

Mass Frontier 8.1 Release Notes

These release notes list the new features in the Thermo Scientific Mass Frontier™ 8.1 software. Also included are the system requirements for the software installation and the known issues in this release of the application.

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For information on installing, configuring, and using the Mass Frontier™ 8.1 software, refer to the installation instructions, user guide, and tutorials available as PDF files.

Features

The Mass Frontier 8.1 release incorporates these new or enhanced features:

- [New Features and Improvements](#)

New Features and Improvements

This release includes several new features and improvements.

Chromatogram Processor

- The new mzCloud library can be used when searching spectra.

Data Manager

- Quick filter/search tool: Using this feature the spectral libraries can be filtered for specific attributes such as Retention time/Retention index, Compound class, Metadata, and structure of a compound.
- Multiple compounds from a library can be saved to a single file.

Library Search and Tools

- Structure and substructure search algorithms have been improved and significantly faster.

SledgeHammer Fragmentation

- The fragmentation module has a new fragmentation algorithm called SledgeHammer.
- SledgeHammer has now increased coverage for fragmentation of negative mode compounds.
- Increased speed of fragmentation.
- Provides 2,068 more fragmentation mechanisms (54,139 fragmentation schemes and ~226,895 decoded mechanisms) in HighChem Fragmentation Library™, which means more fragments are predicted.
- Provides additional general fragmentation schemes for prediction.
- This module uses isotopically labeled atoms in fragment pathways.

Curator

- Curation protocol is now aligned with myLibrary and new mzCloud.
- Supports importing the .sdf file, improving the addition of large list of fragments into curator simpler.

Structure Editor

- Supports multiple charges on multiple atoms for drawing of N-oxides and zwitterions.
- Provides customizable adducts: Using this feature, user can select any adducting species, including multiple species, charges, and neutral losses.
- Increased limit for number of atoms in a structure: Using this feature, users can now draw structures with more than 199 atoms supporting natural products.
- Importing/Exporting SMILES: Structures can now be imported and exported with SMILES IDs in addition to InChI.
- Drawing canvas now supports the use of changing bond colors, addition of stereobonds, and multiple radicals.
- Users can connect and view the Mass Frontier 7.0 libraries if they have the Mass Frontier 7.0 software installed on the computer or network.

GC-MS Support

- Supports component detection GC MS1 data.
- Retention Index (RI) can be used as metadata.

Performance Improvements

- Built on the latest Windows™ architecture and PostgreSQL 15.
- Improved integration of different modules across the application.

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

System	Minimum configuration	Recommended configuration
Hardware	<ul style="list-style-type: none"> • Intel compatible processor with a minimum speed of 1 GHz. • 8GB RAM • 30GB of disk space • Monitor resolution display of 1024 x 768pixels. • DVD-ROM drive (This is optional and not required if you can download from Flexera). 	<ul style="list-style-type: none"> • Intel compatible processor with a minimum speed of 2.5 GHz. • 32GB RAM • 100GB of solid-state drive disk space • Dual monitor resolution display of 1920 x 1080pixels. DVD-ROM drive (This is optional and not required if you can download from Flexera).
Software	<ul style="list-style-type: none"> • Microsoft Windows™ 10 (English) 64bit. • Microsoft™ .NET Framework 4.7.2 • Adobe™ Acrobat Reader DC • Google Chrome version 81.0 or higher. 	<ul style="list-style-type: none"> • Microsoft Windows™ 10 LTSC 64bit. • Microsoft™ .NET Framework 4.7.2 • Adobe™ Acrobat Reader DC • Google Chrome version 81.0 or higher.
Computer	<ul style="list-style-type: none"> • To run processing workflows with online mass spectral database searches, the computer must have an unblocked access to the mass spectral data via the internet . • The time and date settings in computer must be synchronized with the internet time. . • Set the Region and Language setting to English (United States). 	

The following topics contain important information.

General

The Mass Frontier 8.1 application can process LC/MS and infusion data files produced by high-resolution accurate-mass (HRAM) and nominal mass Thermo Scientific™ instruments such as:

- Thermo Scientific™ Tribrid™ mass spectrometers:

- Orbitrap IQ-X™
- Orbitrap Eclipse™
- Orbitrap Ascend™
- Orbitrap Fusion Lumos™
- Thermo Scientific™ hybrid mass spectrometers:
 - Orbitrap Exploris
 - Q-Exactive
- Thermo Scientific™ nominal mass spectrometers
 - LTQ™

It is compatible with Windows 10 (64-bit) operating systems.

Installation

You must have administrator rights to install Mass Frontier 8.1 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.

To install Mass Frontier 8.1 software, do one of the following:

- Download Mass Frontier 8.1 from Flexera <https://thermo.flexnetoperations.com/control/thmo/login> to your local processing computer.
- Install the software from the DVD:
 - Insert the Mass Frontier 8.1 DVD into the DVD/CD-ROM drive.
 - Install Mass Frontier 8.1.
 - Follow on screen instructions (see *Mass Frontier 8.1 Installation Instructions manual*).
 - Activate license (see *Mass Frontier 8.1 Installation Instructions manual*).

Licenses

The demo version comes with the Mass Frontier 8.1 Base plus Curator trial license that is active for 60 days.

If you purchase the Mass Frontier 8.1 application, you can set permanent license using the activation code provided through the Flexera™ account. See *Mass Frontier 8.1 Installation Instructions manual*.

For a permanent license, there are two purchase options:

- **Mass Frontier 8.1 Base**—Provides a permanent license for only the Mass Frontier software.
- **Mass Frontier 8.1 Base + Curator**—Provides a permanent license for the Mass Frontier software and the additional Curator module.

If you purchase only the base license, you can purchase the **Curator License for Mass Frontier 8.1** option at a later date. Contact your local Thermo Fisher sales representative for a quote. This option gives you a license key to permanently activate the Curator module in the Mass Frontier 8.1 software

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

The Mass Frontier 8.1 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 8.0, 8.0 SR1

To install Mass Frontier 8.1 software on a processing computer that has previous versions, you do not need to uninstall the earlier versions. Mass Frontier 8.1 and earlier versions such as Mass Frontier 8.0, 8.0 SR1 can coexist on the same computer.

Migrating Spectral Libraries from Mass Frontier 8.0, 8.0 SR1

- The library file format in Mass Frontier 8.1 has changed compared to previous versions. Server Manager 8.1 allows you to migrate Mass Frontier 8.0 spectral libraries into Mass Frontier 8.1 format.
- Mass Frontier 8.1 software does not support the features Uninstall and Reinstall library.

Migrating Spectral Libraries from Mass Frontier 7.0

- Mass Frontier 8.1 does not support migration of Mass Frontier 7.0 libraries. However, user can connect and view the Mass Frontier 7.0 libraries if they have the Mass Frontier 7.0 software installed on the computer or network.

Note For more information regarding migrating Mass Frontier 8.0, and 8.0 SR1 libraries to Mass Frontier 8.1 format, refer to the *Migrating Spectral Libraries* section in the *Mass Frontier 8.1 User Guide*.


Multiple Monitor Support

Mass Frontier 8.1 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 8.1 comes with seven step-by-step tutorials that are available from the application window. Follow the tutorials to get started with the application.

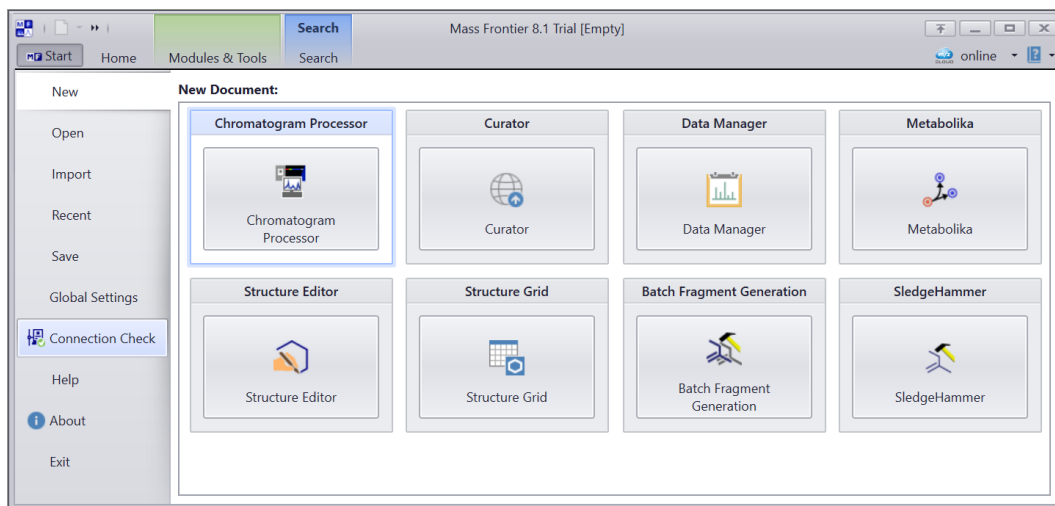
❖ To access the tutorials and the user guide

Click the **Help** icon, , in the upper right corner of the application window.

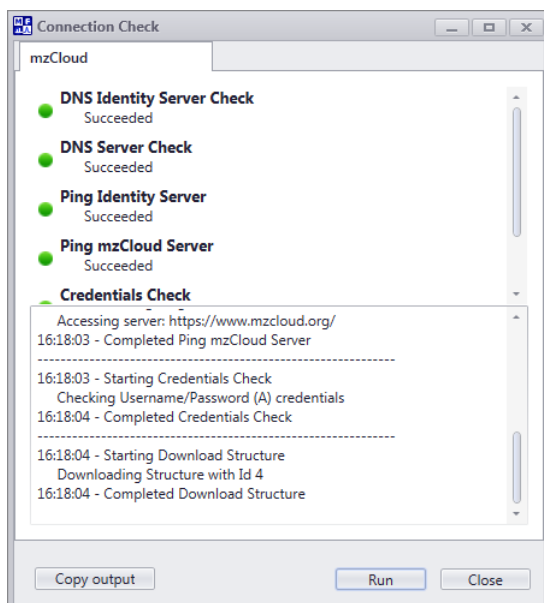
A typical Mass Frontier analysis that identifies unknown compounds or retrieves structures and metadata searches databases on the Internet. To run these searches, the application must have unblocked Internet access to these databases. To test the application's access to the online mass spectrum databases,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

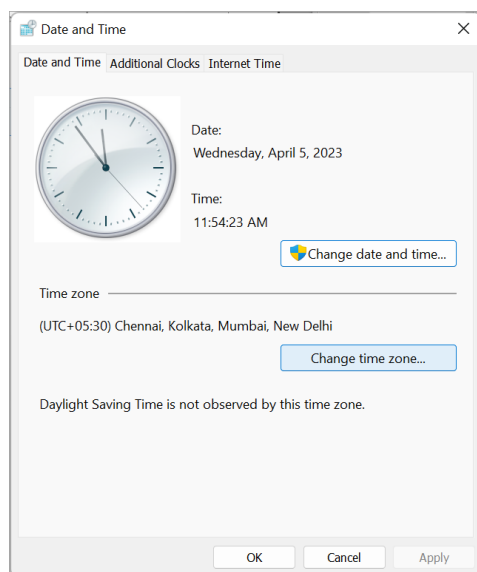
2. If a connection check fails, check the following:
 - The computer's physical connection to the Internet
 - The computer's time and time zone settings

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.

Known Issues

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.

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
Chromatogram Processor	Minor	Sometimes Custom Profile is displayed in the Search Type drop down list in the Component Search view.	Low	MFEIGHT3082
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	Major	The Curator removes m/z values higher than the precursor ions (when it is a doubly charged ion) from MS2 spectra.	Medium	MFEIGHT3079
SledgeHammer and Batch Fragmentation	Major	Knowledge-based fragmentation using fragmentation libraries ignores isotopically labeled hydrogens in structures.	Medium	MFEIGHT2779
SledgeHammer 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

Resolved Issues

Table 1. Known defects (Sheet 3 of 3)

Software section	Severity	Abstract	Risk	Item ID
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
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

Table 2 contains resolved issues in the software, categorized by software section, with a brief abstract related to each defect. The Item ID is the internal number assigned to each issue.

Table 2. Known defects (Sheet 1 of 3)

Software section	Abstract	Item ID
Batch Fragmentation	Improved progress for Batch Fragmentation.	MFEIGHT-2316
Batch Fragment Generation	Request to use the name of the structure as the default name for the generated sdf files	MFEIGHT-2848

Table 2. Known defects (Sheet 2 of 3)

Software section	Abstract	Item ID
Batch Fragment Generation	Batch Fragment Generation does not auto import from Structure Grid if SMILES is included.	MFEIGHT-3056
Curator	Curator shows NaN for Correlation at the Recalibrate step.	MFEIGHT-2794
Chromatogram Processor	Missing Scan Data dialog box needs improvement	MFEIGHT-2062
Chromatogram Processor	Component Search Settings dialog box change.	MFEIGHT-2270
Chromatogram Processor	Copy keyboard shortcut and the Copy button do not paste the same thing.	MFEIGHT-2274
Chromatogram Processor - FISh Filter	Input m/z List dialog box needs improvement	MFEIGHT-2844
Chromatogram Processor	Query spectra are not synchronized with Library spectra in "Show Details".	MFEIGHT-2623
Chromatogram Processor - FISh filter	Input m/z list- sorting on m/z does not work as expected.	MFEIGHT-2765
Chromatogram Processor - FISh Modification dialog box	Columns are not sortable	MFEIGHT-2842
Chromatogram Processor	Incorrectly assigned MS2 scans to component.	MFEIGHT-2827
Chromatogram Processor	In the Download MetaData wizard, the Previous and Next buttons are not available on some laptops.	MFEIGHT-2839
Chromatogram Processor	TIC line is not shown in mzML file format.	MFEIGHT-2892
Chromatogram Processor - Component Search view	Request to include Component# in the title.	MFEIGHT-2840
Chromatogram Processor	In the Filter Editor dialog box for the Components table, "Match" "Contains" does not work.	MFEIGHT-2901
Chromatogram Processor	FISh Modification dialog box: Typographical error. Change "domethylation" to "demethylation".	MFEIGHT-2940
Chromatogram Processor	Threshold Ion Intensity in DICD is not applied.	MFEIGHT-2946
Chromatogram Processor - Reporting	Export to Grid or Export to Spreadsheet— the mzCloud link is missing or it links to the wrong compound.	MFEIGHT-2973
Chromatogram Processor - Scans list	MS2 scans are sometimes randomly ordered when MS3 data are present.	MFEIGHT-2981
Chromatogram Processor	Cannot click on New Chromatogram after canceling.	MFEIGHT-3029
Data Manager - Compare Spectra View	Request to always show scan filter label for query and library spectra.	MFEIGHT-3070
Data Manager	Add full precursor info to spectrum in clipboard.	MFEIGHT-2850
Data Manager	Auto annotation of a MS2 spectrum requires the MS1 spectrum.	MFEIGHT-2920
Data Manager	Mass Frontier crashes after manually pasting an MS3 spectrum to an existing spectral tree.	MFEIGHT-2956
Data Manager	Auto fragment annotation shows inconsistent color coding.	MFEIGHT-2961
Data Manager	The message that appears when you save a curated spectral tree to a local library needs improvement.	MFEIGHT-3057

Table 2. Known defects (Sheet 3 of 3)

Software section	Abstract	Item ID
Formula Generator	The Generate button in Formula Generator looks like a table header not an action button.	MFEIGHT-3049
Formula Generator	Hide the Clear Existing Labeling check box in Formula Generator.	MFEIGHT-3059
General - Homepage	Delete all Recent Items and Delete Selected Recent Item are reversed on the startup screen.	MFEIGHT-3034
General	Typographical errors and inconsistent terminologies. (Partially fixed).	MFEIGHT-3038
General - Homepage	User needs a visual indicator for the Mass Frontier Service Status in the main application window.	MFEIGHT-3071
Structure Editor	Improvement of speed for loading large collection of structures.	MFEIGHT-2855
Structure Editor	Sometimes the metadata are not read for a MOL file.	MFEIGHT-2888
Structure Editor	Rename the Insert button to Open in Structure Editor and Structure Grid.	MFEIGHT-3069
Structure Grid	Mass Frontier crashes if Structure Grid is saving a large SDF file and at the same time the same SDF file is being opened in another Structure Grid module.	MFEIGHT-2874
Structure Grid	Initial structure counting issue.	MFEIGHT-3053
Search	Peak Search does not populate with the user picked m/z from spectrum.	MFEIGHT-3008
SledgeHammer	Fragmentation prediction failed with attached saponin compound.	MFEIGHT-2939
SledgeHammer	Error occurs when fragmenting Digitonin with Fragmentation Library.	MFEIGHT-2845
SledgeHammer	Problem with copying m/z values in fragments and mechanisms.	MFEIGHT-2851
SledgeHammer	The Generate button is not available in the untabbed view of the Reactions and Restrictions dialog box on some laptops.	MFEIGHT-2919
SledgeHammer - Reaction Restrictions dialog box	Set the tabbed view as the default layout.	MFEIGHT-2929
SledgeHammer	Auto fragment annotation does not work as expected for fragmentation scans of doubly charged ions.	MFEIGHT-3050
SledgeHammer	Nothing happens when clicking the text "Double-click to define the structure".	MFEIGHT-3058

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