School of Chemistry

Aims and Objectives: Session 2023-2024, Semester 1

Module CH3716: Quantitative Aspects of Medicinal Chemistry

Course Title: Thermodynamics in Medicinal Chemistry

Duration: 4 hours

Lecturer: Professor P. A. Wright

Aims: The course is intended to build on students' knowledge of thermodynamics and solutions; to introduce some thermodynamic concepts relevant to solutions and to apply these to biochemically important phenomena such as osmosis and non-cooperative and cooperative ligand binding to proteins ligand binding at equivalent binding sites.

Objectives:

1. To understand the importance of Gibbs energy in medicinal chemistry and the concepts of partial molar quantities and chemical potential.

2. To understand osmosis, osmotic pressure and dialysis and their physiological and biochemical importance; to calculate solute molar masses; to recognise and deal with anomalies due to charge and solute molecular size, eg., proteins in solution and to understand the Donnan effect.

3. To understand how thermodynamic parameters reveal information on the physical processes involved in the binding reaction; to be able to use experimental data relating to the binding of ligands and metal ions to macromolecules to extract information on binding sites and dissociation constants.

4. To be familiar with experimental methods of obtaining binding parameters and thermodynamic data.