MS/MS Viewer

Function:

Generate a mass spectrum figure based on the metabolomics raw data in the XML file and the provided peptide sequence, to aid the user in determining whether or not the peptide is a good match to the spectrum.

XML file was from experiment. The values of peptide sequence are theoretical calculation values.

Instructions:

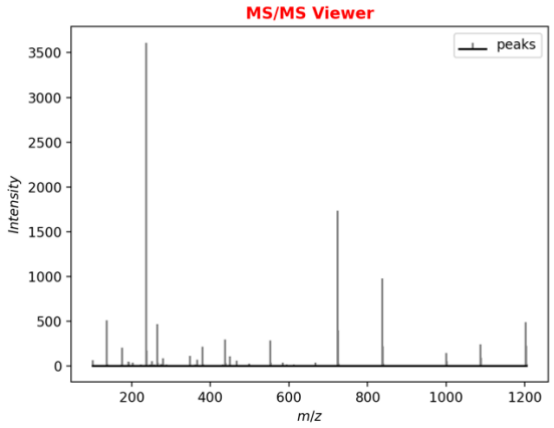
Provide xml file name, scan number and peptide sequence.

e.g.: python Viewer.py 17mix_test2.mzxml.gz 1301 TYDSYLGDDYVR

One figure will be return in output.

Methods:

1. xml file analysis
   read the xml file and extract the needed information,
   (peaks). Because the type of peaks is base64. Then, use python modules to read the peaks values. Plot the figure.

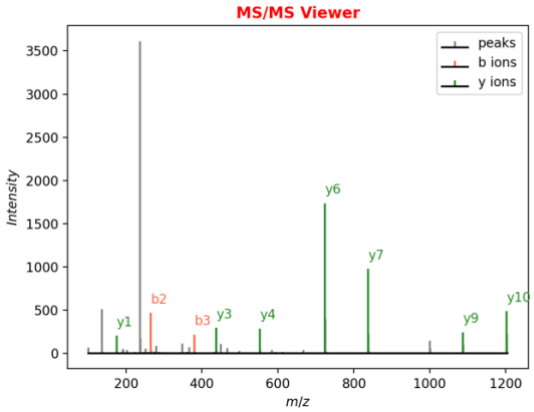


2. Calculate the molecules weight of b ions and y ions of peptide sequence.

$$bi = \left[\sum_{1}^{i} mw(AA)\right] + 1$$

$$yi = \left[\sum_{i}^{i-1} mw(AA\right] + 19$$

3. If difference between xml values and peptide sequence is not significate, they are matched values. Plot them.


MS/MS Viewer
peaks
b ions
y ions
Intensity
m/z
y1
b2
b3
y3
y4
y6
y7
y9
y10