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AG Algorithmische Bioinformatik

Algorithmische Bioinformatik

10. Übungsblatt WS 11/12

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Name:

Matrikelnummer:

Übungsgruppe:

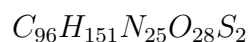
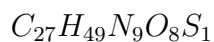
1 2 3

1 Isotopic distribution

1.1 Computation

Now it's up to you to calculate, with your programming language of choice, the isotopic distribution of some peptides. If you have the code, you can try different masses, and see what happens to the distribution when you have lower and higher masses of the peptides.

For this exercise (to compare our results) consider the following two sum formulas:



Glu-Pro-Met-Lys-Arg-Ser-Thr-Glu-Ala-Leu-Asn-Phe-Val-Ile-Ser-Gln-Met-Trp

As we have depicted in the end of our lecture, use the information and the formula which you can find in these slides. The main part of information for you starts at slide 12.

Isotopes:

isotopes	mass [Da]	% abundance
¹ H	1.007825	99.985
² H	2.014102	0.015
¹² C	12.0	98.90
¹³ C	13.003355	1.10
¹⁴ N	14.003074	99.63
¹⁵ N	15.000109	0.37
¹⁶ O	15.994915	99.76
¹⁷ O	16.999131	0.038
¹⁸ O	17.999159	0.20
³² S	31.972072	95.02
³³ S	32.971459	0.75
³⁷ S	33.967868	4.21

Once you have computed the distributions, plot them and see what you got.

1.2 Running time

What is the running time of the naive algorithm of calculating the isotopic distribution of a given sum formula if you take into account all possible isotopic masses that have a probability greater than zero? What is the running time if you just take the first ten isotopic masses?

2 Proteinidentifizierung

2.1 Suche

Im Wiki finden sich zwei Spektren eines zu identifizierenden Proteins. Zur Analyse können Sie Mascot¹ verwenden. Geben Sie die Sequenzen der Peptide, den besten Treffer in einem Protein sowie den Score-Wert des Treffers an. Hinweis: um Signifikanz zu erreichen, müssen die Spektren zu einer Datei kombiniert werden. Hinweise dazu finden sich in der Mascot-Hilfe zu Dateiformaten. Die Daten sind im SEQUEST-Format.

¹http://www.matrixscience.com/search_form_select.html