

thermoscientific

Release Notes

Chromeleon 7 Chromatography Data System

Software Version 7.3.2 • April 2023

thermo scientific

Copyright and trademarks

© 2023 Thermo Fisher Scientific Inc. All rights reserved.

ACQUITY, Alliance, and Waters are trademarks of Waters Corporation.

Agilent is a trademark of Agilent Technologies.

Microsoft, Windows, Excel, .NET Framework and SQL Server are trademarks of Microsoft Corporation.

PerkinElmer and Clarus are trademarks of PerkinElmer Inc.

Shimadzu is a trademark of Shimadzu Corporation.

Kori-xr is a trademark of Markes International Ltd.

WibuKey is owned by Wibu Systems.

ReSpect[™] Deconvolution Algorithm © 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. This document is copyright protected and any reproduction of the whole or any part of this document is strictly prohibited, except with the written authorization of Thermo Fisher Scientific Inc.

The contents of this document are subject to change without notice. All technical information in this document is for reference purposes only. System configurations and specifications in this document supersede all previous information received by the purchaser.

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.

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

Table of Contents

1	Intr	oduction	.5
2	Oth	er Documentation	.6
3	Wh	at's New in Chromeleon 7.3.2	.7
	3.1	New and Updated Thermo Scientific Instrument Drivers	.7
	3.2	IQ/OQ/PQ	.8
	3.3	New and Updated Third Party Instrument Drivers	.8
	3.4	Other Instrument Related Enhancements	.9
	3.5	New Database Scheme [234582]	. 10
	3.6	Compliance and Auditing Updates	. 10
	3.7	Chromeleon Console Updates	. 14
	3.8	Chromeleon Studio Updates	. 15
	3.9	Data Processing Updates	. 18
	3.10	Chromeleon Administration Console Updates	. 20
	3.11	Working with Two Sequences Together in the Studio [192030]	. 20
	3.12	Other Client Updates	. 23
	3.13	Reporting Updates	. 23
	3.14	Reporting 2.0	. 26
	3.15	Data Import/Export Updates	.31
	3.16	Peptide Analysis Enhancements	. 33
	3.17	Non-Targeted MS Processing Enhancements	. 34
	3.18	Protein/Oligonucleotide Deconvolution Enhancements	. 36
	3.19	Discovery Service Enhancements	. 38
	3.20	Support in CM Console for large sequence transfer between Data Vaults	. 39
	3.21	MS Performance Enhancements	. 39
	3.22	Chromeleon XPS Enhancements [281641]	. 45
	3.23	Process Analyzer Auto-Export [350504]	. 47
	3.24	Local Data Vaults based on SQL Server Express 2022	. 47
4	Res	olved Issues	. 48
5	Lim	itations and Known Issues	. 57
	5.1	Limitations with Thermo Scientific Instruments	. 57
	5.2	Limitations with Waters Instruments	. 64
	5.3	Limitations with Agilent ICF	. 64
	5.4	Limitations with Agilent Drivers for Chromeleon	. 67
	5.5	Limitations with Other Third-Party Instruments	. 68
	5.6	Limitations With Setup	. 70
	5.7	Other Limitations	.72
	5.8	Obsolete Instrument Drivers	. 79
6	Bac	kward/Forward Compatibility Issues	. 80

	6.1	Thermo Scientific Vanquish Charged Aerosol Detector [CM6-23499]	80
	6.2	Thermo Scientific Vanquish Autosampler [CM6-23405]	80
	6.3	Thermo Scientific TriPlus RSH	80
	6.4	Thermo Scientific TriPlus 300 HS	80
	6.5	Thermo Scientific TriPlus LS-100	80
	6.6	TSQ Quantiva and Endura Instrument Method [CM7-18759]	80
	6.7 Dom	Chromeleon Enterprise Compatibility of different versions of Chromeleon install nain Controller, Clients and Instrument Controllers	led on 80
7	Арр	pendix	82
	7.1	Release Notes	82
	7.2	Online Help	82
	7.3	Contributed Content	82

1 Introduction

Chromeleon[™] 7.3.2 is the latest version of the Thermo Scientific[™] Chromatography Data System (CDS). Chromeleon delivers superior compliance tools, networking capabilities, instrument control, automation, data processing, and much more, providing 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 features a modern user interface, comprehensive 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 release provides updated and new instrument control for instruments from Thermo Fisher Scientific and third-party manufacturers. Improvements and enhancements have been made in several areas including ease of use, compliance, data reporting, and peptide analysis. Please see below for more details on these and other enhancements in this release.

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 in the Documents folder of the installation kit.

Please refer to the Chromeleon 7.3.2 installation media for information regarding:

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

For Enterprise Chromeleon systems, a full set of Enterprise Documents are available. These describe the process for installation of enterprise systems based on Chromeleon 7.3.2.

3 What's New in Chromeleon 7.3.2

In addition to new and updated control for both Thermo Scientific and third-party instruments, Chromeleon 7.3.2 implements a number of new features and enhancements to existing features, including new granular privileges, , dual sequence/injection workflow, 64-bit reporting engine, redesigned client/server for faster data processing, usability enhancements and improved BioPharma workflows This document can only give a short overview of all features. 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 7.3.2. 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 7.3.2 installation kit.

Thermo Scientific Vanquish Autosampler – Automatic rack recognition [231935]

This release provides support for a custom bar code for tray identification for the Thermo Scientific Vanquish Autosampler. This feature provides a tighter connection between the sequence and the tray, thereby preventing errors caused by the user accidentally placing the tray into the wrong tray holder. Custom variables specify a unique bar code for each tray and a relative inject position on the tray. The automatic rack recognition automatically identifies the segment on which the rack is located and adapts the injection position accordingly.

Note: The Vanquish Charger (VH-A90-A) is not supported.

Thermo Scientific Vanquish Integral Fraction Collector FT [238643]

This release introduces support for the Vanquish Integral Fraction Collector FT (VF-F20-A).

Please note that the driver for the Vanquish Integral Fraction Collector FT is not included in the Chromeleon 7.3.2 installation media and needs to be downloaded and installed separately. Support for the Vanquish Integral Fraction Collector FT (VF-F20-A) under Chromeleon 7.3.2 requires Vanquish Fraction Collector Driver Package V1.4, which can be downloaded at the Digital Science Support Resource Center (<u>https://support.thermoinformatics.com/downloads/</u>) under Chromeleon > Related Drivers.

Thermo Scientific EXTREVA ASE [370263]

This release introduces support for the EXTREVA ASE Accelerated Solvent Extractor.

Thermo Scientific Vanquish Flex – Diagnostics [269627]

This release introduces an additional diagnostic test (Intensity Test) for the Vanquish Diode Array Detector FG and additional diagnostic tests (Intensity Test, Shutter Motor Test and Grating Motor Test) for the Vanquish Variable Wavelength Detector F. A firmware update may be required to make use of this new functionality.

This release introduces an additional diagnostic test (Basic Tightness Test) for the Vanquish Flex Pumps in combination with selected Vanquish Flex Split Samplers. A firmware update for both modules may be required to make use of this new functionality.

ISQ EC/EM driver removed from installation package

As part of our strategy to improve support for instrument releases and support within enterprise environments we have decided to remove the ISQ EC/EM driver from the installation package. This will help remove the burden for customers to upgrade their base Chromeleon version whenever new instruments are released, it will also enable us to decouple the defect fixing and development effort. As a replacement for the drivers which are removed, we now provide a driver which consolidates several Thermo Fisher Scientific single quadrupole and triple quadrupole mass spectrometers in one, native, Chromeleon specific driver. For more details, please contact your local representative.

3.2 IQ/OQ/PQ

HPLC Instruments IQ

New HPLC Instruments IQ tools are available in Chromeleon CDS. HPLC Instruments IQ version 5.7 adds support for the Vanquish Fraction Collector (VF-F20-A) and addresses an issue with the ISQ detector: Support of new model number "ISQ ICMS Family". For details, please refer to the document \Documents\HPLC Instruments IQ V.5.7 - Release Notes.pdf on the Chromeleon CDS disk.

HPLC Instruments OQ/PQ

New HPLC OQ/PQ tools are available in Chromeleon CDS. HPLC OQ/PQ version 9.9 addresses an issue with the ISQ detector: Support of new model number "ISQ ICMS Family". For details, please refer to the document \Documents\HPLC OQ PQ V.9.9 - Release Notes.pdf on the Chromeleon CDS disk.

3.3 New and Updated Third Party Instrument Drivers

Waters Driver Pack removed from the Chromeleon Installation Package [272090]

Responsibility for the drivers to control Waters Chromatography Systems in Chromeleon has been transferred from Thermo Fisher to Waters. Please contact your local Waters representative to obtain Waters Driver Packs and corresponding Waters Support Layers as well as licenses to control Waters Chromatography Systems in Chromeleon.

When upgrading to Chromeleon 7.3.2 there are several possible scenarios:

- If the earlier Chromeleon version had the optional Waters Driver Pack installed, upgrading to Chromeleon 7.3.2 removes the Waters Driver Pack. The drivers for the Waters 2487 Detector, 2690/2695 Separations Module, 996/2996 PDA Detector, and 474 Fluorescence Detector are still part of the installation after the upgrade.
- If the earlier Chromeleon version had the Waters Driver Pack manually installed, the upgrade to Chromeleon 7.3.2 will not keep the installed Waters Driver Pack intact. The upgrade will trigger an uninstallation of the previous Chromeleon version. The final state after this uninstallation depends on the existence of the Waters Driver Pack:
 - If the Waters Driver Pack can be accessed via System Package Cache or directly from the DVD image, it will use the uninstaller of the Waters Driver Pack to remove the Waters Driver Pack entirely.

 Otherwise, the Chromeleon Setup will report an error that it cannot uninstall an optional component. This will require a manual repair of the existing Waters Driver Pack installation.

The drivers for the Waters 2487 Detector, 2690/2695 Separations Module, 996/2996 PDA Detector, and 474 Fluorescence Detector are still part of the installation after the upgrade.

The upgrade in this scenario for Waters Driver Pack 2019 R1 as well as a guide to re-installing the corresponding Waters Support Layer is available as a separate document. Please request this document from your local Thermo Scientific representative.

• If the earlier Chromeleon version did not have Waters Driver Pack installed, the drivers for the Waters 2487 Detector, 2690/2695 Separations Module, 996/2996 PDA Detector, and 474 Fluorescence Detector are still part of the installation after the upgrade.

Waters Driver Pack 2019 R1 and the corresponding Waters Support Layer are supported with Chromeleon 7.3.2.

A guide to help install the appropriate Waters Support Layer alongside Waters Driver Pack DP 2019 R1 is available as a separate document. Please request this document from your local Thermo Scientific representative.

Note: Responsibility for maintenance of the Waters Driver Pack 2019 R1 and Waters Support Layer has transferred to Waters.

Silicon Labs CP210x USB to UART Bridge Virtual COM Port – New Driver

This release introduces support for the Silicon Labs CP210x USB to UART Bridge Virtual COM Port (VCP) driver, which allows for use of CP210x adapter products to facilitate USB to serial port connections. This driver can be installed from the Advanced Options page of the Chromeleon installer.

Shimadzu LC Driver / GC Driver – Updated Driver

Shimadzu LC Driver (Version 3.20) for Chromeleon 7 are available on DVD under folder "Drivers\Shimadzu Driver Pack\DeploymentManager\ShimadzuLC".

Release Notes, Quick Start Guide and ReadMe files are located "Drivers\Shimadzu Driver Pack\DeploymentManager\ShimadzuLC\Documents\ENG\"

Shimadzu GC Driver (Version 2.30) for Chromeleon 7 are available on DVD under folder "Drivers\Shimadzu Driver Pack\DeploymentManager\ShimadzuGC"

Release Notes, Quick Start Guide, LAN Adapter Installation Manual and ReadMe files are located "Drivers\Shimadzu Driver Pack\DeploymentManager\ShimadzuGC\Documents\ENG\"

Agilent LC/Agilent GC – Updated Driver

This release includes an updated driver, provided by Agilent Technologies, for control of Agilent LC and GC instruments (ADC 2.5). More details are available in the Resolved Issues section, and in the release notes document provided in the \packages\Agilent Chromeleon Drivers\Documentation folder on the Chromeleon CDS disk.

3.4 Other Instrument Related Enhancements

Support for Virtual Channels for peak-based Fraction Collection [229709]

HPLC Fraction collection: A Virtual Channel can now be used as an input to peak-based fraction collection.

3.5 New Database Scheme [234582]

Chromeleon 7.3.2 comes with a new database scheme 7.3.2.106 for datavaults which improves the performance when using custom variables, especially when executing injection queries in large multiuser datavaults and having query conditions for such sequence or injection custom variables. The database scheme also implies an improved serialization framework when saving or loading processing methods with lots of components.

Database Scheme Update

When a new Chromeleon version is installed local data vaults are automatically upgraded to the newest database scheme. For Chromeleon 7.3.2 this is only "partially" applied. Installing Chromeleon 7.3.2 Local data vaults are automatically upgraded to database scheme 7.3.2.9. In order to use the database scheme with the improved performance you need to use the Chromeleon Data vault Manager. After clicking on the <Upgrade scheme> button a dialog appears where you must confirm the upgrade to the newest database scheme 7.3.2.106. The latter is not compatible with prior releases anymore. Chromeleon clients from prior releases as 7.3.1 or earlier cannot connect to such data vaults.

For multi-user data vaults the upgrade to database scheme 7.3.2.106 might take quite some time, even multiple hours. During this time a dedicated dialog shows the progress of the upgrade. Any update in the data vault from a Chromeleon client during such a database scheme upgrade might either fail or could stop the upgrade. It is strongly recommended to disconnect any Chromeleon client or IPC from the data vault during the scheme upgrade to avoid such complications.

3.6 Compliance and Auditing Updates

Sequence Acquisition Approval [28121]

This release includes an option to require that users receive approval before submitting a sequence for acquisition. This provides the opportunity for a second person to review a sequence for completeness and accuracy, reducing the possibility of wasting valuable time and samples.

3.6.1.1 New user privileges

This release introduces several new privileges related to approving sequences for acquisition:

Acquire Sequences Without Approval

This privilege is granted by default to all existing Roles. Users without this privilege must submit their sequences for review before they may be run.

∠ Sequences	
 Create Sequence via Wizard 	Create new sequences using the wizard.
 Create Sequence via eWorkflows 	Create new sequences using eWorkflows.
 Create Sequence via Save As 	Create new sequences using Save As.
 Create Sequence via Save As with Raw Data 	Create new sequences using Save As, including Raw Data.
 Create Sequence from Injection Query Results 	Create sequence from injection query results.
 Create Sequence from Worklist 	Create new sequences by importing LIMS worklists.
Create Sequence	Create sequences by another method, e.g. running a Station Qualification or storing Monitor Baseline data.
Modify Sequence	Modify existing sequences (but not rename them).
Modify Running Sequence	Modify sequences while they are running.
Rename Sequence	Rename existing sequences.
Rename Sequence with Raw Data	Rename existing sequences that contain raw data.
Copy Sequence	Copy sequences.
Move Sequence	Move sequences.
Delete Sequence	Delete or overwrite sequences, including the respective raw data, audit trails and associated items.
Delete Read-Only Sequence	Delete Read-Only sequences.
Make Sequence Read-Only	Make sequences Read-Only.
Remove Sequence Read-Only	Remove sequences Read-Only.
 Manage Sequence Variables 	Change the column assignment in the sequence and/or define sequence report columns or add new ones (al
 Modify when Visible Views Are Updated 	Modify the sequence Update Visible Views property to Automatically or On-demand.
Manual Upload	Upload the sequence manually.
 Modify Sequence Auto Reporting Settings 	Modify the Auto Reporting settings of the sequence properties.
Acquire Sequences Without Approval	Allows the user to acquire sequences without requiring approval.

Approve Sequences for Acquisition

Users with this privilege can approve a pending sequence for acquisition.

Remove Sequence Approval for Acquisition

Users with this privilege can revoke approval for a pending sequence.

 Electronic Signature 	
 Sign as Submitter 	Submit results.
 Sign as Reviewer 	Review results.
Sign as Approver	Approve results.
 Remove Signature when Submitted 	Remove electronic signature of submitted results.
Remove Signature when Reviewed	Remove electronic signature of reviewed results.
 Remove Signature when Approved 	Remove electronic signature of approved results.
 Modify Signature Requirements 	Modify the signature requirements of sequences.
 Approve Sequences for Acquisition 	Approve sequences for acquisition.
 Remove Sequence Approval for Acquisition 	Remove sequence approval for acquisition.

3.6.1.2 Requiring a Separate Approver

A new option is available to require that the sequence submitter and the sequence approver be different. This option is found in the User Database Policies of the Admin Console (User Database > User Database Policies > Electronic Signature)

Electronic Signature			
Sequence Acquisition Approval			
Submitter and Approver must be different			

3.6.1.3 Sequence Creation and Modification

When a user lacking the "Acquire Sequences Without Approval" privilege creates or edits a sequence, then when it is saved, instead of the Start/Resume button, a "Request Acquisition Approval" button will appear above the sequence table.

							Sequence 'BY(
	New	Request	Acquisition Approv	al 🔻			
	Save 🧿 Studio	🛃 Print 🕞 📩 U	p 🛛 🔤 Insert Rov	v 👻 💵 Fill Down	🔒 Lock 🛛 🍸 Filterin	g 冒 Grouping 📋	f_{χ} Custom Columns
#	Chromatogram 🕨	Name	Туре	Position	Volume	Instrument Method	Processing Method
1	None	Sample	Unknown	RA1	1.000	U3000 - 0.5 min	3D Quantitative
2	None	🔋 Sample	Unknown	RA2	1.000	U3000 - 0.5 min	3D Quantitative
3	None	🛜 Sample	Unknown	RA3	1.000	U3000 - 0.5 min	3D Quantitative
4	None	🔋 Sample	Unknown	RA4	1.000	U3000 - 0.5 min	3D Quantitative
5	None	🔋 Sample	Unknown	RA5	1.000	U3000 - 0.5 min	3D Quantitative
6	None	🔋 Sample	Unknown	RA6	1.000	U3000 - 0.5 min	3D Quantitative
							Click here

3.6.1.4 Approving Sequences for Acquisition

When a user with the "Approve Sequences for Acquisition" privilege clicks the "Request Acquisition Approval" button, they will be prompted to enter their eSignature username and password. If authenticated, then the Start/Resume button will appear above the sequence table, and the sequence may be acquired as normally done.

Once a sequence has been approved for acquisition, if a user lacking the "Acquire Sequences Without Approval" privilege edits the sequence in any way, then it will revert to its "Request Acquisition Approval" state.

Users lacking the "Acquire Sequences Without Approval" privilege are not able to edit a sequence that is running of is in the run queue.

Granular Processing Method Privileges [90548]

With this release support has been added to restrict editing of specific portions of the processing method.

The support is implemented by means of a **<u>Ruleset</u>**, which is defined in the User Database section of the Admin Console.

Ruleset Name:		
Limited Component Table Columns	The ruleset name must have 1 t	o 32 characters
Ruleset Description:		angle quotea.
Editing limited to a few MS Component Table co	lumns	
Privileges:		
Privilege	Privilege Description	
Managed Custom Variables:	List custom variables here sepa	rated by commas
Detection Threshold, MaximumCV	e.g. cv1,cv2,cv3	,
Chromatogram Subtraction		
Composite Scoring		
General and Advanced Settings		
MC Cattions		
Peak and Component Tables		
Add/Pamous Components	Add or romovo rowo of the posk and composed to	blog
Name	Modify the name	DICS.
	Modify the retention time	
Mindow.	Modify the neak window	
	Modify the channel	
Peak Type	Modify the neak type	
Comment	Modify the comment	
Charge	Modify the charge	
Left/Right Limit	Modify the left/right limit	
Eactor	Modify the factor	
Ret Index	Modify the retention index	
Reference UV Spectrum Settings	Modify reference UV spectrum settings	
	Modify the concentration unit	
Prev. Retention	Modify the previous retention.	
Mol. Mass	Modify the molecular mass.	
CAS	Modify the CAS.	
Chem. Formula	Modify the chemical formula.	
Extracted Ion Chromatograms	Modify the extracted ion chromatograms.	
Peptide Group	Modify the peptide group.	
Reference MS Spectrum Settings	Modify reference MS spectrum settings.	
RTS Ratio Tolerance	Modify the RTS ratio tolerance.	
Modify Managed Custom Variables	Modify the custom variables named in the managed	list (above).
Modify All Custom Variables	Modify all custom variables.	
Peak Groups		
Peak Tracking		
D QD Calibration		
▷ SST/IRC		
UV Settings		
D UV Spectral Library Screening		

The ruleset is then applied to a role using a new privilege:



CSV Export for Data and Instrument Audit Trails [116800]

This release adds two new commands to export the Data and Instruments Audit Trails to a CSV File. The new commands are available in the Data category of the Chromeleon Console. After selecting the data vault root or any folder in a data vault the context menu in the tree view area offers the two new commands 'CSV Export Data Audit Trail ...' and 'CSV Export Instrument Audit Trails...'. A dedicated new privilege 'CSV Export Audit Trail' provided in the 'Reporting' category controls which users can execute these export commands.

Note: This CSV Export capability has been already present in Chromeleon 7.2.10 MUa and later 7.2.10 MU-releases, but not in 7.3 or 7.3.1. For details about this new feature see the release notes document for 7.2.10 MUa.

3.7 Chromeleon Console Updates

Displaying helper tooltips in sequence tables

By default, there is a tooltip displayed over cells of the sequence table in Chromeleon Console and Studio depending on the position of the mouse cursor. As more experienced users are familiar with sequence tables, a new configurable option was introduced allowing them to turn off displaying of these helper tooltips.

This option can be configured via Chromeleon Console's main menu: Tools->Preferences...

Import of Chromeleon data and Bulk import via the context menu

Context menu of the Navigation pane of the Data category was updated to include a possibility for user to perform import of Chromeleon data from an external location and bulk import.

Till now user could perform these actions only via the Menu Bar and the menu option: File.

Command line parameter allowing opening of instrument's ePanel upon launch of Console

A new command line parameter was introduced to Chromeleon Console executable (Chromeleon.exe) that allows automatic opening of ePanel of specific instrument upon launch of Chromeleon Console.

Example: Chromeleon.exe cm-instrument://localhost/TestInstrument/

Injection Query Enhancements [179597]

With this release, it is now possible to query for injection based on comments in the instrument method. The option is contained within the Computed Criteria section of the injection query definition.

3.8 Chromeleon Studio Updates

Ribbon customization of Data Processing category

Users having "Modify View Settings" privilege can from now on customize their ribbons within the Data Processing category and all its contexts using the Ribbon Editor.

Ribbon Editor can be launched from the context menu of the Chromeleon Studio ribbon.

Ribbon customization is stored within the currently selected View Settings of the sequence, so user may define have different ribbons for different View Settings.

User may also import ribbon customization from other View Settings and reset the ribbon in case user needs to revert ribbon to the factory settings state.

Category Bar items

There was a change implemented in the displaying of Category Bar items in Chromeleon Studio so that only those items are shown which are relevant and which logged in user's license and UI settings permit:

- Non-Targeted MS Processing if the sequence being worked on doesn't contain any MS data, Non-Targeted MS Processing category bar item isn't shown.
- Intact Protein Deconvolution if the sequence being worked on doesn't contain any MS data, Intact Protein Deconvolution category bar item isn't shown.
- **UV Spectral Library** if the sequence being worked on doesn't contain any 3D UV data or Spectral Library associated items, UV Spectral Library category bar item isn't shown.

In case of empty sequences or sequences containing idle injections only, all these Category Bar items are displayed.

Improved Navigation Pane Grouping and Filtering [192030]

With this release, it is now possible to group injections by type. The grouping option is available in both the Data Processing and the Report Designer categories.

ata Processing	•
Injections	Filter Y
▲ Blank - 2 Ungr	oup
27 🗂 blank 🖌 Grou	p by Injection Type
31 🗂 solvent_blank	C)-
Calibration Standard - 5	
1 🟅 level1	C)-
2 📱 level2	C)-
3 🖉 level3	C)-
4 📱 level4	C3-
5 📱 level5	C]-
Check Standard - 1	
26 🛐 chk_std_50	C}-
Unknown - 23	
6 🛐 mv 1	C)-
7 🔋 mv 2	C)-
8 🛐 mv 3	C)-
9 🛐 mv 4	C3-
10 🛐 mv 5	C]-
11 🔂 mdl 1	r1-

It is also now possible to filter both the injections and components by any desired criteria:

Data Processing	**	Conditions
Injections	Filter	Include Injection Types
4 Unknown - 23	Edit	
6 🛐 mv 1	Clear Cl-	Check Sandard Soled
7 👸 mv 2	c3-	
8 🛐 mv 3	c3-	
9 👸 mv 4	C3-	Custom Conditions
10 👸 mv 5	c3-	Also include injections that match the following conditions:
11 👸 mdl 1	C)-	Match ALL v of the following sules:
12 🛐 mdl 2	c3-	
13 👸 mdl 3	C3-	Comment v - v v +
14 🛐 mdl 4	c3-	and
15 🛐 mdl 5	c3-	
16 👸 mdl 6	⇔	OK Orosel
17 🛐 mdl 7	C3-	UN Carce
18 👸 mdl 8	C3-	
10 5 mdl 0	m .	

Overriding Automatic Confirmation of Component Identification [23580]

The Composite Scoring parameters in the processing method are used to automatically confirm the identified status of a component. With this release, it is now possible to override that automatic confirmation.

3.8.1.1 New user privilege

The ability to override the automatic confirmation status of component identification is controlled by a new user privilege:

⊿ 🗹 Manual Data Processing	
✓ Modify Peaks	Manually modify the peak integration and identification.
 Delete Peak Modifications 	Delete manual peak integration and identification.
 Edit Injection Specific XIC Detection Settings 	Use and edit XIC detection settings specific to a particular injection.
Manually Assign Confirmation Status	Manually assign the Composite Scoring status of a component.

3.8.1.2 New Privileged Action

A new privileged action may be associated with overriding the automatic confirmation status of component identification.

3.8.1.3 Context menu

Users with the appropriate privilege can right-click on a component and change the identification state of the component.

▲ Components 🗮 👻 🗞	Filter Y	
🔛 Nonanal	c1−	
🔛 Decanoic acid, methyl e	ster 🛛 🖓	
🔏 Undecanoic acid, meth	Open	Enter
🆋 Dodecanoic acid, methy	Overlay	Space
🚼 Benzenamine, 2,6-dime	Manually Confirm	n Identification
M Phenol, 2,5-dimethyl-	Manually Overrid	e Confirmation

3.8.1.4 Report Variables

Two new report variables

peptide.IsCompScoreManuallyAssigned and **peak.compScoring.IsCompScoreManuallyAssig ned** are now available to report if the identification status of a component was manually assigned.

Peak/Component Navigation

The Peak Mode Menu within the 'Data Processing Home>Navigation' ribbon in Chromeleon Studio has been enhanced to allow switching between the Peak and Component navigation.

When the 'MS Quantitation' channel is selected, the Peak Mode navigation in the ribbon is automatically switched to the component one.

New shortcuts (F6 and Shift-F6) have been introduced to allow switching between the Previous and Next Peaks/Components.

Improved Named Peak Group Selection

Named Peak Group selections and deselections within the Navigation Pane have been improved. A user is now able to achieve more precise selection/deselection of individual Named Peak Groups by using the left mouse button click and the CTRL key or their combination.

Overlay of manual modified chromatograms with the automatic integration [185883]

The chromatogram plot for 2D-signal offers a new option to overlay a manually integrated chromatogram with the corresponding chromatogram being automatically integrated with the current processing method parameters. The new option can be found on the page 'Comparison', section 'Overlay', in the Chromatogram Plot Properties dialog.

Overlay	
Overlay with peak characterization	
Overlay with right signal axis	
Mirror last overlaid chromatogram	
Overlay with automatically integrated chromatogram	

Optional Comment for Manually Integrated Peaks [185887]

If a peak in a chromatogram is affected by a manual integration you can now enter a comment for just this peak. The comment can be entered in various ways:

- The context menu of a selected peak in the chromatogram plot offers a new command 'Manually Integrated Peak Comment ...' which opens a dedicated dialog to enter the comment.
- The property page 'Manual Peak Identification' of the Chromatogram Plot Properties is extended with a new input field labeled '**Manually Integrated Peak Comment'**. The same input field is also offered in the page 'Peak' of the Peak Properties Pane.

The comment for all peaks is stored together with the manually integrated chromatogram. With the new report variable 'Manipulated Comment', formula **peak.manipComment**, the comment can be put into corresponding report tables.

If the sequence contains a customer variable named **CM7:Peak_Comments** of type list the input field to enter the comment will offer all possible values of the customer variable in a dedicated combobox.

Show Formulas Option for Read-Only Sequences [88921]

The option 'Show Formulas' in the Home Ribbon of the Report Designer category is now enabled also for read-only Sequences. Currently this option has been disabled in this case.

NIST MS Search Version Update [28071]

With this release, MS library search has been updated to use the 2014 version NIST search tools. The installer for the standalone AMDIS and MS Search utilities on the distribution media has also been updated to this version. Note that, although NIST 2014 release offers additional search and filtering options as compared to NIST 2008, the additional options are not yet available in the Studio UI.

3.9 Data Processing Updates

Delete All Selected Peaks in One Step [298819]

The chromatogram plot pane in the Data Processing category of the Chromeleon Studio window allows to select multiple peaks pressing the **<Ctrl>-key** when clicking into the peak(s) with the left mouse button. Having selected multiple peaks, the **-key** or using the **Delete Peak / Delete Peaks** command in the Processing Ribbon will now delete all selected peaks in one step.

The **Delete All Peaks** command in the Processing Ribbon is still deleting all peaks of the currently selected chromatogram.

3.9.1.1 Extended use case for MS Component Plot Pane [218307]

The MS Component Plot Pane for XIC (Extracted Ion Chromatogram)-Based Chromatograms has been extended to support multiple selection of component tiles if the SmartLink option is enabled. This can be done by clicking in the tile of a component and holding the <Ctrl>-key at the same time. The background color of such component tiles is colored to a darker blue (see screenshot below).



In the Processing Ribbon the Delete Peak(s) command is labeled as **Delete Component Peak(s)** and will delete all Component Peaks, i.e., peaks which are currently assigned to the selected component, in the selected XIC (Quantitation, Confirmation 1, etc...) for all selected components. The **Delete All Peaks** deletes all detected peaks in the selected XIC for all selected components.

If multiple injections are selected or pinned in the navigation area of the studio window there is also the capability to select all tiles of all components for one injection or all tiles of one component for all injections by selecting the corresponding tile row or column header.



New Cobra Detection Parameter to control threshold of 2nd derivate [107812]

Cobra is using the 2nd derivate of the raw data signal automatically applying a threshold whether a signal portion could be regarded as a peak or not. This threshold is mainly based on the automatic noise detection and the smoothing width which is either fixed or also automatic.

With Chromeleon7.3.2 this 2nd derivative threshold can be modified by multiplying it with a userdefinable factor. The corresponding Cobra detection parameter is called '**Curvature Sensitivity Factor'**. When the factor value is smaller than 1, the Cobra algorithm will tend to detect more peaks; a value greater than 1 will detect fewer peaks.

Note: The new Cobra detection parameter is only available if the newest version of the Cobra algorithm is applied for the processing method. Already existing processing methods doesn't offer this new detection parameter initially.

3.10 Chromeleon Administration Console Updates

Displaying status of connection to Chromeleon domain controller

In Chromeleon Administration Console, the connection status to Chromeleon domain controller is now indicated on each screen as icon displayed in the bottom right corner of the status bar.

3.11 Working with Two Sequences Together in the Studio [192030]

The release introduces support for working with two related sequences in a single Chromatography Studio session. This functionality facilitates cross sequence analysis of samples run using multiple techniques (e.g., LCMS and GCMS)

Linking Sequences

To enable two sequences to be loaded together in a single Studio session, they must be explicitly linked. Linking is defined on the General tab of the sequence properties:

quence l	Properties						
General	Features	Locks	Signature	Auto Reporting	Notifications	Raw Data Statis	tics
Name	: G(CMS - Or	ganic Honey				
Locat	ion: ch	rom://tf-	9997648450	91/ChromeleonLo	cal/zSandbox/	Pesticides/LCMS-	GCMS/GCM
Acc	ess Informa	ation:					
	Created:		6/4/2020 3	:39:43 PM +02:00	benedicte.gaur	iat	
	Last update	e:	12/6/2022	12:53:39 PM -05:0	00 Frank		
	Version:		12/6/2022	12:53:39 PM -05:0	0 Frank	N	o. 8
Comr	nent:						
Instru	ment:	<dei< td=""><td>MO></td><td></td><td></td><td></td><td></td></dei<>	MO>				
Defa	ault Report	Template	e & Channel:				
1	Report Tem	plate:					· · · · ·
1	/iew Setting	js:					· · · · ·
(Channel:	I	MS Quantitati	ion			•
F	Read-Only						
						ОК	Cancel

When an eWorkflow with linked instruments is executed, the resulting two sequences will be automatically linked.

Working with Linked Sequences in the Studio

When linked sequences are opened in the Studio, several functional enhancements become available.

Chromeleon 7

Data Processing		Clonyrali	d	1	Clopyralid Eq:y	=0.0 x ² 186 x + 2206 F	R ² =0.9011	Apex Clopyralid Scan: #	1997 RT: 3.17 min NL: 1	.92E
	1.0e5	counts		14	counts*min		120]	%	~	
Sequences				12		\mathbf{O}	100	112.00 - 70.00	(4)	
A 📅 GCMS - Organic Renev 🛛 🖊	7.5e4	·	4	10	000 -	•	75	112 00 > 76 00		
B 📅 LCMS - Organic Honey 🛛 🕪		R	=3.17		1	_ /	Pa (* 1	112.00 - 10.00		
🔺 Injecti 📴 🎁 🕶 Filter 🍸	5.0e4			Clopyn	500		50 DO	112.00 576.00	148.90 -> 114.	.00
Blank - 3	≤ 2.5e4			₹ 5	••••		25			
Calibration Standard - 21			-	2	500		0			
Unknown - 22	0.0e0		min	v						m/z
M Organic_Honey_BIPEA C-	-1.084	2.64 3.00	3.50 3	64	0.0 20.0	40.0	60.0 60	.0 75.0	100.0	130
200 5746 αl−		Clopyralic	đ	60	Clopyralid Eq	y=0.0 x ² 0 x + 2 F	R ² =0.4321	Apex Clopyralid Scan: #	730 RT: 4.24 min NL: 3.9	90E
28 (3) ^{Ω−}	4.0e2 ·	counts	1.24	4	counts*min			% 191.90 -> 145.90		
1535/5A C-			1	5.0	io 🗍		100 -	101.00 - 140.00		
286 Clasuralid Ch	3.0e2 ·				1	+	75-			
B1 MIEL BLANC CH	- Pie			3.7	75 -		38			
B7 T MIEL BLANC C1-	_ a 2.0e2 ·		200	opyr			in 50-	Juar		
B9 7 Ech Bipea 0.5 uL CI-	801		\sim	C 2.6	50 -			Ĩ	189.84 -> 145.9	96
A19 7 Organic Honey	1.0e2 ·				+		25-			
A20 7 BIPEA DIL2 CI-	1.002		$\sim \sim$	1.2	25 -		6			
A22 🖥 5746 DIL2 💦 🛛	A		- ~ min		1					m/z
A24 👸 6228 DIL2 💙 🖓	0.0e0	950 4250	45	50 0.0	00 200	40.0	60.0 145	880 145 900	145 950	145.98
A26 🛐 153575A DIL2 ଘ⊢						a				
A28 🖥 6145 DIL2 ಬಿ-	.원 Dete	ection MS Detection MS Co	omponent Table	Calibration	MS Settings MS Library	Screening Composite Sc	oring			
A30 🔁 Clopyralid DIL2 🛛 🖓 –	e C	omponent Table								0
▷ Channels 🔤 🕶 Filter 🍸		Group Area Drag a	column header h	ere to group t	by that column. Run (Component Table Wizard.	Show Propertie	s		
A Comp 🗮 🗙 🗙 🔻 Filter 🍸	Ö 📕	Name	Ret.Time +	Window	MS Quantitation Peak	MS Confirming Peak 1	MS Confirming Peak 2	MS Confirming Peak 3	MS Confirming Peak 4	4 [≜
		Copyralid	3.140	0.200 AN	146.90 / 76.00	112.00 / 76.00	148.90 / 114.00	148.90 / 76.00		0.1
	ents	2 4-DMA	3.840	0.200 AN	120.00 / 79.80	121.10 / 119.90	120.00 / 76.90	120.00 / 119.20		0.! =
	8 3	DEET	5.770	0.100 AN	190.10 / 115.00	190.10 / 145.00	191.10 / 190.10	191.10/91.00		0.1
	8 4	Dimethoate	6.330	0.200 AN	124.90 / 46.30	93.00 / 63.00	87.00 / 42.10	93.00 / 62.20	87.00 / 45.90	0.!
	5	Chlorpyriphos-methyl	6.890	0.200 AN	285.84 / 93.00	124.90 / 47.00	287.90 / 209.90	285.90 / 270.80		0.!
M Data Processing	6	Chlorpyriphos_GC_Quan	7.210	0.200 AN	198.90 / 171.10	315.90 / 259.70	196.90 / 107.00	198.90 / 108.30	313.90 / 257.10	0.!
Data Hocessing	7	Imidacloprid	7.330	0.200 AN	210.90 / 181.90	210.90 / 139.50	212.90 / 183.20			0.!
Report Designer	8	Thiamethoxam	7.330	0.200 AN	212.00 / 139.00	182.00 / 148.80	247.00 / 181.10	212.00 / 125.10		0.1
										the second se

1. Sequence Selector

Use the pins in the new Sequences section of the Navigation Pane to toggle the display of either or both sequences.

2. Annotation Indicating Source Sequence

Injection numbers are prefixed with a letter indicating the source sequence.

3. Automatic Linking of Injections and Components

When injections or components have the same name, they are considered the same and are linked.

The sequence/injection annotation for linked injections is hidden but is visible in a popup when hovering over the injection.

In the same way, the sequence annotation for linked components is hidden but is visible in a popup when hovering over the component.

4. Split Panes When Viewing Linked Components

When a linked component is selected in the Navigation Pane, the following panes will be split in the Studio work area:

- MS Components
- Calibration
- MS Spectrum
- Processing Method

A label in the left margin of the pane indicates the source sequence.

Extensions to Report Variables

To support report generation with linked sequences, a new report variable qualifier seq.LinkedSequence() is now available. The variable supports a parameter which species the source

sequence for the data. For example, seq.LinkedSequence("A").name returns the name of the selected injection in sequence A.

Extensions to Report Tables

To support report generation with linked sequences, several report tables now have an additional tab called "Linked Sequence" on their properties dialog. The sequence selection on this tab determines the top-level source for records in the object. (For example, the list of injections in a summary table). Unless the "seq.LinkedSequence()" qualifier (see previous section) is used, the sequence selection on this tab also implicitly applies to any column definitions or other report variable-based values in the table.

Note that this additional tab is only visible when a linked sequence is open in the Studio session.

The following report tables now support the using data from either or both sequences:

- Peak Summary Table (applies to injections)
- Integration Table (applies to components)
- Consolidated Table (applies to both components and injections)

The following report tables now support the using data from either (but not both) sequences:

- Test Cases Table
- MS Raw Spectra
- Tentative Identification
- Component Table
- Peak Group
- Calibration History Table
- Audit Trail
- Data Audit Trail Table
- Audit Trail Event
- Audit Trail Event Configuration
- MS Status Log

Extensions to Report Plots

To support report generation with linked sequences, several report plots tables now have an additional tab called "Linked Sequence" on their properties dialog. The sequence selection on this tab determines the source of the data to be plotted. Unless the "seq.LinkedSequence()" qualifier (see previous section) is used, the sequence selection on this tab also implicitly applies to any other report variable-based values in the table.

Note that this additional tab is only visible when a linked sequence is open in the Studio session.

The following report plots now support the using data from either or both sequences (potentially resulting in a split pane):

- Calibration Plot
- Mass Spectra Plot
- MS Component Plot

The following report plots now support the using data from either (but not both) sequences:

- Chromatogram Plot
- MS Chromatogram Plot

Report Templates and Linked Sequences

When working with linked sequences, report templates from both sequences are available in the following locations:

- Printing data from the Console
- Exporting data from the Console
- Creating an Electronic Report
- Editing Report Templates in the Studio

3.12 Other Client Updates

Support for 4K Graphics Cards [228592]

This release adds support for 4K graphics cards and higher-resolution monitors. The UI has been tested at display settings of Scaling=200% and Resolution= 3840x2400. Other settings combinations are also possible, though the visual quality of every permutation cannot be guaranteed.

Scheduler Task List Improvement [255802]

Graphical representation of the status of Scheduler tasks in the Task List has been improved in this release. Checkboxes have been replaced by icons – the 'tick' icon indicates status 'Enabled'; the 'cross' icon indicates status 'Disabled'.

Chromeleon System Status Report [354155]

3.12.1.1 Limiting the number of included IQ Reports

A new optional command line parameter /IQReports has been introduced to allow a user to specify the number of most recent IQ reports to be included in the report.

3.12.1.2 TxpStore subfolder

Users can now create a System Status report that includes the subfolder "TxpStore" that is located under C:\ProgramData\Dionex\Chromeleon\Replication. To enable this, the additional option "Replication Folder" needs to be checked.

3.13 Reporting Updates

New Composite Scoring Report Tables [237391]

This release introduces two new default report tables.

The Ion Ratios table reports expected values, observed values, and pass/fail for ion ratios:

Name	Ret.Time	Overall Ion Ratio		Ion Ratio #1			Ion Ratio #2	
	min	Result	Expected	Observed	Result	Expected	Observed	Result
Nonanal	3.64	Not confirmed	68.47	185.23	Not confirmed	58.52	59.39	Confirmed
Decanoic acid, methyl ester	4.91	Confirmed	53.36	61.32	Confirmed	16.65	19.24	Confirmed
Undecanoic acid, methyl ester	5.64	Not confirmed	57.44	39.81	Not confirmed	21.23	19.37	Confirmed
Dodecanoic acid, methyl ester	6.38	Not confirmed	62.08	48.53	Not confirmed	14.80	11.60	Not confirmed
Benzenamine, 2,6-dimethyl-	6.72	Confirmed	80.02	74.38	Confirmed	74.24	70.56	Confirmed
Phenol, 2,5-dimethyl-	7.08	Not confirmed	100.31	126.12	Not confirmed	41.13	40.84	Confirmed

The Composite Scoring Results table reports thresholds, observed values and pass/fail for all other composite scoring categories:

		Filter Isotopes				Apex Alignment			Mass Accuracy			Isotopic Dot Product	
Name	Composite Score	Rule	Threshold (counts)	Alignment Type	Threshold Value	Observed Value(s)	Pass/Fail	Threshold PPM	Observed PPM	Pass/Fail	Threshold Value	Observed Value	Pass/Fail
(+3) ALEWLADIWWDDK	Confirmed	Exclude peaks whose Height is < 7.40E+007	7400000	Within Charge State	0.1000	n.a.	Pass	5.00	n.a., n.a., n.a.	Pass	0.9000	n.a.	Pass
ALEWLADIWWDDK	Confirmed	Exclude peaks whose Height is < 7.40E+007	7400000		•		Pass	-		Pass	•		Pass
(+3) ALEWLADIWWDDK[Glycation]K	Confirmed	Exclude peaks whose Height is < 7.40E+007	7400000	Within Charge State	0.1000	n.a.	Pass	5.00	n.a., n.a., n.a.	Pass	0.9000	n.a.	Pass
ALEWLADIWWDDK[Glycation]K	Confirmed	Exclude peaks whose Height is < 7.40E+007	74000000		-		Pass	-	-	Pass	-	-	Pass
(+2) DTLMISR	Confirmed	Exclude peaks whose Height is < 7.40E+007	7400000	Within Charge State	0.1000	0.000	Pass	5.00	1.27, -2.46, n.a.	Pass	0.9000	1.0000	Pass
DTLMISR	Confirmed	Exclude peaks whose Height is < 7.40E+007	7400000		•		Pass	-		Pass	•		Pass
(+2) DTLM[Oxidation]ISR	Not confirmed	Exclude peaks whose Height is < 7.40E+007	7400000	Within Charge State	0.1000	n.a.	Fail	5.00	n.a., n.a., n.a.	Fail	0.9000	n.a.	Fail
DTLM[Oxidation]ISR	Not confirmed	Exclude peaks whose Height is < 7.40E+007	7400000	-	-		Fail	-	-	Fail		-	Fail

Report variable peak.response

A new report variable called peak.response was introduced. It reports the value that had to be plugged into the equation of the calibration curve (of the given component) to calculate its Amount value.

Report variable peak.calFunction

A new report variable called peak.calFunction was introduced. Its value represents the formula of calibration function. Number of decimal places of coefficients and intercept can be configured.

Option to display calibration function formula in calibration plot

A new option was added to the Frame & Axes Page in the Properties Calibration Plot window allowing user to turn on/off displaying of calibration function formula in their calibration plots with the possibility to set decimal places.

Report variable to aggregate numerical results of multiple injections [174120]

A new report variable called 'Select Injections' in the Sequence category, formula expression seq.sellnjections, allows aggregation of numerical results from multiple injections in the currently selected sequence. In the parameter dialog of the new report variable, you can define criteria for which injections in the sequence the aggregation should be computed. As aggregation formulas the report variable offers Average, Count, Maximum, Minimum, Range, Relative Range, Standard Deviation, Relative Standard Deviation and Sum. In the aggregation formula itself you need to define the numerical formula as a parameter which will be evaluated for the injections.

Example: seq.selInjections("Comment";"contains";"AG").average("peak.area")

This formula will compute the average of the area for the selected peak covering all injections in the sequence where the comment field contains the text AG.

Multi-line Peak labels in Chromatograms and MS Component plots

Feature allowing user to define Peak labels in Chromatograms and MS Component plots was enhanced to support multi-line labels. User may define the Peak label to reside on 1, 2, 3 or 4 lines.

Integration and Consolidated tables

For each new Integration and Consolidated table that user creates, the default configuration of 'Filter Peaks' setting is now the following:

- Identified Peaks enabled,
- Unidentified Peaks disabled,
- Undetected Components enabled.

Furthermore, in case user selects MS quantitation channel, newly created Integration and Consolidated tables will by default not contain columns: No., Rel. Area, Rel. Height, Resolution. These can be later added to these tables, if user needs them, via the Table Properties > Report Column section.

Computing Masses from Chemical Formulas [260483]

The report variable **injection.chemical_formula_and_adduct_masses()** has been extended as follows:

- A new parameter for the report variable allows the monoisotopic mass of the given chemical formula to be returned. Previously only the mass of the most abundant isotope was returned.
- It is now possible to specify 'No adducts' when computing the mass from the chemical formula.
- The report variable returns a string representing the calculated mass. Previously, the precision of the values was fixed to 5 decimal places. Now, number of decimal places is based on the Mass Precision decimal places value from the MS Settings tab of the processing method.

Extended Filter Options for the Data Audit Trail Report Table [56254]

The Data Audit Trail Report Table is extended with extended filter capabilities. In the section Custom Conditions of the report table property dialog any property of the data audit trail record can be used for a dedicated filter condition. Multiple such conditions can be combined so that either all conditions or at least one condition need to become true so that the corresponding data audit trail record appears in the report table.

Example:

Properties Data A	Audit Trail	x
Properties Data A Filter Sort Order Report Column	Audit Trail	×
	Data Audit Ti v Operation v is any v Aborted Run;Changed;Deleted v (+) and)
	Close	

In the screen shot above only audit trail record of the sequence appear in the report table which have the operation value Aborted Run, Changed or Deleted.

3.14 Reporting 2.0

Reporting in Chromeleon 7 using Report Templates or Interactive Results in the Data Processing Category of the Studio Window is based on an Excel compatible spreadsheet component. Although still supported by current Excel versions this spreadsheet format (MicroSoft Excel 5.0/95 workbook (*.xls)) is a rather old one with quite some limitations, such as:

- Maximum number of columns: 256
- Maximum number of rows: 16384
- Maximum number of characters in a single cell: 255
- Support of Unicode character set
- Limited number of spreadsheet functions

With Chromeleon 7 Version 7.3.2 there is now an option to use an up-to-date Excel compatible component which overcomes this kind of limitations. Every time a new report template or view settings data object is created the user has the option to select the old or the new spreadsheet component.

Report Templates 2.0

In the dialog to create a new report template the user can select in the combo-box 'Category' to use either the old spreadsheet component (Thermo Scientific Templates) or the new one (Thermo Scientific Templates (2.0)).

Create Choose a	a report template a report template that i	s copied to the current sequ	ience.	
Category Default	Thermo Scientific Te Thermo Scientific Te Thermo Scientific Te Other Templates	emplates (2.0) emplates emplates (2.0)		V
	The second secon	Default DAD	2.0 Empty Template	

Once a report template with the new spreadsheet component is created the corresponding label in the data browser is **Report Template (2.0)**. Old report templates are still labeled with just **Report Template.** In the navigation area of the Report Designer report templates with the new spreadsheet component got a **2.0** label right to their name.

Name	Туре	Date Modified	Report Designer «
🔯 Blank review	View Settings (2.0)	06.03.2023 12:31:02 +01:00	▶ Injections 🔤 🕶 🎁 🕶 (Filter 🖤)
🔯 Default	View Settings	08.09.2020 13:18:14 +02:00	Channels
Default - New	Report Template (2.0)	13.03.2023 14:03:37 +01:00	Components
Default - Old	Report Template	13.03.2023 14:03:52 +01:00	Report Templates
A QuEChERS-Test	Processing Method	20.10.2022 11:31:22 -07:00	Default - New 2.0
M procmeth	Processing Method	22.07.2020 10:23:45 +02:00	l Default - Old
h			

Report Templates (2.0) can be used in parallel with report templates using the old spreadsheet component. They provide also more or less the same functionality as report templates using the old spreadsheet component. In the corresponding Report Designer category there are some new and/or modified UI-elements supporting capabilities supported by the new Excel format, such as 'Merge Cells and 'Conditional Formatting'. See section 3.14.5 for more details.

3.14.1 View Settings 2.0

Similar to Report Templates there is a new option to create View Settings where the Interactive Results pane is using the new spreadsheet component. When triggering the Create -> View Settings command the user can select to create either a view settings data object with Interactive Results using the old spreadsheet component or the new one.



Analogue to report templates view settings with interactive results using the new spreadsheet component will be labeled with **View Settings (2.0)** in the type-column of the data browser and with an additional **2.0** label in the navigation area of the studio window.

Note: Report Templates (2.0) / View Settings (2.0) appear as ordinary Report Templates / View Settings when looking at such new data items in the Chromeleon Console using a Chromeleon version prior to 7.3.2 (e.g., Chromeleon 7.3.1). Trying to open or using such Report Templates (2.0) / View Settings (2.0) will raise error dialogs or lead to an unexpected behavior of Chromeleon.

Report Tables in Reporting 2.0

Reporting 2.0 supports the most important Chromeleon report tables (Integration Report, Peak Summary, etc...). When inserting new report tables into a report template 2.0 you cannot pick from various templates as in the report designer for old report templates. You will get just the same list of report table types as you would insert a report table into the Interactive Results pane in the Data Processing category if the Studio window.

The following report tables which are currently available for report templates with the old spreadsheet component are not available for Report Templates (2.0) yet:

- Fraction Report
- Tube Report
- Audit Trail Events
- Audit Trail Event Configuration
- Tentative Identification
- Component Table
- System Suitability IRC
- Peptide Table
- Composite Scoring Table
- Chromeleon 6 History Table
- MS Raw Spectra
- Sieve Frame Table
- Sieve Processing Parameter Table
- NTMS BioPharma Finder Results
- Mass Analyser Processing Parameters Table
- IPD Component Table
- IPD Processing Parameters Table

3.14.1.1 Spreadsheet Filter for Report Tables

Report tables in Reporting 2.0 with an arbitrary number of columns (Integration Report, Peak Summary, etc...) offer a spreadsheet based customized filter for every report column. In the context menu for the report table there are new options to (de)activate the filter and/or change the filter settings for the currently selected column.

Integr	Integration Results		Release Column			
No.	Peakname	Y	Table Filter On/Off		Height mAU	
	value STARTS WITH "A"		Set Column Filter	i i		
1 2	Acetanilide Acetophenone	X	Clear Column Filter	599 586	73,715 83,460	
Total:			Table Properties	f	157,175	

Graphical Object (Plots) in Reporting 2.0

Reporting 2.0 also supports many graphical objects (Chromatogram Plot, Calibration Plot, etc...). When inserting new graphical objects into a report template 2.0 you cannot pick from various templates as in the report designer for old report templates. You will get just a list of available objects.



The following graphical objects which are currently available for report templates with the old spreadsheet component are not available for Report Templates (2.0) yet:

- SIEVE Frame Plot
- BPF Component Results Plot
- IPD Chromatogram
- IPD Source Spectrum
- IPD Deconvoluted Spectrum

Export Formats in Reporting 2.0

Not all export formats (Text, Excel, PDF, ...) are available with Reporting 2.0. The following export options are disabled in the Export Settings dialog in the corresponding Report Designer.

- GAML file format (*.gaml)
- AnDi/NetCDF file format (*.cdf)
- Chromeleon data file format (*.cmbx)
- Allotrope data file format (*.adf)
- Call Extern Program
- Enable Notifications.

If you want to use these export formats you need to use a report template with the old spreadsheet component.

Using PDF or Excel as export format Reporting 2.0 offers further options.

PDF-Export Option	Excel-Export Option
-------------------	---------------------



UI options in Report Designer 2.0 vs. Report Designer using the old Spreadsheet Component

The Report Designer UI elements and options for Report Templates 2.0 and those for the Report Designer with the old spreadsheet component differ in various areas, mainly due to new or different capabilities of the spreadsheet component. Here a list of such differences worth mentioning:

3.14.1.2 Formula Bar

The formula bar in Reporting 2.0 provides a spreadsheet formula picker triggering a dialog to pick a spreadsheet function similar to the UI which is well known when using Excel. The report designer with the old spreadsheet component doesn't have such an UI element.



When editing spreadsheet formulas in a report template 2.0 the cell range which is referenced in the formula is highlighted in a similar way as in Excel.

By Co	omponent	Acetanilide	(
No	Injection Name	Ret.Time	Area
		min	mAU*min
		UV_VIS_1	UV_VIS_1
		Acetanilide	Acetanilide
1	Alkylphenones 1	0,170	0,694
2	Alkylphenones 2	0,172	1,370
3	Alkylphenones 3	0,174	2,749
4	Alkylphenones 4	0,176	4,127
5	Alkylphenones 5	0,178	5,507
6	Alkylphenones 6	0,180	6,856
7	Alkylphenones 7	0,172	5,223
	Average:	=AVERAGE(C	15:C21)

3.14.1.3 Spreadsheet Formulas in Report Tables

When applying spreadsheet formulas in Chromeleon Report Tables users can enter such formulas directly in the respective report column. When using Reporting 2.0 you need to insert a so-called empty column first before you can enter any spreadsheet formula in this report column. There is a dedicated comment in the context menu for report tables to create such an empty column.



3.14.1.4 Home Ribbon

The home ribbon in the Report Designer for Reporting 2.0 contains two new formatting options 'Merge Cells' and 'Conditional Formatting'.



The commands 'Check for Errors' and 'Custom Formulas' are currently (7.3.2) only available for Report Templates using the old spreadsheet component. Custom Formulas can be used nevertheless with Reporting 2.0 when editing Chromeleon formulas, e.g., for report columns in report tables.

3.14.1.5 Insert Ribbon

In Report Designer 2.0 the ribbon commands for Insert All Tables, All Plots and All Charts do not open a wizard dialog where you can select between different (custom) templates. This has been and is still applied when using the report designer using the old spreadsheet component. Instead a plain list of table, plot or chart object types is offered.

General Charts in Reporting 2.0 are now Excel compatible where you can use far more chart types than before yet with a limited UI to modify the properties of a chart once it is inserted.

3.14.1.6 Page Layout Ribbon

Reporting 2.0 does not provide the capability to visualize automatic page breaks via dotted grid lines in the currently selected spreadsheet. The corresponding option in the Peak Setup ribbon tab is not available.

3.14.1.7 Print Preview

The Navigation Ribbon in Reporting 2.0 provides a Next/Previous Peak/Component command instead of Next / Previous Page. There is also no Zoom Ribbon tab. For the latter you can use the mouse wheel, for next / previous page you can use the scroll bar next to the preview window.

The Autorepeat Ribbon in Reporting 2.0 offers a new option to apply Auto Repeating in the Print Preview.

3.15 Data Import/Export Updates

Orbitrap Exploris MS Inclusion Lists [241733, 353224]

With this release, it is now possible to import inclusion lists exported from Thermo Scientific Exploris MS instrument methods into the MS Component Table of a processing method. It is also possible to export components from a processing method into a format compatible with the Exploris method editor.

XIC Import Limit Increased [270548]

In previous releases, component import from external sources was limited to 1500 XICs. With this release, it is now possible to import up to 10,000 XICs.

Component Transfer Using TraceFinder CSV Format [235648]

TraceFinder supports import and export of component information using a CSV file format. This format includes name, chemical formula, and CAS number, as well as quantitation and confirming ion definitions.

With this release, it is now possible for Chromeleon to also import and export this component information using the same CSV file format. This feature is accessed via the Compound Data Import and Export buttons on the Processing method toolbar.

Compound Data Import	×	
Data Source	۲	
Compound Data Store Path:	Browse 🔻	
	MS Raw Data	
	Compound Data Store	
	NIST Library	
	Acquisition List	
	BioPharma Finder Peptide List	
Select All Unselect All Expand All Collapse All Import	BioPharma Finder Workbook	
	PinPoint Workbook	
	TraceFinder CSV	

Save As					×
$\leftarrow \rightarrow {\cdot} \uparrow$	늘 > This PC > Desktop	> New folder	~ C	🔎 Search New	folder
Organize 🔻 New	w folder				≣ • 😗
This PC	Name	^	Status	Date modified	Туре
E Desktop		No items m	atch your searc	:h.	
Documents					
🚽 Downloads					
🕖 Music	1				
Pictures					
🛂 Videos					
🛀 Windows (C:))				
🕳 TOSHIBA EXT	(G				
- TOSHIBA EXT (0	G:)				
** Drophox					
File name:					~
Save as type:	TraceFinder 3.3 (*.csv)				~
▲ Hide Folders	Exactive Orbitrap LCMS and G ISQ SQ GCMS Family (*.csv) TSQ QqQ GCMS Family (*.csv) TSQ QqQ LCMS Family (*.csv)	iCMS Family (*.csv))			
	ISQ SQ LCMS Family (*.csv)	CMS Eamily (* ccu)			
	TraceFinder 3.3 (*.csv)	Civio Family (ICSV)			

3.16 Peptide Analysis Enhancements

Synchronized Editing of Peptides in the MS Component Table [270561]

When working with Peptides, many attributes in the MS Component Table apply equally to all the charge states as well as the master peptide. With this release, when editing such parameters in the MS Component Table, the change will automatically be propagated to the Master Peptide as well as all charge states of the peptide.

New Target Tolerance Sequence Table Column [260483]

A new built-in column called 'Target Tolerance' has been added to the sequence table. This value is not currently used in any calculations. However, it can be used as a reference value in reports. A new report variable **Inj.TargetTolerance** has been created to report the value of this setting. This column is only available when the 'Show injection target mass detection columns' option is enabled in the Admin Console (Global Policies > UI Customizations)

Improvements to Composite Scoring Settings

3.16.1.1 Composite Scoring Settings Improvements Per Component [233580]

With this release, the 'General MS' option of the Composite Scoring parameters tab has been replaced by two options – 'Basic' and Advanced'. In addition, it is now possible to define general injection and peak-based criteria.

Detection	MS Detection	MS Component Tab	le Calibration	MS Setting	gs MS Library Screening	SST/IRC	Advanced Settings	Composite Scori
MS Crite	eria							
Ba	sic	•						
Cri	teria							
	Confirming ion	ratio passed						
	Peak apex alig	nment ≤ 0.50	min					
	Mass accuracy	≤ 5.00	PPM	Ψ.	Mass Accuracy Calculati <u>o</u> n:	Greatest	Mass Intensity	$\overline{\mathbf{v}}$
	Match ALL 🔻	of the following rule	s:					
)	•			• + -
	and							

3.16.1.2 Composite Scoring Settings Per Component [133528]

In previous releases, one set of Composite Scoring criteria (used to confirm the identification of a component) applied to all components in the processing method.

With this release, it is possible to set the criteria differently on a component-by-component basis. A new checkbox is available on the Composite Scoring tab of the processing method. When checked, the tab settings are disabled and a new column in the processing method is enabled. Double-clicking the cell or opening the Properties page allows the criteria to be adjusted independently for each component.

MS Detection	MS Component Table	MS Settings	SST/IRC	Peptide Table	Composite Scoring			
Composite Scoring								
Per Component Composite Scoring								
Specify composite scoring per component Apply settings to all components								
Scoring result on checked criteria								

ſ	MS	Detection	MS Component Table	MS Setting	s SST/IRC	Peptide T	able Composite Scoring	
l	С	Component Table						
		Group Are	sa Drag a colu	mn header l	here to group	by that colu	nn. Run Component Table Wizard	
1	#		Name		Ret.Time 🔺	Window	Component Composite Scoring	
	3	eeqyn[a	2G2F]STYR		9.647	0.074 AG		
	4	(+2) EEQ`	YN[A2G2F]STYR		9.647	0.074 AG	PS: 2; FS: 2; NTMS; ION; APEX: 0.5; ALIGNMENT: WithinChargeState; ISO: 0.9; ACC: 5; UNIT: PPM; CALC: GreatestMassIntensity;	
	5	(+3) EEQ`	YN[A2G2F]STYR		9.647	0.074 AG	PS: 2; FS: 2; NTMS; ION; APEX: 0.5; ALIGNMENT: WithinChargeState; ISO: 0.9; ACC: 5; UNIT: PPM; CALC: GreatestMassIntensity;	

3.17 Non-Targeted MS Processing Enhancements

Results Filtering Based on A Custom Exclusion List [194215]

With Chromeleon 7.3.1, when performing NTMS New Peak Detection using the BioPharma Finder algorithm, it was possible to filter the list of new peaks to exclude CQAs (peptides defined in the MS Component Table).

With this release, it is now additionally possible to exclude peptides which are not in the MS Component Table. The new option appears in the Filtering sub-pane of the Component Results table of the NTMS Studio category.

Known components may be added manually to the table or may be imported from a csv file. As with CQA components, retention time and m/z match criteria are specified to enable the filtering.

	m/z: O 100.00 am	<u>1</u> O 5.00 PP <u>M</u>	1		
no	wn Components:				
#	Name		Retention Time	m/z	4
1	(+1) LASGVPSR		10.210	786.44683	
		Add Component			

The same filtering option is also available in the Component Results report table in the Report Designer category.

Display Options for New Peak Detection Results [194215]

With this release, when performing NTMS New Peak Detection using the BioPharma Finder algorithm, it is now possible to view the list of new peak detection is multiple ways. Use the radio button set at the top of the Component Results table to see all detected peaks, filtered peaks or peaks that were not filtered.

Show	: O <u>N</u> ew Peaks	│ <u>Id</u> entified/Filte	red Peaks 💿 All Peaks			
	Component Number	Matching Component	Matching Component Source	RT (min)	m/z	Charge State
	109			10.179	428.24896	1
	110		•	10.179	515.29211	1
	111			10.179	301.66568	2
	112		•	10.179	602.32373	1
	113	(+1) LASGVPSR	Known Component Table	10.220	808.42596	2
	114	(No Match)	(No Match)	10.179	393.58322	4
	115			10.185	805.41748	2

In addition, additional columns are now available in the table to report the why a peak was filtered (excluded) from the list of new peaks.

The same filtering option is also available in the Component Results report table in the Report Designer category.

Report Object for XIC Plot [237389]

When NTMS data has been processed using the BioPharma Finder algorithm, a new plot object in the Report Designer is now available for the XIC results plot. Similar to the already existing plot in in the interactive "Non-Targeted MS Processing" category of the Studio, this report object shows the XIC plots of the control and sample injections for the selected results component.

To insert the plot, right-click on a cell and select *Insert > All Plots* and select *BioPharma finder XIC Plot* from the Peptides section. To configure the plot, right-click on it can select *Properties.*



Updated BioPharma Finder New Peak Detection Engine [293887]

With this release, the BioPharma Finder algorithm used for NTMS new peak detection has been updated to the same version as is used by BioPharma Finder 5.1.

New Default Report Templates for NTMS Analysis [35397]

This release includes a new default report template for NTMS (MAM) analysis. Instructions are included in the template itself explaining how to customize the report sheets for the specific components being analyzed.

New NTMS-Related Report Variables [133039]

With this release, the following report variables related to NTMS data have been added:

Report Variable	Context	Description		
SummedTotalPeakArea	Peak	The sum of the peak areas of all the charge states of all the isotopes (confirming ions)		
Summed Group Total Peak Area Master Peptide	Peak	The sum of the peak areas of the Quan lons for the master peptide from all components in the Peptide group		
SummedGroupConfirmingPea kArea(x,y)	Peak	The sum of the peak areas for isotope x (confirming ion) across all components in a Peptide Group.		
SummedGroupChargeStateCo nfirmingPeakArea(y)	Peak	The sum of the peak areas of all the isotopes (confirming ions) per charge state across all components in a Peptide Group.		
SummedGroupTotalPeakArea(y)	Peak	The sum of the areas of all the isotopes (confirming ions) for all charge state across all components in a Peptide Group.		
component Results (n). Matche d Name	nontargetedms_bpf	The name of the component from the MS Component Table which matched the selected NTMS peak		
componentResults(n).Matche dSource	nontargetedms_bpf	Reports "MS Component Table" if the selected NTMS peak matched a component from the MS Component Table		

3.18 Protein/Oligonucleotide Deconvolution Enhancements

New Deconvolution-Related Report Variables [53529, 228855]

With this release, the following report variables related to intact deconvolution data have been added:

Report Variable	Context	Description
intactDeconvolution.ipdCompon ent.matchingTargetComponent	Deconvolution Results	Returns the name of the target component that matches the specified IPD result peak. If no component matches the IPD result, then it returns "(No match)"
intactDeconvolution.ipdCompon	Deconvolution	Returns the average mass of the
-------------------------------	---------------	---------------------------------
ent(n).AverageMass	Results	deconvolved result peak

Expanded Processing Parameters Pane and Report Table [260483]

The Processing Parameters pane in the Intact Protein Deconvolution category as well as the corresponding report table have been extended to report all the effective IPD processing method parameters.

*	Chromatogram Parameters				
	Chromatogram Type	TIC			
	End Scan Number	431			
	End Time	12.001 [min]			
	Is High Sensitivity	True			
	Mass Range High	4000.0000 [m/z]			
	Mass Range Low	2000.0000 [m/z]			
	Range Display Type	Time Limits			
	Relative Intensity Threshold	1			
	Restricted Time	True			
	Start Scan Number	1			
	Start Time	0.000 [min]			
~	Deconvolution Parameters				
	Algorithm Type	ReSpect			
	Spectra Selection Type	Whole Retention Time			
>	ReSpect Advanced Parameters				
~	ReSpect Parameters				
	Choice Of Peak Model Index	Intact Protein			
	Do Use Isotopic Profiles	True			
	End Time	7.298 [min]			
	Is Calculate XIC	True			
	Is Ppm Tolerance	True			
	Mass Tolerance	20			
	Output Mass High	160000			
	Output Mass Limit High	160000			
	Output Mass Limit Low	10000			
	Output Mass Low	10000			
	Resolution At 400 m/z	10607			
	Start Time	5.188 [min]			

IPD Autoprocessing and Autoreporting [35387]

In previous releases, reporting processed Intact Protein Deconvolution (IPD) data required opening the sequence in the Chromatography Studio and manually processing the data.

With this release, it is possible to automatically process and report the results.

This option for preprocessing is enabled on the Auto Reporting tab of the Sequence Properties dialog.

Sequence Properties	5					×
General Features	Locks Signature	Auto Reporting	Notifications	Raw Data Statistics		
MS data processin	ng settings ————					
Perform <u>N</u> TMS	S preprocessing					
Perform IPD p	reprocessing					
Auto reporting setti	ings					
Save electroni	ic report					
Print report						
Export report						
Print/Export report:	After whole sequence	e			•	
Printer: No printe	er selected				$\overline{\mathbf{v}}$	
				ОК	Cance	

Similar options also exist in the New Sequence Wizard and in the eWorkflow editor.

Updated Intact Protein Deconvolution Engine [181601]

With this release, the algorithm used for intact protein deconvolution has been updated to the same version as is used by BioPharma Finder 5.1.

Additional Injection Specific Option for Oligonucleotide Analysis [260483]

When using the Xtract algorithm for intact deconvolution analysis, the existing 'Nucleotide' option for the 'Isotope Table' parameter on the 'Algorithm Parameters' tab of the IPD Processing Method has been renamed 'Nucleotide/ Sequence Specific'. When this option is selected, on a per-injection basis:

- If the 'Target Formula or Mass' column of the sequence is empty or contains a (numeric) mass value, the existing built-in Nucleotide isotope table is passed to the IPD engine (Note: this is the current behavior)
- If the 'Target Formula or Mass' column contains a chemical formula, then a custom isotope table is computed from the chemical formula.

New Default Processing Method for Oligonucleotide Analysis [260483]

This release includes a new default processing method for Sulfur-modified Oligonucleotide analysis.

New Default Report Templates for Oligonucleotide Analysis [35397]

This release includes a new default report template for Sulfur-modified Oligonucleotide analysis. Instructions are included in the template itself explaining how to customize the report sheets for the specific components being analyzed.

3.19 Discovery Service Enhancements

Discovery Web Service

This release introduces a new Discovery Web Service based on gRPC and hosted within the Internet Information Service (IIS). This will replace the existing WCF based Discovery Service to provide a more efficient dissemination of the Chromeleon domain resources. For more in depth information about the Discovery Web Service, please see our Enterprise documentation.

Regional Proxy Servers

In large Chromeleon domains consisting of hundreds of connected Chromeleon clients there might be times when the Chromeleon domain controller becomes less responsive affecting Chromeleon users' productivity.

From Chromeleon v7.3.2 on, Chromeleon Administrator can now setup so called **Regional Proxy Servers** to improve overall Chromeleon domain performance.

Usage of Regional Proxies:

- reduces the network traffic between the Chromeleon workstations and the Chromeleon domain controller,
- improves the performance of the Chromeleon domain controller by decreasing load it needs to handle related to discovery of domain resources,
- makes the discovery of domain resources located within your labs/sites faster,
- allows Chromeleon domain to grow and go beyond 1000+ of connected users/instruments/workstations without any major decrease in performance.
- The Regional Proxy Servers utilize the new Discovery Web Service.

For more in depth information about the Regional Proxy feature, please see our Enterprise documentation.

3.20 Support in CM Console for large sequence transfer between Data Vaults

A new capability allowing Chromeleon Console users to perform safe and reliable transfer of very large sequences (up to 64GB of size) via Copy&Paste has been introduced in 7.3.2.

It can be turned on and configured by Chromeleon Administrator via Global Policies.

3.21 MS Performance Enhancements

With this release, processing of mass spectral data has been redesigned, resulting in significant improvements in both usability and performance.

The majority of MS data processing is now done in the background and, in Enterprise deployments, on the data vault server, meaning that the user interface is much more responsive while processing.

Background Processing of Electronic Reports and Data Export [262814]

In previous releases, when the user requested a data export or created an electronic report, the software user interface was blocked while the operation was completed. With this release, the processing occurs in a background service, meaning the Console and Studio are still responsive to user inputs.

Backward Compatibility

A new option has been added to the Features tab of the Sequence Properties dialog:

Sequence Properties	Х
General Features Locks Signature Notifications Raw Data Statistics	
- NTMS New Peak Detection Algorithm	
○ SIEVE	
Peptide Display Mode	
Show Master Peptides and Charge States	
MS Processing Compatibility Mode	
Chromeleon 7.3.1 and earlier Ochromeleon 7.3.2 and later	
OK Cancel	

This option determines the algorithm to be used when reading MS data. The new algorithm ("Chromeleon 7.3.2 and later") offers increased performance but extracted data may differ slightly from the older algorithm. To ensure backward compatibility, only sequences created using Chromeleon 7.3.2 will have the new algorithm chosen by default.

Note: This setting should not be changed while sequences are acquiring or when the sequence is open in the Chromatography Studio

Update Visible Views Deprecated [355257]

With the introduction of an improved workflow and performance for MS data, there is no longer a need for the "Update Visible Views" functionality in the Chromatography Studio.

Application	UI Elements Removed	Comment
Admin Console	User privilege to modify "Update Visible Views" setting	
Console	"Update Visible Views" option on the Features tab of the Sequence Properties dialog	Parameter value is treated as 'Automatically' for all old and new sequences to ensure backward compatibility
Console	"Update Visible Views" option on the MS Features tab of the MS Properties dialog in the New Sequence wizard	Parameter value is treated as 'Automatically' for all old and new sequences to ensure backward compatibility

As a result, the following have been removed from the client UI:

Console	"Update Visible Views" option on the MS Features tab of the MS Properties dialog in the eWorkflow editor	Parameter value is treated as 'Automatically' for all old and new sequences to ensure backward compatibility
Chromatography Studio	User interface for manually updating data in panes	

Improved UI-Workflows for Processing MS Data Sets

3.21.1.1 General Comments about Chromeleon, Automatic Processing and Cached Primary Peak Results

Every time a Chromeleon formula (e.g., peak.area) is evaluated or results are presented in a Chromeleon window (e.g., Chromatogram Plot, Interactive Results, Console Window Injection List) Chromeleon evaluates automatically whether a corresponding data processing needs to be executed. Processing in this case means that based on the current processing settings

- Peak Detection for 2D-Signals or XICs is executed providing a list of peaks and the corresponding baseline.
- For all detected peaks the so-called **primary peak results** such as peak area, height, width, etc... are computed.
- Peaks are assigned to components of the Processing Method. The component assignment also included in the primary peak results.

The primary peak results are automatically saved as cached results if a studio window is closed and the corresponding processing settings have been saved as well. The automatically triggered processing is always executed on the Chromeleon client process even if the processing settings are not saved yet.

For XICs the cached primary peak results are stored as Custom Raw Files for every injection. These Custom Raw Files can be seen when trying to delete raw data for a sequence (see the following figure).

Delete Raw Data for 'MSDefault'?							
○ <u>A</u> II raw data (incl. 3D fields, si ● <u>S</u> elected raw data	gnals and injection audit trails)						
Name	Туре						
Audit	Audit Trail						
Chromatogram Cache Data	Custom Raw File						
MSDevice	Mass Spectrometry File						
PTV Pressure readback	Signal						
PTV temp	Signal						
Septum Flow	Signal						
Split Flow	Signal						
Warning: This operation will permanently delete the raw data and is not reversible.							
	OK Cancel						

Every time Chromeleon needs any result related to primary peak results if reads the cached chromatogram data and checks whether these results fit to the currently used processing settings. If yes it will just use the cached results, otherwise it will automatically trigger data processing. The cached primary results also contain the mass accuracy results if the corresponding composite scoring option is enabled in the processing method.

3.21.1.2 Background Processing for MS Data Sets

When running Chromeleon versions up to 7.3.1 the processing for the primary peak results has been executed in the Chromeleon client process in a way that it blocked any user action while the processing was running. Having lots of component records and corresponding XICs the processing of all XICs can take quite some time, especially if the XIC peak results are shown or used in a studio window layout and/or if the sequence is located on a network datavault. In this case the XIC raw data which is necessary to execute the processing needs to be copied to the client computer.

With the new Chromeleon version 7.3.2 user actions are not blocked anymore while the processing is running. If a studio window (Data Processing and Report Designer category only!) detects that the cached primary results are not present or that the results are not up-to-date, i.e., that results have been computed with a different processing parameter set, it will automatically trigger a processing for all component XICs and the TIC channel(s) for all injections. In the studio window a corresponding blue notification message will appear:

Out-of-date results have been detected. Reprocessing has been started in the background. You may continue to review data in the studio.

The processing of the XICs and TIC channel(s) is now executed in the background. In the navigation area of the studio window the injection list shows the current processing state of every injection. This processing state is visualized via a dedicated colored icon. Here, a screen shot shows how this looks:

Data Processing					
Injections		11 -	Filter	Y	^
1 🛐 Blank				🔵 ಜಿ-	
2 📱 Std_5ppb_1				🔵 ಜಿ-	
3 📱 Std_5ppb_2				🔵 ಜಿ-	
4 🐺 Std_5ppb_3				🔵 ಜಿ-	
5 📱 Std_10ppb_1				🔵 ಜಿ-	
6 🐺 Std_10ppb_2				🔵 ಜಿ-	
7 📱 Std_10ppb_3				🔵 ಜಿ-	
8 📱 Std_20ppb_1				🔵 ಭ-	
9 🦉 Std_20ppb_2				🔵 ಭ-	
10 📱 Std_20ppb_3				🔵 ಭ-	
11 📱 Std_50ppb_1				3,€ C}-	
12 📱 Std_50ppb_2				<u>}</u> * ⊂⊢	
13 📱 Std_50ppb_3				: <u>}</u>	
14 🦉 Std_100ppb_1				: 아	
15 📱 Std_100ppb_2				꽃 다	
16 🦉 Std_100ppb_3				🔴 ಭ-	
17 🛐 Carryover-Blank	C C			🔴 ಭ-	
18 👸 RSD_10ppb_1				🔴 ಭ-	
19 👸 RSD_10ppb_2				🔵 ಭ-	
20 👸 RSD_10ppb_3				🔵 ಭ-	
				7	

Possible processing states, the corresponding icons, and its colors:

0	Processing for the injection is pending.
	Processing is currently running.
•	Processing is completed and the primary results cache file has been updated.
	Processing was not necessary. Primary results are still up-to-date.

While the processing is running in the background the user can still use the studio window of this sequence to select other injections and review chromatograms and results. As soon as the processing is completed for a sequence the newly computed primary results are immediately rendered in the corresponding panes or in the component list of the navigation area. For injections which are still not processed yet the old primary results are shown. The UI is only blocked while new or old results are rendered in the studio window.

There are two different ways how and where the background processing is executed. This depends on the MS Processing Compatibility Mode setting of the sequence (see section 3.21.2):

- **Chromeleon 7.3.1 and earlier:** background processing is executed on the client in a separate background thread of the studio window for the sequence. If this studio window is closed while the processing is still running the user is asked to confirm that because the processing will be stopped as soon as this window is closed.
- **Chromeleon 7.3.2 and later:** background processing is executed via a dedicated new Windows service (**Application Processing Service**) on the computer where the data vault service is running. This might be a different computer than the one where the Chromeleon

client is running. In this case the processing continues after the Studio Window for the sequence or even the Chromeleon client is closed.

As soon as all injections are completely processed the processing icons disappear from the navigation area of the Studio Window.

Notes:

- This new UI-Workflow for background processing is only present for MS data sets. Non MS Data Sets are not affected. The standard automatic processing is still in place (see previous section 3.21.4.1 - General Comments about Chromeleon, Automatic Processing and Cached Primary Peak Results).
- Using the sequence property MS Processing Compatibility Mode Chromeleon 7.3.2 and later will provide a better performance than Chromeleon 7.3.1 and earlier. In this case (Chromeleon 7.3.2 and later) processing of multiple injections can run in parallel, XIC raw data doesn't need to be copied to the client computer and therefore the time spent for processing a complete sequence with many injections is much faster compared to Chromeleon 7.3.1 and earlier.

3.21.1.3 Automatic Processing on the Instrument Controller (IPC)

If a sequence is running, the instrument controller automatically executes the data processing for the primary peak results once an injection is finished. Now with version 7.3.2 this also includes the mass accuracy results if the corresponding composite scoring parameter is enabled. Thus, after the sequence run is completed and the sequence is later opened in the studio there is normally no need to trigger an automatic background processing. All cached primary peak results are up-to-date at this point.

3.21.1.4 Improved UI Workflow while Changes are Pending

Background and Automatic Processing on the IPC as described in the previous sections is only applied for changes to the sequence which have been saved. If you change a processing parameter (e.g., MS Detection Settings) in a Studio Window Chromeleon will automatically trigger processing in the client before you change the changes (Pending Modifications). This processing for pending modifications is executed on the client and blocks any UI activities until the results presented in the studio window are up-to-date in regards of the pending modifications.

With Chromeleon 7.3.2 there is now an option to cancel the automatic processing of MS data sets to review the currently processed and rendered results. When Chromeleon is starting the automatic processing for pending modifications it estimates the processing time. If this above 3 seconds a progress window appears where the user has the chance to stop the automatic processing.

📭 Update Chromatogram Results				
Processing chromatograms				
Std_5ppb_2 Processing chromatogram 520/610				
	Cancel			

After pressing Cancel a yellow notification bar appears on top of the studio window

Data Processing is paused and results may be not up-to-date. Save processing settings to start background processing or continue data processing in the studio using unsaved settings.

At this point automatic processing is not applied anymore. Any further change to processing parameters is not applied. Clicking on the link continue data processing in the studio automatic processing will resume. The link Save processing settings will open the save dialog to save the pending modifications which will then trigger background processing as described in the previous sections.

In any case automatic processing of MS data sets will be visualized in the navigation area of the studio window. Analogue to background processing the processing state is visualized via a dedicated colored icon. Here, a screen shot shows how this looks:



Possible processing states, the corresponding icons, and its colors:

-	Processing for the injection is pending. Results of this injections which contribute to the studio window are not up-to-date in regards of the pending modifications.
	Processing is currently running.
•	Processing in regards of the pending modifications is completed for all XICs of the injection which contribute to results in the studio window.

3.22 Chromeleon XPS Enhancements [281641]

Chromeleon XPS is a simple-to-use walk up open access user interface for the Chromeleon client, based on Chromeleon eWorkflows. This release of Chromeleon includes several enhancements to Chromeleon XPS

Overriding the Default Starting Vial Position

In previous releases, Chromeleon XPS would automatically compute the next available vial position for the samples, based on pending sequences in the run queue. With this release, it is now possible to override that selection and specify a different starting vial position.

Chromeleon 7

🎼 Cł	nromeleon XPS					– o ×
		🕂 Log off	Launch Chromeleon	Launcl Instrume Dashboa	h ent ard	Administration Mode
			# <u>V</u> ials (max. 1 Sampler start posit	100): 6 tion <u>R:A1</u>		Jse Sample Names from eWorkflow Manually specify vial positions
#	Sample Name	Position	SampleSource	R:A2 B:A3		
1	Sample-0001	R:A1		R:A4		
2	Sample-0002	R:A2		R:A6		
3	Sample-0003	R:A3		R:A7 R:A8		
4	Sample-0004	R:A4		R:A9 B:410		
5	Sample-0005	R:A5		R:A11		
6	Sample-0006	R:A6		R:A12 R:B1 R:B2 R:B3 R:B4 R:B5 R:B6 R:B7 R:B8 R:B7 R:B8 R:B9 R:B10 R:B11 R:B11 R:B11 R:B12 R:C1 R:C2 R:C2 R:C2 R:C4 R:C5 R:C6		Import
	Help					Back Next
						Frank

Using Sample Names and Vial Positions Present in the eWorkflow

When an eWorkflow includes injection blocks with fixed sample names and vial positions (e.g., for a calibration curve) Chromeleon XPS now includes the option to use those names and positions instead of auto-computed values.

Support for Instruments with Two or More Injection Devices

When using an instrument with more than one injection device (e.g., dual GC inlets or a manual injector + an autosampler), Chromeleon XPS will now prompt the user for which sampling to use.

Select Sampler	×
There is more than one sampler/injector device installed on the selected instrument	
Please select the sampler/injector to use.	
Inject Using:	_
AS1310 Manual_Injection	
OK Cancel)

3.23 Process Analyzer Auto-Export [350504]

The Chromeleon 7 Process Analyzer ("CM7 PA") now supports the automatic export of data at the end of an injection. In the CM7-PA client, the configuration page for each instrument now includes an option titled "Export End-of-Run Report"

3.24 Local Data Vaults based on SQL Server Express 2022

With this release, Chromeleon now ships with SQL Server Express 2022 for local Data Vaults and XVaults.

As before, Chromeleon will only install SQL Server Express if it is not already present on the computer. If a previous installation of Chromeleon already installed SQL Server Express 2014, the installer will <u>not</u> automatically upgrade the SQL Server Express version.

Please note: SQL Server Express version >= 2017 no longer supports Windows 7 or 32bit OS systems. On those systems, the installation of SQL Server Express version >= 2017 can be skipped, and local Data Vaults or XVaults are not available. To install Chromeleon >= 7.3.0 on Windows 7 or a 32bit OS, please manually install and configure SQL Server Express 2014 first (see Installation Guide).

4 Resolved Issues

This chapter describes the issues that have been resolved with the release of Chromeleon 7.3.2.

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
135619	eWorkflow Audit Trail: If an associated data object (Instrument / Processing Method, Report Template, etc) is embedded in an eWorkflow and not a link, any change of such methods led to 2 audit trail records in the eWorkflow. The 1 st one recorded a Delete operation and the 2 nd one a Create or Copy operation. Now with Chromeleon 7.3.2 there will be only a single audit trail record with the operation 'Changed'.
139606, 172750	Vanquish Autosampler: The configuration options "Support for external rack transfer" enabled (on the "Options" tab) and the charger option (on the "General" tab) can be checked and unchecked at any time now. The hardware can support only one option, therefore it is not possible to save the configuration with both options enabled.
143052	Console and Studio: Various UI elements had display issues on monitors set at high DPI Screen Resolution.
145433	System Suitability Report Templates: Using a SST report table from a Thermo Scientific Template, e.g., Default View Settings, Report Template 'Default' or 'Default DAD', the Total Result is computed via an Excel Formula referring Test results of every single SST in the report table. This excel formula was not correct. If a single SST couldn't be evaluated and is configured to return a failed result (NA -> Failed) the Total Result reported Passed. For report tables in the Interactive Results pane the formula is now correct. In Report Templates the Excel Formula has been replaced by the Chromeleon formula injection.sst_result.
148927	Detailed Changes of Manual Chromatogram Integrations: for certain unknown manual integrations of a chromatogram one could not view the detailed changes in the data audit trail. When pressing <show changes=""> for the corresponding data audit trail record Chromeleon runs into an error message "An error occurred while comparing the items". It was also not possible to create an audit trail report including changes for the sequence or to open a read-only studio session for the sequence version which contains the problematic manual chromatogram integration.</show>
151272	Dostmann P750: Continued and uninterrupted data logging into the file *.dostm is now enabled again. Previously, the data logging was randomly interrupted.
166994	UltiMate 3000 Autosampler: After changing the rack configuration on the ePanel for an UltiMate 3000 Autosampler it was not possible to write a sequence as the new rack configuration was not available. Now the rack preview in the sequence is updated correctly after a tray change.
172039 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.
172747, 120000	Vanquish Core: When creating new instrument methods in the wizard the current gradient delay volume is no longer used to create a method. Instead, a default value is used. The method transfer option is deactivated by default, a specific gradient delay volume has to be defined by the user, if desired.

ID	Description				
177708	Waters Acquity: When using Waters Acquity Driver Pack 4 and trying either to create a new instrument method or to open the Acquity console from the ePanel, in some instances a problem occurred. A message appeared informing the user that launching the application had failed, and maybe the Acquity driver pack was not installed. This issue has been addressed in Driver Pack 2017 R2.				
177731	DDK Drivers: If a DDK driver (e.g., a Shimadzu driver or Agilent Chromeleon Driver) was running in overlapped mode and the processing method was changed, this would trigger a sequence abort of the driver. Changes to the processing method no longer cause a sequence abort of the driver.				
183309	Calibration Levels for Peak Groups and Fixed Calibration: If Fixed Calibration is enabled or updated in the Processing Method all values of all calibration levels for peak groups have been reset to 1.00000.				
184758	Create User Database: After activating the User Mode for a newly installed Chromeleon the privileges 'Modify Processing Method' and 'Modify Processing Method – Restricted' in the Full Access role were both enabled even though they are designed to be mutually exclusive. With Chromeleon 7.3.2 only the privilege 'Modify Processing Method' is enabled. The other one is disabled by default.				
192357	Baseline monitoring: If a user started baseline monitoring on one PC and then this user or another user tried to stop baseline monitoring on another PC, or the console was re- opened after restarting Chromeleon on the same PC, baseline monitoring would stop, but the "Save Monitor Baseline Data To" dialog didn't open. Now, the "Save Monitor Baseline Data To" dialog opens.				
193502	Injection Query: Grouping query results by Instrument while the query was still in progress would sometimes place injections in a group which contained no instrument information.				
202077	In previous Chromeleon versions moving a remote sequence back to the network data vault to resolve a failed upload scenario sets the sequence to "read-only" even though the user did not have the privilege to do so. The main idea is to lock that sequence to prevent further modifications to that sequence before it is finally uploaded. Therefore, using the "Manual Upload" or " Manual Move" to remove sequences from the instrument sequence queue requires the additional sequence privilege "Make sequence read-only". If the user does not have that privilege a warning message will be presented and sequence will stay in the Instrument sequence queue.				
202533	Download Failure: A data vault configured for load balancing occasionally reports a download failure. Failed" error. The DataError.log would contain the message "Data Vault Service on'' <localhostname'' as="" balancer="" caching="" configured="" data="" discovery="" for="" information="" is="" load="" not="" of="" outdated="" removed.<="" service="" th="" url".="" vault=""></localhostname''>				
209601	In previous versions of Chromeleon, it was observed that the Station Performance Qualification Report had shown inconsistent date/time notation and an unexpected duration. The two timestamps are consistent, and the duration time format has been fixed to display days.				
209265	Chromeleon crashing and strange behavior when using precision higher than 14 digits in Sequence Table columns				
209944	Restore Sequence Version: After restoring a previous version of a sequence via the Data Audit Trail Window Restore operation all injection records which have been finished in the current version but not yet finished in the version to be restored were reset to Idle with an empty injection time. After completing (saving) the restore operation in the corresponding studio window the raw data of such injection records were deleted without any warning or any privilege checks. With 7.3.2 the restore operation will not reset such injection records back to Idle. Instead injection status and injection time are preserved and already acquired raw data are not silently deleted.				

ID	Description			
209969	Component Table: CSV component import would fail if a compound name contained a regex special character, e.g., "+" in (+1) SLSLSP.			
217346	Rheodyne: The ePanels for the Rheodyne MXII and LabPRO now support a maximum of four valve instances.			
217728, 264423, 269153	For Thermo Scientific MS instruments raw data were not saved to the raw data file. This has been fixed. Now the MS driver uses the .NET Writer to create and write to the MS raw file.			
219518	Vanquish Flex Autosampler, firmware versions before 2.06: While executing a pump purge, executing the needle wash twice on the autosampler can cause the issue of erroneously connecting the drainage flow path to the column which may lead to column damage. With firmware version 2.06 and newer, this issue is fixed.			
219747	It was observed that the Chromeleon 7 domain discovery information is not fully removed if Chromeleon software gets uninstalled from a Chromeleon domain member machine. Orphan records must be removed manually using the Administration Console.			
226492	Append Injections via a Worklist (.wlex-Files): Appending new injections to an already existing sequence via a worklist (.wlex-File) failed if the sequence contained custom variables for the injections which were also set in the worklist file showing the error message 'The given key was not present in the dictionary'.			
227053	Shimadzu GC Control: When a connected to a GC-2014, the 'ModelNo' property for the instrument and its ePanel reported the model as "GC-2010A".			
227741 <i>,</i> 248389	For a driver on TDS5 controlled via Terminal Server it was not possible to connect to the ePanel. An error message "Value cannot be null, Parameter name: format" was shown.			
227846	Comparison Details for Report Templates: If a report template contains sheets with more than 1 report table, the first report table having a dynamic number of rows (e.g., summary report, integration report) and one of the subsequent report tables further down in the spreadsheet having report columns with excel formulas, a detailed version comparison of such report templates might have shown differences in these report columns regarding a deviation for a single cell or a cell range reference in these formulas although such differences were not present if the different versions of this report template at all.			
229725	User Management and Services Manager: Local Chromeleon Service Managers will check, according to poll settings, if the User Management, Discovery, and Licensing Services are running on the Chromeleon Domain Controller. If there is large number of concurrent Service Managers connected, e.g., with more than 500 IPCs, the possible high load caused by this number could result in connection failures. With 7.3.2 the communication to check this connection has been revised. The frequency for this check and the corresponding workload for the User Management service is reduced now. Note : After installing Chromeleon on a computer the Services Manager is added to the Windows System Tray. When this computer is started the Services Manager is automatically started and running. For large Chromeleon domains with lots of IPCs and/or			
	workstations it's highly recommended to remove the Services Manager from the Windows System Tray. The Chromeleon Services Manager can be always started manually if necessary.			
232813	Sequence: Occasionally, instrument method references were deleted from the injection list. This occurred even if the user had no privilege to change finished injections.			

ID	Description
234621	The PerkinElmer Clarus 680 GC accepts up to 10 volume values (10%, 20%, 100% of the nominal syringe capacity) for the 10µl and 50µl syringe and 5 values (20%, 40% 100%) for the 5µl syringe. However, the Chromeleon sequence editor would allow entry of different volume values, which would then fail in the Ready Check. This has been resolved. To change to a different syringe, carry out the following steps: Disconnect the GC in Chromeleon Console ePanel and leave the Chromeleon Console open. Change the syringe volume at the physical instrument. Connect the GC in Chromeleon. The syringe volume is updated. Close and reopen the Chromeleon console again to also update the range of allowed volume values.
235168	Privileged Actions: It is now possible to delete entries from t'e 'recent comme'ts' pick list by right-clicking and selecti'g 'Del'te'.
238086	Report Designer: In certain seldom scenarios a report template might become damaged and couldn't be opened anymore. Selecting the Report Designed category in the Studio window for such a report template showed the error message "Object reference not set to an instance of an object".
238339	Email Notifications: If email notifications (for example, for completion of a sequence) were configured to be sent to a user, and the user was retired (but not deleted), notifications were still emailed to the retired user.
238876	UltiMate 3000 WPS-FC: For an UltiMate 3000 WPS-FC with for example, RedTray= 40_Vials, GreenTray= 40_Vials and BlueTray= 96_Wells configured, on the ePanel for the sampler, SamplesFractionsSplitPoint is initially shown as "RA1". Changing this value, for example to "BA1", the ePanel would show a different Split Point "RB9".
239132	PerkinElmer Clarus GC: With an unreliable RS232 connection, signal raw data points can get lost. This could lead to a shift in the retention time of parts of the chromatogram, even though the sequence was not interrupted. This issue has been resolved. If signal raw data is lost, the sequence is aborted at the current injection with a relevant error message displayed.
239150	User Management: Retired user accounts have been still available when creating new ACL- records in the Access Control page of the properties dialog for a datavault or folder. Retired accounts will no longer be available to select when creating Access Control Groups.
241244	Missing audit trail comment for Save As operation: If a Save As operation is executed for a signed sequence the comment entered for this operation has not been saved in the corresponding audit trail record.
242871	Data File Integrity: When a file integrity check detects a discrepancy, the audit trail message now includes both the injection/sequences of the data as well as advice on whether the error was only transitory.
243965	Console: If a sequence contained injections with injection properties (for example, inject volume) that were outside their allowed limits, then the sequence could not be copied to another location in the data vault.
244384	Report Designer: When inserting multiple new sheets into an existing report template during a single Studio Window session Chromeleon may have encountered an 'Out of Memory' exception message.
244394	Data Audit Tra–I - Version Comparison: For sequences located on a multi-user datavault the version comparison of two sequence versions via the "Show Changes" button in the Data Audit Trail window could display the wrong version for the comparison if one of the selected Data Audit Trail entries belonged to an Instrument Controller operation (for example" "Downloa"ed"), and the other to a user operation. As a result, changes were shown that actually belonged to a different Data Audit Trail entry.

ID	Description
245911, 26219	PerkinElmer Clarus GC: When initially configuring a PerkinElmer Clarus GC, entering an invalid setting on the auxiliary pneumatics page would not allow proceeding to the next page even after the settings had been corrected. Now, once the settings have been corrected, it is possible to proceed to the next page.
245913, 28062	PerkinElmer Clarus 580 GC: While it was possible to specify the detector gas flow with one decimal (for example, 2.4 ml/min), the flow was only interpreted as an integer. Now the detector gas flow is executed in the sequence to one decimal. The instrument method wizard now only accepts an integer for the air flow.
249010	Vanquish DAD, MWD and VWD detectors and UltiMate 3000 DAD, MWD and VWD detectors: The online help now states that if the UVLampOperationTime.Limit or VISLampOperationTime.Limit is reached the system issues a warning and if the UVLampOperationTime.Warning or VISLampOperationTime.Warning is reached the system issues a message.
250819	Peak Group Calibration Levels: If peak groups, within a processing method, contained calibration levels withnon empty values and a sequence on a network datavault containing such a processing method had been downloaded to a XVault, the amount values of these calibration levels of the peak groups would be automatically set to empty values. If this processing method was subsequently modified by a user while the sequence was still downloaded, the amount values were also set to empty values for the original sequence on the network datavault, even if the user h'dn't changed anything within the peak group table. Similar behaviour was observed when creating a CMBX-File with a processing method containing calibration levels for peak groups. Restoring such CMBX-Files reset the amount values for all calibration levels of peak groups to 1. See also the impact of the CMBX-File use case in section 4.7 Other Limitations, same ID 250819.
251644	DDK Drivers: A Smart Startup during a sequence run that resulted in a failed equilibration would lead to an access violation.
252790, 281282	Licensing: The first time a user logged into a Chromeleon domain from a remote client, "a "No License Availa"le" error message was displayed. This applied to AWS and Citrix clients as well as thin clients.
257138	Agilent 7890: The ePan'l 'Conn'ct' button would sometimes be disabled and indicate that the instrument was not connected, even though the instrument was in fact connected. Resolution requires updating to version 2.5 of the Agilent Drivers for Chromeleon.
258175	Remote Inject Device: The inject volume range of the remote inject device has been limited to 2 mL. The inject volume range has been increased to 10 mL.
252854, 252856	Export: Exporting a report template which contains many references to the report variables ms.spectrum and peak.mspec would sometimes take hours to complete. This could occur for example when repeatedly using these variables in calculations, when doing large numbers of library searches or when repeatedly evaluating these variables as part of an SST (System Suitability Testing). The same issue was observed with report template which contain many references to the report variables ms.statusLog or ms.tune().
253095	Admin Conso–e - Scheduler: Audit section – in order to provide more clarity, "Audit Trail Settings" was renamed to "Scheduler Service and Task Audit Trail settings"

ID	Description
254875	The Scheduler Service logs of Chromeleon version prior 7.3.2 only keep three rolling backups, and the maximum log file size was limited to 1MB. There was no possibility of adjusting the logging configuration using the common log4net.config and changing the values of maxSizeRollBackups and maximumFileSize. This limited the ability to troubleshoot large scheduled tasks as the amount of logging done exceeds the content captured in three 1 MB log files.
259247	Services: Stopping and restarting the Microsoft Cryptographic Services would cause several Chromeleon services to stop running, thereby causing Chromeleon to stop functioning on that PC.
261139	MS Processing: When identifying peaks using 'Spectrum-only matching ', if the peak window was wide and the chromatogram contained many peaks, switching between injections was very slow.
261494	SCION 450 GC: Configuring the SCION 450 GC driver would fail with a fatal error displaying an error message "Chromeleon Instrument Configuration: The configuration cannot be changed. Driver 450 GC (SCION450GC.Driver.dll) has terminated. This is a fatal error, you need to restart the Instrument Controller to recover."
261970	Atlas Peak Detection: With certain chromatograms, applying Atlas peak detection could cause the channel to become unavailable. The same issue could arise with some imported Atlas workbooks.
262075	eWorkflows: Sequences generated using an eWorkflow did not populate the Replicate ID Column when replicates were specified. Now, if the ReplicateId field in the eWorkflow is empty, the Replicate ID will be set to the vial position. If the ReplicateId field in the eWorkflow is not empty, Replicate IDs will be based on the entered template. The template supports the same field codes as the InjectionName field.
262284	Administration Audit Trail Query: Certain Administration Audit Trail Queries with Advanced Search Criteria combining rules with logic operators AND and OR couldn't be opened anymore once they have been saved.
262854	Export: Exporting a report template which references the TIC channel would sometimes take hours to complete.
267370	Copying Signed Sequences: It was not possible to copy or move signed sequences having injection records containing raw data to a different data vault if these injection records also had different versions. The copy operation would report an exception with the error messa'e 'Object reference not set to an instance of an obj'ct'.
267560	Custom Variables of Peak Groups: When a new custom variable has been created for the peak group table in a processing method and the component table contained lots of component records (for example, >200) the studio window was blocked for an extended time period (2 minutes and more) until the user could continue working in this Chromeleon session. This performance bottleneck has been removed. Creating new custom variable for peak group tables is now executed immediately even for processing methods with many components.
268343	Instrument Audit Trail: When viewing or printing a report of the Instrument Audit Trail, the instrument name was not included in the report header.
269056	Injection Locking: When multiple users had opened the same sequence in a chromatography studio window and one user locked an injection the other user could still modify the same injection by manually integrating a chromatogram. The save operation for the injection was not prevented in this case although the injection has been already locked.

ID	Description			
271095	SCION 450 GC: It was not possible to configure a SCION 450 GC with more than one methanizer. When trying to connect the SCION 450 GC the driver would disconnect with an audit trail ent"y "{450GC} The device could not be connected (Sequence contains no elemen"s)".			
272764	SCION 450 GC: A value entered for the column flow in Constant Flow mode in the Instrument Method Wizard was not visible in the Instrument Method Editor. A value entered for the column flow would disappear when saving the method.			
273802	Vanquish HPLC: Smart Startup no longer forces the user to open the pump purge valve when the option to purge is not selected in the Smart Startup settings of the instrument method.			
273614	Vanquish Dual Split Sampler with Charger: The sequence is no longer aborted when opening/closing the charger door during a queue run. This abort only occurred if more than one sample rack has been transported from the Vanquish Charger to the Vanquish Dual Split Sampler for injection.			
278758	Injection Query: Position of Custom Variable Columns was not preserved or saved when injection query was re-executed			
280360	Instrument Controller: Following an instrument audit trail save error it could happen that the home data vault was changed to another data vault if the original home data vault was not available.			
285145	ICS-2100, ICS-3000, ICS-5000 and ICS-6000: For the ICS-2100, ICS-3000, ICS-5000 and ICS- 6000 it could happen that the driver would repeatedly log a message at high frequency (several thousand messages per second) to the Instrument Audit Trail. This would result in the (Daily) Instrument Audit Trail growing to a size of several dozen MBs. Trying to open such a large Daily Instrument Audit Trail crashed the client with a System.OutOfMemoryException. In addition, Chromeleon could no longer write to the Instrument Audit Trail, which ultimately resulted in the loss of audit trail entries after 48 hours.			
286258	SCION 430/450 GC: The Instrument Method Wizard for the SCION 430/450 GC the Fluidic Setup page would show empty check list boxes for the selection of GC components. It was not possible to select any components. When continuing through the Wizard and closing it, an exception was thrown.			
286750	Licensing: Moving an Instrument Control PC from the Global group to an Org Unit, or from one Org Unit to another would result in duplicate entries in the Instrument Controller section of the Admin Console License Manager. These duplicate entries incorrectly consumed additional licenses.			
287469	Injection Query: Rerun of unsaved queries ended up with an error.			
287779	Studio Wind–w - Component Identification Status: The identification status of a component was not reported when viewing the corresponding status in the navigation area of a studio window for a sequence, section Components. Instead of showing either the status Detected or Not Detected for the currently selected injection, the navigation area always report'd 'Not Evalua'ed' for all components. For sequences with MS data this problem d'dn't occur.			
288104	Calibration plot: After viewing the calibration plot for an undetected component, it was sometimes observed that the y-axis autoscale setting would become unchecked, causing improperly scaled plots. This applied to both the Interactiv' ('Data Process'ng') plot and the Report Designer plot.			

ID	Description
288554	Vanquish Sampler: Instrument methods created for the Vanquish Sampler (VH-A10-A, VF-A10-A, VC-A10-A) using the Instrument Method Wizard in Chromeleon 7.3.1 would fail when overlapped sample preparation (PrepareNextInjection) was used. This has been resolved.
290350	Version Comparison: Changes made to the Statistics portion of the SST/IRC rules were recorded in the data audit trail, but the details of the changes were not visible in the version comparison window.
291396	XPS: Chromeleon XPS would crash if injection or sequence custom variables were left blank
291965	Processing Method: When certain MS Components were copied from one processing method and pasted into another, it was then no longer possible to delete the component.
297153	Autoreporting: The Chromeleon Autoreporting Service would stop wh"n "Log On"As" was configured to use a user account not in the local Administrator group. In addition, a Windows admin user may also need to manually delete the PrintServiceActiveJobs.xml file, found in C:\ProgramData\Dionex\Chromeleon\.
298191	System Printers: Adding/Editing system printers did not require t'e 'Modify Global Security Setti'gs' privilege
299133	Vanquish FLD: While runni"g "ValidateRa"an" "r "CalibrateRa"an""a "not ready st"te" was reported. Now, if a data acquisition is launched during the aforementioned processes, a more appropriate error message is reported. The previous error messa"e "Cannot start acquisition "0}" is not shown anymore.
299216	Vanquish FLD: Changing the response time settings during an actively running data acquisition is now rejected with an appropriate error message.
302261	Report Variables: When no adducts were specified, the report variabl"s "injection.chemical_formula_and_adduct"()" a"d "injection.chemical_formula_and_adduct_masse"()" would return "n.a"
305697	Markes Thermal Desorber: Submitting a sequence with the SampleGas sequence variable set to 'o "ir' would result in the sequence failing to start due to a Ready Check Error.
307089	Vanquish Fraction Collector (VF-F11-A): The firmware version reported by the driver was alwa"s "1"03", independent of the actual firmware version running in the device. This has been corrected, the property now reports the appropriate value, for examp"e "1"11".
309236	Spectra Plots and Fixed Channel: Using the Fixed Channel option in spectra plots (UV, MS, FLD or I-T) in the Report Designer did not work. The peaks for the corresponding spectra plot were always picked from the currently selected channel in the Studio window or the default channel of the sequence.
314297	Administration Console: All Resources: Manually removed resources reappeared after a short time.
331148	Elemental Composition: Due to differences in hidden default settings, the Chromeleon list of matching chemical formulas would sometimes differ from those reported by the Thermo Scientific FreeStyle software.
313597	Online help was updated to include information about the menu opti'n 'Sh"w "Push Notificat"on" subscriber I'st' appearing on the Domain Resources>Computers screen in the Administration Console.
326668	NTMS Data Processing: Filtering of target components from the new peaks list did not work properly when target components were defined using relative retention time.

ID	Description		
328136	Solvent composition and "Diagnostics" screen. According to Waters this issue has been addressed in 2695 Firmware version 3.0. From Waters Release Notes: Previously, if you used the Menu/Status key to gain access to the Diagnostics screen, and then you pressed the Menu/Status key to return to the original screen without closing the Diagnostics screen, a change in solvent composition could occur. The Menu/Status key is now disabled on all the front panel diagnostics screens except Keypad Diagnostic. You must properly close the Diagnostics screen by pressing the Exit key before returning to the original screen.		
328345	netCDF Import: If a netCDF (AIA) file was missing a value f"r "peak_retention_t"me", then the import would fail with" a "Value cannot be nu"l." error.		
333545	Atlas Data import: Importing an Atlas workbook into Chromeleon 7.3.1 would fail to import peak integration and peak results if the channel name contained bracke"s""(" a"d"")".		
333563	Atlas Data Import: Importing an Atlas workbook would fail with the messa"e "value out of ra"ge" if a calibration level was reported "s ""/A".		
347320	Exporting an instrument configuration no longer triggers a privileged acti"n "Modify Instrument Configurat"on".		
350650	Electronic Signature: If a sequence contains a processing method with reference mass spectra for components, the verification for such a sequence after a successful submit always failed. With Chromeleon 7.3.2 the verification of sequences submitted with prior Chromeleon releases still fail. For successful verification, the applied signature needs to be removed and reapplied.		
356631	Orbitrap Exploris 240: The Instrument Method Editor would not display the MS settings page upon re-entry to that page. Note that this only partially resolves the issue: Displaying the MS settings page is still slow.		
356898	Scheduler: Before Chromeleon 7.3.2 copy/move tasks did copy/move sequences from the Chromeleon 7 recycle bin.		
360163	Agilent 7890 GC: In instrument configuration, clicking OK did not save changes to the settings for detector signal factor, offset or TCP port.		
364318	Running sequence icon not displayed in Chromeleon console on sequence folder		
365309	DDK Drivers: A Smart Startup during a sequence run that resulted in a failed equilibration would lead to an access violation.		
377962	On a system with a DDK driver the Instrument Audit Trail and the Injection Audit Trail contained an unusual amount of entries due to repeating recorded error messages for some injections. Submitting a sequence would fail with a System.OutOfMemoryException. It was not possible to apply an electronic signature to a sequence. The error message indicated "Cannot load data for it'm 'chrom:///xxxx.smp/Audit.au'i"'." and the Data Audit Trail indicated: "ERROR Data.DbConnectionAdapt-r - [] GetRawDataHash and Exception of ty'e 'System.OutOfMemoryExcept'on' was thrown".		
379505	GCMS TSQ: Editing a scan list in the Instrument Method Editor, for example deleting a large number of entries, was slow.		
379506	Vanquish Core: The retention time would continue to increase after the completion of "a "Purge needle w"sh".		
379509	Dionex / Shodex RI-101 detector: Instead of a warning messa'e 'detector has lost acquisition d'ta' the audit trail now reports an error message.		

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
172030	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.
CM7-25370	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 7.3.2 does not support Smart Startup, Smart Standby or Smart Shutdown settings for inverse (or tandem) gradient methods. Hence in Chromeleon 7.3.2, 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.
CM7-25447	Vanquish Drivers: Vanquish Duo Autosampler: When adjusting the needle height, this is only adjusted for the left-hand sampler unit, and not for both sampling units as would be expected. Use the property Sampler2.SampleHeight to adjust the needle height for the right-hand sampling unit
148280	VH-D10-A Vanquish DAD HL: In very rare cases, the injection is running continuously, and the UV signal is not recorded.
171456	 When migrating from Chromeleon 6.8 to Chromeleon 7.3.2 (under Windows 10), UltiMate 3000 system(s) connected via USB may result in the PC to which these instruments are connected not starting. Workaround: Disconnect the USB cables for the UltiMate 3000 system(s) before starting the PC, start the PC, then connect the UltiMate 3000 system(s) via USB.
171977	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). 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. 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
172022	Accela Open Autosampler: Sequences cannot be run when the sampler does not include the DIW option. This configuration is not supported and requires a custom script.
172067	Accela Open Autosampler: When using this autosampler, a dot ('.') must be used as decimal separator.

344723	UltiMate VWD-3x00(RS) and Dionex ICS-VWD: On an UltiMate system with two detectors, an idle VWD-3x00(RS) can cause a sequence interruption with an error messa"e "No response from VWD-3000 @ USB- <id> for 300.000000 seco"ds"). Similar for the Dionex ICS-VWD. Workaround: If you are using VWD firmware version < 4.10, try upgrading to VWD firmware version 4.10. With VWD firmware version 4.10 the stability of the USB-handling has been improved. However, even with VWD firmware version 4.10, if the UltiMate VWD-3x00(RS) (or Dionex ICS-VWD) is not in use for an extended period of time a spontaneous disconnect can occur. For VWD firmware version 4.10 and earlier: If the VWD-3x00(RS) (or Dionex ICS-VWD) is not in use for an extended period of time, disconnect it form Chromeleon and only connect it when actually using it. If a spontaneous disconnect of the VWD-3x00(RS) (or ICS-VWD) has occurred, reconnect the VWD-3x00(RS) (or ICS-VWD) to resume communication.</id>
172041	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.
СМ6-22760	TRACE 1300 GC: The autozero function does not work correctly for the FID, NPD, ECD and FPD detector types.
CM7-25600	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)". The workaround is to close the Virtual Terminal on GC1 before attempting to start the run on GC2.
CM6-23614	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.
CM6-24043	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.
172735	TriPlus 500 HS: When acquiring a sequence with overlapping sample preparation, the system may create an audit trail log event regarding a vial/injection that is not the current injection. When this occurs, the event is logged to the current injection rather than the preparing injection to which it relates.
CM7-25760	MS Drivers: When working with MS devices, the raw file must 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.
CM7-15632	TSQ Quantiva and Endura: When removing the source from a TSQ Quantiva or Endura in mid-acquisition, the sequence does not abort.
СМ7-16030	TSQ Quantiva and Endura: With these instruments the standby state reports that the instrument is on, regardless of the real instrument state.
CM7-16154	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.
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.
СМ7-21967	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.
СМ7-16557	MSQ Plus and Tune Application: When using the MSQ Plus with Chromeleon the user must 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.
172740	There are known issues where saving or modifying MSQ Plus instrument methods or Tune files fail. This change in operation has been linked to applying monthly Microsoft Quality updates to Windows 10 and Windows 7 operating systems. Removing the Windows KB Updates will resolve the issues in most cases. However, in certain situations, it may be necessary to restore the system to an earlier point before the Windows Updates were applied. It is strongly recommended that automatic updates for Windows be disabled on systems running MSQ Plus instruments. Any Windows Updates that are planned for application on systems running these instruments should be tested at the installation site before they are installed on a system in active use.
СМ7-20295	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.
СМ7-17500	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 this process, please consult with your local MS field service engineer.
114502	MS Tuning: When one or more MS Tune Reports are deleted from their default folder (/Instrument Data/(Instrument Name)/MS Tune Reports) the list of available Tune Reports on the MS ePanel will not be automatically refreshed to reflect the change. This can occur if the reports are deleted manually as well as if they are deleted automatically (when automatic archiving is enabled) The workaround is to close and reopen the Chromeleon Console.

245918	MS Tune: The embedded tune window in Chromeleon can be closed while running a calibration by exiting Chromeleon. The Chromeleon window closes and the calibration continues. An invalid entry will be added to audit trail e.g., 'Diagnostic run finished with result passed'. Restarting Chromeleon immediately will open Tune to allow the user to start a new calibration while the previous calibration could still be running. This in turn means that the results of both calibrations can be unreliable. This is different from the behavior of the stand-alone Tune application. When closing the stand-alone Tune application, a warning "Calibration is in progress. Do you want to close Tune application?" is shown allowing the user to confirm or cancel closing the stand-alone Tune application.
28276	LC Drivers: A Vanquish instrument with two Column Compartments cannot be configured. The underlying cause for this issue may be insufficient USB bandwidth to fulfill the bandwidth reservations made by the instrument modules. When a second Column Compartment driver instance is configured with the USB address that is already used by the first Column Compartment, an error message indicates that the selected USB address is already in use.
35925	Vanquish Variable Wavelength Detector: If the shutter is opened or closed manually (e.g., via ePanel), no firmware download is possible afterwards. The audit trail message is "Error: Cannot start firmware installation. The module is still busy." Workaround: After opening or closing the shutter manually (e.g., via ePanel), disconnect and reconnect the Vanquish VWD before downloading the firmware.
53052	TSQ MS Tuning/Calibration: If the instrument is disconnected while a tune/calibration operation is in progress, the tune will not automatically fail or abort. It may be an hour or more before the instrument audit trail reports that the MS is disconnected. If the instrument is reconnected, the calibration will automatically resume.
115504	Vanquish Core modules require a minimum firmware version 2.01 or 2.02 for pumps, respectively. Please also use firmware version 2.01 (FW version 2.02 for pumps) for any new modules of the Vanquish Flex and Vanquish Horizon series. Vanquish Core modules can be combined with Vanquish Flex and/or Vanquish Horizon modules in one instrument as long as firmware version 2.01 (FW version 2.02 for pumps) or higher is used for all modules. For existing Vanquish Flex and Horizon modules, firmware version 2.01 (FW version 2.02 for pumps) as stated in the List of Supported Instruments.
142047	MS driver: TSQ Altis: There is no report variable available for the module serial number.
162479	Vanquish Driver: For the Vanquish DAD FG/CG and MWD CG, the wellness properties for the UV/VIS lamp operation time limit and warning were transmitted enlarged by a factor of 4 to the instrument. Warnings and limits are now transmitted correctly to the instrument.
	operation lifetimes, these will now be read out from the firmware at 4 times the intended value. If you wish to remain with the initial settings, you will need to adapt the values set for the UV/VIS lamp operation time limits and/or warnings in Chromeleon by reducing them to their initial value (25% of new value).
	Example: With Chromeleon 7.3 (or earlier), 7.2 SR5 MUk (or earlier) or 7.2.10 MUa, a setting of UV/VIS lamp operation time limit of 2,500 hours would be transmitted to the firmware as 10,000 hours. After an upgrade to Chromeleon 7.3.2, the value of 10,000 hours is read out from the firmware and set as the UV/VIS lamp operation time limit in Chromeleon. If the intended limit is 2,500 hours, you will need to adjust the limit in Chromeleon to 2,500 hours.

163499	In very rare cases the injection status of an injection stays on "Running" and subsequent injections are not started. Proceeding to the next injection requires a restart of the Instrument Controller. Upon restart of the Instrument Controller the status of the injection is changed from "Running" to "Interrupted" (although "Finished" would be appropriate).
167481	Trying to acquire the pump pressure signal for 24 hrs. with a high data rate (100 Hz) results in an instrument crash. This was seen with an UltiMate 3000 pump HPG-3400RS. This is due to the fact that the signal acquired at 100 Hz for 24 hrs. results in 8.64 million points. The console memorizes these points and increases the size of the respective PointList, which leads to System.OutOfMemoryExceptions in the console. The only way to fix this is to stop the instrument controller and close down Chromeleon.
172736	Vanquish Drivers: In rare circumstances if a transport error occurs with the Vanquish Autosampler (VH-A40-A or VF-A40-A) with a charger (VH-A90-A), it's not possible to bring the system into an operational state using the commands "Reset" or "Cleanup". An instrument controller restart is necessary.
172738	Vanquish DAD HL: Using the command "UV.Shutter Closed" in an instrument method after the Acquisition Off commands, the Method Check does not trigger a warning or error. Using this instrument method in a sequence does not elicit a warning or error in the Queue Ready Check. However, starting the queue fails and Chromeleon reports in the instrument audit trail: "Can't change the 'Shutter' property during data acquisition, or during autozero, calibration and validation procedures." The command "UV.Shutter Closed" can only be inserted after the acquisition off commands using the instrument method script editor by an expert user, who should be aware that the "UV.Shutter Closed" cannot be inserted after the acquisition off commands. Workaround: Use an instrument method without any acquisition or a trigger that waits for the acquisition to end.
172742	IQ/OQ/PQ: For the OQ/PQ for the UltiMate 3000 NCS-3500RS in the warmup and oven test sequence Solvent B shows a wrong value on the specification sheet. Instead of "water + 0.x% acetone" the sheet shows "Caffeine" as the value for solvent B for gradient (correct reference is line 375 instead of 372).
172746	The Vanquish Charger is only supported with Vanquish Autosamplers with temperature control.
172749	The Troubleshooting Guide for the Vanquish Binary Pump VH-P10-A (hardware revision 2) can be found under C:\Program Files (x86)\Thermo\Chromeleon\bin\Troubleshooting Guides English: Man-LC-VQ-PumpH-Operation-DOC4820-4411-EN-1-0 French: Man-LC-VQ-PumpH-Utilisation-DOC4820-4411-FR-1-0 German: Man-LC-VQ-PumpH-Betrieb-DOC4820-4411-DE-1-0
172751	Vanquish Autosampler: The option "External Rack Transfer" is not compatible with Chromeleon User-Defined Programs (UDP's).

195521	GCMS Single Quadrupole instruments (ISQ and ISQ 7000 families) and GCMS Triple Quadrupole instruments (TSQ 8000/9000 families) provide several options (e.g., timed SRM mode) for which the permission to use the option is stored in the flash RAM of the MS hardware. If you purchase the option at the time of the MS instrument purchase, the flash RAM has the option included. If you purchase the option after the MS instrument purchase, Thermo Fisher ships you a small ini file, which you then upload to the MS flash RAM. If a Chromeleon instrument method requires such a GCMS instrument option, but the permission for the GCMS instrument option is not available in the flash RAM of the MS hardware, the Sequence Ready Check and Instrument Audit Trail show an error message. (For example: "Instrument method cannot be run: Timed mode is not allowed under the current license. To enable timed mode acquisitions, please upgrade your software to include time mode.") This error message is somewhat misleading, as it is the flash RAM of the MS hardware that needs to be updated with the relevant permission, not Chromeleon itself.
205589	UltiMate 3000 WPS: Changes to the tray configuration on the ePanel are not immediately relayed to the sequence wizard. When changing a tray configuration on the ePanel, the tray configuration in the sequence wizard is only updated after making another change to the tray configuration on the ePanel.
205590	Vanquish Dual Pump (DGP): If a Vanquish Dual pump is configured with the option "shared bottle" selected, it should not be possible to set different eluent monitoring properties (%A/%B/%C_WarningLimit and %A/%B/%C_Level.LowerLimit) for the two pump units. However, it is possible to set the WarningLimit and Level.LowerLimit to different values for both pumps. This results in different RemainTime values for both pumps, which is not possible with a shared bottle. In addition, %A/%B/%C_Level.Value is divided by a factor of 2. That is, the system switches the pump off at half the intended Level.Value.This limitation is not applicable in cases where a Vanquish Solvent Monitor module is part of the instrument. Workaround: Set the same eluent monitoring properties (%A/%B/%C_WarningLimit and %A/%B/%C_Level.LowerLimit) for both pump units.
238872	Vanquish ISQ Family: If the device name of Vanquish ISQ Family is using Unicode characters (e.g., if it is localized in Japanese) the Ready Check fails.
238873	UltiMate 3000 PCM-3000: For UltiMate Detectors DAD, MWD and VWD with the PCM- 3000, the automatic gain adjustment of the PCM-3000 frequently leads to wrong conductivity channel values.
254951	MS Method Editor: When trying to open the MS method part of multiple instrument methods Chromeleon Studio crashes with "System out of memory".
279701	Exploris 120: Opening the method editor or opening the online help results in an error: "Error in sample changed event handler of object Processing Method Editor. Exception of type 'System.OutOfMemoryException' was thrown." Workaround: Close and re-open Chromeleon Studio regularly when opening / examining MS methods.
296042	Vanquish Core DAD: In very rare cases, when two Vanquish instruments are configured with a Vanquish Core Diode Array Detector each, switching off one of two DAD detectors may lead to a negative interference with the second DAD. The second DAD may stop sending data, and the chromatogram stops to display detector data. As a consequence, the sequence may abort after a time delay.
282028	UltiMate VWD-3400(RS): In the data collection section for the UV portion of a method, the peak width value will change to 0.02 min if the method is saved and reopened. The Data Collection Rate and Time Constant will change according to the Peak Width entered in the Instrument Method Editor and stay at the desired value after the method is saved and reopened.

297798	Orbitrap Exploris: On a system where the Orbitrap Exploris 4.0 SP1 driver has been installed, it is not possible to modify the instrument configuration of the Orbitrap Exploris in the Chromeleon Instrument Configuration Manager. When launching the Chromeleon Instrument Configuration Manager where the configuration was previously created, it stops responding and then closes. Workaround: Delete the instrument controller configuration file from the folder ProgramData, then add the module again or import a saved instrument controller configuration file. If the MS device is clicked again in the Instrument Configuration Manager, the issue is seen again.
298674	Method Translation from UltiMate 3000 to Vanquish: The temperature of the sampler cabin is not correctly translated in case a temperature for the column compartment is set.
299110	Fraction Collector: In the instrument method for a system with an UltiMate AFC-3000 or Vanquish Fraction Collector FT, under the Fraction Collection section the preview window will display the error "Can't determine pump flow as it is not constant over method duration. Parametername: Pump Left" even if the pump flow for the entire method is constant. This occurs when the fraction collection time starts with no set flow around the time it starts, while the collection end time has a pump flow around the time it ends.Workaround: The error only appears when the Pump.Flow.Nominal Command is exactly on the "End Time" and if there is no other Pump.flow command present within the Collection Time Frame. Add another Pump.flow.Nominal command at the Fraction Collection "Start Time" in the Script Editor:954 9,000 PumpModule.PumpLeft.Flow.Nominal PractionCollector.FractionCollection.Collections By_Peak PractionCollector.FractionCollection.Collections Py FractionCollector.FractionCollection.Collection 5 Py PumpModule.PumpLeft.%B.Value Py PumpModule.PumpLeft.%B.Value Py PumpModule.PumpLeft.%B.Value Py PumpModule.PumpLeft.%B.Value Py PumpModule.PumpLeft.%B.Value Py PumpModule.PumpLeft.%B.Value Py PumpModule.PumpLeft.%B.Value Py PumpModule.PumpLeft.%B.Value Py PumpModule.PumpLeft.%B.Value Py PumpModule.PumpLeft.%B.Value
344351	Thermo ISQ and TSQ GCMS: Instrument methods developed for the Thermo ISQ or TSQ GCMS using a driver version older than 5.0 will not be readable or usable when version 5.0 or higher of the driver is installed. The workaround is to either downgrade the driver to the older version of re-create them using the version 5 driver.
347230	Thermo Exploris Series ePanel: On the Thermo Exploris Series ePanel the "MS Parameters" panel is missing.
347312	For a Vanquish instrument it is possible to change the instrument configuration while a diagnostic test is running.
376961	TSQ Fortis: A TSQ Fortis Plus system may throw a memory exception directly after MS data processing. This may also lead to an injection failing. Workaround: Restart the Chromeleon Instrument Controller when the memory of CmDDKHostCL4.exe exceeds 1GB (e.g., before a new Queue is started). This will restart the drivers.

ID	Description
148624	Waters 2690/2695: In very rare cases, a sequence is interrupted with the error message: "Acquisition finished by Chromeleon before first data point could be transferred. Maybe the run time is too short in case of blank run."
172741	Waters Alliance 2695: It is not possible to control a column selection valve installed in a Waters Alliance 2695.
181345	Waters 2690/2695 and 2489: Very rarely a sequence interruption with an error message "Acquity System state has changed to error during run." is seen.
256747	Waters Alliance 2487 absorbance detector: Changing properties on the Alliance 2487 detector ePanel does not apply in the firmware. It is not possible to set the Data_Collection_Rate, AutozeroOnEventIn , AutozeroOnWlChange, FilterTimeConstant, FilterType or Wavelength from the ePanel or from the Command (F8) window. These properties were removed from the ePanel. Only the property Lamp On/Off can be set from the ePanel and from the Command (F8) window.
279507	Waters eAlliance 2695 HPLC and 2998 Detector: When trying to collect data, after the first injection the acquisition stops with an error message: "Acquisition finished by Chromeleon before first data point could be transferred. Maybe the run time is too short in case of blank run". Workaround: The Waters eAlliance separation module and the detector need to be connected via a contact closure cable.
299266	Waters eAlliance 2695 with Waters RID 2414 or PDA 2998: In rare cases with a Waters eAlliance 2695 with a Waters RID 2414 or PDA 2998 data acquisition is not possible and an error message "Acquisition finished by Chromeleon before first data point could be transferred. Maybe the runtime is too short in case of blank run." is shown. Workaround: After inserting the remote signal cables for the detectors, data acquisition starts to work properly.
317906	Waters eAlliance: The curve parameter is handled differently in the GPIB and LAN driver for the Waters eAlliance. For the eAlliance LAN driver if the curve is set to "6" in the Chromeleon IME, a linear gradient is performed. This is the same behavior seen with Waters Empower. Please note that by default the curve parameter is set to "5". The value needs to be actively set to "6" to perform a linear gradient. Also, instrument methods created with the eAlliance GPIB driver are not compatible with the eAlliance LAN driver with respect to the curve setting. Workaround: If no equilibration stage is involved, the curve can be set to 5 at time 0.0 [min] and for times > 0.0 [min] following times to the demanded curve value +1. Note: The IME graphical view of the curve applying to the eluents should be ignored.
331239	Waters eAlliance LAN driver: With an instrument method in which the parameter "HPLC_System.Pump.Curve" is placed right after the parameter "HPLC_System.Pump.Flow.Nominal" in the gradient script, Channel %A switches to 100% right after inject. This can only be observed on the eAlliance display. Workaround: Set the parameter "HPLC_System.Pump.Curve" as the last parameter for a given gradient step. This is achieved when using the IME to create the gradient.

5.2 Limitations with Waters Instruments

5.3 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
СМ7-19347	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.
СМ7-20047	Agilent VWD G1314B: When using a G1314B VWD, occasionally the chromatogram is half the expected length.
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.
CM7-21427	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
CM7-22567	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.</channel>
СМ7-19540	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.
СМ7-25781	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.
CM7-23242	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.
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.
CM6-24004	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.
СМ6-24005	Agilent 7697A: When 7697A headspace instrument method parameters are included in a report, the "fill pressure" parameter is rounded to the nearest integer.
СМ6-24007	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.
СМ6-24009	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.
165661	Agilent 1290 ELSD: For an Agilent 1290 ELSD controlled by Agilent ICF drivers, the sequence interrupts with an error message: "Error 155: An error occurred during data collection. Data integrity compromised." This issue has been reported to Agilent.
165966	Using an Agilent LC system with a sampler and the Agilent LC-ICF Drivers on a Japanese, Chinese or Brazilian Portuguese O/S, the sequence wizard does not allow creating a sequence.
	Workaround: This issue is caused by a language satellite DLL provided by Agilent Technologies (Agilent.LCDrivers.Sampler.BusinessObjects.resources.dll). Removing this satellite DLL addresses the issue, while presenting the user interface in English language. For example, on a Japanese O/S remove "C:\Program Files (x86)\Agilent Technologies\Instrument Control Framework\ja\Agilent.LCDrivers.Sampler.BusinessObjects.resources.dll". Alternatively, use Agilent Chromeleon Drivers instead of Agilent LC-ICF Drivers to control the instrument.

172059	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 1 is already acquiring, and the Abort option has been selected, the entire sequence will be aborted, including the acquiring sample 1.
172753	Privileges: The privilege "Control Instrument While Queue is Running" does not apply to ICF controlled instruments. This privilege only applies to actions through Chromeleon properties or commands (command box or standard ePanel elements). It does not apply to actions through the Agilent Status UI.
192715	Agilent LC ICF: Aborting an injection after the start of a sequence but before the injection results in an error, requiring the instrument controller to be restarted.
224052	Logging off from the Instrument Configuration Manager is now reported in User Management Audit Trail.
222538	Agilent ICF driver: When reconfiguring ICF-based LC System, then opening the instruments page in the Console, the ePanel no longer shows the status windows for the individual submodules. Clicking on the ePanel control results in the crash. This is also seen with Agilent Drivers for Chromeleon.
259115	Agilent LC System: Using an Agilent LC system with the ICF driver, a running sequence may be interrupted with an error "Undefined complex Type 'LCMethodBaseType' is used as a base for complex type extension." Workaround: We recommend using Agilent Drivers for Chromeleon.

5.4 Limitations with Agilent Drivers for Chromeleon

ID	Description
143713	Agilent 12xx LC: If an Agilent 12xx LC configuration includes the Agilent 1290 Infinity Flexible Cube, the Flexible Cube needs to be enabled in the instrument method. When creating an Instrument Method, Chromeleon provides an option (check box) to select if the Flexible Cube is used. If this check box is cleared, the sequence will interrupt. Workaround: Remove the Flexible Cube from the Instrument Configuration to run a sequence for which the Flexible Cube is not needed.
216488	Agilent LC Autosampler: When using pretreatment method for an Agilent LC Autosampler it is not possible to use a command like "Eject 40.0µL to seat with 200µL/min" via the user interface as this results in an error message. Agilent confirmed that this is known issue, which has been addressed with LC Driver 3.4. However, LC Driver 3.4 is incompatible with ADC driver (version 1.x and 2.x) due to .NET restrictions. Workaround: It is possible to set this parameter from within the method script. However, reviewing the method via the graphical user interface different parameters are displayed.

280985	Agilent ADC 2.5: For a sampler with a long sampler device name, in the message indicating 'waiting for inject response from <samplername>' the sampler's device name is truncated to 15 characters. If two injectors are used on the same instrument both with device names exceeding 15 characters (and equal in the first 15 characters), this will lead to a crash during driver initialization.</samplername>
	Workaround: Use sampler names with less than 16 characters, minimally ensure that the sampling devices can be identified uniquely based on the first 15 characters of the sampling device name.

5.5 Limitations with Other Third-Party Instruments

ID	Description
172044	Agilent 1100 Obsolete Driver: Occasionally, when using a combination of older and newer modules, the raw data was not correctly acquired.
171971	Agilent 6850: Instrument Configuration Manager does not report mismatches between the hardware and the Chromeleon configuration.
CM7-12366	Agilent 5890 DICE Card: Please note the following when using the19257 DICE card with the Agilent 5890 GC: Control and acquisition using the DICE card is only supported via the serial interface. The
	GPIB interface is not supported.
	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.
	Currently, it is possible to select certain illegal combinations in the Configuration Dialog such as:
	Digital acquisition with the 19254 card. This is not supported.
	Digital acquisition on one detector and analog acquisition on the other. Acquisition needs to be exclusively digital or exclusively analog.
	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.
	Note that when performing analog acquisition, the 5890 INET mode should still be set to "LOCAL" (as described in the online help).
СМ7-9675	Agilent 7890 GC (legacy driver): 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.
CM7-24724, 26224	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.
27896	Privileges: The privilege "Control Instrument While Queue is Running" does not apply to ICF controlled instruments.

CM7-15400, CM7-15556, CM7-15734, CM7-15736	PerkinElmer LC200 Autosampler: When upgrading from earlier versions of Chromeleon 7 CDS to Chromeleon CDS 7.3.2, 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.			
172037	PerkinElmer Clarus 400 GC: Some users must select AutoSystem XL in configuration in order to communicate with the PerkinElmer Clarus™ 400.			
161617	Shimadzu LC 20 native driver: If the flow rate for a pump has exceeded upper limit, the sequence aborts with an error "HPLC_System Fatal Instrument Error (-1073708575, 1)." The Shimadzu documentation states the following for the error code C00081E1 (hexadecimal converted from the decimal -1073708575):			
	0x81E1	Pump: Flow rate has exceeded upper limit.	The binary/ternary gradient system is configured with pumps of different flow rate ranges.	Check the instrument configuration.
172062	Shimadzu L instrument unexpected	.C-10A, LC-2010: If th and then, for examp d effects during the r	ne user cancels the key lock state of ole, stops a manual acquisition, this next operation such as sudden abor	the front panel of the is likely to lead to t of the sample run.
171991	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. 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. Several of the Shimadzu devices can be controlled by obtaining an updated driver directly from Shimadzu (see the "List of Supported Instruments" for details).			
141735	Shimadzu F Timeout wi Workarour driver versi acquisition volume to 0	Shimadzu Prominence-i Series: A sequence was interrupted with the error "Abort Error: Timeout while waiting for the instrument to finish, the current injection will be aborted." Workaround: The Release Notes provided by Shimadzu describe a workaround for LC driver version 2.20 or later: When the system is waiting to start a blank run, the data acquisition may be interrupted in some cases. As a workaround, please set injection volume to 0.0 and change the type to "unknown".		
171972	Shimadzu L activated d	.C: For the Shimadzu uring a run from the	LC-10, LC-20 and LC-30 the instrum instrument front panel.	ent standby can be
172024	Shimadzu L the 'Advan command.	.C: Unlike most drive ced' filter in the Com	rs, some Shimadzu UV detectors rea mand (F8) window in order to acce	quire that you select ss the Lamp On/Off
194996	Shimadzu 2 negative nu Workaroun signal to 1. problem or separator a	2030: When collectin umber. nd: In the driver conf 000 manually. Seems n some systems with are swapped).	g UV data, in rare cases the signal d iguration set the signal factor for th s to be 1000 in some cases (most lik specific languages, in which separa	rops to a very large e PDA_Spectrum ely a localization tor and thousand

228857	Shimadzu LC 2030: Setting the instrument method to use "DataAcquisition=False" in the sequence run, may result in sequence interruption on the Shimadzu LC 2030 with an error message: "The following device is blocking the injection run termination: HPLC_System". This is an issue with the Shimadzu LC Driver. Workaround: Set the instrument method to use "DataAcquisition=True".
227295	Markes TD: If an instrument configuration includes a Kori-xr, then methods created in Chromeleon versions prior to 7.3.2 will fail a 'Ready Check' when submitted as part of a sequence. To resolve this issue, open the method in the editor and, on the script page, delete the command(s) that reference the "KoriTrapHeatingRate".
256522	Bruker Scion GC: Installing the drivers Bruker Scion 430 GC and Scion 450 GC causes a number of warnings in the Chromeleon IQ Report stating "The file was not installed by any of the known packages." These warnings can safely be ignored. SCION 450 GC: Warnings for the following files in the directory C:\Program Files (x86)\Thermo\Chromeleon\Bin\DDK\V1\Drivers\SCION\450GC: 450GC_20.bmp, 450GC- Help-en.chm, ACE.dll, DDK.dll, DriverCert.xml, ECC.dll, ECC_Client.dll, GC450_Node.dll, General.dll, iconv.dll, libxml2.dll, log4net.dll, lua51.dll, Lua51.dll, MultiLanguage.dll, Node.dll, Node_Client.dll, NodeView.dll, NodeXML.dll, Observer.dll, OSX_Layer_ACE.dll, SCION450GC.Common.dll, SCION450GC.ConfigUI.dll, SCION450GC.DDKInterface.dll, SCION450GC.Driver.dll, SCION450GC.Shared.dll, and zlib1.dll, and for the following files in the directory C:\Program Files (x86)\Thermo\Chromeleon\Bin\DDK\V2\Drivers\SCION\450GC: 450GC-Help-en.chm, DriverCert.xml, log4net.dll, SCION450GC.Common.dll, SCION450GC.EditorPlugin.dll, and SCION 430 GC: Warnings for the following files in the directory C:\Program Files (x86)\Thermo\Chromeleon\Bin\DDK\V1\Drivers\SCION\430GC 430GC_20.bmp, 430GC- Help-en.chm, DriverCert.xml, SCION430GC.Common.dll, SCION430GC.ConfigUI.dll, SCION430GC.Driver.dll, and SCION430GC.Common.dll, SCION430GC.ConfigUI.dll, SCION430GC.Driver.dll, and SCION430GC.Common.dll, SCION430GC.ConfigUI.dll, SCION430GC.Driver.dll, and SCION430GC.Shared.dll, and for the following files in the directory C:\Program Files (x86)\Thermo\Chromeleon\Bin\DDK\V2\Drivers\SCION\430GC: 430GC-Help-en.chm, DriverCert.xml, SCION430GC.Common.dll, SCION430GC: 430GC-Help-en.chm, DriverCert.xml, SCION430GC.Common.dll, SCION430GC: 430GC-Help-en.chm, DriverCert.xml, SCION430GC.Common.dll, SCION430GC: 430GC-Help-en.chm, DriverCert.xml, SCION430GC.Common.dll, SCION430GC.EditorPlugin.dll, and SCION430GC.Shared.dll.
335233	Markes TD: After running a method that specifies tube recollection using sequence variables (i.e., custom injection variables in the sequence), if the next method (same or subsequent sequence) supports recollection, but it leaves the sequence variables section blank, then it will continue to recollect on the last tube recollected. The workaround is to add a SeqVar_RecollectionType=None to the method script to ensure recollection is disabled.
335233	Markes TD: Running a sequence with a recollect method and then setting RecollectionType to "None" or "SameTube", but leaving the RecollectionTube blank will cause a ready check error. The workaround is to always specify a RecollectionTube. The value will be ignored when RecollectionType = "None" or "SameTube"
335233	Markes TD: The Online Help and eWorkflow provided on the DVD both specify the possible values for RecollectionType as "None", "Same" and "Tube". The driver doesn't support the value "Same"; instead, it expects "SameTube". The workaround is to specify "SameTube" instead of "Same" when setting up the custom injection variable for RecollectionType.

5.6 Limitations With Setup

п	
u	_

Description

CM7-21780	Setup: NIST MS Search and Demo Library No Longer Automatically Installed: Incompatibilities of the NIST 2008 MS Demo Library installer with Window 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. Note that MS library searching within the Chromatography Studio is not affected by this issue.
CM7-23341	Setup: When Agilent ICF is installed, un-install of either Chromeleon or Agilent ICF fails if the Instrument Controller is running:
	 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. To avoid this issue, stop the Instrument Controller before uninstalling
226887	As part of the Chromeleon installation, the Microsoft Edge WebView2 Runtime will be installed, and its installation package is added to the package cache of the machine so that it can be reused for the repair/modify scenarios of Chromeleon. When uninstallation Chromeleon the corresponding package of the WebView2 Runtime component will be removed from the package cache of that machine. It is expected that this package is kept in the package cache as this system component is kept on the system after the uninstallation of the Chromeleon software. Workaround: Select the Microsoft Edge WebView2 Runtime entry of the Add/Remove program dialog of the Windows OS system and click on the repair/uninstall option. Clicking Repair will connect to the Internet. The package cache is NOT recreated, but Microsoft Edge WebView2 Runtime is properly installed afterward. Clicking Uninstall will remove the Microsoft Edge WebView2 Runtime component from the machine.
254867	Depending on the state of the machine GAC the IQ of Chromeleon 7.3.2 may report the following recommendation: "C:\Programme (x86)\Thermo\Chromeleon\bin\System.ValueTuple.dll: The file is a shared library and a different version (System.ValueTuple, Version=4.0.0.0, Culture=neutral, PublicKeyToken=cc7b13ffcd2ddd51) of it is also installed into the global assembly cache including a binding redirect. The redirected library will always be loaded from the shared files location and never this one. Please ensure that this is by intent and does not cause any unwanted side effects." The compatibility of these two different "System.ValueTuple.dll" file versions is very high, it is not expected that it causes any issue in Chromeleon and the recommendation can be ignored.
367826	Setup in combination with Waters Driver Pack: Chromeleon versions 7.3.1 and older on a system with Waters Drivers Pack preinstalled; try to uninstall the optional component Waters Driver Pack during uninstallation of that Chromeleon version. During the upgrade installation from an older Chromeleon version to Chromeleon 7.3.2, this uninstallation routine of the pre-installed Chromeleon version (mentioned before) is executed before installing the new Chromeleon 7.3.2 components. Although the 7.3.2 setup did not request this component Waters Driver Pack, the uninstaller of the older Chromeleon version removes or tries to remove the Waters driver pack (depending on if the CM7 ISO file is mounted or not). After the installation of Chromeleon 7.3.2, the pre-installed Waters Driver Pack installation needs to be reinstalled.

5.7 Other Limitations

ID	Description
CM7-22986	During stress tests with multiple, very long sequences with more than 1000 injections, the queue was aborted with an unexpected error: "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". 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." As a workaround it is recommended that automatic upload be disabled when running very large sequences and uploading them manually instead.
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 has to restart the corresponding Chromeleon 7 Scheduler Service to get this kind of deadlock being resolved.
CM7-23051	In a few cases Sequences have been reported to abort with messages in the audit trail that were not conclusive, such as: "The injection audit trail / signal "" cannot be saved. Error detail: The transaction has aborted. The transaction commit operation failed." 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.
СМ7-25508	Upload: In very rare cases, an upload may succeed, however the sequence remains locked (redirected to the XVault).
SWFR-248	 Waters Empower Import: The following limitations apply to the import of data from Waters Empower: 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.
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 μ L as their default volume unit. If one of these devices is configured in the same instrument that also includes an injection device that uses μ L, problems may be observed with volume validation in the sequence table as well as units associated with volumes in reports.
120335	Queries: When using Oracle as a data vault server, text-based queries (e.g., searching for an injection name) are case sensitive. So, for example searching for "Extract" would not return matches for "EXTRACT" or "extract". This limitation does not apply to SQL Server data vaults since SQL Server text searches are case insensitive.
138190	Opening an instrument method that is assigned to a not available instrument takes up to 40 seconds for the first attempt. Subsequent attempts are faster. The issue is caused by DNS resolution of the host name. Workaround: Create an instrument in simulation mode and assign the method to this
---------------------	---
	instrument. Afterwards the instrument can be deleted. The DNS look-up will be faster as the physical PC is still existing.
147417	Report Variables: The report variables peak.evaluate, chm.evaluate and injection.evaluate expect a formula in the invariant format (e.g., ',' as list separator, '.' as decimal symbol). The evaluation does not work if other regional settings (e.g., ';' as list separator, ',' as decimal symbol) are used in the formula text.
150978	Console: Data: Dragging the height of an injection row to make it too small for the text can result in the line being hidden until the console is restarted. This behavior has been seen only intermittently and only on a few PCs.
168759	Instrument Method Editor – Gradient Plot: If the time stamp of the first line (white background) in the equilibration stage (e.g., t = -3.00 min, Eluent = 100% B) is different from the one of the equilibration stage header line (orange background, e.g., t = -5.00 min), the gradient plot indicates that an equilibration with the eluent combination selected for the first (white) line in the equilibration stage (e.g., t = -3.00 min). However, the actual gradient starts at the time indicated (e.g., t = -5.00 min) with 100% A and ramps to 100% B at t = -3.00 min. Workaround: Fully define the equilibration stage. Ensure that the first step of the equilibration stage (white background) has the same time stamp as the equilibration stage header line (orange background)
169879	In rare cases, a sequence completes and some injections contain raw data, but the status shows "Interrupted" or "Idle" and the Inject Time field is empty. 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. Workaround: Remediation for this incident is manually re-executing the data upload from the local IPC to the Central Data Vault. Note: If you are affected by this problem, please contact your local Thermo Fisher representative for assistance with recovery of the missing injection details.
171965 CM7-25633	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.
171967 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
171968 CM7-25551	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.</sequence_name>
171969 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.
171974 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.

171986 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 procMeth.version.time.
171987 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. However, 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 gen.currentTime or gen.reportTime together with the necessary format, e.g., {gen.currentTime; "dd.mm.yyy hh:mm"}. Note: the formula gen.currentTime 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 gen.reportTime.
171976 CM7-24600	Spectral Library: If a Chromeleon version older 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 dialog with OK will result in an exception being thrown.
171993 CM7-23033	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 must 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. Thermo Fisher Scientific recommends enabling the replication framework with Chromeleon 7.2 SR5 or a later version to avoid the problem.
171994	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. Note: If you are affected by this problem, please contact your local Thermo Fisher representative for assistance with recovery of the missing injection details.
171997 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.
172001 CM7-21783	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.
172004 CM7-21399	Queries: 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).
172011 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.
172016 CM7-19836	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.

172018 CM7-19336	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.
172020 CM7-18252	Export: 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.
172023	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.
172025 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.
172028 CM7-17465	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.
172029 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.
172047 CM7-11692	Console: Instruments: When monitoring the baseline with an overlay chromatogram added to the signal plot, the overlay may disappear after changing to a different ePanel and back.
172727	eSignatures: For sequences containing manually manipulated XICs saved in a software version older than 7.2.6, if the sequence was signed in a later software version without viewing the manually manipulated XICs, then verification could fail if the XICs were subsequently viewed before the verification. To resolve this situation, remove the signature, view the manipulated XIC, and re-sign the sequence. Then view the manipulated XICs once more before verification.
172732	Console: It might happen that when a sequence is directly started from the Console, the sequence "running icon" (green arrow) is not shown in the tree view of the data vault (in the left pane). This is likely a status reporting issue with the Discovery service and does not interfere with actual acquisition. The proper status is still shown in the instrument queue and in the view of the sequence itself.
172734	NTMS: Due to limitations in the Sieve processing engine, it is only possible to perform NTMS processing on system with en US localization (i.e., non-US localized systems are not supported) (This is also documented in the Sieve Release Notes)

174091	Console: Data: It was observed that while a sequence is being added to the instrument sequence queue, there was a very short time slot where its parent folder got renamed while the "adding to queue" operation was in progress. Afterward, the queued sequence got stuck in the instrument sequence queue. It will cause an upload failure at the end of the acquisition using the automatic upload as the original folder name cannot be resolved anymore and breaks the data transfer link to the central data vault. In addition, the folder name cannot be reverted to resolve the upload failure because the sequence once it is queued is marked as redirected. Once the sequence is redirected, it locks the folder to prevent the renaming folder operation. Workaround: To remove the sequence from the queue a manual move operation needs to be executed.
183709	Queries: In an Enterprise environment, if the Injection Query is not saved before running, then query results for a sequence in the same folder as the unsaved query may not be accessible (since the folder contents cannot be refreshed due to the pending change). Therefore, when those injections are opened in the Studio, they might not appear or might have an incorrect name. In addition, opening the sequence containing that injection from the query results list may fail. To prevent this problem, either create the query in a different folder or save it before running it.
215589	NTMS: When processing NTMS data using the SIEVE algorithm, at time the molecular weights of similar samples may differ, even though the molecular masses are very similar. This is a consequence of how the SIEVE algorithm analyzes the data and is to be expected.
231359	Import of CMBX-Files by previous Chromeleon releases or into datavaults with an old database scheme: Chromeleon 7.3.2 is using a new database scheme for datavaults which records the logon role in the data audit trail. If a data object (e.g., sequence) contains data audit trail records with a role and the data object is exported to a CMBX-File the import of such a CMBX-File by a previous Chromeleon release is still possible. Yet the imported data object cannot be modified anymore. Any attempt to modify it runs into a corresponding error message. A similar scenario is also present if you import the CMBX-File by the Chromeleon 7.3.2 into a datavault with an old database scheme.
231464	MS Plot: When viewing profile mode mass spectra, Chromeleon labels peaks with the actual apex m/z of the profile data. In contrast, the FreeStyle and Qual Browser software will label profile mode mass spectra with the centroided m/z. This can result in minor differences in the displayed data between these applications.
231883	eWorkflows: The sequence layout in an eWorkflow for a pair of linked instruments must only contain a Sample Block. If the eWorkflow contains Header, Footer, or Bracket blocks, then the eWorkflow can only be run in 'single instrument' mode.
232285	Queries, and NTMS Frame/Results Filters: Rules that compare floating point parameters to a fixed value using the "=" condition will not round or truncate values when performing the comparison. This means for example, that the rule "mass = 123.4" will not match a mass of 123.42.
234256	Queries: If a user is not a member of an access group assigned to a folder, attempting to create an injection or audit trail query will fail with a misleading error about a missing privilege, even if the user does indeed have the required privilege.
236172	Chromeleon 7.2x and Chromeleon 7.3.0x client machines need to disable option "Receive push notifications" in the discovery configuration dialog to be able to join a Chromeleon 7.3.2 domain. Chromeleon 7.2x and Chromeleon 7.3.0x client machines that are already part of a Chromeleon 7.3.2 domain and have "Receive push notifications" enabled will not receive any push notifications as this feature has been removed with Chromeleon 7.3.2. It is required to enable "Poll for updates every <number> seconds" to receive that lasted discovery information.</number>

238857	The error message "Could not connect the replication service. A TCP error (10051: A socket operation was attempted to an unreachable network) occurred while transmitting data. A socket operation was attempted to an unreachable network" that appears during sequence interruption has nothing to do with the customer network and means that data cannot be saved locally therefore the sequence is interrupted.
240632	Interactive Results: Trying to insert a report table without header rows (e.g., MS Instrument Method (XRAW), Instrument Method / Overview) in the Interactive Results pane leads to an error message 'Invalid cell reference' in the upper left corner (A1) of the inserted new sheet". Such report tables can still be successfully inserted in the Report Designer.
245276	DDK Driver: An injection may not terminate when an Abort error happens at AcqOn time for 3D channels.
250819	CMBX-Files and Peak Group Calibration Levels: if a CBMX-File has been created by a Chromeleon Version 7.2.10 Mua(b,c,d) for a sequence containing a processing method with peak groups, the amount values for the calibration levels of the peak groups were not saved into this CBMX-File. If such a CMBX-File is now restored by any Chromeleon Version being able to read this CMBX-File the amount values for the calibration levels of peak groups are reset to 1.0.
254003	Custom variables: A sequence with the invisible character 0x1F (unit separator) in a custom field text of a custom injection variable aborts with an error message "hexadecimal value 0x1F, is an invalid character". Workaround: Do not use the invisible character 0x1F (unit separator) in a custom field value.
264434	Hardware OQ: Turkish region setting causes values to disappear for Hardware OQ files. When trying to run a Hardware OQ on an instrument in Turkey, the OQ fails with the error message "Unexpected character(s) at end of line." In addition, values in the instrument method disappear, e.g., "Infinite" for PumpModule.Pump.MaximumFlowRampDown and PumpModule.Pump.MaximumFlowRampUp.
267233	ePanels: While editing ePanels, the ePanel Editor (under unknown circumstances) occasionally and spontaneously changes the background color of Edit Field controls to LightPink and sometimes the Edit Field controls look empty.
275608	Sequence: If the sequence name contained a foreign character that was not part of the regional language code page (for example, α on an English-US system), the respective sequence could be started, but the sequence bar turned orange and showed "Disconnected".
276956	Instrument Controller: OnlineExtract for MS Channel does not perform smoothing when programmed in a script. While the command "OnlineExtract" provides smoothing parameters, these are nor applied to MS mass trace signals created with the "OnlineExtract" command.
282151	Instrument Method: If the chromatographic portion of an instrument method is changed without changing the MS portion of the method, the instrument method and MS instrument method can show a different date/time modified. This is due to the nature of the integration of the MS Instrument Method Editor into the overall instrument method and is to be expected.
299483	A special character (e.g., the Unicode control character "Record Separator") in the comment for an injection (in the injection table) will cause a Ready Check error. A sequence run aborts with an error message "hexadecimal value 0x1F, is an invalid character".

307368	Orbitrap Exploris: Method Translation does not recognize the difference between Orbitrap Exploris™ models. When opening a Chromeleon instrument method created on an Orbitrap Exploris 240 on an Orbitrap Exploris MX instrument, no warning is presented to indicate the difference between the model the instrument method was created for and the actual instrument. Instead, the Ready Check fails with a method mismatch error and suggested solution. Workaround: After opening the instrument method re-enter a single MS parameter to trigger the 'Save' action.
336304	On a system where the data vault "ChromeleonLocal" is not present or not accessible and a local data vault is mounted, but not accessible, trying to import an instrument configuration shortly after the start of the Instrument Controller results in an error: "Chromeleon Instrument Configuration: Remote instrument controller can't save configuration. The Instrument Controller does not respond. It is probably very busy." Workaround: Wait several minutes after the start of the Instrument Controller before saving or importing an instrument configuration.
353518	Chromeleon XPS: If an eWorkflow is defined for multiple instruments and the instrument name is the same for two or more of the instruments, then in Chromeleon XPS only one occurrence of the instrument will be shown. Workaround: Do not add more than one instrument with the same name to an eWorkflow being used in Chromeleon XPS.
356523	Unicode characters (such as greek letters or special characters) are not properly displayed in the Console and in the Instrument Configuration. However, Chromeleon can handle Greek characters on a Greek system and Chinese characters on a Chinese system, but e.g., not Greek characters on an English system.
364515	MS Component Pane: When displaying the XICs of a reference injection in pane, if the reference XICs are zoomed, then the tile containing the sample XICs will disappear.
373730	IPD: If the Output Mass Range on the Algorithm Parameters page exceeds the range of the data, the x-axis range of the Deconvoluted Spectrum plot will be limited to that of the available data.
375765	 Processing Method: If a processing method created in version 7.3.1 or earlier is opened in version 7.3.2, repeated edits and saves within the same Studio session may cause the UI of some tabs (e.g., MS Settings, Calibration or Advanced) to be incorrectly scaled, obscuring some of the controls on the tab. To prevent this from occurring: Select 'Processing Ribbon' >> 'Layouts' >> 'MS Quantitation'. Add or remove any tabs as desired.
377930	Driver issues (and possibly using Triggers) can lead to huge Instrument Audit Trails if messages are logged repeatedly at high frequency (several thousand messages per second) in the Instrument Audit Trail. This results in the (Daily) Instrument Audit Trails growing to a size of several dozen MBs. Trying to open such a large Daily Instrument Audit Trail crashes the client, e.g., with a System.OutOfMemoryException and can even lead to the Chromeleon client crashing immediately after start.
391086	Linked Sequences: When viewing the Calibration plots for a component present in both sequences, zooming in on the plot for one sequence will also zoom the pot for the other sequence.
391202	Linked sequences are copied via copy&paste incorrectly in CM Console in case copying is carried out by large transfers feature enabled in Global Policies.
391203	Copying of sequences carried out by large transfers feature enabled in Global Policies doesn't work well when source or destination data vault become dismounted.

391805 Filter Table Property is not offered for these reporting 2.0 tables: MS Detection Settings, MS Status Log, MS Device Information, MS Instrument Method, MS Tune Table.

5.8 Obsolete Instrument Drivers

Chromeleon includes a number of obsolete instrument drivers which are included to provide backward compatibility with existing installations. The complete list of drivers may be found in the Obsolete category of the 'Add module to Instrument dialog' in the Instrument Configuration Manager:

Martinatutes. Perkin Elmer Polymer Laboratories Rainin Rheodyne Shimadzu SofTA Transcat (Martel) URG Corporation Valco Varian VICI Waters Obsolete Agilent/HP CTC Thermo Scientific IC Thermo Scientific GC	Accela PDA Accela PDA Aglient/HP 1200 HPLC System ASI-100 Autosampler Corona Charged Aerosol Detector D C Detector/Chromatography (ICS-3000 D DP-3600 Pump D DGP-3600 Pump D DF-3600BM Pump D DP Jual Pump (ICS-3000) D P Jual Pump (ICS-3000) D P Jual Pump (ICS-5000) E G Elivert Generator (ICS-5000)
--	--

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.

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 MUc 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 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.

6.7 Chromeleon Enterprise Compatibility of different versions of Chromeleon installed on Domain Controller, Clients and Instrument Controllers

Whilst, in general, it is possible for a Chromeleon Enterprise with a domain controller running one version of Chromeleon to work with instrument controllers and client PCs running a different version of Chromeleon, we would not recommend this kind of 'mixed' environment for customers with a fully validated Chromeleon system.

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. For details of processing parameters which will not be available, refer to all the release notes issued for all versions between the oldest and newest versions you are combining.

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 section contains general Information about Release Notes, Online Help, and Contributed Content.

7.1 Release Notes

The Release Notes list the new features and improvements of the current release.

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 7.3.2 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
- View Settings

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.

www.thermofisher.com

© 2009-2023 Thermo Fisher Scientific Inc. All rights reserved.

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

