Thermo Scientific Orbitrap Exploris 4.3 Instrument Control Software (OES 4.3 ICSW) –

Overview

February 2024

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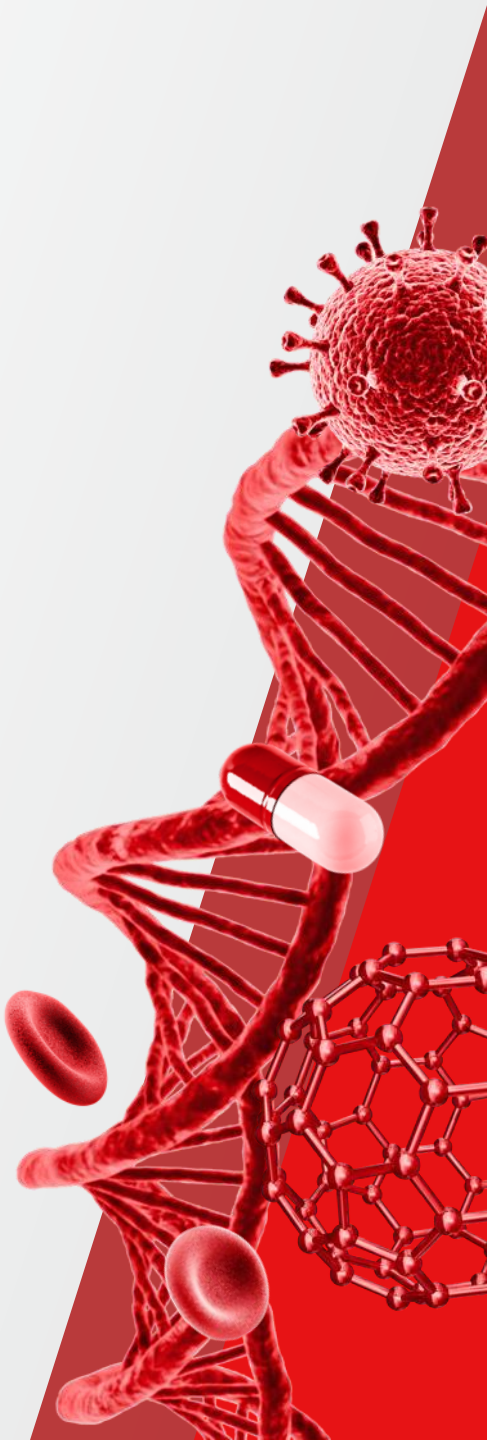
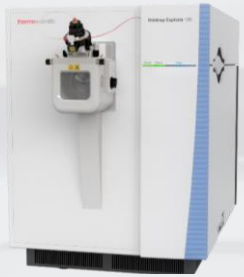
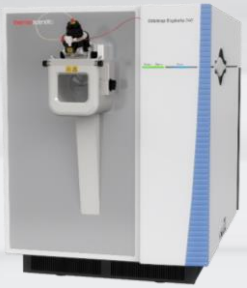


Thermo Scientific Orbitrap Exploris MS Portfolio – one ICSW

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

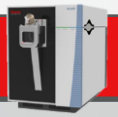
Thermo Scientific™ Orbitrap Exploris™ GC
Mass Spectrometer

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**		
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:	• 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, AcquireX AB TMT @ 45k resolution setting	• 16 msec transient (7,500 min resolution) • System Templates supporting BoxCar and SureQuant approaches • TurboTMT with TMT reagents up to 18-plex

Release Notes

Thermo Scientific Orbitrap Exploris Series 4.3 Instrument Control Software Release Notes							
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	✓	✓	✓	✓	✓	✓
4.2 SP2	4.2.362.26	✓	✓	✓	✓	✓	✓
4.2 SP3	4.2.362.36	✓	✓	✓	✓	✓	✓
4.2 SP4	4.2.362.42	✓	✓	✓	✓	✓	✓
4.3	4.3.458.15	✓	✓	✓	✓	✓	✓

Source: Release Notes for OES 4.3 ICSW

System Requirements

Thermo Scientific Orbitrap Exploris Series 4.3 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 4.3 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, 2019 LTSC or 2021 LTSC Thermo Scientific Xcalibur 4.7

Tip The Orbitrap Exploris Series 4.3 Instrument Control Software was only tested within the delivered composition.

Note:
Xcalibur 4.7 software applies Foundation 3.1 SP9.

Source: Release Notes for OES 4.3 ICSW

List of New Features and Improvements in OES 4.3 ICSW

New Features

General

- Operating Manual, Pre-Installation Requirements Guide, and Software manuals are updated
- Additional resolution settings are also accessible for OE 120 and OE MX (11.25k, 22.5k, and 90k) in Tune and Method Editor

Method Editor

- Display of absolute AGC target
- MaxIT dynamic for FSddMS2 experiments
- Lock Mass injection per experiment

OE GC:

- ME: User Defined LM correction - RunStart mode
- ME: Production Ions Scan - Product Ion Window Modes
- Tune: improved Manual Calibration tables separated by polarity
- Tune: Improved Leak Check

Improvements

General

- Scheduled one-point mass calibration (via Tune Preferences)
  - Addition of a Calendar view

Tune

- System calibration
- Tune Preferences: Hotlink function is now limited to the Ion Source settings

Method Editor

- EASY-IC “On/Off” available for all experiments in the timeline
- EASY-IC “On/Off” available for Lock Mass Correction Mode: Timed (for all experiments in the timeline
- Method Execution: the instrument now preserves the Ions Source settings and polarity after the sample acquisition has finished.

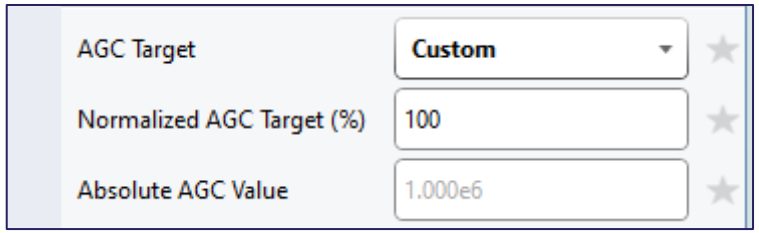
Diagnostics

- All MALDI related functionalities are now applicable to OT Exploris MX as well

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

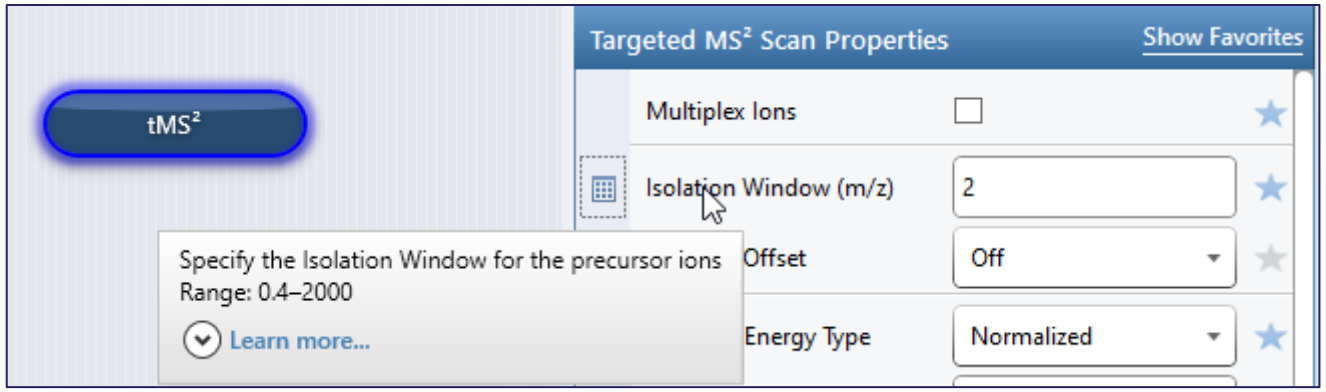
Source: Release Notes for OES 4.3 ICSW

Display of the Absolute AGC Value



- If the user chooses AGC Target „Custom“, the absolute AGC Value will be displayed underneath.
- The absolute AGC target value is a conversion of the AGC percentage target set in the method into absolute values. This read-only value will be automatically updated according to the scan type and the target percentage.

Isolation width for DDA/tMS2 for OE240 is extended



- In tMS2 and FSddMS2 experiments the isolation width has been extended to 2000 Da

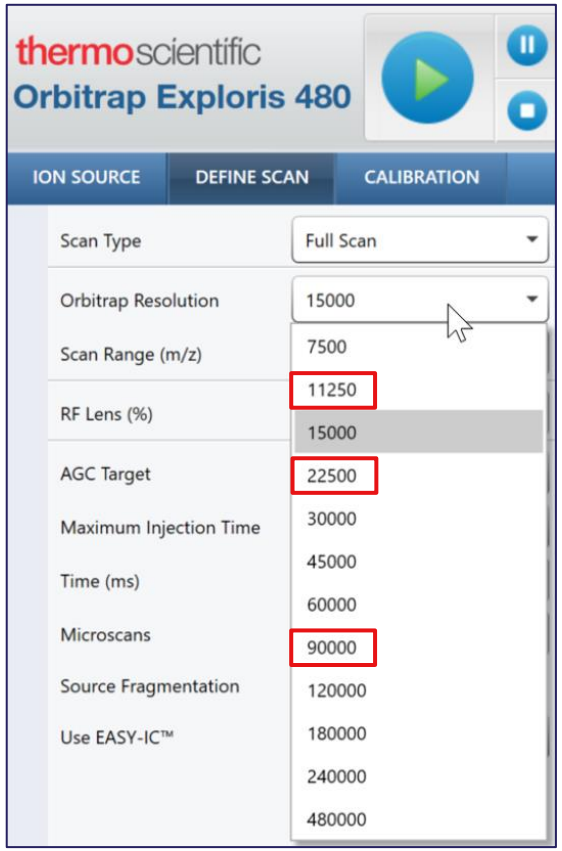
Additional Resolution Settings
→ now also for OE120 and MX

LSMS

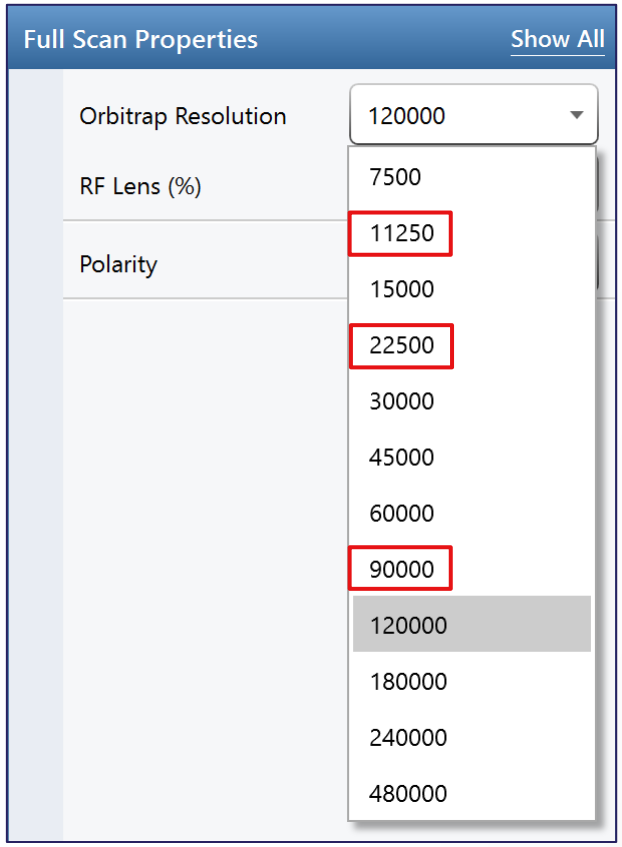
ThermoFisher SCIENTIFIC

Added Resolution to Provide More Flexibility in Short LC Gradient Analysis

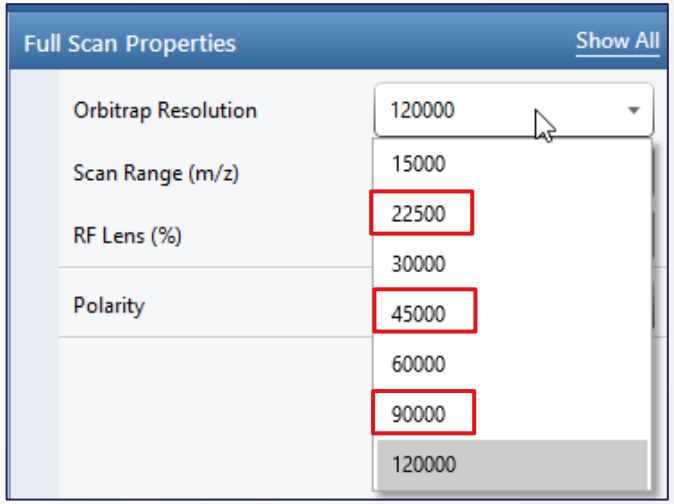
Tune



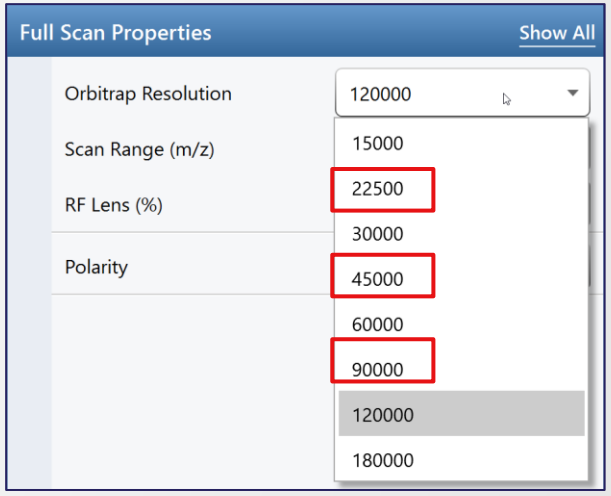
Method Editor



OE120



OE MX



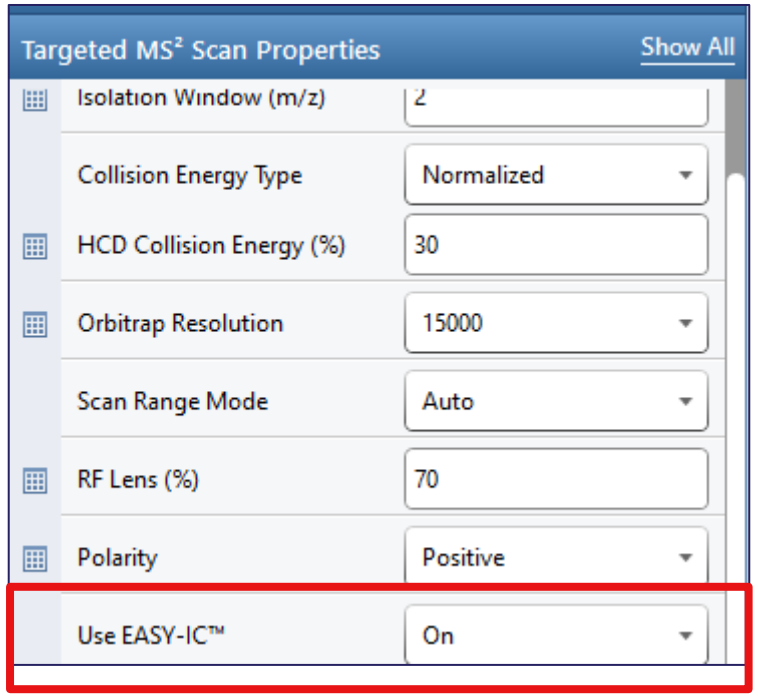
System calibration

- Reminder
  - General concept → Only when the full calibration is passed calibration values are stored
  - If a procedure does not pass, repeating the „system calibration“ will resume from a checkpoint before the not passed procedure
  - Update of the date for the next recommended System calibration when ALL procedures have passed

- NEW: In negative mode the calibration values get saved even if the ICS HV calibration has not passed. The recommended date will not be updated until also the ICS HV calibration has passed.

„Use EASY-IC“ On/Off

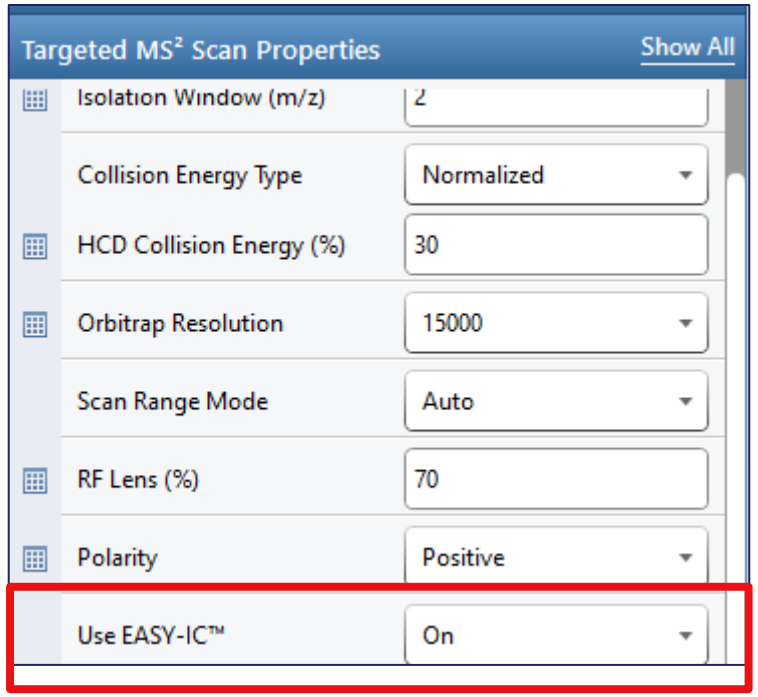
Improvement: for EACH experiment



- If On is selected, it provides an internal reference mass that is used for mass correction during a run (Lock Mass Correction: EASY-IC™, Mode ≠ RunStart)
- Now available for each experiment in the timeline – here displayed for a tMS2 experiment
- This provides the possibility in mixed experiments to perform Scan-to-Scan EASY-IC only in the FullScan experiment and not in an e.g. additional tMS2 experiment
- If no lock mass is found in one scan, the system will apply the last successful locking information to this scan. Time duration of last locking and lock mass correction are provided in the scan header of the individual scan.

„Use EASY-IC“ On/Off - Timed

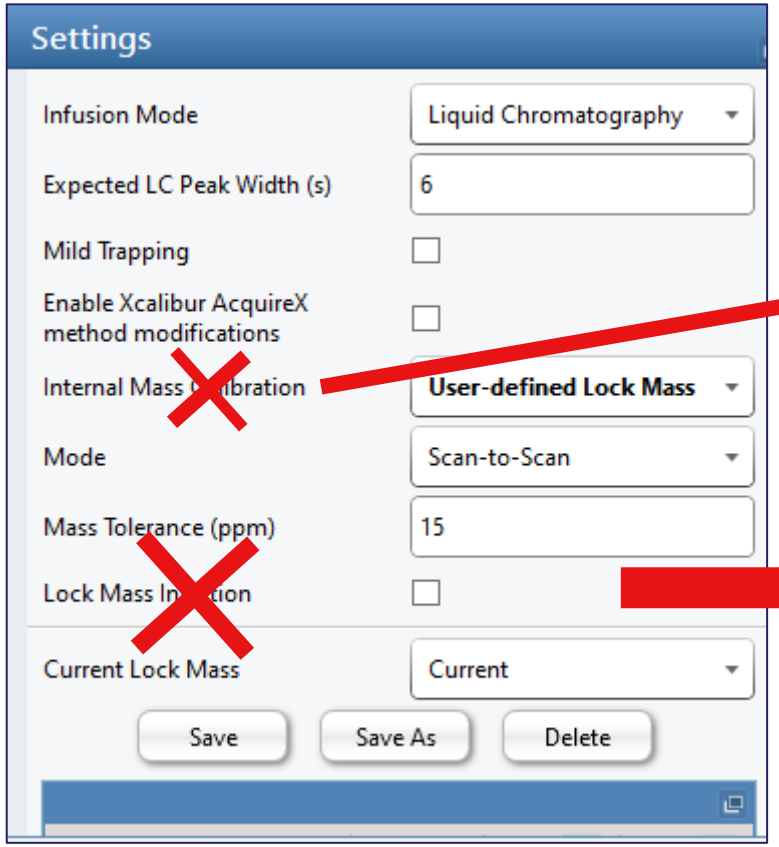
Improvement: also for Timed EASY-IC “On/Off“ can be chosen



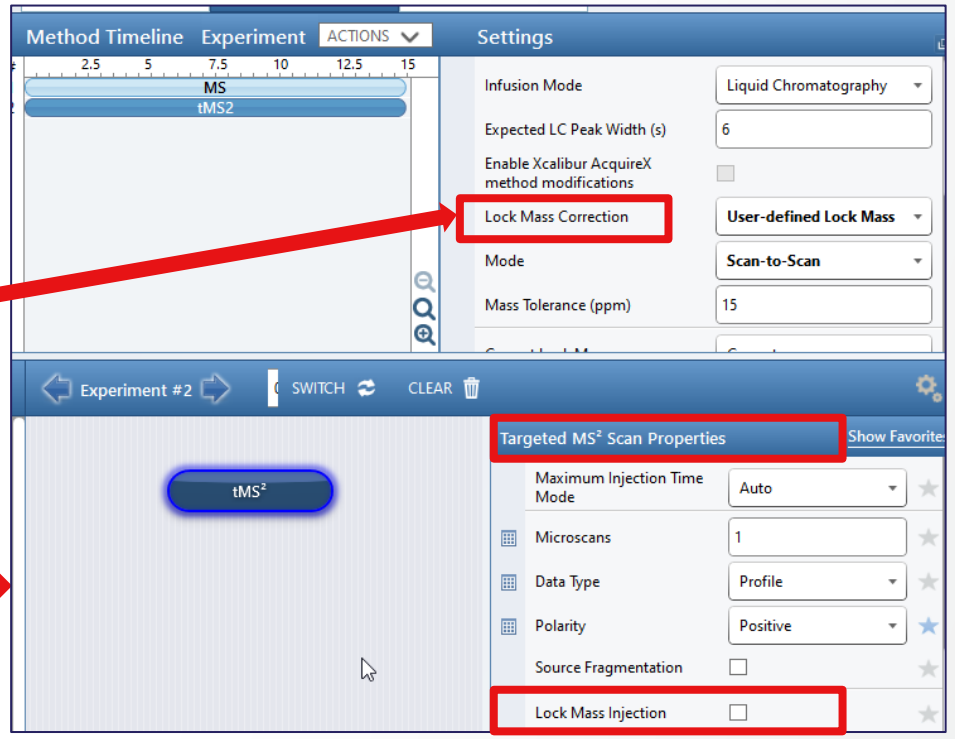
- If “On” is selected, it provides an internal reference mass that is used for mass correction during the defined time window
- If no lock mass is found in one scan, the system will apply the last successful locking information to this scan. Time duration of last locking and lock mass correction are provided in the scan header of the individual scan.

Lock Mass Injection parameter moved to scan properties

≤ OES 4.2



OES 4.3



- Lock Mass Injection function available for every experiment in the timeline
- Whereas a FullScan might not need the custom lock mass to be injected (no time penalty) the lock mass could be injected for tMS2 experiments.
- Please Note: EASY-IC™ injects the lock mass to every chosen experiment (see previous slide)

- Additionally we renamed „Internal Mass Calibration“ to „Lock Mass Correction“ as the old naming was confusing for many customers.

MaxIT Mode „Dynamic“ for FSddMS2*

No additional properties are exposed when selecting dynamic Max IT but method execution is affected

Number of Scans

- Max IT for every scan in the experiment is scaled by (1+TopN)/(1+SumCand)
- TopN = user-defined max. number of dd scans, SumCand = sum of actually available candidates from master scan,
- Increment of 1 to account for the master scan itself
- Scaling factor must be >1 to take effect.
- **Example:**
  with TopN=100 but only 50 available candidates in a cycle, the expected max. IT values that result from parallel acquisition of scans would be scaled by a factor of ~2
- → for a Resolution of 15k (ddMS2) the maxIT will be extended from 32 ms to ~2 x 32 = ~64 ms (minus overheads)

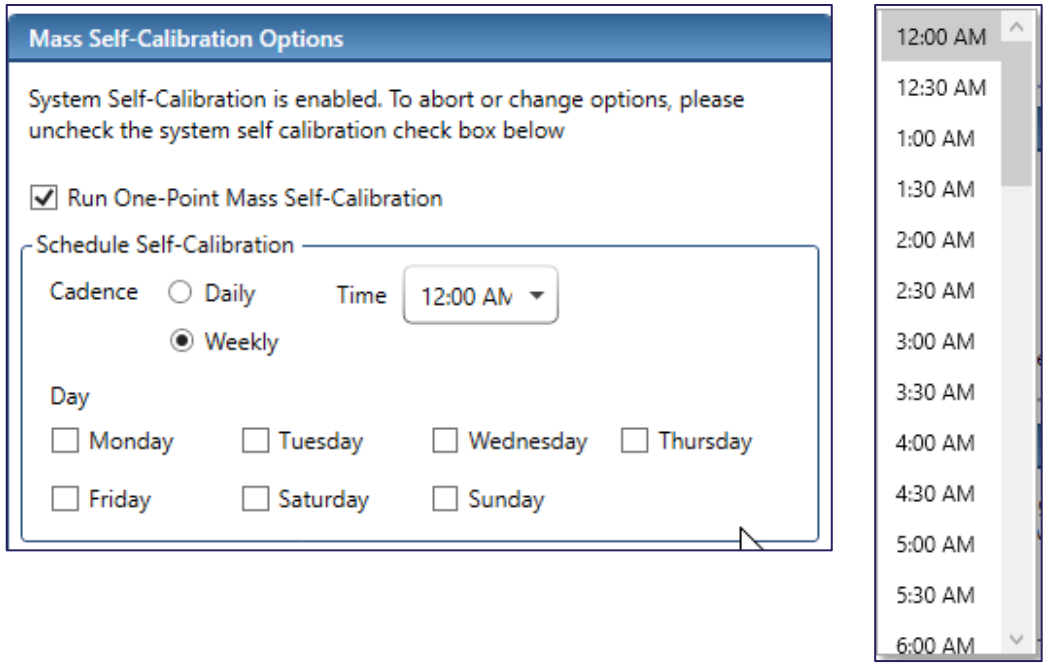
Cycle time

- MaxIT for every scan is determined as max(“Expected_max_IT”, Cycle Time/ SumCand)
- With “Expected_max_IT” = maxIT value pertaining to parallel acquisition.
- **Example:**
  Cycle Time: 0.6 sec; 15k Res – 32 ms transient length
  → ~18 MS2 spectra (theoretical) with a maxIT of 32 ms
  If only 9 candidates available → maxIT extended by a factor of ~2

*previously only available for targeted experiments.

One-Point Self Calibration

Improved Capabilities – Calendar View



- The One-point Self-calibration can be set up in a more detailed way
- E.g. it can be set to be performed every Monday, Wednesday and Friday.
- Also, there are more options for the timing.

Updates to Manuals for Orbitrap Exploris Series

Pre-Installation Requirements Guide

Operator Manuals

Model specific Software Manuals and online help

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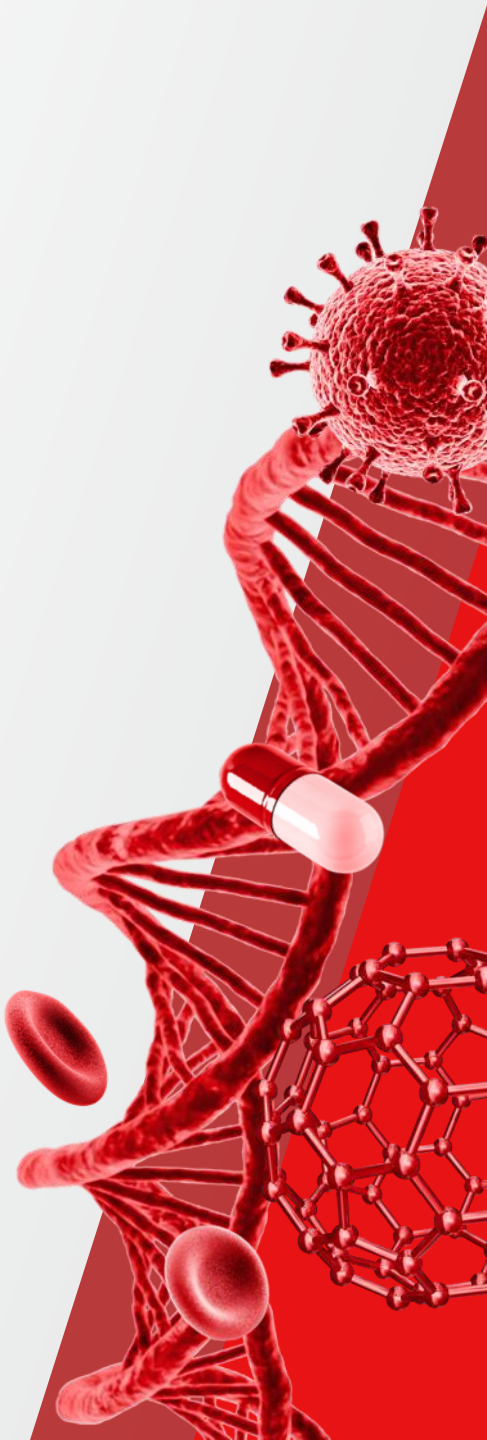
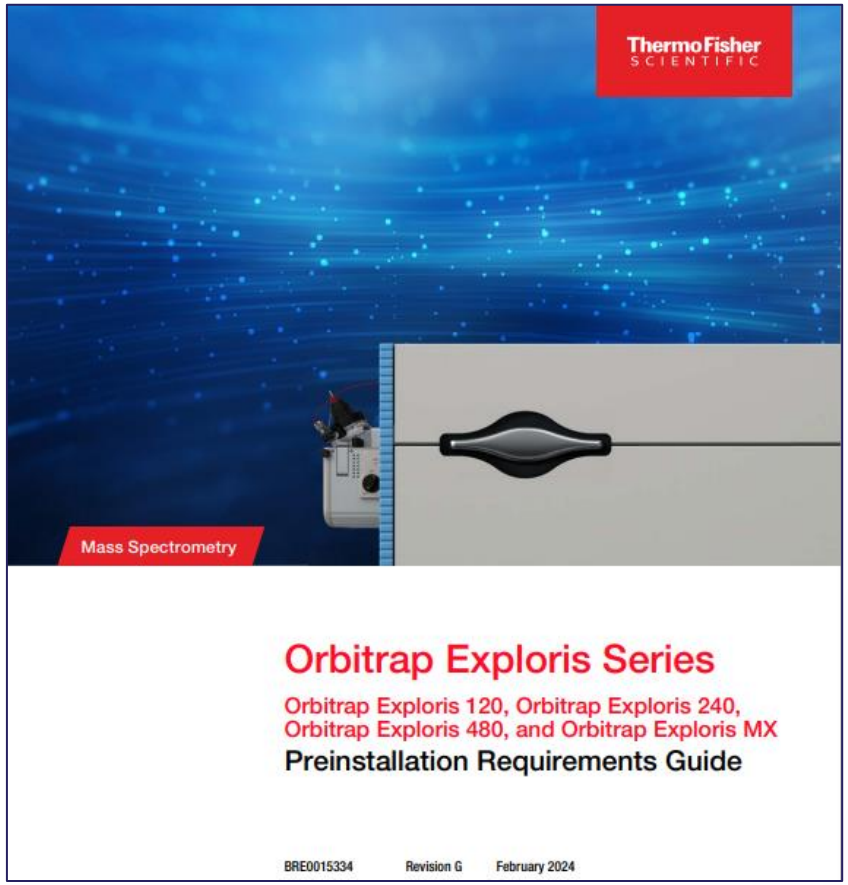


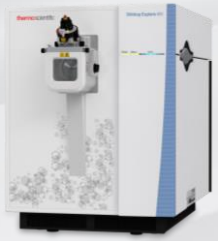
Pre-Installation Requirements Guide And Operating Manual

Pre-Installation Requirements Guide

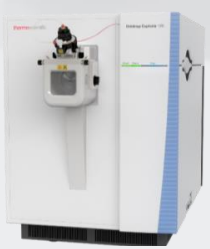


Operating Manual

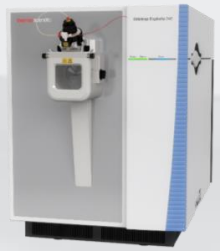
Software Manuals for these Orbitrap Exploris models



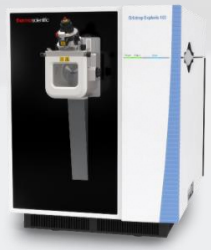
Thermo Scientific™
Orbitrap Exploris™ MX Mass Detector



Thermo Scientific™ Orbitrap Exploris™ 120
Mass Spectrometer



Thermo Scientific™ Orbitrap Exploris™ 240
Mass Spectrometer



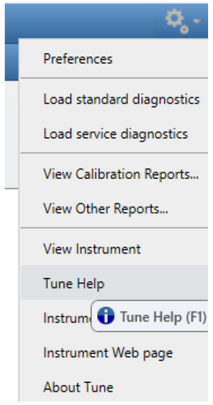
Thermo Scientific™ Orbitrap Exploris™ 480
Mass Spectrometer

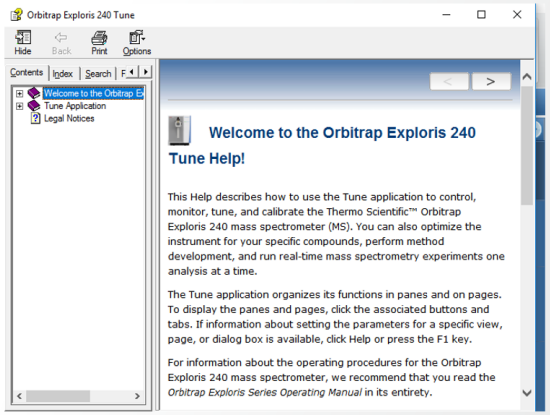
Updated Software Manuals and updated online help are part of the delivered ISO-Image and installed upon the installation of OES 4.3 ICSW

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

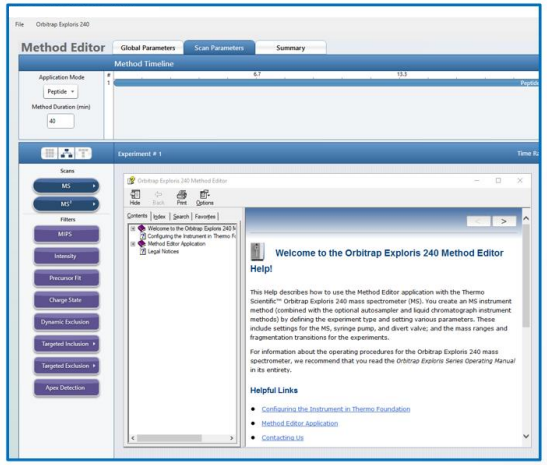
Display online help – of Tune - via Fct F1 key

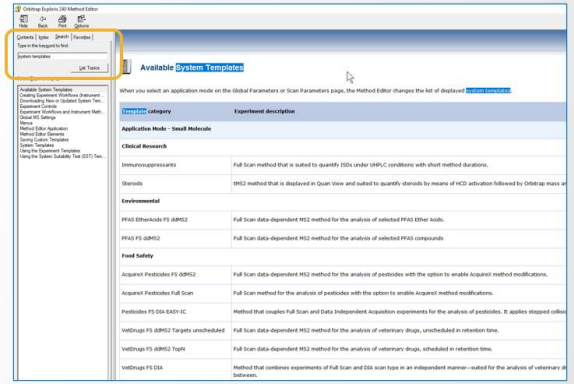
or via the gear wheel symbol in Tune – located to the right (top) corner in Tune

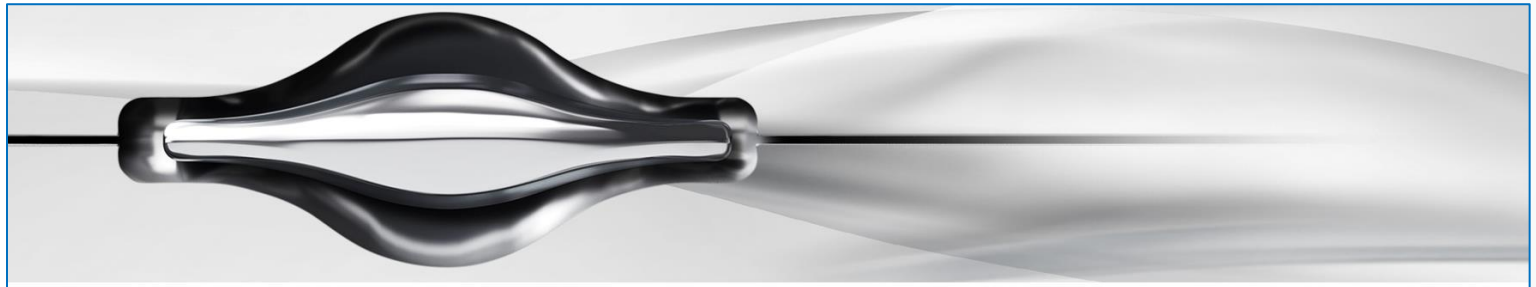




Display online help – of Method Editor - via Fct F1 key







- **Working under Chromeleon CDS * software**

* CDS = Chromatography Data System

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OES 4.3 ICSW and Chromeleon CDS Software

LC-MS data acquisition under Chromeleon

- **OES 4.3 driver** validated for use with Chromeleon CDS 7.2.10 MUh software and Chromeleon CDS 7.3.2 MUb

- Defect fixes:
  The previous issue that the OT Exploris model difference in Chromeleon is not recognized is 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**.