

Thermo Scientific Exactive Series 2.8 SP1 Release Notes

This document lists all new features, improvements, fixed defects, and known issues that exist in the Thermo Scientific Exactive Series 2.8 SP1 release. For information regarding the installation, features, functionality, and use of this product, refer to the following sources of information:

- DVD Insert
- Operating Manual
- Online Help
- Software Manual
- Quick Start Guide

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Installation Notes

Supported Target Systems

- Thermo Scientific Exactive GC mass spectrometer
- Thermo Scientific Exactive Plus mass spectrometer
- Thermo Scientific Exactive Plus EMR mass spectrometer
- Thermo Scientific Q Exactive mass spectrometer
- Thermo Scientific Q Exactive Focus mass spectrometer
- Thermo Scientific Q Exactive GC mass spectrometer
- Thermo Scientific Q Exactive HF mass spectrometer
- Thermo Scientific Q Exactive Plus mass spectrometer

System Requirements

The minimum hardware and software configurations required for Exactive Series 2.8 SP1 operation are as follows:

System	Requirements
PC	2.40 GHz Dual Core Processor 4 GB RAM 512 GB Hard Drive DVD-ROM Drive Display Monitor Resolution of 1680 × 1050 2 nd Network Interface Card (NIC), 100 MBit/s
Software	Microsoft™ Windows™ 7 SP1 Professional (32-bit or 64-bit) Microsoft Office 2010 or 2013

NOTICE The Exactive Series Instrument Software Kit 2.8 SP1 was only tested within the delivered composition. ▲

Installation

NOTICE Prepare the computer in advance of any new installation! ▲

This guidance addresses a standard installation of a computer suitable to act as a data system for Exactive Series based instruments. The current software version is 2.8 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 are different. The current explanations have Windows 7 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 Exactive Series instruments is highly recommended for setting up a new PC.

Technical Requirements

Choose a PC with Microsoft Windows 7 as operating system. Windows XP is partially tested for older instruments. Vista or Windows 8 have not been tested, but are expected to work in principle. The PC should have 4 GB or more RAM, a 2 GHz CPU, better more than one CPU core and a dedicated, separate network interface card (NIC) for communication with the instrument and LC devices, if present.

There are small differences in using 32 bit or 64 bit operating systems. Check the list of supported operating systems for a particular Exactive Series Instrument Software Kit.

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

More than one NIC may 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. 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 5e 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 ExactiveService.exe (file locations see below) needs access to incoming and outgoing network traffic. Remind 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

NOTICE Do not start software installation before network setup has been completed! See “[Network Setup](#)” on [page 2](#). ▲

File Locations

Depending on various conditions, the typical installation folders on the computer can be either

- C:\Xcalibur\system\Exactive
- C:\Program Files (x86)\Thermo\Exactive
- C:\Program Files\Thermo\Exactive

This instruction list uses C:\Xcalibur\system\Exactive for easy reading, but depending on the installation package like Exactive Series Instrument Software kit or Chromeleon, this may be different.

Once the Exactive software has been installed on a system, the folder of the first 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:\Xcalibur\system\Exactive\instrument\msx_instrument_files
- C:\Xcalibur\system\Exactive\instrument\ExactiveLicenses.txt
- C:\Xcalibur\system\Exactive\instrument\reports
- Various Tune files at user-selected locations

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

Uninstalling

Previous versions of Thermo Exactive should be removed using Control Panel operation. Present configuration settings will remain.

Installation

Install using the DVD or a copy of it. 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 Exactive 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 may be different to that of the installation. Either use Instrument Configuration and look where files are located or check the folders appearing at “[File Locations](#)” on [page 2](#).

NOTICE It is important to stop the only program that interacts with the files coming from the backup. That is ExactiveService. ▲

❖ To stop ExactiveService

1. In Windows Explorer, right-click **Computer**.
2. Select **Manage > Services and Applications > Services > Thermo Exactive Series**.
3. Right-click it and select **Stop**.
Keep the dialog open.
4. Replace the **msx_instrument_files** folder, because it already exists. All other files of the backup should not exist on the new system. Copy them.
5. Use the open dialog to start the **Thermo Exactive Series** service again. Alternatively, reboot the computer. In doubt, contact the Exactive support team of Thermo Fisher Scientific.

Set the power setting to maximal performance.

NOTICE Automatic updates of any kind, those of the operating system in particular, are usually set to **automatic**, but this may disturb instrument data acquisition. We strongly recommend setting all updates to **manual** and checking for updates regularly. ▲

Software Compatibility Matrix

This table shows the supported instrument control software versions for various Exactive Series instrument models.

	Q Exactive	Exactive Plus	Q Exactive Plus	Exactive Plus EMR	Q Exactive HF	Q Exactive Focus	Q Exactive GC	Exactive GC
2.0	✓							
2.0 SP1	✓							
2.0 SP2	✓							
2.1	✓	✓						
2.2 SP1	✓	✓						
2.3	✓	✓	✓	✓				
2.3 SP1	✓	✓	✓	✓				
2.4	✓	✓	✓	✓	✓			
2.5	✓	✓	✓	✓	✓	✓		
2.6	✓	✓	✓	✓	✓	✓	✓	
2.7	✓	✓	✓	✓	✓	✓	✓	
2.7 SP1	✓	✓	✓	✓	✓	✓	✓	
2.8	✓	✓	✓	✓	✓	✓	✓	✓
2.8 SP1	✓	✓	✓	✓	✓	✓	✓	✓

New Features and Improvements

The following tables list improvements and defects fixes in the Exactive Series 2.8 SP1 release ([Table 1](#)); new features, improvements and defects fixes in the Exactive Series 2.8 release ([Table 2](#)); improvements and defects fixes in the Exactive Series 2.7 release ([Table 3](#)); improvements and defects fixes in the Exactive Series 2.6 release ([Table 4](#)); an improvement in the Exactive Series 2.5 SP1 release ([Table 5](#)); improvements and defects fixes in the Exactive Series 2.5 release ([Table 6](#)); new features, improvements and defects fixes in the Exactive Series 2.4 release ([Table 7](#)); improvements and defects fixes in the Exactive Series 2.3 SP1 release ([Table 8](#)); new features, improvements and defects fixes in the Exactive Series 2.3 release ([Table 9](#)); new features, improvements and defects fixes in the Exactive Series 2.2 SP1 release ([Table 10](#)); new features and improvements in the Exactive Series 2.1 release ([Table 11](#)); improvements and defect fixes in the Exactive Series 2.0 SP2 release ([Table 12](#)); and improvements and defect fixes in the Exactive Series 2.0 SP1 release ([Table 13](#)).

[Table 1](#) lists improvements and defects fixes in the Exactive Series 2.8 SP1 release that were implemented since the Exactive Series 2.8 release. For details, please refer to the Online Help or the Software manual.

Table 1. Changes from Exactive Series 2.8 to Exactive Series 2.8 SP1

Abstract	SCR
Improvement: Exactive GC is added as new instrument of the Exactive Series.	36326
Improvement: Improved cooling of turbomolecular pump - allow new high-speed fan to run on Exactive Series.	36330
Defect fix: normal mode eFT calibration and HMR eFT calibration as well as EMR eFT calibration interfere each other.	37111
Defect fix: manipulating a license key in the “Add license” window results in a crash of Tune.	36549
Defect fix: HMR eFT calibration makes normal mode mass calibration “void” (traffic light is yellow).	37113
Defect fix: Quadrupole Endurance Test saves Quad default values to master_cal	38338

Table 2 lists new features, improvements and defects fixes in the Exactive Series 2.8 release that were implemented since the Exactive Series 2.7 release. For details, please refer to the Online Help or the Software manual.

Table 2. Changes from Exactive Series 2.7 to Exactive Series 2.8

Abstract	SCR
New feature: Support of High Mass Range (HMR) mode for Q Exactive Plus and Q Exactive HF enabled by a license 'High Mass Range' for improved analysis of monoclonal antibodies: • Increase the m/z range to last mass 8000. • Increase S-lens RF level to maximum value 200. • Increase In-Source CID max value to 150 eV (HESI source) or 200 eV (NSI source). • Access to 'Averaging' feature. • Access to 'Trapping Gas Pressure' settings from 1.0 to 1.5. • HMR mode Calibration and Evaluation procedures using ammonium hexafluorophosphate (AHFP) as calibration solution. • HMR experiments in Method Editor: 'HMR - Full MS' and 'HMR - AIF'.	DEU-2501
Improvement: Calibration Report: Plot history values of the Isolation Transmission Endurance Test.	DEU-1980
Improvement: Make PDF Reports for Evaluations available.	DEU-2106
Improvement: PDF Reports for Calibrations: Include Report of Failed Calibration results.	DEU-2580
Improvement: Q Exactive, Q Exactive Plus and Q Exactive HF: Make Loop count user accessible in PRM experiment.	DEU-2519
Improvement: Modified bakeout procedure. Maximum bakeout time set to 30 h.	DEU-2623
Improvement: Q Exactive Plus and Q Exactive HF: Improve robustness of HCD gas supply when using Protein Mode.	DEU-2637
Improvement: Modified bakeout procedure. Switch off Trapping Gas during bakeout.	DEU-2676
Improvement: Q Exactive GC: Reduce default lock mass tolerance in Tune to ± 5 ppm.	HR-232
Improvement: Q Exactive GC: Make C-Trap Energy Offset editable in instrument method.	HR-236
Improvement: Q Exactive GC: Hide Lock mass filter in Tune Spectrum view and raw file scan headers.	HR-237
Improvement: Q Exactive GC: Do not restore heater set values after changing in a method.	HR-239
Defect fix: Q Exactive GC: Help File has wrong release history.	DEU-2486
Defect fix: Q Exactive GC: Collection of manuals within Windows Start menu and corresponding links are not complete/correct.	DEU-2556
Defect fix: TIC Variation is not calculated correctly for all Q Exactive instruments.	DEU-2518
Defect fix: QE Focus: Method Editor help description box text shows wrong loop count.	DEU-2524
Defect fix: Rephrase Method Editor help description box text for (N)CE.	DEU-2523
Defect fix: Exactive Plus EMR: Method Editor: In-source CID values > 100 eV fall back to 100 eV after saving the method.	DEU-2562
Defect fix: Instrument Configuration: Special Characters in the Public Name prevent Reports from being generated.	DEU-2613
Defect fix: Q Exactive GC: AGC Issues when doing low mass scanning.	HR-233
Defect fix: Q Exactive GC: Tuning issue with low mass scanning.	HR-234

Table 3 lists all improvements and fixed defects in the Exactive Series 2.7 release that were implemented since the Exactive Series 2.6 release. For details, please refer to the Online Help or the Software manual.

Table 3. Changes from Exactive Series 2.6 to Exactive Series 2.7

Abstract	SCR
Improvement for Q Exactive, Q Exactive Plus, Q Exactive HF, Q Exactive Focus, Q Exactive GC: new property (N)CE / stepped (N)CE is available to switch between absolute collision energy (CE) and normalized collision energy (NCE).	DEU-2376
Improvement: Scan filters show precursor m/z as well as scan ranges with four decimal places.	DEU-2382
Improvement Q Exactive Focus: new experiment AIF is available.	DEU-2387
Improvement Q Exactive Focus: Full MS experiment can be combined with the experiments SIM, PRM or AIF.	DEU-2388
Improvement Q Exactive Focus: loop count up to three available for • Full MS - discovery • Full MS - confirmation • SIM • SIM - confirmation.	DEU-2398
Improvement Q Exactive Focus: msx count up to 10 in SIM experiment.	DEU-2399
Improvement Q Exactive Focus: scan range m/z 50-3000 for Full MS experiment and AIF experiment is supported.	DEU-2400
Improvement Q Exactive GC: enable low mass scanning.	DEU-2410
Defect fix Exactive Plus (EMR): intensity threshold now accepts all set values.	DEU-2370
Defect fix Q Exactive GC: repaired link to Operating Manual in Windows Start Menu.	DEU-2390
Defect fix: Carry-over of Full MS ions into subsequent fragmentation scan is prevented.	DEU-2403
Defect fix: DAQ board throws error when switching to acquisition mode too early after instrument reset.	DEU-2405
Defect fix Tune: When fragmentation CE is selected, field for charge state will be grayed out.	DEU-2421
Defect fix Method Editor Global Lists: Fragmentation Energy values are now accepted when typing in combo box.	DEU-2425
Defect fix Method Editor: PreselectedTuneFileChooser does update renamed or deleted folders.	DEU-2433
Defect fix Q Exactive GC: Method Editor summary shows correct ion source.	DEU-2450

Table 4 lists all improvements and fixed defects in the Exactive Series 2.8 SP1 release that were implemented since the Exactive Series 2.5 SP1 release. For details, please refer to the Online Help or the Software manual.

Table 4. Changes from Exactive Series 2.5 SP1 to Exactive Series 2.6

Abstract	SCR
Improvement: Method Editor: Help description boxes briefly explain each property setting.	DEU-0718
Improvement: Tune: Better messages and help procedures are provided when Inject Flatapol calibration or Quadrupol Isolation Mass/Resolution Calibrations fail.	DEU-1069
Improvement: Method Editor: Minimum AGC target value instead of Underfill ratio is shown in Data Dependent settings.	DEU-1103
Improvement: Tune: UHV warn level is increased when a DART™ ion source is configured (Instrument System Configuration settings > DART Ion Source Compatibility).	DEU-1522
Improvement: Spray current standard deviation is reported in status log.	DEU-1832
Improvement: Online Help: Better description of Method Editor Experiments.	DEU-1871
Improvement: Online Help: Experiment pane is directly linked with Online Help. In Online Help, experiment symbols show hyperlinks to parameter descriptions.	DEU-2041

Table 4. Changes from Exactive Series 2.5 SP1 to Exactive Series 2.6, continued

Abstract	SCR
Improvement: Xinstaller: Newer IQ report template is available for IQ Report of the Installer.	DEU-2303
Defect Fix: Monoisotopic Peak Determination Algorithm is setting the wrong monoisotopic m/z in Scan Header.	DEU-2204
Defect Fix: Xcalibur Sequence Editor: Used file names that include special characters will create empty acquisitions raw files.	DEU-2213
Defect Fix: Tune About Window text block scaling is unfavorable when no MS Office is installed.	DEU-2252
Defect Fix: Method Editor TuneFileChooser: Show file time as local time.	DEU-2265
Defect Fix: Tune: CTCDD calibration is dependent on sheath gas flow.	DEU-2269
Defect Fix: Exactive Plus EMR: For support of calibrating an instrument with Advion NanoMate™ ion source, the background noise check procedure was removed for the following calibration procedures: C-trap charge detection scaling and mass calibrations.	DEU-2284
Defect Fix: Q Exactive instruments: MS1 ions carry over into MS2 after CTCDD scan.	DEU-2294
Defect Fix: Q Exactive Focus Method Editor: When 'min AGC Target' Trigger is switched off, the Intensity threshold is shown differently for dd-MS2 modes.	DEU-2330
Defect Fix: Q Exactive Focus: Wrong Scan Ranges are acquired for Full MS with Segmented Master Scans and Polarity switching.	DEU-2345
Defect Fix: Method Editor: Unfavorable Font is loaded when no MS Office is installed.	DEU-2350

Table 5 lists an improvement in the Exactive Series 2.5 SP1 release that was implemented since the Exactive Series 2.5 release. For details, please refer to the Online Help or the Software manual.

Table 5. Changes from Exactive Series 2.5 to Exactive Series 2.5 SP1

Abstract	SCR
Improvement: Transfer of messages from Exactive Series Tune and Method Editor is adjusted to the Chromeleon audit trails.	DEU-2059

Table 6 lists all improvements and fixed defects in the Exactive Series 2.5 release that were implemented since the Exactive Series 2.4 release. For details, please refer to the Online Help or the Software manual.

Table 6. Changes from Exactive Series 2.4 to Exactive Series 2.5

Abstract	SCR
Improvement: Calibration Report has to be generated for "Customized Mass Calibration".	DEU-1907
Improvement: Q Exactive instruments: Optimize reporting of quadrupole and injection filter calibrations.	DEU-1958
Improvement: Q Exactive, Q Exactive Plus, Q Exactive HF: Provide correct "Last Locking" information in scan header with regard to time.	DEU-2179
Defect fix: Method Editor: the MS/MS data dependent first mass switches to '-' when $m/z < 50$ is entered.	DEU-735
Defect fix: Quad iso/res calibration (rough) plot: Coloring of primary and secondary axis should be different.	DEU-1929
Defect fix: Q Exactive Plus/HF: During evaluation of the Injection flatapole, the message on the graph header shows Injection flatapole calibration.	DEU-1961
Defect fix: Method Editor Global Lists: Empty fields are not supported for (N)CE when a value was set.	DEU-2042
Defect fix: Method Editor Global Lists: Cannot delete field values in a table.	DEU-2043

Table 6. Changes from Exactive Series 2.4 to Exactive Series 2.5, continued

Abstract	SCR
Defect fix: Electronics evaluations in Extra Evaluation procedures are not called when root node is selected.	DEU-2085
Defect fix: CE/NCE: Tune Analysis Graph does not support plotting CE energies.	DEU-2087
Defect fix: Tune Analysis graph / Scan HCD Energy: The Activation Energy Scan Range must be increased from (1-100) to (1-200).	DEU-2089
Defect fix: Exactive Plus EMR: Tune Analysis graph / Scan In-Source-CID Energy: The Activation Energy Scan Range must be increased from (1-100) to (1-200).	DEU-2090
Defect fix: Q Exactive Plus/HF: Mass Traces / Scan CE, NCE and in-source CID energy do not show real-time plot.	DEU-2097
Defect fix: CE/NCE: Charge state info is displayed when CE is selected.	DEU-2101
Defect fix: Q Exactive Plus: Full MS / PRM: PRM scan events are delayed with Full MS Enhanced Resolution.	DEU-2104
Defect fix: Method Editor Properties: Minimum value in a range is not honored if entered in a property grid in the edit field “mass width”.	DEU-2121
Defect fix: Method Editor TopN: Avoid using Periodic Prescan (PPS) mass ranges other than the full scan range.	DEU-2137
Defect fix: The use of Q Exactive Tune files must be forbidden on Q Exactive Plus and Q Exactive HF instruments in both Tune and Method Editor.	DEU-2145
Defect fix: Exactive Plus without HCD shows CE fragmentation in Tune.	DEU-2182

[Table 7](#) lists all new features, improvements and fixed defects in the Exactive Series 2.4 release that were implemented since the Exactive Series 2.3 SP1 release. For details, please refer to the Online Help or the Software manual.

Table 7. Changes from Exactive Series 2.3 SP1 to Exactive Series 2.4

Abstract	SCR
New feature: Q Exactive, Q Exactive Plus, Q Exactive HF: Grouping in MSX Scans For spectrum multiplexed experiments, an inclusion list MSX ID defines the candidates to be multiplexed in one scan event.	DEU-1995
New feature: Q Exactive, Q Exactive Plus, Q Exactive HF: Enable switching between NCE and CE. Enable switching between normalized collision energy (NCE) and absolute collision energy (CE), which is supported in Tune Editor (“Instrument Control Fragmentation” and “Mass Traces Scan and Plot”) and in the global “Inclusion” list of the Method Editor	DEU-2003
Improvement: TIC Intensity Compensation Factors are extended for target values higher than 2.25E6	DEU-1479
Improvement: Instrument Configuration: Audit trailing maximum text size is configurable	DEU-1956
Improvement: Q Exactive, Q Exactive Plus, Q Exactive HF: Instrument method “Targeted-MS2” is renamed to “PRM”	DEU-1962
Improvement: Tune: Save/open custom calibration lists	DEU-1978
Improvement: Q Exactive Plus/HF: Workflow FS / AIF / NL-dd MS ² workflow has to be supported for Protein Mode licensed systems if instrument is currently not in Protein Mode	DEU-1979
Improvement: Q Exactive Plus/HF: Enable averaging functionality of scans for Protein Mode	DEU-1983
Improvement: Q Exactive, Q Exactive Plus, Q Exactive HF: Stepped NCE values are displayed individually in the raw file scan header	DEU-2047
Defect fix: Quad RF Frequency Fine Adjustment Procedure does not detect intermittent large dips in isolation profile	DEU-1785

Table 7. Changes from Exactive Series 2.3 SP1 to Exactive Series 2.4, continued

Abstract	SCR
Defect fix: Exactive Plus without HCD shows AIF experiments	DEU-1954
Defect fix: targeted-MS ² (PRM): Acquisition of more than one experiment of this type in one method does not work properly	DEU-2058

Table 8 lists all improvements and fixed defects in the Exactive Series 2.3 SP1 release that were implemented since the Exactive Series 2.3 release. For details, please refer to the Online Help or the Software manual.

Table 8. Changes from Exactive Series 2.3 to Exactive Series 2.3 SP1

Abstract	SCR
Improvement: Support for Windows standard service accounts	DEU-1458
Improvement: Outdated log files will be automatically deleted after 18 months	DEU-1780
Improvement: Q Exactive Plus: Quadrupole isolation shape check procedure	DEU-1825
Improvement: Q Exactive, Q Exactive Plus: Improvement for isolation calibration	DEU-1862
Improvement: Automated inject time calculation for highly concentrated samples is improved	DEU-1863
Improvement: Q Exactive Plus: Optimize HCD cell parameters in protein mode	DEU-1905
Defect fix: Tune: In rare cases the spectrum view can freeze requiring a restart of the Tune	DEU-926
Defect fix: Data system runs out of memory on unexpected stop of Windows Explorer	DEU-1809
Defect fix: Acquisition freezes occasionally in methods with complex sample and big number of dependent scans	DEU-1830
Defect fix: After running a method from the tune page, some tune settings are not restored	DEU-1841
Defect fix: Exactive Plus EMR: Allow running HCD transfer tuning procedure	DEU-1846
Defect fix: Method setup: Restrict lock mass input range	DEU-1851
Defect fix: Exactive Plus EMR: Re-initialize the CTCD parameters when switching EMR mode on/off, reducing equilibration times	DEU-1856
Defect fix: Q Exactive Plus: Run-time error at end of Quad Transmission Evaluation	DEU-1864
Defect fix: Use custom max IT setting for customized mass calibration procedure	DEU-1865
Defect fix: Method setup: Customized Tolerances Dialog Boxes: Typing separators does not work as expected	DEU-1867
Defect fix: Internal rounding error for maximum ion time setting under certain conditions	DEU-1872
Defect fix: False nitrogen gas warning may appear on 0 psi set point	DEU-1932
Defect fix: Exactive Plus without HCD shows AIF experiments	DEU-1954

Table 9 lists all new features, improvements and fixed defects in the Exactive Series 2.3 release that were implemented since the Exactive Series 2.2 SP1 release. For details, please refer to the Online Help or the Software manual.

Table 9. Changes from Exactive Series 2.2 SP1 to Exactive Series 2.3

Abstract	SCR
New feature: Mass accuracy improvements by lock mass injection	DEU-1742
New feature: User-adjustable mass tolerances for methods	DEU-1744
New feature: More flexible stepped collision energy	DEU-1745
New feature: Support of API programs	DEU-1750
New feature: User-selectable isolation window offset	DEU-1752
Improvement: For Q Exactive Plus, tuning of transfer optics voltages is not necessary; therefore, the "Tune" pane is removed from the Tune program for Q Exactive Plus	DEU-951

Table 9. Changes from Exactive Series 2.2 SP1 to Exactive Series 2.3, continued

Abstract	SCR
Improvement: Improved quadrupole isolation/resolution narrow calibration	DEU-1370
Improvement: Tune “Plot Mass Traces” mass tolerance changed to 10ppm	DEU-1555
Improvement: Logic of inclusion list runtime-order changed	DEU-1556
Improvement: Lock mass validity restricted to single run	DEU-1561
Improvement: Broader isolation windows for MS/MS allowed	DEU-1579
Improvement: Improved Isolation Transmission Endurance Test	DEU-1697
Defect fix: Scan filter is doubly displayed by running msx dd experiments	DEU-51
Defect fix: There is no validation for entering Start time > End time	DEU-810
Defect fix: The “Setup Complete” window hides behind another window	DEU-841
Defect fix: “Vacuum not ready” failure may show up after instrument startup	DEU-853
Defect fix: Method Editor: User role wrongly displayed after switching settings in properties	DEU-1431
Defect fix: PDF reporting issues after CTCDC calibration	DEU-1533
Defect fix: Customized mass calibration is not saved in master cal file	DEU-1540
Defect fix: Mass calculator does not store last used formula	DEU-1615
Defect fix: Double-click on Method start brings up busy messages	DEU-1640
Defect fix: Method Editor: TopN: dd-SIM is not available	DEU-1645
Defect fix: Change record missing when pasting a table	DEU-1723

[Table 10](#) lists all new features, improvements and fixed defects in the Exactive Series 2.2 SP1 release that were implemented since the Exactive Series 2.1 release. For details, please refer to the Online Help or the Software manual.

Table 10. Changes from Exactive Series 2.1 to Exactive Series 2.2 SP1

Abstract	SCR
New feature: Implement a Data Independent Acquisition (DIA) MS/MS experiment in the Method Editor.	DEU-904
New feature: Widen the isolation window width limit to 50 Da.	DEU-1004
AGC improvements are needed to support faster chromatography in targeted experiments	DEU-995
New feature: Chromatographic peak width (FWHM) definable in method setup to automatically adapt instrument timings. By setting the full width half maximum (FWHM) of the persistent or expected elution profiles of your chromatographic setup, the instrument software can adapt the frequency in which AGC information will be delivered. Especially for quantification experiments at fast chromatography, the AGC information needs to be updated much faster to get the correct response areas.	DEU-1412
New feature: Implement an Exact Mass Calculator. Based on the analytes chemical formula or sequence (e.g. peptides), species (e.g. +Na adduct) and charge state, the exact mono isotopic mass is calculated and used for a target definition in inclusion lists. Additionally it is available in Tune, so one can directly calculate the needed isolation center mass for SIM and MS/MS scan types and check the current spectral data for expected candidates and species.	DEU-1262
Improvement: Optimized quadrupole RF timing pattern	DEU-1316
Improvement: Inclusion list entries are applied in the defined order (unsorted processing, valid for DIA)	DEU-1321
New feature: Method setup shall allow selecting centroid mode for data acquisition.	DEU-956
New feature: Implemented PDF-Reports for calibration	DEU-1265

Table 10. Changes from Exactive Series 2.1 to Exactive Series 2.2 SP1, continued

Abstract	SCR
New feature: Provide a .NET based Instrument Application Programming Interface (API).	DEU-1266
New feature: Improvement of Tune for Direct Control for LC systems (supported are: Accela Pump 1250, Accela autosampler Open AS, CTC PAL autosampler)	DEU-1383
New feature: Implemented Quadrupole Transmission Evaluation	DEU-1085
New feature: To improve robustness, the sweep gas can be turned on when in standby mode.	DEU-1260
Defect fix: Exactive Series instruments overwrite Accela Pump pressure traces in RAW files with voltages if analog channel data is acquired by the instrument.	DEU-1094
Defect fix: Under certain conditions invalid values for CTCD scaling can occur.	DEU-1258

Table 11 lists all new features and improvements in the Exactive Series 2.1 release that were implemented since the Exactive Series 2.0 SP2 release. For details, please refer to the Online Help or the Software manual.

Table 11. Changes from Exactive Series 2.0 SP2 to Exactive Series 2.1

Abstract	SCR
New feature: Extended mass range to 50–6000.	DEU-1046
New feature: Increased speed of polarity switching; applies for Exactive Plus and for all Q Exactive instruments that are shipped after May 2012.	DEU-1088
New feature: Additional AGC target value of 5e6	DEU-989
New feature: Added AIF method	DEU-1123
New feature: Additional logic for “peptide match” trigger criteria: “preferred”	DEU-1031
New feature: Automatic source identification for DART	DEU-1010
New feature: Automatic source identification for AP-MALDI	DEU-1079
New feature: Calibration report for printout	DEU-1080
Improvement: Modified maximum inject time setting concept	DEU-1102

Table 12 lists all new features, improvements and fixed defects in the Exactive Series 2.0 SP2 release that were implemented since the Exactive Series 2.0 SP1 release. For details, please refer to the Online Help or the Software manual.

Table 12. Changes from Exactive Series 2.0 SP1 to Exactive Series 2.0 SP2

Abstract	SCR
Improved AGC performance via C-trap charge detection	DEU-631
Improved quadrupole calibrations and evaluations	DEU-961
Data Dependent experiment cycle improvements	DEU-632
Improved HCD RF amplitude settings (depend now on frequency readback)	DEU-943
Improvement: Separate quadrupole calibration for negative ion mode	DEU-879
Improved fan error message: Added hint to check the air filters	DEU-894
Improvement: Added voltage range checks for IOS HV supply	DEU-934
Improved scan header: Inject time now shown as integer	DEU-916
Improvement: Increased decimal places in “Neutral Loss” and “Tag Masses” lists from 3 to 5	DEU-875
Defect fix: The isolation window width can not be set to an odd number in one decimal place	DEU-938
Defect fix: Error on removing the last line in the table editor	DEU-846
Defect fix: Precursor m/z value cannot be easily set in the Instrument Control window	DEU-895

Table 13 lists all new features, improvements and fixed defects in the Exactive Series 2.0 SP1 release that were implemented since the Exactive Series 2.0 release. For details, please refer to the Online Help or the Software manual.

Table 13. Changes from Exactive Series 2.0 to Exactive Series 2.0 SP1

Abstract	SCR
Online Help: Calibrate and Evaluate do not launch Online Help when pressed F1 if one of the sub-windows is active	DEU-844
Orbitrap: In rare cases, the mass RF amplitude dependency calibration fails in negative ion mode	DEU-896
Improvement of the Data Dependent “exclude isotopes” feature	DEU-428
Improvement of the isolation overlap control for targeted workflows	DEU-859

Known Issues

This table lists all known issues that exist in the Exactive Series 2.8 SP1 release.

Abstract	SCR
The divert valve numbering in the instrument software is not consistent with the numbering on the valve itself.	DEU-264
Tune Editor does not show correct scan types during ME data acquisition.	DEU-949
Method Editor global lists changes in a saved method are not saved automatically.	DEU-1191
Remedy: Once a method including a global list was saved as Xcalibur *.meth file and this global list is edited again, save the *.meth file again.	
System does sometimes not boot automatically when Tune version is updated.	DEU-1789
Significant drop in signal every 2.5 sec using “Protein Mode”.	DEU-2075
Remedy: Average several microscans or switch off C-Trap Charge Detector Support (Instrument Status Control Settings).	

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