# Exercise 2
Algorithmic problems in HPLC/MS

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 excercise (to compare our results) consider the following 2 sum formulas:

$$C_{27}H_{49}N_9O_8S_1$$

$$C_{96}H_{151}N_{25}O_{28}S_2$$
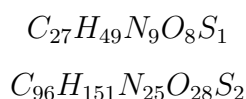
As we have depicted in the end of our lecture, use the information and the formula which you can find in these slides. The main part of information for you starts at slide 12.

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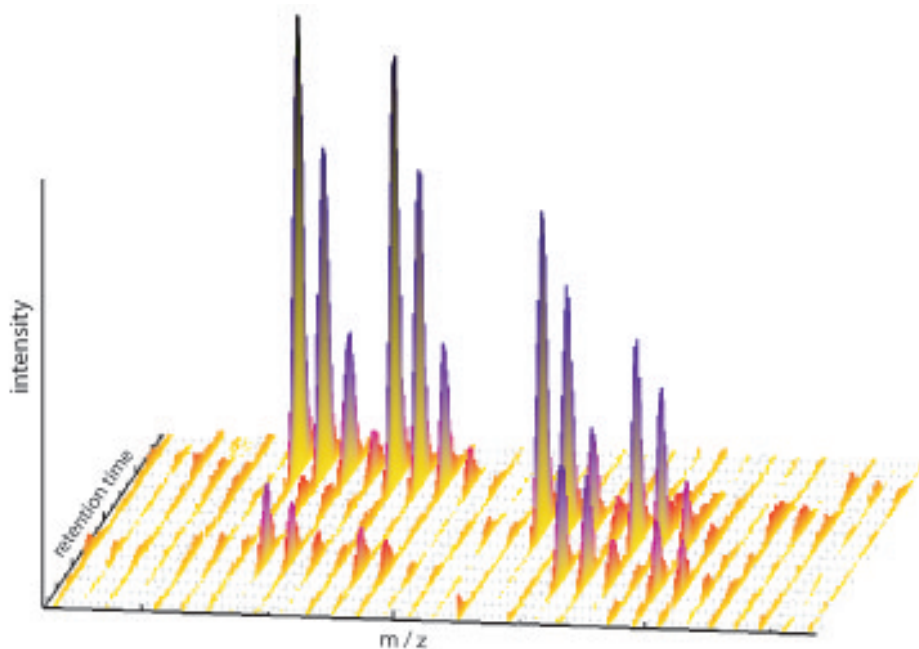
1.3 Sufficiency

Is it always sufficient/reasonable to take just the first ten isotopic masses?
Why, why not? How can you check that?

2 LC/MS map

2.1 Masses and labels

We have not talked about labeling peptides/proteins but what is probably done in the following picture? (The distance of these peaks is just 1 Da on the m/z axis).

Hint: The slides are very useful to do the other exercies as well ;-)