Exploring and mining MSI data with Python

Involved package:

pyimzml	https://pyimzml.readthedocs.io/en/latest/
numpy	https://numpy.org/
matplotlib	https://matplotlib.org/3.1.1/index.html
molmass	https://github.com/cgohlke/molmass/

Exercice 1: Extract information from imzml

1/ Open imzML file with pyimzml package

2/ get X and Y pixels counts

3/ get a list of XY coordinates

4/ Extract MS spectrum from the pixel 5, 50, 500, 5000

5/ Store m/z and intensity lists from pixel 5

Exercice 2: Parse MS spectra for each pixel

Exercice 3: Create TIC matrix

Exercice 4: Plot TIC and Base peak MSI image

1/ Create TIC image

2/ Create Base Peal image

Exercice 5: Function isolation

1/ Isolate the calculation function from the main code

2/ Plot TIC and BPC plot

Exercice 6: Plot XIC image

1/ Create XIC image for m/z between 780 and 785

2/ Create XIC image for m/z 782.561 with a tolerance of 5ppm

3/ Create XIC image for m/z 773.542 with a tolerance of 5ppm

Exercice 7: Create the XIC image from formula

1/ Create XIC image of of $C_{51}H_{69}N_6OH$

2/ Create XIC images of $C_{51}H_{69}N_6O$ with 4 different adducts (H, Na, K, NH_4)

3/ Save XIC images as .PNG files

Exercice 8: Automatic XIC MSI data generation from formula in text file