Thermo Scientific Orbitrap Exploris Series 4.2 SP1 Instrument Control Software Release Notes

This document lists installation notes, new features and improvements regarding the Thermo Scientific™ Orbitrap Exploris™ Series 4.2 SP1 Instrument Control Software release. For information regarding the installation, features, functionality, and use of this product, refer to the following sources of information:

- *Orbitrap Exploris Series Operating Manual*
- *Orbitrap Exploris GC and Orbitrap Exploris GC 240 Operating Manual*

Contents

Installation Notes

Supported Target Systems

Thermo Scientific Orbitrap Exploris 120 mass spectrometer

Thermo Scientific Orbitrap Exploris 240 mass spectrometer

Thermo Scientific Orbitrap Exploris 480 mass spectrometer

Thermo Scientific Orbitrap Exploris MX mass spectrometer

Thermo Scientific Orbitrap Exploris GC mass spectrometer

Thermo Scientific Orbitrap Exploris GC 240 mass spectrometer

System Requirements

The minimum hardware and software configurations required for the Orbitrap Exploris Series 4.2 SP1 Instrument Control Software operation are as follows:

System	Requirements
PC	3.0 GHz Quad Core Intel™ Processor 32 GB RAM 512 GB SSD Hard Drive Display Monitor Resolution of 1920 × 1080 Two Network Interface Cards (NIC), 1000 MBit/s
Software	Microsoft™ Windows™ 10 Enterprise 2016 LTSB, 2019 LTSC or 2021 LTSC Thermo Scientific Xcalibur 4.6

Tip The Orbitrap Exploris Series 4.2 SP1 Instrument Control Software was only tested within the delivered composition.

Tip Support for Chromeleon™. The Chromeleon driver compatibility matrix reflects the tested compatibility for combinations of Orbitrap Exploris Series instrument control software versions, Chromeleon software versions, and instrument models. For more information and to view the compatibility matrix, sign on to support.thermoinformatics.com/downloads/default.aspx, and then select **Chromeleon > Chromeleon > Related Drivers > Driver Compatibility Matrix**.

Installation

Note for FAIMS Users Please reboot the FAIMS unit after the installation of the Orbitrap Exploris Series 4.2 SP1 Instrument Control Software (switch Main Control Box off and on).

The new Orbitrap Exploris Series 4.2 SP1 Instrument Control Software provides a firmware update for the FAIMS unit, which is mandatory to support the new improvements and defect fixes for FAIMS Pro and the new FAIMS Pro Duo interface.

This guidance addresses a standard installation of a Windows computer acting as an access point for Orbitrap Exploris Series based instruments. The current software version is 4.2 SP1. The guidance is valid at least up to this version. There are differences between nearly all computers, so even if you have a receipt of installation, be aware that the operating system or language settings might be different. The current explanations have Microsoft Windows 10 Enterprise LTSB 2016, LTSC 2019 or LTSC 2021 and English in focus.

Thermo Fisher Scientific does not accept any warranty claims about the completeness of this instruction list. Consulting a Thermo Fisher Scientific support team member of Orbitrap Exploris Series instruments is highly recommended for setting up a new PC.

Technical Requirements

Choose a PC equipped as described at "System Requirements" on .

Operating System Language

English is the only tested language. It is recommended to switch to English language before installation. This installation instruction refers to names of English operating systems.

Network Setup

At least two NICs must be present in the system. The one connected to the instrument must not be connected to the regular Internet connection. Only the instrument to be driven by this particular PC may be connected to the PC using a 1 GBit switch or hub. Additional devices like autosampler or LC or GC systems may be connected to that switch, too.

Configure the IPv4 interface as follows:

- address 172.16.0.101
- network mask 255.255.0.0
- manual DNS selection with empty fields

Physical Links

Use at least a Cat 6 patch cable. Double-check the quality of the cable if errors occur.

Virus Scanner and Firewall

Disable virus scanner and firewall during installation. Virus scanning can happen in advance and may stay turned on, if it is guaranteed that the firewall is turned off. The installation program informs only the built-in firewall of Windows properly. Other firewalls have to be informed that the program Thermo Exploris Core Service (file locations see below) needs access to incoming and outgoing network traffic. Remember that the dedicated NIC is usually considered to be a "public network." Firewall and virus scanner can be turned on after installation. Reboot the instrument to be sure that everything works.

Software Installation

File Locations

The default installation folder on the computer is C:\ProgramData\Thermo\Exploris.

This instruction list uses C:\ProgramData\Thermo\Exploris for easy reading, but depending on the installation package like Orbitrap Exploris Series Instrument Control Software kit or Chromeleon, this may be different.

When the Orbitrap Exploris Series software has been installed on a system, the folder of the previous installation will be reused.

Backup

Several files and folders require a backup for later installation, either for crash recovery or for replacing the computer. The backup can be performed during normal operation.

These files and folders (see "File Locations" on page 2) should be saved if present:

- C:\ProgramData\Thermo\Exploris\instrument\msx_instrument_files
- C:\ProgramData\Thermo\Exploris\Licenses.txt
- C:\Thermo\Instruments\Exploris\[version]\System\Programs\dependencies\msi\TNGConfig.xmb

Setup of a new computer without any backup requires assistance of the Orbitrap Exploris support team of Thermo Fisher Scientific. The computer may require licenses or some extra configuration files.

Uninstalling

The Installer will automatically remove outdated versions prior to the installation of a new version.

Installation

Install using the ISO image or a copy of its content by executing the installation program OrbitrapExplorisFullSetup.exe. Use the regular way of installation for best results. It detects several problems, if they exist at all.

Restoring a Backup

This step is not needed, if the installation was just an upgrade of the Orbitrap Exploris Series software. All present configuration settings remain on uninstalling.

For setting up a replacement computer or after a disk crash, the restore procedure needs to be performed. The procedure requires administrator privileges. The restore procedure should happen after installation of the new software.

The installation place in the backup may be different to that of the present installation. Either use Instrument Configuration and look where files are located or check the folders appearing at "File Locations" on page 2.

Tip It is important to stop the only program that interacts with the files coming from the backup. That is Thermo Exploris Core Service.

❖ **To stop the Thermo Exploris Core Service**

1. In Windows 10 desktop, open **Computer Management** (<⊞> + <X>).
2. Select **Computer Management (Local) > Services and Applications > Services > Thermo Exploris Core Service**.
3. Right-click it and select **Stop**.

    Keep the dialog open.

4. After a new installation, the instrument already created the msx_instrument_folder with default content. Replace the content of that folder by the files from the backup.
5. Use the open dialog to start the **Thermo Exploris Core Service** again. Alternatively, reboot the computer. In doubt, contact the Orbitrap Exploris support team of Thermo Fisher Scientific.

Operation

Set the power setting to maximal performance.

Tip Automatic updates of any kind, those of the operating system in particular, are usually set to **automatic**, but this may disturb instrument data acquisition. To not disturb your data acquisitions by automatic updates, we strongly recommend setting all updates to **manual** and checking for updates regularly.

Put the computer to sleep: Never (Control Panel\Hardware and Sound\Power Options\Edit Plan Settings).

Software Compatibility Matrix

Table 1 shows the supported instrument control software versions for various Orbitrap Exploris Series instrument models.

Table 1. Software compatibility matrix

Version	Version No.	Orbitrap Exploris 480	Orbitrap Exploris 240	Orbitrap Exploris 120	Orbitrap Exploris GC	Orbitrap Exploris GC 240	Orbitrap Exploris MX
1.0	1.0.77.7	✓	—	—	—	—	—
1.1	1.1.117.22	✓	—	—	—	—	—
1.1 SP1	1.1.117.26	✓	—	—	—	—	—
2.0	2.0.182.18	✓	✓	✓	—	—	—
2.0 SP1	2.0.182.25	✓	✓	✓	—	—	—
2.0 SP2	2.0.182.35	✓	✓	✓	—	—	—
3.0	3.0.261.13	✓	✓	✓	✓	✓	—
3.1	3.1.279.9	✓	✓	✓	✓	✓	—
4.0	4.0.309.27	✓	✓	✓	✓	✓	✓
4.0 SP1	4.0.309.28	✓	✓	✓	✓	✓	✓
4.1	4.1.335.19	✓	✓	✓	✓	✓	✓
4.2	4.2.362.16	✓	✓	✓	✓	✓	✓
4.2 SP1	4.2.362.21	✓	✓	✓	✓	✓	✓

New Features and Improvements

Table 2 lists defect fixes in the Orbitrap Exploris Series 4.2 SP1 Instrument Control Software release that were implemented since the Orbitrap Exploris Series 4.2 Instrument Control Software release.

Table 2. Changes realized with Orbitrap Exploris Series 4.2 SP1 Instrument Control Software relative to Orbitrap Exploris Series 4.2 Instrument Control Software

Defect Fixes	
ID	Title
356984	Method execution Full Scan DDA with Targeted Mass Filter and Fixed/Stepped Collision Energies (CEs): fixed CEs in the Targeted Mass Filter are erroneously executed as stepped CEs
347689	Method transfer: Cannot open certain older methods with Orbitrap Exploris Series 4.2 ICSW – index out of range error message
351444	Orbitrap Exploris GC: License Error with 60k GCHCD license prevents running methods
356173	Orbitrap Exploris GC: Method Editor: Corrected acquisition delay tooltip in Global Settings
356170	Orbitrap Exploris GC: Method Editor: Factor 10x UI recommendation rule is erroneously applied to all GC System Templates
356174	Orbitrap Exploris GC: Method Editor: Restore Default context menu does not work for parameters under Ion Source Properties
364748	Full Scan acquisition with Mild Trapping option (Small Molecule Application Mode) leads to signal drop in positive mode

Table 3 lists new features, improvements and defect fixes in the Orbitrap Exploris Series 4.2 Instrument Control Software release that were implemented since the Orbitrap Exploris Series 4.1 Instrument Control Software release.

Table 3. Changes realized with Orbitrap Exploris Series 4.2 Instrument Control Software relative to Orbitrap Exploris Series 4.1 Instrument Control Software

New Features	
ID	Title
153451	AcquireX support is provided for peptide mapping (AcquireX Ab) with Orbitrap Exploris 240 and Orbitrap Exploris 480
221915	Method Editor: New management of tables in DIA scan
168318	Method Editor: New table format is available for SIM scan. SIM with multiple broad scan ranges is provided for Orbitrap Exploris 120, 240 and GC.
153788 286667	Method Editor: Options are provided to select the order with which precursors are selected for data-dependent scans
186364	Method Editor: TMT 18-plex is supported by TurboTMT on Orbitrap Exploris 480
235118	Method Editor: The new option "Auto-Extended" is provided for MS2 Scan Range Mode (Small Molecule Application Mode)
285925	Orbitrap Exploris GC: Method Editor provides a "Run Start Mass Calibration" template in system template
290954	Orbitrap Exploris GC: Tune Calibration pane provides a Manual Calibration panel
284960	Orbitrap Exploris GC: Tune Preferences provides a panel for Self-Calibration Options
235073	Tune and Method Editor: Additional resolution settings are accessible for Orbitrap Exploris 240 and Orbitrap Exploris 480 (11.25k, 22.5k, and 90k)
214828	Tune: Scheduled one-point mass calibration (via Tune Preferences)

Improvements	
ID	Title
302210	Diagnostics: FlexMix Spray Optimization (neg+pos) applies Source Gases independent from polarity
310820	FAIMS: Tune Calibration pane enables One-Point Mass and Customized Mass procedures which are compatible with FAIMS attached
208815	Method Editor: User experience is enhanced when changing "Max. number of multiplexed ions"
254731	Method Execution: Spray Voltage stays "On" during the execution of Run Start EASY IC
154537	Orbitrap Exploris GC: Chromeleon: Data Audit Trail exposes 'MS Tune Reports' from Thermo Exploris Series ePanel **Note** This improvement is available only on Chromeleon versions ≥ 7.3.2.
318301	Orbitrap Exploris GC: Tune and ion source optimization reports contain a leak check history plot, filament current and emission current plots, and an emission current set value plot
327864	Tune and Method Editor: Optimized default ESI/HESI gas flow settings for Orbitrap Exploris 120, 240, MX
302209	Tune: Source gas and temperature are set independently from polarity
153260	Tune: Calibration Status panel: reworked the update of Recommended Calibration dates depending on the procedure outcome
308704	Tune: Calibration Status panel: clarified display of Last Successful Calibration to 'Outdated' after Venting and Bake-out
302209	Tune: Source gas and temperature are set independently from polarity
152982	Tune: Status pane: Added an exception for the "Temperature change since calibration" monitoring for automatically started bake-outs after venting the instrument

Table 3.   Changes realized with Orbitrap Exploris Series 4.2 Instrument Control Software relative to Orbitrap Exploris Series 4.1 Instrument Control Software, continued

280624	The Orbitrap Exploris Series 4.2 Installer updates the MongoDB from version 4.06 to version 4.0.28. **Note** MongoDB needs to be uninstalled manually when downgrading from version 4.2 to an older version. The ISO image contains a MongoDB uninstaller.

Defect Fixes	
ID	**Title**
291191	AcquireX: Method Editor needs to mark incompatible Mass List Types in red
203732	Chromeleon: Method Editor menu bar is missing
302180	Method Editor / Instrument Configuration: Settings "Contact Closure" are named the same but refer to different functions (Digital Input/Output)
245745	Method Editor: MSX ID in Mass List Table changes when switching between Quan and Qual Views
221534	MongoDB uses too large memory (>3GB) at background
318660	TurboTMT: Method Editor needs to mark the incompatible MS2 property "Scan Range Mode = Auto" in red
329295	Workstation method editor cannot be launched without Foundation installed (affects Chromeleon Enterprise)
322914	Installation of workstation OES removes previously installed workstation version
297887	System Calibration: Electronics Smart Calibration is checking against the wrong frequency range in interference peak removal procedure

Table 4 lists improvements and defect fixes in the Orbitrap Exploris Series 4.1 Instrument Control Software release that were implemented since the Orbitrap Exploris Series 4.0 SP1 Instrument Control Software release.

Table 4.   Changes realized with Orbitrap Exploris Series 4.1 Instrument Control Software relative to Orbitrap Exploris Series 4.0 SP1 Instrument Control Software

Improvements	
ID	**Title**
270859	FAIMS Pro and Pro Duo: Adjusted fan speed monitoring thresholds
254371	FAIMS Pro and Pro Duo: DV Tune and DV Check procedures operate at a wider DAC range to support FAIMS operation at altitudes > 2000 m
263849	FAIMS Pro and Pro Duo: Improved gas control to conserve cooling gas
218222	Instrument Manuals: PDF documents provide translations of the English Operating Manual and Pre-Installation Requirements Guide in Chinese, French, German (Operating Manual only), Italian, Japanese, and Spanish
229906	Tune System Calibration includes a reworked noise-canceling procedure (Interference Peak Removal) as part of the Electronics Smart Calibrations
154508	Tune System Calibration runs independent from selected Application Modes (Small Molecules, Peptide, Intact Protein)
250289	Tune System Calibration/Check: Improved robustness of the HCD Fragmentation and Trapping Efficiency Check
242936	Tune System Calibration: Further improvements of the Isolation Shape Analysis algorithm to obtain a shorter duration of system calibration procedure
232380	Tune System Calibration: HCD Fragmentation and Trapping Efficiency Check is now also part of the System Calibration
243124	Tune: The About Tune box now shows active licenses for all Orbitrap Exploris models
156731	Tune: The Status pane (By Function / By Board) displays Turbopump readbacks in the Vacuum System node

Table 4. Changes realized with Orbitrap Exploris Series 4.1 Instrument Control Software relative to Orbitrap Exploris Series 4.0 SP1 Instrument Control Software, continued

152982	Tune: The Status pane (By Function) indicates the ambient temperature change since last calibration in the new Performance node
633	Orbitrap Exploris GC: Apply a yellow warning when a fullscan range is beyond the 15x rule in method editor
622	Orbitrap Exploris GC: Remember the last used polarity to an added new line in the internal lock mass table in method editor
653	Orbitrap Exploris GC: Enable MSMS and all resolutions on the Standalone Workstation

Defect Fixes

ID	Title
164799	Chromeleon: The instrument method of extracted raw files now shows the Orbitrap Exploris model as instrument name
245000	Chromeleon: Method Editor shows AcquireX UI Elements when instrument is operated by Chromeleon
153267	Chromeleon: Method Editor: Cannot edit Mass List Tables when maximized as popup window
267594	Method Editor: Added 45000 resolution for DIA Scans
233648	Method Editor (Full Installation): RF Level Conversion is erroneous when importing methods between Orbitrap Exploris 120/240/MX and Orbitrap Exploris 480
258112	Method Editor Ion Source Properties: Gas Mode settings are available when Source Type is NSI
243767	Method Editor: Orbitrap Exploris 120 Mass List Tables: MSX-IDs are changed when saving and reopening the method
263755	Method Editor: tMS2 Scan: Method Download Validation fails with stepped Collision Energy
280344	Method Editor: When "RunStart" is selected in the global MS Settings, scan properties show "Use EASY-IC" parameter
258279	Method Execution: Multiplexing in tMS2 negative mode is not executed when polarity is a table value
261532	Tune Calibration Status: Recommended Calibration Dates need to reset after Venting and Bake-out event
258076	Thermo Foundation Instrument Configuration: The Contact Closure configuration dropdown list labels are now aligned with the Method Editor (Transition close-to-open, Transition open-to-close)
258413	Nanospray Flex Ion Source: Source interlock does not always prohibit acquisition mode
625	Orbitrap Exploris GC: Correct "Collision Energy Type" in MS2 Scan type in Tune
627	Orbitrap Exploris GC: Correct "HCD collision energy" tooltips in Method Editor
632	Orbitrap Exploris GC: Correct "Negative Quad Isolation Check" error message
636	Orbitrap Exploris GC: Add "Ion Source Optimization Report" Header to the optimization report in Tune
637	Orbitrap Exploris GC: Default "Hot link" is unchecked in Tune Preferences
640	Orbitrap Exploris GC: Change default mass and mass range under Optimization in Tune
661	Orbitrap Exploris GC: Correct "Injection Flatapole DC and Inter Flatapole Lens" names that associate to the corresponding procedures in Tune
208147	Orbitrap Exploris GC: Plot Chromatogram is not active when the system is on
250789	Orbitrap Exploris GC: User saved "Favorites" settings in Tune are not loaded if MS2 scan is defined with normalized collision energy
265908	Tune Diagnostics: Removed "ICD Calibration (No Ions Required)" from Partial Calibration tree
153053	Tune Plots: All plots need to clear when going to the next sub procedure

Table 4. Changes realized with Orbitrap Exploris Series 4.1 Instrument Control Software relative to Orbitrap Exploris Series 4.0 SP1 Instrument Control Software, continued

| 154440 | Tune Plots: Context menu "Copy to Clipboard" needs to be functional outside the graph plot area |
| 276236 | TNG Tune: Set Value Positive Ion Spray Voltage shows value "0" instead of actual set value when running sequences |

Table 5 lists defect fixes in the Orbitrap Exploris Series 4.0 SP1 Instrument Control Software release that were implemented since the Orbitrap Exploris Series 4.0 Instrument Control Software release.

Table 5. Changes realized with Orbitrap Exploris Series 4.0 SP1 Instrument Control Software relative to Orbitrap Exploris Series 4.0 Instrument Control Software

Defect Fixes	
ID	**Title**
252969	System Calibration: eFT calibration may fail due to wrong fit
253113	Orbitrap Exploris MX System Check: Negative HCD Fragmentation and Trapping Efficiency Check may fail on too low *m/z* 1506 intensity

Table 6 lists new features, improvements and defect fixes in the Orbitrap Exploris Series 4.0 Instrument Control Software release that were implemented since the Orbitrap Exploris Series 3.1 Instrument Control Software release.

Table 6. Changes realized with Orbitrap Exploris Series 4.0 Instrument Control Software relative to Orbitrap Exploris Series 3.1 Instrument Control Software

New Features	
ID	**Title**
188489	Tune: Customized Mass Calibration and Check run the Mass Calibration with User-definable mass lists.
190826	Tune: Calibration pane provides a One-Point Mass Calibration procedure using fluoranthene.
152876	Tune: Fore Vacuum supervision: The user needs to be informed if transfer tube is clogged.
153034	Method Editor: Global Settings - Internal Mass Calibration provides various internal calibration modes (RunStart, Scan-to-Scan, Timed).
154268	Method Editor: Global Settings - Internal Mass Calibration offers Lock Mass Injection functionality for user-defined lock masses.
153449	Raw file spectra provide access to extended peak data supported by FreeStyle 1.8 and higher.
Improvements	
ID	**Title**
235608	Tune and Method Editor Precursor *m/z*: Quadrupole Isolation Range checking needs to consider the first mass of the quadrupole isolation window.
236947	Tune and Method Editor Scan Range checking needs to restrict Full Scan ranges to the Factor 15 rule (Orbitrap Exploris 120, 240, 480, and MX).
214822	Tune Diagnostics: rearranged the Tools tree for improved access to the toggles and settings separated by category: Calibration, Define Scan, Application Mode, Method Setup, Peripherals.
193411	Tune System Calibration: Faster, more robust Isolation Shape Analysis algorithm results in shorter duration of system calibration procedure.
557	Tune: Mass Calibration Due Time is active in Diagnostics Pane also for Orbitrap Exploris GC.
629	Orbitrap Exploris GC Tune: Move "Quadrupole Isolation Check" and "Quadrupole Calibration" to Diagnostics Pane.
604	Orbitrap Exploris GC Tune: improvements in the Quad Iso Calibration procedure.
195617	Chromeleon: ePanel Thermo MS Tuning: Instrument Audit Trail logs information about Tune events.
225995	FAIMS Pro Duo: a firmware update mitigates 'overcooling' of the FAIMS electrodes.

Table 6. Changes realized with Orbitrap Exploris Series 4.0 Instrument Control Software relative to Orbitrap Exploris Series 3.1 Instrument Control Software, continued

ID	Title
214725	Software Manuals / Online help: New website https://www.analyteguru.com/ succeeds deprecated PlanetOrbitrap.com.
156632	Thermo Foundation Instrument Configuration: Ion Source: When toggle "Enable Sweep Gas for NSI Source" is disabled, the sweep gas will disappear from the Tune and Method Editor user interface, and inactivate the sweep gas flow.
243744	Method Editor: Full Scan: added a recommendation to set the first mass to values ≤2500 *m/z*.
203331	Method Editor: Targeted Mass Filter: Property 'Collision Energy Mode' is removed and HCD Collision Energy (% or V) allows access to 1 (fixed), and 2, 3, 4, 5 (stepped) set values.
211730	Method Editor: Targeted Scans: Property 'Collision Energy Mode' is removed and HCD Collision Energy (% or V) allows access to 1 (fixed), and 2, 3, 4, 5 (stepped) set values.
559	Orbitrap Exploris GC Method Editor: Add property "Isolation offset" to SIM scan.
217910	Method Execution: EASY-IC applies the same lock mass correction behavior for ddMS2 scans as with User Defined Lock masses.
213667	Orbitrap Exploris 120 provides access to precursor m/z isolations up to *m/z* 2500 in ddMS2/tMS2 and SIM scan types.

Defect Fixes	
ID	**Title**
204120	Tune Diagnostic procedure for ICS Burn-in and HV Current Calibration unexpectedly requires FlexMix infusion.
533	Orbitrap Exploris GC Tune: Limited the mass range in plot chromatogram and monitor mass accuracy tables.
555	Orbitrap Exploris GC: Reorder repeller and source offset values recorded in raw files under Optics table of Instrument Method section.
153327	Chromeleon: AcquireX UI Elements show in Method Editor when instrument is operated by Chromeleon.
233966	FAIMS and tSIM ddMS2 - Method Execution: MS2 scans are collected at the same CV, regardless of the CV used as a table value in the master SIM scan.
245244	FAIMS: Tune Ion Source pane: Sweep Gas is set when using "Get Default" function.
153573	Thermo Foundation Instrument Configuration: Behavior of "Enable Sweep Gas for NSI" differs from Tribrid Series Instrument Control Software.
235015	Method Editor: 45000 resolution is missing for Full MS and SIM.
153360	Method Editor: Ion Source Properties: UI validation formula for gas flows is incorrect.
243792	Method Editor: Mass List Tables: Within the same User-defined MSX ID group, different HCD Collision Energies and Adducts are restricted erroneously.
243763	Method Editor: Mass List Tables: Collision Energies (CE) are not imported when CE types (Absolute, Normalized) are different.
218273	Method Editor: tSIM + MSX methods with adjacent mass ranges are correctly validated but not executed.
237786	Method Execution: EASY-IC does not correct masses in ddMS2 scans.

Table 7 lists new features, improvements and defect fixes in the Orbitrap Exploris Series 3.1 Instrument Control Software release that were implemented since the Orbitrap Exploris Series 3.0 Instrument Control Software release.

Table 7. Changes realized with Orbitrap Exploris Series 3.1 Instrument Control Software relative to Orbitrap Exploris Series 3.0 Instrument Control Software

New Features	
ID	**Title**
153032	FAIMS Pro Duo Interface: Tune and Method Editor support Highflow LC/MS applications using HESI/APCI sources

Table 7. Changes realized with Orbitrap Exploris Series 3.1 Instrument Control Software relative to Orbitrap Exploris Series 3.0 Instrument Control Software, continued

152894	Tune: Calibration pane user interface is aligned with Tribrid Series 3.4
186434	Orbitrap Exploris 120 Method Editor provides more options: up to five experiments per method, Microscans, Multiplexing of up to 20 targets, Custom AGC Target
174361	Method Editor provides an Isotope Exclusion Filter to choose assigned or unassigned isotopes for triggering data dependent scans

Improvements

ID	Title
190370	FAIMS Pro Duo: improved AGC performance when method applies different Compensation Voltages (CV)
199341	FAIMS Pro Duo: High resolution mode definition: inner electrode temperature increased from 70 °C to 80 °C
156627	Data acquisition: Intensity display correction for very low precursor isolation widths
155669	Tune: System Calibration: improved resume function from the last valid checkpoint if procedure has failed
194014	Tune: System Calibration: improved Injection Filter Low-m/z RF Calibration to enhance ion transmission for m/z values < m/z 150 on some systems
209230	Tune: Calibration option 'Skip Spray Stability Evaluation for Mass Calibration' moved to the Diagnostics pane
189067	Tune and Method Editor support MALDI and DART sources for Orbitrap Exploris 120, 240, 480
202700	Tune: improved readability of PDF Reports for calibration, check, and diagnostics procedures
174997	Method Editor: Targeted MS2 scans and Targeted SIM scans support Polarity as a table value also when multiplexing in tSIM and tMS2 experiments
153453	Method Editor: Targeted MS2 scans support Fixed and Stepped Collision Energies as a table value also in multiplexing tMS2 experiments
166860	Method Editor: Targeted Mass Filter supports Stepped Collision Energy
187465	Method Editor: RunStart EASY-IC scans are moved to the "Prepare for Run"-time and consider more than the very last lock mass correction for a more reliable lock mass correction at the beginning of the data acquisition
155244	Method Editor: Mass List Table UI recommendations are aligned with Tribrid Series 3.4
175638	Orbitrap Exploris 480 Method Editor: Dynamic Exclusion Filter supports prefiltering data dependent scans with multiple branches

Defect Fixes

ID	Title
201250	Data Acquisition: Missing masses in Full MS when first mass is set > m/z 2500
202960	FAIMS Pro Duo: DV Tune procedure gives temporary false error alert
177971	Tune: Calibration: System always switches to Low Pressure after procedure run if in Intact Protein mode regardless of prior pressure
204120	Tune: Diagnostic procedure for ICS Burn-in and HV Current Calibration unexpectedly requires FlexMix infusion
152898	Tune: Error message for HESI vaporizer readback is incorrect on certain instruments due to wrong delta value
153397	Tune: System Calibration: When calibration fails, Recommended Date info gets lost and Performance Status shows an Error
183927	Handshake: When recording a RAW file triggered by handshake mode, one extra scan is added into RAW file
190496	Method Editor Summary: Error when printing (complex) instrument methods

Table 7. Changes realized with Orbitrap Exploris Series 3.1 Instrument Control Software relative to Orbitrap Exploris Series 3.0 Instrument Control Software, continued

198382	Method Editor: DIA method does not start because calculated window lies outside precursor mass range when Window Placement Option is active
207283	Method Execution Orbitrap Exploris 480: Cycle time is longer than defined in the method when multiple ddMS2 branches use scan priority
546	Orbitrap Exploris GC - Tune: Leak Check fails when Scans to Average is turned on in Tune.
540	Orbitrap Exploris GC - Tune: Incorrect Theoretical Masses for Negative Ions are shown in Customize Calibration within Tune.
541	Orbitrap Exploris GC - Tune: Users cannot run a normal mass calibration after a custom calibration. Customize Calibration runs even if it is not selected.
186	Orbitrap Exploris GC - Tune: Selecting "Abort" does not stop all selected Ion Source Optimizations.

Table 8 lists new features, improvements and defect fixes in the Orbitrap Exploris Series 3.0 Instrument Control Software release that were implemented since the Orbitrap Exploris Series 2.0 SP2 Instrument Control Software release.

Table 8. Changes realized with Orbitrap Exploris Series 3.0 Instrument Control Software relative to Orbitrap Exploris Series 2.0 SP2 Instrument Control Software

New Features	
ID	**Title**
152951	FAIMS Pro: Data acquisition optimizes FAIMS CV post-switching delay time when using multiple CV Voltages per experiment
153796	FAIMS Pro: Total Carrier Gas Flow succeeds FAIMS User Gas to enable lower flow rates for improved nano spray (NSI) stability
153696	FAIMS Pro: Instrument configuration supports user-defined IP addresses for FAIMS
152892	Tune Diagnostics provides restructured procedures separated by category (Partial Calibration, Optional Calibration) and polarity (Positive, Negative)
152877	Tune Diagnostics provides Low *m/z* Spectral Mass Accuracy Calibration and Check to obtain high mass accuracy also in the low mass range
154453	Tune Diagnostics provides a tool to change the Mass Calibration Due Time
153319	Tune supports Collaborator interfaces via license
153450	Method Editor supports TMTpro Reagent (TMT-16-plex) for Orbitrap Exploris 480
163618	Method Editor supports variable collision energies in a Mass List Table for multiplexing experiments
Improvements	
ID	**Title**
153497	Tune: Instrument Status pane displays vacuum pressures in a separate heading "Vacuum System"
152895	Tune: System Calibration and Check stop the syringe pump when procedure has finished to save consumption of FlexMix
152998	Tune: System Calibration: Calibration Solution Pre-Check forces the ion transfer tube to 320 °C for optimal spectral quality of FlexMix
152997	Tune: System Calibration includes an Interference Peak Removal procedure (only run after Venting and Bake-out)
152996	Tune: System Calibration provides an improved Quadrupole Main and End Segment DC Calibration
185621	System Calibration Negative: Improved robustness of ICS Active HV Current calibration subprocedure so that the procedure runs successfully after the first attempt
152994	Tune: System Check checks HCD Fragmentation/Trapping in both ion polarities
152978	Tune Diagnostics provide Tooltips for the whole diagnostics procedure tree

Table 8. Changes realized with Orbitrap Exploris Series 3.0 Instrument Control Software relative to Orbitrap Exploris Series 2.0 SP2 Instrument Control Software, continued

152897	Tune Diagnostics provide High Mass Range Calibrations (AHFP) also for Negative polarity when using Application Mode 'Intact Protein'
153051	Tune Diagnostics provides an improved Quadrupole Maintenance Check procedure
152983	Tune Diagnostics provides an improved Transfer Tube Maintenance Check procedure
154542	Tune Diagnostics procedure "Disable AGC" disables PrOSA when AGC mode = fixed
155647	Help Files: Method Editor provides an Online Help
155646	Help Files: Tune provides an Online Help
164760	AcquireX: Improved robustness for running experiments with Mass List Tables >5000 entries
152995	BioPharma: Improved eFT phase calibration to improve mass accuracy for High Mass Range applications
173884	tSIM Isolation Offset: the user can define an isolation offset for the isolation windows. The parameter is accessible as table value
152874	Method Editor: user needs to access updated System Templates as applies with the upcoming release OES 3.0
152875	Method Editor: Global MS Settings provide optimized default values per selected Application Mode (Small Molecule, Peptide, Intact Protein)
152979	Data Acquisition: RAW files include signal instability warnings in the Error Log

Defect Fixes

ID	Title
152969	Chromeleon: User cannot open Method Editor Workstation Standalone from client computer
153344	Data Acquisition: Instrument still scanning in Standby and Off mode
183927	Data Acquisition: When recording a RAW file triggered by handshake mode, one extra scan is added into RAW file
153308	EASY-IC: In Polarity Switching experiments, ICS AGC is not done for each polarity separately
166232	Method Editor: DIA peak lists do not give original values when Mass Defect is set back to 1.0005 m/z
180523	Method Editor: Could not run Quan View DIA methods when Precursor Mass Range exceeded last mass m/z 524
166862	Method Editor: DIA scan Window Placement Optimization not properly applied for non-zero Window Overlap value
153270	Method Editor: Incorrect RF Lens Value Shown when Importing Methods between Orbitrap Exploris models
152940	Method Editor: Targeted Mass Filter does not support Fixed Collision Energy as table value (SureQuant)
170714	Method Execution: Dynamic exclusion filter: Mass tolerance mode "m/z" not working
153420	Method Validation: Mismatch of Ion Source type configuration during sequence submission
153577	Tune: System Calibration: Not all 'after venting procedures' run after venting - and 'after venting procedures' run although no venting took place
162574	Tune: Ion Source pane calls wrong default (H)ESI settings when 'Current LC Flow' = 500 µL/min

Table 9 lists improvements and defect fixes in the Orbitrap Exploris Series 2.0 SP2 Instrument Control Software release that were implemented since the Orbitrap Exploris Series 2.0 SP1 Instrument Control Software release.

Table 9. Changes realized with Orbitrap Exploris Series 2.0 SP2 Instrument Control Software relative to Orbitrap Exploris Series 2.0 SP1 Instrument Control Software

Improvements	
ID	**Title**
9783	Orbitrap Exploris 120 Method Editor: Extend Data Dependent MS2 Method to create TopN experiments with N = 1,2,3,4 in DDA
9781	Orbitrap Exploris 120 Method Editor: Provide System Templates for TopN experiments with N = 1,2,3,4
Defect Fixes	
ID	**Title**
9667	BioPharma: Application Mode "Intact Protein" uses unsafe Extended Trapping 1 eV
9849	EASY-IC: ICS Prechecks should give dedicated error for extreme mass deviation
9683	EASY-IC: Issues with ICS ion intensities after prolonged idle time
9817	RunStart EASY-IC: Miscorrection when polarity switching is active
9844	System Calibration: C-Trap RF Frequency Calibration should avoid 3.2 MHz

Table 10 lists improvements and defect fixes in the Orbitrap Exploris Series 2.0 SP1 Instrument Control Software release that were implemented since the Orbitrap Exploris Series 2.0 Instrument Control Software release.

Table 10. Changes realized with Orbitrap Exploris Series 2.0 SP1 Instrument Control Software relative to Orbitrap Exploris Series 2.0 Instrument Control Software

Improvements	
ID	**Title**
9409	Limit maximum C-Trap RF for increased robustness
9261	BioPharma: Provide AHFP calibration in TNG Tune Diagnostics
Defect Fixes	
ID	**Title**
9228	BioPharma Orbitrap Exploris 240: Loss of signal at maximum S-lens RF amplitude during intact mAb LC-MS analysis
9498	DIA: Method transfer from Orbitrap Exploris Series ≤1.1 SP1 to Orbitrap Exploris Series 2.0 does not consider the new AGC Target Normalized Base 1e5
9267	Diagnostics: Quadrupole Maintenance Test switches rod configuration but does not apply rod-specific calibration set
9524	FAIMS communication LED remains off when ion source is removed and reconnected
9242	FAIMS DV Tune and Check are not always shown in Tune Diagnostics pane
9461	FAIMS: In-source CID together with FAIMS results in a defect raw file
9464	Method Execution: In-source CID is not applied for data-dependent scans
9341	System Calibration: Checkpoint "Inject Filter (IF) Calibration" separates IF Isolation Calibration and Check, trapping users with poor IF calibrations
9470	UI: Method Editor crashes when deleting Targeted Mass Exclusion Filter from the method
9283	UI: Tune: Ion Source tab: "Get Defaults" ion source values for "Current LC flow" does not work

Table 11 lists new features, improvements and defect fixes in the Orbitrap Exploris Series 2.0 Instrument Control Software release that were implemented since the Orbitrap Exploris Series 1.1 SP1 Instrument Control Software release.

Table 11. Changes realized with Orbitrap Exploris Series 2.0 Instrument Control Software relative to Orbitrap Exploris Series 1.1 SP1 Instrument Control Software

New Features	
ID	**Title**
4846	AcquireX: Orbitrap Exploris 240 and 480 support AcquireX workflows for Application Mode "Small molecule"
765	iAPI provides access to real-time control of Orbitrap Exploris 480
7514	Method Editor provides access to latest System Templates updates directly via the Thermo Fisher Cloud
8144	Method Editor: Application Mode 'Small Molecule' provides optionally access to Mild Trapping settings to reduce MS1 fragmentation of labile compounds
7513	Method Editor: Ion Source pane provides access to time-dependent ion source gas flows
5121	Method Editor: RunStart EASY-IC allows for internal mass calibration only at the beginning of the data acquisition
7512	Method Editor: tMS2 and DIA scans use isochronous injection times for multiplexing experiments
322	Method transfer: Method Editor is able to open and save methods from all Orbitrap Exploris Series instruments
7953	Tune Calibration pane: System Calibration provides improved help text in gray box, Alert Window and Calibration Reports
8174	Chromeleon: Orbitrap Exploris Series 2.0 shall run under Chromeleon 7.2.10
8173	Chromeleon: Orbitrap Exploris Series 2.0 shall run under Chromeleon 7.3

Improvements	
ID	**Title**
5012	EASY-IC: Method Execution and Tune operate IC Source in idle mode when EASY-IC is not use
8090	EASY-IC: Thermo Foundation Instrument Configuration provides the possibility to switch off the IC Source
7545	FAIMS Pro provides same optimized CV values aligned with Tribrid Series and TSQ Series instruments
7121	Method Editor: DIA Scan AGC target is aligned with Tribrid Series - Normalized Base (100%) is equal to 1e5
8542	Method Editor: Mass List Tables: MRFA is default compound aligned with Tribrid Series
8816	Method Editor: Mass List Tables: Pop-up Warning 'Columns don't match' has improved messages when importing Exactive Series Global Lists
7119	Method Editor: Targeted MS2 Scans: 'Dynamic RT' provides a Retention Time Standards Table for Pierce PRTC Mixture (Orbitrap Exploris 240 and Orbitrap Exploris 480 models)
7410	Scan Filter: Methods using Internal Mass Calibration hide "lock" to improve generating XICs from the same scan filter
8001	Tune Calibration pane: Recommended Date of a mass calibration updates after successful system calibration
643	Tune: Ion Source pane provides improved default Ion Source Parameters

Defect Fixes	
ID	**Title**
7919	Installer: Uninstallation report of Orbitrap Exploris Series 1.1 shows content of installation
7840	Instrument stays in Off mode after Data System Computer Reset
6605	Method Editor: Audit trail shows wrong number of data dependent scans
8747	Method Execution: Too much precursor ion intensity is remaining when using stepped (N)CE

Table 11. Changes realized with Orbitrap Exploris Series 2.0 Instrument Control Software relative to Orbitrap Exploris Series 1.1 SP1 Instrument Control Software, continued

ID	Title
8555	RAW file Scan Header: Precursor Fit Filter: 'Error in isotopic envelope fit' is not recorded
4972	RAW files: Instrument Method settings do not reflect Method Editor Summary content
8489	Tune cannot start because TNGConfig.xmb file gets corrupted sporadically
6095	Tune Diagnostics pane shows FAIMS procedures although FAIMS is not attached with the instrument
8869	Tune: Application Mode 'Intact Protein': Trapping voltage of Continuous acquisition is misaligned with Instrument Method acquisition

Table 12 lists improvements and defect fixes in the Orbitrap Exploris Series 1.1 SP1 Instrument Control Software release that were implemented since the Orbitrap Exploris Series 1.1 Instrument Control Software release. For details, please refer to the Online Help or the Software Manual.

Table 12. Changes realized with Orbitrap Exploris Series 1.1 SP1 Instrument Control Software relative to Orbitrap Exploris Series 1.1 Instrument Control Software

Improvements	
ID	**Title**
8053	Instrument Configuration: Check box "Enable Minimum Gas Flow Requirement for Ion Source" replaces the previous text field.
8348	System Calibration: Improved Bent Flatapole RF calibration.
8162	System Calibration: Improved Quad Transm./Rod Config Calibration.
8115	System Calibration: Removed checkpoint after quadrupole isolation calibration.
Defect Fixes	
ID	**Title**
8128	Alerts Console: Low OT temperature readback raises "Temperature too high" failure.
8297	Chromeleon: MS Tuning ePanel: Passed calibration file is named as Failed.
8180	Instrument Status: Electronics does not recognize readbacks being outside possible set range.
8284	Instrument Status: Threshold for warning "UHV gauge not ignited" is too high.
8070	Method Editor: System Templates: SureQuant method is not fully functional.
8031	Method Editor: TopN with multiple outcomes and ddSIM: Method Editor closes after appending a Targeted Mass Filter.
8040	System Calibration: Wrong threshold used in IF Low m/z RF Calibration.

Table 13 lists new features, improvements and defect fixes in the Orbitrap Exploris Series 1.1 Instrument Control Software release that were implemented since the Orbitrap Exploris Series 1.0 Instrument Control Software release. For details, please refer to the Online Help or the Software Manual.

Table 13. Changes realized with Orbitrap Exploris Series 1.1 Instrument Control Software relative to Orbitrap Exploris Series 1.0 Instrument Control Software

New Features	
ID	**Title**
7538	System Calibrations must provide improved user experience.
	User Story 4140—Tune: Diagnostics provide single-component sub procedures of system calibration.
	User Story 6961—Tune Calibration: System calibrations are resume-able. Intermediate results are saved as checkpoints. This allows for optimizing spray conditions or refilling the syringe.
365	The user must be able to define favorite scan settings for easy access to sets of parameters.
	User Story 748—Tune: Favorites pane: System Settings: Favorite settings for ESI source provide default ion source and define scan properties for calibration and diagnostics procedures.

Table 13. Changes realized with Orbitrap Exploris Series 1.1 Instrument Control Software relative to Orbitrap Exploris Series 1.0 Instrument Control Software, continued

ID	Title
7084	The Dynamic Exclusion filter must support a global list option (exclusion across experiments and outcomes).
	User Story 819—Method Editor: Dynamic Exclusion Filter provides global functionality across all experiments in the method time line (new property "Share dynamic exclusion list with other selected dynamic exclusion filters").
7126	Method Editor: Must have import list functionality from QE exported lists.
	User Story 7339—Method Editor: Import of Exactive Series mass lists (CSV files) into Orbitrap Exploris Series 1.1 mass list tables is supported.
	• Exactive Series global inclusion lists can be imported into Orbitrap Exploris Series mass list tables of scans (tMS2, Product Ion Scan, SIM Scan) and filters (Targeted Mass Filter).
	• Exactive Series global exclusion lists can be imported into Orbitrap Exploris Series Targeted Mass Exclusion Filter.
762	The instruments must be able to interface with Chromeleon Software.
	User Story 3174—Chromeleon: Tune and Method Editor are integrated in Chromeleon 7.2.10 (please install Chromeleon 7.2.10 hotfix files from thermo.flexnetoperations.com or from support.thermoinformatics.com).

Improvements	
ID	**Title**
7297	FAIMS: Acquisition sequence will pause if system recognizes a DV drop. This gives the opportunity to run a DV Check or DV Tune procedure before resuming the sequence.
7538	System Calibrations must provide improved user experience.
	User Story 6227—Tune Diagnostics: improved bake-out procedure.
	User Story 6228—Tune Calibration: System calibrations are improved regarding robustness.
	User Story 7167—Tune Diagnostics: improved ICS calibrations (EASY-IC option).
	User Story 7295—Tune Calibration: Additional calibration information is displayed in gray box.
	User Story 7328—Tune Diagnostics: "FlexMix Solution Evaluation" procedure to check for contaminated FlexMix.
7231	Tune Diagnostics: improved ion optics maintenance check.
7587	Tune Alert Window: improved messages about instrument status, calibration/check and diagnostics.
371	Users must have access to user manuals and online Help.
	User Story 2145—UI: Tune shall display tooltips for each UI element.
	User Story 2146—UI: Method Editor shall display Tooltips for each UI element.
7098	Updated system templates must be applied
	User Story 7420—Method Editor: Templates tab provides updated system templates for all application modes and for all models of Orbitrap Exploris Series MS systems.

Defect Fixes	
ID	**Title**
6490	Tune: APCI Source Optimization: Pos and Neg ion discharge current not supported.
6493	Tune: APPI Lamp of APPI ion source not controlled.
6733	Chromeleon: Data Acquisition via MS Tune panel is not supported.
6736	Chromeleon: Instrument Status ePanel needs to be configured manually.
6760	Chromeleon: Anomaly on first sequence acquisition in a series of sequences.
6790	Chromeleon: User mode selection anomaly.
6799	Instrument needs to be set to standby manually after reboot.
6812	ME and Tune GUI allows isolation low being higher than 2500.
6817	User does not reliably get a message when vacuum is not ready for instrument electronics to be set to "On" or "Standby."

Table 13. Changes realized with Orbitrap Exploris Series 1.1 Instrument Control Software relative to Orbitrap Exploris Series 1.0 Instrument Control Software, continued

6819	Tune: Define Scan: Collision Energy Mode: Stepped CE is not supported.
6821	PDF Reports: Diagnostics: Quadrupole Maintenance Check Plot not included.
6850	Tune: Status Pane: Peripheral Devices: "Turbo Pump 1" show Status "Not Connected" although turbo pump is connected.
6877	Data Acquisition via Method: Source type "ESI" not supported.
6929	After boot, Orbitrap Supply throws a warning (Device Limit exceed and Status-Warn), which can be ignored.
6930	Sometimes system calibration can fail due to unstable spray.

Known Issues

Table 14 lists all known issues that exist in the Orbitrap Exploris Series 4.2 SP1 Instrument Control Software release.

Table 14. Known Issues

ID	Severity	Title
153093	3 - Medium	Divert Valves need to be Configured for USB Control.
		Remedy: The divert valves can be controlled through interfacing with a computer. Download the MX Series II™ Control Software Program to configure the divert valves for Orbitrap Exploris: www.idex-hs.com/literature-tools/software-drivers/
153505	3 - Medium	Installer blocks workstation installation (Method Editor standalone) if there is already a Full Installation on the data system PC.
		Remedy: Run Workstation installation on a different computer. Installer supports simultaneous Workstation installation of all Orbitrap Exploris instrument models.
153665	3 - Medium	Orbitrap Exploris 480 DVD ISO image: Software Uninstallation Error.
153050	3 - Medium	Tune: Define Scan: RF Lens: Scan Range (*m/z*) may apply false parameters when hotlink is active.
		Remedy: Deselect the hotlink check box in Tune Options > Tune Preferences.
154441	3 - Medium	Tune: Display imperfect on 4 k monitor.
153627	3 - Medium	Tune: Under certain conditions, wrong number of errors and warnings is shown.
332442	4 - Low	Tune Preferences: Self-Calibration check box is enabled by default after upgrade from Orbitrap Exploris version 4.1 to 4.2.
		Remedy: Deselect the check box in Tune Options > Tune Preferences > Self-Calibration Options. New installations are not affected.
153432	2 - High	UI: Method Editor: MIPS filter incompatible with Targeted Mass filter.
		Remedy: Do not use MIPS Filter with Targeted Mass Filter.
214267	3 - Medium	Chromeleon: sporadic communication loss to Thermo Exploris Series ePanels.
		Remedy: This may happen sporadically during standby or after a sequence has finished. Restarting Chromeleon allows regain control of Thermo Exploris Series ePanel.
280624	3 - Medium	MongoDB needs to be uninstalled manually when downgrading from Orbitrap Exploris Series 4.2 to an older version.
		Uninstallation instruction:
		Right-click MongoDBUninstaller.exe and choose **Run as administrator**.
		To also uninstall MongoDB data and log files:
		1. Open command prompt in administrator mode
		2. Go to folder containing copied uninstaller
		3. Run MongoDBUninstaller.exe with argument "-f", e.g. C:\Uninstall> MongoDBUninstaller -f