

Table 7-4 shows thermodynamic changes for the transfer of hydrocarbons from water to nonpolar solvents.

Table 4-1 indicates two scales which attempt to indicate the relative hydrophobicity and hydrophilicity of the a.a..

The hydrophilicity refers to a favorable interaction with water.

The combined behavior of the a.a. toward water is referred to as the hydrophathy.

The more + the number, the more hydrophobic the a.a..

The more - the number, the more hydrophilic the a.a..

These scales were derived by a combination of experimental and empirical observations.

Measurements have been made of the relative tendency of a.a. or their side chain analogues to partition between aqueous and nonaqueous solvents-

Empirical observations have considered where each of the side chains is distributed between inner nonpolar and outer polar regions of water soluble proteins.

Table 1 is an amalgam of these two approaches developed by Kyte and Doolittle.

The relative hydrophathy of the amino acids has been scaled to range from +4.5 for the most hydrophobic amino acid (Ile) to -4.5 for the most hydrophilic amino acid (Arg).

These values are commonly used to predict which portions of a polypeptide chain are inside a protein, not exposed to water, and which portions are outside exposed to the aqueous solvent.

An additional property of a.a. is their ability to reversibly bind metal ions as represented by the following equilibrium-

Metal ions associate with anionic and neutral ligands. Bond formation involves both electrostatic interactions and the donation of nonbonded ligand electron pairs to vacant metal orbitals.

The following basic forms of the ionizable groups of a.a. as well as the sulfur of methionine can bind metal ions:

Metal ions typically found associated with such groups in proteins are Ca^{2+} , Mg^{2+} , Mn^{2+} , $\text{Fe}^{2+,3+}$, Cu^{2+} and Zn^{2+} .

Another property of a.a. is their ability to form salt bonds.

Salt bonds refer to electrostatic interactions between positively and negatively charged groups as shown below for protonated amino and carboxylate groups-

The force of attraction between such groups is given by-

$$F = q_1 * q_2 / Dr^2$$

q is the charge, D the dielectric constant and r the distance between charges.

The dielectric constant is a measure of the ability of a substance to allow electrons to move from one plate to the other with a potential difference between the two plates.

Insulators have low dielectric constants while conductors have high dielectric constants.

The following are dielectric constants for various solvents which indicate how the strength of salt bonds will vary with environment:

The attractive force in an aqueous environment is much smaller than in a nonpolar environment.

As you are aware, salts are generally dissociated in water.

As we will see later however, salt bonds are often important to protein structure where ionic groups have a less polar environment.

Disulfide bond formation is an important property of the a.a. cys.

The side chains of two cys a.a. are often joined in proteins as a result of oxidation to form a disulfide bond-

Consider the stereochemistry of a.a..

All the a.a. except gly have an α - carbon which is chiral and as a result may have two different configurations in space.

The two configurations are referred to as the D and L forms.

The D and L terminology is also based on the D and L forms of glyceraldehyde.

The a.a. found in proteins have an α -carbon configuration corresponding to L glyceraldehyde-

According to the R and S nomenclature, the L configuration of most a.a. corresponds to the S configuration used in organic chemistry.

It should be noted that D-a.a. exist in nature but are not found in proteins.

Lastly consider the UV spectra of aromatic a.a..

Phe, tyr and trp have absorption bands in the UV as shown in Fig 5.6.

Note, as indicated, that the absorbance scale is logarithmic. Trp and tyr absorb much more strongly than phe.

The UV absorption of proteins at 280nm is due to these aromatic a.a. and is occasionally used to estimate the concentration of proteins in a solution.