

Thermo Scientific

GRAMS Suite

Version 9.1

Welcome Guide

Revision A



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Welcome to GRAMS Suite 9.1

I am delighted to present the latest edition of the GRAMS Suite. Based on your feedback we have updated the entire suite to support enhanced data import, provide compatibility for Windows 7 64-bit and simplify its install, uninstall and licensing.

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, and we have retained the legacy export tool for backwards compatibility (under the Data Conversion subfolder accessed from the Start menu).

We have added conversion capabilities for the Analytical Spectral Devices Inc. Indico format files.

Some converters are not yet supported in 64-bit mode due to their legacy 16bit code. The process of upgrading these converters is ongoing and will be prioritized based on user feedback. Currently supported formats can be found in the release notes and on the GRAMSSuite.com website. All converters are accessible when using 32-bit emulation in Windows XP mode. If you wish to run GRAMS in this mode you will require a change to the licence file supplied by Thermo Scientific. Email sales@gramssuite.com for details.

GRAMS can now be deployed directly from a web browser using the optional Thermo WebAccess (TWA). TWA allows GRAMS to be installed on a central server and used remotely via a web browser as if it were running on the user's desktop.

We have added further enhancements to our two standalone products:

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 10

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:

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

Component Applications

The GRAMS Suite 9.1 comprises the following applications:

- GRAMS/AI 9.1
- GRAMS 3D 9.1
- Spectral ID 9.1
- Spectral DB 9.1
- GRAMS Convert 9.1
- GRAMS IQ 9.1
- Active Multifile Tool 9.1
- Excel Exchange 9.1
- IQ Predict 9.1
- QuickQuant 9.1

All of these applications are installed by the GRAMS Suite setup executable.

Validation

This release has been developed in line with Thermo Scientific's Quality Management System and, as part of the development process, has been tested on the following operating systems:

- Windows XP Professional SP3
- Windows 7 64-bit SP1
- Thermo WebAccess 2008 Server 32-bit 4.0.1 SP3

Shipping Content

GRAMS Suite 9.1 will be shipped on request to supported customers. The kit includes the latest GRAMS Suite software, accompanying tools, and product release notes in PDF format.

GRAMS Suite 9.1 can also be installed from the following download site: http://gramssuite.com/downloads

Installation

Comprehensive installation instructions are included in this Welcome Guide. We recommend that you read the instructions carefully prior to installation.

Feedback

Thank you for choosing GRAMS Suite 9.1 and Thermo Scientific.

We are sure you will be extremely pleased with GRAMS Suite 9.1. Our aim, as always, is to deliver high quality software solutions to meet your laboratory requirements. Consequently, we are very interested in any suggestions you wish to make.

Please make comments via email to:

support@gramssuite.com

Alternately, you may reach us via our website:

http://gramssuite.com

Regards,

David Joyce

GRAMS Product Manager

System Requirements

This section contains details of the hardware and software requirements for the GRAMS Suite.

Hardware

The following table provides the minimum hardware requirements for the GRAMS Suite:

Hardware	Required	
Processor	Intel Pentium 600 MHz	
RAM	512 MB	
Hard Disk Space	GRAMS Suite	90 MB
	Microsoft .NET Framework 2.0	200 MB
Display Resolution	1024 x 768 with 256 colors	

Software

The GRAMS Suite runs on the following operating systems:

- Windows XP Professional SP3
- Windows Vista Professional
- Windows 7 (32-bit and 64-bit)

In each case, the Microsoft .NET Framework 2.0 is required. If this is not already installed on your system, the GRAMS Suite's InstallShield wizard will install it for you.

Contents of the Installation Kit

The GRAMS Suite installation kit contains the following items:

• GRAMS Suite setup executable

To install the GRAMS Suite and the GRAMS Converters package, run GRAMSSuiteSetup.exe.

• GRAMS 9.1 Product Release Notes

The release notes for this release, a PDF document, includes details of new functionality, corrected issues, etc.

README file

A text file detailing any late updates and instructions for this release.

Installation Instructions

This section contains instructions for:

- Installing the GRAMS Suite, including the GRAMS Converters package.
- Licensing the GRAMS Suite

Before installation, we strongly recommend that you close all programs (to ensure that files are updated properly), and verify that you have administrator privileges on the target computer.

Installing the GRAMS Suite

To start the installation of the GRAMS Suite

- 1. Locate and run the GRAMSSuiteSetup.exe setup executable.
 - If you have downloaded the file from the Internet, a security warning dialog box may appear. This is a Microsoft feature designed to protect users from downloading files from unknown websites. The download for the GRAMS Suite software install will indicate that its Publisher is Thermo Fisher Scientific.
- 2. Click **Run** (or similar) on any security warning dialog boxes that appear.
- 3. The Self-Extractor opens:
 - Click **Setup** to start the installation process.
 - Click Cancel to stop installation (no changes are made to your system).
 - Click **About** to see the versions of the software packages.

Note If a previous version of GRAMS Converters or the GRAMS Suite is found on your computer, Setup tells you that it will be updated. Click **OK** to uninstall the previous version and begin installation of the current version.

4. The GRAMS Suite InstallShield wizard appears:

Preparing to Install

While the installation package is being prepared, a progress bar is visible.

Note If the Microsoft .NET Framework is not already installed on your system, you are prompted to install it at this point. Follow the instructions in the Microsoft .NET Framework 2.0 Setup wizard.

When the wizard is ready to start the GRAMS Suite installation, the Welcome Screen appears.

Figure 1. GRAMS Suite InstallShield wizard



b. Welcome

Click **Next** to continue.

c. License Agreement

Read and accept the terms of the license agreement, and then click Next to continue.

Note You can click **Print** to print the license agreement.

d. Destination Folder

Either use the default installation location, or click **Change** to install the GRAMS Suite in a different location, and then click **Next** to continue.

Note The GRAMS Suite documentation refers to the default installation location. If a different location is used, please make a note of its path for future reference.

GRAMS Suite Data Destination Folder e.

The data destination folder is the path used by the GRAMS Suite to save all information that can be modified during the operation of the applications.

Either use the default installation location, or click **Change** to specify a different location, and then click **Next** to continue.

IMPORTANT It is critical that the selected folder has write access for all GRAMS Suite users. Be sure to record the path that is selected. In many cases, it may be helpful to place the GRAMSSuiteData folder in a short, easy-to-remember path.

f. Ready to Install the Program

At this point, the InstallShield wizard has all the information it requires for your installation.

Click **Install** to complete the installation, or **Back** if you need to make any changes to your selections.

Note A User Account Control dialog box may appear, requesting permission to continue with the installation. Click Continue.

Installing GRAMS Suite g.

This screen contains a progress bar, indicating the progress of the GRAMS Suite installation.

When all files have been copied to your system, the GRAMS Configuration Manager is started.

Note After you have set up a license using the GRAMS Configuration Manager, you return to the GRAMS Suite InstallShield Wizard.

5. If this is a new installation, the GRAMS Configuration Manager displays the following message:

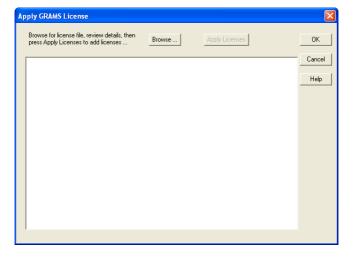
Figure 2. Missing Database message



Click **OK** to continue.

The Apply GRAMS License window appears.

Figure 3. Apply GRAMS License window



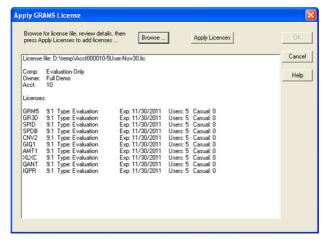
6. Click **Browse** and select the license file for the GRAMS Suite.

If you have purchased the software, you will have received a license file as an email attachment. If you have registered for a trial version, use the downloaded license file. In either case, your license file will have an extension of .lic.

IMPORTANT It is a violation of the GRAMS Suite License Policy to apply a license file to more than one computer. If you need to have any of the GRAMS Suite applications installed on additional machines, please email the Sales department at sales@gramssuite.com.

After selecting the license file, the Apply GRAMS License window displays information about the license:

Figure 4. Apply GRAMS License window – License Information



7. Check the license information to ensure that it is correct, and then click **Apply License** to license the products.

The Apply GRAMS License window updates to show the licenses being applied. If any errors occur, they appear here.

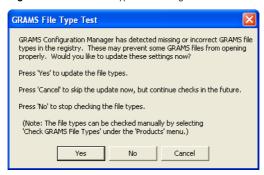
8. Click **OK** to close the Apply GRAMS License window.

9. The GRAMS Configuration Manager now checks the registry to verify that the GRAMS Suite file types are properly registered.

If the Configuration Manager finds any extensions that are incorrectly identified, the following steps occur:

The GRAMS File Type Test dialog box appears.

Figure 5. GRAMS File Type Test dialog box



b. Click **Yes** to register the file types.

> **Note** A User Account Control dialog box may appear, requesting permission for the GRAMSAdmin.exe application to access your computer. Click Allow.

When file type registration is complete, a confirmation message appears.

- Click **OK** to close the message. c.
- 10. From the GRAMS Configuration Manager's File menu, choose **Exit** to close the application and return to the GRAMS Suite InstallShield wizard.

The Installation Wizard Completed screen appears.

11. Click **Finish** to close the InstallShield wizard and complete the installation.