PIERRE WENSEL

PROTEOMICS: EXERCISE 1-DeNOVO

Open the file `Ex-1-HCD-OT-OT.raw` using the SeeMS software. This data has been aquired with high resolution both in MS1 and MS2 using HCD as fragmentation method.

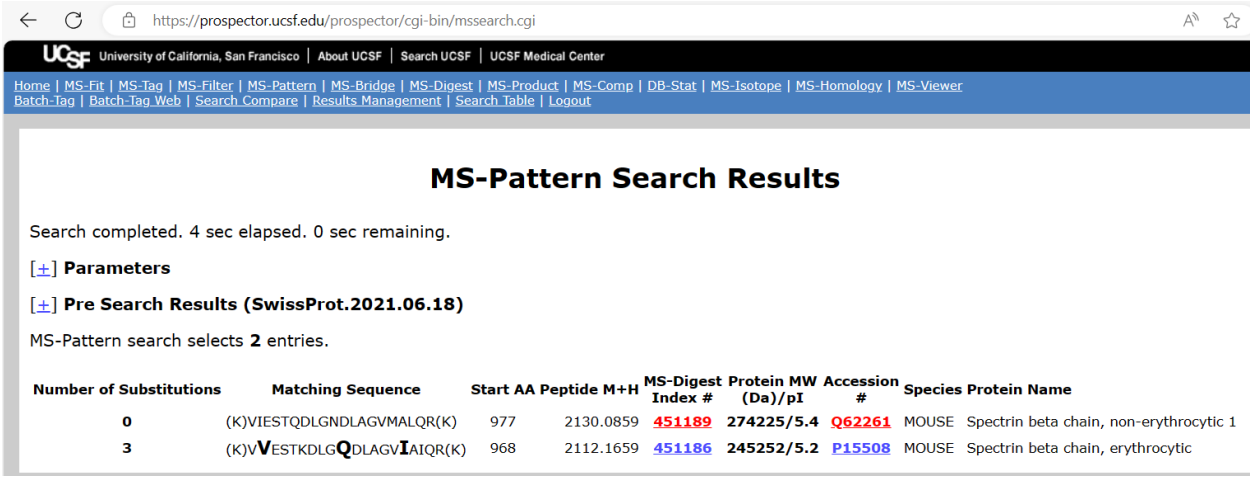
Go to `scan 326` and determine the sequence of this peptide from the MS2 data. Remember to determine the mass of the peptide from the previous MS1 scan. You have a printout of the MS2 spectrum in the next page and a printout of the previous MS1 scan in case you don't have access to the SeeMS software.

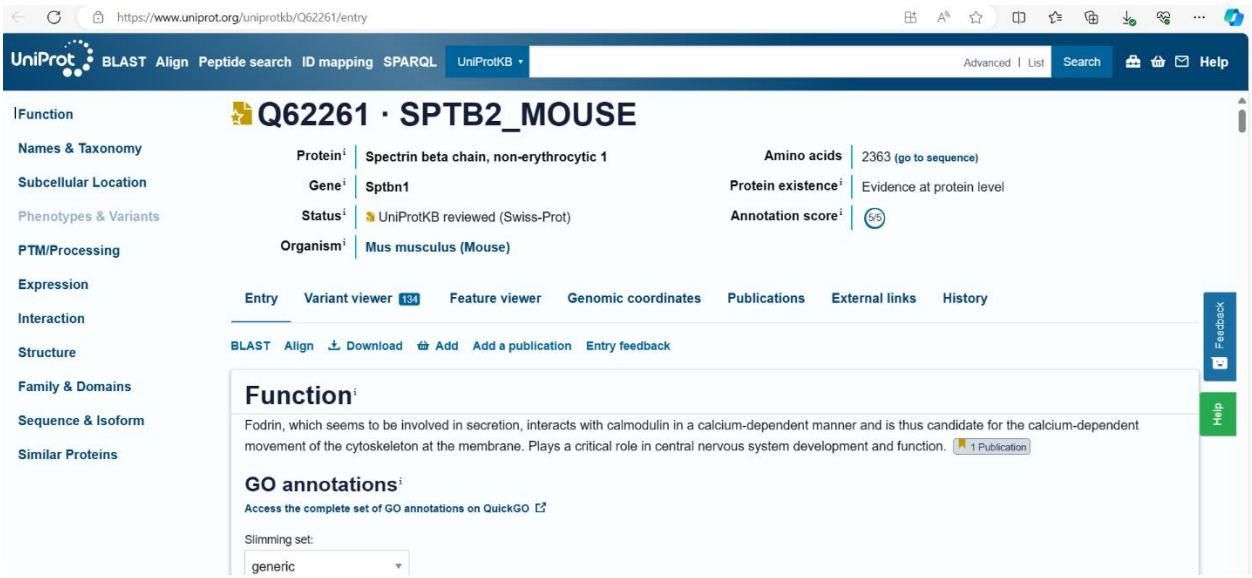
To validate the result use PROSIT (the mass/intensity.information is in the `scan326.xlsx` file located in the `evaluation-task-1-denovo` folder)

The output of the exercise is the sequence (this is a mouse fully tryptic peptide with no missed cleavages) and the explanation on how you have deduced the sequence plus the correlation between the experimental spectrum and the predicted spectrum using PROSIT.

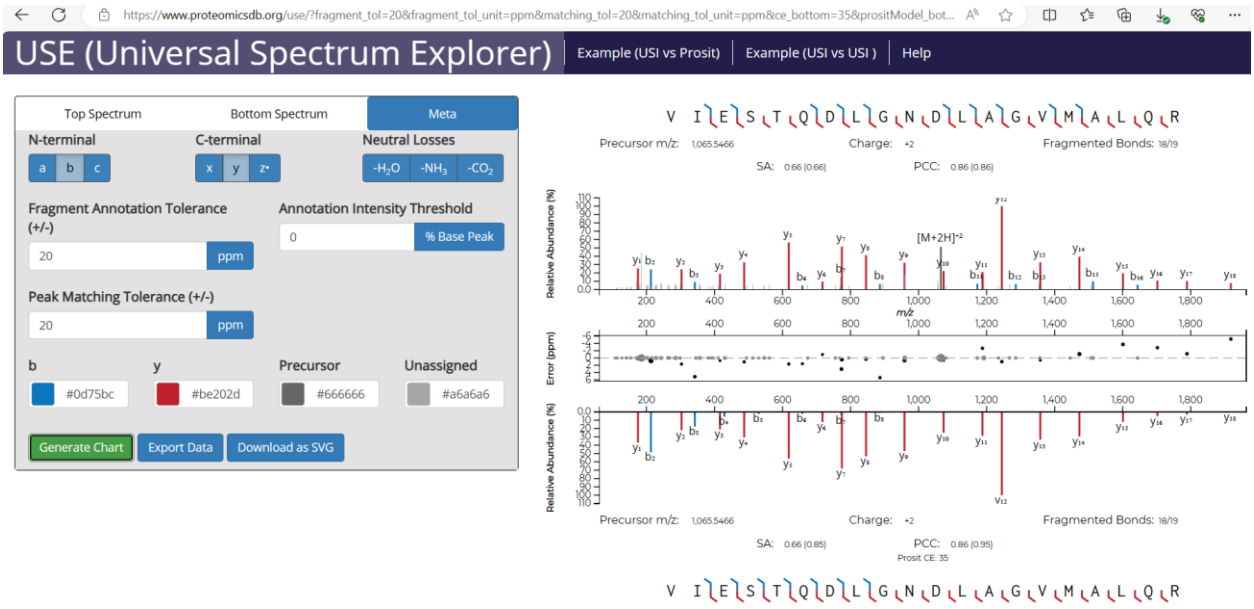
https://prospector.ucsf.edu/prospector/cgi-bin/msform.cgi?form=mspattern

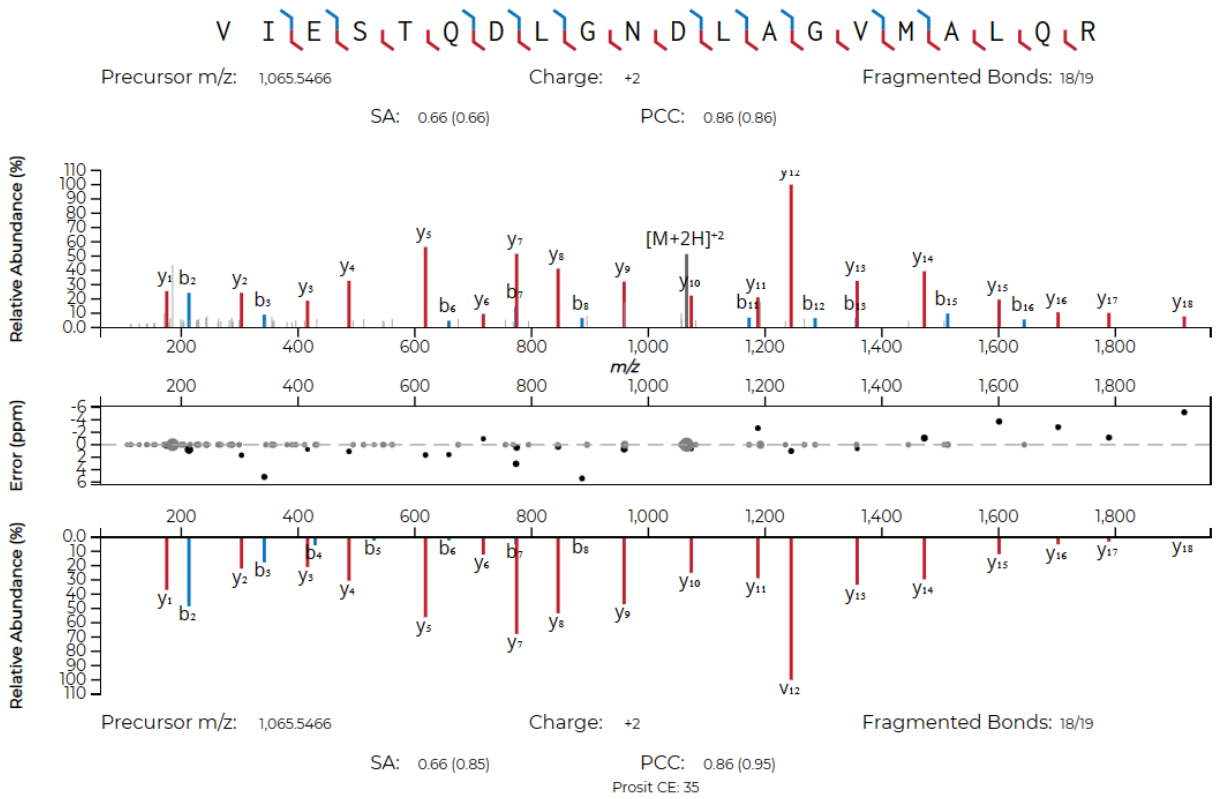
V[IL]EST[QK]D[IL]GND[IL]AGVMA[IL][QK]R

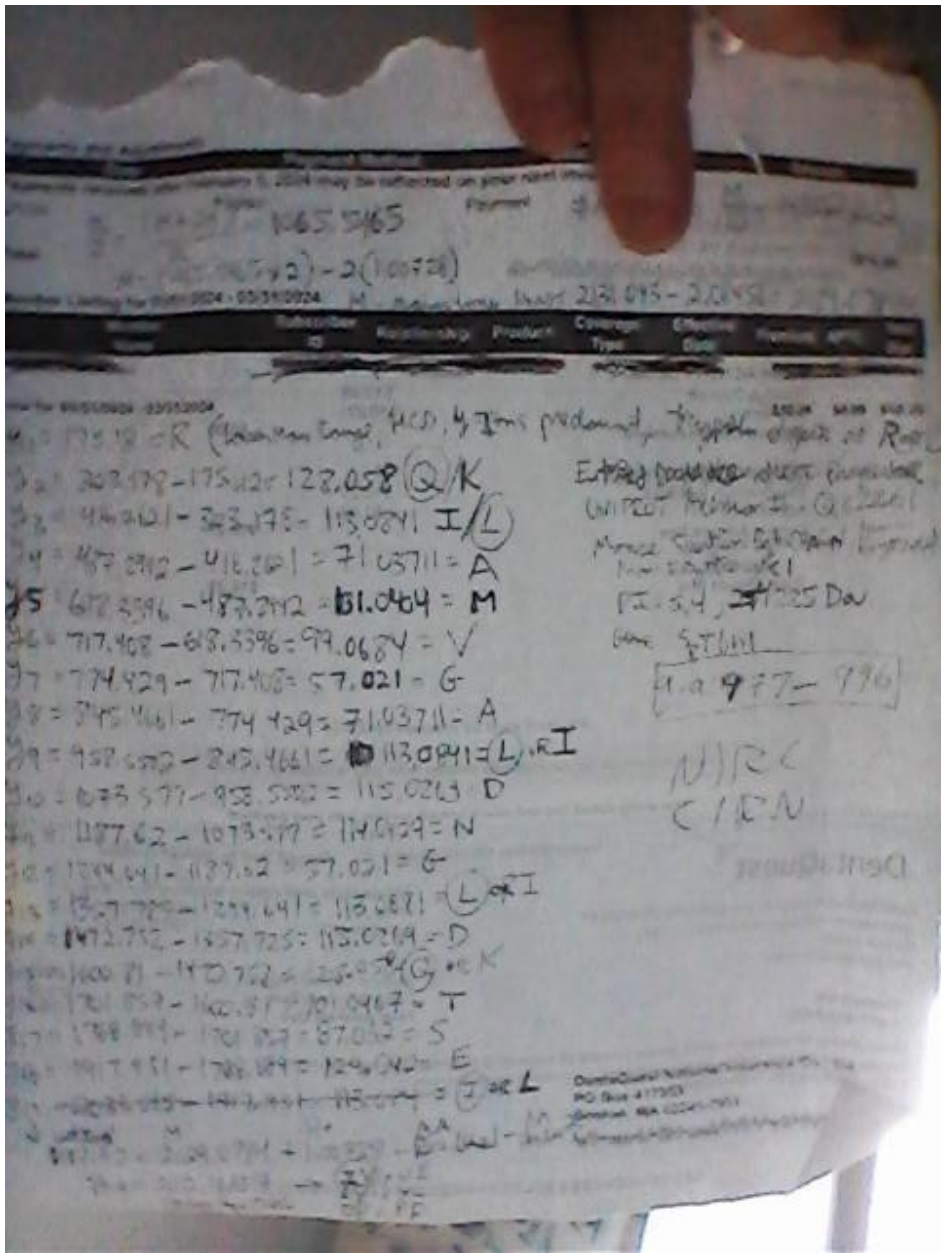


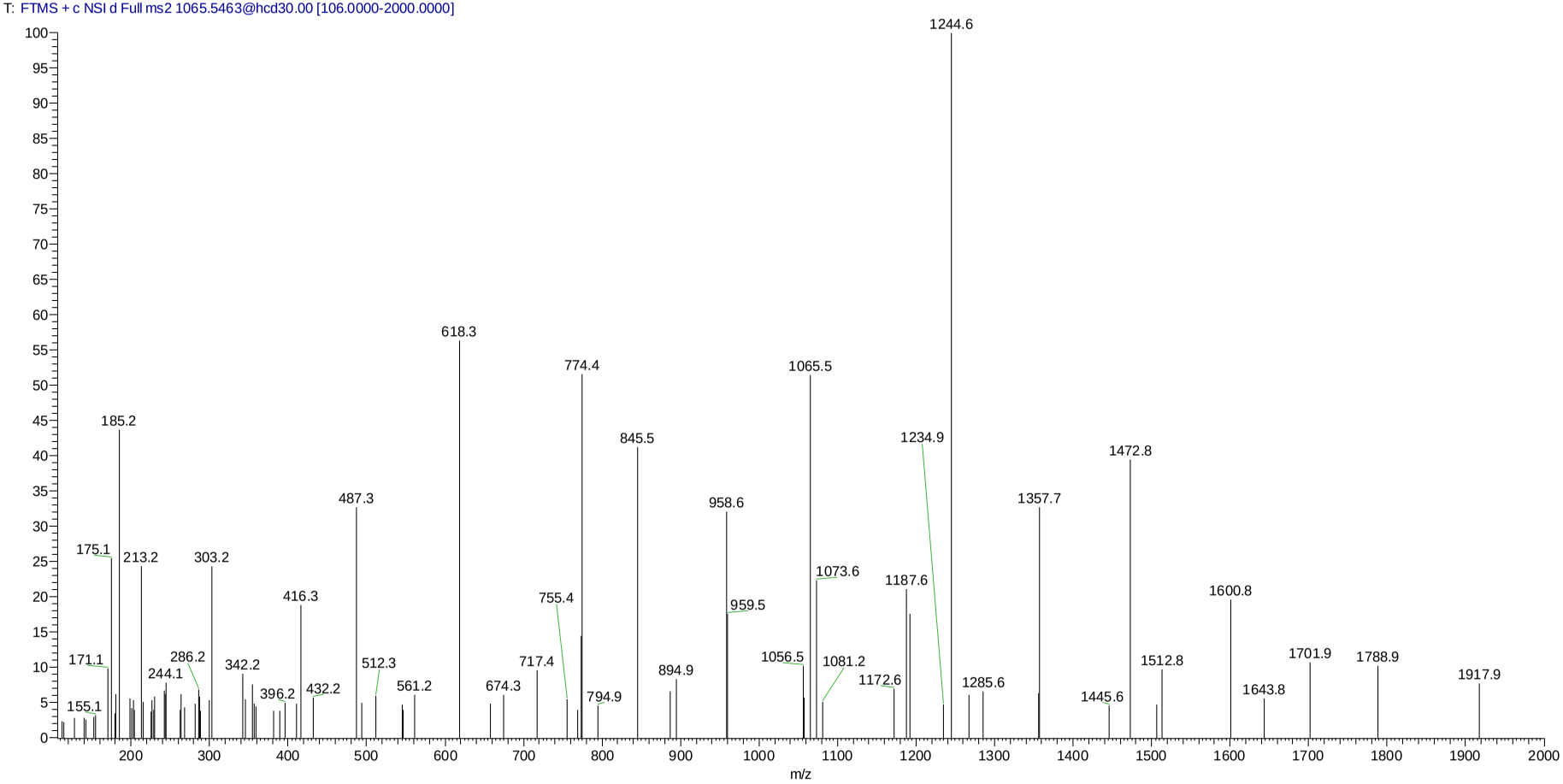


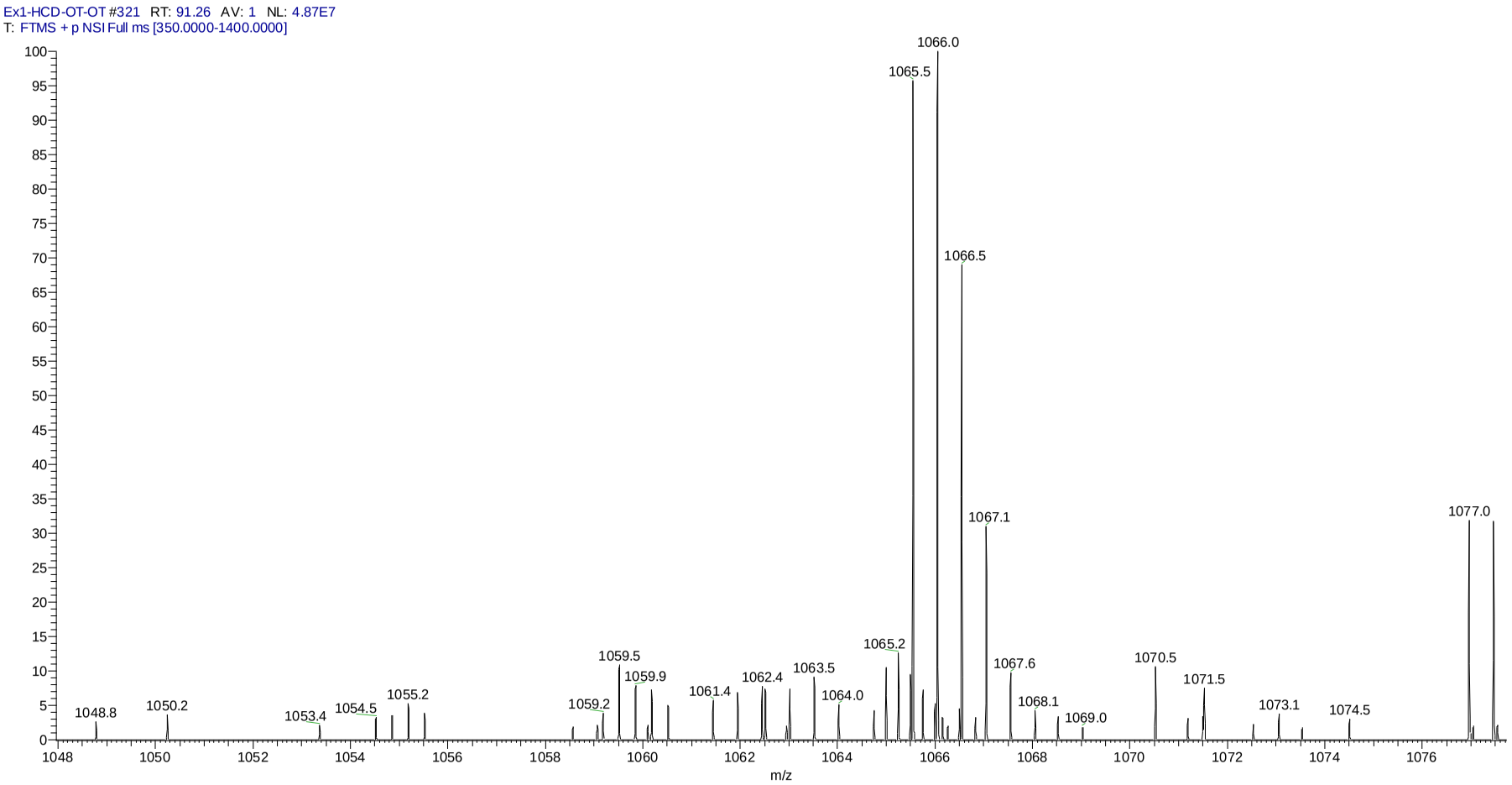
VIESTQDLGNDLAGVMALQR




V I E S T Q D L G N D L A G V M A L Q R
Precursor m/z: 1,065.5466
Charge: +2
Fragmented Bonds: 18/19
SA: 0.66 (0.66)
PCC: 0.86 (0.86)
Relative Abundance (%)
[M+2H]+2
m/z
Error (ppm)
Relative Abundance (%)
Precursor m/z: 1,065.5466
Charge: +2
Fragmented Bonds: 18/19
SA: 0.66 (0.85)
PCC: 0.86 (0.95)
Prosit CE: 35
V I E S T Q D L G N D L A G V M A L Q R




Ex1-HCD-OT-OT #326 RT: 91.26 AV: 1 NL: 9.23E5
T: FTMS + c NSI d Full ms2 1065.5463@hcd30.00 [106.0000-2000.0000]
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
200
300
400
500
600
700
800
900
1000
1100
1200
1300
1400
1500
1600
1700
1800
1900
2000
m/z
1244.6
618.3
774.4
1065.5
185.2
845.5
1234.9
1472.8
487.3
958.6
1357.7
175.1
213.2
303.2
1073.6
1187.6
1600.8
416.3
755.4
959.5
171.1
286.2
342.2
512.3
717.4
894.9
1056.5
1081.2
1512.8
1701.9
1788.9
244.1
396.2
432.2
561.2
674.3
794.9
1172.6
1285.6
1643.8
1917.9
155.1
1445.6


Ex1-HCD-OT-OT #321 RT: 91.26 AV: 1 NL: 4.87E7
T: FTMS + p NSI Full ms [350.0000-1400.0000]
1066.0
1065.5
1066.5
1067.1
1077.0
1065.2
1059.5
1059.9
1067.6
1070.5
1063.5
1062.4
1071.5
1061.4
1064.0
1068.1
1073.1
1074.5
1059.2
1055.2
1054.5
1050.2
1048.8
1053.4
1069.0
m/z