Fasta2MS

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1. Overview

This application digests and fragments fasta proteins into annotated MS spectra.

MS/MS spectra are returned in the standard output in mgf format.

2. Usage

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usage: Fas2MS <fasta> [-a] [-d <arg>] [-f <arg>] [-h] [--no-digestion]
        [-p <arg>] [-q <arg>] [-v]
 -a,--annot-mode             enable peak annot mode.
 -d,--digest-motif <arg>     define the motif for digestion:
                             <pre-cut> <cut-token> <post-cut>
                             <pre-cut> := (<AA> | <AA-class>)+
                             <post-cut> := (<AA> | <AA-class>)+
                             <AA> := [A-Z]
                             <AA-class> := '[' AA+ ']'
                             by default: Trypsin, [KR]|[^P].
 -f,--frag-types <arg>       define the fragment type(s):
                             a,b,c,x,y,z for backbone type fragments
                             i for immonium and p for precursor
                             by default: b,y.
 -h,--help                   print this message.
    --no-dig                 non digestion mode.
 -p,--precision <arg>        define the decimal precision for any
                             mass-to-charge ratio
                             by default: 6.
 -q,--charge-numbers <arg>   define the list of charge for fragments:
                             a sequence of integers like in 1,2,3:5,10:7
                             by default: 1.
 -v,--version                print the version info.
```

3. Releases

The latest version is v1.2 - Download app with java sources.

3.1. Rel1.2

Type	Changes
New	Add new option '--no-digestion' to disable protein digestion.

3.2. Rel1.1

Type	Changes
New	Add new option '-d' to define peptidase for protein digestion.
Change	Change option name for frag_type '-t' -> '-f'.

3.3. Rel1.0

Type	Changes
Bug fixed	Immonium and precursor fragmentation was not working at all.
Bug fixed	Fasta reader was not able to read windows files.
Change	Remove option fasta file input, not optional anymore.
New	Add option 'annot-mode' that enables peak's annotation.
New	Add option 'precision' to specify precision for double display.