

## Exercise Sheet 7 – Computational mass spectrometry

### Introduction to mass spectrometry

#### 1. Mass spectrometry (5.0 points)

a) Name the core components of a mass spectrometer and describe their function briefly (max 4 sentences). (3 points)

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a) Explain concisely (in 2 sentences) what a mass spectrum is and what information it depicts. Use the following terms:  $m/z$ , intensity, peak(s). (2 point)

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## 2. Peptides, fragmentation, peaks and masses (10.0 points)

a) Write a small program/script/function (language of your choice) which calculates and returns all possible tryptic peptides for any protein sequence. The function may look similar to “String[] getTrypticPeptides(String proteinSequence)”. Provide your source code and its output (as PDF at the end) and the number of peptides generated (fill in here) for the protein P00533-1. Download the protein sequence from UniProt.org. (4.0 points) You will re-use the source code in the next exercise.

Number of tryptic peptides: \_\_\_\_\_

b) Write a small program/script/function (language of your choice) which calculates and returns the monoisotopic masses of all possible singly charged y- and b-fragment peaks with at least 7 significant figures for any given input peptide. The function may look similar to “double[] getFragmentMasses(String sequence)”. Provide your source code and its output (as PDF at the end) and the output for the peptide “MAINHTGEK” (fill in table). (4.0 points) You will re-use the source code in the next exercise.

b+	m/z	AAS	m/z	y+
1		M		9
2		A		8
3		I		7
4		N		6
5		H		5
6		T		4
7		G		3
8		E		2
9		K		1

b) The first isotope (peak) of ethanol ( $C_2H_5O_1H_1$ ) contains 1 additional neutron. Let's assume that the neutron is either incorporated in form of a heavy H ( $^2H$ ) or heavy C ( $^{13}C$ ). Assume you pick two molecules from the first isotope, one containing a single heavy H ( $C_2H_5O_1^2H_1$ ) and the other containing

a single heavy C ( $^{13}\text{C}_1\text{C}_1\text{H}_5\text{O}_1\text{H}_1$ ). The difference between the two molecules is which atom contains the additional neutron. With the information at hand, what do you expect the mass of  $^{13}\text{C}_1\text{C}_1\text{H}_5\text{O}_1\text{H}_1$  to be in relation of  $\text{C}_2\text{H}_5\text{O}_1^2\text{H}_1$ ? Smaller, equal or bigger? Explain your reasoning (1 sentence). (2.0 points)

☐  $^{13}\text{C}_1\text{C}_1\text{H}_5\text{O}_1\text{H}_1$  is lighter (smaller m/z) than  $\text{C}_2\text{H}_5\text{O}_1^2\text{H}_1$

☐  $^{13}\text{C}_1\text{C}_1\text{H}_5\text{O}_1\text{H}_1$  is equal (same m/z) than  $\text{C}_2\text{H}_5\text{O}_1^2\text{H}_1$

☐  $^{13}\text{C}_1\text{C}_1\text{H}_5\text{O}_1\text{H}_1$  is heavier (bigger m/z) than  $\text{C}_2\text{H}_5\text{O}_1^2\text{H}_1$

Explanation:

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