CompassXport 4.0.0

Operation Manual

Contents

About CompassXport

CompassXport is a free data export tool from *Bruker Daltonik GmbH*.

It has two main exporting components: a command line tool, for single file export as well as export of multiple analyses across one directory and its subdirectories; and a COM-DLL, which offers single file export to be embedded into scripts and applications.

CompassXport exports Meta data, spectrum data and precursor information. *CompassXport* does not offer peak picking; it can only export existing line spectra information.

The user can also choose to export the original raw data, instead of data that was recalibrated by *Bruker Daltonics' DataAnalysis*.

Installation

CompassXport can be installed from the self-extracting archive which is available for download from http://www.bruker.com. After the extraction, the setup will start automatically and will lead the user through the installation.

Additionally to the files needed for operation, some example files for accessing the *CompassXport* COM component will be installed as well as the latest release notes, this manual and some registry control files.

Please read the release notes for latest changes to *CompassXport* that may not have found their way into this manual.

Source Formats

CompassXport is compatible with the following *Bruker Daltonics* data formats:

Analysis.baf, Analysis.yep

Instrument families: apex, BioTOF, otof series (baf) and amaZon, esquire, HCT series (yep)

fid (XMASS data format)

*Instrument families: BioTOF, flex, apex series (**not** Compass 1.4 for flexSeries container format)*

Note: MALDI data needs parameter definition tables to be successfully exported. Two tables (in xml format) are installed alongside *CompassXport.exe*: FlexVariableTable.xml and ICRVariableTable.xml.

If you plan to call *CompassXport* via COM, you need to copy these 2 XMLs into the same directory as your calling program. E.g. for VBScript this is C:\Windows\System32 or C:\Windows\SysWow32\ (Windows 64 Bit).

Also note that the **container format** supported by *Compass 1.4 for flexSeries* needs to be converted to XMASS format using the *flex Data Converter* supplied with *Compass 1.4 for flexSeries*.

Operation

After installation, the command line tool is registered with Windows and can be accessed from anywhere at the command prompt. To start it, just type the command "`compassxport.exe`".

The following parameters control *CompassXport's* operation:

`-a <INPUTFILE>`

With version 3.0, CompassXport supports the actual raw data file as input, as well as the Analysis.d directory. Both absolute and relative paths are supported. ("-a" comes from A like Analysis)

`-o <OUTPUTFILE>`

The output file is *optional*, if it is not given, the sample name will be used and the output file will be placed in the Analysis directory. If set to ".d" (Bruker's file extension for analyses), the analyses directory will be used as the output filename. An already existing file will be overwritten, so the user is advised to use a custom output file name.
NB: special meaning when exporting to CSV.

`-multi <SOURCE>`

This exports all raw data files that can be found in the *source* directory to the given export format.
The output filename again is optional and will be used for all exports instead of the default output filename

Note that *either* the a-parameter *or* the multi-parameter and their according output file name must be used.

`-raw <1/0>`

This will export either line (`-raw 0`) or profile spectra (`-raw 1`). `-raw` is optional, if not given, line spectra will be exported.

Note that *CompassXport* does no peak picking or data conversion. It can only export line or profile spectra already stored in the original data.

`-log <level>`

Will control the amount of feedback put out on the command line.
Possible options are: **`none`**, **`error`** or **`all`**. "All" is also the default setting.

`-mode <TARGETFORMAT>`

Selects the target format the data will be exported to and also sets the default output file name, if no one is given. See Target Formats for details.

Codes/Formats are:

`0: mzXML 2.1`
`1: mzData 1.05`
`2: mzML 1.1`
`3: JCAMP 6.0`
`4: CSV`

If no target format is given, the default target format is used. See Registry Settings on how to change the default target format.

Target Formats

Currently supported target formats are: *mzXML 2.1*, *mzData 1.05*, *mzML 1.1*, *JCAMP 6.0* and *comma-separated values (CSV).*
The `mode #x` information indicates how to specify this format on the command line and in a COM function call.

mzXML

mzXML was developed by the Sashimi group, now SPC/Institute for Systems Biology. It is an XML based format for ms and ms/ms proteomics data and includes an offset index for faster file access. *mzXML* is no longer in development.

http://tools.proteomecenter.org/wiki/index.php?title=Formats:mzXML

CompassXport supports *mzXML 2.1* since version 1.0. (`mode 0`)

mzData

mzData was introduced by the PSIDEV group at HUPO. It is an XML based format for ms and ms/ms proteomics data. *mzData* is no longer in development.

http://www.psidev.info/index.php?q=node/80#mzdata

CompassXport supports *mzData 1.05* since version 1.3. (`mode 1`)

mzML

mzML is a new XML format and the successor to both *mzXML* and *mzData*. It combines positive aspects from both parent formats and relies heavily on controlled vocabularies (CV).

http://www.psidev.info/index.php?q=node/257

CompassXport supports *mzML 1.1* since version 3.0. (`mode 2`)

JCAMP

JCAMP was developed by International Union of Pure and Applied Chemistry and is a tag-value pair based export format.

http://www.jcamp-dx.org/

CompassXport supports *JCAMP 6.0* since version 3.0. (`mode 3`)

CSV

CompassXport is able to export spectra to *comma separated values*.
Each spectrum is exported to one *CSV* file. These files consist only out of m/z-intensity value pairs. The filename will contain the spectrum number and the retention time in seconds.

> ***Note on operation:*** with CSV, each spectrum will be exported into a single .csv file. The command line parameter `-a` and the target file COM parameter will be used as a prefix to the actual file names, which will be suffixed with an ascending number:
> `-o sampleA` will result in sampleA_001_0.1.csv, sampleA_002_0.2.csv, …

CompassXport supports *CSV* since version 3.0. (`mode 4`)

COM-Interface description

The installation comes with some example files on how to call *CompassXport* programmatically via COM. By default, these should be extracted to a directory next to the *CompassXport* files: e.g. C:\Program Files\Bruker Daltonik\CompassXport\examples.

The COM object needed to be instantiated is "BDal.Xport.mzXML" or "mzXMLCom 1.0 Type Library" in the Visual Studio "Add Reference" dialog (this is the old name from the first release, it was kept to stay backwards compatible). Alternatively use `CreateInstance` with `__uuidof(mzXMLCOMLib::mzXMLConverter)`.

N.B.: VBScript on Windows 7 64 Bit needs to call the 32 Bit version of `wscript` (normally found in %WindowsFolder%\SysWOW64.

Also, as CompassXport is a 32 Bit program, only other 32 Bit programs can call it via COM on 64 Bit Windows.

With a successful COM connection, the following function calls can be used:

`HRESULT ConvertAndLog2([in] BSTR inputFileName, [in] BSTR outputFileName, [in] LONG logLevel, [in] VARIANT_BOOL convertRaw)`

Exports profile (*convertRaw* = true) or line spectra (*convertRaw* = false) *inputFileName* to *outputFileName* (same as using parameter `-a` from command line).

`HRESULT ConvertMultipleAndLog2([in] BSTR inputFileName, [in] BSTR outputFileName, [in] LONG logLevel, [in] VARIANT_BOOL convertRaw)`

Exports all found analyses from the path *inputFileName* into file(s) *outputFileName*, either profile (*convertRaw* = true) or line spectra (*convertRaw* = false) (same as using parameter `-multi` from command line).

Note: the parameter* logLevel *states the detail of messages output into "compassxport.log": 0 = none, 1 = errors, 2 = all. The log file will be placed next to* inputFileName. *See it for error codes.

`HRESULT SetTargetFormat([in] LONG mode)`

(New with CompassXport 3.0, please use this function instead of the old *SetExportMode*)

Defines the target format that COM-CompassXport will export to. Same definitions as with the command line export formats apply:

```
0: mzXML 2.1
1: mzData 1.05
2: mzML 1.1
3: JCAMP 6.0
4: CSV
```

Registry Settings

Some *CompassXport* settings should not be controlled via the command line or COM parameters, so they have been put into the Windows Registry.

The registry key for these settings is:
HKEY_CURRENT_USER\Software\Bruker Daltonik\CompassXport

The following keys are used:

`UseEnhancedMSMS`: Support for Enhanced MSMS data (1 = activated, 0 = deactivated). Initially activated.

`UseRecalibratedSpectra`: Export the latest recalibration of this analysis (1 = activated, 0 = deactivated). Initially activated, the same way DataAnalysis' opens analyses.

`DefaultExportMode`: DWORD with a default file format, uses the number code as described in section Target Formats. This setting **only** applies to the command line program.
If the parameter `-mode` is not used, the chosen registry setting applies. If this also is empty, *CompassXport* will export to mzXML.

`ExportPrecision64Bit`: DWORD, selected export precision (0 = 32bit precision/float, 1 = 64bit precision/double)

The setup puts some easy to use registry files into the "Configuration" folder in the installation directory.

Note: these settings only work for the current user. To change another user's settings, he needs to log on first.

Controlled Vocabularies

(mzML only)

To control which CVs should be used when exporting to mzML, there are additional registry keys: HKEY_LOCAL_MACHINE\Software\Wow6432Node\Bruker Daltonik\CompassXport\CV\...

`MS`: absolute path to the OBO-File for PSI-MS. See http://psidev.info/index.php?q=node/160 for the latest version of this file. This file is absolutely needed for mzML export.

`UO`: absolute path the OBO-File for Unit Ontology. See http://obo.cvs.sourceforge.net/*checkout*/obo/obo/ontology/phenotype/unit.obo for the latest version.

If necessary, both files can be exchanged for newer versions. The registry key has to be changed as well!

To change these settings, the user has to have administrative rights!

Error handling

When encountering errors during the export, *CompassXport* tries to overcome the fault, but most likely, it will cancel the operation and return to the command prompt. The export file will be there and will give clues on why the export was cancelled, but more important is the error code, which will usually get put out with the error message.

Some frequently occurring errors and their solution:

48: Unknown file type given for input or this file type is not supported.

146: When trying to export MALDI data, *CompassXport* could not find the parameter definition tables. See Source Format description: fid for details.

1798: *CompassXport* cannot find the compression software libraries needed to decompress the data, possibly written by *Compass 1.2* or later. Check your installation, there should be several compression DLLs in "C:\Program Files\Common Files\Bruker Daltonik\AIDA\compression\" or "C:\Program Files (x86)\Common Files\Bruker Daltonik\AIDA\compression\".

Support Contact

The contact email for CompassXport is maldi.sw.support@bdal.de. Log files, the data files in question or aborted result files will greatly help us, please attach them or offer us a way to download them.

Note that *Bruker Daltonik GmbH* does not guarantee an answer.