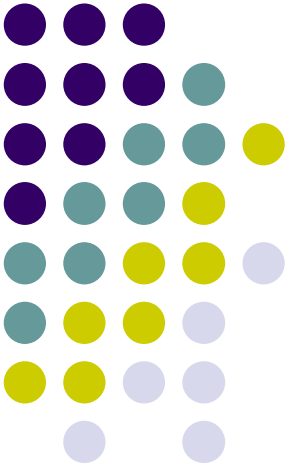
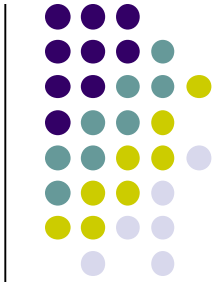
Project Descriptions

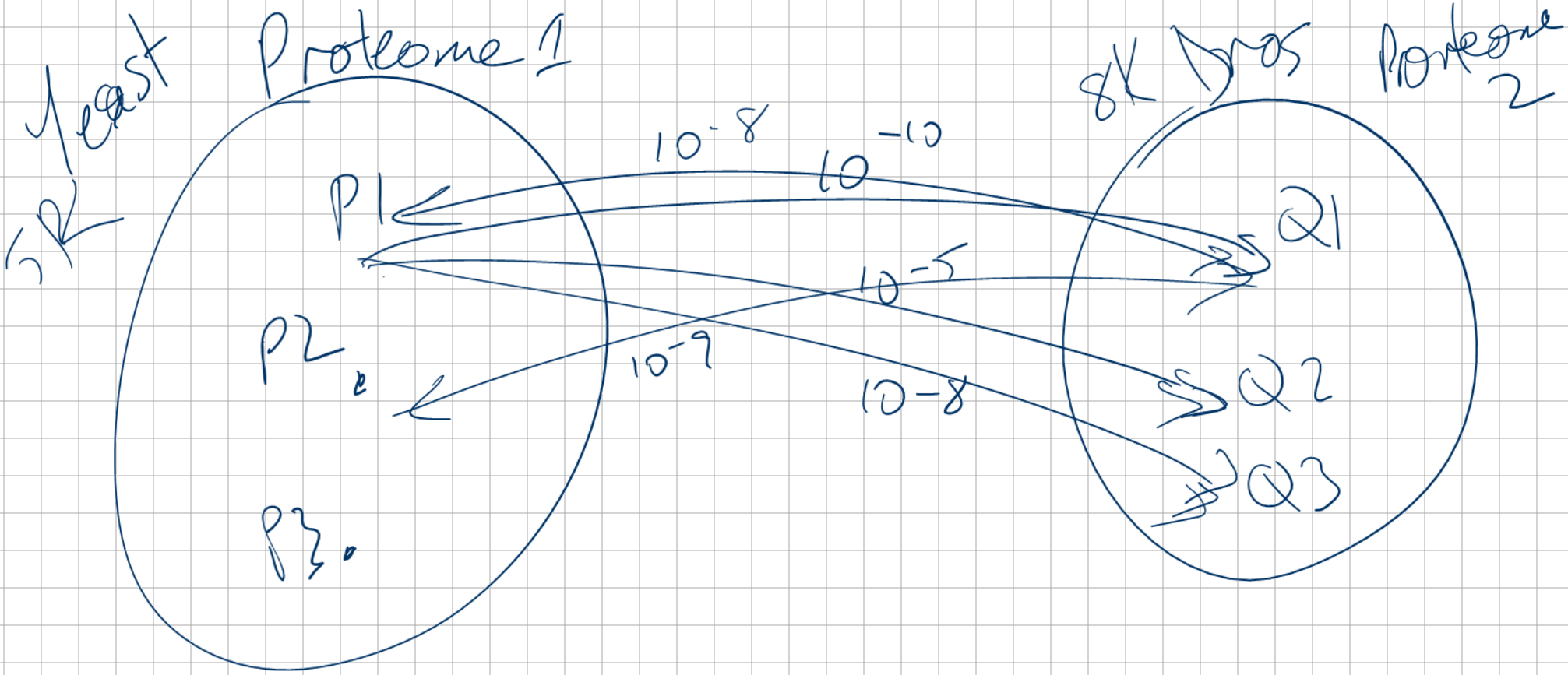
BINF5240
Lecture 18

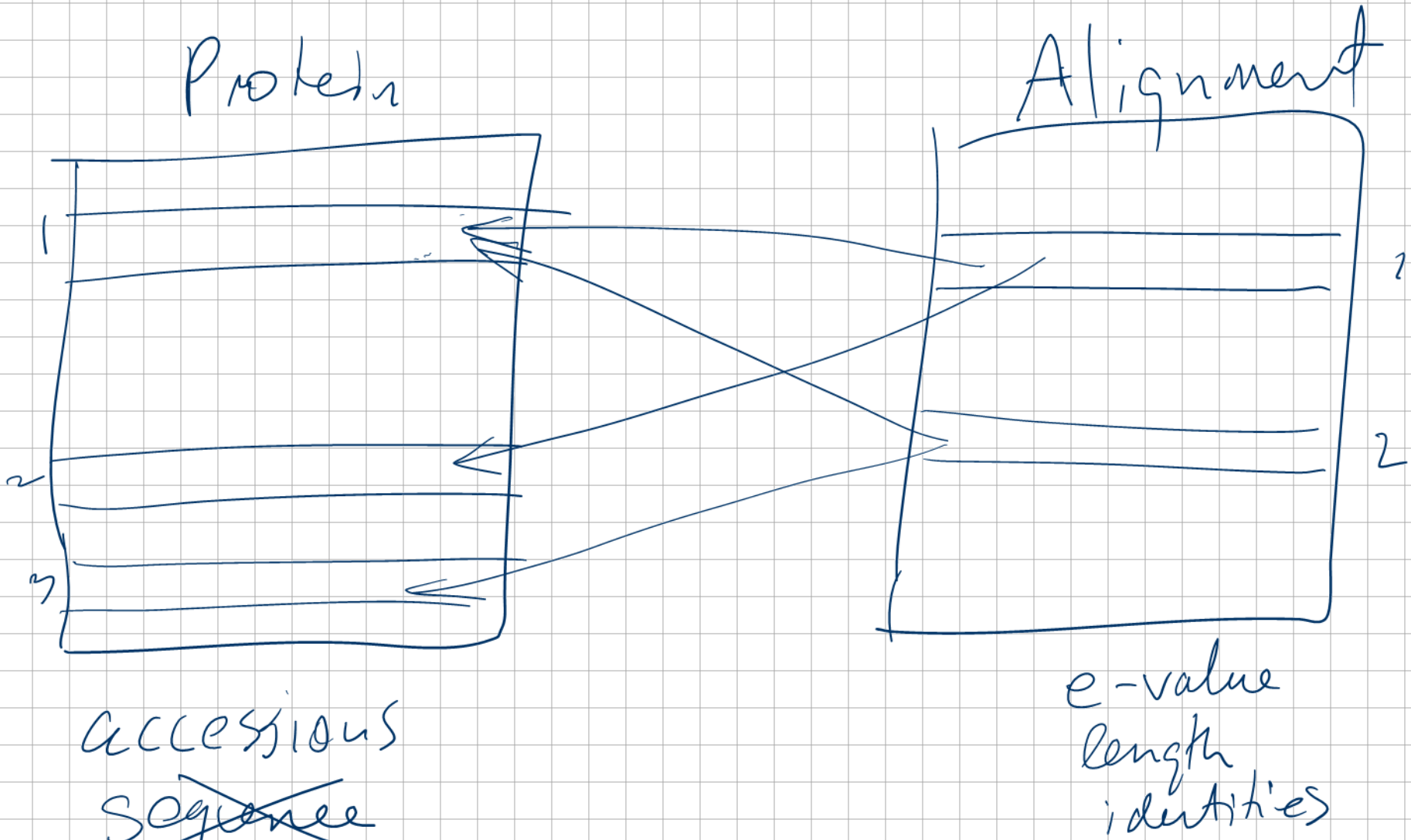


Class Project: Blast Database



1. Write a program that computes all pairwise blast alignments for two species' proteomes and stores the alignments in a relational database.
2. Write a program that retrieves the blast alignment for two proteins (specified by their accessions) from the relational database.
3. Write a program that finds pairs of orthologous proteins that are mutually best hits in the species' proteomes.

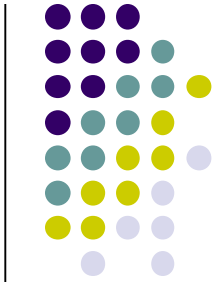

least
Proteome 1
P1
P2
P3
10-8
10-10
10-5
10-9
10-8
St Dros
Proteome 2
Q1
Q2
Q3



accessions
~~sequence~~
description
organism

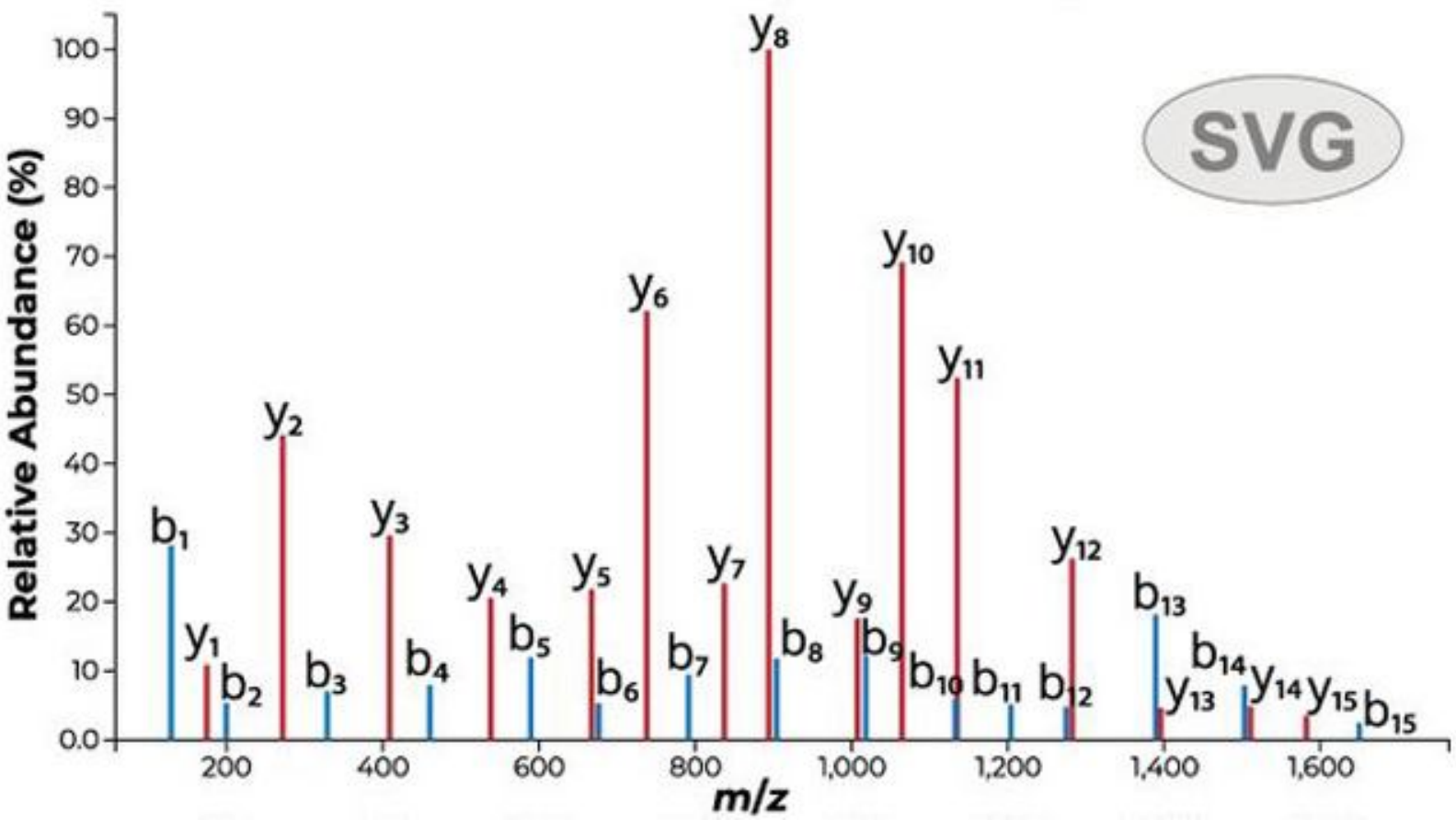
e-value
length
identities

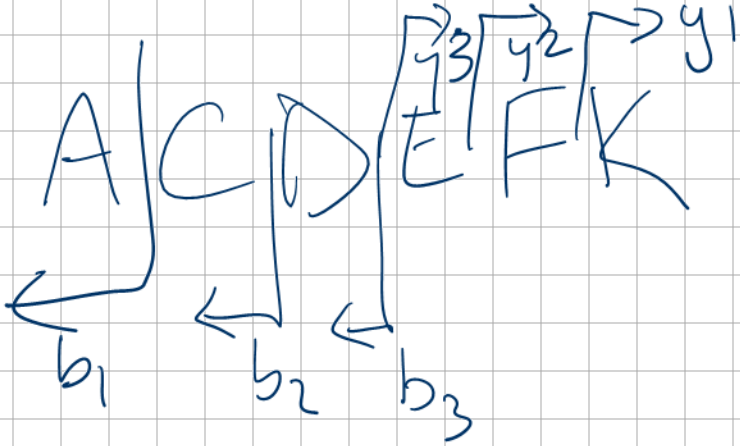
Class Project: MS/MS Viewer



- Write a program to display peptide fragmentation spectra from an mzXML file.
  - The program will take an mzXML file, a scan number, and a peptide sequence as input.
  - The peptide's b-ion and y-ion m/z values should be computed, and peaks matching these m/z values annotated with appropriate labels.
  - The output figure/plot should aid the user in determining whether or not the peptide is a good match to the spectrum.

Example of annotated spectrum





m/2 value (largest int)

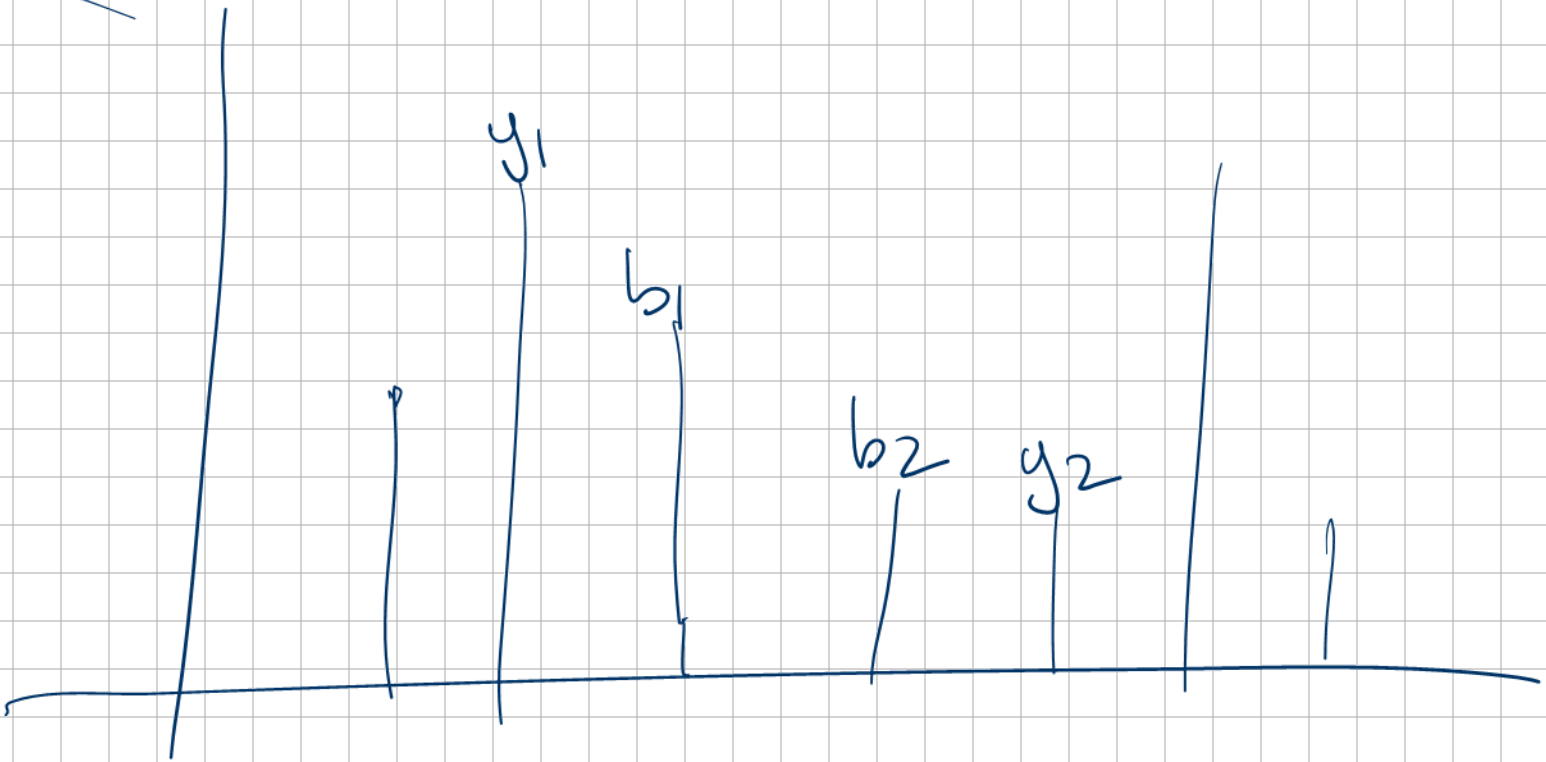
$$m2_{b_i} = \sum_{j=1}^{i} mw_{AA_j} + 1$$

$$m2_{y_i} = \sum_{j=n}^{n-i+1} mw_{AA_j} + 19$$

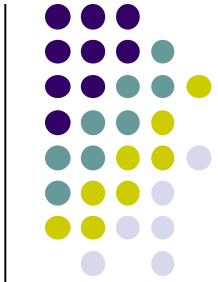
$mw_G = 57$

~~$mw_G = 75$~~

stem

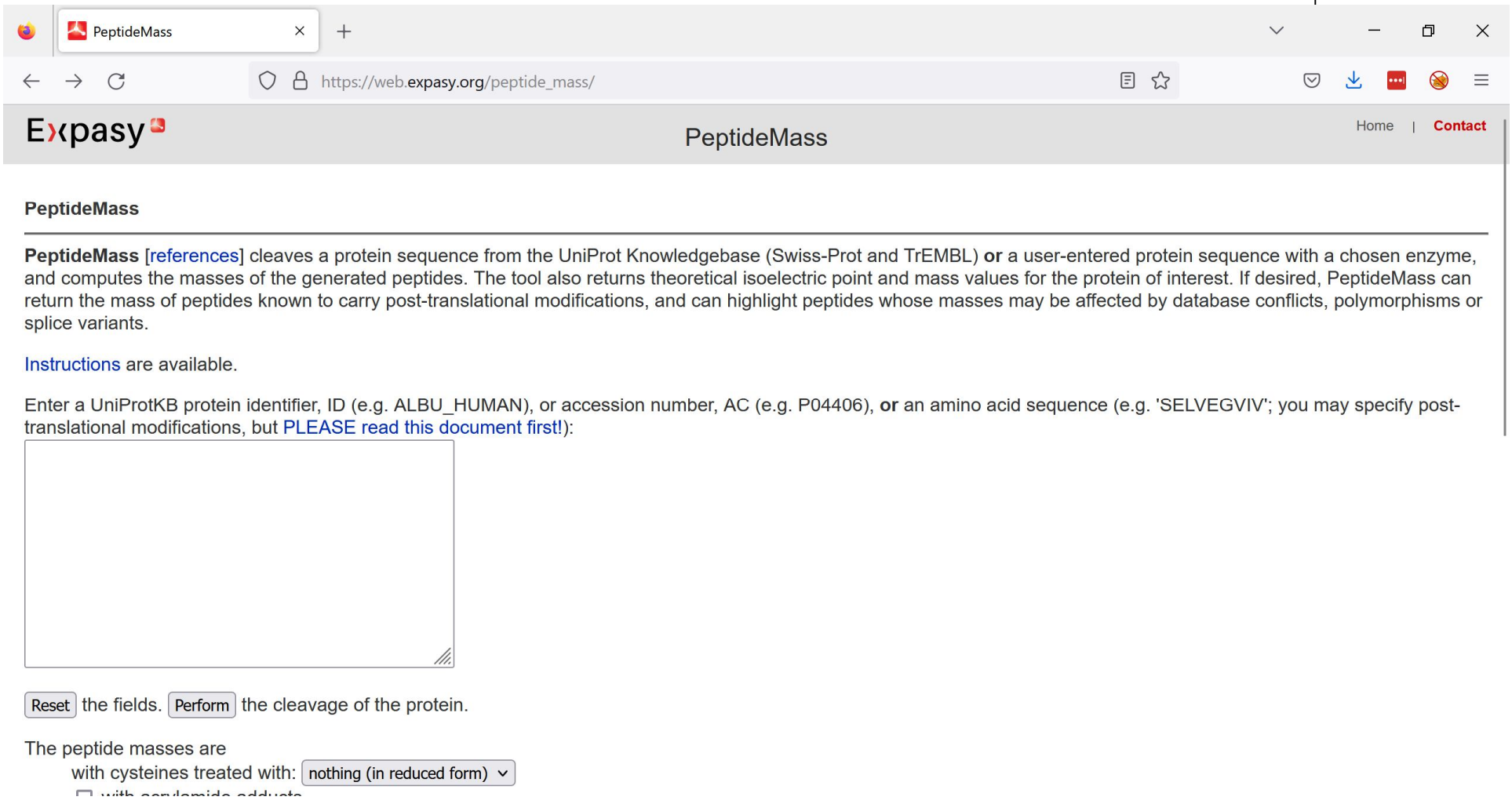


Class Project: Protein Digest



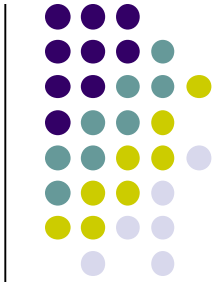
- Write a simple web-server application using TurboGears to carry out an *in silico* enzymatic digest of a user-provided protein sequence.
  - Users should be able to specify min and max length, min and max molecular weight, # of missed cleavages, and specific enzyme.
  - Output should be a table of peptides, with their length, molecular weight, # of missed cleavages, and amino-acids to left and right of each peptide in the protein sequence.

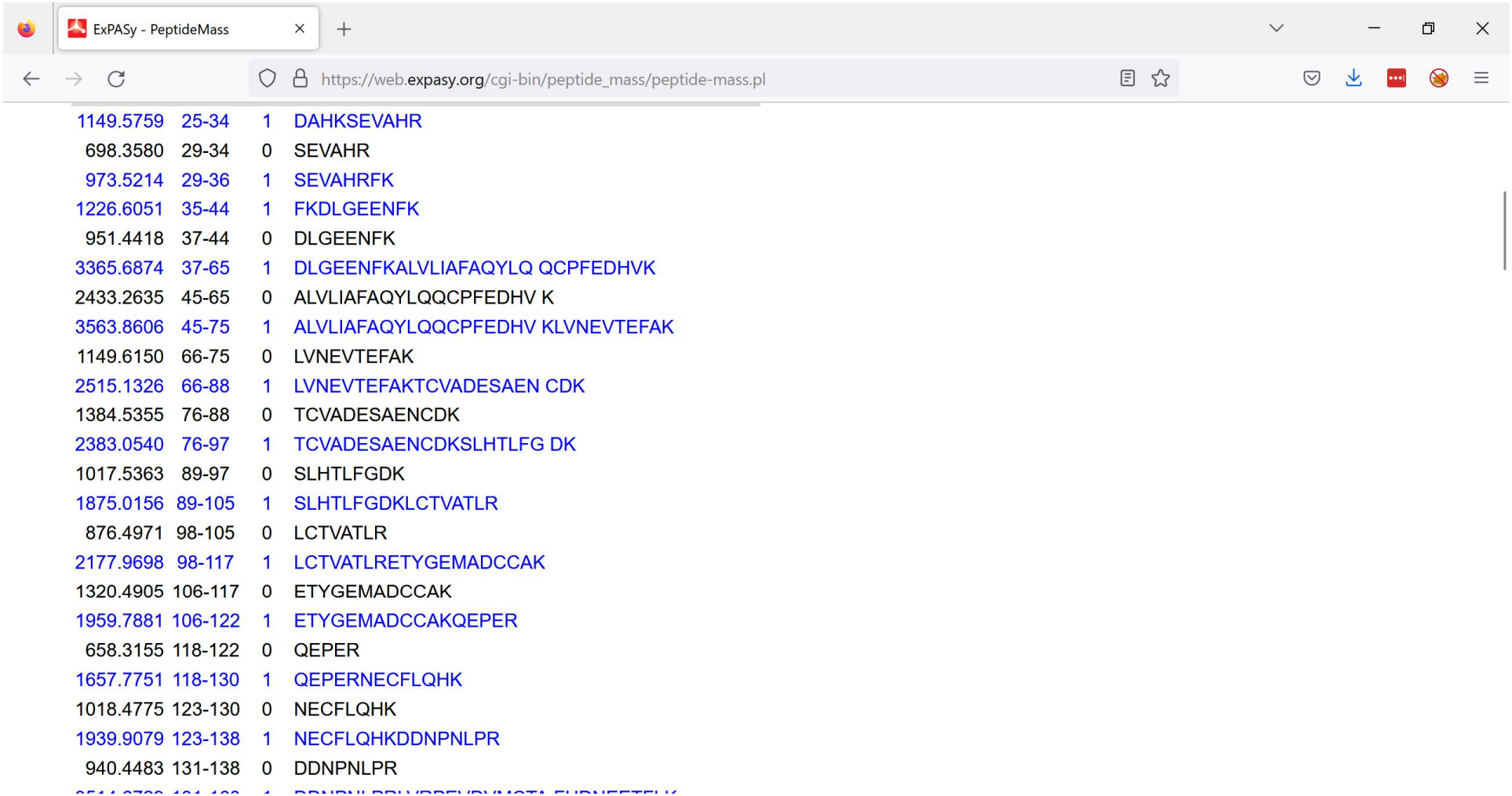
Example: PeptideMass



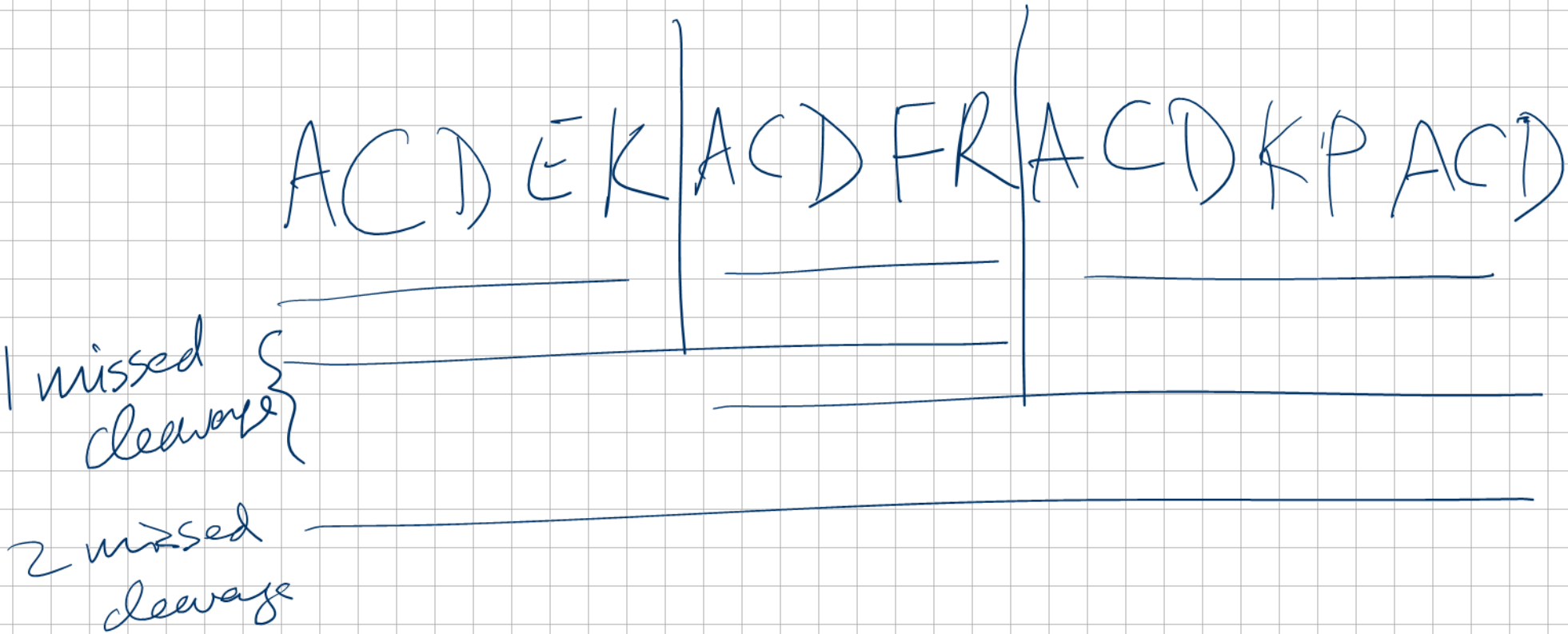
https://web.expasy.org/peptide_mass/

Example: PeptideMass





1149.5759	25-34	1	DAHKSEVAHR
698.3580	29-34	0	SEVAHR
973.5214	29-36	1	SEVAHRFK
1226.6051	35-44	1	FKDLGEENFK
951.4418	37-44	0	DLGEENFK
3365.6874	37-65	1	DLGEENFKALVLIAFAQYLQ QCPFEDHVK
2433.2635	45-65	0	ALVLIAFAQYLQQCPFEDHV K
3563.8606	45-75	1	ALVLIAFAQYLQQCPFEDHV KLVNEVTEFAK
1149.6150	66-75	0	LVNEVTEFAK
2515.1326	66-88	1	LVNEVTEFAKTCVADESAEN CDK
1384.5355	76-88	0	TCVADESAENCDK
2383.0540	76-97	1	TCVADESAENCDKSLHTLFG DK
1017.5363	89-97	0	SLHTLFGDK
1875.0156	89-105	1	SLHTLFGDKLCTVATLR
876.4971	98-105	0	LCTVATLR
2177.9698	98-117	1	LCTVATLRETYGEMADCCAK
1320.4905	106-117	0	ETYGEMADCCAK
1959.7881	106-122	1	ETYGEMADCCAKQEPER
658.3155	118-122	0	QEPER
1657.7751	118-130	1	QEPERNECFLQHK
1018.4775	123-130	0	NECFLQHK
1939.9079	123-138	1	NECFLQHKDDNPNLPR
940.4483	131-138	0	DDNPNLPR



MW(pep) = sum(amino-acids) + 19 # [M+H]