

Tutorial 3: MS Spectrum Interpretation

Bio312

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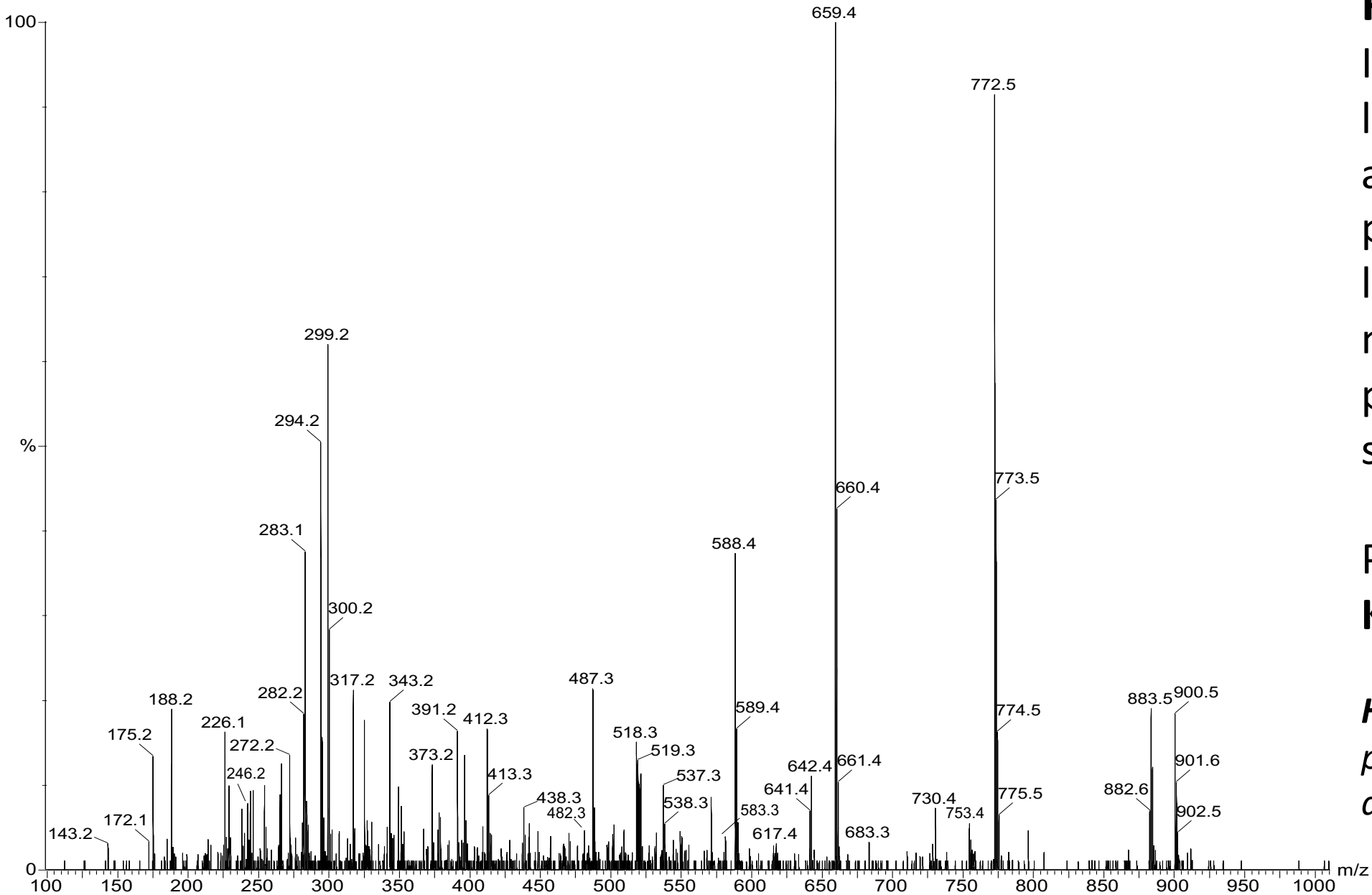
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Practice 1

In this peptide, both lysine residues are acetylated (+42), please use “arrows and labels” to assign as many *b*- and *y*-ions as possible in this MS/MS spectrum.

Peptide Sequence:
K_{ac}QLATK_{ac}AAR

*Hint: write down all the possible masses of *b* ions and *y* ions first.*



Code (1 letter)	Monoisotopic mass
G	57.021 47
A	71.037 12
S	87.032 03
P	97.052 77
V	99.068 42
T	101.047 68
C	103.009 19
I	113.084 07
L	113.084 07
N	114.042 93
D	115.026 95
Q	128.058 58
K	128.094 97
E	129.042 60
M	131.040 49
H	137.058 91
F	147.068 42
R	156.101 12
Y	163.063 33
W	186.079 32

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Peptide Sequence:

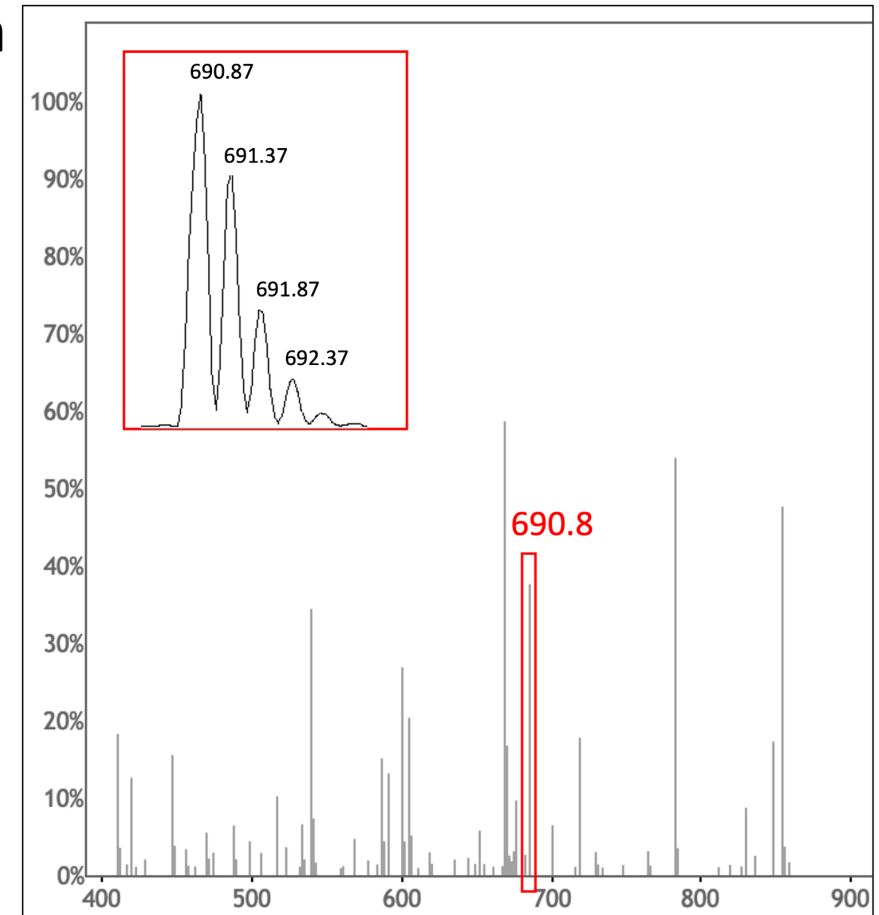
K_{ac}QLATK_{ac}AAR

	AA Sequence	M/z	M/z	AA Sequence	
					y9
b1					y8
b2					y7
b3					y6
b4					y5
b5					y4
b6					y3
b7					y2
b8					y1
b9					

Practice 2

• Figure **a** is the full scan MS1 spectrum of a mixture of tryptic peptides. The inset is the isotopic peak of a modified 12-residue peptide. The modification is either methylation or acetylation. To identify the amino acid sequence and the type of modification, the precursor ions of the modified 12-residue peptide are selected for CID fragmentation and analyzed in the second MS analyzer. The tandem mass spectrum is shown in Figure **b**. Using the spectra and the information provided, answer the following questions:

i) What is the mass of the modified peptide? What is the charge of this peptide?



ii) Determine the type and location of the modification.

iii) Determine the full sequence of the modified sequence. Can you assign the sequence with this data alone? If not, what technique can be used to help you identify the full sequence?

