

## CompassXport 4.0.0

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#### 1 Overview

#### 1.1 Introduction

This document provides information how to install the product. In addition information is given about certain limitations currently found in the CompassXport 4.0.0 software release.

#### 1.2 License Agreement

- A) CompassXportSFX<version>.exe is a self extracting archive, which contains the complete setup.
- B) CompassXport (the "Software") is not Freeware. After unpacking you will find the License text in the setup. The right to use the Software is provided only on the condition that you ("Licensee") agree to this agreement. If you do not agree to the terms of this agreement, you may not install the Software. However, installing the Software indicates your acceptance of this agreement.
- C) CompassXport is an unsupported tool. You are welcome to use the product, but Bruker Daltonik Technical Support cannot guarantee that we'll be able to respond to all requests and fix all issues.

#### 2 Manuals

The operation manual is installed with the software.

## 3 Site Specifications

#### 3.1 Operating Systems

The following operating systems are supported:

- ♦ Windows 7 (32 & 64 Bit)
- ♦ Windows 10 (64 Bit)

Other OS have not been tested.

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#### 4 Installation

#### 4.1 First time Installation

Bruker Daltonik offers an all-inclusive self-extracting archive for download via their website at <a href="http://www.bruker.com">http://www.bruker.com</a>. The archive contains the CompassXport setup program, the Operation Manual and this document.

Before the actual installation process, the archive will extract its content to a temporary directory and will then start the setup program. After CompassXport has been installed successfully, both the archive and the temporary directory may be deleted.

The actual setup process does not require user interaction beyond acknowledging the License Agreement and walking step by step through the setup wizard.

#### 4.2 Upgrade from earlier version

Since CompassXport 3.0 an upgrade from an earlier version of CompassXport is possible. CompassXport 4.0.0 will completely replace the older version.

#### 4.3 Additional Installations

CompassXport 4.0.0 comes as a self-contained installation, separate from other Bruker Daltonics products.

However, parallel installation with Bruker Daltonics analysis software, e.g. DataAnalysis or FlexAnalysis, might update shared component used by CompassXport and this software.

#### 5 Software Issues

- There might be wrong masses and intensities when exporting .yep data with recalibration set to ON - for every export format. See the manual on how to deactivate support for recalibrated data when working with .yep files.
- When exporting data from Bruker esquire, HCT, amaZon and apex instruments, only basic instrument meta information will be available.
- CompassXport is a 32 Bit component. It will run and operate normally on Windows 7 64 Bit, but the COM component can only be called by 32 Bit programs.
- CompassXport 4.0.0 does not support analysis data from Compass 1.4 for flex ("MALDI Compass 1.4") that was saved in "container format". It is still compatible to MALDI compass data in XMASS format.
- CompassXport 4.0.0 cannot access profile data from certain OTOF series instruments, including (at the moment of this release) some maXis, impact and compact instruments.
  Line data access is not affected for these instruments.

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## 6 Filtering of Zero Intensities

Bruker Daltonics' Aqcuisition Software will compress Analysis raw data. To save on operation time and to keep export file sizes small, CompassXport 4.0.0 will filter out zero (0.0) intensities when exporting to mzXML or mzData (both formats do not support compression in the versions supported by CompassXport 4.0.0).

This does not apply to mzML export – CompassXport 4.0.0 supports mzML 1.1 and zlib-compressed data.

## 7 Changes since last release

### 7.1 CompassXport 4.0.0

- Complete update of all used components to support new developments in the acquisition software.
- Updated compiler, needs newer runtimes (included in setup)

#### 7.2 CompassXport 3.0.9.2

- Bugfix release, fixed incorrect XML format for mzXML
- CompassXport could crash in some situations

#### 7.3 CompassXport 3.0.8

- Bugfix release, fixed export of older & non-TOF raw data.
- Fixed XML information on recalibrating program.

#### 7.4 CompassXport 3.0.7

• Bugfix release, changed export of recalibrated data.

#### 7.5 CompassXport 3.0.6

- Now running with VC9.0
- Better support for Windows 7 64 Bit
- Support for new instruments
- UHR instruments require 64bit export as default (see Registry settings)

#### 7.6 CompassXport 3.0.5

- Bugfix release
- C++ examples files
- Support for Windows 7 (will run under 64 Bit, with precautions; see 5: Software Issues)

#### 7.7 CompassXport 3.0.4

- Bugfix release:
  - XMass export fixed

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#### 7.8 CompassXport 3.0.3

- Bugfix release:
  - Resolved several format specific problems
  - Fixed Centroided data export from LCMaldi runs
  - Selecting centroided export for LCMaldi runs will no longer switch to raw export
  - o MSn data export fixed

#### 7.9 CompassXport 3.0.2

- Bugfix release:
  - o Fixed multi export, export files are now again put into analysis directory
  - o Removed -multiName parameter, use -o instead
  - o Fixed empty spectra bug
  - More bugfixes

#### 7.10 CompassXport 3.0.1

- Selectively export with 32 bit or 64 bit precision (see manual)
- Better feedback handling when exporting profile or line spectra
- CSV export fixed
- COM support fixed
- More bugfixes

#### 7.11 CompassXport 3.0

- New export format: mzML 1.1
- New export format: JCAMP 6.0
- New export format: CSV
- Support for OBO ontologies (mzML only)
- COM-Interface extension
- Rewrite of documentation
- Rewrite of commandline parameters
- Lots of bugfixes

#### 7.12 Major releases prior to 3.0

#### CompassXport 1.3.8:

· Added support for recalibrated spectra

#### CompassXport 1.3.0:

• New export format: mzData 1.05

#### CompassXport 1.2.0:

MS/MS-Support for mzXML

#### CompassXport 1.0.0

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## CompassXport 4.0.0

CompassXport 3.0.9.2



• First release, support for mzXML 2.1

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

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