PRIDE Converter 2

Command-Line User Manual

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# 1. Introduction

The PRIDE Converter 2 tool suite is a composed of 4 independent applications:

* The ***PRIDE Converter 2*** application will convert MS search result files containing identification and spectra into PRIDE XML.
* The ***PRIDE mzTab Generator*** will produce skeleton mzTab files from MS search results files. These skeleton files require either manual or scripted editing to add quantitation and/or gel information.
* The ***PRIDE XML Filter*** will remove identifications or spectra from PRIDE XML files based on a series of configurable filters.
* The ***PRIDE XML Merger*** will combine several PRIDE XML files into a single one.

All tools have both a Graphical User Interface (GUI) and a Command-Line Interface (CLI). The GUIs have been designed to provide a rich, user-friendly interface while the CLIs have been developed mainly for tool and pipeline developers to be able to integrate the PRIDE Converter 2 tools in their own software to provide an efficient way to generate PRIDE XML from their own resources.

# 2. *PRIDE Converter 2* Requirements

## 2.1. System Requirements

* Java: JRE 1.5 +
* CPU: 1 gigahertz (GHz) or faster 32-bit or 64-bit processor.
* Memory: 1 gigabyte (GB) RAM.
* Hard Disk: 55 MB available for installation, more if doing file conversions.
* Platform: Tested in Mac OS X, Linux, and Windows (XP, Vista, 7).

## 2.2. Additional Requirements

PRIDE Converter 2 requires Internet access for connection to the Ontology Lookup Service (OLS) web service and automatic access to PubMed records already published.

# 3. *PRIDE Converter 2* CLI User Guide

Using the PRIDE Converter CLI is a multi-step process. Given the enormous complexity and heterogeneity of the data that *PRIDE Converter 2* is trying to capture, it was basically impossible to design a command-line structure that would be suitable to task. Therefore, *PRIDE Converter 2* is designed to work in two modes, *prescan* and *conversion*.

By default, if the converter is launched in from a command-line prompt without arguments, the GUI will start. In order to start the CLI, arguments must be provided and, if unsure of what arguments to use, users can always use ‘-help’ to obtain on-screen assistance:

|  |
| --- |
| C:\pride-converter>java –jar pride-converter-2.0-SNAPSHOT.jar -help  Usage: java -jar pride\_converter.jar [mode]  PRIDE Converter 2  PRIDE Converter can operate in several different modes.  To launch the graphical mode simply specify no parameters.  The following modes are supported by PRIDE Converter:  -converter Launches the PRIDE Converter in convert mode.  This mode allows one to convert several search  engine result files into the PRIDE XML format.  -filter Launches the PRIDE Converter in filter mode.  This mode allows one to remove f.e. unidentified  spectra or a given set of proteins from an existing  PRIDE XML file.  -merger Launches PRIDE Converter in merger mode.  This mode allows one to merge several PRIDE XML files  into a single file.  For mode specific help please use java -jar pride\_converter.jar [mode] -help |

Note that there is no mzTab generator tool. To generate mzTab files, use the converter tool and use ‘-mode mzTab’. To obtain more information for a specific tool, simply follow the instructions. For example, the converter tool:

C:\pride-converter>java –jar pride-converter-2.0-SNAPSHOT.jar -converter -help

usage: PrideConverter -converter [-compress] [-D <property=value>]

[-debug] [-engine <engine>] [-fastafile <file>] [-fastaformat

<format>] [-gel\_identifier <gel identifier>] [-gel\_spot\_identifier

<spot identifier>] [-gel\_spot\_regex <regular expression>]

[-generate\_quant\_fields <nr. of reagents>] [-help] [-mode <mode>]

[-mztabfile <file>] [-outputfile <file>] [-reportfile <file>]

[-reportOnlyIdentifiedSpectra] [-sourcefile <file>] [-spectrafile

<file>] [-submit\_to\_intact] [-useHybridSearchDatabase

<useHybridSearchDatabase>] [-version]

Note that -mode, -engine and -sourcefile are required parameters for conversion.

-compress turn on gzip

compression for

output file

-D <property=value> use value for given

property. If passing

engine-specific

options, this should

only be used with

-mode=PRESCAN. In

mode=SCAN,

engine-specific

configuration

options are parsed

from the report

file.

-debug print debugging

Information

-engine <engine> search engine. Must

be one of the

following values:

[MASCOT, MGF, DTA,

PKL, MS2, mzML,

XTandem, mzIdentML,

mzXML, mzData, MSGF,

crux\_txt, SpectraST,

OMSSA]

-fastafile <file> full path and

filename of FASTA

file used as a

search database

-fastaformat <format> The format of the

FASTA id line.

OPTIONAL. Must be

one of [FULL,

UNIPROT\_MATCH\_ID,

UNIPROT\_MATCH\_AC,

FIRST\_WORD].

Defaults to FULL

-gel\_identifier <gel identifier> sets the gel

identifier to be

used for

identifications in

the generated mzTab

file. This option

only takes effect

when generating

mzTab files.

-gel\_spot\_identifier <spot identifier> sets the gel spot

identifier to be

used for

identifications in

the generated mzTab

file. This option

only takes effect

when generating

mzTab files. This

option is ignored if

gel\_spot\_regex is

set.

-gel\_spot\_regex <regular expression> used to extract the

gel spot identifier

based on the

sourcefile's name.

The first matching

group in the pattern

is used as a spot

identifier.

-generate\_quant\_fields <nr. of reagents> adds (empty)

quantitative fields

to the generated

mzTab file for the

number of specified

reagents.

-help print this message.

If combined with

-engine, will also

output

engine-specific

options

-mode <mode> The mode in which to

run PrideConverter.

Must be one of the

following values:

[PRESCAN, CONVERT,

MZTAB]

-mztabfile <file> full path and

filename of mzTab

file

-outputfile <file> full path and

filename of PRIDE

XML output file.

OPTIONAL. Will

default to

<sourcefile>.xml.gz

-reportfile <file> full path and

filename of report

file. OPTIONAL. Will

default to

<sourcefile>-report.

xml

-reportOnlyIdentifiedSpectra Indicates that only

identified spectra

should be reported

in the generated

PRIDE XML file.

-sourcefile <file> full path and

filename of source

file.

-spectrafile <file> overwrites the path

to the spectrum

file(s) with the set

value. This can

either specifiy a

directory containing

multiple MS data

files referenced in

the search result

file or one MS data

file directly

depending on the

file format.

-submit\_to\_intact Indicates that the

generated XML file

contains interaction

data that should be

submitted to IntAct

-useHybridSearchDatabase <useHybridSearchDatabase> Indicates if the

search database

contains a

combination of valid

and decoy protein

sequences. Must be

[TRUE|FALSE].

Defaults to TRUE.

-version print the version

information and exit

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To obtain DAO-specific help, when and if DAO-specific options are available, add –engine [ENGINE\_NAME] to the command-line. For example, for the Mascot DAO:

C:\pride-converter>java –jar pride-converter-2.0-SNAPSHOT.jar -converter -engine mascot -help

This command would display the help information as shown above, plus the following information:

usage: Mascot engine options

use the -Dproperty=value syntax to use these options

-compatibility\_mode If set to true (default) the

precuror charge will also be

reported at the spectrum level using

the best ranked peptide's charge

state. This might lead to wrong

precursor charges being reported.

The correct charge state is always

additionally reported at the peptide

level.

-decoy\_accession\_prefix An accession prefix that identifies

decoy hits. Every protein with an

accession starting with this

precursor will be flagged as decoy

hit. Furthermore, any decoy hit

who's accession does not start with

this prefix will be altered

accordingly.

-enable\_protein\_grouping Indicates whether the grouping mode

(Occam's Razor, see Mascot

documentation) should be enabled.

This is the default behaviour for

Mascot. This mode is not equivalent

to the protein clustering introduced

in Mascot 2.3.

-homology\_threshold If set to true (default is "false"

the homology instead of the identity

threshold will be used to identify

significant identifications.

-ignore\_below\_ions\_score Peptides with a lower expect ratio

(of being false positives) will be

ignored completely. Set to 1 to

deactivate. Default value is 0.0

-include\_error\_tolerant Indicates whether integrated error

tolerant search results should be

included in the PRIDE XML support.

These results are not included in

the protein scores by Mascot.

-min\_probability Specifies a cut-off point for

protein scores, a cut-off for an

Integrated error tolerant search and

a threshold for calculating MudPIT

scores. This value represents a

probability threshold.

-only\_significant Indicates whether only significant

peptides / (in PMF searches)

proteins should be included in the

generated PRIDE file.

-remove\_duplicates\_different\_query Indicates whether duplicate peptides

having the same sequence (but maybe

different modifications) coming from

different queries (= spectra) should

be removed.

-remove\_duplicates\_same\_query Indicates whether duplicate peptides

having the same sequence and coming

from the same query (= spectrum)

should be removed. These peptides

may have different modifications

reported.

-remove\_empty\_spectra If set to true (default) spectra

without any peaks are ignored and

not reported in the PRIDE XML file.

-use\_mudpit\_scoring Indicates whether MudPIT or normal

scoring should be used.

The *prescan* will generate a report file that contains placeholders for all of the data that requires annotation intervention (software, sample, protocol, instrumentation, PTMs, etc). It is expected that pipeline maintainers will develop their own code to update the report files with their own metadata and then run PRIDE Converter in *conversion* mode, to generate fully-annotated PRIDE XML files.

For most users, the *PRIDE Converter 2* GUI will handle all of the report annotation, but it is essentially working in the same fashion, while doing most of the file I/O in the background. It generates a report file in the background, and then presents the users with a form-based wizard to capture the metadata. It then updates the report file and runs in conversion mode to generate PRIDE XML.

Users who wish to integrate the PRIDE Converter CLI into their own applications are encouraged to read the section entitled “Report File Manual Annotation Guidelines” in the Developer Guide.