



## Chemistry 4/5

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#### MODULE N - BIOPHYSICAL CHEMISTRY

**ORGANISER: DR D. DRYDEN**

[Structures of Biological Macromolecules](#) - Dr. Dryden

[Biophotonics](#) - Dr. Jones

[Macromolecules in Motion](#) - Dr. Egelhaaf

[Macromolecular Structure Determination](#) - Prof. Walkinshaw/Dr. Barran/Dr. Barlow

[Computational Biology and Bioinformatics](#) - Dr. Camp

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#### STRUCTURES OF BIOLOGICAL MACROMOLECULES

**Dr. D.T.F. Dryden**

**10 lectures**

#### AIMS

The aim of this course is to describe the structure and function of biological macromolecules.

#### SYNOPSIS

The structures described will comprise:

1. Proteins.
2. The nucleic acids DNA and RNA.
3. Biological membranes.
4. The genome and the proteome.
5. Large-scale intracellular components: vesicles, the cytoskeleton, the nucleus and chromatin.
6. Extracellular structures such as exoskeletons.

## LEARNING OUTCOMES

The student should be able to describe biological structures from the atomic to the cellular scale.

## READING

1. "Principles of Physical Biochemistry"  
K.E. van Holde, W.C. Johnson and P.S. Ho  
Prentice Hall, 1998.
2. "Biophysical Chemistry", Volumes 1-3  
C.R. Cantor and P.R. Schimmel  
Freeman, 1980.
3. "Biochemistry"  
J.M.Berg, J.L. Tymoczko and L.Stryer  
Freeman, 2002.

or

- "Biochemistry"  
D. Voet and J.G. Voet  
Wiley, 1995.
4. "Physical chemistry: principles and applications in biological sciences"  
I. Tinoco, K. Sauer, J.C. Wang and J.D. Puglisi.  
Prentice Hall, 2002.

## BIOPHOTONICS

**Dr. A. C. Jones**

**5 lectures**

## AIMS

A detailed examination of widely used spectroscopic methods for the study of biomacromolecules, namely, electronic and vibrational spectroscopy.

## SYNOPSIS

1. UV-visible spectroscopy – absorption and chromophores, fluorescence and fluorophores, circular dichroism and fluorescence polarisation.
2. Infra-red and Raman spectroscopy - vibrational spectroscopy in biology.

## LEARNING OUTCOMES

The student should understand the uses of electromagnetic radiation for the analysis of structure, dynamics, interactions and chemical reactions of biological molecules.

### READING

1. "Principles of Physical Biochemistry"  
K.E. van Holde, W.C. Johnson and P.S. Ho  
Prentice Hall, 1998.
2. "Biophysical Chemistry", Volumes 1-3  
C.R. Cantor and P.R. Schimmel  
Freeman, 1980.
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J.M.Berg, J.L. Tymoczko and L.Stryer  
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4. "Physical chemistry: principles and applications in biological sciences"  
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Prentice Hall, 2002.

### MACROMOLECULES IN MOTION

**Dr. S. Egelhaaf**

**5 lectures**

#### AIMS

An introduction to experimental techniques which are frequently used to analyse (and some of them to prepare) solutions of biomacromolecules. These simple methods provide an extraordinary amount of information on biomacromolecules.

#### SYNOPSIS

1. Calorimetric methods, in particular differential scanning calorimetry (DSC) and isothermal titration calorimetry (ITC), are used for the thermodynamic analysis of biomolecules, such as proteins, lipids or biological membranes, as well as interactions between different biomolecules.
2. An introduction to diffusion experiments; sedimentation, electrophoresis and

chromatography. These methods are based on transport processes following the application of external perturbations. These perturbations induce diffusion in a concentration gradient, sedimentation due to external forces (gravitational or centrifugal forces), electrophoretic motion in an electric field, and solvent flux through a medium in the case of chromatography.

## LEARNING OUTCOMES

By the end of the course, the student should be familiar with the different methods, in particular the information which they can provide, but also their limitations.

## READING

1. "Principles of Physical Biochemistry"  
K.E. van Holde, W.C. Johnson and P.S. Ho  
Prentice Hall, 1998.
2. "Biophysical Chemistry", Volumes 1-3  
C.R. Cantor and P.R. Schimmel  
Freeman, 1980.
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I. Tinoco, K. Sauer, J.C. Wang and J.D. Puglisi.  
Prentice Hall, 2002.

## MACROMOLECULAR STRUCTURE DETERMINATION

**Prof. M. Walkinshaw**  
**Dr. P. Barlow**  
**Dr. P. Barran**

**6 lectures**

### AIMS

An introduction to the most complex, but most informative, methods for analysing macromolecules.

### SYNOPSIS

- Protein X-ray Crystallography. How to determine the atomic structure of proteins using X-ray crystallography covering crystallisation, data collection and structure refinement.
- Protein structure and dynamics using nmr spectroscopy. The gross features of a 1-dimensional proton NMR spectrum of a protein and the difficulties of assignment. Preparation of stable and soluble, isotopically enriched, proteins. Structural assignment based on multidimensional triple-resonance NMR

spectra: identification of distance restraints using interproton NOEs, angle restraints based on J-couplings, and other structural restraints based on residual dipolar couplings for the structure calculation. NMR for the analysis of intramolecular motion. Advanced applications of macromolecular NMR: protein-DNA complexes, drug design and membrane proteins.

- Mass Spectrometry for Protein Identification. Recent developments in the use of mass spectrometry coupled with purification techniques to identify proteins and their interactions with other molecules. Peptide mass fingerprinting (PMF) using enzymatic fragmentation of proteins, Matrix assisted Laser desorption Ionisation Time of Flight Mass Spectrometry (MALDI-TOFMS) and electronic databases of protein sequences. Practical examples of the processes will be demonstrated.

## LEARNING OUTCOMES

The student should understand the basic principles of these techniques, the special sample preparation procedures required for their successful application and the importance of these methods in current biological and pharmaceutical science.

## READING

1. "Principles of Physical Biochemistry"  
K.E. van Holde, W.C. Johnson and P.S. Ho  
Prentice Hall, 1998.
2. "Biophysical Chemistry", Volumes 1-3  
C.R. Cantor and P.R. Schimmel  
Freeman, 1980.
3. "Physical chemistry: principles and applications in biological sciences"  
I. Tinoco, K. Sauer, J.C. Wang and J.D. Puglisi.  
Prentice Hall, 2002.

## COMPUTATIONAL BIOLOGY AND BIOINFORMATICS

**Dr. P.J. Camp**

**4 lectures**

### AIMS

The aims of this course are:

1. To describe the computational methods used to analyse the amino-acid and nucleotide sequences of proteins and nucleic acids, respectively.
2. To provide an account of contemporary methods for simulating and predicting

the secondary and tertiary structures of proteins and nucleic acids.

## SYNOPSIS

1. Analysing amino-acid and nucleotide sequences in proteins and nucleic acids
  - a. Analysing individual sequences: the Human Genome Project (1990-2003).
  - b. Comparing pair-wise sequences: dot plots; sequence alignment.
  - c. Multiple sequence alignments.
2. Predicting secondary and tertiary structures of proteins and nucleic acids
  - a. Molecular interactions and force fields.
  - b. Dealing with long-range electrostatic interactions.
  - c. Molecular dynamics and Monte Carlo simulations of biological molecules.
  - d. The IBM Blue Gene project.

## LEARNING OUTCOMES

By the end of the course students should be able to:

1. Describe contemporary techniques for analysing and comparing the sequences of proteins and nucleic acids.
2. Provide a non-technical account of computer 'experiments' on biological systems, as applied to the prediction of secondary and tertiary structures of proteins and nucleic acids.

## READING

1. "Principles of Physical Biochemistry"  
K.E. van Holde, W.C. Johnson and P.S. Ho  
Prentice Hall, 1998.
2. "Introduction to bioinformatics"  
A. M. Lesk  
Oxford University Press, 2002.
3. "Bioinformatics: sequence and genome analysis"  
D. W. Mount  
Cold Spring Harbor Laboratory Press, 2001.
4. "Primer of genome science"  
G. Gibson and S.V. Muse  
Sinauer, 2002.

5. [Bioinformatics Organisation](#) - For links to a huge number of online tutorials, exercises, and demonstrations
6. "Computer simulation of liquids"  
M.P. Allen and D.J. Tildesley,  
Clarendon, 1987.
7. Journals / reviews referred to in lectures.

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