FreeStyle 1.6 Release Notes

These release notes briefly list changes in the Thermo FreeStyle™ 1.6 software, fixes to previously reported issues, and known issues still existing in the FreeStyle 1.6 software release.

Contents

For information on using the FreeStyle 1.6 application, refer to the *FreeStyle 1.6 User Guide*, which is available as a PDF file, or the Help.

Features

This release incorporates a number of new and enhanced features.

New Features

- Experimental spectra labeled with peptide fragments computed for a user-entered amino acid sequence.
- Annotate experimental spectral peaks with structure from a user-selected mol file.
- Create 2D and 3D map view.
- Refresh live .raw file displays during acquisition.

Feature Enhancements

- Separate axis for multi-plot chromatogram views.
- Edit and relocate text and graphic annotations.
- Include MS/MS spectrum with predicted elemental compositions from precursor elemental composition analysis.
- Searches against local mzVault™ libraries include new pre-filter options.

thermo scientific

System Configurations

These are the recommended hardware configuration and required or recommended software configurations for operation of the FreeStyle 1.6 application.

System	Required or *recommended* configuration
Hardware (Recommended configuration)	• *3.6 GHz Quad core processor* • *16 GB RAM* • *Video card and monitor capable of 1920×1080 resolution* • *1 TB hard drive*
Software	• Microsoft™ Windows™ 7 SP1 64-bit or *Windows 10* • Microsoft Office 2013 • Microsoft .NET Framework 4.6.2 • Adobe™ Acrobat™ or Reader™ 10.1 • Adobe Flash™ Player 11 • Xcalibur™4.2 SP1 or higher

Important Information

General

The FreeStyle 1.6 application does not require licensing in any form. It is compatible with Windows 7 SP1 (64-bit) and Windows 10 operating systems.

Installation

You must have administrator rights to install and run the FreeStyle 1.6 software on your computer. The FreeStyle 1.6 application is installed as part of the Thermo Xcalibur 4.3 core software suite.

Resolved Issues

Table 1 lists defects that were resolved in the FreeStyle 1.6 release. The table excludes Help issues and any cosmetic fixes. In some cases, the Abstract has been amended or extended from the original to better describe the reported 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 (Sheet 1 of 3)

ID	Title	Severity
35862	Call out and text disappears while converting a spectrum to a MultiSpectrum.	2 - High
37338	Annotation ribbon menu buttons cannot be "Turned Off".	2 - High
37372	Peak detection on a UV trace with negative absorbance - The peak integration automatically adjusts peak baseline only > 0 absorbance.	2 - High
37384	Text annotation are not getting printed.	2 - High
41850	Opening the "Legend: Scan Header" form, and pressing OK without making any changes causes the scan type to be shown twice on filtered spectra.	2 - High
47493	Application crashes upon using the attached template file.	2 - High
46963	AcquireX™ Component ion detection step failed with the system. Exception "Could not open raw file" when the raw file opens in FreeStyle 1.6.	2 - High
45115	Spectrum plot is not updated "at random" when choosing scan filters from the info bar.	2 - High
50542	Elemental Composition in the info bar displays random mass not corresponding to the base peak of the selected spectrum.	2 - High
52011	Double clicking on the nearby precursor flag shows original spectrum instead of nearby precursor spectrum.	2 - High
52217	Recent File List: Application shows error message when the attached file is opened.	2 - High
46049	On changing the default ITMS mass precision value to 0, Mass value in Ranges column in Chromatogram Ranges still shows 4 decimal digits.	3 - Medium

Table 1.   Resolved issues (Sheet 2 of 3)

ID	Title	Severity
47277	The Peaks List reappears after closing when navigating through a sequence.	3 - Medium
47279	Base Peak chromatogram label does not follow defined sigfigs.	3 - Medium
47442	Peak Baseline Marker not drawn correctly after manual baseline adjustment.	3 - Medium
47471	After performing "Label relative to mass on a spectra" Changing the spectra to wavelength scan retains the relative labeling on wavelength scan.	3 - Medium
48105	User is unable to navigate to different scans in the spectrum when text and graphics annotation tab is selected.	3 - Medium
48287	Undo delete spectrum does not return the averaged and background subtracted values.	3 - Medium
49092	Not able create the EIC for the mass from the spectrum peak when text and graphics annotations tab is selected.	3 - Medium
49093	MultiSpectrum "Release" state in header is not updated for the selected trace if the text and graphics annotations tab is selected.	3 - Medium
49094	Chromatogram averaging is not working when the text and graphics annotations is selected.	3 - Medium
49095	Chromatogram add peak is not working when the text and graphics annotations is selected.	3 - Medium
49096	Chromatogram delete peak is not working when the text and graphics annotations is selected.	3 - Medium
49097	Chromatogram background subtractions is not working when the text and graphics annotations is selected.	3 - Medium
49098	Spectrum EIC Mass from tool box is not working when text and graphics tab is selected.	3 - Medium
49099	Select manual noise range is not working when text and graphics tab is selected.	3 - Medium
49100	Clear manual noise range is not working when text and graphics tab is selected.	3 - Medium
49101	Unable to remove the chromatogram trace when text and graphics tab is selected.	3 - Medium
49102	Unable to remove the spectrum in multi spectrum view when text and graphics tab is selected.	3 - Medium
41929	Unable to close the spectrum having peptide fragment markers.	3 - Medium
44340	Chromatogram and chromatogram ranges are not in sync.	3 - Medium
45044	Text alignment mode is not indicated when adding text annotation.	3 - Medium
37385	When new peaks are manually added after performing peak detection > Append the peak table based on RT sorting.	3 - Medium
41629	Zoom in at mass functionality should be restored and corrected.	3 - Medium
41691	It is not possible to select a mass from a peak label, for a structure, when the annotation tab is open.	3 - Medium
37373	Performing manual peak detection automatically resets the Y-axis zoom.	3 - Medium
35267	Sorting order is not correct for NIST search results.	3 - Medium
35748	When the chromatogram trace is changed to PDA - the spectrum does not update to wavelength scan.	3 - Medium
36247	Chromatogram view 2 does not copy from existing chromatogram view 1.	3 - Medium
36675	Detector Type display error in spectrum ranges.	3 - Medium
36832	MS data shown in absolute scale when not expected.	3 - Medium

Table 1. Resolved issues (Sheet 3 of 3)

ID	Title	Severity
37092	When printing the peak list report - all the values of RT, Peak Height, Peak area etc are displayed to greater than 5 decimal places in the report instead of using exponential display.	3 - Medium
37115	For UV trace - using reset scaling option doubles the Y-axis scaling.	3 - Medium
37176	Undo zoom is not enabled in chromatogram when zoom is performed via ribbon menu.	3 - Medium

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, Thermo Fisher Scientific generally does 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
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.
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.
Medium	A minor error or poor behavior of a product feature. There is probably a workaround.
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 2 contains known defects in the software, categorized by severity with a brief abstract. The Item ID is the internal number assigned to each issue. Product management assesses risk, which can differ significantly from the reported severity.

Table 2. Software defects (Sheet 1 of 4)

ID	Title	Severity
29974	Export workspace as EMF with dimensions does not 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

Table 2. Software defects (Sheet 2 of 4)

ID	Title	Severity
29977	Peak detection is randomly applied when trace is deleted.	3 - Medium
29978	Many spectra are added automatically upon applying layout.	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
29988	Product displays blank screen during remote access.	3 - Medium
47469	Space is wasted above spectrum plots.	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
47203	Custom axis name is not copied when we open new workspace.	3 - Medium
47273	SN display format is not ideal (decimals and scientific notation).	3 - Medium
37166	Display Options- Subtabs corresponding to both chromatogram and spectrum are shown.	3 - Medium
47478	m/z bandwidth text box should not wait for the click of ENTER button.	3 - Medium
47635	Text and annotation is retained even after changing the .raw file for a chromatogram, spectrum, and MultiSpectrum.	3 - Medium
48108	Installer shows up a warning though latest version of MS office is installed.	3 - Medium
50023	Separate axis should be automatically enabled when a new chromatogram trace is added to the chromatogram view.	3 - Medium
50601	MS Paint cannot correctly draw "formula labels" on FreeStyle Spectra when an image is copied to clipboard (but PowerPoint is correct).	3 - Medium
50639	NIST Search: Mass labels are missing in exclusion plot.	3 - Medium
50769	Enabling "Show within the Workspace" for isotope simulation and checking profile resolution triggers simulated isotope plot.	3 - Medium
50834	Toolbox is removed when selecting "text and graphics annotation".	3 - Medium
50835	Units are missing from "Label Threshold".	3 - Medium
51144	Labels from simulated plot (Elemental Composition, NIST) disappear after applying "Show within the Workspace" for isotope simulation.	3 - Medium
51471	Pressing F1 does not direct the user to the respective help page.	3 - Medium
30251	Blank spectrum is displayed when background subtraction 2 range is performed in the new chromatogram view.	3 - Medium
29982	Mass tolerance - different for mzVault verses mzCloud - Example FTMS and ITMS.	3 - Medium
29983	File name alignment is incorrect when many windows are open.	3 - Medium

Table 2. Software defects (Sheet 3 of 4)

ID	Title	Severity
29984	Changing Detector type after overlay is performed does not revert the plots back to stack.	3 - Medium
29985	Mass tolerance is not updated when chemical formula/Peptide sequence is present.	3 - Medium
29986	'Reference' checkbox settings are not preserved upon adding a new chromatogram view.	3 - Medium
29987	Layouts - Spectrum pane is displayed on opening a raw file applied with layout having MultiSpectrum pane floated and no Spectrum pane.	3 - Medium
30469	Layouts: MultiSpectrum position changes and new spectra is added upon performing apply default.	3 - Medium
30470	Splash screen which appears before FS main window on starting application is very small on a 4K 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
30483	RT marker does not move while navigating through keyboard.	3 - Medium
30493	Averaging on spectrum with multi segment data is merged to single segment scan in MultiSpectrum.	3 - Medium
30494	Chromatogram pot title and hover box do not reflect user-selected decimal places.	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
29968	Layout: Isotope Simulation: simulated spectrum is missing.	3 - Medium
29969	Peak detection is not applied from the default layout.	3 - Medium
29970	Installed programs show both the versions of FreeStyle while upgrading from any lower versions to FS 1.5.	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
29391	Missing labels in chromatogram plots during print.	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
29961	Sequence-Auto Filter shows incorrect filters.	3 - Medium
29962	CV Plot cannot be re-enabled if closed while floating.	3 - Medium
29963	CV Plot does not update after re-ordering in Active Traces window.	3 - Medium
29964	Little variation noticed in exported averaged/background subtracted spectrum.	3 - Medium
29965	PPD Chromatogram peak tip occasionally cut off.	3 - Medium
30574	Sum button does not stay active.	3 - Medium

Table 2. Software defects (Sheet 4 of 4)

ID	Title	Severity
30652	Usability Issue - Cursor or RT marker does not 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
30467	Application does not accept decimal values as expected in mass range entry.	3 - Medium
30468	Mismatch in elemental composition result for PPD peak top vs user-selected peak top.	3 - Medium
30662	Layouts are not applied if we open the same raw file or different raw file again.	3 - Medium
30670	Isotope simulation: The plot title does not match with the plot selected.	3 - Medium
30699	FS layout default overrides smoothing, delay time, reference, applies invalid settings to raw files.	3 - Medium
44086	Installer: FreeStyle 1.6 installer should check for Foundation 3.1 SP5.	3 - Medium
30709	Incorrect file name is displayed in the spectrum view title bar.	3 - Medium
30695	Chromatogram display options - RT labels are missing in 'Stick' view.	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
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	Elemental Composition MS/MS scan number 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

Trademarks