

OES 3.0 ICSW - New Features, Improvement and Defect Fix

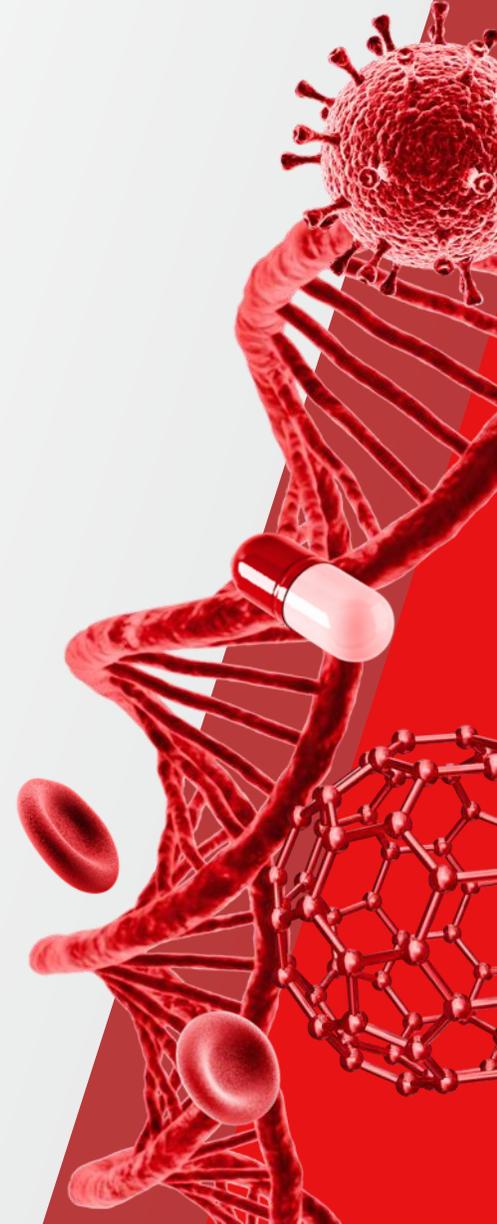
Kerstin Strupat

Product Manager

With contribution from the LSMS Product Management Team

March 2021

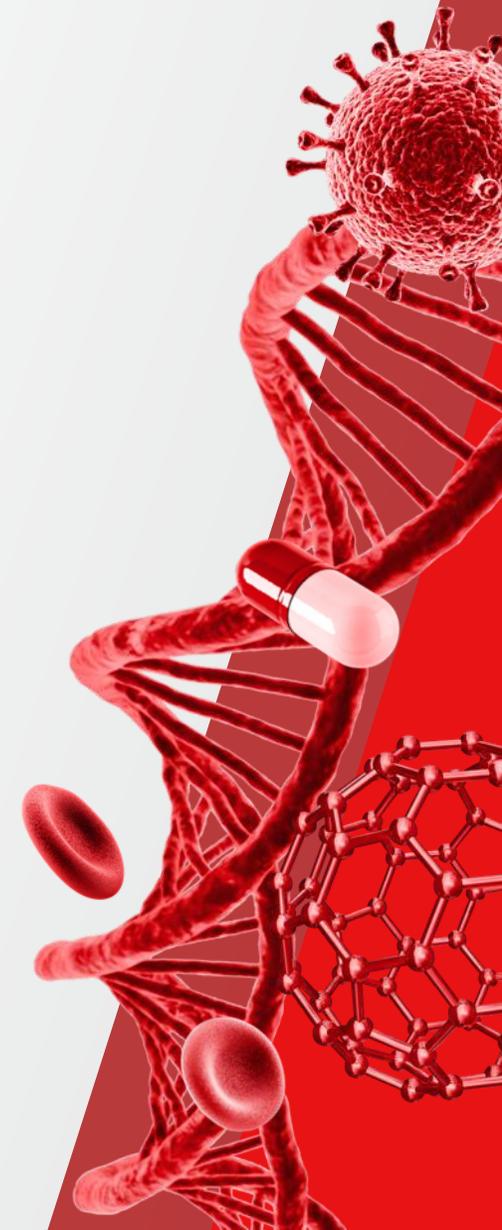
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- **FAIMS Carrier Gas** – update
- **Tune Diagnostics**
 - **Optional Calibration**
 - Low Mass Range
 - High Mass Range
 - **Partial Calibration**
 - Restructured procedures by category and polarity
 - **Tools**
 - Change Mass Calibration Due Time
- **Further Improvements**
 - Tune: Instrument Status pane displays vacuum pressures in a separate heading ‘Vacuum System’
 - Method Editor: TurboTMT supports TMTpro Reagent
- **Software Manuals**
- **Online help** for Tune and Method Editor

FAIMS Carrier Gas – update

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FAIMS Carrier Gas Update

Changes in the User Interface: Now it is possible to **reduce the carrier gas for increased spray stability at nanoflow**

Previously – with and until OES 2.0 SP2 ICSW:

- Carrier gas: hidden parameter, set by capillary type and temperature
- Not possible to reduce the carrier gas below the set value
- **'FAIMS Gas'** in Tune and Method Editor: optional user parameter to apply additional carrier gas

ION SOURCE		DEFINE SCAN		CALIBRATION	
Ion Source		Optimization			
Current LC Flow (µL/min)	0			Get Defaults	
Ion Source Type	ESI				
Pos Ion Spray Voltage (V)	3400			24	
Neg Ion Spray Voltage (V)	2000				
Sheath Gas (Arb)	0			0.00	
Aux Gas (Arb)	7			0.00	
Ion Transfer Tube Temp (°C)	320			320.0	
FAIMS Gas (L/min)	0			0.0	
FAIMS Mode	Standard Resolution				

New with OES 3.0 ICSW:

- **'Total Carrier Gas Flow'** replaces 'FAIMS gas' in Tune and Method Editor UI
- Default **'Total Carrier Gas Flow'** values and ranges dependent on capillary type
- The dependency on capillary temperature has been removed:
 - **Models OE 120, OE 240** - Round bore ion transfer tube: 0.7 to 4.3 L/min, default: 1.2 L/min (e.g. Orbitrap Exploris 240, Orbitrap ID-X, TSQ Quantis)
 - **Model OE 480** - Letterbox ion transfer tube: 3.5 to 7.7 L/min, default: 4.6 L/min (e.g. Orbitrap Exploris 480, Orbitrap Fusion Lumos, TSQ Altis)

ION SOURCE		DEFINE SCAN		CALIBRATION	
Ion Source		Optimization			
Current LC Flow (µL/min)	200			Get Defaults	
Ion Source Type	Heated ESI				
Pos Ion Spray Voltage (V)	3500			22	
Neg Ion Spray Voltage (V)	2500				
Sheath Gas (Arb)	50			0.00	
Aux Gas (Arb)	10			0.00	
Ion Transfer Tube Temp (°C)	320			319.2	
Vaporizer Temp (°C)	350			34.0	
Total Carrier Gas Flow (L/min)	4.6			4.6	
FAIMS Mode	Standard Resolution				

FAIMS Carrier Gas Update

Readbacks

Previously – with and until
OES 2.0 SP2 ICSW:

STATUS	By Function
▷	Current Scan
▷	<input checked="" type="checkbox"/> Ion Source
▷	<input checked="" type="checkbox"/> Atmospheric Interface
▷	<input checked="" type="checkbox"/> HCD Cell
▷	<input checked="" type="checkbox"/> Orbitrap
▷	Internal Calibration
◀	<input checked="" type="checkbox"/> FAIMS
	Compensation Voltage (CV) 0.0 V
	Dispersion Voltage (DV) 0.0 V
	Entrance Plate 0.1 V
	FAIMS User Set Gas Flow 0.0 L/min
	Cooling Gas Flow 5.0 L/min
	<input checked="" type="checkbox"/> Inner Electrode Temperature 100.0 °C
	<input checked="" type="checkbox"/> Outer Electrode 1 Temperature 100.0 °C
	<input checked="" type="checkbox"/> Outer Electrode 2 Temperature 100.0 °C
▷	<input checked="" type="checkbox"/> Alerts
▷	<input checked="" type="checkbox"/> Peripheral Devices

New with OES 3.0 ICSW:

STATUS	By Function
▷	Current Scan
▷	<input checked="" type="checkbox"/> Ion Source
▷	<input checked="" type="checkbox"/> Vacuum System
	Internal Calibration
◀	<input checked="" type="checkbox"/> FAIMS
	Compensation Voltage (CV) 0.1 V
	Dispersion Voltage (DV) 0.0 V
	Entrance Plate 0.1 V
	Total Carrier Gas Flow 1.2 L/min
	Cooling Gas Flow 5.0 L/min
	<input checked="" type="checkbox"/> Inner Electrode Temperature 100.0 °C
	<input checked="" type="checkbox"/> Outer Electrode 1 Temperature 100.0 °C
	<input checked="" type="checkbox"/> Outer Electrode 2 Temperature 100.0 °C
▷	<input checked="" type="checkbox"/> Alerts
▷	<input checked="" type="checkbox"/> Peripheral Devices

FAIMS Carrier Gas Update

Method Conversion / Method Transfer

OES 2.x ICSW methods can be converted/updated to their [usage in OES 3.0 ICSW](#) – using the **same instrument model**

New 'Total Carrier Gas Flow' will be set to the default (by capillary type) + FAIMS gas setting from 2.x method.

Examples:

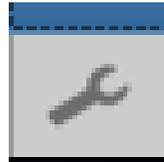
- OE 480, OES 2.0 method with FAIMS gas of 0 L/min will be converted to OE 480, OES 3.0 method with 'Total Carrier Gas Flow' of 4.6 L/min
- OE 480, OES 2.0 method with FAIMS gas of 1.1 L/min will be converted to OE 480, OES 3.0 method with 'Total Carrier Gas Flow' of 5.7 L/min (new 'Total Carrier Gas Flow' can be time-dependent, just like old 'FAIMS Gas')

Note these aspects when converting from OES 2.x ICSW methods to their [usage in OES 3.0 ICSW](#) – when using methods in **different instrument models**

New 'Total Carrier Gas Flow' will be set to the default (by capillary type).

Examples:

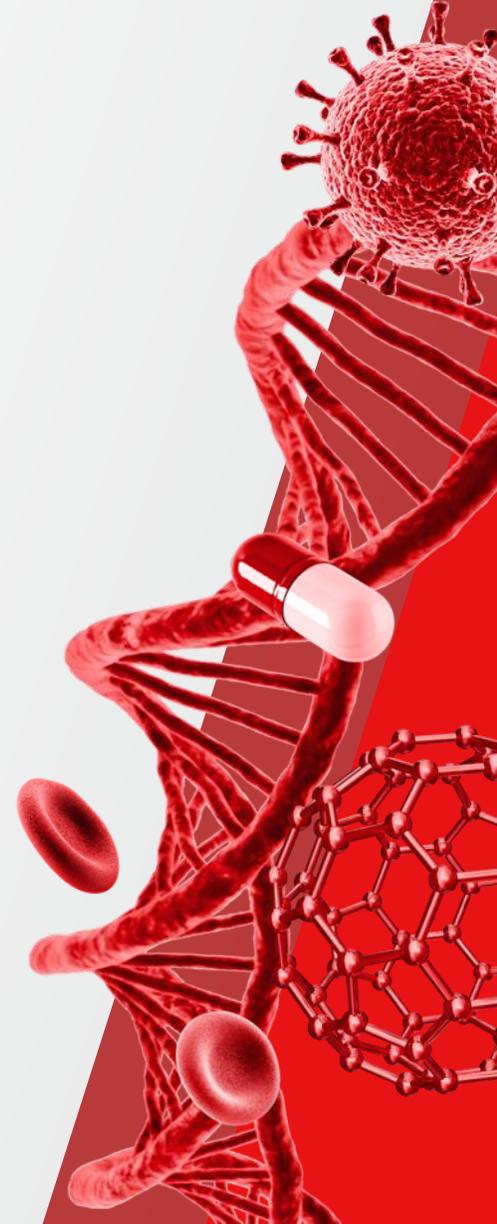
- OE 240, OES 2.0 method with FAIMS gas of 0 L/min will be converted to OE 480, OES 3.0 method with 'Total Carrier Gas Flow' of 4.6 L/min
- OE 240, OES 3.0 method with FAIMS gas of 1.1 L/min will be converted to OE 480, OES 3.0 method with 'Total Carrier Gas Flow' of 4.6 L/min
- OE 480, OES 3.0 method with FAIMS gas of 0 L/min will be converted to OE 240, OES 3.0 method with 'Total Carrier Gas Flow' of 1.2 L/min
- OE 480, OES 2.0 method with FAIMS gas of 2 L/min will be converted to OE 240, OES 3.0 method with 'Total Carrier Gas Flow' of 1.2 L/min



OES 3.0 ICSW – Tune Diagnostics / Optional Calibration

- low m/z mass calibration
- mass calibration / mass check for both polarities

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... Provides Low m/z Spectral Mass Accuracy Calibration & Check

Find the wrench symbol in the bottom left corner of the Tune application to access Tune Diagnostics



Orbitrap Exploris 240 Tune Application 3.0.261.7

thermo scientific
Orbitrap Exploris 240

ION SOURCE | DEFINE SCAN | CALIBRATION

Diagnostics

- System
- Partial Calibration
- Optional Calibration
 - Low Mass Range
 - Low m/z Spectral Mass Accuracy Calibration (for Low m/z Applications) (pos)
 - Low m/z Spectral Mass Accuracy Check (pos)
 - Low m/z Spectral Mass Accuracy Calibration (for Low m/z Applications) (neg)
 - Low m/z Spectral Mass Accuracy Check (neg)
 - High Mass Range
 - Setup Scan for Manual AHFP Spray Optimization (5 min) (pos)
 - High m/z AHFP Spectral Mass Accuracy Calibration (pos)
 - High m/z AHFP Spectral Mass Accuracy Check (pos)
 - Setup Scan for Manual AHFP Spray Optimization (5 min) (neg)
 - High m/z AHFP Spectral Mass Accuracy Calibration (neg)
 - High m/z AHFP Spectral Mass Accuracy Check (neg)
- Tools

Optional Calibration

- Low Mass Range
 - Low m/z Spectral Mass Accuracy Calibration (for Low m/z Applications) (pos)
 - Low m/z Spectral Mass Accuracy Check (pos)
 - Low m/z Spectral Mass Accuracy Calibration (for Low m/z Applications) (neg)
 - Low m/z Spectral Mass Accuracy Check (neg)

This procedure calibrates the spectral mass accuracy for the low m/z range (40 - 310 m/z).

[Learn more...](#)

This procedure improves mass accuracy for low m/z applications. However, the standard m/z mass accuracy (150 - 2000 m/z) may shift in a sub-ppm level after running this procedure. For returning to standard m/z applications, it is highly recommended to run the Mass Calibration from the Calibration pane.

Note:

Per default, with the **System Calibration** in the tab **Calibration** the low masses are calibrated already. If there is particular need for high mass accuracy in the low mass range, then the here displayed **Optional Calibration** can be performed.

Please reflect the content of the tool tips; consider that the standard mass range might have a little higher deviation, when working with the optional low mass range calibration. Re-run a mass calibration under tab **Calibration** if you intend to work with standard mass range.

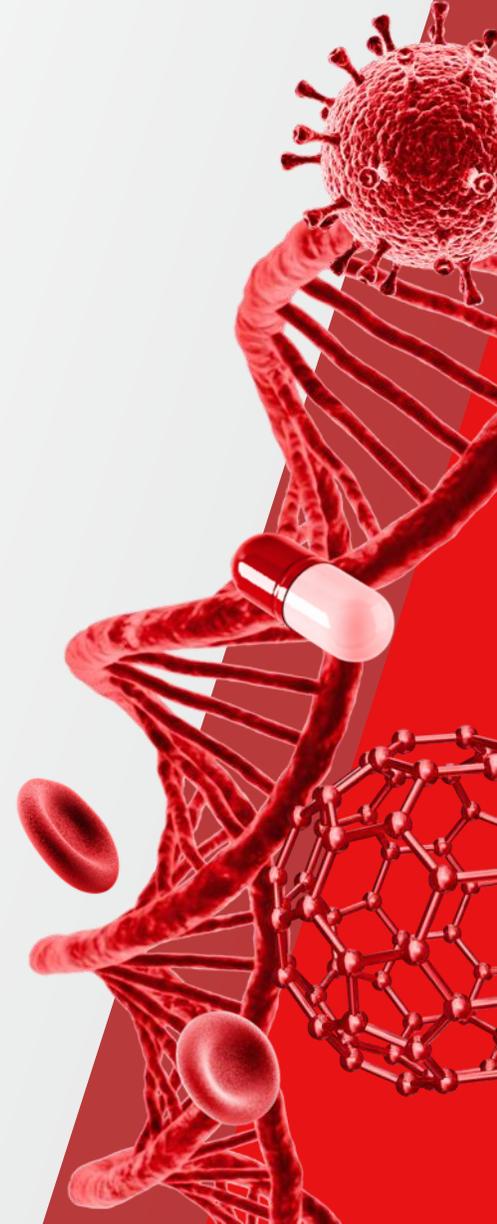
BioPharma update -



OES 3.0 ICSW –Tune Diagnostics / Optional Calibration

- applies an improved eFT calibration
- provides mass calibration / mass check for positive and negative ion modes

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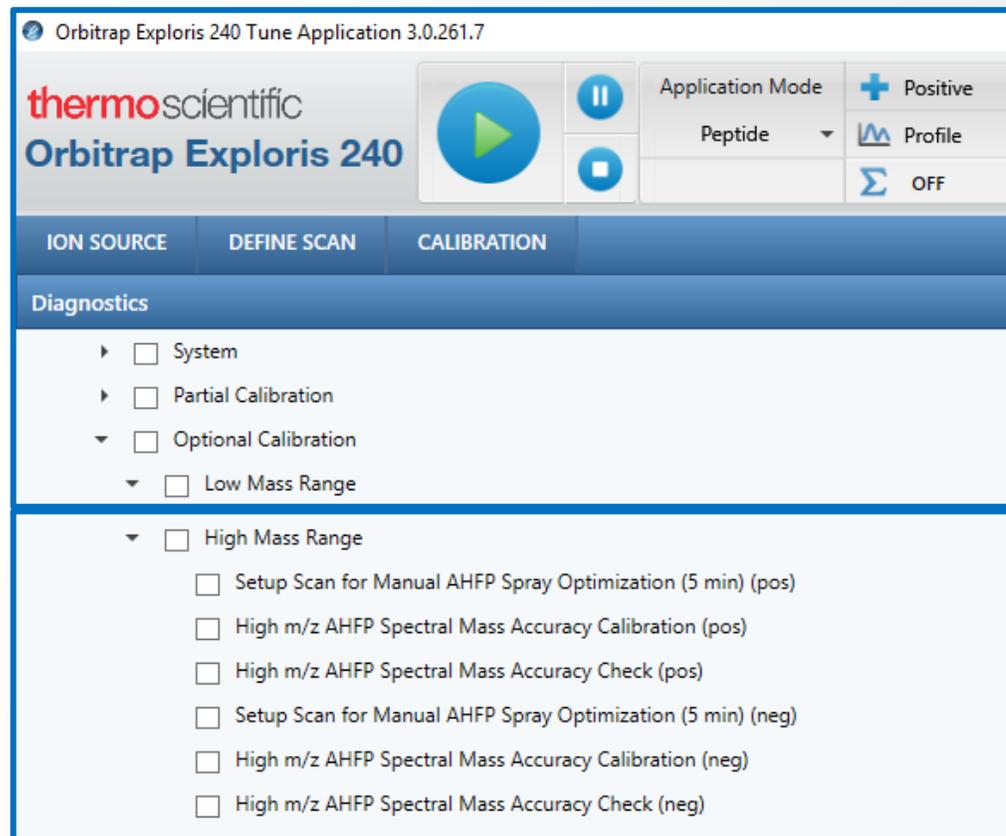
With OES 3.0 ICSW an improvement and a new feature is provided to meet the user's need in BioPharma applications better

Improvement

- Improved eFT phase calibration to improve mass accuracy for High Mass Range applications

New Feature

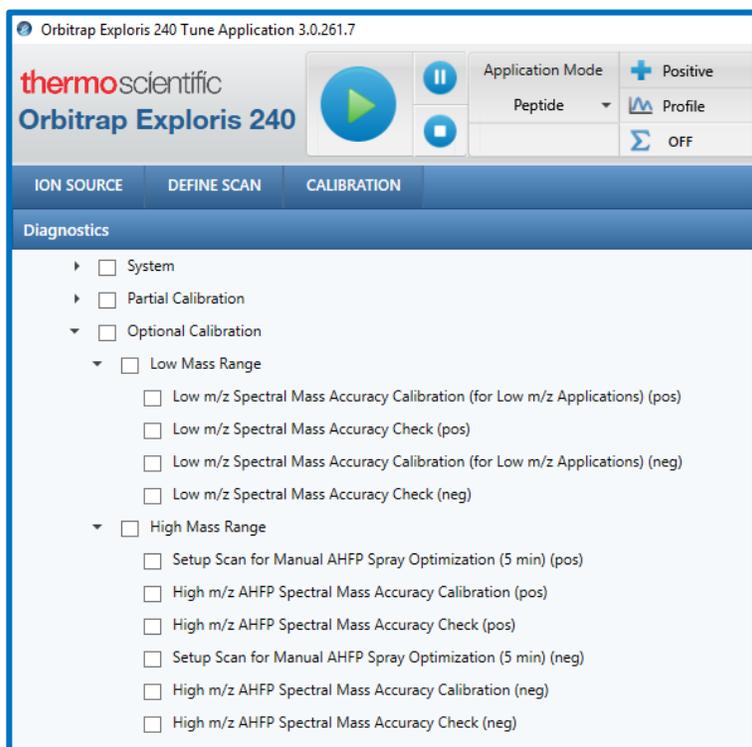
- Tune Diagnostics provide High Mass Range Calibr. (AHFP) for negative polarity when using Application Mode 'Intact Protein'



This functionality is available for Orbitrap Exploris models OE 240, OE 480 when BioPharma mode licensed

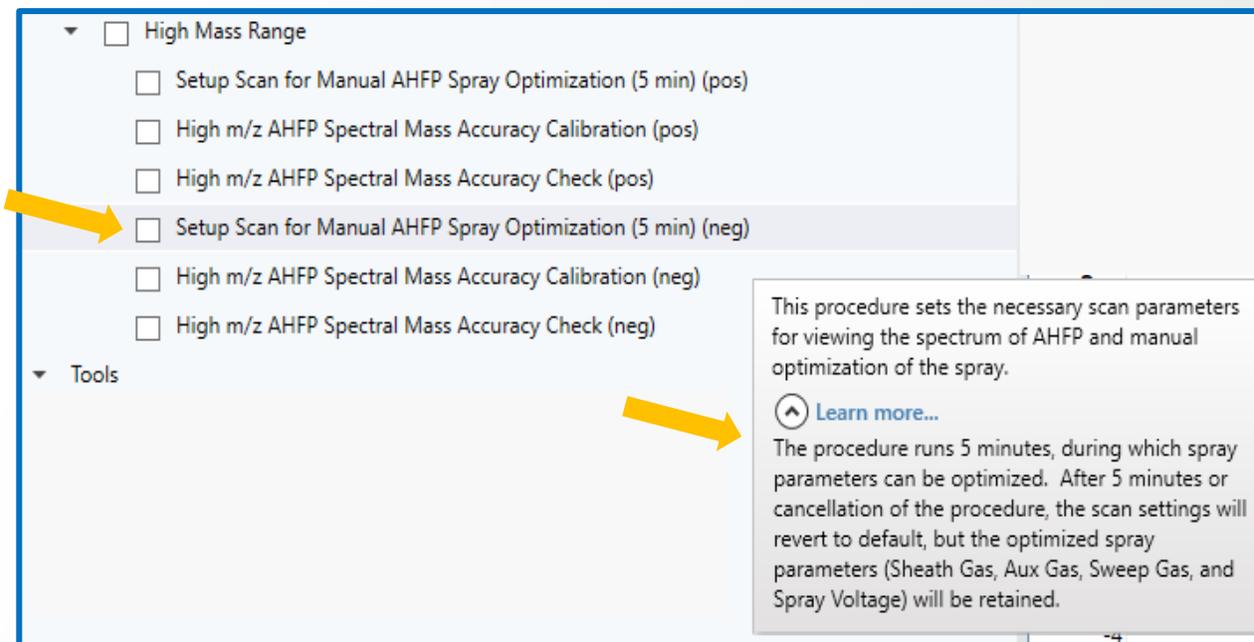
With OES 3.0 ICSW an improvement and a new feature is provided to meet the user's need in BioPharma applications better

Find the wrench symbol in the bottom left corner of the Tune application to access Tune Diagnostics



New Feature

- Tune Diagnostics provide High Mass Range Calibr. (AHFP) for **negative polarity** when using Application Mode 'Intact Protein'

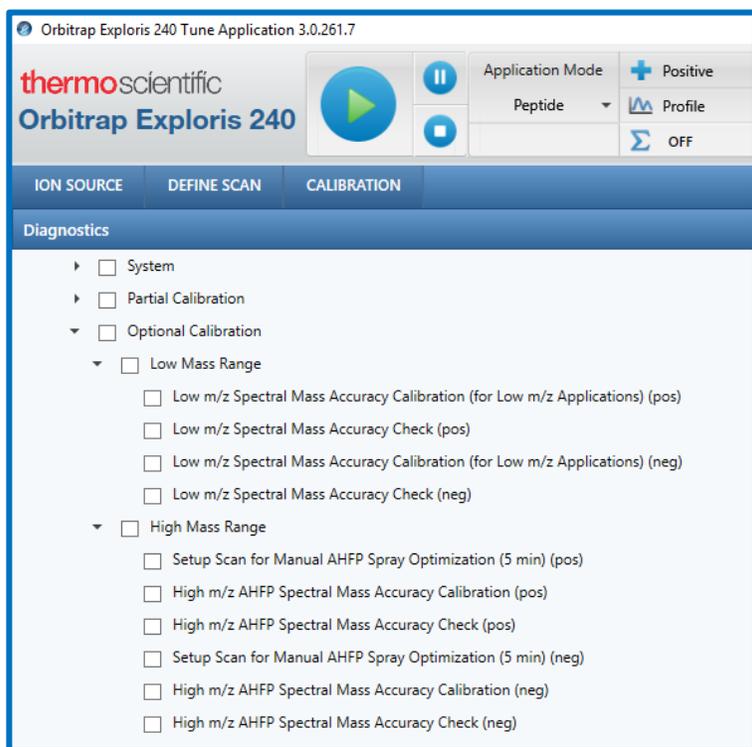


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<https://www.fishersci.com/shop/products/ammonium-hexafluorophosphate-99-5-extra-pure-acros-organics-4/AC202320050>

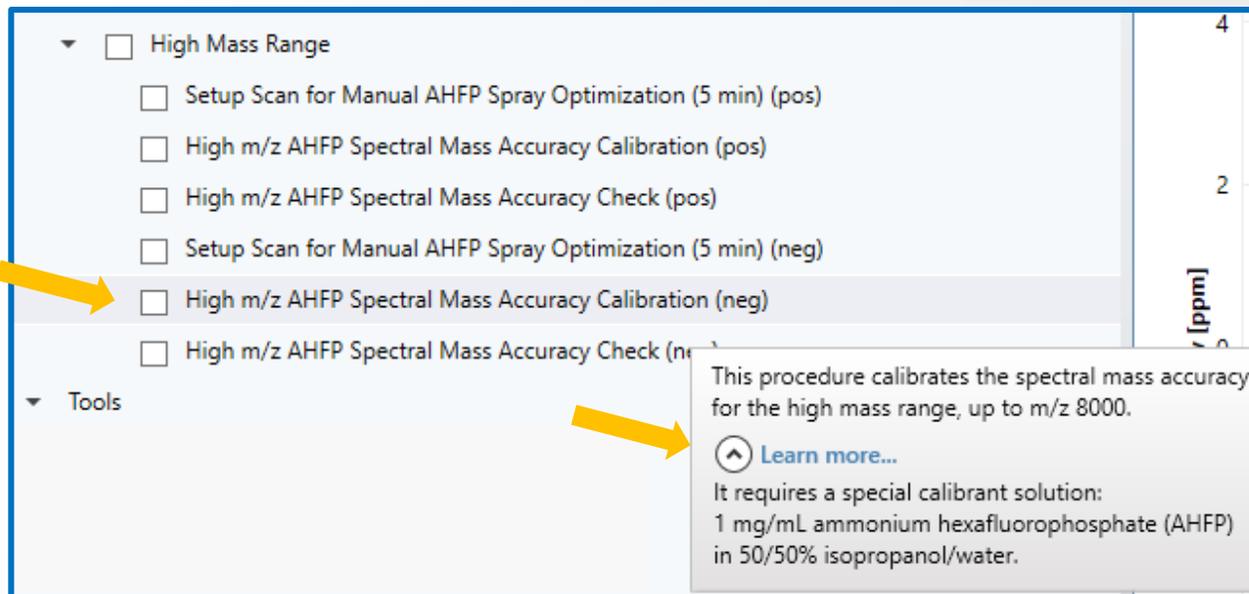
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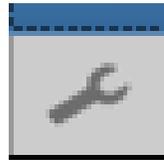
New Feature

- Tune Diagnostics provide High Mass Range Calibr. (AHFP) for **negative polarity** when using Application Mode 'Intact Protein'



This functionality is available for Orbitrap Exploris models OE 240, OE 480 when BioPharma mode licensed

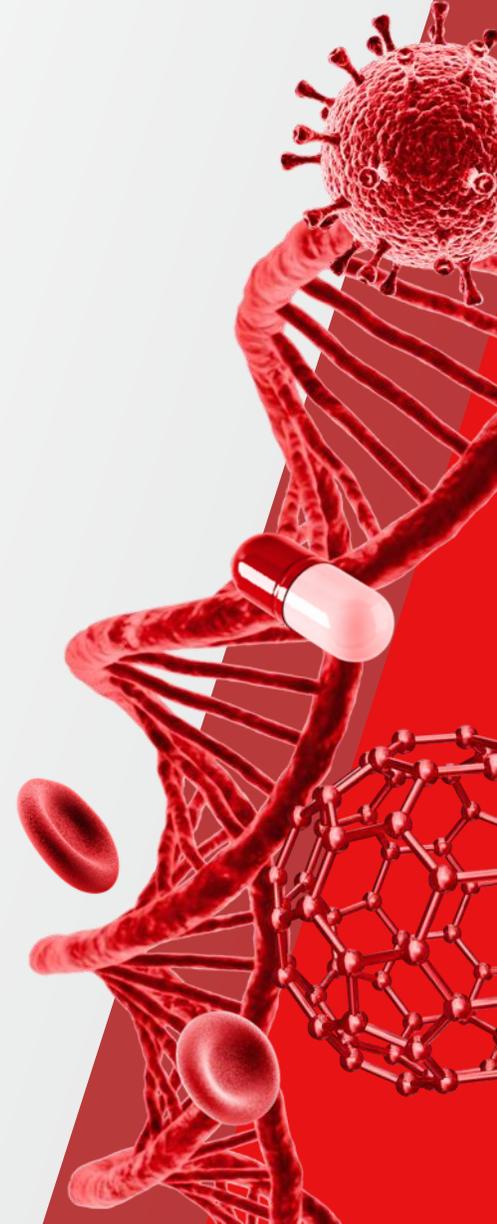
<https://www.fishersci.com/shop/products/ammonium-hexafluorophosphate-99-5-extra-pure-acros-organics-4/AC202320050>



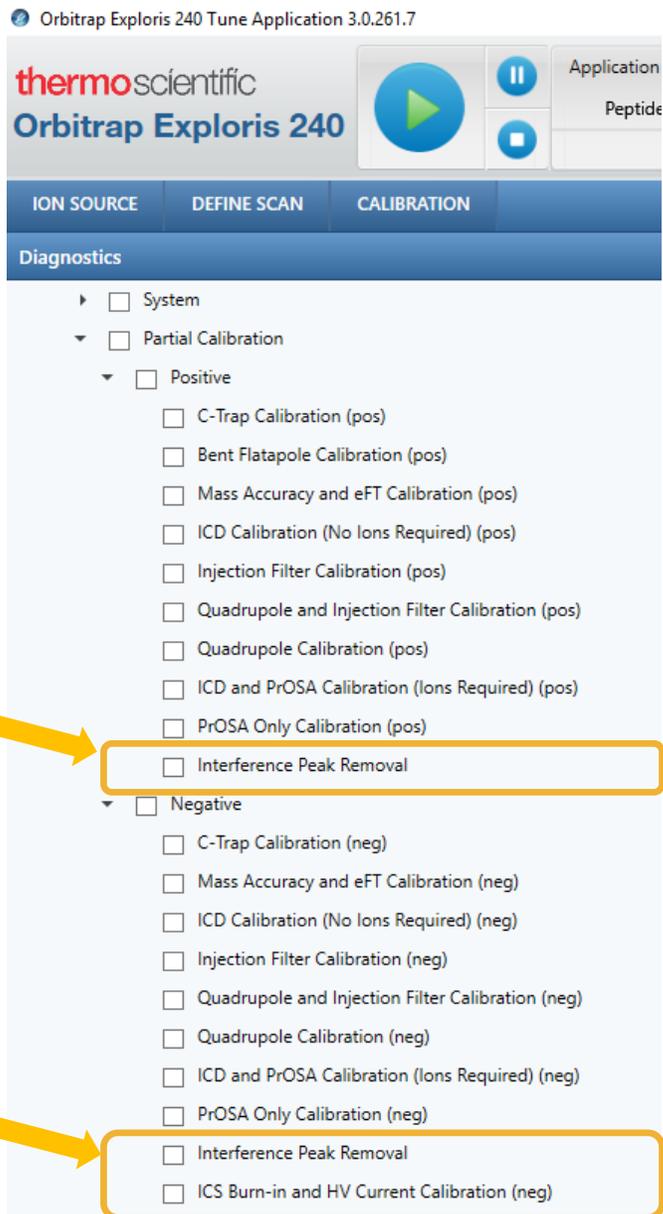
OES 3.0 ICSW – Tune Diagnostics / Partial Calibration

- ‘Partial Calibration’ procedure menu

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... provides restructured procedures separated by category and polarity



Find the wrench symbol in the bottom left corner of the Tune application to access **Tune Diagnostics**



Interference Peak Removal Procedure

1. It is (a) part of the System Calibration, (b) a single procedure (*here*) in Diagnostics/Partial Calibrations.
2. The procedure works similar to active noise cancelling on headphones and helps to further reduce the background noise at known frequencies in the ion optics and the quadrupole.
3. After venting and bakeout, the system calibration will (anyways) additionally process sub-procedures which execute the known RF frequency calibrations (IF, Quad, C-trap) plus the new Interference Peak Removal Calibration.
There is no need to recall the procedure on an individual basis.

ICS Burn-in and HV Current Calibration Procedure

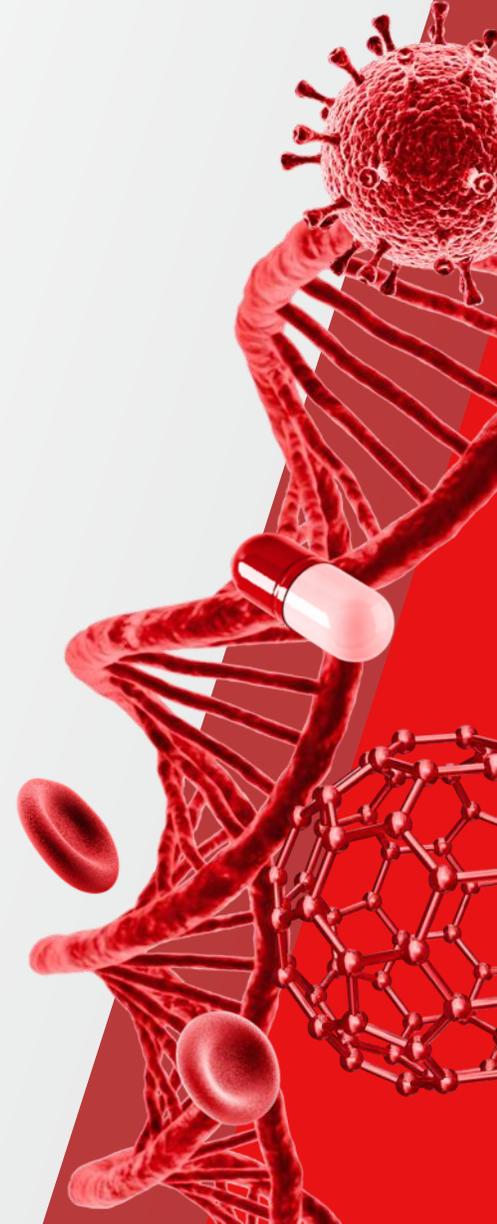
1. The ICS burn-in procedure was further improved and added to the HV Current Calibration (neg).
2. It resolves issues with System Calibration in negative ion mode, especially when EASY-IC was not in use for a longer time.



OES 3.0 ICSW – Tune Diagnostics / Tools

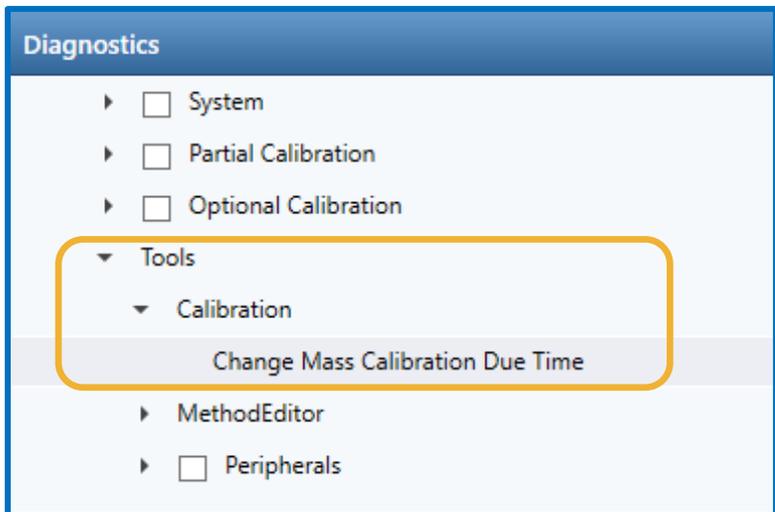
- mass calibration due time can be set by user

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... provides a tool to change the Mass Calibration Due Time

Find the wrench symbol in the bottom left corner of the Tune application to **access Tune Diagnostics**



- Under 'Tools' / 'Calibration' a new parameter '**Change Mass Calibration Due Time**' is available
- At the bottom of the 'Diagnostics tab', the parameter and its set value (in hours) is now accessible for the user (here 25 h, default)

Parameter Name	Parameter Value
Mass Calibration Due Time	25

ION SOURCE DEFINE SCAN CALIBRATION

Diagnostics

- System
- Partial Calibration
- Optional Calibration
- Tools
 - Calibration
 - Change Mass Calibration Due Time
 - MethodEditor
 - Peripherals

Mass accuracy is < 3 ppm within 25 h (Specification). Please evaluate any change in the due time setting ('Recommended Date') . (default: 25h). A change in the due time will adjust the recommended date and thus the time point when a warning message appears in the resulting raw data files.

[Learn more...](#)

Here the due time setting ('Recommended Date') for the next mass calibration can be customized. The user may consider a longer time period (e.g. 75 h/3 days) between two succeeding mass calibrations according to his/her application and experience. It is recommended to evaluate the frequency of performing mass calibrations before changing the due date.

... see next slide for details

Applies to all models – here displayed for Orbitrap Exploris 120 system

... provides a tool to change the Mass Calibration Due Time

Following up from previous slide

Mass accuracy is ≤ 3 ppm within 25 h (Specification). Please evaluate any change in the due time setting ('Recommended Date') . (default: 25h). A change in the due time will adjust the recommended date and thus the time point when a warning message appears in the resulting raw data files.

[Learn more...](#)

Here the due time setting ('Recommended Date') for the next mass calibration can be customized. The user may consider a longer time period (e.g. 75 h/3 days) between two succeeding mass calibrations according to his/her application and experience. It is recommended to evaluate the frequency of performing mass calibrations before changing the due date.

	Recommended	Last Calibrated
<input type="checkbox"/> Mass Calibration	Feb 18, 2021	
<input type="checkbox"/> Positive ion mode	Mar 04, 2021	Mar 03, 2021
<input type="checkbox"/> Negative ion mode	Feb 18, 2021	Feb 17, 2021
<input type="checkbox"/> System Calibration		
<input type="checkbox"/> Positive ion mode	Apr 02, 2021	Mar 03, 2021
<input type="checkbox"/> Negative ion mode	Mar 19, 2021	Feb 17, 2021

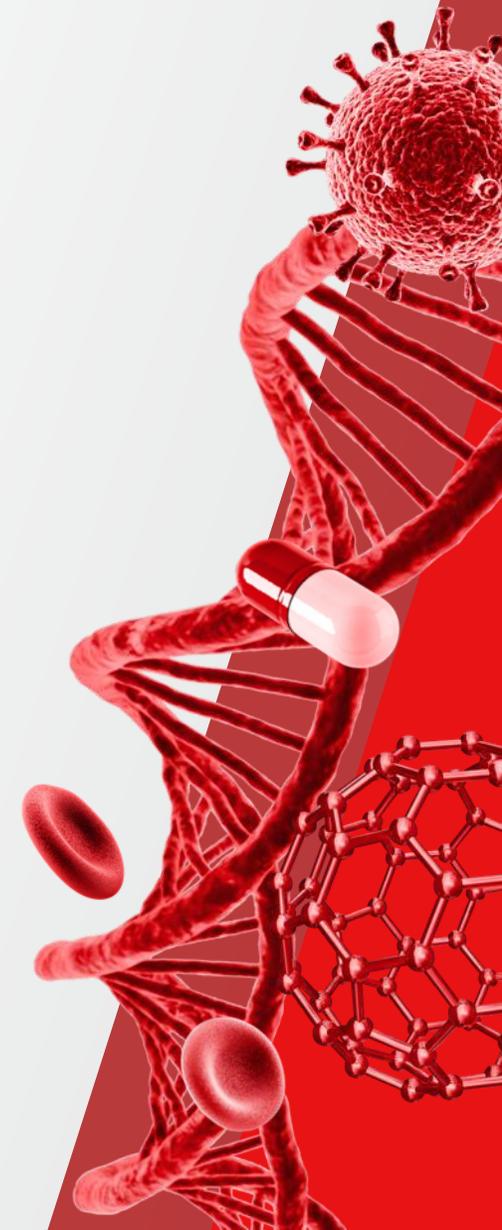
Functionality

- Recommended date and last calibrated dates are updated accordingly – considering user-defined time duration
- Warning messages appear only after the user-defined due time is exceeded
- The modified Mass Calibration Due Date is also reflected in RAW file Status Log and Error Log accordingly
- **Note:** The Tune Diagnostics pane handles 'Change Mass Calibration Due Time' as a procedure.
→ The user needs to **hit** the '**Start**' button to apply the change.

Applies to all models – here displayed for Orbitrap Exploris 120 system

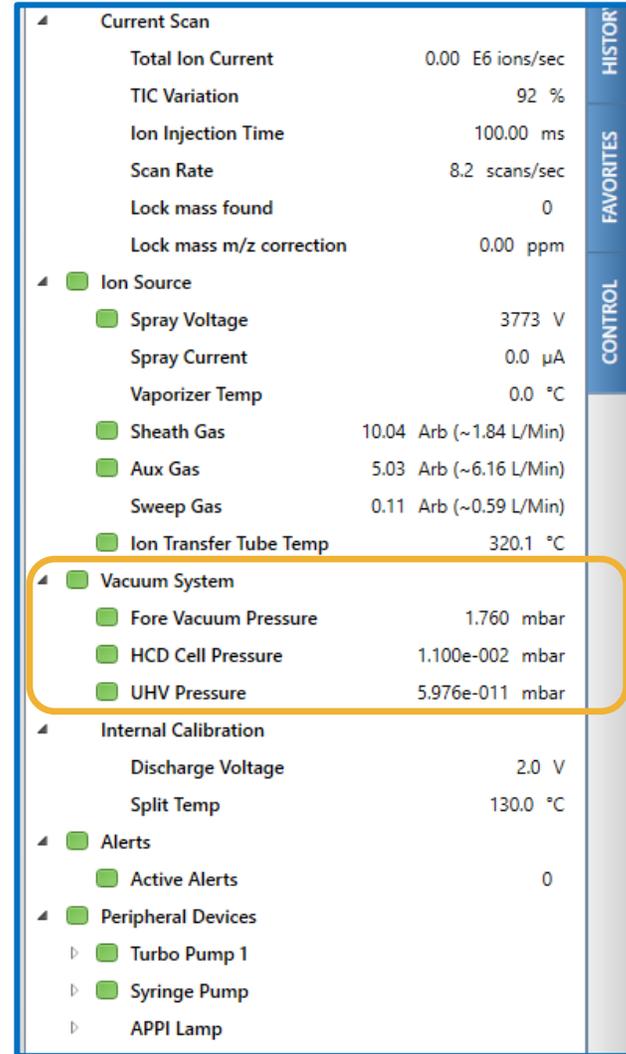
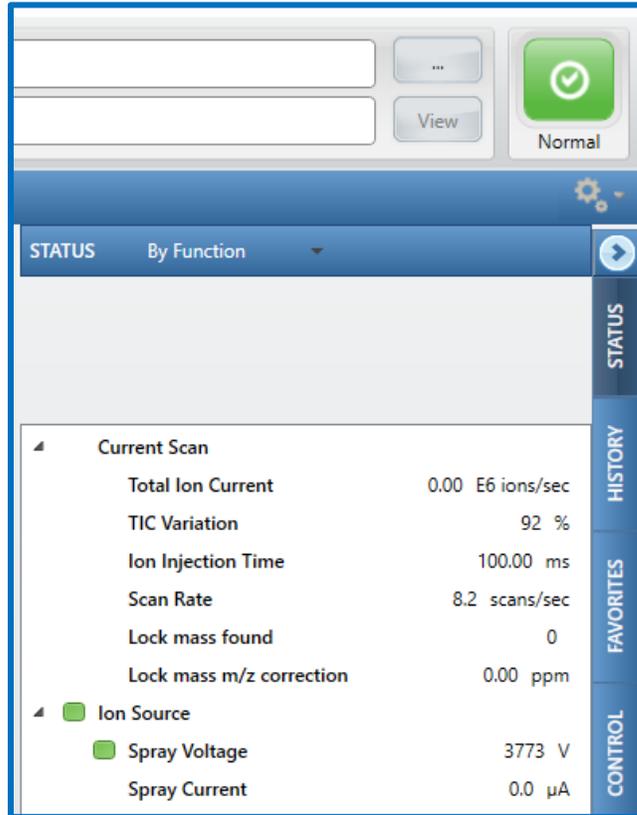
Further Improvements

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Further Improvements

Tune: Instrument Status pane displays vacuum pressures in a separate heading 'Vacuum System'



Take frequent looks at the Vacuum System

Too low fore vacuum pressure is a strong indicator that the ion transfer tube needs to be exchanged.

Background:

When the fore vacuum is too low, the ions are not cooled down enough in the bent flatapole region. This may lead to more MS1 fragmentation influencing the MS2 spectral match.

OE120 / OE240: 1.8 – 2.2 mbar @320 °C

OE480: 3.5 – 3.9 mbar @320 °C

Further Improvements

Method Editor supports TMTpro Reagent (16plex TMT)

Data-Dependent MS² Scan Properties

Multiplex Ions	<input type="checkbox"/>
Isolation Window (m/z)	2
Isolation Offset	Off
Collision Energy Mode	Fixed
Collision Energy Type	Normalized
HCD Collision Energy (%)	30
Orbitrap Resolution	15000
TurboTMT	Off
Scan Range Mode	Off
AGC Target	TMTpro Reagent

Orbitrap Resolution	15000	★
TurboTMT	Off	★
Scan Range Mode	Off	
First Mass (m/z)	TMT Reagents	
	TMTpro Reagent	
AGC Target	Custom	★

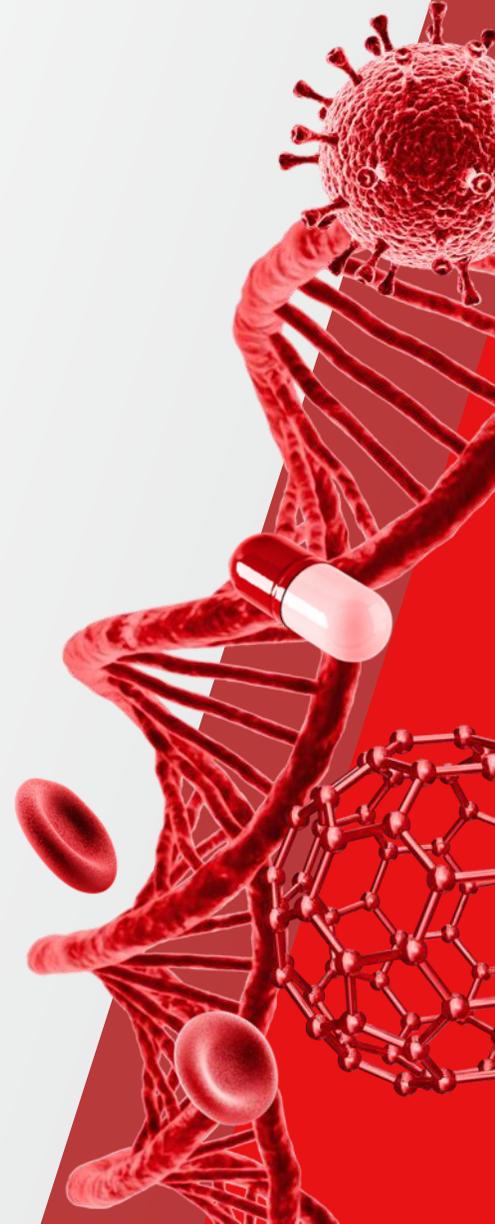
- Off
- Sixplex TMT, 10plex TMT, 11plex TMT
- TMTpro 16plex

This functionality is available for Orbitrap Exploris models OE 480. The scan types tMS2, Product Ion Scan, ddMS2 additionally support 'TMTpro Reagent' for the parameter TurboTMT – when resolution setting 15k or 30k is chosen

Availability of Orbitrap Exploris Series

- Software Manuals
- online help

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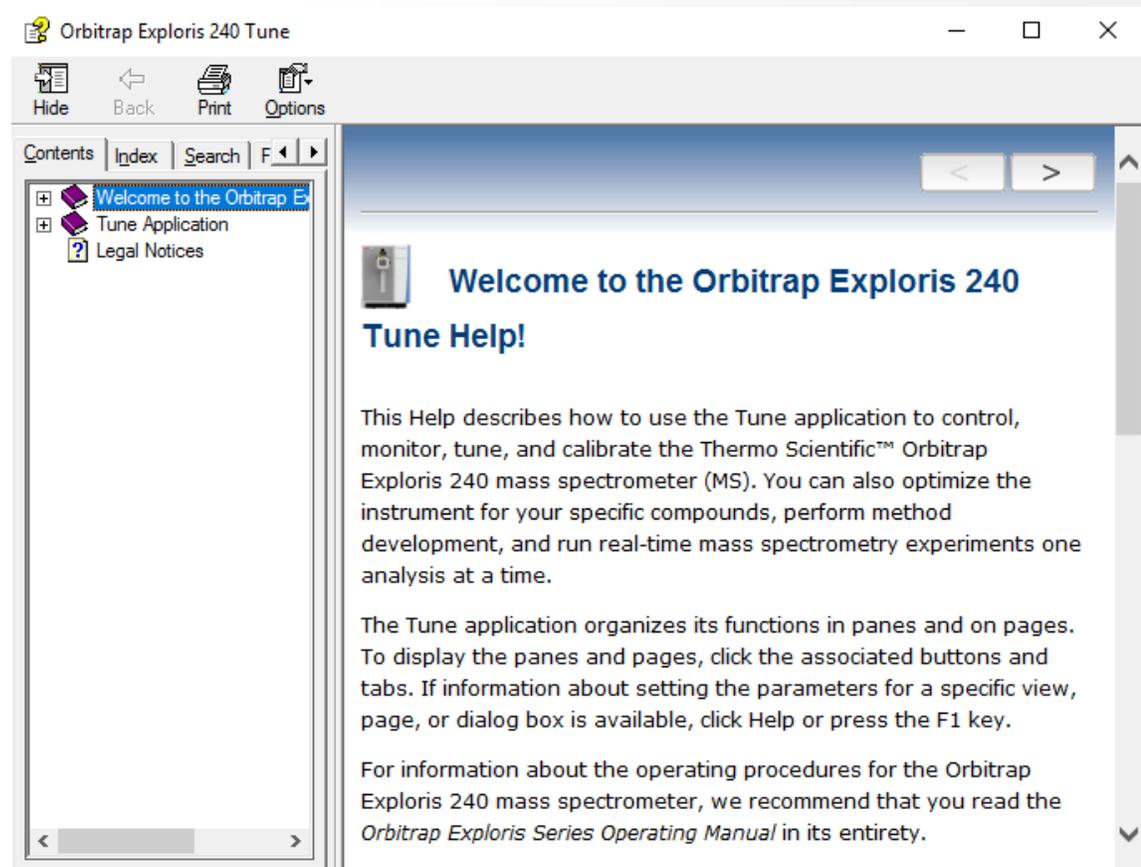
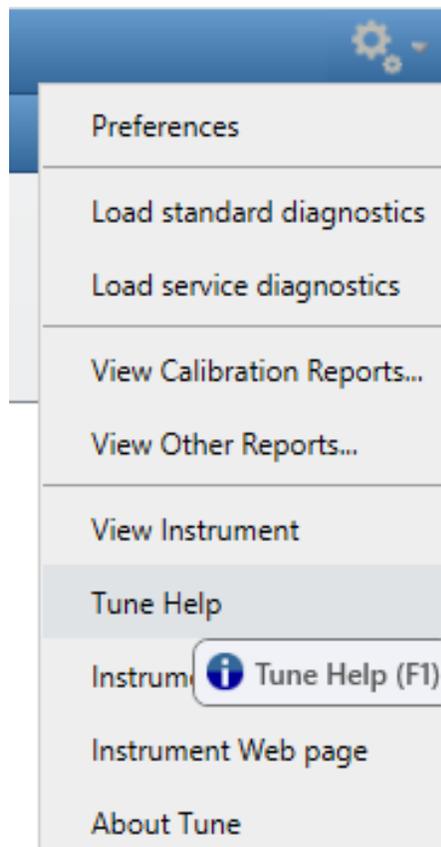


Software Manuals are part of the delivered iso-image and installed upon the installation procedure



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

Orbitrap Exploris 240 Method Editor 3.0.261.9
File Orbitrap Exploris 240

Method Editor Global Parameters Scan Parameters Summary

Method Timeline

Application Mode #1
Peptide

Method Duration (min)
40

Experiment # 1

Scans
MS
MS²

Filters
MIPS
Intensity
Precursor Fit
Charge State
Dynamic Exclusion
Targeted Inclusion
Targeted Exclusion
Apex Detection

Orbitrap Exploris 240 Method Editor

Welcome to the Orbitrap Exploris 240 Method Editor
Help!

This Help describes how to use the Method Editor application with the Thermo Scientific™ Orbitrap Exploris 240 mass spectrometer (MS). You create an MS instrument method (combined with the optional autosampler and liquid chromatograph instrument methods) by defining the experiment type and setting various parameters. These include settings for the MS, syringe pump, and divert valve; and the mass ranges and fragmentation transitions for the experiments.

For information about the operating procedures for the Orbitrap Exploris 240 mass spectrometer, we recommend that you read the *Orbitrap Exploris Series Operating Manual* in its entirety.

Helpful Links

- [Configuring the Instrument in Thermo Foundation](#)
- [Method Editor Application](#)
- [Contacting Us](#)

Orbitrap Exploris 240 Method Editor

Hide Back Print Options

Contents Index Search Favorites

Type in the keyword to find:
system templates

List Topics

Available System Templates

When you select an application mode on the Global Parameters or Scan Parameters page, the Method Editor changes the list of displayed [System Templates](#).

Template category	Experiment description
Application Mode - Small Molecule	
Clinical Research	
Immunosuppressants	Full Scan method that is suited to quantify ISDs under UHPLC conditions with short method durations.
Steroids	tMS2 method that is displayed in Quan View and suited to quantify steroids by means of HCD activation followed by Orbitrap mass analysis.
Environmental	
PFAS EtherAcids FS ddMS2	Full Scan data-dependent MS2 method for the analysis of selected PFAS Ether Acids.
PFAS FS ddMS2	Full Scan data-dependent MS2 method for the analysis of selected PFAS compounds
Food Safety	
AcquireX Pesticides FS ddMS2	Full Scan data-dependent MS2 method for the analysis of pesticides with the option to enable AcquireX method modifications.
AcquireX Pesticides Full Scan	Full Scan method for the analysis of pesticides with the option to enable AcquireX method modifications.
Pesticides FS DIA EASY-1C	Method that couples Full Scan and Data Independent Acquisition experiments for the analysis of pesticides. It applies stepped collision energy.
VetDrugs FS ddMS2 Targets unscheduled	Full Scan data-dependent MS2 method for the analysis of veterinary drugs, unscheduled in retention time.
VetDrugs FS ddMS2 TopN	Full Scan data-dependent MS2 method for the analysis of veterinary drugs, scheduled in retention time.
VetDrugs FS DIA	Method that combines experiments of Full Scan and DIA scan type in an independent manner—suited for the analysis of veterinary drugs.

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