



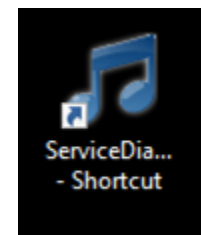
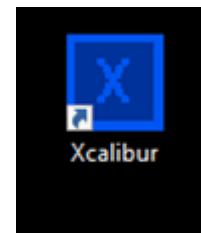
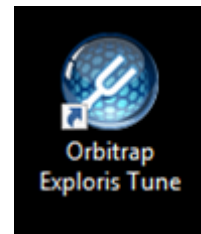
# Orbitrap Exploris 480 Software Introduction

Revision 00 – June 2019

Product Support  
Life Science Mass Spectrometry

# Software

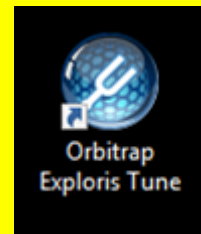
- Orbitrap Exploris Tune
  - Tune Software (similar to Fusion/Lumos)
- Xcalibur:
  - Method Editor
  - ...
- SDT Service Diagnostic Tool
  - Only for Service
  - Can be found in  
C:\Thermo\Instruments\Exploris\1.0\System\Programs



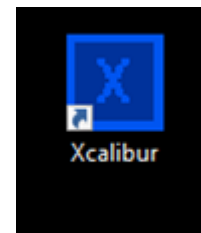
- Exactive Series: Instrument ID received from Embedded PC
  - Issue: when Embedded PC is exchanged, Instrument ID changes. FSE needs to renew licenses. FSE needs to adjust Tune files and master cal file (Diagnostics function “Adapt instrument ID”)
- Orbitrap Exploris 480: Framework ID (chip on HW framework)
  - User Roles in SDT and Licensing implementation is not fully defined, yet

# Software

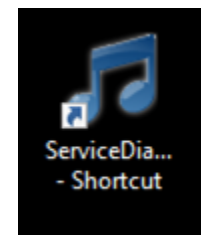
- Orbitrap Exploris Tune
  - Tune Software (similar to Fusion/Lumos)



- Xcalibur:
  - Method Editor
  - ...



- SDT Service Diagnostic Tool
  - Only for Service
  - Can be found in  
C:\Thermo\Instruments\Exploris\1.0\System\Programs



# Orbitrap Exploris 480 InstCtrl Software has the TNG User Interface

The screenshot displays the Thermo Scientific Orbitrap Exploris 480 InstCtrl software interface, which features a TNG (Thermo Navigator) User Interface. The interface is divided into several sections:

- Top Panel:** Includes the Thermo Scientific logo, application mode (Negative), ion source (Peptide), and various instrument parameters like spray voltage (2000 V) and spray gas flow (1.7 L/min).
- Left Panel:** Contains optimization settings for the ion source, including ion source type (NSI), spray voltage, spray gas flow, and ion transfer tube temperature.
- Center Panel:** Displays real-time data plots, including HF amplitude (1667.9 V), LF amplitude (3333.7 V), DV RF ramp check (Low field), and a mass spectrum plot showing relative intensity versus m/z.
- Right Panel:** Features the **Method Editor** with tabs for Global Parameters, Scan Parameters, and Summary. It includes a method timeline, application mode (Peptide), method duration (1 min), and a detailed scan sequence diagram showing a Full Scan followed by two ddMS<sup>2</sup> scans (10 scans and 5 scans).
- Bottom Right Panel:** Shows data-dependent MS<sup>2</sup> scan properties, including scan priority (2), isolation window (m/z), HCD collision energy type (Normalized), HCD collision energy (%), Orbitrap resolution (15000), enhanced resolution mode (TMT Reporter Ions), scan range mode (Auto), maximum injection time mode (Custom), and maximum injection time (ms).

The interface is designed for configuring and controlling the Orbitrap Exploris 480 mass spectrometer, providing a comprehensive view of instrument parameters and data acquisition results.

# No Tune Files

| ION SOURCE                                                      |      |       |
|-----------------------------------------------------------------|------|-------|
| Current LC Flow (µL/min)                                        | 0    |       |
| <button>Get Defaults</button>                                   |      |       |
| Ion Source Type: Heated ESI                                     |      |       |
| Pos Ion Spray Voltage ( V )                                     | 3800 | 46    |
| Neg Ion Spray Voltage ( V )                                     | 3000 |       |
| Sheath Gas (Arb)                                                | 10   | 0.00  |
| Aux Gas (Arb)                                                   | 0    | 0.00  |
| Sweep Gas (Arb)                                                 | 0    | 0.00  |
| <input checked="" type="checkbox"/> Ion Transfer Tube Temp (°C) | 350  | 350.0 |
| Vaporizer Temp (°C)                                             | 0    | 44.6  |

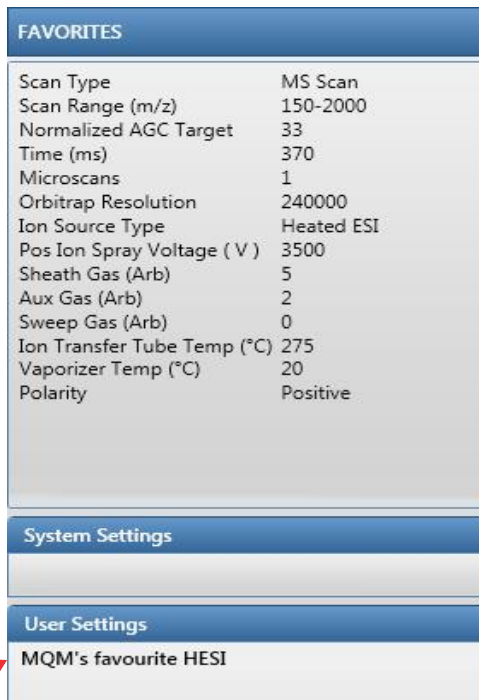
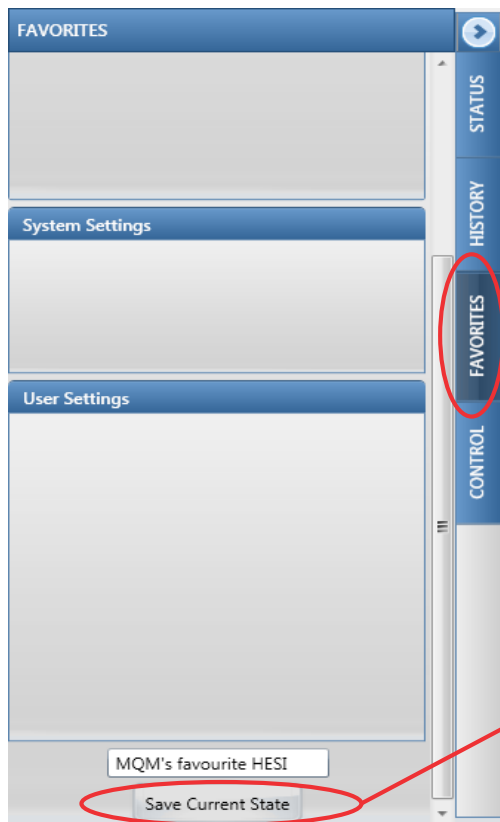
**Finally  
polarity  
independent**

Apply

- Ion Source settings are now part of the instrument method
- Tune file still exists historically, but user has no access and cannot modify
- Gas consumption read back in Status pane

| STATUS                 |  | By Function            |  |
|------------------------|--|------------------------|--|
| Ion Source             |  |                        |  |
| Spray Voltage          |  | 3762 V                 |  |
| Spray Current          |  | 2.0 µA                 |  |
| Vaporizer Temp         |  | 43.0 °C                |  |
| Sheath Gas             |  | 9.67 Arb (~1.63 L/Min) |  |
| Aux Gas                |  | 4.99 Arb (~5.07 L/Min) |  |
| Sweep Gas              |  | 2.03 Arb (~2.75 L/Min) |  |
| Ion Transfer Tube Temp |  | 349.6 °C               |  |
| Fore Vacuum Pressure   |  | 2.000 mbar             |  |

# Missing Tune files – Really?



- Ion Source settings are a **global instrument method parameter**
- **Favorites** allow for saving, deleting, loading, applying **ion source and scan settings**

# Orbitrap Exploris Tune: UI Elements

The screenshot displays the Orbitrap Exploris Tune software interface, which is organized into several functional areas:

- Power Icons:** Located at the top left, this section includes a large green play button and a red stop button.
- Instrument buttons:** This area contains controls for the instrument's state, including a dropdown menu for 'Positive', 'Profile', and 'OFF', and a 'Syringe ON (5 µL/min)' button.
- Data Acquisition buttons:** This section includes a 'Record' button, a file path input field (c:\Thermo\Data), and buttons for 'Rawdata', 'View', and 'Normal'.
- Status Icons:** A green checkmark icon indicating the system is 'Normal'.
- Panes:** The left sidebar contains several panes for configuration, including 'ION SOURCE', 'DEFINE SCAN', and 'CALIBRATION'. The 'DEFINE SCAN' pane is currently active, showing settings for 'View Type' (Qual View), 'Scan Type' (MS Scan), 'Orbitrap Resolution', 'Scan Range (m/z)' (150 - 2000), 'RF Lens (%)' (70), 'AGC Target' (Standard), 'Maximum Injection Time' (Custom), 'Time (ms)' (370), 'Microscans' (1), and 'Source Fragmentation'.
- Easy Access Ribbon:** A horizontal ribbon at the top of the main workspace area.
- Chromatogram / Plotting Views:** The main workspace displays two plots: a chromatogram showing relative intensity versus time (m/z) and a spectrum view showing relative intensity versus m/z.
- Spectrum View:** The bottom plot shows a mass spectrum with peaks labeled with their m/z values and relative intensities. Key peaks include 524.1755 (R=156506, z=1), 731.8350 (R=123606, z=1), 921.8538 (R=113706, z=1), 1121.8075 (R=106206, z=1), 1321.7612 (R=98506, z=1), 1521.7153 (R=91606, z=1), 1721.6700 (R=85706, z=1), and 1921.6252 (R=80306, z=1).
- Options Help About...:** A vertical menu on the right side of the interface, accessible via a gear icon.
- Graph Modes:** A set of icons at the bottom right of the interface, used to switch between different graphing modes.
- Diagnostics Pane:** A small icon at the bottom left of the interface, used to access diagnostic tools.

# Orbitrap Exploris Tune: Status Icons



Normal



Changing Settings



Source Off



Error



Initializing



Disconnected

**Source Off** - grey: This indicates that the ion source is not connected.

**Disconnected** - grey: This indicates that the instrument is disconnected from the Data System PC.

**Initializing** - green (while instrument is booting)

**Normal** - green

**Changing** - orange: This indicates that a new Tune value was set, but the readback is not achieved, yet.

**Error** - red (Readback errors are mapped)

**Warning** - yellow (warnings from alert window mapped to Status Control)

# Orbitrap Exploris Tune: Instrument Status Pane

The screenshot displays the 'STATUS' pane of the Orbitrap Exploris Tune software, which is organized into two main columns: 'By Function' and 'By Board'. A red dashed line highlights the left sidebar and the main content area.

**Left Sidebar (Callouts):**

- Status Icons:** A green checkmark icon labeled 'Normal'.
- Options Help About...:** A gear icon for settings.
- Panes:** A vertical menu with buttons for STATUS, HISTORY, FAVORITES, and CONTROL.
- Graph Modes:** A row of icons for different data visualization modes.

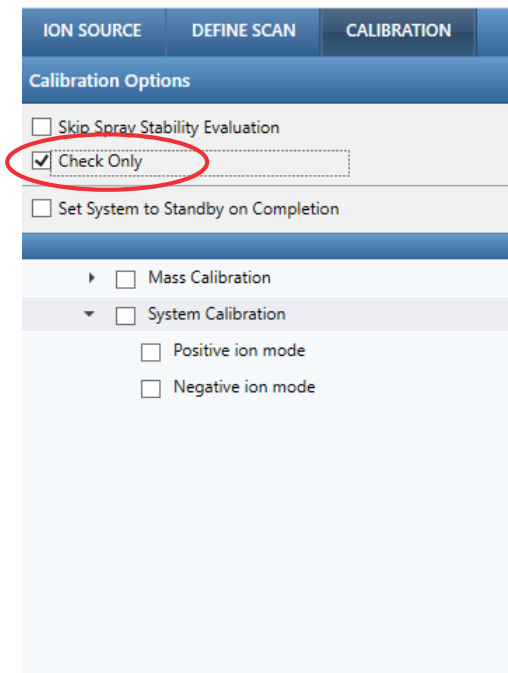
**Main Content Area (Callouts):**

- STATUS By Function:**
  - Current Scan
  - Ion Source
    - Spray Voltage
    - Spray Current
    - Vaporizer Temp
    - Sheath Gas
    - Aux Gas: 0
    - Sweep Gas: 0
    - Ion Transfer Tube Temp
  - Fore Vacuum Pressure
  - HCD Cell
    - HCD Cell Pressure
  - Orbitrap
    - UHV Pressure
  - Peripheral Devices
- STATUS By Board:**
  - Instrument Control
    - Fore Vacuum Pressure
    - HCD Cell Pressure
    - UHV Pressure
  - Source
    - Spray Voltage
    - Spray Current
    - Vaporizer Temp
    - Sheath Gas
    - Aux Gas: 0.13
    - Sweep Gas: 0.02
    - Ion Transfer Tube Temp
    - Discharge Voltage
    - Split Temp
  - Peripheral Devices
    - Turbo Pump 1
    - Syringe Pump
    - APPI Lamp

The 'CONTROL' pane displays a summary of instrument performance. It includes a status bar at the top with an information icon and the text 'Instrument Performance - Affected: MS M'. Below this, a vertical sidebar on the right contains buttons for STATUS, HISTORY, FAVORITES, and CONTROL.

# Calibrations and Checks

- Each Orbitrap Exploris Tune Calibration is accompanied by a Check procedure
- “Check Only” toggle enables Evaluation only, i.e. skips Calibration



The screenshot shows a software interface with three tabs at the top: 'ION SOURCE', 'DEFINE SCAN', and 'CALIBRATION'. The 'CALIBRATION' tab is selected. Below the tabs is a section titled 'Calibration Options'. This section contains three checkboxes: 'Skip Spray Stability Evaluation' (unchecked), 'Check Only' (checked and highlighted with a red circle), and 'Set System to Standby on Completion' (unchecked). Below these options is a blue bar, followed by a section with two expandable/collapsible items: 'Mass Calibration' (expanded, showing an unchecked checkbox) and 'System Calibration' (collapsed, showing a dropdown arrow and an unchecked checkbox). Under 'System Calibration', there are two more unchecked checkboxes: 'Positive ion mode' and 'Negative ion mode'.

# Diagnostics

- IF one or more of the checks OR calibrations are failing you can rerun these particular procedures using "Examine Failed Sub-Procedures" in the Diagnostics Pane

ION SOURCE DEFINE SCAN CALIBRATION

Calibration Options

☐ Skip Spray Stability Evaluation

☒ Check Only

☐ Set System to Standby on Completion

▸ ☐ Mass Calibration

▾ ☐ System Calibration

☐ Positive ion mode

☐ Negative ion mode

ION SOURCE DEFINE SCAN CALIBRATION

Diagnostics

▾ ☐ System

☐ Bake Vacuum Chamber

☒ Examine Failed Sub-Procedure

☐ Ion Optics Connectivity Check

☐ Transfer Tube Maintenance Check

☐ Ion Optics Maintenance Check

☐ Quadrupole Maintenance Check

▾ ☐ FAIMS

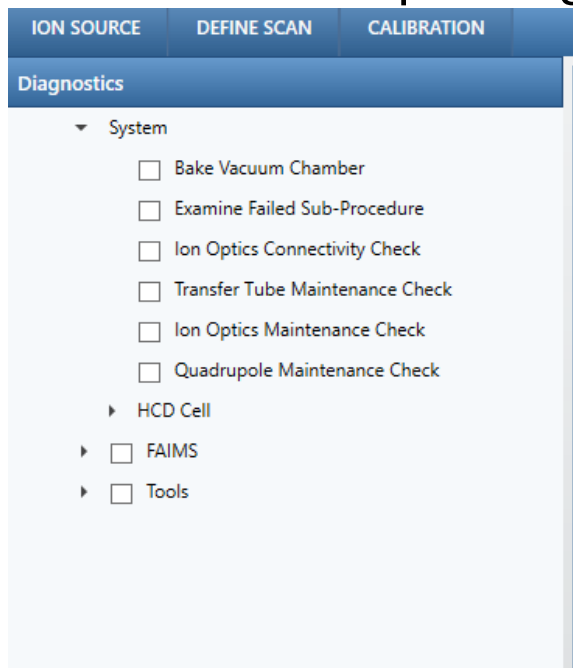
☐ DV Check

☐ DV Tune

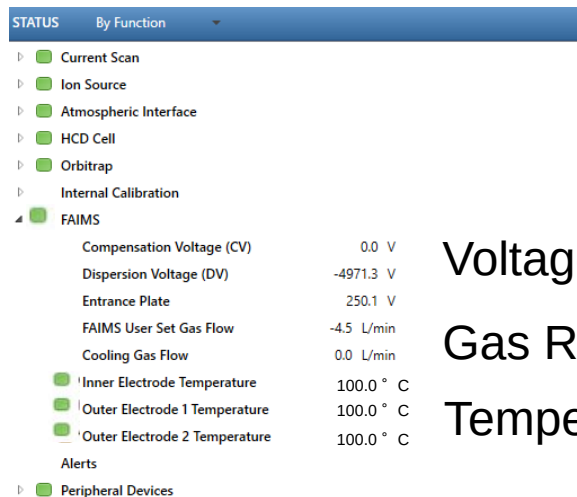
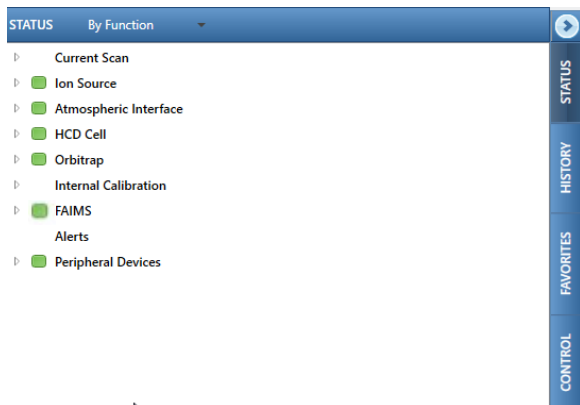
▾ ☐ Tools

▸ ☐ Peripherals

- In Orbitrap Exploris Tune, Diagnostics procedures are provided separately (i.e. procedures w/o corresponding Calibration procedure)



- FAIMS Readback in the Status Tree



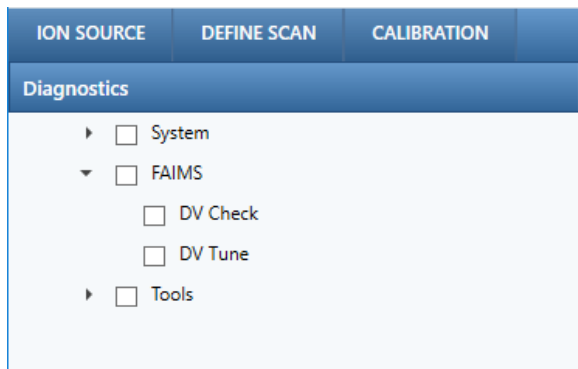
Voltage Readback

Gas Readback

Temperature Readbacks

# FAIMS Calibration

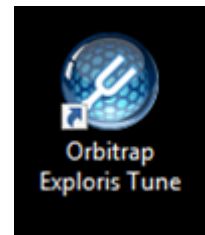
- You can find the calibration in the Diagnostics area of the software



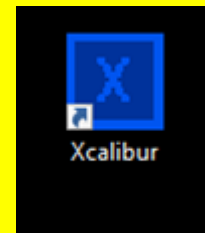
- The DV Tune has to be done:
  - After installation
  - After cleaning
  - After changing the kind of ion source

# Software

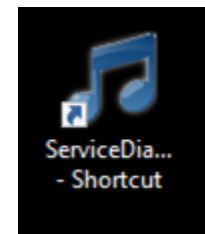
- Orbitrap Exploris Tune
  - Tune Software (similar to Fusion/Lumos)



- Xcalibur:
  - Method Editor
  - ...



- SDT Service Diagnostic Tool
  - Only for Service
  - Can be found in  
C:\Thermo\Instruments\Exploris\1.0\System\Programs



# Orbitrap Exploris Tune



**Settings**

|                            |                       |
|----------------------------|-----------------------|
| Infusion Mode              | Liquid Chromatography |
| Expected LC Peak Width (s) | 30                    |
| Internal Mass Calibration  | Off                   |

**Targeted SIM Scan Properties** [Show Favorites](#)

|                             |                          |   |
|-----------------------------|--------------------------|---|
| Multiplex Ions              | <input type="checkbox"/> | ★ |
| Isolation Window (m/z)      | 2                        | ★ |
| Orbitrap Resolution         | 60000                    | ★ |
| RF Lens (%)                 | 70                       | ★ |
| Maximum Injection Time Mode | Auto                     | ★ |
| Data Type                   | Profile                  | ★ |
| Polarity                    | Positive                 | ★ |
| Source Fragmentation        | <input type="checkbox"/> | ★ |
| Time Mode                   | Retention Time Window    | ★ |

▲ Select table icon to define the property per row

**Settings**

|                           |          |
|---------------------------|----------|
| Infusion Mode             | Infusion |
| Internal Mass Calibration | Off      |

**Targeted SIM Scan Properties** [Show Favorites](#)

|                             |                          |   |
|-----------------------------|--------------------------|---|
| Multiplex Ions              | <input type="checkbox"/> | ★ |
| Isolation Window (m/z)      | 2                        | ★ |
| Orbitrap Resolution         | 60000                    | ★ |
| RF Lens (%)                 | 70                       | ★ |
| Maximum Injection Time Mode | Auto                     | ★ |
| Data Type                   | Profile                  | ★ |
| Polarity                    | Positive                 | ★ |
| Source Fragmentation        | <input type="checkbox"/> | ★ |
| Time Mode                   | Retention Time Window    | ★ |

▲ Select table icon to define the property per row

# Orbitrap Exploris Tune

- Possibility to show and enable/disable favorites<sup>1</sup>
- Possibility to define settings in the table

**Settings**

Infusion Mode: Liquid Chromatography  
Expected LC Peak Width (s): 30  
Internal Mass Calibration: Off

**Targeted SIM Scan Properties** <sup>1</sup> [Show Favorites](#)

<sup>2</sup> Multiplex Ions ☐ <sup>1</sup>

<sup>2</sup> Isolation Window (m/z): 2 <sup>1</sup>

Orbitrap Resolution: 60000

RF Lens (%): 70

Maximum Injection Time Mode: Auto

Data Type: Profile

Polarity: Positive

Source Fragmentation: ☐

Time Mode: Retention Time Window

Select table icon to define the property per row

**Targeted SIM Scan Properties** <sup>1</sup>

☒ Enable Recommendations  
☒ Enable Favorites  
Restore Advanced Template Messages

Multiplex Ions ☐

Isolation Window (m/z): 2

Orbitrap Resolution: 60000

RF Lens (%): 70

Maximum Injection Time Mode: Auto

Data Type: Profile

Polarity: Positive

Source Fragmentation: ☐

Time Mode: Retention Time Window

Select table icon to define the property per row

<sup>2</sup> Select table icon to define the property per row

| Mass List Table |          |           |        |          |   |             |
|-----------------|----------|-----------|--------|----------|---|-------------|
|                 | Compound | Formula   | Adduct | m/z      | z | RT Time (m) |
| 1               | Caffeine | C8H10N4O2 | +H     | 195.0877 | 1 | 30          |

# (Orbitrap Exploris Tune) Method Editor: Overview

**Method Editor** | Global Parameters | Scan Parameters | Summary

Methc 1 line | Experiment | ACTIONS | Settings

Method Duration (min): 60

Global Parameters

Ion Source Properties

Ion Source Type: H-ESI

Spray Voltage: Static

Positive Ion (V): 3500

Negative Ion (V): 2500

Sheath Gas (Arb): 2

Aux Gas (Arb): 2

Sweep Gas (Arb): 2

Ion Transfer Tube Temp (°C): 275

Vaporizer Temp (°C): 0

APPI Lamp: Not in Use

Use Ion Source Settings from Tune: ☐

FAIMS Mode: Not Installed

## Method Editor tabs:

1. Global Parameters
2. Scan Parameters
3. Summary Page

# (Orbitrap Exploris Tune) Method Editor: Global Parameters

**Method Editor** | Global Parameters | Scan Parameters | Summary

**Method Timeline** | Experiment | ACTIONS | Settings

Method Duration (min): 60

**Global Parameters**

1. Ion Source

2. Syringe

3. Divert Valve A

4. Divert Valve B

5. Contact Closure

**Ion Source Properties**

- Ion Source Type: H-ESI
- Spray Voltage: Static
- Positive Ion (V): 3500
- Negative Ion (V): 2500
- Sheath Gas (Arb): 2
- Aux Gas (Arb): 2
- Sweep Gas (Arb): 2
- Ion Transfer Tube Temp (°C): 275
- Vaporizer Temp (°C): 0
- APPI Lamp: Not in Use
- Use Ion Source Settings from Tune: ☐
- FAIMS Mode: Not Installed

## Global Parameters:

1. Ion Source Properties
2. Syringe Properties
3. Divert Valve A Properties
4. Divert Valve B Properties
5. Contact Closure Properties

# (Orbitrap Exploris Tune) Method Editor: Global Method Settings

**Method Editor** | Global Parameters | **Scan Parameters** | Summary

**Method Timeline** | Experiment | ACTIONS | Settings

Method Duration (min): 60

Infusion Mode: Liquid Chromatography  
Expected LC Peak Width (s): 30  
Internal Mass Calibration: Off

Experiment # 1 | Time Range (min): 0-60

Place Scan Here

Scans:

- SRM Scan
- Full Scan
- Product Ion Scan
- SIM Scan
- DIA Scan

Properties

## Scan Parameters:

1. Global Method Settings:
  - Method Duration (min)
  - Method Timeline
  - Infusion Mode
  - Expected LC Peak Width (s)
  - Internal Mass Calibration
2. Experiment Pane View Types:
  - a. Quan View
  - b. Qual View
  - c. Template View

# (Orbitrap Exploris Tune) Method Editor: Experiment Pane View Types

The screenshot displays the Method Editor interface with three experiment pane view types highlighted by yellow circles and labels:

- 1. Global Method Settings:** Located at the top of the interface, including tabs for Global Parameters, Scan Parameters, and Summary. The Scan Parameters tab is active, showing a Method Timeline and various settings like Infusion Mode, Peak Width (s), and Internal Mass Calibration.
- 2. Experiment Pane View Types:** Located on the left side of the interface, showing a list of view types: Scans, SRM Scan, Full Scan, Product Ion Scan, SIM Scan, and DIA Scan.
- a. Scans:** A view type showing a list of scan types: SRM Scan, Full Scan, Product Ion Scan, SIM Scan, and DIA Scan.
- b. Filters:** A view type showing a list of filter types: MS, MS<sup>2</sup>, Intensity, Charge State, Dynamic Exclusion, Targeted Mass, Targeted Mass Exclusion, and Apex Detection.
- c. System Templates:** A view type showing a list of system templates: ISDs, Steroids, Vetdrug Explorer, Pharmaceuticals, and Custom Templates (My Experiments).

## Scan Parameters:

- Global Method Settings:
  - Application Mode
  - Method Duration (min)
  - Method Timeline
  - Infusion Mode
  - Expected LC Peak Width (s)
  - Internal Mass Calibration
- Experiment Pane View Types:
  - Quan View
  - Qual View
  - Template View

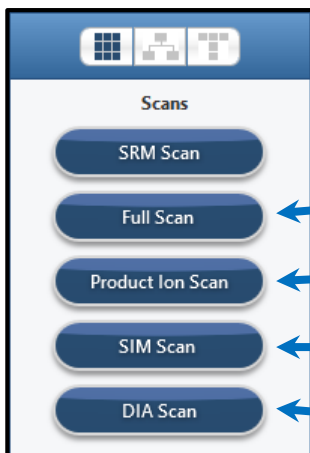
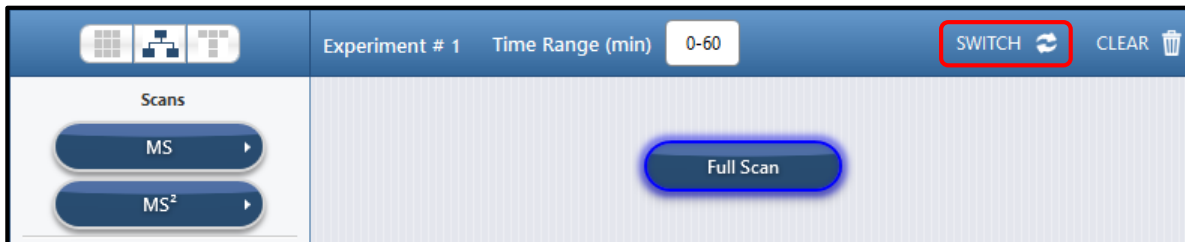
# (Orbitrap Exploris Tune) Method Editor: Scan Parameters

The screenshot displays the 'Method Editor' interface for the 'Scan Parameters' tab. The interface is divided into several sections:

- Method Timeline:** A horizontal timeline at the top showing a duration of 60 minutes. A red dashed box highlights the 'Experiment' label and the 'ACTIONS' dropdown menu.
- Settings:** A panel on the right containing parameters such as 'Infusion Mode' (set to Liquid Chromatography), 'Expected LC Peak Width (s)' (set to 30), and 'Internal Mass Calibration' (set to Off).
- Experiment # 1 Time Range (min):** A section below the timeline showing a time range of 0-60 minutes. It includes a 'Convert Button' and a 'Clear Button' (indicated by a red dashed box).
- Scans:** A section on the left with buttons for 'MS' and 'MS<sup>2</sup>'. A red dashed box highlights the 'Master Scans' and 'MS/MS Scans' labels.
- Filters:** A section on the left with buttons for 'Intensity', 'Charge State', 'Dynamic Exclusion', 'Targeted Mass', 'Targeted Mass Exclusion', and 'Apex Detection'. A red dashed box highlights the 'Filter Types' label.
- Full Scan:** A button in the center of the interface.
- Scan Properties:** A panel on the right containing parameters such as 'Orbitrap Resolution' (set to 60000), 'Scan Range (m/z)' (set to 100-1000), 'RF Lens (%)' (set to 70), 'Maximum Injection Time Mode' (set to Auto), 'Data Type' (set to Profile), 'Polarity' (set to Positive), and 'Source Fragmentation' (unchecked).

# (Orbitrap Exploris Tune) Method Editor: TSQ View

Convert button indicates if switch Quan View ↔ Qual View is possible



## Supported Conversions

SRM (Quan View) and AIF (Qual View) are not convertible

# Qual View: Create a Full Scan data-dependent MS<sup>2</sup> method

The screenshot displays the 'Method Editor' software interface. At the top, there are tabs for 'Global Parameters', 'Scan Parameters', and 'Summary'. Below these is a 'Method Timeline' with a duration of 60 minutes. The main workspace is divided into a left sidebar, a central 'Scans' area, and a right 'Properties' pane. The sidebar contains 'Scans' (MS, MS<sup>2</sup>) and 'Filters' (Intensity, Charge State, Dynamic Exclusion, Targeted Mass, Targeted Mass Exclusion, Apex Detection). The central 'Scans' area shows a sequence of scans: MS, MS<sup>2</sup>, and a 'Full Scan' button. A yellow circle with the number '1' is placed over the 'Full Scan' button. A yellow circle with the number '2' is placed over the 'MS<sup>2</sup>' button. A yellow circle with the number '3' is placed over the 'Full Scan' button in the 'Properties' pane. Arrows indicate the flow from the 'Full Scan' button in the central area to the 'Full Scan' button in the 'Properties' pane, and from the 'MS<sup>2</sup>' button to the 'Full Scan' button in the central area.

## Scan Parameters:

1. Go to MS Scans and add a Full Scan to the experiment pane.
2. Go to MS<sup>2</sup> Scans and append a MS<sup>2</sup> to the Full Scan.
3. A new Full Scan data-dependent MS<sup>2</sup> method is created.

# Qual View: Full Scan data-dependent MS<sup>2</sup> properties

The screenshot displays the 'Method Editor' software interface. At the top, there are tabs for 'Global Parameters', 'Scan Parameters', and 'Summary'. Below these is a 'Method Timeline' with a scale from 0 to 60 minutes. The 'Scan Parameters' tab is active, showing two main panels:

- Panel 1 (Left): Full Scan Properties** (indicated by a yellow circle with the number 1). It contains the following settings:
  - Orbitrap Resolution: 60000
  - Scan Range (m/z): 100-1000
  - RF Lens (%): 70
  - Maximum Injection Time Mode: Auto
  - Data Type: Profile
  - Polarity: Positive
  - Source Fragmentation: ☐
- Panel 2 (Right): Data-Dependent MS<sup>2</sup> Scan Properties** (indicated by a yellow circle with the number 2). It contains the following settings:
  - Multiplex Ions: ☐
  - Isolation Window (m/z): 2
  - Isolation Offset: Off
  - HCD Collision Energy Type: Normalized
  - HCD Collision Energy (%): 30
  - Stepped Collision Energy: ☐
  - Orbitrap Resolution: 15000
  - Scan Range Mode: Auto
  - Maximum Injection Time Mode: Auto
  - Maximum Injection Time (ms): 1
  - Data Type: Profile

On the far right, there is a 'Settings' panel with a dropdown menu set to 'Liquid Chromatography' and various input fields for parameters like '30' and 'Off'.

## Scan Parameters:

1. Full Scan Properties:
  - Orbitrap Resolution
  - Scan Range (m/z)
  - RF Lens (%)
  - Maximum Injection Time Mode
  - Data Type
  - Polarity
2. ddMS<sup>2</sup> Scan Properties:
  - Isolation Window (m/z)
  - Isolation Offset
  - HCD Collision Energy Type
  - HCD Collision Energy (% / eV)
  - Stepped Collision Energy
  - Orbitrap Resolution
  - Scan Range Mode
  - Maximum Injection Time Mode
  - Data Type

# Qual View: Full Scan data-dependent MS<sup>2</sup> - Intensity Filter

The screenshot displays the 'Method Editor' window with the 'Scan Parameters' tab selected. The interface is divided into several sections:

- Method Timeline:** A horizontal bar at the top showing the sequence of scans. An arrow labeled '1' points from the 'Intensity' filter button in the left sidebar to the 'Intensity' scan step in the timeline.
- Left Sidebar:** Contains 'Scans' (MS, MS<sup>2</sup>) and 'Filters' (Intensity, Charge State, Dynamic Exclusion, Targeted Mass, Targeted Mass Exclusion, Apex Detection). The 'Intensity' filter is highlighted with a yellow circle labeled '1'.
- Experiment # 1:** The main workspace showing the scan sequence: Full Scan → Intensity → ddMS<sup>2</sup>. The 'Intensity' scan is highlighted with a yellow circle labeled '2'.
- Settings Panel:** On the right, the 'Intensity Properties' section shows the 'Intensity Threshold' set to 2.0e5.

## Scan Parameters:

1. Go to Scan Filters and add an Intensity Filter to the experiment pane.
2. Intensity Properties:
  - Intensity Threshold

*The minimum signal intensity required to trigger a data dependent scan.*

# Qual View: Full Scan data-dependent MS<sup>2</sup> - Charge State Filter

The screenshot displays the 'Method Editor' interface with the 'Scan Parameters' tab selected. The 'Method Timeline' at the top shows a sequence of scans: Full Scan, Intensity, Charge State, and ddMS<sup>2</sup>. A 'Charge State' filter is highlighted in the 'Filters' list on the left, with an arrow pointing to its configuration in the 'Charge State Properties' panel on the right. The 'Charge State Properties' panel shows two options: 'perform dependent scans on singly charged precursors only' (selected) and 'perform dependent scans on singly charged precursors and precursors with undetermined charge state' (unselected). The 'Scan Parameters' panel on the right shows settings for 'Infusion Mode' (Liquid Chromatography), 'Expected LC Peak Width (s)' (30), and 'Internal Mass Calibration' (Off).

Method Editor

Global Parameters | Scan Parameters | Summary

Method Timeline

Experiment # 1

Time Range (min) 0-60

Scans

- MS
- MS<sup>2</sup>

Filters

- Intensity
- Charge State
- Dynamic Exclusion
- Targeted Mass
- Targeted Mass Exclusion
- Apex Detection

Charge State Properties

- ☒ perform dependent scans on singly charged precursors only
- ☐ perform dependent scans on singly charged precursors and precursors with undetermined charge state

Settings

Infusion Mode: Liquid Chromatography

Expected LC Peak Width (s): 30

Internal Mass Calibration: Off

## Scan Parameters:

1. Go to Scan Filters and add a Charge State Filter to the experiment pane.

2. Charge State Properties:

*perform dependent scans on singly charged precursors only*

*perform dependent scans on singly charged precursors with undetermined charge state*

# Qual View: Full Scan data-dependent MS<sup>2</sup> - Dynamic Exclusion Filter

The screenshot displays the 'Method Editor' window with the 'Scan Parameters' tab selected. The interface includes a 'Method Timeline' at the top, a 'Settings' panel on the right, and a central workspace for building the method. On the left, a 'Filters' sidebar contains buttons for 'MS', 'MS<sup>2</sup>', 'Intensity', 'Charge State', 'Dynamic Exclusion', 'Targeted Mass', 'Targeted Mass Exclusion', and 'Apex Detection'. An arrow labeled '1' points from the 'Dynamic Exclusion' button in the sidebar to a 'Dynamic Exclusion' filter node in the central workspace. The central workspace shows a sequence of steps: 'Full Scan', 'Intensity', 'Charge State', 'Dynamic Exclusion', and 'ddMS<sup>2</sup>'. A 'Dynamic Exclusion Properties' dialog box, labeled '3', is open, showing settings for 'Dynamic Exclusion Mode' (set to 'Custom'), 'Exclude after n times' (1), 'Exclusion duration (s)' (2), 'Mass Tolerance' (ppm), 'Low' (5), 'High' (5), and 'Exclude isotopes' (checked). In the top right 'Settings' panel, 'Dynamic Exclusion Properties' is labeled '2', and the 'Dynamic Exclusion Mode' is set to 'Auto'.

## Scan Parameters:

1. Go to Scan Filters and add a Dynamic Exclusion Filter to the experiment pane.
2. Dynamic Exclusion Properties:  
- Auto Mode / Custom Mode
3. When *Auto* is applied a target will be excluded for (Expected LC Peak width x 1.5) seconds.

In *Custom Mode* the user can define specific values for dynamic exclusion.

# Qual View: Full Scan data-dependent MS<sup>2</sup> - Targeted Mass Filter

**Method Editor** | Global Parameters | Scan Parameters | Summary

Method Timeline | Experiment | ACTIONS | Settings

Method Duration (min): 60

Experiment # 1 | Time Range (min): 0-60 | CLEAR

**Scans:** MS, MS<sup>2</sup>

**Filters:** Intensity, Charge State, Dynamic Exclusion, Targeted Mass, Targeted Mass Exclusion, Apex Detection

**Targeted Mass Filter Configuration:**

- Full Scan
- Intensity
- Charge State
- Dynamic Exclusion
- Targeted Mass** (1)
- ddMS<sup>2</sup>

**Targeted Mass Properties (2)**

MASS LIST

Mass List Type: m/z & z

Time Mode: Retention Time Window

Include Intensity Threshold: ☐

| Compound   | Formula   | Adduct | m/z      | z | RT |
|------------|-----------|--------|----------|---|----|
| 1 Caffeine | C8H10N4O2 | +H     | 195.0877 | 1 | 30 |

Mass Tolerance: ppm

Low: 5

High: 5

Ignore Charge State Requirement in the table for Ions with Undetermined Charge State: ☒

Set Collision Energy per Compound: ☐

Perform dependent scan on most intense Ion if no targets are found: ☐

**Targeted Mass Table:**

| Compound   | Formula   | Adduct | m/z      | z | RT Time (min) | Window (min) | HCD Collision Energy (%) |
|------------|-----------|--------|----------|---|---------------|--------------|--------------------------|
| 1 Caffeine | C8H10N4O2 | +H     | 195.0877 | 1 | 30            | 0.5          | 30                       |

## Scan Parameters:

1. Go to Scan Filters and add a Targeted Mass Filter to the experiment pane.
2. Targeted Mass Properties:
  - Mass List Type
  - Time Mode
  - Include Intensity Threshold
  - Mass Tolerance (Low/High)

*Ignore Charge State Requirement in the table for Ions with undetermined Charge State*

*Set Collision Energy per Compound*

*Perform dependent scan on most intense Ion if no targets are found*

# Qual View: Full Scan data-dependent MS<sup>2</sup> - Targeted Mass Exclusion Filter

**Method Editor** | Global Parameters | **Scan Parameters** | Summary

Method Timeline | Experiment | ACTIONS | Settings

Method Duration (min): 60

Experiment # 1 | Time Range (min): 0-60 | CLEAR

**Scans**

- MS
- MS<sup>2</sup>

**Filters**

- Intensity
- Charge State
- Dynamic Exclusion
- Targeted Mass
- Targeted Mass Exclusion
- Apex Detection

**Targeted Mass Exclusion**

Full Scan

Intensity

Charge State

Dynamic Exclusion

Targeted Mass

Targeted Mass Exclusion

ddMS<sup>2</sup>

**Targeted Mass Exclusion Properties**

MASS LIST

Time Mode: Retention Time Window

Include Intensity Threshold: ☐

| Compound | Formula  | Adduct    | m/z | z        | RT |    |
|----------|----------|-----------|-----|----------|----|----|
| 1        | Caffeine | C8H10N4O2 | +H  | 195.0877 | 1  | 30 |

Exclusion mass width: ppm

Low: 5

High: 5

Ignore Charge State Requirement in the table for Ions with Undetermined Charge State: ☒

## Scan Parameters:

1. Go to Scan Filters and add a Targeted Mass Exclusion Filter to the experiment pane.
2. Targeted Mass Exclusion Properties:
  - Time Mode
  - Include Intensity Threshold
  - Mass Tolerance (Low/High)

*Ignore Charge State Requirement in the table for Ions with undetermined Charge State*

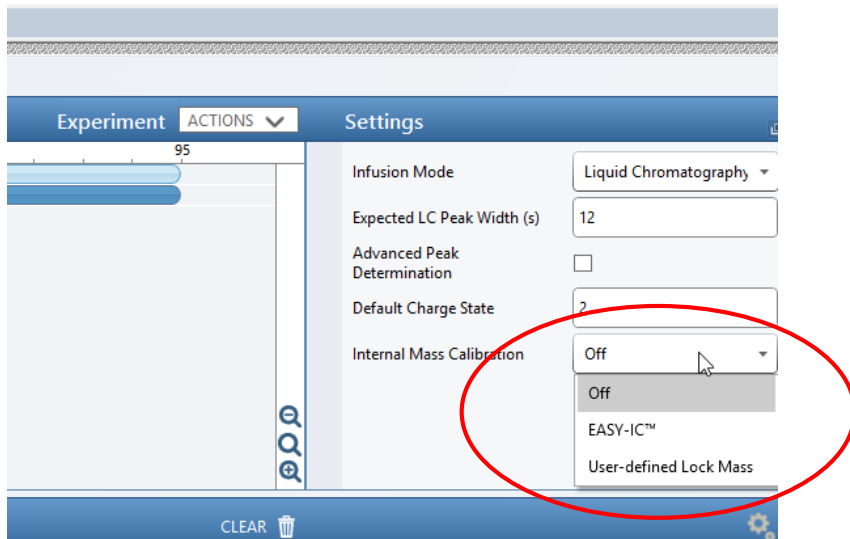
# Qual View: Full Scan data-dependent MS<sup>2</sup> - Apex Detection Filter

The screenshot displays the 'Method Editor' interface with the 'Scan Parameters' tab selected. The 'Method Timeline' at the top shows a 60-minute duration. The 'Settings' panel on the right includes 'Infusion Mode' (Liquid Chromatography), 'Expected LC Peak Width (s)' (30), and 'Internal Mass Calibration' (Off). The main workspace shows a workflow for 'Experiment # 1' with a time range of 0-60 minutes. The workflow starts with 'Full Scan', followed by 'Intensity', 'Charge State', 'Dynamic Exclusion', 'Targeted Mass', 'Targeted Mass Exclusion', 'Apex Detection', and 'ddMS<sup>2</sup>'. A callout box labeled '1' points to the 'Apex Detection' filter in the workflow. Another callout box labeled '2' points to the 'Apex Detection Properties' panel on the right, which shows the 'Desired Apex Window (%)' set to 30. The left sidebar shows 'Scans' (MS, MS<sup>2</sup>) and 'Filters' (Intensity, Charge State, Dynamic Exclusion, Targeted Mass, Targeted Mass Exclusion, Apex Detection).

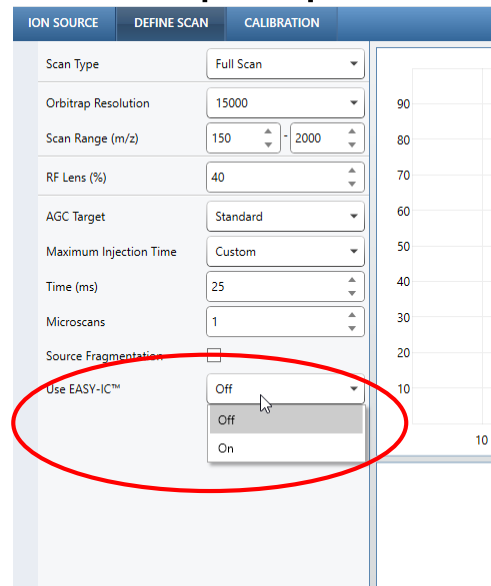
## Scan Parameters:

1. Go to Scan Filters and add a Apex Detection Filter to the experiment pane.
2. Apex Detection Properties:
  - Desired Apex Window (%)

## Method Editor



## Orbitrap Exploris Tune



- Source is automatically recognized
- It automatically appears in the Orbitrap Exploris Tune Software

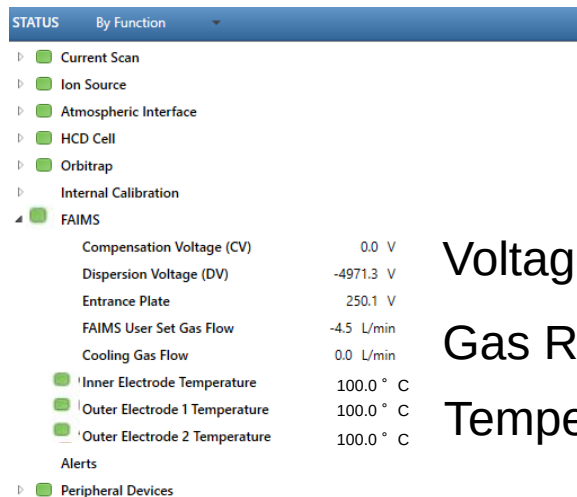
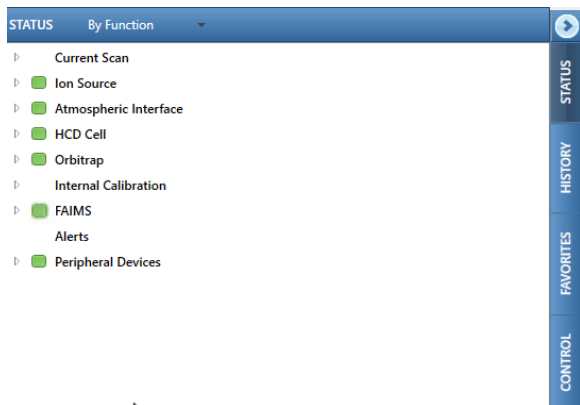
| ION SOURCE             | DEFINE SCAN              | CALIBRATION |
|------------------------|--------------------------|-------------|
| Scan Type              | Full Scan                |             |
| Orbitrap Resolution    | 15000                    |             |
| Scan Range (m/z)       | 150 - 2000               |             |
| RF Lens (%)            | 50                       |             |
| AGC Target             | Standard                 |             |
| Maximum Injection Time | Custom                   |             |
| Time (ms)              | 20                       |             |
| Microscans             | 1                        |             |
| Source Fragmentation   | <input type="checkbox"/> |             |
| Use EASY-IC™           | Off                      |             |
| FAIMS Voltages         | On                       |             |
| FAIMS CV (V)           | 0                        |             |

| ION SOURCE                          | DEFINE SCAN                 | CALIBRATION         |
|-------------------------------------|-----------------------------|---------------------|
| Ion Source Optimization             |                             |                     |
| Current LC Flow (μL/min)            |                             | 0                   |
| <button>Get Defaults</button>       |                             |                     |
| Ion Source Type                     |                             | ESI                 |
| <input checked="" type="checkbox"/> | Pos Ion Spray Voltage (V)   | 4000 3975           |
|                                     | Neg Ion Spray Voltage (V)   | 2200                |
|                                     | Sheath Gas (Arb)            | 0 0.00              |
|                                     | Aux Gas (Arb)               | 0 0.00              |
| <input checked="" type="checkbox"/> | Ion Transfer Tube Temp (°C) | 320 320.5           |
|                                     | FAIMS Gas (L/min)           | 0 -4.5              |
|                                     | FAIMS Mode                  | Standard Resolution |

| STATUS                              | By Function           |
|-------------------------------------|-----------------------|
| <input type="checkbox"/>            | 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              |
| <input type="checkbox"/>            | Internal Calibration  |
| <input checked="" type="checkbox"/> | FAIMS                 |
| <input type="checkbox"/>            | Alerts                |
| <input checked="" type="checkbox"/> | Peripheral Devices    |

STATUS  
HISTORY  
FAVORITES  
CONTROL

- FAIMS Readback in the Status Tree



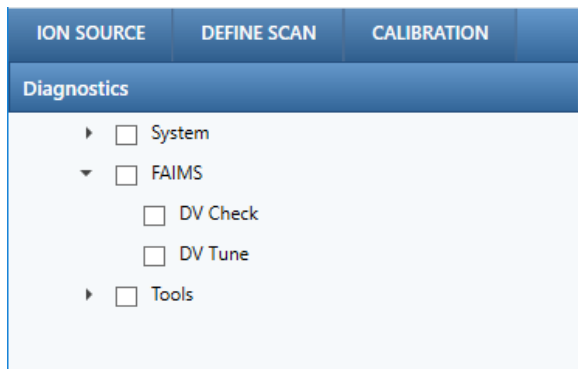
Voltage Readback

Gas Readback

Temperature Readbacks

# FAIMS Calibration

- You can find the calibration in the Diagnostics area of the software



- The DV Tune has to be done:
  - After installation
  - After cleaning
  - After changing the kind of ion source

# (Orbitrap Exploris Tune) Method Editor: Summary Page (1)

**Method Editor** | Global Parameters | Scan Parameters | **Summary**

Document View | Tree View

▼ Method Settings

Application Mode: **Small Molecule**  
Method Duration (min): **60**

▼ Global Parameters

▲ Ion Source

Ion Source Type: **H-ESI**  
Spray Voltage: **Static**  
Positive Ion (V): **3500**  
Negative Ion (V): **2500**  
Sheath Gas (Arb): **2**  
Aux Gas (Arb): **2**  
Sweep Gas (Arb): **2**  
Ion Transfer Tube Temp (°C): **275**  
Vaporizer Temp (°C): **0**  
APPI Lamp: **Not in Use**  
Use Ion Source Settings from Tune: **False**  
FAIMS Mode: **Not Installed**

▲ MS Global Settings

Infusion Mode: **Liquid Chromatography**  
Expected LC Peak Width (s): **30**  
Internal Mass Calibration: **Off**

▼ Experiment#1 [MS]

Start Time (min): **0**  
End Time (min): **60**

Master Scan:

▲ Full Scan

Orbitrap Resolution: **60000**  
Scan Range (m/z): **100-1000**  
RF Lens (%): **70**  
Maximum Injection Time Mode: **Auto**  
Data Type: **Profile**  
Polarity: **Positive**  
Source Fragmentation: **Disabled**

Filters:

▲ Intensity

Intensity Threshold: **2.0e5**

▲ Charge State

**perform dependent scans on singly charged precursors only**

▲ Dynamic Exclusion

Dynamic Exclusion Mode: **Custom**  
Exclude after n times: **1**  
Exclusion duration (s): **5**

# (Orbitrap Exploris Tune) Method Editor: Summary Page (2)

**Method Editor** | Global Parameters | Scan Parameters | **Summary**

Document View | Tree View

Low: 5  
High: 5  
Exclude Isotopes: **True**

Targeted Mass

Mass List

Mass List Type: **m/z & z**  
Time Mode: **Retention Time Window**  
Include Intensity Threshold: **False**

| Compound | Formula   | Adduct | m/z      | z | RT Time (min) | Window (min) | HCD Collision Energy (%) |
|----------|-----------|--------|----------|---|---------------|--------------|--------------------------|
| Caffeine | C8H10N4O2 | +H     | 195.0877 | 1 | 30            | 0.5          | 30                       |

Mass Tolerance: **ppm**  
Low: 5  
High: 5  
Ignore Charge State Requirement in the table for Ions with Undetermined Charge State: **True**  
Set Collision Energy per Compound: **True**  
Perform dependent scan on most intense ion if no targets are found: **False**

Targeted Mass Exclusion

Mass List

Time Mode: **Retention Time Window**  
Include Intensity Threshold: **False**

| Compound | Formula   | Adduct | m/z      | z | RT Time (min) | Window (min) |
|----------|-----------|--------|----------|---|---------------|--------------|
| Caffeine | C8H10N4O2 | +H     | 195.0877 | 1 | 30            | 60           |

Exclusion mass width: **ppm**  
Low: 5  
High: 5  
Ignore Charge State Requirement in the table for Ions with Undetermined Charge State: **True**

Apex Detection  
Desired Apex Window (%): 30

Data Dependent  
Number of Dependent Scans: 4

Scan Event Type 1:

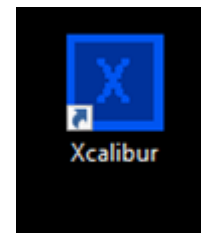
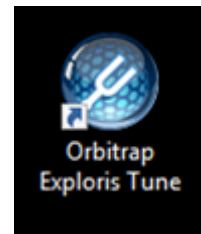
Scan:

ddMS<sup>2</sup>

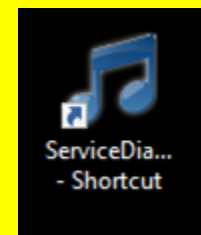
Multiplex Ions: **False**  
Isolation Window (m/z): 2  
Isolation Offset: **Off**  
HCD Collision Energy Type: **Normalized**  
Stepped Collision Energy: **False**  
Orbitrap Resolution: **15000**  
Scan Range Mode: **Auto**  
Maximum Injection Time Mode: **Auto**  
Maximum Injection Time (ms): 1  
Data Type: **Profile**

# Software

- Orbitrap Exploris Tune
  - Tune Software (similar to Fusion/Lumos)
- Xcalibur:
  - Method Editor
  - ...



- SDT Service Diagnostic Tool
  - Only for Service
  - Can be found in  
C:\Thermo\Instruments\Exploris\1.0\System\Programs



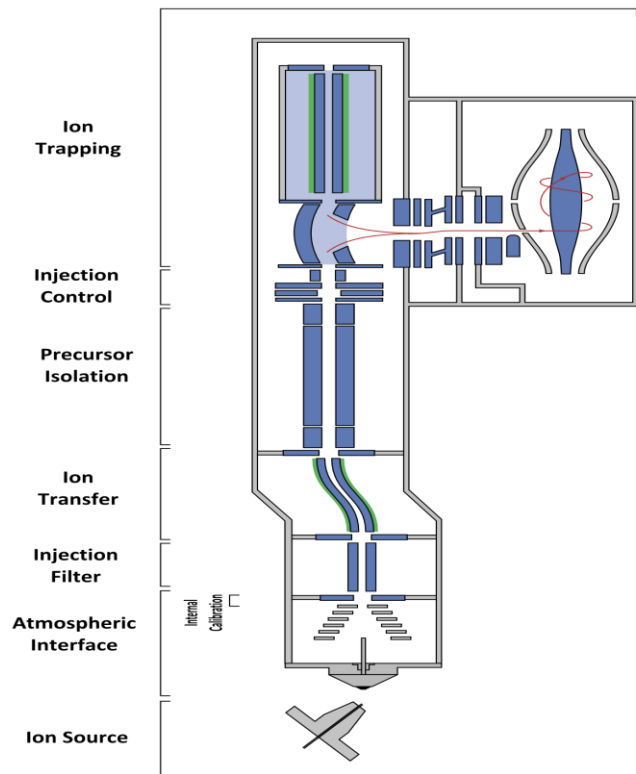
## Status Tree

The screenshot displays the SDT interface with the following components:

- Top Menu:** File, Reports, Help
- Mode/State/Peripherals:** Buttons for Mode, State, and Peripherals.
- Instrument Control:**
  - Scan Parameters:** Scan Range [150-2000], Isolation Range same, Fragmentation none, In-Source CID none, Resolution 15,000, Polarity Positive, Microscans 1, AGC target 1e6, Maximum inject time 10.
  - ESI source:** Sheath gas flow rate 0, Aux gas flow rate 5, Sweep gas flow rate 0, Spray voltage (kV) 3.50, Spray current (uA) 0.40, Ion transfer tube temp. (°C) 320, S-lens RF level 80.0.
  - Acquisition:** Acquisition state Ready, Progress 0.00 min, File in use, Destination file, Acquisition scheme, Sample, Comment, On start don't wait, After acquisition stay on.
- Spectrum:** Scan: #34714, uS 1, IT: 10.0, NL: 6.5167, Type: FTMS - p ESI Full ms [150.0000-2000.0000]. The plot shows Relative Abundance (%) vs m/z with peaks at 202.078, 215.073, 216.080, 204.087, 189.070, 644.320, 625.097, and 904.681.
- Analysis Graphs:** Transients, Frequency View.
- Messages:** Log of system events including connection status and acquisition mode changes.
- Status Tree (Highlighted):**
  - Application/Method
  - Components
  - Settings (DEPRECATED)
  - Configuration settings
  - Storing the last bake out ID for specific calibrations
  - Factory Data
  - System
    - Software
    - Sys-Com Nodes
    - Tune/Values
    - CalibrationValues
    - Version and ID
    - Current User Role
    - HW Parts ID & Tracking
  - Analysis Graph
  - Performance
  - Electronics
    - Instrument Control Board
    - Embedded FTICU
    - Ion Optics Board
    - Source Board
    - LED Panel
    - Data Acquisition Board
    - Pre-Amplifier
    - PCBA Orbitrap Supply
    - PCBA Orbitrap Pulser
    - Quad Supply
    - C-Trap Board
  - Peripheral Devices
  - Procedures
    - Calibrant Masses
    - Custom Masses
    - Pre-Conditions
    - By Functionality
      - Utility
      - General
      - Ion Source
      - Atmospheric Interface

# Reorganization of Instrument Status Tree: Components

## Component definition for instrument control tree

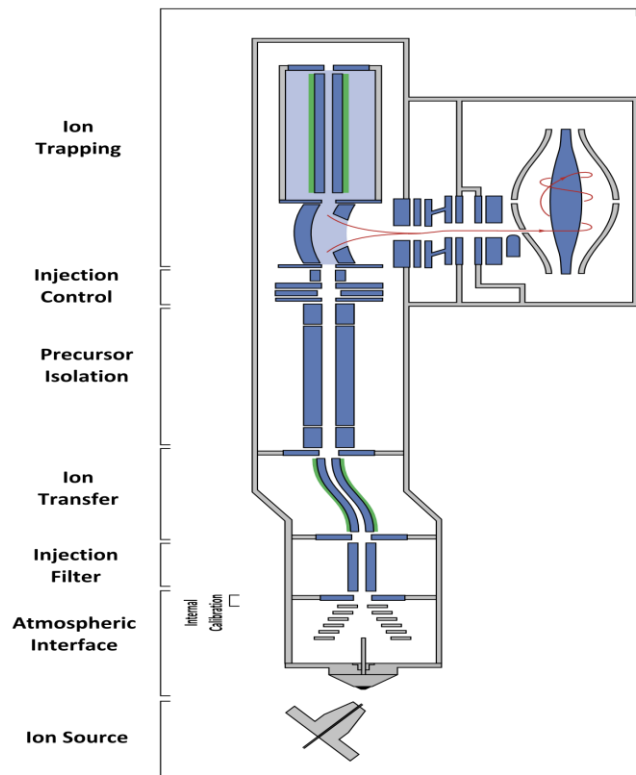


| Status Tree |                             |
|-------------|-----------------------------|
| ▷           | Tree Tools                  |
| ▷           | Current Scan                |
| ✓           | ▲ Control                   |
| ▷           | Define Scan                 |
| ▷           | Application/Method          |
| ✓           | ▲ Components                |
| ▷           | General                     |
| ✓           | ▷ Vacuum System             |
| ✓           | ▷ Ion Source                |
|             | ▷ Atmospheric Interface     |
|             | ▷ Injection Filter          |
|             | ▷ Ion Transfer              |
|             | ▷ Precursor Isolation       |
|             | ▷ Injection Control         |
|             | ▷ Ion Trapping              |
|             | ▷ Timing and Settling Times |

Proprietary & highly confidential!

# Reorganization of Instrument Status Tree: Procedures

## Component definition for instrument control tree



|                             |                              |
|-----------------------------|------------------------------|
| ▲ Procedures                | ::                           |
| ▷ Calibrant Masses          | CalMix                       |
| ▷ Custom Masses             | CalMix                       |
| ▷ Pre-Conditions            |                              |
| ▲ By Functionality          | 1;;By Functionality          |
| ▷ Utility                   | 1;;Utility                   |
| ▷ General                   | 1;;General                   |
| ▷ Ion Source                | 1;;Ion Source                |
| ▷ Atmospheric Interface     | 1;;Atmospheric Interface     |
| ▷ Injection Filter          | 1;;Injection Filter          |
| ▷ Ion Transfer              | 1;;Ion Transfer              |
| ▷ Precursor Isolation       | 1;;Precursor Isolation       |
| ▷ Injection Control         | 1;;Injection Control         |
| ▷ Ion Trapping              | 1;;Ion Trapping              |
| ▷ Internal Calibrant Source | 1;;Internal Calibrant Source |
| ▷ System Level              | 1;;System Level              |
| ▲ By Sequence               | 1;;By Sequence               |
| ▷ User                      | 1;;User                      |
| ▷ Factory                   | 1;;Factory                   |
| ▷ Service                   | 1;;Service                   |
| ▷ Development               | 1;;Development               |
| ▷ Supplier                  | 1;;Supplier                  |
| AutoTune                    | 1;;AutoTune                  |

Proprietary & highly confidential

# Search Function in Status Tree

- FSEs can search status tree entries
- Add hit to favorites node
- Favorites file is stored in msx\_instrument\_files folder and transferrable to another instrument

The screenshot displays the 'Instrument' tree structure with the 'Tree Search & Results' panel expanded. The search filters are set to 'PrOSA' for all fields. Below the filters, a table shows 54 hits for 'PrOSA'. The 'Add hit to favorites' button is highlighted for the third match. At the bottom, a file explorer view shows the 'status\_tree\_favorites' file selected in the 'msx\_instrument\_files' folder.

**Instrument**

- Tree Tools
- Tree Search & Results
  - Search Root: PrOSA
  - Search Control: PrOSA
  - Search Electronics: PrOSA
  - Search Settings (DEPRECATED): PrOSA
  - Search Procedures: PrOSA

**Tree Search & Results** 54 hits for 'PrOSA'

| Match #  | Control | Appli..d | M ICD..s               | M ICD PrOSA D |
|----------|---------|----------|------------------------|---------------|
| Match #1 | Control | Appli..d | M ICD..s               | M ICD PrOSA D |
| Match #2 | Control | Appli..d | M ICD PrOSA Support *  |               |
| Match #3 | Control | Appli..d | M ICD PrOSA Support Ac |               |
| Match #4 | Control | Appli..d | M ICD..s               | M ICD PrOSA D |

**★ Favorites**

Regulated Bake-Out 0;Done.;Regulated Bake-Out

| Name                   | Date modified      | Type        |
|------------------------|--------------------|-------------|
| 2017-16-3-backup       | 3/16/2017 1:09 PM  | File folder |
| obsolete               | 1/4/2017 2:14 PM   | File folder |
| default.mstune.backup  | 6/9/2017 1:13 PM   | BACKUP File |
| inst_config.cfg        | 7/18/2017 11:02 AM | CFG File    |
| procedure_history      | 7/18/2017 8:28 AM  | File        |
| status_tree_favorites  | 7/14/2017 1:13 PM  | File        |
| status_tree_favorites_ | 6/16/2017 8:16 AM  | File        |

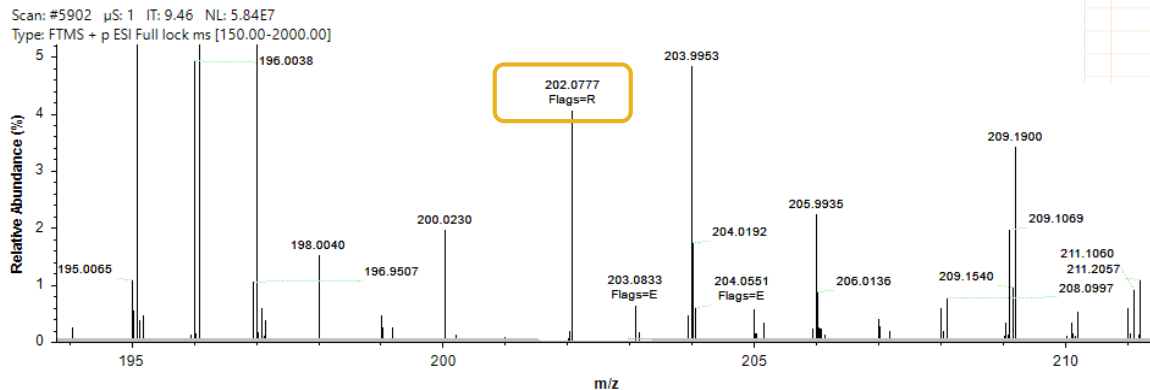
# Activate the ICS

- Controlled through Instrument Configuration (or SDT)
- Should work with default settings
- The oven may take >15 min to reach the set temperature!
  - Settling time is printed at the bottom of the instrument tree

| Status Tree                     |                                      |
|---------------------------------|--------------------------------------|
| Instrument                      | IC Source - Temperature Supervision  |
| Tree Tools                      |                                      |
| Current Scan                    |                                      |
| Control                         |                                      |
| Define Scan                     |                                      |
| Application/Method              |                                      |
| Components                      |                                      |
| General                         |                                      |
| Vacuum System                   |                                      |
| Analyzer Temperature Control    |                                      |
| Ion Source                      |                                      |
| Atmospheric Interface           |                                      |
| Injection Filter                |                                      |
| Ion Transfer                    |                                      |
| Precursor Isolation             |                                      |
| Injection Control               |                                      |
| Ion Trapping                    |                                      |
| Timing and Settling Times       |                                      |
| IC Ion Source                   |                                      |
| ICS Operation Mode *            | On                                   |
| ICS HV current trimmer adjustm  | 0.0                                  |
| ICS active HV current (μA) #    | 5.0                                  |
| ICS idle HV current (μA) #      | 0.05                                 |
| ICS Make-up Gas (psi) #         | 15.0                                 |
| ICS timing                      |                                      |
| ICS Bump HV current (μA) #      | 5.0                                  |
| ICS Bump Duration (ms) #        | 1.0                                  |
| ICS Switch on Delay (ms) #      | 7.0                                  |
| ICS Switch off Delay (ms) #     | 8.0                                  |
| ICS Oven Temperature (°C) #     | 65.0                                 |
| ICS Split Temperature (°C) #    | 130.0                                |
| ICS Calibration m/z #           | 202.0777                             |
| IC Source                       | Temperature Supervision - Actual Ove |
| Status                          | On                                   |
| Settling Time                   | 7.5 min                              |
| IC AGC Status                   | Disabled                             |
| Temperature Supervision         | Actual Oven Heater Temperature - 47  |
| Actual Oven Heater Temperature  | 47.6 °C                              |
| Actual Split Heater Temperature | 129.8 °C                             |
| Alerts                          |                                      |

# Use the ICS lockmass

- Tick EasyIC box in Method Editor
- SDT allows to choose for which mode(s) to use ICS lockmass
  - Added as separate, last injection
- Ensure ICS AGC mode = On
  - Typical ICS IT < 0.5 ms for S/N 75



| Status Tree                        |                                      |
|------------------------------------|--------------------------------------|
| ! Instrument                       | Performance - Affected: System Calib |
| ▶ Tree Tools                       |                                      |
| ▶ Current Scan                     |                                      |
| ✓ Control                          |                                      |
| ▶ Define Scan                      |                                      |
| ▲ Application/Method               |                                      |
| LC peak width (FWHM) *             | 15.0                                 |
| ▶ AGC Details                      |                                      |
| Application mode (requested)       | Standard                             |
| Application mode (actual)          | Standard                             |
| Bigmass Application mode (actual)  | Off                                  |
| Bigmass Calibration Index (actual) | ix0                                  |
| Trapping gas pressure setting *    | 1.0                                  |
| ▲ Lockmass Details                 |                                      |
| Analyte Lockmass injection *       | Off                                  |
| IC Lockmass injection *            | Off                                  |
| ICS (max) inject time (ms) *       | 5.0                                  |
| ICS AGC mode *                     | On                                   |
| ICS AGC target (s/n) *             | 75                                   |
| Lockmass inj iso width (m/z) *     | 2.5                                  |
| Lockmass inj target *              | 2000.0                               |
| Lockmass tolerance * (ppm)         | 15                                   |
| Multi-Lockmass Logic               | Best Peak                            |

## Instrument Control

The screenshot displays the SDT Instrument Control software interface. The left sidebar contains the 'Instrument Control' panel, which is highlighted with a red box. This panel is divided into three sections: 'Scan Parameters', 'ESI source', and 'Acquisition'. The 'Scan Parameters' section includes fields for Scan Range (150-2000), Isolation Range (same), Fragmentation (none), In-Source CID (none), Resolution (15,000), Polarity (Positive), Microscans (1), AQC target (1e6), and Maximum inject time (10). The 'ESI source' section includes fields for Sheath gas flow rate (0), Aux gas flow rate (5), Sweep gas flow rate (0), Spray voltage (3.50), Spray current (0.40), Ion transfer tube temp (320), and S-lens RF level (80.0). The 'Acquisition' section includes fields for Acquisition state (Ready), Progress (0.00 min), File in use, Destination file, Acquisition scheme, Sample, Comment, On start (don't wait), and After acquisition (stay on). The main window displays a mass spectrum plot with Relative Abundance (%) on the y-axis and m/z on the x-axis. The plot shows several peaks, with the base peak at m/z 202.078. Other labeled peaks include 215.073, 216.080, 544.320, 904.681, 204.087, 189.070, and 625.097. The bottom right corner of the interface shows a 'Status Tree' with a hierarchical view of the instrument's components and their status. The 'Messages' panel at the bottom displays a log of system events, including connection status changes and acquisition mode transitions.