



Product Release Notes

GRAMS Suite 9.3 SP1

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Introduction

Thermo Fisher Scientific is pleased to announce the release of Thermo Scientific™ GRAMS Suite™ version 9.3 SP1. The content in this document describes new and/or revised functionality in this version of the product, as well as supported platform combinations, fixed issues and known issues.

Please always be sure to check the support site for any updates to this product.

Supported Platforms

The following section contains information on the platforms currently supported for GRAMS Suite version 9.3 SP1.

Client Operating System

Microsoft® Windows® 10

Features

This product release introduces modified features and fixed issues for GRAMS Suite version 9.3 SP1.

Functional Area(s)

GRAMS IQ Usability Enhancements

The GRAMS IQ application has been enhanced to provide easier methods of entering data, identifying outliers, and saving settings for calibration files.

- A command-line interface has been added to provide automation of the steps to load data and create calibration files.
- New columns have been added to the Training Set grid to display the range of the Y values. This can aid in identifying samples that are outliers.
- The colors used for the traces have been modified to provide better contrast, and users are now able to select samples from the Experiment Setup tab and modify the Type of the sample.
- The template mechanism has been expanded to include the Experiment Setup tab allowing users to save commonly used settings for that page.
- The settings used to create a calibration file can be saved in a separate XML file to help document the creation of the calibration.

For more information, see the GRAMS IQ section of the Thermo Scientific GRAMS Suite Help file.

Requirement	Description
SCR125524	Add command-line parameters to GRAMS IQ to enable creation of experiments and loading of data.
SCR125525	GRAMS IQ should display a progress dialog when loading Training Set data.
SCR125526	Provide a mechanism in GRAMS IQ to save model settings and stats to an XML file.
SCR125548	GRAMS IQ should provide a mechanism to set the type for input data that matches specified criteria.
SCR125549	GRAMS IQ handling of Factors on the Results page should be improved.
SCR125550	GRAMS IQ should provide command line parameters to specify settings for the calibration file.
SCR125551	GRAMS IQ should allow a user to select a trace in the Experiment Setup tab.

Requirement	Description
SCR125721	GRAMS IQ should provide a mechanism to change the type of a sample while on the Experiment Setup tab.
SCR125722	GRAMS IQ should provide templates for the setting on the Experiment Setup tab.
SCR126183	The colors used to display items in GRAMS IQ should be adjusted to avoid conflicts.

Spectral ID Library Management Enhancements

The Spectral ID application has been modified to allow users to export a list of the compounds in a library. Also, when adding files to a search library, a new option allows the filename of each spectrum to be inserted into the comment field.

For more information, see the Spectral ID section of the Thermo Scientific GRAMS Suite Help file.

Requirement	Description
SCR120749	Provide a mechanism in Spectral ID to insert filename into comment field when adding to a search library.
SCR118918	Spectral ID should be enhanced to allow export of library item names.
SCR34571	Allow Spectral ID to output a list of all spectra in a library

IQ Predict

The "Open Unknowns" menu of IQ Predict has been enhanced to include options to import instrument data files. The import mechanism is the same one already used in other GRAMS applications.

For more information, see the IQ Predict section of the Thermo Scientific GRAMS Suite Help file.

Requirement	Description
SCR120070	IQ Predict cannot open non-SPC files.

GRAMS Envision Viewer

The GRAMS Envision Viewer was developed to display instrument data in a modern easy to use interface. It provides modular viewers for 2D, 3D and "linked data". The linked data module allows the user to view a chromatogram and the associated PDA or MS data and interactively look at slices of the data.

In the past, the viewer has been shipped separately or with our Data Manager product. In this release, Envision has been pulled into the GRAMS Suite install and menu items have been added to pass data to/from the Envision viewer.

For more information, see the Thermo Scientific GRAMS Envision Help file.

Requirement	Description
SCR126184	Include Envision Application with GRAMS installation.
SCR126185	Integrate Envision with other GRAMS Suite application menus.
SCR126186	Envision should be updated to use the latest .Net components.

Fixed Issues

The following table details the software issues that have been corrected in this product release.

Issue ID	Summary
SCR117265	Reconvert fails and causes unhandled exception in GRAMS Convert
SCR117752	GRAMS YUnit Conversion fails on customer's data file
SCR117755	GRAMS AI does not pass multifile to Active MultiFile Tool
SCR117765	The GRAMS applications need to be updated to use the new version of the component GImportFile
SCR118917	GRAMS displays a warning message when near support expiration date.
SCR120069	IQ Predict crashes if calibration file has a region with only 1 point.
SCR120267	The GIOSubs component is causing a failure in GRAMS IQ when PLS-2 calibrations are processed.
SCR120469	The GRAMS IQ Threshold field is not saved when changing plots.
SCR120754	The recommended number of factors in GRAMS IQ are not set properly if result templates are loaded
SCR120818	The Predicted Concentration value is missing in some tables of the GRAMS IQ Report Document.
SCR120819	Saving a CFL file in GRAMS IQ from a Training Set that contains Validation data creates an invalid file.
SCR121063	GRAMS Excel Exchange creates a bad SPC file if the input data contains trailing spaces.
SCR121316	GRAMS AMT locks up with large SPC files.
SCR121872	GRAMS IQ plots with Sample Number axis do not display correct sample number.
SCR122366	GRAMS IQ Predict crashes when running a customer calibration file.
SCR122566	GRAMS IQ can crash if a percent symbol ('%') is passed to the tracing routine.

Issue ID	Summary
SCR122755	GRAMS IQ can display the wrong X axis orientation if the first sample is removed.
SCR122757	The Sample Numbers on GRAMS IQ result plots may not line up with the numbers displayed in the Training Set grid.
SCR123241	Several GRAMS applications cannot open files if there is a '#' in the folder name.
SCR123552	Some GRAMS applications fail on Windows 10.
SCR123995	GRAMS IQ fails to open TDFX file if data has a large number of points.
SCR31769	The GRAMS Convert pop-up for the 'Search For' field is empty.
SCR9930	Error in GRAMS Spectral Subtract with multifiles.

Known Issues

There are no known Priority 1 or Priority 2 issues identified within this product version as of 04-March-2022.

Any other known issues, Knowledge Base articles, and workaround details may be obtained via the Thermo Scientific Informatics Support Portal by using the following link:

<https://support.thermoinformatics.com/>.

You must have a valid and current support contract in order to access this information.

Database Changes

This section indicates whether or not changes were made to the database structure as a result of the enhancements and/or issue resolution included in this release.

Yes, changes were made

No, changes were not made

Not applicable