OES 3.0 ICSW -
New Features, Improvement and Defect Fix

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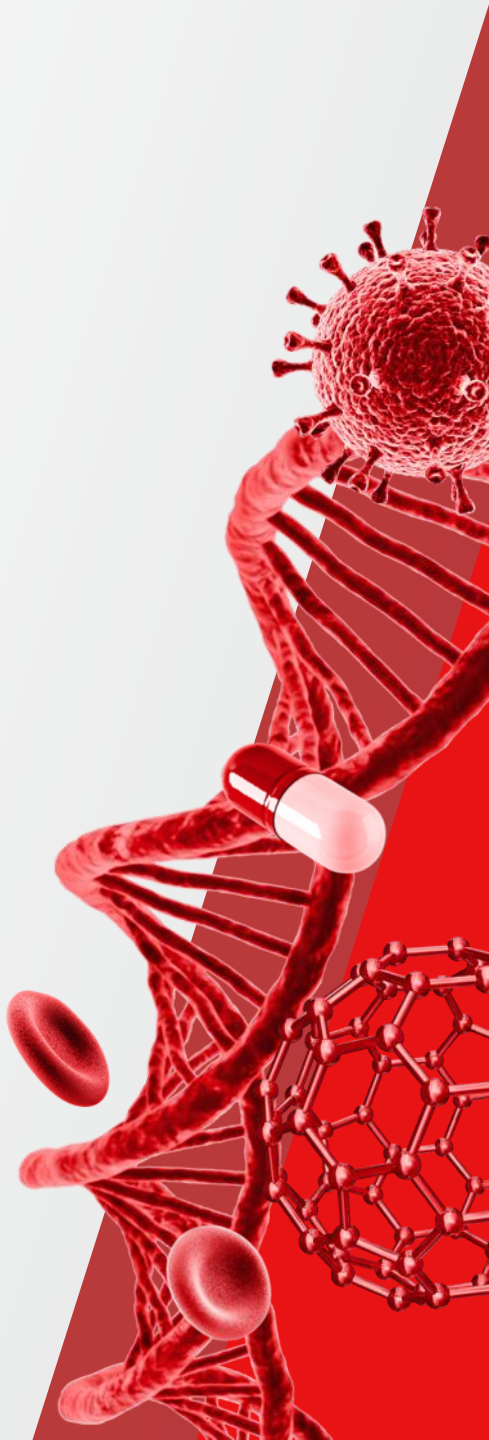
Product Manager
With contribution form the LSMS Product Management Team

March 2021



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- **Tune Diagnostics**
  - **Optional Calibration**
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    - High Mass Range
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- **Further Improvements**
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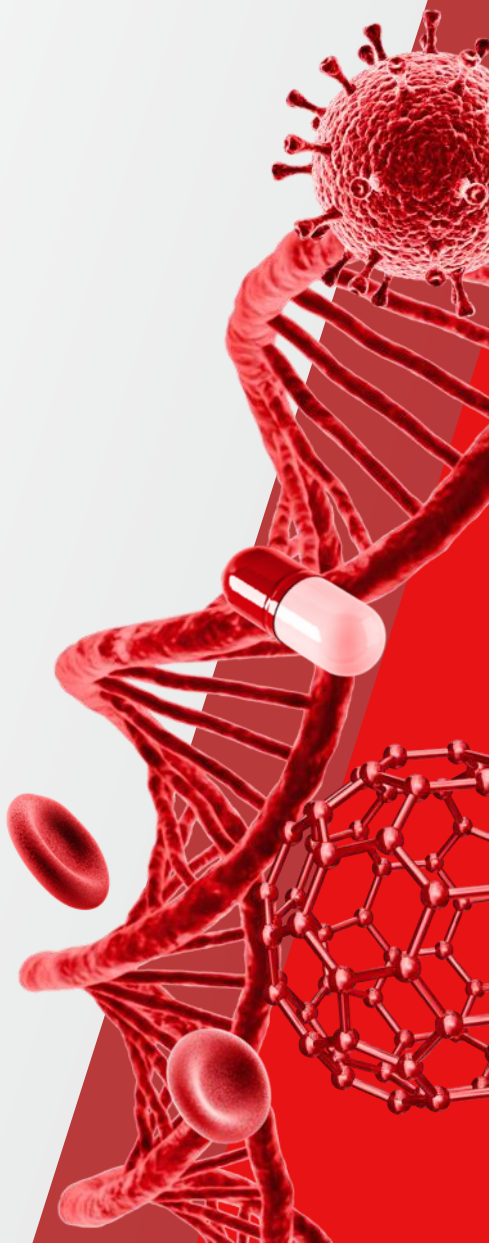
  - Method Editor: TurboTMT supports TMTpro Reagent
- **Software Manuals**
- **Online help** for Tune and Method Editor

FAIMS Carrier Gas – update



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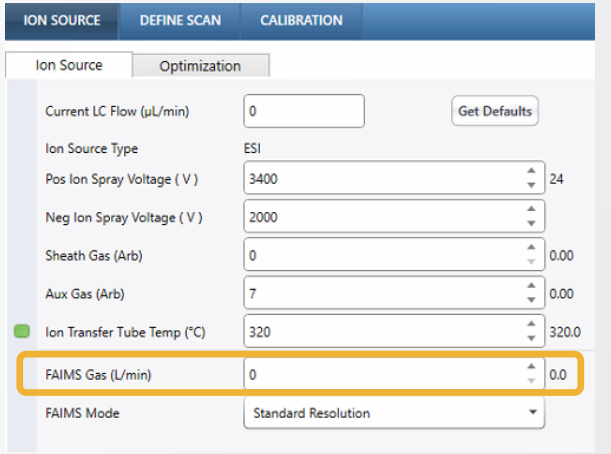
FAIMS Carrier Gas Update

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



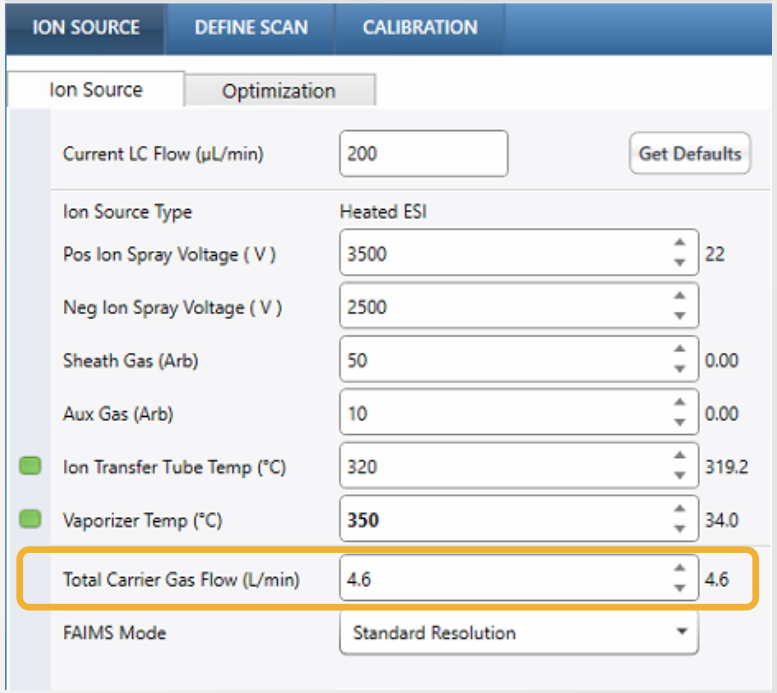
Previously – with and until OES 2.0 SP2 ICSW:

- 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

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

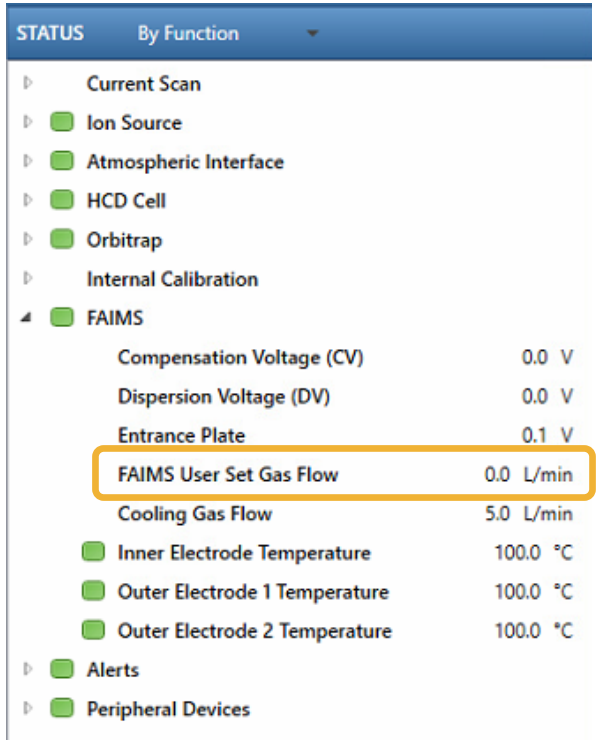
- The dependency on capillary temperature has been removed:
  - **Models OE 120, OE 240 -** Round bore ion transfer tube: 0.7 to 4.3 L/min, default: 1.2 L/min (e.g. Orbitrap Exploris 240, Orbitrap ID-X, TSQ Quantis)
  - **Model OE 480 -** Letterbox ion transfer tube: 3.5 to 7.7 L/min, default: 4.6 L/min (e.g. Orbitrap Exploris 480, Orbitrap Fusion Lumos, TSQ Altis)



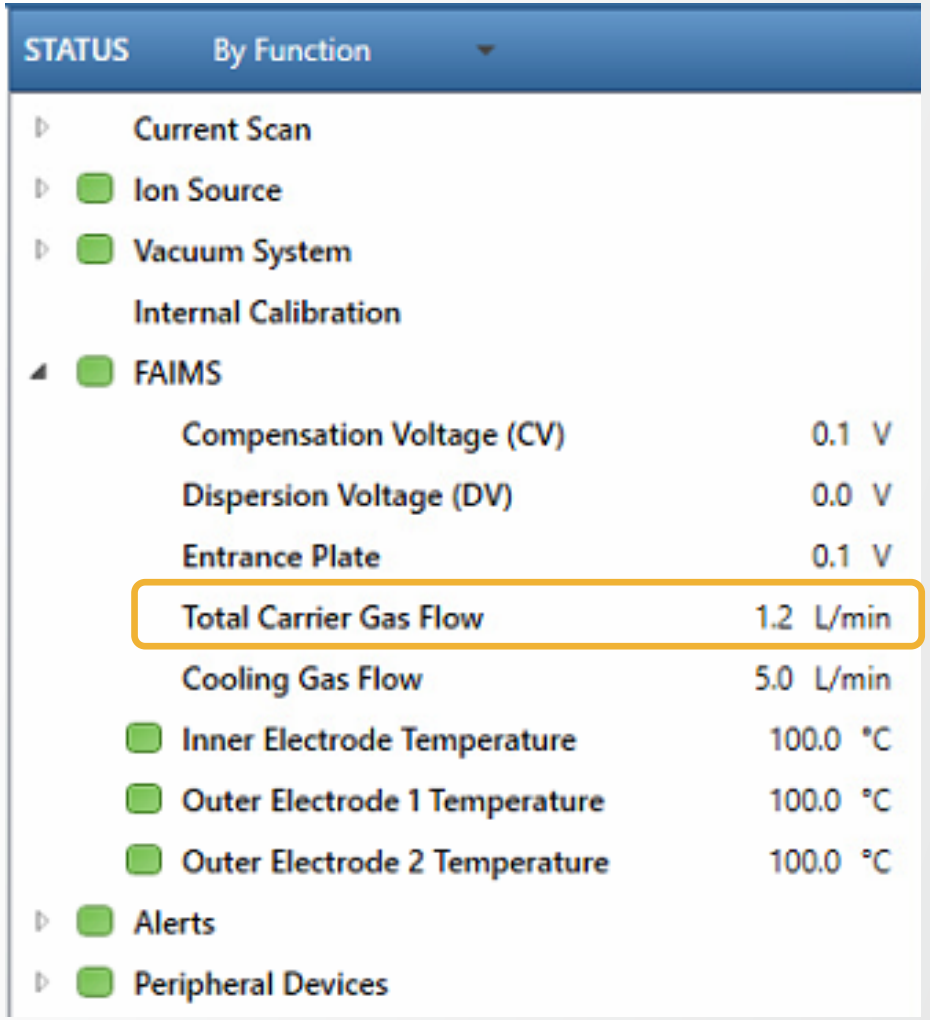
FAIMS Carrier Gas Update

Readbacks

Previously – with and until OES 2.0 SP2 ICSW:



New with OES 3.0 ICSW:



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:

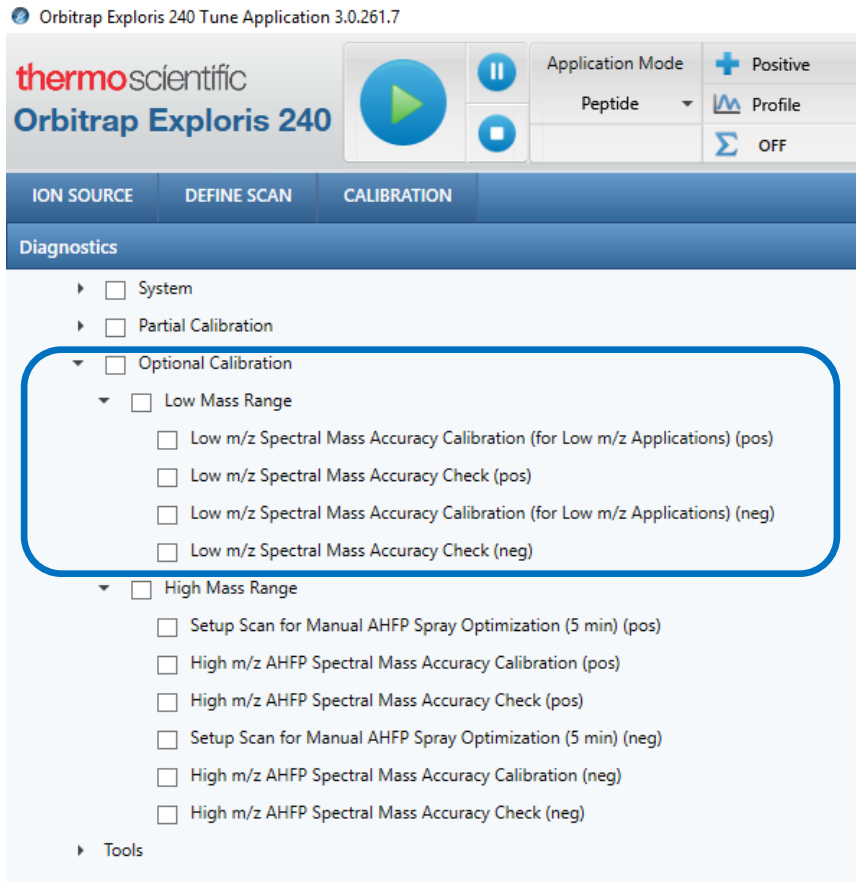
- OE 240, OES 2.0 method with FAIMS gas of 0 L/min will be converted to OE 480, OES 3.0 method with 'Total Carrier Gas Flow' of 4.6 L/min
- OE 240, OES 3.0 method with FAIMS gas of 1.1 L/min will be converted to OE 480, OES 3.0 method with 'Total Carrier Gas Flow' of 4.6 L/min
- OE 480, OES 3.0 method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

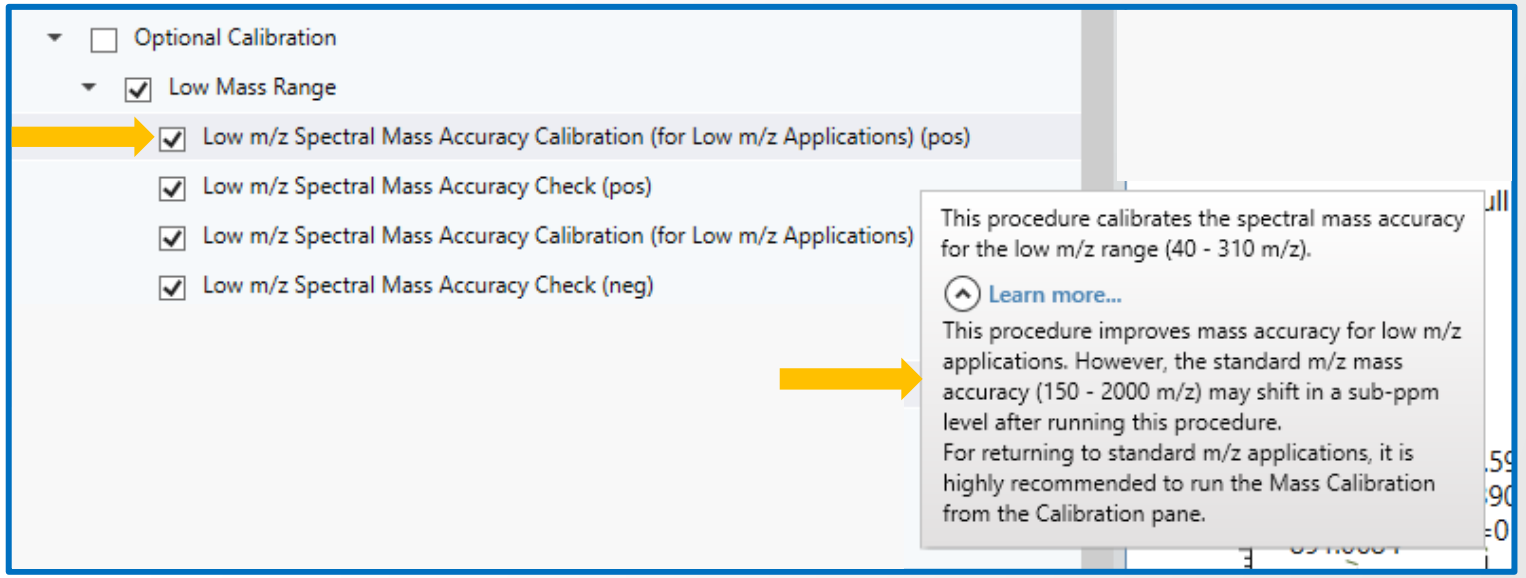
OES 3.0 ICSW – Tune Diagnostics / Optional Calibration

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

… 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





Note:

Per default, with the **System Calibration** in the tab **‚Calibration‘** the low masses are calibrated already.

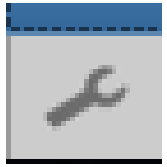
If there is particular need for high mass accurcay in the low mass range, then the here displayed **Optional Calibration** can be performed.

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.

This functionality is available for all Orbitrap Exploris models OE 120, OE 240, OE 480

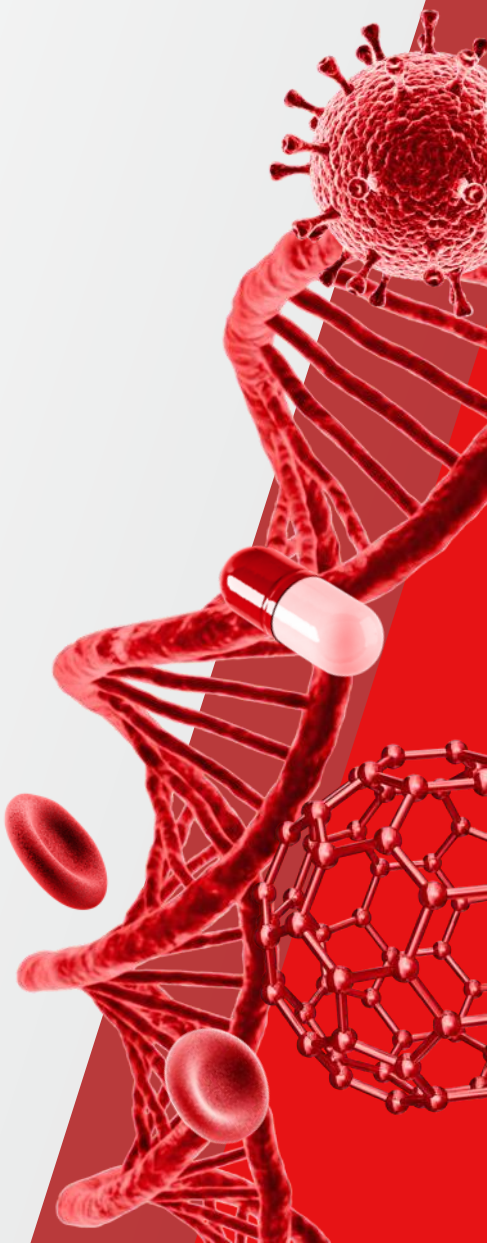
ThermoFisher SCIENTIFIC

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



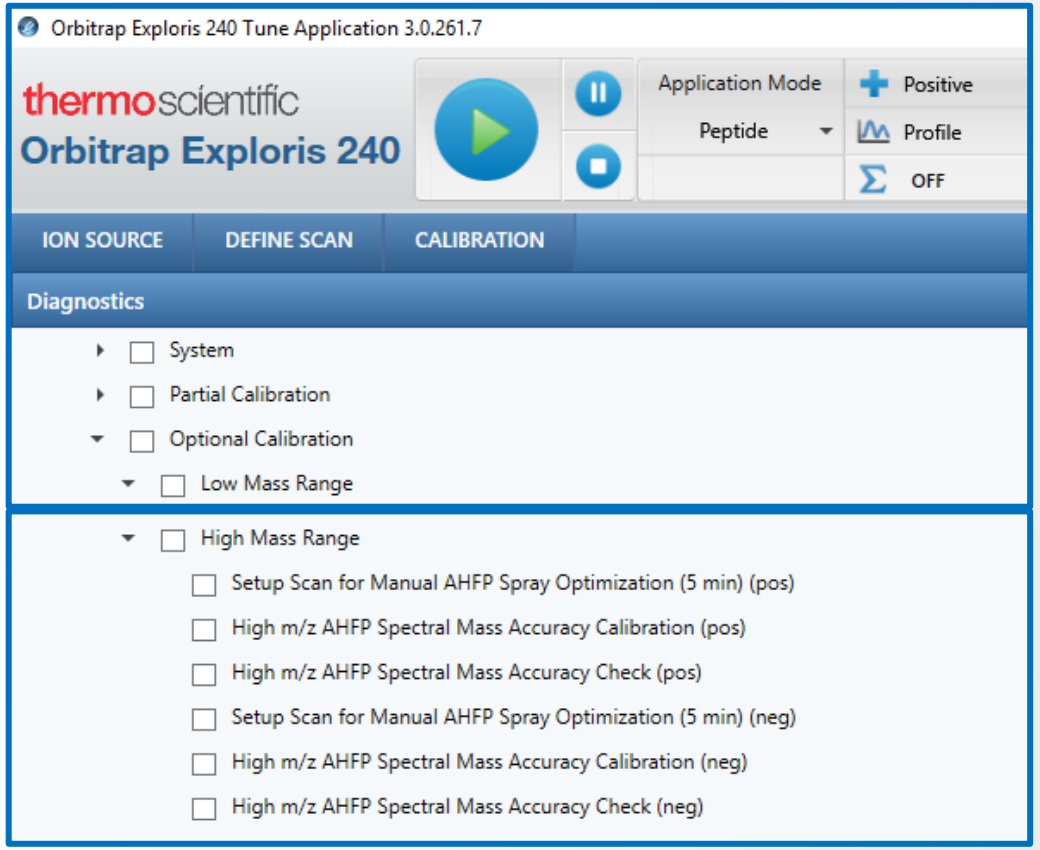
With OES 3.0 ICSW an improvement and a new feature is provided to meet the user's need in BioPharma applications better

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

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

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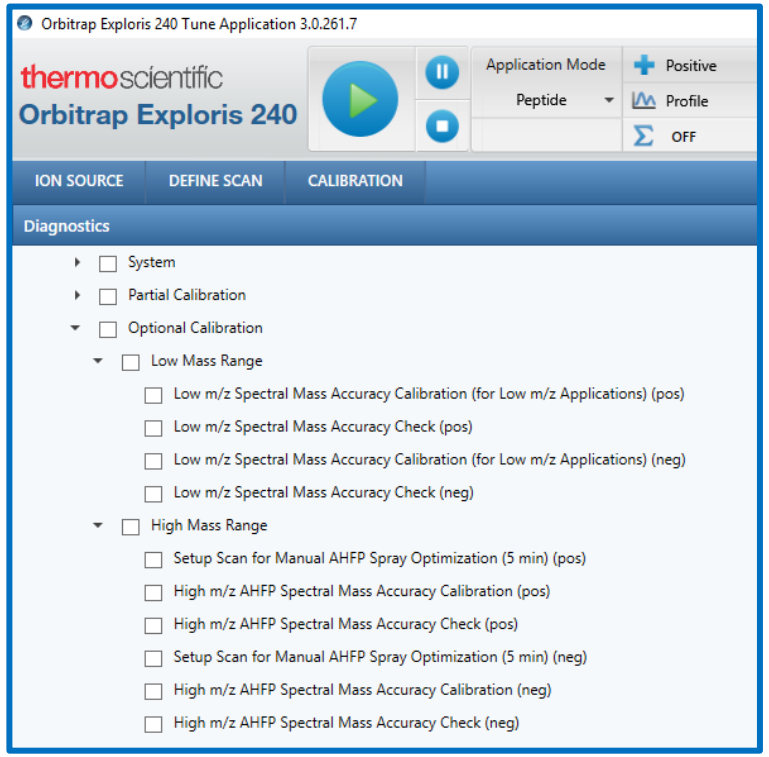
Find the wrench symbol in the bottom left corner of the Tune application to access Tune Diagnostics



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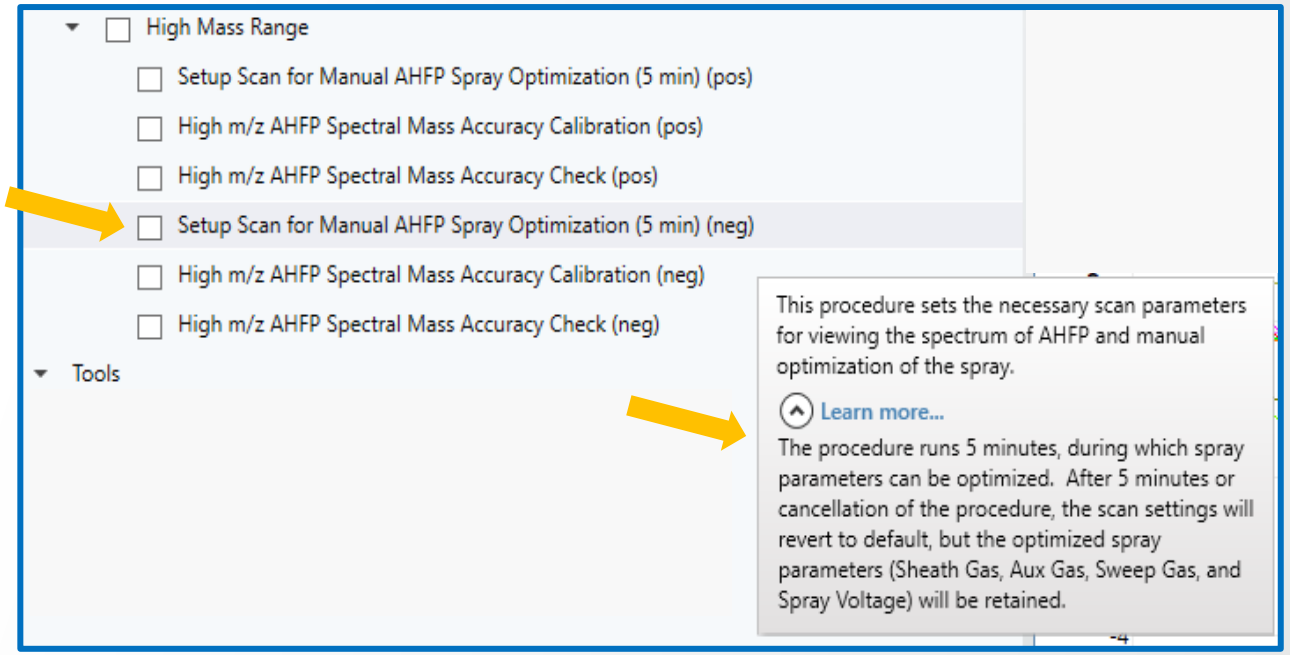

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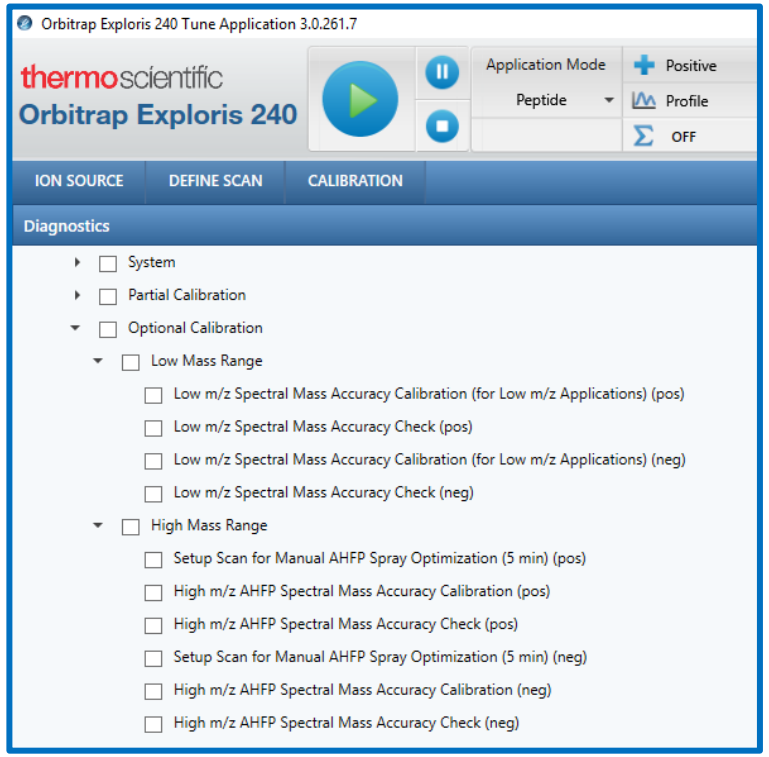

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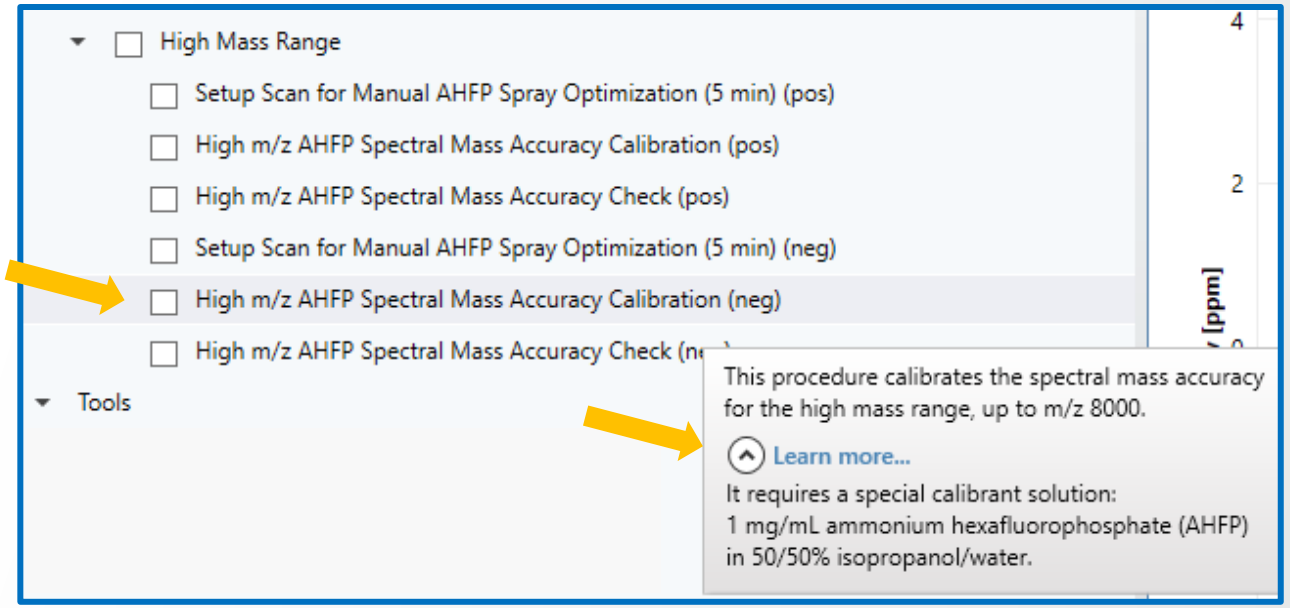

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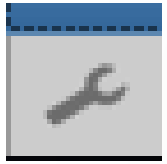

OES 3.0 ICSW – Tune Diagnostics / Partial Calibration - ‘Partial Calibration’ procedure menu

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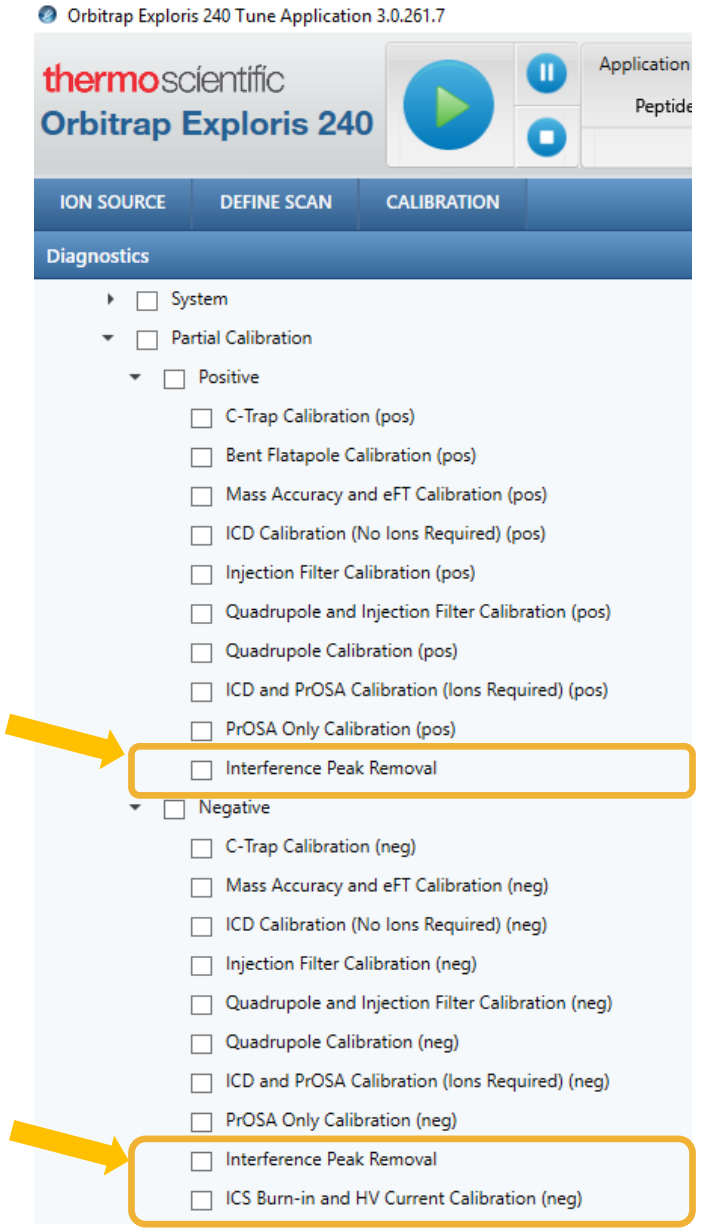
… provides restructured procedures separated by category and polarity



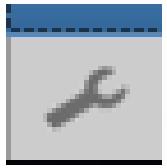
Find the wrench symbol in the bottom left corner of the Tune  application to access **Tune Diagnostics**

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.

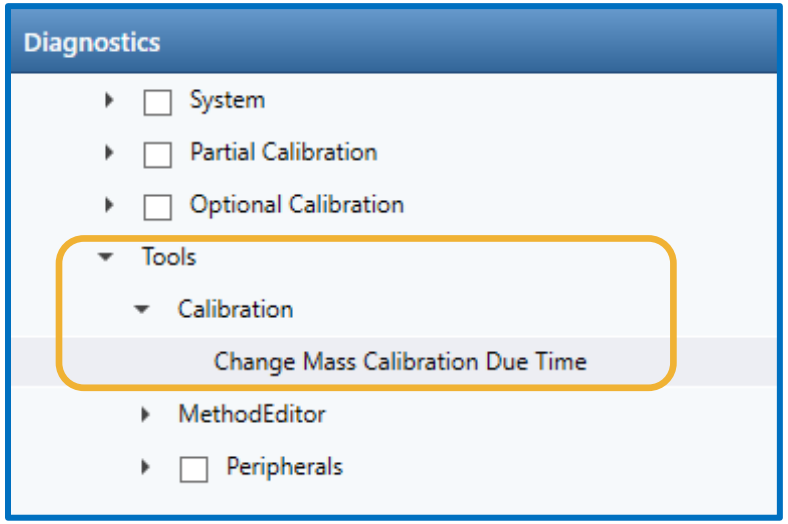


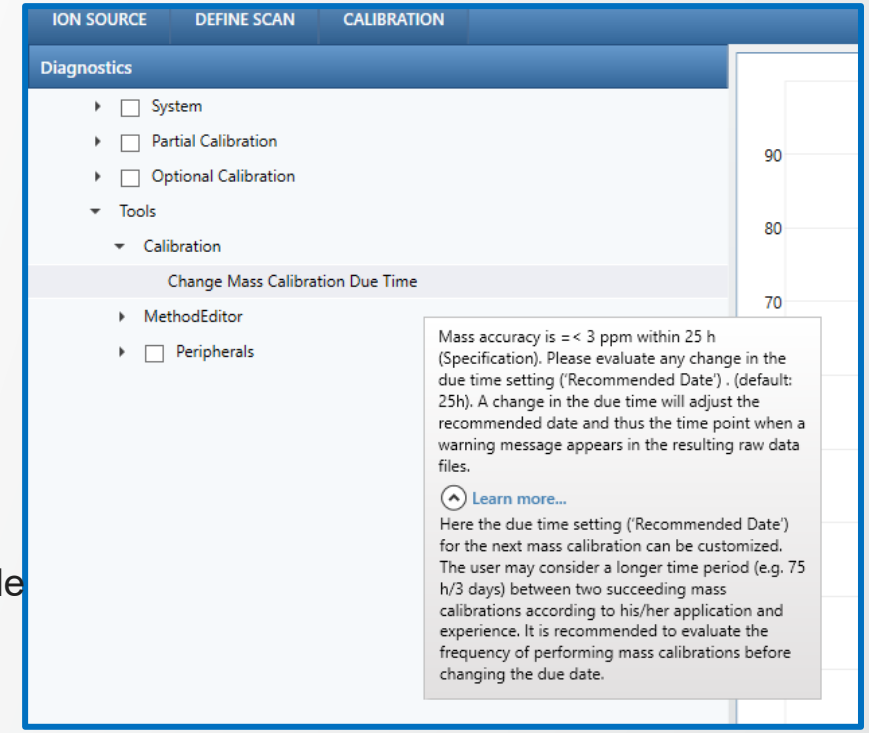
OES 3.0 ICSW – Tune Diagnostics / Tools

- mass calibration due time can be set by user

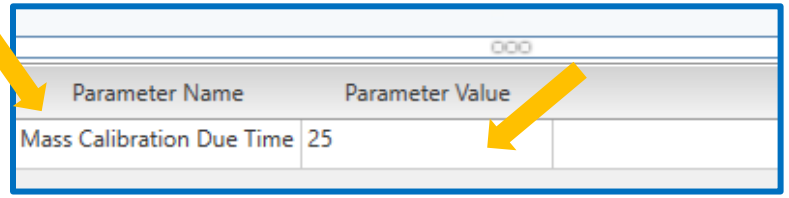
… provides a tool to change the Mass Calibration Due Time

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)

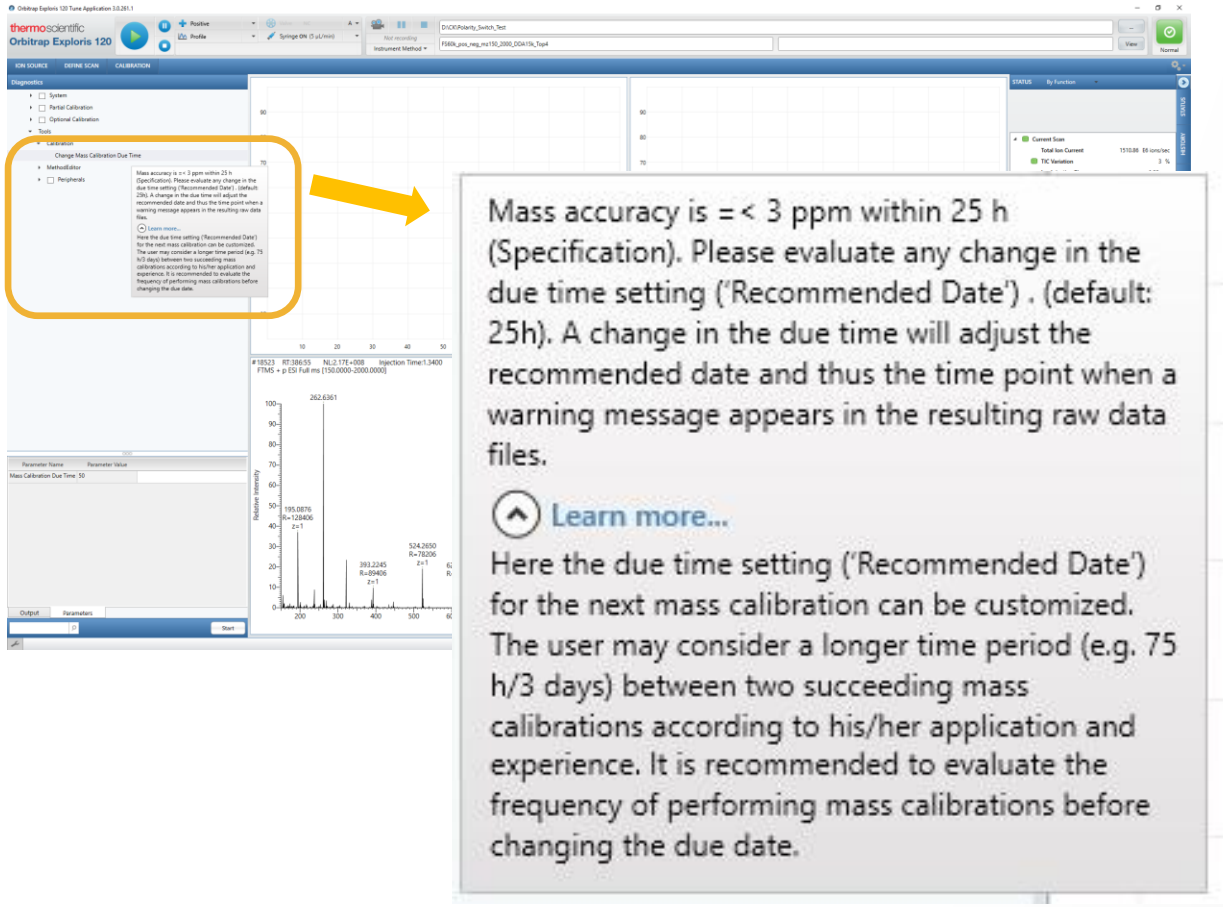


… see next slide for details

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

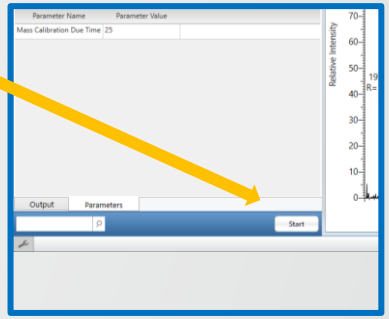
… provides a tool to change the Mass Calibration Due Time

Following up from previous slide



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.



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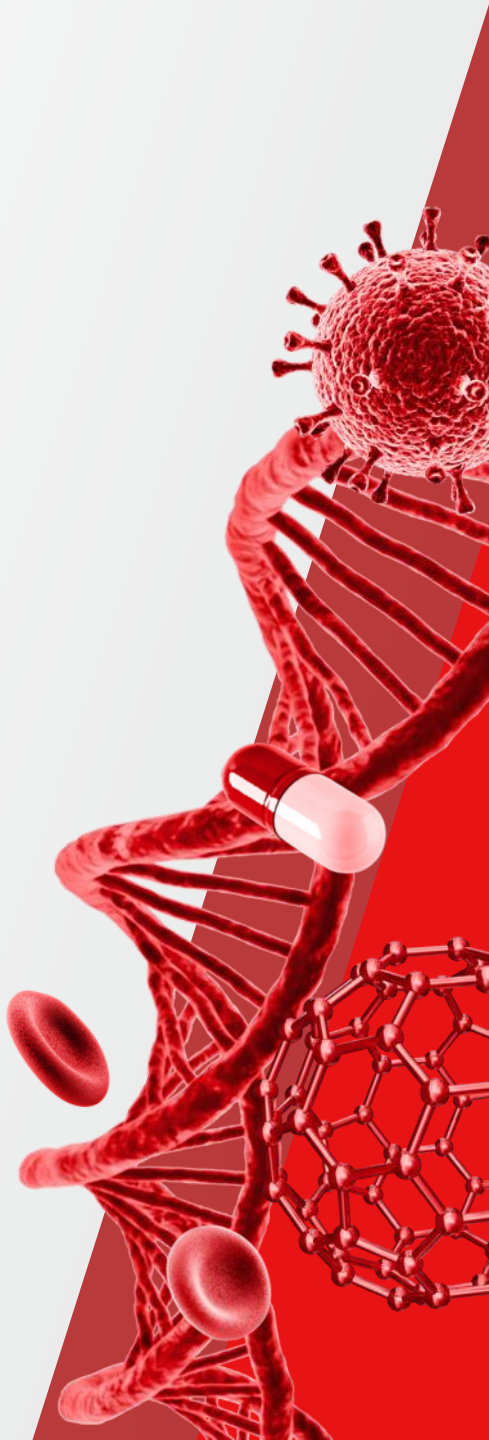
Further Improvements



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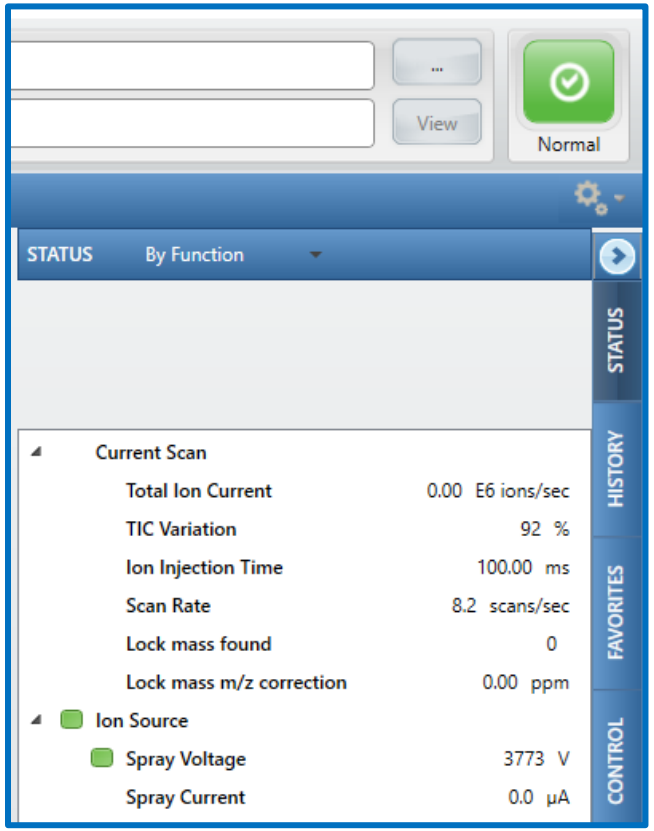
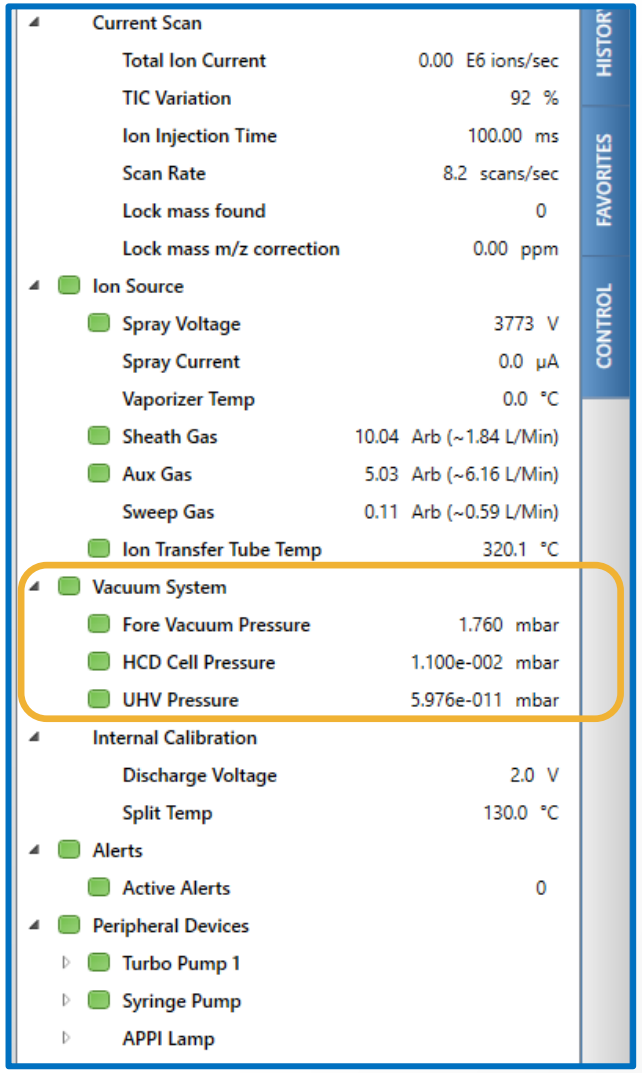
Further Improvements

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.

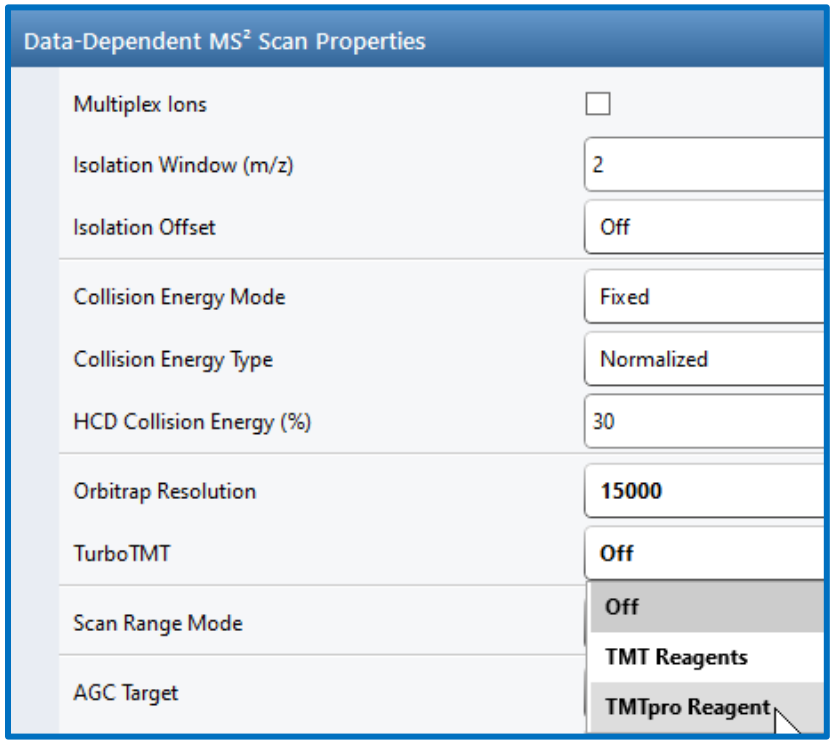
Background:

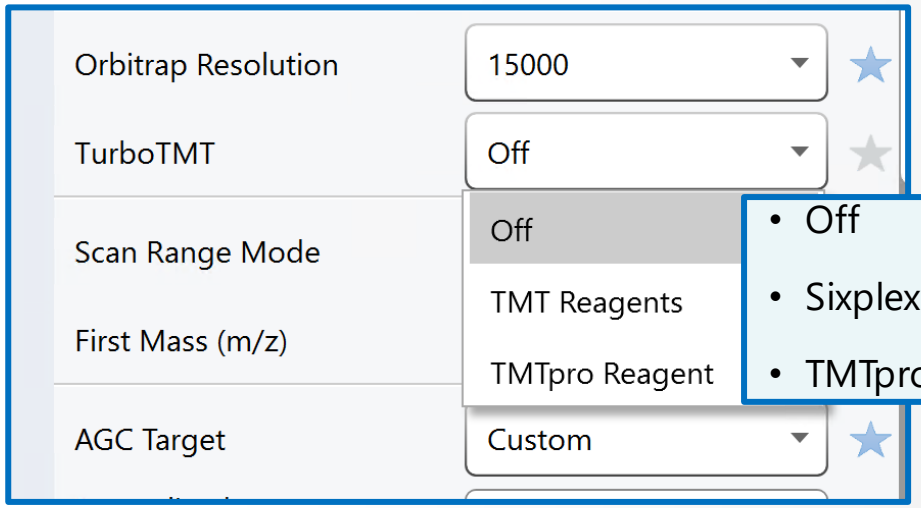
When the fore vacuum is too low, the ions are not cooled down enough in the bent flatapole region.
This may lead to more MS1 fragmentation influencing the MS2 spectral match.

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)





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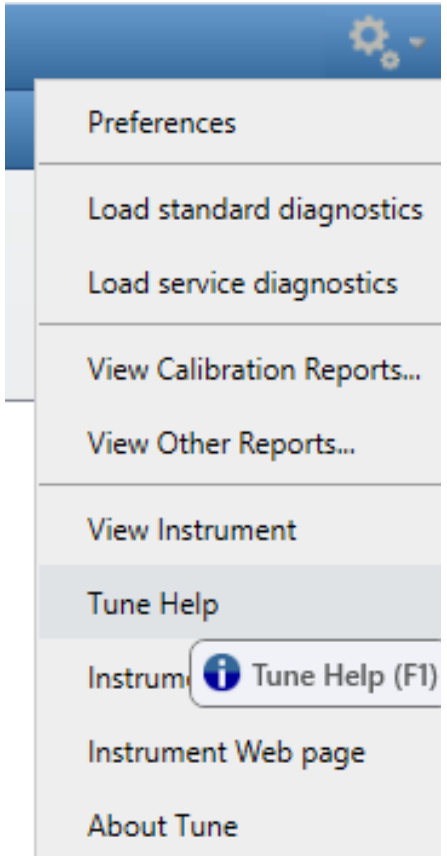
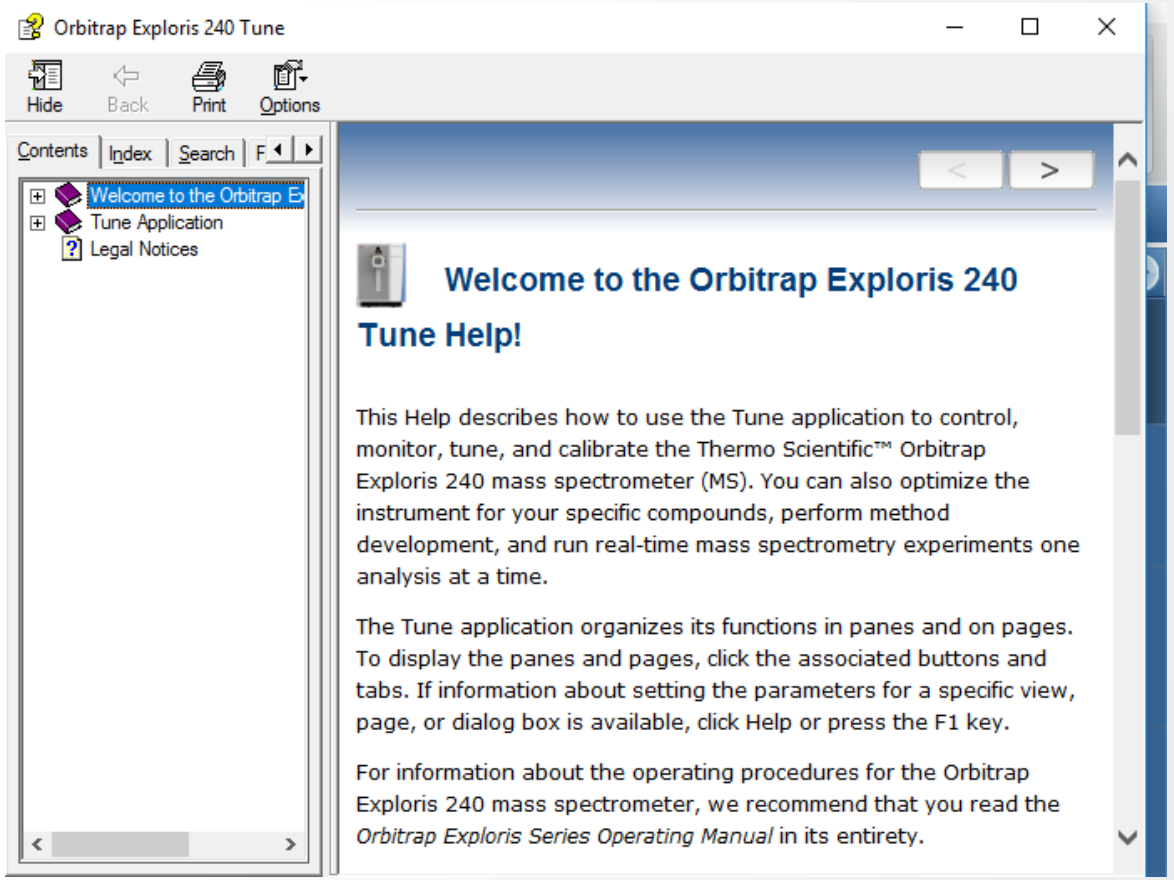
Software Manuals are part of the delivered iso-image and installed upon the installation procedure

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





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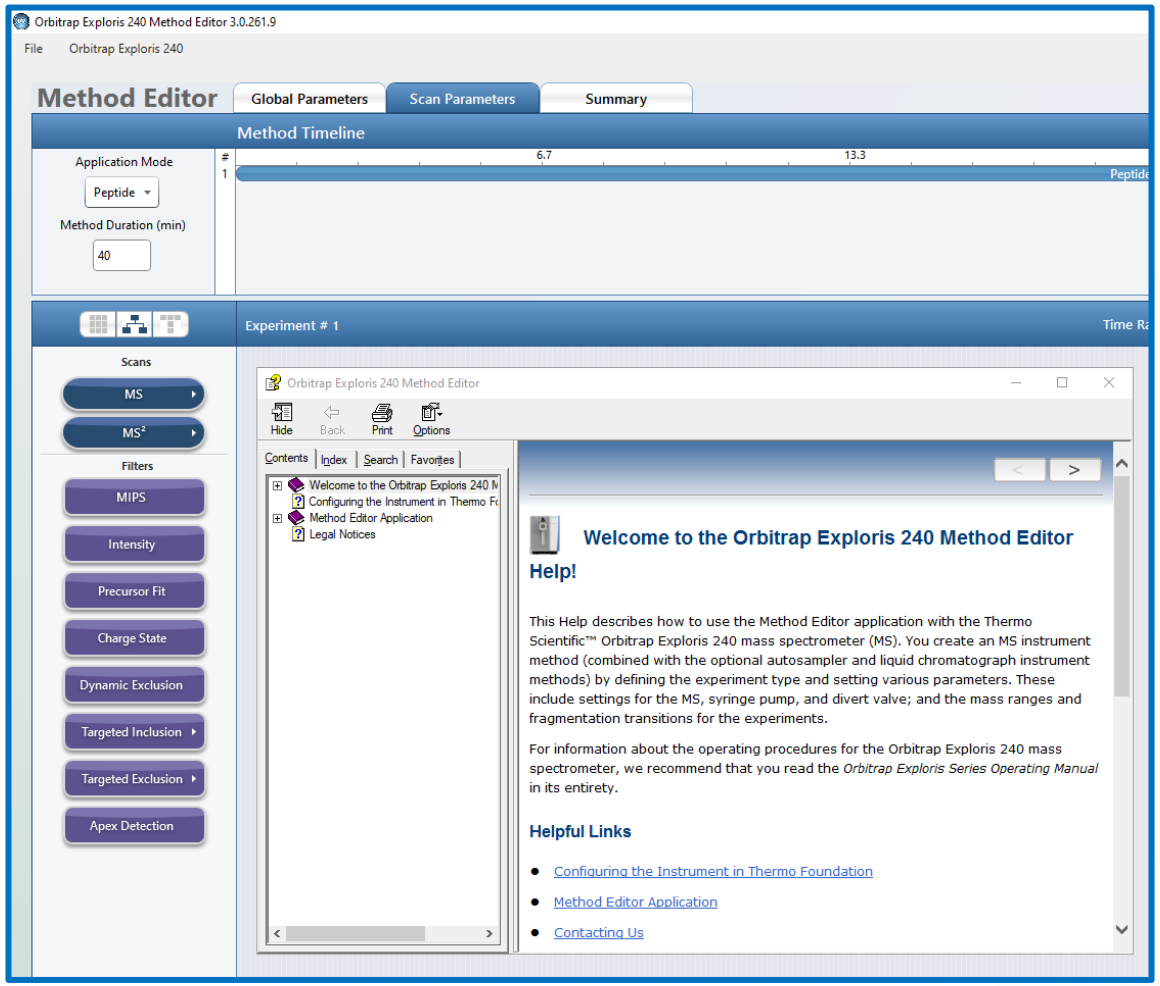

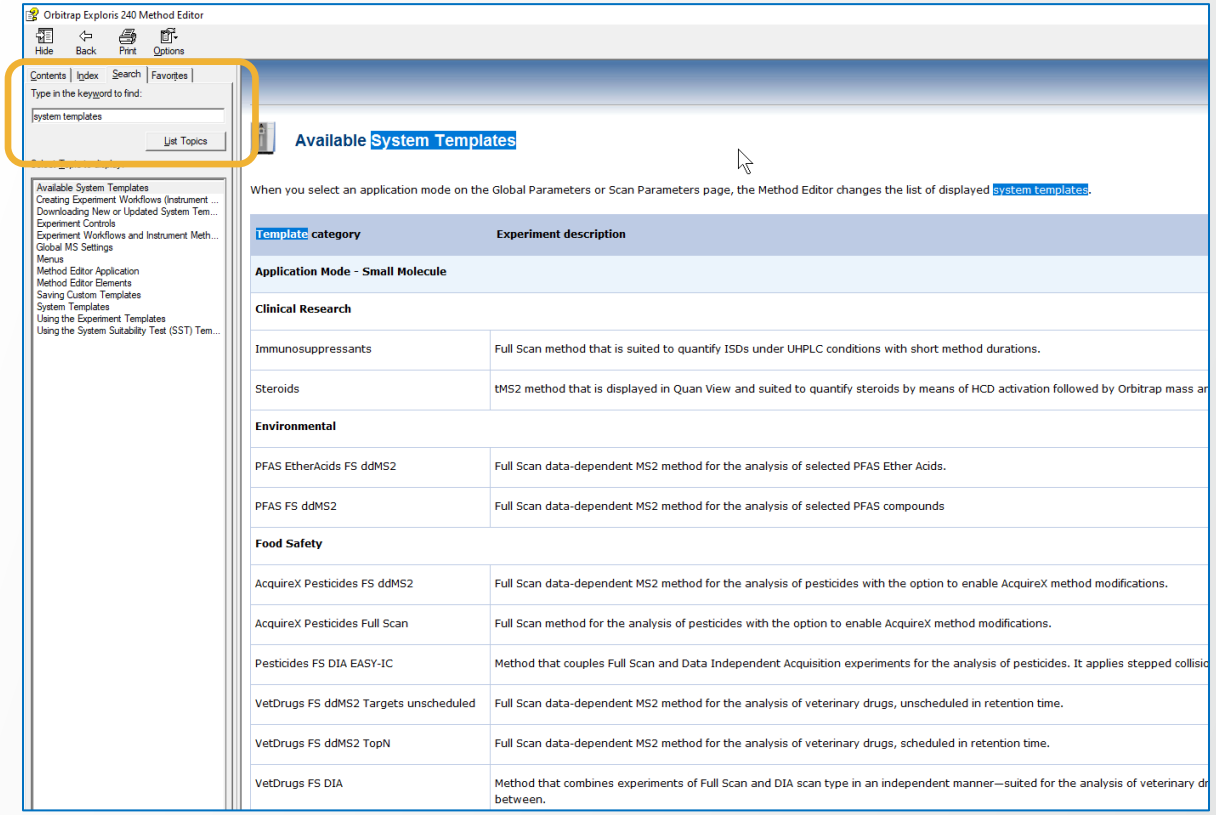

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