browse for the raw file.
3. Select the raw file.
4. If available, select a scan filter.
5. Select a trace type.

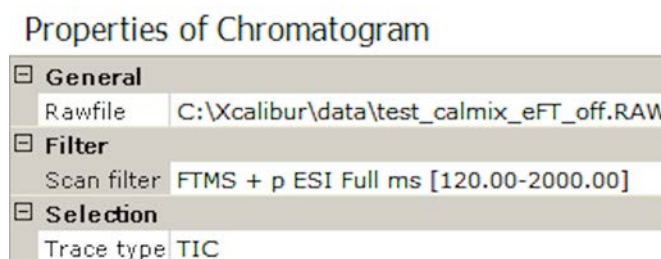


Figure 3-14. Properties of Chromatogram

The software updates the chromatogram immediately after a change.

❖ **To zoom on the chromatogram**

- Position the mouse pointer within the time axis area and drag the mouse across the time area of interest.
- To zoom in, position the mouse pointer within the chromatogram and roll the mouse wheel forward.
- To zoom out, roll the wheel backward.
- To increase the zooming factor by two, keep the <Shift> key pressed while using the mouse wheel.

❖ **To unzoom the chromatogram**

Right-click in the Scan Groups pane to display the shortcut menu. Choose **Unzoom**.

The chromatogram is also zoomed when the time axis of the Scan Groups is zoomed.

❖ **To display this view**

On the External Hardware pane, expand the Chromatogram item.

Scan Groups

In the Scan Groups pane, time bars represent the scan events during the acquisition. The Scan Groups pane is filled when you drag experiment symbols from the Experiment pane to the Graph pane.

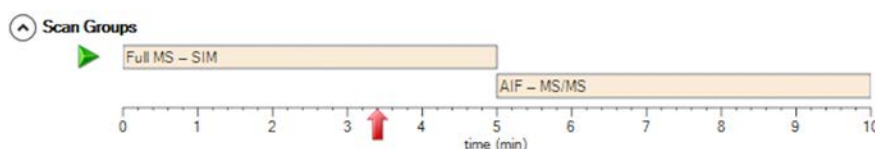


Figure 3-15. Scan Groups

Use the Properties pane of a scan event to control the activities during individual experiments. Red triangles (▶) to the left side of a time bar indicate active scan events.

❖ **To display the active scan events at a certain time**

Click the time line at the position. A red arrow (↑) indicates the selected time. A green triangle (▶) to the left side of the time bar indicates the active scan event. If scan events overlap at the selected time, green triangles appear for each active scan event. The bottom part of the Properties pane shows the parameters for the selected scan event.

❖ **To change start and end time of a scan event**

- Drag the left and right edges of the time bar to the intended positions on the time line.
- Enter the times in the Minimum and Maximum boxes of the runtime parameter on the Properties pane.

❖ **To zoom on the Scan Groups pane**

- Position the mouse pointer within the time axis area and drag the mouse across the time area of interest.
- To zoom in, position the mouse pointer within the pane and roll the mouse wheel forward.
- To zoom out, roll the wheel backward.
- To increase the zooming factor by two, keep the <Shift> key pressed while using the mouse wheel.

❖ **To unzoom the Scan Groups pane**

Right-click in the pane to display the shortcut menu. Choose **Unzoom**.

The Scan Groups pane is also zoomed when the time axis of the chromatogram display is zoomed.

❖ **To display this view**

On the External Hardware pane, expand the Scan Groups item.

Experiment Pane

The Experiment pane is located on the bottom left side of the Experiment Setup page. It gives access to predefined experiment templates. You cannot delete the experiment templates.

Every single experiment is associated with a descriptive icon. This icon can be dragged from the Experiment pane to the Graph pane. When selected, the icon gives an overview to the operator, which experiment and which associated options are active. Therefore, this icon changes depending on the settings. Use the Properties pane to specify the values for your experiment parameters.

Licenses that are installed on your instrument might affect the number of available experiments and the parameters used by them.

UHMR Experiment Templates

The UHMR folder contains predefined templates for experiments.

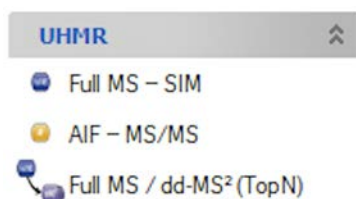
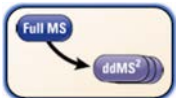


Figure 3-16. Available general templates

The Experiment Setup page allows using several system templates in an instrument method.

Experiment Symbols

Three experiment templates are available on the Experiment pane. Click the experiment symbol in the table to display an overview of the available parameters and values, which are displayed on the [Properties Pane](#).

Template	Experiment Symbol	Description
Full MS – SIM		This experiment comprises a full MS scan or SIM scan without HCD fragmentation.
AIF – MS/MS		This AIF-MS/MS experiment will acquire HCD fragmentation scans with or without prior quadrupole selection. You can set the <i>m/z</i> ranges for the quadrupole isolation window and the analyzer detection window.
Full MS / dd-MS ² (TopN)		This experiment comprises a full MS scan (without collision energy) followed by a set of Data Dependent™ scans with a collision energy applied. Ions of the second scan event enter the HCD collision cell, ions of the first do not. Special feature: Auto value option: Dynamic Exclusion^a Filters for triggering Data Dependent scans are listed under dd Settings.

^a Auto value options: Depending on the experiment type, properties like “Dynamic Exclusion” can be set automatically by the software, dependent on the chromatographic peak width (FWHM).

Graph Pane

The Graph pane is located at the middle bottom side of the Experiment Setup window. It shows a graphic representation of the experiment during the acquisition.

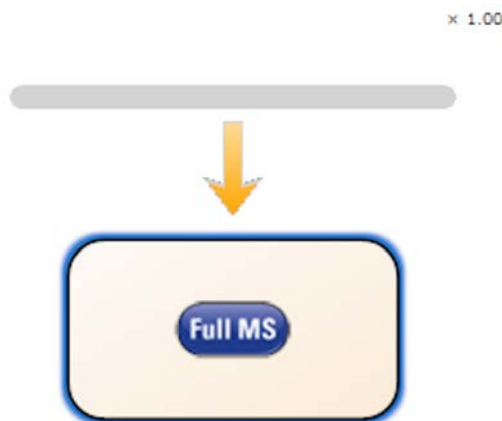


Figure 3-17. Graphic representation of the experiment

❖ To add an experiment to the active method

1. Do one of the following:
 - Double-click an experiment symbol on the Experiment pane.
 - Drag an experiment symbol from the Experiment pane to the gray bar in the Graph pane.

In Xcalibur, the Scan Groups pane shows a corresponding time bar for each symbol.

2. Use the Properties pane of an experiment to control the activities during individual experiments.

❖ To delete an experiment

1. Right-click the experiment symbol to display the shortcut menu.
2. Choose **Delete this <Name of Experiment>**.

Depending on the position of the mouse pointer and on the number of selected experiment symbols, additional commands may be available in the shortcut menu.

❖ To zoom in or out on the Graph pane

- Position the mouse pointer within the pane and roll the mouse wheel forward to zoom in.
- Roll the wheel backward to zoom out.

The zoom factor ranges from 0.25 to 2. The actual zoom factor is displayed in the top right corner of the Graph pane.

Properties Pane

The Properties pane is on the right side of the Experiment Setup page.

Properties

Properties of the method

▼ Global Settings	
User Role	Standard
Use lock masses	best
Chrom. peak width (FWHM)	30 s
▼ Time	
Method duration	5.00 min

User Role
Select the current user role

Properties of Full MS — SIM

▼ General	
Runtime	0 to 5 min
Polarity	positive
▼ Desolvation / Fragmentation	
In-source CID	Off
IST Desolvation	-10
▼ Full MS / SIM	
Resolution	50,000
AGC target	fixed
Maximum IT	200 ms
Scan range	2000 to 10000 m/z
Isolation range	Off

Runtime
Data acquisition start time and end time for selected MS experiment [min] (0.00 to 10,000.00)

Figure 3-18. Properties pane

The pane consists of two parts:

- [Properties of the Method](#)

The upper part is always available. It shows the properties of the active method.

The lower part depends on the item that is selected on the left side of the Experiment Setup page. One of these tables is displayed:

- [Properties of Tunefiles](#)

The table shows the properties of the tune files selected in the Global Settings pane.

- [Properties of Divert Valve A / Divert Valve B](#)

The table shows the properties of the switching valve selected in the Global Settings pane.

- [Properties of Syringe](#)

The table shows the properties of the syringe pump selected in the Global Settings pane.

- [Properties of Contact Closure](#)

The table shows the properties of the contact closure selected in the Global Settings pane.

- The table shows the parameters for the experiment symbol selected in the Graph pane:

- [Properties of Full MS – SIM](#)
- [Properties of AIF – MS/MS](#)
- [Properties of Full MS / dd-MS² \(TopN\)](#)

Properties of the Method

The properties of the method include these parameters:

Parameter	Description
Global Settings	
User Role	Use this field to specify whether the advanced parameters for scan events are displayed or not. To show the advanced parameters, set the field to Advanced . To hide the advanced parameters, set the field to Standard . Double-click into the field to change the status.
use lock masses	Use the list box to specify how lock masses are used in the active instrument method. These options are available: • off No lock masses are used. • best Only the most intense lock mass of the global list that is found in the spectrum is used for a calibration. • if all present Lock masses are used only when all active masses of the global lock mass list are present at the same time. If timed lock masses are used, the mass spectrometer takes into account only those lock masses whose time windows cover the current retention time.

Parameter	Description
Chrom. peak width (FWHM)	Use this box to specify the estimated or determined chromatographic peak width at full width half maximum for the user's chromatographic setup. Based the value in this field, the mass spectrometer may calculate the values of other parameters to optimize the settings for HPLC or UHPLC if they are set to Auto: - Automatic pre-scanning for AGC AGC information will be updated automatically with a high frequency, when setting a lower FWHM (for fast chromatography) - Dynamic exclusion To change the peak width, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, you can enter the time in the spin box text field. The valid range for the peak width is from 1 to 10000 seconds.
Time	
Method duration	Use this box to specify the total mass spectrometer acquire time, in minutes, for the run. The instrument rescales the Segments bar to correspond to the specified acquire time. To change the time, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, you can enter the time in the spin box text field. The valid range for the time is from 0.1 to 10000 minutes.
Customized Tolerances (+/-)^a	
Lock Masses Inclusion Exclusion Dynamic Exclusion	Use the boxes in this group to adjust mass tolerances for global lists in different instrument methods. The tolerance can be set independently for each list type. To change a tolerance, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, you can enter the tolerance in the spin box text field. Available options are: – (use instrument default) 0.1–1000 ppm 0.1–50000 mmu When you directly enter a tolerance in the text field, you can use additional units. The software will convert it to ppm or mmu depending of its nature (absolute or relative definition). Accepted units are (for absolute definition: Da, Th, u, mmu; for a relative definition: ppt, ppb, ppm, %). An empty property value field as well as a set value of 0, -, or off will result in using the instrument default (displayed as -).

^aThis parameter is not available when User Role is set to **Standard**.

Properties of Tunefiles

The properties of the Tune Files item include these parameters:

Parameter	Description
General	
Switch Count	Use this spin box to enter the number of switch positions that are to occur during a run. The valid range of positions is 0 through 50. Entering “0” results in the switch remaining either On or Off throughout the run. Enter a number between “1” and “50” to change the state from Off to On or On to Off at multiple specified times during a run. The number of positions on the Retention Time bar corresponds to the number of switch positions you specify using this spin box. When you enter a number different from 0, a corresponding number of Element parameter groups is displayed on the Properties pane.
Base Tunefile	Use this box to specify the current tune method file. To change the tune method file, click the button next to the box and browse for the new tune method file. A red dot in the left column indicates that no tune file is selected.
Elementn ($n=1-50$)	
Use the parameters of the Element groups to specify properties for the active item during individual switching events. The displayed parameters depend on the active item.	
At	Use this spin box to specify the time of the switching event. To change this value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, enter a value in the spin box text field.
New Tunefile	Use this box to specify the tune method file for the new element. To change the tune method file, click the button next to the box and browse for the new tune method file. A red dot in the left column indicates that no tune file is selected.

❖ To show this view

Click the Tunefiles symbol in the Global Settings pane.

Properties of Divert Valve A / Divert Valve B

The properties of a switching valve include these parameters:

Parameter	Description
General	
Used	Use this field to specify whether the switching valve is used during the acquisition or not. To use the switching valve, set the field to True . To not use the switching valve, set the field to False . Double-click into the field to change the status.

Parameter	Description
Start in 1-2	Use this field to specify whether the initial position of the switch at the start of a run is 1-2 or 1-6. To start the switching valve in position 1-2, set the field to True . To start the switching valve in position 1-6, set the field to False . Double-click into the field to change the status.
Switch Count	Use this spin box to enter the number of switch positions that are to occur during a run. The valid range of positions is 0 through 50. Entering “0” results in the switch remaining either On or Off throughout the run. Enter a number between “1” and “50” to change the state from Off to On or On to Off at multiple specified times during a run. The number of positions on the Retention Time bar corresponds to the number of switch positions you specify using this spin box.
Element n ($n=1-50$)	
Use the parameters of the Element groups to specify properties for the active item during individual switching events. The displayed parameters depend on the active item.	
At	Use this spin box to specify the time of the switching event. To change this value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, enter a value in the spin box text field.
Switches to	This display field shows the status to which the contact closure is switched.

❖ **To show this view**

Click the Divert Valve a / Divert Valve b symbol in the External Hardware pane.

Properties of Syringe

The properties of the Syringe item include these parameters:

Parameter	Description
General	
Used	Use this field to specify whether the syringe pump is used during the acquisition or not. To use the syringe pump, set the field to True . To not use the syringe pump, set the field to False . Double-click into the field to change the status.
Start in Off	Use this field to specify whether the initial state of the switch at the start of a run is On or Off. To start the acquisition with the syringe pump in Off status, set the field to True . To start the acquisition with the syringe pump in On status, set the field to False . Double-click into the field to change the status.
Stop at end of run	Use this field to have the mass spectrometer turn the syringe pump off when the run is completed. To turn the syringe pump off, set the field to True . To not have the mass spectrometer turn the syringe pump off after the run, set the field to False . Double-click into the field to change the status.

Parameter	Description
Switch Count	Use this spin box to enter the number of switch positions that are to occur during a run. The valid range of positions is 0 through 50. Entering “0” results in the switch remaining either On or Off throughout the run. Enter a number between “1” and “50” to change the state from Off to On or On to Off at multiple specified times during a run. The number of positions on the Retention Time bar corresponds to the number of switch positions you specify using this spin box.

Pump Setup

Use the settings in this area to specify the syringe type and flow rate of the syringe pump.

Syringe type	Use this list box to specify the syringe type (Hamilton, Unimetrics, or Other). If you select Hamilton or Unimetrics , you must specify the volume of the syringe in the Volume list box. If you select Other , you must specify the inside diameter of the syringe in the Inner diameter spin box.
Flow Rate	Use this spin box to set the volume of solvent solution passing through the syringe pump per unit time. The acceptable range of values depends on the selected syringe diameter. To change this value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, enter a value in the spin box text field.
Inner diameter	Use this spin box to specify the inside diameter for syringes other than Hamilton and Unimetrics syringes. The acceptable range of values is 0.1 to 35 mm. To change this value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, enter a value in the spin box text field.
Volume (µL)	Use this list box to specify the syringe volume for Hamilton and Unimetrics syringes. The acceptable values depend on the syringe type: - Hamilton: 0.5, 1, 2, 5, 10, 25, 50, 100, 250, and 500 µL. - Unimetrics: 10, 25, 50, 100, 250, 500, 1000, 2500, 5000, 10000, 25000, and 50000 µL.

Element n ($n=1-50$)

Use the parameters of the Element groups to specify properties for the active item during individual switching events. The displayed parameters depend on the active item.

At	Use this spin box to specify the time of the switching event. To change this value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, enter a value in the spin box text field.
Switches to	This display field shows the status to which the syringe pump is switched.

❖ To show this view

Click the Syringe symbol in the External Hardware pane.

Properties of Contact Closure

The properties of the Contact Closure item include these parameters:

Parameter	Description
General	
Used	Use this field to specify whether a timed contact closure program is used in an experiment method or not. To use the contact closure, set the field to True . To not use the contact closure, set the field to False . Double-click into the field to change the status.
Start in Closed	Use this field to specify whether the initial status of the contact closure at the start of a run is On or Off. To start the acquisition with the syringe pump in Closed status, set the field to True . To start the acquisition with the contact closure in Open status, set the field to False . Double-click into the field to change the status.
Switch Count	Use this spin box to select the number of switch positions that are to occur during a run. The valid range of positions is 0 through 50. Selecting "0" results in the switch remaining either Closed or Open throughout the run. Selecting a number between "1" and "50" allows you to change the state from Closed to Open or Open to Closed at multiple specified times during a run. The number of positions on the Retention Time bar corresponds to the number of switch positions you specify using this spin box.
Element n ($n=1-50$)	
Use the parameters of the Element groups to specify properties for the active item during individual switching events. The displayed parameters depend on the active item.	
At	Use this spin box to specify the time of the switching event. To change this value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, enter a value in the spin box text field.
Switches to	This display field shows the status to which the contact closure is switched.

❖ To show this view

Click the Contact Closure symbol in the External Hardware pane.

Properties of Chromatogram

The properties of the Chromatogram item include these parameters:

Parameter	Description
General	
Rawfile	Use this field to select a previously obtained raw data file corresponding to a similar chromatographic separation. Click the button next to the box and browse for the raw file. A red dot in the left column indicates that no raw file is selected.

Parameter	Description
Filter	
Scan filter	Use this field to select a scan description that tells the data system how to filter the raw data.
Selection	
Trace type	Use this field to select a chromatogram plot type. The software updates the chromatogram immediately after a change. These options are available: • TIC Plots the sum of all the ion intensities. • Neutral Fragment Plots the sum of the ion intensities of the ions that produce a neutral fragment with a mass specified in the Neutral Fragment spin box. • Base Peak Plots the ion intensity of the most intense ion in the chromatogram. • Mass Range Plots the sum of the ion intensities only for ions in the mass range or ranges specified in the Range(s) box.
Neutral Fragment	This field is available when you have selected Neutral Fragment as trace type. To enter the m/z value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, enter a value in the spin box text field.
Mass Ranges	Use this field to specify the range or ranges of mass-to-charge ratios (m/z) that the mass spectrometer can analyze. Use a dash (-) to separate the low and high masses of a range. Use a comma (,) to separate ranges. This field is not available when you have selected TIC as trace type.
Mass Tolerance	
Tolerance	For Neutral Fragment, Mass Range, and Base Peak plot types, use the spin box to specify the value of the mass tolerance. Enter a value in the range from 0 to 2000 and select the appropriate option in the Units field. To change this value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, enter a value in the spin box text field.
Unit	Use this field to select the units that are used in processing the raw file. Select either the mmu (millimass units) option or the ppm (parts per million) option.

❖ **To show this view**

Click the Chromatogram symbol in the External Hardware pane.

Properties of Full MS – SIM

The properties of a Full MS – SIM experiment include these parameters:

Parameter	Description
General	
Runtime	Use this box to specify the duration in minutes of the active scan event. Click into the field to display the spin boxes for the start time (Minimum) and the end time (Maximum) of the scan event. To change a value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, you can enter a value in the spin box text field. The valid range for the start time is from 0 to (end time minus 0.01) minutes. The valid range for the end time is from (start time plus 0.01) to 10000 minutes. Or, drag the left and right edges of the corresponding time bar to the intended positions on the time line in the Scan Groups pane.
Polarity	Use this list box to toggle between positive ion and negative ion polarity.
Desolvation / Fragmentation	
In-source CID	Use the spin box to enter the in-source CID collision energy. To change the value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. You can set the CID collision energy to any value from 0.1 to 150 eV (ESI source) or 200 eV (NSI source). Select Off to switch off the collision energy (0 eV).
IST Desolvation	Use the spin box to enter the Desolvation voltage of the Ion Source Trapping. To change the value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. You can set the IST Desolvation voltage to any value from –300 to +300 V. Select Off to switch off the IST Desolvation voltage. If IST Desolvation is used, the AGC is turned off and maximum injection time is used.
Full MS / SIM	
Use the parameters in this group to specify the properties of the master scan.	
Microscans ^a	Use this spin box to select the number of averaged transients for one scan event. To change the value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, you can enter a value in the spin box text field. The minimum number of microscans is 1. The possible maximum number of microscans depends on the active values for Resolution and Maximum IT.
Resolution	Use this list box to select the mass resolution used during the selected scan event. The mass resolution of the Orbitrap analyzer is proportional to $1/\sqrt{m/z}$. The scan time increases with increasing resolution and detect time. Available options are 1563, 3125, 6250, 12500, 25000, 50000, 100000, or 200000.

Parameter	Description
AGC target	Use this list box to select the AGC target value for the selected scan event. The AGC target value controls the number of ions that are injected into the Orbitrap analyzer. Available options are 2e4, 5e4, 1e5, 2e5, 5e5, 1e6, 3e6, or 5e6. If IST Desolvation is used, the AGC is turned off and maximum injection time is used.
Maximum IT	Use this list box to type or click a maximum allowed injection time (in milliseconds) to reach the AGC target value. You can enter either a number between 1 and 1000 or auto. If you enter auto, the mass spectrometer chooses a value that depends on the highest resolution of the active and the previous scan event.
Scan range	Use the spin boxes in this field to set values (in mass-to-charge ratio units) for Minimum, Maximum, Center, and Width for the scan range. To change the value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. • Minimum Select the minimum value for the scan range. You can enter any m/z value from 350.0 to 79995.0. • Maximum Select the maximum value for the scan range. You can enter any m/z value from 355.0 to 80000.0. • Center Select the center mass of the scan range. You can enter any m/z value from 352.5 to 79997.5. • Width Select the width of the scan range. You can enter any m/z value from 5.0 to 79650.0.
Isolation range	Use the spin boxes in this field to set values (in mass-to-charge ratio units) for Minimum, Maximum, Center, and Width for the quadrupole isolation range. To change the value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Select Off to switch off the isolation range. • Minimum Select the lowest value for the isolation range. You can enter any m/z value from 500.0 to 24995.0. • Maximum Select the highest value for the isolation range. You can enter any m/z value from 505 to 25000.0. • Center Select the center mass of the isolation range. You can enter any m/z value from 502.5 to 24997.5. • Width Select the width of the isolation range. You can enter any m/z value from 5.0 to 24500.0.

^aThis parameter is not available when User Role is set to **Standard**.

❖ **To show this view**

Click the Full MS symbol in the Graph pane.

Properties of AIF – MS/MS

The properties of an AIF – MS/MS experiment include these parameters:

Parameter	Description
General	
Runtime	Use this box to specify the duration in minutes of the active scan event. Click into the field to display the spin boxes for the start time (minimum) and the end time (maximum) of the scan event. To change a value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, you can enter a value in the spin box text field. The valid range for the start time is from 0 to (end time minus 0.01) minutes. The valid range for the end time is from (start time plus 0.01) to 10000 minutes. Or, drag the left and right edges of the corresponding time bar to the intended positions on the time line in the Scan Groups pane.
Polarity	Use this list box to toggle between positive ion and negative ion polarity.
Desolvation / Fragmentation	
In-source CID	Use the spin box to enter the in-source CID collision energy. To change the value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. You can set the CID collision energy to any value from 0.1 to 150 eV (ESI source) or 200 eV (NSI source). Select Off to switch off the collision energy (0 eV).
IST Desolvation	Use the spin box to enter the Desolvation voltage of the Ion Source Trapping. To change the value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. You can set the IST Desolvation voltage to any value from –300 to +300 V. Select Off to switch off the IST Desolvation voltage. If IST Desolvation is used, the AGC is turned off and maximum injection time is used. Tip For the fragmentation/desolvation of positive ions, we recommend using negative desolvation voltages. For the fragmentation/desolvation of negative ions, we recommend using positive desolvation voltages.
HCD CE	Use this box to specify the absolute collision energy (CE) in eV. To change a value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. You can enter any value from 1 to 300.

Parameter	Description
AIF	
Microscans ^a	Use this spin box to select the number of averaged transients for one scan event. To change the value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, you can enter a value in the spin box text field. The minimum number of microscans is 1. The possible maximum number of microscans depends on the active values for Resolution and Maximum IT.
Resolution	Use this list box to select the mass resolution used during the selected scan event. The mass resolution of the Orbitrap analyzer is proportional to $1/\sqrt{m/z}$. The scan time increases with increasing resolution and detect time. Available options are 1563, 3125, 6250, 12500, 25000, 50000, 100000, or 200000.
AGC target	Use this list box to select the AGC target value for the selected scan event. The AGC target value controls the number of ions that are injected into the Orbitrap analyzer. Available options are 2e4, 5e4, 1e5, 2e5, 5e5, 1e6, 3e6, or 5e6. If IST Desolvation is used, the AGC is turned off and maximum injection time is used.
Maximum IT	Use this list box to type or click a maximum allowed injection time (in milliseconds) to reach the AGC target value. You can enter either a number between 1 and 1000 or auto. If you enter auto , the mass spectrometer chooses a value that depends on the highest resolution of the active and the previous scan event.

Parameter	Description
Scan range	Use the spin boxes in this field to set values (in mass-to-charge ratio units) for Minimum, Maximum, Center, and Width for the scan range. To change the value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. • Minimum Select the minimum value for the scan range. You can enter any m/z value from 350.0 to 79995.0. • Maximum Select the maximum value for the scan range. You can enter any m/z value from 355.0 to 80000.0. • Center Select the center mass of the scan range. You can enter any m/z value from 352.5 to 79997.5. • Width Select the width of the scan range. You can enter any m/z value from 5.0 to 79997.5.
Isolation range	Use the spin boxes in this field to set values (in mass-to-charge ratio units) for Minimum, Maximum, Center, and Width for the quadrupole isolation range. To change the value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Select Off to switch off the isolation range. • Minimum Select the lowest value for the isolation range. You can enter any m/z value from 500.0 to 24995.0. • Maximum Select the highest value for the isolation range. You can enter any m/z value from 505 to 25000.0. • Center Select the center mass of the isolation range. You can enter any m/z value from 502.5 to 24997.5. • Width Select the width of the isolation range. You can enter any m/z value from 5.0 to 24500.0.

^aThis parameter is not available when User Role is set to **Standard**.

❖ **To show this view**

Click the AIF symbol in the Graph pane.

Properties of Full MS / dd-MS² (TopN)

The properties of a Full MS / dd-MS² experiment include these parameters:

Parameter	Description
General	
Runtime	Use this box to specify the duration in minutes of the active scan event. Click into the field to display the spin boxes for the start time (minimum) and the end time (maximum) of the scan event. To change a value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, you can enter a value in the spin box text field. The valid range for the start time is from 0 to (end time minus 0.01) minutes. The valid range for the end time is from (start time plus 0.01) to 10000 minutes. Or, drag the left and right edges of the corresponding time bar to the intended positions on the time line in the Scan Groups pane.
Polarity	Use this list box to toggle between positive ion and negative ion polarity.
Default charge state	Use this box to specify the default charge state for Data Dependent scans. The mass spectrometer uses the charge state to determine the highest mass-to-charge ratio and HCD energy for the Data Dependent MSⁿ scan. If the mass spectrometer cannot determine the charge state from the preceding scan, it uses the default charge state that you specify here. The valid range for the default charge state is 1 through 100. For typical applications, a charge state of +2 is suitable for tryptic digests in which the peptide has a charge state of +2. If you are running a different experiment, you might want to change the default to a more appropriate value.
Inclusion	Use this field to enable the inclusion masses list that is attached to the active instrument method. Available options are on (inclusion list enabled) and – (inclusion list disabled).
Exclusion	Use this field to enable the exclusion masses list that is attached to the active instrument method. Available options are on (exclusion list enabled) and – (exclusion list disabled).
Desolvation / Fragmentation	
In-source CID	Use the spin box to enter the in-source CID collision energy. To change the value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. You can set the CID collision energy to any value from 0.1 to 150 eV (ESI source) or 200 eV (NSI source). Select Off to switch off the collision energy (0 eV).

Parameter	Description
IST Desolvation	Use the spin box to enter the Desolvation voltage of the Ion Source Trapping. To change the value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. You can set the IST Desolvation voltage to any value from –300 to +300 V. Select Off to switch off the IST Desolvation voltage. If IST Desolvation is used, the AGC is turned off and maximum injection time is used.
Full MS / SIM	
Microscans ^a	Use this spin box to select the number of averaged transients for one scan event. To change the value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, you can enter a value in the spin box text field. The minimum number of microscans is 1. The possible maximum number of microscans depends on the active values for Resolution and Maximum IT.
Resolution	Use this list box to select the mass resolution used during the selected scan event. The mass resolution of the Orbitrap analyzer is proportional to $1/\sqrt{m/z}$. The scan time increases with increasing resolution and detect time. Available options are 1563, 3125, 6250, 12500, 25000, 50000, 100000, or 200000.
AGC target	Use this list box to select the AGC target value for the selected scan event. The AGC target value controls the number of ions that are injected into the Orbitrap analyzer. Available options are 2e4, 5e4, 1e5, 2e5, 5e5, 1e6, 3e6, or 5e6. If IST Desolvation is used, the AGC is turned off and maximum injection time is used.
Maximum IT	Use this list box to type or click a maximum allowed injection time (in milliseconds) to reach the AGC target value. You can enter either a number between 1 and 1000 or auto. If you enter auto, the mass spectrometer chooses a value that depends on the highest resolution of the active and the previous scan event.
Scan range	Use the spin boxes in this field to set values (in mass-to-charge ratio units) for Minimum, Maximum, Center, and Width for the scan range. To change the value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. • Minimum Select the minimum value for the scan range. You can enter any m/z value from 350.0 to 79995.0. • Maximum Select the maximum value for the scan range. You can enter any m/z value from 355.0 to 80000.0. • Center Select the center mass of the scan range. You can enter any m/z value from 352.5 to 79997.5. • Width Select the width of the scan range. You can enter any m/z value from 5.0 to 79997.5.

Parameter	Description
Isolation range	Use the spin boxes in this field to set values (in mass-to-charge ratio units) for Minimum, Maximum, Center, and Width for the quadrupole isolation range. To change the value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Select Off to switch off the isolation range. - Minimum Select the lowest value for the isolation range. You can enter any m/z value from 500.0 to 24995.0. - Maximum Select the highest value for the isolation range. You can enter any m/z value from 505 to 25000.0. - Center Select the center mass of the isolation range. You can enter any m/z value from 502.5 to 24997.5. - Width Select the width of the isolation range. You can enter any m/z value from 5.0 to 24500.0.
dd-MS² / dd-SIM	
Microscans ^a	Use this spin box to select the number of averaged transients for one scan event. To change the value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, you can enter a value in the spin box text field. The minimum number of microscans is 1. The possible maximum number of microscans depends on the active values for Resolution and Maximum IT.
Resolution	Use this list box to select the mass resolution used during the selected scan event. The mass resolution of the Orbitrap analyzer is proportional to $1/\sqrt{m/z}$. The scan time increases with increasing resolution and detect time. Available options are 1563, 3125, 6250, 12500, 25000, 50000, 100000, or 200000.
AGC target	Use this list box to select the AGC target value for the selected scan event. The AGC target value controls the number of ions that are injected into the Orbitrap analyzer. Available options are 2e4, 5e4, 1e5, 2e5, 5e5, 1e6, 3e6, or 5e6. If IST Desolvation is used, the AGC is turned off and maximum injection time is used.
Maximum IT	Use this list box to type or click a maximum allowed injection time (in milliseconds) to reach the AGC target value. You can enter either a number between 1 and 1000 or auto. If you enter auto, the mass spectrometer chooses a value that depends on the highest resolution of the active and the previous scan event.
Loop count	Use this spin box to enter the number of repetitions of the corresponding scan event before continuing with the next scan event or experiment cycle. To change the value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, you can enter a value in the spin box text field. The valid range is from 1 (no repetition) to 5 repetitions.

Parameter	Description
Isolation window	Use this list box to enter the isolation width (in mass-to-charge ratio units) for the precursor ion of interest. The mass range for the peak is centered at the precursor mass and ranges one-half of the isolation width to either side of the precursor mass. You can set the isolation window to any m/z value from 5.0 to 50. Too low a value results in loss of sensitivity because not all of the ions in a mass peak or in neighboring isotopic peaks are isolated. Too high a value causes interference from neighboring peaks.
Isolation offset ^a	Use this spin box to define an absolute offset by which the isolation window is shifted. The resulting window is non-symmetric with regard to the precursor m/z. Thus, more isotopes of a cluster might be covered, without the need of expanding the isolation window. Example: Precursor = m/z 524.265; Isolation window = 5.0 m/z; Isolation offset = +0.5 m/z; Resulting isolation window = m/z 519.765–529.765 To change the isolation offset, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. You can set the isolation offset to any m/z value from -200 to +200. Default is m/z 0.
Fixed first mass	Use this box to specify the first mass of the Data Dependent scan. You can set Fixed first mass either to any m/z value between 350 and 1000. To change the value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value.
HCD (N)CE	Use this box to specify either the absolute collision energy (CE) in eV or the normalized collision energy (NCE). The latter is a dimensionless number that is approximately equivalent to the HCD collision energy (in eV) for a reference ion of mass 500 and charge 1. The actual HCD energy is calculated on basis of mass and charge of either the selected precursor ion (Data Dependent MS2 or AIF scans) or the center mass of an isolation window (targeted MS2 or AIF scans). Specify whether absolute collision energy (CE) or normalized collision energy (NCE) is used. In the box, the software adds the prefix “ce:” or “nce:” to collision energy values (for example, ce:35) to indicate the selected energy type. To change a value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. You can enter any number from 1 to 300. Enter – to switch off the collision energy for Data Dependent SIM scans.
dd Settings	
Use the parameters in this group to specify criteria for selecting one or more ions of interest on which to perform subsequent scans.	
Underfill ratio	Use this box to specify a minimum percentage of the AGC target value. If the mass peak of interest reaches this intensity within the maximum IT, the mass spectrometer initiates a Data Dependent scan. The valid range is from 0 to 100%. Example: AGC Target = $1e5$, maximum IT = 250 ms, underfill ratio = 1%: trigger threshold is 1000 charges in 250 ms.

Parameter	Description
Minimum AGC target	Use this box to specify a minimum value for the AGC target. If the mass peak of interest reaches this intensity within the Maximum IT, the mass spectrometer initiates a Data Dependent scan. Enter the value either as integer or in scientific notation with two decimal places (for example, 3.80e4) in the spin box text field. The valid range is from 0 to the value for the AGC target of the Data Dependent scan event.
Intensity threshold	This field displays the minimum intensity that a mass peak requires to initiate a Data Dependent scan.
Apex trigger	To obtain the highest quality data in the shortest period of time, it is best to defer data acquisition until near the apex of a chromatographic peak. Using the chromatographic peak apex detection provides numerous benefits for Data Dependent LC/MS/MS, including: • Improved MS/MS quality and signal levels • Shorter ion injection times • Reduced MS/MS acquisition of chemical background • Less dependence on static or dynamic exclusion lists • Reduced retriggering of scans on tailing chromatographic peaks Use this box to enter start (Minimum) and end (Maximum) of a retention time window in seconds relative to the occurrence of a precursor. If the mass spectrometer finds an apex within the window, it triggers a Data Dependent acquisition for the corresponding m/z or range of m/z. The mass spectrometer also triggers a Data Dependent scan when the end of the time window is reached without detecting an apex. The apex trigger always depends on other selection criteria (for example, intensity threshold). • Minimum Enter the minimum value for the time window (in seconds). You can enter any value from – (0) to 360. The default value is –. • Maximum Enter the maximum value for the time window (in seconds). You can enter any value from – (0) to 360 as long as it equals or exceeds the Minimum value. The default value is –.
Charge exclusion	Use the check boxes in this field to reject individual charge states or undetermined charge states as precursors for Data Dependent MS/MS scans. These options are available: • – (charge exclusion disabled), • unassigned (charge state not determined) • 1–8 (at least one charge state is selected), • >8

Parameter	Description
Multiple charge states	Use this field to decrease the number of redundant MS2 spectra by limiting them to the most abundant charge state within a charge state distribution. All other criteria for dd-MS2 properties must be met. These options are available: • all (All charge states of a charge envelope are triggered.) • one charge state only (Only the most intense charge state of a charge envelope is triggered.)
Peptide match	Use this field to enable the mass spectrometer to select small molecules with peptide-like isotopic distributions for Data Dependent scanning. The mass spectrometer recognizes the monoisotopic mass of an isotopic distribution by comparing isotopic intensity ratios to typical peptide-like distributions. These options are available: • on (peptide match enabled) • – (peptide match disabled) • preferred (peaks that are determined to belong to peptides are preferred and will be selected prior to those that are not, but still meeting all of the other Data Dependent filter criteria, for example, charge state and intensity) Default setting is preferred.
Exclude isotopes	Use this field to check whether the most intensive isotope of a cluster has been triggered in a Data Dependent scan event. All isotopes of that cluster will be then excluded. Available options are on (isotopes exclusion enabled) and – (isotopes exclusion disabled). Default setting is on. Isotopes exclusion is disabled for inclusion list entries.

Parameter	Description
Dynamic exclusion	Use this box to enter a time (in seconds) to prevent an ion from triggering a subsequent Data Dependent scan after it has already triggered a Data Dependent scan. These input options are available: – (no dynamic exclusion) 0.1 to 50000 - auto [Dynamic exclusion = $2.5 \times \text{Chrom. peak width (FWHM)}$] Dynamic exclusion is valuable if the mass spectrometer has obtained enough data on an ion or if the base peak corresponds to a contaminant or an ion of non interest. If you enable dynamic exclusion, and if the mass spectrometer performs a Data Dependent scan on an ion, that ion is placed on the exclusion list (a temporary reject mass list) for a user-specified period of time. Then, when the mass spectrometer performs another Data Dependent scan on another ion, that ion is also placed on the exclusion list, and so on.
if idle	Use this field to select the behavior of the mass spectrometer when it has finished the Data Dependent scans that were triggered by a mass that meets the established criteria for Data Dependent actions. Available options are do not pick others and pick others. Default setting is do not pick others. This parameter is available only when the parameter Inclusion is set to on.

^aThis parameter is not available when User Role is set to **Standard**.

❖ To show this view

Click the Full MS / dd-MS² symbol in the Graph pane.

Summary Page

The Summary page displays the parameters for mass spectrometer setup, syringe pump, divert valves, and contact closure that you specified on the Experiment Setup page.

❖ To zoom in or out on the Summary page

- Position the mouse pointer within the pane, press the <Ctrl> key, and roll the mouse wheel forward to zoom in.
- Position the mouse pointer within the pane, press the <Ctrl> key, and roll the wheel backward to zoom out.

The content of this page will be printed together with the information for other instruments.

❖ To display this page

In the Instrument Setup window, click the Summary tab.

Dialog Boxes of the Experiment Setup Page

This section provides a reference to the dialog boxes in the Experiment Setup page:

- Use the dialog boxes for global lists to define properties of masses that are used for setting up the experiments in the Experiment Setup page:
 - [Lock Masses Dialog Box](#)
 - [Inclusion List Dialog Box](#)
 - [Exclusion List Dialog Box](#)
- [Mass Calculator](#)

When you import data from csv files or txt files, pay attention to these guidelines:

- Thermo Fisher Scientific recommends pasting the data from comma- or tab-separated files into a table instead of using the Import command. This way, the character encoding is usually transported and special letters like μ or € or 3 appear as intended.
- Empty lines are ignored when pasting.
- The order and content of columns must match the table if no column headers are present. With column headers present, the order is taken from the headers.
- Missing columns enforce usage of the default value.
- If a formula is present, the Method Editor always recalculates the m/z value of a compound. This prevents computational errors or missing significant fractional digits from being carried over.

Lock Masses Dialog Box

Use the Lock Masses dialog box to select a lock mass list for the active instrument method and to edit it. Lock masses are peaks in the spectrum that the mass spectrometer uses for internal mass calibration. Using lock masses improves the mass accuracy of the mass analyzer. If you do not specify any lock masses, the mass spectrometer uses the external mass calibration.

The dialog box allows defining a time window of activity for each lock mass (=timed lock masses). If Start or End is left blank, the lock mass is active from the beginning or until the end of the method, respectively. In the latter case, the End field displays “end.” The usage of lock masses during the active instrument method is specified on the Properties pane of the method.

The table shows the properties of the masses contained in the active lock mass list (*.lock-masses). To change the sort order, click the respective table column header. To invert the sort order, click again.



Figure 3-19. Method Editor—Lock Masses dialog box

The Lock Masses dialog box has these parameters:

Parameter	Description
Mass [m/z]	Enter the mass-to-charge-ratio of the lock mass into the field (with a maximum of five decimals). To change this value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, enter a value in the spin box text field.
Polarity	Use this list box to toggle between positive ion and negative ion polarity. During a scan, the mass spectrometer uses only the lock masses with a polarity that matches the active ion mode.
Start [min]	Enter the start time in minutes. Or, you can enter a time in seconds (by appending the letter <i>s</i>) or in hours (by appending the letter <i>h</i>). The software automatically converts your input into minutes.
End [min]	Enter the end time in minutes. Or, you can enter a time in seconds (by appending the letter <i>s</i>) or in hours (by appending the letter <i>h</i>). The software automatically converts your input into minutes.
Comment	Enter a comment for the lock mass into the field (for example, the compound name). This field is optional.

❖ **To display this dialog box**

1. In the Method Editor, expand the Global Lists pane.
2. Click the  **Lock Masses** button.

Title Bar

The title bar of a global list displays the name of the dialog box. A “modified” indicates a file with unsaved changes.

File Menu

The File menu provides commands for file operations. It has these commands:

Command	Description
Import <Ctrl> + <I>	Opens a dialog box where you can select an existing mass collection. In addition to the program-specific data files, you can select *.csv or *.txt files that meet the requirements of the program. All available masses are replaced by the masses contained in the imported file. Click Open to import the file.
Export <Ctrl> + <S>	Opens a dialog box that you can use to save the active mass collection. In addition to using the program-specific data files, you can save the mass collection as tabulator-separated file (*.txt, for example) or comma-separated file (*.csv, for example). Enter a new file name, select the file type, and select the location (disk and directory) where you want to save it. Or, you can select an existing file. Click Save to save the file.
Export selected <Ctrl> + <Shift> + <S>	Opens a dialog box that you can use to save the selected masses. In addition to using the program-specific data files, you can save the mass collection as tabulator-separated file (*.txt, for example) or comma-separated file (*.csv, for example). Enter a new file name, select the file type, and select the location (disk and directory) where you want to save it. Or, you can select an existing file. Click Save to save the file. This command is available only when at least one line in the dialog box is selected.
Minimize <Ctrl> + <F4>	Closes the dialog box. Your edits will be retained. Or, click the Done button at the right side of the menu bar.

Edit Menu

The Edit menu provides commands for editing the active file. It has these commands:

Command	Description
Undo until last save <Ctrl> + <Z>	Discards all changes to the active file that have not been saved.
Copy <Ctrl> + <C>	Copies the data of the selected mass to the clipboard.
Replace by clipboard <Ctrl> + <V>	Replaces the available masses by the content of the clipboard. The clipboard stores lock mass data as tabulator-separated text files. When the data in the clipboard are not in this format, the command is not available.

Help Menu

Displays the Help for this dialog box.

Inclusion List Dialog Box

Use the Inclusion List dialog box to edit a list of specific masses (inclusion masses) that can activate a Data Dependent action. The dialog box allows defining a time window of activity for each inclusion mass. If Start or End is left blank, the inclusion mass is active from the beginning or until the end of the method, respectively. In the latter case, the End field displays “end.”

To use an inclusion list in a experiment, set the Inclusion parameter on the Parameter pane to **on**. When a inclusion mass list is used in a Data Dependent experiment (Full MS / dd-MS²), the ions will be selected for the Data Dependent scan event, *only* if they are:

1. appearing in the referring master scan (mostly the full scan) and
2. fulfill all of the other defined selection criteria, such as Intensity Threshold.

The table shows the properties of the masses contained in the active inclusion masses list (*.include-masses). To change the sort order, click the respective table column header. To invert the sort order, click again.

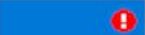
Method editor — Inclusion List									
File Edit Help									Done 
	Mass [m/z]	Formula [M]	Species	CS [z]	Polarity	Start [min]	End [min]	CE	Comment
▶* 1					Positive				

Figure 3-20. Method Editor—Inclusion List dialog box

The Inclusion List dialog box has these parameters:

Parameter	Description
Mass [m/z]	Enter the mass-to-charge-ratio of the inclusion mass into the field (with a maximum of five decimals). If you use the Mass Calculator to edit the Formula field, this field is automatically updated when you exit the editor.
Formula [M]	Use this field to describe the structure of the active compound. In addition to chemical formulas, you can enter amino acid sequences (one letter code) and peptide sequences (if they are structural terminated by H₂O). The different ways of definition are called formula types. You can either enter the formula directly or use the Mass Calculator. To display this editor, click the down arrow in this field. If more than one formula type for your input is possible, the Method Editor chooses the type with the highest priority (chemical formula > peptides > amino acids). Peptide sequences are marked by the prefix "p:" (for example, p: MRFA with $m/z = 524.26496$), amino acids by the prefix "aa:" (for example, aa: MRFA with $m/z = 506.25440$). Enter a prefix directly with the formula to ensure that the right type is applied. Pay attention to these restrictions: • When you enter a valid formula, the Method Editor will set the default values for charge state (1) and Species (+H/-H). Then it will display an automatically calculated value in the Mass [m/z] field. • When you enter a formula that the Method Editor cannot interpret, the Mass [m/z] field will stay empty. When you save the method, the Method Editor will warn you that the method is not in the shape to be executed (due to the missing m/z value). When you reopen the method, the Method Editor will display exactly the formula that was entered. • When you enter a formula, The Method Editor requires a value for the charge state to calculate an m/z value. You can, however, save the method without specifying a charge state for the entry. When you save the method, the Method Editor will warn you that the method is not in the shape to be executed (due to the missing charge state). When you reopen the method, the Method Editor will display exactly the formula that was entered. • Entries of compounds with calculated m/z values outside the measurement specifications of the mass spectrometer ($m/z=350-80000$) can be saved in an instrument method. The instrument software, however, will ignore these entries when it executes the method. • When you change the m/z value that was calculated for the given set of formula, species and charge state, the Method Editor will clear the formula and species definition. The charge state will be preserved. • When you change the polarity for a set of calculated m/z, formula, species and charge state, the Method Editor will clear the Mass [m/z] field if the species definition is not valid for this polarity. You then need to change the species definition.

Parameter	Description
Species	Use this text field to define adducts or modifications of the active compound that are expected to be formed. The default value is +H for positive polarity and –H for negative polarity. The Method Editor will then recalculate the value in the Mass [m/z] field, if possible. The Species field can be used in two ways: - Click the down arrow to display a list of predefined adducts for each polarity: +H, +Na, +K, +NH₄ for positive polarity –H, +Cl, +OH, +HCOO for negative polarity - an empty entry to express adducts (for example, radical cations) for both polarities. The corresponding set will be displayed depending on the selected polarity. Selecting an adduct (A) will result in the strict behavior of applying one unit A to the compound and using “+H” or “–H” adduct depending on the charge state and active polarity. “+K” = $[M + K^+ + (z-1)H^+]^{z+}$; for example, MRFA, +K, CS=2, positive pol. = $[M + K^+ + H^+]^{2+}$ - Enter the modifications of the compound by using squared brackets and at least M as representation of the basic compound (for example, [M + Na + K] or [2M + Na]). The predefined adducts can be entered, too. This definition is used without additional auto dependencies, like adding protons. If you use the Mass Calculator to edit the Formula field, the Species field is automatically filled when you exit the editor.
CS [z]	Use this spin box to enter the charge state of the ion to be fragmented. The valid range is 1–100. The required collision energy for fragmenting an ion depends on its charge state. The higher the charge state, the lower the required collision energy. If this field is left blank, any charge state will be accepted, even unassigned. If you use the Mass Calculator to edit the Formula field, this field is automatically updated when you exit the editor.
Polarity	Use this list box to toggle between positive ion and negative ion polarity. During a scan, the mass spectrometer uses only the inclusion masses with a polarity that matches the active ion mode. If you use the Mass Calculator to edit the Formula field, this field is automatically updated when you exit the editor.
Start [min]	Enter the start of the time window (in minutes) that corresponds to the mass in this row. Or, you can enter a time in seconds (by appending the letter <i>s</i>) or in hours (by appending the letter <i>h</i>). The instrument automatically converts your input into minutes.
End [min]	Enter the end of the time window in minutes. Or, you can enter a time in seconds (by appending the letter <i>s</i>) or in hours (by appending the letter <i>h</i>). The instrument automatically converts your input into minutes.

Parameter	Description
CE	Use the spin box to enter a potential gradient in the HCD cell used to fragment ions. The default collision energy is 35 eV. In the list box, specify whether absolute collision energy CE [eV] is used or normalized collision energy NCE is used. The valid range is 1 to 300 eV for CE or 1 to 300 for NCE. In the list, the software adds the prefix “ce:” to collision energy values (for example, ce:35). A high collision energy value results in more energy deposition (which generally leads to more fragmentation). A low collision energy value results in less energy deposition (which generally leads to less fragmentation).
Comment	Enter a comment for the inclusion mass into the field (for example, the compound name). This field is optional.

❖ **To display this dialog box**

1. In the Method Editor, expand the Global Lists pane.
2. Click the  **Inclusion** button.

Title Bar

The title bar of a global list displays the name of the dialog box. A “modified” indicates a file with unsaved changes.

File Menu

The File menu provides commands for file operations. It has these commands:

Command	Description
Import <Ctrl> + <I>	Opens a dialog box where you can select an existing mass collection. In addition to the program-specific data files, you can select *.csv or *.txt files that meet the requirements of the program. All available masses are replaced by the masses contained in the imported file. Click Open to import the file. When you want to import *.csv or *.txt files with entries that contain formulas, an extra third column "Formula type," which contains the prefix, must specify the formula type. Valid values for the fields that can be (re)interpreted are: - for Peptide type: "Peptide", "p", and "p:" (all case insensitive), - for Amino acid type: "Amino acid", "aa", "aa:" (all case insensitive), - for Chemical formula type: "Chemical formula", "c", "c:" (all case insensitive), and "" (empty).
Export <Ctrl> + <S>	Opens a dialog box that you can use to save the active mass collection. In addition to using the program-specific data files, you can save the mass collection as tabulator-separated file (*.txt, for example) or comma-separated file (*.csv, for example). Enter a new file name, select the file type, and select the location (disk and directory) where you want to save it. Or, you can select an existing file. Click Save to save the file. When you export *.csv or *.txt files with entries that contain formulas, an extra third column "Formula type" specifies the formula type. Values for the fields that are: - for Peptide type: "Peptide", - for Amino acid type: "Amino acid", - for Chemical formula type: "" (empty).
Export selected <Ctrl> + <Shift> + <S>	Opens a dialog box that you can use to save the selected masses. In addition to using the program-specific data files, you can save the mass collection as tabulator-separated file (*.txt, for example) or comma-separated file (*.csv, for example). Enter a new file name, select the file type, and select the location (disk and directory) where you want to save it. Or, you can select an existing file. Click Save to save the file. This command is available only when at least one line in the dialog box is selected.
Minimize <Ctrl> + <F4>	Closes the dialog box. Your edits will be retained. Or, click the Done button at the right side of the menu bar.

Edit Menu

The Edit menu provides commands for editing the active file. It has these commands:

Command	Description
Undo until last save <Ctrl> + <Z>	Discards all changes to the active file that have not been saved.
Copy <Ctrl> + <C>	Copies the data of the selected mass to the clipboard.
Replace by clipboard <Ctrl> + <V>	Replaces the available masses by the content of the clipboard. The clipboard stores lock mass data as tabulator-separated text files. When the data in the clipboard are not in this format, the command is not available.

Help Menu

Displays the Help for this dialog box.

Exclusion List Dialog Box

Use the Exclusion List dialog box to edit a list of specific masses (exclusion masses) that will not trigger a subsequent Data Dependent scan even if they are present. The dialog box allows defining a time window of activity for each exclusion mass. If Start or End is left blank, the exclusion mass is active from the beginning or until the end of the method, respectively. In the latter case, the End field displays “end.”

To use an exclusion list in a experiment, set the Exclusion parameter on the Parameter pane to **on**.

The table shows the properties of the masses contained in the active exclusion masses list (*.exclude-masses). To change the sort order, click the respective table column header. To invert the sort order, click again.

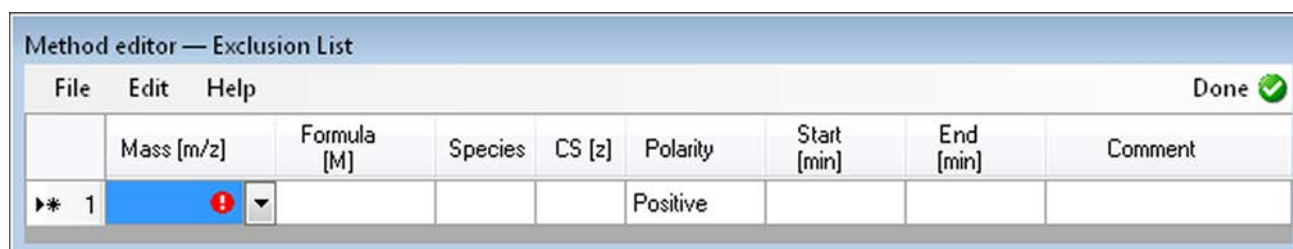


Figure 3-21. Method Editor—Exclusion List dialog box

The Exclusion List dialog box has these parameters:

Parameter	Description
Mass [m/z]	Enter the mass-to-charge-ratio of the exclusion mass into the field (with a maximum of five decimals). If you use the Mass Calculator to edit the Formula field, this field is automatically updated when you exit the editor.
Formula [M]	Use this field to describe the structure of the active compound. In addition to chemical formulas, you can enter amino acid sequences (one letter code) and peptide sequences (if they are structural terminated by H₂O). The different ways of definition are called formula types. You can either enter the formula directly or use the Mass Calculator. To display this editor, click the down arrow in this field. If more than one formula type for your input is possible, the Method Editor chooses the type with the highest priority (chemical formula > peptides > amino acids). Peptide sequences are marked by the prefix “p:” (for example, p: MRFA with $m/z = 524.26496$), amino acids by the prefix “aa:” (for example, aa: MRFA with $m/z = 506.25440$). Enter a prefix directly with the formula to ensure that the right type is applied. Pay attention to these restrictions: • When you enter a valid formula, the Method Editor will set the default values for charge state (1) and Species (+H/–H). Then it will display an automatically calculated value in the Mass [m/z] field. • When you enter a formula that the Method Editor cannot interpret, the Mass [m/z] field will stay empty. When you save the method, the Method Editor will warn you that the method is not in the shape to be executed (due to the missing m/z value). When you reopen the method, the Method Editor will display exactly the formula that was entered. • When you enter a formula, The Method Editor requires a value for the charge state to calculate an m/z value. You can, however, save the method without specifying a charge state for the entry. When you save the method, the Method Editor will warn you that the method is not in the shape to be executed (due to the missing charge state). When you reopen the method, the Method Editor will display exactly the formula that was entered. • Entries of compounds with calculated m/z values outside the measurement specifications of the mass spectrometer ($m/z=350-80000$) can be saved in an instrument method. The instrument software, however, will ignore these entries when it executes the method. • When you change the m/z value that was calculated for the given set of formula, species and charge state, the Method Editor will clear the formula and species definition. The charge state will be preserved. • When you change the polarity for a set of calculated m/z, formula, species and charge state, the Method Editor will clear the Mass [m/z] field if the species definition is not valid for this polarity. You then need to change the species definition.

Parameter	Description
Species	Use this field to define adducts or modifications of the active compound that are expected to be formed. The default value is +H for positive polarity and –H for negative polarity. The Method Editor will then recalculate the value in the Mass [m/z] field, if possible. The Species field can be used in two ways: - Click the down arrow to display a list of predefined adducts for each polarity: +H, +Na, +K, +NH₄ for positive polarity –H, +Cl, +OH, +HCOO for negative polarity - an empty entry to express adducts (for example, radical cations) for both polarities. The corresponding set will be displayed depending on the selected polarity. Selecting an adduct (A) will result in the strict behavior of applying one unit A to the compound and using “+H” or “–H” adduct depending on charge state and active polarity. “+K” = $[M + K^+ + (z-1)H^+]^{z+}$; for example, MRFA, +K, CS=2, positive pol. = $[M + K^+ + H^+]^{2+}$ - Enter the modifications of the compound by using squared brackets and at least M as representation of the basic compound (for example, [M + Na + K] or [2M + Na]). The predefined adducts can be entered, too. This definition is used without additional auto dependencies, like adding protons. If you select or define a species and the Formula field is empty, the species definition will stay grayed out. If you use the Mass Calculator to edit the Formula field, this field is automatically updated when you exit the editor.
CS [z]	Use the spin box to enter the charge state of the ion to be excluded. The valid range is 1–100. The required collision energy for fragmenting an ion depends on its charge state. The higher the charge state, the lower the required collision energy. If you use the Mass Calculator to edit the Formula field, this field is automatically updated when you exit the editor.
Polarity	Use this list box to toggle between positive ion and negative ion polarity. During a scan, the mass spectrometer uses only the exclusion masses with a polarity that matches the active ion mode. If you use the Mass Calculator to edit the Formula field, this field is automatically updated when you exit the editor.
Start [min]	Enter the start of the time window (in minutes) that corresponds to the mass in this row. Or, you can enter a time in seconds (by appending the letter <i>s</i>) or in hours (by appending the letter <i>h</i>). The software automatically converts your input into minutes.

Parameter	Description
End [min]	Enter the end of the time window in minutes. Or, you can enter a time in seconds (by appending the letter <i>s</i>) or in hours (by appending the letter <i>h</i>). The software automatically converts your input into minutes.
Comment	Enter a comment for the exclusion mass into the field (for example, the compound name). This field is optional.

❖ **To display this dialog box**

1. In the Method Editor, expand the Global Lists pane.
2. Click the  **Exclusion** button.

Title Bar

The title bar of a global list displays the name of the dialog box. A “modified” indicates a file with unsaved changes.

File Menu

The File menu provides commands for file operations. It has these commands:

Command	Description
Import <Ctrl> + <I>	Opens a dialog box where you can select an existing mass collection. In addition to the program-specific data files, you can select *.csv or *.txt files that meet the requirements of the program. All available masses are replaced by the masses contained in the imported file. Click Open to import the file. When you want to import *.csv or *.txt files with entries that contain formulas, an extra third column “Formula type,” which contains the prefix, must specify the formula type. Valid values for the fields that can be (re)interpreted are: • for Peptide type: “Peptide”, “p”, and “p:” (all case insensitive), • for Amino acid type: “Amino acid”, “aa”, “aa:” (all case insensitive), • for Chemical formula type: “Chemical formula”, “c”, “c:” (all case insensitive), and “” (empty).
Export <Ctrl> + <S>	Opens a dialog box that you can use to save the active mass collection. In addition to using the program-specific data files, you can save the mass collection as tabulator-separated file (*.txt, for example) or comma-separated file (*.csv, for example). Enter a new file name, select the file type, and select the location (disk and directory) where you want to save it. Or, you can select an existing file. Click Save to save the file. When you export *.csv or *.txt files with entries that contain formulas, an extra third column “Formula type” specifies the formula type. Values for the fields that are: • for Peptide type: “Peptide”, • for Amino acid type: “Amino acid”, • for Chemical formula type: “” (empty).

Command	Description
Export selected <Ctrl> + <Shift> + <S>	Opens a dialog box that you can use to save the selected masses. In addition to using the program-specific data files, you can save the mass collection as tabulator-separated file (*.txt, for example) or comma-separated file (*.csv, for example). Enter a new file name, select the file type, and select the location (disk and directory) where you want to save it. Or, you can select an existing file. Click Save to save the file. This command is available only when at least one line in the dialog box is selected.
Minimize <Ctrl> + <F4>	Closes the dialog box. Your edits will be retained. Or, click the Done button at the right side of the menu bar.

Edit Menu

The Edit menu provides commands for editing the active file. It has these commands:

Command	Description
Undo until last save <Ctrl> + <Z>	Discards all changes to the active file that have not been saved.
Copy <Ctrl> + <C>	Copies the data of the selected mass to the clipboard.
Replace by clipboard <Ctrl> + <V>	Replaces the available masses by the content of the clipboard. The clipboard stores lock mass data as tabulator-separated text files. When the data in the clipboard are not in this format, the command is not available.

Help Menu

Displays the Help for this dialog box.

Mass Calculator

Use the Mass Calculator to specify the properties of compounds that are used in the Inclusion List dialog box and the Exclusion List dialog box.

Figure 3-22. Mass Calculator (Method Editor)

When you display the Mass Calculator, its fields are filled with the values of the active list fields, if available. Otherwise, its fields are filled with the default values. The Method Editor applies the set and calculated values of the Mass Calculator to the active list fields, when you exit the editor by doing one of the following:

- Press **Enter** at any position.
- Click at any position outside of the editor.
- Click the down arrow in the Formula field again.

The Mass Calculator has these parameters:

Parameter	Description
Compound	
Formula	Use the text field to specify the basic composition of the compound. Click the down arrow to display a list of the last entered compounds. The syntax rules and interpretation accept the kind of formula that is also accepted on the Spectrum Simulation page (Isotope Simulation area) of the Qual Browser.

Parameter	Description
Type	Use the Type list to specify the formula type used in the Formula field: • Chemical formula Formula is defined as the resulting elemental composition of the entered formula. This is the default selection. • Peptide Formula is defined as the sum of all of the entered amino acids additionally terminated with H at the N-terminus and OH at the C-terminus. • Amino Acid Formula is defined as the sum of all of the entered amino acids. Independent of the entry in the Species field, the elemental composition and the mass of the compound, Formula is completely determined by the given formula and selected formula type. Determined or defined formulas types are marked by the addition of a text prefix. For peptides it is “p:” (for example, “p: MRFA”). For amino acids it is “aa:” (for example, “aa: MRFA”). No prefix is displayed for chemical formulas.
Species	Use this text field to define adducts or modifications of the active compound that are expected to be formed. The default value is +H for positive polarity and –H for negative polarity. The Species field can be used in two ways: • Click the down arrow to display a list of predefined adducts for each polarity: - +H, +Na, +K, +NH₄ for positive polarity - -H, +Cl, +OH, +HCOO for negative polarity - an empty entry to express adducts (for example, radical cations) for both polarities. The corresponding set will be displayed depending on the selected polarity. Selecting an adduct (A) will result in the strict behavior of applying one unit A to the compound and using “+H” or “-H” adduct depending on the charge state and active polarity. “+K” = $[M + K^+ + (z-1)H^+]^{z+}$; for example, MRFA, +K, CS=2, positive pol. = $[M + K^+ + H^+]^{2+}$ • Enter the modifications of the compound by using squared brackets and at least M as representation of the basic compound (for example, [M + Na + K] or [2M + Na]). The predefined adducts can be entered, too. This definition is used without additional auto dependencies, like adding protons.
Charge state	Use the list box to select the resulting charge state. Available options are 1+ to 100+ for positive polarity and 1– to 100– for negative polarity. The default charge state is 1+ for positive polarity and 1– for negative polarity.
Polarity	Use the option buttons to select the applied polarity. The default polarity is positive.

Parameter	Description
m/z	This text field displays the calculated mass-to-charge ratio, with five decimal places (for example, 524.26496).
Composition	This text field displays the determined total formula (for example, C23 H38 N7 O5 S).

❖ **To display the Mass Calculator**

Click the down arrow in a Formula cell of the Inclusion List dialog box or the Exclusion List dialog box.

Instrument Setup

Dialog Boxes of the Experiment Setup Page

Explore Q Exactive UHMR Tune

This chapter provides information about Q Exactive UHMR Tune, its views, functions, and features.

Contents

- [Q Exactive UHMR Tune Overview](#)
- [Q Exactive UHMR Tune Menus](#)
- [Toolbar](#)
- [Tasks Panel](#)
- [Display Panel](#)
- [Dialog Boxes](#)

Q Exactive UHMR Tune Overview

The Q Exactive UHMR Tune program is used to operate the Q Exactive UHMR mass spectrometer. Figure 4-1 shows Q Exactive UHMR Tune. To access information about Q Exactive UHMR Tune, use the title bar, toolbar, menu commands, display views, and Help.

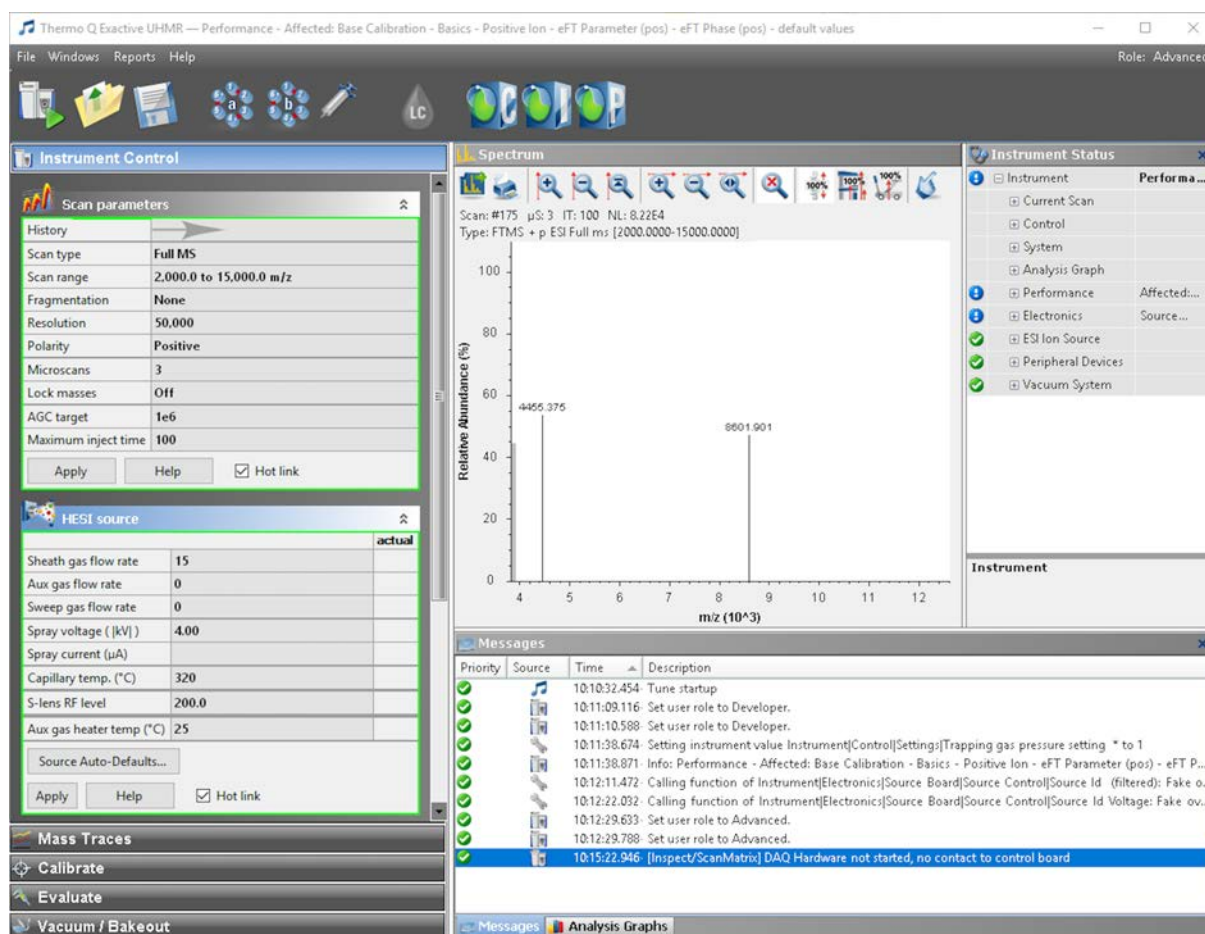


Figure 4-1. Q Exactive UHMR Tune

❖ To display this window

- Choose **Start > Programs > Thermo Exactive Series > Tune**, or
- Click  on the desktop.

When you are running Q Exactive UHMR Tune, a Q Exactive UHMR Tune icon () is displayed in the Microsoft™ Windows™ system tray. Double-click the  icon to display the Q Exactive UHMR Tune window when it is minimized. Right-click the  icon to display a shortcut menu that provides commands for restoring or terminating Q Exactive UHMR Tune.

Title Bar

The Q Exactive UHMR Tune title bar displays the name of the program, the name of the active Tune Method, and the instrument status. An asterisk indicates a Tune Method with unsaved changes.

Menus

The Q Exactive UHMR Tune menu bar displays the available menus. The Q Exactive UHMR Tune menus are as follows:

- [File Menu](#)
- [Windows Menu](#)
- [Reports Menu](#)
- [Help Menu](#)

On the far right side of the menu bar, the active user role is displayed.

Toolbar

The [Toolbar](#) provides symbol shortcuts for frequently used commands. It is located below the title bar of the Q Exactive UHMR Tune window.

Tasks Panel

The tasks panel on the left side of the Q Exactive UHMR Tune window comprises five windows:

- The [Instrument Control Window](#) on the left side of the Q Exactive UHMR Tune window comprises three windows:
 - [Scan Parameters Window](#) for defining a scan depending on the scan mode and scan type combination.
 - API Source window for displaying and editing parameters of the API source. The window adapts name and parameters of the detected source. At present, Q Exactive UHMR Tune provides these API source windows:
 - [HESI Source Window](#)
 - [NSI Source Window](#)
 - [Acquisition Window](#) for acquiring and storing measurement data.
- [Mass Traces Window](#) for selecting mass traces that are displayed in the Analysis Graphs Window.

- [Calibrate Window](#) for performing an automatic optimization of the calibration parameters.
- [Evaluate Window](#) for performing an automatic check of the instrument precision.
- [Vacuum / Bakeout Window](#) for displaying the pressure values at the vacuum gauges and performing an instrument bakeout.

Display Panel

The display panel on the right side of the Q Exactive UHMR Tune window comprises up to five windows:

- [Spectrum Window](#) for displaying a real-time data plot. The spectrum window is always visible.
- [Instrument Status Window](#) for displaying instrument parameters.
- [Messages Window](#) for displaying status information about the instrument, the control service, or other programs.
- [Analysis Graphs Window](#) for displaying a real-time graph.
- [Debug Messages Window](#) for displaying messages that can be used during software development. The debug messages window is not available for standard users.

In addition to these five windows, the display panel may show additional windows for controlling other installed instruments.

Q Exactive UHMR Tune Menus

The Q Exactive UHMR Tune window has these menus:

- [File Menu](#)
- [Windows Menu](#)
- [Reports Menu](#)
- [Help Menu](#)

User Role

On the far right side of the menu bar, the active user role is displayed. The user role specifies the number of parameters that are available for the active experiment. Standard User is the user role with the lowest number of available parameters.

Click the entry (Advanced, for example) to display a list that displays the available user roles. To change the active user role, click the respective entry. The number of available user roles depends on the installed licenses. See “[License Dialog Box](#)” on [page 4-49](#).

File Menu

The File menu provides commands for file and program operations. It has these commands:

Command	Description
Load Tune File	Displays a dialog box that you can use to find and open a tune file (*.mstune) that already exists.
Save Tune File	Saves the active tune file with the active settings. Tip Do not overwrite the default tune file Default_UHMR.mstune!
Save Tune File as	Opens a dialog box that you can use to enter a new file name and to select the location (disk and directory) where you want to save it. Click Save to save the tune file with the active settings.

Command	Description
Export System Settings	Opens a dialog box that you can use to save the active system settings (*.ini) to be imported on another computer that has no instrument attached and is intended for method editing. This computer has to have installed all needed software including Thermo Platform, Thermo Xcalibur and all instrument drivers like HPLC drivers installed. Imported values will be overwritten if an instrument will be attached later.
Terminate	Closes the active window. If the active tune file contains unsaved changes, a dialog box warns about losing data when you terminate the program.

Windows Menu

The Windows menu provides commands for customizing the information displayed in the Q Exactive UHMR Tune window. The system highlights the icon to the left of a command if the window is active. Deselect the command to hide the window.

The Windows menu has these commands:

Command	Description
View > Show all	Displays all windows of Q Exactive UHMR Tune.
 Tooltips	Displays a short description of an item on the Q Exactive UHMR Tune window when you rest the mouse pointer over it.
 Spectrum	Displays the Spectrum window. The Spectrum Window is always visible.
 Instrument Status	Displays/Hides the Instrument Status window.
 Messages	Displays/Hides the Messages window.
 Analysis Graphs	Displays/Hides the Analysis Graphs window.
 Debug Messages	Displays/Hides the Debug Messages window. The debug messages window is not available for standard users.

Command	Description
 Mass Calculator	Displays the Mass Calculator, which helps you to calculate the mass of an compound of interest.
Installed instruments	Depending on the individual configuration of your system, additional commands may allow displaying windows for controlling other installed instruments.

Q Exactive UHMR Tune may open some windows (the analysis graphs window, for example) without user interaction if new important information is available.

Reports Menu

The Reports menu provides access to various calibration reports. The individual commands are available only when the respective reports have been created. If no reports exist (in a new system, for example), the Reports menu is shown grayed out and has no commands.

The Reports menu has these commands:

Command	Description
Calibration > Latest	Opens the latest complete calibration report in PDF format.
Calibration > List	Displays the list of up to five (5) complete calibration reports. To open a report, double-click any of the items from the list.
Spectral Mass Calibration (neg) > Latest	Opens the latest negative mode calibration report in PDF format.
Spectral Mass Calibration (neg) > List	Displays the list of up to five (5) negative mode calibration reports. To open a report, double-click any of the items from the list.
Spectral Mass Calibration (pos) > Latest	Opens the latest positive mode calibration report in PDF format.
Spectral Mass Calibration (pos) > List	Displays the list of up to five (5) positive mode calibration reports. To open a report, double-click any of the items from the list.
Evaluation > Latest	Opens the latest complete evaluation report in PDF format.

Command	Description
Evaluation > List	Displays the list of up to five (5) complete evaluation reports. To open a report, double-click any of the items from the list.
Spectral Mass Evaluation (neg) > Latest	Opens the latest negative mode evaluation report in PDF format.
Spectral Mass Evaluation (neg) > List	Displays the list of up to five (5) negative mode evaluation reports. To open a report, double-click any of the items from the list.
Spectral Mass Evaluation (pos) > Latest	Opens the latest positive mode evaluation report in PDF format.
Spectral Mass Evaluation (pos) > List	Displays the list of up to five (5) positive mode evaluation reports. To open a report, double-click any of the items from the list.
All Reports	Opens a file manager window with a list of all previously acquired reports.

Help Menu

The Help menu groups commands that provide information about Q Exactive UHMR Tune. It has these commands:

Command	Description
Help Overview	Displays Q Exactive UHMR Tune Help.
Help Content	Displays the table of contents for Q Exactive UHMR Tune Help.
Help Index	Displays the index for Q Exactive UHMR Tune Help.
About	Displays the About dialog box with information about the instrument and the Q Exactive UHMR Tune version.

Toolbar

The toolbar provides symbol shortcuts for frequently used commands. It is located below the title bar of the Q Exactive UHMR Tune window. To activate a toolbar function, click the corresponding toolbar button.

Some symbols provide information about the statuses of respective instrument components either by their color or by displaying a tooltip when you rest the mouse pointer on them.

These functions are available:

Button	Description
	General instrument state On / Standby / Off
	Run by Xcalibur
	Click to toggle between the instrument operating statuses On, Standby, and Off. The button reflects the instrument status: - When the mass spectrometer is On, Q Exactive UHMR Tune displays . - When the mass spectrometer is in Standby, Q Exactive UHMR Tune displays . - When the mass spectrometer is Off, Q Exactive UHMR Tune displays .
	The status of this button controls also the statuses of gas flow and syringe pump use (if present). If the mass spectrometer is controlled by an Xcalibur sequence, Q Exactive UHMR Tune displays . The acquisition can only be stopped from Xcalibur Sequence Setup View.
IMPORTANT When you start an acquisition while the instrument is in Off position, the instrument begins acquiring data after a delay of about 30 seconds.	
	Open Click to display a dialog box that you can use to find and open a *.mstune file that already exists. Or, choose File > Load Tune File.
	Save Click to open a dialog box that you can use to select the location (disk and directory) where you want to save the tune file. Or, choose File > Save Tune File as. This button is not available when the settings of the active tune file are not changed.

Button		Description
 	Divert Valve A Position 1 or Position 2	Click to switch the valve position directly. The button reflects the valve status (connected positions, Valve “a”).
 	Divert Valve B Position 1 or Position 2	Click to switch the valve position directly. The button reflects the valve status (connected positions, Valve “b”).
  	Syringe Pump Settings Syringe Pump On or Syringe Pump Off	Click to switch on/off the syringe pump (if present). A symbol in the lower right corner of the button indicates the status of the syringe pump: - When the syringe pump is On, Q Exactive UHMR Tune displays . - When the syringe pump is Off, Q Exactive UHMR Tune displays . - When the syringe pump is in an unknown status, Q Exactive UHMR Tune displays . Click the down arrow to display the Syringe Pump Settings dialog box. Here, you can specify syringe pump parameters or manually operate the syringe pump.
	Direct Instrument Control	Click to display additional commands that allow displaying windows for controlling other installed instruments.
  	Communication Status	Shows the actual communication status of the system: - Green: communication with instrument is OK. - Yellow: only service is accessible (no instrument). - Red: communication is broken (no instrument, no service).

Button		Description
 	Hardware Status	Shows the actual hardware status of the system (top instrument tree state): - Green: all readbacks are in specifications (green hooks). - Red: one or more readbacks are out of range.
  	Performance Status	Shows the actual performance status of the system: - Green: the last evaluation/calibration was successful. - Yellow: the last evaluation/calibration was successful, but is out of date. - Red: the evaluation/calibration was not successful. By default, the performance status icon turns yellow 25 hours after the last successful mass calibration or check. Advanced users can change this value in the System node of the instrument status window according to their mass accuracy requirements.
	Procedure active	If a procedure is active (for example, system bakeout or tune) Q Exactive UHMR Tune displays an animated icon next to the performance status button.
	Acquisition indicator	If the mass spectrometer is acquiring data, Q Exactive UHMR Tune displays an animated icon next to the performance status button.

Tasks Panel

Use the windows of the tasks panel to perform procedures that maintain the quality of measurements with the Q Exactive UHMR mass spectrometer.

The tasks panel is always visible. The windows in the tasks panel can be minimized or maximized. Click the title bar of an individual window to display it.

- [Instrument Control Window](#)
- [Mass Traces Window](#)
- [Calibrate Window](#)
- [Evaluate Window](#)
- [Vacuum / Bakeout Window](#)

Instrument Control Window

Use the windows of the Instrument Control window to enter individual physical settings and to acquire scans. These windows are available:

- [Scan Parameters Window](#)
- API Source Window (one of the following)
 - [HESI Source Window](#)
 - [NSI Source Window](#)
- [Acquisition Window](#)

The Instrument Control window is always visible. Click the title bar of an individual window to display it. Click again to hide it. To change the order of windows within the Instrument Control window, drag individual windows by their title bars to the new places.

Scan Parameters Window

Use the Scan Parameters window to define a scan depending on the selected scan mode and scan type combination. The mass spectrometer updates the scan parameters only after you click **Apply** or select the Hot link check box.

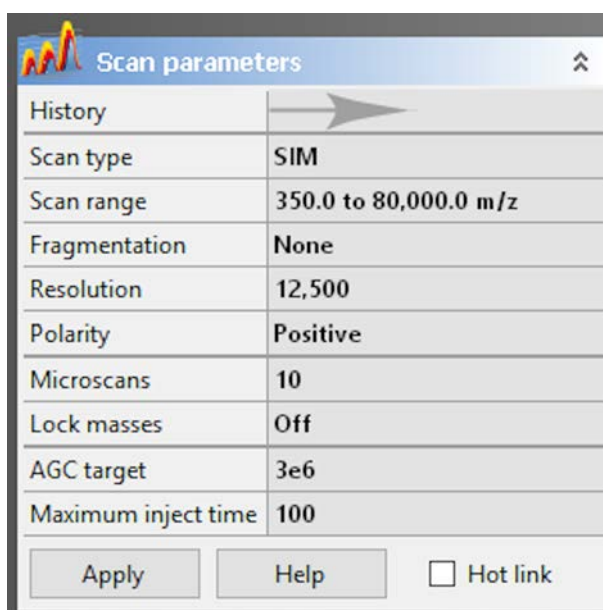


Figure 4-2. Scan Parameters window

The Scan Parameters window has these parameters:

Parameter	Description
History	Click to display the Scan Parameters History dialog box. Here, select from a list of recent scans based on short scan descriptions. The maximum number of list items is 100. After a change of parameters, the history is updated when you click Apply or when you change the status of the Hot link check box.
Isolation Range	Displays the active quadrupole isolation range. To change the settings, click into the field to display the Isolation Range dialog box.
Scan Range	Displays the active scan range. To change the settings, click into the field to display the Scan Range dialog box.
Fragmentation	Displays the settings for HCD fragmentation and in-source CID fragmentation. If no fragmentation type is selected, the text field shows <i>None</i> . To change the settings, click into the field to display the Fragmentation dialog box. Automatic tuning is disabled when in-source CID fragmentation is on.
Resolution	Use this list box to select the mass resolution for FTMS analysis. The mass resolution of the Orbitrap analyzer is proportional to $1/\sqrt{m/z}$. The scan time increases with increasing resolution and detect time. Available options are 1563, 3125, 6250, 12500, 25000, 50000, 100000, or 200000.
Polarity	Use this list box to toggle between positive ion and negative ion polarity.

Parameter	Description
Microscans	Use this spin box to select the number of averaged transients for one scan event. To change the value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, you can enter a value in the spin box text field. The minimum number of microscans is 1. The possible maximum number of microscans depends on the active values for Resolution and Maximum inject time.
Lock masses	Displays the active lock masses. During a scan, the mass spectrometer uses only the lock masses with a polarity that matches the ion mode. If no lock masses are selected, the text field shows <i>Off</i>. To change the settings, click into the field to display the Lock Masses dialog box. Q Exactive UHMR Tune allows using active lock masses in user-defined calibration mass lists.
AGC target	Use this list box to select the AGC target value. The AGC target value controls the number of ions that are injected into the Orbitrap analyzer. Available options are 2e4, 5e4, 1e5, 2e5, 5e5, 1e6, 3e6, and 5e6.
Maximum inject time	Use this list box to type or click a maximum injection time for AGC. For example, type 160 . The valid range is from 1 to 1000 milliseconds.
Buttons	
Apply	Sends all changes to the instrument.
Help	Displays the Help for this window.
Hot Link	Select the Hot link check box to allow Q Exactive UHMR Tune to send any changes immediately to the instrument. A green frame around the parameter box indicates an active hot link.

❖ To display this window

Click the Scan Parameters window title bar in the Instrument Control window.

HESI Source Window

Use the HESI source window to specify heated-electrospray ionization (H-ESI) source parameters. See [API Source Settings for Various LC Flow Rates](#) for recommended settings. The mass spectrometer updates the H-ESI source parameters only after you click **Apply** or with the Hot link check box being selected.

HESI source		actual
Sheath gas flow rate	5	
Aux gas flow rate	0	
Sweep gas flow rate	0	
Spray voltage ([kV])	3.00	
Spray current (μA)		
Capillary temp. (°C)	320	
S-lens RF level	50.0	
Aux gas heater temp (°C)	30	

Source Auto-Defaults...

Apply Help ☒ Hot link

Figure 4-3. HESI source window

This window is available only when the mass spectrometer has detected an installed H-ESI source. The H-ESI source is the standard API source of the Q Exactive UHMR mass spectrometer.

The HESI source window has these parameters:

Parameter	Description
Sheath Gas Flow Rate	Displays the setpoint H-ESI source sheath gas flow rate (in arbitrary units). To change the setpoint flow rate, click the arrows in the Sheath Gas Flow Rate spin box to increase [up arrow] or to decrease [down arrow] the value. You can set the sheath gas flow rate to any value from 0 to 80 units. Or, you can enter a value in the spin box text field. The mass spectrometer changes the flow rate when you click Apply or with the Hot link check box being selected. The Sheath Gas Flow Rate readback is to the right of the spin box. This readback displays the actual flow rate (in arbitrary units).
Aux Gas Flow Rate	Displays the setpoint H-ESI source auxiliary gas flow rate (in arbitrary units). To change the setpoint flow rate, click the arrows in the Aux Gas Flow Rate spin box to increase [up arrow] or to decrease [down arrow] the value. You can set the flow rate to any value from 0 to 40 units. Or, you can enter a value in the spin box text field. The mass spectrometer changes the flow rate when you click Apply or with the Hot link check box being selected. The Aux Gas Flow Rate readback is to the right of the spin box. This readback displays the actual flow rate (in arbitrary units).

Parameter	Description
Sweep Gas Flow Rate	Displays the setpoint H-ESI source sweep gas flow rate. To change the setpoint flow rate, click the arrows in the Sweep Gas Flow Rate spin box to increase [up arrow] or to decrease [down arrow] the value. You can set the flow rate to any value from 0 to 10 units. Or, you can enter a value in the spin box text field. The mass spectrometer changes the flow rate when you click Apply or with the Hot link check box being selected. The Sweep Gas Flow Rate readback is to the right of the spin box. This readback displays the actual flow rate (in arbitrary units).
Spray Voltage	Displays the setpoint H-ESI source spray voltage (absolute value, in kilovolts). To change the setpoint spray voltage, click the arrows in the Spray Voltage spin box to increase [up arrow] or to decrease [down arrow] the value. You can set the spray voltage to any value from 0.0 to 8.0 kV. The sign of the spray voltages changes automatically with the ion polarity mode: positive for positive ions and negative for negative ions. Or, you can enter a value in the spin box text field. The mass spectrometer changes the spray voltage when you click Apply or with the Hot link check box being selected. The Spray Voltage readback is to the right of the spin box. This readback displays the actual spray voltage (absolute value, in kilovolts).
Spray Current	This readback displays the actual H-ESI source spray current (in microamperes). The H-ESI spray current is typically less than 5 μA.
Capillary Temperature	Displays the setpoint H-ESI source heated capillary temperature (in degrees Celsius). To change the setpoint heated capillary temperature, click the arrows in the Capillary Temp spin box to increase [up arrow] or to decrease [down arrow] the value. You can set the heated capillary temperature to any value from 0 to 450 °C. Or, you can enter a value in the spin box text field. The mass spectrometer changes the heated capillary temperature when you click Apply or with the Hot link check box being selected. The Capillary Temperature readback is to the right of the spin box. This readback displays the actual temperature (in degrees Celsius) of the heated capillary.

Parameter	Description
S-Lens RF Level	Displays a numerical factor that the mass spectrometer uses, along with the lowest and highest mass, to calculate the S-lens RF amplitude. The magnitude of the S-lens RF level affects the mass spectrum as follows: - Decreasing the S-lens RF level will decrease the amount of fragmentation of fragile ions in the S-lens. - Decreasing the S-lens RF level will decrease the transmission of high m/z ions through the S-lens and increase the transmission of the low m/z ions. - Increasing the S-lens RF level will increase the amount of fragmentation of fragile ions in the S-lens. - Increasing the S-lens RF level will increase the transmission of high m/z ions through the S-lens and decrease the transmission of the low m/z ions. To change the S-lens RF level, click the arrows in the S-Lens Level spin box to increase [up arrow] or to decrease [down arrow] the value. You can set the S-lens RF level to any value from 0 to 200. Or, you can enter a value in the spin box text field. The mass spectrometer changes the S-lens RF level when you click Apply or with the Hot link check box being selected. For stable ions, the default value, 100, provides a good starting point.
Aux. Gas Heater Temperature	Displays the setpoint temperature (in degrees Celsius) of the H-ESI source heater, which heats the auxiliary gas. To change the setpoint vaporizer temperature, click the arrows in the Heater Temp spin box to increase [up arrow] or to decrease [down arrow] the value. You can set the vaporizer temperature to any value from 0 to 600 °C. Or, you can enter a value in the spin box text field. The mass spectrometer changes the vaporizer temperature when you click Apply or with the Hot link check box being selected. The Heater Temperature readback is to the right of the spin box. This readback displays the actual temperature (in degrees Celsius) of the vaporizer.
Buttons	
Source Auto-Defaults	Displays the Autoselect ion source values dialog box.
Apply	Sends all changes to the instrument.
Help	Displays the Help for this window.
Hot Link	Select the Hot link check box to allow Q Exactive UHMR Tune to send any changes immediately to the instrument. A green frame around the parameter box indicates an active hot link.

❖ **To display this window**

Click the HESI source window title bar in the Instrument Control window.

NSI Source Window

Use the NSI source window to specify nanospray ionization (NSI) source parameters. The mass spectrometer updates the NSI source parameters only after you click **Apply** or with the Hot link check box being selected.

NSI source		actual
Sheath gas flow rate	0	
Aux gas flow rate	0	
Sweep gas flow rate	0	
Spray voltage ([kV])	1.50	
Spray current (μA)		
Capillary temp. (°C)	250	
S-lens RF level	50.0	

Source Auto-Defaults...

Apply Help ☒ Hot link

Figure 4-4. NSI source window

This window is available only when the mass spectrometer has detected an installed NSI source.

The NSI source window has these parameters:

Parameter	Description
Sheath Gas Flow Rate	Displays the setpoint NSI source sheath gas flow rate (in arbitrary units). To change the setpoint flow rate, click the arrows in the Sheath Gas Flow Rate spin box to increase [up arrow] or to decrease [down arrow] the value. You can set the sheath gas flow rate to any value from 0 to 80 units. Or, you can enter a value in the spin box text field. The mass spectrometer changes the flow rate when you click Apply or with the Hot link check box being selected. The Sheath Gas Flow Rate readback is to the right of the spin box. This readback displays the actual flow rate (in arbitrary units).
Aux Gas Flow Rate	Displays the setpoint NSI source auxiliary gas flow rate (in arbitrary units). To change the setpoint flow rate, click the arrows in the Aux Gas Flow Rate spin box to increase [up arrow] or to decrease [down arrow] the value. You can set the flow rate to any value from 0 to 40 units. Or, you can enter a value in the spin box text field. The mass spectrometer changes the flow rate when you click Apply or with the Hot link check box being selected. The Aux Gas Flow Rate readback is to the right of the spin box. This readback displays the actual flow rate (in arbitrary units).

Parameter	Description
Sweep Gas Flow Rate	Displays the setpoint NSI source sweep gas flow rate. To change the setpoint flow rate, click the arrows in the Sweep Gas Flow Rate spin box to increase [up arrow] or to decrease [down arrow] the value. You can set the flow rate to any value from 0 to 10 units. Or, you can enter a value in the spin box text field. The mass spectrometer changes the flow rate when you click Apply or with the Hot link check box being selected. The Sweep Gas Flow Rate readback is to the right of the spin box. This readback displays the actual flow rate (in arbitrary units).
Spray Voltage	Displays the setpoint NSI source spray voltage (absolute value, in kilovolts). To change the setpoint spray voltage, click the arrows in the Spray Voltage spin box to increase [up arrow] or to decrease [down arrow] the value. You can set the spray voltage to any value from 0.0 to 8.0 kV. The sign of the spray voltages changes automatically with the ion polarity mode: positive for positive ions and negative for negative ions. Or, you can enter a value in the spin box text field. The mass spectrometer changes the spray voltage when you click Apply or with the Hot link check box being selected. The Spray Voltage readback is to the right of the spin box. This readback displays the actual spray voltage (absolute value, in kilovolts).
Spray Current	This readback displays the actual NSI source spray current (in microamperes). NSI spray current is typically less than 5 μA.
Capillary Temperature	Displays the setpoint NSI source heated capillary temperature (in degrees Celsius). To change the setpoint heated capillary temperature, click the arrows in the Capillary Temp spin box to increase [up arrow] or to decrease [down arrow] the value. You can set the heated capillary temperature to any value from 0 to 450 °C. Or, you can enter a value in the spin box text field. The mass spectrometer changes the heated capillary temperature when you click Apply or with the Hot link check box being selected. The Capillary Temperature readback is to the right of the spin box. This readback displays the actual temperature (in degrees Celsius) of the heated capillary.

Parameter	Description
S-Lens RF Level	Displays a numerical factor that the mass spectrometer uses, along with the lowest and highest mass, to calculate the S-lens RF amplitude. The magnitude of the S-lens RF level affects the mass spectrum as follows: - Decreasing the S-lens RF level will decrease the amount of fragmentation of fragile ions in the S-lens. - Decreasing the S-lens RF level will decrease the transmission of high m/z ions through the S-lens and increase the transmission of the low m/z ions. - Increasing the S-lens RF level will increase the amount of fragmentation of fragile ions in the S-lens. - Increasing the S-lens RF level will increase the transmission of high m/z ions through the S-lens and decrease the transmission of the low m/z ions. To change the S-lens RF level, click the arrows in the S-Lens Level spin box to increase [up arrow] or to decrease [down arrow] the value. You can set the S-lens RF level to any value from 0 to 200. Or, you can enter a value in the spin box text field. The mass spectrometer changes the S-lens RF level when you click Apply or with the Hot link check box being selected. For stable ions, the default value, 100, provides a good starting point.
Buttons	
Source Auto-Defaults	This parameter is not available for this ion source type.
Apply	Sends all changes to the instrument.
Help	Displays the Help for this window.
Hot Link	Select the Hot link check box to allow Q Exactive UHMR Tune to send any changes immediately to the instrument. A green frame around the parameter box indicates an active hot link.

❖ To display this window

Click the NSI source window title bar in the Instrument Control window.

Acquisition Window

Use the Acquisition window to enter parameters for acquiring and storing scan data as well as to monitor the progress of the active acquisition.

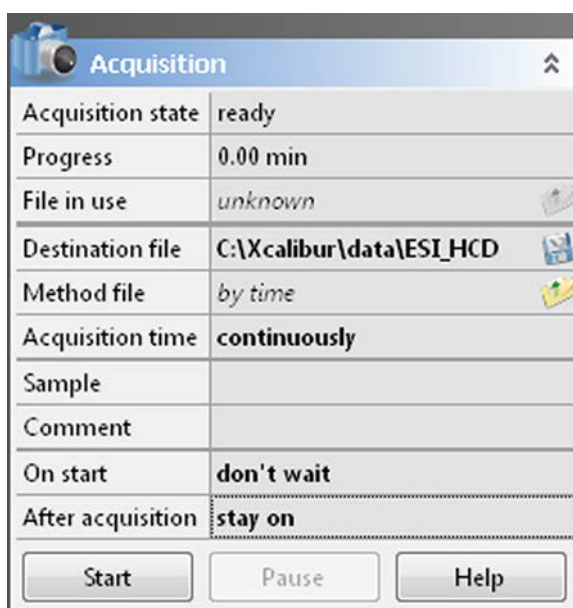


Figure 4-5. Acquisition window

The Acquisition window has these parameters:

Parameter	Description
Acquisition state	Displays the status of the active acquisition.
Progress	Displays the elapsed time of the active acquisition.
File in use	Displays the name of the raw file to be acquired to disk for the active sample. To display the file in Qual Browser, click the  button. This value is up to date even when Q Exactive UHMR Tune is acquiring data under control of Xcalibur.
Destination file	Displays the full path of the folder where your *.raw files will be saved. To change the path, type the full path (Drive:\path) in the text box or click the  button to the right of the text box to browse your directories and select the folder where your *.raw files should be saved. Saving raw files on network drives typically causes problems. Preferably select a local path (for example, C:\Xcalibur\data).
Method file	Displays the name of the instrument method (*.meth) to be used during the active acquisition. The tune file used in that instrument method will be used for your scan but other devices configured in that instrument method will not be included. Type in the name of the instrument method, or click the  button to the right of the text box to browse your computer for an instrument method file (typically saved in C:\Xcalibur\methods). When the active acquisition is controlled by the settings of the parameter Acquisitions time, this parameter is not available. Instead, the text field shows <i>by time</i>.
Sample	Displays the name of the active sample. To change the sample name, type the new name in the text field.

Parameter	Description
Comment	Displays a comment on the active sample, if available. To change the comment, type the new name in the text field.
Acquisition time	Displays the duration of the acquisition time. Use the option buttons to select one of these settings: - Continuously The acquisition, once it is started, will continue until you stop (Stop button) or pause (Pause button) it. - Scans Specify the number of scans for the acquisition. You can set the number of scans to any value from 1 to 1000000. To change this value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, enter a value in the spin box text field. - Minutes Specify the time in minutes for the acquisition. You can set the acquisition time from 0.01 to 15000.00 minutes. To change this value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, enter a value in the spin box text field. When the active acquisition is controlled by a method file, this parameter is not available. Instead, the text field shows <i>by method</i>.
On start	Use the list box to set the start mode of the data acquisition. The options are as follows: - don't wait Initiates acquisition of the raw file immediately when you click Start in the Acquisition window. - wait for contact closure When you click Start in the Acquisition window, the acquisition pauses. Q Exactive UHMR Tune initiates acquisition of the raw file either when it receives a contact closure signal (for example, from an analog autosampler) or when you click Resume.
After acquisition	Use the list box to set the instrument mode after the data acquisition has stopped. The options are as follows: - stay on The instrument remains On when the active acquisition is completed. - enter standby mode Sets the instrument to Standby when the active acquisition is completed. - switch off Switches Off the instrument when the active acquisition is completed.
Buttons	

Parameter	Description
Start / Stop	Use this button to start and stop the data acquisition. When no acquisition is in progress, Q Exactive UHMR Tune displays Start. When an acquisition is in progress, Q Exactive UHMR Tune displays Stop. To start an acquisition, click Start. To stop an acquisition, click Stop. To pause an acquisition, click the Pause / Resume button. No Q Exactive UHMR Tune controlled data acquisition is possible if the instrument is controlled by Xcalibur. IMPORTANT When you start an acquisition while the instrument is in Off position, the instrument begins acquiring data after a delay of about 30 seconds.
Pause / Resume	Use this button to pause and resume an acquisition in progress. When no acquisition is in progress, the button is inactive (gray). When an acquisition is in progress, Q Exactive UHMR Tune displays Pause. When an acquisition is paused, Q Exactive UHMR Tune displays Resume. To pause an acquisition in progress, click Pause. To resume an acquisition that is paused, click Resume. To stop an acquisition in progress, click the Start / Stop button. The acquisition can be started by clicking Resume if the mass spectrometer is waiting for contact closure.
Help	Displays the Help for this window.

❖ **To display this window**

Click the Acquisition window title bar in the Instrument Control window.

Mass Traces Window

Use the Mass Traces window to display mass traces for the total ion current and up to five m/z values in the Analysis Graphs window. You can plot mass traces when you manually adjust source parameters like gas flows or spray voltage. You can also optimize collision energy/normalized collision energy or in-source CID energy.

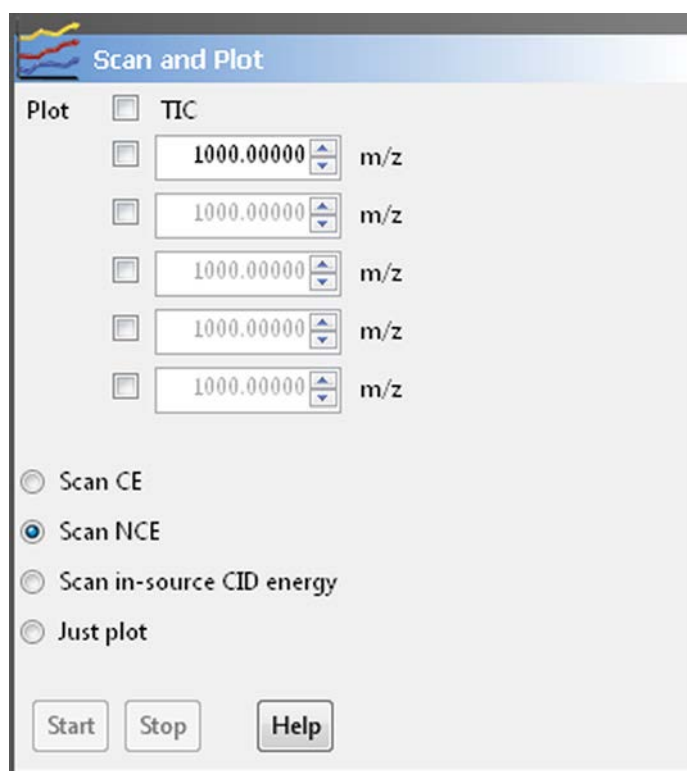


Figure 4-6. Mass Traces window

The Mass Traces window has these parameters:

Parameter	Description
Plot	
TIC	Select this check box to plot the total ion current.
Masses to plot	Select a check box for each m/z value that you want to plot (up to five). When you select a check box, the spin box becomes available. The spin box displays the mass-to-charge ratio to plot. You can set the mass-to-charge ratio to any m/z value from 350 to 80000. To change this value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, enter a value in the spin box text field.
Scan CE	Select this option button to optimize the collision energy on the total ion current.
Scan NCE	Select this option button to optimize the normalized collision energy on the total ion current.
Scan in-source CID energy	Select this option button to optimize the in-source CID energy on the total ion current.
Just plot	Select this option button to plot the mass trace without optimization.

Parameter	Description
Buttons	
Start	Click Start to start plotting the mass traces. The instrument needs to be in On status to start a plotting procedure. When plotting is in progress, Q Exactive UHMR Tune displays Stop .
Stop	Click Stop to stop plotting the mass traces.
Help	Displays the Help for this window.

Calibrate Window

Use the Calibrate window of the tasks panel to perform an automatic optimization of the calibration parameters. Calibration parameters are instrument parameters whose values do not vary with the type of experiment.

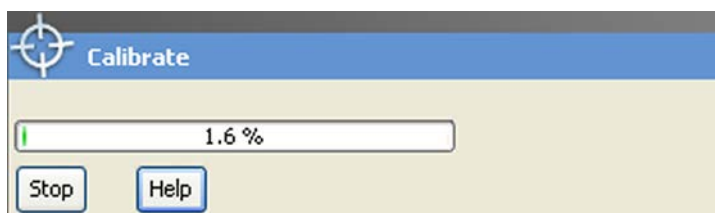


Figure 4-7. Calibrate window

Standard users can choose the ion mode they want to calibrate in the CsI Calibration window. Advanced users can use the CsI Calibration window to calibrate the instrument with the cesium iodide calibration solution. Or, they can use the Customized Calibration window to enter parameters for a calibration with a calibration solution of their choosing.

Tip If the system was in Off mode before, it is necessary to put the instrument into On mode for at least 90 minutes before a mass calibration is performed.

The calibrating procedure requires that you introduce calibration solution into the mass spectrometer at a steady rate for several minutes (or longer). You can introduce the solution directly from the syringe pump. Refer to the *Exactive Series Operating Manual* for information.

The Calibrate window has these parameters:

Parameter	Description
Progress bar	Displays the elapsed percentage of the active calibration procedure.

Parameter	Description
Buttons	
Calibrate	Click Calibrate to start an automatic calibration of the mass spectrometer. The instrument needs to be in On status to start a calibration. The duration of the automatic calibration depends on the selected check boxes. A complete automatic calibration requires about four minutes. When calibration is in progress, Q Exactive UHMR Tune displays Stop .
Stop	Click Stop to stop a calibration in progress.
Help	Displays the Help for this window.

❖ **To display this window**

Click  **Calibrate** in the tasks panel.

CsI Calibration Window

Use the CsI Calibration window to select parameters and ion modes when you perform an automatic calibration with the cesium iodide calibration solution. The window displays the statuses of the individual calibration items on the right side.

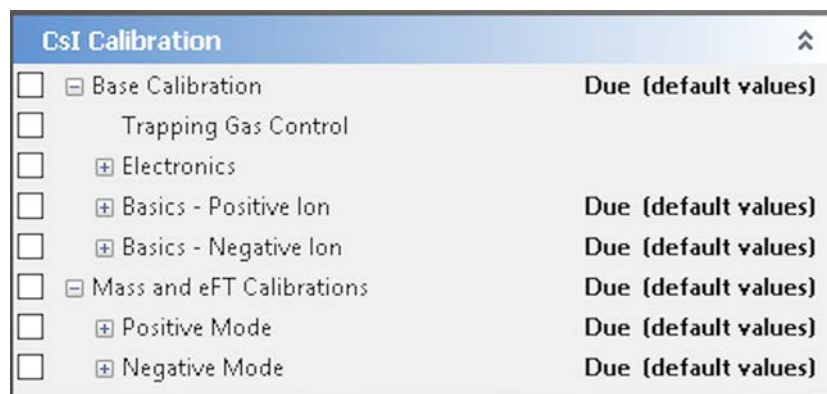


Figure 4-8. CsI Calibration window (for advanced users)

The CsI Calibration window has these parameters:

Parameter	Description
In a hierarchical list of items in a tree view, advanced users can select individual parameters that they want to calibrate. If the check box is not selected, no subentry is selected. If the check box is selected, all subentries are selected. If the check box is filled, some subentries are selected.	
Base Calibration	The Base Calibration item displays a hierarchical list of items in a tree view. This parameter is not available for standard users.
-Basics - Positive Ion -Basics - negative Ion	Select this check box to perform an automatic calibration for isolation mass and resolution of the quadrupole in the respective ion mode.
Mass and eFT Calibrations	Select this check box to perform an automatic calibration for the calibration parameters in all ion modes. Select the check boxes of subentries to perform an automatic calibration for specific parameters. Refer to the <i>Exactive Series Operating Manual</i> or the <i>Q Exactive Plus QuickStart Guide</i> for information about the required calibration solution. Tip You must perform the mass calibrations and the eFT calibrations in both low m/z detector mode and high m/z detector mode.

Evaluate Window

Use the Evaluate window of the tasks panel to perform an automatic check of the instrument calibration.

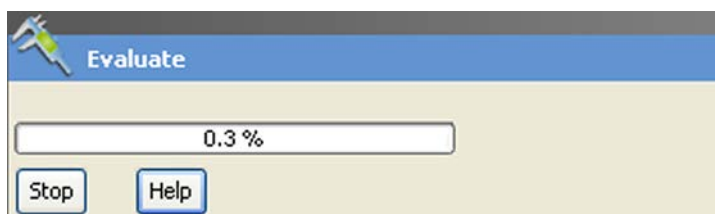


Figure 4-9. Evaluate window

To enable an evaluation, standard users must select at least one check box in the CsI Evaluation window. Advanced users must select at least one check box either in the CsI Evaluation window or in the Customized Evaluation window.

The evaluation procedure requires that you introduce calibration solution into the mass spectrometer at a steady rate for several minutes (or longer). You can introduce the solution directly from the syringe pump. Refer to the *Exactive Series Operating Manual* for information.

The Evaluate window has these parameters:

Parameter	Description
Progress bar	Displays the elapsed percentage of the active evaluation procedure.
Buttons	
Evaluate	Click Evaluate to start an automatic evaluation of calibration parameters. The instrument needs to be in On status to start an evaluation. When evaluation is in progress, Q Exactive UHMR Tune displays Stop .
Stop	Click Stop to stop an evaluation in progress.
Help	Displays the Help for this window.

❖ **To display this window**

Click  **Evaluate** in the Tasks window.

CsI Evaluation Window

Use the CsI Evaluation window to enable the evaluation with the cesium iodide calibration solution.

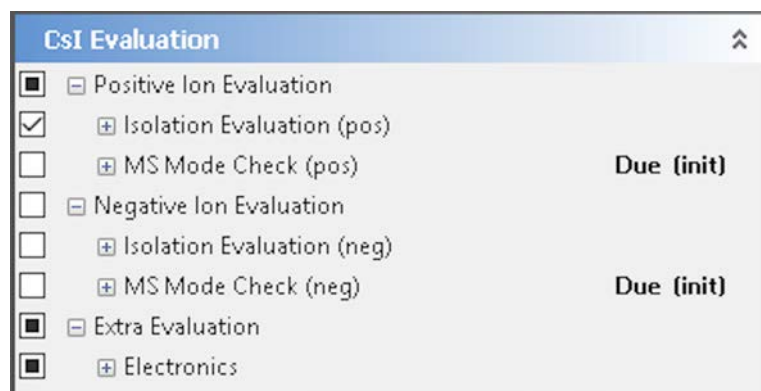


Figure 4-10. CsI Evaluation window (for advanced users)

The CsI Evaluation window has these parameters:

Parameter	Description
In a hierarchical list of items in a tree view, you can select individual parameters that you want to evaluate. If the check box is not selected, no subentry is selected. If the check box is selected, all subentries are selected. If the check box is filled, some subentries are selected.	
Positive Ion Evaluation	
Select the check boxes to evaluate various parameters for the positive ion mode.	
-Isolation Evaluation (pos)	Evaluates the performance of the quadrupole in positive ion mode.
--Quadrupole isolation shape check (pos) ^a	Evaluates the quadrupole transmission against minimum requirements in positive ion mode. This evaluation requires a calibrated quadrupole and a stable calmix spray.
-MS Mode Check (pos)	Evaluates the basic performance of the instrument in UHMR mode.
--UHMR Spectral Mass Accuracy Test (pos) ^a	Performs a mass accuracy test for the UHMR mode.
Negative Ion Evaluation	
Select the check boxes to evaluate various parameters for the negative ion mode.	
-Isolation Evaluation (neg)	Evaluates the performance of the quadrupole in negative ion mode.
--Quadrupole isolation shape check (neg) ^a	Evaluates the quadrupole transmission against minimum requirements in negative ion mode. This evaluation requires a calibrated quadrupole and a stable calmix spray.
-MS Mode Check (neg)	Evaluates the basic performance of the instrument in UHMR mode.
--UHMR Spectral Mass Accuracy Test (neg) ^a	Performs a mass accuracy test for the UHMR mode.
Extra Evaluation	
Select the check boxes to evaluate various parameters that are not contained in the standard evaluations.	
Electronics	Evaluates the performance of electronic components.
-Quadrupole RF Frequency ^a	Checks the quadrupole RF voltage.
-Inject Flatapole RF ^a	Checks the inject flatapole RF voltage.
-Bent Flatapole RF ^a	Checks the bent flatapole RF voltage.
-HCD RF ^a	Checks the RF voltage of the collision cell.

^aThis parameter is not available for standard users.

Vacuum / Bakeout Window

The Vacuum / Bakeout window of the tasks panel reads back the pressure values at the vacuum gauges and allows performing an instrument bakeout.

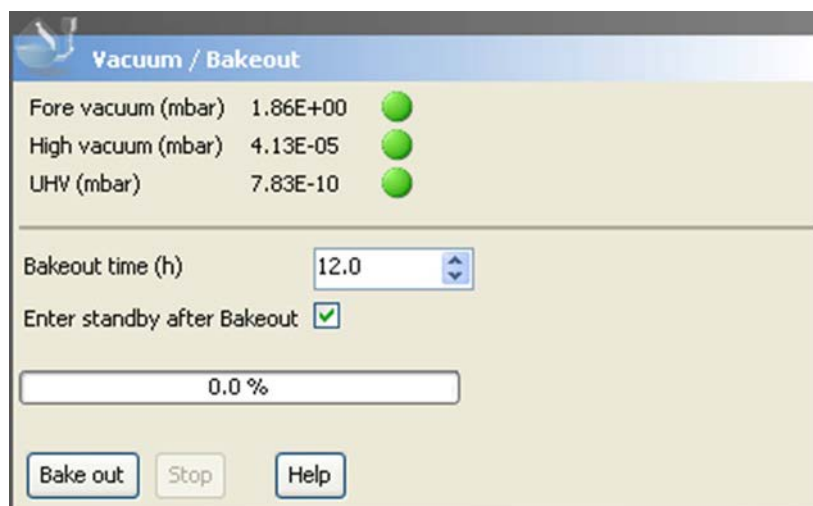


Figure 4-11. Vacuum / Bakeout window

Tip After the bakeout time has expired, the instrument requires a cooling and stabilization time of about three hours.

The Vacuum / Bakeout window has these parameters:

Parameter	Description
Vacuum	
Green LEDs indicate that the readback values are sufficient for operating the mass spectrometer. If an LED indicates a vacuum problem, use the instrument status window for error diagnosis.	
Fore vacuum	This readback displays the actual pressure (in mbar) in the forevacuum line and ion source region as read by the Pirani gauge.
High vacuum	This readback displays the actual pressure (in mbar) in the high vacuum chamber as read by the ion gauge. This parameter is visible only when the ion gauge in the high vacuum chamber is switched on. Advanced users can switch on this gauge by using the shortcut menu of the Vacuum System node of the instrument status window.
UHV	This readback displays the actual pressure (in mbar) in the Orbitrap chamber as read by the ion gauge.
Bakeout	
Bakeout time	Enter the baking duration (in hours) into the spin box. The range is 4 to 30 hours. When you click Bake out , the mass spectrometer starts the baking routine. The baking script is stopped after the preset duration. Click Stop to abort the baking routine. The instrument has to cool down for another three hours before it can be used.
Enter standby after Bakeout	Select the check box to set the instrument to standby mode after the bakeout procedure is finished.

Parameter	Description
Progress bar	Displays the elapsed percentage of the active baking procedure.
Bake out	Click Bake out to start the bakeout routine. To stop a bakeout in progress, click the Stop button. Bakeout is possible only when the instrument status is Off.
Stop	Click Stop to abort the bakeout routine. The instrument has to cool down for another three hours before it can be used.
Help	Displays the Help for this window.

❖ **To display this window**

Click  **Vacuum / Bakeout** in the tasks panel.

Display Panel

The windows in the display panel provide real-time information about the instrument status, the Q Exactive UHMR Tune software, or other programs.

These windows are available:

- [Spectrum Window](#)
- [Instrument Status Window](#)
- [Messages Window](#)
- [Analysis Graphs Window](#)
- [Debug Messages Window](#)

The spectrum window is always visible. The debug messages window is not available for standard users.

Depending on the individual configuration of your system, additional windows may allow controlling other installed instruments.

Q Exactive UHMR Tune offers various ways to arrange windows in the display panel:

❖ **To display a window in the display panel**

Choose the respective command in the Windows menu.

❖ **To hide a window in the display panel**

- Choose the respective command in the Windows menu.
- Right-click the title bar of a window to display the shortcut menu. Choose **Hide**.

❖ **To change the position of a window in the display panel**

- Use the mouse to drag the window by its title bar to the new location, which can be even outside the Q Exactive UHMR Tune window.
- Within the display panel, you can dock the window to any one of the four sides. While you drag the window, Q Exactive UHMR Tune displays icons to indicate the available docking positions.
- Right-click the title bar of a *docked* window to display the shortcut menu. Choose **Floating** to undock the window.

Or, double-click on the title bar of the window.

- Right-click the title bar of an *undocked* window to display the shortcut menu. Choose **Floating** to dock the window to its last docking position.

Or, double-click the title bar of the window.

Spectrum Window

The spectrum window displays real-time data generated during calibration, tuning, and diagnostic tests. The spectrum window is always visible.

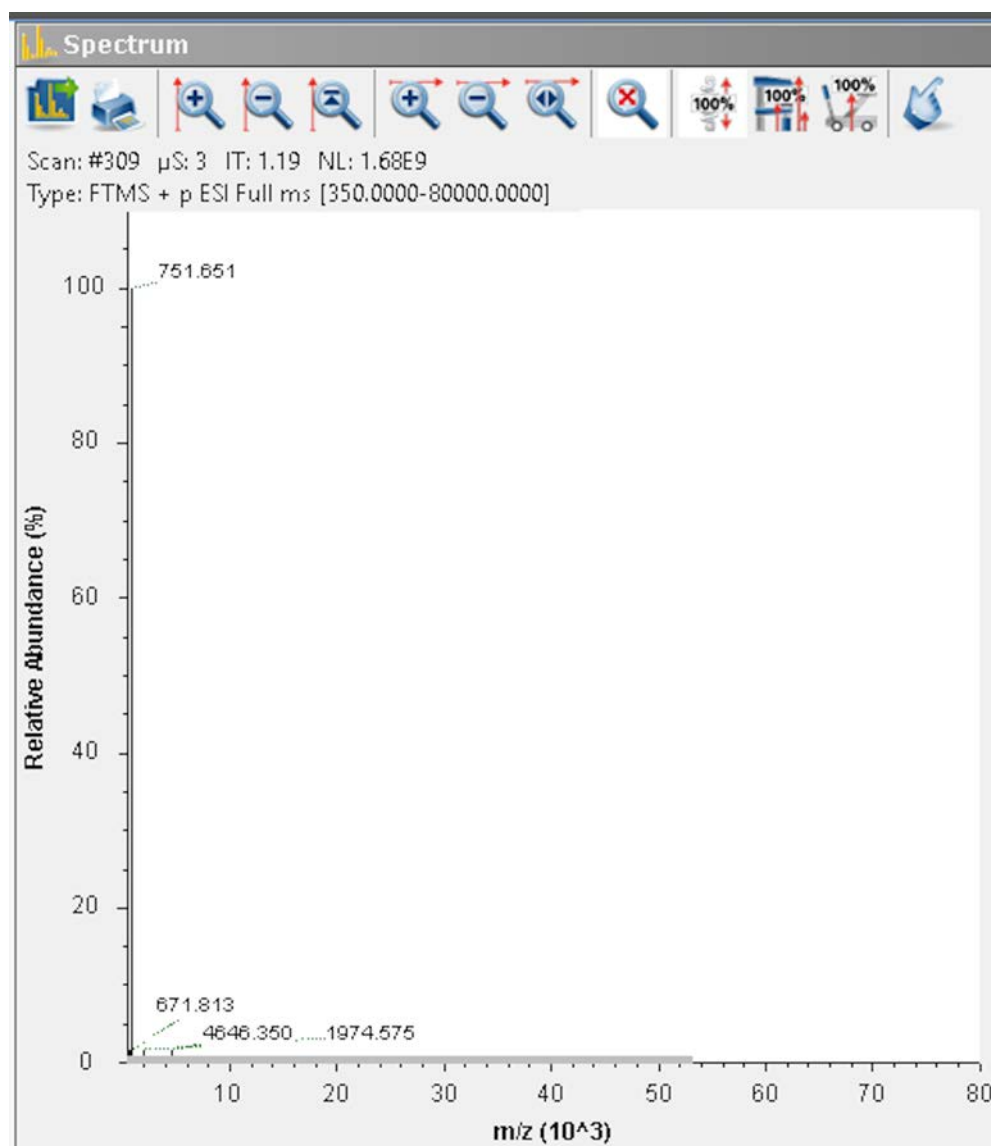


Figure 4-12. Spectrum window

The spectrum window allows using the mouse for zooming.

❖ To zoom in or out on a spectrum

- Click and drag with the left mouse button (hand cursor) from the beginning to the end of the portion you want to see enlarged.
- Or, use the mouse wheel for zooming. Position the mouse pointer within the spectrum and roll the wheel forward to zoom in on the spectrum area.
- To zoom in on the spectrum with respect to one axis only, position the mouse pointer within the axis area and roll the mouse wheel forward. Roll the wheel backward to zoom out.
- To increase the zooming factor by two, keep the <Shift> key pressed while using the mouse wheel.

To return to a display of the full spectrum, click the  button in the toolbar or choose **Unzoom** in the shortcut menu.

Press the <Shift> key to enable mouse panning. When mouse panning is active (mouse pointer changes to hand cursor), you can shift the spectrum along the X-axis while keeping the left mouse button pressed.

The spectrum window has these parameters:

Parameter	Description
Header	
Scan #	The number of scans since the beginning of the last acquisition (or since the last time the mass spectrometer was rebooted)
μS	Number of microscans
IT	Inject time (in milliseconds)
NL	Normalization level
Type	Scan type The scan type information comprises ion polarity, source type, fragmentation type and energy (if active), and scan range. When the acquisition is controlled by an instrument method, the information includes the active scan segment and the active scan event.

❖ To display this window

Choose **Windows > Spectrum**.

Toolbar

Use the buttons in the toolbar to manipulate the spectrum display.

The toolbar of the spectrum window has these parameters:

Parameter	Description
	Click to copy the active spectrum into the clipboard.
	Click to plot the active spectrum. You can view a print preview before the spectrum is printed. In a Page Setup dialog box, you can set up printer's parameters (paper size and orientation, for example).
	Click to zoom in on the Y-axis (factor 2).
	Click to zoom out on the Y-axis (factor 2).
	Click to normalize the Y scale: Q Exactive UHMR Tune always displays the largest peak in the spectrum at full scale (vertical scale = largest peak in spectrum).
	Click to zoom in on the X-axis (factor 2).
	Click to zoom out on the X-axis (factor 2).
	Click to display the entire mass range.
	Click to normalize the display (X-axis, Y-axis).
	Click to set to fixed mode: the height of the Y-axis is set equal to the height of the largest peak in the active spectrum and remains fixed even if larger peaks occur.
	Click to set the Y-axis to the height of the highest peak so that the largest peak in the spectrum is always displayed at full scale.

Parameter	Description
	Click to set to creep mode: the Y scale of the mass spectrum automatically increases if the peak intensity increases, but does not decrease if the peak intensity decreases.
	Click to toggle between mouse panning and mouse zooming: - When mouse panning is active, you can shift the spectrum along the X-axis while keeping the left mouse button pressed (hand cursor). - When mouse zooming is active, you can zoom in the spectrum by using the mouse.

Shortcut Menu

Right-click the spectrum window to display the shortcut menu. It has these commands:

Command	Description
Save Image As	Saves the active graph as image file. A Save As dialog opens and you can enter the file name, file type, and the directory.
Unzoom	Reverts the zoom action.
Display options	Opens the Display Options dialog box.

Instrument Status Window

The instrument status window displays real-time status information for the instrument components. All parameters are arranged in a tree view. The Control node and the System node are not available for standard users.

[-] Control	
[-] Settings	
[-] Define Scan	
[+] Misc.	
Averaging	0
Detector m/z Optimization *	High m/z
[+] Processing	
AGC mode *	prescan
[-] Ion transfer	
Source DC Offset * (V)	21.0
[-] In-Source Trapping Mode	
In-Source Trapping On/Off *	Off
Desolvation Voltage (V) *	0
[-] Ion Transfer m/z Optimization	
Ion Transfer Target m/z	High m/z
Inj. Fl. RF Ampl. *	700
Bent. Fl. RF Ampl. *	940
Trans. MP and HCD-cell RF Ampl. *	900
C-Trap RF Ampl. *	2950
Injection Flatapole DC * (V)	5.0
Inter Flatapole Lens * (V)	4.0
Bent Flatapole DC * (V)	2.0
Transfer Multipole DC * (V)	0
C-Trap Entrance Lens Inject * (V)	1.8
[+] Quad	
[+] HCD event	
Trapping gas pressure setting *	7.0
C-Trap Charge Detector Support *	On
[+] Mass Calibration Data	

Figure 4-13. Instrument status window, detail (Advanced User)

When expanded, some nodes provide shortcut menus that are displayed when you right-click an item. The available commands depend on the selected node and the user privileges. Generally, the shortcut menus allow changing the active settings.

Tip For normal operation, it is not necessary to change the settings in the instrument status window. It just allows monitoring the system in more detail (more readbacks etc.) than the other windows.

The following table contains an overview about parameters in the instrument status window that are frequently used.

Instrument

- **Current Scan**
- - **Total Ion Current**
- - - **TIC Variation**
- - - **Inject time**
- - - **AGC Target reached**
- - - **AGC Prescan Mode**
- - - **Scan Rate**
- - **Lock Masses**
- - - **Lock mass found**
- - - - **Lock mass m/z correction**
- **Control**
- - **Settings**
- - - **Define Scan**
- - - - **Misc**
- - - - - **Extended trapping * (eV) UHMR**
If the value is positive, ions are transported to the HCD cell during a Full MS scan. The value entered here defines the injection energy by which the ions enter the HCD cell. If HCD fragmentation energy is applied, this value is overridden.
- - - - **Averaging**
If the value is positive, averaging lowers the noise level by performing a cumulative rolling average of the time domain signal using the specified number of transients.
- - - - - **Detector m/z Optimization ***
Changes the detector pulsing scheme to be optimized for low or high m/z ions.
- - - - - **Processing**
- - - - - **Noise threshold**
Use this parameter to set the number of standard deviations for sigma clipping-based determination of the local noise level of the spectrum.
- - - - **AGC Mode ***
“Prescan” optimizes the ion inject time for the target number of charges. “Fixed” uses the maximum inject time as the injection time for every scan.
- - - **Ion Transfer**
- - - - **Source DC Offset * (V)**
Use this parameter to set the DC bias of the S-Lens. Possible entries are values between -100 and +100 V.
- - - - **In-Source Trapping Mode**
- - - - - **In-Source Trapping On/Off**
Use this parameter to turn on or off In-Source Trapping. When In-Source Trapping is on, AGC Mode is set to Fixed.

Desolvation Voltage (V) *

Use this parameter to set the DC bias of the injection flatapole rods during the trapping step of In-Source Trapping. For desolvation/fragmentation, negative desolvation voltages are recommended for positive ions and positive desolvation voltages are recommended for negative ions. Possible entries are values between -300 and +300 V.

- - - **Ion Transfer m/z Optimization**

- - - **Ion Transfer Target m/z**

Setting this value to “Low m/z” or “High m/z” optimizes the RF settings of the transfer ion optics for this m/z range. A setting of “Manual” reflects that manual tuning has been performed for the RF Ampl. below.

Inj. Fl. RF Ampl. *

Use this parameter to set the RF voltage of the injection flatapole. Possible entries are values between 150 and 700 V.

Bent. Fl. RF Ampl. *

Use this parameter to set the RF voltage of the bent flatapole. Possible entries are values between 300 and 940 V.

Trans. MP and HCD-cell RF Ampl. *

Use this parameter to set the RF voltage of the transfer multipole and the HCD cell. Possible entries are values between 250 and 900 V.

C-Trap RF Ampl. *

Use this parameter to set the RF voltage of the C-Trap. Possible entries are values between 600 and 2950 V.

- - - **Injection Flatapole DC * (V)**

Use this parameter to set the DC voltage that is applied to the injection flatapole.

Inter Flatapole Lens * (V)

Use this parameter to set the DC voltage that is applied to the inter flatapole lens. Possible entries are values between -50 and +50 V.

Bent Flatapole DC * (V)

Use this parameter to set the DC voltage that is applied to the bent flatapole. Possible entries are values between -50 and +50 V.

Transfer Multipole DC * (V)

Use this parameter to set the DC voltage that is applied to the transfer multipole. Possible entries are values between -30 and +30 V.

C-Trap Entrance Lens Inject * (V)

Use this parameter to set the DC voltage that is applied to the C-Trap entrance lens during C-Trap filling. Possible entries are values between -15 and +15 V.

- - - **Quad**

- - - - **Isolation Limit Low # (m/z)**

This parameter shows the lowest m/z that can be isolated with the current quadrupole calibration. Standard CsI calibration has a m/z 2000 limit.

Isolation Limit High # (m/z)

This parameter shows the highest m/z that can be isolated with the current quadrupole calibration. Standard CsI calibration has a m/z 25000 limit.

Quad Calibration Inject Time

Use this parameter to set the injection time that is used during quadrupole calibration. 30 ms is default for CsI, but the value can be varied for custom calibrations. Possible entries are values between 6 and 200 ms.

Quad Calibration uScans

Use this parameter to set the microscans used during quadrupole calibration. 2 microscans is default for CsI, but the value can be varied for custom calibrations. Possible entries are values between 1 and 20 microscans.

User Mass List: Rough Quad Calibration

Use this parameter to edit the entries for the mass list that is used for the rough quadrupole calibration procedure. Editing and successful calibration changes the isolation limits.

User Mass List: Wide Quad Calibration

Use this parameter to edit the entries for the mass list that is used for the wide quadrupole calibration procedure. Editing and successful calibration changes the isolation limits.

- - - **HCD Event**

- - - - **Purge Time * (ms)**

Use this parameter to edit the time that ions are ejected from the HCD cell. The time can be increased at the expense of scan speed to increase transmission of high m/z ions out of the HCD cell.

C-Trap Exit Lens: Purge * (V)

Use this parameter to edit the voltage that is applied to the C-Trap exit lens when ions are moving from the HCD cell to the C-Trap.

HCD Field Gradient --- Purge * (V)

Use this parameter to edit the electrical field by which ions are ejected from the HCD cell. the voltage can be increased to increase transmission of high m/z ions out of the HCD cell.

In addition to showing numerical values of parameters, the instrument status window uses icons to indicate the statuses of system components. Thus, you can use the instrument status window for a quick error diagnosis.

❖ **To display this window**

Choose **Windows > Instrument Status**.

Messages Window

The messages window displays real-time information about the statuses of the instrument, the control service, or other programs.

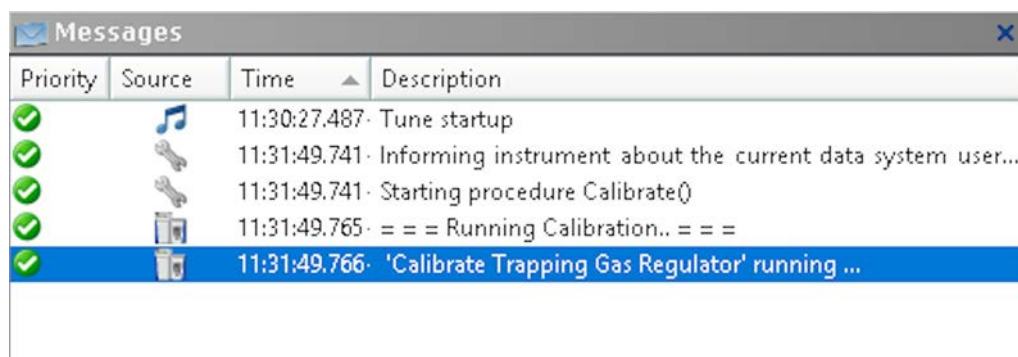


Figure 4-14. Messages window

For further analysis, you can copy the content of the messages window to a text editor.

❖ To copy content from the messages window to a text editor

1. Select part of the content with the mouse, or press **<Ctrl> + <A>** to select the complete content of the messages window.
2. Press **<Ctrl> + <C>** to copy the text to the clipboard.
3. Open a document in the text editor.
4. Press **<Ctrl> + <V>** to insert the copied text into the document.

The messages window has these parameters:

Parameter	Description
The messages are sorted with respect to time. To change the sort order, click the respective table column header. To invert the sort order, click again.	
Priority	The message priority is indicated by symbols: - Info; status is normal / command successful - Warning; no user action required - Error; user action required - Fatal error; program cannot proceed
Source	The message source is indicated by symbols: Message from Q Exactive UHMR Tune program

Parameter	Description
	Message from instrument
	Message from service
Time	Time and date of the message
Description	Displays the message text.

❖ **To display this window**

Choose **Windows > Messages**.

Analysis Graphs Window

The analysis graphs window displays real-time data generated during calibration, tuning, and diagnostic tests. To save data displayed in the window, choose **Save Image As** in the shortcut menu of the window.

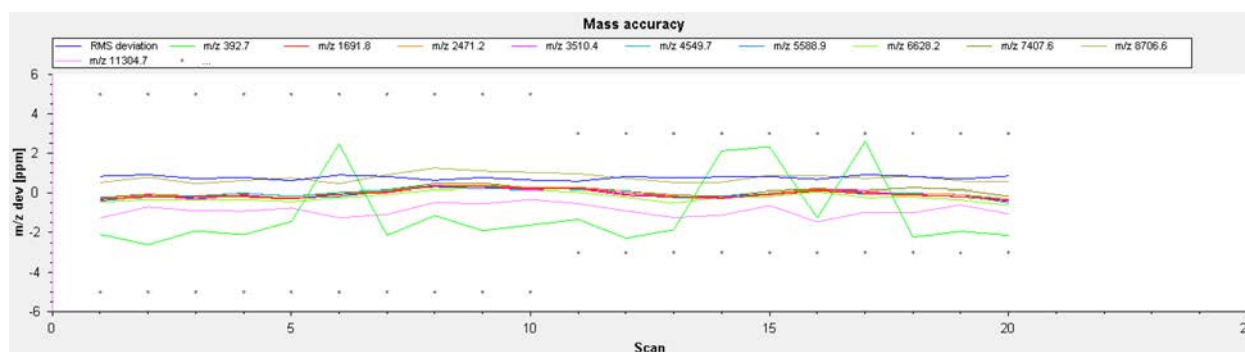


Figure 4-15. Analysis Graphs window

The analysis graphs window allows using the mouse for zooming.

❖ **To zoom in or out on an analysis graph**

- Click and drag with the left mouse button (hand cursor) from the beginning to the end of the portion you want to see enlarged.
- Or, use the mouse wheel for zooming. Position the mouse pointer within the graph and roll the wheel forward to zoom in on the graph area.
- To zoom in on the graph with respect to one axis only, position the mouse pointer within the axis area and roll the mouse wheel forward. Roll the wheel backward to zoom out.
- To increase the zooming factor by two, keep the **<Shift>** key pressed while using the mouse wheel.

To return to a display of the full spectrum, click the  button in the toolbar or choose **Unzoom** in the shortcut menu.

Press the <**Shift**> key to enable mouse panning. When mouse panning is active (mouse pointer changes to hand cursor), you can shift the graph along both axes while keeping the left mouse button pressed.

❖ **To display this window**

Choose **Windows > Analysis Graphs**.

Toolbar

The toolbar of the analysis graphs window has these parameters:

Parameter	Description
	Click to copy the active graph into the clipboard.
	Click to plot the active graph. You can view a print preview before the graph is printed. In a Page Setup dialog box, you can set up printer's parameters (paper size and orientation, for example).
	Click to normalize the display (X-axis, Y-axis).

Shortcut Menu

Right-click the analysis graphs window to display the shortcut menu. It has these commands:

Command	Description
Save Image As	Saves the active graph as image file. A Save As dialog opens and you can enter the file name, file type, and the directory.
Unzoom	Reverts the zoom action.

Debug Messages Window

The debug messages window displays messages that can be used during method development. The debug messages window is not available for standard users.

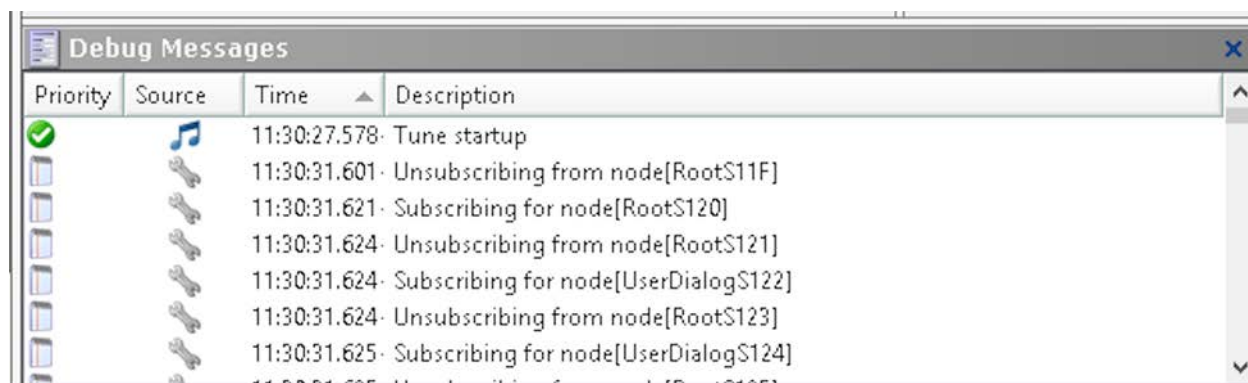


Figure 4-16. Debug Messages window

For further analysis, you can copy the content of the debug messages window to a text editor.

❖ **To copy content from the debug messages window to a text editor**

1. Select part of the content with the mouse, or press **<Ctrl> + <A>** to select the complete content of the messages window.
2. Press **<Ctrl> + <C>** to copy the text to the clipboard.
3. Open a document in the text editor.
4. Press **<Ctrl> + <V>** to insert the copied text into the document.

The debug messages window has these parameters:

Parameter	Description
The messages are sorted with respect to time. To change the sort order, click the respective table column header. To invert the sort order, click again.	
Priority	The message priority is indicated by symbols: 📁 Debugging message ✓ Info; status is normal / command successful ⚠ Warning; no user action required ✖ Error; user action required 💀 Fatal error; program cannot proceed
Source	The message source is indicated by symbols: 🎵 Message from Q Exactive UHMR Tune program. 📁 Message from instrument. 🔑 Message from service.

Parameter	Description
Time	Time and date of the message
Description	Displays the message text.

❖ To display this window

Choose **Windows > Debug Messages**.

Shortcut Menu of the Debug Messages Window

The debug messages window has a shortcut menu that is displayed when you right-click into the window. Use the commands of the shortcut menu to configure the scope of the messages displayed in the window. Click a command to activate it. Click it again to deactivate it.

These message priorities can be displayed:

- Debug
- Log
- Info
- Warning
- Error
- Fatal

For each message priority, these message sources are available:

- Instrument
- Service
- Application

A  icon in front of a message source shows that it is selected. A  icon in front of a message priority shows that it is shown for all three message sources. A  icon in front of a message priority shows that it is shown for one or two message sources.

In addition to the commands for configuring the content of the debug messages window, the **Clear list** command allows removing the complete content of the window.

Dialog Boxes

This section provides a reference to the dialog boxes in Q Exactive UHMR Tune.

Dialog Boxes Displayed from the Menu Bar

- [About Dialog Box](#)
- [License Dialog Box](#)
- [Mass Calculator](#)

Dialog Boxes Displayed from the Toolbar

- [Syringe Pump Settings Dialog Box](#)

Dialog Boxes Displayed from the Scan Parameters Window

- [Fragmentation Dialog Box](#)
- [Isolation Range Dialog Box](#)
- [Scan Parameters History Dialog Box](#)
- [Scan Range Dialog Box](#)

Dialog Boxes for Editing Lock Masses

- [Collection Modification Dialog Box](#)
- [Delete Lock Mass Collection Dialog Box](#)
- [Lock Masses Dialog Box](#)
- [Lock Mass Removal Dialog Box](#)
- [Lock Mass Replacement Dialog Box](#)
- [Name Change Dialog Box](#)
- [New Lock Mass Collection Dialog Box](#)

Dialog Boxes Displayed from the Spectrum Window

- [Display Options Dialog Box](#)

About Dialog Box

Use the About dialog box to display information about the instrument, the software version, and the active licenses. To copy the instrument identification to the clipboard, click the  button.

The About dialog box has these parameters:

Parameter	Description
Buttons	
OK	Saves your changes and closes the dialog box.
Add license	Displays the License dialog box.
Back / Next	Display various dialog boxes with legal information and information about third party licenses used by Q Exactive UHMR Tune.
Help	Displays the Help for this dialog box.

❖ To display this dialog box

Choose **Help > About**.

Autoselect Ion Source Values Dialog Box

Use the Autoselect ion source values dialog box to automatically apply suitable parameters for a HESI ion source in dependence on a LC flow rate.

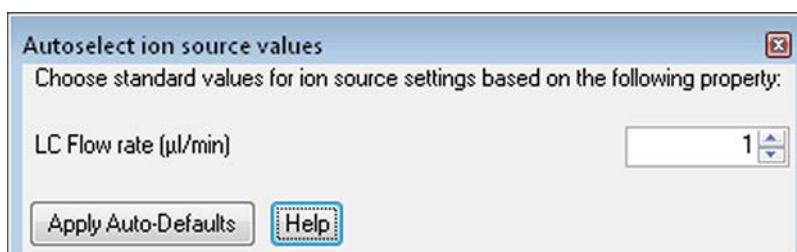


Figure 4-17. Autoselect ion source values dialog box

See “[Default Parameters and Ranges for HESI-2](#)” on [page 6-5](#) for a list of the involved parameters and their values.

The Autoselect ion source values dialog box has these parameters:

Parameter	Description
LC Flow rate (µl/min)	Use this spin box to specify the volume of solvent solution passing through the liquid chromatography system per unit time (in microliters per minute). To change this value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, enter a value in the spin box text field. The acceptable range of values is 0 to 2000.
Buttons	
Apply Auto-Defaults	Applies suitable values for these source parameters: • Capillary temperature • Vaporizer temperature • Sheath gas flow • Auxiliary gas flow • Sweep gas flow • Spray voltage (for HESI)

❖ To display this dialog box

On the HESI source window, click **Source Auto-Defaults**.

Isolation Range Dialog Box

Use the Isolation Range dialog box to specify the settings for the quadrupole isolation.

Figure 4-18. Tune—Isolation Range dialog box

The Isolation Range dialog box has these parameters:

Parameter	Description
No Isolation	Select this option to switch off the quadrupole isolation.
Isolation	Select this option to switch on the quadrupole isolation. Use the spin boxes to set values (in mass-to-charge ratio units) for Minimum, Maximum, Center, and Width for the quadrupole isolation range. To change the value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. • Minimum Select the lowest value for the isolation range. You can enter any m/z value from 500.0 to 24995.0. • Maximum Select the highest value for the isolation range. You can enter any m/z value from 505 to 25000.0. • Center Select the center mass of the isolation range. You can enter any m/z value from 502.5 to 24997.5. • Width Select the width of the isolation range. You can enter any m/z value from 5.0 to 24500.0.

❖ **To display this dialog box**

In the Scan Parameters window, click the Isolation range field.

License Dialog Box

Use the License dialog box to enter licenses that activate additional features.



Figure 4-19. License dialog box

The License dialog box has these parameters:

Parameter	Description
License key	Use the text box to enter the license key.

Parameter	Description
Buttons	
OK	Saves your changes and closes the dialog box.
Cancel	Discards your changes and closes the dialog box.
Help	Displays the Help for this dialog box.

❖ **To display this dialog box**

1. Choose **Help > About** to display the About dialog box.
2. In the About dialog box, click **Add license**.

Mass Calculator

Use the Mass Calculator to calculate the exact mass of an compound of interest.

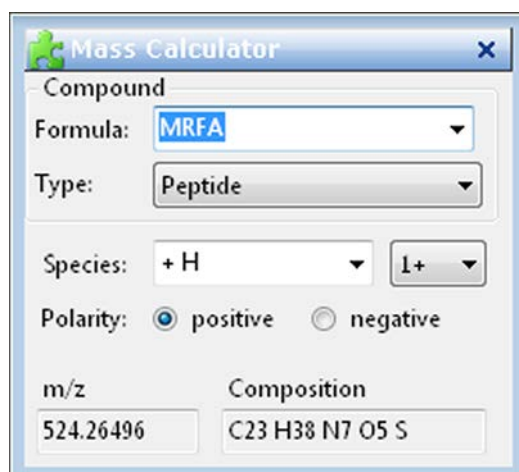


Figure 4-20. Mass Calculator (Tune)

The Mass Calculator has these parameters:

Parameter	Description
Compound	
Formula	Use the text field to specify the basic composition of the compound. Click the down arrow to display a list of the last entered compounds. The syntax rules and interpretation accept the kind of formula that is also accepted on the Spectrum Simulation page (Isotope Simulation area) of the Qual Browser.

Parameter	Description
Type	Use the Type list to specify the formula type used in the Formula field: • Chemical formula Formula is defined as the resulting elemental composition of the entered formula. This is the default selection. • Peptide Formula is defined as the sum of all of the entered amino acids additionally terminated with H at the N-terminus and OH at the C-terminus. • Amino Acid Formula is defined as the sum of all of the entered amino acids. Independent of the entry in the Species field, the elemental composition and the mass of the compound, Formula is completely determined by the given formula and selected formula type.
Species	Use this text field to define adducts or modifications of the active compound that are expected to be formed. The Species field can be used in two ways: • Click the down arrow to display a list of predefined adducts for each polarity: - +H, +Na, +K, +NH₄ for positive polarity - -H, +Cl, +OH, +HCOO for negative polarity - an empty entry to express adducts (for example, radical cations) for both polarities. The corresponding set will be displayed depending on the selected polarity. Selecting an adduct (A) will result in the strict behavior of applying one unit A to the compound and using “+H” or “-H” adduct depending on the charge state and active polarity. “+K” = $[M + K^+ + (z-1)H^+]^{z+}$; for example, MRFA, +K, CS=2, positive pol. = $[M + K^+ + H^+]^{2+}$ • Enter the modifications of the compound by using squared brackets and at least M as representation of the basic compound (for example, [M + Na + K] or [2M + Na]). The predefined adducts can be entered, too. This definition is used without additional auto dependencies, like adding protons.
Charge state	Use the list box to select the resulting charge state. Available options are 1+ to 100+ for positive polarity and 1– to 100– for negative polarity. The default charge state is 1+ for positive polarity and 1– for negative polarity.
Polarity	Use the option buttons to select the applied polarity. The default polarity is positive .
m/z	This text field displays the calculated mass-to-charge ratio, with five decimal places (for example, 524.26496).
Composition	This text field displays the determined total formula (for example, C ₂₃ H ₃₈ N ₇ O ₅ S).

❖ **To display the Mass Calculator**

Choose **Windows > Mass Calculator**.

Syringe Pump Settings Dialog Box

Use the Syringe Pump Settings dialog box to specify parameters of the syringe and the syringe pump. Additionally, use the dialog box to manually operate the syringe pump.

Syringe type	Other
Volume (µL)	10
Syringe inner diameter (mm)	2.300
Flow rate (µL / min)	5.000

Apply Help

Manual control Start Stop

Figure 4-21. Syringe Pump Settings dialog box

Tip Advanced users can select the syringe pump type and enter parameters for the syringe pump in the instrument status window.

The Syringe Pump Settings dialog box has these parameters:

Parameter	Description
Syringe type	Use this list box to specify the syringe type (Hamilton, Unimetrics, or Other). If you select Hamilton or Unimetrics, you must specify the volume of the syringe in the Volume list box. If you select Other, you must specify the inside diameter of the syringe in the Syringe inner diameter spin box.
Volume (µL)	Use this list box to specify the syringe volume for Hamilton and Unimetrics syringes. The acceptable values depend on the syringe type: - Hamilton: 0.5, 1, 2, 5, 10, 25, 50, 100, 250, and 500 µL. - Unimetrics: 10, 25, 50, 100, 250, 500, 1000, 2500, 5000, 10000, 25000, and 50000 µL.
Syringe inner diameter (mm)	Use this spin box to specify the inside diameter for syringes other than Hamilton and Unimetrics syringes. The acceptable range of values is 0.1 to 35 mm. To change this value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, enter a value in the spin box text field.

Parameter	Description
Flow rate (μL/min)	Use this spin box to specify the volume of solvent solution passing through the syringe pump per unit time (in microliters per minute). The acceptable range of values depends on the selected syringe volume or syringe inner diameter. To change this value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, enter a value in the spin box text field.
Buttons	
Apply	Sends all changes to the instrument.
Help	Displays the Help for this window.
Manual Control	Sets the syringe pump to manual control. Use the buttons on the syringe pump to switch it on and off. When the syringe pump is under manual control, Q Exactive UHMR Tune displays .
Start	Switches on the syringe pump. When the syringe pump is On, Q Exactive UHMR Tune displays .
Stop	Switches off the syringe pump. When the syringe pump is Off, Q Exactive UHMR Tune displays .

❖ To display this dialog box

In the toolbar, right-click the  symbol.

Scan Parameters History Dialog Box

Use the Scan Parameters History dialog box to select from a list of recent scans based on short scan descriptions. Select a scan from the list to populate all scan parameters in the Scan Parameters window with the parameters from that scan.

If the Hot link check box is selected in the Scan Parameters window, selecting another list item immediately changes the instrument parameters.

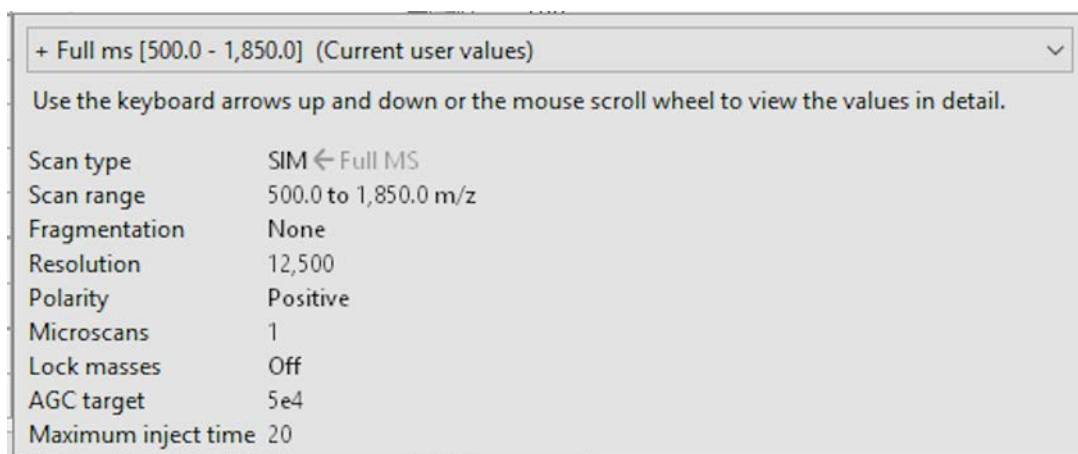


Figure 4-22. Scan Parameters History dialog box

❖ **To display this dialog box**

In the Scan Parameters window, click the History field.

Scan Range Dialog Box

Use the Scan range dialog box to specify the scan range of the data acquisition. The scan range affects the amount of stored and transmitted data.

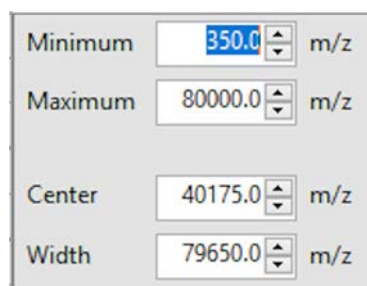


Figure 4-23. Scan range dialog box

The Scan Range dialog box allows setting either minimum and maximum or center and width of the scan range. If you change one pair of values, the other pair is changed accordingly.

The Scan range dialog box has these parameters:

Parameter	Description
Minimum	Use this spin box to select the minimum value for the scan range (in mass-to-charge ratio units) used during the selected scan event. To change the value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. You can enter any m/z value from 350.0 to 79995.0.
Maximum	Use this spin box to select the maximum value for the scan range (in mass-to-charge ratio units) used during the selected scan event. To change the value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. You can enter any m/z value from 355.0 to 80000.0.
Center	Use this spin box to select the center mass (in mass-to-charge ratio units) of the scan range. To change the value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. You can enter any m/z value from 352.5 to 79997.5.
Width	Use this spin box to select the width of the scan range (in mass-to-charge ratio units) used during the selected scan event. To change the value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. You can enter any m/z value from 5.0 to 79650.0.

❖ **To display this dialog box**

In the Scan Parameters window, click the Scan range field.

Fragmentation Dialog Box

Use the Fragmentation dialog box to activate a fragmentation with in-source CID or the HCD collision cell. You can specify the fragmentation voltages to be used.

Figure 4-24. Tune—Fragmentation dialog box

The Fragmentation dialog box has these parameters:

Parameter	Description
In-source CID	Activates the in-source CID. To change the CID collision energy, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. You can set the CID collision energy to any value from 0.1 to 150 eV (ESI source) or 200 eV (NSI source). Automatic tuning is disabled when in-source CID fragmentation is on. To use automatic tuning, clear this check box.
HCD	
	Activates the HCD collision cell. When you select this check box, Q Exactive UHMR Tune automatically changes the scan type, if necessary. When HCD fragmentation is on, automatic tuning comprises only HCD relevant parameters.
NCE / CE	Use the option buttons to specify whether to use normalized collision energy (NCE) or collision energy (CE) for HCD fragmentation. Thus, you can apply the same absolute HCD collision energy for internal standards (ISTDs) and the corresponding analytes. NCE is a dimensionless number that is approximately equivalent to the HCD collision energy (in eV) for a reference ion of mass 500 and charge 1. The actual HCD energy is calculated on basis of mass and charge of the selected precursor ion. To change the value, click the arrows in the spin box to increase [up arrow] or to decrease [down arrow] the value. You can enter any value from 1 to 300.
Charge	Enter the charge state of the ion to be fragmented. The available range is 1 to 100. The required collision energy for fragmenting an ion depends on its charge state. The higher the charge state, the lower the required collision energy. The algorithm for calculating the absolute collision energy is based on empirical data taken from measurements on peptides. For example, the required absolute collision energy to fragment a $[M+2H]^{2+}$ ion is about 90 percent of that of the corresponding $[M+H]^+$ ion. For a $[M+3H]^{3+}$ ion, the value decreases to 85 percent. The spin box is available only if the HCD check box is selected.

❖ To display this dialog box

In the Scan Parameters window, click into the Fragmentation field.

Collection Modification Dialog Box

Use this dialog box to modify a lock mass collection by importing lock masses from an xml file. . This dialog box appears only when the xml file contains information about lock mass collections that differs from the available lock mass collections.



Figure 4-25. Collection Modification dialog box

The Collection Modification dialog box has these parameters:

Parameter	Description
OK	Saves your changes and closes the dialog box. The lock mass collection is updated with the data contained in the xml file.
Cancel	Discards your changes and closes the dialog box.
Help	Displays the Help for this dialog box.

❖ To display this dialog box

1. Choose **Import > Merge with file content** in the shortcut menu of the Lock Masses dialog box.
2. In the file selection dialog box, select an xml file to import from.

Lock Masses Dialog Box

Use the Lock Masses dialog box to edit lock mass lists. The table shows all available lock masses. Lock mass collections store information about lock mass usage.

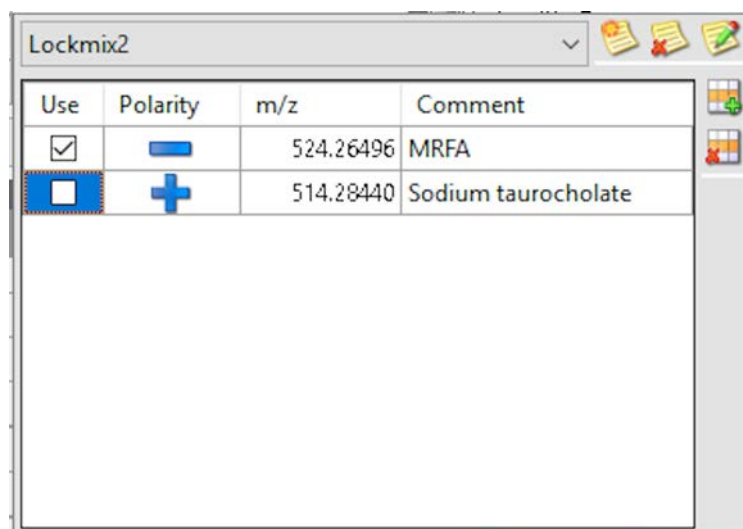


Figure 4-26. Tune—Lock Masses dialog box

The Lock Masses dialog box has these parameters:

Parameter	Description
Lock mass lists	
Lock mass lists	Use the list box to select an existing lock mass collection.
	Displays the New Lock Mass Collection dialog box where you can enter the name for a new lock mass collection.
	Deletes the active lock mass collection. The lock masses themselves are still available.
	This button is not available when no lock mass collection is selected.
	Displays the Name Change dialog box where you can edit the name of the active lock mass collection.
	This button is not available when no lock mass collection is selected.

Parameter	Description
Available lock masses	
The table displays the properties of the available lock masses and whether they are used in the selected lock mass collection. To change the sort order, click the respective table column header. To invert the sort order, click again.	
Lock mass table	• Use Select the check box to use the lock mass. A ☒ indicates that the lock mass is used in the active lock mass collection. The lock mass is displayed in the Lock masses field of the Scan Parameters window. • Polarity Click the symbol to change the polarity of the lock mass. During a scan, the mass spectrometer uses only the lock masses with a polarity that matches the active ion mode. • m/z Enter the mass of the lock mass into the field (with a maximum of five decimals). • Comment Enter a comment for the lock mass into the field. This field is optional.
	Creates a new lock mass.
	Deletes the selected lock masses.

❖ To display this dialog box

In the Scan Parameters window, click into the Lock Masses field.

Shortcut Menu of the Lock Masses dialog box

The Lock Masses dialog box has a shortcut menu that is displayed when you right-click into the dialog box.

It has these commands:

Command	Description
Select all masses in use	Selects all masses used in the active lock mass collection. This command is not available when no lock mass is used.
Import > Merge with clipboard	Appends the content of the clipboard to the available lock masses. The clipboard stores lock mass data as tabulator-separated text files. When the data in the clipboard are not in this format, the command is not available.
Import > Replace by clipboard	Replaces the available lock masses by the content of the clipboard. The clipboard stores lock mass data as tabulator-separated text files. When the data in the clipboard are not in this format, the command is not available.

Command	Description
Import > Merge with file content	Opens a dialog box so that you can select a .csv, .txt, or .xml file that contains a list of lock masses. The content of the file is appended to the available lock masses. See Exporting and Importing Lock Masses for information about the format of lock mass files.
Import > Replace by file content	Opens a dialog box so that you can select a .csv, .txt, or .xml file that contains a list of lock masses. All available lock masses are replaced by the masses contained in the imported file. The present lock masses are removed from all existing lock mass lists. You have to confirm your action in the Lock mass replacement dialog box. See Exporting and Importing Lock Masses for information about the format of lock mass files.
Export > Copy selected to clipboard	Copies the data of the selected lock mass to the clipboard.
Export > Copy all to clipboard	Copies the data of all available lock masses to the clipboard.
Export > Copy selected to file	Opens the dialog box, where you can save the data of the selected lock mass(es) as a .csv, .txt, or .xml file. See Exporting and Importing Lock Masses for information about the format of lock mass files.
Export > Copy all to file	Opens the dialog box, where you can save the data of all available lock masses as a .csv, .txt, or .xml file. See Exporting and Importing Lock Masses for information about the format of lock mass files.

Lock Mass Removal Dialog Box

Use this dialog box to delete one or more lock masses that are selected in the Lock Masses dialog box.

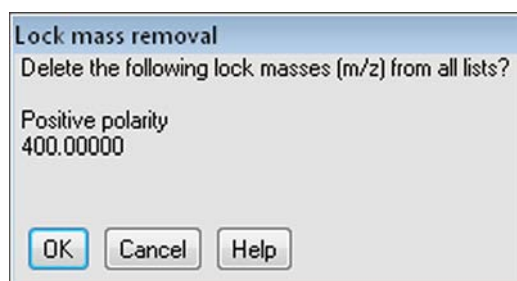


Figure 4-27. Lock Mass Removal dialog box

The Lock Mass Removal dialog box has these parameters:

Parameter	Description
OK	Saves your changes and closes the dialog box. The lock masses are now removed from the table in the Lock Masses dialog box.
Cancel	Discards your changes and closes the dialog box.
Help	Displays the Help for this dialog box.

❖ **To display this dialog box**

In the Lock Masses dialog box, click the  button.

Lock Mass Replacement Dialog Box

Use this dialog box to replace all available lock masses by masses contained either in a csv, txt, or xml file or in the clipboard.

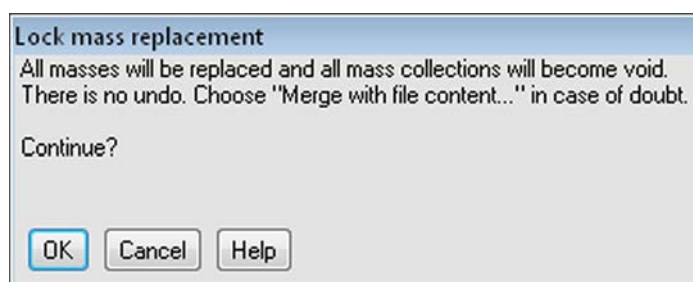


Figure 4-28. Lock Mass Replacement dialog box

The Lock Mass Replacement dialog box has these parameters:

Parameter	Description
OK	Removes the lock masses and replaces them by the imported lock masses. The present lock mass collections become void.
Cancel	Closes the dialog box.
Help	Displays the Help for this dialog box.

❖ **To display this dialog box**

Choose **Import > Replace by file content** or **Import > Replace by clipboard** in the shortcut menu of the Lock Masses dialog box.

New Lock Mass Collection Dialog Box

Use this dialog box to enter a name for the lock mass collection that is displayed in the Lock Masses dialog box.

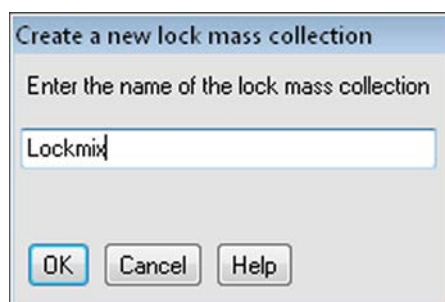


Figure 4-29. New Lock Mass Collection dialog box

The New Lock Mass Collection dialog box has these parameters:

Parameter	Description
Name of lock mass collection	Use this text field to enter the name for the new lock mass collection.
Buttons	
OK	Saves your changes and closes the dialog box. The name of the lock mass collection is now displayed in the list box of the Lock Masses dialog box.
Cancel	Discards your changes and closes the dialog box.
Help	Displays the Help for this dialog box.

❖ To display this dialog box

In the Lock Masses dialog box, click the  button.

Delete Lock Mass Collection Dialog Box

Use this dialog box to delete an existing lock mass collection. The lock masses themselves are not deleted.

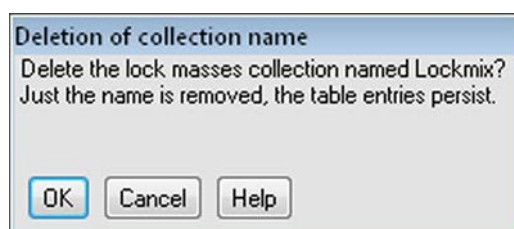


Figure 4-30. Delete Lock Mass Collection dialog box

The Delete Lock Mass Collection dialog box has these parameters:

Parameter	Description
OK	Saves your changes and closes the dialog box. The name of the lock mass collection is now removed from the list box of the Lock Masses dialog box.
Cancel	Discards your changes and closes the dialog box.
Help	Displays the Help for this dialog box.

❖ **To display this dialog box**

In the Lock Masses dialog box, click the  button.

Name Change Dialog Box

Use this dialog box to change the name of an existing lock mass collection.

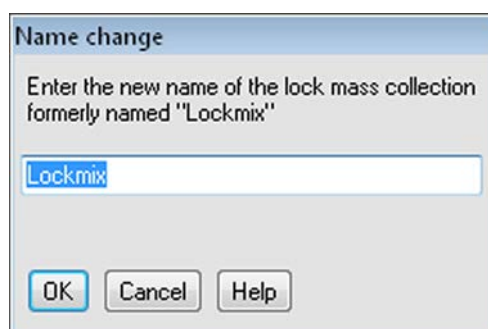


Figure 4-31. Name Change Dialog Box

The Name Change dialog box has these parameters:

Parameter	Description
Name of lock mass collection	Use this text field to enter the new name for the lock mass collection.
Buttons	
OK	Saves your changes and closes the dialog box. The name of the lock mass collection is now displayed in the list box of the Lock Masses dialog box.
Cancel	Discards your changes and closes the dialog box.
Help	Displays the Help for this dialog box.

❖ **To display this dialog box**

In the Lock Masses dialog box, click the  button.

Display Options Dialog Box

Use this dialog box to modify the appearance of the displayed mass spectrum in the spectrum window.

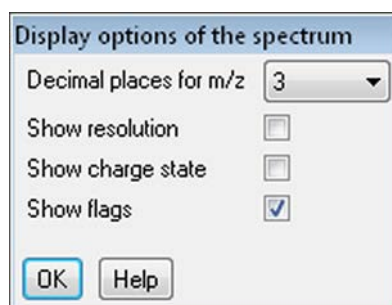


Figure 4-32. Display Options Dialog Box

The Display Options dialog box has these parameters:

Parameter	Description
Decimal places for m/z	Use this list box to set how many decimal places of precision are shown when mass positions are annotated on mass spectra. The valid range is 0 to 5.
Show resolution	Select this check box to have Q Exactive UHMR Tune annotate mass peaks with the mass resolution.
Show charge state	Select this check box to have Q Exactive UHMR Tune annotate mass peaks with the charge state.
Show flags	Select this check box to have Q Exactive UHMR Tune indicate peaks that are contained in the active lock mass collection. The scan parameters window must show entries for lock masses.
Buttons	
OK	Saves your changes and closes the dialog box.
Help	Displays the Help for this dialog box.

❖ To display this dialog box

In the shortcut menu of the spectrum window, choose **Display options**.

Procedures in Q Exactive UHMR Tune

This chapter describes procedures that you may need when using Q Exactive UHMR Tune.

Contents

- [Adding a License](#)
- [Using Lock Masses and Lock Mass Collections](#)
- [Performing a System Bakeout](#)
- [Changing Default Settings of Q Exactive UHMR Tune](#)
- [Using Specific Settings in Q Exactive UHMR Tune](#)

Adding a License

Use the License dialog box to enter licenses that activate additional features.

❖ To add a license

1. Copy the license key that you received from Thermo Fisher Scientific to the clipboard.
2. In Q Exactive UHMR Tune, choose **Help > About** to display the About dialog box.
3. In the About dialog box, click **Add license** to display the License dialog box.
4. Paste the license code from the clipboard into the text field.
5. Click **OK** to save your input and close the License dialog box.

The About dialog box now displays the expiration date of the new license.

Using Lock Masses and Lock Mass Collections

This section provides instructions for using lock masses and lock mass collections.

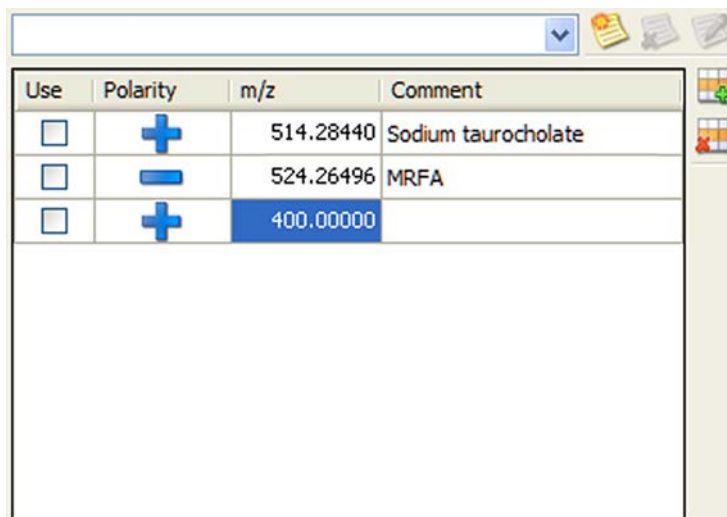
These topics are available:

- [Adding a Lock Mass](#)
- [Deleting Lock Masses](#)
- [Exporting and Importing Lock Masses](#)
- [Creating a new Lock Mass Collection](#)
- [Renaming a Lock Mass Collection](#)
- [Adding a Lock Mass to a Lock Mass Collection](#)
- [Removing a Lock Mass from a Lock Mass Collection](#)
- [Deleting a Lock Mass Collection](#)

Adding a Lock Mass

❖ To add a lock mass

1. In the Lock Masses dialog box, click the  button. A new row appears at the end of the lock mass table.



Use	Polarity	m/z	Comment
☐	+	514.28440	Sodium taurocholate
☐	-	524.26496	MRFA
☐	+	400.00000	

Figure 5-1. Adding a new lock mass

2. Enter the data for the new lock mass into the new table row:
 - a. Select the Use check box if you want to use the new lock mass in the active lock mass collection.

- b. Click the cell in the Polarity column until the correct sign appears:  for positive or  for negative.
- c. Enter the m/z value for the new lock mass (with a maximum of five decimals).
- d. Optionally, enter a comment for the new lock mass.

The new lock mass is now available to be used.

Deleting Lock Masses

❖ To delete lock masses

1. In the Lock Masses dialog box, select one lock mass or several lock masses:
 - To select a single lock mass, click into the respective table row.
 - To select adjacent lock masses, click the first table row. Then hold down the **<Shift>** key while you click the last row.
 - To select nonadjacent lock masses, click the first table row. Then hold down the **<Ctrl>** key while you click the other rows that you want to add to the selection.
2. Click the  button. The Lock Mass Removal dialog box appears and requests your confirmation for deleting the listed lock masses.
3. Click **OK** to confirm your input and to close the dialog box. All selected lock masses are removed from the list in the Lock Masses dialog box.

Exporting and Importing Lock Masses

Q Exactive UHMR Tune allows exporting lock mass data to the clipboard or to a file. Other applications can then use the data. You can also copy the export files to other computers where Q Exactive UHMR Tune is installed. So you can reuse the lock masses without having to recreate them. To reuse the lock masses, import the data either from the clipboard or from a lock mass file.

With a spreadsheet, a text editor, or an XML editor, you can create lock mass files even without using Q Exactive UHMR Tune.

Lock Mass Files

Q Exactive UHMR Tune uses these file formats for exporting and importing lock mass data:

- Comma-separated value lists (.csv)

- Tabulator-separated text files (.txt)
- XML files (.xml)

Lock mass data are stored in this order:

1. Usage status: True for used, False for unused
2. Ion polarity: positive mode or negative mode
3. m/z: up to five decimals
4. Comment: optional

The clipboard stores lock mass data as tabulator-separated text files. In contrast to .csv and .txt files, .xml files additionally store information about lock mass collections and lock mass usage.

Exporting Lock Masses

Q Exactive UHMR Tune allows exporting lock mass data to the clipboard or to a file.

❖ To export selected lock masses to the clipboard

1. In the Lock Masses dialog box, select the lock masses you want to export:
 - To select a single lock mass, click into the respective table row.
 - To select adjacent lock masses, click the first table row. Then hold down the **<Shift>** key while you click the last row.
 - To select nonadjacent lock masses, click the first table row. Then hold down the **<Ctrl>** key while you click the other rows that you want to add to the selection.
2. Right-click into the dialog box to display the shortcut menu.
3. Choose **Export > Copy selected to clipboard** to copy the selected lock mass to the clipboard.

❖ To export all lock masses to the clipboard

1. In the Lock Masses dialog box, right-click into the dialog box to display the shortcut menu.
2. Choose **Export > Copy all to clipboard** to copy all available lock mass to the clipboard.

❖ **To export some lock masses to a file**

1. In the Lock Masses dialog box, select the lock masses you want to export:
 - To select a single lock mass, click into the respective table row.
 - To select adjacent lock masses, click the first table row. Then hold down the <Shift> key while you click the last row.
 - To select nonadjacent lock masses, click the first table row. Then hold down the <Ctrl> key while you click the other rows that you want to add to the selection.
2. Right-click into the dialog box to display the shortcut menu.

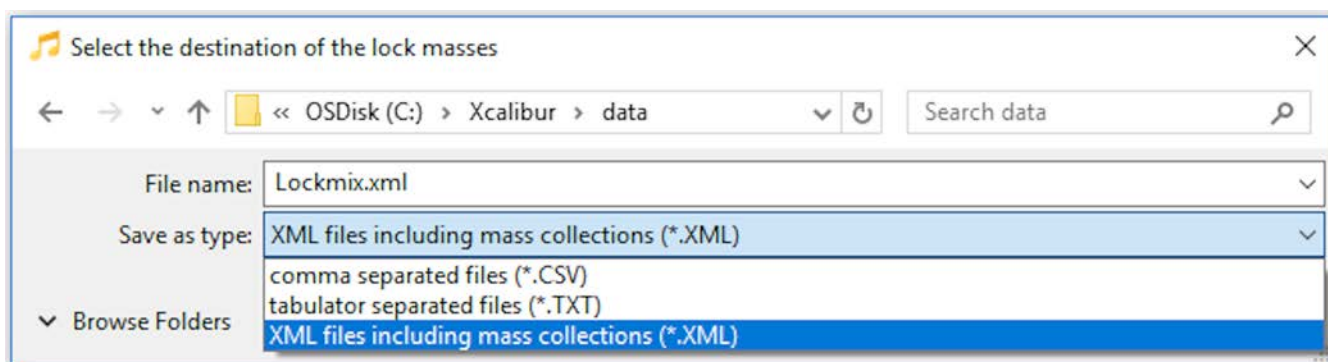


Figure 5-2. Selecting the lock mass export file

3. Choose **Export > Copy selected to file** to open the file selection dialog box.
 - a. Browse to the destination of the export file.
 - b. Select the format of the export file.
 - c. Enter a new name for the export file or select an existing file.
 - d. Click **Save** to export the selected lock masses to the file. If you want to overwrite an existing file, you have to confirm your action in a dialog box. The file selection dialog box is closed.

❖ **To export all lock masses to a file**

1. In the Lock Masses dialog box, right-click into the dialog box to display the shortcut menu.

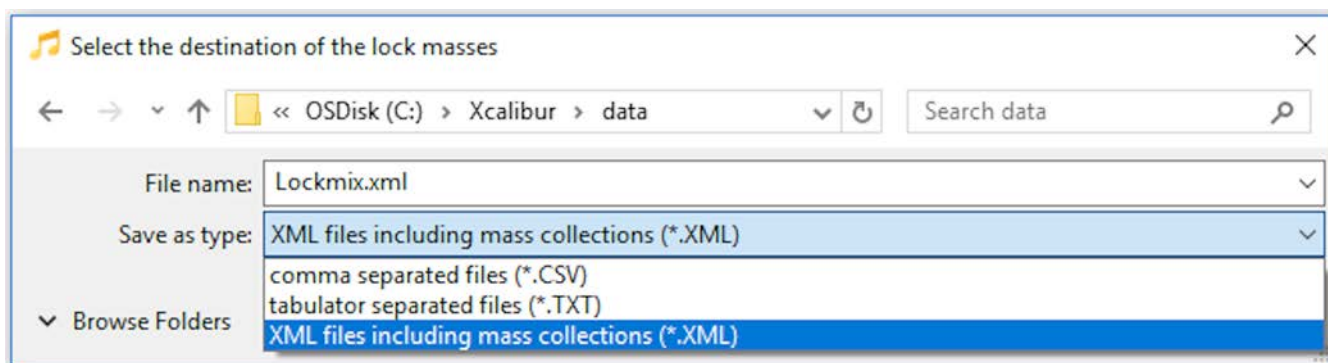


Figure 5-3. Selecting the lock mass export file

2. Choose **Export > Copy all to file** to open the file selection dialog box.
 - a. Browse to the destination of the export file.
 - b. Select the format of the export file.
 - c. Enter a new name for the export file or select an existing file.
 - d. Click **Save** to export the lock masses to the file. If you want to overwrite an existing file, you have to confirm your action in a dialog box. The file selection dialog box is closed.

Importing Lock Masses

Q Exactive UHMR Tune allows importing lock mass data from the clipboard or from a file. The imported lock masses either are added to the present lock masses or they replace them.

❖ To add lock masses from the clipboard

1. Copy lock mass data in an appropriate format to the clipboard. See [Lock Mass Files](#) for information about the requirements.
2. In the Lock Masses dialog box, right-click into the dialog box to display the shortcut menu.
3. Choose **Import > Merge with clipboard** to import the lock mass data from the clipboard to the lock mass table.

The clipboard stores lock mass data as tabulator-separated text files. When the data in the clipboard are not in this format, the command is not available.

4. The lock mass list in the Lock Masses dialog box displays additional rows for the imported lock masses.

❖ **To add lock masses from a file**

1. In the Lock Masses dialog box, right-click into the dialog box to display the shortcut menu.
2. Choose **Import > Merge with file content** to open the file selection dialog box.
 - a. Browse to the destination of the import file.
 - b. Select the format of the import file.
 - c. Select one of the displayed files.
 - d. Click **Open** to import the lock masses to Q Exactive UHMR Tune. The dialog box is closed.
3. If you are importing an xml file that contains information about lock mass collections that differs from the present lock mass collections, the Collection modification dialog is displayed. Click **OK** to confirm the operation and to close the dialog box.

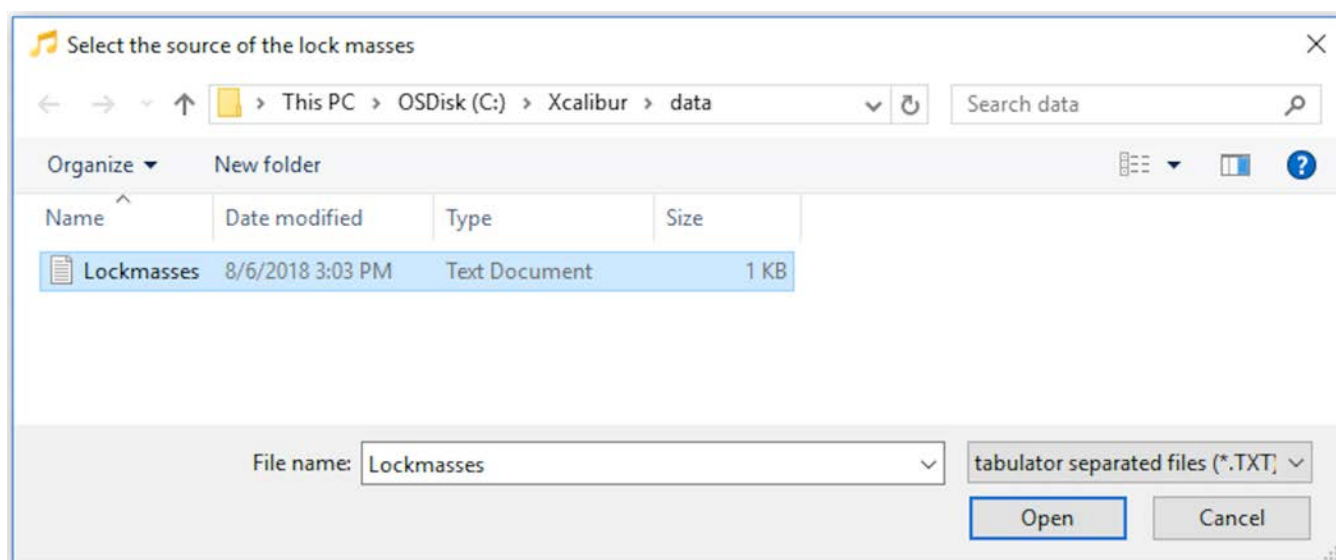


Figure 5-4. Selecting the lock mass import file

4. The lock mass list in the Lock Masses dialog box displays additional rows for the imported lock masses.

❖ **To replace all lock masses by clipboard data**

1. Copy lock mass data in an appropriate format to the clipboard. See [Lock Mass Files](#) for information about the requirements.
2. In the Lock Masses dialog box, right-click into the dialog box to display the shortcut menu.
3. Choose **Import > Replace by clipboard** to import the lock mass data from the clipboard to the lock mass table.

The clipboard stores lock mass data as tabulator-separated text files. When the data in the clipboard are not in this format, the command is not available.

4. The Lock Mass Replacement dialog box is displayed. Click **OK** to confirm the import.
5. The Lock Mass Replacement dialog box is closed. The lock mass list in the Lock Masses dialog box displays only the imported lock masses.

❖ **To replace all lock masses from a file**

1. In the Lock Masses dialog box, right-click into the dialog box to display the shortcut menu.
2. Choose **Import > Replace by file content**.
3. The Lock Mass Replacement dialog box is displayed. Click **OK** to confirm the import.

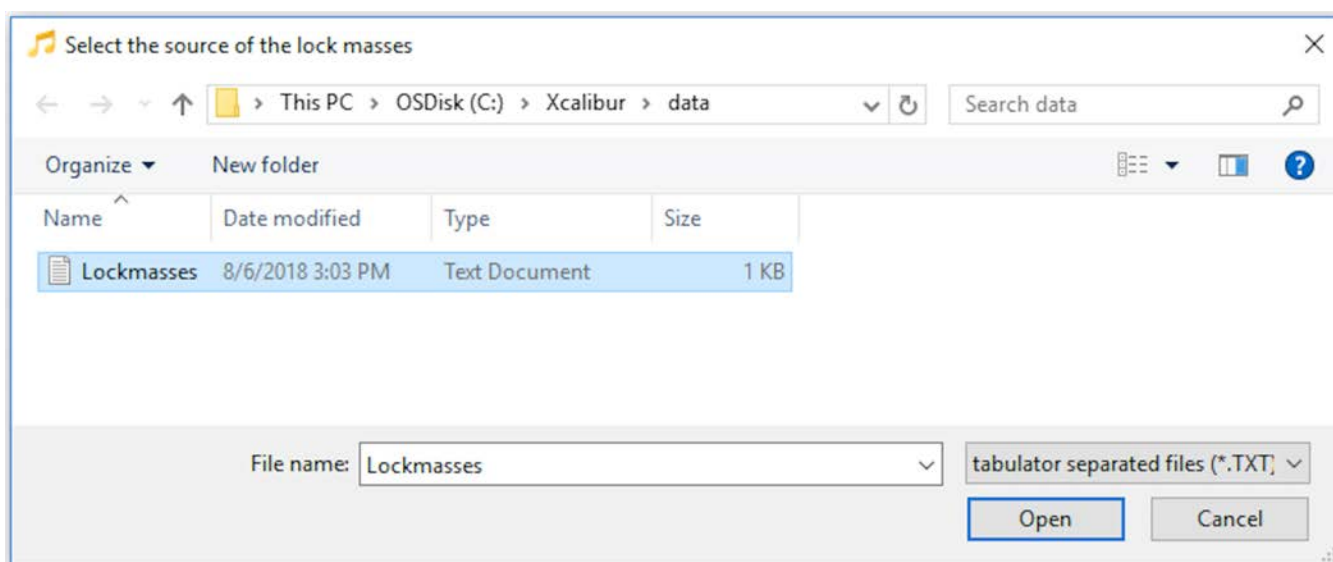


Figure 5-5. Selecting the lock mass import file

4. The Lock Mass Replacement dialog box is closed. The file selection dialog box is displayed.
 - a. Browse to the destination of the import file.
 - b. Select the format of the import file.
 - c. Select one of the displayed files.
 - d. Click **Open** to import the lock masses to Q Exactive UHMR Tune. The dialog box is closed.
5. The lock mass list in the Lock Masses dialog box displays only the imported lock masses.

If you have imported lock mass data from an xml file that contained information about lock mass collections and lock mass usage, the dialog box displays the corresponding information.

Creating a new Lock Mass Collection

❖ To create a lock mass collection

1. In the Lock Masses dialog box, click the  button.
2. In the New Lock Mass Collection dialog box, enter a name for the new lock mass collection.

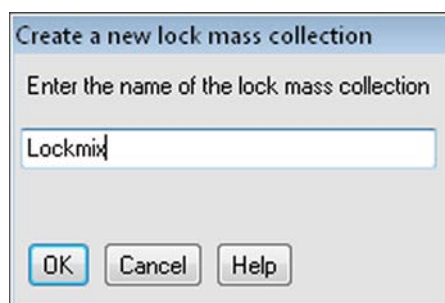


Figure 5-6. Creating a lock mass collection

3. Click **OK** to confirm your input and to close the dialog box.
4. The name of the new lock mass collection appears in the list box of the Lock Masses dialog box.

Renaming a Lock Mass Collection

❖ To rename a lock mass collection

1. In the Lock Masses dialog box, select an existing lock mass collection in the list box.
2. Click the  button. The Name Change dialog box is displayed.

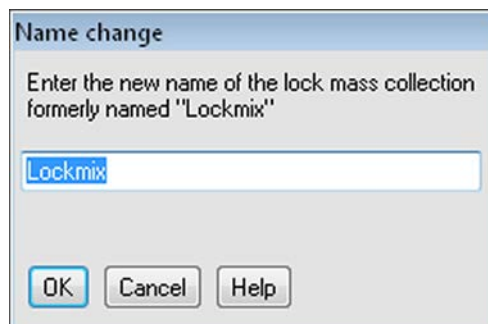


Figure 5-7. Changing the name of a lock mass collection

3. In the text field, replace the old name of the lock mass collection with the new name.
4. Click **OK** to confirm your input and to close the dialog box.
5. In the Lock Masses dialog box, the new lock mass collection is displayed in the list box.

Adding a Lock Mass to a Lock Mass Collection

❖ To add a lock mass to a lock mass collection

1. In the Lock Masses dialog box, select an existing lock mass collection in the list box.
2. Select the Use check box in the table row of the lock mass.
3. A ☒ indicates that the lock mass is used in the active lock mass collection.

Removing a Lock Mass from a Lock Mass Collection

❖ To remove a lock mass from a lock mass collection

1. In the Lock Masses dialog box, select an existing lock mass collection in the list box.
2. Clear the Use check box in the table row of the lock mass.
3. A ☐ indicates that the lock mass is not used in the active lock mass collection.

Deleting a Lock Mass Collection

❖ To delete a lock mass collection

1. In the Lock Masses dialog box, select an existing lock mass collection in the list box.
2. Click the  button.
3. In the Delete Lock Mass Collection dialog box, click **OK** to confirm your action and to close the dialog box.
4. The name of the lock mass collection is removed from the list box of the Lock Masses dialog box.

Performing a System Bakeout

The system bakeout of the mass spectrometer removes unwanted gases or molecules (collected or remaining) from the high vacuum region of the instrument. Ions can collide with those gases or molecules resulting in lower overall sensitivity. Therefore, Thermo Fisher Scientific recommends baking out the instrument if the high vacuum decreases noticeable during routine operation.

Bakeout is mandatory after maintenance or service work is performed in the analyzer region where the system is vented. You should bake out an instrument that has been vented for at least twelve hours (12 hours) before you can start using it again.

In case the system has been vented during a power failure, it is necessary to bake out the system to obtain the operating vacuum.

Tip Before you start the bakeout, make sure that the pumps are up and running at their operating speed. If you have just switched on the mass spectrometer, this will take about 10 minutes. To check the pump speed, open the Instruments Status window and expand the Vacuum System node of the Instrument tree

❖ To perform a system bakeout

1. In the Q Exactive UHMR Tune window, click the **On/Standby** button () to put the instrument in Off condition.
2. In the Tasks panel, click  to display the Vacuum / Bakeout window.
3. Enter the baking duration (in hours) into the spin box. The range is 4 to 30 hours.

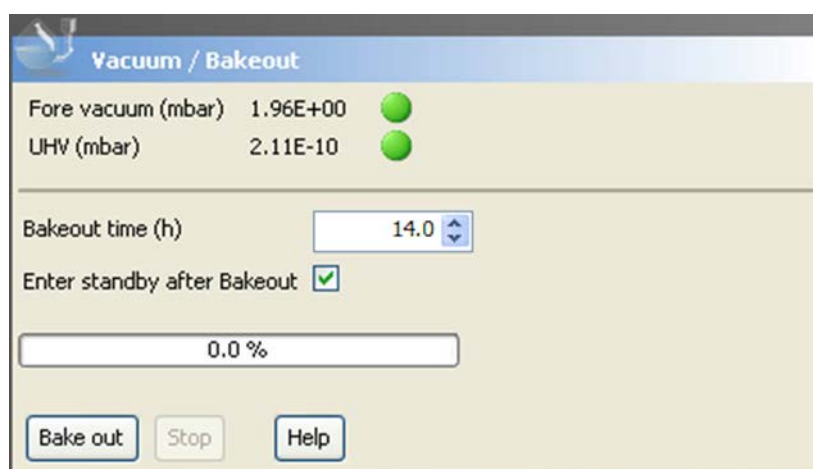


Figure 5-8. Vacuum / Bakeout window

4. Click **Bake out**. A dialog box shows the duration of the baking procedure. Click **Yes** to confirm the message.

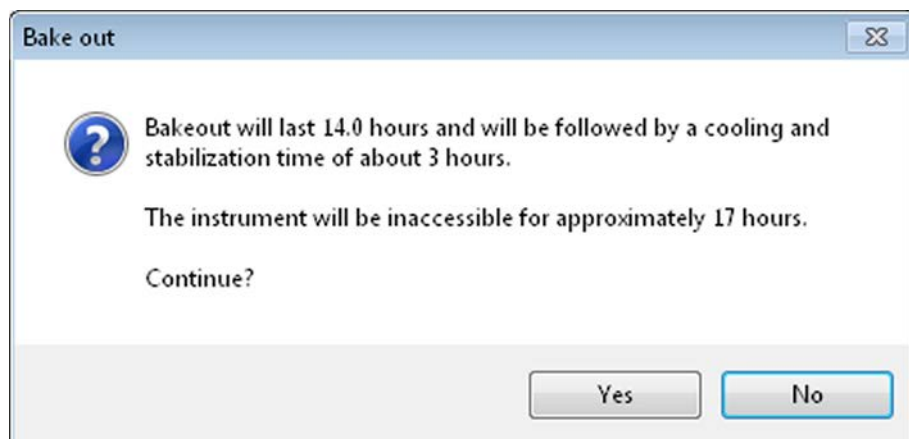


Figure 5-9. Bakeout message box

5. The message box disappears and the baking procedure starts. The instrument indicates the active bakeout procedure by a flashing Vacuum LED at the front side. Additionally, the Q Exactive UHMR Tune software displays a corresponding message box.
6. The baking of the instrument stops after the preset duration. The Vacuum LED keeps flashing until the cooling and stabilization time (of about 3 hours) is finished.

Click **Stop** in the Vacuum / Bakeout window to abort the baking routine before the preset time.

Changing Default Settings of Q Exactive UHMR Tune

Advanced users can use the instrument status window to change default settings of Q Exactive UHMR Tune.

These topics are available:

- [Displaying the High Vacuum Readback](#)
- [Entering Parameters for the Syringe Pump](#)
- [Changing the Settings for the Performance Status Check](#)
- [Changing the Sweep Gas Flow in Standby Mode](#)

Displaying the High Vacuum Readback

The High Vacuum readback in the Vacuum / Bakeout window is visible only when the ion gauge in the high vacuum chamber is switched on. Advanced users can switch on this gauge manually.

Tip Thermo Fisher Scientific recommends that you do not switch on the high vacuum gauge at elevated (>1) trapping gas pressure settings.

❖ To switch on the High Vacuum readback in the Vacuum / Bakeout window

1. Click  **Vacuum / Bakeout** in the tasks panel to display the Vacuum / Bakeout window.
2. If the instrument status window is not visible, choose **Windows > Instrument Status**.
3. In the instrument status window, click **Instrument > Vacuum System**.
4. Right-click the High Vacuum parameter to display the shortcut menu.
5. Choose **Turn on** to switch on the ion gauge in the high vacuum chamber.
6. The Vacuum / Bakeout window now displays the High Vacuum readback.

To extend the lifetime of the ion gauge in the high vacuum chamber, it is switched off again after a preset time of about thirty minutes.

Entering Parameters for the Syringe Pump

The syringe contact of the Q Exactive UHMR mass spectrometer allows controlling established syringe pumps by Q Exactive UHMR Tune by means of the RS-232 serial interface. Suitable syringe pumps are the Chemyx Fusion 100 pump (available from Thermo Fisher Scientific) and the Harvard Apparatus Model 11 Plus Advanced pump. Advanced users can select the syringe pump type and enter parameters for the syringe pump in the instrument status window.

❖ To enter parameters for the syringe pump

1. If the instrument status window is not visible, choose **Windows > Instrument Status**.
2. In the instrument status window, click **Instrument > System > Configuration settings > Peripherals**. The Peripherals node displays parameters for the syringe pump.

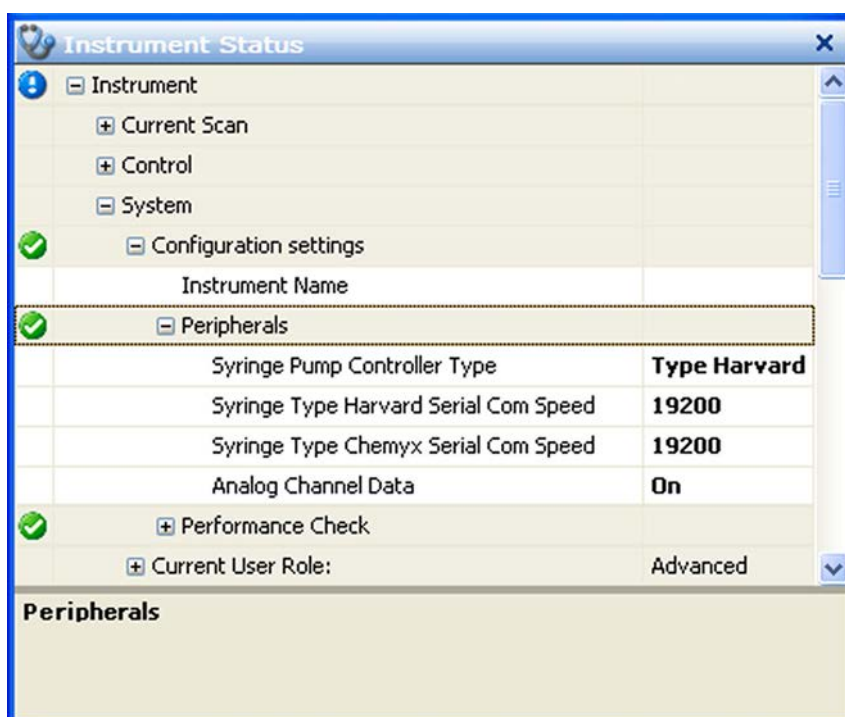


Figure 5-10. Instrument status window—Peripherals node

3. To change the settings for a parameter, right-click the parameter entry to display the shortcut menu. If necessary, change the values of these parameters:
 - Syringe Pump Controller Type: In the list box, select either **Type Harvard** (for Harvard Apparatus Model 11 Plus Advanced pump) or **Type Chemyx** (for Chemyx Fusion 100 pump).

- Syringe Type Harvard Serial Com Speed: Enter the baud rate for the interface into the input field. Available options are 1200, 2400, 4800, 9600, and 19200 bauds. Press the **<Enter>** key to confirm your input.
- Syringe Type Chemyx Serial Com Speed: Enter the baud rate for the interface into the input field. Available options are 1200, 2400, 4800, 9600, and 19200 bauds. Press the **<Enter>** key to confirm your input.

See the manual that came with the syringe pump for the correct baud rate.

Changing the Settings for the Performance Status Check

By default, the performance status icon on the toolbar turns yellow 25 hours after the last successful mass calibration or check. Advanced users can change this value in the System node of the instrument status window according to their mass accuracy requirements.

❖ To change the settings for the performance status check

1. If the instrument status window is not visible, choose **Windows > Instrument Status**.
2. In the instrument status window, click **Instrument > System > Configuration settings > Performance Check**. The Mass calibration due time (h) field displays the active validity period of the mass calibration (25 hours, for example).

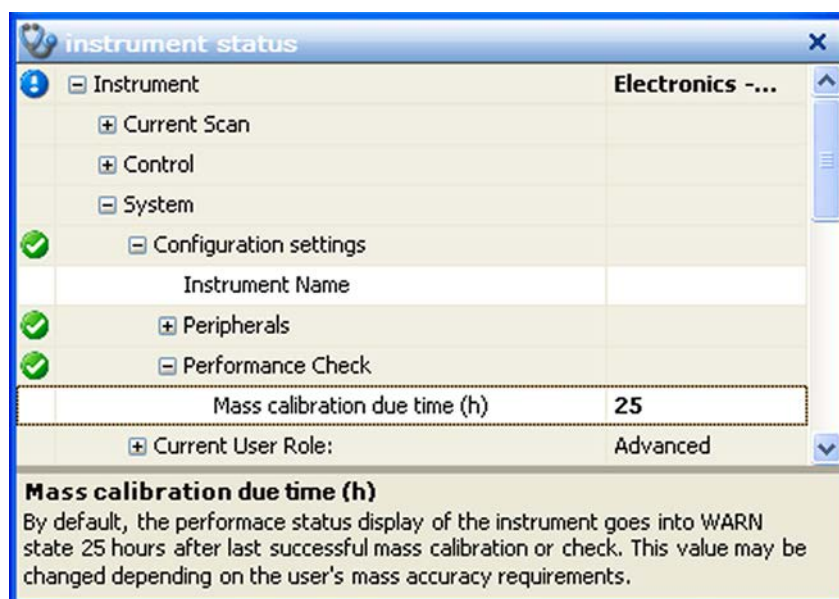


Figure 5-11. Instrument status window—Performance Check node

3. To change the value, right-click the number in the text field to display the shortcut menu.
4. In the Set text field, enter the new validity period (40, for example). You can enter a value between 1 and 500 hours.



Figure 5-12. Changing the calibration validity period

5. Press the <Enter> key to confirm your input. The shortcut menu disappears and the new value is displayed in the instrument status window.

Changing the Sweep Gas Flow in Standby Mode

Advanced users can leave some sweep gas on during standby to positively pressurize the ion source. Studies have shown that this can reduce the amount and size of the particles that get into the system and onto the ion optics.

Users who use nitrogen gas from a limited supply (gas bottles, for example) may want to switch off the sweep gas flow during standby.

❖ To change the sweep gas flow during standby

1. If the instrument status window is not visible, choose **Windows > Instrument Status**.
2. In the instrument status window, click **Instrument > System > Configuration settings > Sweep Gas Flow During Standby**.

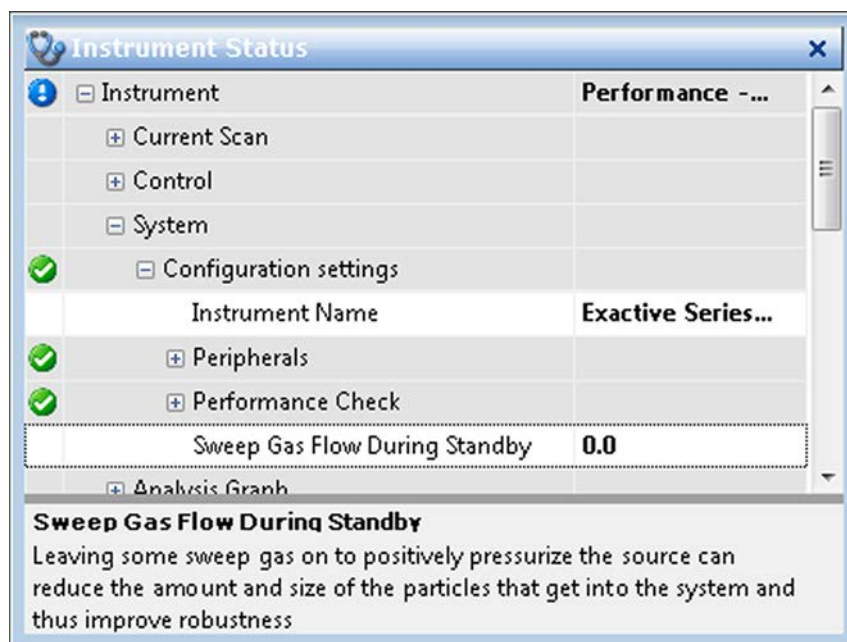


Figure 5-13. Instrument status window—Sweep gas flow during standby

3. To change the value, right-click the number in the text field to display the shortcut menu.
4. In the Set text field, enter the new value (2, for example). You can enter a value between 0 (no sweep gas) and 10 arbitrary units.



Figure 5-14. Changing the sweep gas flow

5. Press the **<Enter>** key to confirm your input. The shortcut menu disappears and the new value is displayed in the instrument status window.

Using Specific Settings in Q Exactive UHMR Tune

The instrument status window provides various parameters that are available for advanced users.

Averaging Spectra

Advanced users can use the instrument status window to enable the rolling averaging of the acquired spectra. If the value is positive, averaging lowers the noise level by performing a cumulative rolling average of the time domain signal by using the specified number of transients.

❖ To enable the averaging of spectra

1. If the instrument status window is not visible, choose **Windows > Instrument Status**.
2. In the instrument status window, click **Instrument > Control > Settings > Define Scan > Averaging**.

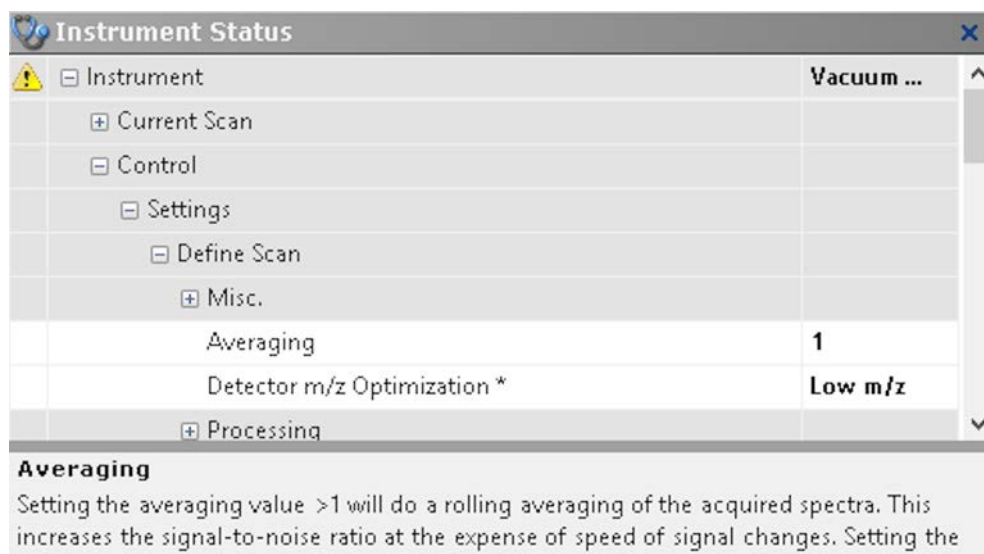


Figure 5-15. Instrument status window—Averaging

3. To change the value, right-click the number in the text field to display the shortcut menu.
4. In the Set text field, enter the new value (100, for example). You can enter either 0 or 1 (no averaging) or an integer between 2 and 1000.



Figure 5-16. Enabling averaging spectra

5. Press the **<Enter>** key to confirm your input. The shortcut menu disappears and the new value is displayed in the instrument status window.

Displaying the Mass Calibration List for UHMR Mode

Advanced users can use the instrument status window to display the list of masses used for mass calibrations and evaluations in UHMR mode. They can also change the used masses, if necessary.

❖ To display the UHMR mass list

1. If the instrument status window is not visible, choose **Windows > Instrument Status**.
2. In the instrument status window, click **Instrument > Control > Procedures > UHMR Mass List**. A list of ten positive masses in the range between m/z 392.7 and m/z 11304.7 and a list of ten negative masses in the range between m/z 386.7 and m/z 11298.7 are displayed.

Setting the HCD Trapping Gas Pressure

HCD trapping enables a better trapping of large molecules. The trapping gas pressure is normalized to the standard operating pressure difference in the trapping region. A value <1 decreases the pressure compared to the standard pressure, a value >1 increase the pressure compared to the standard pressure.

❖ To change the HCD trapping gas pressure

1. If the instrument status window is not visible, choose **Windows > Instrument Status**.
2. In the instrument status window, click **Instrument > Control > Settings**.

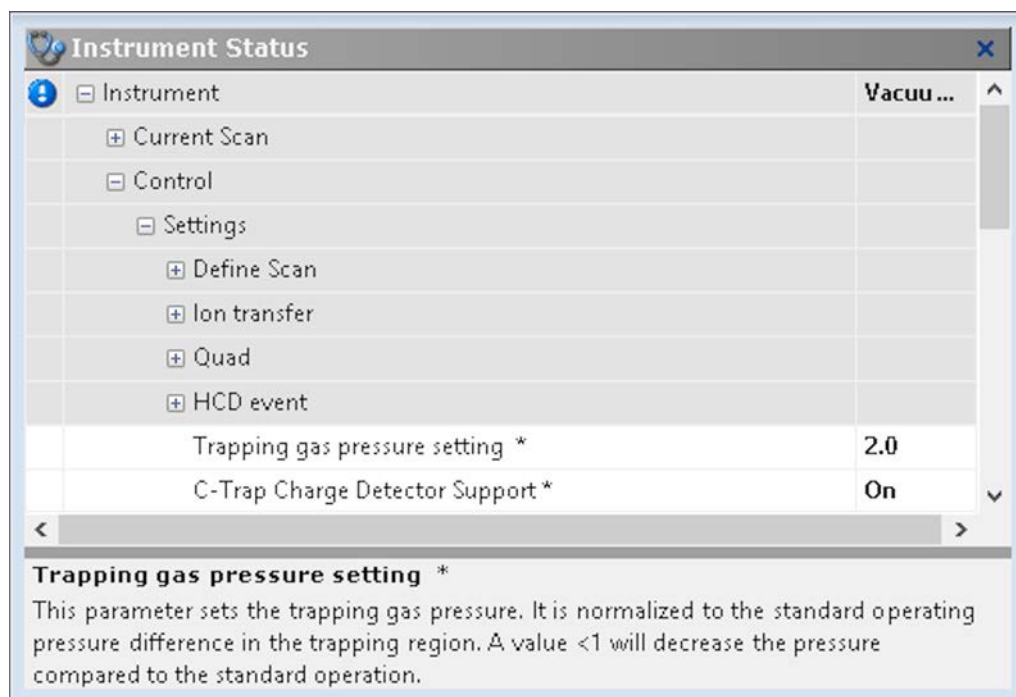


Figure 5-17. Instrument status window—Trapping gas pressure

3. Right-click **Trapping gas pressure setting** to display the shortcut menu.
4. In the Set rel. pressure field, enter the new value (1, for example).

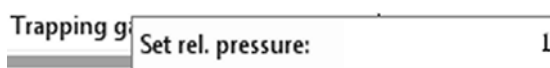


Figure 5-18. Changing the trapping gas pressure

5. Press the <Enter> key to confirm your input. The shortcut menu disappears and the new value is displayed in the instrument status window.

Switching the Detector Mode

Advanced users can use the instrument status window to select the detector mode for the mass calibrations and the eFT calibrations.

❖ To switch the detector mode

1. If the instrument status window is not visible, choose **Windows > Instrument Status**.
2. In the instrument status window, click **Instrument > Control > Settings > Define Scan**.

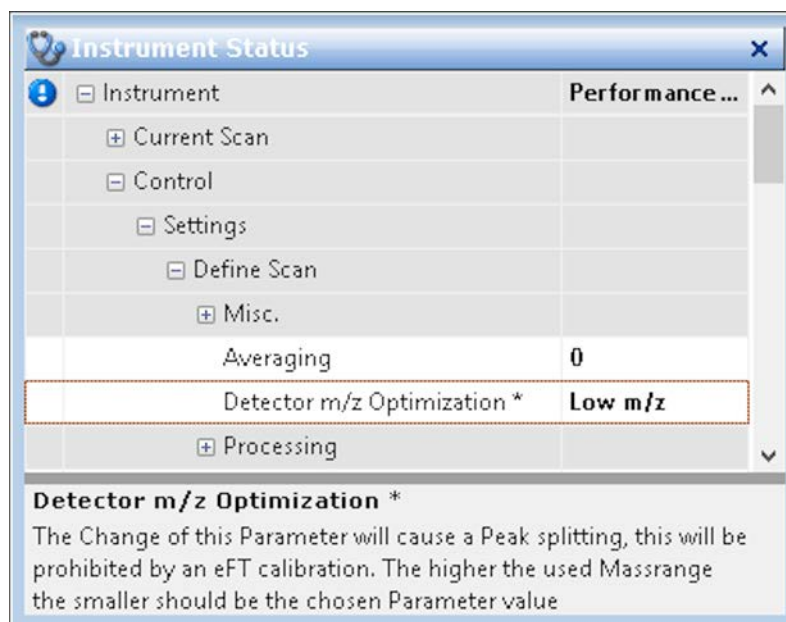


Figure 5-19. Instrument status window—Detector *m/z* Optimization

3. Right-click **Detector *m/z* Optimization** to display the shortcut menu.
4. In the Set field, select the mass range (High *m/z*, for example). You can select either Low *m/z* or High *m/z*.

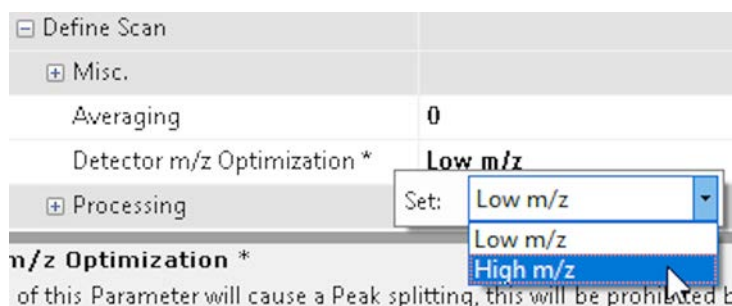


Figure 5-20. Selecting the detector mode

5. Press the **<Enter>** key to confirm your input. The shortcut menu disappears and the new value is displayed in the instrument status window.

Reference Information

This topic provides reference information for the Q Exactive UHMR instrument software.

Contents

- [Log Files](#)
- [Tune Files and Calibration Files](#)
- [API Source Settings for Various LC Flow Rates](#)
- [One-Letter Abbreviations for Amino Acids](#)

Log Files

Log files (*.log) are created for a Q Exactive UHMR mass spectrometer. The default directory for the log files is C:\Xcalibur\system\Exactive\log. The Instrument Configuration window shows the actual path.

Additional log files are created every time the Exactive window service starts. The file name shows date and time of the service start, as shown in this example:

Thermo Exactive--2008-10-22--08-17-22.log

The system automatically deletes all log files that are older than 18 months.

Each line in a log file is a message. A message has several properties that are listed at the beginning of the line, followed by the message body.

Properties are enclosed in brackets. A property is a property name followed by an equal sign followed by the property value. These properties exist:

Abbreviation	Meaning
Time	Time of the message. The local time is displayed followed by the time offset to UTC.
Acc	Windows™ account name that caused this message; “(none)” is used for an instrument source. Other known values are “ExactiveUser” and “Xcalibur_System”.
User	User name description of the Windows account
Comp	Computer name on which this message was caused, “(none)” is used for an instrument source.
App	Application name that caused this message; “(none)” is used for an instrument source.
PID	Process identifier of the application process
Inst	Instrument affected
Conn	Connection in charge for the communication with the instrument
Type	Type of the message. Message types are “info”, “warning”, “error” and “FATAL error”

Access to the log files is regulated by the Microsoft™ Windows user account or group account. Full access to the log files is granted to Administrators. Members of the Power User group can read, delete, and modify these files. Standard users can read these files.

Tune Files and Calibration Files

Tune files and calibration files contain information for operating the instrument.

Tune Files

Tuning optimizes the voltage settings for the API source and the ion transfer optics to ensure highest sensitivity. The resulting tune file (*.mstune) is specific to a particular analyte and solvent flow rate.

During the installation of the instrument, the service engineer creates a tune file in the folder C:\Xcalibur\methods\. Use this file as a starting point for optimizing the mass spectrometer for your specific measurement requirements. Use this folder to store your personal tune files.

Calibration File

Calibrate the Q Exactive UHMR mass spectrometer to ensure the mass accuracy of the measurement results. Calibration parameters are instrument parameters whose values do not vary with the type of experiment. They are stored *automatically* in a calibration file (*.mscal) in the folder

C:\Xcalibur\system\Exactive\instrument\msx_instrument_files\.

The file master_cal.mscal contained in this folder is the calibration file used for operating the instrument. It will be overwritten with new calibration values every time a calibration procedure is successful.

Tip Do not save or change files in the folder C:\Xcalibur\system\Exactive\instrument\msx_instrument_files\! Files in this folder are automatically managed by the instrument software.

API Source Settings for Various LC Flow Rates

The ESI, H-ESI, and HESI-II probes can generate ions from liquid flows of 1 $\mu\text{L}/\text{min}$ to 1.0 mL/min . With this flow rate range, you can use a variety of separation techniques: capillary LC, microbore LC, and analytical LC. An optional nanospray ion source is available for sub-microliter analysis.

As you change the rate of flow of solvents entering the mass spectrometer, you must adjust several of the mass spectrometer parameters:

- For ESI, adjust the temperatures of the ion transfer tube and adjust the gas flow rates for the sheath gas and auxiliary gas.
- For H-ESI, adjust the temperatures of the ion transfer tube and the vaporizer, and adjust the gas flow rates for the sheath gas and auxiliary gas.

In general, the higher the rate of liquid flowing into the mass spectrometer, the higher the temperature of the ion transfer tube (and vaporizer) and the higher the gas flows.

Table 6-1 provides guidelines for setting H-ESI operating parameters for various LC solvent flow rates. Table 6-2 provides guidelines for setting ESI operating parameters.

Table 6-1. Guidelines for setting operating parameters for LC/H-ESI/MS

Liquid flow rate ($\mu\text{L}/\text{min}$)	Capillary (ion transfer tube) temperature ($^{\circ}\text{C}$) ^a	Vaporizer temperature ($^{\circ}\text{C}$) ^b	Sheath gas pressure (arbitrary units)	Auxiliary gas flow (arbitrary units)	Spray voltage (V)
5	275	Off to 50	5	0 to 10 ^c	+3500 (-2500) ^d
200	275	300 to 400	45	30 (H-ESI probe) 10 (HESI-II probe)	+3500 (-2500)
500	300	300 to 400 (H-ESI probe) 300 to 500 (HESI-II probe)	55	50 (H-ESI probe) 15 (HESI-II probe)	+3500 (-2500)
1000	325	350 to 450 (H-ESI probe) 500 (HESI-II probe)	65	60 (H-ESI probe) 20 (HESI-II probe)	+3500 (-2500)

^aAlways optimize the S-lens RF voltage when you change the temperature of the ion transfer tube.

^bCompound dependent

^cAux gas flow must be greater than 0 if the vaporizer is on.

^dNegative ion mode

Table 6-2. Guidelines for setting operating parameters for LC/ESI/MS

Liquid flow rate (μL/min)	Suggested column ID size (mm)	Spray voltage (V)	Capillary temperature (°C)	Sheath gas (arbitrary units)	Auxiliary gas (arbitrary units)
less than 10	Capillary	3000 (-2500) ^a	200 to 250	5 to 30	Off
50 to 100	1.0	3000 (-2500)	250 to 300	10 to 30	5 to 10
200 to 400	2.1 to 4.6	3500 (-2500)	300 to 350	20 to 40	10 to 20
greater than 400	4.6	4000 (-3500)	350	30 to 75	10 to 40

^aNegative ion mode

Default Parameters and Ranges for HESI-2

Table 6-3 lists the parameters and values that Q Exactive UHMR Tune uses when you click **Source Auto-Defaults** in the HESI source window.

Table 6-3. Default Parameters and Ranges for HESI-2

Liquid flow rate (μL/min)	Capillary temp. (°C)	Vaporizer temp. (°C)	Sheath gas press. (arbitrary units)	Auxiliary gas flow (arbitrary units)	Sweep gas flow (arbitrary units)	Spray voltage (V)
5	275	50	5	3	0	+3500 (-2500)
10	275	100	15	5	0	+3500 (-2500)
50	275	150	30	10	1	+3500 (-2500)
100	275	200	35	10	1	+3500 (-2500)
200	275	400	45	10	2	+3500 (-2500)
600	300	450	55	15	3	+3500 (-2500)
1000	325	500	65	20	4	+3500 (-2500)

Spray Voltage is a “tunable” parameter, which can optimize at low voltages (for example, 500–1000 V) for some compounds.

One-Letter Abbreviations for Amino Acids

The table assists you in using the Mass Calculator.

One letter	Name	Formula
A	Alanine	C ₃ H ₅ NO
C	Cysteine	C ₃ H ₅ NOS
D	Aspartate	C ₄ H ₅ NO ₃
E	Glutamate	C ₅ H ₇ NO ₃
F	Phenylalanine	C ₉ H ₉ NO
G	Glycine	C ₂ H ₃ NO
H	Histidine	C ₆ H ₇ N ₃ O
I	Isoleucine	C ₆ H ₁₁ NO
K	Lysine	C ₆ H ₁₂ N ₂ O
L	Leucine	C ₆ H ₁₁ NO
M	Methionine	C ₅ H ₉ NOS
N	Asparagine	C ₄ H ₆ N ₂ O ₂
O	Ornithine	C ₅ H ₁₁ N ₂ O
P	Proline	C ₅ H ₇ NO
Q	Glutamine	C ₅ H ₈ N ₂ O ₂
R	Arginine	C ₆ H ₁₂ N ₄ O
S	Serine	C ₃ H ₅ NO ₂
T	Threonine	C ₄ H ₇ NO ₂
V	Valine	C ₅ H ₉ NO
W	Tryptophan	C ₁₁ H ₁₀ N ₂ O
Y	Tyrosine	C ₉ H ₉ NO ₂

Glossary

This section lists and defines terms used in this manual. It also includes acronyms, metric prefixes, symbols, and abbreviations.

A B C D E F G H I J K L M N O P Q R S T U V W X Y Z

A

A ampere

AC alternating current

ADC analog-to-digital converter; a device that converts data from analog to digital form.

adduct ion An ion formed by the joining together of two species, usually an ion and a molecule, and often within the ion source, to form an ion containing all the constituent atoms of both species.

AGC See [Automatic Gain Control \(AGC\)](#).

AIF All Ion Fragmentation

API See [atmospheric pressure ionization \(API\)](#).

API atmospheric pressure region The first of two chambers in the API source. Also referred to as the spray chamber.

API capillary-skimmer region The area between the capillary and the skimmer, which is surrounded by the tube lens. It is also the area of first-stage evacuation in the API source.

API heated capillary A tube assembly that assists in desolvating ions that are produced by the ESI probe.

See also [API heated capillary voltage](#).

API heated capillary voltage The DC voltage applied to the heated capillary. The voltage is positive for positive ions and negative for negative ions.

See also [API source](#) and [API heated capillary](#).

API ion transfer capillary A tube assembly that assists in desolvating ions that are produced by the ESI probe or the NSI probe.

See also [API ion transfer capillary offset voltage](#) and [API ion transfer capillary temperature](#).

API ion transfer capillary offset voltage A DC voltage applied to the ion transfer capillary. The voltage is positive for positive ions and negative for negative ions.

See also [API source](#) and [API ion transfer capillary](#).

API ion transfer capillary temperature The temperature of the ion transfer capillary, which should be adjusted for different flow rates.

See also [API source](#) and [API ion transfer capillary](#).

API source The sample interface between the LC and the mass spectrometer. It consists of the API probe and the API stack.

See also [atmospheric pressure ionization \(API\)](#), [ESI source](#), [ESI probe](#), and [API stack](#).

API spray chamber The first of two chambers in the API source. In this chamber the sample liquid exits the probe and is sprayed into a fine mist (ESI or NSI) as it is transported to the entrance end of the ion transfer capillary.

API spray shield A stainless steel, cylindrical vessel that, in combination with the ESI flange, forms the atmospheric pressure region of the API source.

See also [atmospheric pressure ionization \(API\)](#).

API stack Consists of the components of the API source that are held under vacuum and includes the [API spray shield](#), [API ion transfer capillary](#), [API tube lens](#), the ion transfer capillary mount, and the tube lens and skimmer mount.

See also [atmospheric pressure ionization \(API\)](#) and [API source](#).

API tube lens A lens in the API source that separates ions from neutral particles as they leave the ion transfer capillary. A potential applied to the tube lens focuses the ions toward the opening of the skimmer and helps to dissociate adduct ions.

See also [API tube lens offset voltage](#), [API source](#), [API ion transfer capillary](#), and [adduct ion](#).

API tube lens and skimmer mount A mount that attaches to the heated capillary mount. The tube lens and skimmer attach to the tube lens and skimmer mount.

API tube lens offset voltage A DC voltage applied to the tube lens. The value is normally tuned for a specific compound.

See also [API tube lens](#), [adduct ion](#), and [source CID](#).

ASCII American Standard Code for Information Interchange

atmospheric pressure ionization (API) Ionization performed at atmospheric pressure by using [electrospray ionization \(ESI\)](#) or [nanospray ionization \(NSI\)](#).

atomic mass unit Atomic Mass Unit (u) defined by taking the mass of one atom of carbon-12 as being 12u; unit of mass for expressing masses of atoms or molecules.

Automatic Gain Control (AGC) Sets the ion injection time to maintain the optimum quantity of ions for each scan. With AGC on, the scan function consists of a prescan and an analytical scan.

See also [ion injection time](#).

auxiliary gas The outer-coaxial gas (nitrogen) that assists the sheath (inner-coaxial) gas in dispersing and/or evaporating sample solution as the sample solution exits the ESI nozzle or the H-ESI nozzle.

auxiliary gas flow rate The relative rate of flow of [auxiliary gas](#) (nitrogen) into the API source reported in arbitrary units.

auxiliary gas inlet An inlet in the API probe where auxiliary gas is introduced into the probe.

See also [auxiliary gas](#) and [atmospheric pressure ionization \(API\)](#).

auxiliary gas plumbing The gas plumbing that delivers outer coaxial nitrogen gas to the ESI nozzle.

auxiliary gas valve A valve that controls the flow of auxiliary gas into the API source.

B

b bit

B byte (8 b)

baud rate data transmission speed in events per second

BTU British thermal unit, a unit of energy

C

°C degrees Celsius

CE central electrode (of the Orbitrap analyzer);

European conformity. Mandatory European marking for certain product groups to indicate conformity with essential health and safety requirements set out in European Directives.

centroid data Data used to represent mass spectral peaks in terms of two parameters: the centroid (the weighted center of mass) and the intensity. The data is displayed as a bar graph. The normalized area of the peak provides the mass intensity data.

cfm cubic feet per minute

CID See [collision-induced dissociation \(CID\)](#).

cm centimeter

cm³ cubic centimeter

collision gas A neutral gas used to undergo collisions with ions.

collision-induced dissociation (CID) An ion/neutral process in which an ion is dissociated as a result of interaction with a neutral target species.

comma-separated values text file A comma-delimited text file. The extension of a comma-separated values text file is csv. This file format can be read by a text editor program, such as Microsoft™ Notepad, or by a spreadsheet program, such as Microsoft Excel™.

CPU central processing unit (of a computer)

C-Trap curved linear trap

<Ctrl> control key on the terminal keyboard

D

d depth

Da dalton

DAC digital-to-analog converter

data-dependent scan A scan mode that uses specified criteria to select one or more ions of interest on which to perform subsequent scans, such as MS/MS or ZoomScan.

DC direct current

divert/inject valve A valve on the mass spectrometer that can be plumbed as a divert valve or as a loop injector.

DS data system

DSP digital signal processor

E

electrospray ionization (ESI) A type of atmospheric pressure ionization that is currently the softest ionization technique available to transform ions in solution into ions in the gas phase.

EMBL European Molecular Biology Laboratory

<Enter> Enter key on the terminal keyboard

ESD ElectroStatic Discharge. Discharge of stored static electricity that can damage electronic equipment and impair electrical circuitry, resulting in complete or intermittent failures.

ESI See [electrospray ionization \(ESI\)](#).

ESI flange A flange that holds the [ESI probe](#) in position next to the entrance of the heated capillary, which is part of the API stack. The ESI flange also seals the atmospheric pressure region of the API source and, when it is in the engaged position against the spray shield, compresses the high-voltage safety-interlock switch.

ESI probe A probe that produces charged aerosol droplets that contain sample ions. The ESI probe is typically operated at liquid flows of 1 µL/min to 1 mL/min without splitting. The ESI probe includes the ESI manifold, sample tube, nozzle, and needle.

ESI source Contains the ESI probe and the API stack.

See also [electrospray ionization \(ESI\)](#), [ESI probe](#), and [API stack](#).

ESI spray current The flow of charged particles in the ESI source. The voltage on the ESI spray needle supplies the potential required to ionize the particles.

ESI spray voltage The high voltage that is applied to the spray needle in the ESI source to produce the ESI spray current. In ESI, the voltage is applied to the spray liquid as it emerges from the nozzle.

See also [ESI spray current](#).

eV Electron Volt. The energy gained by an electron that accelerates through a potential difference of one volt.

Extensible Markup Language See [XML \(Extensible Markup Language\)](#).

external lock mass A lock that is analyzed in a separate MS experiment from your sample. If you need to run a large number of samples, or if accurate mass samples will be intermingled with standard samples, you might want to use external lock masses. These allow more rapid data acquisition by eliminating the need to scan lock masses during each scan.

See also [internal lock mass](#).

F

f femto (10^{-15})

°F degrees Fahrenheit

ft foot

Fast Fourier Transform (FFT) An algorithm that performs a Fourier transformation on data. A Fourier transform is the set of mathematical formulas by which a time function is converted into a frequency-domain function and the converse.

FFT See [Fast Fourier Transform \(FFT\)](#).

firmware Software routines stored in read-only memory. Startup routines and low-level input/output instructions are stored in firmware.

forepump The pump that evacuates the foreline. A rotary-vane pump is a type of forepump.

fragment ion A charged dissociation product of an ionic fragmentation. Such an ion can dissociate further to form other charged molecular or atomic species of successively lower formula weights.

fragmentation The dissociation of a molecule or ion to form fragments, either ionic or neutral. When a molecule or ion interacts with a particle (electron, ion, or neutral species) the molecule or ion absorbs energy and can subsequently fall apart into a series of charged or neutral fragments. The mass spectrum of the fragment ions is unique for the molecule or ion.

FT Fourier Transformation

FTMS Fourier Transformation Mass Spectrometry

full-scan type Provides a full mass spectrum of each analyte or parent ion. With the full-scan type, the mass analyzer is scanned from the first mass to the last mass without interruption. Also known as single-stage full-scan type.

FWHM See [peak width at half height](#).

G

g gram

G Gauss; giga (10^9)

GUI graphical user interface

H

h hour

h height

handshake A signal that acknowledges that communication can take place.

HCD See [higher energy collision-induced dissociation \(HCD\)](#).

header information Data stored in each data file that summarizes the information contained in the file.

H-ESI probe Heated-electrospray ionization (H-ESI) converts ions in solution into ions in the gas phase by using [electrospray ionization \(ESI\)](#) in combination with heated [auxiliary gas](#).

higher energy collision-induced dissociation (HCD)

Collision-induced dissociation that occurs in the HCD cell of the [Orbitrap mass analyzer](#). The HCD cell consists of a straight multipole mounted inside a collision gas-filled tube. A voltage offset between C-Trap and HCD cell accelerates parent ions into the collision gas inside the HCD cell, which causes the ions to fragment into product ions. The product ions are then returned to the Orbitrap analyzer for mass analysis. HCD produces triple quadrupole-like product ion mass spectra.

high performance liquid chromatography (HPLC)

Liquid chromatography in which the liquid is driven through the column at high pressure. Also known as high pressure liquid chromatography.

HPLC See [high performance liquid chromatography \(HPLC\)](#).

HV high voltage

Hz hertz (cycles per second)

I

ID inside diameter

IEC International Electrotechnical Commission

IEEE Institute of Electrical and Electronics Engineers

in. inch

instrument method A set of experiment parameters that define Xcalibur operating settings for the autosampler, liquid chromatograph (LC), mass spectrometer, divert valve, syringe pump, and so on. Instrument methods are saved as file type .meth.

internal lock mass A lock that is analyzed during the same MS experiment as your sample and is contained within the sample solution or infused into the LC flow during the experiment. Internal lock masses provide the most accurate corrections to the data.

See also [external lock mass](#).

I/O input/output

ion gauge Measures the pressure in the mass analyzer region (high vacuum region) of the vacuum manifold.

ion injection time The amount of time that ions are allowed to accumulate in the ion trap mass analyzer when AGC is off. With AGC on, the ion injection time is set automatically (up to the set maximum ion injection time) based on the AGC target value.

See also: [Automatic Gain Control \(AGC\)](#).

ion optics Focuses and transmits ions from the API source to the mass analyzer.

ion source A device that converts samples to gas-phase ions.

ion sweep cone A removable cone-shaped metal cover that fits on top of the [API ion transfer capillary](#) and acts as a physical barrier to protect the entrance of the capillary.

ion sweep gas Extra nitrogen gas that flows along the axis of the API ion transfer capillary (between the ion sweep cone and the capillary block) towards the API spray. The sweep gas flow is thus countercurrent to the flow of the ions.

See also [ion sweep gas pressure](#).

ion sweep gas pressure The rate of flow of the sweep gas (nitrogen) into the API source. A measurement of the relative flow rate (in arbitrary units) to provide the required flow of nitrogen gas out from the Ion Sweep cone towards the API spray.

See also [ion sweep gas](#).

K

k kilo (10³, 1000)

K kilo (2¹⁰, 1024)

KEGG Kyoto Encyclopedia of Genes and Genomes

kg kilogram

L

l length

L liter

LAN local area network

lb pound

LC See [liquid chromatography \(LC\)](#).

LC/MS See [liquid chromatography / mass spectrometry \(LC/MS\)](#).

LED light-emitting diode

liquid chromatography (LC) A form of elution chromatography in which a sample partitions between a stationary phase of large surface area and a liquid mobile phase that percolates over the stationary phase.

liquid chromatography / mass spectrometry (LC/MS) An analytical technique in which a high-performance liquid chromatograph (LC) and a mass spectrometer (MS) are combined.

lock mass A known reference mass in the sample that is used to correct the mass spectral data in an accurate mass experiment and used to perform a real-time secondary mass calibration that corrects the masses of other peaks in a scan. Lock masses with well-defined, symmetrical peaks work best. You can choose to use [internal lock mass](#) or [external lock mass](#).

log file A text file, with a log file extension, that is used to store lists of information.

M

μ micro (10⁻⁶)

m meter; milli (10⁻³)

M mega (10⁶)

M⁺ molecular ion

MB Megabyte (1 048 576 bytes)

MH⁺ protonated molecular ion

microscan One mass analysis (ion injection and storage or scan-out of ions) followed by ion detection. Microscans are summed, to produce one scan, to improve the signal-to-noise ratio of the mass spectral data. The number of microscans per scan is an important factor in determining the overall scan time.

min minute

mL milliliter

mm millimeter

MRFA A peptide with the amino acid sequence methionine–arginine–phenylalanine–alanine.

MS mass spectrometer; mass spectrometry

MS scan modes Scan modes in which only one stage of mass analysis is performed. The scan types used with the MS scan modes are [full-scan type](#) and [selected ion monitoring \(SIM\) scan type](#).

MSDS Material Safety Data Sheet

MS/MS Mass spectrometry/mass spectrometry, or tandem mass spectrometry is an analytical technique that involves two stages of mass analysis. In the first stage, ions formed in the ion source are analyzed by an initial analyzer. In the second stage, the mass-selected ions are fragmented and the resultant ionic fragments are mass analyzed.

MSⁿ scan mode The scan power equal to 1 to 10, where the scan power is the power *n* in the expression MSⁿ. MSⁿ is the most general expression for the scan mode, which can include the following:

- The scan mode corresponding to the one stage of mass analysis in a single-stage full-scan experiment or a selected ion monitoring (SIM) experiment
- The scan mode corresponding to the two stages of mass analysis in a two-stage full-scan experiment or a selected reaction monitoring (SRM) experiment
- The scan mode corresponding to the three to ten stages of mass analysis (*n* = 3 to *n* = 10) in a multi-stage full-scan experiment or a consecutive reaction monitoring (CRM) experiment

See also [MS scan modes](#) and [MS/MS](#).

multipole A symmetrical, parallel array of (usually) four, six, or eight cylindrical rods that acts as an ion transmission device. An RF voltage and DC offset voltage are applied to the rods to create an electrostatic field that efficiently transmits ions along the axis of the multipole rods.

m/z Mass-to-charge ratio. An abbreviation used to denote the quantity formed by dividing the mass of an ion (in u) by the number of charges carried by the ion. For example, for the ion C₇H₇²⁺, *m/z* = 45.5.

N

n nano (10⁻⁹)

nanospray ionization (NSI) A type of electrospray ionization (ESI) that accommodates very low flow rates of sample and solvent on the order of 1 to 20 nL/min (for static nanospray) or 100 to 1000 nL/min (for dynamic nanospray).

NCBI National Center for Biotechnology Information (USA)

NIST National Institute of Standards and Technology (USA)

NMR Normal Mass Range

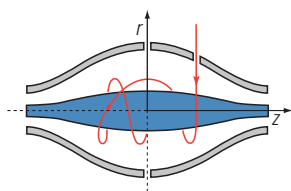
NSI See [nanospray ionization \(NSI\)](#).

O

octapole An octagonal array of cylindrical rods that acts as an ion transmission device. An RF voltage and DC offset voltage applied to the rods create an electrostatic field that transmits the ions along the axis of the octapole rods.

OD outside diameter

Orbitrap mass analyzer The Orbitrap™ mass analyzer consists of a spindle-shape central electrode surrounded by a pair of bell-shaped outer electrodes. Ions inside the mass analyzer orbit in stable trajectories around the central electrode with harmonic oscillations along it.



Two detection electrodes record an image current of the ions as they undergo harmonic oscillations. A Fourier transformation extracts different harmonic frequencies from the image current. An ion's mass-to-charge ratio m/z is related to the frequency f of its harmonic oscillations and to the instrumental constant k by: $m/z = k/f^2$

OT Orbitrap

See [Orbitrap mass analyzer](#).

OVC outer vacuum case

Ω ohm

P

p pico (10^{-12})

Pa pascal

parent ion An electrically charged molecular species that can dissociate to form fragments. The fragments can be electrically charged or neutral species. A parent ion can be a molecular ion or an electrically charged fragment of a molecular ion. Also called a precursor ion.

parent mass The mass-to-charge ratio of a parent ion. The location of the center of a target parent-ion peak in mass-to-charge ratio (m/z) units. Also known as precursor mass.

See also [parent ion](#).

PCB printed circuit board

PDA detector Photodiode Array detector is a linear array of discrete photodiodes on an integrated circuit chip. It is placed at the image plane of a spectrometer to allow a range of wavelengths to be detected simultaneously.

PE protective earth

peak A maximum in a graph of intensity versus time or intensity versus mass. The position of the maximum is said to be the position of the peak.

peak end The end of a chromatographic peak occurs when the detection signal decreases to a value less than the current threshold criteria.

See also [peak start](#).

peak height (peak dimension) The distance from the peak maximum to the peak base, measured perpendicular to the ordinate.

peak start The start of a chromatograph peak occurs when the detection signal increases to a value greater than the current threshold criteria.

See also [peak end](#).

peak width The distance across a peak measured at a selected peak-height level, in minutes or mass units. The peak-height level is usually specified as a percentage of the maximum peak height.

See also [peak width at half height](#).

peak width at half height The full width of a peak at half its maximum height, sometimes abbreviated FWHM.

See also [peak width](#) and [peak end](#).

PID proportional / integral / differential

P/N part number

p-p peak-to-peak voltage

ppm parts per million

precursor ion An electrically charged molecular species that can dissociate to form fragments. The fragments can be electrically charged or neutral species. A precursor ion (PR) can be a molecular ion or an electrically charged fragment of a molecular ion. Also known as parent ion.

precursor mass Mass of the corresponding precursor (or parent) ion or molecule.

profile data Data representing mass spectral peaks as point-to-point plots, with each point having an associated intensity value.

psig pounds per square inch, gauge

PTM posttranslational modification

Q

quadrupole A symmetrical, parallel array of four hyperbolic rods that acts as a mass analyzer or an ion transmission device. As a mass analyzer, one pair of opposing rods has an oscillating radio frequency (RF) voltage superimposed on a positive direct current (DC) voltage. The other pair has a negative DC voltage and an RF voltage that is 180 degrees out of phase with the first pair of rods. This creates an electrical field (the quadrupole field) that efficiently transmits ions of selected mass-to-charge ratios along the axis of the quadrupole rods.

R

RAM random access memory

raw data Uncorrected liquid chromatograph and mass spectrometer data obtained during an acquisition. Xcalibur and Xcalibur-based software store this data in a file that has a .raw file extension.

resolution The ability to distinguish between two points on the wavelength or mass axis.

retention time (RT) The time after injection at which a compound elutes. The total time that the compound is retained on the chromatograph column.

RF radio frequency

RF lens A multipole rod assembly that is operated with only radio frequency (RF) voltage on the rods. In this type of device, virtually all ions have stable trajectories and pass through the assembly.

RF voltage An AC voltage of constant frequency and variable amplitude that is applied to the ring electrode or endcaps of the mass analyzer or to the rods of a multipole. Because the frequency of this AC voltage is in the radio frequency (RF) range, it is referred to as RF voltage.

RMS root mean square

ROM read-only memory

rotary-vane pump A mechanical vacuum pump that establishes the vacuum necessary for the proper operation of the turbomolecular pump. (Also called a roughing pump or forepump.)

RS-232 An accepted industry standard for serial communication connections. This Recommended Standard (RS) defines the specific lines and signal characteristics used by serial communications controllers to standardize the transmission of serial data between devices.

RT An abbreviated form of the phrase *retention time (RT)*. This shortened form is used to save space when the retention time (in minutes) is displayed in a header, for example, RT: 0.00-3.75.

S

s second

scan mode and scan type combinations A function that coordinates the three processes in the MS detector: ionization, mass analysis, and ion detection. You can combine the various scan modes and scan types to perform a wide variety of experiments.

selected ion monitoring (SIM) scan type A scan type in which the mass spectrometer acquires and records ion current at only one or a few selected mass-to-charge ratio values.

See also [selected reaction monitoring \(SRM\) scan type](#).

selected reaction monitoring (SRM) scan type A scan type with two stages of mass analysis and in which a particular reaction or set of reactions, such as the fragmentation of an ion or the loss of a neutral moiety, is monitored. In SRM a limited number of product ions is monitored.

Serial Peripheral Interface (SPI) hardware and firmware communications protocol

serial port An input/output location (channel) for serial data transmission.

sheath gas The inner coaxial gas (nitrogen), which is used in the API source to help nebulize the sample solution into a fine mist as the sample solution exits the ESI nozzle.

sheath gas flow rate The rate of flow of sheath gas into the API source. A measurement of the relative flow rate (in arbitrary units) that needs to be provided at the sheath gas inlet to provide the required flow of [sheath gas](#) to the ESI nozzle.

sheath gas inlet An inlet in the API probe where [sheath gas](#) is introduced into the probe.

sheath gas plumbing The gas plumbing that delivers [sheath gas](#) to the ESI nozzle.

sheath gas pressure The rate of flow of sheath gas (nitrogen) into the API source. A measurement of the relative flow rate (in arbitrary units) that needs to be provided at the sheath gas inlet to provide the required flow of inner coaxial nitrogen gas to the ESI nozzle. A software-controlled proportional valve regulates the flow rate.

See also [sheath gas](#).

sheath gas valve A valve that controls the flow of [sheath gas](#) into the API source. The sheath gas valve is controlled by the data system.

signal-to-noise ratio (S/N) The ratio of the signal height (S) to the noise height (N). The signal height is the baseline corrected peak height. The noise height is the peak-to-peak height of the baseline noise.

SIM See [selected ion monitoring \(SIM\) scan type](#).

source CID A technique for fragmenting ions in an [atmospheric pressure ionization \(API\)](#) source. Collisions occur between the ion and the background gas, which increase the internal energy of the ion and stimulate its dissociation.

SPI See [Serial Peripheral Interface \(SPI\)](#).

SRM See [selected reaction monitoring \(SRM\) scan type](#).

sweep gas Nitrogen gas that flows out from behind the sweep cone in the API source. Sweep gas aids in solvent declustering and adduct reduction.

See also [sweep gas flow rate](#).

sweep gas flow rate The rate of flow of sweep gas into the API source. A measurement of the relative flow rate (in arbitrary units) to provide the required flow of nitrogen gas to the sweep cone of the API source.

See also [sweep gas](#).

syringe pump A device that delivers a solution from a syringe at a specified rate.

T

T Tesla

target compound A compound that you want to identify or quantitate or that a specific protocol (for example, an EPA method) requires that you look for. Target compounds are also called analytes, or target analytes.

TIC See [total ion current \(TIC\)](#).

TMP See [turbomolecular pump](#).

Torr A unit of pressure, equal to 1 mm of mercury and 133.32 Pa.

total ion current (TIC) The sum of the ion current intensities across the scan range in a mass spectrum.

tube lens offset The voltage offset from ground that is applied to the tube lens to focus ions toward the opening of the skimmer.

See also [source CID](#).

Tune Method A defined set of mass spectrometer tune parameters for the ion source and mass analyzer. Tune methods are defined by using the instrument software's tune window and saved as tune file.

A tune method stores tune parameters only. (Calibration parameters are stored separately, not with the tune method.)

tune parameters Instrument parameters whose values vary with the type of experiment.

turbomolecular pump A vacuum pump that provides a high vacuum for the mass spectrometer and detector system.

TWA time weighted average

U

u atomic mass unit

UHV ultra high vacuum

ultra-high performance liquid chromatography (U-HPLC) See [high performance liquid chromatography \(HPLC\)](#).

Ultramark 1621 A mixture of perfluoroalkoxycyclotriphosphazenes used for ion trap calibration and tuning. It provides ESI singly charged peaks at m/z 1022.0, 1122.0, 1222.0, 1322.0, 1422.0, 1522.0, 1622.0, 1722.0, 1822.0, and 1921.9.

UMR Universal Mass Range

V

V volt

VAC volts alternating current

VDC volts direct current

vacuum manifold A thick-walled, aluminum chamber with machined flanges on the front and sides and various electrical feedthroughs and gas inlets that encloses the API stack, ion optics, mass analyzer, and ion detection system.

vacuum system Components associated with lowering the pressure within the mass spectrometer. A vacuum system includes the vacuum manifold, pumps, pressure gauges, and associated electronics.

vent valve A valve that allows the vacuum manifold to be vented to air or other gases. A solenoid-operated valve.

vol volume

W

w width

W watt

WEEE European Union Waste Electrical and Electronic Equipment Directive. Provides guidelines for disposal of electronic waste.

X

XML (Extensible Markup Language) A general-purpose markup language that is used to facilitate the sharing of data across different information systems, particularly via the Internet.



Index

Symbols

.csv file 4-60–4-61, 5-5
.exclude-masses file 3-52
.include-masses file 3-47
.ini file 4-6
.lock-masses file 3-45
.log file 6-2
.meth file 4-21
.mscal file 6-3
.mstune file 4-5, 4-9, 6-3
.raw file 3-18, 4-21
.txt file 4-60–4-61, 5-5
.xml file 4-57, 4-60–4-61, 5-5

A

About dialog box 1-2, 4-47, 5-2
Access audit database 1-2
acquisition time 4-22
Acquisition window 4-20
AGC target value 3-32, 3-34, 3-37–3-38, 4-14
All Ion Fragmentation (AIF) 3-21
analysis graphs window
 description 4-42
 shortcut menu 4-43
 toolbar 4-43
 zooming 4-42
apex trigger 3-40
asterisk, in the title bar 4-3
Audit Trail 3-3–3-4
auditing 1-2
autosampler 4-22
Autoselect ion source values dialog box 4-47
auxiliary gas
 H-ESI 4-15
 NSI 4-18
averaging, spectra 5-19

B

bakeout
 duration 4-30
 purpose 5-12

C

Calibrate window 4-25

calibration
 file 6-3
 High Mass Range 5-20
 of quadrupole 4-27
 parameters 4-25
 reports 4-7
 solution 4-25, 4-27
capillary temperature 4-16, 4-19
center mass 3-32, 3-35, 3-37, 4-55
charge exclusion 3-40
charge state 3-40, 3-49, 3-54, 4-56
charge state distribution 3-41
chromatogram display 3-18
Chromeleon 1-2
clipboard 3-46, 3-52, 3-56, 4-41, 4-47, 4-59–4-60
collision energy (CE) 3-33, 3-39
comma separated values text file 5-4
comment, on active sample 4-22
communication status 2-2, 4-10
connection status 1-2
contact closure 3-16, 4-22–4-23
cooling and stabilization time 4-30
creep mode 4-36
CsI Calibration window 4-26
CsI Evaluation window 4-28

D

data acquisition 4-23
debug messages window 4-43
default charge state 3-36
dialog boxes 3-44, 4-46
Display Options dialog box 4-64
display panel 4-4
Divert Valves page 3-11
duration, of bakeout 4-30
dynamic exclusion 3-42

E

elapsed time
 of active acquisition 4-21
 of active procedure 4-25, 4-28, 4-31
error diagnosis 4-30, 4-40
Evaluate window 4-27
evaluation procedure 4-27
Exactive window service 6-2
Exclusion List dialog box 3-52

exclusion masses list [3-36](#)
Experiment pane [3-20](#)
Experiment Setup page [3-7](#)
exporting lock masses [5-4–5-5](#)

F

File menu [3-3, 4-5](#)
File Summary Information Dialog Box [3-5](#)
first mass [3-39](#)
flow rate [3-28, 4-53](#)
forevacuum line [4-30](#)
fragmentation
 settings [4-13, 4-55](#)
 type [4-34](#)
Fragmentation dialog box [4-55](#)

H

hardware status [2-2, 4-11](#)
HCD cell
 activating [4-56](#)
HCD trapping [5-20](#)
header information [3-4–3-5](#)
Help menu [3-4](#)
H-ESI
 heater temperature [4-17](#)
 sheath gas flow rate [4-15](#)
 source [4-14](#)
 spray current [4-16](#)
 spray voltage [4-16](#)
 sweep gas flow rate [4-16](#)
HESI source window [4-14](#)
high vacuum chamber [4-30, 5-14](#)
Home Page window [2-1](#)
Hot link [4-12, 4-14](#)

I

image files [4-36, 4-43](#)
importing
 data from csv files or txt files [3-44](#)
 lock masses [5-7](#)
Inclusion List dialog box [3-47](#)
inclusion masses list [3-36](#)
inject time [4-34](#)
inside diameter, for syringes [4-52](#)
in-source CID
 activation [4-55](#)
 collision energy [3-31, 3-33, 3-36, 4-56](#)
 settings [4-13](#)
installed instruments [4-4, 4-7, 4-10, 4-32](#)
instrument bakeout [4-29](#)

Instrument Configuration program [3-2–3-3](#)
Instrument Configuration window [1-1](#)
Instrument Control panel [4-12](#)
instrument files [1-2](#)
instrument identification [4-47](#)
instrument method [3-4–3-5, 4-21, 4-34](#)
Instrument Setup window [3-2](#)
instrument status [1-2, 4-9](#)
instrument status window
 shortcut menus [4-37](#)
 Vacuum System node [4-30](#)
instrument type [1-2](#)
ion polarity [4-34](#)
ion source region [4-30](#)
Ion Source Trapping [3-31, 3-33, 3-37](#)
IP address [1-2](#)
isolation offset [3-39](#)
isolation range [3-32, 3-35, 3-38, 4-49](#)
Isolation Range dialog box [4-48](#)
isolation width [3-39](#)
isolation window [3-39](#)
isotope clusters [3-41](#)

L

license
 key [4-49, 5-2](#)
 settings [4-47, 5-2](#)
License dialog box [4-49, 5-2](#)
list, of recent scans [4-13](#)
lock mass collection
 deleting [4-62](#)
 name [4-62–4-63](#)
Lock Mass Replacement dialog box [4-61](#)
lock masses
 creating [4-59](#)
 editing [3-44, 3-47, 3-52, 4-57](#)
 exporting [5-4](#)
 usage [3-24, 4-14, 4-64](#)
Lock Masses dialog box [3-44, 4-57](#)
log file [1-2](#)
Loop count [3-38](#)

M

mains failure [5-12](#)
manual control, of syringe pump [4-53](#)
mass accuracy [5-16](#)
Mass Calculator [3-57, 4-7, 4-50](#)
mass calibration [5-16](#)
mass resolution [3-31, 3-34, 3-37–3-38, 4-13, 4-64](#)
Mass Traces window [4-23](#)
maximum audit record length [1-2](#)

- maximum injection time 3-32, 3-34, 3-37–3-38, 4-14
- maximum value, for apex trigger 3-40
- maximum value, for scan range 3-32, 3-35, 3-37, 4-55
- menu bar 4-3
- messages window 4-41
- Method Editor 3-6
- microscan 3-31, 3-34, 3-37–3-38, 4-14, 4-34
- minimum value, for apex trigger 3-40
- minimum value, for scan range 3-32, 3-35, 3-37, 4-55
- most abundant charge state 3-41
- mouse
 - panning 4-34, 4-36, 4-43
 - wheel 4-34, 4-42
 - zooming 4-36
- multiple charge states 3-41

N

- nanospray ionization 4-18
- network address 1-2
- network drives 4-21
- noise level 4-34
- normalized collision energy (NCE) 3-50, 4-56
- NSI
 - sheath gas flow rate 4-18
 - source 4-18
 - source window 4-18
 - spray current 4-19
 - spray voltage 4-19
 - sweep gas flow rate 4-19
- number, of scans 4-34

O

- Oracle audit database 1-2
- Orbitrap chamber 4-30

P

- page setup 3-4
- peptide-like isotopic distributions 3-41
- performance status 2-2, 4-11, 5-16
- Pirani gauge 4-30
- polarity 3-31, 3-33, 3-36, 3-45, 3-49, 3-54, 4-13
- precision, of mass positions 4-64
- pressure values 4-29
- print preview 4-35, 4-43
- printer's parameters 4-35, 4-43
- printing 3-4, 3-43
- pumping, the system 5-12

Q

- quadrupole
 - calibration 4-27
 - transmission 4-29
- quadrupole isolation range 4-48
- Qual Browser 4-21

R

- removing, gases 5-12
- Reports menu 4-7
- resolution 3-31, 3-34, 3-37–3-38, 4-13
- RS-232 5-15

S

- sample name 4-21
- scan event 4-34
- Scan Groups pane 3-19
- Scan Parameters History dialog box 4-53
- Scan Parameters window 4-12
- scan range 4-13, 4-34, 4-54
- Scan range dialog box 4-54
- scan segment 4-34
- scan type 4-13, 4-34
- Sequence Setup View 4-9
- setup parameters 3-2
- shortcut menus
 - analysis graphs window 4-43
 - debug messages window 4-45
 - instrument status window 4-37
 - Lock Masses dialog box 4-59
 - spectrum window 4-36
 - Status page 2-1
 - tray icon 4-2
- S-lens RF amplitude 4-17, 4-20
- software version 4-47
- source type 4-34
- spectrum window
 - display options 4-64
 - toolbar 4-35
 - visibility 4-32
 - zooming 4-34
- standby mode 4-30
- Status page, of Information view 2-1
- status, of active acquisition 4-21
- Summary page 3-43
- sweep gas flow, during standby 5-17
- switch positions
 - of switching valves 3-27
 - of syringe pump 3-26–3-28
 - of tune files 3-26
- syringe

- diameter [3-28](#)
- type [3-28](#), [4-52](#)
- volume [3-28](#), [4-52](#)
- syringe pump
 - interface [5-15](#)
 - manual control [4-53](#)
 - operating status [3-27](#), [4-10](#)
 - parameters [4-52](#)
- system bakeout [5-12](#)
- system settings [4-6](#)
- system tray, in Microsoft Windows [4-2](#)

T

- tasks panel [4-3](#), [4-12](#)
- text editor [4-41](#)
- third party licenses [4-47](#)
- title bar [3-45](#), [3-50](#), [3-55](#), [4-3](#)
- toggling, between mouse panning and mouse zooming [4-36](#)
- toolbars
 - analysis graphs window [4-43](#)
 - spectrum window [4-35](#)
 - Tune window [4-9](#)
- tooltip [4-6](#)
- TopN [3-21](#), [3-36](#)
- total ion current (TIC)
 - plotting [4-24](#)
- trapping gas pressure [5-20](#)
- tune file [4-5](#), [6-3](#)
- Tune Method [4-3](#), [4-5](#), [4-9](#)
- Tune window [4-2](#)

U

- UHMR mass list [5-20](#)
- underfill ratio [3-39](#)
- user role [4-3](#), [4-5](#)

V

- Vacuum / Bakeout window [4-29](#)
- vacuum gauges [4-29](#)
- Vacuum System node [4-30](#)
- validity period, of mass calibration [5-16](#)
- valve position [4-10](#)
- View bar [3-3](#)

W

- width, of scan range [3-32](#), [3-35](#), [3-37](#), [4-55](#)
- Windows menu [4-6](#)

X

- Xcalibur [4-9](#), [4-21](#), [4-23](#)

Z

- zooming
 - analysis graphs window [4-34](#), [4-42](#)
 - spectrum window [4-34](#)

