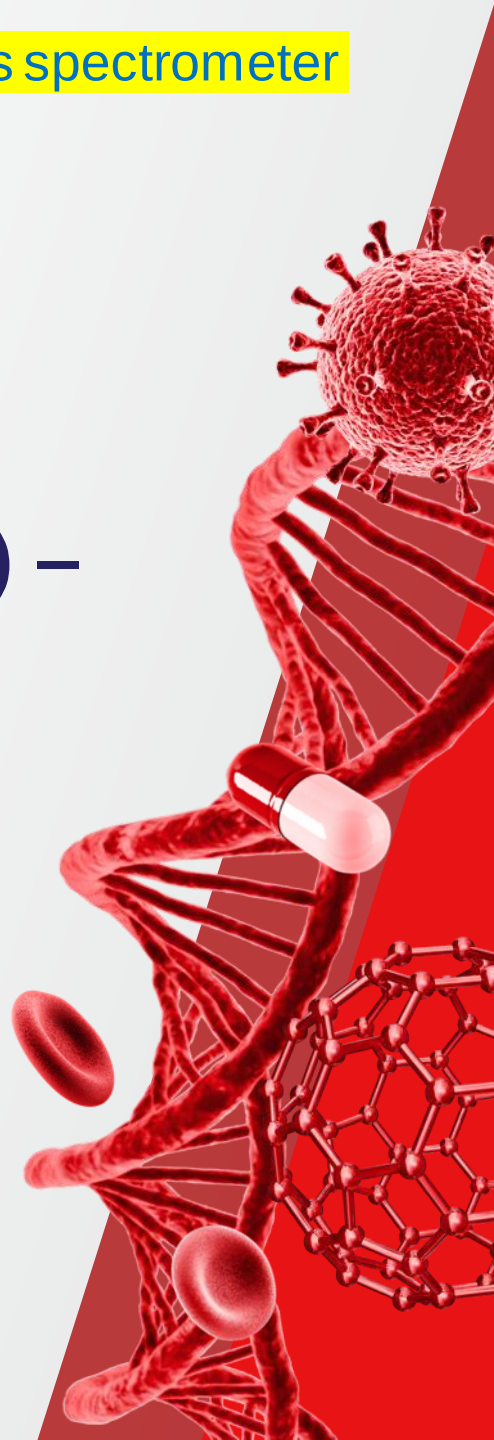
We recommend to install **OES 4.0 SP1 ICSW** with your mass spectrometer to take full advantage of all capabilities.

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 form Product Management Team LSMS

Q4 2021



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

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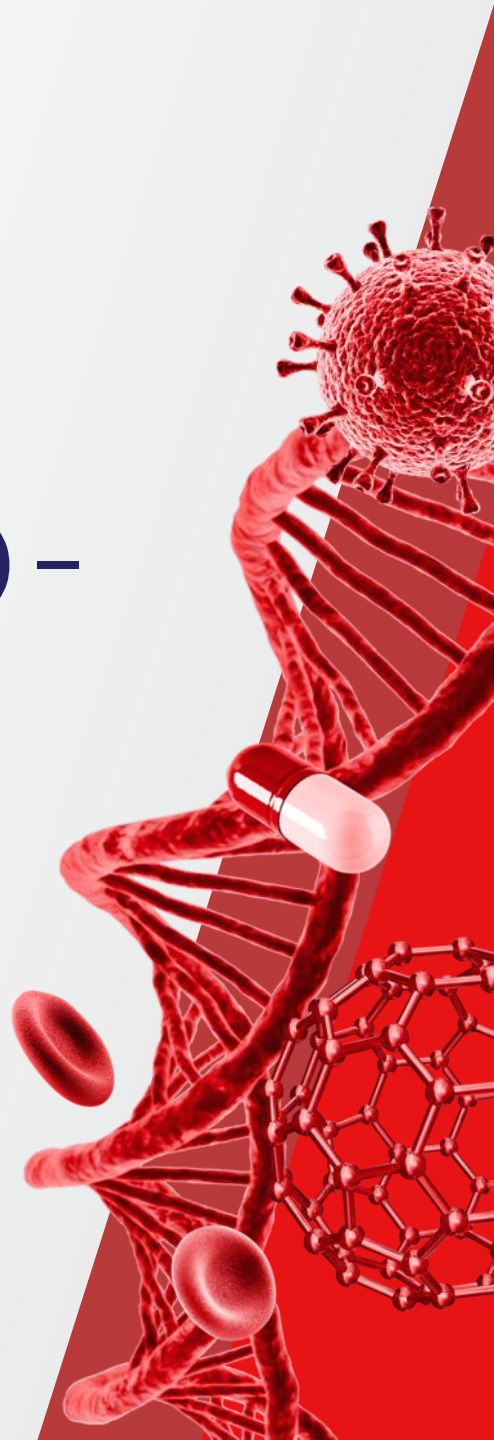

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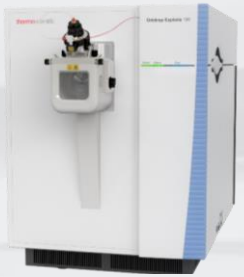
Thermo Scientific Orbitrap Exploris MS Portfolio – one ICSW

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

ThermoFisher SCIENTIFIC

	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 **harmonization and improved user experience across all TNG platforms** (TSQs, Hybrids, Tribrids)			
One-Point Mass Calibration	One-Point Mass Calibration achieves < 3 ppm RMS drift over at least 4 weeks **- new with OES 4.0 ICSW**			
Scan modes **Full MS** **AIF** **t-SIM** **DIA** **MS2** combinable within in one single experiment, such as:	• Full Scan In addition, multiple experiments can be created combining various Full Scan experiments	• Full Scan ddMS2 (Top1-4) • tSIM (targeted mass list) ddMS2 (Top1-4) • Full Scan ddMS2 (targeted list) (Top1-4) In addition, up to 5 experiments can be created combining the above listed scan types	• Full Scan ddMS2 (topN) • Full Scan ddSIM • tSIM (targeted mass list) ddMS2 • Full Scan ddMS2 (targeted mass list) With options for • 'Number of Scans' (= TopN) • 'Cycle Time' In addition, multiple experiments can be created combining the above listed scan types	• Full Scan ddMS2 (topN) • Full Scan ddSIM • tSIM (targeted mass list) ddMS2 • Full Scan ddMS2 (targeted mass list) With options for • 'Number of Scans' (= TopN) • 'Cycle Time' • 'Scans per Outcome' (branching) In addition, multiple experiments can be created combining the above listed scan types
Advanced acquisitions	APD	AcquireX (chargeable option)	AcquireX, APD TMT @ 45k resolution setting	• 16 msec transient (7,500 min resolution) • System Templates supporting BoxCar and SureQuant approaches • TurboTMT with TMT reagents up to 16-plex

Release Notes

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 LTSB 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 ≤ 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 ≤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

Source: Release Notes for OES 4.0 ICSW – available with the installation using the ISO-image

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

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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New Functionalities enabled w/ OES 4.0 ICSW

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

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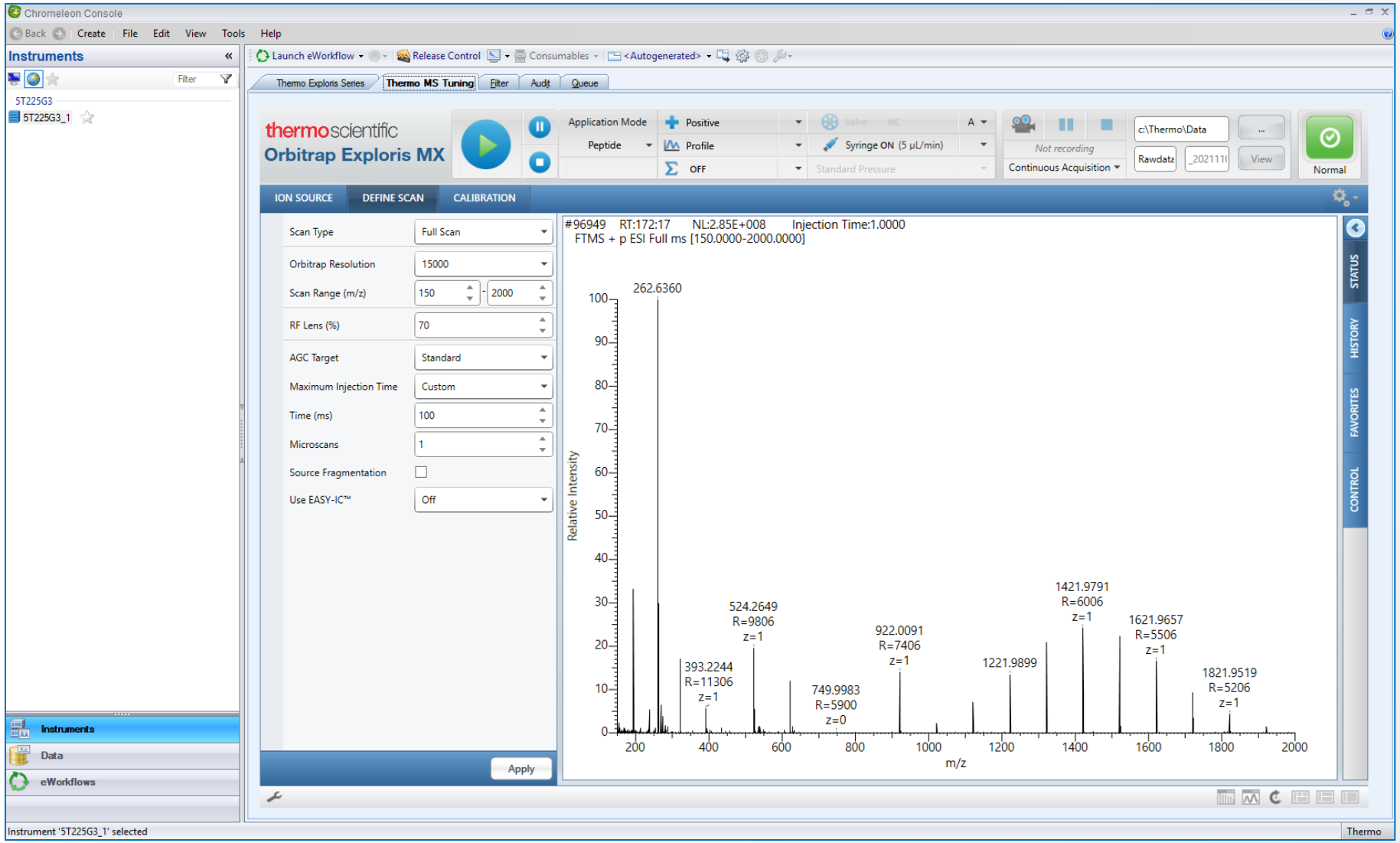
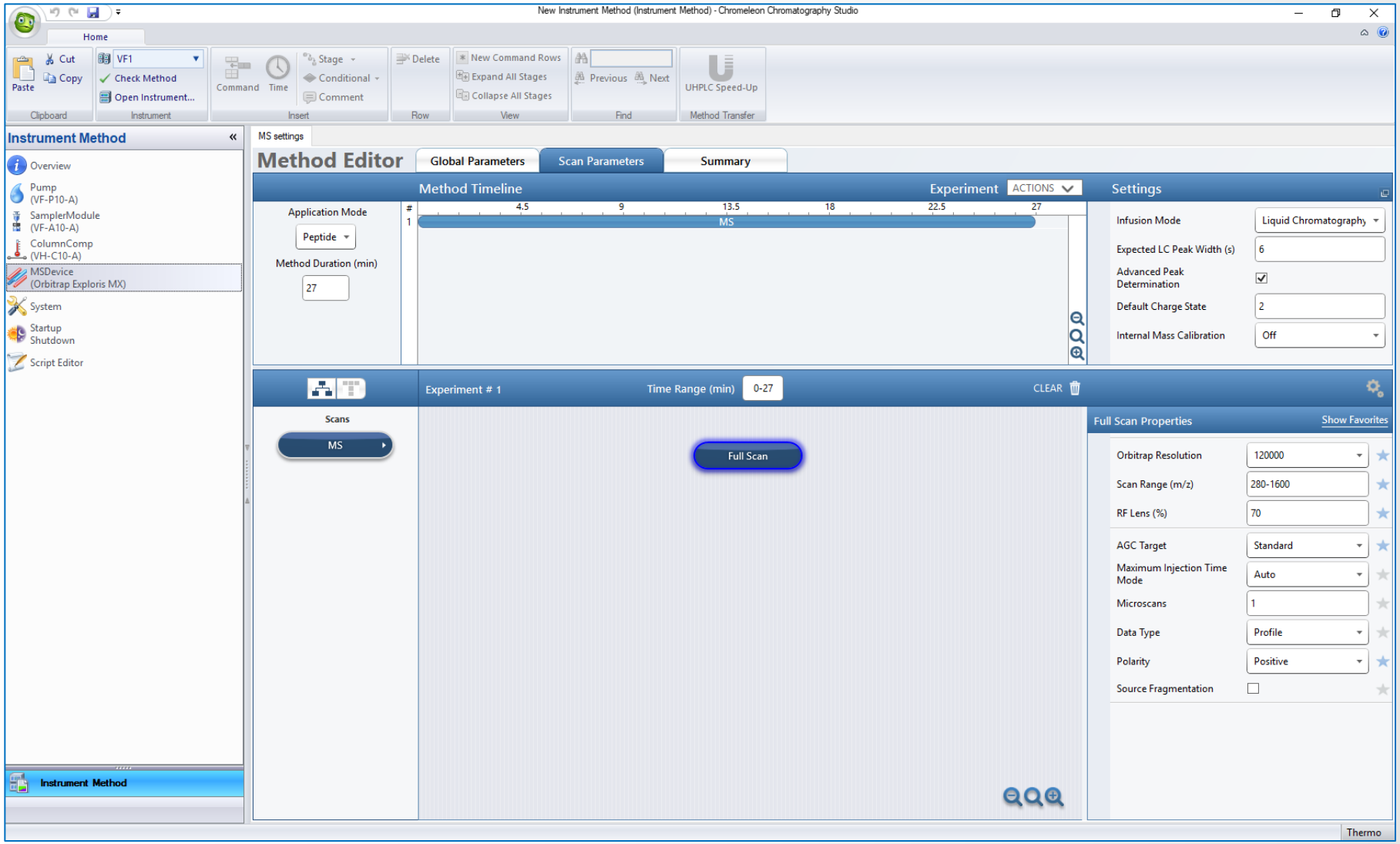
Full integration of Orbitrap Exploris MX MS into OES ICSW

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



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

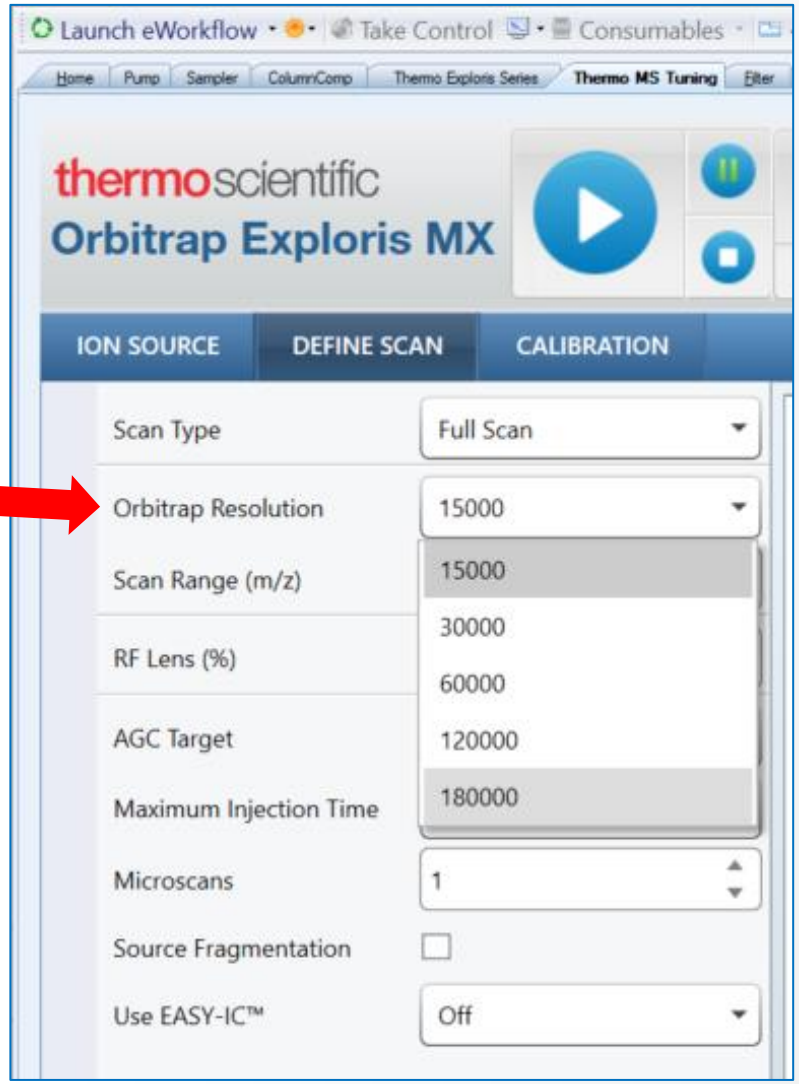
For **Full Scan** type,

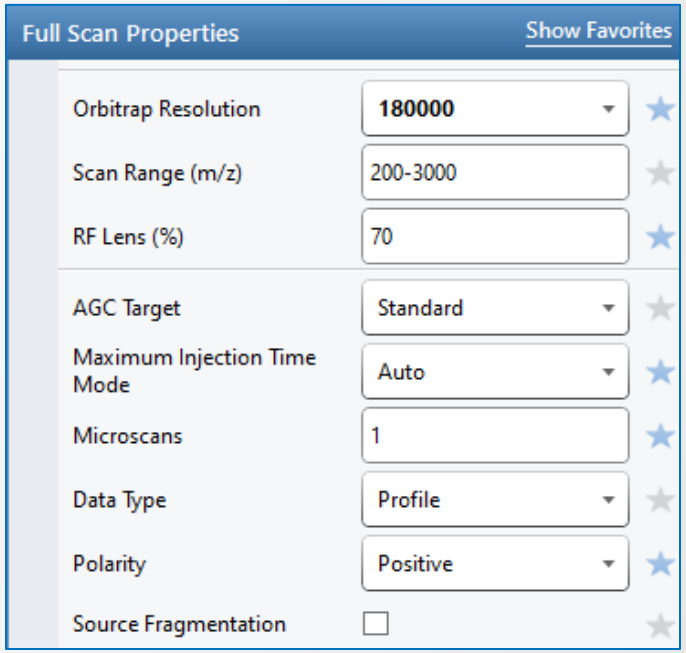
- Tune Application and
- Method Editor Application

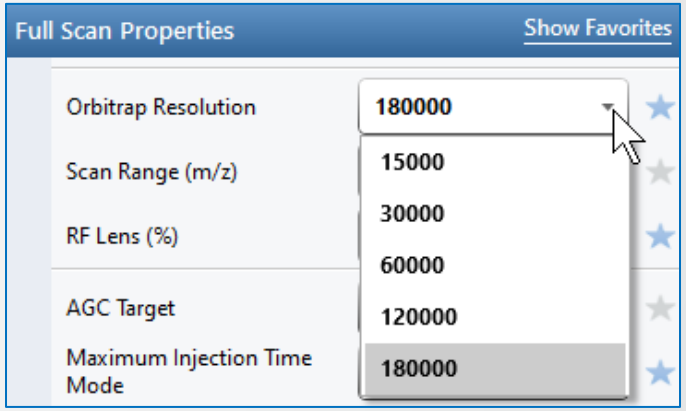
allow to choose an Orbitrap Resolution of 180 k (set value) for these models:

- 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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Thermo Scientific™ Orbitrap Exploris™ MX Mass Detector

Thermo Scientific™
Orbitrap Exploris™ 240 Mass Spec

Thermo Scientific™
Orbitrap Exploris™ 480 Mass Spec

New Functionalities enabled w/ OES 4.0 ICSW

2. One-Point Mass Calibration

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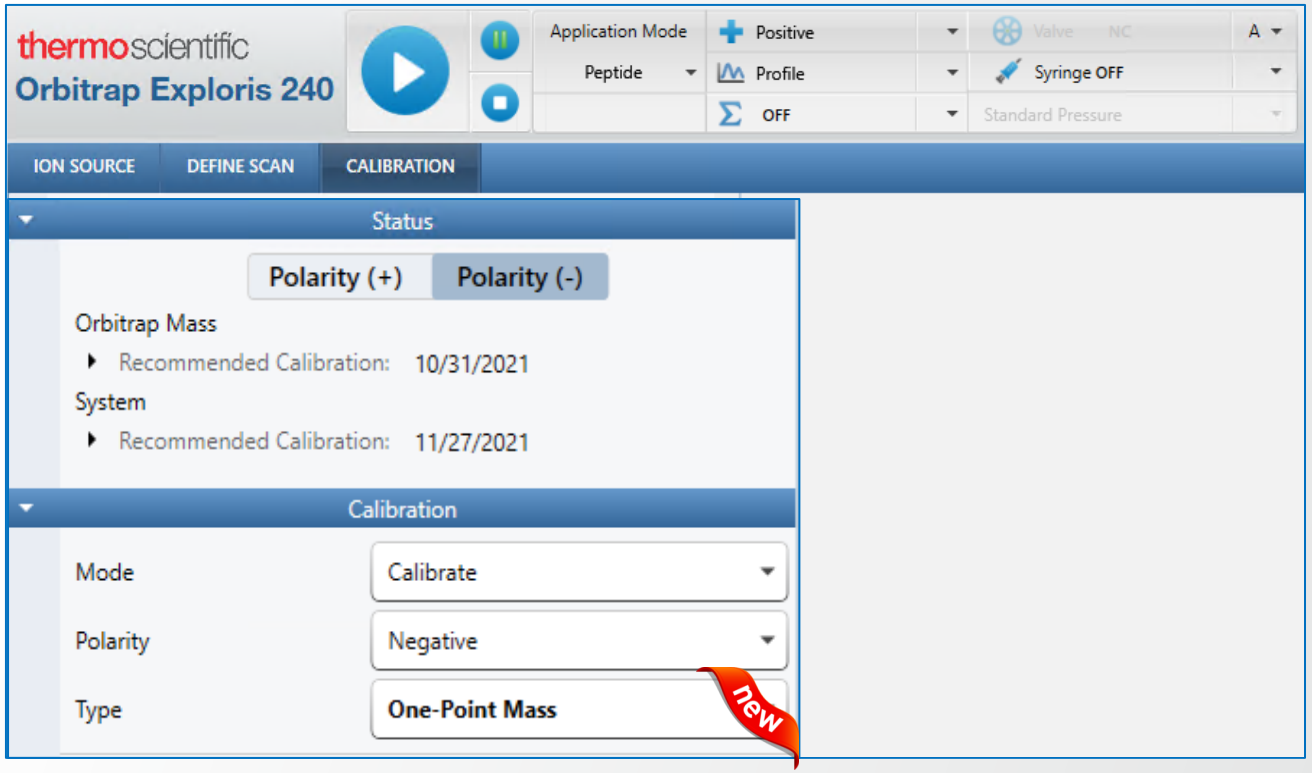
One-Point Mass Calibration – in Tune application

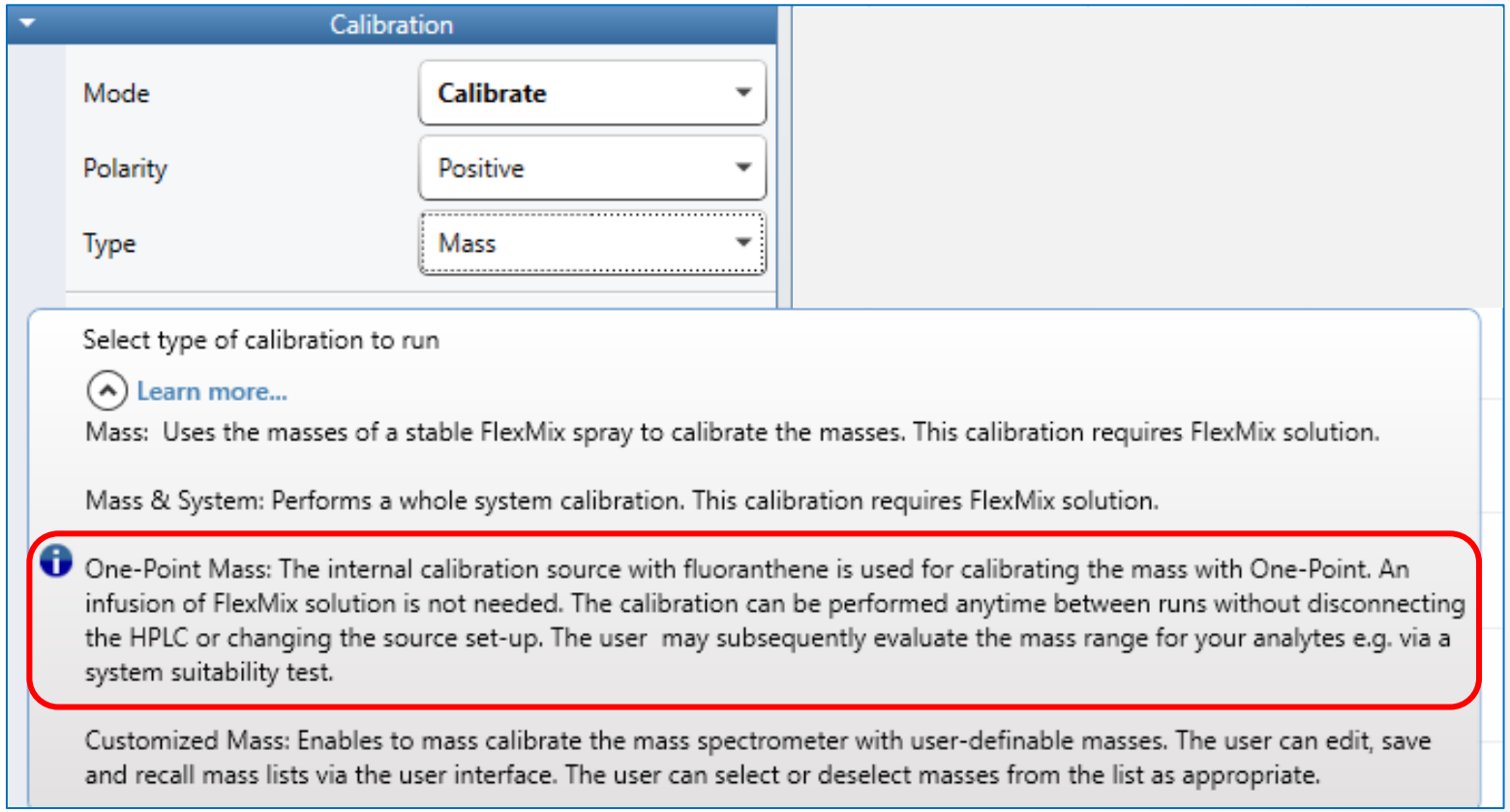
Available with OES 4.0 ICSW → Calibration tab → Calibration panel

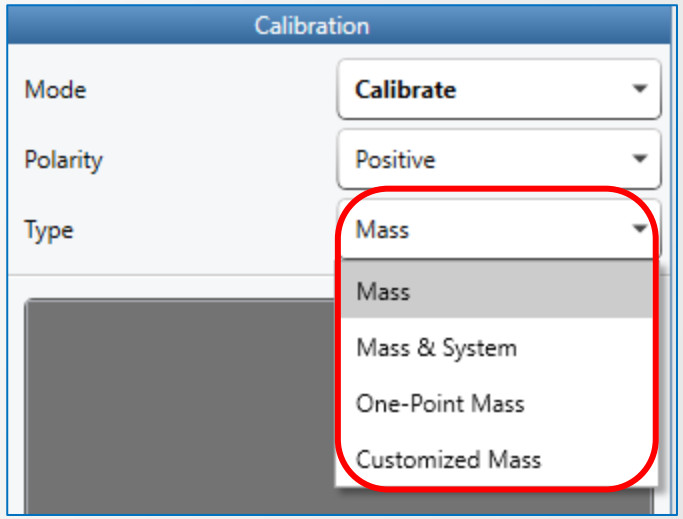
- **'One-Point Mass'** Calibration Procedure calibrates positive and negative ion mode
- Fluoranthene from the EASY-IC source is used for the '**One-Point Mass**' calibration procedure
- **Important Note:** running the '**One-Point Mass**' calibration procedure updates the master calibration file. Its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

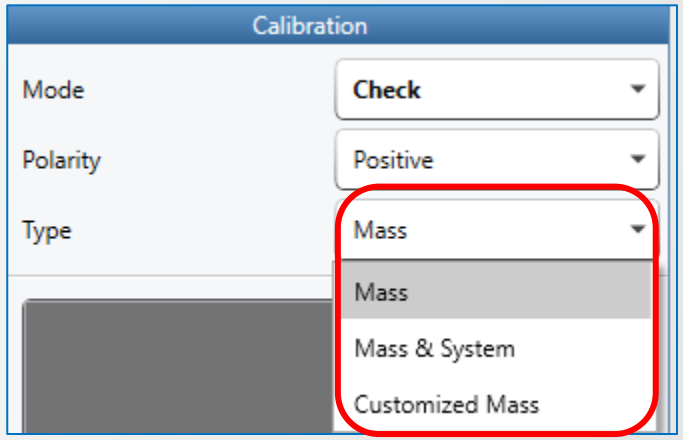


In more depth:
One-Point Mass Calibration – in Tune application

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



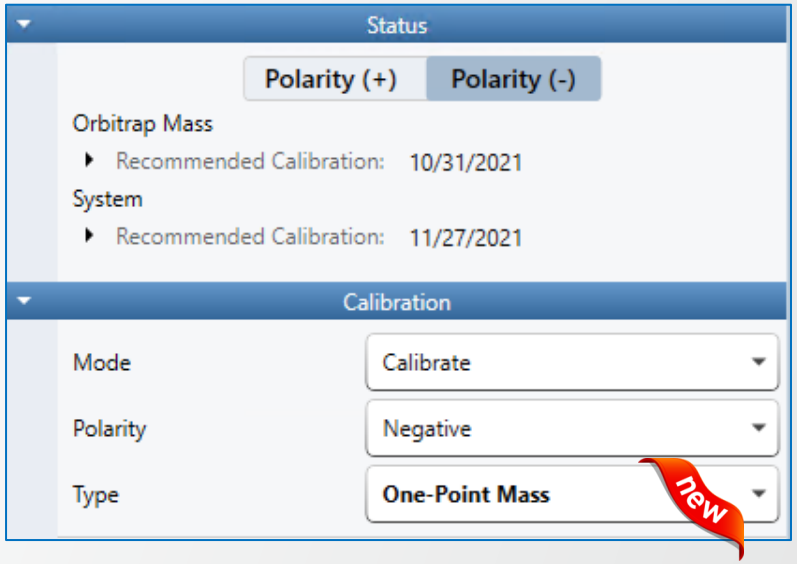




One-Point Calibration – in Tune application

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)



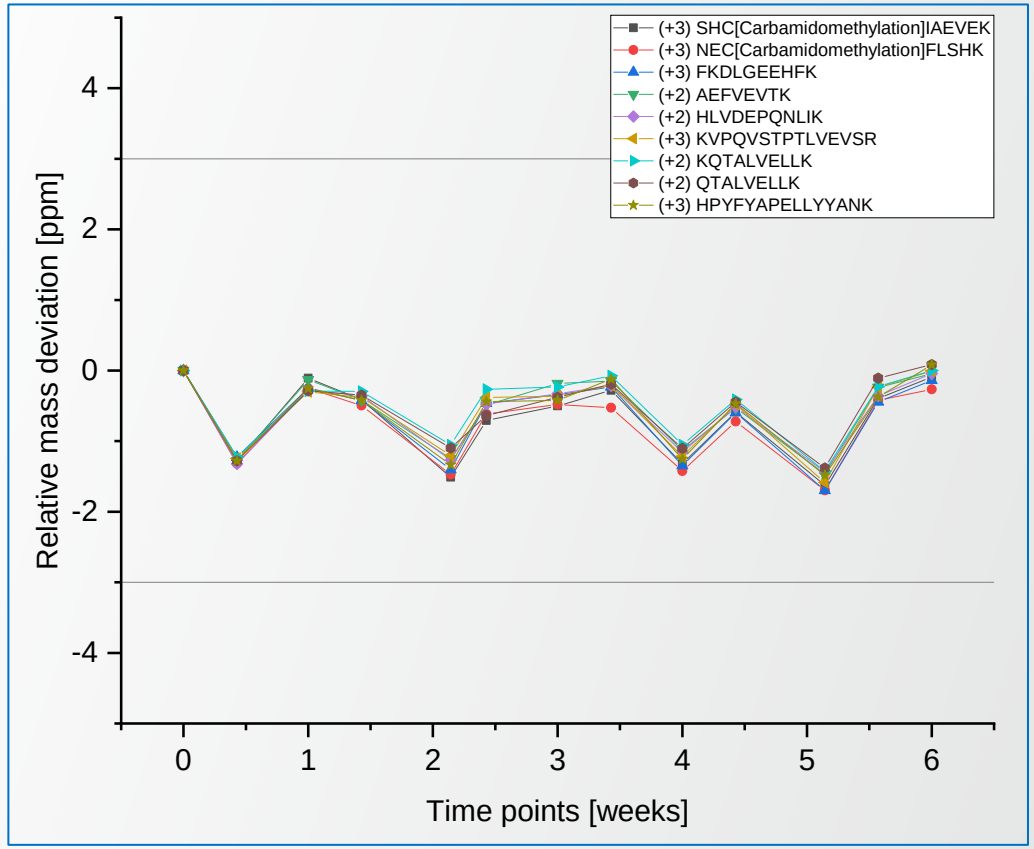
- The user may subsequently evaluate the mass range of interest e.g. via a system evaluation test
- **Important Note:** running the '**One-Point Mass**' calibration procedure updates the master calibration file. Its updated content is applied to upcoming scans and raw data files w/o further user interaction. 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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New Functionalities enabled w/ OES 4.0 ICSW

3. Customized Mass Calibration / Check Functionality

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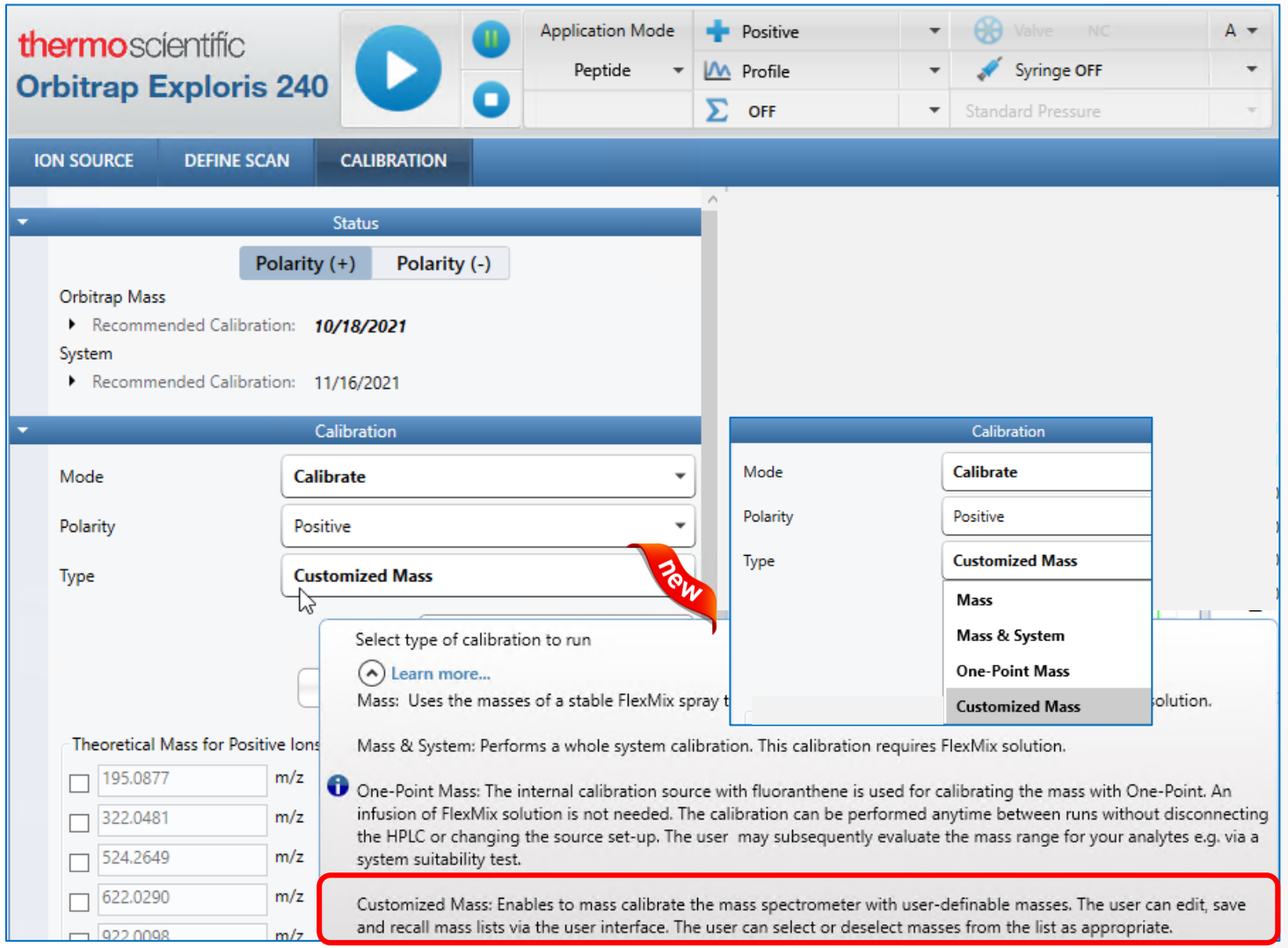
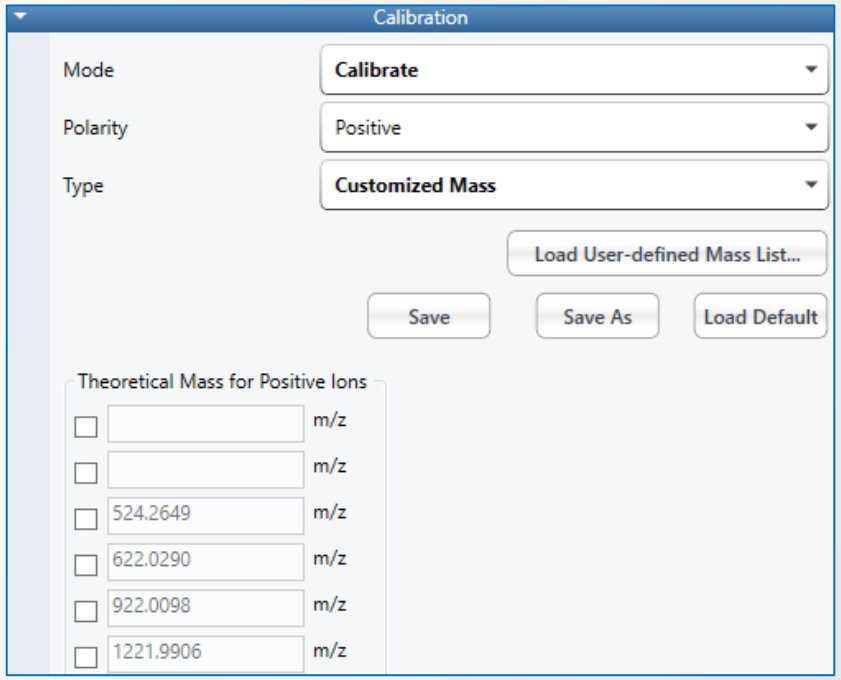
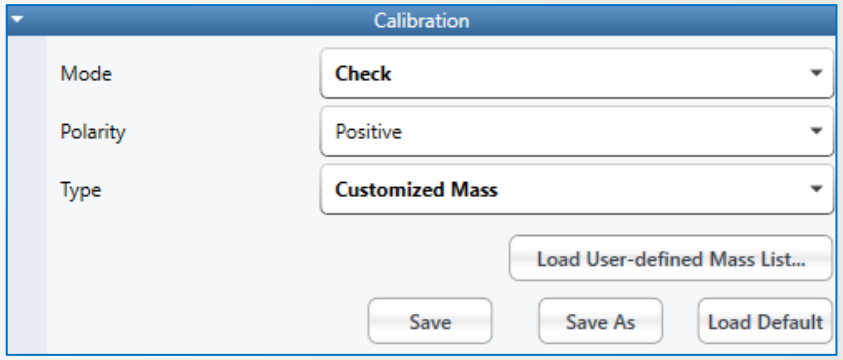
Customized Mass Calibration – in Tune application

new

Available with OES 4.0 ICSW → Calibration tab → Calibration panel

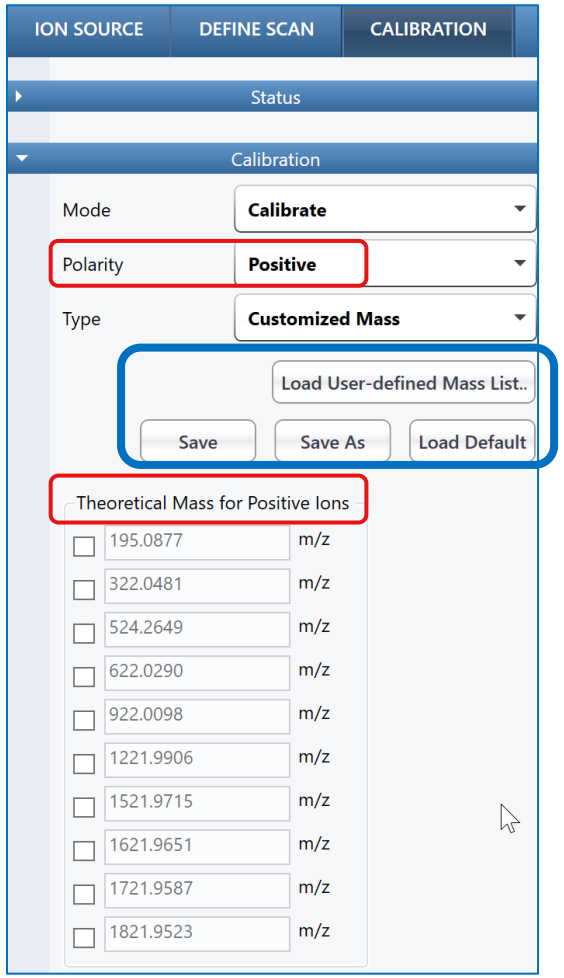


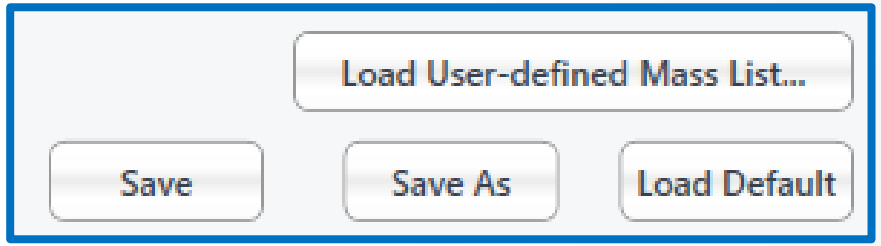




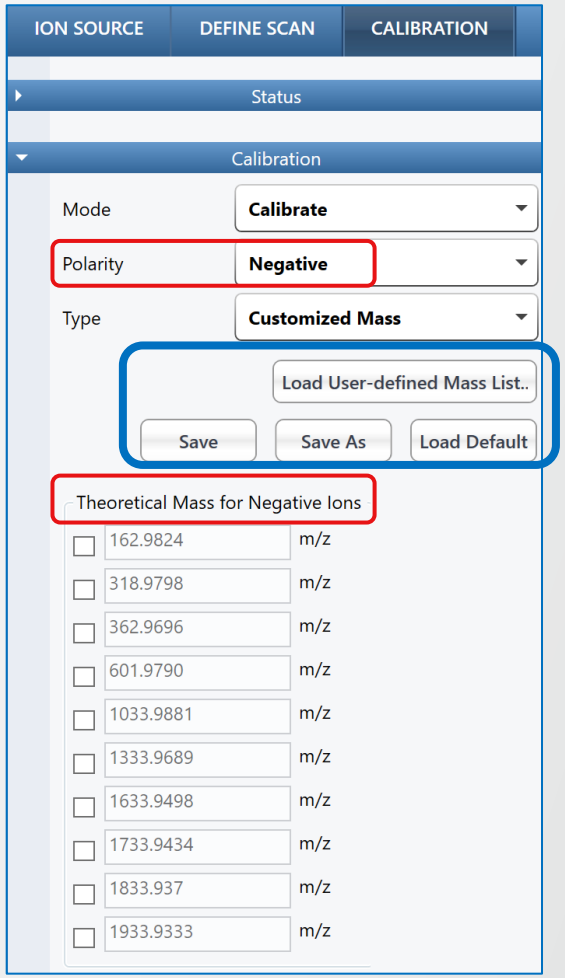
Customized Mass Calibration – in Tune application

Available with OES 4.0 ICSW → Calibration tab → Calibration panel



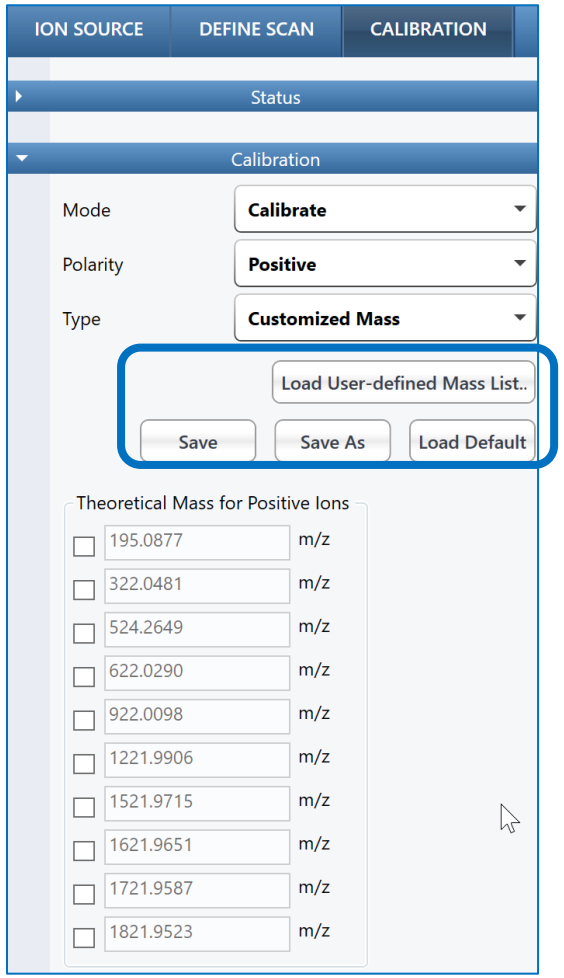


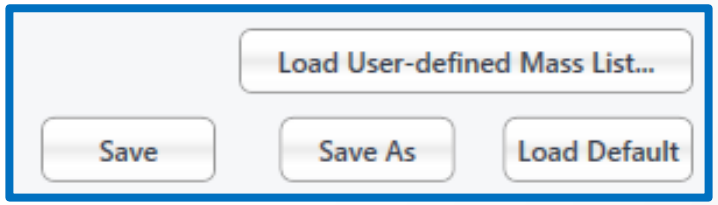
- **'Load Default'**
- **'Load User-defined Mass List'**
- **'Save'**
- **'Save As'**



Customized Mass Calibration – in Tune application

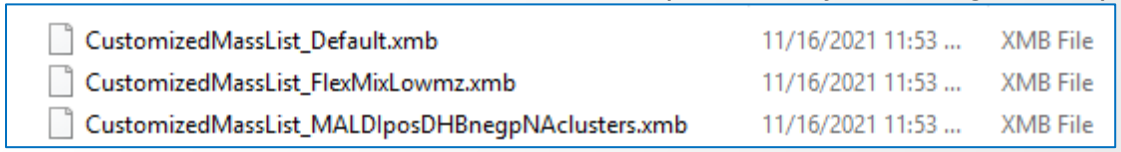
Available with OES 4.0 ICSW → Calibration tab → Calibration panel





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



- **'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

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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

new

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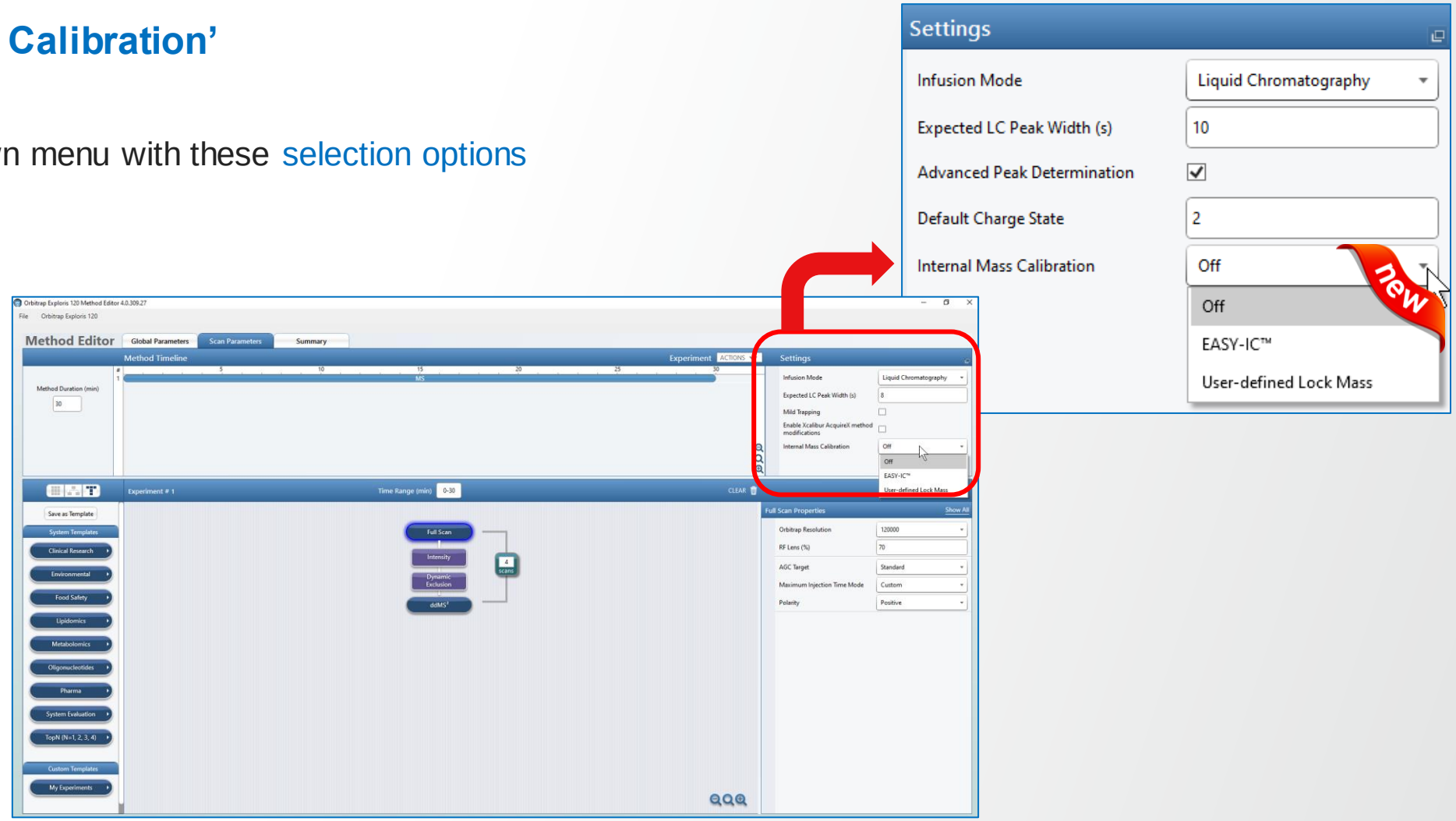
In Method Editor – Global Settings

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



In Method Editor – Global Settings

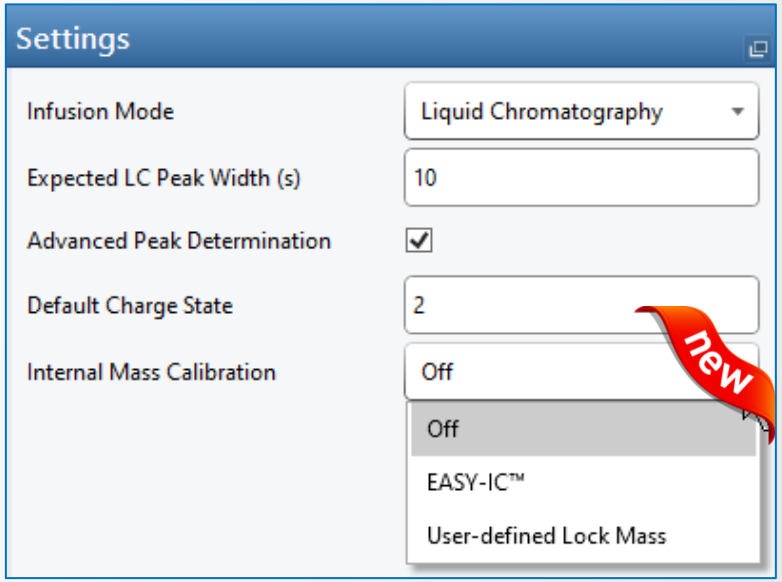
Available with OES 4.0 ICSW

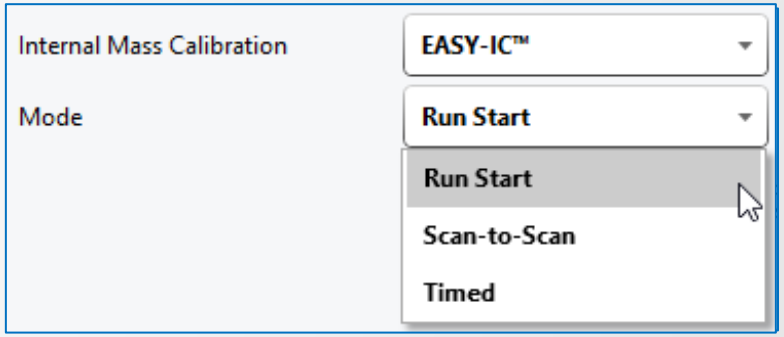
Parameter 'Internal Mass Calibration'

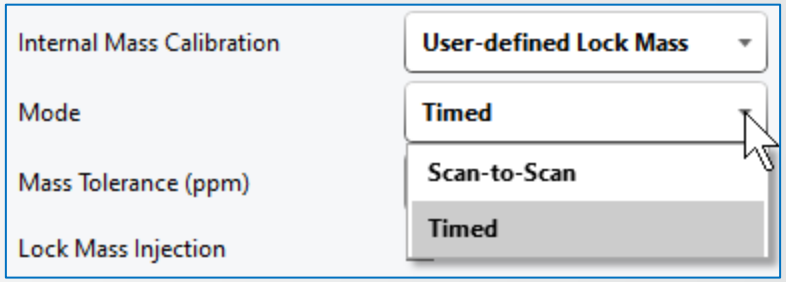
- UI is tidied up
  - Parameter has drop down menu with these selection options
    - off
    - EASY-IC
    - User-defined Lock Mass

- 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** new

  - With Mode 'User-Defined Lock Mass' selected, the user has access to two **Modes**
    - Scan-to-Scan(as earlier)
    - **Timed** new



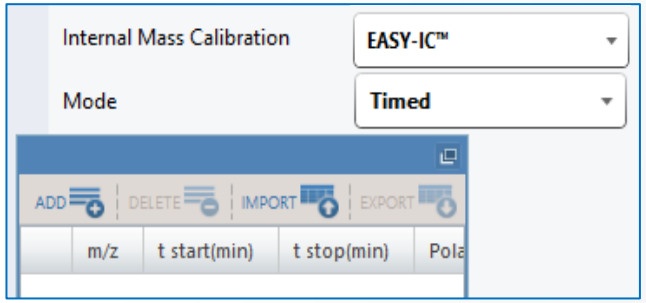


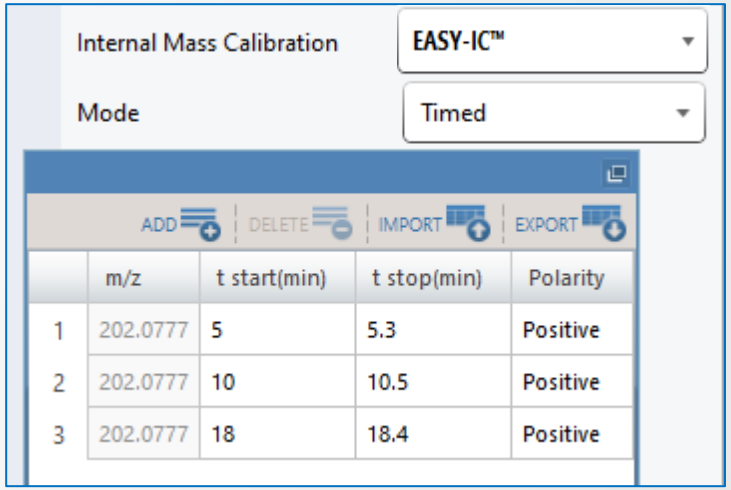


An example w/ ‘EASY-IC’ selected

Available with OES 4.0 ICSW

- With Internal Mass Calibration ‘**EASY-IC**’ selected, and
  Mode ‘**Timed**’ selected, a table appears

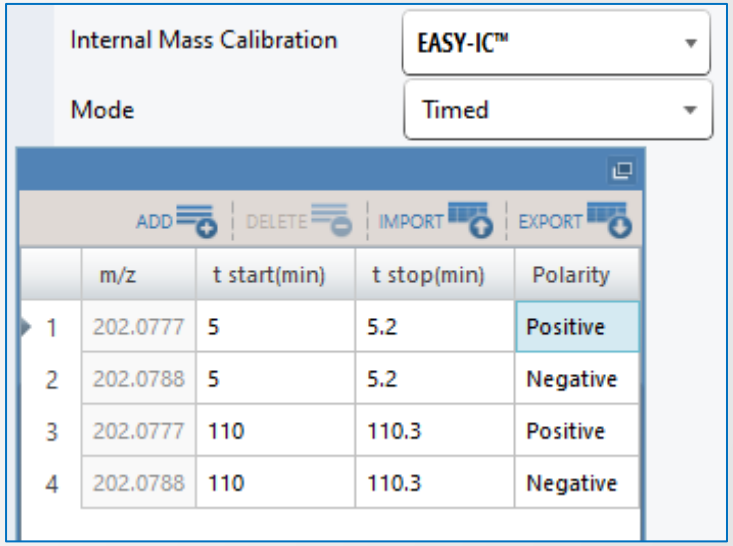




- User-definable retention time windows can be set by the user during which the locking takes place: $t_{start\ (min)}$, $t_{stop\ (min)}$

- 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

An example w/ User-defined Lock Mass' selected

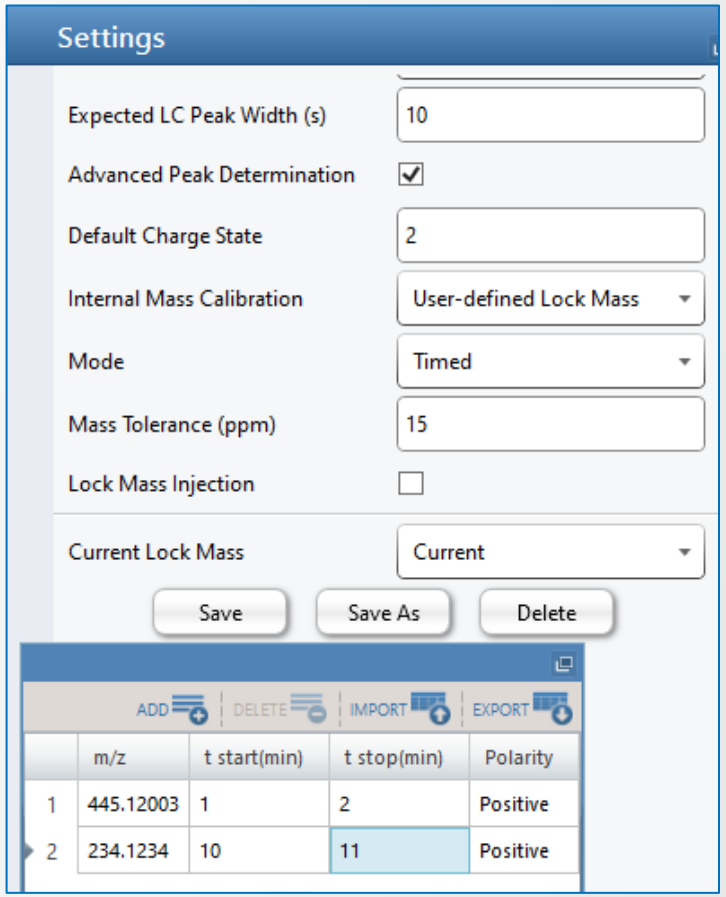
Available with OES 4.0 ICSW

- 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



	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

Some Comments

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

new

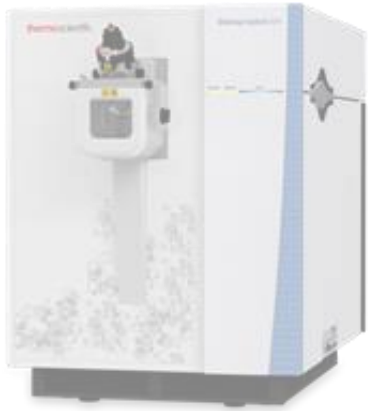
- The new options – introduced with OES 4.0 ICSW release - enlarge the capabilities of the Global Setting Parameter 'Internal Mass Calibration' significantly
- The new options apply to
  - locking w/ EASY-IC (fluoranthene) and
  - locking w/ User-defined Lock Masses

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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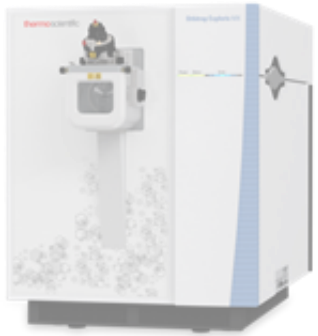
Thermo Scientific™
Orbitrap Exploris™ 120 Mass Spec



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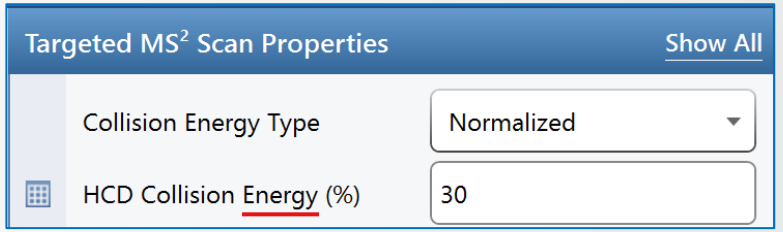
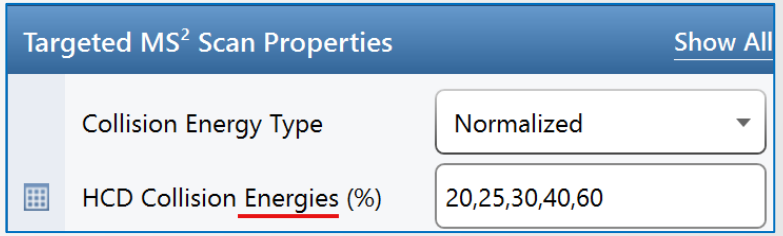
'Collision Energy Mode' is removed for an improved UX:

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'





'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‘
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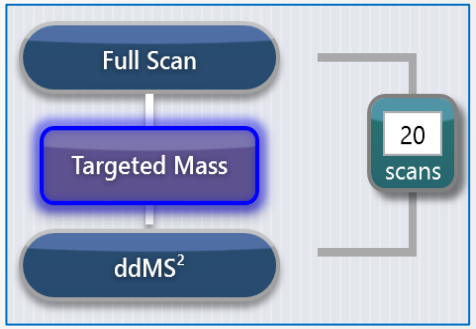
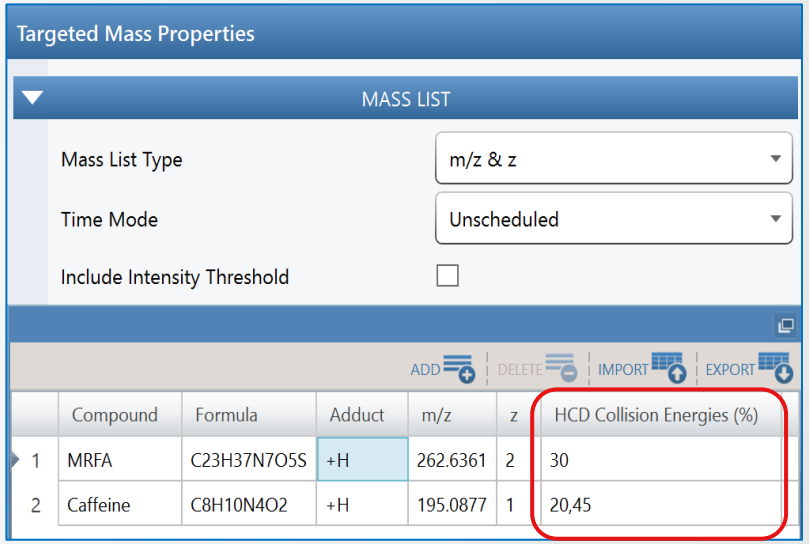


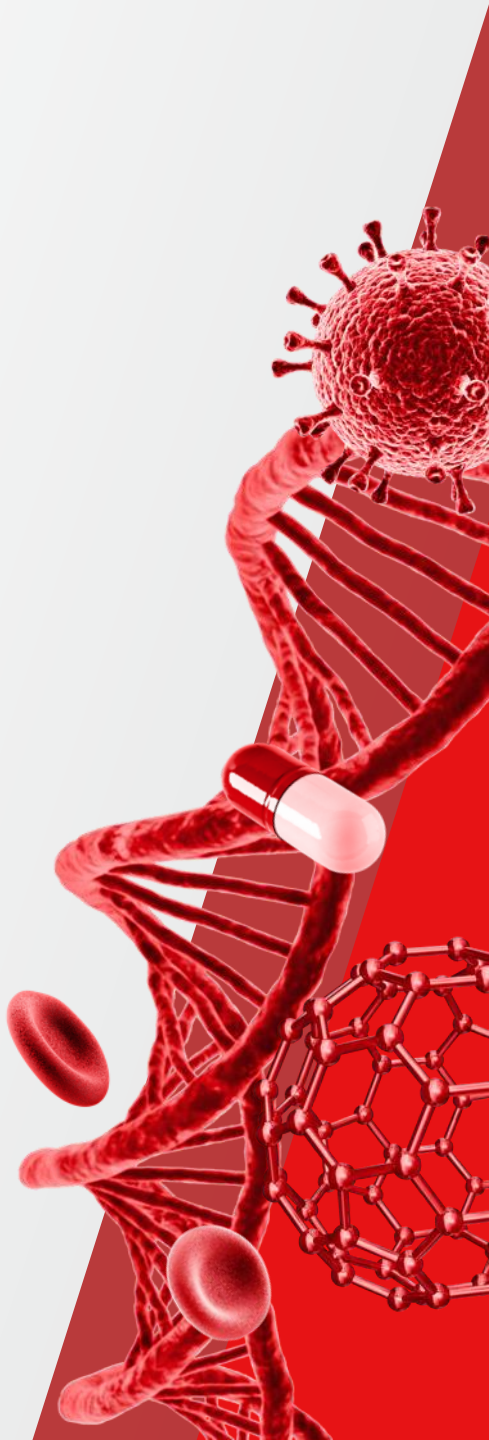


Updates to Manuals for Orbitrap Exploris Series

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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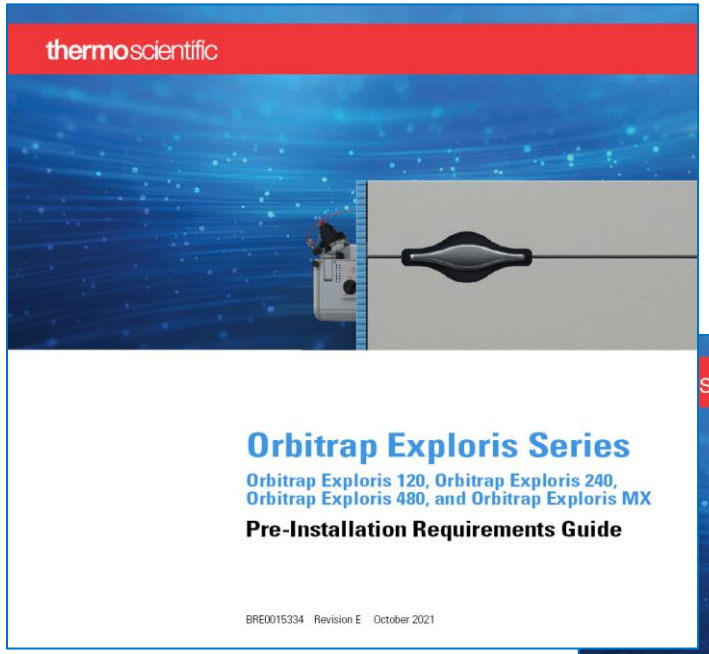
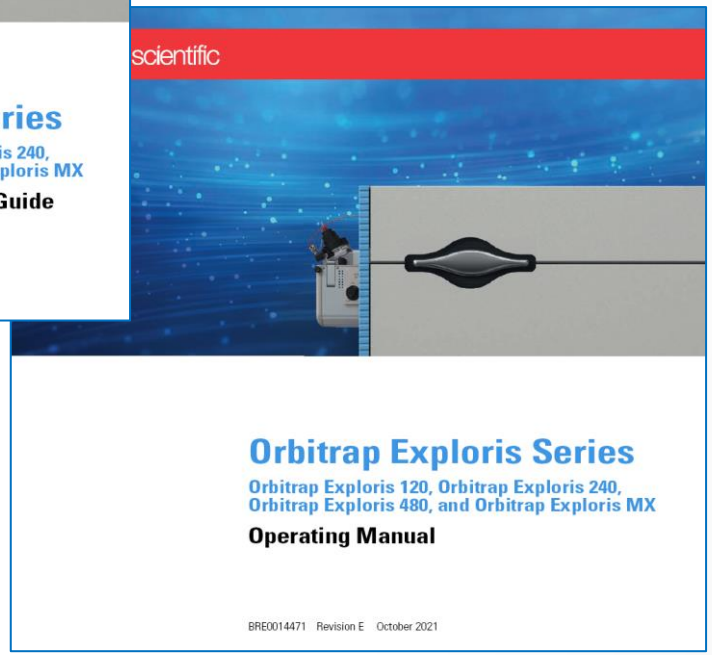
PRG and OE manuals

Pre-Installation Requirement Guide



Operator Manual



	Language	Additional languages
Preinstallation Requirements Guide	English	- Chinese - Japanese - French - Italian New: Spanish
Operating Manual Hardware	English	- Chinese - Japanese - French - Italian 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

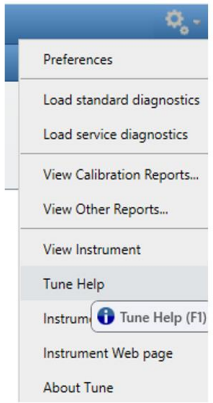
Updated Software Manuals and updated online help are part of the delivered ISO-Image and installed upon the installation of OES 4.0 ICSW

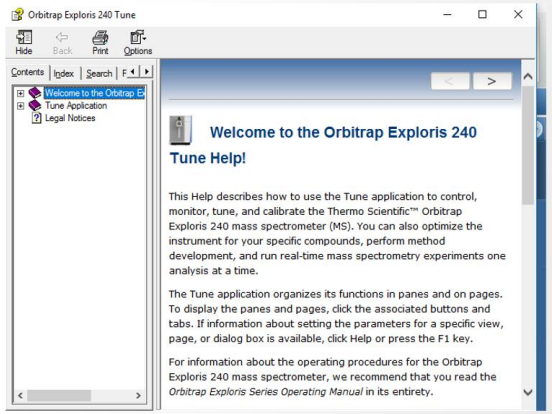
For updates check also the new website https://www.analyteguru.com/ which succeeds deprecated PlanetOrbitrap.com.

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

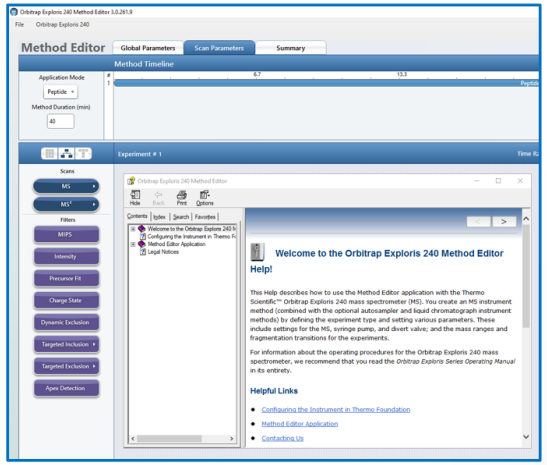
Display online help – of Tune - via Fct F1 key

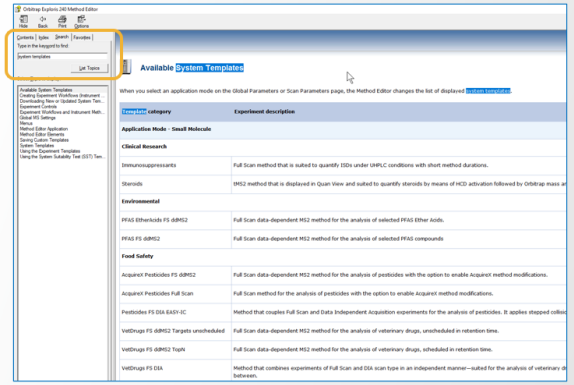
or via the gear wheel symbol in Tune – located to the right (top) corner in Tune

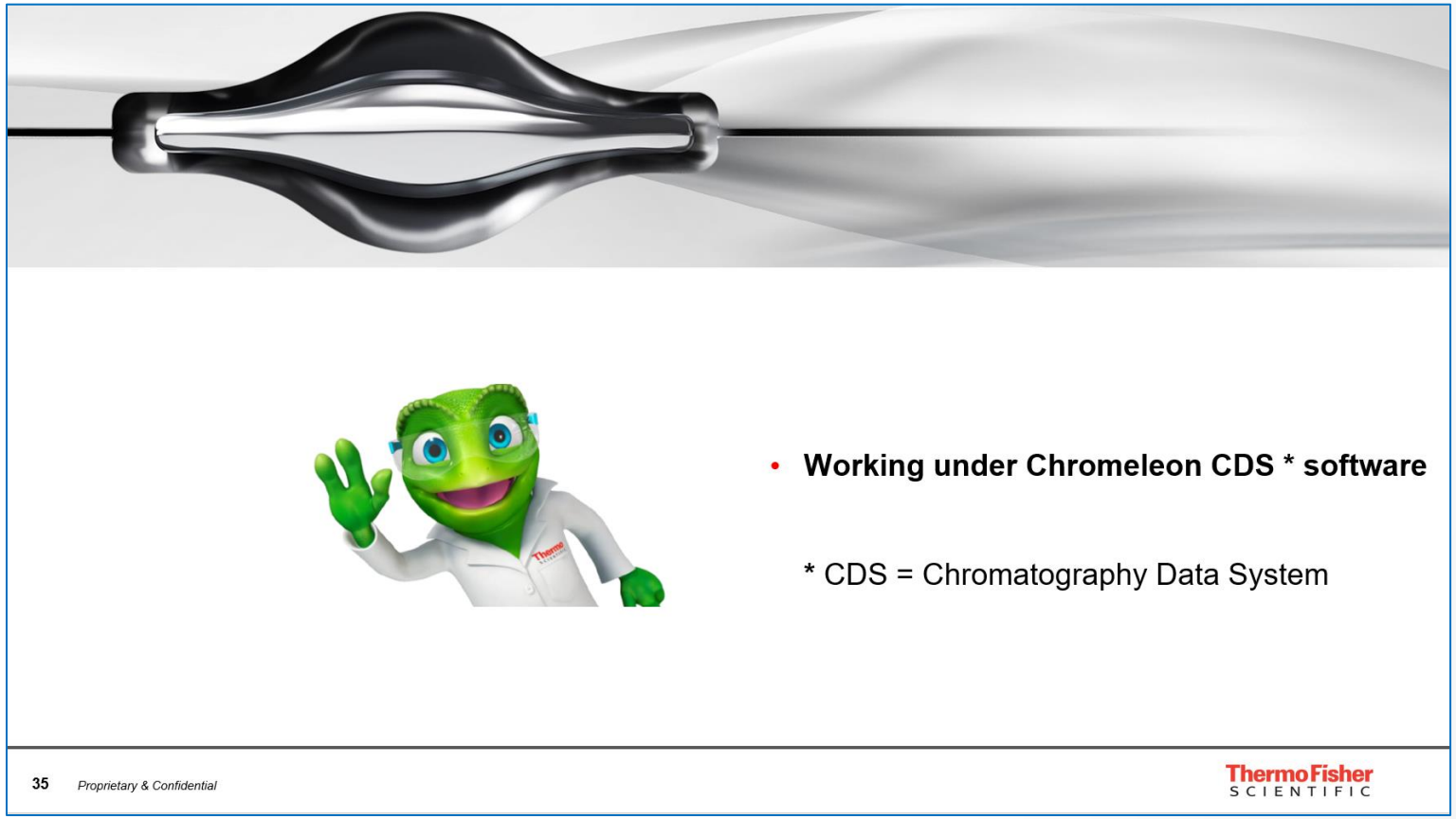




Display online help – of Method Editor - via Fct F1 key







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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

FSE: Field Service Engineer