MSDataFilter

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1. Overview

This application read MS spectra, apply filters and generate new file.

> **Note:**
> By now, it filters only msp/sptxt spectra with only one available filter JPLIntensityAttenuator.

2. Algorithm

```
BEGIN
1.  parse the file with spectra lib
2.  compute MS1/MS2 peaks distributions over all spectra (here is an
example for precursor charge +3)
    [2 types of more local distributions through mz precursor intervals]
2.1 mz distributions of all mzs (example[1])
2.2 mz distributions at precursors neighborhood (from 1 to z) (example[1])
END

[1] these histograms are rendered (with R) with option -r (see command line
below).
```

3. Usage

```
 usage: MSDataFilter <fasta> [-b <arg>] [--bp] [-e <arg>] [-g <arg>] [-h]
        [-i <arg>] [--no-norm] [-o <arg>] [-p <arg>] [-q] [-r] [-s <arg>]
[-t
        <arg>] [-v]

 -b,--bin-width <arg>          set the width of interval in histograms
                               by default: 1.0.
    --bp <arg>                 set base peak intensity for normalization
                               process.
 -e,--export-ratios <arg>      export ratios in filename
                               by default: null.
 -g,--group-number <arg>       set the number of peak list partitions by
                               precursor charge
                               by default: 10.
 -h,--help                     print this message.
 -i,--setting-file <arg>       give a property file with all input
                               settings.
    --no-norm                  disable base peak intensity normalization.
 -o,--output <arg>             set the output filename
                               by default: null.
 -p,--precision <arg>          define the decimal precision for any
                               mass-to-charge ratio
                               by default: 6.
```

```
-q,--quiet                      quiet mode (verbose off).
-r,--render                     export and render MS histograms in /tmp/hist
                                by default: false.
-s,--sliding-window <arg>       set the sliding window value to compute
                                baseline histogram
                                by default: 20.
-t,--threshold-ratio <arg>      set the ratio threshold for the attenuator
                                filter
                                by default: 2.0.
-v,--version                    print the version info.
```

4. Example

5. Releases

The latest version is v0.2 - Download app with java sources.