

TraceFinder 5.1 SP1 Release Notes

These release notes briefly list features in the Thermo TraceFinder™ 5.1 SP1 data system and known issues that still exist in the TraceFinder application.

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For information on installing TraceFinder 5.1 SP1 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:

- Time-range peak enhancements
 - Support for confirming ion ratios
 - Option to select how to report RT (center or highest)
 - Option to zero the baseline
- Support for VeriSpray™ data processing
- Support for mzVault 2.3 and multiple library selection
- Report designer improvements

These are the minimum hardware and software configurations required for TraceFinder 5.1 operation.

Table 1. System requirements

System	Requirements
Hardware	<ul style="list-style-type: none">• 3.1 GHz Quad core processor with 16 GB RAM• Video card and monitor capable of 1920 × 1080 resolution• 1 TB hard drive• CD/R-ROM drive (or DVD)
Software	<ul style="list-style-type: none">• Microsoft™ .NET Framework 4.6.2• Adobe™ Reader™ 10.1• Thermo Scientific™ software:<ul style="list-style-type: none">– Xcalibur™ data system 4.3– Foundation™ platform 3.1 SP7– mzVault™ 2.3– FreeStyle™ 1.6• Operating system (one of the following):<ul style="list-style-type: none">– Microsoft Windows™ 7 Professional SP1– Microsoft Windows 10 x64 IoT Enterprise 2016LTSC– Microsoft Windows 10 x64 IoT Enterprise 2019LTSC

Important Information

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 were resolved after the TraceFinder 5.1 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
General	Major	TraceFinder might slow down after a certain amount of time related to temporary files not being removed as expected.	116517
Acquisition	Major	Insert copy of a sample can cause the batch to no longer be openable. Requires a new batch to be created for the data files.	117926
Data Review	Major	Multiple threading can lead to Calibration lock up and batches unopenable. Requires a new batch to be created for the data files.	120209
Data Review	Major	TraceFinder runs into an "Out of Memory" error after many method changes in a batch. Computer must be restarted to clear it.	122679
Acquisition	Major	Reinjection of a sample can cause the batch to no longer be openable. Requires a new batch to be created for the data files.	124272
Acquisition	Major	Injection volume might change to zero when submitted for processing while acquisition is still ongoing.	126611
Data Review	Minor	NIST library results disappear for adjusted compound when working with multiple batches.	113900
Real Time Status	Minor	TraceFinder will not launch FreeStyle 1.7 from Real Time Status.	115378
Acquisition	Minor	TraceFinder will not launch FreeStyle 1.6/1.7 or Qual Browser from Quick Acquisition mode.	115379
Acquisition	Minor	Incorrect maximum injection volume of 100uL is applied for all injections greater than 100uL.	118960
Legacy Data Converter	Minor	TraceFinder 5.0 master method converted to 5.1 gives error when submitted for acquisition.	120797
Data Review	Minor	Cannot reselect an 'Active' compound following processing.	122675
Data Review	Minor	TraceFinder takes a long time to open when a repository has many batches.	124565
Data Review	Minor	Update Master Method from Local Method is not working if the master method is on the D: drive.	128574
Method Development	Major	Unable to save the master method anywhere except to the C: drive.	128572
Acquisition	Minor	Acquisition batch template is not saving the correct batch location if it is directly on the drive; it must be on a folder at least one level down.	128570
Legacy Data Converter	Minor	The Legacy Data Converter changes calibration levels from blank to zero.	128567
Data Review	Major	User peak settings do not apply or persist when the local method is set to Global for that parameter.	61692
Data Review	Major	If the Range Integrated is larger than the Extraction window, TraceFinder does not detect any peaks.	61673
Data Review	Minor	Disappearing dropdown menu can persist when a bad template is saved.	61685
Processing	Minor	Manually integrating a peak while in Time Range Peak does not reprocess the Fragment\Library\Isotope test.	61672

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.

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 (Sheet 1 of 2)

Software section	Severity	Abstract	Risk	Item ID
Acquisition	Major	Selecting to open a network batch while the network is down causes an unexpected exception error.	Low	61668
Admin Console	Medium	Removing/Renaming a mapped network drive prevents the user from opening batches.	Low	59588
Compound Database	Minor	Swapping Target and Confirming ion types might cause duplicate entries.	Low	59480
Data Review	Major	Isotope delta is not calculated correctly if it is set to less than 2 ppm because of a hard-coded default setting.	Low	61677
Data Review	Minor	Expanded display collapses when you choose another sample.	Low	59553
Data Review	Major	Taking batch ownership of a network batch leaves the batch open and usable on the original computer.	Medium	61702
Data Review	Medium	Unknown peak has missing monoisotopic mass if there was trouble identifying a good MS/MS scan.	Low	59512
Data Review	Medium	Default view does not display the sample- or compound-centric view correctly when opened for the first time.	Low	59514
Data Review	Major	User peak setting area/height thresholds do not apply when the local method is set to global.	Low	61675
Data Review	Medium	IR flags might not be correct when evaluating multiple targets.	Low	59494
Data Review	Medium	Batch processing for an unknown peak is canceled if you manually integrate a peak during processing.	Low	59503
Data Review	Medium	RMB of local method does not integrate peaks if no raw data files were associated with the master/local method.	Low	59475
Local Method	Major	Chromatogram labels in the master method, local method, and data review are missing due to peak size.	Low	59527
Master Method	Minor	Selecting Update Ion Ratios while adding a new compound will update ratios for all compounds.	Low	59574
Master Method	Minor	RT is not cleared when reassociating a raw data file with the expected RT turned off.	Low	59589
Master Method	Major	Isotope pattern does not work for multiple charge states when it is set to Global.	Medium	59418
Predictor Tool	Minor	You must enter protein data by importing a FASTA file. You must manually enter peptide data.	Low	59564
Predictor Tool	Minor	Hiding modifications from a table requires an application restart.	Low	59549
Real Time Status Display	Medium	Stopping processing in the Real Time Status display does not close the batch and prevents others from opening it until the original user opens/closes it.	Low	59544
Report Designer	Medium	Target and confirming ions swap places in reports when Integration mode in Data Review is changed.	Low	59487

Table 3. Known defects (Sheet 2 of 2)

Software section	Severity	Abstract	Risk	Item ID
Processing	Crash	Unknown Screening might crash when processed from a network location.	Low	58675
Processing	Major	Unknown Screening might throw errors when processed from a network location.	Low	58676
Data Review	Minor	Target Screening Library results with the same score are not sorted properly.	Medium	61686
Processing	Major	Processing might not continue for unacquired samples when a batch is closed after a Local Method Change.	Medium	83233
Audit Trail	Major	Real Time Viewer changes are not audited in local or master methods.	Medium	61680
Audit Trail	Minor	Ending <i>m/z</i> default value is not audited correctly.	Medium	59097
Audit Trail	Cosmetic	Change made from Autocalc initial events is recorded as 0/1 instead of off/on.	Low	59130
Data Review	Minor	Under a user-defined peak, changing the expected RT of the target peak also sets confirming peaks to user-defined.	Medium	59287
Compound Database	Minor	An ExactFinder™ compound database does not import into TraceFinder 4.0.	Minor	58394
Processing	Minor	Copies of the same batch are being updated when one of them is processing and the copy is also open.	Low	58382
Data Review	Minor	Spectral plot does not show all Peptide labels.	Low	58232
Quick Acquisition	Minor	In Quick Acquisition, stopping a batch from acquiring doesn't release the samples for editing.	Low	58233
Audit Trail	Minor	Converted Legacy Methods can update Avalon settings to latest when the user edits a different parameter.	Low	58337
Processing	Minor	Fragment Ratios are not evaluated for Required.	Medium	58334
Processing	Minor	Confirming ion coelution is not evaluated for Required.	Medium	58335
Master Method / Data Review	Minor	Accessing remote repositories with a large number of batches or methods can be slow to open.	Medium	58344
Audit Trail	Minor	When the user closes the Audit Viewer while logging off of Windows, there is no audit record of the audit viewer closing.	Low	58483
Data Review	Minor	Selecting a New Master Method does not clear out all old information until it is reprocessed.	Medium	58341
Data Review	Minor	Quan+Unknown batch - quan results in the grid are cleared during processing for unknown as well.	Medium	38346
Method Forge	Minor	Method Forge Target List is ignoring the start RT.	Medium	61699
Data Review	Cosmetic	Reinjected samples from Intelligent Sequencing are sorted out of order until the batch is reopened.	Low	58338
Reports	Minor	Calibration curves might not show up on the first couple of requested reports.	Medium	58276
Processing	Minor	Confirming peak test is still run when target peak is not found for type Range Integrated.	Medium	111629
Processing	Minor	GCMS Decon - If there is a mismatch in the submission request, a separate RT Alignment will be run.	Low	85468
Processing	Minor	For mzVault, Reverse Search not forced for AIF data if exact scan filter selected.	Low	88210

Trademarks

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