

Product Release Notes

GRAMS 9.1

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Introduction

Purpose

The objective of the release notes is to describe new and revised functionality in this version of the product, as well as platform combinations used in formal testing, fixed defects and known defects.

Inventory of Materials

1. GRAMS Suite 9.1 Setup executable. Includes:
 - a. GRAMSSetup.exe: Version 9.1 of the GRAMS Suite installation
 - b. GRAMSConvertersPackage.msi: Version 9.1 of the GRAMS Converters Package installation.
2. Welcome Guide (PDF file)
3. Release Notes (PDF file)

Testing Information

The following platform combinations were used in testing.

Primary Testing Platform

Server	Platform	OS	OS version
	Intel PC	Windows 7 64 bit	SP1

Secondary Platform Testing

Server	Platform	OS	Version
Client	Intel PC	Windows XP	SP3
Server	Intel PC	Citrix	XenApp 5
	Platform	OS	OS version
Client	Intel PC	Windows XP	SP3
Server	Intel PC	Thermo Web Access 2008 Server 32 bit	4.0.1 SP3

New/Modified Functionality

This section describes the new and modified functionality for GRAMS 9.1. This release also features an update to the GRAMS converters package.

For details of fixed defects, see the Fixed Defects section.

Operating Platforms

The GRAMS Suite has been tested against Microsoft Windows 7 (32-bit and 64-bit). It now supports concurrent users on a Citrix server.

GRAMS Suite can also now be run remotely, in a web browser window, using the optional Thermo Web Access client.

We have increased the speed of a number of Array Basic programs and provided command-line access to the GRAMS file conversion capabilities. The ability to export as ASCII, JCAMP, and ANDI formats directly from the file menu has returned, although we have retained the legacy export tool for backwards compatibility (in the Data Conversion subfolder accessed from the Start menu).

We have added further enhancements to our two new standalone products:

GRAMS IQ

GRAMS IQ is a simple graphical tool for chemometric model creation, maintaining the industry standard functionality of PLSplus/IQ and adding a step-by-step graphical interface:

- Import sample data using GRAMS Converters
- Reference data through a new matching wizard.
- Analyze the data graphically to determine the most informative regions and modelling parameters.
- Define plots to test the model by self-reference or validation sets to identify outliers and areas for improvement.
- Build calibrations and user-definable reports.

GRAMS Convert

GRAMS Convert allows the bulk transformation of any supported instrument data files on your system to the industry standard GRAMS SPC format. It can intelligently scan multiple directories, converting known file formats into SPC format.

GRAMS Converters

The following updates have been made to the GRAMS converters for this release:

- A new converter has been provided to support the ASD Indico format.
- The ASCII converters have been upgraded to run in a 64-bit environment. Both import and export are supported.
- The J-Camp converter has been upgraded to run in a 64-bit environment. Both import and export are supported.
- The AnDI/ newCDF (AIA) Chromatography converter has been updated to support export.

See the section "Converter Support" for information on all supported converters.

Fixed Defects

The following list details the software changes (defects) that have been implemented in this product release.

Issue Number	IR Number (If applicable)	Category	Issue Description
11487	IR-GAML-0000059	General	The SpecID icon in the toolbar and on the Taskbar is the wrong colour depth.
27559	IR-GAML-0000054	General	Spectral ID Close menu item does not work.
27560	IR-GAML-0000053	General	'Create Plot' button is not enabled properly.
27561	IR-GAML-0000052	General	GRAMS IQ does not recognize 'Excluded Constituents' in a .tdf file.
27562	IR-GAML-0000051	General	GRAMS IQ crashes when running experiment with additional data from CFL or Synthetic Data generator
27564	IR-GAML-0000049	General	GRAMS IQ Sample names in 'Create Document' rtf file are incorrect.
27565	IR-GAML-0000048	General	The 'Linked Applications' menu item in AMT is disabled.
27566	IR-GAML-0000047	General	The region band in GRAMS IQ is sometimes displayed on the Training Set spectral display.
28106	IR-GAML-0000009	General	GSpCIOLib crashed with DEP error reading/writing "fixed point" values.
28172	IR-GAML-0000045	General	Some of the GRAMS add-on applications fail to open if they have been closed while minimized.

Issue Number	IR Number (If applicable)	Category	Issue Description
28897	IR-GAML-0000044	General	Drag-and-drop of SPC file with period and space in path fails to open in GRAMS/AI.
28898	IR-GAML-0000043	General	The File > Open Trace dialog box in GRAMS/AI fails to open if too many files are selected.
28918	IR-GAML-0000042	General	Overlapping regions do not combine in GRAMS IQ if the X values are running high to low.
28919	IR-GAML-0000041	General	GRAMS IQ can crash trying to save the calibration file if the file is opened by another application.
28920	IR-GAML-0000040	General	Cut-and-paste wizard copies the last row of the input to all selected rows in the Training Set table.
28921	IR-GAML-0000039	General	Removing a constituent from an Experiment can affect values of other constituent columns.
28922	IR-GAML-0000038	General	Experiment hierarchy is broken when more than three Experiments deep.
28923	IR-GAML-0000037	General	Create Document function can crash if samples are excluded from the training set.
28924	IR-GAML-0000036	General	Changes made to Constituent values are not saved.
28926	IR-GAML-0000035	General	The X values of Sample Data in GRAMS IQ are inaccurate.

Issue Number	IR Number (If applicable)	Category	Issue Description
28928	IR-GAML-0000034	General	Using the DELETE key to remove a sample from the Training Set table can result in a corrupt TDFX file.
28933	IR-GAML-0000033	General	Invalid calibration files if number of factors is changed when adding calibration.
28949	IR-GAML-0000032	General	GRAMS IQ will not return to normal size if it has exited when minimized.
28955	IR-GAML-0000031	General	Remove All Samples in Training Set menu causes errors when trying to add new samples.
28956	IR-GAML-0000030	General	The "Apply Flexnet License" menu item of GRAMS Config does not validate the input file.
28957	IR-GAML-0000029	General	The GRAMS AI "Invalid SPC Data" error message does not provide additional details.
28959	IR-GAML-0000027	General	The "Correlation" and "Determination" statistics plots are not being displayed.
28967	IR-GAML-0000025	General	Spectral ID fails to open if converters are not installed.
28984	IR-GAML-0000024	General	The Equation Editor and Legend Display items on the Object menu of GRAMS AI are disabled.
29127	IR-GAML-0000023	General	The GRAMS IQ application may fail to save the TDFX file on exit.

Issue Number	IR Number (If applicable)	Category	Issue Description
29970	IR-GAML-0000065	GAML Converters	OMNIC converter missing date field.
29972	IR-GAML-0000066	GAML Converters	OMNIC converter generates data files that are misidentified as Raman by Spectral ID.
29973	IR-GAML-0000078	General	Replicates in GRAMS IQ are not rotated out correctly for CrossValidation.
29974	IR-GAML-0000077	General	IQ does not remember Column sizes in Training Grid.
29975	IR-GAML-0000076	GAML Converters	PE TurboChrom is missing SUIT_TAILING_FACTOR parameters.
29976	IR-GAML-0000075	General	The Paste Wizard of GRAMS IQ cannot paste into Name and Memo field.
29977	IR-GAML-0000074	General	Changing the number of factors on the Experiment tab of GRAMS IQ has no effect on the output.
29978	IR-GAML-0000073	General	GRAMS IQ error for mismatched data should not have Yes/No buttons.
29979	IR-GAML-0000072	General	Remove the "stub" converter help file, and add an error message to the apps that have converter help on Help menu.
29980	IR-GAML-0000071	General	AMT fails if converters not installed.
29981	IR-GAML-0000070	General	The Array Basic DOS command does not properly wait for the command to complete.

Issue Number	IR Number (If applicable)	Category	Issue Description
29982	IR-GAML-0000069	General	The base name of the output files generated by GRAMS Convert does not match the base names of the input file.
29983	IR-GAML-0000068	GAML Converters	Some Masslynx data files fail to convert.
29984	IR-GAML-0000067	General	The result plots in GRAMS IQ do not display the default number of factors.
29873	IR-GAML-0000079	GAML Converters	ChromQuest Converted data has missing peaks: c.f. the ChromQuest UI.
31446	N/A	General	The Active Multifile Tool does not preserve the Spare values in SPC files.

Known Defects

The following section contains all known issues with a severity level of 4 or 5, as well as issues with a severity level of 3 identified within this release. The defects are listed with a severity rating where available and a workaround if known.

A complete listing of known issues and Knowledge Base articles can be obtained in the eService Portal by using the following link: <http://eservice.thermo.com/>. You must have a valid and current support contract in order to access this information.

Issue Number	Description	Severity
31773	Converter install may prompt for reboot causing GRAMS install to be skipped.	3-Moderate

Converter Support

Converter Name	Type	Status
AIA/ANDI Chromatography	32-bit (GAML)	Will run on all supported operating systems.
AIA/ANDI FT-IR	32-bit	Will run on all supported operating systems.
AIA/ANDI Mass Spectrometry	32-bit	Will run on all supported operating systems.
ANDO AQ Optical Spectrum Analyzer	32-bit (GAML)	Will run on all supported operating systems.
ASCII X,Y (Constant X Spacing)	32-bit (GAML)	Will run on all supported operating systems.
ASCII X,Y (High Precision X)	32-bit (GAML)	Will run on all supported operating systems.
ASCII X,Y (Variable X Spacing)	32-bit (GAML)	Will run on all supported operating systems.
ASCII Y (Single Column)	32-bit (GAML)	Will run on all supported operating systems.
ASD PSII UV-Vis	16-bit	Will not run on Windows 7 64-bit
ASYST V1.5+ Data File	16-bit	Will not run on Windows 7 64-bit
AVIV UV-Vis/CD	16-bit	Will not run on Windows 7 64-bit
Acorn NMR NUTS	32-bit	Will run on all supported operating systems.
Agilent ChemStation (LC/GC/PDA/MS)	32-bit (GAML)	Will run on all supported operating systems.
Alton Instruments LS2000	16-bit	Will not run on Windows 7 64-bit
Amersham Bioscience UNICORN	32-bit (GAML)	Will run on all supported operating systems.
Analect FT-IR	32-bit	Will run on all supported operating systems.
Ando AQ-6312B	16-bit	Will not run on Windows 7 64-bit
Applied Automation Optichrom	16-bit	Will not run on Windows 7 64-bit
Atlas Chromatography Data System	32-bit (GAML)	Will run on all supported operating systems.
Beckman DU60 ASCII UV-Vis	16-bit	Will not run on Windows 7 64-bit
Beckman FT1000/2000 FT-IR	16-bit	Will not run on Windows 7 64-bit
Beckman Gold Chromatography	32-bit (GAML)	Will run on all supported operating systems.
Beckman Gold Diode Array	16-bit	Will not run on Windows 7 64-bit
Beckman PeakPro Chromatography Data System	32-bit (GAML)	Will run on all supported operating systems.
Beckman UV-Vis/Fluorescence	16-bit	Will not run on Windows 7 64-bit
Bio-Rad BioDimension DAD	16-bit	Will not run on Windows 7 64-bit

Converter Name	Type	Status
Bio-Rad Digilab 3200 FT-IR	16-bit	Will not run on Windows 7 64-bit
Bio-Rad Digilab IMX FT-IR	16-bit	Will not run on Windows 7 64-bit
Bio-Rad Sadtler IR	16-bit	Will not run on Windows 7 64-bit
Bomem DA3/DA8 FT-IR	16-bit	Will not run on Windows 7 64-bit
Brimrose AOTF NIR	16-bit	Will not run on Windows 7 64-bit
Bruker ATS FT-IR (Aspect)	16-bit	Will not run on Windows 7 64-bit
Bruker AXS DIFFRACplus/AT XRD	32-bit	Will run on all supported operating systems.
Bruker Aspect NMR	32-bit	Will run on all supported operating systems.
Bruker ESP300 ESR	16-bit	Will not run on Windows 7 64-bit
Bruker OPUS FT-IR (OS/2)	32-bit	Will run on all supported operating systems.
Bruker UXNMR (X32)	16-bit	Will not run on Windows 7 64-bit
Bruker WIN-NMR	16-bit	Will not run on Windows 7 64-bit
Bruker XWIN-NMR	32-bit (GAML)	Will run on all supported operating systems.
Chemagnetics CMX NMR	16-bit	Will not run on Windows 7 64-bit
Chemagnetics SpinSight NMR	32-bit	Will run on all supported operating systems.
Data Interchange Format (DIF)	16-bit	Will not run on Windows 7 64-bit
Dilor Microdil 28 Raman (V2)	16-bit	Will not run on Windows 7 64-bit
Dilor Microdil 28/Z24 Raman (V1)	16-bit	Will not run on Windows 7 64-bit
Dionex Chromeleon Chromatography Data System	32-bit (GAML)	Will run on all supported operating systems.
Dionex-Lee Scientific 600	16-bit	Will not run on Windows 7 64-bit
EG&G PAR CCD Spectrum	16-bit	Will not run on Windows 7 64-bit
EG&G PAR OMA88 CCD Spectrum	16-bit	Will not run on Windows 7 64-bit
EG&G PAR ProcessVision	16-bit	Will not run on Windows 7 64-bit
EG&G Spectrum Master Maestro II	16-bit	Will not run on Windows 7 64-bit
EZChrom Elite Chromatography	32-bit (GAML)	Will run on all supported operating systems.
Finnigan MAT ITDS GC-MS	16-bit	Will not run on Windows 7 64-bit
GBC Spectral UV-Vis	32-bit	Will run on all supported operating systems.
GE Omega NMR	16-bit	Will not run on Windows 7 64-bit
GE/Nicolet NMR (1280)	16-bit	Will not run on Windows 7 64-bit
Gilson Unipoint Chrom.	32-bit	Will run on all supported operating systems.
Groton Tech. PF1 DAD	16-bit	Will not run on Windows 7 64-bit
Groton Tech. SoloNet DAD	16-bit	Will not run on Windows 7 64-bit
Guided Wave NIR	16-bit	Will not run on Windows 7 64-bit
HP 1040 Diode Array (PAWS)	16-bit	Will not run on Windows 7 64-bit

Converter Name	Type	Status
HP 1090 Diode Array (PAWS)	32-bit (GAML)	Will run on all supported operating systems.
HP 8452 Time Scan (DOS)	16-bit	Will not run on Windows 7 64-bit
HP 8452 UV-Vis (DOS)	16-bit	Will not run on Windows 7 64-bit
HP ChemStation Chromatogram	32-bit (GAML)	Will run on all supported operating systems.
HP ChemStation Diode Array	32-bit (GAML)	Will run on all supported operating systems.
HP ChemStation IRD GC-IR	16-bit	Will not run on Windows 7 64-bit
HP ChemStation MSD GC-MS	32-bit (GAML)	Will run on all supported operating systems.
HP LAS Converter	32-bit (GAML)	Will run on all supported operating systems.
Hitachi D-7000 HPLC System	32-bit (GAML)	Will run on all supported operating systems.
Hitachi R-1200/1100 NMR	32-bit	Will run on all supported operating systems.
Hitachi R-1500 NMR	16-bit	Will not run on Windows 7 64-bit
Horiba FT-IR	16-bit	Will not run on Windows 7 64-bit
IBM 9420/9430 UV-Vis	16-bit	Will not run on Windows 7 64-bit
IBM IR30 FT-IR	16-bit	Will not run on Windows 7 64-bit
ISA PRISM Raman	16-bit	Will not run on Windows 7 64-bit
ISA SPEX Raman	16-bit	Will not run on Windows 7 64-bit
ISA SpectraMax Raman	16-bit	Will not run on Windows 7 64-bit
Interspectrum/Spectrolab PFS2000	32-bit	Will run on all supported operating systems.
JCAMP-DX Data File	32-bit (GAML)	Will run on all supported operating systems.
Jasco J-600 CD	16-bit	Will not run on Windows 7 64-bit
Jasco J-700 CD	16-bit	Will not run on Windows 7 64-bit
Jasco Spectra Manager	32-bit (GAML)	Will run on all supported operating systems.
Jeol GX/EX NMR	32-bit	Will run on all supported operating systems.
Jeol Generic NMR	32-bit	Will run on all supported operating systems.
Jeol WinSpec FT-IR	32-bit	Will run on all supported operating systems.
Kontron DS-450 Chromatogram	16-bit	Will not run on Windows 7 64-bit
Kratos MACH3 GC-MS	16-bit	Will not run on Windows 7 64-bit
LDC Analytical SM5000 DAD	16-bit	Will not run on Windows 7 64-bit
LTI SpectraMetrix/PowerScan	16-bit	Will not run on Windows 7 64-bit
LabControl SPECTACLE File	32-bit	Will run on all supported operating systems.

Converter Name	Type	Status
LeCroy 7200 Oscilloscope	16-bit	Will not run on Windows 7 64-bit
LeCroy 8818A Digitizer/Catalyst	16-bit	Will not run on Windows 7 64-bit
LeCroy 94xx Oscilloscopes	16-bit	Will not run on Windows 7 64-bit
Linear Instruments DAD	16-bit	Will not run on Windows 7 64-bit
Lotus 123 Worksheet (V1.0a)	16-bit	Will not run on Windows 7 64-bit
Lotus 123 Worksheet (V2.0)	16-bit	Will not run on Windows 7 64-bit
Mattson FIRST/WinFIRST FT-IR	16-bit	Will not run on Windows 7 64-bit
Mattson ICON FT-IR	16-bit	Will not run on Windows 7 64-bit
Micromass MassLynx Chromatography Data System	32-bit (GAML)	Will run on all supported operating systems.
NIRSystems NSAS/Vision	32-bit	Will run on all supported operating systems.
NIST MSP Text	32-bit	Will run on all supported operating systems.
Nicolet PCIR FT-IR	16-bit	Will not run on Windows 7 64-bit
Nicolet SX/DX FT-IR (1280)	16-bit	Will not run on Windows 7 64-bit
Oriel DOS InstaSpec	16-bit	Will not run on Windows 7 64-bit
Oriel Runes II	16-bit	Will not run on Windows 7 64-bit
Otsuka Diode Array	16-bit	Will not run on Windows 7 64-bit
PE Nelson 2600 Chromatogram	16-bit	Will not run on Windows 7 64-bit
PE Nelson Access*Chrom	32-bit (GAML)	Will run on all supported operating systems.
PE Nelson TurboChrom (V3.3)	16-bit	Will not run on Windows 7 64-bit
PE Sciex Analyst (WinNT LC-MS)	32-bit (GAML)	Will run on all supported operating systems.
Perkin Elmer PIONIR	16-bit	Will not run on Windows 7 64-bit
Perkin Elmer TurboChrom	32-bit (GAML)	Will run on all supported operating systems.
Perkin-Elmer 7000 FT-IR & UV-Vis	16-bit	Will not run on Windows 7 64-bit
Perkin-Elmer IR Data Manager	16-bit	Will not run on Windows 7 64-bit
Perkin-Elmer PC137 SAM	16-bit	Will not run on Windows 7 64-bit
Perkin-Elmer Spectrum/Winlab	32-bit (GAML)	Will run on all supported operating systems.
Perkin-Elmer TurboMass LC/GC-MS	32-bit	Will run on all supported operating systems.
Perkin-Elmer UV/FL Data Manager (B)	16-bit	Will not run on Windows 7 64-bit
Perkin-Elmer UV/FL Data Manager	16-bit	Will not run on Windows 7 64-bit
Perten Instruments PerCon NIR	32-bit	Will run on all supported operating systems.
Pharmacia LKB Gelscan XL	16-bit	Will not run on Windows 7 64-bit
Phillips IR/40 FT-IR	16-bit	Will not run on Windows 7 64-bit
Polymer Laboratories Cirrus GPC/Triple Detection Converter	32-bit (GAML)	Will run on all supported operating systems.

Converter Name	Type	Status
Princeton Instruments CCD	16-bit	Will not run on Windows 7 64-bit
Radiomatic FLO-One ASCII File	16-bit	Will not run on Windows 7 64-bit
SLM Aminco 3000 UV-Vis	16-bit	Will not run on Windows 7 64-bit
SLM Aminco Universal File	16-bit	Will not run on Windows 7 64-bit
Shimadzu HyperIR FT-IR	32-bit	Will run on all supported operating systems.
Shimadzu QP5000 GC-MS	16-bit	Will not run on Windows 7 64-bit
Shimadzu UV160/265	16-bit	Will not run on Windows 7 64-bit
Siemens AXS DIFFRACplus/AT XRD	32-bit	Will run on all supported operating systems.
Spectra Physics ChromStation	16-bit	Will not run on Windows 7 64-bit
Spectra Physics DAD	16-bit	Will not run on Windows 7 64-bit
Spectra Physics Memory Module	16-bit	Will not run on Windows 7 64-bit
Spectronic SLM-Aminco Bowman 2	32-bit (GAML)	Will run on all supported operating systems.
Stanford Research SR265	16-bit	Will not run on Windows 7 64-bit
TA Instruments Universal Analysis (DSC & TGA only)	32-bit	Will run on all supported operating systems.
Target Chromatography Analysis Software	32-bit (GAML)	Will run on all supported operating systems.
TechMag MacNMR	16-bit	Will not run on Windows 7 64-bit
Teknivent GC-MS	16-bit	Will not run on Windows 7 64-bit
Telos Labs Spectrogram FT-IR	16-bit	Will not run on Windows 7 64-bit
Temet Instruments FT-IR	16-bit	Will not run on Windows 7 64-bit
Thermo Elemental Solaar Converter	32-bit (GAML)	Will run on all supported operating systems.
Thermo Finnigan Xcalibur Converter	32-bit (GAML)	Will run on all supported operating systems.
Thermo Fisher ASCII File with Header	32-bit (GAML)	Will run on all supported operating systems.
Thermo Fisher GAML	32-bit (GAML)	Will run on all supported operating systems.
Thermo Fisher IEEE 32-bit Float File	16-bit	Will not run on Windows 7 64-bit
Thermo Fisher SPC	32-bit (GAML)	Will run on all supported operating systems.
Thermo LabSystems Multichrom	32-bit (GAML)	Will run on all supported operating systems.
Thermo Nicolet Omnic	32-bit (GAML)	Will run on all supported operating systems.
Thermo Spectronic Helios	32-bit (GAML)	Will run on all supported operating systems.
Tracor Northern TN-6500	16-bit	Will not run on Windows 7 64-bit
Tracor Northern TN-6600	16-bit	Will not run on Windows 7 64-bit
VG Plasma-Quad ICP-MS	16-bit	Will not run on Windows 7 64-bit

Converter Name	Type	Status
Varian Cary UV-VIS-NIR	32-bit (GAML)	Will run on all supported operating systems.
Varian Cary UV-Vis (OS/2)	16-bit	Will not run on Windows 7 64-bit
Varian Chemagnetics NMR	32-bit	Will run on all supported operating systems.
Varian Galaxie /JMBS DIAMIR/Bio-Tek KromaSystem 3000	32-bit (GAML)	Will run on all supported operating systems.
Varian Saturn 3 GC-MS	16-bit	Will not run on Windows 7 64-bit
Varian Saturn 5 GC-MS	32-bit	Will run on all supported operating systems.
Varian Star GC	32-bit	Will run on all supported operating systems.
Varian VNMR	32-bit	Will run on all supported operating systems.
Varian XL/XR/Gemini NMR	16-bit	Will not run on Windows 7 64-bit
Waters 990 DAD	16-bit	Will not run on Windows 7 64-bit
Waters Maxima 820 Chromatogram	16-bit	Will not run on Windows 7 64-bit
Zeiss ASCII File	16-bit	Will not run on Windows 7 64-bit