Biochemistry (BT351)
Second Semester 2023/24
Problem Set II (Due on 06/05/2024 by 11:30 pm)

Important Notes:

- No late work will be accepted
- You should work the problem set as groups of THREE students
- Only hand-written and hard copies will be accepted
- You need to download PS1 pdp files folder
- You need to show all your calculations and units for all questions
- Good luck

Question 1

View the PyMOL peptide associated with your serial number. **PSII pdp files**

A) Write the correct sequence of your peptide.
B) Using the pKa values in table 4-1. Draw the titration curve for your peptide. Use equivalents for the x-axis.
C) Draw the structure of your peptide at pH 3, 8 and 12
D) Using arrows, indicate peptide bonds
E) Circle atom(s) that can act as hydrogen acceptor. Draw a water molecule forming a hydrogen bond with this atom.
F) Circle atom(s) that can act as hydrogen donor. Draw a water molecule forming a hydrogen bond with this atom.

Question 2

Open the helix structure in file **Helix.pdb**. Show all the backbone hydrogen bonds (i.e. between C=O and H-N) and the distances (dashes and numbers in black).
Change the lines to stick:
From **H** (Right menu), select **lines** then from **S** (Right menu) select **sticks**
Change the background to white:
From **Display** tab (Top menu), go to **Background** then select **White**
Finding and drawing the hydrogen bonds:
From **Wizard** tab select **Measurements.** Choose the first **O (or H),** and then select the **H (or O).** In PyMOL, nitrogen is represented as blue and oxygen as red
Changing the color of dashed H-bond from yellow to black and hiding the distance:
Select from the right menu each **measure (e.g measure01)**, from **C** (right menu) choose **greys** then **black.** Record all distances from N- to C- terminal and from **H** (Right menu), select **labels.**

A) What is the type of this helix (α, π or 3_{10})? **Explain your answer.**
B) Prepare a figure of this helix showing the H-bonds as dashed lines. Choose the best view that will show most of the H-bonds and attach the figure to your answers.

Question 3

Open the structure in file **Q3.pdb** (PS1 pdp files)**.** Answer the following questions.

A) This type of structure is called _____and it's composed of _____ chains.
B) Write down the amino acid sequence for each chain.
C) Determine the length of each chain.
D) Draw the helical wheel structure for residues 231-248 using the following website (http://rzlab.ucr.edu/scripts/wheel/wheel.cgi?sequence=ABCDEFGHIJLKMNOP&subm).
Copy the One-letter amino acid sequence and paste it in the sequence box and hit submit. Include the generated figure in your report and show the regions of the hydrophobic core, the hydrophilic surface and the ion pair.

Question 4

Open the structure in file **Q4.pdb** (PSII pdp files)**.** Use PyMOL to determine the phi and psi angles of residues 225-230 of the helix.

Residue	Phi (ϕ)	Psi (ψ)
225		
226		
227		
228		
229		
230		

A) The phi and psi values. **Make sure you are measuring angles for the right residues.**

Finding the dihedral angles Phi (ϕ) and Psi (ψ):

From **Wizard** tab select **Measurements.** Click **Distance** and select **Dihedral.** The phi angle for each residue is measured by selecting atoms C_{i-1} (carboxyl carbon), N_i (amino nitrogen), $C_{i\alpha}$ (chiral carbon), and C_i (carboxyl carbon of the next residue). The psi angle for each residue is measured by selecting atoms N_i (amino nitrogen), $C_{i\alpha}$ (chiral carbon), C_i (carboxyl carbon), and N_{i+1} (amino nitrogen of the next residue). Both angles values will appear in yellow color.

B) Plot the phi and psi values for each residue to produce a Ramachandran plot **(Use Excell).** In which part of the plot the residues cluster? Did the residues cluster in the part of the plot you expected? **Explain why?**

Question 5

The following peptide can fold to give a unique 3D structure.
SACVDVNPGSSKNAFEDVSKRFVDDNPGSRKVEFKYA

A) Use the following folding data for this peptide to determine ΔH^o and ΔS^o [Hint: Plot a van't Hoff plot ($\ln(k_{eq})$ vs 1/T)

Temperature (K)	Fraction unfolded
290	0.01
295	0.05
300	0.09
305	0.19
310	0.38
315	0.57
320	0.78
325	0.87
330	0.94
335	0.97

B) Using the **PSIPRED Protein Sequence Analysis Workbench (Google it)**, predict the secondary and super-secondary structure of this peptide. Draw the topology of this peptide using the result obtained from PSIPRED.

1. Copy the peptide sequence to input sequence
2. Choose PSIPRED v3.3 (Predict Secondary Structure)
3. Fill the Short identifier for submission
4. Press Predict
5. You might have to wait for 30 minutes.
6. Choose the PSIPRED tap