Waters™

waters_connect MS Quan 1.11.1

Release Notes

General information

Copyright notice

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About these release notes

This document contains information about the features and functions introduced, changed, or removed in this version of the product. It contains a list of major feature changes as well as descriptions of known defects, resolved defects, and observed product behaviors (concessions) that Waters deems of importance to customers. This document does not include:

- An exhaustive list of all changes to this version of the product

- Descriptions of defects that were not known to Waters at the time of the product's release

- Descriptions of defects that cannot be reproduced by Waters

- Information about customer requests for enhancements to the product
- Specific details of changes to proprietary aspects of product components, features, computational algorithms, and software code

The changes listed in this document are relative to the previous version of the product. If you are updating an older version of the product, review the release notes for all the intervening versions to ensure that you understand the cumulative impact of the product changes.

Carefully review the information in this document before the product is installed. If you have questions about how installing this product might affect your environment or if you need more information about this product, contact your Waters representative.

Compliance recommendations

Any time you install, change, or uninstall software or system modules in a regulated environment, Waters recommends that you follow your organization's approved change control procedure.

You should assess the impact of the changes described in the release notes on the qualification status and validation for the intended use of your system, including any impact on personnel, methods, laboratory workflows, or connected equipment, and scale your activities accordingly.

Manufacturer information

Manufacturer:

▟	Waters Corporation 34 Maple Street Milford, MA 01757 USA

Customer comments

We seriously consider every customer comment we receive. Help us better understand what you expect from our documentation so that we can continuously improve its accuracy and usability. To report any errors that you encounter in this document or to suggest ideas for otherwise improving it, reach us at tech_comm@waters.com.

Contacting Waters

Contact Waters with technical questions regarding the use, transportation, removal, or disposal of any Waters product. You can reach us through the Internet, telephone, fax, or conventional mail.

Contact method	Information
www.waters.com	The Waters website includes contact information for Waters locations worldwide.
iRequest	iRequest is a secure Web service form that allows you to request support and service for Waters instruments and software or to schedule a planned service activity. These types of support and services may be included as part of your maintenance plan or support plan. You may be charged for the requested service if you do not have appropriate plan coverage for your product. **Note:** In areas managed by authorized distributors, iRequest may not be available. Contact your local distributor for more information.
Local office contact information	For worldwide locations, telephone, fax, and conventional mail information is available at the Local Offices website.
Corporate contact information	Waters Corporation 34 Maple Street Milford, MA 01757 USA From the USA or Canada, phone 800-252-4752 or fax 508-872-1990.

Updated information

Refer to the Waters website (www.waters.com) and click **Support** > **Support Documents and Downloads** for updates to this document.

Obtaining Waters software and software updates

To digitally obtain the software application and licenses that you purchased, use the Waters Digital Software Delivery and License Entitlement platform. With an active Waters Software

Maintenance Plan, the platform gives you email notifications of and immediate access to newly released software. This delivery platform allows you to securely search and share software entitlements and instrument drivers, and it provides a secure search document link to www.waters.com that details all relevant documents for the specific software product and version.

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If you have not yet arranged for access to this platform, work with your Waters sales representative to begin the secure onboarding process.

Access the software delivery and license entitlement platform through your www.waters.com user profile at **waters.com** > **My Account [Hello, *username*]** > **Profile** > **Download Software Entitlements**.

Table of contents

waters_connect MS Quan overview

waters_connect MS Quan is a Web-based application that launches from the waters_connect application hub.

The MS Quan application enables you to process mass spectrometry data collected using Multiple Reaction Monitoring (MRM) methods.

You can use the MS Quan Processed Data Review workflow to efficiently review processed data.

New features and enhancements

MS Quan 1.11.1 includes the following new features and enhancements since the previous commercially released version of the product:

New feature or enhancement	Details
New save, edit, and discard behavior	To clarify the situation when saving and editing within MS Quan, we introduced edit, save, and discard buttons to all entities (such as result sets, methods, rule sets, and reporting templates). Entities now open in a read-only state and can only be edited if transitioned to the edit mode by use of the edit button.
Internal standards % recovery	A % recovery value is now calculated for all internal standards (primary and secondary) and shown in the data summary table and reports.
Report template chromatogram settings	Additional options are now available in the report template to allow users to select the size and determine the axis ranges, both x and y, of their chromatograms in the PDF report.
Report filtering	Users can now generate reports with a filtered set of the data. At the point of report generation, injections and analytes can be filtered out of the PDF to give a more concise report. This functionality is controlled by a role permission that is configured in the administration app.

Deployment notes for MS Quan

Ensure that you complete the following prerequisites before you install the MS Quan application:

- Installed waters_connect Platform 7.1.0 or waters_connect Platform 7.2.0 on your workstation or network server.

- Installed UNIFI 3.6.0 or UNIFI 3.8.0.

- Uninstalled previous versions of MS Quan.

See also: For information on waters_connect systems that include this application, search www.waters.com for "waters_connect with UNIFI supported systems".

Issues resolved in this release

This section lists problems that were resolved since the previous commercial release of the product. The numbers identify issues that Waters personnel monitor within a system change request tracking tool.

INFMSQ-9584

Previously, users encountered difficulties when specifying sample positions involving tray numbers and well positions. Specifically, the format "10:C,1" triggered an error message, "Sample Position not in the correct format". This issue was resolved by refining the sample position handling logic. Now, you can seamlessly set up an Acquire and Process method that includes all trays within the Sample Organizer. Whether you are analyzing complex matrices or routine samples, the new workflow accommodates your needs.

INFMSQ-9776

Previously, there was an issue with the advanced ion ratio calculations related to determining the appropriate tolerance for comparing ion ratios with their expected values. This issue has been resolved. An improved approach now ensures more accurate assessments:

- Tolerance Calculation: The tolerance is now determined by examining the expected value and converting it to a relative percentage. If the value is less than 1, it is first inverted.

- Importance of Discrepancy: Ion ratios with larger discrepancies between the two peaks have a correspondingly larger tolerance.

This enhancement improves the accuracy of ion ratio assessments and enhances the reliability of results.

INFMSQ-10084

When an analyte uses a calibration reference compound, there is no concept of Quan Reference (QR) values. However, previously, when the expected ion ratios for analytes were updated using values from the QR injections, these analytes had their values set to 0. This issue has been resolved, and the values are not updated.

Known issues in this release

This section lists the known issues and solutions for this release. The numbers identify issues that Waters personnel monitor within a system change request tracking tool.

INFMSQ-3435

When pasting SVG downloads into Microsoft Word, they do not display correctly.

Solution: Convert the downloads to another file format such as PNG with a third-party application, and then paste into the original target application.

INFMSQ-3937

When two users are active at the same time through the identity server login page bookmark, MS Quan switches from the original user to the new user. This may lead to a user working under the wrong account.

Solution: Avoid having the identity server login page as a bookmark, and sign in a different way.

INFMSQ-4379, PMFCR-1090, PMFCR-2114

When returning to MS Quan after leaving it open overnight, an error message appears and you must relaunch the application.

Solution: If you leave MS Quan unlocked overnight, close the application tab, and then relaunch it from the Hub. MS Quan then functions correctly and any unsaved data is in a recovered state.

INFMSQ-4531

When you have access to Company but not company-level folders, the add new folder button is unavailable.

Solution: Select a folder you have access to before clicking the add new folder button.

INFMSQ-4667, PMFCR-912

When importing a method from TargetLynx, if all analytes are set to TIC for the quantitation trace, an empty method is created.

Solution: Before importing the method, update the TargetLynx method to specify MRM transitions.

INFMSQ-4951

When you disable an internal standard rule on the Dashboard overview page, there is no placeholder for the IS widget.

Solution: None.

INFMSQ-5080

When you navigate away from a step, the analyte filter does not restore the analyte name.

Solution: Select an analyte from the filter again, and then delete it from the box.

INFMSQ-5293, PMFCR-946

When you have multiple instances of the same analyte transition in different channels, you must resolve the ambiguity in MS Quan by assigning a channel to each analyte. However, the channel numbers displayed in the Resolve duplicate transitions dialog box do not always match the function number in the Acquisition Method Editor (AME) method.

Solution: There is no solution at this time for the mismatch in channel and function numbers. However, the online Help topic "Resolving duplicate transitions" contains advice to assist you in resolving ambiguities using other information.

INFMSQ-5356

When you import a MassLynx sample list (using waters_connect Explorer) with the "Quan Reference" option set to True for an injection, and then analyze the data in MS Quan, the MS Quan field "Quan reference" is not selected.

Solution: After processing the results set, open the Injections page and change the "Quan reference" setting for the relevant injections. When the data is reprocessed, the results include the correct reference values.

INFMSQ-5437, PMFCR-1115

When you use the "Create MS Quan processing method" option in waters_connect Acquisition Method Editor to create an MS Quan method, with "Start MS Quan on completion" selected, MS Quan fails to launch. When you open MS Quan from the waters_connect Hub, the method is present in the "(Recovered)" state.

This defect only occurs the first time you use this option in a session. If you repeat the process, MS Quan launches correctly.

Solution: After you use the "Create MS Quan processing method" option in waters_connect Acquisition Method Editor for the first time in a session, open MS Quan from the waters_connect Hub to view the method.

INFMSQ-5515, PMFCR-1121

In a method, when adding levels to an analyte, you see a nonspecific error. This occurs after creating new analyte rows on the Levels tab. For example, the following steps produce the error:

1. Create a method.
2. On the Analytes page, in the Analytes tab, specify an analyte name, precursor mass, and product mass.
3. Click the **Levels** tab and select to add a row to the table.
4. Delete the added row.
5. Select to add a new level to the table.

Solution: Always create new analyte rows on the Analytes tab. To remedy the error if you performed the steps above, navigate to the home page using the link provided within the error message or the home page button. The method is present in the recovered state and you can open it again.

INFMSQ-5631, PMFCR-1156

In MS Quan, when you create a new method and select to create a new folder, the check mark and cross buttons next to the folder are hidden, preventing you from creating the folder.

Solution: Resize the Create Method dialog box to make it larger. You can now see the check mark and cross buttons.

INFMSQ-5769, PMFCR-1215

When you view calibration data on the Cals & QCs page using the quadratic fit type, an apparently valid calibration curve can appear without data for the calibration and QC data points. In this situation, you see the messages "No available calibration standards to display" and "No available QCs to display".

This happens when the quadratic curve increases to a maximum response ratio and then decreases within the charted concentration range. In this situation, some values on the Response Ratio (y) axis can match more than one value on the Concentration (x) axis, because they intersect the curve in two places either side of the maximum. Because of this, the curve is not usable.

Solution: Select a different fit type. A Linear or Average RF fit avoids this possible issue.

INFMSQ-5775, PMFCR-1239

When you have multiple instances of the same analyte transition in different channels, you must resolve the ambiguity in MS Quan by assigning a channel to each analyte. However, the channel numbers displayed in the Resolve duplicate transitions dialog box do not always match the function number in the Acquisition Method Editor (AME) method.

Solution: Use other information to assign the channels (for example, cone voltage and collision voltage, which are displayed as part of the channel information). If this information is not sufficient to resolve the ambiguity, use all possible assignments to determine which produces the correctly detected peak.

INFMSQ-7293

When you create a method, the values are specified to a certain number of decimal places, and this data format is not configurable. When a result set is created from that method, if any changes are made to the display settings in the embedded rule set, those display settings are applied to the embedded method as well.

Solution: None.

INFMSQ-7863

Result sets created in previous versions of MS Quan with names longer than 50 characters cannot be opened in MS Quan version 1.9.0 or later.

Solution: Recreate the result set from the processing method and sample set and type a name with fewer than 50 characters.

INFMSQ-7949

If you include an open curly bracket "{" in the name of a reporting template, results set, method, or rule set, an "Oops! Something went wrong" error occurs when you try to browse the objects.

Solution: Use waters_connect Explorer to delete the object.

INFMSQ-8315

On a network system, when two users have the same result set open and a report is generated, an "Oops! Something went wrong" error occurs.

Solution: None.

INFMSQ-8338, PMFCR-2017

When you create a folder policy in waters_connect Administration that requires a user-defined audit reason for App Report actions Create and Delete, and then apply the policy to the Company folder and attempt to generate a report from MS Quan, you are not asked to supply a reason, and the report generation fails with the error "An error has occurred while processing your request. Please contact support and mention this error token *token_GUID*. Conflict: The given audit log reason is missing or empty."

Solution: Remove the folder policy from the admin app.

INFMSQ-8813, PMFCR-2083

The CSV sample list import for SSUB does not work properly for the MS Quan sample type Quality Control.

Solution: In the CSV that you are importing, use the term CheckStandard as the sample type for injections that you want to be processed as Quality Control samples. Alternatively, set the sample type correctly on the injections tab in MS Quan after processing the data.

INFMSQ-8814, PMFCR-2057

The right-click context menu for ignoring QC points is not correctly disabled for users who do not have permission to ignore QCs. If these users attempt to ignore a QC using this method, the application displays a 403 error. Refreshing the page clears the error, but the QC point is not ignored.

Solution: Log in as a user with the required permission.

INFMSQ-8860

When you specify multiple new values into a rule set before waiting for the initial value to complete, the values are not always stored.

Solution: Specify the values one at a time and wait for the sync to complete each time.

INFMSQ-8890

The installation of MS Quan fails if predefined reasons are created for MS Quan specific permission-based actions (for example, modify integration settings) under the result set category.

Note: This defect is not seen if there are predefined reasons for modify or delete actions.

Solution: Delete the predefined reason for any custom action before the new version of MS Quan is installed.

INFMSQ-8968

When you log in to MS Quan as a user with the report content filter permission and clear the search text from the search field, the search box returns to its state before a filter was applied but the table is still filtered.

Solution: When the search text is removed (using backspace or delete), press the Enter key on the keyboard to ensure that the search filtering on the table is also cleared.

INFMSQ-8987

When cancelling the Audit reason dialog for Select peak, the UI stops responding.

Solution: Select another step and click **Back**.

INFMSQ-9015

When changing an embedded method in a result set, a Processing dialog box appears but is then followed by an Impossible to Change dialog box. Processing is completed, but you must select **Refresh** in the Impossible to Change dialog box.

Solution: None.

INFMSQ-9068

When you create a MS Quan Result Set using the default rule set and default reporting template, generate a report, and open the report, the rule set version is reported as 0.

Solution: None.

INFMSQ-9135

When you open a published Result Set and transition to edit mode, the read-only toaster message reappears.

Note: This defect is not seen for other item types.

Solution: None.

INFMSQ-9143

When you modify the ion ratios rule in the Result Set by changing it from Quan/Qual to Qual/Quan, there is no warning triangle similar to the warning triangle for retention time and ion ratios.

Solution: None.

INFMSQ-9152

When migrating from version 1.9.0 to 1.11.0, the Generated Reports list is empty even though users generated reports in version 1.9.0.

Solution: None.

INFMSQ-9156

When updating an advanced Ion Ratio in the Rule Set, if you leave the cursor in the cell when you click **Save**, an "Oops! Something went wrong" error occurs.

Solution: None.

INFMSQ-9167

When you manually lock the MS Quan application when a rule set is open in an edit mode, the application fails and the home button does not work.

Solution: None.

INFMSQ-9169

When you perform field validation in an embedded method, the existing number cannot be removed, and changing the text locks the cell.

Note: This works as expected for a method opened from the MS Quan landing page. Only an embedded method within a result set seems to cause issues.

Solution: Select one of the other sub-tabs (for example, Levels), and then go back to the Analytes tab.

INFMSQ-9195

When you go the MS Quan homepage, lock MS Quan, and then unlock MS Quan, the MS Quan version disappears.

Solution: Refresh the page to bring back the version number.

INFMSQ-9198

When you press the Discard changes button, the calibration graph disappears.

Solution: Move the pointer around the card header area where the R^2 value is located.

INFMSQ-9330

When you cancel the overwrite warning message of manual integration settings, the values in the integration parameters are not cleared.

Solution: Select System Suitability (or any other item in the panel) and switch back to Cals & QCs. This clears the values.

INFMSQ-9528

When Qual ion is manually integrated, the signal-to-noise (S/N) values of Qual ions change to N/A.

Solution: Manually apply S/N regions to a standard and to all the injections.

INFMSQ-9852

In a Result Set from the **Unknowns** page, when you click a **By analyte** graph, the labels on the top and bottom axes do not align correctly. This inconsistency can lead to confusion for users interpreting the data.

Solution: Refer only to the top axis for the correct scale.

INFMSQ-10062

When users delete the Quan Reference injection, the ion ratios and associated deviation calculations are not consistently updated. This behavior can lead to discrepancies in data analysis.

Solution: None.

INFMSQ-10068

When users manually modify the expected ion ratios and then click the **Update Expected Ion Ratios** button, a synchronization issue occurs on the front end. The issue is that the peak is still being displayed as manually integrated, and it should not be.

Solution: Reload the page or navigate to a new page and return to see the correct peak.

INFMSQ-10120

When a user with permission to modify result sets accesses the Blanks page in a Read-Only result set, the tooltip displays incorrect information.

Solution: None.

INFMSQ-10132

When manually dragging the start and end points of baseline markers on the Cals & QCs page, the markers are not correctly rendered on the plot. This issue affects the visualization of baseline information for specific analytes.

Solution: Click **Apply** to add the manually altered peak, and the markers reappear.

INFMSQ-10189

The ID for the method and reporting template consistently defaults to version 1, regardless of the version used to create the report.

Solution: None.

Calculating standard deviation

Standard deviation can be calculated as either population standard deviation or sampling standard deviation.

- If the data is considered a population on its own, it is known as population standard deviation and is divided by the number of data points.

- If the data is a sample from a larger population, it is known as sampling standard deviation and is divided by one fewer than the number of data points in the sample.

Standard deviations in MS Quan are calculated as population standard deviation.

Signing in to MS Quan

After you install MS Quan, you can open this application from the waters_connect Hub. When you sign in to waters_connect Hub or MS Quan, you are signed in to all waters_connect applications.

To sign in to MS Quan:

1. Double-click the waters_connect Hub icon and, if it is not present, do the following depending on your installation type:

   - On a workstation, open Chrome to *https://localhost:1234*.

   - On a network client, open Chrome to *https://<server_name>:1234*, where <server_name> is the fully qualified domain name of the server.

2. On the waters_connect Authentication page, type your username and password, and then click **Sign in**.

3. In the waters_connect Hub, click **MS Quan**.