

TSQ Series II 3.4 SP2 Release Notes

These release notes document improvements to the Thermo TSQ Series II¹ instrument control software version 3.4 SP2.

You can use the TSQ Series II application to collect high-quality mass spectrometry data on the TSQ Series II mass spectrometer. Control of the instrument is through two application packages: Tune and Method Editor.

- The Tune application displays acquired mass spectra in a continuous loop, and reports the observed values of various instrument parameters that indicate the instrument status. The application includes a variety of scan types, scan modes, ion polarities, scan rates, and resolution settings, which you can use to tune and calibrate your instrument for optimal performance. The application also provides a host of diagnostic functions for easy troubleshooting, and contains features that you can use to manage peripheral devices (such as a divert valve and a syringe pump) through a USB connection. Finally, for output documentation purposes, this application supports the generation of reports that cover various diagnostics, calibrations, and optimizations.
- In the Method Editor, you can set up and run experiments using the entire complement of scan types such as the SRM scan mode (commonly used for quantitation). You can also specify peripheral device controls (such as a divert valve) to be used as part of the experiment.

Methods constructed using the Method Editor can be executed in high-level applications such as the Thermo Xcalibur™ data system, the Chromeleon CDS (Chromatography data system), or the Thermo TraceFinder™ software.

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¹ TSQ Series II refers to the following Thermo Scientific mass spectrometry systems: TSQ Altis™, TSQ Altis Plus, TSQ Quantis™, TSQ Quantis Plus, TSQ Fortis™, TSQ Fortis Plus, TSQ Quantiva™, and TSQ Endura™.

Features

The TSQ Series II instrument control software has the following features, listed by the latest to earliest version.

TSQ Series II 3.4 SP2

This service pack will:

- Address various bug fixes (see [Resolved issues](#))
- Not support any new features

TSQ Series II 3.4 SP1 QF1

This service pack with Quick Fix will:

- Address the issues in the reporting format of the Japanese operating system
- Not enforce the installation of Almanac Agent with TNG installer

TSQ Series II 3.4 SP1

This service pack supports the following new features:

- Refined Compound Optimization Tool
- Improved FAIMS™ diagnostics for service

TSQ Series II 3.4

This release supports the following Series II models of triple quadrupole mass spectrometers:

- TSQ Altis and TSQ Altis Plus
- TSQ Quantis and TSQ Quantis Plus
- TSQ Fortis and TSQ Fortis Plus
- TSQ Endura
- TSQ Quantiva

TSQ Series II 3.4 also supports the following hardware items:

- FAIMS Pro Duo™
- Calibration Spray Insert (Calibration Probe)

New software features with TSQ Series II 3.4 include the following:

- mzCloud™ Conversion Tool
- Dwell Time Factor Option
- Simplified System Check and Calibration Options
- FAIMS CV Optimization Tool
- The selection of cycle time or points per peak for easy method setup
- Extension of the source fragmentation range to 140V (TSQ Altis Plus, TSQ Altis, TSQ Quantis, TSQ Quantis Plus, TSQ Endura, TSQ Quantiva) and 80V (TSQ Fortis and TSQ Fortis Plus)
- Extension of the collision energy to 90V in the TSQ Plus portfolio.

TSQ Series II 3.2 SP1

This service pack addresses the following issues:

- Electrometer baseline drift
- Japanese localization for Chromeleon
- Extended mass range down to m/z 2
- Robust TSQ Fortis mass calibration procedure at high altitude
- Improved charging diagnostics for service

TSQ Series II 3.2

This release supports the existing TSQ Series II models of triple quadrupole mass spectrometers—TSQ Altis, TSQ Quantis, TSQ Fortis, TSQ Quantiva, and TSQ Endura—and adds support for the newly released VeriSpray™ ion source.

Enhancements include support for the following:

- Running PaperSpray™ analyses with the VeriSpray ion source.
- Controlling the LC/MS system from the Chromeleon 7.2.10 CDS, which has an integrated Thermo MS Tuning ePanel.
- Monitoring the mass spectrometer's calibration status. The Tune Status pane includes the mass spectrometer's calibration status, and the Tune Status icon indicates an error state when the mass spectrometer is due for calibration or the Check Mass Calibration routine fails.

TSQ Series II 3.1

This release supports the existing TSQ Series II models of triple quadrupole mass spectrometers, the TSQ Endura, TSQ Quantiva, TSQ Quantis, and TSQ Altis—and adds support for the newly released TSQ Fortis.

Enhancements include the following:

- Support for the TSQ Fortis MS
- New, fast, and easy installation program
- FAIMS support
- Improved calibration and optimization procedures

TSQ Series II 3.0

This release supports the new TSQ Series II models of triple quadrupole mass spectrometers, the TSQ Altis and TSQ Quantis.

Enhancements include support for segmented quads and improvements in the following: the electron multiplier lifetime, mass and resolution calibration, and service diagnostics.

The application integrates with the Xcalibur 4.1 data system, which contains Foundation™ platform 3.1 SP4 and deploys the .NET-based raw file reader and writer.

TSQ Series II 2.1

- The Tune interface provides a new compound optimization tool for source optimization, precursor RF-lens optimization, selection of the *n*-most intense product ions from a product ion spectrum, specifying exclusion mass losses, collision energy (CE) breakdown curves for selected fragments, and reports using loop injection and infusion. With the introduction of this new tool in the Tune interface, the older optimization interface on the Source and Scan tabs has been removed.
- The Method Editor provides a visualization component for concurrent SRMs within a method.
- The application can dynamically update the scheduled SRM retention time during method acquisition if a reference mass peak is assigned.
- The Chromatogram Filter value is automatically calculated based on the chromatographic peak width.
- An alerts console in the Tune interface shows errors, warnings, and other information.

TSQ Series II 2.0

- Improved reports for calibration, compound optimization, auto tune, and diagnostics with the addition of results tables and targeted formatting of report artifacts.
- Ability to import and export certain methods as XML files and apply mass list modifications to the methods by using a defined XML schema.
- Mixed scan mode that enables you to run multiple different scan types in the same time window.
- Enhancements to compound optimization so that you can specify Source CID values and choose either the stepped collision energy or the ramped collision energy option.

- Improved calibration and tuning including faster calibrations, more auto-tuned lenses, higher scan rate calibrations done in Q3 mode, and automatic coarse calibration
- Availability of time-dependent source voltage settings in the method definition
- Event transition states directed to the Foundation platform to eliminate the time lost in state polling cycles
- Chrom-filter support for SRM methods when using the dwell time option
- Improvements to QED method that add a limit to the threshold values and enable dynamic DDCE calculations
- Support for scan rate- and dwell time-based SIM scans
- Integration and support for compound optimization through the QuickQuan™ application
- Support for additional APPI lamp for both H-ESI and APCI sources

TSQ Series II 1.1

- Audit of the method and system changes
- Extended mass calibration with Extended Mass Reference Solution (EMRS)
- Support interfaces for integration with the Thermo Chromeleon™ platform
- QED data-dependent scan
- Ion source recognition with combo sources
- Instrument calibration date included in raw data files
- Changes to the calibration options in Tune
- System and user method templates
- Remote diagnostics

TSQ Series II 1.0

- TSQ instrument configuration: This feature is available through the Thermo Xcalibur/Foundation interface as a modal dialog box, and the configured values are stored by the instrument software. Instrument configuration supports system information, instrument warnings, and historical data retention policies; it also supports configurations for the inlet and the ion source, and those that relate to field services.
- Tune Ion Source page: Use this page to configure the ion source's related gases, temperature, and voltage, or change current parameters. You can configure the following ion sources: H-ESI, APCI, or NSI. You can also get the default parameter values based on the matrix of the LC flow rate for both H-ESI and APCI.
- Tune Define Scan – Scan page: Use this page to tune the scan parameters for your mass spectrometer. You can edit a set of scan parameters applicable to the experiment of interest. The scan will result in updated graphs and a spectrum that is displayed in the Tune application. Supported scans include SRM, SIM, full scan, neutral loss scan, and product and precursor scans.
- Tune Calibration Options pane: Use this pane to perform calibration in a separate area that handles mass position, resolution, and multiplier gain calibration. You can also check the spray stability in both positive and negative ion modes.
- The instrument can control devices from the instrument host computer using a USB interface for these devices: the turbo pump for readbacks, the syringe pump for both control and readbacks, and divert valves A and B for both control and readbacks.
- Tune Data Acquisition pane:
 - Acquire scan data from perpetual scans or method runs into a designated raw data file. This view presents a Record icon and the ability to enter a file path for method specification.
 - Start an acquisition loop with a contact closure signal from the LC system at the start of the gradient.
- Tune History and Favorites panes (vertical tabs): Use these two panes for access to saved instrument state information that you can reapply at any time.
- Tune buttons and icons: This topmost area consists of buttons and icons that report on the overall status of the instrument. The Status pane displays readback values for By Optics or By Board selections.

Minimum requirements

- Tune application:
 - You can select the positive or negative ion mode for the system; move the instrument into start, pause, or stop mode; and choose profile or centroid options for scanning.
 - You can copy the compound/LC-flow optimized source settings.
- Method Editor Scan Parameters page: Part of Method Editor, which also has the Global Parameters and Summary pages. A method can have experiments and each experiment can have multiple, timed rows for any type of scan. The supported scan types include SRM scan, SIM scan Q1, SIM scan Q3, full scan, product scan, precursor scan, and neutral loss scan.
- Method Editor validation: Performs extensive validation on the method parameters and warns you if a method is in error, even after you have saved it. The Method Editor will not execute invalid methods when they download to the instrument.
- Method Editor Global Parameters page: Use this page to configure a timeline-based source and peripheral settings that are applied during the method run and include parameters for method duration, ion source settings, syringe pump, divert valve A, divert valve B, and contact closure.
- Method Editor Summary page: This page is also included in the raw data file.
- Support for exporting and importing XML files: For processing applications like Thermo TraceFinder™, LCquan, and third-party applications, the TSQ Series II application supports the export and import of XML files for the mass list and method setup.

These are the minimum hardware and software configurations recommended for TSQ Series II 3.4 SP2 operation.

System	Recommendation
Computer	<ul style="list-style-type: none"> • 3.1 GHz Quad core processor with 16 GB RAM • Video card and monitor capable of 1920 x 1080 resolution • 1 TB hard drive • DVD drive • USB ports
Mass spectrometer	TSQ Series II
Software	<ul style="list-style-type: none"> • Microsoft™ Windows™ 10 Enterprise LTSC 64-bit OS (Shipping configuration); Windows 10 Enterprise 2016 LTSC 64-bit OS or Windows 10 Enterprise (Supported) • Thermo Scientific™ software: <ul style="list-style-type: none"> – Foundation 3.1 SP9 or later – Xcalibur 4.6 or later – FreeStyle™ 1.8 SP2 or later – SII for Xcalibur 1.7 or later – LC Devices 3.2 SP3 or later – Chromeleon 7.2.10 MUF or later – Chromeleon 7.3.1 MUA or later

Resolved issues

Table 1 lists defects that are resolved in the TSQ Series II 3.4 SP2 application. 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 1. Resolved issues (Sheet 1 of 2)

Item ID	Abstract
229776	TSQ software should display the status information of dry pump when it's connected with a special cable to communicate with mass spec
275114	Missing scans in QQQ methods using cycle time
276692	Wrong SRIG RF settings in product ion mode
281704	Early TSQ Quantiva instruments with older style SRIG PCBs will cause the instrument to go into error mode
297777	Mismatch between summary table entry and detail result data table for Calibration Check report
298692	Dip Ion Funnel diag missing from customer facing diagnostics (3.4/3.4 SP1)
310032	FAIMS Pro Diag "Entrance Plate Voltage Ramp Test" issues with compensation and inner plate voltage
314086	Upgrade MongoDB to 4.0.28 for TNG and CO
314087	Add authentication to MongoDB
326362	TSQ Plus Q2 RF Dip throws run-time error and exit when the resonance frequency (well-developed maximum point) is not being found
326967	Cannot launch workstation Method Editor without Foundation installed for TSQ Series II instruments v 3.4 SP1 QF1
330287	Remove Optimization service entry from version info and Add/remove programs
331288	Remove Almanac Agent and UDA Identify server from TNG installer
332570	MongoDB needs to be uninstalled manually when downgrading from 3.4 SP2

Table 1. Resolved issues (Sheet 2 of 2)

Item ID	Abstract
335954	Jagged Scans when using pos/neg switching
336863	Update EULA (installer and Tune) to remove obsolete 3rd party license
341342	Update the calibration report - reference to more information
343704	Update the Hardware User Manual to add reference to calibration requirement on user
347362	When Pump is reconnected, console shows Fore Pump: Exception code: Illegal data address
349194	Installing TSQ Series II Workstation on Windows Server 2012 - incorrect error message
351014	Hardware User Manual: Need to correct TM symbol and Spray stability figure

Known issues

When using any of the commands in the toolbars, you must click outside the area for the action to take effect.

Suggested recovery actions

- For some issues like connectivity problems, restarting the application is the appropriate recovery action.
- In some cases (particularly issues that arise during data acquisition), restarting applications such as the Home Page might not ensure complete recovery. Typically, restarting the data system computer resolves issues, 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.

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 could compromise operation if it occurs.
Low	Issue is minor; however, the software could operate differently from a user's expectations. A workaround may 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, 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 2. Known defects

Software section	Severity	Abstract	Risk	Item ID
Chromeleon (embedded Tune)	Medium Problem	Calibration or Diagnostics Report is not displayed in the Chromeleon Tune Results Page.	Low	136030
Compound Optimization	Minor Problem	A combination of earlier versions of VAS software and SII might result in SII being stuck in an error state after multiple, consecutive stoppages of a Compound Optimization run. You can correct this error by right-clicking the SII device in Xcalibur and resetting the VI state command.	Low	42233
Compound Optimization	Minor Problem	The Prelude SPLC™ and Transcend™ Systems are not supported for compound optimization within TNG Tune application.	Low	43429
Chromeleon (embedded Tune)	Major Problem	Verispray source recognition does not function using TSQ software controlled through Chromeleon	High	361173

Trademarks

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