

**Biophysics - BIO361**  
**RUBRICS Quiz-2**

**Total Marks : 20**  
**Duration : 1h**

**Part1- Multiple Choice Questions**

**Total marks - 5\*1=5 marks**

**Each Question is for one mark. Correct answers are written in BOLD letters.**

1. Which one of the following is not a Multiple Sequence alignment tool?
  - a. MUSCLE
  - b. T-Coffee
  - c. WebPRANK
  - d. **Water**
  
2. What does a negative change in Helmholtz free energy indicate in the context of protein interactions?
  - a. **Spontaneous binding or folding**
  - b. Decreased stability
  - c. Unfavorable reaction
  - d. No change in system energy
  
3. Which of the following is not a tool for calculating the hydrogen bond interactions?
  - a. FoldX
  - b. Chimera
  - c. PIC
  - d. **Stitch**
  
4. Which of the following statements regarding the Helmholtz and Gibbs free energies, and their relationship with volume and pressure, is true?
  - a. The Helmholtz free energy is solely dependent on the energy (E) of the system and does not consider the effects of temperature(T) or entropy(S).
  - b. **At low pressures for solids or liquids, the correction term PV is much smaller compared to the thermal energy of the body, making it negligible for these systems.**
  - c. The Helmholtz free energy is calculated for a system with a constant pressure.
  - d. The value of PV is significantly higher for solids and liquids compared to gasses, due to the compact nature of molecules in solids and liquids.
  
5. Which of the following phase transitions of a typical non-polar molecule is energetically least expensive?
  - a. **Liquid to crystals**
  - b. Crystals to aqueous solution
  - c. Liquid to aqueous solution

- d. All are equal

## **Part 2 - Short Answer-type Questions (3 marks each)**

**Total marks -  $5 \times 3 = 15$  marks**

**6. What is the difference between Helmholtz and Gibbs free energy? Write the difference between 'energy' and 'free-energy'.**

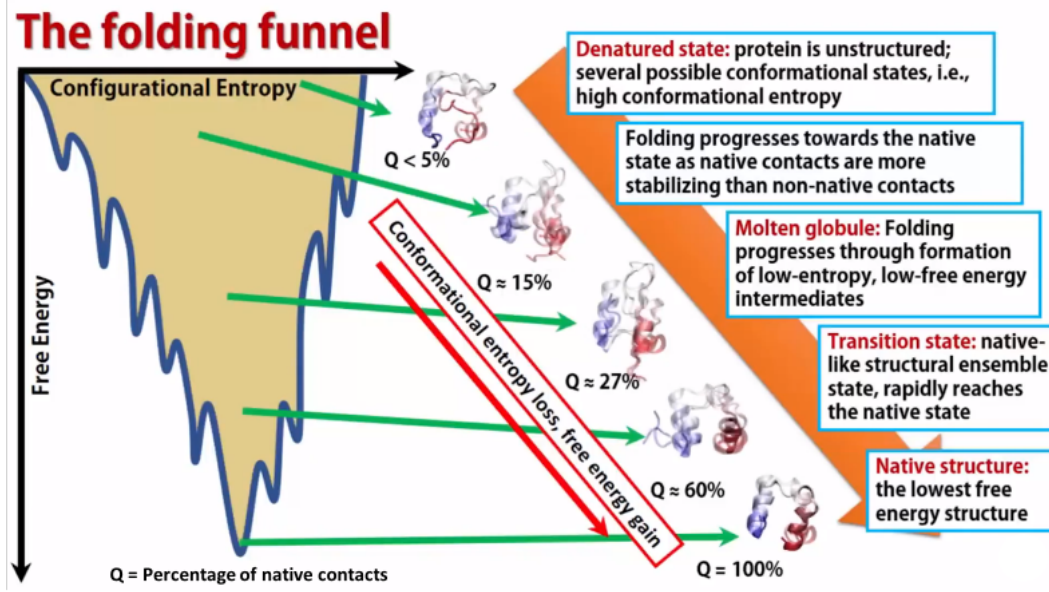
The Gibbs free energy is the energy available to do non-PV work in a thermodynamically-closed system at constant pressure and temperature. The Helmholtz free energy is the maximum amount of "useful" (non-PV) work that can be extracted from a thermodynamically-closed system at constant volume and temperature.

Energy is the measure of work done on a certain object at normal temperature conditions whereas free energy is the work a system can perform at the constant temperature.

The "free energy" is a natural generalization of the regular "energy" for the case when the system exchanges heat with the environment. A change in the energy,  $E_b - E_a$ , is the work required to transfer a body from state "a" into state "b" when there is no heat exchange with the environment. And a change in the free energy  $F_b - F_a$  is the work required to transfer a body from state "a" into state "b" when the body keeps exchanging heat with the environment.

**7. What are energy landscapes with respect to protein folding, and is it related to entropy? Explain with a diagram.**

Free energy landscape describes the energy of a system in terms of certain parameters, with respect to protein folding it will show the transition in energy as a protein goes from unfolded to most stably folded state.



When the protein tends to move from a denatured to a folded state, the percentage of native contacts increases, which reduces the entropy of the structure, making it energetically stable. decrease as it goes from the unfolded to the most stably folded state.

## 8. What are the 3 laws of thermodynamics?

- 1st Law of Thermodynamics - Energy cannot be created or destroyed.
- 2nd Law of Thermodynamics - For a spontaneous process, the entropy of the universe increases.
- 3rd Law of Thermodynamics - A perfect crystal at zero Kelvin has zero entropy.

## 9. Why are nonpolar molecules like cyclohexane hydrophobic? Explain its relationship with entropy in an aqueous environment.

The reason is that, unlike water molecules, nonpolar molecules are **incapable of H-bonding**.

When hydrophobic molecules are added to an aqueous solution, the water molecules **arrange** around them in a favorable position to avoid loss of H bonds, thereby partially freezing their thermal motion. So, when a hydrophobic molecule is added to an aqueous solution its **entropy will reduce**.

## 10. Explain the differences between basic and advanced modeling using Modeller.

Basic Modelling	Advanced Modelling
<ul style="list-style-type: none"> <li>Used for modelling smaller proteins for which good query coverage is</li> </ul>	<ul style="list-style-type: none"> <li>Used for modelling complex structures with no accurate template available</li> </ul>

<p>available.</p> <ul style="list-style-type: none"><li>- Uses single template structure</li><li>- Gives less precise and accurate model</li><li>- Uses basic alignment and no refinement techniques are used.</li><li>- Query and template is aligned to build the model</li></ul>	<ul style="list-style-type: none"><li>- Uses multiple template structures</li><li>- Gives more precise and accurate model</li><li>- Models complex structures with loop modeling, and refinement.</li><li>- Templates are aligned and then the query is aligned with the template structures</li></ul>
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