FreeStyle 1.7 SP2 Release Notes

These release notes briefly list the changes in the Thermo FreeStyle ™ 1.7 SP2 software, new features and enhancements, fixes to the previously reported issues, and known issues that exist in the FreeStyle 1.7 SP1 software release. Additionally, system requirements for the software installation are included in these release notes.

Contents

- Features
- System Requirements
- Important Information
- Resolved Issues
- Known Issues
- Trademarks

For information on using the FreeStyle 1.7 SP2 application, refer to the user guide available as PDF file, or the embedded Help.

Features

This release incorporates the following fixed issues, and new and enhanced features.

Issues fixed in FreeStyle 1.7 SP2

The FreeStyle 1.7 SP2 application includes the following fixes:

- Chemical formula not saved in Layout.
- Background subtraction followed by Averaging does not apply correctly on Spectrum when Elemental Composition is applied.
- Application crashes when Elemental Composition for Selected Scan is applied for a spectrum where averaging and background subtraction was applied.
- Wrong scan header and scan data are shown when elemental composition (selected scan) is applied after performing Background subtraction followed by Averaging.
- Print to A4 size does not work as expected.

Issues fixed in FreeStyle 1.7 SP1

The FreeStyle 1.7 SP1 application includes the following fixes:

- NIST™ search: Unable to get results using In-source HiRes search mode in NIST search within FreeStyle
- NIST search: Exception seen for custom library used for NIST search in FreeStyle
- Export: Missing simulation (within workspace) on export of spectrum to .EMF
- Isotope simulation: Decimal places cannot be increased for simulated profile spectrum plot

Additional resolved issues are listed in Table 2.



Features and Enhancements in FreeStyle 1.7

Features

- New Data Analytics view that displays Trailer Extra and Status Log information as a Histogram or Trend plot in a separate window
- New Mass Defect Filtered (MDF) Chromatogram view for one or more user-defined Mass and Mass Defect Ranges
- Mass Defect Filtered Spectrum views linked to MMDF chromatograms
- Custom periodic table with editable isotope abundance for use in elemental composition calculation and isotope simulations
- A new customizable File Header view

Enhanced Features

- Save and Apply Text and Structure Annotations in the Spectrum View.
- Theoretical Spectral Distance Isotope Pattern now overlaid on Spectrum View and includes Theoretical Mass, Delta Mass, and support for Isotope Simulation.
- Map Ranges available as a right-click option in the Map View and includes Mass Range and Retention Time value fields.
- New peak identification group section in the Peak Detection Info bar page to select Nearest, Highest, or All Peaks detection mode.
- Import component parameters from the processing method to the current or copy of the selected trace.

System Requirements

These are the minimum required and recommended hardware and software configurations for operation of the FreeStyle 1.7 SP2 application.

System	Required or <i>recommended</i> configuration
Hardware	• 3.6 GHz Quad core processor with a minimum of 8 GB RAM (16 GB recommended)
	CD/R-ROM or DVD drive
	• 1 TB hard drive
	 Video card and monitor capable of 1920×1080 resolution
Software	 Adobe[™] Flash[™] Player (to view the demonstration animations in Help)
	 Adobe Acrobat[™] Reader[™] 10.1 or later
	 Microsoft[™] .NET Framework 4.7.2
	Microsoft Office 2013 (for exported data)
	 Microsoft Windows[™] 7 SP1 (64-bit) or Windows 10 Enterprise 2016 LTSB or Windows 10 Enterprise LTSC (64-bit)
	 Thermo Xcalibur[™] 4.3 or later (for the NIST Library Browser)
	• Thermo Foundation™ Platform 3.1 SP7 or later

Important Information

General

The FreeStyle 1.7 SP2 application does not require licensing in any form. The software may be installed on Windows 7 SP1 64-bit or Windows 10 operating systems.

Installation

You must have administrator rights to install and run the FreeStyle 1.7 SP2 software on your computer.

Compatibility

FreeStyle 1.7 SP2 is compatible with the Xcalibur data system, version 4.3 or later.

Upgrade Installation from FreeStyle 1.6, FreeStyle 1.7, and FreeStyle 1.7 SP1

- To upgrade your FreeStyle 1.7 SP1 installation to FreeStyle 1.7 SP2
- To upgrade your FreeStyle 1.7 installation to FreeStyle 1.7 SP2
- To upgrade your FreeStyle 1.6 installation to FreeStyle 1.7 SP2

To upgrade your FreeStyle 1.7 SP1 installation to FreeStyle 1.7 SP2

- 1. Download FreeStyle 1.7 SP2 from Flexera, https://thermo.flexnetoperations.com/control/thmo/login, to your local processing computer.
- 2. Open the Windows Control Panel, and navigate to the Uninstall or Change a Program screen.
- 3. Uninstall FreeStyle 1.7 SP1.
- 4. Install FreeStyle 1.7 SP2.

To upgrade your FreeStyle 1.7 installation to FreeStyle 1.7 SP2

- 1. Download FreeStyle 1.7 SP2 from Flexera, https://thermo.flexnetoperations.com/control/thmo/login, to your local processing computer.
- 2. Open the Windows Control Panel, and navigate to the Uninstall or Change a Program screen.
- 3. Uninstall FreeStyle 1.7.
- 4. Install FreeStyle 1.7 SP2.

❖ To upgrade your FreeStyle 1.6 installation to FreeStyle 1.7 SP2

1. Download FreeStyle 1.7 SP2 from Flexera https://thermo.flexnetoperations.com/control/thmo/login to your local processing computer.

Note You must uninstall previous versions and install the Xcalibur data system, version 4.3 or later.

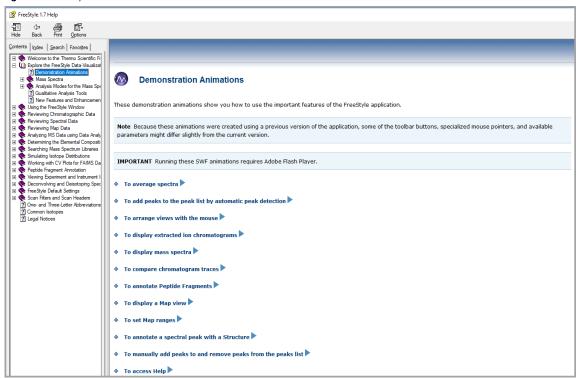
- 2. Open the Windows Control Panel, and navigate to the **Uninstall or Change a Program** screen.
- 3. Uninstall FreeStyle 1.6.
- 4. Uninstall previous version of Xcalibur.
- 5. Uninstall previous version of Foundation.
- 6. Install Xcalibur 4.3 or later.
- 7. Install FreeStyle 1.7 SP2.

Getting Started Demonstration Animations

To learn how to use the FreeStyle application, refer the demonstration animations in FreeStyle Help

- 1. In the FreeStyle application window, click **File > Help**.
- 2. In the FreeStyle 1.7 Help window, open the Explore the FreeStyle Data-Visualization Application chapter.

Figure 1. FreeStyle Demonstration Animations



- 3. Open the **Demonstration Animations** section.
- 4. From the list of animations, click the animation that you want to view.

Resolved Issues

Table 1 lists the defects that were resolved in the FreeStyle 1.7 SP2 release. The table excludes Help issues and any cosmetic fixes. In some cases, the Title has been amended or extended from the original to better describe the reported issue. The ID is the internal number assigned to each issue. Both an engineering fix and follow-up testing (verified by our product evaluation department) have resolved each of these issues.

Table 1. Resolved issues in FreeStyle 1.7 SP2

ID	Title	Severity
142951	Chemical formula not saved in Layout.	3 - Medium
143581	Background subtraction followed by Averaging does not apply correctly on Spectrum when Elemental Composition is applied.	2 - High
147401	Application crashes when Elemental Composition for Selected Scan is applied for a spectrum where averaging and background subtraction was applied.	1 - Critical
147411	Wrong scan header/ scan data shown to the user when elemental composition (selected scan) is applied after performing Background subtraction followed by Averaging.	2 - High
150705	Print to A4 size does not work as expected.	3 - Medium

Table 2 lists the defects that were resolved in the FreeStyle 1.7 SP1 release. The table excludes Help issues and any cosmetic fixes. In some cases, the Title has been amended or extended from the original to better describe the reported issue. The ID is the internal number assigned to each issue. Both an engineering fix and follow-up testing (verified by our product evaluation department) have resolved each of these issues.

Table 2. Resolved issues in FreeStyle 1.7 SP1 (Sheet 1 of 2)

ID	Title	Severity
129498	Exception seen for a custom library used for NIST search in FreeStyle.	2 - High
129899	Chromatogram not plotted for ICAL01 file for certain trace type selections.	2 - High

Table 2. Resolved issues in FreeStyle 1.7 SP1 (Sheet 2 of 2)

ID	Title	Severity
129906	Map View shows blank for ICAL01 file for all trace type selections.	2 - High
130271	Unable to get results using In-source HiRes search mode in NIST search within FreeStyle.	2 - High
129365	Missing simulation on export of spectrum to EMF.	2 - High
129493	FreeStyle sporadically fails to extend raw file chromatogram graph line to scans 1-2.	3 - Medium
29977	Peak detection is randomly applied when trace is deleted.	3 - Medium
30670	Isotope simulation: The plot title does not match with the plot selected.	3 - Medium
30709	Incorrect file name is displayed in the spectrum view title bar.	3 - Medium
51144	Labels from simulated plot (Elemental Composition, NIST) disappear after applying "Show within the Workspace" for Isotope Simulation.	3 - Medium
115443	"Show Peptide Results Table" is disabled for spectrum 1 when spectrum 2 is closed.	3 - Medium
134564	FreeStyle:[1.6] [Cannot increase the number of decimals for isotope simulation].	3 - Medium
133597	Null Value exception seen when performing Peptide fragments and subsequently adding Mass Ranges with Peptide.	2 - High
135326	Manufacturing layout: Application crashes during "apply layout".	1 - Critical

Known Issues

Suggested Recovery Actions

- For some issues, restarting the application is the appropriate recovery action.
- In some cases (particularly issues that arise during data acquisition), restarting applications such as the Home Page might not ensure complete recovery. Typically, restarting the data system computer resolves issues, but some devices with error conditions might require power cycling.
- 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

Risk	Interpretation
1 - Critical	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.
2 - High	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.
3 - Medium	A minor error or poor behavior of a product feature. There is probably a workaround.
4 - Low	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.

Known Defects

Table 3 table contains known defects in the software, categorized by severity with a brief abstract. The ID is the internal number assigned to each issue. Product management assesses risk, which can differ significantly from the reported severity.

 Table 3.
 Known defects (Sheet 1 of 3)

ID	Title	Severity
29391	Missing labels in chromatogram plots during print.	3 - Medium
29953	Adjusting the Chromatogram Range window to a certain size shows the chemical formula window - partially hidden the chemical formula floating window.	3 - Medium
29954	Performing mzVault/NIST search on Multispectrum - Opens new spectrum window each time search is performed.	3 - Medium
29955	Elem Comp MSMS Scan no. accepts SRM scan filters.	3 - Medium
29956	PPD Chromatogram Copy to Clipboard does not reflect PPD peak.	3 - Medium
29957	Template can cause m/z range to be set to 0-1 if raw file is outside template m/z range.	3 - Medium
29958	Scrolling up Vertically for chromatogram and multiSpectrum hides the Horizontal scrollbar.	3 - Medium
29959	Manual peak detection for UV data files.	3 - Medium
29960	PPD Chromatogram peak label missing for 1 peak but those adjacent OK.	3 - Medium
29964	Little variation noticed in exported averaged/background subtracted spectrum.	3 - Medium
29965	PPD Chromatogram peak tip occasionally cut off.	3 - Medium
29966	The chromatogram RT marker stops tracking, after releasing a spectrum.	3 - Medium
29967	Legends > Scan header options do not work for composite & average spectra.	3 - Medium
29971	Averaging and background subtraction icons in the toolbox disappear when chromatogram is zoomed.	3 - Medium
29972	Sequence file name is not synced with current chromatogram view.	3 - Medium
29973	Mass labels appear for every profile point from ITMS profile file.	3 - Medium
29974	Export Workspace as EMF with Dimensions Doesn't Work Correctly on Windows 10.	3 - Medium
29975	Minimum trace height feature does not work correctly on 4K screens.	3 - Medium
29976	Multispectrum: Unable to change the color from 9th plot onwards.	3 - Medium
29979	Toolbox will not relocate to my cursor position: moves about twice as fast as mouse	3 - Medium
29980	Manufacturing layouts: Position of chromatogram and spectrum are changed.	3 - Medium
29981	PPD S/N Threshold Sometimes not Applied to Filtered Chromatograms for some raw files.	3 - Medium
29982	mass tolerance - different for mzvault verses mzcloud - Example FTMS and ITMS.	3 - Medium
29985	Mass tolerance is NOT updated when chemical formula/Peptide sequence is present.	3 - Medium
29988	Product displays blank screen during remote access.	3 - Medium
30251	Blank spectrum is displayed when background subtraction 2 range is performed in the new chromatogram view.	3 - Medium
30467	Application does not accept decimal values as expected in mass range entry.	3 - Medium
30468	Mismatch in Elemental Comp Result for PPD peak top vs User selected peak top.	3 - Medium
30469	Layouts: Multispectrum position changes and new spectra is added upon performing apply default.	3 - Medium

 Table 3.
 Known defects (Sheet 2 of 3)

ID	Title	Severity
30470	Splash screen which appears before FS main window on starting application is very small on a $4\mathrm{K}$ screen.	3 - Medium
30473	Window placement arrows are disabled.	3 - Medium
30480	Layout - Peak List - Empirical formula is NOT displayed upon Apply Default although settings is 'Saved as Default'.	3 - Medium
30493	Averaging on spectrum with multi segment data is merged to single segment scan in MultiSpectrum.	3 - Medium
30494	Chromatogram Plot Title and Hover Box do not reflect User Selected Decimal Places.	3 - Medium
30574	Sum button does not stay active.	3 - Medium
30652	Usability Issue - Cursor Or RT marker doesn't move when Delay Time is given in Chromatogram Ranges and move to End RT using keyboard Arrow keys.	3 - Medium
30658	Deleting Unselected, Unreferenced Chromatogram Plot Affects Selected, Reference Plot.	3 - Medium
30660	Average with multiple Chromatogram - RT value within limits but looks like limit is for second chromatogram.	3 - Medium
30661	.Raw file name is replaced by selected file name from sequence when both .raw and .sld files are opened together.	3 - Medium
30662	Layouts are not applied if we open the same raw file or different raw file again.	3 - Medium
30695	Chromatogram display options - RT labels are missing in 'Stick' view.	3 - Mediun
30699	FS Layout Default overrides Smoothing, Delay Time, Reference, applies invalid settings to raw files.	3 - Medium
37166	Display Options- Subtabs corresponding to both chromatogram and spectrum are shown.	3 - Medium
44777	Unchecking and rechecking the trace from chromatogram ranges makes to the annotated text to disappear.	3 - Medium
44875	Instrument method view does not correctly show which method is being displayed.	3 - Medium
44883	Text annotation: Add/Edit text is NOT working for a long statement.	3 - Medium
47273	SN display format is not ideal (decimals and scientific notation).	3 - Mediun
47478	m/z Bandwidth text box should not wait for the click of ENTER button.	3 - Medium
48108	Installer shows up a warning though latest version of MS office is installed.	3 - Mediun
50023	Separate axis should be automatically enabled when a new chromatogram trace is added to the Chromatogram view.	3 - Medium
50639	NIST Search: Mass labels are missing in Exclusion plot.	3 - Medium
56308	Write to .raw does not include reference / exception peak information.	3 - Mediun
61791	Layout: Incorrect averaging done upon applying layout.	3 - Mediun
62330	Chemical Formula or Peptide Sequence EIC Info not retained in Layout.	3 - Mediun
63283	HRAM Data not Exported if Quick, Normal Search Types Selected.	3 - Mediun
63563	Undo Zoom does not function when chromatogram has been averaged followed by zoomed.	3 - Medium
82778	Chromatogram becomes blank for a particular trace type.	3 - Medium
86938	Reports - Configured width and height is not used in "To Clipboard in EMF".	3 - Medium
107758	NIST similarity search type Neutral Loss results mismatch in FreeStyle and NIST browser.	3 - Medium

Table 3. Known defects (Sheet 3 of 3)

ID	Title	Severity
113322	Cannot export tab delimited data to clipboard.	3 - Medium
113915	Elemental results table does not track selected spectrum.	3 - Medium
115117	Layout: Blank Map view window is displayed on applying layout for an invalid filter but Map ranges displays no filter as shown in default scenario.	3 - Medium
115599	Columns in the Elemental Composition Results table cannot be resized.	3 - Medium

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