## 060113 Quiz 1 Morphology of Complex Materials

- 1) Explain how a protein displays structural hierarchy.
  - a) List 4 levels of structure for a protein
  - b) Describe each of these levels of structure
  - c) Explain what self-assembly means in the context of a protein.

d) How is structure related to function in a protein? (For example in a membrane protein.)

- e) How could evolution act on the structural hierarchy of a protein?
- 2) Amino acids are the mer units of a protein.
  - a) Give the generic chemical structure for an amino acid (labeling the alpha carbon).

b) Show how a condensation reaction could proceed between two amino acids to result in a dipeptide. Label the C and N ends of this dipeptide.

c) Cystine is an important amino acid. Sketch the structure of cystine and explain the importance of cystine in protein structure.

d) Proline is an important amino acid. Sketch the structure of proline and explain the importance of proline to protein structure.

e) Give the structure of glycine and explain where glycine units might occur in the secondary structure of a protein.

3) In polymers and in proteins bond rotation angles have been found to govern, to some extent, chain conformation. In polymers bond rotation angle is the basis of the rotational isomeric state model (RISM) of Flory that, through matrix math, describes short-range interactions; and in proteins bond rotation angles are the basis of Ramachandran plots for elucidation protein conformation. (We will, hopefully, see that these two implementations of bond rotation angle have some similarities but also striking differences which parallel the similarities and differences between Polymer Science and Structural Biology.)

a) Sketch a protein chain labeling the three bond rotation angles of importance to chain conformation.

b) Explain why one of these angles is generally ignored in the Ramachandran plot.

c) The following plot (Figure 1 below) shows a Ramachandran plot for a protein displaying a prominent feature (upper left black enclosing line and black crosses) and a weaker feature (central left black enclosing line and grey crosses). The little squares to the right are glycines. Explain what these two features are and why glycines might be located away from these two features.

d) What typically holds an  $\alpha$ -helix or a  $\beta$ -sheet together? Show how this feature is shown in Figures 3 and 4 below and explain what the structures are (Label the atoms you can).

e) The native state of protein G is shown to the right below, Figure 2. Where would you expect hydrophobic and hydrophilic groups to occur in this structure? Sketch one hydrophobic and one hydrophilic amino acid which might be expected in these two regions of the protein.





Figure 1

Figure 2



Figure 3



Figure 4

## ANSWERS: 060113 Quiz 1 Morphology of Complex Materials

1) a) Primary Structure- Sequence arrangement of amino acids

Secondary Structure- Hydrogen bonded structures such as alpha helix, beta sheet and super secondary structures such as beta barrels.

Tertiary Structure- Larger scale structures composed of secondary structures bonded by disulfide bonds, by hydrophilicity, hydrogen bonds and by static charge. Tertiary structure defines the difference between a folded native state protein and an unfolded protein. Tertiary structure refers to the final native state of a single protein molecule.

Quaternary Structure- Generally a collection of proteins and other organic and inorganic species that are bound by hydrogen bonds, hydrophilicity and static charge to produce a single functional unit such as a ribosome.

- b) above
- c) Self-assembly, in the context of a protein, indicates that once the amino acid primary structure is produced at the ribosome there is limited external organizational control over the formation of secondary structures by hydrogen bonds, or of tertiary structure. The tertiary and quaternary structures of the final protein are encoded to a large extent in the amino acid sequence and the higher level structures assemble themselves.
- d) The spatial location of hydrophilic and hydrophobic groups in the native state folded protein decided by the primary, secondary and tertiary structure determines the functionality of a protein. For example, a membrane protein might be expected to display two hydrophilic end domains with a hydrophobic central domain that could be embedded in an amphiphilic membrane. The quaternary structure might involve a beta barrel with a hydrophilic core that could allow transport of polar molecules through the cell membrane.
- e) Evolution simply observes the functionality of basically random modifications of the amino acid sequence associated with random modification of DNA in terms of survivability of the organism as a whole. Enhancement in survivability encourages a particular modification (mutation) since the carrier of this modification (organism) will be more likely to reproduce and pass on the modification to later generations. The evolutionary model has become a major pathway to understanding protein morphology (generally 20% of most current textbooks on proteins).

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the horized of the is hopded such the flexibility of the flexibility o 2e) State 2 1 w C 1. 11 L K 1. psi 39) 6) wis 180° (or -180°) due to parhal charge + steric efferts HS+ -C 7 1 B-sheet in top left is the dominant feature with on x-helix in the middle Left. The little squares are B-turns. Elycne are fletible units upeful in turns. turns ¢ 1800 Ó

d) Dashed lines are hydrogen bonds between NH, dark grey ball and O, Light ball end of dashed line. Top are two Beta strands hydrogen bonded together and bottom is an apha helix.

e) Hydrophobic where the two structures touch, hydrophilic towards the outside of the structure.

C00 <sup>-</sup> H <sub>2</sub> N-C-H	COO <sup>-</sup> HaN-C-H	CO0⁻ H∍N-C-H	СОО <sup>-</sup> Н₀№-С-Н	С00 <sup>-</sup> НN-С-Н
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Alanine	Valine	н <sub>3</sub> с сн <sub>3</sub>	CH3	Proline
A	v	Leucine	Isoleucine	Р
.C00-	C00-	, Ç00-	C00-	Ç00 <sup>-</sup>
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H <sub>3</sub> N-Ç-H	H <sub>3</sub> N-Ç-H	H <sub>3</sub> N-Ç-H	H <sub>3</sub> N-Ç-H	H <sub>3</sub> N-Ċ-H
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C	CH2	CH2	CH2	HC=C
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hydrophilic.

Top group are hydrophobic. All others are