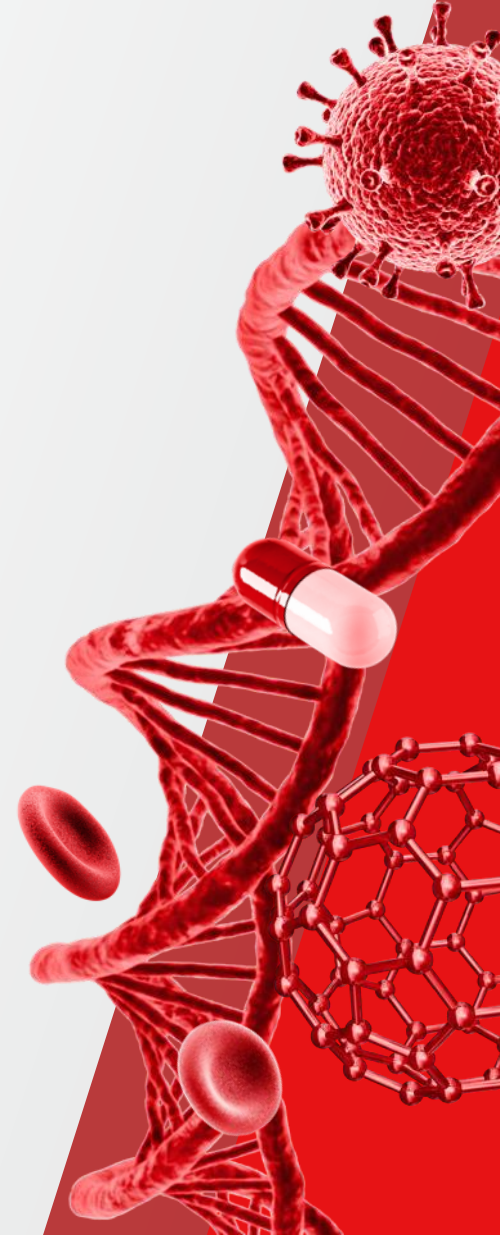


Thermo Scientific Orbitrap Exploris 4.2 Instrument Control Software (OES 4.2 ICSW) –

Overview – Updated With Defect Fixes in SP1

February 2023

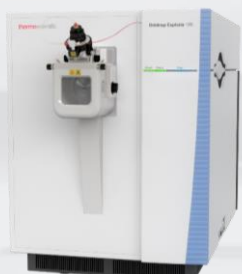
 The world leader in serving science



Thermo Scientific Orbitrap Exploris MS Portfolio – one ICSW



Thermo Scientific™ Orbitrap Exploris™ MX
Mass Detector



Thermo Scientific™ Orbitrap Exploris™ 120
Mass Spectrometer



Thermo Scientific™ Orbitrap Exploris™ 240
Mass Spectrometer



Thermo Scientific™ Orbitrap Exploris™ 480
Mass Spectrometer



Thermo Scientific™ Orbitrap Exploris™ GC
Mass Spectrometer

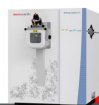


For Research Use Only. Not for use in diagnostic procedures.



Thermo Scientific™ Orbitrap Exploris™ GC 240
Mass Spectrometer

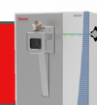
Comparison of Orbitrap Exploris Portfolio



Orbitrap Exploris MX



Orbitrap Exploris 120



Orbitrap Exploris 240



Orbitrap Exploris 480

	Orbitrap Exploris MX	Orbitrap Exploris 120	Orbitrap Exploris 240	Orbitrap Exploris 480
Max Resolution (FWHM) @ m/z 200	180,000	120,000	240,000	480,000
Mass range	40 – 3,000 (8,000 *)	40 – 3,000	40 – 6,000 (8,000 *)	
Precursor ion selection	n/a	≤ 2,500		
Sensitivity		S/N 250 @ 200 fg reserpine (tSIM)		S/N 150 @ 50 fg reserpine (tSIM)
MSMS scan rate (Hz)	22 Hz (Full Scan)	22 Hz		40 Hz
Mass accuracy - external	< 3 ppm RMS drift over 24 hours			
Mass accuracy w/ EASY-IC - internal	< 1 ppm over 5 days			
Spectral multiplexing	n/a	20		
Polarity switching * : one cycle equals (pos./switch/neg./switch)	60 k Full Scan* < 700 ms (equals > 1.4 Hz)	60 k Full Scan* < 700 ms (equals > 1.4 Hz) 60 k tSIM Scan* < 600 ms (equals > 1.6 Hz)		
Calibration	One-click calibration with FlexMix and dedicated calibration probe - with harmonization and improved user experience across all TNG platforms (TSQs, Hybrids, Tribrids)			
One-Point Mass Calibration	One-Point (Self) Mass Calibration achieves < 3 ppm RMS drift over at least 4 weeks			
Scan modes Full MS AIF t-SIM DIA MS2 combinable within in one single experiment, such as:	<ul style="list-style-type: none"> Full Scan <p>In addition, multiple experiments can be created combining various Full Scan experiments</p>	<ul style="list-style-type: none"> Full Scan ddMS2 (Top1-4) tSIM (targeted mass list) ddMS2 (Top1-4) Full Scan ddMS2 (targeted list) (Top1-4) <p>In addition, up to 5 experiments can be created combining the above listed scan types</p>	<ul style="list-style-type: none"> Full Scan ddMS2 (topN) Full Scan ddSIM tSIM (targeted mass list) ddMS2 Full Scan ddMS2 (targeted mass list) <p>With options for</p> <ul style="list-style-type: none"> 'Number of Scans' (= TopN) 'Cycle Time' <p>In addition, multiple experiments can be created combining the above listed scan types</p>	<ul style="list-style-type: none"> Full Scan ddMS2 (topN) Full Scan ddSIM tSIM (targeted mass list) ddMS2 Full Scan ddMS2 (targeted mass list) <p>With options for</p> <ul style="list-style-type: none"> 'Number of Scans' (= TopN) 'Cycle Time' 'Scans per Outcome' (branching) <p>In addition, multiple experiments can be created combining the above listed scan types</p>
Advanced acquisitions	APD	AcquireX (chargeable option)	AcquireX, APD, AcquireX AB TMT @ 45k resolution setting	<ul style="list-style-type: none"> 16 msec transient (7,500 min resolution) System Templates supporting BoxCar and SureQuant approaches TurboTMT with TMT reagents up to 18-plex

Software Release

Flexera Orbitrap Exploris Series ICSW 4.2 SP1 is available to customers using Flexera software distribution site.

Customers new to the Flexera site should use the following link:

<https://thermo.flexnetoperations.com/control/thmo/RegisterMemberToAccount>

After setting up an account, customers can access the site using the following link:

<https://thermo.flexnetoperations.com/control/thmo/login>

In the 'Product List' page, find 'Instrument – Orbitrap Exploris Series' and identify Orbitrap Exploris Series 4.2 SP1 in the subfolder.

The screenshot shows the 'Software Download and Licensing Portal' for 'Life Sciences Mass Spectrometry'. The page title is 'Orbitrap Exploris Series 4.2'. A left-hand navigation menu includes categories like 'Software & Services', 'Licensing', 'Administration', 'Information', and 'Sessions'. The main content area features a 'Product Download' section with a table of files. A 'Download Selected Files' button is visible below the table. A disclaimer is present above the table, and a 'Download Help' link is in the top right of the content area.

<input type="checkbox"/>	File Description	File Size	File Name
<input type="checkbox"/>	Orbitrap Exploris Series 4.2	1.7 GB	ExplorisSeries4.2.iso
<input type="checkbox"/>	Orbitrap Exploris Series 4.2 Workstation	1.1 GB	ExplorisSeriesWorkstation4.2.iso

Thermofisher.com & AnalyteGuru

Learn more about LC-MS Data Acquisition software

You can use the instrument control software to collect high-quality mass spectrometry data on the Thermo Scientific mass spectrometers. Control of the instruments is through two application packages: Tune and Method Editor.

For questions about the software, to request features, or to report defects, send an email by clicking [here](#).

Orbitrap Tribrid MS series | Orbitrap Exploris MS series | Exactive MS Series

Orbitrap Exploris MS series control software version 4.0 SP1

Release date	Build number	Instruments	Software requirements
December 17, 2021	4.0.309.28	Orbitrap Exploris 480 MS, Orbitrap Exploris 240 MS, Orbitrap Exploris 120 MS, Orbitrap Exploris GC MS, and Orbitrap Exploris GC 240 MS	Microsoft™ Windows™ 10 Enterprise 2016 LTSC or 2019 LTSC Thermo Scientific Xcalibur 4.5

Follow the upgrade instructions provided: Orbitrap Exploris MS series Instrument Control Software v.4.0 SP1 [Release Notes](#)

Orbitrap Exploris MS series ICSW v.4.0 SP1 and Xcalibur 4.5 software: [Download the software](#)

Orbitrap Exploris MS series ICSW v.4.0 SP1 Overview: [Download the Update Overview](#)

New features
The Orbitrap Exploris MS series instrument control software version 4.0 & 4.0 SP1 incorporates the following new and improved features from version 3.1

- Tune: Customized Mass Calibration and Check run the Mass Calibration with User-definable mass lists.
- Tune: Calibration pane provides a One-Point Mass Calibration procedure using fluoranthene.
- Fore Vacuum supervision: The user needs to be informed if transfer tube is clogged.
- Method Editor: Global Settings - Internal Mass Calibration provides various internal calibration modes (RunStart, Scan-to-Scan, Timed).

- Updates: [AnalyteGuru.com](https://www.analyteguru.com)

To receive focused updates, subscribe to the pertinent labels (e.g., *Orbitrap Exploris MS Instrument Control Software*)

AnalyteGuru > Knowledgebase > Scientific Library > Download Orbitrap Exploris Series Instrument Contr...

Download Orbitrap Exploris Series Instrument Control software 4.0 SP1 here

Peter
Team TFS

on 06-29-2022 07:24 AM

I'm excited to announce that the Orbitrap Exploris Series Instrument Control software update is now available to download from Thermofisher.com. Please find the link below to the software and associated release notes:

[LC-MS Data Acquisition Software | Thermo Fisher Scientific - UK](#)

Orbitrap | Orbitrap Exploris MS Instrument Control Software | Software

- Information: [Thermofisher.com](https://www.thermofisher.com)

- Software information
- Links for download
- New Features
- Known Issues
- Discovered issues
- Fixed Defects

Thermo Scientific Orbitrap Exploris Series 4.2 SP1 Instrument Control Software Release Notes

This document lists installation notes, new features and improvements regarding the Thermo Scientific™ Orbitrap Exploris™ Series 4.2 SP1 Instrument Control Software release. For information regarding the installation, features, functionality, and use of this product, refer to the following sources of information:

- *Orbitrap Exploris Series Operating Manual*
- *Orbitrap Exploris GC and Orbitrap Exploris GC 240 Operating Manual*

Version	Version No.	Orbitrap Exploris 480	Orbitrap Exploris 240	Orbitrap Exploris 120	Orbitrap Exploris GC	Orbitrap Exploris GC 240	Orbitrap Exploris MX
1.0	1.0.77.7	✓	—	—	—	—	—
1.1	1.1.117.22	✓	—	—	—	—	—
1.1 SP1	1.1.117.26	✓	—	—	—	—	—
2.0	2.0.182.18	✓	✓	✓	—	—	—
2.0 SP1	2.0.182.25	✓	✓	✓	—	—	—
2.0 SP2	2.0.182.35	✓	✓	✓	—	—	—
3.0	3.0.261.13	✓	✓	✓	✓	✓	—
3.1	3.1.279.9	✓	✓	✓	✓	✓	—
4.0	4.0.309.27	✓	✓	✓	✓	✓	✓
4.0 SP1	4.0.309.28	✓	✓	✓	✓	✓	✓
4.1	4.1.335.19	✓	✓	✓	✓	✓	✓
4.2	4.2.362.16	✓	✓	✓	✓	✓	✓
4.2 SP1	4.2.362.21	✓	✓	✓	✓	✓	✓



Source: Release Notes for OES 4.2 SP1 ICSW

System Requirements

Thermo Scientific Orbitrap Exploris Series 4.2 SP1 Instrument Control Software Release Notes

Installation Notes

Supported Target Systems

Thermo Scientific Orbitrap Exploris 120 mass spectrometer
Thermo Scientific Orbitrap Exploris 240 mass spectrometer
Thermo Scientific Orbitrap Exploris 480 mass spectrometer
Thermo Scientific Orbitrap Exploris MX mass spectrometer
Thermo Scientific Orbitrap Exploris GC mass spectrometer
Thermo Scientific Orbitrap Exploris GC 240 mass spectrometer

System Requirements

The minimum hardware and software configurations required for the Orbitrap Exploris Series 4.2 SP1 Instrument Control Software operation are as follows:

System	Requirements
PC	3.0 GHz Quad Core Intel™ Processor 32 GB RAM 512 GB SSD Hard Drive Display Monitor Resolution of 1920 × 1080 Two Network Interface Cards (NIC), 1000 MBit/s
Software	Microsoft™ Windows™ 10 Enterprise 2016 LTSP, 2019 LTSC or 2021 LTSC Thermo Scientific Xcalibur 4.6

Tip The Orbitrap Exploris Series 4.2 SP1 Instrument Control Software was only tested within the delivered composition.

Note:
Xcalibur 4.6 software applies
Foundation 3.1 SP9.

List of New Features and Improvements Realized With OES 4.2 ICSW

New Features

General

- Operating Manual, Pre-Installation Requirements Guide, and Software manuals are updated
- AcquireX support is provided for peptide mapping (AcquireX Ab) with OE 240 and OE 480
- Scheduled one-point mass calibration (via Tune Preferences)
- Additional resolution settings are accessible for OE 240 and OE 480 (11.25k, 22.5k, and 90k) in Tune and Method Editor

Tune

- OE GC: Tune Calibration pane provides a Manual Calibration panel
- OE GC: Method Editor provides a “Run Start Mass Calibration” template in system template

Method Editor

- New management of tables in DIA scan
- New table format is available for SIM scan. SIM with multiple broad scan ranges is provided for OE 120, 240 and GC
- Options are provided to select the order with which precursors are selected for data-dependent scans
- TMT 18-plex is supported by TurboTMT on OE 480
- New option “Auto-Extended” is provided for MS2 Scan Range Mode (Small Molecule Application Mode)

Improvements (selection)

Tune and Method Editor : Optimized default ESI/HESI gas flow settings for OE 120, 240, and MX

Tune Diagnostics : FlexMix Spray Optimization (neg+pos) applies Source Gases independent from polarity

Tune

- Calibration pane enables One-Point Mass and Customized Mass procedures which are compatible with FAIMS attached
- Source gas and temperature are set independently from polarity
- OE GC: Tune and ion source optimization reports contain a leak check history plot, filament current and emission current plots, and an emission current set value plot
- Calibration Status panel: reworked the update of Recommended Calibration dates depending on the procedure outcome
- Calibration Status panel: clarified display of Last Successful Calibration to ‘Outdated’ after Venting and Bake-out

Method Editor : User experience is enhanced when changing “Max. number of multiplexed ions”

Method Execution : Spray Voltage stays “On” during the execution of Run Start EASY IC

General : The Orbitrap Exploris Series 4.2 Installer updates the MongoDB from version 4.0.6 to version 4.0.28

Note: MongoDB needs to be uninstalled manually when downgrading from version 4.2 to an older version. The ISO image contains a MongoDB uninstaller.

Note: It is recommended upgrading the system to benefit from these improvements

Source: Release Notes for OES 4.2 SP1 ICSW

Resolved Issues in OES 4.2 SP1

- **Resolved Issues between OES 4.2 and OES 4.2 SP1**

- Method execution Full Scan DDA with Targeted Mass Filter and Fixed/Stepped Collision Energies (CEs): fixed CEs in the Targeted Mass Filter are erroneously executed as stepped CEs
- Method transfer: Cannot open certain older methods with Orbitrap Exploris Series 4.2 ICSW – index out of range error message
- Orbitrap Exploris GC: License Error with 60k GCHCD license prevents running methods
- Orbitrap Exploris GC: Method Editor: Corrected acquisition delay tooltip in Global Settings
- Orbitrap Exploris GC: Method Editor: Factor 10x UI recommendation rule is erroneously applied to all GC System Templates
- Orbitrap Exploris GC: Method Editor: Restore Default context menu does not work for parameters under Ion Source Properties
- Full Scan acquisition with Mild Trapping option (Small Molecule Application Mode) leads to signal drop in positive mode

Scheduled One-Point Mass Calibration

Setting up Mass Self-Calibration

Under Tune Preferences



Tune Preferences

General

- Clear Calibration check boxes when complete
- Clear Diagnostics check boxes when complete
- Enable Hotlink for Define Scan and Ion Source Panel

Report Options

Calibration Reports

- Automatically generate reports
- Path: C:\Thermo\Instruments\Reports\
- Show Report Generation Options dialog box
- Do not generate reports

Other Reports

- Automatically generate reports
- Path: C:\Thermo\Instruments\Reports\
- Show Report Generation Options dialog box
- Do not generate reports

Report Content Options

- Show Console
- Show graph
- Show spectrum
- Show system configuration
- Show embedded system configuration

Alerts Console Options

- Show warnings
- Show recovered errors and warnings
- Show information
- 300 Minutes included in the log file before error detected
- 300 Minutes included in the log file after error detected

Mass Self-Calibration Options

System Self-Calibration is enabled. To abort or change options, please uncheck the system self calibration check box below

- Run One-Point Mass Self-Calibration

Schedule Self-Calibration

Day: **Fridays** Time: **2 PM**

OK Cancel

- ‘One-Point Mass Self-Calibration’ Procedure calibrates positive and negative ion mode - Unattended
- Fluoranthene from the EASY-IC source is used for the ‘One-Point Mass’ calibration procedure
- Infusion of FlexMix solution is not needed
- Running the ‘One-Point Mass Self-Calibration’ procedure updates the master calibration file. Its updated content is applied to upcoming scans and raw data files without further user interaction. The *Recommended Calibration* date (and color indicator) is updated accordingly.

Mass Self-Calibration Options

System Self-Calibration is enabled. To abort or change options, please uncheck the system self calibration check box below

- Run One-Point Mass Self-Calibration

Schedule Self-Calibration

Day: **Fridays** Time: **2 PM**

Mass Self –Calibration Options

- ‘Run One-Point Mass Self-Calibration’ can be activated
- Day and time for Self-Calibration is defined

Scheduled One-Point Mass Calibration

Self-Calibration Pre-Conditions

- Self-Calibration procedure is pursued only if
 - The instrument is in standby or scanning (“On”)
 - ‘Run One-Point Mass Self-Calibration’ can be activated in Tune Preferences
- Self-Calibration procedure is deferred and subsequently run if
 - There is an acquisition in progress (acquisition sequence or tune recording) at the time of scheduled Self-Calibration
 - Acquisition queue gets empty within the next 24 hours of scheduled Self-Calibration (check every 5 min)
- Self-Calibration is executed when MS is controlled under Xcalibur or Chromeleon

Scheduled One-Point Mass Calibration

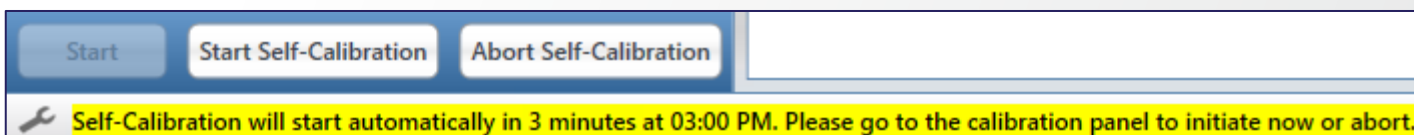
Self-Calibration Procedure

- 5-min delay Self-Check preparation
- Notification is displayed in Tune bottom panel that Self-Check is about to start; text is updated every minute



Self-Calibration will start automatically in 5 minutes at 03:00 PM. Please go to the calibration panel to initiate now or abort.

- 'Start Self-Calibration' / 'Abort Self-Calibration' buttons displayed and 'Start' button in calibration panel disabled



- Self-Calibration execution
 - Started after 5-min preparation has elapsed
 - Instrument is switched to 'On' if currently in standby
 - During preparation, calibration UI is disabled
 - During Self-Calibration execution
 - Tune operations are disabled, procedure can be aborted by pressing relevant button (aborted Self-Calibration not run until next scheduled calibration)
 - Self-Calibration running status is displayed (progress bar, notification panel)

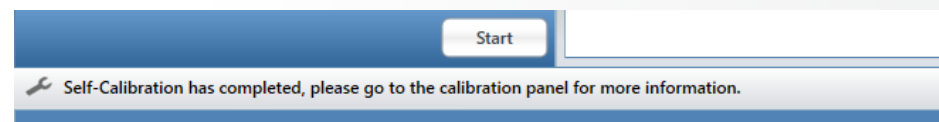
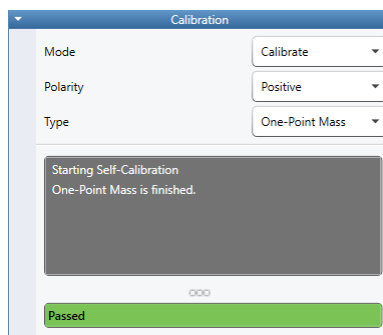
Scheduled One-Point Mass Calibration

After Completion of Self-Calibration

- PDF report is generated

Self-Calibration Report		thermo		scientific	
Date & Time	Wednesday, October 5, 2022 09:15:01 AM				
Instrument Model	Orbitrap Exploris 240				
Instrument Serial	MM10003C				
Software Version	4.2.357.0				
Name	Result	Comment			
OnePointMass Calibration (positive and negative Mode)	Passed				
OnePointMass Calibration (positive and negative Mode)					
Name	Result	Value	Range	Comment	
Type		-	-	Calibration	
ICS Mass Calibration passed.					
System Configuration					
Name	Value				
Ion Source Type	ESI				
Internal Calibration (EASY-IC) Source	enabled				
Options	EASY-IC, BioPharma				
Embedded System Information					
Label	Version				
Instrument Embedded Software	4.2.316.0				
Instrument Hardware Hash	c9463e6c4c2a1872414bd80b2d74da4e4f5c724a				

- Notification in Tune bottom panel and notification area of calibration tab



Best Practice to Work With One-Point Mass (Self) Calibration and EASY-IC

For a good and reliable mass accuracy/stability:

- Run experiments with RunStart EASY-IC
- Schedule unattended self-calibration: daily
- Run a system calibration once per month

Internal Mass Calibration	EASY-IC™
Mode	Run Start

Mass Self-Calibration Options	
System Self-Calibration is enabled. To abort or change options, please uncheck the system self calibration check box below	
<input checked="" type="checkbox"/> Run One-Point Mass Self-Calibration	
Schedule Self-Calibration	
Day	Daily
Time	9 AM

System	
Recommended Calibration:	11/19/2022
Last Successful Calibration:	10/20/2022
Calibration	
Mode	Calibrate
Polarity	Positive
Type	Mass & System

AcquireX Data Acquisition Workflow Enhancements

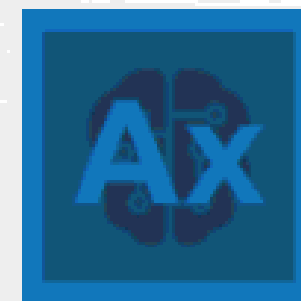
New Features

- New intelligent data acquisition workflow for Biopharma applications: AcquireX Ab
 - Available with Xcalibur 4.6 in Peptide Application Mode of Orbitrap Exploris 240 and 480 MS systems
 - One AcquireX Ab workflow: Custom Workflow

- New AcquireX workflow for Small Molecule applications: Custom Workflow
 - Available with Xcalibur 4.6 in Small Molecule Application Mode of Orbitrap Exploris 240 and 480 MS systems (chargeable option for Orbitrap Exploris 120)
 - Custom Workflow replaces Advanced Deep Scan Workflow



AcquireX Ab



AcquireX

New AcquireX Ab Workflow for Peptide Mapping

New Features in Method Editor

Orbitrap Exploris 480 Method Editor 4.2.361

File Orbitrap Exploris 480

Method Editor Global Parameters Scan Parameters Summary

Application Mode # 1
Peptide
Method Duration (min) 60

Method Timeline Experiment ACTIONS Settings

Infusion Mode Liquid Chromatography
Expected LC Peak Width (s) 10
Advanced Peak Determination
Default Charge State 2
Enable Xcalibur AcquireX Ab method modifications
Internal Mass Calibration Off

Experiment #1 0-60 CLEAR

Targeted Mass Properties

MASS LIST

Mass List Type m/z
Time Mode Start/End Time
Include Intensity Threshold
Add Mass List Targets Determined by Xcalibur AcquireX Ab

20 scans

Compound	m/z	t start (min)	t stop (min)	Intensity Threshold
1 MRFA	524.265	0	60	0.0e0

- AcquireX Ab workflows introduced with Xcalibur 4.6
- AcquireX Ab available in Peptide Application Mode
- Controls implemented in
 - Global Settings
 - Targeted Mass and Targeted Mass Exclusion filters
- Constraints
 - Time Mode = Start/End Time
 - Include Intensity Threshold = TruePrecursor Mass Range
 - Mass List Type = m/z OR m/z & z

Targeted Mass Exclusion Properties

MASS LIST

Mass List Type m/z & z
Time Mode Start/End Time
Include Intensity Threshold
Add Mass List Targets Determined by Xcalibur AcquireX Ab

Compound	Formula	Adduct	m/z	z	t start (min)	t stop (min)
1 MRFA	C23H37N7O5S	+H	524.265	1	0	60

Xcalibur: Acquire X Custom Workflows

Small molecules

- Advanced Deep Scan has been replaced by Custom Workflows
 - Allows for the use of multiple groups in a single workflow
 - Reuse and combine inclusion and exclusion lists from previous groups
 - Reminder: option to use new component detection from Thermo Scientific™ Compound Discoverer™ software



The screenshot shows the 'CUSTOM WORKFLOWS' interface. At the top, a flowchart displays the workflow steps: 'MS OT' (blue), 'Targeted Mass (Optional)' (purple, highlighted with a red border), 'Targeted Mass Exclusion' (purple), and 'ddMS² OT HCD' (blue). Below the flowchart, the text 'CUSTOM WORKFLOWS' is centered. Underneath, it says 'Create workflows specific to your requirement'. A section titled 'What Xcalibur Does:' contains a bulleted list of features. At the bottom, there is a blue 'SELECT' button.

MS OT

Targeted Mass (Optional)

Targeted Mass Exclusion

ddMS² OT HCD

CUSTOM WORKFLOWS

Create workflows specific to your requirement

What Xcalibur Does:

- Generates an inclusion or exclusion list by combining up to 5 injections per group
- Provides options to reuse inclusion and exclusion lists from previous groups
- Incorporates various experiment types in a single experiment
- Submits an experiment with several groups

SELECT

Xcalibur: Acquire X Custom Workflows

The screenshot shows the AcquireX Workflow Editor interface. On the left, there is a sidebar with 'CUSTOM WORKFLOWS' and a list of workflow components: MS-OT, Targeted Mass, Targeted Mass Exclusion, and ddMS⁺-OT-HCD. Below this is a section for 'Experiment Details' with fields for 'Experiment Folder' and 'Experiment Name', each with a 'Browse' button. The 'Group Parameters' section includes a 'Group #' dropdown set to '1' and an 'Apply To All Groups' button. Under 'Instrument Methods', there are three sections: 'Full Scan Method', 'MSn Template Method', and 'Experiment Parameters' (with 'Exclusion Override Factor (default = 3)').

The main area is titled 'AcquireX Workflow Editor' and shows a table for 'AcquireX Template Injections'. The table has columns: #, Name, Type, Group, Instrument Method, Apply Excl. ..., Apply Incl. List, Vial, and Vol (µl). Above the table, there are controls for 'Blanks 0', 'Excl. Ref 0', 'Incl. Ref 0', 'ID Injections 0', and '# Groups Add 0'. A note above the table states: 'Adding or removing template injections auto-populates this table'. At the bottom of the editor are buttons for 'Back', 'Cancel', 'Export', 'Import', 'Save', 'Save As', and 'Submit'. A 'Mode' dropdown is set to 'Low'.

Callouts provide the following information:

- Use double blue arrow and check box to select new compound detection (recommended)
- Full customization of number of each sample type added to each group.
- Low- reuse exclusion and/or inclusion list from Group 1 only. High- reuse use any list (even multiple) from any previous group
- Acquire X sequence can be exported as a .csv and imported later

Xcalibur: Acquire X Custom Workflows

Group 1
"Deep Scan"

Group 2
"Iterative precursor exclusion"

AcquireX Workflow Editor

Mode **High**

AcquireX Template Injections **Group 2** | Blanks 2 | Excl. Ref 1 | Incl. Ref 0 | ID Injections 4 | # Groups to Add 1 | Add

#	Name	Type	Group	Instrument Method	Apply Excl. List	Apply Incl. List	Vial	Inj Vol (µl)
1	Blank_01	Blank	1	Instrument Method			R:A1	10.00 µl
2	ExclusionRef_01	Exclusion	1	Instrument Method			R:A1	10.00 µl
3	Sample_01	Inclusion	1	Instrument Method			R:A1	10.00 µl
4	ID_01	Id	1	Instrument Method	[1]	[1]	R:A1	10.00 µl
5	ID_02	Id	1	Instrument Method			R:A1	10.00 µl
6	ID_03	Id	1	Instrument Method			R:A1	10.00 µl
7	Blank_01	Blank	2	Instrument Method			R:A1	10.00 µl
8	Blank_02	Blank	2	Instrument Method			R:A1	10.00 µl
9	ExclusionRef_01	Exclusion	2	Instrument Method			R:A1	10.00 µl
10	ID_01	Id	2	Instrument Method	1, [2]	1	R:A1	10.00 µl
11	ID_02	Id	2	Instrument Method			R:A1	10.00 µl
12	ID_03	Id	2	Instrument Method			R:A1	10.00 µl
13	ID_04	Id	2	Instrument Method			R:A1	10.00 µl

Right click allow for copy down, insert injection, and undo

In High mode- Option to choose exclusion list from group 1 and 2

- Insert Inj Above
- Insert Inj Below
- Copy Down
- Undo
- Display Comment Column
- Apply Name Extension

Xcalibur: Acquire X Ab Custom Workflows

Peptide and protein workflows

- New workflow for peptides/proteins, and other biopharma applications
- 1 workflow called “Custom Ab Workflow”
- Component detection is based on Thermo Scientific™ Biopharma Finder™ software Mass Analyzer algorithm
- Use MSn methods for exclusion/inclusion generation
- Reuse and combine exclusion and inclusion lists from previous groups



```
graph TD; MSOT[MS OT] --> TM[Targeted Mass (Optional)]; TM --> TME[Targeted Mass Exclusion]; TME --> ddMS[ddMS² OT HCD];
```

CUSTOM Ab WORKFLOWS

Create peptide mapping workflows specific to your requirement

What Xcalibur Does:

- Creates one exclusion list per group to reduce background fragmentation in your ID runs
- Creates one inclusion list per group to fragment more relevant precursor ions in multiple ID injections
- Injects ID samples iteratively for groups with an inclusion list until all ions in the inclusion list are fragmented or a user-defined number of ID injections is reached
- Injects ID samples iteratively for groups without an inclusion list until all ions in the sample are fragmented or a user-defined number of ID injections is reached
- Provides options to reuse inclusion and exclusion lists from previous groups
- Submits an experiment with several groups

Xcalibur: Acquire X Ab Custom Workflows

The screenshot shows the 'AcquireX Ab Workflow Editor' interface. On the left, there is a sidebar with 'CUSTOM Ab WORKFLOWS' and 'Experiment Details' (Experiment Folder, Experiment Name), 'Group Parameters' (Group # 1, Apply To All Groups), 'Instrument Methods' (Method for Blank/Exclusion/Inclusion samples, Template method for ID samples), and 'Experiment Parameters' (Component Detection Settings, Exclusion List Parameters, Inclusion List Parameters). A bracket on the left labels these as 'Fully customizable detection parameters'. The main area is a table for 'AcquireX Template Injections' with columns: #, Name, Type, Group, Instrument Method, Apply Excl. List, Apply Incl. List, Vol, and Inj Vol (µl). Callouts point to the 'Blanks', 'Excl. Ref', 'Incl. Ref', and 'ID Injections' fields, stating: 'Full customization of number of each sample type added to each group.' and 'Low- reuse exclusion and inclusion list from Group 1 only. High- reuse use any list (even multiple) from any previous group'. A callout points to the 'Method for Blank/Exclusion/Inclusion samples' field, stating: 'Method for Blank/Exclusion/Inclusion can be MSn not ONLY MS'. A callout points to the 'Export' button, stating: 'Acquire X Ab sequence can be exported as a .csv and imported later'. The bottom bar contains buttons: Back, Cancel, Export, Import, Save, Save As, Submit.

Mode Low

AcquireX Template Injections

Blanks 0 Excl. Ref 0 Incl. Ref 0 ID Injections 0 # Groups to Add 0 Add

#	Name	Type	Group	Instrument Method	Apply Excl. List	Apply Incl. List	Vol	Inj Vol (µl)
Adding or removing template injections auto-populates this table								

Experiment Details

Experiment Folder Browse

Experiment Name

Group Parameters

Group # 1 Apply To All Groups

Instrument Methods

Method for Blank/Exclusion/Inclusion samples Browse New

Template method for ID samples Browse New

Experiment Parameters

Component Detection Settings

Exclusion List Parameters

Inclusion List Parameters

Back Cancel Export Import Save Save As Submit

Fully customizable detection parameters

Full customization of number of each sample type added to each group.

Low- reuse exclusion and inclusion list from Group 1 only.
High- reuse use any list (even multiple) from any previous group

Method for Blank/Exclusion/Inclusion can be MSn not ONLY MS

Acquire X Ab sequence can be exported as a .csv and imported later

Xcalibur: Acquire X Ab Custom Workflows

Experiment Name

Group Parameters

Group # 1 Apply To All Groups

Instrument Methods

Method for Blank/Exclusion/Inclusion samples Browse New

Template method for ID samples Browse New

Experiment Parameters

Component Detection Settings

User-defined Exclusion Settings On

MS Noise Level 2.00e+4 S/N Threshold 2.50e+1 |MS| Signal Threshold 5.00e+5

User-defined Inclusion Settings Off

User-defined Start/End Time On

Start (min) 0 End (min) 600

Exclusion List Parameters

Inclusion List Parameters

AcquireX Ab Workflow Editor Mode Low

AcquireX Template Injections Blanks 0 Excl. Ref 0 Incl. Ref 0 ID Injections 0 # Groups to Add 0 Add

#	Name	Type	Group	Instrument Method	Apply Excl. List	Apply Incl. List	Vial	Inj Vol (µl)
Adding or removing template injections auto-populates this table								

Back Cancel Export Import Save Save As Submit

This workflow uses the detection algorithm from Biopharma Finder software.

Options to use default values or individually customize several settings

Xcalibur: Acquire X Ab Custom Workflows

AcquireX Ab Workflow Editor

Mode **High** ⓘ

AcquireX Template Injections **Group 2** ✎ 🗑️ | Blanks 2 Excl. Ref 1 Incl. Ref 1 ID Injections 3 # Groups to Add 1 **Add** 🗄️

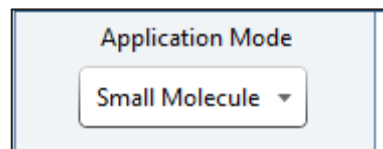
#	Name	Type	Group	Instrument Method	Apply Excl. List	Apply Incl. List	Vial	Inj Vol (µl)	
1	Blank_01	Blank	1	Instrument Method			R:A		
2	ExclusionRef_01	Exclusion	1	Instrument Method			R:A		
3	Sample_01	Inclusion	1	Instrument Method			R:A		
4	ID_01	Id	1	Instrument Method	[1]	[1]	R:A		
5	ID_02	Id	1	Instrument Method			R:A		
6	Blank_01	Blank	2	Instrument Method			R:A1	10.00 µl	
7	Blank_02	Blank	2	Instrument Method			R:A1	10.00 µl	
8	ExclusionRef_01	Exclusion	2	Instrument Method			R:A1	10.00 µl	⋮
9	Sample_01	Inclusion	2	Instrument Method			R:A1	10.00 µl	⋮
10	ID_01	Id	2	Instrument Method	1, [2]	[2]	R:A1	10.00 µl	⋮
11	ID_02	Id	2	Instrument Method	<input checked="" type="checkbox"/> 1 <input checked="" type="checkbox"/> 2		R:A1	10.00 µl	⋮
12	ID_03	Id	2	Instrument Method			R:A1	10.00 µl	⋮

Right click allow for copy down, insert injection, and undo

In High mode- Option to choose exclusion list from group 1 and 2

Each group can have a different number to sample types

Scan Range Mode - Auto-Extended (tMS2 or ddMS2)

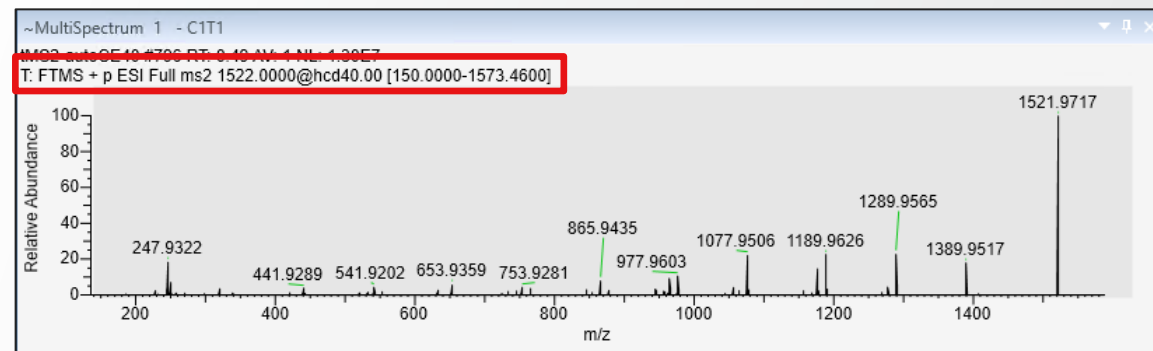


- Scan Range Mode „Auto-Extended“
- Applies factor 15 rule for all precursor masses
- Low fragments for precursor masses between 500 and 1500 are integrated in the scan filter (better comparability with Q Exactive spectra for low fragment masses)

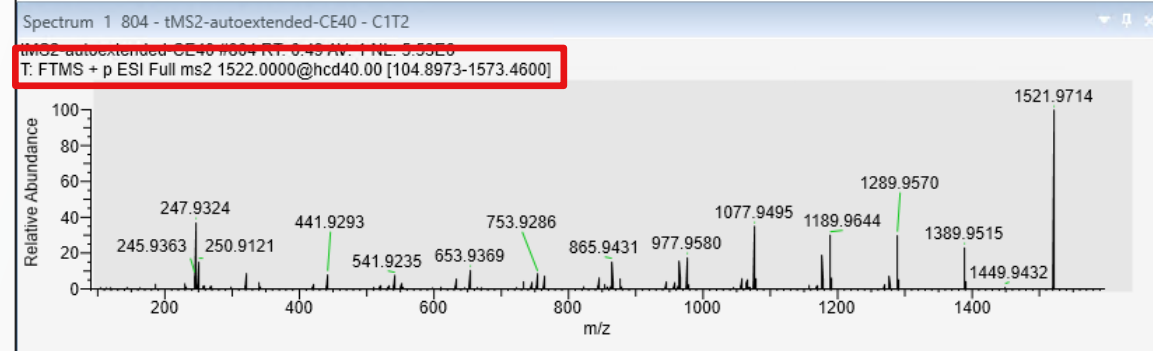
Targeted MS² Scan Properties

Isolation Window (m/z)	2
Isolation Offset	Off
Collision Energy Type	Normalized
HCD Collision Energy (%)	40
Orbitrap Resolution	15000
Scan Range Mode	Auto-Extended
RF Lens (%)	Auto
AGC Target	Define First Mass
Maximum Injection Time Mode	Define m/z Range
	Auto-Extended

Auto



Auto-extended



Examples – Auto vs. Auto-Extended

Last mass/ Precursor Mass [m/z]	Rule in Scan range mode „Auto“	Scan Range Mode „Auto“	Scan Range Mode Auto “Auto-Extended” (Factor 15 rule)
200	Factor 5	40	40
240	Factor 5	48	40
250	Factor 5	50	40
260	Factor 10	50 < 50 → fm increase to 50 (note not to 40!)	40
400	Factor 10	50 < 50 → fm increase to 50	40
900	Factor 10	90	60
1000	Factor 10	100	67
1500	Factor 10	150	100
1600	Factor 15	150 < 150 → fm increase to 150	107
2000	Factor 15	150 < 150 → fm increase to 150	133

Management of Tables in DIA Scan

New DIA Window Type

- DIA Window Type = Auto
 - DIA windows calculated from
 - Precursor Mass Range
 - Isolation Window
 - Window Overlap
 - DIA windows in Table cannot be
 - Modified by direct typing
 - Modified by adding / deleting rows
 - Modified by importing files
- DIA Window Type = User Defined
 - DIA windows defined by
 - Direct typing
 - Adding / deleting rows
 - Importing files

DIA Window Type = Auto

Data-Independent Acquisition Properties Show Favorites

Precursor Mass Range (m/z)	100-1100	★
DIA Window Type	Auto	★
Multiplex Ions	<input type="checkbox"/>	★
Isolation Window (m/z)	100	★
Window Overlap (m/z)	0	★
Window Placement Optimization	Off	★
Number Of Scan Events	10	★
DIA Window Mode	m/z Range	★
Collision Energy Type	Normalized	★

DIA Window Type = User Defined

Data-Independent Acquisition Properties Show Favorites

DIA Window Type	User Defined	★
Multiplex Ions	<input type="checkbox"/>	★
DIA Window Mode	m/z Range	★
Collision Energy Type	Normalized	★

DIA m/z window ADD DELETE IMPORT EXPORT

	m/z range
1	100-200
2	200-300
3	300-400
4	400-500
5	500-600
6	600-700
7	700-800
8	800-900
9	900-1000
10	1000-1100

DIA m/z window ADD DELETE IMPORT EXPORT

	m/z range
1	100-200
2	200-300
3	300-400
4	400-500
5	500-600
6	600-700
7	700-800
8	800-900
9	900-1000
10	1000-1100

Management of Tables in DIA Scan

New DIA Window Mode

- DIA Window Mode = m/z Range
 - One column in Table
 - m/z Range
- DIA Window Mode = Center Mass
 - Two columns in Table
 - Center Mass
 - Window Width
- DIA Windows are converted when switching between the two modes
- The two DIA Window Modes are compatible with the two DIA Window Types

DIA Window Mode = m/z Range

Data-Independent Acquisition Properties Show Favorites

DIA Window Type: User Defined

Multiplex Ions:

DIA Window Mode: m/z Range

Collision Energy Type: Normalized

DIA m/z window

	m/z range
1	100-200
2	200-300
3	300-400
4	400-500
5	500-600
6	600-700
7	700-800
8	800-900
9	900-1000
10	1000-1100

DIA Window Mode = Center Mass

Data-Independent Acquisition Properties Show Favorites

DIA Window Type: User Defined

Multiplex Ions:

DIA Window Mode: Center Mass

Collision Energy Type: Normalized

DIA m/z window

	Center Mass (m/z)	Window Width (m/z)
1	150	100
2	250	100
3	350	100
4	450	100
5	550	100
6	650	100
7	750	100
8	850	100
9	950	100
10	1050	100

New Table Format For SIM Scan

New SIM Window Mode

Mass List Table					
	Compound	Formula	Adduct	Center Mass (m/z)	z
1				524.2649	1
2				262.6	1
3				922	1

Targeted SIM Scan Properties	
Multiplex Ions	<input type="checkbox"/>
Isolation Window (m/z)	2
Isolation Offset	Off
SIM Window Mode	Center Mass

Mass List Table						
	Compound	Formula	Adduct	Center Mass (m/z)	z	Isolation Window (m/z)
1				524.2649	1	2
2				262.6	1	2
3				922	1	2

Targeted SIM Scan Properties	
Multiplex Ions	<input type="checkbox"/>
Isolation Window (m/z)	Defined in Table
Isolation Offset	Off
SIM Window Mode	Center Mass

Mass List Table	
	m/z Range
1	523.2649-525.2649
2	261.6-263.6
3	921-923

Targeted SIM Scan Properties	
Multiplex Ions	<input type="checkbox"/>
SIM Window Mode	m/z Range
Orbitrap Resolution	60000
RF Lens (%)	50

- SIM Window Mode = m/z Range
 - One column in Table
 - m/z Range
- SIM Window Mode = Center Mass
 - Two columns in Table
 - Center Mass
 - Window Width (with Table icon selected)
- SIM Windows converted when switching between the two modes

Multiple Full Scan Ranges (tSIM)

Time Range (min) 0-15 SWITCH CLEAR

tSIM

Mass List Table			
	m/z Range	RT Time (min)	Window (min)
1	100-300	7.5	15
2	300-600	7.5	15
3	600-1000	7.5	15

Targeted SIM Scan Properties

- Multiplex Ions
- SIM Window Mode **m/z Range**
- Orbitrap Resolution 60000
- RF Lens (%) 70
- AGC Target Standard
- Maximum Injection Time Mode Auto
- Microscans 1
- Data Type Profile
- Polarity Positive
- Source Fragmentation
- Scan Description
- Time Mode Retention Time Windo

Select table icon to add property to mass list table.

Mass List Table			
	m/z Range	RT Time (min)	Window (min)
1	100-300	7.5	15
2	300-600	7.5	15
3	600-1000	7.5	15

- Multiple Scan ranges can be entered in the new table format for tSIM
- Extension of "Isolation Window" width from 0.4-50 to 0.4-2000 m/z units on OE120 and OE240
- Possibility to set parameters scan range dependent

Advantages:

- Increase dynamic range of the calibration curve
- Better overview – parameters for all scan ranges are on one view (opposed to setup the experiment with different experiments in the timeline)

Note: For Full Scan ranges consider to set the AGC Target value to 1000 (1e6). Standard = 100 \cong 1e5

Additional Resolution Settings

Added Resolution to Provide More Flexibility in Short LC Gradient Analysis

Tune

thermo scientific
Orbitrap Exploris 480

ION SOURCE DEFINE SCAN CALIBRATION

Scan Type: Full Scan

Orbitrap Resolution: 15000

Scan Range (m/z): 7500

RF Lens (%): 11250

AGC Target: 22500

Maximum Injection Time: 30000

Time (ms): 45000

Microscans: 90000

Source Fragmentation: 120000

Use EASY-IC™: 180000

240000

480000

Method Editor

Full Scan Properties Show All

Orbitrap Resolution: 120000

RF Lens (%): 7500

Polarity: 11250

15000

22500

30000

45000

60000

90000

120000

180000

240000

480000

- Available for OE 480 and OE 240
- Available for all scan types

TMT 18-plex Support by TurboTMT

One More Window Covered by TurboTMT / TMTpro Reagent

- TurboTMT only available for OE 480
- Additional reporter ions
 - TMTpro-134C: 134.154565 (covered by existing window 134.0414 – 134.2614)
 - TMTpro-135N: 135.151600 (covered by new window 135.0446-135.2646)

TurboTMT is specifically applied to increase the resolving power to six windows of 0.22 Da width, centered around the reporter masses for TMT and TMTpro in the mass range of 125-136 Da.

[Learn more...](#)

TurboTMT uses an advanced spectral processing algorithm that increases resolving power within a specified reporter ion mass range without requiring a longer transient acquisition. Using TurboTMT specifically to the Tandem Mass Tags™ (TMT™) reporter ions increases the resolution sufficient to baseline resolve isotopologues even when using transients that produce a 30,000 resolution.

For TMT Reagent, Turbo TMT is specifically applied to 6 windows of 0.22 Da centered around the masses 126.1309, 127.1279, 128.1313, 129.1346, 130.1380, 131.1413.

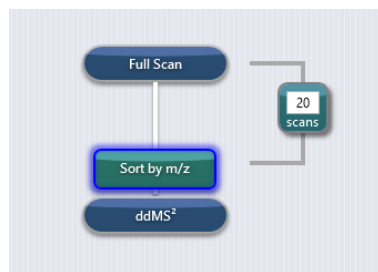
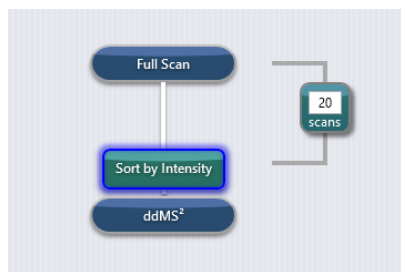
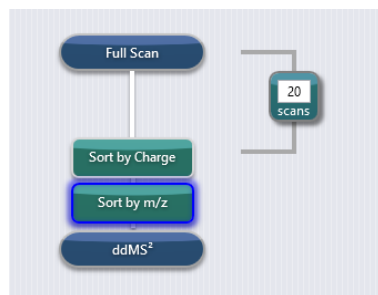
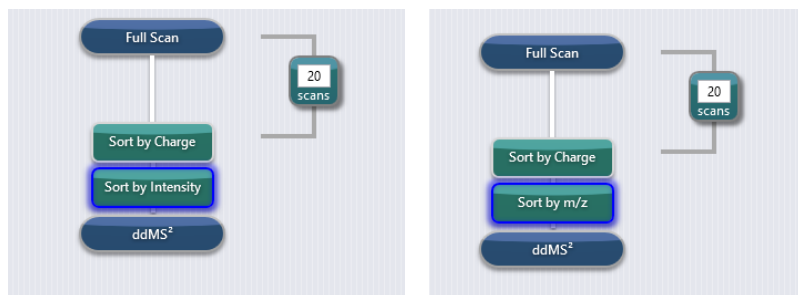
For TMTpro Reagent, Turbo TMT is specifically applied to 10 windows of 0.22 Da centered around the masses 126.1309, 127.1279, 128.1313, 129.1346, 130.1380, 131.1413, 132.1447, 133.1480, 134.1514, 135.1546)

Note: Using 15,000 resolving power may require additional data analysis tools.

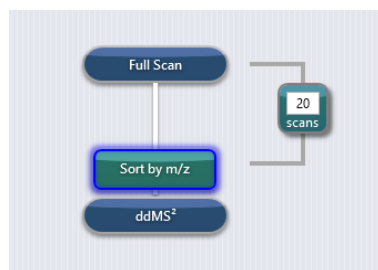
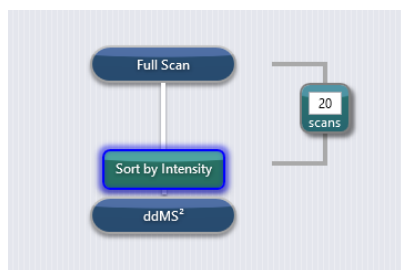
Alternate Precursor Sorts

Additional Options to Define Precursor Selection Priority in DDA

OE 480, OE 240



OE 120

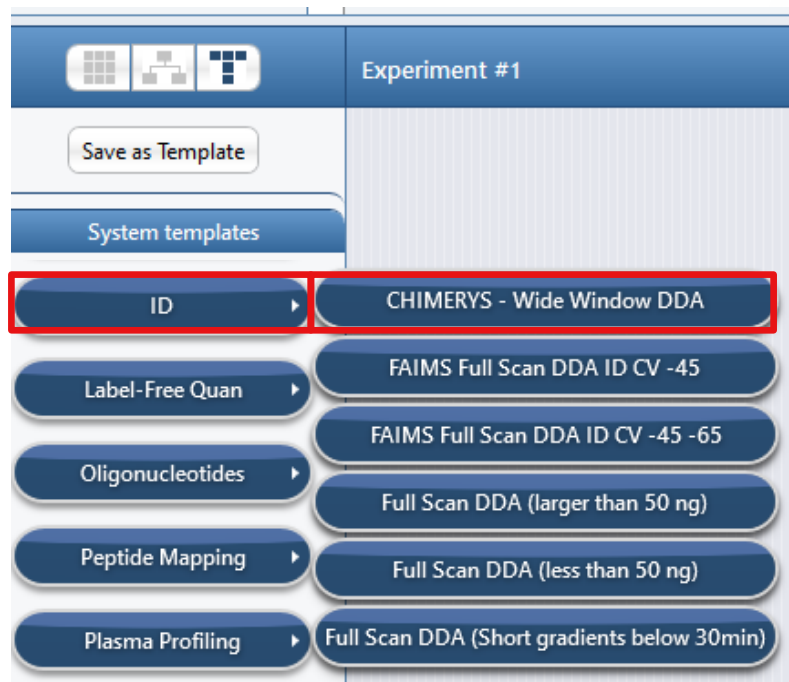


- Alignment with Orbitrap Tribrid Series ICSW
- No sorting for OE MX
- No Charge State Sorting for OE 120
- Allowed combinations
 - OE 480, OE 240: Sort by Charge (1st) AND Sort by Intensity OR Sort by m/z
 - OE 120: None

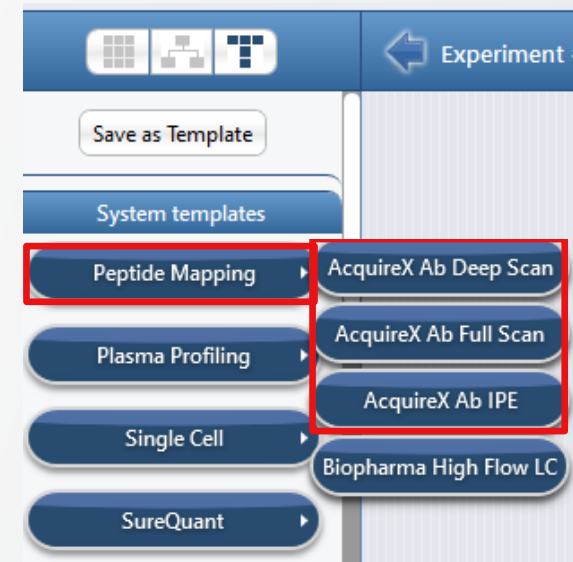
New and Updated Templates

- New Chimerys templates (Peptide Application Mode)
- New AcquireX Ab templates (Peptide Application Mode)
- Updated/Corrected Ion Source settings for several small molecule templates

Chimerys



AcquireX Ab



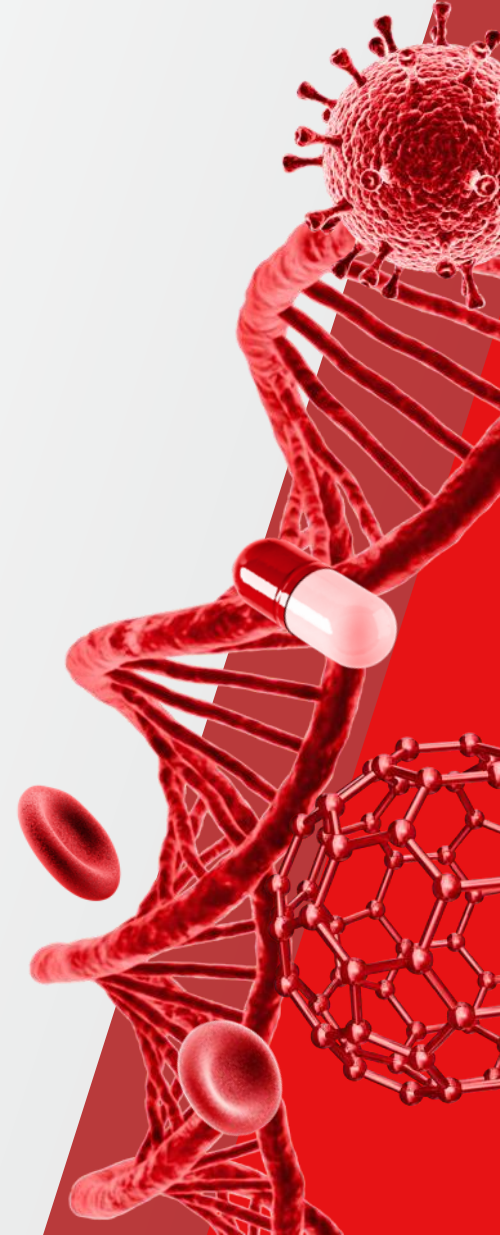
Updates to Manuals for Orbitrap Exploris Series

Pre-Installation Requirements Guide

Operator Manuals

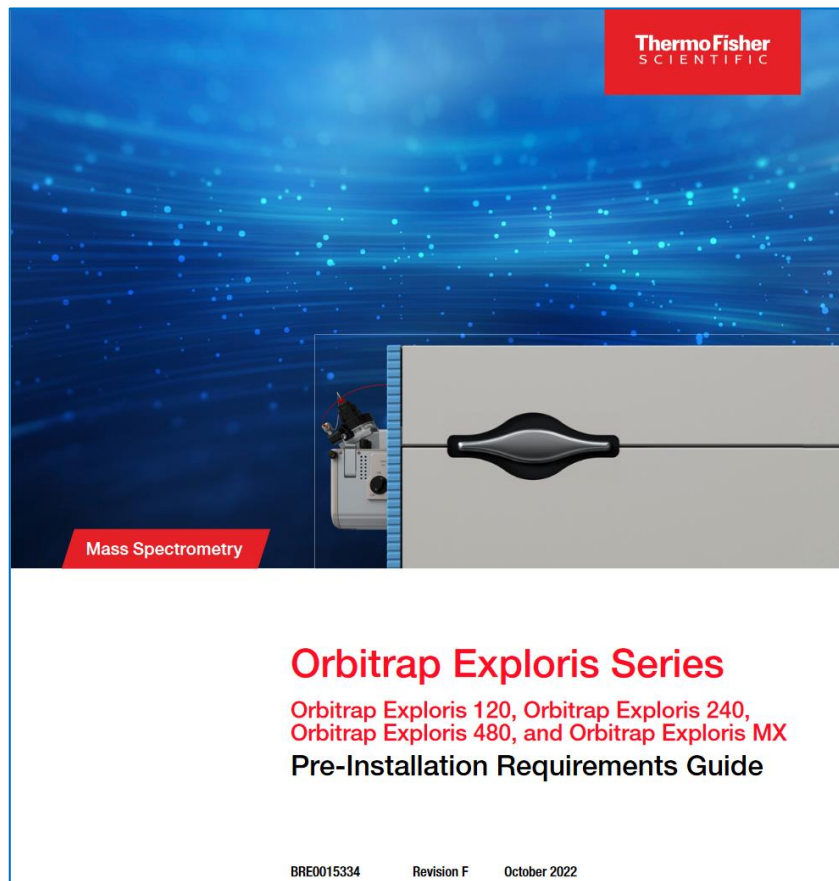
Model specific **Software Manuals** and **online help**

 The world leader in serving science



Pre-Installation Requirements Guide And Operating Manual

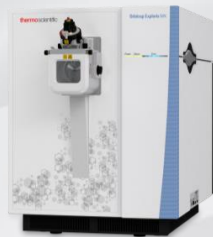
Pre-Installation Requirements Guide



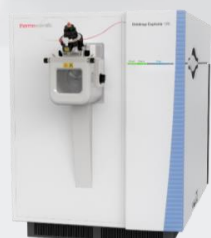
Operating Manual



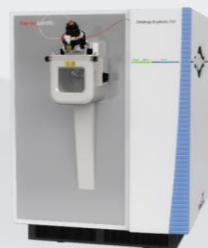
Software Manuals for these Orbitrap Exploris models



Thermo Scientific™
Orbitrap Exploris™ MX Mass Detector



Thermo Scientific™ Orbitrap Exploris™ 120
Mass Spectrometer



Thermo Scientific™ Orbitrap Exploris™ 240
Mass Spectrometer



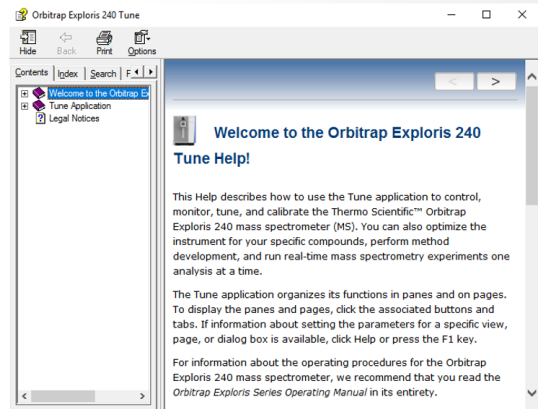
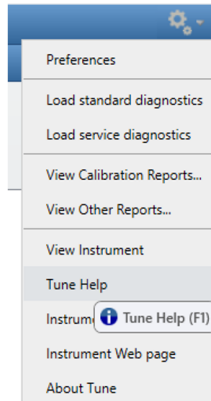
Thermo Scientific™ Orbitrap Exploris™ 480
Mass Spectrometer

Updated Software Manuals and updated online help are part of the delivered ISO-Image and installed upon the installation of OES 4.2 SP1 ICSW

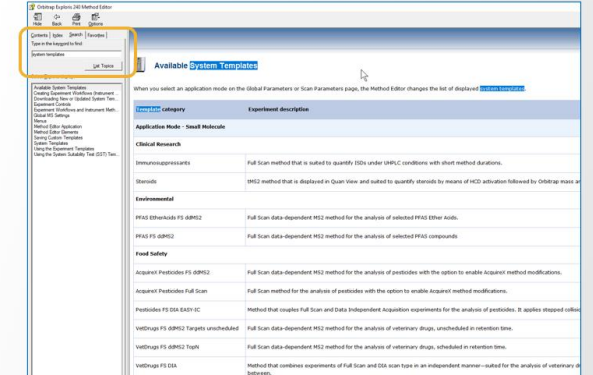
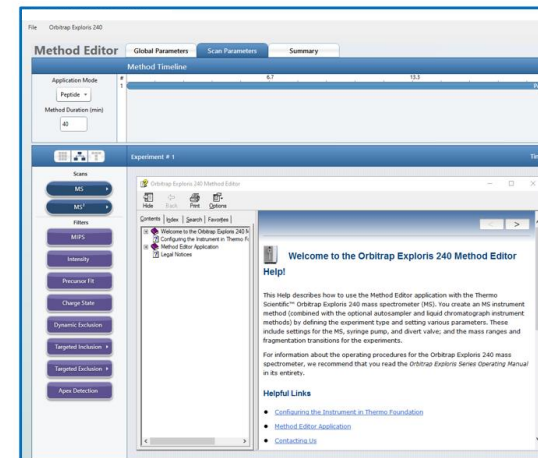
Display Online Help – of Tune – and – of Method Editor - via Fct F1 Key

Display online help – of Tune - via Fct F1 key

or via the gear wheel symbol in Tune – located to the right (top) corner in Tune



Display online help – of Method Editor - via Fct F1 key

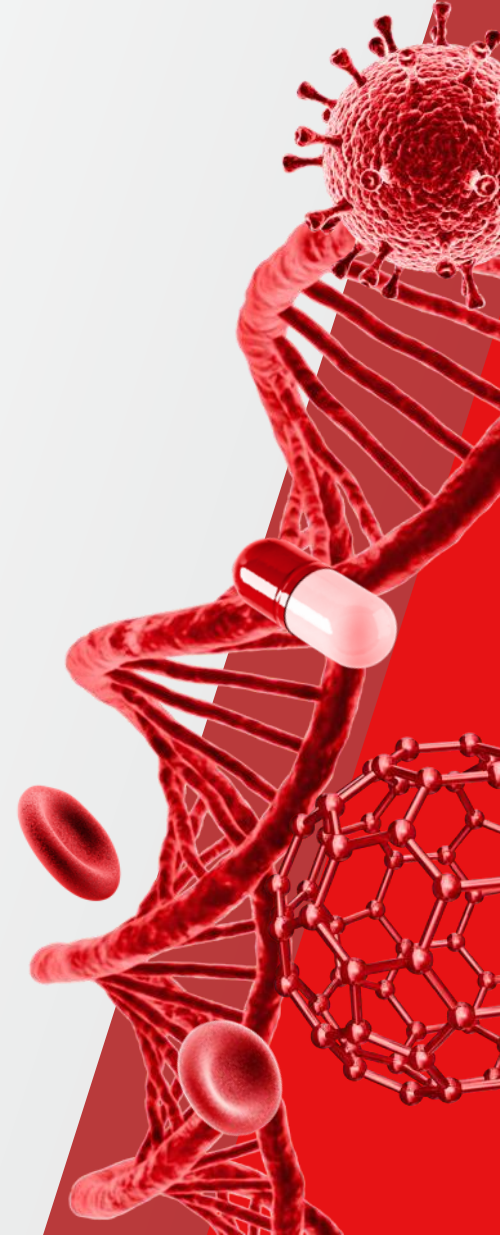




- Working under Chromeleon CDS * software

* CDS = Chromatography Data System

 The world leader in serving science



OES 4.2 SP1 ICSW and Chromeleon CDS Software

LC-MS and GC-MS data acquisition under Chromeleon

- **OES 4.2 SP1 driver** validated for use with Chromeleon CDS 7.2.10 MUg software and Chromeleon CDS 7.3.1 MUa
- Improvements : Method Editor menu bar is now available and allow
 - Import Method from Raw Data File
 - Import Mass Lists from Q Exactive Method File
- Defect fixes: The previous issue observed with Orbitrap Exploris Series 4.1 ICSW, which prevented Workstation Method Editor to be launched without Foundation installed and therefore the use of the MS client driver on Chromeleon enterprise systems using Terminal Server / Citrix clients, has been fixed.
- The Chromeleon Driver Compatibility matrix is updated when new combinations of software versions are tested. For more information and to view the compatibility matrix, sign on to <https://support.thermoinformatics.com/downloads/default.aspx>, and then select **Chromeleon > Chromeleon > Related Drivers > Driver Compatibility Matrix**.

