

We recommend to install **OES 4.0 SP1 ICSW** with your mass spectrometer to take full advantage of all capabilities.

# Thermo Scientific Orbitrap Exploris 4.0 and 4.0 SP1 Instrument Control Software (OES 4.0 and 4.0 SP1 ICSW) –

## New Features, Improvement and Defect Fixes

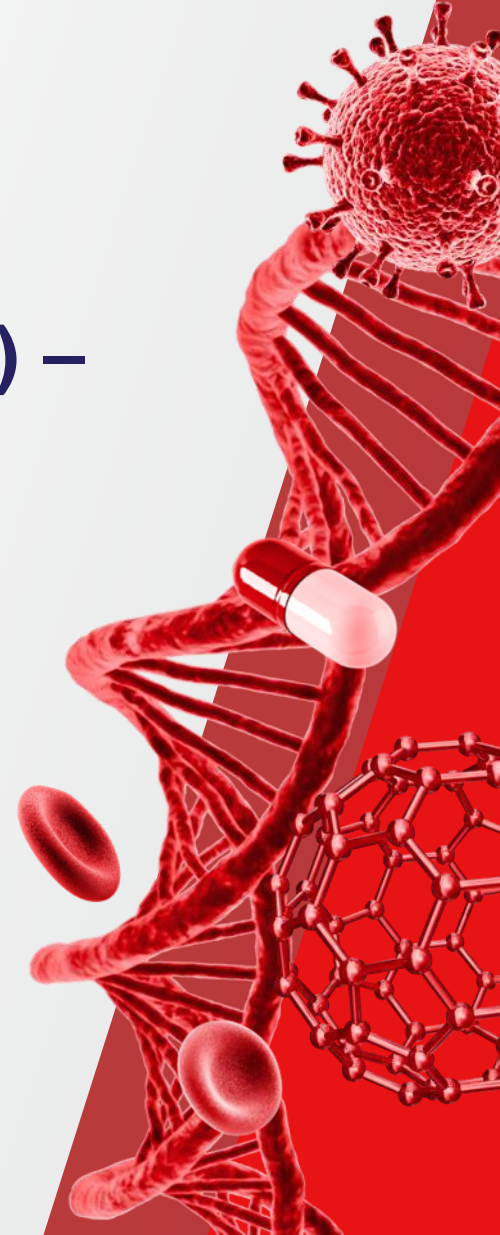
**Kerstin Strupat**

Product Manager

With contribution from Product Management Team LSMS

Q4 2021

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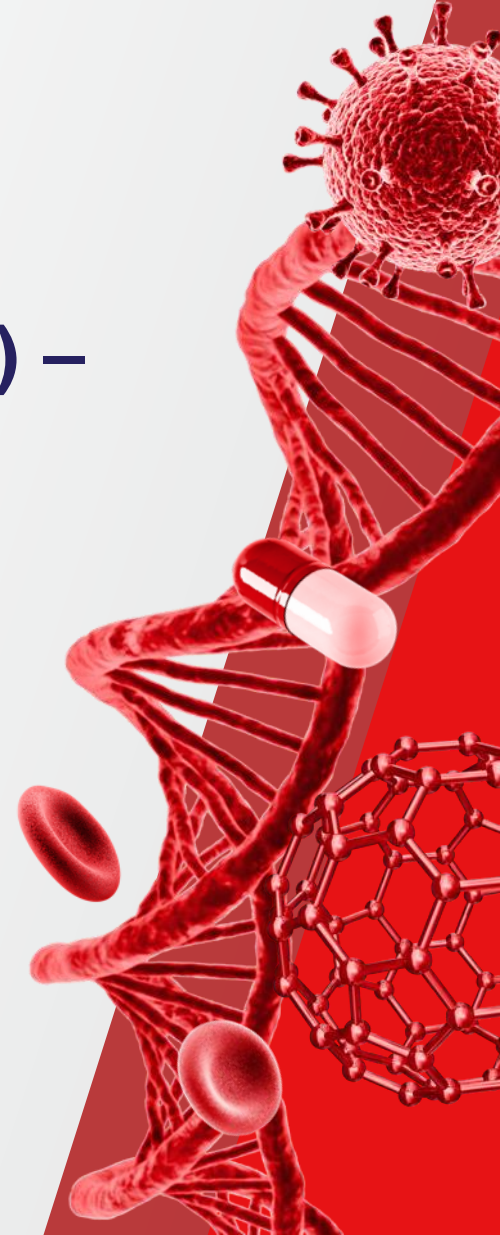
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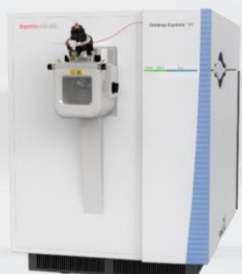
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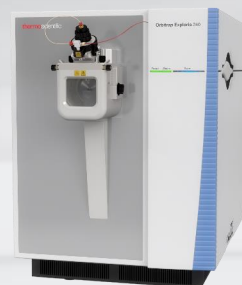
# Thermo Scientific Orbitrap Exploris MS Portfolio – one ICSW



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 - new with OES 4.0 ICSW		
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* > 1.4 Hz	60 k Full Scan* > 1.4 Hz 60 k tSIM Scan* > 1.6 Hz		
Calibration	One-click calibration with FlexMix and dedicated calibration probe - with <b>harmonization and improved user experience across all TNG platforms</b> (TSQs, Hybrids, Tribrids)			
One-Point Mass Calibration	One-Point Mass Calibration achieves < 3 ppm RMS drift over at least 4 weeks - <b>new with OES 4.0 ICSW</b>			
Scan modes  Full MS AIF t-SIM DIA MS2  combinable within in one single experiment, such as:	<ul style="list-style-type: none"> <li>Full Scan</li> </ul> <p>In addition, multiple experiments can be created combining various Full Scan experiments</p>	<ul style="list-style-type: none"> <li>Full ScanddMS2 (Top1-4)</li> <li>tSIM (targeted mass list) ddMS2 (Top1-4)</li> <li>Full ScanddMS2 (targeted list) (Top1-4)</li> </ul> <p>In addition, up to 5 experiments can be created combining the above listed scan types</p>	<ul style="list-style-type: none"> <li>Full ScanddMS2 (topN)</li> <li>Full ScanddSIM</li> <li>tSIM (targeted mass list) ddMS2</li> <li>Full ScanddMS2 (targeted mass list)</li> </ul> <p>With options for</p> <ul style="list-style-type: none"> <li>'Number of Scans' (= TopN)</li> <li>'Cycle Time'</li> </ul> <p>In addition, multiple experiments can be created combining the above listed scan types</p>	<ul style="list-style-type: none"> <li>Full ScanddMS2 (topN)</li> <li>Full ScanddSIM</li> <li>tSIM (targeted mass list) ddMS2</li> <li>Full ScanddMS2 (targeted mass list)</li> </ul> <p>With options for</p> <ul style="list-style-type: none"> <li>'Number of Scans' (= TopN)</li> <li>'Cycle Time'</li> <li>'Scans per Outcome' (branching)</li> </ul> <p>In addition, multiple experiments can be created combining the above listed scan types</p>
Advanced acquisitions	APD	AcquireX (chargeable option)	AcquireX, APD  TMT @ 45k resolution setting	<ul style="list-style-type: none"> <li>16 msec transient (7,500 min resolution)</li> <li>System Templates supporting BoxCar and SureQuant approaches</li> <li>TurboTMT with TMT reagents up to 16-plex</li> </ul>

## Thermo Scientific Orbitrap Exploris Series 4.0 Instrument Control Software Release Notes

This document lists installation notes, new features and improvements regarding the Thermo Scientific™ Orbitrap Exploris™ Series 4.0 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	✓	✓	✓	✓	✓	✓



Source: Release Notes for OES 4.0 ICSW

# System Requirements

## Thermo Scientific Orbitrap Exploris Series 4.0 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 4.0 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 LTSC or 2019 LTSC Thermo Scientific Xcalibur 4.5

**Tip** The Orbitrap Exploris Series 4.0 Instrument Control Software was only tested within the delivered composition.

**Note:**  
Xcalibur 4.5 software applies  
Foundation 3.1 SP8.

Source: Release Notes for OES 4.0 ICSW

# List of new Features and Improvements realized with OES 4.0 ICSW

## New Features

### General

- Full Integration of Orbitrap Exploris MX into the platform

### Tune

- 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.
- Tune: Fore Vacuum supervision: The user needs to be informed if transfer tube is clogged.

### Method Editor

- Method Editor: Global Settings - Internal Mass Calibration provides various internal calibration modes (RunStart, Scan-to-Scan, Timed).
- Method Editor: Global Settings - Internal Mass Calibration offers Lock Mass Injection functionality for user-defined lock masses.
- Raw file spectra provide access to extended peak data supported by FreeStyle 1.8 and higher.

## Improvements (selection)

**Orbitrap Exploris 120 model:** access to precursor  $m/z$  isolations  $\leq m/z$  2500 in ddMS2 / tMS2 and SIM scans

### Tune and Method Editor

- Precursor  $m/z$ : Quadrupole Isolation Range checking considers the first mass of quadrupole isolation window
- Scan Range checking restricts Full Scan ranges to the Factor 15 rule (OE 120, 240, 480, and MX models)

### Tune Diagnostics

- rearranged the 'Tools' tree for improved access to toggles and settings separated by category: Calibration, Define Scan, Application Mode, Method Setup, Peripherals

### Tune System Calibration

- Faster, more robust Isolation Shape Analysis algorithm results in shorter duration of system calibration

### Method Editor

- Full Scan: recommendation to set the first mass to values  $\leq 2500$   $m/z$  is added
- Method Editor: Targeted Mass Filter: Property 'Collision Energy Mode' is removed and HCD Collision Energy (%) allows access to 1 (fixed), and 2, 3, 4, 5 (stepped) set values
- Targeted Scans: Property 'Collision Energy Mode' is removed and HCD Collision Energy (% or V) allows access to 1 (fixed), and 2, 3, 4, 5 (stepped) set values
- Method Execution: EASY-IC applies the same lock mass correction behavior for ddMS2 scans as with User Defined Lock masses

**Chromeleon:** Chromeleon: ePanel Thermo MS Tuning: Instrument Audit Trail logs information about Tune events.

**FAIMS Pro Duo:** a firmware update mitigates 'overcooling' of the FAIMS electrodes



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Orbitrap Exploris™ MX  
Mass Detector



Thermo Scientific™  
Orbitrap Exploris™ 240 Mass Spec

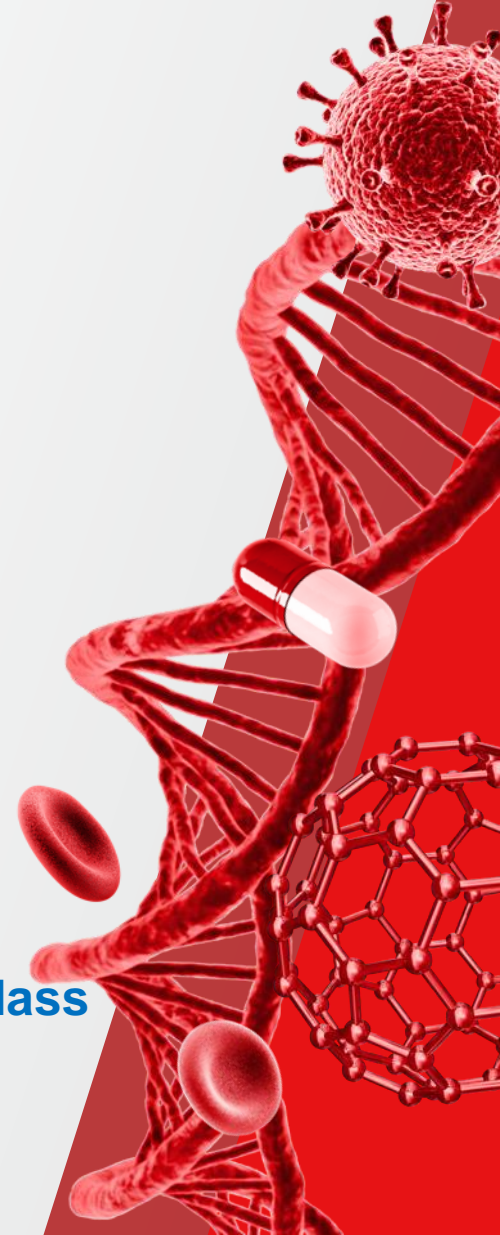


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## New Functionalities enabled w/ OES 4.0 ICSW

1. Full integration of Orbitrap Exploris MX mass detector into OES ICSW
2. One-Point Calibration
3. Customized Mass Calibration
4. Various 'Internal Calibration' options – applicable to EASY-IC or User-Defined Lock Mass

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Thermo Scientific™  
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Mass Detector



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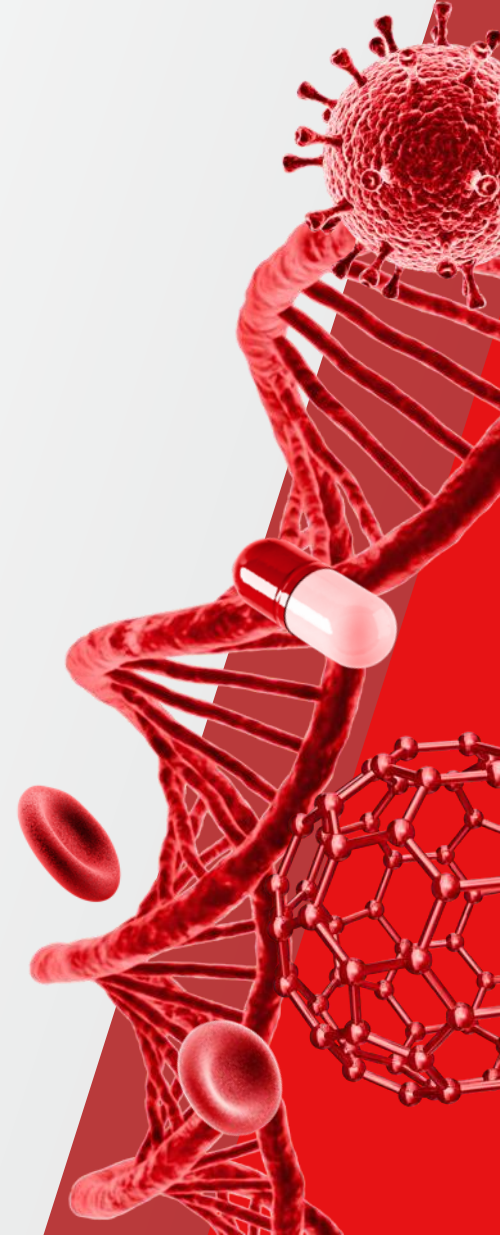


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## New Functionalities enabled w/ OES 4.0 ICSW

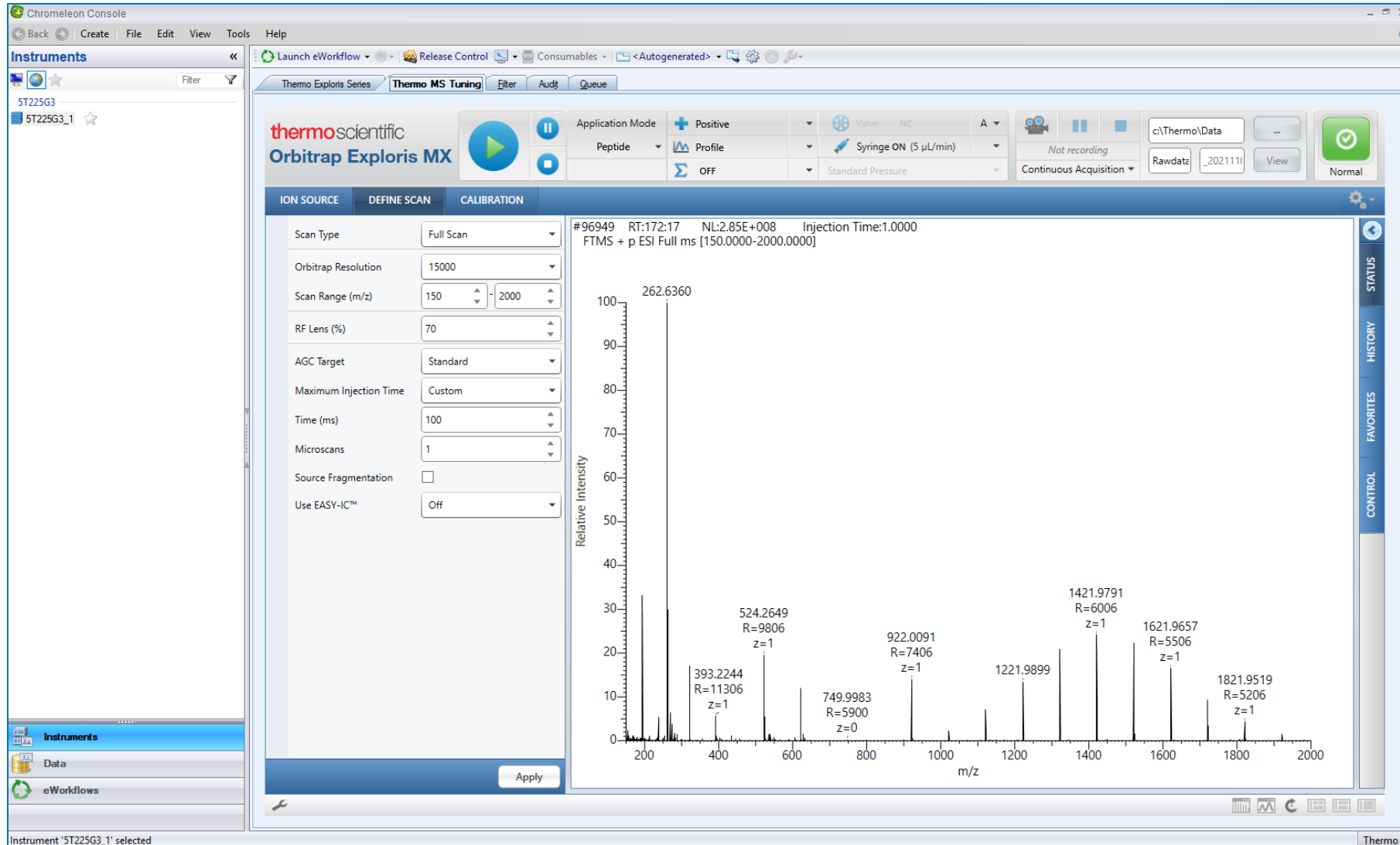
### 1. Full integration of Orbitrap Exploris MX mass detector into OES ICSW

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# Full integration of Orbitrap Exploris MX MS into OES ICSW

Available with OES 4.0 ICSW – Integration of **Tune Application** as ePanel in Chromeleon CDS sw



# Full integration of Orbitrap Exploris MX MS into OES ICSW

Available with OES 4.0 ICSW – Integration of **Method Editor Appl.** as ePanel in Chromeleon CDS sw

The screenshot displays the 'New Instrument Method (Instrument Method) - Chromeleon Chromatography Studio' window. The interface is divided into several sections:

- Toolbar:** Contains icons for Home, Cut, Copy, Paste, Check Method, Open Instrument..., Command, Time, Stage, Conditional, Comment, Delete, New Command Rows, Expand All Stages, Collapse All Stages, Previous, Next, Find, UHPLC Speed-Up, and Method Transfer.
- Instrument Method Panel (Left):** Shows a tree view with categories like Overview, Pump (VF-P10-A), SamplerModule (VF-A10-A), ColumnComp (VH-C10-A), MSDevice (Orbitrap Exploris MX), System, Startup Shutdown, and Script Editor.
- Method Editor (Center):** Features tabs for Global Parameters, Scan Parameters, and Summary. It includes a 'Method Timeline' with a graph showing a single 'MS' scan from 0 to 27 minutes. Below the timeline is a 'Scans' section with a 'Full Scan' button.
- Settings Panel (Right):** Contains various configuration options:
  - Infusion Mode: Liquid Chromatography
  - Expected LC Peak Width (s): 6
  - Advanced Peak Determination:
  - Default Charge State: 2
  - Internal Mass Calibration: Off
  - Orbitrap Resolution: 120000
  - Scan Range (m/z): 280-1600
  - RF Lens (%): 70
  - AGC Target: Standard
  - Maximum Injection Time Mode: Auto
  - Microscans: 1
  - Data Type: Profile
  - Polarity: Positive
  - Source Fragmentation:

# New for certain models is now access to 180 k resolution setting

Available with OES 4.0 ICSW – Parameter **Orbitrap Resolution** allows to set **180 k** set value

For **Full Scan** type,

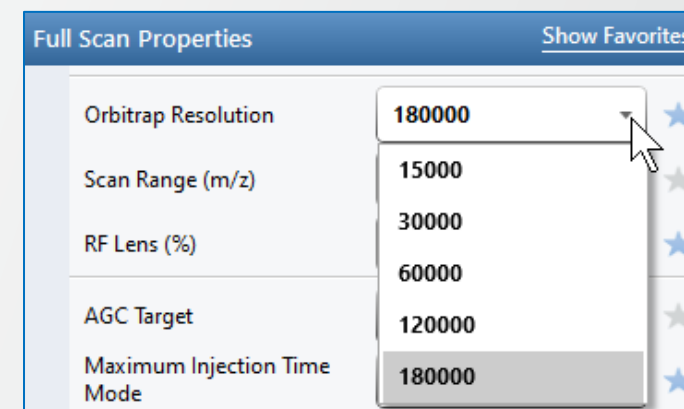
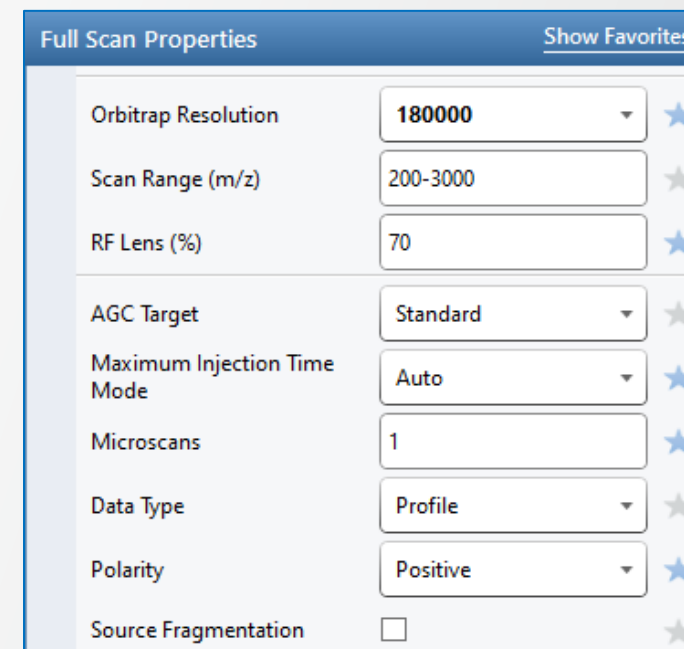
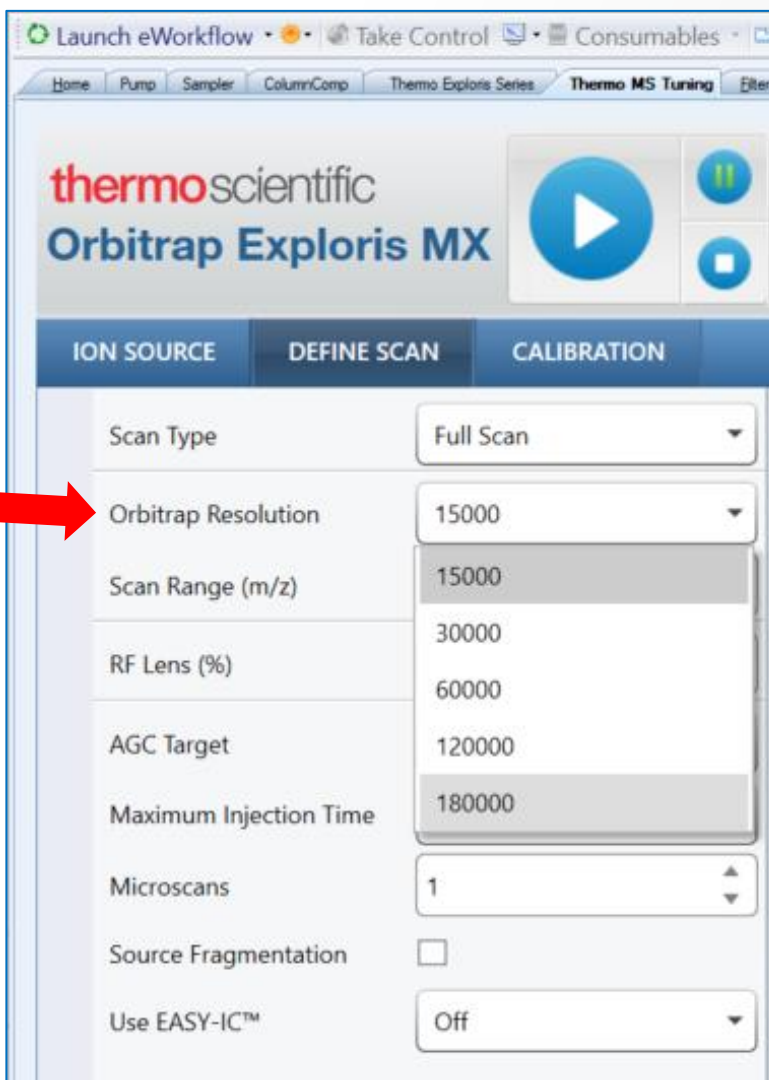
- **Tune Application** and
- **Method Editor Application**

allow to choose an

**Orbitrap Resolution of 180 k** (set value) for these models:

- Orbitrap Exploris MX (shown to the right)
- Orbitrap Exploris 240
- Orbitrap Exploris 480

Additionally, the **Tune Application** provides access to **Orbitrap Resolution of 180 k** for **MS2** and **SIM Scan** types for models Orbitrap Exploris 240, Orbitrap Exploris 480. (not shown here)





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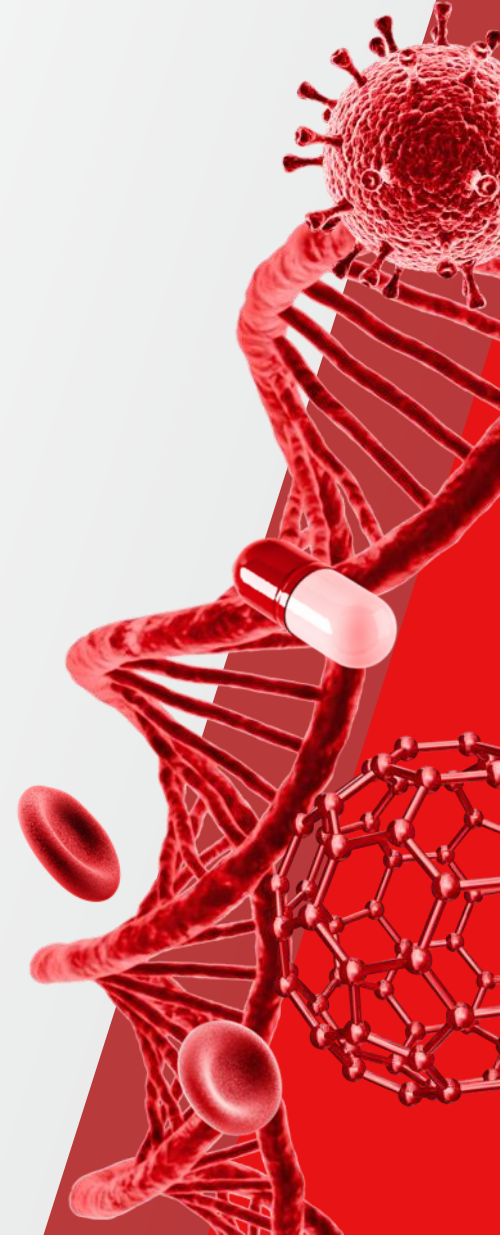
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## New Functionalities enabled w/ OES 4.0 ICSW

### 2. One-Point Mass Calibration



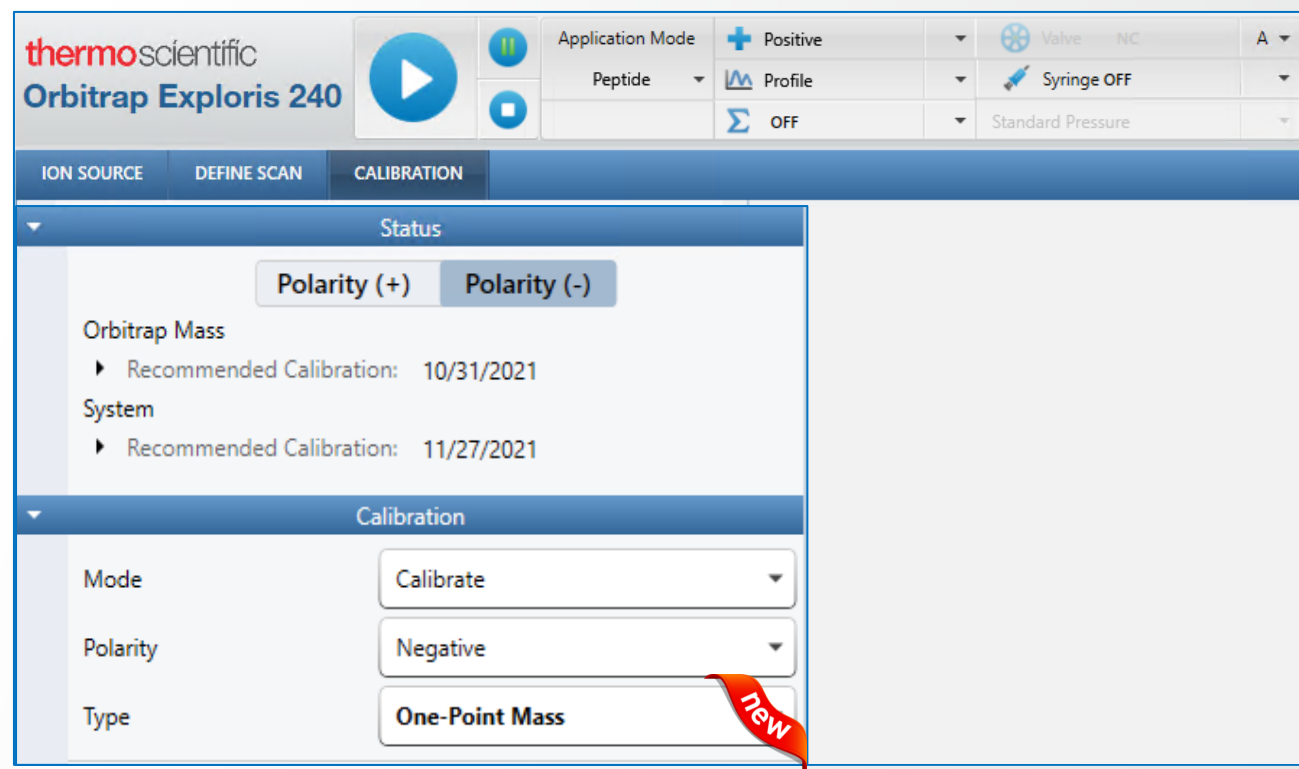
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# One-Point Mass Calibration – in Tune application

Available with OES 4.0 ICSW → Calibration tab → Calibration panel

- **‘One-Point Mass’** Calibration Procedure calibrates positive and negative ion mode
- Fluoranthene from the EASY-IC source is used for the **‘One-Point Mass’** calibration procedure
- **Important Note:** running the **‘One-Point Mass’** calibration procedure updates the master calibration file. Its updated content is applied to upcoming scans and raw data files w/o further user interaction.



# In more depth: One-Point Mass Calibration – in Tune application

Available with OES 4.0 ICSW → Calibration tab → Calibration panel → Mode: Calibrate / Check, Types

Calibration

Mode: Calibrate

Polarity: Positive

Type: Mass

Select type of calibration to run

[Learn more...](#)

Mass: Uses the masses of a stable FlexMix spray to calibrate the masses. This calibration requires FlexMix solution.

Mass & System: Performs a whole system calibration. This calibration requires FlexMix solution.

**i One-Point Mass: The internal calibration source with fluoranthene is used for calibrating the mass with One-Point. An infusion of FlexMix solution is not needed. The calibration can be performed anytime between runs without disconnecting the HPLC or changing the source set-up. The user may subsequently evaluate the mass range for your analytes e.g. via a system suitability test.**

Customized Mass: Enables to mass calibrate the mass spectrometer with user-definable masses. The user can edit, save and recall mass lists via the user interface. The user can select or deselect masses from the list as appropriate.

Calibration

Mode: Calibrate

Polarity: Positive

Type: Mass

- Mass
- Mass
- Mass & System
- One-Point Mass
- Customized Mass

Calibration

Mode: Check

Polarity: Positive

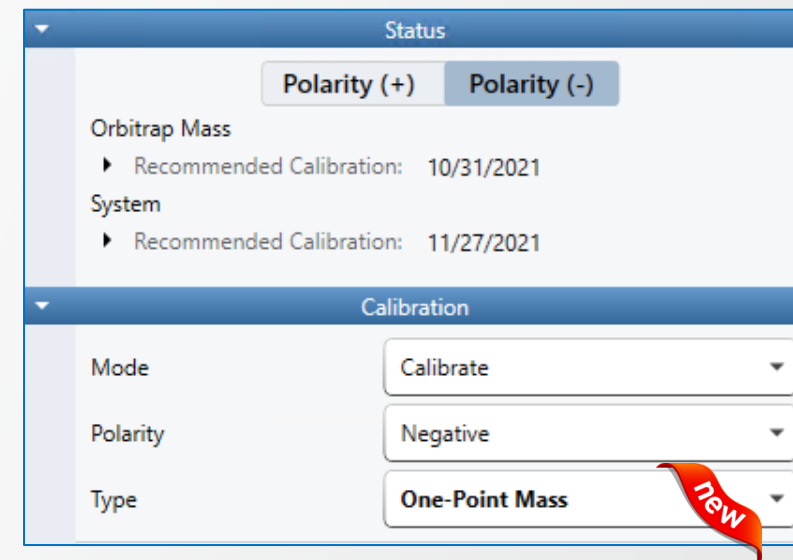
Type: Mass

- Mass
- Mass
- Mass & System
- Customized Mass

# One-Point Calibration – in Tune application

Available with OES 4.0 ICSW → Calibration tab → Calibration panel

- ,One-Point Mass' calibration Procedure calibrates positive and negative ion mode
- Fluoranthene from the EASY-IC source is used for the 'One-Point Mass' calibration procedure
- Infusion of FlexMix solution is not needed
- → calibration can be performed anytime between runs
- → no need to disconnect the LC line
- → no need to change the source set-up (to e.g. the calibration sprayer)
- The user may subsequently evaluate the mass range of interest e.g. via a system evaluation test
- **Important Note:** running the '**One-Point Mass**' calibration procedure updates the master calibration file. Its updated content is applied to upcoming scans and raw data files w/o further user interaction. The *Recommended Calibration* date is updated accordingly. **In contrast:** With '**Internal Mass Calibration**' (w/ EASY-IC or User-defined Lock Mass) the master calibration file is NOT updated, but the recognized correction upon locking is remembered within a given raw file acquisition\*. The *Recommended Calibration* date is NOT updated with 'Internal Mass Calibration'.



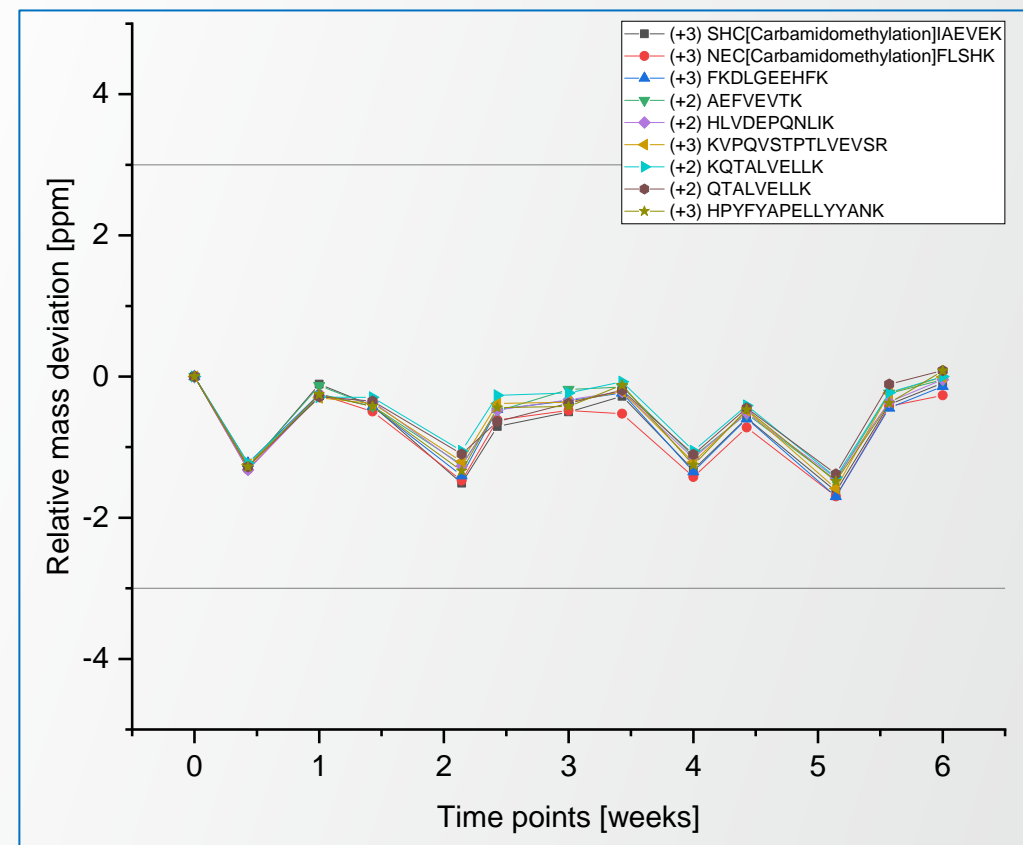
\* see section 'New Functionalities w/ OES 4.0 ICSW - Internal Mass Calibration Options'



# One-Point Mass Calibration

Maintains Mass Accuracy over a long duration >> 24 h

- 9 Peptides of a BSA digest were analyzed
- Prior to each data point a **One-Point Mass Calibration** procedure was performed
- One data point represents an average of 19 individual injections
- **Exceptional mass accuracy over a period of 6 weeks** of repeated injections of BSA digest during regular operation



Data shows the mass deviation in ppm relative to the first data point and displayed for the various monitored BSA peptides monitored over several weeks.



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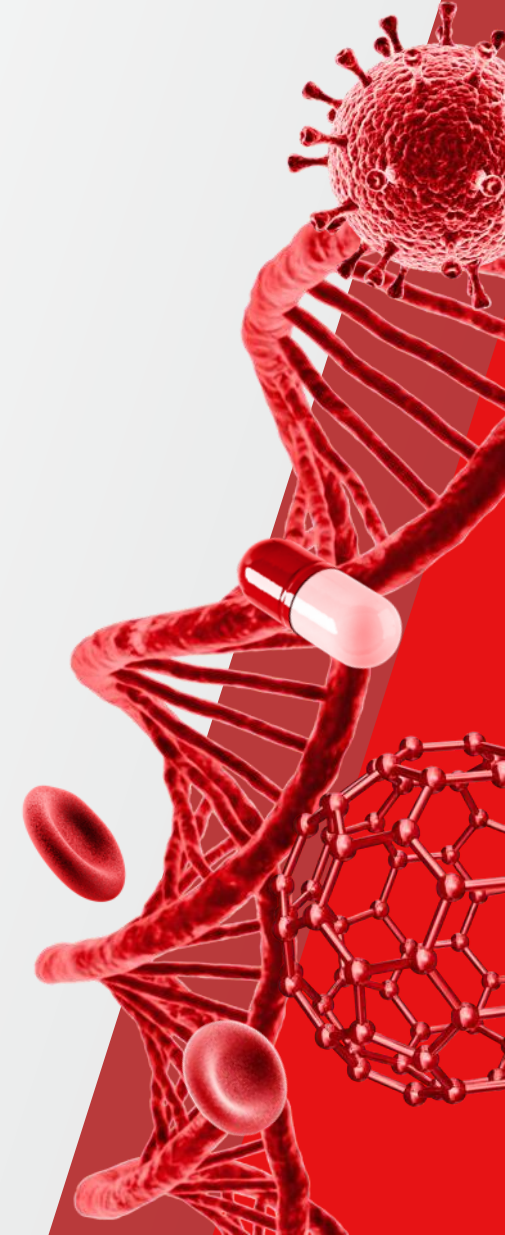
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## New Functionalities enabled w/ OES 4.0 ICSW

### 3. Customized Mass Calibration / Check Functionality



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# Customized Mass Calibration – in Tune application



Available with OES 4.0 ICSW → Calibration tab → Calibration panel

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Orbitrap Exploris 240

Application Mode: + Positive, Peptide, Profile, OFF, Valve: NC, Syringe: OFF, Standard Pressure

ION SOURCE | DEFINE SCAN | **CALIBRATION**

Status: Polarity (+) | Polarity (-)

Orbitrap Mass: Recommended Calibration: 10/18/2021  
System: Recommended Calibration: 11/16/2021

Calibration Panel:

Mode: Calibrate  
Polarity: Positive  
Type: Customized Mass

Theoretical Mass for Positive Ions:

<input type="checkbox"/>		m/z
<input type="checkbox"/>		m/z
<input type="checkbox"/>	524.2649	m/z
<input type="checkbox"/>	622.0290	m/z
<input type="checkbox"/>	922.0098	m/z
<input type="checkbox"/>	1221.9906	m/z

Calibration Type Selection:

- Mass
- Mass & System
- One-Point Mass
- Customized Mass**

One-Point Mass: The internal calibration source with fluoranthene is used for calibrating the mass with One-Point. An infusion of FlexMix solution is not needed. The calibration can be performed anytime between runs without disconnecting the HPLC or changing the source set-up. The user may subsequently evaluate the mass range for your analytes e.g. via a system suitability test.

**Customized Mass: Enables to mass calibrate the mass spectrometer with user-definable masses. The user can edit, save and recall mass lists via the user interface. The user can select or deselect masses from the list as appropriate.**

Calibration

Mode: Calibrate  
Polarity: Positive  
Type: Customized Mass

Buttons: Load User-defined Mass List..., Save, Save As, Load Default

Theoretical Mass for Positive Ions:

<input type="checkbox"/>		m/z
<input type="checkbox"/>		m/z
<input type="checkbox"/>	524.2649	m/z
<input type="checkbox"/>	622.0290	m/z
<input type="checkbox"/>	922.0098	m/z
<input type="checkbox"/>	1221.9906	m/z

Calibration

Mode: Check  
Polarity: Positive  
Type: Customized Mass

Buttons: Load User-defined Mass List..., Save, Save As, Load Default

# Customized Mass Calibration – in Tune application

Available with OES 4.0 ICSW → Calibration tab → Calibration panel

ION SOURCE DEFINE SCAN CALIBRATION

Status

Calibration

Mode **Calibrate**

Polarity **Positive**

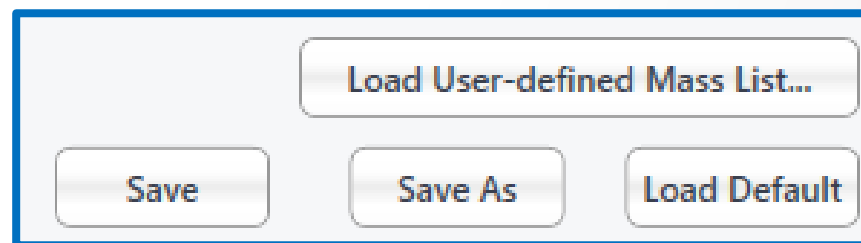
Type **Customized Mass**

Load User-defined Mass List..

Save Save As Load Default

Theoretical Mass for Positive Ions

<input type="checkbox"/>	195.0877	m/z
<input type="checkbox"/>	322.0481	m/z
<input type="checkbox"/>	524.2649	m/z
<input type="checkbox"/>	622.0290	m/z
<input type="checkbox"/>	922.0098	m/z
<input type="checkbox"/>	1221.9906	m/z
<input type="checkbox"/>	1521.9715	m/z
<input type="checkbox"/>	1621.9651	m/z
<input type="checkbox"/>	1721.9587	m/z
<input type="checkbox"/>	1821.9523	m/z



- 'Load Default'
- 'Load User-defined Mass List'
- 'Save'
- 'Save As'

ION SOURCE DEFINE SCAN CALIBRATION

Status

Calibration

Mode **Calibrate**

Polarity **Negative**

Type **Customized Mass**

Load User-defined Mass List..

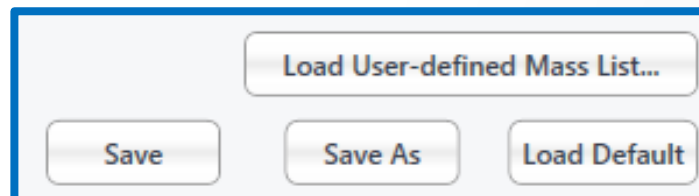
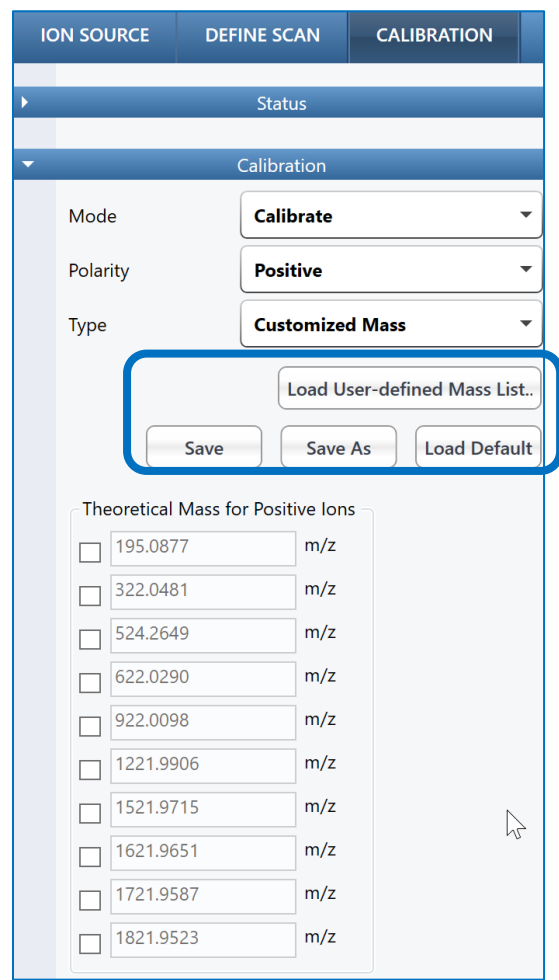
Save Save As Load Default

Theoretical Mass for Negative Ions

<input type="checkbox"/>	162.9824	m/z
<input type="checkbox"/>	318.9798	m/z
<input type="checkbox"/>	362.9696	m/z
<input type="checkbox"/>	601.9790	m/z
<input type="checkbox"/>	1033.9881	m/z
<input type="checkbox"/>	1333.9689	m/z
<input type="checkbox"/>	1633.9498	m/z
<input type="checkbox"/>	1733.9434	m/z
<input type="checkbox"/>	1833.937	m/z
<input type="checkbox"/>	1933.9333	m/z

# Customized Mass Calibration – in Tune application

Available with OES 4.0 ICSW → Calibration tab → Calibration panel



Mass lists for customized calibration or check are accessed with:

- **Load Default:**

- FlexMix list (positive / negative) - *not modifiable*
- other specific lists - *not modifiable*; \*.xmb format:  
e.g.: 'FlexMix Low Masses', 'MALDI Matrix clusters'

find these here, FYI: C:\Thermo\Instruments\Exploris\4.0\System\Programs\dependencies\msi\Merkur

CustomizedMassList_Default.xmb	11/16/2021 11:53 ...	XMB File
CustomizedMassList_FlexMixLowmz.xmb	11/16/2021 11:53 ...	XMB File
CustomizedMassList_MALDIposDHBnegNAclusters.xmb	11/16/2021 11:53 ...	XMB File

- **'Load User-defined Mass List'**

- user-definable, savable, and later editable; **xml format**
- Comes along with '**Save**' and '**Save As**', for updating user-defined mass lists  
find here: C:\Thermo\Instruments\Exploris\4.0\System\Programs\dependencies\msx



Thermo Scientific™  
Orbitrap Exploris™ 120 Mass Spec



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Mass Detector



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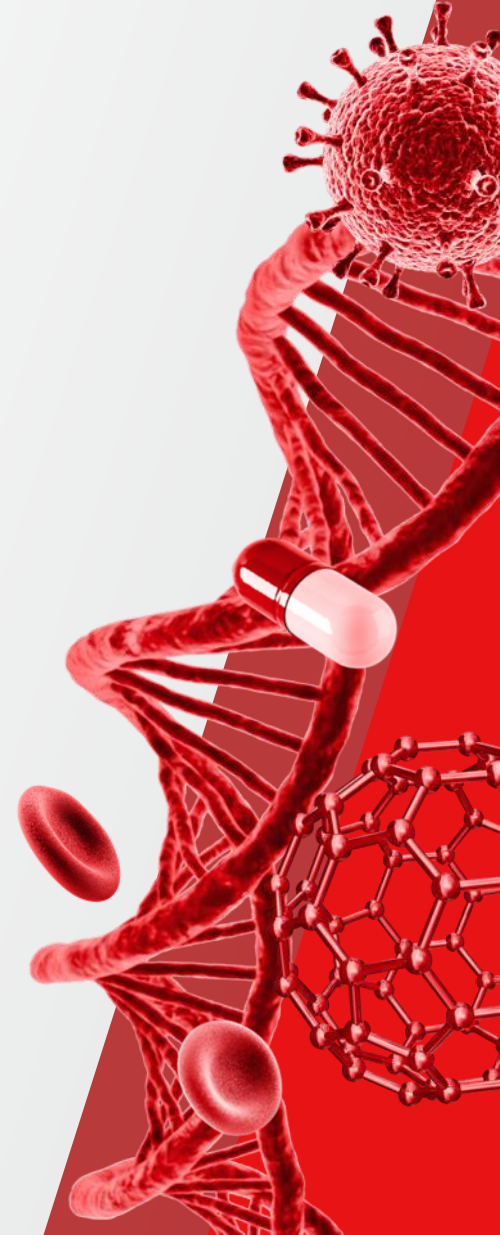


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## New Functionalities enabled w/ OES 4.0 ICSW

4. Various 'Internal Mass Calibration' options –  applicable to EASY-IC or User-Defined Lock Mass

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# In Method Editor – Global Settings

Available with OES 4.0 ICSW

Method Editor, **Global Settings** (top right corner)

## Parameter ‘Internal Mass Calibration’



- UI is tidied up
  - Parameter has drop down menu with these selection options
    - off
    - EASY-IC
    - User-defined Lock Mass

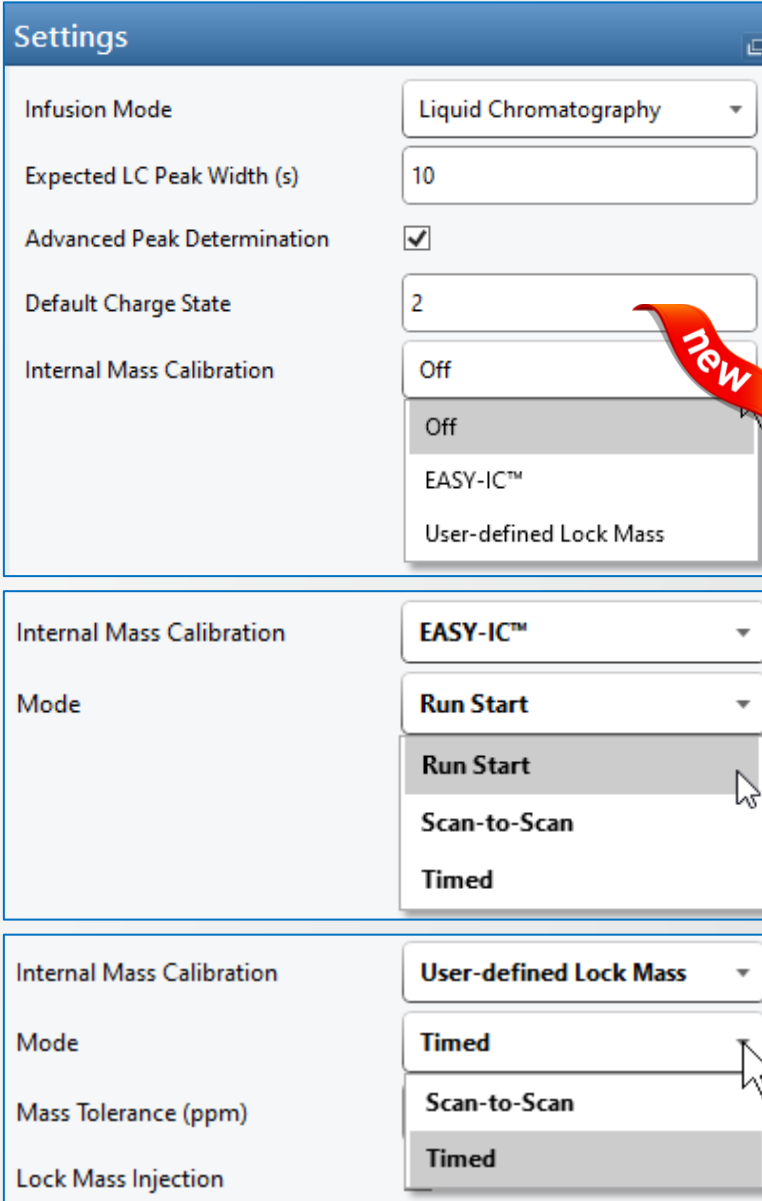
The screenshot displays the 'Method Editor' software interface. A 'Settings' panel is open in the top right corner, showing various parameters. The 'Internal Mass Calibration' parameter is highlighted with a red box and a red arrow pointing to a detailed view of its options. The options are: 'Off', 'EASY-IC™', and 'User-defined Lock Mass'. A red 'new' banner is overlaid on the 'User-defined Lock Mass' option. The main interface shows a 'Method Timeline' at the top, a 'Full Scan' workflow diagram in the center, and a 'Full Scan Properties' panel on the right.

# In Method Editor – Global Settings

Available with OES 4.0 ICSW

## Parameter ‘Internal Mass Calibration’

- UI is tidied up
  - Parameter has drop down menu with these selection options
    - off
    - EASY-IC
    - User-defined Lock Mass
- UX is enhanced and improved w/ more capabilities
  - With Mode ‘EASY-IC’ selected, the user has access to three **Modes**
    - RunStart (as earlier)
    - Scan-to-Scan(as earlier)
    - **Timed** 
  - With Mode ‘User-Defined Lock Mass’ selected, the user has access to two **Modes**
    - Scan-to-Scan(as earlier)
    - **Timed** 



The image displays three screenshots of the 'Settings' window in the Method Editor, illustrating the configuration of the 'Internal Mass Calibration' parameter.

**Top Screenshot:** Shows the 'Internal Mass Calibration' parameter set to 'Off'. A red ribbon with the word 'new' is positioned over the dropdown menu. The dropdown menu is open, showing three options: 'Off', 'EASY-IC™', and 'User-defined Lock Mass'.


**Middle Screenshot:** Shows the 'Internal Mass Calibration' parameter set to 'EASY-IC™'. The 'Mode' dropdown menu is open, showing three options: 'Run Start', 'Scan-to-Scan', and 'Timed'. A mouse cursor is pointing at the 'Run Start' option.

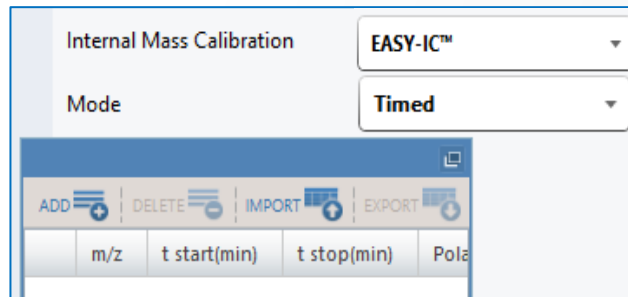
**Bottom Screenshot:** Shows the 'Internal Mass Calibration' parameter set to 'User-defined Lock Mass'. The 'Mode' dropdown menu is open, showing three options: 'Timed', 'Scan-to-Scan', and 'Timed'. A mouse cursor is pointing at the 'Timed' option.



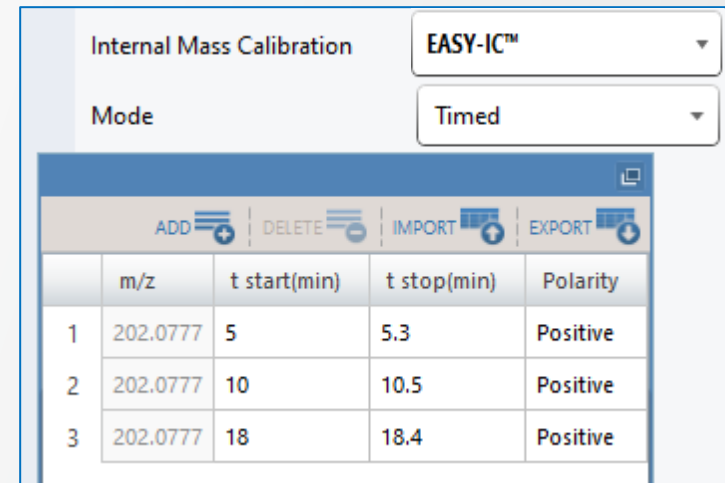
# An example w/ 'EASY-IC' selected

Available with OES 4.0 ICSW

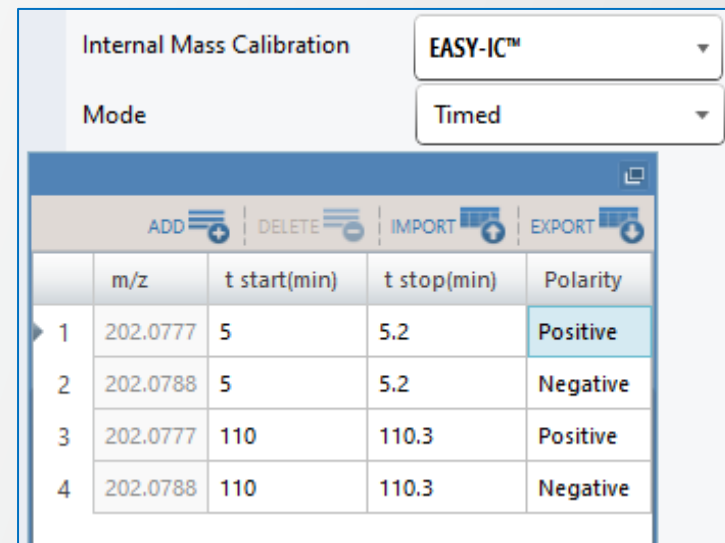
- With Internal Mass Calibration '**EASY-IC**' selected, and Mode '**Timed**' selected, a table appears
- User-definable retention time windows can be set by the user during which the locking takes place:  $t_{\text{start}}(\text{min})$  ,  $t_{\text{stop}}(\text{min})$
- See examples to the right 
- Up to **8 rows** can be added to the table
- As introduced with OES 3.1 ICSW release already – and continues to apply with OES 4.0 ICSW: RunStart EASY-IC scans are moved to the "**Prepare for Run**"-time and consider more than the very last lock mass correction for a more reliable lock mass correction at the beginning of the data acquisition



m/z	t start(min)	t stop(min)	Polarity
-----	--------------	-------------	----------




m/z	t start(min)	t stop(min)	Polarity
202.0777	5	5.3	Positive
202.0777	10	10.5	Positive
202.0777	18	18.4	Positive

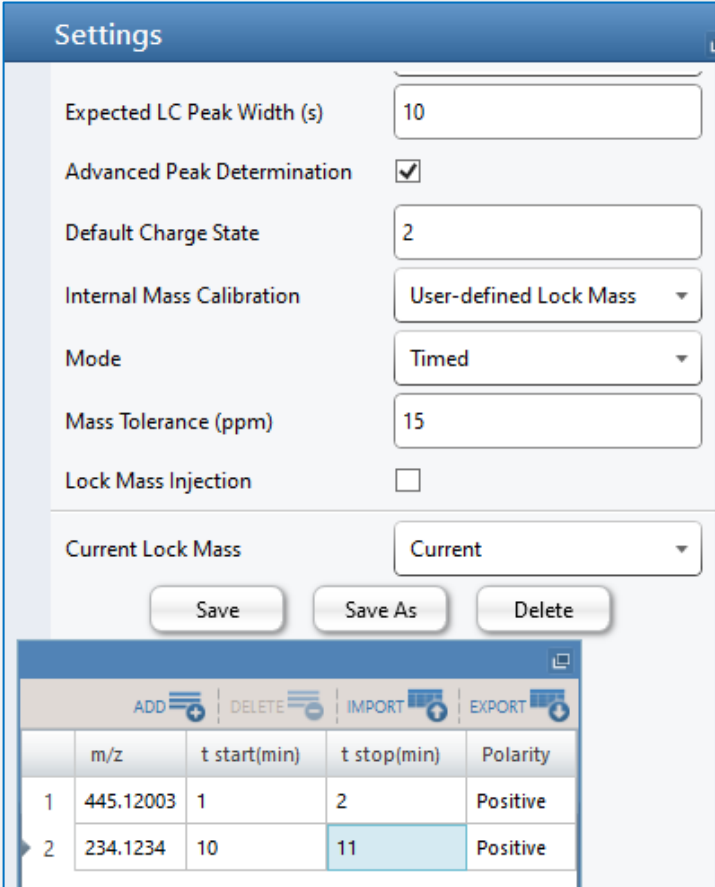


m/z	t start(min)	t stop(min)	Polarity
202.0777	5	5.2	Positive
202.0788	5	5.2	Negative
202.0777	110	110.3	Positive
202.0788	110	110.3	Negative

# An example w/ User-defined Lock Mass' selected

Available with OES 4.0 ICSW

- With Internal Mass Calibration 'User-Defined Lock Mass' selected, and Mode 'Timed' selected, a table appears which can be filled correspondingly
- User-definable retention time windows can be set by the user during which the locking takes place:  $t_{start}$  (min) ,  $t_{stop}$  (min)
- See examples to the right 
- Up to 8 rows can be added to the table



Settings

Expected LC Peak Width (s) 10

Advanced Peak Determination

Default Charge State 2

Internal Mass Calibration User-defined Lock Mass

Mode Timed

Mass Tolerance (ppm) 15

Lock Mass Injection

Current Lock Mass Current

Save Save As Delete

	m/z	t start(min)	t stop(min)	Polarity
1	445.12003	1	2	Positive
2	234.1234	10	11	Positive

	m/z	t start(min)	t stop(min)
5	445.12003	200	201
6	445.12003	300	301
7	445.12003	400	401
8	445.12003	450	451

- The new options – introduced with OES 4.0 ICSW release - **enlarge the capabilities** of the Global Setting Parameter 'Internal Mass Calibration' significantly
- The new options apply to
  - locking w/ EASY-IC (fluoranthene) and
  - locking w/ User-defined Lock Masses

In any case ...

- w/ locking, the m/z is **corrected** for the individual scan or raw file given \*
- if locking is applied during the raw file acquisition, the correction is applied to all scans until the next locking within the same raw file takes place
- if locking cannot be applied according to the method (e.g. when the User-defined Lock Mass is n/a in the expected retention time window), the locking information from the previous locking continues to apply
- the individual scan header of a raw file reports unambiguously about the last successful locking and the correction (ppm) applied

\* w/ locking, the master calibration file is *not* updated – in contrast to the newly introduced 'One-point mass' calibration procedure which updates the master calibration file and all subsequent raw data file acquisitions apply the settings of the master calibration file accordingly.



Thermo Scientific™  
Orbitrap Exploris™ 120 Mass Spec



Thermo Scientific™  
Orbitrap Exploris™ MX  
Mass Detector



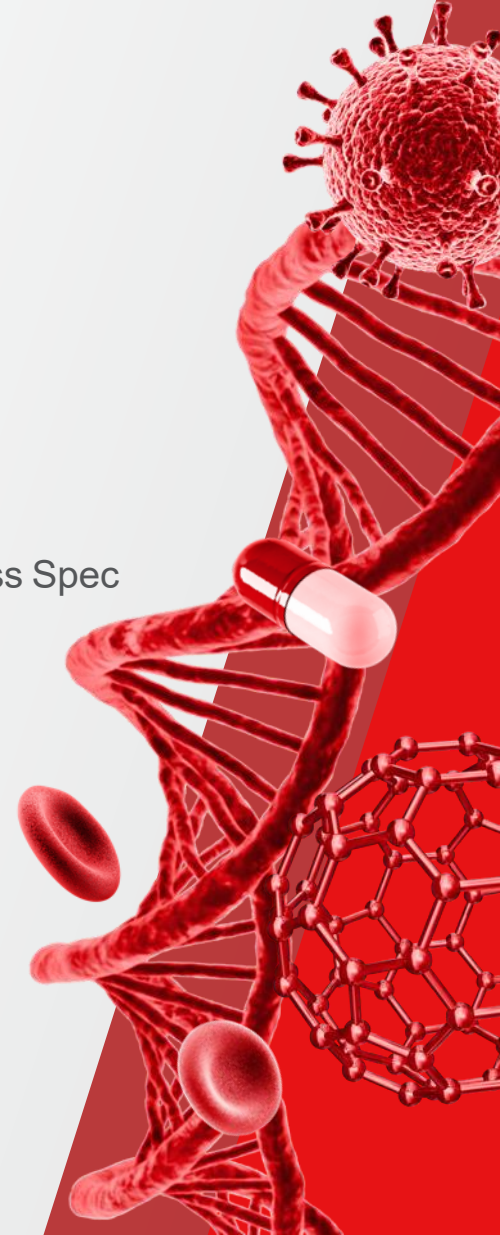
Thermo Scientific™  
Orbitrap Exploris™ 240 Mass Spec

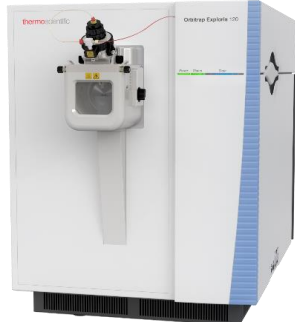


Thermo Scientific™  
Orbitrap Exploris™ 480 Mass Spec

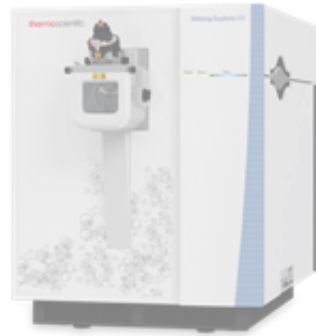
**Improvements** – applying to models OE 120, OE 240 and OE 480 MS -  
enabled w/ **OES 4.0 ICSW**

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Thermo Scientific™  
Orbitrap Exploris™ 120 Mass Spec



Thermo Scientific™  
Orbitrap Exploris™ MX  
Mass Detector



Thermo Scientific™  
Orbitrap Exploris™ 240 Mass Spec

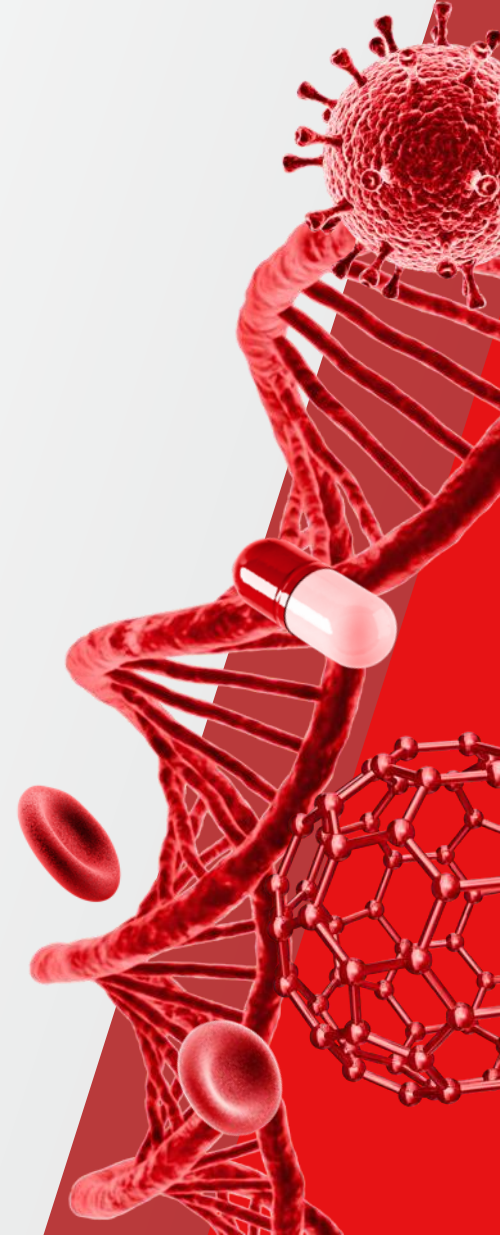


Thermo Scientific™  
Orbitrap Exploris™ 480 Mass Spec

## Improvements enabled w/ OES 4.0 ICSW

'Collision Energy Mode' is removed for an improved UX:  
*fixed* (1 set value) and *stepped* (2, 3, 4, 5 set values) energies are now accessible  
via 'HCD Collision Energy (% or V)' and  
applicable to *Mass List Table* and to *Targeted Mass Filter*

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# 'Collision Energy Mode' is removed for an improved UX:

Functionality for 'fixed' and 'stepped' energies is now available in Parameter 'HCD Collision Energy'

- Applies in Tune and Method Editor Application
- **Applies to tMS2 type - w/ Targeted Mass List Tables**
- Applies to ddMS2 type experiments - w/ Targeted Mass List Filters
- 1 (N)CE Energy value succeeds the (N)CE Mode ,Fixed'
- 2 to 5 (N)CE Energies succeed the (N)CE Mode ,Stepped'



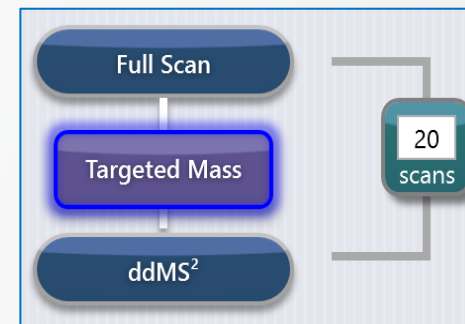
Targeted MS <sup>2</sup> Scan Properties		<a href="#">Show All</a>
Collision Energy Type	Normalized	
HCD Collision <u>Energy</u> (%)	30	

Targeted MS <sup>2</sup> Scan Properties		<a href="#">Show All</a>
Collision Energy Type	Normalized	
HCD Collision <u>Energies</u> (%)	20,25,30,40,60	

# 'Collision Energy Mode' is removed for an improved UX:

Functionality for 'fixed' and 'stepped' energies is now available in Parameter 'HCD Collision Energy'

- Applies in Tune and Method Editor Application
- Applies to tMS2 type experiments - w/ Targeted Mass List Tables
- **Applies to ddMS2 type - w/ Targeted Mass List Filters**
- 1 (N)CE Energy value succeeds the (N)CE Mode ,Fixed'
- 2 to 5 (N)CE Energies succeed the (N)CE Mode ,Stepped'



Targeted Mass Properties

MASS LIST

Mass List Type: m/z & z

Time Mode: Unscheduled

Include Intensity Threshold:

	Compound	Formula	Adduct	m/z	z	HCD Collision Energies (%)
1	MRFA	C <sub>23</sub> H <sub>37</sub> N <sub>7</sub> O <sub>5</sub> S	+H	262.6361	2	30
2	Caffeine	C <sub>8</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub>	+H	195.0877	1	20,45

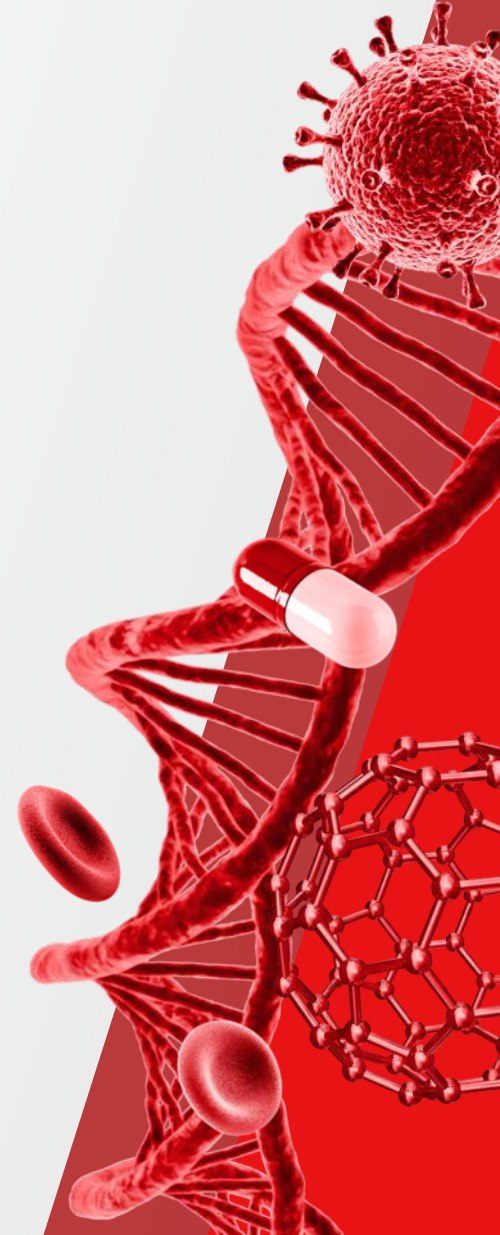
## Updates to Manuals for Orbitrap Exploris Series

**Pre-Installation Requirements Guide**  
and its translations into other languages

**Operator Manuals**  
and its translations into other languages

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

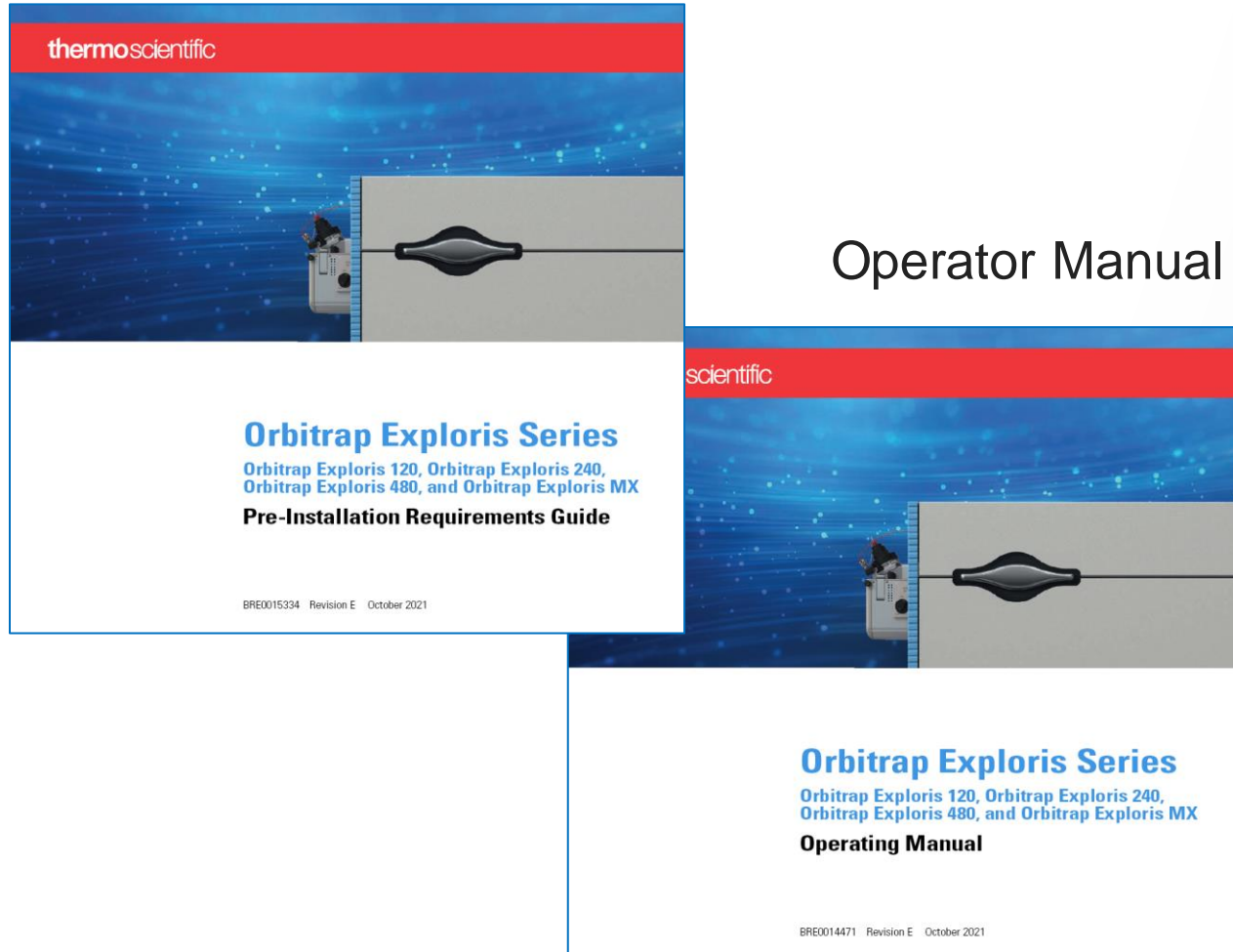
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# PRG and OE manuals

## Pre-Installation Requirement Guide



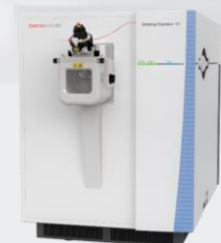
	Language	Additional languages
<b>Preinstallation Requirements Guide</b>	English	<ul style="list-style-type: none"> <li>- Chinese</li> <li>- Japanese</li> <li>- French</li> <li>- Italian</li> </ul> New: Spanish
<b>Operating Manual Hardware</b>	English	<ul style="list-style-type: none"> <li>- Chinese</li> <li>- Japanese</li> <li>- French</li> <li>- Italian</li> </ul> New: Spanish

Manuals in English language are available with the installation of the ISO-Images  
Translations will be made available soon

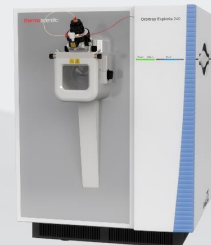
# Software Manuals for these Orbitrap Exploris models



Thermo Scientific™  
Orbitrap Exploris™ MX Mass Detector



Thermo Scientific™ Orbitrap Exploris™ 120  
Mass Spectrometer



Thermo Scientific™ Orbitrap Exploris™ 240  
Mass Spectrometer



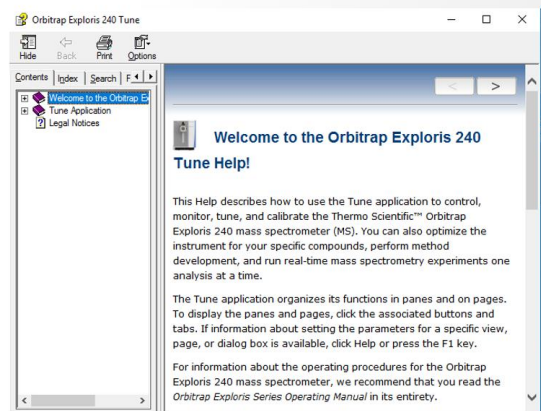
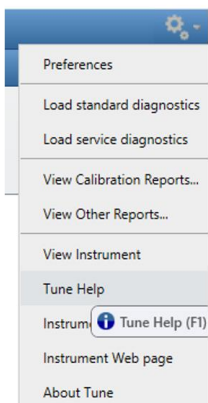
Thermo Scientific™ Orbitrap Exploris™ 480  
Mass Spectrometer

Updated Software Manuals and updated online help are part of the delivered ISO-Image and installed upon the installation of OES 4.0 ICSW  
For updates check also the new website <https://www.analyteguru.com/> which succeeds deprecated PlanetOrbitrap.com.

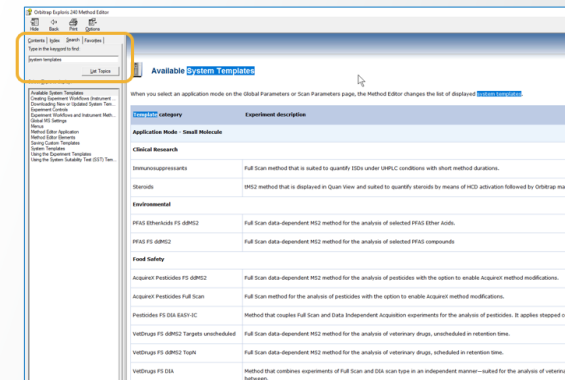
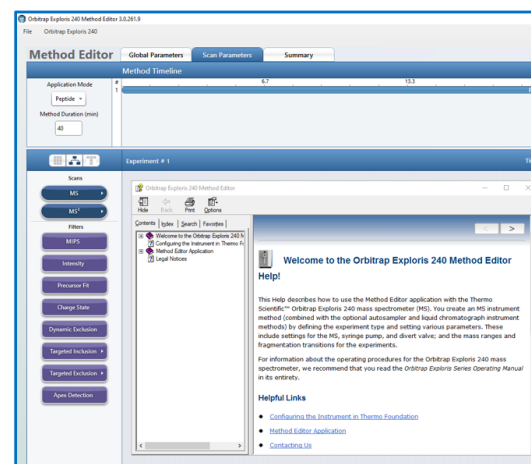
# Display online help – of Tune – and – of Method Editor - via Fct F1 key

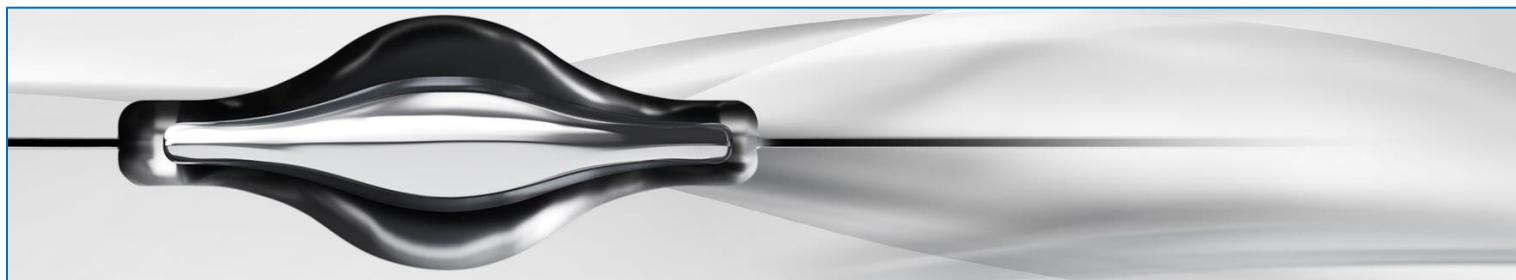
## Display online help – of Tune - via Fct F1 key

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

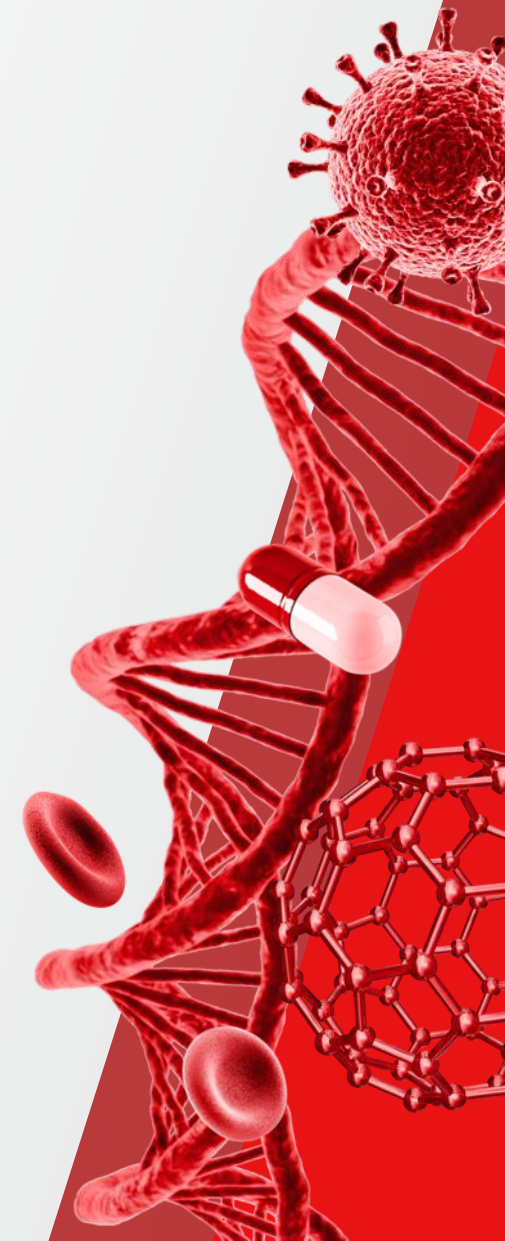




- Working under Chromeleon CDS \* software

\* CDS = Chromatography Data System

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# OES 4.0 ICSW and Chromeleon CDS Software

## LC-MS and GC-MS data acquisition under Chromeleon

The **OES 4.0 drivers** for the six models of the **Orbitrap Exploris Series platform** are validated for use with

- Chromeleon CDS 7.2.10 \*1 software,
- Chromeleon CDS 7.2.10 MUa software
- Chromeleon CDS 7.2.10 MUd software
- upcoming Chromeleon CDS 7.2.10 MUe software
- upcoming Chromeleon CDS 7.3.1 software

All these require working with **Foundation 3.1 SP8**; it is found on **Flexera**.

It is recommended to also check <https://support.thermoinformatics.com/> for more details, incl. the compatibility matrix.

\*1: Chromeleon 7.2.10 requires a hotfix, see PSB.SW-2019-044

