

Release Notes

Chromeleon 7 Chromatography Data System

Software Version 7.2.9 • April 2019

Document Revision 2.0

Copyright

Copyright © 2009-2019 Thermo Fisher Scientific Inc. All rights reserved.

Trademarks

ACQUITY, Alliance and Waters are registered trademarks of Waters Corporation. Agilent is a registered trademark of Agilent Technologies. Microsoft, Windows 8.1 Pro, .NET Framework and SQL Server are registered trademarks of Microsoft Corporation. PerkinElmer and Clarus are registered trademarks of PerkinElmer Inc. Shimadzu is a trademark of Shimadzu Corporation. Air Server-xr, TD100-xr UNITY-xr and Kori-xr are trademarks of Markes International Ltd. WibuKey is owned by Wibu Systems.

ReSpect (tm) Deconvolution Algorithm (c) 2013 by Positive Probability Ltd.

All other trademarks are property of Thermo Fisher Scientific Inc. and its subsidiaries.

Thermo Fisher Scientific Inc. provides this document to its customers with a product purchase to use in the product operation. The document is copyright protected; any reproduction of the whole or any part of this document is strictly prohibited, except with the written authorization of Thermo Fisher Scientific Inc.

This document is provided “as is”. The contents of this document are subject to being changed, without notice, in future revisions.

Thermo Fisher Scientific Inc. makes no representations that this document is complete, accurate, or error-free. Thermo Fisher Scientific Inc. assumes no responsibility and will not be liable for any errors, omissions, damage, or loss that might result from any use of this document, even if the information in the document is followed properly.

This document is not part of any sales contract between Thermo Fisher Scientific Inc. and a purchaser. This document shall in no way govern or modify any Terms and Conditions of Sale. The Terms and Conditions of Sale shall govern all conflicting information between the two documents.

Release History

Revision	Date	Comment
1	September 2018	Initial Product Release
2	April 2019	Updated section Error! Reference source not found. ; added section 3.7.3; Add Known Limiation reagrding Functional Specifications; corrected typographical errors.

For Research Use Only. Not for use in diagnostic procedures.

Table of Contents

1	Introduction	5
2	Other Documentation	6
3	What's New in Chromeleon 7.2.9	7
3.1	New and Updated Thermo Scientific Instrument Drivers	7
3.2	New and Updated Third Party Instrument Drivers	8
3.3	Compliant MS Tuning Features	9
3.4	Vanquish and Ultimate 3000 Features	9
3.5	Chromeleon Server And 247 Instrument Controller Enhancements	10
3.6	Chromeleon Client Enhancements	12
3.7	Other Enhancements	14
4	Resolved Issues	15
5	Limitations and Known Issues	23
5.1	Limitations with Thermo Scientific Instruments	23
5.2	Compatibility with Foundation 3.1	26
5.3	Limitations with the Waters Driver Pack	26
5.4	Limitations with Agilent ICF	27
5.5	Limitations with Other Third Party Instruments	29
5.6	Limitations With Setup	31
5.7	Other Limitations	32
5.8	Obsolete Drivers	36
5.9	Functional Differences between Chromeleon 7.2 and Chromeleon 6.8	36
6	Backward/Forward Compatibility Issues	37
6.1	Thermo Scientific Vanquish Charged Aerosol Detector [CM6-23499]	37
6.2	Thermo Scientific Vanquish Autosampler [CM6-23405]	37
6.3	Thermo Scientific TriPlus RSH	37
6.4	Thermo Scientific TriPlus 300 HS	37
6.5	Thermo Scientific TriPlus LS-100	37
6.6	Thermo Scientific TSQ Quantiva	37
6.7	Thermo Scientific TSQ Quantiva and Endura	37
6.8	TSQ Quantiva and Endura Instrument Method [CM7-18759]	37
6.9	Signed Sequences [CM7-16374]	38
6.10	Improved Peak Grouping	38
6.11	Chromeleon Enterprise Compatibility of a Chromeleon 7.2 SR5 Domain Controller with Newer Versions of Chromeleon Clients and Instrument Controllers	39
7	Appendix	40
7.1	Release Notes	40
7.2	Online Help	40
7.3	Contributed Content	40

7.4 Improved Peak Grouping – A Comparison With Prior Releases..... 40

1 Introduction

The Thermo Scientific™ Chromeleon™ 7 Chromatography Data System (CDS) is a new-generation chromatography data system that provides the fastest path from samples to results. Building upon market-leading innovations of prior Chromeleon software releases – such as dynamic interactive data displays, an integrated database for rapid data retrieval, and spreadsheet-based reporting – Chromeleon 7 features a modern user interface, comprehensive new tools for peak detection, and an innovative workflow management framework, all of which speed up learning, simplify operation, and deliver results with greater efficiency than any other chromatography data system.

This new version, Chromeleon 7.2.9 CDS, provides updated and new instrument control for instruments from Thermo Fisher Scientific. Improvements and enhancements have been made in several areas related to ease of use, data processing and visualization. Please see below for more details on these and other enhancements present in this release.

The software is developed using modern software development tools and technologies that improve performance, sustainability and extendibility.

Backward compatibility with Chromeleon 6 is maintained to the greatest practicable extent, to provide an easy migration path.

2 Other Documentation

Chromeleon is provided with many other documents that will help you to learn more about the software. These documents can also be found in electronic form on the installation disk in the Documents folder.

Please refer to the Installation Guide for information regarding:

- System Requirements
- Supported Operating Systems and Databases
- Required Third-Party Software
- Compatibility with Previous Versions
- Installing and configuring the Chromeleon software

Also available are the Enterprise Documents that were released for Chromeleon 7.2 SR5, which describe the process for installation of enterprise systems based on Chromeleon 7.2 SR5. These documents are also applicable for Chromeleon 7.2.9.

3 What's New in Chromeleon 7.2.9

Chromeleon 7.2.9 implements a number of new features, including support for the new ISQ-EM single quadrupole mass spectrometer and support for the Vanquish Charger with the Vanquish Dual Split Samplers. Significant improvements have been made to MS data processing performance and a new workflow has been added for Intact Protein Deconvolution analysis. Also included are several updated instrument drivers and other core Chromeleon enhancements as well as a new data and evaluation model for peak grouping. This document will only give a short overview of all features without going into much detail. For more details, refer to the Online Help.

3.1 New and Updated Thermo Scientific Instrument Drivers

This chapter lists new and updated Thermo Scientific™ drivers added to Chromeleon 7.2.9. For details on supported options, required licenses, installation, and control, refer to the Online Help or the List of Supported Instruments document found on the Chromeleon 7.2.9 DVD.

3.1.1 Vanquish Duo UHPLC - Updated Driver [CM-2302]

This release includes support for the Vanquish Charger (VH-A90-A) with the Vanquish Dual Split Sampler HT (VH-A40-A) and the Dual Split Sampler FT (VF-A40-A). For more detail see section 3.4.3.

3.1.2 Vanquish UHPLC - Updated Driver [CM-12582]

This release introduces inject synchronization between the Vanquish HPG-Horizon (VH-P10) and the Vanquish Autosampler (VH-A10, VF-A10, VH-A40, VF-A40). For more detail see section 9.

3.1.3 ISQ EM Single Quadrupole MS For IC and HPLC – New Driver [CM-11901]

This release includes support for the new Thermo Scientific ISQ EM, which is a single quadrupole mass spectrometer for HPC and IC. The ISQ-EM is based on the ISQ-EC SQMS, but features:

- An extended mass range (up to 2000 Da)
- An optional APCI source

3.1.4 Exactive / Q-Exactive LC – Updated Driver [CM-2158]

This release includes support for version 2.9 SP2 of the Thermo Scientific Exactive and Q-Exactive Orbitrap™ family of LC and GC mass spectrometers. This includes the following models:

- Exactive Plus
- Exactive Plus EMR
- Q Exactive
- Q Exactive Focus
- Q Exactive Plus (including Biopharma)
- Q Exactive HF (including Biopharma)
- Q Exactive HFX (including Biopharma)

3.1.5 Exactive GC / Q-Exactive GC – New Driver [CM-11854]

This release includes support for the Thermo Scientific Exactive-GC and Q-Exactive-GC Orbitrap™ mass spectrometers.

3.1.6 Integral SS/SP - New Driver [CM-15145, CM-13643, CM-13621, CM-39, CM-13632, CM-13654]

This release includes driver support for the Stream Selector and Sample Preparer modules in the Integral product line. The Integral SS and SP modules can be configured and operated with any system supported in Chromeleon 7.2.9. This includes the ICS-6000, Integriion, and Aquion product lines. Their stand-alone capabilities can be useful for many single-system process monitoring applications.

Note: The additional functionality of the CM-PA Analyzer and CMOPC Server programs are not yet migrated to CM 7.2. These include features such as multi-system parallel operation, automatic sequence generation, sample-prep overlap, conditional branching, and OPC connectivity.

3.2 New and Updated Third Party Instrument Drivers

This chapter lists new and updated third party instrument drivers added to Chromeleon 7.2.9. For details on supported options, required licenses, installation, and control, refer to the Online Help or the List of Supported Instruments document found on the Chromeleon 7.2.9 DVD.

3.2.1 Agilent 7890 GC – Updated Driver [CM-11856]

This release adds support for the following devices for the Agilent 7890 GC:

- MMI (Multi-Mode Inlet)
- NPD (Nitrogen Phosphorus Detector)

3.2.2 Waters Acquity System Driver – Updated Driver [SWFR-206, SWFR-52, SWFR-724, SWFR-2512]

With this release, the Waters Acquity system driver has been updated to provide support for the following modules:

- Waters 2414 Refractive Index Detector
- Waters 2475 Fluorescence Detector
- Waters Acquity Evaporative Light Scattering Detector
- Waters Acquity Arc Quaternary Solvent Manager-R
- Waters Acquity Arc Sample Manager

3.2.3 Agilent G7100 CE – Updated Driver [SWFR-726]

This release adds support for the following Agilent 7100 Capillary Electrophoresis modules:

- 7150A Mainframe
- 7151A DAD

3.3 Compliant MS Tuning Features

This release extends the compliance related functionality of Chromeleon to cover on-demand Autotuning of the ISQ-EC and ISQ-EM SQ mass spectrometers for IC and HPLC. Future releases of Chromeleon will expand this functionality to cover manual tuning and to other Thermo Scientific mass spectrometers.

3.3.1 User Privilege for On-demand MS Autotuning [CM-17266, CM-18688]

A new user privilege called “Execute On-demand Auto tune” has been added to the list of available privileges for a user role. This privilege controls access to the on-demand autotune feature of the ISQ-EC/EM. Without this privilege, a user is not permitted to perform an autotune from the ePanel.

3.3.2 Secure Storage of MS Tune Reports [CM-19659]

After the user performs an on-demand autotune of the ISQ-EC/EM, a copy of the tune report is automatically saved in the local data vault, in the following folder:

/Instrument Data/(InstrumentName)/ MS Tune Reports/

Note: In order to prevent unauthorized manipulation of the tune results, it is recommended that the Chromeleon system administrator limit user access to the folder to ‘read-only’, using the Access Control functionality of Chromeleon.

3.3.3 Display of Tune Report after MS Autotuning [CM-16017]

The ePanel for performing an on-demand autotune of the ISQ-EC/EM now includes a list of recent tune reports for the instrument. When an autotune completes, the list is updated. Double-clicking on a report will display the report

3.4 Vanquish and Ultimate 3000 Features

3.4.1 Vanquish Duo

For the Vanquish Duo for Tandem LC or LC-MS and the Vanquish Duo for Inverse Gradient, the ready check has been improved to check the method workflow integrity [CM-7445, CM-11145]. For the inverse gradient configuration, the integrity check checks for a valid instrument configuration, a valid fluidic description and manual changes in the gradient that result in a mismatch between the inverse gradient and the analytical gradient. [CM-7445] For the tandem configuration, the integrity check checks for a valid instrument configuration and a valid tandem fluidic description. [CM-11145]

For the Vanquish Duo for Tandem LC or LC-MS the Instrument Method Wizard for the tandem gradient now provides an indication on the single pump gradient page that the tandem gradient split point can be moved. [CM-2797]

For the Vanquish Duo for Tandem LC or LC-MS the documentation now provides some conceptual information on Tandem operation. [CM-5714]

3.4.2 Vanquish Horizon

This release introduces inject synchronization between the Vanquish HPG-Horizon (VH-P10) and the Vanquish Autosampler (VH-A10, VF-A10, VH-A40, VF-A40). It is now possible to synchronize the injection of the autosampler with the pump strokes in Chromeleon similar to the Vanquish LPG/DGP-Flex (VF-P20 / VF-P32). This improves the retention time reproducibility for a Vanquish HPG-Horizon (VH-P10) with a Vanquish Autosampler (VH-A10, VF-A10, VH-A40, VF-A40) when running shallow gradient profiles. [CM-12582]

3.4.3 Vanquish Charger

For the Vanquish Charger support, this release introduces the possibility to configure the number of rack positions reserved for rack transfers [CM-2302]. This can increase the performance and reliability in cases in which the rack is changed often within a sequence.

3.4.4 Updated Translation for UltiMate 3000 Methods to the Vanquish Platform [SWFR-2884]

The instrument method translation workflow has been enhanced to include support for further Thermo Scientific UltiMate 3000 and Vanquish series instruments. Details of the supported translations are available in the Online Help.

3.5 Chromeleon Server And 247 Instrument Controller Enhancements

3.5.1 64 Bit Server Based Data Processing [CM-12134, CM-12200, CM-55]

When installed on a PC with a 64-bit version of Microsoft Windows, operating system the Chromeleon setup kit will automatically enable a new data processing service optimized for large data sets, which will significantly improve data processing performance.

To further improve performance in Enterprise environments, the data processing service may be installed on the PC which is hosting the Chromeleon Data Vaults, eliminating time intensive network access of raw data for calculations.

3.5.2 System Printers and Central Reporting [CM-2505, CM-14197, CM-4582, CM-16209, CM-16220, CM-3022]

Chromeleon 7.2.8 introduced a number of enhancements in the way Chromeleon performs post-acquisition printing and exporting:

- The Instrument Queue tab no longer needed to be opened for reporting to take place
- Reporting would be performed even if the Chromeleon Client was closed after starting the sequence acquiring
- Post-injection and post-sequence report options could now be selected in the Sequence and/or pre-defined in the eWorkflow

- A new 'enforce' option to allow Chromeleon System Administrators to apply reporting options to all sequences acquired on each configured Instrument. Enforced options cannot be modified by users in the sequence.

Chromeleon 7.2.9 further enhances this functionality in the following ways:

- A new Print Service can be enabled on a Chromeleon Server (normally a Data Vault Server or a dedicated Printer Server) to handle reporting tasks centrally. This means that the Windows session on the Chromeleon client no longer needs to stay running after a user has started a sequence which needs post-acquisition printing.
- Chromeleon Administration Console now allows 'System Printers' to be configured and associated with a Printer Server. During configuration the Chromeleon System Administrator provides a unique name for each System Printer, which can then be referenced from any Chromeleon client when setting up post-acquisition processing. This means that the Chromeleon client computer(s) or IPC(s) no longer needs to have a local printer configured.
- If the printer hardware needs to be replaced for any reason (e.g. printer failure or upgrade), the System Printer in Chromeleon can simply be associated with the new printer. Any Report Templates which reference the System Printer will automatically print to the replacement printer without requiring any changes in the Report Template.
- A new option "Save Electronic Report" has been added to the Auto-reporting section of the Sequence Properties dialog box. If this option is ticked, Chromeleon will automatically generate an Electronic Report and save it to the Sequence once the Sequence has finished acquiring. This action can be performed on its own or in combination with post-acquisition printing and/or exporting.
- In the same way as Printing and Reporting can be enforced for all Sequences on an instrument, the new Save Electronic report can also be enforced.
- When Auto-reporting options have been enforced by a Chromeleon System Administrator for an instrument, any Sequence created on that instrument will have the option selected and greyed out in the Sequence properties dialog box, so users can clearly see what actions have been enforced and will be performed for that Sequence.

Notes:

- If a non-system printer (i.e. a printer connected to the Chromeleon client computer or IPC), printing will be performed locally rather than centrally by a background process, ReportManager.exe. In this situation, the Windows session must remain logged-in in order for the printing to be performed.
- If post-acquisition exporting is configured and no printing option is selected, the export will be performed by ReportManager.exe and the Windows session must remain logged-in.
- If post-acquisition exporting is configured, and printing is also configured, and a System Printer has been selected, both printing and exporting will be performed on the Print Server. In this situation, you should take care to ensure that the location of the exported file is accessible to the account running the Print Service.

3.5.3 Automated Roll-out of Chromeleon Updates

Chromeleon 7.2.9 introduces the first phase of a new mechanism for updating clients, IPCs and 247 Instrument Controllers in an Enterprise environment. This will enable Chromeleon Administrators to manage the process of rolling-out Chromeleon software updates across their entire Chromeleon

domain from within the Chromeleon Administration Console. Phase One features new options to decide *what* will be installed and *when* the installation will be performed.

Administrator users with the necessary privileges can create an “Updater Package” from a Chromeleon Service Release (SR), Maintenance Update (MU), or Hotfix, then determine which computers in the Chromeleon Domain will receive this Updater Package, and also define a Maintenance Window during which the kit will be available for installing.

Before the defined start of the maintenance window, Chromeleon automatically downloads the Updater Package to the target computer(s). The progress of the download(s) can be monitored in the Chromeleon Administration Console. The maintenance window prevents Sequences from being started during the maintenance period on any IPCs or 247 Instrument Controllers to which it has been applied. When the maintenance window begins the Client, IPC or 247 Instrument Controller access to the computer is restricted, the updater package is available for installation, and the computer is ready to be updated.

3.6 Chromeleon Client Enhancements

3.6.1 Intact Protein Deconvolution [CM-11556, CM-10570, CM-10470, CM-10469, CM-11924, CM-12289]

With this release, a new category has been added to the Chromatography Studio to support a workflow for Intact Protein Deconvolution. The workflow is based on the similar workflow found in the Thermo Scientific BioPharma Finder software, but is also tightly integrated with the compliance, reporting and other functionality of Chromeleon.

Included in this workflow are:

- Import and export of BioParma Finder 3.1 workbook files, which contain protein/peptide component lists and deconvolution processing method parameters
- Analysis using both the ReSpect™ and Xtract deconvolution algorithms
- The processing method parameters are saved as part of the Chromeleon processing method
- New report objects and report variable have been created to facilitate reporting of raw data and results
- Full support for audit trails and versioning is included

Notes:

1. A specific Chromeleon client license must be purchased In order to use the Intact Protein Deconvolution workflow.
2. During setup, the deconvolution engine must be installed by selecting the option on the ‘Advanced’ page of the Chromeleon setup program.
3. Intact protein deconvolution analysis is limited to data acquired using Thermo Scientific Orbitrap LCMS hardware.

3.6.2 On-Demand Updating of View Panes in the Studio [CM-12013]

In order to improve software responsiveness when working with large MS sequences containing many XICs, a new sequence property is now available to defer real-time updating of data and results in calculation intensive panes of the Chromatography Studio. The option applies to both the Data Processing and Report Designer categories of the Studio. Views may be refreshed by clicking a ribbon toolbar button.

This functionality may be enabled for individual sequences (in the Sequence Properties dialog or eWorkflow settings) as well as on a global basis (in the Global Policies of the Administration Console).

3.6.3 Improved Peak Grouping [CM-41]

Chromeleon 7.2.9 introduces a new data and evaluation model for peak grouping with more flexibility and capabilities. In the processing method there is a new Peak Group Table replacing the former Unidentified Peak Group Table. Existing processing methods and their evaluations will be processed in a compatible way, meaning peak group-related results of existing sequences will not be changed in 7.2.9.

For a detailed explanation of the differences in functionality, see Section 7.4

For an explanation of incompatibilities between the old and new peak grouping models, see Section 6.10

3.6.4 Supporting Multiple ISTDs with Variable Amounts [CM-14073]

Chromeleon 7.2.9 supports multiple ISTD components with variable amount values. To enable this functionality, an injection custom variable with the reserved name **CM7:IntStd_Level** of type **List** needs to be added to the sequence / eWorkflow. The list of possible values for this custom variable must be filled with the calibration level names you want to use for entering reference amounts of the ISTD components. An example of such a sequence / injection list is the following:

Name	Type	Level	*CM7:IntStd_Level
Blank	Blank		
Blank	Blank		
EN:1948 CSL/4	Calibration Standard	CSL/4	CSL/4
EN:1948 CSL/2	Calibration Standard	CSL/2	CSL/2
EN:1948 CSL	Calibration Standard	CSL	CSL
EN:1948 CS1	Calibration Standard	CS1	CSL
EN:1948 CS2	Calibration Standard	CS2	CSL
EN:1948 CS3	Calibration Standard	CS3	CSL
EN:1948 CS4	Calibration Standard	CS4	CSL
EN:1948 CS5	Calibration Standard	CS5	CSL
Blank	Blank		
EN:1948 CSL/2	Unknown		Sample
EN:1948 CSL	Check Standard	QC	QC

Figure 1 - Sequence with custom variable 'CM7:IntStd_Level'

If this custom variable is present in the sequence, the values in the **IntStd** column of the injection list are no longer used to evaluate the ISTD components with variable amounts. Instead the values of the corresponding concentration levels in the component table are used in this case, allowing references to multiple ISTD components with variable amount setting. The following is an example of a component table which corresponds to the sequence / injection list in the above sequence:

Component Table													
Group Area													
Drag a column header here to group by that column. Run Component Table Wizard... Show Properties...													
#	Name	Ret.Time	Level "CS1"	Level "CS2"	Level "CS3"	Level "CS4"	Level "CS5"	Level "CS6"	Level "CSL"	Level "CSL2"	Level "CSL4"	Level "QC"	Level "Sample"
1	1234-TCDD IS	19.024							16.000000	8.000000	4.000000	2.000000	16.000000
2	2378-TCDF IS	19.174							16.000000	8.000000	4.000000	5.000000	8.000000
3	2378-TCDF	19.184	0.200000	0.800000	4.000000	16.000000	80.000000	320.000000	0.040000	0.020000	0.010000		
4	2378-TCDD IS	19.616							16.000000	8.000000	4.000000	5.000000	8.000000
5	2378-TCDD	19.634	0.200000	0.800000	4.000000	16.000000	80.000000	320.000000	0.040000	0.020000	0.010000		
6	12378-PeCDF IS	22.358							16.000000	8.000000	4.000000	5.000000	8.000000
7	12378-PeCDF	22.364	0.400000	1.600000	8.000000	32.000000	160.000000	640.000000	0.080000	0.040000	0.020000		

Figure 2 - Component Table with ISTD components with variable amounts

Beyond the calibrations levels CS1...5, CSL/2 and CSL/4 there are also the levels **QC** and **Sample**, which are used in the sequence for the Unknown and Check Standard injections. For the ISTD components with variable amounts (e.g. 1234-TCDD IS and 2378-TCDF IS in the example above) you can now enter different values. In 7.2.8 you could only enter a single value for all ISTD components with variable amounts in the IntStd field of an injection.

All concentration levels that you want to pick in the **CM7:IntStd_Level** column need to be added to the list of the corresponding custom variable. In the processing method all concentration levels beyond the calibration/check standard ones need to be added manually.

3.7 Other Enhancements

3.7.1 Chromeleon Data Vaults on Microsoft SQL-Server 2016

Chromeleon 7.2.9 supports the Microsoft SQL-Server 2016. The Chromeleon Data Vault Manager allows to create Multiuser and Standard Data Vaults on any SQL-Server 2016 instance. Chromeleon 7.2.9 needs to be installed not only on the computer where the Data Vault Service is running but also on all Chromeleon instances (e.g. Client, Instrument Controller, and Scheduler) which need or want to access such Data Vaults.

3.7.2 'Show Logon Events' Option in the Audit Trail Viewer

In the Chromeleon Administration Console the 'Show Logon Events' option has been already been available in the audit trail viewer of the user database. With 7.2.9 this option is now also available in the audit trail viewer on the root level of the Administration Console and the Organizational Unit.

3.7.3 Enhancements for SampleManager Link [CM-193]

This release of Chromeleon supports the following new functionality for SampleManager Link:

- Define when results are ready for automatic transfer to SampleManager LIMS
- Check User Training Record and/or Instrument Maintenance Status Before Starting Acquisition

Note: SampleManager 12.1 SP1 or later is required.

4 Resolved Issues

This chapter describes the issues that have been resolved with the release of Chromeleon 7.2.9.

Many trivial and minor issues have been resolved but are not mentioned here. If you require information about the status of an issue observed in a Chromeleon 7 release, but which is not listed here, please contact your local Thermo Fisher Scientific representative for more information.

The numbers in the first column of the table below refer to the Thermo Fisher Scientific tracking IDs.

ID	Description
CM7-14014	Client: Console: Data: Import External: The Convert button in the Console view, which converts a Chromeleon 6 Sequence to use the Chromeleon 7 algorithm, was not disabled when an Electronic Report was generated using the imported Chromeleon 6 results.
CM7-14673	For some devices, configuring with a name longer than twelve characters would prevent a connection between the instrument and the Chromeleon client. Chromeleon now supports names of up to 20 characters for these devices. Affected devices include: DC-6000 (including detectors), DP-6000, SP-6000, EG-6000, Integrion, Aquion, and any discontinued equivalent instruments, e.g., the ICS-5000 series, ICS-2100, etc.
CM7-16546	Instrument Control Localization/Globalization: Foreign characters in e.g., the sequence name, sequence path, injection name and instrument method name were displayed as question marks in ready check result messages and instrument audit trail messages.
CM7-17291	Import Electronic Report: After importing a Chromeleon 6 signed sequence certain electronic reports (called SOR-File in Chromeleon 6) did not show up completely. For some report sheets the electronic report content was truncated. The fix also corrects already imported sequences and their electronic reports.
CM7-18970	Client: Import/Export: The Undo/Redo option was not available in either the Console or Studio view after converting an imported Chromeleon 6 Sequence to use the Chromeleon 7 processing algorithm.
CM7-19041	Client: Studio: Processing Method: An error in the calculation for 1st and 2nd derivatives resulted in data points being plotted on the derivative channel chromatogram which did not match the slope of the original chromatogram.
CM7-19104	Instruments: Controller: If the number of IRC re-injects exceeded the maximum, the sequence would incorrectly abort and an unhelpful error message would be reported.
CM7-19395	Setup: When ejecting the DVD during installation, Setup would finish without any error. However, Configuration and Installation Qualification were not executed.
CM7-19511	Setup: using "Modify" to install or remove the Thermo Exactive driver would fail with an error: Setup cannot continue because some required components failed [...] Failed to verify package Thermo Exactive Services [...]
CM7-19828	Client: Studio: Processing Method: Attempting to add a Custom Condition to an SST/IRC test case in a Processing Method outside of a Sequence would cause an unhandled exception.
CM7-19831	Client: Studio: Processing Method: Attempting to move a row in the SST/IRC method would cause an unhandled exception.

ID	Description
CM7-19918	Version Comparison: Processing Method: If a custom variable in the component table of a processing method is renamed a new version of the processing method is created. However, the comparison details did not mention this rename operation. Only a layout change was reported.
CM7-20501	User Management: The privilege "Modify Status of Already Finished or Interrupted Injection" and its description have been rephrased. The new name is "Change Status of Injections With Raw Data Back To Idle" with the description "Change status of injections with raw data including deletion of raw data if reset to idle". This was done to clarify that existing raw data are deleted when the status of an injection is reset back to idle.
CM7-20616	Report Designer: Having multiple chromatogram plot objects in a report template and changing the time axis to a fixed time range for one chromatogram plot object a subsequent change to a fixed time range for another chromatogram plot object did not work. The fixed time range for the second chromatogram was not updated automatically.
CM7-21115	Results: Peak Grouping: If multiple components in the Processing Method are assigned to the same peak group the components were always calibrated and evaluated according the calibration of the peak group. Having the freedom to set the value of the property "Factor" for the respective components arbitrarily one could get different group amount values in report tables. It is now possible to choose whether components of one and the same peak group should be calibrated on their own or via dedicated peak group settings. Thus the computation of the group amount will always result in one and the same value and does not depend on the component for which the group amount is reported.
CM7-21451	Results: Formula Evaluation: When using Matrix Correction in the Processing Method peak width results at a custom peak height value, e.g. peak.width(15), were computed after applying the matrix correction. For the built-in height values 5%, 10% and 50% the values were computed before applying the matrix correction. This is harmonized now. Any peak width value is now computed before the matrix correction is applied and thus always based on the original peak height.
CM7-21589	Installation Qualification (IQ): In the Nano IQ Report in the RT calculation table on the MS sheet the RT column was filled with numbers. The column is now filled with the string "Fill in".
CM7-21920	Studio: Data Processing: When Fixed Calibration Mode was selected in the Processing Method the Cobra Wizard was disabled and couldn't be used in the corresponding sequence. The Cobra Wizard is now enabled again for all chromatograms which belong to the corresponding sequence. If the currently selected chromatogram belongs to the injection list of the fixed calibration sequence the Cobra Wizard still remains disabled, since those chromatograms cannot be modified.
CM7-21993	Studio: For sequences with injections containing both UV and MS 3D raw data, the Time Spectra Tool didn't open the UV-Vis Spectra pane automatically for UV channels. Only the Mass Spectra pane was opened.
CM7-22302	User Management: For the user name in the user database Chromeleon didn't allow single quote characters. This restriction has been removed.
CM7-22314	<p>Console: In an installation with more than one Organizational Unit, only users with the "Modify Global Security Settings" were permitted to view all Data Vaults across all of the Organizational Units. This has now been changed to allow any user in the Global Organizational Unit to see all of the Data Vaults, barring any access restrictions.</p> <p>Because this change may reveal Data Vaults to users for whom they were not formerly visible, access privileges for those Data Vaults should be reviewed and changed, if necessary.</p>
CM7-22445	Instrument Control: When executing on-line commands for 3rd party drivers, a ready check of a sequence queue was blocking the execution of these commands. In some instances, this led to an interruption of the connection to the console. This issue has been resolved.

ID	Description
CM7-22775	If two users added and deleted injections to the same sequence concurrently, the deletion was not always executed properly. While the deleted injection would appear to be deleted, in some cases it would still be found in injection queries, and cause a "Object reference not set to an instance of an object" error. This affected only Data Vaults with versioning disabled.
CM7-22839	Instrument Controller: In rare cases, requesting on-line signal points of uploaded signals would result in a loss of the connection to the instrument. Chromeleon would try to establish a connection to the instrument and fail with the error message "Timeout. The internal communication pipe for the instrument controller request cannot be connected."
CM7-23034	Client: Import/Export: Attempting to backup an Instrument Audit Trail to a target path which didn't exist would cause an error message. In these cases, the necessary folder(s) are now created.
CM7-23053	Client: Import/Export: Data exported from Chromeleon to AnDI/CDF was exported as mAU*sec instead of mAU*min.
CM7-23162	MS Processing: The rounding used when computing Mass Accuracy was not documented in the help file, resulting in concerns about the correctness of the value.
CM7-23526	UltiMate WPS-FC: It was possible to enter an incorrect value for the initial tube for fraction collection, and thereafter to run the sequence, resulting in incorrect fraction collection.
CM7-23569	Client: Console: Instruments: If a printer other than the 'default' printer on the Chromeleon client was selected for post-injection/post-sequence printing, the selection would not be retained if the Chromeleon Console was closed and reopened.
CM7-23620	UltiMate WPS-3000: If USB communication was lost, following reconnection the sequence did not restart correctly
CM7-23667	AS-AP: Occasionally, a USB communication issue would cause the following injection to get stuck towards the end, preventing the sequence from continuing to subsequent injections.
CM7-23740	Query: When searching for injections by date using the operator "Is Not During Previous", the query result would also return injections created/modified during the current day.
CM7-23884	UltiMate VWD-3x00: In rare circumstances, the instrument would stop communicating with the driver, but this was not acknowledged in the software. A warning is now provided after 90 seconds, and the acquisition aborts after 5 min without communication.
CM7-23903	A2D: Occasionally A2Ds with a serial number lower than 007000, especially when acquiring sequences with a large number of injections, would fail to acquire data for a sample, with a "Zero data points acquired" error.
CM7-23956	Scheduler: The audit trail option "Delete entries older than" was not evaluated correctly. Instead of applying the specified number of months the Scheduler always applied 3 months.
CM7-24222	CM6 Data Import: Chromeleon 6 sequences which contained SST test cases restricted to specific sample types (Unknown, Standard, etc.) and which were created or edited by a Japanese or Chinese Chromeleon 6 client could not be imported. Trying to read or import such a Chromeleon 6 sequence led to an error message stating, "Cannot read Chromeleon 6 data (Injection Type: Unknown Chromeleon 6 enumeration value)".
CM7-24298	Markes Thermal Desorber: If the Sample Volume or Sample Position was calculated using a number that wasn't a custom variable, an incorrect volume could get sent to the instrument.

ID	Description
CM7-24450	Administration Console, Discovery: Chromeleon did not correctly handle the existence of multiple Data Vaults or Data Vault servers with the same ID. This condition usually results from renaming or cloning a computer. Now, when a duplicate Data Vault ID or Data Vault server ID is detected a "Discovery Publishing Error", containing the names of the conflicting Data Vaults, is written to the Station Audit Trail (if enabled in the Global Policies) and the problem is also logged in DataError.log, thereby informing the Chromeleon Administrator that the conflict requires resolution, e.g. by removing the duplicate resources from the Chromeleon domain in the Administration Console.
CM7-24550	Reporting: The Calculated Mass report variable was incorrectly calculated using the most abundant rather than the monoisotopic mass.
CM7-24695	Processing Method: Injections added by the IRC auto-dilution action did not put any context information into the "Additional Information" column of the Sequence Data Audit Trail.
CM7-25130	Console: Data: A "Raw data failed integrity check" error message could be incorrectly reported for custom raw data files.
CM7-25162	GC Drivers: If a disconnect command was sent to an AI-1310 Autosampler while a Sequence was acquiring on another instrument connected to the same Instrument Controller, the other Sequence(s) would incorrectly get aborted.
CM7-25163	System Status Report: IF a UNC path as used, creation of the SSR would fail with the error message "Unable to obtain required reports. Object must be a root directory ("C:\") or a drive letter ("C").".
CM7-25190	ICS-5000+: The Suppressor Current setting on the DC ePanel now displays properly. It was inadvertently removed in Chromeleon 7.2.8.
CM7-25271	Data Audit Trail: When a Sequence is exported to a .cmbx file Chromeleon adds an "Exported. Sent to:" record in the original Sequence. However, that record was not also added to the .cmbx, so when the .cmbx was imported into Chromeleon, the imported Sequence did not contain a record of the "Exported" event.
CM7-25295	Vanquish Drivers: For the Vanquish Dual Split Sampler (VH-A40-A-02 and VF-A40-A-02) relays are shared between instruments. Manual changes on one instrument also affect the other instrument. Now, If a sequence is running on the other instrument, a warning is issued.
CM7-25296	Vanquish Drivers: For the Vanquish Dual Pump F (VF-P32-A-01) relays are shared between instruments. Manual changes on one instrument also affect the other instrument. Now, if a sequence is running on the other instrument, a warning is issued.
CM7-25300	Agilent 7890: When used with certain LAN cards that are slow to initialize, the GC would sometimes fail to connect if the acquisition service was set to automatically start on system start.
CM7-25306	Agilent ICF: In rare cases, up-to-date tray configuration information was not received from ICF. Chromeleon would then improperly request the instrument to perform runs without injecting samples. This condition is now detected and results in an Error during Queue Ready Check.
CM7-25314	ASTM Noise: The online help incorrectly implied that the ASTM method was used to compute noise, Signal/Noise and Signal-to-Noise Ratio. Although the principles of noise calculation according to ASTM are used, noise is calculated only over a single segment. The online help has been updated to reflect this.
CM7-25321	eWorkflow Editor: Under some scenarios, an eWorkflow was immediately marked as "changed" after opening (i.e., the "Save" button is enabled). These changes were internal updates related to metadata like injection volume range, available positions, and available methods. If these changes resulted in invalid values for the user-editable fields volume, position, or instrument/processing method, they were also updated. These automatic updates are no longer performed.

ID	Description
CM7-25325	Installation of KB4041083 "Security and Quality Rollup for the .NET Framework 3.5.1, 4.5.2, 4.6, 4.6.1, 4.6.2, and 4.7 for Windows 7 SP1 and Windows Server 2008 R2 SP1: September 12, 2017" or any .NET Security and Quality Rollup released between September 2017 and March 2018 on a PC with the Agilent ICF framework caused the Chromeleon Instrument Configuration Manager to crash.
CM7-25334	Console: Data: Using the Merge option when re-importing a cmbx file could result in the deletion of Sequences which had been created since the cmbx was created
CM7-25337	Vanquish Drivers: For an instrument with the Vanquish Dual Split Sampler (VF-A40-A or VH-A40-A) and an instrument method configured for the left sampling unit using the default Smart Shutdown settings, Smart Shutdown would purge the right sampling unit (and vice versa).
CM7-25371	SDK: Formula Evaluation: Calling an SDK method to evaluate formulas of the detection parameter category (e.g. det.minRelativeArea) caused an error message "Unknown report variable".
CM7-25375	Exactive/Q-Exactive Data Acquisition: Under very rare circumstances, it had been observed that during data acquisition from the Exactive/Q-Exactive family of LCMS improperly indexed (duplicate) scan data might be returned by the instrument, which rendered the MS data unreadable. A message was displayed that "The data points are not sorted in ascending order". This was caused by a defect in the MS firmware associated with version 2.8 of the driver. The error message and help file have been updated to clarify the situation. However, in order to ensure the issue does not recur it is strongly recommended to upgrade to version 2.9 or later of the Exactive driver.
CM7-25392	eWorkflow Import: After importing an eWorkflow, the audit trail contained an additional "changed" entry, although the user hadn't make any changes. This was due to Tags in the eWorkflow that were not present in the destination domain being removed. Now a comment similar to "Unknown tags automatically removed on import: Tag-1, Tag2." is added to the audit trail. Note that the user can also edit the tags during import. These changes were included in the same audit trail entry. Now a separate entry is being generated, listing the changes made by the user.
CM7-25413	Instrument Method Editor: Changing the stage time for an inverse gradient resulted in a notification that synchronization had stopped. The inverse gradient now adapts to the changed stage time.
CM7-25414	Instrument Method: For a method translation of an instrument method for a finished sequence the method review would fail. After the instrument method was assigned to an instrument, a review of the method would fail and "Loading plug-ins" was displayed. The instrument method is now opened for review.
CM7-25424	Vanquish Driver: With a Vanquish dual autosampler shared on two instruments, if the autosampler was deleted from one of the instruments using the option "Move to other instrument", the configuration plug-in still reported the sampler as shared.
CM7-25425	ISQ EC: If "Use this detector" was unchecked in the instrument method, a Ready Check error stating that properties were missing was generated.
CM7-25430	SDK: Formulas evaluating Mass Spec related results, e.g. peak area of a MS Quantitation Peak, didn't work when using the corresponding SDK methods.
CM7-25455	Vanquish Drivers: When configuring a Vanquish Autosampler, entering an invalid character for the relay name resulted in a fatal error and the instrument controller had to be restarted. Now the entry of an invalid character is rejected.
CM7-25460	Chromatogram Plot: When choosing seconds instead of minutes for the time axis unit of the chromatogram the tangents of peaks were still drawn applying minutes for the time axis.
CM7-25463	Upload: In very rare cases, under high load and when using IRC to create additional channels, uploading a sequence after acquisition would hang.

ID	Description
CM7-25487	Processing Method: Fixed Calibration: When setting up a fixed calibration processing method, assigning a large MS Calibration sequence as the fixed sequence sometimes resulted in a timeout error stating "Could not load raw data for item".
CM7-25506	Data Audit Trail: When a Sequence is exported to a .cmbx by use of drag-and-drop, an "Exported. Sent to:" record was not added to the Data Audit Trail.
CM7-25553	Instrument Method: Method Translation: The method translation was not working when attempting to translate an instrument method for a Waters UPLC instrument, when a module was deleted after the instrument method was created.
CM7-25556	ED-6000: Several missing SmartX settings have been added, including Mode, pH lower/upper limits, waveform name, DC voltage, and the DC voltage command is now added where appropriate.
CM7-25532, CM7-25560, CM7-25563	Instrument Method: Method Translation: When creating an instrument method for a given instrument configuration, then removing a module from the instrument configuration and using the Method Translation Tool to update the instrument method, in some cases there was no indication in the Method Translation Tool that the initial instrument method contained settings for the removed module. The Method Translation Tool now also reports settings for removed modules.
CM7-25567	ISQ EC: Under some circumstances, Smart Startup parameters were not sent to the hardware.
CM7-25570	In rare occurrences, an instrument could appear twice in the instrument category navigation, or a data vault could momentarily disappear during startup.
CM7-25586	In Chromeleon 7.2.8, reporting was performed by a separate 'background' process on the Chromeleon Client or IPC where the Sequence was added to the queue. The Windows session on this computer needed to remain logged-in until reporting had completed. If the user logged out of the Windows session, the background process would be exited and reports would not be generated for any queued or acquiring Sequences. Reporting is now performed by a Windows Service rather than a background process.
CM7-25592	Instrument Controller: When the XVault was unavailable, sequences were downloaded to a regular local data vault instead of the XVault. Now, if the XVault is unavailable, the download is not possible.
CM7-25597	Integrion: When two systems were configured under one Chromeleon 7 Instrument, newly detected consumables could not be approved via the Consumables Inventory interface, thus preventing a sequence from running.
CM7-25598	Data Import: It was possible for a user without the Import CMB/CMBX privilege to import data by using Drag and Drop instead of the File > Import menu item.
CM7-25614	Custom Variables: When changing the capitalization (but not the name) of a custom variable stored at the data vault level, an error message "The short name is already used by the custom field..." was displayed and the data vault would become inaccessible.
CM7-25619	Component Table: Importing peptides that have modification tags would fail if the modification name contained spaces, e.g. ["Heavy K"].
CM7-25630	Electronic Report: When an electronic report was printed and the checkbox "Save report" was also selected, the saved version was created a few seconds after the printed version, meaning the time stamps were a few seconds different.
CM7-25634	UV Spectrum Pane: Unlike Chromeleon 6, the normalization settings of the plot were only used for displaying the curve on the plot. When computing the difference spectrum, the actual (unnormalized) data was used. Chromatographic analysis spectra are now evaluated from the normalized source spectrum, and subtraction is now from the target spectrum.

ID	Description
CM7-25660	User Manager: When creating a new organization unit you could enter only 32 characters in the description field. Modifying the description field later this input limit has been removed. Now there is no limit during the creation procedure as well.
CM7-25681	Reporting: Internal Standard (ISTD): if a component referring to an ISTD is not detected in the chromatogram but nevertheless included in the report (e.g. via the integration report table filter option 'Include Undetected Components') all report variables in the report categories peak.istdChm or peak.istdChm returned n.a. although the ISTD chromatogram did exist and the corresponding ISTD component had been successfully detected.
CM7-25686	Console: Data: It was possible to use Copy and Paste in the Injection List to delete the Instrument Method assignment for an acquired injection.
CM7-25687	Licensing: The dongle grace period expired immediately after the dongle was removed, if the dongle had been plugged in more than 7 days prior to the removal. Now the grace period of 7 days starts with the date/time when Chromeleon detects that the dongle is removed or damaged.
CM7-25712	Processing Method Editor: Removing the "Manage Component Variables" privilege from the logon role of a user did not prevent the user from selecting the "Page Selector" dialog via the Processing Method > Layouts ribbon or the context menu in any editor page. This would allow the user to display new pages and thus also new component columns into the processing method editor view.
CM7-25720	<p>Report Designer: When a report table is rendered, new rows might need to be inserted automatically, e.g. for additional injections in a summary table. This temporarily changed the cell formats of all columns in the sheet for the inserted rows and thus marked all columns as used by the report in certain cases. If this happened during the printout or the export of a sequence, Chromeleon created sometimes many empty pages or the exported file was bigger than expected. If this happened for a consolidated report table, automatic repetition of table columns was blocked, which resulted in columns being omitted and showing "..." instead of actual values.</p> <p>Note: If this issue is still observed after upgrading to Chromeleon 7.2.9, it will be necessary to update the report template. Select the complete cell range right of the problematic report table(s) and clear it using the "Clear/Clear All" button on the "Home" tab of the report designer ribbon. Then save the changes.</p>
CM7-25729	Audit trail: The filtering/grouping toolbar is now visible where for Chromeleon 7.2.8 it had to be accessed via a context menu.
CM7-25734	TRACE 1300 GC: Aux Carrier Controller Flow was incorrectly divided by 10 when downloaded to the instrument
CM7-25739	Markes Thermal Desorber: When running a TD100 2-3StageDesorb method using 'InjectType = Dry Purge', the instrument would get stuck at "Lead Test Low Pressure".
CM7-25741	eWorkflow Editor: A user logged on with a role without the "Modify eWorkflow" privilege could open, modify and save an eWorkflow by using the Edit-button in the toolbar of the eWorkflow-category.
CM7-25755, CM7-25968	The ShimCRComm component that Chromeleon uses to control Shimadzu instruments used an older version of MFC than Chromeleon does, which could result in unhandled access violation messages. An updated version of ShimCRComm is now included with Chromeleon.
CM7-25757	Reporting: For ISTD components using Variable Internal Standard, the variable component.amount did not return the value in the IntStd column of the corresponding injection record.
CM7-25774	Instrument Configuration: When a computer was given a name exceeding 15 characters, launching the local instrument configuration manager resulted in an error message: "Error connecting to instrument controller: The network address is invalid."

ID	Description
CM7-25783	An emergency method including an inject command would overwrite the inject time of the injection run just previously.
CM7-25808	ISQ-EC: During an OQ/PQ/IQ analysis, the wrong Serial Number was displayed.
CM7-25809	User Management: The description of the privilege "Create eWorkflow" incorrectly stated that it enabled the user to create a new eWorkflow or save existing ones under new names. In fact, the "Modify eWorkflow" privilege is required to save an eWorkflow under a new name. The description has been updated to reflect this.
CM7-25812	Waters Acquity: In cases where Chromeleon was unable to download the instrument method to the instrument, data acquisition would still continue. This scenario now results in an aborted sequence.
CM7-25835	Chromeleon XPS: On slower systems, the Instrument Selection view could show status "Unknown" due to a communication timeout. A new setting in the ChromeleonXPS.exe.config file allows the timeout to be lengthened to ensure the correct instrument status is displayed.
CM7-25836	Import/Export: Chromeleon did not prevent users without the "Send to File" privilege from creating a .cmbx file using the "Send to File" option from right pane of the Chromeleon Console.
CM7-25847	User Management: When the Chromeleon logon password had expired and the user needed to enter a new password during the logon procedure one could close the corresponding dialogs without entering a new password, and the user could still continue to work with the Chromeleon Console.
CM7-25866	Using a Chromeleon 7.2.8 client, running an eWorkflow with an empty sample block col not be finished and didn't create a sequence.
CM7-25885	If automatic configuration was selected in Instrument configuration with a Perkin Elmer GC driver instance while a Console was online and an ePanel set linked to that instrument was active, in some instances the instrument server would switch to a 'busy' status so that it was not possible to save the changed configuration.
CM7-25919	Processing Methods: When using multiple processing methods with Fixed Calibration in a sequence, editing more than one processing method and the corresponding fixed calibration settings at the same time in the Chromeleon Studio could result in the raw data files for the fixed calibration injections being automatically deleted 24 hours after the fixed calibration changes were saved. Modifying and saving the fixed calibration for just a single processing method did not cause this problem.
CM7-25939	Vanquish DAD-HL: If the reference channel was set to either of the physical boundaries (190nm or 680nm) then the calculated wavelengths for all channels including the 3D channel were incorrect.
CM7-25947	Processing Method: Composite Scoring: Editing and then reverting composite scoring criteria sometimes resulted in the scoring results for components to change.
CM7-25961	In rare cases the filter selection settings for Non-Targeted MS Processing (NTMS) would not be saved. In addition, NTMS data processing now prevents processing when no Scan Filters are selected. Saving is allowed with scans unchecked however an error notifying the user that at least one filter must be selected to process the date will appear if method is re-opened.
CM7-25965	IQ: Japanese Windows: When installed Chromeleon 7.2.8 (English version) on a computer running a Japanese Windows OS the corresponding Chromeleon IQ failed with 2 errors referring to a missing firewall registration.
CM7-26038	MS Component Table: After importing HRAM data into the MS Components Table and editing the XIC definitions, it was possible that mass precision could be truncated to 2 decimal places.

5 Limitations and Known Issues

The following sections list known issues and limitations. The numbers in the first column of the table below refer to the Thermo Fisher Scientific tracking IDs.

5.1 Limitations with Thermo Scientific Instruments

ID	Description
CM7-25895	The Secure Boot feature of Windows 10 and Windows 8 blocks some USB drivers used by Chromeleon when Windows Defender Application Control (WDAC) is activated. This prevents any communication between Chromeleon and the USB-connected instrument. The drivers affected are CMUSB64.sys and MOTUSB64.sys, used by the UltiMate and Vanquish ranges of HPLC. The workaround is to leave WDAC disabled on any IPC which is connected to an instrument which uses these drivers.
CM7-16851	UltiMate 3000 MWD-3000 and DAD-3000: In the Instrument Method Editor for these devices, the script page offers one additional option for the data collection rate (20 Hz) that is not present in the Instrument Method Wizard. This additional option is a valid value for this parameter. Although it is possible to manually type in a value for the data collection rate that is not in the list, these values will be rejected by the Ready Check when a sequence is submitted.
CM7-21342	Vanquish Variable Wavelength Detector: For acquiring data on a single channel only using the Vanquish VWD it is necessary to use channel UV_VIS_1.
CM7-25370	Vanquish Duo: Instrument Method, Electronic Report: An inverse gradient method created on Chromeleon 7.2.7 (or earlier) can be run on Chromeleon 7.2.8 or later. However, Chromeleon 7.2.8 does not support Smart Startup, Smart Standby or Smart Shutdown settings for inverse (or tandem) gradient methods. Hence in Chromeleon 7.2.8, for an inverse gradient method created on Chromeleon 7.2.7 (or earlier) any Smart Startup, Smart Standby and/or Smart Shutdown settings included in the method are neither executed nor reported with Chromeleon 7.2.8.
CM7-25447	Vanquish Drivers: Vanquish Duo Autosampler: If the user adjusts the needle height, this is only adjusted for the left hand sampler unit, and not for both sampling units as would be expected. The user should use the property Sampler2.SampleHeight to set the height for the right hand sampling unit
CM7-25818	For some autosamplers, in particular the Vanquish Autosampler, the following problem can occur: For an instrument method with a Position assignment (Instrument Setup, Equilibration, Inject Preparation or Inject stage, e.g. Position G:G5) and a sequence with more than one injection (Position e.g. R:A1, R:A2, R:A3 ...), while all injections are performed from the correct Position (G:G5), it can happen that an incorrect Position (e.g. R:A1) is reported in the sequence, both in the audit trail and sequence information. Two possible workarounds exist: 1) Use the 'Position' parameter of the Inject command to specify the sample position within the method or 2) Add an equilibration stage of a few seconds and specify 'Position' in the initialization stage of the method.

ID	Description
CM7-24471	<p>Shared Devices: When configuring an Ultimate 3000 DGP or a Vanquish Dual Pump, a Vanquish Dual Autosampler, or Vanquish Column Compartment that is shared between two instruments, make sure to use non-identical device names for the instrument devices (e.g., PumpLeft and PumpRight).</p> <p>If an Ultimate 3000 DGP or a Vanquish Dual Pump, a Vanquish Dual Autosampler, or Vanquish Column Compartment are shared between two instruments with identical device names (e.g., "Pump") in both instruments, removing the driver from one instrument and moving it to the other instrument results in a fatal error.</p> <p>Workaround: Rename the instrument devices to non-identical device names (e.g., rename the pump units to PumpLeft and PumpRight). Save the instrument configuration and restart the server. Alternatively, remove the driver, save the configuration, restart the server and re-add the driver again.</p>
CM7-25466	<p>Shared Devices: When using a Vanquish Dual Autosampler in shared mode, if the two instrument methods have different temperatures set, the temperature setting of the sequence started first is overwritten by the setting of the sequence started second.</p>
CM7-18098	<p>Accela Open Autosampler: Sequences cannot be run when the sampler does not include the DLW option. This configuration is not supported and requires a custom script.</p>
CM6-21321	<p>Accela Open Autosampler: When using this autosampler, a dot ('.') must be used as decimal separator.</p>
CM7-15457	<p>ESA Drivers: Coulochem III: Before setting the cell state to ON manually, please ensure that eluent is flowing into the detector. Otherwise the detector can be damaged.</p>
CM6-22760	<p>TRACE 1300 GC: The autozero function does not work correctly for the FID, NPD, ECD and FPD detector types.</p>
CM7-25600	<p>TriPlus RSH / TriPlus 100: When running the TriPlus RSH or TriPlus 100 in Clone mode (Autosampler serves two GCs), if the Virtual Terminal is opened from the ePanel of one of the GCs and a Sequence is started for the other, the Sequence fails with an error; "Sample - Error while validating script. (Trayplate 1: Slot 1:3)". This can be worked-around by closing the Virtual Terminal on GC1 before attempting to start the run on GC2.</p>
CM6-23614	<p>TriPlus RSH: When using the TriPlus RSH in constant double pro headspace mode, starting a sequence that includes a constant double pro method will generate a validation error.</p>
CM6-24043	<p>TriPlus RSH: If firmware version 2.2 is installed on the TriPlus RSH autosampler, then tool changes on the instrument are not immediately recognized in Chromeleon. It is necessary to disconnect and reconnect the instrument after such changes are made; they will then be detected.</p>
CM7-25760	<p>MS Drivers: When working with MS devices, the raw file must of necessity be created prior to the injection taking place. It is therefore expected that the time stamp in the raw file header differs slightly from the injection time noted in Chromeleon.</p>
CM7-15632	<p>TSQ Quantiva and Endura: When removing the source from a TSQ Quantiva or Endura in mid-acquisition, the sequence does not abort.</p>
CM7-16030	<p>TSQ Quantiva and Endura: With these instruments the standby state reports that the instrument is on, regardless of the real instrument state.</p>
CM7-16154	<p>TSQ Quantiva and Endura: When creating an Instrument Method for the TSQ Endura or TSQ Quantiva, the MS run time is not the same as the Chromeleon run time. The user should enter the correct run time on the MS page of the Wizard.</p>

ID	Description
CM7-17668	TSQ Quantiva and Endura: TSQ Endura and TSQ Quantiva instruments are usually shipped with a PC ("Endura/Quantiva PC") that includes all the necessary instrument data files, such as calibration files, for operating the MS instrument. If you want to control an instrument using a different PC, make sure that the specific instrument data files residing on the Endura or Quantiva PC are backed up and transferred to the new PC. For details on performing this process, please consult with your local MS field service engineer.
CM7-18129	TSQ Quantiva and Endura: After an upgrade of the TSQ Endura/Quantiva instrument driver, an error may occur when opening the Chromeleon Instrument Configuration. To resolve the error, remove the Chromeleon Mass Spectrometer driver from the configuration and then add it again. This will update the configuration information in Chromeleon to match the updated TSQ Endura/Quantiva instrument driver version.
CM7-21967	TSQ Quantiva and Endura: The TSQ Endura and Quantiva mass spectrometer method editor is supported on English operating systems with English/United States regional settings only.
CM7-24445	TSQ Quantiva and Endura: Instrument methods written with an earlier version of the method editor cannot be opened with a newer version thereof.
CM7-23138	MSQ Plus: It is recommended to use only the MS driver provided on the Chromeleon installation medium. Other versions of the MSQ Plus driver may not be compatible with Chromeleon. Please consult your local field service engineer for additional details.
CM7-16557	MSQ Plus and Tune Application: When using the MSQ Plus with Chromeleon the user has to wait for the Chromeleon Instrument Controller to be in idle mode before opening the Tune application. Without waiting, the MSQ Plus will not be able to change the operating mode (On, Off, Standby), or it will not be possible to run injections. To recover from this error both the PC and the MSQ Plus would have to be restarted.
CM7-20295	TSQ 8000 and ISQ Series: When a GC-MS instrument method includes a scan event containing multiple SIM ions (e.g. "SIM 115, 152, 188") then data from matching filters collected at different time ranges will not be combined into a single filter in the data for that injection.
CM7-23669	TSQ 8000 Series: If you attempt to abort an acquisition of multiple timed acquisitions while the MS is acquiring data, the MS will not cycle back to a Ready state and the sequence will not end. It is necessary to stop and restart the Instrument Controller to regain access to the instrument.
CM7-22490	Exactive Series: When setting the divert valve parameters for an Exactive Series MS with a 2-position valve, the valve positions are recorded in the MS raw data opposite of how the divert valve parameters were configured.
CM7-17500	Exactive Series: Exactive Series instruments are usually shipped with a PC ("Exactive PC") that includes all the necessary instrument data files, such as calibration files, for operating the instrument. If you want to control an Exactive instrument using a different PC, make sure that the specific instrument data files residing on the Exactive PC are backed up and transferred to the new PC. For details on performing the data backup on the Exactive PC, refer to the Thermo Exactive Series 2.5 SP1 Release Notes, section Backup provided on the Chromeleon installation disk in the Packages\Thermo Exactive\Documentation folder.
CM7-20547	247 Instrument Controller: TDS4: Due to the smaller internal storage space available on TDS4 models of 247 Instrument Controller, and the larger data files created by 3D acquisition, TDS4 models of 247 should only be used to acquire 2D data. To acquire 3D data, a TDS5 model of 247 should be used.

5.2 Compatibility with Foundation 3.1

Chromeleon is only compatible with Thermo Foundation 3.0 SP2. Users may encounter situations where PCs provided with mass spectrometers come pre-installed with Foundation 3.1 or newer. In these instances, the factory procedure to uninstall any MS instrument control component software must first be followed before reinstalling Foundation 3.0 SP2 and the mass spectrometer driver.

This procedure must only be carried out by individuals that have completed the necessary software and hardware training.

5.3 Limitations with the Waters Driver Pack

ID	Description
CM7-25485	The Waters Driver Pack 2017 R2 cannot be installed on a PC running Windows Server 2016. The corresponding option is greyed out and cannot be selected during the Chromeleon setup.
CM6-24164	When the Waters Driver Pack 4 is installed in a Citrix environment, the World Wide Web Publishing Service is automatically disabled, so that after restarting the PC, the Citrix web application is no longer reachable. The service should be reset to automatic start, after which the application can be reached
CM7-25782	Waters Acquity: During long-running sequences it is possible that the PDA can get into or remain in a running state, thus preventing further injections from starting. A workaround is to add a post run stage with a delay of 90 seconds after the acquisition stop to prevent this error.
CM7-19830	Waters Acquity: When using the Waters Acquity driver in a Citrix environment, the Acquity console does not update correctly and therefore doesn't show current log file entries. This is due to a problem in the Acquity console, and can be mitigated by using the instrument audit trail on remote clients.
CM7-20374	Waters Acquity: If the user attempts to open an Instrument method on a PC where the Waters Driver Pack is installed, but then selects "work offline", an error message will be shown. This is a problem of the Waters Driver Pack, the workaround is to ensure that the instrument can be reached, i.e. work online.
CM7-22872 CM7-15225	Waters Acquity - Console: When using the Waters Acquity driver, some Chromeleon screens may not appear properly, such that text from the previous screen is still visible. This has been observed with the Sequence Properties and the Chromeleon Log on screen.
CM7-23504	Waters Acquity: In rare circumstances when the user configures and then deletes an Acquity PDA, the module will still be shown in the Acquity Console. If a command is then executed (e.g. lamp on), the module disappears from the console, after which the user then needs to reconfigure the instrument in the Chromeleon Instrument Configuration Manager in order e.g. to turn off the lamp.
CM7-23730	Waters Acquity: When using the Waters Acquity Driver Pack4 and trying either to create a new instrument method, or to open the Acquity console from the ePanel a problem sometimes occurs. A message appears informing the user that launching the application had failed, and that the Acquity driver pack may not be installed. If this occurs, the user should contact Thermo Fisher Scientific for further advice.
CM7-24022	Waters Acquity: If the user has two Acquity systems connected to one Instrument Controller, the range for the column temperature in the Waters method editor does not always match the hardware configuration. This is affecting the method editor only, and occurs when opening a method for instrument A while the Acquity console for instrument B is open.

ID	Description
CM-9703	Waters Driver Pack 2017 R2: When installing Waters Driver Pack 2017 R2 ensure that Microsoft Windows Universal C Runtime (KB2999226) is installed. This is to avoid failure of Waters Driver Pack 2017 R2's DM.exe application, which depends on the Windows Universal C Runtime that this hotfix provides for older Windows platforms.
CM6-21112	Waters 2998 PDA: Localization to a non-English regional setting for the PC (e.g., German) does not function correctly for the timed events table, e.g., using a Waters 2998 PDA detector and setting a timed event in the program file (e.g., wavelength change at 5 minutes). The event is recorded, but without the event time.
CM6-21180	After removing the Sample Organizer from the Instrument Configuration, the plate setup is not updated correctly. Manually updating the plate settings in the plate setup configuration dialog avoids this issue.
CM6-24158	Waters 2489 PDA: After changing the Instrument Method from single to dual-wavelength mode (without changing Channel A wavelength), the data rate for Channel B is set incorrectly and incomplete data collection occurs.
CM6-24191	In extremely rare cases the Acquity PDA server stops working, which then causes the running sequence to be interrupted.

5.4 Limitations with Agilent ICF

For a general overview regarding the Agilent Instrument Control Framework, please refer to the document Chromeleon and Agilent ICF - Quick Start Guide - Chromeleon 7.2 .pdf, found in the \Documents\ folder of the Chromeleon 7.2 CDS DVD. For Agilent drivers, please refer to Agilent documentation.

ID	Description
CM7-25840	Instrument Configuration: In rare instances on a Microsoft Windows 7 or Windows 10 PC Agilent for Chromeleon Drivers 1.1 cannot be added. The Windows application event log will contain the following error message: "Cannot create an instance of IConfigurationPlugin." In order to solve the issue please upgrade Agilent for Chromeleon Drivers to version 1.2.
CM7-19347	Agilent G1312B DAD: When using this device in combination with an old JetDirect card, problems may occur collecting data at 80Hz. Users affected by this issue should contact their local Thermo Fisher Scientific representative for advice on possible solutions.
CM7-20047	Agilent VWD G1314B: When using a G1314B VWD, occasionally the chromatogram is half the expected length.
CM7-19863	Agilent ICF: The Agilent LC System Configuration dialog includes entries to configure the following devices, which are not supported by the release: All ELS Detectors (While the ELS Detectors can be configured, they are not supported). Multi-sampler and DAD HDR (Although configurable, they have several known issues and are therefore not supported)
CM7-20991	Agilent ICF: Occasionally when performing injections with ICF controlled instruments the injection volume is incorrectly displayed, although the injection itself was performed correctly.
CM7-21172	Agilent ICF: If the user has the monitor DPI settings on their PC set at greater than 100%, then some parts of the Agilent LC system device ePanel are not visible.

ID	Description
CM7-21427, CM7-18984	Agilent ICF with 1100 or 1200 LC DAD: When acquiring data from an Agilent 1100 or 1200 LC DAD, the signal trace may be shifted to the start of the run, and the end time is inconsistent. No data points are lost with a data rate of 10 Hz and slower (≥ 0.025 min 0.5 sec) 20 Hz and a low number of spectra (all other than ALL Spectra) 20 Hz and spectrum range 190- 400 step 2
CM7-22051	Agilent ICF: Aborting an injection after the start of a sequence but before the injection resulted in an error, requiring the instrument controller to be restarted
CM7-22567	Agilent ICF: When using a Diode Array Detector with the Agilent ICF, it is necessary to enable spectra collection initially (this also allows to specify the wavelength range to be used in this run). If no spectra are needed for a specific time window during the run, use the timetable to temporarily set the mode to "None".
CM7-23096	Agilent ICF: If a Fraction Collector with Thermostat is installed, the channel mapping is not correct. This can be resolved by removing the <Channel name="FC: Delay Sensor"> node from DefaultConfiguration.xml before adding the driver. After this, the user can configure the mapping for the two channels manually on the Signals (2D) tab of the configuration dialog.
CM7-19540	Agilent ICF: The Agilent GC System Configuration dialog includes entries to configure the 7697A Headspace, G1888A Headspace, 7890 GC, 6890 GC, 68550 GC, and 7820 GC. Currently, it is only possible to configure the 7697A Headspace sampler. Attempting to configure any of the other modules will result in a message indicating that the modules are not supported.
CM7-25781	Agilent 7697A: The "Sample Bar Code Reader with data tracking" option on the Agilent 7697A sampler is not currently supported in Chromeleon.
CM7-19975, CM7-20451	Agilent 7697A: The Soft Config option, available via the ICF for Agilent LCs, is not supported for the Agilent 7697 HS. It should not be added to any custom ePanel as its use can cause issues by allowing configuration changes to be applied to the sampler during acquisition.
CM7-19993	Agilent 7697A: If the 7697A loses its connection to the network, an audit trail message is added indicating this fact. However, the ePanel will still show the unit as 'Ready'.
CM7-23242	Agilent 7697A: Running multiple 7697A Headspace autosamplers on a single 247 Instrument Controller can cause Windows "Out Of Memory" errors, requiring a reboot of the 247 to resolve. Thermo Fisher therefore recommends that only one 7697A is connected to any 247 Instrument Controller.
CM6-23980	Agilent 7697A: When starting a sequence while the 7697A Headspace Sampler is in an 'Error', 'Running', or 'Not Connected' state, the ready check does not give an error message. After the sequence starts, the following happens: If the sampler is in error state, the sequence starts without getting interrupted If the sampler is running, the sequence stops with audit trail message "Sequence stopped by user" If the sampler is not connected, the sequence interrupts with audit trail messages "Lost connection to Agilent 7697A Headspace Sampler", and "The instrument is offline. Check power to all modules, cabling between modules and whether the configuration matches the list of modules."
CM6-23992	Agilent 7697A: The 7697 Headspace Sampler has two versions; 111- and 12-vial capacity configurations. The Chromeleon driver is written and tested with the 111 vial capacity version. Though not tested, the driver is expected to work with the 12-vial capacity module. The user should not use vial positions greater than 12 in this case. The rack view always shows 111 vial positions.

ID	Description
CM7-20259	Agilent 7697A: Although the vial position may be assigned in the instrument method script, unless this is done in the Instrument Setup Stage, the sequence table will not be updated. This can result in misleading information in reports and should be avoided.
CM7-20259	Agilent 7697A: Although the vial position may be assigned in the instrument method script, unless this is done in the Instrument Setup Stage, the sequence table will not be updated. This can result in misleading information in reports and should be avoided.
CM6-23996, CM7-19940, CM7-21324	Agilent 7697A: The 7697 Headspace Autosampler has two options for handling missing vials: Pause and Abort. An issue has been observed when the Abort option has been selected. In either mode, the autosampler overlaps sample preparation, i.e.: sample 2 is prepared while sample 1 is acquiring. If the autosampler finds that the sample 1 vial is missing, it will Abort or Pause the sequence at the point it discovers the vial is missing. However, if the autosampler finds that the sample 2 vial is missing, while sample 1 is already acquiring, and the Abort option has been selected, the entire sequence will be aborted, including the acquiring sample 1.
CM6-24004	Agilent 7697A: Using the instrument front panel, the allowed range for Transfer Line Diameter is 200-600 microns. However, when setting this value in the Chromeleon instrument configuration the limit is 250-530 microns.
CM6-24005	Agilent 7697A: When 7697A headspace instrument method parameters are included in a report, the "fill pressure" parameter is rounded to the nearest integer.
CM6-24007	Agilent 7697A: Some parameters logged to the instrument audit trail are rounded to nearest integer. However, all values are downloaded to the instrument with the proper precision.
CM6-24008	Agilent 7697A: When editing an existing 7697A Headspace instrument method, if the values for Purge Flow, Purge Time or Leak Flow are changed, the Save button is not enabled until the user changes tabs.
CM6-24009	Agilent 7697A: When configuring an Agilent 7697A, there is an option in the user interface to "Upload Config from Instrument". This option does not work. Instead, you will need to manually configure the instrument settings.
CM7-19993	Agilent 7697A: If the 7697A loses its connection to the network, an audit trail message is added indicating this fact. However, the ePanel will still show the unit as Ready.

5.5 Limitations with Other Third Party Instruments

ID	Description
CM7-20464	Varian 3800 GC: It is not possible to start a manual data acquisition if the GC is not ready (i.e. all temperatures, pressures and so on are at their set points). Trying to do so will generate a Ready Check message detailing what is not ready.
CM7-15293, CM7-18463	Agilent 1100 Obsolete Driver: Occasionally, when using a combination of older and newer modules, the raw data was not correctly acquired.
CM7-25343	Agilent 6850: Instrument Configuration Manager does not report mismatches between the hardware and the Chromeleon configuration.

ID	Description
CM7-12366	<p>Agilent 5890 DICE Card: Please note the following when using the 19257 DICE card with the Agilent 5890 GC:</p> <p>Control and acquisition using the DICE card is only supported via the serial interface. The GPIB interface is not supported.</p> <p>Digital data acquisition via the serial interface of the DICE card is only supported for a single channel; dual channel digital acquisition is not supported.</p> <p>Currently, it is possible to select certain illegal combinations in the Configuration Dialog such as:</p> <p>Digital acquisition with the 19254 card. This is not supported.</p> <p>Digital acquisition on one detector and analog acquisition on the other. Acquisition needs to be exclusively digital or exclusively analog.</p> <p>When using the DICE card to acquire data digitally, the 5890 INET mode must be set to "GLOBAL" not "LOCAL". Failure to do so will result in a "No response from GC" message following the AcqOn command in the audit trail.</p> <p>Note that when performing analog acquisition, the 5890 INET mode should still be set to "LOCAL" (as described in the online help).</p>
CM7-9675	<p>Agilent 7890 GC: There is a backward compatibility issue that affects the Agilent 7890 GC Sampler Positions. When using a 7890 GC in combination with a 7693 sampler, certain positions in the sampler could give a misspelled value to a move command. This has now been corrected and could in rare cases lead to Instrument Method files needing to be updated to avoid errors.</p>
CM7-24724	<p>Agilent 7890B GC: With certain firmware versions, the GC does not properly send abort information to the software, meaning that events such as FID flame out, pressure errors, hardware faults and so on, will not be recognized or reported by Chromeleon. The problem is seen in FW versions B.02.01, B.02.04.2 and B.02.05, but not versions A.01.xx.x. The 7890A GC does not seem to have this problem.</p>
CM7-15400, CM7-15556, CM7-15734, CM7-15736	<p>PerkinElmer LC200 Autosampler: When upgrading from earlier versions of Chromeleon 7 CDS to Chromeleon 7.2 CDS SR3, it is necessary to reload the PerkinElmer LC200 Autosampler driver and configure the loop size within the configuration. The user should then check all instrument methods using this autosampler to ensure that they continue to function correctly.</p>
CM7-15716	<p>PerkinElmer Clarus 400 GC: Some users must select Autosystem XL in configuration in order to communicate with the PerkinElmer Clarus™ 400.</p>
CM7-24840	<p>PerkinElmer Clarus 580 GC: For the PerkinElmer Clarus 580 GC without an internal autosampler the automatic type recognition of the PerkinElmer GC driver configuration module fails for the 580 type. The automatic type recognition detects a 500 series instead. Setting the GC type to 580 manually does not allow to connect to the instrument.</p> <p>Workaround: Leaving the setting on 500 (or 600) allows to connect to the instrument and to control it properly.</p>
CM7-25156	<p>PerkinElmer Autosystem XL GC: Chromeleon is currently not able to control or change the signal source of a channel. Such settings must be controlled by the user at the GC display and it must be verified that the channels are linked to the correct detector before the method is used for Chromeleon control.</p> <p>Workaround: The PerkinElmer Autosystem XL GC allows to set the channel to detector link at the GC display for the method that is used for Chromeleon control. In the pane 'Output' setting, verify that the correct detector is linked to the signal channel. See also chapter 'routing detector output' in the GC user manual. Note: It is not possible with Chromeleon to alter the output link during analysis with timed events</p>
CM7-17948	<p>Shimadzu LC: Unlike most drivers, some Shimadzu UV detectors require that you select the Advanced filter in the Command (F8) window in order to access the Lamp On/Off command.</p>

ID	Description
CM6-23947	Shimadzu LC-10A, LC-2010: If the user cancels the key lock state of the front panel of the instrument and then, for example, stops a manual acquisition, this is likely to lead to unexpected effects during the next operation such as sudden abort of the sample run.
CM7-24868	Shimadzu LC-2010A: If using a large injection volume, samples could remain in a running state until interrupted manually by the user. The need to configure the loop volume in two places was not correctly documented in the help.
CM7-23099	<p>Shimadzu LCs: The Microsoft Visual C++ 2005 Run Time component is no longer supported by Microsoft. However, this component is required for the Shimadzu LC-2010A and Shimadzu LC-10A/20A/30A drivers and is therefore installed by Chromeleon.</p> <p>If you don't use these drivers, it is possible to uninstall the Visual C++ 2005 Run Time component from the 'Programs and Features' page of the Windows Control Panel. Alternatively, during the installation of Chromeleon, it is possible to suppress the installation of the Visual C++ 2005 Run Time component by using a response file and excluding the "__MicrosoftVisualC2005_SP1__" package. Please refer to the Installation Guide for details.</p> <p>Several of the Shimadzu devices can be controlled by obtaining an updated driver directly from Shimadzu (see the "List of Supported Instruments" for details).</p>

5.6 Limitations With Setup

ID	Description
CM7-21780	<p>Setup: NIST MS Search and Demo Library No Longer Automatically Installed: Incompatibilities of the NIST 2008 MS Demo Library installer with Window 7 and 10 could cause the main Chromeleon installer to hang or crash. To address this, the NIST Demo library, and the associated AMDIS and MS Search software are no longer automatically installed when you install Chromeleon. If desired, this package may be installed manually using the setup program found in the /Tools/ folder of the Chromeleon DVD. Alternatively, one may install AMDIS and MS Search using the full (licensed) NIST library installer.</p> <p>Note that MS library searching within the Chromatography Studio is not affected by this issue.</p>
CM7-23341	<p>Setup: When Agilent ICF is installed, un-install of either Chromeleon or Agilent ICF fails if the Instrument Controller is running:</p> <p>Failed to execute package Agilent Instrument Control Framework A.02.04. Another application has exclusive access to the file 'C:\ProgramData\Agilent Technologies\Instrument Control Framework\RCDriver.log'. Please shut down all other applications, then click Retry.</p> <p>To avoid this issue, stop the Instrument Controller before uninstalling</p>
CM7-24384	<p>Setup: When Chromeleon 7.2 SR5 is installed on a Windows 10 PC, upgrading that PC to Chromeleon 7.2.6 will appear to complete successfully, with no IQ errors or warnings. However, attempting to export a sequence to PDF will fail with an error stating "Printer not activated, error code – 30".</p> <p>To resolve this problem, rerun the Chromeleon 7.2.6 setup, selecting 'Repair' on the opening screen of the setup program.</p>

5.7 Other Limitations

ID	Description
CM-21182	Functional Specification: The functional specification document on the Chromeleon DVD has not be updated to reflect the new functionality available in Chromeleon 7.2.9. The updated document is however available online for download.
CM7-25151	Scheduler: Copy/Move Sequences: Scheduler jobs copying or moving sequences to a network data vault might run into a state where the jobs cannot be completed anymore. One must restart the corresponding Chromeleon 7 Scheduler Service to get this kind of deadlock being resolved.
CM7-15588	Discovery: The Discovery service failed to start if the PC name included non-standard characters. Now, the Discovery service will not crash and will log the PC name to help troubleshoot why it is not listed in the Console or Administration Console.
CM7-22111	<p>Discovery: Mixed Installations with Chromeleon 7.2 SR5 Domain Controller: If you have an existing installation of Chromeleon < 7.2 SR1, the following limitations apply during an upgrade:</p> <ul style="list-style-type: none"> • Stations that have Chromeleon 7.2 or below installed will not see any data vaults or instruments that have been created with Chromeleon 7.2 SR5, until after those stations are upgraded to 7.2 SR5. • It is not possible for a Chromeleon 7.2 (and below) station to join a Chromeleon 7.2 SR5 domain. • Stations that have Chromeleon 7.2 or below will not receive any updates from the Discovery Service after the Chromeleon domain controller has been upgraded to 7.2 SR5, and will only see resources that were already in existence and cached. <p>Please refer to the Enterprise Documentation for guidance on upgrading an older installation of Chromeleon 7 to Chromeleon 7.2 SR5.</p>
CM7-24042	Instrument Configuration Manager: The .NET 4.7 framework is installed by Windows Update. For Windows 7 it is a recommended update, but for Windows 10 it is a mandatory update. This release of Chromeleon has been validated against .NET 4.7. However, under rare circumstances, the installation of .NET 4.7 could lead to malfunctioning or crashes of the instrument configuration manager or configuration plug-ins. If this occurs, please contact your Chromeleon support desk for assistance in correcting the problem.
CM7-20449	User Management: Login "Role" dropdown box becomes empty after upgrading to Chromeleon 7.2 SR4. This is due to the fix for CM7-18178 "Roles were offered in the Logon dialogue, even if they were not specified as Logon roles". To work around this issue, enable the "Logon Role" property in the user database for all logon roles that users need to be able to select.
CM7-11692	Console: Instruments: When monitoring the baseline with an overlay chromatogram added to the signal plot, the overlay disappeared after changing to a different ePanel and back.
CM7-17966	Console: Instruments: Online Plot: For the Vanquish CAD, some properties and two channels are recorded where the data is transmitted as aA, and scaled to pA with 6 digits resolution. The online plot displays these numbers for the current signal value with 2-digit precision only.
CM7-25480	Console: Data: If a Data Vault is unavailable, it is not shown as collapsed in the data explorer tree despite its sub-folders and items being inaccessible.

ID	Description
CM7-22738	<p>Console: Data: Empty Inject Time and GUID fields have been seen in a few single injections. Raw data have been successfully acquired and stored on the local Instrument PC. The Injection Audit Trail on the Instrument PC contains complete information, including the missing details. Too few instances have been reported to identify the root cause of this problem.</p> <p>Note: If you are affected by this problem, please contact your local Thermo Fisher representative for assistance with recovery of the missing injection details.</p>
CM7-21399	<p>Console: Data Query: Injection Variables 'Auto Dilution Ratio' and 'Retention Time Standard': Auto Dilution Ratio and Retention Time Standard columns are not available in the custom filter conditions for injection records (e.g., in the IRC editor or summary report).</p>
CM7-19836	<p>Console: eWorkflows: The eWorkflows wizard fails with a message "Failed to retrieve the required Data Vault" when there is more than one Data Vault with the same name in the Chromeleon Domain.</p>
CM7-24058	<p>Console: eWorkflows: The new eWorkflow option "Preserve Layout", introduced in Chromeleon 7.2.6 is not backwards compatible with older versions of Chromeleon. If a client with an earlier version attempts to open an eWorkflow for which this option is enabled, the error message "Cannot load, as the data was created with a newer Chromeleon version." Is displayed.</p>
CM7-19336	<p>Import Chromeleon 6: Due to changes in Auditing between Chromeleon 6 and Chromeleon 7, when a Chromeleon 6 Sequence is imported into Chromeleon 7, some of the text displayed in the Instrument Audit trail will not appear exactly as it did in Chromeleon 6. Refer to the topic "Viewing Chromeleon 6 Data" in the online help for further information.</p>
SWFR-248	<p>Waters Empower Import: The following limitations apply to the import of data from Waters Empower:</p> <ol style="list-style-type: none"> 1. Time zone information is not supplied by the Waters toolkit API, so dates and times will be imported as if they were local. 2. Empower allows injections that are not contained in sample sets. These are not visible to the importer and cannot be imported unless added to a sample set. 3. Some peak results fields show incorrect units in Chromeleon since there is currently no mechanism to change the units on 'core' fields. They are included correctly in custom fields that by default are hidden.
CM7-25551	<p>Import/Export: If two (or more) users simultaneously attempt to export a Sequence to the same location, a "Cannot export <sequence_name>" error is displayed for all.</p>
CM7-18252	<p>Export MS Raw Data: When acquiring MS data, Chromeleon acquires MS data and all other signal data, such as UV, FLD, and pump pressure signals, in separate formats. As a result, when MS data is exported, non-MS data is not exported with the MS raw data file.</p>
CM7-15455	<p>Processing Method: Without data in the first injection, it is not possible to select the 2nd or 3rd Detector for Dead/Delay Time.</p>
CM7-17465	<p>Processing Method: On the MS Settings page, It can happen the spectral bunching value for Peak Dependent Correction that is displayed as an annotation on the chromatogram plot does not match the value entered in the processing method on the MS setting page. This is by design, because the method setting defines the maximum number of spectra for averaging. The actual number of spectra used is determined the number of MS spectra which fit the filter used for the chromatogram. This is not correctly documented in the Chromeleon online help.</p>
CM7-21783	<p>Processing Method: Performance When Importing Fixed Calibration Standards for MS Sequences: When working with sequences of MS data, importing injections for use in a fixed calibration can take 1-2 minutes to complete, depending on the data.</p>

ID	Description
CM7-24825	Processing Method: A sample with a processing method created in Chromeleon 7.2.7 when opened in the Chromeleon 7.2.6 in the Studio should show a notification bar indicating that the evaluation results may differ from those using the version which was used to create/save the processing method. This notification bar is not displayed. This issue affects only qualification sequences; regular sequences are not affected.
CM7-20335	Comparison of Old Report Versions Shows Change in CmbxExportParameters: If a report which was created in Chromeleon 7.2 SR2 or earlier, and modified in SR3, has its history compared in SR4, the history will appear to show that the "Cmbx Export Parameters" value has changed from True to False. This is due to a change in the default value of this field and does not represent any user-modification of the report.
CM7-17203	Report Designer: With some date/time formatting settings in the report, the order of month and day changes for some formats automatically. The settings in the Report Template can change based on the Windows regional settings. For example it is not possible to set m.d.yy as format with German regional settings. The Report Template replaces this with d.m.yyyy. The substitution occurs for report variables and non-report variable entries.
CM7-22145	Reporting: Discrepancy in "Last Modified" Time: Owing to differing rounding methods used, it is possible that the value of the "last modified" time for an object in a sequence has a difference of 1 second between the client display and the value shown in a report. For more details, please see the on-line help.
CM7-17841	Report Designer: If using a non-Chinese format as the regional setting in Windows, and Chinese as the setting for Non-Unicode programs, then the header on a Chromeleon report is not correctly displayed for variables. If the format is changed to Chinese, then everything is correctly displayed.
CM7-21331	Reporting: The mass spectrum resolution report variable returns an internally used processing value instead of the resolution setting defined in the MS instrument method. It is recommended to discontinue use of this report variable until further notice.
CM7-23442	Reporting: In order to display the date and time in the Header/Footer of reports one can use the spreadsheet placeholders &D and &T respectively. During report creation these placeholders are replaced by the current date and time and formatted via the regional settings of the currently logged on Windows user account. Yet this doesn't work correctly for every regional settings, e.g., 24 hour time formatting. Instead of using &D and &T one can use the Chromeleon report formula <code>gen.currentTime</code> or <code>gen.reportTime</code> together with the necessary format, e.g. <code>{gen.currentTime; "dd.mm.yyy hh:mm"}</code> . Note: the formula <code>gen.currentTime</code> is replaced by the current date/time during the electronic report creation. If you want to display the date/time when the electronic report is really printed or exported you have to use the formula <code>gen.reportTime</code> .
CM7-24972	Reporting: When applying a two level Autorepeat rule with double grouping to a plot object, if the sequence contains a large number of injections and a large number of components, it is possible that software performance will degrade significantly. This has been observed when applying Autorepeat to an MS Components plot for a sequence with 27 injections and 292 components.
CM7-23484	Reporting: In order to display the last updated date and time for a locked injection it is necessary to use the Chromeleon report formula <code>procMeth.version.time</code> .
CM7-25590	Chromatogram Plot: When creating a Virtual Channel, the Power Factor only increments in steps of 0.5, which does not provide sufficient flexibility for controlling the scale of the extracted data.

ID	Description
CM-14128	<p>Non-Targeted MS Processing: When performing Non-targeted MS data processing, Chromeleon uses a disk-based cache to increase processing performance. Over time, this cache can grow to consume large amounts of local hard disk space. To flush the cache and release the disk space, a utility is included on the Chromeleon distribution DVD in the \Tools\CacheCleaner\ folder. Double-click on CacheCleaner.exe to manage the content of the cache.</p>
CM7-22986	<p>During stress tests with multiple, very long sequences with more than 1000 injections, the queue was aborted with an unexpected error:</p> <p>"Queue End 24.12.2016 16:27:22 +01:00 Stopped the sequence queue run. Sequence End 24.12.2016 16:27:22 +01:00 End of sequence "Simple Vanquish Test 2016-12-21 19_37".</p> <p>Abort Error 24.12.2016 16:27:21 +01:00 The injection audit trail cannot be saved. Error detail: Die Transaktion wurde abgebrochen. The transaction commit operation failed. The save operation failed for data item(s) "'chrom://c-germoefelein/XVault/Vanquish-H/6/Simple Vanquish Test 2016-12-21 19_37.seq/277.smp/Audit.audit'". Execution of txp [05f69eb4-c9ed-11e6-9598-005056c00008] failed. Error message : The command 'UPDATE CJ_VERSION SET VERSION_LAST_SIBLINGS_TXN_NO = @P0 WHERE CJ_VERSION.VERSION_INVALIDATE_TXN_NO > @P1 AND CJ_VERSION.PARENT_ID IN (@P2)' failed."</p> <p>As a workaround it is recommended that automatic upload be disabled when running very large sequences and uploading them manually instead.</p>
CM7-23033	<p>Legacy Upload: With replication framework disabled, when trying to modify a sequence while the automatic upload is already in progress the upload may fail in very rare cases and it is not possible to remove the sequence from the instrument queue by retry of the upload. To recover the sequence a copy of the sequence has to be stored manually. Chromeleon 7.2 SR5 adds an audit trail entry to the manually uploaded sequence that refers to the original sequence so that traceability is ensured.</p> <p>Thermo Fisher Scientific recommends to enable the replication framework with Chromeleon 7.2 SR5 to avoid the problem.</p>
CM7-23051	<p>In a few cases Sequences have been reported to abort with messages in the audit trail that were not conclusive, such as:</p> <ul style="list-style-type: none"> • "The audit trail was unavailable for some time. Several audit trail messages are lost. They have been logged to the file "Dionex\Chromeleon\Log\AuditTrailMessages.log" in the (common) application data folder." • "The injection audit trail / signal "... " cannot be saved. Error detail: The transaction has aborted. The transaction commit operation failed." <p>However, the SQL Server ERRORLOG files of the affected Instrument Controller PCs revealed errors due to slow file operations on the local hard drive. Thus, it is assumed that these failures were caused by poor disk drive performance. Chromeleon 7.2 SR5 introduced additional internal error reporting so that similar errors can be identified more easily in the future.</p>
CM7-25508	<p>Upload: In very rare cases, an upload may succeed, however the sequence remains locked (redirected to the Xvault).</p>
CM7-25633	<p>Services: In very rare cases if the Oracle database disk is running out of disk space and in addition an IPC cannot be connected properly, it may happen that that a sequence cannot be uploaded automatically. When trying to reboot the IPC a retry of the upload may result in an error message "A transaction package is missing on the hard disk. The order of transaction packages which should be sent to the network data vault can't be accomplished." The sequence can't be removed from queue automatically. It needs to be removed manually.</p>

ID	Description
SWFR-2543	Sampling Devices That Do Not Use uL As Units for Volume: Although most liquid injection devices expect volumes to be entered in uL, there are a few devices (e.g. Thermo AS-HV and PerkinElmer GC Autosampler) which do not use µL as their default volume unit. If one of these devices is configured in the same instrument that also includes an injection device that uses µL, problems may be observed with volume validation in the sequence table as well as units associated with volumes in reports.
CM7-24600	Spectral Library: If an older Chromeleon version than Chromeleon 7.2.7 is used to create and name components from library screening results, then upon selecting the folder reference attempts to close the dialogue with OK will result in an exception being thrown.

5.8 Obsolete Drivers

Chromeleon includes a number of obsolete drivers in order to provide backward compatibility of existing installations:

- Agilent/HP 1200 HPLC System
- AI 1310/3000 GC Sampler - 10ul
- AI 1310/3000 GC Sampler - 5ul
- AI 1310/3000 GC Sampler - 5ul - 155 Vials
- AI 1310/3000 GC Sampler - 5ul - 105 Vials
- AI 1310/3000 GC Sampler - 10ul - 155 Vials
- AI 1310/3000 GC Sampler - 10ul - 105 Vials
- PAL Sampler for GC
- PAL Sampler for LC
- TRACE 1300 Series GC (First generation driver that has been superseded by TRACE 1300 Series GC II driver)

Please note that issues reported for any of these drivers will no longer be addressed. If you are using one of these drivers Thermo Fisher Scientific recommends migrating to a supported driver as soon as possible.

5.9 Functional Differences between Chromeleon 7.2 and Chromeleon 6.8

Chromeleon 7.2.9 implements the vast majority of Chromeleon 6.8 features, and in general, has a richer feature set than Chromeleon 6.8. However, a few Chromeleon 6.8 features remain to be implemented on the Chromeleon 7 platform and a few will never be implemented, since they are now obsolete or no longer relevant. If a particular missing feature is important to you, please contact your local Thermo Fisher Scientific representative to find out if that feature is in the product development plans.

6 Backward/Forward Compatibility Issues

6.1 Thermo Scientific Vanquish Charged Aerosol Detector [CM6-23499]

Any Instrument Methods created for the Vanquish Charged Aerosol detector with Chromeleon 7.2 SR2 MUa and earlier may need to be updated due to changes in the driver introduced in Chromeleon 7.2 SR2 MUb.

6.2 Thermo Scientific Vanquish Autosampler [CM6-23405]

Any Instrument Methods created for the Vanquish Autosampler with Chromeleon 7.2 SR2 MUb and earlier will need to be updated if they contain the WashSpeed property. The WashSpeed value needs to be divided by 0.06 in order for the Instrument Method to work correctly.

6.3 Thermo Scientific TriPlus RSH

The current driver for this instrument is incompatible with firmware older than version 2.4.

6.4 Thermo Scientific TriPlus 300 HS

The current driver for this instrument is incompatible with firmware older than 2001.9.0.

6.5 Thermo Scientific TriPlus LS-100

The current driver for this instrument is incompatible with firmware older than version 2.4.

6.6 Thermo Scientific TSQ Quantiva

The driver version 1.1 QF1 for this instrument, included in this Service Release, may not be compatible with existing TSQ Quantiva mass spectrometers running driver version 1.0 without a hardware update. Please contact your local MS service engineer before attempting to upgrade the unit.

Note: New TSQ Quantiva modules from the factory are not affected by this issue.

6.7 Thermo Scientific TSQ Quantiva and Endura

The driver version 1.1 SP1 for these instruments may not be compatible with existing TSQ Quantiva and Endura mass spectrometers running driver version 1.0 without a hardware update. Please contact your local MS field service engineer before attempting to upgrade the unit.

Note: New TSQ Quantiva and Endura modules from the factory are not affected by this issue.

6.8 TSQ Quantiva and Endura Instrument Method [CM7-18759]

Instrument methods created with older versions of the TSQ Quantiva and Endura instrument method editor cannot be opened with newer versions of the method editor. If a large number of instrument methods have already been created for regular use, upgrade of the TSQ Quantiva and Endura driver

is not recommended. Contact your local Thermo Fisher Scientific representative for additional details.

6.9 Signed Sequences [CM7-16374]

Sequences that have been signed within Chromeleon 7.2 SR1 will fail verification after copying within later versions of Chromeleon 7.2 CDS.

6.10 Improved Peak Grouping

6.10.1 Processing Method

With the new data model for peak grouping, processing methods created in Chromeleon 7.2.9 which contain peak groups are not compatible with prior Chromeleon versions (e.g. 7.2.8). Opening these processing methods in Chromeleon 7.2.8 or older will result in an error message. Processing methods created in Chromeleon 7.2.9 that do not contain peak groups are still compatible with prior Chromeleon versions.

When opening older processing methods with Chromeleon 7.2.9, the parameters are re-mapped such that the evaluation for group related results is identical to prior Chromeleon versions. If such processing methods are changed and saved, Chromeleon tries to save the processing method in a way that prior versions can read it. However, for the following modifications in the peak group and component table this is not possible:

- When new peak group is added to the peak group table.
- Any field of a named group is changed except for the peak group name.
- A field of a timed group that is not present in the prior Chromeleon versions is modified, e.g. "Group Type", "Group Evaluation" and "Concentration Values".
- All peak group assignments of components or timed groups to a named group are removed.
- The name of a timed group is changed to use more than 64 characters.
- Any calibration type setting of any peak group is changed.
- Any calibration type setting of a component that belongs to a (named) peak group is changed.

Any of the modifications listed above will make the processing method incompatible with prior Chromeleon versions.

6.10.2 Peak Grouping Results

Evaluating and reporting peak grouping-relevant results is fully compatible with prior Chromeleon versions: if you create a report of a sequence with a processing method from a prior Chromeleon version you will get the same results in 7.2.9.

6.11 Chromeleon Enterprise Compatibility of a Chromeleon 7.2 SR5 Domain Controller with Newer Versions of Chromeleon Clients and Instrument Controllers

In general, it is possible for a Chromeleon Enterprise with a domain controller running Chromeleon 7.2 SR5 (including any MUs) to work with instrument controllers and client PCs running newer versions of Chromeleon (7.2.6 and later).

For customers with a fully validated Chromeleon 7.2 SR5 system, we would not recommend connecting clients or IPCs with a later version of Chromeleon installed.

However, should you choose to create a 'mixed' Chromeleon environment, the following restrictions apply:

Opening Processing Methods Created on Newer Versions on an Older Client

These processing methods may be opened, edited and saved without losing any parameters specific to the newer version. However, the new parameters will not be applied to data processing, will not be accessible as report variables and will be completely 'invisible' on the older client. The new parameters include:

- Peak Identification by Reference Mass Spectrum
- Time based specification of the Cobra Wizard the integration parameters 'Smoothing Width', 'Baseline Noise Range' and 'Consider Void Volume'
- UV Spectrum Search Across Multiple Libraries
- Variable Amount ISTD quantitation Based on Ratio (Response) vs Ratio (Amount)

Enterprise Functionality Specific to Newer Chromeleon Versions

Features such as email notification, automated results export, post-sequence reporting with Chromeleon Client closed, and Chromeleon XPS will not function, even if accessed from a client running a newer version of Chromeleon.

Support for Instrument Control Specific to Newer Chromeleon Versions

In general, it is possible to control these instruments. However the following restrictions apply:

- The instrument controller PC must be running the newer version of Chromeleon
- Older client PCs will not be able to create, edit or view instrument methods for the new driver
- Older client PCs will not be able to view ePanels related to the new driver
- Some instrument view toolbar items such as 'Consumables' and 'Troubleshooting' may be disabled (or have fewer sub-options) on the older client.
- Older client PCs will not be able to perform manual tuning or do real-time scanning for remote mass spectrometers

Additional restrictions may also apply. If you have any questions or concerns, please contact your local Chromeleon support channel.

7 Appendix

This chapter contains general information about Service Releases, Release Notes, Online Help, and Contributed Content.

7.1 Release Notes

The Release Notes list the new features and improvements of the current release. Included in these Release Notes are all of the functionality and bug fixes from Chromeleon 7.2 SR5 MUa through MUF. For details about Chromeleon 7.2 SR5 and other previous releases, refer to the relevant release notes which can be found on the Chromeleon 7.2.9 DVD.

7.2 Online Help

In general, new features, updates and drivers that are introduced with this release are described in an updated Online Help that is distributed with the release.

7.3 Contributed Content

The Chromeleon 7 disk contains a folder titled Contributed Content. This folder contains:

- Demonstration Material
- Localized Documents
- Localized ePanels
- Localized Report Templates
- eWorkflow Templates
- User Management Example
- Charlie Mouse Pointer

Note: The files in the Contributed Content folder have not been tested and validated according to Thermo Fisher Scientific Software Development Cycle guidelines modeled after ISO 9001:2008 standards. Thermo Fisher Scientific assumes no responsibility for any errors that may appear in the content provided in the Contributed Content folder.

7.4 Improved Peak Grouping – A Comparison With Prior Releases

Chromeleon 7.2.9 introduces a new data and evaluation model for peak grouping. In the processing method there is a new Peak Group Table replacing the former Unidentified Peak Group Table. Existing processing methods and their evaluations will be processed in a compatible way, meaning peak group-related results of existing sequences will not be changed in 7.2.9.

7.4.1 The “Old” Data and Evaluation Model

Chromeleon 7.2.8 and earlier offered two different ways to use Peak Groups.

7.4.1.1 “Named” Peak Groups in the Component Table

Component records can be assigned to a peak group by simply setting the group field with an arbitrary group name. These “named” peak groups are calibrated implicitly using the calibration-relevant properties of the corresponding components Calibration Type, Evaluation Type, Standard Method and Concentration Levels. The values for Calibration Type, Evaluation Type and Standard Method are set automatically to identical values for all components belonging to the same peak group. The following screenshot is an example of such a component table with two named peak groups A and P.

Component Table							
Group Area		Drag a column header here to group by that column.				Run Component Table Wizard...	Show Prop
#	Name	Group	Eval.Type	Cal.Type	Stand.Meth.	Level "A_75"	Level "A_100"
1	Acenaphthylene	A	Height	Lin, WithOffset	External	9.900000	13.200000
2	Fluorene		Area	Lin, WithOffset	External	20.100000	26.800000
3	Phenanthrene	P	Area	Lin, WithOffset, 1/A	External	27.900000	37.200000
4	Anthracene	A	Height	Lin, WithOffset	External	12.150000	16.200000
5	Pyrene	P	Area	Lin, WithOffset, 1/A	External	18.900000	25.200000

Figure 3 - Component Table (7.2.8)

The components ‘Acenaphthylene’ and ‘Anthracene’ belong to peak group ‘A’, components ‘Phenanthrene’ and ‘Pyrene’ belong to peak group ‘P’.

7.4.1.2 “Timed” Peak Groups in the Unidentified (UI) Peak Group Table

A UI peak group is defined by a dedicated time range (Start/End Time) in the corresponding records. All unidentified peaks in this time range are automatically members of this UI peak / time group. The following screenshot is an example of such a UI peak group table with two “timed” peak groups – UI Peak Group 1 and 2.

Unidentified Peak Group Table								
Group Area		Drag a column header here to group by that column.						
#	Name	Start Time	End Time	Group	Eval.Type	Cal.Type	Factor	Channel
1	UI Peak Group 1	0.800 [min]	1.500 [min]	P	Area	Lin, WithOffset, 1/A	1.000000	All Channels
2	UI Peak Group 2	2.000 [min]	3.100 [min]		Area	None	1.000000	All Channels

Figure 4 - Unidentified Peak Group Table (7.2.8)

Via the property ‘group’, UI peak groups can also be assigned to named groups. In the example above, UI Peak Group 1 belongs that way to the named peak group P. In this case calibration relevant parameters (Evaluation Type, Calibration Type) for the UI group record are also identical to the corresponding values of the component records which belong to the same named peak group.

7.4.1.3 Calibration and Amount Computation of Peak Groups

When calibrating a peak group, the calibration relevant parameters are either picked from any component (or UI peak group) that belongs to the named group or from the UI peak group record itself. UI Peak Group records do not have concentration levels and the corresponding values. Therefore for those UI Peak Groups that do not belong to a named group (see UI Peak Group 2 in the Figure 4) the calibration type can only be set to ‘None’, ‘Manual’ or ‘Calibration of other component’.

Components and unidentified peaks that belong to a named peak group are automatically calibrated together as a group. This means that for the X-values of the (group) calibration points - depending on the Integration Type (Area, Height, etc.) - e.g. the areas of all peaks that belong to the same named

group are added together. For the Y-values of the calibration points the values of concentration level are added.

When calculating the amount of a component or unidentified peak that is member of peak group (named or timed), the area of the corresponding peak in the chromatogram is evaluated against the corresponding group calibration. For the report variable 'Group Amount' (Formula peak.groupAmount) the sums of all peak areas that belong to the peak group are evaluated against the group calibration.

7.4.1.4 Peak Group Results

Beneath the basic group membership of a peak/component in a chromatogram (Formula peak.group), Chromeleon can report the group area (Formula peak.groupArea) and height (Formula peak.groupHeight), summing the areas and height values of the peaks that belong to the same group. The Group Amount (Formula peak.groupAmount) is already mentioned in the previous chapter.

7.4.2 The "New" Data and Evaluation Model

7.4.2.1 "New" Peak Group Table in the Processing Method

The "old" Unidentified Peak Group Table has been replaced in Chromeleon 7.2.9 by the new **Peak Group Table**. The main difference is that the new peak group table additionally contains separate records for named groups. There are also new properties in the new peak group table, which allow evaluation of named or timed groups as in Chromeleon 7.2.8, as well as offering additional capabilities. The Processing Method Editor provides new pages for the Peak Group Table. The following shows the new Peak Group Table of the same processing method as in the previous section.

Peak Group Table											
Group Area Drag a column header here to group by that column.											
#	Name	Group Type	Start Time	End Time	Peak Group(s)	Group Evaluation	Eval.Type	Cal.Type	Stand.Meth.	Level "A_75"	Level "A_100"
1	UI Peak Group 1	Timed Group	0.800 [min]	1.500 [min]	P	Calibration	Area	Use P	External		
2	UI Peak Group 2	Timed Group	2.000 [min]	3.100 [min]		Calibration	Area	None	External		
3	P	Named Group				Calibration	Area	Lin, WithOffset, 1/A	External		
4	A	Named Group				Calibration	Height	Lin, WithOffset	External		

Figure 5 - Peak Group Table (7.2.9)

"Old" UI peak group records (as UI Peak Group 1 and 2 in the screenshot) are kept with the group type "Timed Group". The "old" named groups A and P are now present with dedicated new records.

The peak group record contains the following properties/columns. In the following the **(New!)** label marks those properties which were not present in the old data model. The label **(Partially New!)** is used if the property has been already present in the old data model but with extended options in the new one.

- **Name:** Defines the group name.
- **Group Type (New!):** Possible values are Timed Group and Named Group. Depending on this value, other properties and columns are enabled or disabled.
- **Start / End Time:** This columns are only valid for timed peak groups. They define the time range for unidentified peaks in the chromatogram which should belong to the peak group.
- **Peak Group(s) (Partially New!):** This column is only valid for timed peak groups. Here you can also define to which named group this timed group should belong. In the old data model this

column has been named 'Group'. In the new data model you can also assign multiple named groups.

- **Group Evaluation (New!):** Possible values are 'Calibration', 'Reporting' and 'None'. 'Calibration' is always used for old processing methods. The value 'Reporting' means that such peak groups are not calibrated and cannot be used when selecting the calibration type 'Calibration of other component or peak group' (see description of 'Cal.Type' column below). For peak groups with evaluation 'None' Chromeleon doesn't report any peak group results, e.g. group area. Such peak groups can't be used for calibration purpose neither.
- **Eval. Type:** This column defines the evaluation type (Area/Height, etc.) when calibrating a peak group and / or calculating the amount of a component or peak which belongs to this group.
- **Cal. Type (Partially New!):** This column defines the calibration type (Linear, Linear with Offset, etc.) for the peak group. The corresponding edit field is only valid if the group evaluation is set to 'Calibration'. In 7.2.9 the calibration type lets you refer to the calibration of a named peak group which is marked for calibration (Group Evaluation = Calibration). In 7.2.8 this calibration type could only refer to a component. The following screenshot shows the extended capability having selected the named group 'P'.

Figure 6 - Calibration Type Dialog (7.2.9)

- **Standard Method (Partially New!):** This column defines the standard method used for calibration and amount computation. Possible values are "External" or "Internal" referring to an ISTD component. The corresponding edit field is only valid if the group evaluation is set to 'Calibration'. In the old data and evaluation mode Chromeleon always used the Standard Method value of the components that belong to the same named group. For pure timed groups this calibration parameter was not available.
- **Concentration Levels (New!):** Similar to the concentration levels for a component, you can set dedicated concentration level values for peak groups as well. For old processing methods these values are left empty. The Peak Group Table offers exactly the same concentration level columns as the component table. Having a named group, the concentration level values of a peak group and the corresponding values of the component record are not "mixed". This means that if a peak group record contains a non-empty value for the concentration level, this value alone is used for the calibration. The values of the components belonging to this peak group are ignored in this case. If the peak group record contains an empty value for the concentration value, the corresponding values of the component records are added together (this is also how the old evaluation model worked).

- **Factor:** An arbitrary multiplication factor used in the amount formula for peak groups (Formula: groupAmount).
- **Include Identified Peaks (New!):** This property is only valid for timed peak groups. Its value (Yes/No) defines whether identified peaks in the time range of the timed group should belong to this peak group or not.
- **Channel:** This property specifies whether a peak group should be valid only for a certain channel (e.g. UV_VIS_1) or all channels (All Channels) of the sequence.
- **Comment:** Free text for user comments.
- **Custom Variables:** Analogous to the component table, the Peak Group Table can be extended by custom variables.

7.4.2.2 Named Peak Groups in the Component Table

Components in the component table can only be assigned to named peak groups. The corresponding group-column in the old data model has been replaced by a dedicated column called **'Peak Group(s)'**. This column follows the same workflow as the corresponding column in the Peak Group Table:

- Only Named Groups can be selected.
- Multiple selection is possible, so a component may belong to multiple named peak groups.

Currently new named peak groups can be created only in the Peak Group Table editor. In versions of the processing method editor up to 7.2.8, named peak groups could be created by just entering the corresponding name in the group column.

There is also a new page in the processing method editor called **'Component Table and Peak Groups'** where components and peak groups can be viewed and edited on one page. The following figure shows this page for the processing method we used in Figure 3 and Figure 4.

Component Table										
Drag a column header here to group by that column. Run Component Table Wizard... Show Properties...										
#	Name	Peak Group(s)	Ret.Time	Window	Channel	Peak Type	Stand.Meth.	Cal.Type	Level "A_75"	Level "A_100"
1	Acenaphthylene	A	1.400	0.030 AG	All Channels	Autodetect	External	Use A	9.900000	13.200000
2	Fluorene		1.910	0.030 AG	All Channels	Autodetect	External	Lin, WithOffset	20.100000	26.800000
3	Phenanthrene	P	2.020	0.030 AG	All Channels	Autodetect	External	Use P	27.900000	37.200000
4	Anthracene	A	2.170	0.030 AG	All Channels	Autodetect	External	Use A	12.150000	16.200000
5	Pyrene	P	2.880	0.030 AG	All Channels	Autodetect	External	Use P	18.900000	25.200000
* Click here to add a new component										

Peak Group Table											
Drag a column header here to group by that column.											
#	Name	Start Time	End Time	Channel	Group Type	Peak Group(s)	Group Evaluation	Stand.Meth.	Cal.Type	Level "A_75"	Level "A_100"
1	UI Peak Group 1	0.800 [min]	1.500 [min]	All Channels	Timed Group	P	Calibration	External	Use P		
2	UI Peak Group 2	2.000 [min]	3.100 [min]	All Channels	Timed Group		Calibration	External	None		
3	P			All Channels	Named Group		Calibration	External	Lin, WithOffset, 1/A		
4	A			All Channels	Named Group		Calibration	External	Lin, WithOffset		
* Click here to add a new peak group											

Figure 7 - Editor Page 'Component Table and Peak Groups'

This new editor page can be selected in the Page Selector dialog of the Processing Method editor. Using this page it is possible to create a new named peak group and assign it to a component without the need to switch between pages.

Similar to peak groups, the calibration type for components now offers the capability to select a named peak group. Therefore you can choose whether a component that belongs to named peak group is calibrated and evaluated on its own, or via the corresponding group calibration. In versions up to 7.2.8 only the latter choice was possible.

7.4.2.3 New Peak Group Results in 7.2.9

7.4.2.3.1 Peak Group Report Table

In Chromeleon 7.2.9 peak group results are primarily available in a dedicated new report table called the '**Peak Group Table**' which replaces the former Unidentified Peak Group Table in versions up to 7.2.8. The new report table can list all or a filtered list of peak group records. In the corresponding report table properties dialog you can filter the resulting peak group records by channel (All Channels or a specific one) and group type (Show all groups, Show only timed groups, Show only named groups).

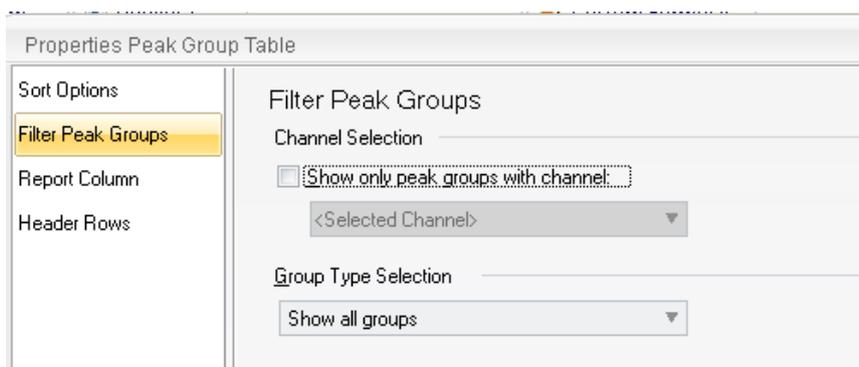


Figure 8 - Properties Peak Group Report Table

The former report table Unidentified Peak Group Table is no longer present. Old report templates containing such report tables are still valid. Old report tables are simply replaced by the new one with the filter option 'Show only timed groups'.

In the columns of this report table you can select any column of the peak group record in the processing method. A dedicated report category '**Peak Group**' allows selection of any of the corresponding properties (peakGroup.name, peakGroup.type, etc.).

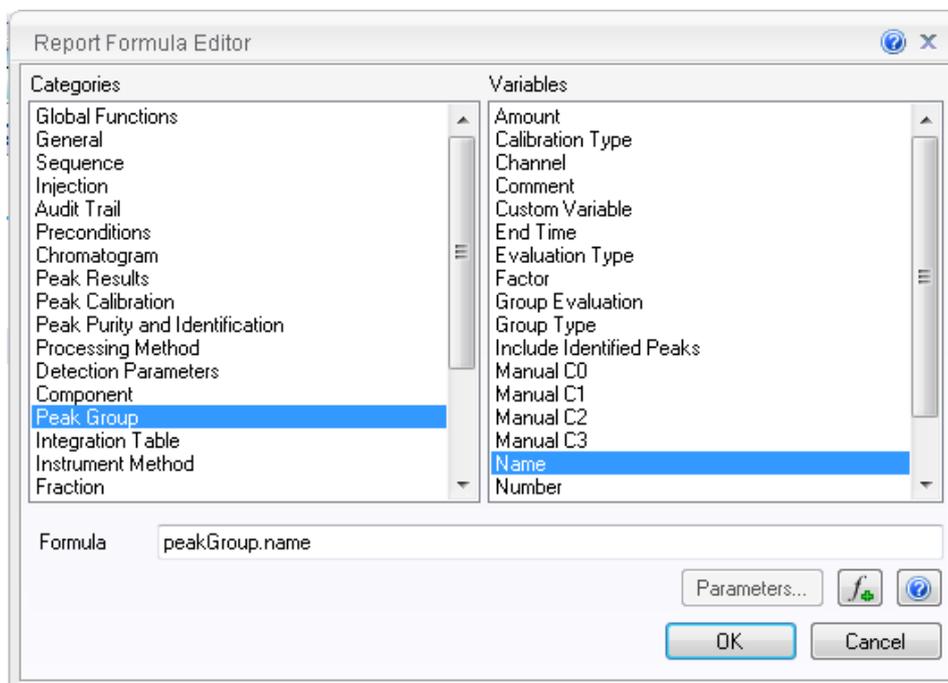


Figure 9 - Report Category 'Peak Group'

The former report category Unidentified Peak Group and the corresponding formulas (starting with UIPeakGroup) are still evaluated in a compatible way, but are no longer available in the Report Formula Editor.

7.4.2.3.2 Peak Group Results using the Peak Results / Calibration Category

The new report table can also be used to report peak group evaluation results. For this purpose the formulas of the peak report category are evaluated in a dedicated way, e.g. the formula peak.area will return the sum of all areas of all peaks in the currently selected chromatogram belonging to the peak group. **Such a group-evaluation of peak-formulas is currently only available in this new report table!** Not all peak formulas provide a reasonable value for the corresponding peak group. There is also the group evaluation property (Calibration, Reporting, None), which limits the usage of peak-formulas, e.g. for group evaluation 'None', there is no peak-formula evaluation at all. Below is a list of valid peak-formulas and their corresponding evaluations in this context, i.e. as a report column in a peak group result table:

Peak formula	Group Evaluation 'Calibration'	Group Evaluation 'Reporting'
peak.amount, peak.groupAmount	The area/height of the peak group is evaluated against the peak group calibration. The resulting value is multiplied with the Factor-value of the peak group record.	Sum of all amount values of all peaks which belong to the peak group are added together.
peak.amount_deviation	The deviation of peak.amount vs. the reference group amount	Sum of all amount_deviation values of all peaks which belong to the peak group.
peak.area, peak.groupArea	Returns the area of the peak group, i.e. the sum of all area values of all peaks which belong to the peak group.	Same as for Group-Evaluation 'Calibration'.
peak.calCoefficient et al.	Specific result of the group calibration as calCoefficient, calMode, calPointFx, etc.	n.a.
peak.concentration	The peak.amount value divided by the injection volume.	Similar to peak.amount all peak.concentration values of peaks which belong to the peak group are added together.
peak.height, peak.groupHeight	Returns the height of the peak group, i.e. the sum of all height values of all peaks which belong to the peak group.	Same as for Group-Evaluation 'Calibration'.
peak.rel_amount	Returns the relative amount where the groupAmount (see above) is the nominator of the relative value.	Returns the relative amount where the groupAmount (see above) as the nominator relative value.
peak.rel_area	Returns the relative amount where the groupArea (see above) is the nominator relative value.	Same as for Group Evaluation 'Calibration'.
peak.rel_height	Returns the relative amount where the groupHeight (see above) is the nominator relative value.	Same as for Group Evaluation 'Calibration'.

Peak formula	Group Evaluation 'Calibration'	Group Evaluation 'Reporting'
<p>For all "relative value" formulas above the reference value (denominator) depends on the corresponding parameter setting. For 'All peaks of the same group' the corresponding values (Amount, Area, and Height) of all peaks which belong to the same peak group are added together. In 7.2.9 you can also select a fixed group via 'Fixed component or group' and the corresponding group name. In this case the groupAmount of the specified group is the reference value.</p>		
peak.name	Returns the name of the peak group. Identical to peakGroup.name. This formula is also valid for Group Evaluation 'None'.	Same as for Group Evaluation 'Calibration'.
peak.group	Returns the list of all assigned named groups to the peak group. Identical to peakGroup.group. This formula is also valid for Group Evaluation 'None'.	Same as for Group Evaluation 'Calibration'.

Peak group results are also available in other report tables as Integration, Summary and Consolidated Report Tables. The following peak-formulas return group relevant results:

- **peak.name:** If an unidentified peak belongs to a timed group, peak.name returns the name of this timed group. If such a peaks belongs to multiple timed groups, the name of timed group with the smallest start time value is returned.
- **peak.group:** Returns the list of all named groups (possibly separated by list separator) where the peak belongs to.
- **peak.groupAmount:** Returns the peak.groupAmount value as described in the previous table for the peak group where the peak belongs to. If a peak belongs to more than one peak group, the group amount of the first assigned peak group (lexicographic order) is returned.
- **peak.groupArea:** Returns the peak.groupArea value as described in the previous table for the peak group where the peak belongs to. If a peak belongs to more than one peak group, the group area of the first assigned peak group (lexicographic order) is returned.
- **peak.groupHeight:** Returns the peak.groupHeight value as described in the previous table for the peak group where the peak belongs to. If a peak belongs to more than one peak group, the group height of the first assigned peak group (lexicographic order) is returned.
- **peak.rel_amount, peak.rel_area, peak.rel_height:** Similar to the "relative" peak formulas in the table above but now using the single peak amount, area or height values as the nominator. The reference value (denominator) for the option 'All peaks of the same group' comes always from the first peak group to which the peak is assigned to (lexicographic order).

www.thermofisher.com

© 2009-2019 Thermo Fisher Scientific Inc. All rights reserved.

Thermo Fisher Scientific Inc.
168 Third Avenue
Waltham, MA 02451
USA

ThermoFisher
SCIENTIFIC