Thermo Scientific Orbitrap Astral Series 2.0 Instrument Control Software Release Notes

This document lists installation notes, new features and improvements regarding the Thermo Scientific™ Orbitrap Astral™ Series 2.0 Instrument Control Software release. For information regarding the installation, features, functionality, and use of this product, refer to the following sources of information:

- *Orbitrap Astral Operating Manual*
- *Orbitrap Astral Zoom Operating Manual*

Installation notes

This section describes the supported target systems and the system requirements.

Supported target systems

- Thermo Scientific Orbitrap Astral mass spectrometer
- Thermo Scientific Orbitrap Astral Zoom mass spectrometer

System requirements

The minimum hardware and software configurations required for Orbitrap Astral Series 2.0 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
	DVD-ROM Drive
	Display Monitor Resolution of 1920 × 1080
	Two Network Interface Cards (NIC), 1000 MBit/s
Software	Microsoft™ Windows™ 10 Enterprise 2021 LTSC
	Thermo Scientific™ Xcalibur™ 4.7 SP1

TIP: The Orbitrap Astral Series 2.0 Instrument Control Software was only tested within the delivered composition.

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Installation

TIP: Prepare the computer in advance of any new installation.

NOTE: **All Users**
Please perform a System Calibration or a Mass Calibration after a software upgrade or downgrade.

NOTE: **FAIMS Users**
Please reboot the FAIMS unit after the installation of the Orbitrap Astral Series 2.0 Instrument Control Software (switch Main Control Box off and on).

This guidance addresses a standard installation of a Windows computer acting as an access point for Orbitrap Astral based instruments. The current software version is 2.0. 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 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 Astral Series instruments is highly recommended for setting up a new PC.

Technical requirements

Choose a PC equipped as described at “System requirements”.

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 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

> **TIP**: Do not start the software installation before the network setup has been completed. See “Network Setup”.

File locations

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

This instruction list uses C:\ProgramData\Thermo\Astral for easy reading, but depending on the installation package like Orbitrap Astral Instrument Control Software kit, this may be different. When the Orbitrap Astral 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”) should be saved if present:

- C:\ProgramData\Thermo\Astral\instrument\msx_instrument_files
- C:\ProgramData\Thermo\Astral\Licenses.txt
- C:\Program Files\Thermo Scientific\Instruments\Astral\2.0\System\Programs\dependencies\msi\TNGConfig.xmb

Setup of a new computer without any backup requires assistance of the Orbitrap Astral 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 OrbitrapAstralFullSetup.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 Astral 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”.

> **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

Procedure

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 has 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. If in doubt, contact the Orbitrap Astral 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.

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

Supported instruments

The instruments listed in the table below are supplied and supported in this release.

Table 1 Supported instruments

Instrument Control Software Version	Version No.	Instrument	
		Orbitrap Astral	Orbitrap Astral Zoom
1.0	1.0.100.11	✓	–
1.0 SP1	1.0.100.14	✓	–
1.0 SP2	1.0.100.28	✓	–

Instrument Control Software Version	Version No.	Instrument	
		Orbitrap Astral	Orbitrap Astral Zoom
1.0 SP3	1.0.100.40	✓	–
1.1	1.1.477.46	✓	–
2.0	2.0.690.11	✓	✓

New features and improvements

The table below lists new features, improvements and defect fixes in the Orbitrap Astral Series 2.0 Instrument Control Software release that were implemented since the Orbitrap Astral Series 1.1 Instrument Control Software release.

Table 2 Changes realized with Orbitrap Astral Series 2.0 Instrument Control Software relative to Orbitrap Astral Series 1.1 Instrument Control Software

ID	Severity	Title
New features		
488673	—	Orbitrap Astral Zoom: Faster Ion Optics Switching: Higher acquisition rate with improved ion optics switching times
740686	—	Orbitrap Astral Zoom: Faster Ion Processor Timings: Higher acquisition rate due to faster ion transfer in the Ion Processor
491850	—	Orbitrap Astral Zoom: Pre-Accumulation: The user needs bent-flatapole pre-accumulation
595718	—	Orbitrap Astral Zoom: Application Mode: The user needs a "Low Input" Application Mode
595715	—	Orbitrap Astral Zoom: TMT 32-Plex: The user needs a TMT HR mode to resolve the signal of all reporter ions
449007	—	Orbitrap Astral Zoom: Peak Picking: The user needs Full Astral MS2 Spectrum Peak Picking
491831	—	Orbitrap Astral Zoom: SureQuant Hybrid DIA: The user needs to perform SureQuant type and derived Hybrid DIA acquisition using Astral analyzer
747451	—	Orbitrap Astral Zoom: Faster Stepped NCE in IRM: The user needs faster Astral MS2 acquisition when using stepped Collision Energy
424340	—	Orbitrap Astral Zoom: The user needs Top-Down Acquisition with Astral MS2 scans
169738	—	Orbitrap Astral Zoom: eDR: The user needs to perform eDR Full Scan-type ion detection
650535	—	Orbitrap Astral Zoom: tSIM msx: The user needs the ability to execute methods with multiplex tSIM with Orbitrap analyzer

ID	Severity	Title
Improvements		
745468	—	Astral MS2 Scan Range: The user needs expanded functionalities of Astral MS2 Scan Range
745777	—	System Calibrations must provide improved user experience
749850	—	Add "Exclude isotopic cluster" option to Targeted Mass Exclusion filter
749864	—	The user needs individual maxIT settings in DDA w/ inclusion list (directed-ddA)
778704	—	RAW File Scan Header: The user needs the ability to differentiate tMS2 and DIA scans via the scan header
Defect fixes		
639247	3 - Medium	UI: ME: Orbitrap Astral Method Summary for DIA does not report the correct parameter used for Loop Control
747865	3 - Medium	UI: ME: Factor 15 Rule is applied for Astral MS2 scan range unexpectedly
784006	3 - Medium	UI: ME: RAW File Instrument Method erroneously reports Astral Resolution
808914	3 - Medium	UI: XML Method Modification has dysfunctions
639762	3 - Medium	After changing at setting in Tune, while the Instrument is in Intact Protein mode, Injection Time is unregulated
631487	3 - Medium	Method Execution: nCE values are translated in CE values above 200 V
763179	1 - Critical	RunStart ICS degrades mass accuracy
776401	1 - Critical	Automatic Ion Foil Offset Adjustment leads to failing mass evaluations with large mass errors
779710	4 - Low	Tune: Calibration and Diagnostics Start button - procedure "cancelled by user", after internal error

The table below lists new features, improvements and defect fixes in the Orbitrap Astral Series 1.1 Instrument Control Software release that were implemented since the Orbitrap Astral Series 1.0 SP3 Instrument Control Software release.

Table 3 Changes realized with Orbitrap Astral Series 1.1 Instrument Control Software relative to Orbitrap Astral Series 1.0 SP3 Instrument Control Software

ID	Severity	Title
New features		
491821	—	Stepped CE Astral: The user needs the ability to perform the acquisition of single MS2 scan with multiple Collision Energy values when using Astral detector Type

ID	Severity	Title
425845	—	Full Profile OT: The user needs the ability to perform Orbitrap MS1 and MS2 acquisition with Full Profile in Intact Protein Mode
Improvements		
610911	—	NSI: The user needs an updated default value of Positive Spray Voltage for NSI in ME and Tune
431751	—	Orbitrap Astral shall automatically correct the ion foil voltage using the ICS
597081	—	FAIMS CV switching performance shall be improved
496128	—	UI: ME: The user needs the "Lock mass injection" to be a parameter in the scan properties for each scan type
407868	—	Method Editor: The System Templates must be saved in "Astral" folder
434211	—	UI: ME: The user needs the possibility to choose "Use EASY-IC" On/Off for each experiment/scan type in Timed Mode
469200	—	UI: ME: The user needs to be able to see the displayed absolute AGC target values
408025	—	Tune: Favorites/UserSettings and History information must be saved in "Astral" folders
448670	—	The user needs the ability to monitor pressure readbacks for Astral Analyzer in Tune
Defect fixes		
458725	3 - Medium	MongoDB uses large memory (>3GB) at background
459860	3 - Medium	If in DIA experiments (using Astral detector) a Loop Time is defined, as shorter than the Orbitrap transient time set in another experiment of the method, the instrument schedules not enough DIA scans to match the expected loop control time
594611	3 - Medium	Fluxscans are not used in edge cases (fm/lm +/- isolation width)
597496	3 - Medium	DIA: Methods miswriting mass window centres as 524.265 in raw file instrument method
598230	3 - Medium	Missing Plot: Mass Calibration
591844	3 - Medium	Tune: Pressure Mode always set to Standard Pressure after startup
592082	3 - Medium	Tune UI: Astral Turbo pumps readbacks are swapped
467823	3 - Medium	Issue with DIA Windows Definition with Windows Optimization "On" under certain conditions

ID	Severity	Title
470082	3 - Medium	Max IT information is not copied when using copy/paste functionality of MS2 information - instead default max IT (10 ms) is used
439849	3 - Medium	"Use EASY-IC" dropdown is not available if LM correction mode is set to "timed"
412392	2 - High	Instrument reported to be set to standby because of open source, but continued the sequence
424847	3 - Medium	The search window for the EASY-IC lockmass is shifted by outliers
426171	3 - Medium	"Bakeout cooling time" and other ICB/HICB timers are reset by software update
415413	3 - Medium	Astral Mass Stabilization is performed at different timepoints within a LC-MS run
455566	3 - Medium	Syringe does not get turned off during Electronics Smart Calibration in User System Calibration
456040	2 - High	Setting the Funnel RF Level to default is not in Astral Default Scan Settings

The table below lists defect fixes in the Orbitrap Astral Series 1.0 SP3 Instrument Control Software release that were implemented since the Orbitrap Astral Series 1.0 SP2 Instrument Control Software release.

Table 4 Changes realized with Orbitrap Astral Series 1.0 SP3 Instrument Control Software relative to Orbitrap Astral Series 1.0 SP2 Instrument Control Software

Defect Fixes		
ID	**Severity**	**Title**
466217	1 - Critical	Large Time Gap between MS1 and data-dependent MS2 scan.
553186	2 - High	Insufficient IRM settling time causing unstable fragmentation pattern in Orbitrap MS2 scans.
452322	1 - Critical	Ion Control not working well under low intensity, high background conditions.
414707	3 - Medium	False positive initial bus error warnings from DPRTrap Board.
427472	2 - High	Detector Calibration failing with “Too few ions in focused peak.”
449905	2 - High	Suboptimal setting of channel saturation threshold.
234095	2 - High	Astral analyzer pressure readbacks not displayed in Tune.

The table below lists defect fixes in the Orbitrap Astral Series 1.0 SP2 Instrument Control Software release that were implemented since the Orbitrap Astral Series 1.0 SP1 Instrument Control Software release.

Table 5 Changes realized with Orbitrap Astral Series 1.0 SP2 Instrument Control Software relative to Orbitrap Astral Series 1.0 SP1 Instrument Control Software

Defect Fixes		
ID	**Severity**	**Title**
357681	4 - Low	Method execution waits for temperatures to stabilize while 'Wait for Temperatures to stabilize' option is unchecked in Instrument Configuration.
361874	3 - Medium	Missing fields in the scan header/trailer.
398882	3 - Medium	AGC calculations for method using more than one FAIMS CV (delta>1) are based on single CV.
403091	3 - Medium	Raw file: Scan headers of ASTMS scans report irrelevant FT resolution.
407881	3 - Medium	Data Acquisition using lock mass correction is not aborted while Internal Calibrant Source is faulty/ defective.
396718	1 - Critical	Data Acquisition: FAIMS occasionally returns “source is open” right after the start of a method while source is closed.
416835	1 - Critical	Both the restart from an error as well as quick system restart fail with a restart loop.
418457	1 - Critical	Orbitrap mode scan rate too low after reboot of system.
424800	3 - Medium	Orbitrap easyIC lockmass correction (timed / Scan-to-Scan modes) is not functional if the first mass of the scan range is above *m/z* 275.
424984	1 - Critical	Failing Signal Stability Evaluation - high TIC variations in Orbitrap signal.
425564	3 - Medium	Bake-out plot is not redisplayed after the system entered standby.
427904	3 - Medium	Block voltage insufficient for Curve Corrector on systems with large non-zero curve corrector settings.
428554	3 - Medium	Activating microscans shifts the mass centroid in Astral spectra.
429956	3 - Medium	TNG System Check Negative: system
429981	3 - Medium	“Short burn-in of ICS” is always run during System Check.
430132	3 - Medium	Previous plot is not redisplayed after Astral analyzer polarity switch.
430259	1 - Critical	Discharge evaluation not actually setting to negative mode during discharge event.
431767	3 - Medium	Missing Quick Gas Capillary Check to allow the user to assess if a capillary is blocked.

Defect Fixes		
433742	3 - Medium	Scan Start Timing fallback option may lead to out of order retention times.
434485	3 - Medium	Missing checks in Tune Diagnostics.
436967	3 - Medium	Astral service bundle mostly empty (no astral data).
442099	2 - High	System Calibration: Quad RF DDS frequency does not get set always on boot.
450428	1 - Critical	After performing Mass and System check from Tune, a drift of about 1 *m/z* unit may be observed in mass spectra acquired with Astral detector.

The table below lists defect fixes in the Orbitrap Astral Series 1.0 SP1 Instrument Control Software release that were implemented since the Orbitrap Astral Series 1.0 Instrument Control Software release.

Table 6 Changes realized with Orbitrap Astral Series 1.0 SP1 Instrument Control Software relative to Orbitrap Astral Series 1.0 Instrument Control Software

Defect Fixes		
ID	**Severity**	**Title**
412822	1 - Critical	Occasionally spikes can be observed in ion chromatogram while ion spray stable.
419732	1 - Critical	EASY-IC: Lockmass expected position does not change with polarity.
421872	1 - Critical	XML method modification interface is not functional.
419661	2 - High	System Calibration/Check: Change PrOSA Scaling specifications.
416053	3 - Medium	System Calibration/Check: HCD Fragmentation and Trapping Efficiency Check leads to a SW internal failure (occasionally).

Known issues

The table below lists all known issues that exist in the Orbitrap Astral Series 2.0 Instrument Control Software release.

Table 7 Known Issues

ID	Severity	Title
347288	4 - Low	Tune: Setting incorrect Syringe Pump flow rate displays wrong message “the syringe may be out of sample”. Remedy: Remove and place the syringe again into the pump to release the backpressure.
375776	3 - Medium	Tune: “Continue to batch reports” option is not available after running diagnostic/optimization procedure.
362826	3 - Medium	ME: Selection of scan nodes is not possible when Method Editor window is not maximized.

ID	Severity	Title
357067	3 - Medium	Isolation m/z range below *m/z* 40 does not trigger a validation error when resulting from an inappropriate isolation offset setting. Remedy: Enter an isolation offset value that complies with accepted isolation range.
387627	4 - Low	RF values are not converted to account for differences between S-lens and funnel when importing OE120/240/MX methods. Remedy: Please manually adjust the RF value accordingly.
402163	3 - Medium	When Internal Calibrant Source is faulty/defective, the warning message is incomplete, missing the following text: “The mass accuracy performance may be slightly lower than in regular conditions.”
402347	4 - Low	With Fine Astral Mass Calibration (part of System Calibration), result messages are not located below the associated plots in PDF report.
404844	3 - Medium	Xcalibur: If the file name contains the symbol µ, two raw data files are generated instead of one. Remedy: Do not use symbol µ in file name.
614321	3 - Medium	Ion Foil Correction and Astral Mass Stabilization can fail due to uncalibrated ICS source. Remedy: Perform Negative Polarity System Calibration from time to time even if not using the system in negative polarity mode.
503511	3 - Medium	Multiple error messages about ion foil adjustment in Xcalibur. Remedy: Please close manually windows reporting the error messages.
676639	3 - Medium	FAIMS: Temperature differences above 20° between inner and outer electrode might not be reachable and cause timeouts. Remedy: When using "User Defined" FAIMS Mode in Method Editor, adjust FAIMS Inner Electrode Temp/ FAIMS Outer Electrod Temp in order keep the temperature difference between the two electrodes below 20°C.
813657	3 - Medium	Acquisition time not properly reported in rawfile with tMS2-only method not starting acquisition at t=0 min. Remedy: Accept the incorrect report of acquisition time in rawfile (not affecting acquisition) or modify the method so that actual acquisition is started at t=0 min (e.g., by including a full scan experiment starting at t=0 min).

ID	Severity	Title
820630	3 - Medium	UI: ME: tSIM and tMS2: setting maxIT and microscans in table/scan property. Remedy: Revert "Maximum Injection Time" or "Microscan" as a scan property.
824228	3 - Medium	DDA performed in small molecule application mode and with m/z of selected precusor ion varying substantially may result in instable TIC for full scan MS and ddMS2 overfilling (for high mass precursor ion). Remedy: Restrict the full scan mass range by using, ideally, a last m/z value not exceeding five times the first m/z value.
827732	2 - High	UI: ME: TMT HR Mode available in Small Molecule and Intact Protein Modes. Remedy: Do not use TMT HR Mode in "Small Molecule" and "Intact Protein" modes as it is not relevant.
814458	3 - Medium	Scan Range mode set to "Auto-Extended" in some of the scans of a formerly saved method (using small molecule application mode) is changed to "Define m/z Range" when re-opened. Remedy: The method works as expected at the time of saving. If the method is re-opened for modification, make sure Scan Range mode is set again to "Auto-Extended" before saving the method.
829920	3 - Medium	Methods including eDR m/z windows having first mass higher than m/z 25000 with "eDR Window Type" set to "Auto" do not report error and can be saved without warning, but do not pass method validation when executing a sequence in Xcalibur. Remedy: Set "eDR Window Type" to "User Defined" before saving the method to confirm m/z window values are in accepted range.
830065	3 - Medium	DIA methods using "DIA Window Mode" set to "Center Mass" report DIA m/z windows table with headers "m/z" and "Q1 Resolution (m/z)" instead of "Center Mass (m/z)" and "Window Width (m/z)", respectively, in summary section.
830395	2 - High	When preparing a method which contains Orbitrap MS2 scan using Profile data type, modifying subsequently the Application Mode before saving will change data type to Centroid (only visible when re-opening the method). Remedy: Set application mode first when creating a method.

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