

Problem Set 1: Due Sunday, Sept 1 - 5:30 PM.

Total time required ~50 min (If you take more than twice this time, there is likely an issue regarding how you are approaching the problem, please seek help).

Calculate – use a formula to give quantitative answers.

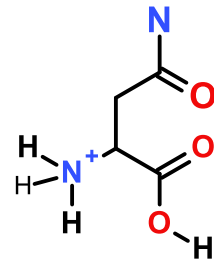
Sketch - you need not calculate the curve, just try to reproduce its general features. However, take care in representing certain 'landmarks', such as inflection points, etc. Fully label the axis with units and scale.

Unless instructed otherwise, please include plots or sketches with your problem set, the graphs should have:

- i) Brief title
- ii) The axis labeled, with units if appropriate
- iii) If there are multiple datasets on the same plot they should be clearly distinguished using a legend.

1. (5 points, 10 min) The structure shown to the right is that of the amino acid asparagine.

- a) Add any protons that may be missing from this structure. You can assume that the ionizable groups are fully protonated, as indicated on the diagram (2 pts).
- b) Circle the atoms that are unique to asparagine (the sidechain atoms). What is the name of the functional group on the sidechain? (1 pt)
- c) Add one H₂O molecule to your drawing that donates a H-bond to the **sidechain** of asparagine. Clearly label the hydrogen bond donors and acceptors (2 pts).

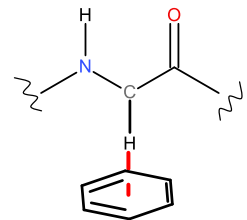


[Draw the waters as "H-O-H", with approximate bond angles and bond lengths.]

2. (4 pts, 5 min) What is the electronic configuration of the most stable form of Ca? Is it ionized and if so what is its charge? Briefly justify your answer.

3. (5 points, 5 min) Rank, from highest to lowest, the hydrogen bond strength of the following groups; assume the H-bond acceptor is the carbonyl (C=O) group. a) -N-H b) -O-H c) -S-H d) -C-H. Briefly justify your answer. [Hint: A table of electronegativities may be helpful, see lecture 2 notes. The electronegativity of S is 2.58].

4. (5 pts, 10 min) The interaction shown on the right is often observed in protein structures, where the C α -H group is positioned above the middle of an aromatic ring, as drawn on the right. What features of this interaction lead to its stability? Be sure that you discuss the role of all the atoms on the amino acid.



5. (5 pts, 10 min) Open the JSmol page associated with this problem set. In order to answer this question, you will have to look at the structures of amino acids that are given in lecture 5 of OLI.

- a) Draw the chemical structure that is displayed in JSmol (2 pts).
- b) State whether the compound shown in JSmol is polar or non-polar (or both); briefly justifying your answer (2 pts).
- c) What amino acid contains this functional group (1 pt)?

6. (6 pts, 15 min) Use Excel to determine the best linear fit to the following data points.

- a) Submit a chart with your problem set that has the following features (2 pts):
 - i) The data where the points are indicated by filled circles and they are not connected by a line.
 - ii) The linear fit is on the chart, shown as a dotted line.
 - iii) The chart has a title "Enzyme Velocity"
 - iv) The x- and y-axis are labeled appropriately.
 - v) the range for the x-axis is 1-5.

[S] mM	V (uM/sec)
0	0.00
1	1.15
2	2.10
5	3.80

b) In the legend to the figure, include a brief description of the plot and the values for the equation of the line (2 pts)

c) Do you feel that the data is well fit to a straight line? Justify your answer (2 pts).