Mass Frontier 8.0 Release Notes

These release notes list the new features in the Thermo Scientific Mass Frontier™ 8.0 application. Also included are the system requirements for the software installation and the known issues in this release of the application.

Contents

For information on installing, configuring, and using the Mass Frontier 8.0 application, refer to the installation instructions, user guide, and tutorials available as PDF files.

Features

This release incorporates these new modules and these new or enhanced features:

- New Modules
- New Features and Improvements

New Modules

The Curator and Metabolika modules are new.

Curator

- Curates spectral trees for building high-quality mass spectral libraries.
- Uses a wizard to guide you through the curation process.

Metabolika

- Creates and edits reaction pathways, for example, biochemical, drug metabolism, or biodegradation pathways.
- Integrates with other modules such as Fragmentation & Mechanisms, Structure Editor, Structure Grid, and Structure / Substructure Search.
- Includes 370+ curated biochemical pathways of various organisms with annotated reactions and corresponding metadata in Pathway Explorer.
- Provides publication-quality graphics for use in presentations.

New Features and Improvements

This release includes several new features and improvements.

Chromatogram Processor

- Reading and processing common format mzML files
- Show Neutral Loss command to automatically suggest neutral losses for spectral peaks
- Subtract Blank File command to subtract ion profiles of supplied background file (blank) from the active chromatogram (sample)
- Contaminants Elimination Filter command to filter the chromatographic data for any known and unwanted substance

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- Integrated component and mzLogic search inside Chromatogram Processor
- Significantly faster JCD component detection to handle large size raw files

Library Search and Tools

- Integration of the online mzCloud™ mass spectral database. Access to the mzCloud database from Data Manager and Chromatogram Processor.
- New similarity search algorithms including Similarity Forward and Similarity Reverse. Improved matching algorithms for Identity, Identity Substructure, Tree Search, and SubTree Search library searches.
- New probability-based confidence-score calculations trained on the extensive mzCloud database.
- MolGate ™ structure search in a new aggregator of relevant public databases comprising 40 million chemical compounds.
- mzLogic™ analysis for ranking structure candidates using spectral similarity and structure similarity matching against the mzCloud database.

Fragments and Mechanisms

Provides more fragmentation mechanisms (>52,000 fragmentation schemes and ~220,000 decoded mechanisms) in HighChem Fragmentation Library™, which means more fragments are predicted.

Structure Editor

Supports two-way conversion of MOL to InChi string and InChi key.

Server Manager 3.0

- Supports migration of Mass Frontier 7 libraries to the new Mass Frontier 8.0 format.
- Provides backup and restore capabilities for spectral libraries.

Usability Improvements

- Multiple monitor support.
- New user interface inspired by Microsoft Office™.

Performance Improvements

- Built on the latest Windows™ architecture and SQL Server 2014.
- Extensive use of parallelization for faster processing of CPU intensive tasks.
- Improved integration of different modules across the application.

New Flexera Licensing System

Licensing activation and deactivation through the Flexera™ licensing server.

System Requirements

These are the minimum required and recommended hardware and software configurations for the Mass Frontier 8.0 application.

System	Minimum configuration	Recommended configuration
Hardware	• Intel™ compatible processor with a minimum speed of 1 GHz • 8 GB RAM • 30 GB of disk space • DVD-ROM drive • Monitor resolution display of 1024×768 p	• Intel™ compatible processor with a minimum speed of 2.5 GHz • 32 GB or higher of RAM • 100 GB of solid-state drive (SSD) disk space • DVD-ROM drive • Dual monitors with resolution display of 1920×1080 p
Software	• Microsoft Windows 7 Professional (English) SP1 (64-bit) or Windows 10 Professional (64-bit) • Microsoft .NET 4.6.1 • Microsoft Office 2010 • Adobe™ Acrobat™ Reader™ DC • Microsoft Windows Internet Explorer™ 11 or later	• Windows 10 Enterprise LTSB 2016 (64-bit) with latest updates • Microsoft .NET Framework 4.6.1 or higher • Microsoft Office 2016 • Adobe™ Acrobat™ Reader™ DC • Microsoft Windows Internet Explorer™ 11 or later
System	• To run processing workflows with online mass spectral database searches, ensure the computer has unblocked access to the mass spectral databases on the Internet. • Ensure that the computer has the correct time and date settings and is synchronized with Internet time. • Set the Region and Language setting to English (United States).	

Important Information

The following topics contain important information.

General

The Mass Frontier 8.0 application can process LC/MS and infusion data files produced by high-resolution accurate-mass (HRAM) Thermo Scientific™ instruments, such as the Orbitrap ID-X™, Orbitrap Fusion™, Orbitrap™ hybrids, Q Exactive™, and Exactive™ mass spectrometers, and nominal mass Thermo Scientific instruments, such as the LTQ™ series mass spectrometers. It is compatible with Windows 7 SP1 (64-bit) and Windows 10 (64-bit) operating systems.

Installation

You must have administrator rights to install Mass Frontier 8.0 software on your computer. For detailed installation instructions, refer to the Installation Instructions located on the software media or downloaded as a ZIP file from Flexera.

Licenses

The demo version comes with the Mass Frontier 8.0 Base plus Curator trial license that is active for 60 days.

For a permanent license, there are two purchase options:

- **Mass Frontier 8.0 Base**—Provides a permanent license for only the Mass Frontier application.
- **Mass Frontier 8.0 Base + Curator**—Provides a permanent license for the Mass Frontier application and the additional Curator module.

If you purchase only the base license, you can purchase the **Curator License for Mass Frontier 8.0** option at a later date. Contact your local Thermo Fisher sales person for a quote. This option gives you a license key to permanently activate the Curator module in the Mass Frontier 8.0 application.

Supported Local Language and Date/Time Format for the Data System Computer

The Mass Frontier 8.0 application was tested and is therefore only supported for US-English Only locale settings. To change the format on your computer, go to **Control Panel > Region and Language**.

Upgrading from Mass Frontier 7.0, 6.0, or Earlier

To install Mass Frontier 8.0 software on a processing computer that has previous versions, you do not need to uninstall the earlier versions. Mass Frontier 8.0 and earlier versions such as Mass Frontier 7.0 can coexist on the same computer.

Migrating Spectral Libraries from Mass Frontier 7.0, 6.0 or Earlier

The library file format in Mass Frontier 8.0 has changed compared to previous versions. Server Manager 3.0 allows you to migrate Mass Frontier 7.0 spectral libraries into Mass Frontier 8.0 format. Migrating spectral libraries from Mass Frontier 6.0 or earlier versions is a two-step process. First migrate the Mass Frontier 6.0 spectral libraries into the Mass Frontier 7.0 format, and then migrate the Mass Frontier 7.0 libraries into the Mass Frontier 8.0 format.

> **Note** For more information regarding migrating Mass Frontier 7.0 libraries to Mass Frontier 8.0 format, refer to the *Migrating Spectral Libraries* section in the *Mass Frontier 8.0 User Guide*.

Multiple Monitor Support

Mass Frontier 8.0 software supports multiple monitors. To connect the data system computer to two monitors, use the two display ports on the back of most computers.

Tutorials

Mass Frontier 8.0 comes with seven step-by-step tutorials that are available from the application window. Follow the tutorials to get started with the application.
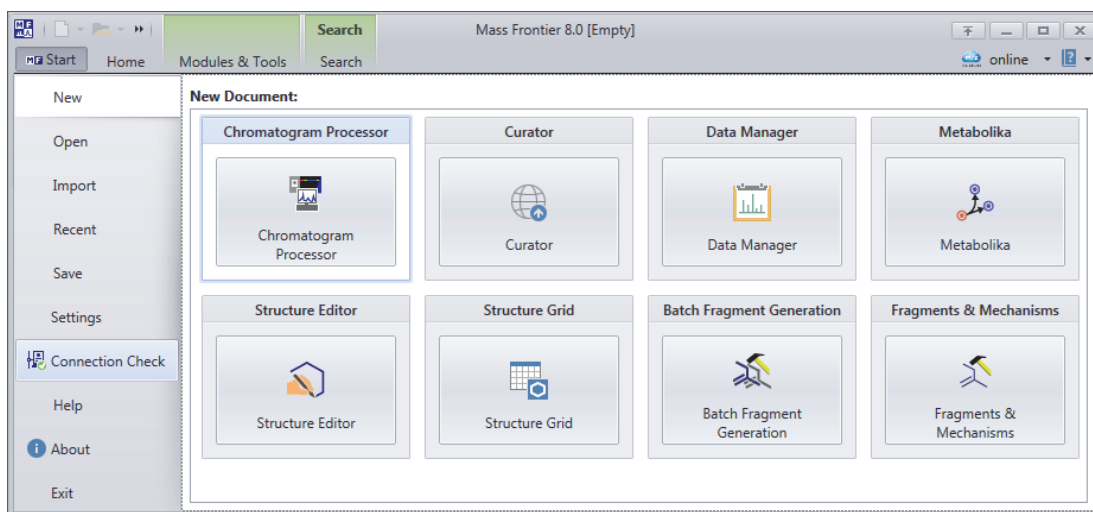
❖ **To access the tutorials and the user guide**

Click the **Help** icon, [?] , in the upper right corner of the application window.
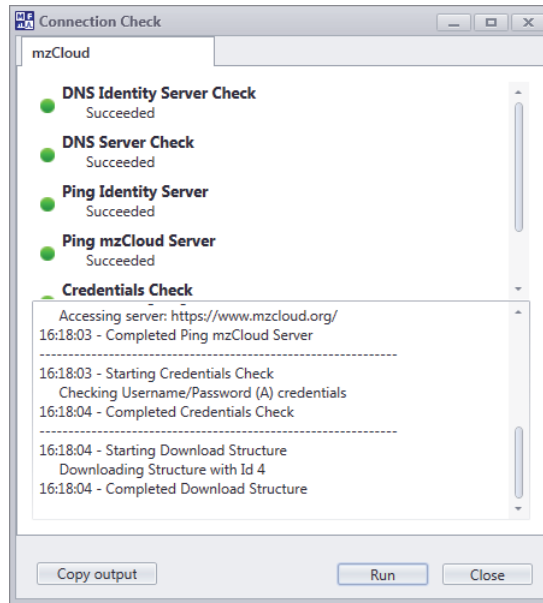
Ensuring Access to the Online Databases

A typical Mass Frontier analysis that identifies unknown compounds or retrieves structures and metadata searches databases on the Internet. To run these searches, the application must have unblocked Internet access to these databases. To test the application's access to the online mass spectrum databases, follow this procedure.

❖ **To test and troubleshoot the application's access to the mzCloud and MolGate server**

1. Run the connection check from the Mass Frontier Start menu as follows:
   a. Choose **Connection Check**.

b. In the Connection Check dialog box, click **Run**.

If the connection checks succeed, the application has access to the mzCloud and MolGate server.
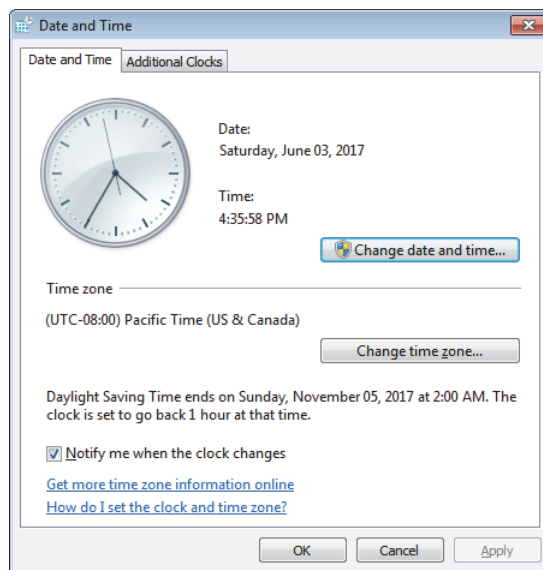
2. If a connection check fails, check the following:

- The computer's physical connection to the Internet
- The computer's time and time zone settings

The mzCloud connection check includes a validation of the date and time settings on the processing computer.

❖ **To check the time and time zone settings**

1. Open the Date and Time dialog box.

> **Tip** For the Windows 7 operating system, open the Control Panel. In the View By list, select **Category**. Then choose **Clock, Language, and Region > Date and Time**.

2. Make sure that the date, time, and time zone settings are correct.

3. If the Internet Time tab is available, synchronize the Internet time.

> **Note** The Internet tab is only available when your computer is not part of a network domain. If your computer is not part of a network domain that synchronizes the computer's clock to the network server, you can use an Internet server to synchronize the computer's clock.

Known Issues

Suggested recovery actions

- For some issues, restarting the application is the appropriate recovery action.
- As a fix we generally do not recommend reinstalling the software or the operating system, which more commonly occurs after you install a new hard drive.

Feature requests and other removed items

- We do not include issues where there is insufficient information logged to successfully reproduce the reported problem.
- We do not list feature requests as software issues, regardless of the reported significance or severity of the request. Product managers evaluate logged feature requests for future releases.
- We report only discrepancies in the documented software as known issues.

Terminology

Severity	Interpretation
Crash/Data Loss	A problem that renders the system unusable because either an entire function is unusable and no workaround exists, or use of the current system compromises data integrity or results in data loss. Catastrophic problems also include significant and non-obvious quantitative errors, and all human and instrument safety issues.
Major Problem	A serious issue that does not affect data integrity (meaning data loss, corruption of data, or the wrong answer), but affects the customer's ability to use the product as designed. It can be a failure, design issue, or documentation error or omission. A workaround might or might not exist.
Minor Problem	A minor error or poor behavior of a product feature. There is probably a workaround.
Cosmetic	An issue that has a limited effect on customer usage of the product; for defects with visibility so low that a customer might never see it; or for ease of use issues or other items not causing any performance degradation.

Risk	Interpretation
High	Occurrence is likely to happen and can compromise operation.
Medium	Occurrence is uncommon, but if it occurs, can compromise operation.
Low	Issue is minor; however, the software might operate differently from a user's expectations. A workaround is often available.
No Risk	This issue causes no problems but is commonly an inconsistency or a 4- Low issue.

Known defects

Table 1 contains known defects in the software, categorized by software section, with a brief abstract and information related to each defect's severity and risk. The Item ID is the internal number assigned to each issue. Product management assesses risk, which can differ significantly from the reported severity.

Table 1. Known defects (Sheet 1 of 3)

Software section	Severity	Abstract	Risk	Item ID
Chromatogram Processor	Minor	Neutral Loss annotations are sometimes displayed out of spectrum area and cropped.	Low	MFEIGHT2716

Table 1. Known defects (Sheet 2 of 3)

Software section	Severity	Abstract	Risk	Item ID
Chromatogram Processor	Minor	New Contaminant window cannot be canceled or closed if the Name field is empty. See workaround in the Troubleshooting section.	Low	MFEIGHT2692
Component Tree Search	Major	Tree Search not able to differentiate some flavonoid compounds if the MS2 spectrum has only one or two significant peaks	Medium	MFEIGHT2704
Contaminants Elimination Filter	Minor	When running commands from Command Window, the progress bar sometimes does not disappear and window cannot be closed. See workaround in the Troubleshooting section of the user guide.	Low	MFEIGHT2778
Curator	Minor	NaN is sometimes displayed for Correlation at the Recalibrate step.	Low	MFEIGHT2794
FISh Detection	Minor	FISh filter: Input m/z list sorting on m/z column not working as expected.	Low	MFEIGHT2765
Fragments & Mechanisms and Batch Fragmentation	Major	Knowledge-based fragmentation using fragmentation libraries ignores isotopically labeled hydrogens in structures.	Medium	MFEIGHT2779
Fragments & Mechanisms and Batch Fragmentation	Major	No fragments for H- Electron Impact (EI, EC) ionization when starting from neutral structure. As a workaround, manually specify the "Unspecified H⁻" charge site prior the fragment generation.	Low	MFEIGHT2792
Licensing	Minor	Demo license expiration date not updated after successful activation of the demo extension key. The new expiration date only kicks in after the previous demo or trial license expires.	Low	Bug 76909
Main Application	Minor	Intensive CPU or GPU utilization when processing or redrawing makes application unresponsive for a while and a black box appears. See workaround in the Troubleshooting section of the user guide.	Low	MFEIGHT1601
Main Application Settings	Minor	mzCloud enable/disable check box in mzCloud section does not work when clicking OK button and Apply button is disabled. As a workaround, change any other field in the settings and click Apply.	Low	MFEIGHT2789
Monoisotopic Mass Search	Major	If the search matches compound structure in the user libraries, only the compound is shown in the result table without any underlying spectral trees or records.	Medium	MFEIGHT2776

Table 1. Known defects (Sheet 3 of 3)

Software section	Severity	Abstract	Risk	Item ID
mzLogic and MolGate	Major	MolGate does not support charged structures.	Medium	MFEIGHT2703
mzLogic Component Search	Minor	No warning message when conflicting polarity of adduct selected.	Low	MFEIGHT2738
mzLogic Component Search	Minor	The name of the Similar Structures does not include special characters and the long names are not displayed fully.	Low	MFEIGHT2724
mzLogic and MolGate Tool	Minor	In some cases, the Results Preview pane does not show correct number of structures when using Structure grid as Workspace.	Low	MFEIGHT2683
mzLogic and MolGate Tool	Minor	The Accuracy edit box sometimes shows value with 15 decimal places.	Low	MFEIGHT2730
Precursor Search	Major	The search results are shown for recalibrated spectral trees by default, if they are not present on the matched precursor ion, no spectral trees are shown initially. To display spectral trees, the user has to manually change the view to filtered or raw trees.	Low	MFEIGHT2776
Server Manager	Major	Migrating Mass Frontier 7 libraries with spectral trees having data reduced chromatograms, all components in those chromatograms are inserted as new empty compounds in Mass Frontier 8.0. See workaround in the Troubleshooting section of the user guide.	Low	MFEIGHT2767
Structure and Monoisotopic Mass Search	Major	Individual fragments in the fragmentation schemes are not searched.	Medium	MFEIGHT2791
Structure Editor	Major	^{18}F is not supported in Structure Editor	Low	MFEIGHT2762

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