Xcalibur™ 4.3 Release Notes

These release notes briefly list changes in the Xcalibur 4.3 software, fixes to previously reported issues, and known issues still existing in the Xcalibur 4.3 software release.

Contents

For information on installing the Xcalibur 4.3 application, refer to the DVD insert. For information on using the Xcalibur 4.3 software, refer to the manuals available as PDF files or the Help.

Features

This release is a minor version release that incorporates a number of new and enhanced features and resolves bugs listed in Resolved Issues section

New features in this release include the following:

- Enhancement of the AcquireX Deep Scan workflow to use TopN DDA methods
- Addition of a TopN DDA AcquireX workflow
- Improvements to AcquireX component detection performance and data quality
- Integration of Thermo Scientific™ Almanac as an Xcalibur widget
- Direct access of the Thermo Scientific mass spectrometer Tune application from the Xcalibur homepage

System Requirements

These are the minimum required (or recommended) data system computer hardware and software configurations for operation of the Xcalibur 4.3 application.

System	Requirements
Hardware	• (Recommended) 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
Software	• Microsoft™ Windows™ 10 Enterprise 2016 LTSB or Windows 7 Professional SP1 (64-bit) • .NET Framework 4.6.2 • Thermo Foundation™ 3.1 SP7 or later • Microsoft Office 2013 • Adobe™ Acrobat™ or Reader™ 10.1

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General

Xcalibur 4.3 does not require licensing in any form. You can install Xcalibur 4.3 on either Windows 10 or Windows 7 SP1 64-bit operating systems (see System Requirements for details).

Installation

You must have administrator rights to install Xcalibur software on your computer.

Xcalibur 4.3 installs Foundation version 3.1 SP7, Almanac 1.3, and FreeStyle 1.6. Any older versions are removed prior to installation. See below for detailed installation instructions.

- To perform a new installation of Xcalibur 4.3
- To upgrade an existing installation of Xcalibur 4.2 SP1, 4.2, or 4.1

❖ **To perform a new installation of Xcalibur 4.3**

1. Click **ThermoLauncher.exe**.
2. Click **Adobe Reader 10.1** to install the Adobe Reader application.
3. Click **Xcalibur 4.3**.

   Xcalibur 4.3 (build 4.3.73.11) installs on the data system computer, and includes Foundation 3.1 SP7 (build 3.1.300), FreeStyle 1.6 (build 1.6.75.20), and Almanac 1.3 (build 1.3.250).

❖ **To upgrade an existing installation of Xcalibur 4.2 SP1, 4.2, or 4.1**

1. Using the Foundation Instrument Configuration window, remove all configured instruments.
2. Uninstall Xcalibur and Foundation using Windows "Add and Remove Programs" in the following order:
   a. Xcalibur
   b. Foundation
3. Click **ThermoLauncher.exe**.
4. Click **Adobe Reader 10.1** to install the Adobe Reader application.
5. Click **Xcalibur 4.3** and proceed as follows:
   a. Follow the installer instructions to have the installer to install Foundation 3.1 SP7, Xcalibur 4.3, Almanac 1.3, and FreeStyle 1.6.
   b. When prompted, restart the data system computer.
6. (For users of mzVault with FreeStyle only) Click **mzVault 2.2** to install the Thermo mzVault™ 2.2 application.
7. (For users of NIST 17 with FreeStyle or Qual Browser only) Click **NIST 17** to install the NIST™ MS Search Program 2.3 application.

Resolved Issues

Table 1 describes the defects that were resolved in the Xcalibur 4.3 release. 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 (Sheet 1 of 2)

Item ID	Abstract	Severity
50748	Submission fails for Background exclusion and Component Inclusion and Background Exclusion due to incorrect error message.	Critical
8949	MS gets disconnected in pre-acquiring state of ID_01 when running 60 min method of Background Exclusion and Component Inclusion experiment.	High
16108	In some instances, AcquireX stop responding on ID injections.	High
51399	AcquireX sequence grid disappears during acquisition monitoring if sequence is stopped.	High

Table 1. Resolved issues (Sheet 2 of 2)

Item ID	Abstract	Severity
45961	In some instances, AcquireX stops responding during blank injection processing.	High
48912	In some instances, component detection stops while processing.	High
47238	Invalid Modification XML error upon running ID_02 run even though ID_01 completed without errors with AcquireX.	High
32299	Recent Experiments, Last Accessed Experiments, or Open Experiments do not open the saved or acquired experiments correctly.	High
52470	Stopping ID_01 at the processing stage deletes the rest of the AcquireX runs.	High
38049	When FreeStyle is opened from the Xcalibur home page, it cannot find the user manual.	High
54189	The XSLD file is not created when the AcquireX experiment is saved and submitted in some instances.	High
34053	Injection volume of -1 used with the EASY-nLC can give an error that prevents the sequence from being submitted.	Medium
52469	Deleting all of the AcquireX samples does not delete the last sample.	Medium
48972	AcquireX creates a duplicate folder under Experiments when the Save button is clicked after the sequence is submitted.	Medium
56163	The AcquireX Deep Scan experiment workflow encounters a processing error after first ID run when a MS is not the last device in the instrument method section of the raw file.	Medium
53509	AcquireX submissions fail if the injection volume is a decimal value.	Medium
44404	AcquireX experiments with long names—more than 120 characters—are not saved, preventing them from being opened in the recent experiments list.	Medium
47681	The preferred ion list in the AcquireX design experiment page is mismatched between (M-H+H2O) and (M+H-H2O).	Medium
49639	The Real Time Plot displays a blank screen.	Medium
51121	ThermoFisher.Foundation.AcqSupportTray.exe does not start automatically at windows startup.	Medium
50102	Xcalibur freezes after stopping or deleting an Acquire X experiment that is in progress.	Medium

Known Issues

Suggested recovery actions

- For some issues, restarting the application is the appropriate recovery action.

- In some cases (particularly issues that arise during data acquisition), restarting applications such as the Roadmap might not ensure complete recovery. Typically, restarting the data system computer resolves issues, or opening and then closing the Foundation Instrument Configuration, 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.

- In some instances QuanBrowser might disappear from Xcalibur under Microsoft Windows 10. This is a result of a missing or incompatible universal C runtime library from Microsoft. To resolve this issue, install Windows 10 SDK b26624 with all of the default options enabled.

- When configuring instruments under Xcalibur 4.3 for the first time after a clean installation, the user might encounter the message "Acquisition service is not running". This can be resolved by rebooting the data system.

Feature requests and other removed items

- Issues are excluded when there is insufficient information logged to successfully reproduce the reported problem.

- Feature requests are not listed as software issues, regardless of the reported significance or severity of the request. Product managers evaluate logged feature requests for future releases.

- Only discrepancies in the documented software are reported as known issues.

Terminology

Severity	Interpretation
Critical	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.
High	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.
Medium	A minor error or poor behavior of a product feature. There is probably a workaround.
Low	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.

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 2 contains known defects in the software identified by ID number, a brief abstract, and severity level. The Item ID is the internal number assigned to each issue. Product management assesses risk, which can differ significantly from the reported severity.

Table 2. Known defects

Item ID	Abstract	Severity
52652	Installer appears to report an incorrect number of files installed due to counting of files which are also moved to the Windows system global assembly cache.	High
54555	Validation missing on the invalid experiment folder and template method path upon Save and Submit.	High
38310	Remove duplicates in the exclusion list for the Iterative Precursor Exclusion AcquireX experiment.	Medium
50052	EULA Text Alignment issue for Foundation 3.1.	Medium
51152	Multiple instances of the Xcalibur installer might be spawned if user attempts to start the installation multiple times.	Medium
52728	Report an Issue function does not open Microsoft Outlook by default.	Medium
52869	AcquireX can access and run some AcquireX experiments with incorrect file extensions from "Open experiment" but not from "Last accessed experiment".	Medium
53131	AcquireX user interface will not display the "Stopped" label in the acquisition queue under certain circumstances.	Medium
53516	Instrument Configuration window might be improperly sized for certain instruments.	Medium
53856	If Xcalibur is upgraded while acquisition is in progress, the installer might uninstall the Almanac Agent and FreeStyle applications.	Medium
54545	QuanBrowser Audit Trail records a Microsoft Excel™ export event incorrectly.	Medium
54797	Clicking Help on the authentication window does not open the online Help file.	Medium
55722	Some AcquireX experiment cards might not be visible from the Select Experiment Page without scrolling the window.	Medium
56315	Error message (popup) does not appear when entering wrong path in Recent Experiments.	Medium
61382	Context-sensitive Help is not displayed for "Designing an AcquireX Experiment".	Medium
48898	Xcalibur 4.3 installation might leave Foundation 3.1 SP6 assemblies in the Windows Global Assembly Cache during the upgrade process.	Low
53898	Authorization Manager incorrectly displays "Supervisor" as "SuperVisor".	Low
54188	The AcquireX Iterative Precursor Exclusion Card Text has incorrect grammar.	Low
61365	Attempting to print from Processing Setup will cause Processing Setup to stop if Microsoft Office is not installed.	Medium