School of Chemistry

Aims and Objectives: Session 2022-2023

Module CH5616: Molecular Recognition

Duration: 20 hours

Lecturers: Dr E. R. Kay and Professor D. Philp*

(*Module Convenor)

Aims: The principal aim of this course is to introduce the student to the principles and applications of non-covalent interactions of molecules in solution. It will provide a fundamental understanding of intermolecular interactions and introduce the fundamental concepts and processes of molecular recognition in solution. The course will provide the basis for the characterisation, quantification, and analysis of molecular associations and illustrate how this knowledge can be applied to understand small molecule–small molecule associations and to engineer specific molecular recognition interactions.

The course will illustrate and expand on these principles through a series of short case studies from the recent literature.

Objectives:

1. To understand the basic definitions of host–guest chemistry and supramolecular chemistry.
2. To understand the basic principles of molecular interaction thermodynamics in solution, and the fundamental electrostatic interaction: pole–pole, pole–dipole, dipole–dipole, dispersion.
3. To recognise of hydrogen bonds and understand the features determining their strength, directionality and origins.
4. To be able to encode and decode patterns of hydrogen bonds and appreciate the role and importance of secondary interactions.
5. To recognise the strength, directionality and origins of interactions between π-systems and between π-systems and cations.
6. To recognise the strength and origins of the hydrophobic effect.
7. To understand the basic principles involved in thermodynamic description of intermolecular binding phenomena, and an awareness of experimental methods that may be used to measure these experimentally.
8. To appreciate how features including molecularity and cooperativity affect binding phenomena.
9. To appreciate the basic principles required for selective molecular recognition, including complementarity and preorganization.
10. To appreciate the design, binding affinities and binding selectivity of crown ethers and other ion–dipole recognition systems.
11. To appreciate the design, binding affinities and binding selectivity of cyclodextrins.
12. To appreciate the design, binding affinities and binding selectivity of cyclophanes.
13. To appreciate the design, binding affinities and binding selectivity of molecular clefts.
14. To appreciate the application of design principles to create selective molecular recognition systems for neutral molecules using hydrogen bonds.

15. To appreciate the design and function of supramolecular catalysts.
16. To appreciate the role of self-assembly in the construction of large ordered molecular and supramolecular assemblies in the natural and unnatural world.
17. To understand the principles of self-assembly of unnatural systems.
18. To understand the principles of template-assisted synthetic strategies for the construction of macrocyclic and interlocked molecular structures.
19. To appreciate how covalent bond formation under thermodynamic control may be combined with noncovalent interactions to drive selection from dynamic combinatorial libraries and to facilitate the efficient template-assisted construction of complex molecular architectures.
20. To appreciate the use of environmental stimuli to modify host-guest interactions and understand the design and operation of simple molecular switches and molecular machines.
21. To be aware of the experimental methods which are useful in determining the presence and strength of molecular associations, and understand the application of these methods for characterizing supramolecular systems.