Orbitrap Tribrid Series 4.2 QF1 Release Notes

These release notes list the new features of the Thermo Scientific[™] Orbitrap[™] Tribrid[™] Series 4.2 QF1 instrument control software, provides details of resolved issues, and details of the known issues that still exist in the software.

The instrument control software is used to collect high-quality mass spectrometry data on the following Thermo Scientific Orbitrap Tribrid Series mass spectrometers.

- Orbitrap Ascend[™] Editions
 - Orbitrap Ascend[™] BioPharma
 - Orbitrap Ascend[™] MultiOmics
 - Orbitrap Ascend[™] Structural Biology
- Orbitrap Ascend™

- Orbitrap Eclipse™
- Orbitrap IQ-X™
- Orbitrap Fusion Lumos™
- Orbitrap ID-X™
- Orbitrap Fusion™

The instrument control software consists of the Tune and Method Editor application packages that enable control of the instrument.

• The Tune application displays acquired mass spectra in a continuous loop and sequentially 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 valve 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.

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

For more information, see the following topics:

- Features
- Minimum requirements
- Resolved issues
- Known issues

Features

The Orbitrap Tribrid Series 4.2 QF1 instrument control software incorporates the following new and improved features:

- New Hardware support (Orbitrap Ascend Editions only)
 - High-Quad for controlled isolation up to 8,000 m/z
 - High mass calibration support (High-Quad only)
 - Quadrupole frequency switching support (High-Quad only)
- **New** Tune Alert window
- New Fragment ion indexing for RTLS
- New Extended enzyme list for RTS searches
- New Exclude isotopes for Targeted Mass Exclusion and Targeted Loss Exclusion filters
- New Resolving power options for Orbitrap scans 90K and 75k (not for ID-X and IQ-X)
- New Support for TMT 32plex
- Enhanced Unclog routine to unclog Auto-Ready source emitter
- Enhanced Input for HCD scan types in Tune. Input field now accepts 1–5 values to control single or stepped collision energy mode

Usability enhancements:

- Improved injection time parallelization
- Improvement to SPS calibration routine
- Improved template management (Orbitrap Ascend Editions only)

Minimum requirements

System	Requirements
Computer	 3.1 GHz Intel[™] Quad-Core processor
	16 GB RAM (32 GB recommended)
	1 TB hard drive
	Two Ethernet gigabit network ports
	DVD-ROM drive
	 Monitor display resolution of 1920 × 1080
Software	 Microsoft[™] Windows[™] 10 Enterprise LTSC 2019
	Thermo Scientific software:
	 Foundation 3.1 SP9
	 – Xcalibur™ 4.7
	 – FreeStyle™ 1.8 SP2 QF1

The minimum hardware and software system requirements are as follows:

Resolved issues

The following tables lists defects that were resolved between the different releases of the Orbitrap Tribrid Series instrument control software. Engineering fixes have resolved the issues with follow-up testing performed by the Product Evaluation department.

NOTE: The information excludes Help issues and cosmetic fixes. In some cases, the abstract description has been amended or extended from the original to better describe the reported issue.

 Table 1
 Resolved issues between Orbitrap Tribrid Series 4.2 and Orbitrap Tribrid Series 4.2 QF1

Item ID	Abstract
633841	Resolved issue of the wrong polarity being applied during ETD calibration. This prevented the anion calibration of trap to trap transfers.

Table 2 Resolved issues between Orbitrap Tribrid Series 4.1 SP1 and Orbitrap Tribrid Series 4.2

Item ID	Abstract
441169	Resolved issue of incorrect polarity being applied to ddMS ² when negative polarity was added to the table.
456319	Fixed issue of pressure mode automatically switching after a reboot. System now retains pressure mode state after reboot.
373773	Fixed issue of ETD reagent mass and isolation width being improperly applied after ETD Quad Transmission check.

Item ID	Abstract
436417	Fixed error that displayed an incorrect validation error during method download.
487154	Resolved issue of incorrect prescan window being applied for tMS ² scans.
489989	Aligned collision energy units between error warning and set value.
494904	Improved the mass list for isotope interactions calculation.
495431	Fixed issue of incorrect injection time when using Orbitrap for MS ¹ and MS ² scans for ddMS ² scan types.
600362	Resolved issue of IAPI ignoring AGC targets for intermittent scans.
598094	Fixed issue of TNG manger crashing when raw files are being saved during manual acquisition with insufficient disk space.
597507	Resolved naming issue of Activation type in scan header as to not interfere with downstream processing tools.

 Table 3
 Resolved issues between Orbitrap Tribrid Series 4.1 and Orbitrap Tribrid Series 4.1 SP1

Item ID	Abstract
453071	Orbitrap losing signal after instrument reboot has now been resolved.
464862	Addressed issue of UHV bearing temperature reporting inaccurate change rate and causing Bakeout procedure to stop.
465458	Resolved issue of RTLS method validation error on IQ-X systems.
465755	Resolved incorrect handling of charge state while using ETD, UVPD, and PTR activation types for MS ⁿ scans.
466029	Resolved issue of Ion guide 3 RF level being incorrectly set during MS ³ methods.
489984	Addressed issue of incorrect HCD energy being displayed in the scan header for multiplex experiments.
467505	Corrected issue of DIA optimized windows calculation.
466518	Resolved issue of incorrect collision energy being applied during tMS ² methods.

Item ID	Abstract
396880	Resolved issue of FAIMS cooling gas going too high even though temperature and source settings are reasonable.
421851	Addressed issue of improper ppm tolerance warning when using CE per compound in an inclusion list.
448902	Addressed issue of HESI and Auto-Ready spray voltage being on during Evaluate Long Term Mass Accuracy.
440635	Resolved issue of comet sometimes carrying over variable modifications when sequential RTS methods were ran.

 Table 4
 Resolved issues between Orbitrap Tribrid Series 4.0 SP1 and Orbitrap Tribrid Series 4.1

Item ID	Abstract
331259	Improved speed of quadrupole transmission check.
446282	Resolved issue of incorrect injection times when using API for targeted methods.
437495	Issue of source voltage optimization not working with ESI source resolved.
416244	Resolved loss of ions during tMS ⁿ OT scans due to poor RF settings applied.
317498	Addressed a shift in Mass Accuracy observed when user changes scan conditions during "Monitoring Mass accuracy" plot.
427125	Resolved issue where user defined target, set in diagnostic, for Internal Cal was not being applied.
416243	Addressed issue of incorrect scan range being applied to tMS ⁿ methods.
393025	Addressed issue of multiple tMS ⁴ experiments in sequence slowing down instrument scan time.
375264	Resolved issue on ID-X of inaccurately reporting fail on Q0 ID Diagnostic.
356288	Resolved intermittent issue of system checking the syringe pump when Auto-Ready source is being used.
350110	Resolved issue of not being able to toggle full profile view in diagnostics after Evaluate Modulation or Evaluate Second Harmonic diagnostics had been run.
349547	Resolved issue of system shutdown when UHV reported vacuum was too good.
337388	Addressed intermittent issue of Self-Check not confirming Auto-Ready was configured.
336512	Addressed issue of reports being generated before diagnostic completed.

Table 5	Resolved issues	between Orbitrap	Tribrid Series 4.0) and Orbitrap	Tribrid Series 4.0 SP
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Item ID	Abstract
357099	Addressed an issue in which injection time may oscillate during LC-MS runs of intact proteins on Orbitrap Ascend system.
357152	Addressed an issue in which Discharge Pressure Check fails due to readback error on Orbitrap Fusion ETD system.
357636	Modified accepted range for energy dependency on Orbitrap Ascend system.
358602	Addressed incorrect application of isolation waveforms in MS ⁿ experiments when ion trap isolation is used for more than one stage.
363649	Addressed an issue in which new changes in "Peak Selection and Threshold Settings" properties are not properly synchronized across multiple Real-Time Search filters after re-opening a method previously saved with "Use Common Peak Selection and Threshold Settings" option selected.

Item ID	Abstract
219580	Corrected IQ-X 7.5k RP default maximum injection time to 11ms (instead of 22ms).
262323	Addressed an issue preventing the display of Method Editor menu bar in Chromeleon.
266405	Modified reference volume of Auto-Ready vial to 4mL (instead of 5mL).
281784	Addressed an issue related to mislabeled Contact Closure options in Instrument Configuration.
296415	Addressed an issue related to the validation of methods including Dynamic Exclusion filter.
315166	Modified messages in calibration reports generated with Auto-Ready Ion Source.
320242	Added 'Calmix Evaluation Toggle' in Diagnostics.
326968	Addressed an issue in which workstation method editor could not be launched without Foundation installed (affects Chromeleon Enterprise).
328502	Added 'Set Spray Voltage' in Diagnostics for Auto-Ready.
276030	Addressed an issue in which ion transfer efficiency may be reduced during acquisition from Tune following the execution of a "View EASY-ETD Reagent" scan in Tune ("Define Scan" tab).
300995	Addressed an issue in which ion current maybe lower than expected in polarity switch experiments.
279631	Addressed a memory consumption issue with methods using Assisted Collision Energy in conjunction with Easy-IC.
279373	Addressed an issue related to inaccurate HCD fragment efficiency calculation.
215549	Addressed an issue in which multiple API licenses are reported in Tune.
269263	Addressed an issue related to FAIMS Pro fan speed out of range.
270254	Addressed an issue related to FAIMS DV status check.

Table 6 Resolved issues between Orbitrap Tribrid Series 3.5 SP2 and Orbitrap Tribrid Series 4.0

Known issues

Discrepancies in the documented software are reported as known issues. Items that are not included as part of the known issues are as follows:

- Issues where there is insufficient information logged to successfully reproduce the reported problem.
- Software feature requests, regardless of the significance or severity. The product management team evaluates feature requests for future releases.

Follow these general recommended recovery actions, as applicable:

NOTE: Do not reinstall the instrument control software or the operating system as a general fix. Contact Thermo Fisher Scientific Technical support for assistance.

- Restart the instrument control software for connectivity issues.
- Restart the data system computer for issues that arise during data acquisition. Devices that display an error state may also require a power cycle.

Review the severity levels and risks levels of the known issues as defined in the following tables.

Table 7 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 user'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 8Risk 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.

The following table lists the known issues in the instrument control software. The table is categorized with an Item ID (the internal number assigned to the issue), severity and risk levels, and a brief abstract description of the issue. The product management team assesses the risk, which can differ significantly from the reported severity.

Item ID	Severity	Description	Risk
607398	Minor Problem	Incorrect UVPD activation time applied in targeted methods. The scaling factor for UVPD activation is not consistently applied between MS ² and MS ³ when the combination of "Use molecular weight calibrated UVPD activation time" and user defined UVPD activation % is set.	Medium
405168	Minor problem	FAIMS CV readback in Tune show -16V when no voltage is applied. This is a readback error only and corrects itself after an initial injection.	Low
606058	Minor problem	UVPD data missing from method summary report in raw data. When UVPD is not added to a mass list table the method summary shows the UVPD as not active.	Medium
603712	Cosmetic	When Enable recommendations is active, MIPS is not showing an error within the Method Editor when being used with lon trap scans.	No risk

Item ID	Severity	Description	Risk
595670	Cosmetic	Alerts Console does not freeze scrolling when active warnings are reported in the Tune alerts window.	Low
595669	Cosmetic	IQ-X only, Tune alerts window repeatedly triggers and clears N2 gas warning when the nitrogen supply is turned off. This fills the alerts window and can't be cleared until nitrogen supply is returned.	Low
507203	Cosmetic	MS ² and MS ⁿ scans briefly show a validation error for ETD when polarity is switched.	Low
468631	Minor problem	Number of average scans not being correctly displayed in the scan title when a method is acquired from Tune. The average data is not impacted but the number of scans used is not captured correctly in the scan header.	Low
547944	Minor problem	After downgrading from Orbitrap Tribrid Series (OTS) 4.2 to an older version, reports are no longer generated. This is because the OTS 4.2 installer updates the MongoDB with unique password, which is different from single hardcoded password used in older versions. Due to this the authentication fails and database is inaccessible.	Low
		Workaround: Manually uninstall the MongoDB when downgrading OTS 4.2 to an older version by using the MongoDB uninstaller provided with OTS 4.2. Follow these steps:	
		Open a command prompt	
		 Navigate to the folder containing the uninstaller 	
		 Type MongoDBUninstaller -f and press Enter (e.g., C:\[folder]\MongoDBUninstaller -f) 	
591027	Minor problem	Turbo pump 1 status not updated when system is spinning down. In short the power consumption will correctly show the 0 watts and the status as green but it should show a warning.	Low
611503	Minor problem	Some AcquireX templates will cause the system to crash if they are run through the Tune application. The reason for the crash is templates do not contain any targeted masses. User should run template methods via the Method Editor.	Medium
626319	Minor problem	UVPD activation energy is displayed incorrectly when "use calibrated value" is used in conjunction with a percentage of the value. This is only for tMS ⁿ scan and DIA scans. The user can ensure the correct value is used by simply applying a standardized reaction time value for UVPD.	Medium
641505	Minor problem	Ardia platform users may encounter an error where the DDI server is clogging the DS log file. TNG is putting unexpected calls into DDI service with invalid device key repeatedly logging every few seconds.	Medium
		Workaround: FSE/Tech support needed to assist.	
		Uninstall Ardia	
		Delete C:\ProgramData\Thermo Scientific\Ardia directory	
		 Reinstall same version of Ardia 	