TraceFinder 5.3 Release Notes

These release notes briefly list features in the Thermo TraceFinder™ 5.3 data system and known issues that still exist in the TraceFinder application.

Contents

- Features
- System Requirements
- Important Information
- Resolved Issues
- Known Issues
- Trademarks

For information on installing TraceFinder 5.3 software, refer to the DVD insert. For information on configuring and using Thermo Scientific™ detection devices, refer to their individual manuals available as PDF files or the Help.

Features

This release incorporates the following new or enhanced features:

- Windows 11, 64-bit IoT Enterprise edition (LTSC 2024)
- MSn support for Thermo Scientific Stellar Mass Spectrometer

System Requirements

These are the minimum hardware and software configurations required for TraceFinder 5.3 operation.

Table 1. System requirements

System	Minimum requirements	Recommended requirements
Hardware	• 3.1 GHz Quad core processor with 16 GB RAM • Video card and monitor capable of 1280 × 1024 resolution • 256 GB memory	• 8 GHz Quad core processor with 32 GB RAM • Video card and monitor capable of 1920 × 1080 resolution • 1 TB SSD hard drive
Software	• The operating system must be either Windows 10 LTSC 2019 LTSC 2021 or Window 11, 64-bit IoT Enterprise edition (LTSC 2024). • Adobe™ Reader™ 10.1 or later • Thermo Scientific™ software: – Xcalibur™ data system 4.7 SP1 – Foundation platform 3.1 SP10 – mzVault™ 2.3 SP1 – FreeStyle™ 1.8 SP2	• Windows 11, 64-bit IoT Enterprise edition (LTSC 2024) • Microsoft .NET Framework 4.8 (x64) • Adobe™ Reader™ 20.1 or later • Thermo Scientific™ software: – Xcalibur™ data system 4.7 SP1 – Foundation platform 3.1 SP10 – mzVault™ 2.3 SP1 – FreeStyle™ 1.8 SP2

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Important Information

Xcalibur™ 4.8 requires Windows® 11 IoT Enterprise LTSC 2024 for installation. Xcalibur™ 4.8 is not supported on Windows® 10 operating systems.

For all Windows® 10 environments, install of Xcalibur™ 4.7 SP1 is required (Xcalibur™ 4.7 SP1 is not included with the TraceFinder™ 5.3 installation media).

CAUTION The TraceFinder application supports only US English versions of Windows and Office, with the English locale settings.

Apart from date localization in reports, no other locale settings (such as change of decimal separator or change of list separator) are supported. To avoid failure of data acquisition and processing, be sure to test all settings.

Resolved Issues

The following table lists defects that are resolved in the TraceFinder 5.3 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.

Table 2. Resolved issues

Software section	Severity	Abstract	Item ID
Data Review	Major	Failure to update ion ratio upon manual peak integration	818225
Data Review	Major	Failure to update flag status upon manual peak integration	818228
Data Review	Major	Library matching score displays NaN after batch save, close, reopen	818230
Data Review	Major	Intermittent R^2 display of greater than 1.000 when Calibration Curve origin setting is set to force through zero	818242
Data Review	Major	Loss of manual peak integration results with peak detect unchecked	818244
Data Review	Major	Manual integration of confirming peak is lost when manual integration of the quan peak is performed	818247
Data Review	Major	XIC overlay not displayed in Unknown Screening data review	857646
Data Review	Medium	Intermittent failure to update Quan Peak chromatogram within the Compound Details panel within Data Review	864073
Data Review	Medium	Intermittent failure to display Library Match spectra within the Compound Details panel within Data Review	864074
Local Method	Major	Intermittent acquisition list display update failure upon opening of existing method in both the master and local method.	864075
Reporting	Medium	Duplicate display of samples with Batch Report when sample batch contains a greater number of samples than batch template.	845549
Master Method	Major	Initial database selection not saved upon Targeted Screening master method creation	846128
Data Review	Medium	Data display sync - Peak Area values for Retention Time Reference compounds.	845545
Data Review	Medium	Failure to apply sample sorting within the Sample Results table to Compound Centric Plot view when sample display selection is updated	836288
Data Review	Medium	Incorrect R^2 calculation display when calibration level table contains zero values and weighting is applied	836334
Master Method	Medium	Application error generated upon selection of Export selected compounds to mass list in the Acquisition List of the Master Method	829218
Intelligent Sequencing	Major	Failure to perform sample reinjection when failure action is set to reinject.	830584

Table 2. Resolved issues

Software section	Severity	Abstract	Item ID
Data Review	Medium	Within Targeted Screening Data Review table filters automatically reset when new compound is selected for display	818232

Known Issues

Suggested recovery actions

- For multiplexing, you must set the data window in both the MS method and the MUXvi Data window. The MS method must be equal to or less than the MUXvi data window.
- You can export CSV files, but only cells and columns for grids in the Method Development section can be pasted back into the application.
- When you use MUXvi, the Startup and Shutdown methods are deactivated.
- Instrument methods must reside in the TraceFinder methods folder.
- LCquan™ methods are not imported directly into the TraceFinder application.
- Loss of scroll bars and windows might occur in some of the views. Installing the latest stable video driver and Windows update (at support.microsoft.com/kb/2670838) fixes this issue.
- Microsoft Excel™ style reports that contain more than 10 000 rows of data or that exceed 1024 pages might hang the OpenOffice™ application or show an Excel corruption error. You can open the file in the Excel application, but it removes formatting as part of the repair. To open in the OpenOffice application requires a smaller report to be created.
- Converted legacy data target screening batches might require reprocessing to show data correctly.
- If a user has not been given folder permissions to repositories that the TraceFinder application has access to, the application crashes. Give all users access to at least the default locations set in the Administrator Console.
- Converted quantitative batches will require reprocessing to correctly show quan flags.
- Windows 10 update released on June 9, 2020 causes report generation to crash. Windows has fixed the issue with later updates.
- When table filtering is performed within the Compound Results table of the Targeted Screening workflow, intermittent delays may occur before display updates are completed. All display updates for the applied filter criteria must finish before sample filters can be cleared using the Clear Filter icon within the Sample Results table.
- Signal to noise calculation can vary between method and manual integration due to algorithms differences within the two peak integration modes.
- Upon removal of pending samples from the acquisition queue, existing samples within the Sample List of the Batch view are no longer locked and grayed out, allowing potential edits to the vial position.
- Customer report generation contains multiple dependencies upon the installed Microsoft Office version, minor variations in report output may be observed dependent on the MS Office version utilized for report generation.
- Within the TraceFinder 5.3 release updates of underlying application components have been implemented resulting in minor differences in decimals values relative to the output generated within previous release versions. Minor decimal differences are observed due to decimal rounding changes provided by the underlying application components and cannot be modified or controlled by the TraceFinder application.
- Method forge functionality for data files generated by the Scientific Orbitrap Astral and Astral Zoom Mass Spectrometers is highly dependent upon data file size and target number of components. Performance may vary and can be slower when processing large file sizes or extensive target lists.
- Intermittent issues have been observed during PDF report generation when LibreOffice is installed prior to TraceFinder. This issue is often resolved by uninstalling and reinstalling both applications, followed by a system restart..
- Intermittent issues have been observed when performing Data Review or navigating within the application while the Real-time Status is displayed during data acquisition. The issue can be mitigated by undocking the real-time display from the main display frame or by closing the Real-time Status view while performing data analysis.

- Intermittent failure to display mouse-over tooltips may occur within the Data Review section of the application when running on Windows 11. The issue can often be resolved by navigating away from the current sample and then returning to refresh the display.
- Within the XIC Overlay view in the Sample View display under Data Review > Show Peaks by Selected, chromatograms may not automatically update when compounds are selected sequentially. To refresh the view for individually selected compounds, navigate away from the current file by selecting another file within the batch, then reselect the original file for display. Alternatively, the Top 20 or All display options can be utilized as a workaround.
- Within the Acquisition List of the Master Method, the MS Order dropdown selection is not applied until focus is moved to another cell or the Enter key is pressed. This behavior may affect the intended MS Order value in the acquisition list and the corresponding scan filter selection. To ensure the correct MS Order is applied, after value selection, press Enter or click into another cell to confirm the selection.
- On Windows 11 systems, the TraceFinder application display and window sizing may be affected by system screen resolution and display settings, with the scale setting having the most significant impact. A scale setting of 100% and a display resolution of 1920×1080 typically provide the most consistent results, though the optimal values will vary depending on the monitor's size and resolution.
- When using Intelligent Sequencing and selecting the Autosample and Reinject option under Failure Action, TraceFinder creates the samples in the Sample List with the Reinject listed before the Autosample. However, the actual injection order is correct — the Autosample is injected first, followed by the Reinject sample. The order displayed within the Sample List is reversed from the true injection sequence. This issue was observed following the resolution of issue number 830584.

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

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.

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

Known Defects

Table 3 contains known defects in the software, categorized by software section, with a brief abstract and information related to each defect's severity and risk. The Item ID is the internal number assigned to each issue. Product management assesses risk, which can differ significantly from the reported severity.

Table 3. Known defects

Software section	Severity	Abstract	Risk	Item ID
Administrator Console	Major	Continuous TraceFinder log overfilled hard drive.	High	267423
Method Development	Medium	Manual Peak Creator Panel error in TF 5.1 SP3.	Medium	273855
Method Development	Medium	When an error is made creating a CDB, and an attempt is made to export it, a confusing error message is displayed.	Medium	277464
Acquisition	Medium	Startup and Shutdown methods are not recognized unless the batch is saved prior to submitting.	Low	275200
Administrator Console	Medium	TF does not currently warn the user if disk fills up on Batch Save As.	Medium	272934
Analysis	Medium	Support – Report generated has incorrect value for calculated amount.	Medium	216424
Method development	Medium	Some CDBs have duplicate compounds, which prevents those compounds from being read by MS method editors.	Medium	279374
Administrator Console	Medium	Setting date back on PC will force error message when launching TF, but option provided in error message is not working correctly.	Medium	283666
Acquisition	Medium	When a Calibration Group batch is saved with another name (Save As), all calibration curves are lost.	Medium	318722
Real time status	Medium	Active sample list under acquisition becomes editable including Name and Vial Position after removing samples from the Acquisition Queue	Low	818245
Reporting	Medium	Failure to generate .pdf reports after new install on systems with existing Libre OpenOffice already installed.	Low	832770
Real time status	Medium	Application instability caused by simultaneous display of Real time status and Data Review	Low	845548
Data Review	Medium	Intermittent failure to display mouse-over tooltips may occur within the Data Review section of the application when running on Windows 11.	Low	846218
Data Review	Medium	XIC Overlay view fails to up chromatogram display when Show Peaks by Selected is chosen.	Low	857745
Master Method	Medium	MS Order dropdown selection is not applied until focus is moved to another cell or the Enter key is pressed	Low	864497
Application	Medium	Windows 11 system screen resolution and display settings may affect the layout and window display throughout the application.	Low	855867
Intelligent Sequencing	Medium	When using the Autosample and Reinject option under Failure Action, TraceFinder creates the samples in the Sample List in reverse order, with the Reinject listed before the Autosample.	Low	855867

Trademarks

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