QuickMod

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1. Overview

QuickMod is a spectral library search based MSMS data analysis tool, designed to identify modified peptides.

Please cite:

Ahrne# E., Nikitin F., Lisacek F., Mu#ller, QuickMod: A Tool for Open Modification Spectrum Library Searches, J. Proteome Res., 2011, 10 (7), pp 2913–2921

Note:

A short description of the tool is available here.

Warning:

Fixing for `Windows` users (if `cygwin` is not installed)

2. Algorithm

A spectral library is a database of already identified MSMS spectra. Typically a peptide entry in the library is represented by a consensus spectrum; an averaged spectrum compiled from multiple, same precursor charge state, spectra representing the same peptide species.

The QuickMod algorithm assumes that the precursor mass difference between a query spectrum and a candidate library spectrum can be explained by a modification. Based on this assumption the two spectra are aligned and a list of similarity measures calculated. In a second step the most likely attachment position of the modification is determined. The QuickMod scoring scheme was developed by carefully examining and combining various peak intensity and peak coverage based scoring features.

QuickMod provides efficient means to evaluate the quality of a MS/MS dataset by revealing modifications induced by sample handling and preparation such as oxidation, pyro-Glu and salt adducts. More importantly, the search algorithm is capable of identifying known PTMs while suggesting a list of previously unknown or unexpected PTMs, to be verified in targeted experiments.

3. Usage

```
usage: java -jar QM-x.x.jar -h
           ---QuickMod Options---
 -h           Print  QuickMod help
 -i <arg>     Absolute path to parameters file, (Required)
```

```
 -s <arg>    library name for binary file creation
 -sN <arg>   binary library batch size (# spectra)
 -sO <arg>   binary library out directory
 -v          verbose mode

To increase memory of JVM try java -Xmx2048M -jar QM-x.x.jar
```

4. Releases

The latest version is v1.03 - Download app with the default properties file or access the online version.

4.1. Rel1.03

Type	Changes
Bug Fixed	MGF reader bug fixed!

4.2. Rel1.01

Type	Changes
Bug Fixed	The dependencies for MzML reader were missing!

4.3. Rel0.9

Type	Changes
Bug Fixed	*java.lang.NumberFormatException* thrown while flushing results. QM was crashing when decimal separator was not '.' (i.e. LANG=fr_FR.utf8).

4.4. Rel0.7

Type	Changes
Import	support zip and tar.gz type files in "libraryPath" and "expDataPath" params .

4.5. Rel0.6

Type	Changes
Export Change	now generates only one pepxml file .

4.6. Rel0.4

Type	Changes
Bug Fixed	QM was crashing due to an internal error in PepXML exporter (threw java.lang.illegalArgumentException - bad format <mzdata-filename.start-scan.end-scan.charge>) .

4.7. Rel0.2

Type	Changes
New	Add PepXML format export (set new tag 'pepXmlExport=true' in parameters file).