

Proteomics

WS 2014/15

Exercises 1

1. Mass

- What is the average and monoisotopic mass [u] of CO_2 ?
- What is the nominal mass of deuterium?
- Consider the peptide ACDEFGH. How many peptides with exactly the same mass (=isobaric peptides) exist that have same length and composition of amino acids (e.g. can be created by swapping amino acid positions)?

2. Mass difference of isotopologues

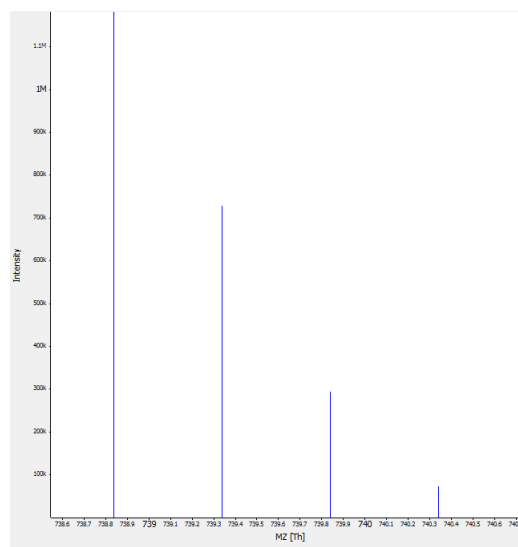
What mass difference in [kg] needs to be resolved in order to distinguish $^{13}C^{16}O$ and $^{12}C^{17}O$?

3. Mass-to-charge calculation

Given an atomic mass of 180.0 Da and a charge of +3. What is the mass-to-charge ratio?

4. Isotope patterns

Given a spectrum,



- (a) determine the charge of your peptide using the distance between isotopic peaks,
- (b) report the monoisotopic m/z and average m/z . (Hint: For average m/z , only a rough estimate is needed).

5. Isotopic fine structure

How many peaks form the isotopic fine structure of C_aN_b ? (Multiple Choice Question (Single Answer))

- (a) $(a + 1) + (b + 1)$
- (b) $(a + 1)^{b+1}$
- (c) $a + b$
- (d) $(a + 1) * (b + 1)$
- (e) a^b
- (f) $a * b$

6. Alanine

At which pH does alanine not move in an electric field?

7. Tryptic digestion

Determine all tryptic peptides of DASLTESTLPEPTIDKWARHIER (mind the the proline rule).

8. Post-translational modifications

- (a) Given n phosphorylation sites (S,T or Y) in a protein. Given a formula for the total number of protein isoforms.
- (b) Identify all eukaryotic phosphorylation sites in the peptide TESTPEPTIDEYEAH
- (c) Given the peptide TESTPEPTIDEYEAH. How many different proteins are there if you consider the eukaryotic phosphorylation sites (S,T or Y) as potentially phosphorylated?

9. Protein database

Download a protein fasta database of *E. coli* from the net and cite your source. How many protein sequences are contained?