Alkaloids_extraction

July 9, 2023

1 Target Peak Extraction with ms-mint

1.1 Importing libraries

```
[13]: # ms-mint: Instance for MS spectrometry data
      from ms_mint.Mint import Mint
      #from ms_mint.notebook import Mint
      mint = Mint()
```

1.2 Selecting files

In this first example, we are going to use the QC files to exemplify how the targeted extraction is going to be conducted for all the samples.

```
[14]: mint.load_files('./Data/QC_*')
      mint.ms_files
```

```
[14]: ['Data/QC_pos_11.mzML',
       'Data/QC_pos_12.mzML',
       'Data/QC_pos_19.mzML',
       'Data/QC_pos_29.mzML',
       'Data/QC_pos_39.mzML',
       'Data/QC_pos_49.mzML',
       'Data/QC_pos_59.mzML',
       'Data/QC_pos_69.mzML',
       'Data/QC_pos_79.mzML',
       'Data/QC_pos_89.mzML',
       'Data/QC_pos_99.mzML',
       'Data/QC_pos_109.mzML',
       'Data/QC_pos_119.mzML',
       'Data/QC_pos_129.mzML',
       'Data/QC_pos_139.mzML',
       'Data/QC_pos_149.mzML',
       'Data/QC_pos_159.mzML',
       'Data/QC_pos_169.mzML',
       'Data/QC_pos_179.mzML',
       'Data/QC_pos_189.mzML',
       'Data/QC_pos_195.mzML',
```

```
        'Data/QC_pos_202.mzML',
        'Data/QC_pos_203.mzML']
```

1.3 Import list of targets

```
[15]: mint.load_targets('targets.csv')
      mint.targets
```

```
[15]:                       mz_mean  mz_width     rt   rt_min  rt_max rt_unit  \
      peak_label
      Dehydrotomatidine    414.3367        10  315.6    309.6   321.6       s
      Tomatidine           416.3531        10  322.2    316.2   328.2       s
      Dehydrotomatine     1032.5379        10  316.2    310.2   322.2       s
      Tomatine            1035.5589        10  321.6    315.6   327.6       s
      Hydroxytomatine     1050.5485        10  327.0    321.0   333.0       s

                          intensity_threshold target_filename
      peak_label
      Dehydrotomatidine                  1000     targets.csv
      Tomatidine                         1000     targets.csv
      Dehydrotomatine                    1000     targets.csv
      Tomatine                           1000     targets.csv
      Hydroxytomatine                    1000     targets.csv
```

1.4 Run data extraction

```
[16]: mint.run()
```

```
maxtasksperchild: None

ERROR:root:process_ms1_files_in_parallel(): invalid literal for int() with base
10: 'scanId=2702'
ERROR:root:process_ms1_files_in_parallel(): invalid literal for int() with base
10: 'scanId=2456'
ERROR:root:process_ms1_files_in_parallel(): invalid literal for int() with base
10: 'scanId=2711'
ERROR:root:process_ms1_files_in_parallel(): invalid literal for int() with base
10: 'scanId=2499'
ERROR:root:process_ms1_files_in_parallel(): invalid literal for int() with base
10: 'scanId=2551'
ERROR:root:process_ms1_files_in_parallel(): invalid literal for int() with base
10: 'scanId=2854'
ERROR:root:process_ms1_files_in_parallel(): invalid literal for int() with base
10: 'scanId=2708'
ERROR:root:process_ms1_files_in_parallel(): invalid literal for int() with base
10: 'scanId=2692'
ERROR:root:process_ms1_files_in_parallel(): invalid literal for int() with base
```

```
10: 'scanId=2681'
ERROR:root:process_ms1_files_in_parallel(): invalid literal for int() with base
10: 'scanId=2878'
ERROR:root:process_ms1_files_in_parallel(): invalid literal for int() with base
10: 'scanId=2871'
ERROR:root:process_ms1_files_in_parallel(): invalid literal for int() with base
10: 'scanId=2696'
ERROR:root:process_ms1_files_in_parallel(): invalid literal for int() with base
10: 'scanId=2557'
ERROR:root:process_ms1_files_in_parallel(): invalid literal for int() with base
10: 'scanId=2870'
ERROR:root:process_ms1_files_in_parallel(): invalid literal for int() with base
10: 'scanId=2422'
ERROR:root:process_ms1_files_in_parallel(): invalid literal for int() with base
10: 'scanId=2666'
ERROR:root:process_ms1_files_in_parallel(): invalid literal for int() with base
10: 'scanId=2693'
ERROR:root:process_ms1_files_in_parallel(): invalid literal for int() with base
10: 'scanId=2712'
ERROR:root:process_ms1_files_in_parallel(): invalid literal for int() with base
10: 'scanId=2714'
ERROR:root:process_ms1_files_in_parallel(): invalid literal for int() with base
10: 'scanId=2435'
ERROR:root:process_ms1_files_in_parallel(): invalid literal for int() with base
10: 'scanId=2634'
ERROR:root:process_ms1_files_in_parallel(): invalid literal for int() with base
10: 'scanId=2667'
ERROR:root:process_ms1_files_in_parallel(): invalid literal for int() with base
10: 'scanId=2738'
```

[16]: <ms_mint.Mint.Mint at 0x2b2adaebc370>

[8]: