DataAnalysis 4.1

Release Notes

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1 Overview

1.1 Introduction
Description: This document provides information on how to install the product. In addition, information is given about certain limitations currently identified in the ESI Compass DataAnalysis 4.1 software release.

Compass DataAnalysis 4.1 supports processing of analyses acquired on ion trap (esquire/HCT/amaZon), ESI-TOF (micrOTOF/micrOTOF-Q/maXis) and FTMS (apex/solariX) series instruments.

1.2 Using this document
This document should be reviewed with the key instrument operator during installation of the ESI Compass software release.

1.3 Manuals
This software package does not install any manuals.

1.4 Operating Systems
The following operating systems are supported:
Windows XP Professional SP 3 (32-bit), US-English (Firewall disabled)
Windows 7 Ultimate (32-bit and 64-bit), US-English (Firewall disabled)
All other operating systems or languages are not supported.

1.5 Software Configurations
Compass DataAnalysis 4.1 software includes the following components:
DataAnalysis 4.1 (Build 359)
QuantAnalysis 2.1 (Build 359)
LibraryEditor 4.1 (Build 359)
ReportDesigner 5.1 (Build 346)
AutomationEngine 4.1 (Build 359)
BuildingBlockEditor 1.6 (Build 359)
LibraryServer 2.1 (Build 359)
CompoundCrawler 2.0 (Build 106)
ESI Tutorial Data 1.0.37

1.6 General Limitations
The number of spectra in an LC run should not exceed 250,000 spectra. Otherwise, “out-of-memory” situations may occur.
2 Installation

2.1 General

- *DataAnalysis 4.1* is tested and released for PCs delivered by Bruker Daltonics with the instrument.
- It is not possible to install and run different versions of Compass software side-by-side. Especially, it is not possible to install different versions of *DataAnalysis* on one PC.
- You will need administrator permissions under Windows XP to initiate installation.
- Hard disk drive partitions – following partitions are recommended:
  - **Drive C:** This partition contains the operating system and the *Compass* software.
  - **Drive D:** It is recommended that this drive partition should be used for the storage of all Method and Data files. It should be the largest partition.

2.2 First Time Installation

2.2.1 Installing DataAnalysis 4.1

- The installation does not require any previous version of *DataAnalysis* to be installed. Any previous version of *DataAnalysis* will removed by this installation. It is not necessary to uninstall a previous version first.
- The *Compass* browser will launch automatically when the CD is loaded into the CD-ROM drive
- Select 'install', then click on ‘DataAnalysis 4.1’.
- The *DataAnalysis 4.1* setup dialog will pop up. Press the "Next" button and follow the instructions.

2.2.2 Installing LibraryServer 2.1

- This installation is not necessary if *DataAnalysis 4.1* software is already installed. It is only necessary on a computer which contains mass spectra libraries, yet, no *DataAnalysis* processing software.
2.2.3 Licensing

- The *DataAnalysis 4.1* registration key (license) is required in order to use this software.
- Additional functionalities in the software require the *DataAnalysis 4.1, Charge Deconvolution Option* and *DataAnalysis 4.1, Maximum Entropy Deconvolution Option* registration keys (licenses).
- Temporary licenses of 60 days duration are issued once upon initial installation
- License keys of previous *DataAnalysis* versions are no longer valid. Except for the, *Charge Deconvolution* and *Maximum Entropy Deconvolution Option* of the *DataAnalysis 3.4* or *ESI Compass 1.3* versions, which are equivalent to the respecting *DataAnalysis 4.1 Option* licenses above.

2.2.4 Installation Qualification

- It is recommended that you run 'Installation Qualification' from the Start menu Programs/Bruker Daltonics/Utilities after complete installation. The result is saved under 'C:\BDal\System\Data\IQReports' and indicates if your installation is correct. If a file is corrupt (missing or modified) it is marked red. A fresh installation or repair will generally fix any problems. There might be some warnings if a newer version of a program or program part is installed. The warnings are marked in yellow and are not critical to the usability of the program.

2.3 Upgrading from a Previous Version

2.3.1 Upgrading from *DataAnalysis 4.0* (or lower) or from *DataAnalysis 4.1 Preliminary Release*

- *DataAnalysis 4.0*, or any previous version, is uninstalled by the *DataAnalysis 4.1* installation. If a previous version needs to be uninstalled, a message and confirmation to continue is displayed before the uninstallation of that version starts. If denied, the installation of *DataAnalysis 4.1* will not continue.

2.3.2 Upgrading from *DataAnalysis 4.1 Beta* (after Preliminary Release)

- The *DataAnalysis 4.1* final version is installed without prior uninstallation of the beta version.

2.3.3 Upgrading problems

- If the installer displays an error message “Error 1935. An error occurred during the installation of assembly component” the following procedure is recommended:
  - Terminate all applications including this installation
  - Close all applications; let the system idle for approx. 10 minutes; also, do not interact with the PC by Remote Desktop
  - If a restart from Microsoft Update is pending, do so now
Repeat the installation
- If the installer displays an error message noting missing access privileges for the folder “C:/BDalSystemData”, please abort the installation, reboot the computer and redo the installation.

2.4 Uninstallation, Downgrade to Previous Version

In case DataAnalysis 4.1 needs to be uninstalled and a previous version of DataAnalysis is to be installed, proceed as following:

- Uninstall DataAnalysis 4.1.
- Install the previous version DataAnalysis 4.0.
- Check if DataAnalysis 4.0 can be launched normally w/o error messages.
- If error messages are displayed, run the Installation Qualification. Check for modules stated as “newer than expected”. Manually delete those files and rerun the installation of DataAnalysis 4.0 in “Repair” mode. This should remove any downgrading problems.
- If BioTools or MetaboliteTools are installed, the installations of BioTools and MetaboliteTools need to be repaired or uninstalled and reinstalled, too.

2.5 Switching between a 32-bit and a 64-bit Installation

- If a 64-bit version of DataAnalysis 4.1 is installed on a 32-bit version of DataAnalysis 4.1, or vice versa, the installed version needs to be uninstalled. A message and confirmation to continue is displayed before the uninstallation of that version starts. If denied, the installation of DataAnalysis 4.1 will not continue.

Note: The 64-bit version of DataAnalysis 4.1 can only be installed on a 64-bit operating system. The 32-bit version of DataAnalysis 4.1 can be installed on a 32-bit or 64-bit operating system.

Note: The 64-bit version of DataAnalysis 4.1 is currently not yet available and will be made available at a later time.

2.6 Additional Installations

To make full use of the automation and scripting capabilities in DataAnalysis it is necessary to install a specific component from Microsoft which cannot be included on this CD.

The component is:
- ActiveX Control Pad 1.0
  The installation of this component may not be necessary, e.g., if Microsoft Office is installed. 
  ActiveX Control Pad 1.0 is used for designing dialogs for scripting in DataAnalysis or AutomationEngine.
ActiveX Control Pad 1.0 can be downloaded from:
http://download.microsoft.com/download/activexcontrolpad/Install/4.0.0.950/WIN98MeXP/EN-US/setuppad.exe

- If ActiveX Control Pad 1.0 is not installed, DataAnalysis will inform you and ask for installation from the above location when the script editor is opened.

  Note: On Windows 7 this setup needs to executed in compatibility mode for Windows XP SP 3. If in doubt how to achieve this, please contact your local IT specialist.

Also, please make sure, at least one printer driver is installed on the system. Otherwise, printing directly to a PDF document will fail. Yet, it is not necessary to connect a printer to the system.
3  Software Issues

3.1  DataAnalysis 4.1

3.1.1  Loading an analysis with a large result (containing several thousand spectra) may take considerably longer if the unit for retention time has changed. (e.g.: An analysis with a large result has been saved with retention time units displayed in 'seconds', yet, the analysis is opened again, with retention time units displayed in 'minutes'.)

3.1.2  The Send Report to PDF Document command and the scripting command PrintToPDF fails, if no printer is installed. Please make sure, that at least one printer driver is installed on the system. It is not necessary to connect a printer to the system.

3.1.3  The Acquisition Parameter Layouts may show some acquisition parameters from previous instruments revisions as “n/a”. Usually, the Acquisition Parameter Layouts are set up for the latest instrument revision of a series. For full compatibility with previous instrument revisions duplicate and modify such a layout to list desired parameters again.

3.1.4  Malfunction when continuing processing of results from previous versions of DataAnalysis. DataAnalysis can load results saved by previous of DataAnalysis. However, if processing is continued from such previous results in rare cases wrong results may be observed. In such cases, please load the ‘raw data’ again and redo the complete processing.

3.1.5  SmartFormula calculates wrong values for ‘Mean Error [ppm]’ and ‘Standard Mean (m/z)’ if the ‘Automatically locate monoisotopic peak’ option is set.

3.1.6  The DataAnalysis Server option is not working as desired. If the ‘Online processing server’ is activated, the interactive DataAnalysis cannot open an analysis while the DataAnalysis Server is processing an analysis. Do not activate the ‘Online processing server’ or open the analysis while the DataAnalysis Server is currently idling.

3.1.7  Replacing a method report layout with a layout of the same name fails without further notification. Name the new method report layout (filename of *.layout) differently than the currently attached method report layout.

3.2  LibraryEditor 4.1

3.2.1  Opening a library fails with the error message: “You do not have permission to open the library '<mlb-file>'. The following rights are missing: Right to write data to file”, although the user has write access to that file and folder. This error likely occurs if the library is not located in a subfolder of “D:\Data\”. The reason is that the current user does not have write access here. Instead, the ‘Authenticated User’ does have write access. Effectively, the user can write to files and folders, e.g., when acting from the explorer. Yet, the LibraryEditor specifically checks
access rights given to the named user.
To resolve this issue, grant the named user full access rights for this or a base folder of it. This can be done from the ‘Security’ tab of the ‘Properties’ dialog. The installation already grants full access to ‘Everybody’ for the folder und subfolders of “D:\Data\”.

3.3 QuantAnalysis 2.1

3.3.1 If Calibration Blocks are interrupted by a Sample, Blank or Quality Control, the software will assume that the next calibration sample in the sequence will start a new calibration block. The Calibration Type currently allows choosing between New and Replace in the Worktable.

3.3.2 For importing the correct values for Inj.Vol. and Dil.Factor with a HyStarSequenceFile (*.seq), the decimal symbol in your language settings must be a point or period (.).

3.4 Compatibility

3.4.1 BioTools 3.2.
If BioTools is installed also, the InstallationQualification for BioTools will report a newer “AnalysisCoreInterface.dll” file.

3.4.2 ProfileAnalysis.
DataAnalysis 4.1 is not compatible with ProfileAnalysis 1.0 or 1.1; it is only fully compatible with ProfileAnalysis 2.1. If ProfileAnalysis 1.1 is used, DataAnalysis 4.0 (no SP) must be used.
(Missing compatibility means: If an analysis has been processed with DataAnalysis 4.1, the analysis can no longer be opened in ProfileAnalysis 1.1.)

Descriptions and specifications supersede all previous information and are subject to change without notice

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