



**University of
Zurich** ^{UZH}



Swiss Institute of Allergy &
Asthma Research

Proteomics Exercise solutions

31.10.2023

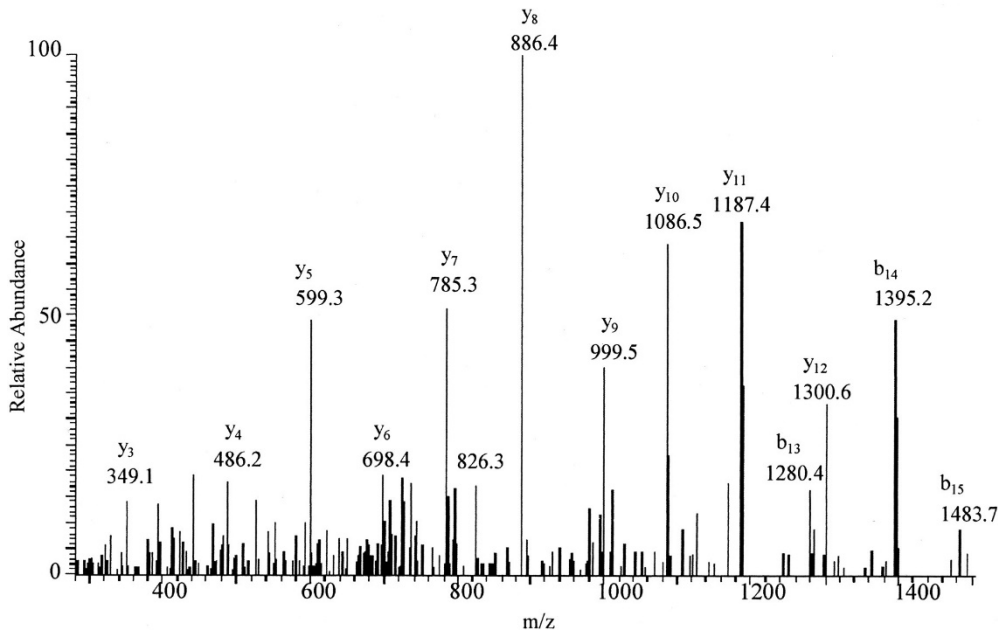
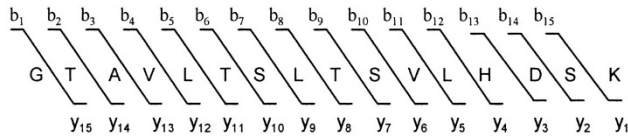
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Swiss Institute of
Bioinformatics

Given the following peptide with the indicated fragment ions,

- 1) What ions will change their m/z when Serin 7 will be phosphorylated?
- 2) What ions will change their m/z when the peptide N-terminus is acetylated?
- 3) What ions will change their m/z when the C-terminal lysine is isotopically labeled?



<https://pwa.klicker.uzh.ch/join/kbaere>



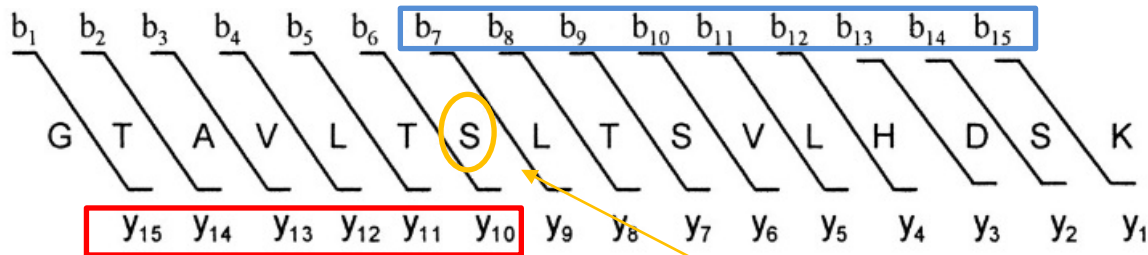
Nisar *et al.*, *Drug Metabolism and Predisposition*, 2004
<https://doi.org/10.1124/dmd.32.4.382>

Given the following peptide with the indicated fragment ions,

1) What ions will change their m/z when Serin 7 will be phosphorylated?

2) .

3) .



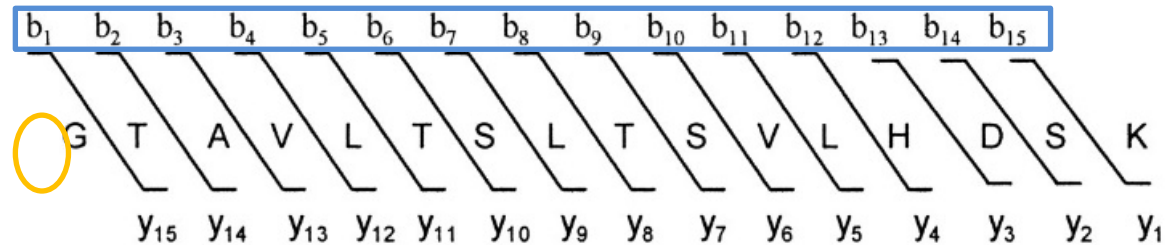
When serine 7 (in orange) is phosphorylated, all peptides containing this serine will change their m/z . E.g. when the peptide bond between S7 and L8 breaks, the b7 and the y9 ion will be generated of which the b7 ion gets the modified serine.

- For the b-ion series that starts from the peptide N-terminus at the left, all the b-ions from b7 to b15 will contain the serine and therefore change their m/z : **b7, b11, b15**

- For the y-ion series that starts from the peptide C-terminus at the right, all the y-ions from y10 to y15 will contain the serine and therefore change their m/z : **y10, y14**

Given the following peptide with the indicated fragment ions,

- 1) .
- 2) What ions will change their m/z when the peptide N-terminus is acetylated?
- 3) .

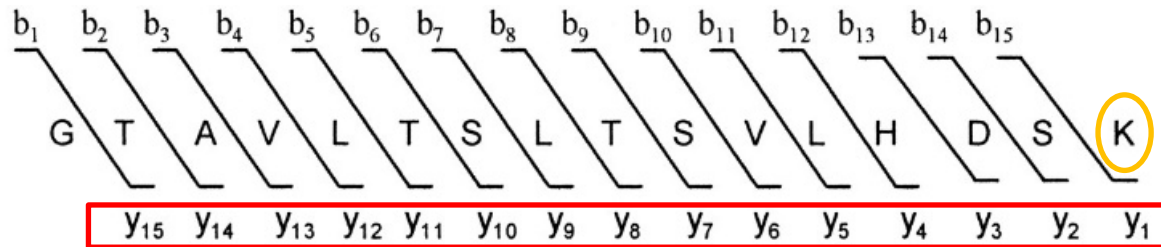


When the peptide N-terminus gets acetylated, all the peptides containing the peptide N-terminus will change their m/z .

- This will be all the b-ions, and none of the y-ions: **b2, b7, b11, b15**

Given the following peptide with the indicated fragment ions,

- 1) .
- 2) .
- 3) What ions will change their m/z when the C-terminal lysine is isotopically labeled?



When the C-terminal lysine is isotopically labeled, all the peptides containing the peptide C-terminus will change their m/z .

- This will be all the y-ions, and none of the b-ions: **y1, y6, y10, y14**

In a PeptideProphet Search applying a 95% probability cut-off, 1500 spectra were matched to peptides; of these, 30 were matched against peptides from the decoy database.

How many incorrect peptide spectrum matches against the target database do you expect?

→ It can be assumed that the number of noticeable wrong hits against the decoy database equals the number of non-noticeable wrong hits against the target database, **one would therefore expect 30 incorrect peptide spectrum matches against the target database.**