

THERMODYNAMICS ASSIGNMENT

1. Hydrophobic interactions:

- a. The forces that hold the nonpolar regions of the molecules together are called Hydrophobic interactions.
- b. The strength of hydrophobic interactions results from the system's achieving greatest thermodynamic stability by minimizing the number of ordered water molecules required to surround hydrophobic portions of the solute molecules.
- c. Hydrophobic interactions between nonpolar amino acids also stabilize the three-dimensional structures of proteins.
- d. These amino acids orient themselves toward the centre of the polypeptide to avoid the water.

2. Hydrogen bonds:

- a. An electrostatic attraction between the oxygen atom of one water molecule and the hydrogen of another is called a hydrogen bond.
- b. Polar R groups on the amino acids form bonds with other Polar R groups.

3. Ionic interaction:

- a. Ionic interactions arise from electrostatic attraction between two groups of opposite charge.
- b. Ionic interactions are among the forces that stabilizes a protein molecule.
- c. Protein structure is stabilized by multiple weak interactions
- d. Hydrophobic interactions are the major contributors to stabilizing the globular forms of most soluble proteins.
- e. Hydrogen bonds and ionic interactions are optimized in the specific structures that are thermodynamically most stable.

4. Van der Waals interaction:

- a. Van der Waals interaction occurs when the two dipoles weakly attract each other, bringing the two nuclei closer. These weak attractions are called van der Waals interactions.

5. Di-sulphide bonds:

- a. It is a special type of covalent bond that can contribute to tertiary structure of a protein.
- b. Disulphide bonds are the covalent linkages between the sulphur containing side chains of cysteines.
- c. It forms cross-links between different regions of polypeptide chains.

6. Nucleic acids – DNA & RNA

- a. Nucleic acids perform a variety of crucial functions in organisms.
- b. The two classes of nucleic acids are Deoxyribonucleic acid (DNA) and Ribonucleic acid (RNA).
 - i. DNA stores and transfers genetic information; it serves as the template for the synthesis of new DNA and RNAs.
 - ii. RNA carries out protein synthesis.
 - iii. The difference in DNA and RNA at a molecular level is:
 1. The presence of uracil in RNA instead of thymine in DNA

2. DNA is a polymer of deoxyribonucleotides and RNA is polymer of ribonucleotides.
3. DNA is double stranded (except for certain viral DNAs which are single stranded) and RNA is single stranded mainly except when self-complementary sequences are there it forms a double stranded structure (Hair pin structure).

7. Carbohydrates:

- a. Carbohydrates are organic molecules found in nature. They have empirical formula $(CH_2O)_N$ made up of molecules of carbon (C), hydrogen (H) and oxygen (O). Exceptions contain nitrogen, phosphorus or sulphur.
- b. Carbohydrate with an aldehyde group is called an Aldose while carbohydrate with a ketone group is called a ketose. Both can be written as $C_3H_6O_3$ or $(CH_2O)_3$.
- c. Carbohydrates are classified into three subtypes: Monosaccharides, disaccharides, and polysaccharides. The simplest carbohydrates that cannot be hydrolysed into simpler units are monosaccharides.
- d. Simple carbohydrates are small polar molecules, containing several – OH functional groups, which makes them hydrophilic (they dissolve well in water)
- e. Polysaccharides, also called complex carbohydrates, are large non polar molecules, and they are not hydrophilic.
- f. Slight changes in structural arrangements are detectable by living things and influence the biological significance of isomeric compounds. For example, the degree of sweetness of various sugars differs according to the arrangement of the hydroxyl groups (-OH) that compose part of the molecular structure.

Q. How Thermodynamics plays a role in molecular interaction. Comment on the below given terms and their role in interaction studies along with their inter-relationship with each other?

1. Entropy:

- Entropy is a measure of disorder of system.
- At the molecular level, entropy can be described in terms of the possible number of different arrangements of particle position and energies, called microstates. The more microstates the system has, the greater its entropy.
- Formula: $S = k \ln W$ (Where, S is the entropy, k is the Boltzmann constant and W is the no. of microstates).

2. Enthalpy:

- Enthalpy, also called as the total energy of the system is released/absorbed during a reaction because the energy from the original bonds is released as the bonds are broken and then the new bonds absorb some energy.
- Formula: $H_{\text{system}} = U_{\text{system}} + (PV)_{\text{system}}$

3. Gibbs free energy:

- Gibbs free energy is the available energy in a system that is capable of doing work. It indicates the spontaneity of a reaction at certain specified conditions purely based on the parameters of the reaction.
- Formula: $\Delta G_{\text{reaction}} = \Delta H_{\text{reaction}} - T_{\text{reaction}} \Delta S_{\text{reaction}}$
- If this value turns out to be negative, the reaction is spontaneous.

- i. Thermodynamics is mainly concerned with its change in free energy and also with change in entropy of the molecule.
- ii. The folding of a protein proteins and examples of the ΔH and $-T\Delta S$ terms competing with each other to determine the G of the folding process.
- iii. In protein folding if the number of conformations is high, i.e., there is more number of unfolded proteins, the entropy and energy will become high because the protein is not ordered.
- iv. But, as the unfolded protein undergoes conformational adjustments residue interactions takes place, protein become ordered which decreases the entropy. The final folded form of protein thus indicates minimum randomness, i.e., entropy and energy are low.
- v. Entropy decreases from the unfolded state to its native state, i.e., the folded protein.
- vi. The free energy also decreases along with the entropy.
- vii. Also, in addition to entropic effects there are enthalpic contributions to protein folding. These include the hydrogen bonding, ionic salt bridges and Van der Waals forces.
- viii. An input of heat energy is required to disrupt these forces and when these interactions form during protein folding, they release heat, therefore, enthalpy is negative.
- ix. The free energy of protein folding is negative and protein folding is a spontaneous process.
- x. Proteins or the polypeptide chain fold via series conformational adjustments that reduces their free energy and entropy until native state is reached.
- xi. The conformational adjustments of protein take place until it reaches the lowest Gibbs free energy.
- xii. These conformational adjustments of protein are generally coupled with processes that produce free enthalpy such as ATP hydrolysis or increases entropy such as wate exclusion during dimerization.