University of Glasgow | School of Chemistry

2022–2023

Module Outlines

MSc Chemistry

MSc Chemistry with Medicinal Chemistry

Please note:

This handbook contains outlines for the modules comprise the lecture courses for all the MSc Chemistry and Chemistry with Medicinal Chemistry courses. The outline is also posted on Moodle for each lecture module. If there are any updates to these published outlines, this will be posted on the Level 4 Moodle, showing the date, to indicate that there has been an update.

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Module Topics for Lecture Courses

The **Course Information Table** below shows, for each of the courses (e.g. Organic, Inorganic, etc), the lecture modules and associated lecturer. Chemistry with Medicinal Chemistry students take modules marked # in place of modules marked ¶.

Organic Chem (o)	Organic Course Modules	Lecturer	Chem	CMC
o1	Pericyclic Reactions	Prof Sutherland	Y	Y
o2	Heterocyclic Systems	Prof Cooke	Y	Y
o3	Advanced Organic Synthesis	Dr Prunet	Y	Y
o4	Polymer Chemistry	Dr Schmidt	Y	Y
o5m	Asymmetric Synthesis	Prof Clark	Y	Y
o6m	Organic Materials	Dr Draper	Y	Y

Inorganic Chem (i)	Inorganic Course Modules	Lecturer	Chem	CMC
i1	Metals in Medicine	Prof Cronin	Y	Y
¶i2	Inorganic Mechanisms	Dr Miras	Y	
¶i3	Industrial Catalysis Chemistry	Prof Jackson	Y	
i4	Applied Coordination Chemistry	Dr Sproules	Y	Y
i5m	Inorganic Materials Design	Prof Gregory	Y	Y
i6m	Chemistry of the f-block	Dr Price	Y	Y

Physical Chem (p)	Physical Course Modules	Lecturer	Chem	CMC
p1	Macromolecules and Colloids	Dr Magennis	Y	Y
¶p2	Surface Chemistry	Prof Lennon	Y	
¶p3	Advanced Chemical Thermodynamics	Dr Hedley	Y	
p4	Modern NMR Spectroscopy	Dr Odedra	Y	Y
p5m	Statistical Mechanics & Reaction Dynamics	Dr Docherty	Y	Y
¶p6m	Theoretical & Computational Chemistry	Dr Senn	Y	

Medicinal Chem (M)	Medicinal Chemistry Course Modules	Lecturer	Chem	CMC
#M1o	Biopolymers Chemistry and Synthesis	Prof Jamieson		Y
#M2cmc	Industrial Medicinal Chemistry	Dr Humphreys GSK + Dr Scott AZ		Y
#M3o	Medicinal Chemistry of Cancer	Dr Watts		Y
#M4o	Chemical Biology	Prof Hartley		Y

Special Topics (S)	Special Topics Course Modules	Lecturer	Chem	CMC
S1o	Organometallics in Synthesis	Dr France	Y	Y
S2o	Organic Supramolecular Chemistry	Prof Adams	Y	Y
S3i	Molecular Magnetism	Prof Murrie	Y	Y
S4i	Electrochemistry for a Sustainable Future	Prof Symes	Y	Y
S5p	Surface Structure & Spectroscopy	Dr Karimullah	Y	Y
S6p	Dynamics of Molecular Clusters and Fluids	Prof Wynne	Y	Y

Code: **o1**

Title: **Pericyclic Reactions**

Lecturer: Prof. Andrew Sutherland

Aims: To develop an understanding of cycloadditions and pericyclic rearrangement reactions, and their importance in organic chemistry, based on frontier orbital interactions and the Woodward-Hoffmann rules.

Module Outline

Topics generally covered in this module include:

1. Description of cycloaddition and rearrangement reactions in terms of frontier orbital interactions.
2. Types of pericyclic reaction; terms such as conrotatory", "suprafacial"; Woodward-Hoffmann Rules.
3. Diels-Alder cycloadditions, including stereospecificity, regioselectivity, and stereoselectivity, in terms of primary and secondary orbital interactions.
4. Other cycloaddition reactions, including 1,3-dipolar and [2+2] cycloadditions, cheletropic reactions, and the ene reaction. Understand, recall and apply the Woodward-Hoffmann Rules to cycloaddition reactions in thermal or photochemical conditions.
5. Chemical outcomes of electrocyclic reactions in terms of orbital interactions and/or the Woodward-Hoffmann Rules.
6. Chemical outcomes of [1,*n*]-, [2,3]- and [3,3]-sigmatropic rearrangements, in terms of primary and secondary orbital interactions and the Woodward-Hoffmann Rules. Rationalise and predict stereoselectivity in [2,3]- and [3,3]-sigmatropic rearrangement reactions in terms of chair-like transition states.
7. Synthetic importance of the above cycloaddition and rearrangement reactions, and give disconnections of target compounds corresponding to these reactions.
8. Apply understanding of the above to examples published in the chemical literature.

Code: **o2**

Title: **Heterocyclic Systems**

Lecturer: Prof. Graeme Cooke

Aims: Heterocycles are crucial components of molecules found across all facets of chemistry. This module aims to provide a rigorous foundation of heterocyclic chemistry. It will cover heterocycle identification and nomenclature, reactivity and synthesis. The module covers all the most commonly encountered heterocycles and will provide the tools for students to design syntheses and predict the properties of any heterocycle.

Module Outline

Topics generally covered in this module include:

1. Various heterocyclic motifs and the names of the most commonly encountered heterocycles.
2. The concept of aromatic bonding for aromatic heterocycles, and the different ways in which a heteroatom can contribute to aromaticity.
3. Electron-rich and electron-poor heterocyclic aromatic systems and their reactivity as electrophiles and nucleophiles.
4. Impact of electronic configuration in the reactivity of heterocycles at the α-positions of the ring.
5. Lithiation and Diels-Alder reactions with heterocyclic systems.
6. The role of ring substituents on the reactivity of heterocycles.
7. The mechanism for the formation of key heterocycles based upon the most commonly encountered syntheses.
8. Synthesis of substituted or complex heterocyclic compounds based upon pattern matching with the syntheses discussed within the course.
9. Importance of heterocyclic units in the function of molecules, and their role in pharmaceutical and materials-chemistry.

Code: **o3**

Title: **Advanced Organic Synthesis**

Lecturer: Dr Joëlle Prunet

Aims: To introduce new methods and extend previously encountered strategies for the preparation of organic molecules with a particular focus on alkenes. To illustrate these methods with syntheses of structurally complex molecules.

Module Outline

Topics generally covered in this module include:

1. Analyse heteroatom containing organic molecules and predict the hybridisation of both carbon and heteroatoms.
2. The effect of hybridisation on reactivity.
3. Reagents employed for the olefination of carbonyl compounds; their mechanisms and application to synthesis.
4. Metathesis and palladium-catalysed reactions in organic synthesis.
5. Olefin geometry, and products from a range of olefination reactions.
6. Mechanisms for the reactions of allylboranes and allylsilanes, apply these reagents to synthesis and explain diastereoselectivity in crotylation reactions.

Code: **o4**

Title: **Polymer Chemistry**

Lecturer: Dr Berhard Schmidt

Aims: Polymers are important materials in everyday life. This module aims for a basic introduction into polymer chemistry. After an introduction into the field, the foundations of polymer synthesis will be discussed based on three basic polymerisation methods (step growth, free radical and anionic). Finally, the basics of the main analytical method for polymers, size exclusion chromatography, will be introduced and polymer properties discussed.

Module Outline

Topics generally covered in this module include:

1. The importance of polymer chemistry in the chemical sciences and nomenclature of the subject.
2. Polymer structure and isomerism discussed with examples.
3. Collection of common polymers.
4. Description of basic polymerisation mechanisms and their differences: Step-growth polymerisation and chain-growth polymerisation.
5. Polymerisation methods (polycondensation, free radical polymerisation, anionic polymerisation) and their effect on molecular mass.
6. Discussion on polymerisation kinetics with respect to the polymerisation method.
7. Explanation of the size-exclusion chromatography method and the underlying separation mechanism.
8. Application of polymers in the real world, i.e. commodity polymers, technical polymers and functional polymers.

Code: **o5m**

Title: **Asymmetric Synthesis**

Lecturer: Prof. Stephen Clark

Aims: To introduce some of the most important asymmetric reactions available to the organic chemist. To discuss in detail asymmetric oxidation reactions (epoxidation, dihydroxylation and aminohydroxylation of alkenes), reduction reactions (hydrogenation of C=C and C=O bond, transfer hydrogenation and hydroboration), and asymmetric C–C bond forming reactions using chiral auxiliaries, chiral Lewis acids and organocatalysts.

Module Outline

Topics generally covered in this module include:

1. The importance of asymmetric reactions in organic synthesis and the fundamental concepts and nomenclature.
2. Sharpless asymmetric epoxidation of allylic alcohols including kinetic resolution of secondary allylic alcohols.
3. Jacobsen-Katsuki asymmetric epoxidation of simple unfunctionalised alkenes.
4. Asymmetric hydrogenation and transfer hydrogenation catalysed by Ru and Rh complexes and recall Corey's oxazaborolidine reduction of carbonyl compounds.
5. Sharpless asymmetric dihydroxylation and aminohydroxylation reactions and their use in synthesis, and use the mneumonic to predict the stereoselectivity of these reactions.
6. Organocatalysis as an alternative to metal-based methods, and application in asymmetric Diels-Alder reactions and Friedel-Crafts alkylations.
7. Asymmetric aldol reactions and factors that can be used to control enolate geometry and stereochemical outcome of the reactions with reference to Zimmerman-Traxler transition states and chiral Lewis Base catalysis.

Code: **o6m**

Title: **Organic Materials**

Lecturer: Dr Emily Draper

Aims: An introduction into the chemistry behind the design, synthesis and processing of organic based materials. Understanding how the state-of-the-art organic materials work and how to design materials for our future.

Module Outline

Topics generally covered in this module include:

1. Structural and performance characterisation techniques for organic materials.
2. General processing techniques.
3. Design principles and considerations when designing new materials.
4. State-of-the-art organic materials.

Code: **i1**

Title: **Metals in Medicine**

Lecturer: Prof. Lee Cronin

Aims: To discuss the increasingly important role played by metallo-organic compounds, in particular those of certain transition metals, in both diagnostic and therapeutic medicine. To introduce some of the more important medical applications of transition metals, and to explore the underlying chemistry that makes a particular element useful in a particular application.

Module Outline

Topics generally covered in this module include:

1. The roles of the metallic elements in biology are briefly considered to provide a context for, and contrast to, the uses of transition metal compounds in medicine.
2. The concentration of ions, and establishing gradients in ion concentration are crucial for cell function. This section describes the basic processes and explains the concept of membrane potential.
3. The nuclear properties of radioisotopes used in medical applications are reviewed and the applications for which they are suited are considered. The use of non-radioactive paramagnetic metal ions as contrast agents in Magnetic Resonance Imaging (MRI) will be included.
4. The treatment of two contrasting ailments; human deficiencies of certain metals and the use of sequestering agents to remove excess or unwanted metals from patients.
5. The use of platinum complexes in the treatment of certain cancers is well establish and models for the mechanism of active are well developed. A variety of other metallo-organic systems also show anti-tumour activity and are finding their way to clinical trials.

Code: **i2**

Title: **Inorganic Mechanisms**

Lecturer: Dr Harry Miras

Aims: To describe and place in context, the factors that are important in determining reaction pathways and mechanisms of metal-centred coordination compounds in solution. To demonstrate how kinetic and non-kinetic evidence can be used to derive or to substantiate a reaction mechanism. To give examples taken from both main group and transition element chemistry. To make use of ideas and concepts presented in previous years, particularly in the areas of kinetics, ligand field theory and acid/base relationships.

Module Outline

Topics generally covered in this module include:

1. Revision of some fundamentals including, dissolution of salts, metal ions in solution, solvation, solvation numbers and their determination, thermochemistry.
2. Kinetics *vs.* thermodynamics; solvent exchange.
3. Complex formation, the Eigen-Wilkins mechanism.
4. Substitution reactions at complex ions, and non-metal centres.
5. Outer sphere and inner sphere electron transfer reactions; Marcus-Hush theory.

Code: **i3**

Title: **Industrial Catalytic Chemistry**

Lecturer: Prof. David Jackson

Aims: To provide an introduction to large scale industrial processes and the links between them.

Module Outline

Topics generally covered in this module include:

1. The interlinks between a number of large scale industrial processes.

2. Definition of the difference in process requirements of endothermic and exothermic equilibrium limited reactions.

3. Different catalytic processes and be able to compare and contrast the catalysts and methodologies used in these processes.

4. Catalytic cycles, including the rate determining steps and specific promotors, used in different processes.

5. An explanation of the roles of catalysts in multi-step processes and how they link to generate the overall process.

Code: **i4**

Title: **Applied Coordination Chemistry**

Lecturer: Dr Stephen Sproules

Aims: To elucidate the electronic structure of coordination complexes of d-block elements using ligand field and MO theory, and advanced experimental techniques; to understand the importance of ligand design in small molecule activation and reactivity.

Module Outline

Topics generally covered in this module include:

1. The concepts of ligand field theory, coordination geometry, formal and physical oxidation states, spin ground state, electronic structure, ligand type and strength.

2. Application of group theory to the construction of molecular orbital diagrams for six-coordinate complexes possessing octahedral, tetragonal and trigonal symmetry.

3. Illustration of the molecular orbitals involved in metal-ligand multiple bonds and summarisation of the “oxo wall”.

4. The role of ligand design and the desired electronic structure for complexes that activate small molecules such as O_2, N_2, and H_2.

5. Description of the basic principles of electrochemistry, magnetometry, electron paramagnetic resonance and Mössbauer spectroscopy, and their application to determining the electronic structure of coordination complexes.

6. The concept of radical ligands, and the use of experimental data to diagnose electronic structure of complexes with redox-active ligands.

7. The properties of transition metal dithiolene complexes and their applications.

Code: **i5m**

Title: **Inorganic Materials Design**

Lecturer: Prof. Duncan Gregory

Aims: To provide an introduction and insight into some of the topics at the forefront of contemporary inorganic solid state and materials chemistry research. The focus of the course is on the link between synthesis, structure and properties and the underpinning concept of materials design. Examples from various areas will illustrate how the concept can lead to both new and improved materials from all parts of the periodic table.

Module Outline

Topics generally covered in this module include:

1. Descriptions of the structures of important binary and ternary oxides and non-oxides.

2. Explanation of the principles of synthesis in the solid state and evaluations of the applicability of various synthesis routes to inorganic solids.

3. Some of the important physical properties in solid state materials and how these properties are interconnected with structure and bonding.

4. How the structure within key materials families, such as Perovskites, relate to properties such as ferroelectricity and colossal magnetoresistance.

5. Explanation of the basic functionality of fast ionic conducting materials and their application as electrodes in rechargeable batteries.

6. Description of the effects of size and morphology on materials functionality and assessment of how these effects impact on the structures and properties of inorganic nanomaterials.

Code: **i6m**

Title: **Chemistry of the f-block**

Lecturer: Dr Daniel Price

Aims: The chemistry of the f-block elements is introduced. The course will examine both chemical and physical properties of these elements and their compounds, with an emphasis on the relationship between properties and underlying electronic structure.

Module Outline

Topics generally covered in this module include:

1. The name, symbol and position in the periodic table of f-block elements
2. Description of the shape and extent of 4f and 5f orbitals
3. Explanation of the origin of the lanthanide contraction.
4. Description of the coordination geometries of lanthanide and actinide ions.
5. Description of the trends in redox chemistry of the f-block elements
6. Explanation of the differences and similarities between the chemistry of the lanthanides, the actinides and the d-block transition metal elements.
7. Discussion of the limitations of coupling schemes and the influence of relativistic effects in describing the electronic structures of these elements.
8. Correlation of electronic, magnetic and optical properties with the electronic structures of the 4f elements.
9. Description of the uses of lanthanides and actinides in the nuclear industry.
10. Assessment of the likely decay mechanisms for given actinide isotopes.
11. Description of the basic chemistry of more stable actinides, thorium to americium.

Code: **p1**

Title: **Macromolecules and Colloids**

Lecturer: Dr Steven Magennis

Aims: To provide an overview of the structure and properties of macromolecules (with a focus on biomacromolecules) and self-assembled aggregates (colloids, micelles and vesicles), and to examine common methods used to study them.

Module Outline

Topics generally covered in this module include:

1. Explanation of the different levels of macromolecular structure.

2. Calculation of the length of a random coil structure from radius of gyration measurements.

3. Explanation of the solution properties of colloids, particularly related to their attraction/repulsion, and the difference between colloids, micelles and vesicles.

4. Evaluation of the difference between number average and weight average calculations that are used to obtain mean molar masses for mono- and poly-dispersed molecules.

5. The use of mass spectrometry to determine the mass of a macromolecule.

6. Application of the principles of static light scattering to determine the radius of gyration of a macromolecule.

7. Explanation of how and why the polarization properties of fluorescence light are measured.

8. Description of the FRET process and how it is used it to measure nanoscale distances.

9. Description of the differences between ensemble and single-molecule methods and explain how the techniques of confocal and TIRF microscopy allow detection of single molecules and particles.

Code: **p2**

Title: **Surface Chemistry**

Lecturer: Prof. David Lennon

Aims: To recognise fundamental concepts of heterogeneous catalysis through the study of the chemistry and kinetics of reactions occurring at the catalyst surface. Particular emphasis will be given to the importance of mechanism and the identification of the adsorption complexes active in the catalytic sequence.

Module Outline

Topics generally covered in this module include:

1. The significance of economic and industrial factors in modern heterogeneous catalysis.

2. Connections and constraints on chemisorption and catalysis by metals.

3. Langmuir-Hinshelwood kinetic expressions for simple hydrogenation reactions.

4. The Horiuti-Polanyi mechanism for the gas phase hydrogenation of alkenes and the link between reaction kinetics and reaction mechanism.

5. A multi-technique approach for the elucidation of reaction mechanism; the kinetic isotope effect for mechanistic insight for heterogeneously catalysed reaction systems.

6. Structure/activity relationships in heterogeneous catalysis.

7. Langmuir adsorption isotherm for competitive adsorption to understand the concept of catalyst poisoning.

Code: **p3**

Title: **Advanced Chemical Thermodynamics**

Lecturer: Dr Gordon Hedley

Aims: To explore advanced thermodynamic theories, including how thermodynamic laws govern ideal energy cycles, the breakdown of ideally, and how advanced thermodynamic concepts control atomic and molecular diffusion. Special emphasis will be given to the applications of each area examined: how does advanced chemical thermodynamics impact upon problems and processes in the world around us, scientific research and societal problems.

Module Outline

Topics generally covered in this module include:

1. Chemical potentials. We will look at what they are, how we define and derive them, and what they are useful for.

2. The Debye–Huckel law. Beginning our examination of ideality, we will look at what happens in dilute solutions, where deviation from expected behaviour occurs, including usage of the Debye–Huckel equation in applied systems.

3. (A)diabatic processes. Continuing investigations of ideality, we will study what happens in systems where it only does work, without transferring heat or mass, and how this compares with systems that do.

4. Carnot & Stirling Cycles. We will build ideal and realistic cycles that do work, examining how they operate, why true ideallity can never be reached, and what real-world applications these can be used for.

5. Maxwell-Boltzmann Distributions. We will examine and understand the statistical laws that underpin how elements are organised according to statistical distribution, and how this can be used in applied contexts.

6. Fickian Diffusion. Finally, we will examine the laws that govern and the processes that result from statistical redistribution. We will explore practical examples of where these laws play an important role.

Code: **p4**

Title: **Modern NMR Spectroscopy**

Lecturer: Dr Smita Odedra

Aims: To review the physical basis of NMR spectroscopy and the interactions that determine the appearance of NMR spectra of both liquids and solids. To introduce the vector model of NMR and use it to describe experiments to measure longitudinal and transverse relaxation. To introduce methods for enhancing the sensitivity and resolution of NMR spectra of solids. To introduce the concept of coherence selection and define the rules of phase cycling.

Module Outline

Topics generally covered in this module include:

1. Review the physical basis of NMR spectroscopy and related techniques such as MRI.

2. Explain key points relating to instrumentation, signal acquisition and signal processing.

3. Describe the origin and influence of the major interactions that determine the appearance of NMR spectra, such as the chemical shift, J-couplings, the dipolar interaction and quadrupolar couplings. Distinguish between the effects of these in solution-state and solid-state NMR.

4. Describe the vector model of NMR and use it to explain experiments including those used to measure transverse and longitudinal relaxation; manipulate experimental data to calculate relaxation rate constants.

5. Describe methods of obtaining high-resolution NMR spectra of solids with high sensitivity and resolution.

6. Recognise the importance of coherence selection and apply the rules of phase cycling to select particular changes in coherence order within a pulse sequence.

7. Apply the theory and techniques introduced during this course to related exercises.

Code: **p5m**

Title: **Statistical Mechanics & Reaction Dynamics**

Lecturer: Dr Frances Docherty

Aims: To build upon existing knowledge of classical thermodynamics, spectroscopy and quantum mechanics such that an understanding of the statistical behaviour of bulk samples is developed. Quantitative methods for describing reaction dynamics and how this relates to kinetics and transition states will also be described.

Module Outline

Topics generally covered in this module include:

1. Define the Boltzmann distribution through concepts such as instantaneous configurations and employ the Boltzmann law for a system of particles.

2. Be able to derive, recall and apply the equations that define the molecular partition function with respect to populations and internal energy.

3. Differentiate between the molecular and canonical partition functions and use them in obtaining thermodynamic information (including some derivations).

4. Demonstrate how statistical thermodynamics can be applied to gain insight into a number of physical, chemical, and biological processes.

5. Express, derive and apply quantitative theories for the dynamics of a reaction, including collision theory, transition state theory, and potential energy surfaces.

Code: **p6m**

Title: **Theoretical & Computational Chemistry**

Lecturer: Dr Hans Senn

Aims: To introduce basic elements of quantum chemistry and molecular electronic structure theory, including computational aspects.

Module Outline

Topics generally covered in this module include:

1. Formulate the connection between classical and quantum mechanics using the correspondence principle.
2. Recall and apply the postulates of quantum mechanics.
3. Explain the properties of (electronic) wavefunctions. Describe the construction of Slater determinants.
4. Recall and describe the molecular Schrödinger equation.
5. Describe and apply the variation principle for the ground state.
6. Describe the Born–Oppenheimer approximation and the concept of potential-energy surfaces.
7. Describe the principles of the self-consistent field (SCF) method and Hartree–Fock theory.
8. Explain the phenomenon of electron correlation and its consequences on solving the Schrödinger equation.
9. Summarize the principles of approximate methods to recover the correlation energy.
10. Summarize the principles and features of density functional theory.

Code: **M1o**

Title: **Biopolymer Chemistry and Synthesis**

Lecturer: Prof. Andrew Jamieson

Aims: To introduce two classes of biopolymers namely nucleic acids and peptides/proteins. Their properties, chemistry and approaches for synthesis will be discussed.

Module Outline

Topics generally covered in this module include:

1. Recall, summarise and explain the structure of nucleic acids and peptide/proteins.

2. Derive, explain and predict the physical and chemical properties of these biopolymers from the presence of their characteristic functional groups.

3. Recall the structures, names and abbreviated names of amino acids and explain their properties.

4. Recall and explain the structure, properties, introduction and cleavage of the protection groups commonly used in peptide synthesis and in nucleic acid synthesis

5. Recognise, recall and explain the structure of coupling reagents and conditions commonly used in peptide synthesis and nucleic acid synthesis.

6. Recall, summarise, explain and classify the different methods for peptide synthesis (solution, solid-phase, enzymatic).

7. Devise the step-wise synthesis of a peptide, or nucleic acid in solution and on the solid-phase.

8. Devise the convergent synthesis of a peptide by coupling of fragments, for example using native chemical ligation.

9. Recall, identify and explain the presence of amino acid sequences, which can be problematic in physical/chemical behaviour of peptides and/or peptide synthesis.

10. Recall, explain and summarise the properties and introduction of the most important post-translational modifications including the selective formation of disulfide bridges.

Code: **M2o**

Title: **Industrial Medicinal Chemistry**

Lecturers: Dr Jamie Scott (AstraZeneca), Dr Phil Humphreys (GlaxoSmithKline)

Aims: To establish an appreciation of modern drug identification approaches and the multiparameter nature of optimisation in modern drug discovery research. In particular, the central importance of control of lipophilicity in generating high quality candidates. This will be illustrated by recent examples of pharmaceutical research programs.

Module Outline

Topics generally covered in this module include:

1. Define lipophilicity and how it is measured, differentiate between logP and logD and suggest changes to a structure that will modulate its lipophilicity.

2. Describe some of the factors that need to be optimised in drug discovery (e.g. potency/solubility/metabolism/plasma-protein-binding/toxicity) and how they are correlated with lipophilicity.

3. Define terms such as Ligand Efficiency (LE), Ligand Lipophilicity Efficiency (LLE) and calculate these when provided with the appropriate data.

4. Explain basic pharmacokinetic principles (ADME), describe metabolic processes and suggest changes to a structure that will modulate its metabolism.

5. Discuss the importance of hERG as an anti-target and suggest changes to a structure that will modulate its hERG liabilities.

6. Describe the factors important in designing drugs for use in the central nervous system.

7. Describe how to use fragment-based drug design strategies to identify and optimize potential drug molecules.

8. Be familiar with the molecular interactions drugs typically make with their protein targets and be able to describe strategies for optimizing these interactions.

9. Describe the factors important in designing and synthesising drugs with the lowest odds of toxicity and promiscuity.

Code: **M3o**

Title: **Medicinal Chemistry of Cancer**

Lecturer: Dr Ciorsdaidh Watts

Aims: To introduce the different types of anticancer drugs, their design, synthesis and mode of action, together with new ways of discovering and optimising drug candidates.

Module Outline

Topics generally covered in this module include:

1. Recall, summarise and explain abnormal cell growth, its causes and possible treatments.

2. Recognise, recall, and classify different types of targets and potential targets for anticancer therapies, and different types of anticancer drugs and potential anticancer drugs.

3. Recall, summarise and explain the synthesis (or partial synthesis) of different types of anticancer drugs and potential anticancer drugs, and their mechanisms of action and pharmacology.

4. Design syntheses of novel compounds structurally related to known anticancer compounds.

5. Evaluate chemical structures for their potential as anticancer agents.

6. Summarise and explain chemical genetics, the design of libraries for screening and the role of chemical biology in drug discovery.

7. Recall the purpose and use of fragment-based design in drug discovery.

8. Define terms including *ligand efficiency* and PIC_{50} and be able to use the associated equations to calculate these.

Code: **M4o**

Title: **Chemical Biology**

Lecturers: Prof. Richard Hartley

Aims: To introduce the main concepts of chemical biology and the tools for elucidating biological processes through synthetic chemistry.

Module Outline

Topics generally covered in this module include:

1. Structure of cells and the processes within them.

2. The structures, names and abbreviated names of amino acids and recall and explain their roles in proteins including mechanisms for reactions involving them.

3. Mechanisms involved in the synthesis of peptides.

4. Molecular biological tools for incorporating labels, tags and sensors, and manipulating biological processes (e.g. unnatural amino acids, SNAP-tag).

5. Classification of the different ways of identifying, sensing, reporting, quantifying, locating, and determining the temporal control of biological molecules and processes.

6. Structures of, syntheses of and mechanisms of sensors, in particular ROS and calcium sensors.

7. Structures, syntheses and mechanisms involved in bio-orthogonal reactions, tagging, labelling and pull down technologies.

8. Structures, syntheses and mechanisms involved in photoactivation (e.g. in photoaffinity labelling, uncaging, and photoswitching) and how it is used to understand biological processes and identify biomolecules.

9. Chemical species with application as tags, labels, molecular probes, sensors or functional molecules.

10. Novel compounds structurally related to known labels, molecular probes, sensors or functional molecules to behave in similar ways.

11. Chemical genetics and competing techniques

Code: **S1o**

Title: **Organometallics in Synthesis**

Lecturer: Dr David France

Aims: To develop a mechanistic understanding of reactions of organic molecules with transition metal complexes, and a working knowledge of transition metal-mediated methods that are of particular importance to organic synthesis.

Module Outline

Topics generally covered in this module include:

1. The recognition and description of fundamental organometallic processes (*e.g.* coordination/dissociation, oxidative addition/reductive elimination, insertion).

2. How to predict the product oforganometallic reactions based on fundamental principles.

3. The mechanisms of transition metal-mediated reactions in organic chemistry.

4. Description of the specific reaction conditions required for catalytic cycles to be efficient.

5. Design syntheses of target organic molecules that make use of transition metals.

Code: **S2o**

Title: **Organic Supramolecular Chemistry**

Lecturer: Prof. Dave Adams

Aims: To describe, illustrate and use the basic principles of supramolecular chemistry.

Module Outline

Topics generally covered in this module include:

1. Discussion and use of the fundamental principles of non-covalent interactions.
2. Illustration on how to use the principles of molecular recognition and self-assembly.
3. Illustration of how the principles of supramolecular chemistry can be used in the development of enzyme models and mimics.
4. Illustration of how the principles of supramolecular chemistry can be used to develop self-replicating systems, in the construction of molecular machines and devices.

Code: **S3i**

Title: **Molecular Magnetism**

Lecturer: Prof. Mark Murrie

Aims: To provide an overview of molecular magnetism, from the magnetic properties of transition metal ions to those of transition metal complexes, and more complex molecular systems such as single-molecule magnets.

Module Outline

Topics generally covered in this module include:

1. Summarise the magnetic properties of the first row transition metal single-ions and contrast with those of simple transition metal complexes.

2. Explain magnetic properties based upon molecular structure.

3. Predict the magnetic properties of large molecular systems.

4. Explain the origins of magnetic anisotropy and recall the properties of single-molecule magnets.

Code: **S4i**

Title: **Electrochemistry for a Sustainable Future**

Lecturer: Prof. Mark Symes

Aims: This module will examine the applications of electrochemistry in a variety of contexts of relevance to sustainable chemical processes. We shall investigate electrochemical methods for water purification, metal extraction and energy (harvesting, storage and conversion). Many of the examples shown are at the cutting edge of scientific and technological research. The emphasis throughout the course will be on the interplay between fundamental concepts and the materials required to perform the tasks of interest.
No previous knowledge of electrochemistry is assumed: all the concepts we will require to describe the relevant systems will be explained.

Module Outline

Topics generally covered in this module include:

Lecture 1: *Introduction to Electrochemistry.* After this lecture you should be familiar with the concepts of electrochemical potential and basic electrochemical processes such as bulk electrolysis and cyclic voltammetry.

Lecture 2: *Fuel Cells.* After this lecture you should be familiar with the concepts of the fuel cell and be able to explain how fuel cells work and which material properties are desirable when designing such devices.

Lecture 3: *Electrolysis of Water.* After this lecture you should understand why electrolytic production of hydrogen from water is important and be able to compare different methods of electrolysis and different materials for this purpose.

Lecture 4: *Batteries.* After this lecture you should be able to describe, explain and evaluate the concepts behind and performance of a selection of battery technologies, including lead-acid batteries, Li-ion batteries and redox flow batteries.

Lecture 5: *Photo-electrochemistry.* After this lecture you should understand what a photo-electrochemical cell is and how it works in terms of its materials of construction, and be able to assess the relative performance of different cells.

Lecture 6: *Water Purification.* After this lecture you should be able to explain the various electrochemical methods of water purification and be able to give a reasoned account of their various merits and demerits.

Lecture 7: *Metal Extraction.* By the end of this lecture you should be able to explain the different electrochemical strategies used to obtain metals from their ores and be able to assess these in terms of their relative efficiency and environmental impact.

Lecture 8: *Electrochemical Fuel Production.* In this final lecture we will examine current research in the direct synthesis of fuels using electrochemistry, looking in particular at the electrochemical reduction of CO_2. We will use the skills and knowledge acquired during the previous seven lectures to assess the prospects for this avenue of research.

Code: **S5p**

Title: **Surface Structure & Spectroscopy**

Lecturer: Dr Affar Karimullah

Aims: To serve as an introduction into surface science, to describe modern spectroscopic techniques of surface analysis and how they can be applied to model systems.

Module Outline

Topics generally covered in this module include:

1. The discussion of why UHV techniques are necessary to study model systems.

2. The nomenclature of surface structure and its use to explain concepts such as surface relaxation and reconstruction.

3. The discussion of low energy electron diffraction and how it can be applied in the determination of surface structure.

4. The description of adsorption at surfaces, and the importance of physisorption and chemisorption.

5. The reasons for the employment of electron based spectroscopic techniques in surface science, highlighting the most commonly used techniques.

6. The explanation of the technique of temperature programmed desorption and its kinetics.

7. The description of vibrational spectroscopy at surfaces and the associated selection rules.

Code: **S6p**

Title: **Dynamics of Molecular Clusters and Fluids**

Lecturer: Prof. Klaas Wynne

Aims: To introduce a time-resolved picture of spectroscopy and the molecular world. Various kinds of common spectroscopy will be described in terms of correlations in time, while not so common time-resolved spectroscopies will be introduced. The motions of molecules – vibrations, tumbling, diffusion, and flowing of liquids – will be described as well as ideas related to crystallisation, jamming, supercooling, clustering, supersaturation, *etc*. Finally, it should become clear that the dynamics of molecules is intimately related to those of sand, paint, and car jams on the motorway.

Module Outline

Topics generally covered in this module include:

1. A formal description of time resolved dynamics and time-resolved spectroscopy
2. Description of the dynamics in liquids: the types of motions, characteristic timescales, viscosity, and diffusion
3. Description of jamming and glass formation: cooperativity, critical behaviour, jamming, and relaxation.
4. Solutions: the effect of solute molecules (including proteins) on the surrounding medium
5. Introduction to “weird” liquids: room temperature ionic liquids, liquids crystals, liquid proteins, etc.
6. Description of crystal nucleation: supersaturation, etc.