SHIFTS-4

Every SHIFTS module uses configuration files (INI), but some of the parameters it contains can also be specified through the command line. Run each module with the help option, ***-h***, (e.g. `python DMcalibrator.py -h`) for a list of parameters that are available through the command line and their description.

1. SHIFTSadapter

This module adapts a Comet-PTM or Recom file so that it can be analyzed with SHIFTS.

- Input:
  - A tab-separated file from Comet-PTM or Recom output (with header).
  - A configuration file (INI). There is a default INI in the "config" folder.
- Output:
  - A tab-separated file (without header).
  - A log file containing the header information.

2. DMcalibrator

This module calculates the calibrated values for experimental masses and deltamasses.

- Input:
  - A file from SHIFTSadapter output.
  - A configuration file (INI). There is a default INI in the "config" folder.
  - A mass file (INI). There is a default INI in the "config" folder.
- Output:
  - The same file with additional columns for theoretical MH and MZ, calibrated MH and MZ, calibrated deltamass MH and MZ, absolute error, ppm error, sequence with calibrated deltamass.
  - A log file containing systematic error before and after calibration, alpha, StdDevMAD_ppm, number of PSMs before and after filtering.

3. PeakModeller

This module concatenates a group of files, generates a histogram grouped by deltamass bins of a user-specified width, and calculates the frequency and slopes (first and second derivatives) for each bin.

- Input:
  - A text file containing a list of calibrated files to be modelled together.
  - A configuration file (INI). There is a default INI in the "config" folder.
- Output:
  - A tab-separated file containing all the input files together (DMTable)
  - A tab-separated file containing the histogram (DMHistogram)
  - A log file.

4. PeakSelector

This module filters a histogram of deltamasses according to user-specified thresholds for slope and frequency, and calculates a list of apexes using the given number of points.

- Input:
  - A DMHistogram to be filtered.
  - A configuration file (INI). There is a default INI in the "config" folder.
- Output:
  - A text file containing the apex list.
  - A log file containing the number of apexes that were calculated.

5. PeakAssignator

This module will assign every PSM to a peak from the provided apex list or identify it as an orphan.

- Input:
  - A DMtable.
  - An apex list.
  - A configuration file (INI). There is a default INI in the "config" folder.
- Output:
  - A DMtable with additional columns for the closest peak, assignation as peak or orphan, assigned deltamass, ppm error, sequence with assigned deltamass.
  - A log file.

6. PeakFDRer

This module will calculate global, local, and peak FDR values for a DMtable subdivided by experiment. For the global FDR, rather than taking an entire experiment, this module will separate it in two deltamass regions (defined by the parameter ***dm_region_limit***, default value -56) and calculate a global FDR for each region.

- Input:
  - A DMtable.
  - A tab-separated file containing a column with the experiment name and another with the file path (must match the file paths in the ***Filename*** column of your DMtable).
  - A configuration file (INI). There is a default INI in the "config" folder.
- Output:
  - A DMtable with additional columns for the global, local and peak FDR ranks and values.
  - A log file.