

Orbitrap Tribrid Series 3.5 SP1 Release Notes

These release notes refer to the features of the Thermo Scientific™ Orbitrap™ Tribrid™ Series version 3.5 instrument control application and provide details regarding the resolved issues and known issues that still exist in the Thermo Scientific Orbitrap Tribrid Series 3.5 SP1 instrument control application.

You can use the Orbitrap Tribrid Series instrument control software to collect high-quality mass spectrometry data on the Thermo Scientific Orbitrap Tribrid Series mass spectrometers (MSs), including Orbitrap Eclipse™, Orbitrap Fusion Lumos™, Orbitrap Fusion™, Orbitrap IQ-X™, or Orbitrap ID-X™ MS systems. Control of the instrument is through two application packages: Tune and Method Editor.

- The Tune application displays acquired mass spectra in a continuous loop and continuously reports the observed values of various instrument parameters that indicate instrument status. Tune is used not only to view spectra but to provide tools to tune and calibrate the instrument for maximum performance with a variety of scan types, scan modes, ion polarities, scan rates, and resolution settings.

The Tune application provides a host of diagnostic functions for easy troubleshooting. You can also use features to manage the USB-connected devices, for example, the external divert valves and the syringe pump. Finally, this application supports report generation so that you can document the outcome of various diagnostics, calibrations, and optimizations.

- In the Method Editor application, you can set up experiments by using the entire complement of scan types, advanced filters, and conditional logic, designing customized sequences of scans to interrogate complicated samples. For example, one method might have a full scan followed by one or more filters and then a data-dependent MSⁿ level scan on the reduced mass list. You have the choice of using your preferred fragmentation technique for MSⁿ scans.

Using the Method Editor application, you can also specify peripheral device controls as part of an experiment. Methods constructed in the Method Editor can be executed in high-level applications such as the Thermo Xcalibur™ data system.

With the Thermo Foundation™ Instrument Configuration options, you can set up conditions specific to your instrument and the experiment run.

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For information about installing the Orbitrap Tribrid Series instrument control software, refer to the DVD insert or the installation instructions provided with the application. For information about configuring and using the Orbitrap Tribrid Series systems, refer to the manuals available as PDF files or the Help.

Features

The Orbitrap Tribrid Series instrument control software version 3.5 incorporates the following new and improved features:

- Support for the Orbitrap IQ-X mass spectrometer
- Support for Real-Time Library Search (Orbitrap IQ-X and Orbitrap Eclipse small molecule application mode only), facilitating decision-based triggering of MSⁿ scan events in small molecule applications
- (Orbitrap IQ-X only) Support for Auto-Ready ion source, enabling automated and remote calibration
- Support for Chromeleon™. Compatibility between Orbitrap Tribrid Series 3.5 and Chromeleon 7.2.10 MUD has been fully tested for Orbitrap IQ-X. The Chromeleon Driver Compatibility matrix is updated when other Tribrid Series models and configurations are fully tested. For more information and to view the compatibility matrix, sign on to <https://support.thermoinformatics.com/downloads/default.aspx>, and then select **Chromeleon > Chromeleon > Related Drivers > Driver Compatibility Matrix**.
- Support for the new AcquireX workflow, “Advanced Deep Scan”, including more flexible parameter settings through the Xcalibur data system 4.5.
- Support for FAIMS Pro Duo Interface through the support of additional sources (HESI/APCI)
- Data acquisition optimizes FAIMS CV post-switching delay time when using multiple CV Voltages per experiment
- FAIMS Pro: Total Carrier Gas Flow succeeds FAIMS User Gas to enable lower flow rates for improved nanospray (NSI) stability
- Advanced Peak Determination (APD) is now standard for all Orbitrap Tribrid products and benefits from application-mode specific optimization
- Support for Extended Low Mass range m/z 40 in MSⁿ scans
- (Small molecule application mode only) The Mild Trapping option is available to reduce MS1 fragmentation of labile compounds

Usability enhancements:

- Refined guidance for setting scan ranges
- Support for target-specific HCD collision energy in Targeted Mass Filter Table to improve flexibility in directed DDA
- Support for absolute and normalized HCD collision energies

Minimum requirements

These are the minimum hardware and software configurations required for Orbitrap Tribrid Series 3.5 SP1 operation.

System	Requirements
Computer	<ul style="list-style-type: none">• 3.1 GHz Quad core processor with 16 GB RAM• Video card and monitor capable of 1920 × 1080 resolution• 1 TB hard drive• DVD drive <p>Note To expedite processing time for some AcquireX workflows, Thermo Fisher Scientific recommends 32 GB of memory, even though the minimum requirement for Instrument Control Software version 3.5 SP1 is 16 GB.</p>
Mass spectrometer	Orbitrap Tribrid Series
Software	<ul style="list-style-type: none">• Microsoft™ Windows™ 10 Enterprise 64-bit Long-Term Servicing Channel (LTSC) 2019• MongoDB Community Version 4.0.6• Thermo Scientific software:<ul style="list-style-type: none">– Foundation 3.1 SP7, or later– Xcalibur 4.3 or later– FreeStyle™ 1.6 or later

General

If there are network, connectivity, or security issues, contact Thermo Fisher Scientific Technical Support to ensure that the security settings, firewalls, and antivirus software are compatible with Thermo Scientific specifications.

Installation

You must have administrator privileges to install the Thermo Scientific Orbitrap Tribrid Series instrument control software version 3.5 SP1 for the Orbitrap IQ-X, Orbitrap Eclipse, Orbitrap Fusion Lumos, Orbitrap Fusion, or Orbitrap ID-X mass spectrometers.

Before installing the instrument control software, run the calibration tests from the Tune application.

Note For any failures, run the applicable calibration procedure. If the system does not pass all calibrations, contact Thermo Fisher Scientific Technical Support.

❖ To install the Orbitrap Tribrid Series instrument control software

1. (For a new installation only) Install the Xcalibur™ data system version 4.5, as follows:
 - a. Click **ThermoLauncher.exe**.
 - b. Click **Adobe Acrobat Reader DC** to install the Adobe Reader application.
 - c. Click **Xcalibur 4.5**.

Xcalibur 4.5 installs on the data system computer and includes Foundation 3.1 SP8, FreeStyle 1.8 SP1, and Almanac agent 1.6.
 - d. Go to [step 4](#).
2. To upgrade from Xcalibur 4.3 or 4.4 to Xcalibur 4.5, do the following:
 - a. Remove all configured instruments by using the Foundation Instrument Configuration.
 - b. If SII for Xcalibur 1.4 or earlier is installed, uninstall it.
 - c. Click **ThermoLauncher.exe**.
 - d. Click **Adobe Acrobat Reader DC** to install the Adobe Reader application.
 - e. Click **Xcalibur 4.5** and proceed as follows:
 - i. Follow the installer instructions and uninstall older versions of FreeStyle, Almanac, Xcalibur, and Foundation.
 - ii. Continue installing Foundation 3.1 SP8, Almanac 1.6, Xcalibur 4.5, and FreeStyle 1.8 SP1.
 - iii. Restart the data system computer.
 - f. Go to [step 4](#).
3. To upgrade from Xcalibur 4.2 SP1 and earlier to Xcalibur 4.5, do the following:
 - a. Using the Foundation Instrument Configuration window, remove all configured instruments.
 - b. If SII for Xcalibur 1.4 or earlier is installed, uninstall it.
 - c. From the Control Panel, uninstall Xcalibur, and then uninstall Foundation.
 - d. When prompted, restart the data system computer.
 - e. Click **ThermoLauncher.exe**.
 - f. Click **Adobe Acrobat Reader DC** to install the Adobe Reader application.
 - g. Click **Xcalibur 4.5**.

Xcalibur 4.5 installs on the data system computer and includes Foundation 3.1 SP8, FreeStyle 1.8 SP1, and Almanac agent 1.6.
4. (Optional) Install SII for Xcalibur 1.6 (including Hotfix 146255) or later.
5. Start the Orbitrap Tribrid Series 3.5 SP1 installer to install the software, view the documentation, and download the release notes.
6. In the Foundation Instrument Configuration window, add and configure the system devices.

7. Open the Tune application and follow the Upgrade Diagnostic prompts:
 - a. Run **Upgrade Diagnostic – No Sample**.
 - b. Infuse the calibration solution.
 - c. With a stable spray of calibration solution, run **Upgrade Diagnostic – Calmix/FlexMix**.
8. After completing the upgrade diagnostics, run the Check Calibration tests. For any failures, run the applicable calibration procedure.

Note Contact Thermo Fisher Scientific Technical Support if the system does not pass all calibrations.

Resolved issues

Table 1 lists defects that were resolved between the Orbitrap Tribrid Series 3.4 and Orbitrap Tribrid Series 3.5 applications. Table 2 lists defects that were resolved between the Orbitrap Tribrid Series 3.5 and Orbitrap Tribrid Series 3.5 SP1 applications.

The table excludes Help issues and any cosmetic fixes. In some cases, the abstract has been amended or extended from the original to better describe the reported issue. Both an engineering fix and follow-up testing (verified by our product evaluation department) have resolved these issues.

Table 1. Resolved issues between Orbitrap Tribrid Series 3.4 and Orbitrap Tribrid Series 3.5

Item ID	Abstract
114907	Addressed a communication error associated with the UVPD laser controller, leading to a CLOL fault.
178345	Addressed an issue associated with the coarse calibration adjustment.
178144	Addressed a problem in which split peaks could be observed only after instrument bootup.
207169	Addressed an issue associated with possible signal intensity fluctuation under specific acquisition conditions (DDA MS2 OT analysis used with resonance CID activation type and Auto Mass Range setting).
200364	Addressed shortcomings in IC Make-up Flow calibration.
189920	Addressed an issue associated with instrument methods including data dependent MS2 triggered MS2 acquisition using UVPD activation.
193188	Addressed a problem in which when creating a new acquisition method from a previously saved method, if the “Internal Mass Calibration” setting is switched from “User-defined Lock Mass” in the previously-saved method to “Off” in the newly created acquisition method, the application of the “User-defined Lock Mass” remains active in subsequent runs performed with the new acquisition method.
211560	Addressed an issue when combining UVPD and assisted CE in the same method (crash). Modification made to obtain method validation failure under these conditions.
145263	Addressed a possible issue in acquisition when combining MIPS and Targeted Mass filters.
165217	Modified recommended date for calibration of pAGC from 7 to 28 days after last successful calibration.
166911	Addressed an issue with defining several static modifications on a given site within Real-Time search node. Modification made to obtain method validation failure under these conditions.
167131	Modified auto turn on/off behavior of syringe pump in order to automatically switch it off after running long auto calibration procedures (> 10 mins).
198523	Modified inner electrode temperature in FAIM high resolution mode from 70 °C to 80 °C.
212811	Addressed an issue in which multiple observed peaks can be associated to common theoretical fragment ions in database search results, leading to overlapping SPS windows and therefore lower SPS match efficiency in TMT SPS MS3 acquisition.
208427	Addressed an issue in methods which include multi-level ddSIM scans. Modification made to avoid creation of such methods and obtain validation failure of such already existing methods.

Known issues

Table 2. Resolved issues between Orbitrap Tribrid Series 3.5 and Orbitrap Tribrid Series 3.5 SP1

Item ID	Abstract
241607	Addressed an issue that occurs when running the diagnostic Calibration > Main Calibration > Optics > Calibrate Source RF Scaling using traditional Cal Mix calibration solution.
241708	Addressed a problem in which after polarity switching and during a long-term mass stability test run, some masses are missing and result in a test failure.
230940	Addressed an issue associated with over-cooling of the FAIMS inner electrode under certain conditions, which prevents the system from achieving the FAIMS Standard Resolution setting.

Suggested recovery actions

- For some issues like connectivity problems, restarting the application is the appropriate recovery action.
- In some cases (particularly issues that arise during data acquisition), restarting applications such as the Xcalibur data system might not ensure complete recovery. Typically, restarting the data system computer resolves issues, but some devices with error conditions might require power cycling.
- As a fix we generally do not recommend reinstalling the software or the operating system, which more commonly occurs after you install a new hard drive.

Feature requests and other removed items

- We do not include issues where there is insufficient information logged to successfully reproduce the reported problem.
- We do not list feature requests as software issues, regardless of the reported significance or severity of the request. Product managers evaluate logged feature requests for future releases.
- We report only discrepancies in the documented software as known issues.

Terminology

Table 3. Severity levels

Severity	Interpretation
Crash/Data Loss	A problem that renders the system unusable because either an entire function is unusable and no workaround exists, or use of the current system compromises data integrity or results in data loss. Catastrophic problems also include significant and non-obvious quantitative errors, and all human and instrument safety issues.
Major Problem	A serious issue that does not affect data integrity (meaning data loss, corruption of data, or the wrong answer), but affects the customer's ability to use the product as designed. It can be a failure, design issue, or documentation error or omission. A workaround might or might not exist.
Minor Problem	A minor error or poor behavior of a product feature. There is probably a workaround.
Cosmetic	An issue that has a limited effect on customer usage of the product; for defects with visibility so low that a customer might never see it; or for ease of use issues or other items not causing any performance degradation.

Table 4. Risk levels

Risk	Interpretation
High	Occurrence is likely to happen and can compromise operation.
Medium	Occurrence is uncommon, but could compromise operation if it occurs.
Low	Issue is minor; however, the software could operate differently from a user's expectations. A workaround might be available.
No Risk	This issue causes no problem but is commonly an inconsistency or cosmetic issue.

Known defects

Table 5 contains a known defect in the software, categorized by software section, with a brief abstract and information related to the defect's severity and risk, if applicable. The Item ID is the internal number assigned to the issue, if applicable. Product management assesses risk, which can differ significantly from the reported severity.

Table 5. Known software issues

Item ID	Severity	Abstract	Risk
57094 (73337)	Minor Problem	<p>Raw files under Windows 10 do not open properly by using the View Raw File button or by directly double-clicking the raw file.</p> <p>To open a raw file, navigate to it, right-click the file, and then browse to the FreeStyle application. Select the check box to always open a raw file with FreeStyle. FreeStyle is now the default application to open raw files.</p>	Low
210023	Minor Problem	<p>When running Orbitrap Tribrid Series software version 3.5 SP1 under Chromeleon 7.2.10 MUD, an error message appears in the Chromeleon audit trail: "Double Property Bearing_Temperature cannot be updated with TP_RUNNING".</p> <p>The error occurs when first opening Chromeleon or when adding the mass spectrometer to the Chromeleon instrument configuration.</p> <p>Note This error does not affect the operation of the Orbitrap Tribrid instrument.</p>	Low
249802	Major Problem	<p>Following acquisition with Orbitrap Tribrid Series software version 3.5 SP1 under Chromeleon 7.2.10 MUD while using a method in which Application Mode is set to Peptide, the resulting file created cannot be opened or exported.</p> <p>When attempting to export the file in RAW format, the error, "Cannot load raw data for item", appears. In this case, you will not be able to view the file in Chromeleon, Xcalibur, or FreeStyle.</p> <p>Workaround: Set the Application Mode to Small Molecule <i>before</i> saving the methods (you can create MS Methods in the Peptide Application Mode from the available scans, filters, and templates).</p>	High

Trademarks

AcquireX, Almanac, Chromeleon, Orbitrap Eclipse, Eclipse, Orbitrap IQ-X, IQ-X, Orbitrap ID-X, ID-X, FlexMix, Foundation, and FreeStyle are trademarks; and Orbitrap, Orbitrap Fusion, Orbitrap Fusion Lumos, Thermo Scientific, Tribrid, and Xcalibur are registered trademarks of Thermo Fisher Scientific Inc. and its subsidiaries in the United States.

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