School of Chemistry

OÉ Gaillimh
NUI Galway

Scoil na Ceimice

School of Chemistry

Medicinal Chemistry Pathway - 3rd Year

Information Booklet

Academic Year 2019 – 2020

Compiled by Dr. Luca Ronconi
Revised: August 2019

Contents

Summary of Course Structure and Schedule

	Module (ECTS Credits)	Examination/Assessment	
		Two-Hour Exam Paper	Continuous Assessment
Semester I	CH311 - Organic Chemistry (5)	90%	10%
	CH326 - Analytical Chemistry & Molecular Structure (5)	90%	10%
	CH332 - Drug Design & Drug Discovery (10)	50%	50%
	CH333 - Experimental Chemistry I (5)	-	100%
	Core Module outside the School of Chemistry PM311 - Introduction to Toxicology (5; further details at www.nuigalway.ie/course-information/module/PM311)		
Semester II	CH307 - Inorganic Chemistry (5)	90%	10%
	CH313 - Physical Chemistry (5)	90%	10%
	CH334 - Experimental Chemistry II (5)	-	100%
	CH3101 - Computers in Chemical Research (10)	-	100%
	CH3103 - Validation in the Pharmaceutical and Medical Devices Industry (5, elective)	65%	35%

Semester I Schedule

CH311 First lecture in Dillon Theater on Monday, September 9th 2019 at 9am

CH326 First lecture in Dillon Theater on Tuesday, September 10th 2019 at 10am

CH332 First lecture in Dillon Theater on Tuesday, September 10th 2019 at 9am
First practical class in Software Engineering Suite on Monday, September 16th 2019 at 2pm

CH333 First practical class in Organic Chemistry Teaching Laboratory on Tuesday, September 17th 2019 at 2pm (registration during the first CH311 lecture, final timetable to be provided in due course)

Semester II Schedule

CH307 First lecture in Dillon Theater on Tuesday, January 14th 2020 at 10am

CH313 First lecture in Dillon Theater on Monday, January 13th 2020 at 9am

CH334 First practical class in Inorganic Chemistry Teaching Laboratory on Tuesday, January 14th 2020 at 2pm (details on registration and final timetable to be provided in due course)

CH3101 First practical class in Finnegan PC Suite on Friday, January 17th 2020 at 2pm

CH3103 First lecture in Dillon Theater on Wednesday, January 15th 2020 at 9am

While every effort has been made to ensure that this booklet is accurate, students should contact Module Coordinator(s) with queries.

CH311 - Organic Chemistry

Instructors: Prof. Peter Crowley, Prof. Paul Murphy (Coordinator), Dr. Eddie Myers, Dr. Miriam O'Duill

MODULE DELIVERY

1. Heterocyclic Chemistry (9 h MOD)

Aliphatic heterocycles
- The reactivity difference between cyclic and acyclic molecules (nucleophilicity and basicity).
- Stereoelectronic effects on conformation and reactivity in heterocycles, *e.g.* the anomeric effect.
- Kinetics and thermodynamics of ring-closing reactions (ring strain, Thorpe-Ingold effect, Baldwin's rules).

Aromatic heterocycles
- An understanding of what makes a molecule aromatic.
- An understanding of the effect of the N atom in pyridine and pyrrole on reactivity in comparison to benzene.
- Reactivity differences and mechanisms of nucleophilic and electrophilic aromatic substitution onto pyridine and pyrrole; Vilsmeier and Mannich reactions.
- Pyridine and DMAP as nucleophilic catalysts.
- Compare and contrast electronic structure, aromaticity and reactivity of pyrrole, furan and thiophene.
- Diels-Alder reaction: orbital theory, mechanism, kinetic and thermodynamic control.
- An understanding of the effect of the N atom of diazoles, triazoles and tetrazoles on electronic structure (aromaticity), basicity (acidity) and reactivity towards electrophiles.
- Biological significance of imidazole (enzymes), nitroimidazoles (antibiotics) and tetrazoles (isosteres of carboxylic acids).
- Synthesis of aromatic heterocycles.

2. Physical Organic Chemistry (8 h, PM)

At the end of this lecture series students should be able to:
- Write expressions for K_a and pK_a.
- Use K_a and pK_a to draw conclusions about acid and base strength.
- To know or predict a molecule or functional groups protonation state at a defined pH.
- To understand and explain chemical factors that have an effect on acidity and basicity.
- To be able to relate pK_a to other properties (*e.g.* leaving group ability, nucleophilicity).
- To understand how various types of experiments are used to study reaction mechanism, including kinetics, kinetic isotope effects, substituent effects (Hammett plots & LFERs), product identification, trapping & competition experiments, cross-over experiments, isotope scrambling & labelling, stereochemical analysis.
- To be able to write reasonable mechanistic proposals for well-known reactions such as acid- and base-promoted hydrolysis of esters; acid-catalyzed formation/hydrolysis of acetals/ketals.

3. Biomolecular Chemistry (9 h, PC)

This aspect of the course focuses on biological molecules in particular, proteins. "*Foundations of Chemical Biology*" (Oxford Primer) is an excellent textbook that will also be useful for fourth year.

Amino acids, peptides and proteins
- Structures and properties of the amino acids.
- Primary, secondary, tertiary and quaternary structures of proteins.
- Isoelectric point.
- The hydrophobic effect.
- Interactions between proteins and small molecules (*e.g.* carbohydrates, lipids).

Carbohydrates
- Monosaccharides: classification and configuration.
- Reactions at the anomeric center.

Lipids
- Biological lipids, bilayers and membranes.
- Chemical structures of terpenes and steroids.

4. Synthesis and Stereochemistry (9 h, EM)

Synthesis
- A general understanding of what organic synthesis involves, and of the difficulties associated with the synthesis of a polyfunctional molecule which can exist in different stereoisomeric forms.
- An understanding of the reason why the synthesis of a complex organic molecule is undertaken.
- A recognition of the different classes into which syntheses can be divided.

- The ability to calculate the yield of a multistep synthesis.
- The ability to distinguish between linear and convergent syntheses, and an appreciation of the advantages of the former.
- An understanding of the basic concept underpinning retrosynthetic analysis.
- The ability to describe what the following terms involve and to provide simple examples of each one: disconnection, functional group interconversion, synthon, synthetic equivalents.
- The ability to carry out multistep retrosynthetic analyses based on the use of Grignard reactions, redox reactions involving carbonyl groups, catalytic hydrogenation, alkyl halide/alcohol interconversions, Friedel-Craft reactions, aldol reactions and Michael reactions.
- The ability to carry out the retrosynthetic analyses of six-membered carbocylic rings based on Diels-Alder reactions and Robinson annulations.
- A general understanding of the protecting group approach, of why it may be necessary, of what is involved, and of the disadvantages associated with it.
- An understanding of the circumstances under which the carbonyl groups in ketones and aldehydes need to be protected, and of how this is done.
- An understanding of the circumstances under which alcohol groups need to be protected, and of how this is done.

Stereochemistry

- The ability to distinguish between constitutional isomers and stereoisomers.
- An understanding of the difference between conformational and configurational stereoisomers.
- An understanding of the stereochemical possibilities, chirality/enantiomerism, in systems containing one asymmetric carbon.
- An appreciation of the concepts of absolute configuration, specific rotation and enantiomeric excess.
- The ability to interpret the significance of the stereochemical descriptors, (+), (-), R and S, both on their own and in combination.
- An understanding of the structural possibilities in systems containing more than one asymmetric carbon: identical, enantiomers and diastereomers.
- A recognition of the importance of a plane of symmetry in a molecule: meso stereoisomers.
- The ability to define and recognize racemization, epimers, epimerization and anomers.
- The recognition that chirality can arise in molecules containing tetrahedral atoms other than carbon: sulfoxides, etc.
- The recognition that chirality can arise in non-tetrahedral systems: allenes, atropisomers (biphenyls), helicenes.
- An understanding of the concept of resolution, the separation of enantiomers.
- The ability to describe, and to discuss the advantages and disadvantages of the three methods by which resolution can be achieved: mechanical separation, decomposition and the use of a resolving agent.
- The ability to recognize and distinguish between enantioselective and diastereoselective reactions.
- The ability to describe a number of diastereoselective reactions and to explain why they are stereoselective.
- An appreciation of why the synthesis of chiral molecules (asymmetric synthesis) is important.
- An understanding of the difficulties involved in carrying out reactions with chiral molecules in terms of retaining chirality.
- An appreciation that there are three different methods of making a chiral molecule: starting with a chiral pool molecule, carrying out a resolution, or using an enantioselective reaction.
- The ability to describe, and to discuss the advantages and disadvantages of, asymmetric synthesis involving chiral pool molecules.
- The ability to describe, and to discuss the advantages and disadvantages of, asymmetric synthesis involving resolution.
- The recognition that enantioselective reactions occur under the influence of a chiral group (chiral auxillary) which can be in the reagent, the substrate or the catalyst.
- The ability to provide examples of all the above methods of carrying out asymmetric synthesis.

Related practicals are included in the laboratory-based Module CH333 - Experimental Chemistry I. Experience will be gained in a range of synthetically important reactions, techniques associated with biological chemistry, as well as analytical techniques, both spectroscopic and chromatographic. Molecular modelling and database searching are also introduced (see description of the CH333 Module for details).

CH326 - Analytical Chemistry & Molecular Structure

Instructors: Dr. Erica Burnell, Dr. Andrea Erxleben, Dr. Patrick O'Leary, Prof. Alan Ryder, Prof. Olivier Thomas (Coordinator)

MODULE DELIVERY

1. **Surface Analysis (4 lectures, AR)**
   - A basic understanding of the workings of: a secondary ion mass spectrometer (SIMS), an X-ray photoelectron spectrometer (XPS), a scanning electron microscope (SEM), and an energy dispersive X-ray analysis system (EDS).
   - An understanding of the kinds of chemical and structural information that these instruments can provide about the surface of materials.
   - Their application to the analysis of the surface of biomaterials.
2. **Crystal Diffraction (4 lectures, AE)**
   - An understanding of the following terms: unit cell, crystal system, Bravais lattice, space group, Miller indices.
   - An understanding of the information that can be obtained from X-ray powder diffraction data.
   - The ability to index simple X-ray powder diffraction patterns and to calculate the unit cell parameters from X-ray powder data of cubic structures.
   - An understanding of the relevance of polymorphism.
3. **Nuclear Magnetic Resonance (NMR) Spectroscopy (8 lectures, OT)**
   - An understanding of how some nuclei, behaving like tiny bar magnets, can line up with and against an external magnetic field and so exist in two energy states.
   - An understanding of how the size of the external field affects the energy gap between these two states.
   - An understanding of how the movement of nuclei between these energy state gives rise to the absorption and emission of energy and thus to the production of a spectrum.
   - The ability to describe how an NMR spectrum of a molecule is obtained in terms of the basic structure of the spectrometer and of sample preparation.
   - An understanding of how the environment of a nucleus in a molecule affects the signal it produces and that thus the environment of a nucleus in a molecule can be determined from the signal it produces.
   - An understanding that the electron cloud surrounding the nucleus lowers the effective magnetic field in the vicinity of the nucleus, thus shielding it.
   - The ability to characterize signals in an NMR spectrum as being shielded/upfield/low frequency or deshielded/downfield/high frequency.
   - The ability to recognize the effect of symmetry on the number of sets of chemically equivalent protons and thus on the number of signals produced by a molecule.
   - The ability to predict the number of signals that would be observed in the ^{1}H NMR spectrum of a molecule on the basis of its structure.
   - An understanding that the position, or frequency, of a signal in the spectrum is determined relative to that of a standard, TMS, added to the sample, and is referred to as the chemical shift (δ) of the signal and/or of the nucleus responsible for it.
   - The ability to use a ^{1}H NMR correlation table to relate the δ value of a signal to the type of proton responsible for it.
   - The ability to use the integration (area) of the signals in a ^{1}H NMR spectrum to determine the relative number of protons responsible for each signal.
   - An understanding that the splitting of a signal for a proton is due to an interaction (vicinal coupling) of that proton with the protons attached to the atom (usually a carbon atom) next to the atom (again usually a carbon atom) carrying the proton producing the signal.
   - The ability to deduce the number of protons on an adjacent carbon based on the multiplicity of the splitting shown by a particular proton (none, doublet, triplet, quartet), given that the multiplicity is equal to (2n +1), where n is the number of protons on the adjacent carbon.
   - An understanding that the standard form of ^{13}C NMR spectrum does not show C-H coupling and, thus, consists of a series of lines in which each set of chemically equivalent carbons appears as a single line.
   - An appreciation that the chemical shift of a carbon signal is affected by the same factors that determine the shift of a proton signal.
   - The ability to use a ^{13}C NMR correlation table to relate the δ value of a signal to the type of carbon responsible for it.
   - The ability to determine the number of hydrogens attached to a particular carbon using a ^{13}C NMR DEPT spectrum.
   - The ability to deduce the structure of simple molecules based on NMR data, usually in the form of actual spectra, the above concepts and simple spectroscopic correlation tables.

- An appreciation of the existence of long-range and geminal coupling, and of the concept of diastereotopic protons.
- An appreciation of the issues relating to the ^{1}H NMR spectra of molecules containing N-H and O-H bonds.
- The ability to describe how ^{1}H NMR spectroscopy is used in medicine in the form of magnetic resonance imaging (MRI).
- An appreciation of what is meant by a 2D NMR spectrum.
- Definition and use of a homonuclear COSY experiment.
- Definition and use of a heteronuclear HSQC experiment.
- Definition and use of a heteronuclear HMBC experiment.
- Logics in the structure elucidation of an organic compound using 1D and 2D NMR analysis.

4. Chromatography (8 lectures, EB)

- Gas Chromatography (GC)
  - Discussion of how, on a molecular level, separation occurs in chromatography, emphasizing how this chromatographic principle underpins all forms of chromatography.
  - GC instrumentation: injections systems, columns and detectors.
  - Quantifying column performance: column efficiency.
  - Applications.
- High Performance Liquid Chromatography (HPLC)
  - The ability to describe the chromatographic separation process in terms of a stationary phase (SP) and a mobile phase (MP).
  - An understanding that the number of peaks in a chromatogram indicates the number of components in the sample and of the reasons why this is not always true.
  - An understanding that the area of a peak is proportional to the amount of a substance in a sample.
  - An understanding of how the retention time of a component in a sample can be used to identify it, and of the limitations of this approach to identifying a substance.
  - An understanding of what preparative chromatography involves.
  - An understanding of the advantages and disadvantages of classical liquid chromatography (LC).
  - An understanding of the advantages and disadvantages of gas chromatography (GC).
  - A particular understanding of why the analysis of involatile/water soluble substances, a group which includes most biological substances/pharmaceuticals, is difficult/impossible by GC.
  - An appreciation that the importance of HPLC in the pharmaceutical industry is due to its ability to efficiently analyze such of involatile/water soluble substances.
  - An appreciation that the separating ability of a chromatography system is directly related to SP surface area, and thus to the size of the particles in packed columns.
  - An appreciation that HPLC is more efficient than classical LC because of the smaller particles used, but that this requires a powerful pump to establish an adequate mobile phase flow.
  - The ability to describe a simple isocratic HPLC system in terms of solvent reservoir/pump, injection valve, column, detector, and PC/data system.
  - An understanding of what a gradient HPLC system involves and what advantages it provides.
  - An understanding of why an injection valve is required and how it operates.
  - A knowledge of the various types of HPLC columns available in terms of their physical size and that of the packing material used.
  - An appreciation of how a fixed wavelength UV/visible detector operates.
  - An appreciation of how a variable wavelength UV/visible detector operates.
  - An appreciation of how a diode array detector operates.
  - An appreciation of how a fluorescence detector operates.
  - An understanding of the relative merits of UV/visible, diode array and fluorescence detectors.
  - An appreciation of the relative merits of GC and HPLC as analytical tools.
  - The ability to identify the key experimental features in a published HPLC method with a view to using it.
  - An understanding of what an adsorption HPLC column is, and of the retention mechanism through which it operates.
  - An understanding of what is implied by the term “chemically bound stationary phase”.
  - An understanding of what a normal phase HPLC column is, and of the retention mechanism through which it operates.
  - An understanding of what a reverse phase (RP) HPLC column is, and of the retention mechanism through which it operates.
  - A precise understanding of why RP columns are the most commonly used HPLC column.
  - An understanding of how chiral HPLC operates and of how it can be used to determine the enantiomeric excess of a compound.

5. Mass Spectrometry (4 lectures, POL)

- A basic understanding of the workings of the basic forms of mass spectrometer including:
  - Sample introduction (direct insertion probe, GC, LC systems).

- Ionization methods (electron impact, chemical, electronspray, laser desorption).
- Mass analyzers (magnetic sector, double focusing including kinetic filter, time of flight including reflectron, quadrupolar).
- Ion detection.

- An understanding of the basics of fragmentation, when and how it occurs and its prevalence with different molecule types and ionization techniques.
- An ability, given a molecule and its mass spectrum (EI or CI) to deduce the fragmentations, and their mechanisms, leading to the main peaks; fragmentations covered will center on alpha radical initiated cleavage, adjacent bond cleavage, and Mc Clafferty type rearrangement.
- An understanding and ability to recognize or apply the isotope effect.
- An appreciation of the importance of resolution as applied to HRMS.

6. XRF and Thermal analysis (4 lectures, AR)

- A basic understanding of the fundamental theory underpinning workings of X-Ray Fluorescence (XRF).
- A basic understanding of the workings and operation of an Energy Dispersive XRF (ED-XRF) and Wavelength Dispersive XRD (WD-XRF).
- An understanding of the major matrix effects (absorption and intensity enhancement) that occur in XRF measurements.
- A basic understanding of the workings of thermogravimetric analysis (TGA, DTA) and scanning calorimetry (DSC) instruments.
- An understanding of the chemical information that these instruments can provide.
- Their application to the understanding of thermal transitions occurring inorganic, organic, polymeric, and biological materials.

The practicals related to the topics dealt with within the course are included in the laboratory-based Module CH333 - Experimental Chemistry I (see description of the CH333 Module for details).

CH332 - Drug Design & Drug Discovery

Instructors: Dr. Erica Burnell, Dr. David Cheung (Coordinator), Prof. Olivier Thomas

MODULE DELIVERY

The Module is delivered in 24 lectures (2 one-hour lectures per week) and 8 practicals (5 Computational Approaches and 3 Natural Products practicals on Mondays 2-5pm) and a continuous assessment exercise for Approaches to Drug Discovery.

1. Computational Approaches to Drug Design (12 lectures + 2 tutorials, DC)

- Role of modelling in drug design.
- Describing molecular structure.
- Molecular Models and Force Fields.
- Molecular Docking.
- Challenges of modelling proteins and prediction of protein structure.
- Molecular Dynamics.
- Thermodynamics of protein-ligand binding.

Learning outcomes

Students will gain an appreciation of:

- Applications of molecular modelling in drug design.
- The importance of three-dimensional molecular structure.
- Potential energy surfaces and how these relate to the structure of molecule.
- Molecular mechanics force fields.
- Molecular docking and molecular dynamics calculations.
- Challenges in modelling biomolecular structure and function.

Practicals

The Molecular Modelling practical component will take place over a ten-week period (3 h per week). Attendance records are taken at practical classes and performance at each laboratory class will be assessed on a weekly basis. Part of the marks will be awarded for this Continuous Assessment.

The principal objectives of the laboratory course are:

- To develop a practical capability to visualize and modify molecular structures on a computer.
- To be able to compute binding energies.
- To be able to perform and analyze data from MD simulations.
- To illustrate the principles dealt with in the lecture course.

Recommended readings

Students may consult the following textbooks (available in the library):

- A.R. Leach, *Molecular Modelling: Principles and Applications*
- A: Hinchliffe, *Molecular Modelling for Beginners*

2. Natural Products in Drug Discovery (6 lectures + 1 tutorial, OT)

This lecture series covers relevant topics relating to modern natural products chemistry and its role in drug discovery and development. Main outcomes are:

- Historical and current importance of natural products as drugs and drug leads, anti-infective, anticancer but also others.
- The most important natural sources for bioprospection and drug discovery: plants, microbes.
- Natural product chemistry: principles for the extraction, isolation and structure elucidation steps.
- Basic concepts of bioactivity guided isolation process.
- Main metabolic pathways leading to specialized metabolites or natural products.
- New perspectives for natural products in drug discovery: sources like the marine biodiversity, extreme environments; dereplication processes, collaborative databases.

Practicals

The Natural Products Chemistry practical component will take place over a six-week period (2 groups, 3 laboratory sessions each, 3 h per week). Attendance records are taken at practical classes and performance will be assessed at the end of the practical. Part of the marks will be awarded for this Continuous Assessment.

- Extraction of the metabolites from a common marine macroalga *Halidrys siliquosa*.
- Fractionation of the extract into families of metabolites of different polarities. Use of solid phase extraction and applications of basic principles of chromatography: normal and reversed phase. Polarity of solvents.
- Analysis of some fractions by mass spectrometry and nuclear magnetic resonance. Drawing of the isolated molecules and structure elucidation.

- Propose metabolic pathways of the isolated metabolites based on basic rules.

Recommended readings
Students may consult the following textbooks (available in the library):
- P.M. Dewick, *Medicinal Chemistry, a Biosynthetic Approach*
- G.M.L. Cragg; D. Kingston, D.J. Newman, *Anticancer Agents from Natural Products*

3. Approaches to Drug Discovery (6 lectures +1 tutorial, EB)
This lecture series deals with the Quantitative Structure-Activity Relationships (QSAR).

Learning outcomes
By the end of the course, students should be able to identify and quantify the physiochemical parameters of compounds and deduce the effects of certain properties on drug activity.

Continuous Assessment
Students will be given data on a series of bioactive analogues to analyze using a QSAR approach and write a report on their findings. This report will be marked as part of the continuous assessment for the module.

Recommended readings
Students may consult the following textbooks (available in the library):
- G.L. Patrick, *An Introduction to Medicinal Chemistry*
- C.H. Hansch, A. Leo, D. H. Hoekmans*, Exploring QSAR*

CH333 - Experimental Chemistry I

Instructors: Dr. Erica Burnell, Prof. Peter Crowley, Dr. Andrea Erxleben, Dr. Eddie Myers, Prof. Alan Ryder, Prof. Olivier Thomas (Coordinator)

COURSE OUTLINE WITH LEARNING OUTCOMES

This laboratory-based Module complements the 3rd Year Organic Chemistry (CH311) and Analytical Chemistry & Molecular Structure (CH326) lecture-based Modules (which students **must** also take).

Attendance to laboratory sessions is **mandatory**.

On successful completion of this Module, the learner will be able to:

- Demonstrate an understanding in protein handling and purification.
- Demonstrate competence in setting up organic and organometallic reactions, work up and standard purification techniques, such as distillation, chromatography and recrystallization.
- Demonstrate competence in mole and yield calculations.
- Demonstrate competence in reaction rate monitoring and reporting.
- Demonstrate competence in organic compound characterization techniques, and analysis of spectroscopic data such as HPLC, GC, IR, UV, MS and NMR spectroscopy.
- Demonstrate competence in report writing, interpretation of laboratory results, and relate experimental data with theoretical and mechanistic aspects covered in the associated lectures (*i.e.* Modules CH311 and CH326).
- Carry out procedures in solving crystal structures.
- Demonstrate competence in the thermal analysis of polymers.

The Module is graded through Continuous Assessment by submission of written reports to laboratory class supervisors with each experiment graded out of 100%. At the end of the course each student will undergo a 10 minute interview assessment, which is also graded out of 100% (equivalent to the grade for one laboratory experiment).

CH307 - Inorganic Chemistry

Instructors: Dr. Andrea Erxleben, Dr. Pau Farras, Dr. Constantina Papatriantafyllopoulou, Dr. Luca Ronconi (Coordinator)

COURSE OUTLINE WITH LEARNING OUTCOMES (LO)

This Module will provide insights into the specific roles of metals and ligands in the broad field of coordination chemistry. Specific areas to be discussed include the coordination and organometallic chemistry of transition metals, inorganic kinetics and principles of nuclear chemistry.

Related practicals are included in the laboratory-based Module CH334 - Experimental Chemistry II (see description of the CH334 Module for details).

On successful completion of this Module, the learner will be able to:

LO1 recognize the basic principles of radioactivity and nuclear chemistry, to include radioactive decays, the interaction of radiations with matter, nuclear reactions and common applications of radioisotopes;
LO2 explain the bonding and structural features of transition metal coordination compounds based on the Crystal Field Theory (CFT) and the Molecular Orbitals (MOs) models;
LO3 predict the spectroscopic properties of transition metal coordination compounds using theoretical models;
LO4 describe the structure, bonding and reactivity of organometallic complexes of d-block elements;
LO5 classify the types of organometallic complexes on the basis of the coordinated ligands;
LO6 illustrate the catalytic activity of selected organometallic complexes and draw the associated mechanisms of reaction;
LO7 explain the structure, bonding and reactivity of transition metals in the various oxidation states;
LO8 discuss in detail the mechanisms of dissociative, associative, interchange, ligand substitution and electron transfer reactions of selected transition metals.

MODULE DELIVERY

The Module is delivered in 30 lectures (normally 3 one-hour lectures per week) and 4 one-hour tutorials (normally grouped at the very end of the course).

Specifically, the following topics will be dealt with.

1. **3rd Year Inorganic Chemistry Laboratory Induction (2 lectures, LR1)**
   This lecture series will provide a general introduction to the experimental work to be carried out.
   The practical experiments include:
   - an investigation of the oxidation states of vanadium;
   - oxidation of ethanol by chromium(VI);
   - synthesis and IR characterization of acetylacetonate derivatives of vanadium(IV) and copper(II);
   - synthesis, IR characterization and redox behavior of cobalt heteropolytungstates;
   - synthesis, spectroscopic characterization and reactivity of acetylacetonate derivatives of cobalt(III).

   See description of the CH334 Module for details.

2. **Organometallic Compounds of the d-Block Elements (8 lectures + 1 tutorial, CP)**
   This lecture series will deal with the structure, bonding and reactivity of organometallic complexes based on d-block elements.
   Specifically, the following topics will be covered:
   - description and classification of the most common types of organometallic complexes based on the various organic ligands (*e.g.* CO, NO, PR_3) used in their construction;
   - use of the MOs theory to describe the bonding in organometallic complexes;
   - the 18-electron rule, its limitations, and its application to organometallic species;
   - description of the common reaction mechanisms observed for organometallic complexes (*e.g.* β-H elimination, alkyl migration, oxidative addition);
   - the catalytic activity of selected organometallic complexes (*e.g.* Grubbs and Schrock types) and the associated mechanisms of reaction.

3. **Comparative Chemistry and Kinetics of Transition Metals (6 lectures + 1 tutorial, AE)**
   This lecture series is comprised of two parts.

   The first part will give an introduction to the chemistry of chromium and vanadium and will cover the following specific topics:
   - general properties of V and Cr in different oxidation states;
   - the pH-dependent equilibria of V species in aqueous solution;
   - balancing the chemical equations to the formation and reactions of V and Cr halides, oxides and oxohalides;

- coordination chemistry of V and Cr;
- the biological relevance of V;
- description of Cr-Cr multiple bonds;
- interpretation of the related Frost-Ebsworth diagrams.

The second part will deal with the kinetics and reaction mechanisms of ligand substitution and electron transfer reactions in transition metal complexes, and will cover the following specific topics:

- description of the dissociative, associative and interchange mechanisms for substitution reactions in coordination compounds;
- plotting the reaction profiles for the dissociative, associative and interchange mechanisms;
- interpretation of kinetic data in terms of the type of mechanism;
- derivation and application of the rate law for substitution reactions in Pt(II) complexes;
- application of the *trans*-effect concept to predict substitution products in Pt(II) complexes;
- description of the Eigen-Wilkins and the conjugate base mechanisms;
- description of the inner-sphere and outer-sphere mechanisms for electron-transfer reactions;
- application of the Marcus-Hush equation.

4. Complex Formation by the Transition Metals (8 lectures + 1 tutorial, PF)

This lecture series will deal with the exploitation of the Crystal Field Theory (CFT) and the Molecular Orbitals (MOs) models to explain the properties of transition metal coordination compounds.
Specifically, the following topics will be covered:

- use of the point group character tables and orbital repulsion considerations to explain the d orbital splitting patterns and the symbolism used in labelling for common geometries found in coordination compounds of the transition metals;
- calculation of the crystal field stabilization energies for coordination compounds of the transition metals in a variety of oxidation states, using a number of common ligands and for common geometries;
- use of laboratory measured properties in conjunction with CFT to predict the geometry adopted by coordination compounds of transition metals in a variety of oxidation states, using a number of common ligands;
- drawing of MOs energy level diagrams and pictorial representations for the bonding in coordination compounds with σ-donor, π-donor and π-acceptor ligands;
- comparison of CFT and MOs approaches to describing the bonding in coordination compounds;
- correlation of MOs diagrams with spectroscopic properties of coordination compounds and accounting for the order of ligands in the spectrochemical series.

5. Nuclear and Isotopic Chemistry (6 lectures + 1 tutorial, LR2)

This lecture series will deal with the basic concepts of nuclear chemistry and radioactivity.
Specifically, the following topics will be covered:

- the nuclear structure and its involvement in the origin of radioactivity and nuclear reactions;
- the nuclide symbolism and definitions (isotopes, nuclear binding energy, nuclei stability band, half-life);
- the radioactive decays and the interaction of radiations with matter;
- radiation measurement and detection;
- natural radioactivity and the radioactive series;
- nuclear reactions (fission and fusion) and nuclear waste handling and cleanup;
- isotopic labelling;
- applications of radioisotopes (radiotracers, radiometric dating, nuclear medicine).

TEXTBOOK AND REFERENCE MATERIAL

- C.E. Housecroft, A.G. Sharpe, *Inorganic Chemistry*, 5th Ed., Pearson Education Ltd., 2018
- Lecture notes, slides and literature papers provided in due course on Blackboard

CH313 - Physical Chemistry

Instructors: Dr. David Cheung, Prof. Henry Curran (Coordinator), Prof. Donal Leech, Prof. Alan Ryder

TEXTBOOK

P.W. Atkins, J. De Paula, *Elements of Physical Chemistry*, 5th Ed. (available in the library)

MODULE DELIVERY

1. **Molecular Interactions (5 h, HC, Chapter 15 of the textbook)**
   Students will understand that:
   - Van der Waals force is an attractive interaction between closed-shell molecules with a potential energy that is inversely proportional to the sixth power of the separation.
   - A polar molecule is a molecule with a permanent electric dipole moment; the magnitude of the dipole moment is the product of the partial charge and the separation.
   - Dipole moments are approximately additive.
   - The equations for potential energies of interaction for (i) charge/charge, (ii) charge/dipole, (iii) dipole/dipole, (iv) London (dispersion) interaction.
   - A hydrogen bond is an interaction of the form X–H···Y, where X and Y are N, O, or F.
   - The Lennard-Jones (6,12)-potential is a model of the total intermolecular potential energy.

2. **Chemical Kinetics (5 h, HC, Chapters 10 & 11 of the textbook)**
   Students will be able to:
   - Derive the rate law for a first- and second-order reaction and from that determine the half-life for a reaction and the rate of reaction.
   - Determine the kinetics for an elementary reaction.
   - Explain the kinetics associated with flow reactors and jet-stirred reactors.
   - Understand how the rate constant of a reaction varies with temperature, and derive the frequency A-factor and activation energy of a reaction given the rate constant and different temperatures.
   - Appreciate and understand the dependence of kinetics on thermodynamics of reactants and products.

3. **Phase Diagrams of Mixtures (5 h, DL, Chapter 6 of the textbook)**
   Students will understand that:
   - The equilibria between phases (at constant pressure) are represented by lines on a temperature-composition phase diagram, and the relative abundance of phases is obtained by using the lever rule.
   - A regular solution is one in which the entropy of mixing, but not the enthalpy of mixing, is the same as an ideal solution.
   - An azeotrope is a mixture that vaporizes and condenses without a change in composition; an eutectic is a mixture that freezes and melts without change of composition.

4. **Macromolecules (5 h, DC, Chapter 16 of the textbook)**
   Students will understand that:
   - Polymers are typically organic molecules made from man copies of small repeating units (monomers).
   - Polymers are typically polydisperse.
   - The definitions of number-average molar mass and weighted-average molar mass and the difference between the two.
   - Techniques for the determination of the mean molar masses of molecules and in particular viscosity measurements and gel permeation chromatography.
   - The classification of polymers and the main properties of thermoplastics, elastomers and thermosets.
   - The properties of amorphous and crystalline polymers.
   - How crystallinity in a polymer influences the physical properties.
   - An understanding of the meaning of the glass transition temperature (T_g) and the main factors such as chain flexibility, steric effects, molar mass and branching and cross-linking which influence its magnitude.

5. **Self-Assembly (5 h, DC, Chapter 16 of the textbook)**
   Students will:
   - Understand that self-assembly is the spontaneous formation of organized structures through a reversible process involving pre-existing components that is controlled by the design of these components, a driving force, and the environment (external input).
   - Understand the formation of surfactant micelles as an example of self-assembly.
   - Predict the morphology of surfactant aggregates based on the relative geometries of the head and tail groups.

- Understand the nature of liquid crystals, nematic and smectic types, and how they self-assemble as a result of packing and intermolecular forces.
- Appreciate how external control of molecular behavior can make a simple twisted nematic liquid crystal display cell.

6. Electrochemistry (5 h, DL, Chapter 16 of the textbook)

Students will understand that:

- An electric double layer consists of a sheet of positive charge at the surface of the electrode and a sheet of negative charge next to it in the solution (and vice versa).
- The Galvani potential difference is the potential difference between the bulk of the metal electrode and the bulk of the solution.
- The current density, j, at an electrode is expressed by the Butler-Volmer equation, $j = j_0\left\{e^{(1-\alpha)f\eta} - e^{-\alpha f\eta}\right\}$, where η is the overpotential $\eta = E' - E_i$, α is the transfer coefficient, and i_0 is the exchange current density.
- A Tafel plot is a plot of the logarithm of the current density against the overpotential; the slope gives the value of α and the intercept at $\eta = 0$ gives the exchange-current density.
- Voltammetry is the study of the current through an electrode as a function of the applied potential difference.
- To induce current to flow through an electrolytic cell and bring about a non-spontaneous cell reaction, the applied potential difference must exceed the cell emf by at least the cell overpotential.

7. Quantum Chemistry (5 h, AR, Chapter 12 of the textbook)

Students will understand that:

- Wien's Law states that $T\lambda_{max}$ = constant; the Stefan-Boltzmann law states that the emission of a black body is proportional to T^4. Planck proposed that *electromagnetic oscillators* of frequency ν could acquire or discard energy in quanta of magnitude $h\nu$. Einstein proposed that *atoms* oscillating in a solid with frequency ν could acquire or discard energy in quanta of magnitude $h\nu$.
- The photoelectric effect is the ejection of electrons when radiation of greater than the threshold frequency is incident on a metal; the kinetic energy of the ejected electrons and frequency of the incident radiation are related by $E_k = h\nu\phi$ where ϕ is the work function of the metal. The de Broglie relation for the wavelength, λ, of a particle of linear momentum p is $\lambda = \eta/p$.
- A wave function, Ψ, contains all the dynamical information about a system and is found by solving the appropriate Schrödinger equation, $-(\bar{h}^2/2m)\mathrm{d}^2\psi/\mathrm{d}x^2 + \mathrm{V}\psi = \mathrm{E}\psi$, subject to constraints on the solutions known as boundary conditions.
- According to the Born interpretation, the probability of finding a particle in a small region of space of volume δV is proportional to $\psi^2\delta V$, where ψ is the value of the wave function in the region.
- According to the Heisenberg uncertainty principle, it is impossible to specify simultaneously, with arbitrary precision, both the momentum and position of a particle.
- The energy levels of a particle of mass m in a 1-D box of length L are $E_n = n^2h^2/8mL^2$, with n = 1, 2,… and the wave functions are $\Psi_n(x) = (2/L)^{1/2}\sin(n\pi x/L)$.
- The energy levels of a particle of mass m in a 3-D box of length L are $E_n = (n_1^2/L_1^2 + n_2^2/L_2^2 + n_3^2/L_3^2)(h^2/8m)$, with n = 1, 2,… and the wave functions are $\Psi_n(x) = (2/L)^{1/2}\sin(n\pi x/L)$.
- Because wave functions do not decay abruptly to zero, particles may tunnel into classically forbidden regions. Two aspects of tunneling include radioactivity and scanning tunneling microscopy.
- The energy levels of a particle of mass m on a circular ring of radius r are $E_{m_I} = m_I^2\hbar^2/2I$ where *I* is the moment of inertia, $I = mr^2$ and $m_l = 0, \pm1, \pm2$, etc.
- The angular momentum of a particle on a ring is quantized and confined to the values $J_z = m_l\hbar$, $m_l = 0, \pm1, \pm2$, etc.
- A particle undergoes harmonic motion if it is subjected to a Hooke's-law restoring force and has a parabolic potential energy, $V(x) = 1/2kx^2$.
- The energy levels of a harmonic oscillator are $E_v = (v + ½)h\nu$, where $\nu = (1/2\pi)(k/m)^{1/2}$ and v = 0, 1, 2,…

8. Spectroscopy (5 h, AR, Chapter 19 of the textbook)

Students will understand that:

- A spectrometer consists of a source of radiation, a dispersing element, and a detector.
- One contribution to the linewidth is the Doppler effect, which can be minimized by working at low temperatures. Another contribution to linewidth is lifetime broadening: $\delta E \approx \hbar/T$, where T is the lifetime of the state.
- The intensity of a transition is proportional to the square of the transition dipole moment.
- A selection rule is a statement about when the transition dipole is non-zero.
- A gross selection rule specifies the general features that a molecule must have if it is to have a spectrum of a given kind.
- A specific selection rule is a statement about which changes in quantum number may occur in a transition.

- The rotational energy levels of a linear rotor and a spherical rotor are given by $E_J = hBJ(J+1)$ with J = 0, 1, 2, ..., where B = fl/4nl is the rotational constant of a molecule with moment of inertia I.
- The Pauli principle states for fermions $\Psi(B,A) = -\Psi(A,B)$ and for bosons $\Psi(B,A) = \Psi(AB)$. The consequences of the Pauli principle for rotational states are called nuclear statistics.
- The populations of rotational energy levels are given by the Boltzmann distribution in connection with noting the degeneracy of each level.
- The gross selection rule for rotational transitions is that the molecule must be polar.
- The specific selection rules for rotational transitions are $\Delta J = \pm 1$, $\Delta K = 0$; a rotational spectrum of a polar linear molecule and of a polar symmetric rotor consists of a series of lines at frequencies separated by 2B.
- In a Raman spectrum lines shifted to lower frequency than the incident radiation are called Stokes lines and lines shifted to higher frequency are called anti-Stokes lines.
- A Raman spectrometer consists of a monochromatic light source (usually a laser), sampling optics, a dispersive element (spectrometer), and a detector (usually a multi-channel CCD).
- The gross selection rule for rotational Raman spectra is that the polarizability of the molecule must be anisotropic.
- The specific selection rules for the rotational Raman transitions of linear molecules are $\Delta J = +2$ (Stokes lines), $\Delta J = -2$ (anti-Stokes lines).
- The vibrational energy levels of a molecule $E_v = (v + 1/2)hcv$ with v = 0, 1, 2,..., where $v = (1/2\pi c\}(k/\mu)^{1/2}$ and $\mu = m_A m_B/(m_A + m_B)$.
- The gross selection rule for vibrational absorption spectra is that the electric dipole moment of the molecule must change during the vibration.
- The specific selection rule for vibrational transitions is $\Delta v = \pm 1$.
- The number of vibrational modes of non-linear molecules is 3N-6; for linear molecules the number is 3N-5.
- Rotational transitions accompany vibrational transitions and split the spectrum into a P branch ($\Delta J = -1$), a Q branch ($\Delta J = 0$), and an R branch ($\Delta J = +1$). A Q branch is observed only when the molecule possesses angular momentum around its axis.
- The gross selection rule for the vibrational Raman spectrum of a polyatomic molecule is that the normal mode of vibration is accompanied by a changing polarizability.
- The exclusion rule states that if the molecule has a center of inversion, then no modes can be both infrared and Raman active.

Related practicals are included in the laboratory-based Module CH334 - Experimental Chemistry II (see description of the CH334 Module for details).

CH334 - Experimental Chemistry II

Instructors: Prof. Henry Curran (Co-Coordinator/Physical Chemistry Practicals), Dr. David Cheung, Dr. Pau Farras, Dr. Constantina Papatriantafyllopoulou, Dr. Yury Rochev, Dr. Luca Ronconi (Co-Coordinator/Inorganic Chemistry Practicals)

COURSE OUTLINE WITH LEARNING OUTCOMES (LO)

This laboratory-based Module complements the 3rd Year Inorganic Chemistry (CH307) and Physical Chemistry (CH313) lecture-based Modules (which students **must** also take).

This course will involve the carrying out of experiments in areas such as inorganic syntheses, analysis and spectroscopic studies of coordination compounds, chemical kinetics, viscosity, temperature dependence of equilibrium, miscible liquids, rotational-vibrational spectra and electrochemistry.

Attendance to laboratory sessions is **mandatory**.

On successful completion of this Module, the learner will be able to:

LO1 set up and carry out a range of inorganic syntheses (*e.g.* coordination compounds, polyoxometallates);
LO2 relate laboratory results to the properties (*e.g.* oxidation states, structures) and reaction mechanisms of compounds of the transition metals (*e.g.* coordination compounds, polyoxometallates) covered in the associated inorganic chemistry lectures;
LO3 demonstrate competence in the spectroscopic characterization (*e.g.* IR, UV-Vis, NMR spectroscopy) of coordination compounds;
LO4 demonstrate competence in stoichiometric calculations;
LO5 set up and perform tests to verify fundamental physical chemistry theories in the laboratory;
LO6 relate experimental results to the physico-chemical principles dealt with in the associated physical chemistry lectures;
LO7 recognize the scientific method of planning, developing, conducting and reporting experiments to a scientifically acceptable standard;
LO8 apply important synthetic and analytical techniques relevant to the professional practice of chemistry;
LO9 implement safe work practices in a chemistry laboratory, to include awareness of common hazards and appropriate safety precautions.

MODULE DELIVERY

The Module is delivered in 10 practical sessions of 4 hours each (1 practical per week) split into two blocks (inorganic chemistry: practicals 1-5; physical chemistry: practicals 6-11).

The week following each block of practicals students will undergo an individual ten-minute oral examination related to the laboratory work carried out.

Specifically, the following practical experiments will be carried out.

1. **Inorganic Chemistry**
   - An Investigation of the Oxidation States of Vanadium
   - Oxidation of Ethanol by Chromium(VI)
   - Synthesis and IR Characterization of Acetylacetonate Derivatives of Vanadium(IV) and Copper(II)
   - Polyoxometallates: Synthesis, IR Characterization and Redox Behavior of a Cobalt Heteropolytungstate
   - Acetylacetonates of Cobalt(III): Synthesis, Characterization and Reactions
2. **Physical Chemistry**
   - Arrhenius Equation
   - Polymer Viscosity
   - Determination of an Equilibrium Constant
   - Miscible Liquids
   - Rotational-Vibrational Spectrum of HCl
   - Cyclic Voltammetry of the Ferrocyanide/Ferricyanide Redox Couple

To derive full benefit from the course students should read details of the experiments to be performed **prior to attending the laboratory** and refer to the **literature resources** indicated in the laboratory manual.

TEXTBOOK AND REFERENCE MATERIAL

- Experimental Chemistry II Laboratory Manual 2019 - 2020
- Lecture notes, slides and literature papers provided in due course on Blackboard

CH3101 - Computers in Chemical Research

Instructors: Dr. David Cheung, Prof. Peter Crowley, Prof. Henry Curran, Dr. Andrea Erxleben, Dr. Pau Farras (Coordinator), Dr. Eddie Myers, Dr. Patrick O'Leary, Dr. Constantina Papatriantafyllopoulou

COURSE OUTLINE WITH LEARNING OUTCOMES

The course provides an opportunity for the student to become familiar with a wide range of software relevant to the working life of a professional chemist or biopharmaceutical chemist. It involves a workshop approach which gives the student practical, hands-on experience of the software. The course will also allow the student to develop their communication skills in terms of both writing and oral presentation.

On successful completion of this Module, the learner will be able to:

- produce scientific written reports for the communication and presentation of chemical information in terms of structures, tables of data and other figures, such as molecular graphics;
- produce spreadsheets and graphs using Excel for inclusion in reports and for analyzing data;
- source information from the primary scientific literature using various resources such as online libraries, search engines, databases (*e.g.* SciFinder, Reaxys), and other related technology;
- prepare a chemistry or biopharmaceutical chemistry presentation, and use it to communicate knowledge to an audience;
- use various sources of chemical knowledge to independently research a topic and write a critical essay or report;
- carry out basic molecular modelling;
- demonstrate increased knowledge and understanding within chemistry and biopharmaceutical chemistry;
- use protein and other structural databases;
- produce a poster suitable for a scientific conference;
- give a PowerPoint presentation.

MODULE DELIVERY

The Module is delivered in 15 lectures (normally 2 three-hour lectures per week), finishing with an oral presentation.

Schedule (Semester II): computer workshops in the Finnegan PC Suite at 2.00-5.00pm.

ASSESSMENT

Continuous assessment based on two workshop reports each week. An extended essay, poster and presentation on an individual topic (assigned to each student at the beginning of the semester) are also part of the assessment process.

Week	Monday			Friday		
	Task	**Software**	**Lecturer**	**Task**	**Software**	**Lecturer**
1				Introduction and project assignment		PF
2	Molecular graphics	ChemDraw	POL	Report writing	MS Word	AE
3	Spreadsheets in the lab	MS Excel	HC	Technical writing	MS Word	EM
4	Data fitting and plotting	MS Excel	HC	Plagiarism	Turnitin	PF
5	Molecular modelling 1: structure building and optimization	Spartan ‘10	DC	Referencing	EndNote	PF
6	Molecular modelling 2: conformational analysis and conformational searching	Spartan ‘10	DC	Presentations	MS PowerPoint	PC
7	e-Searching chemical literature	Reaxys, SciFinder & Web of Knowledge	POL	Presentations	MS PowerPoint	PC
8	Working with proteins	PDB	PC	Posters and how to produce them	MS PowerPoint	CP
9	Visualization of molecular structures	Visual Molecular Dynamics	DC	Project report and presentation preparation		
10	Project report and presentation preparation					
11	Project presentations					
12	Project presentations					

CH3103 - Validation in the Pharmaceutical and Medical Devices Industry

Instructors: Dr. Martin Conneely, Prof. Michael J. Hynes, Dr. Constantina Papatriantafyllopoulou (Coordinator)

MODULE DELIVERY AND ASSESSMENT

The Module is delivered in 15 lectures (normally 3 one-hour lectures per week) and 1 two-hour practical.

The Module is assessed through a formal written examination at the end of Semester II (worth 65%) and Continuous Assessment (Project to be undertaken along with a presentation, worth 35%).

Attendance to lectures and the practical session is **mandatory**.

COURSE OUTLINE WITH LEARNING OUTCOMES

This module will cover relevant topics concerning validatory requirements within the (bio)pharmaceutical and chemical industries. Detailed insights into the inner workings of industry are also given.

On successful completion of this Module, the learner will:

- Be introduced to the concept of Validation and its role in the pharmaceutical industry; the Validation Masterplan (VMP) will then be discussed and its benefits outlined.
- Be introduced to the concept of Good Manufacturing Practice (GMP) and Good Laboratory Practice (GLP) in relation to the pharmaceutical and chemical industries.
- Learn of the numerous and pertinent aspects of Cleaning Validation with respect to the manufacturing industry.
- Apply the basic concepts of the course in a laboratory exercise.
- Be provided with a broad knowledge of the subject of Equipment qualification including Design, Installation, Process and Performance Qualification).
- Be introduced to the cutting-edge field of Process Analytical Technology (PAT) and understand its fundamental relevance to the future of pharmaceutical manufacturing.
- Be introduced to Medical Devices and will glean knowledge in the practical aspects of Quality Control, Good Manufacturing Practices and Drug Development in relation to the Medical Device Industry.

Third Year Chemistry 2019/20 - Semester I

Week beginning		9-Sep	16-Sep	23-Sep	30-Sep	7-Oct	14-Oct	21-Oct	28-Oct	4-Nov	11-Nov	18-Nov	25-Nov
Week no.		**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**
CH311 - Organic Chemistry													
Mon	**9am**	Biomol. Chem.			Heterocyclic			Syn. & Stereo.	***Bank***	Syn. & Stereo.		Phys. Org. Chem.	
Dillon		*PC*			*MOD*			*EM*	***Holiday***	*EM*		*PM*	
CH332 - Drug Design & Drug Discovery													
Tue	**9am**	Computational Approaches to Drug Design											
Dillon		*DC*											
CH326 - Analytical Chemistry & Molecular Structure													
Tue	**10am**	NMR			MS	XRF/TA		GC/HPLC		Cryst. Diff.		Tut.	Surf. Anal.
Dillon		*OT*			*POL*	*AR*		*EB*		*AE*		*OT*	*AR*
CH326 - Analytical Chemistry & Molecular Structure													
Wed	**11am**	NMR			MS	XRF/TA		GC/HPLC		Cryst. Diff.	Surf. Anal.	Tut.	Surf. Anal.
Dillon		*OT*			*POL*	*AR*		*EB*		*AE*	*AR*	*TBA*	*AR*
CH332 - Drug Design & Drug Discovery													
Thu	**9am**	Natural Products						Approaches to Drug Discovery					
Dillon		*OT*						*EB*					
CH311 - Organic Chemistry													
Fri	**10am**	Biomol. Chem.			Heterocyclic			Syn. & Stereo.			Phys. Org. Chem.		
Dillon		*PC*			*MOD*			*EM*			*PM*		
CH311 - Organic Chemistry													
Fri	**11am**	Biomol. Chem.			Heterocyclic			Syn. & Stereo.			Phys. Org. Chem.		
Dillon		*PC*			*MOD*			*EM*			*PM*		
CH326 - Analytical Chemistry & Molecular Structure													
Fri	**12pm**	NMR		MS		Tut.		XRF/TA	GC/HPLC	Cryst. Diff.	Surf. Anal.	Tut.	Tut.
Dillon		*OT*		*POL*		*OT*		*AR*	*EB*	*AE*	*AR*	*TBA*	*TBA*
Practicals													
Mon	**2pm**	**CH332 Labs**											
			Computational Approaches & Natural Products Practicals						***Bank Holiday***	*Computational and Drug Design Practicals*			
Tue or Wed or Thu	**2pm**	**CH333 Labs**											
			Organic Practicals						*Analytical Chemistry & Molecular Structure Practicals*				

Third Year Chemistry 2019/20 - Semester II

Week beginning		13-Jan	20-Jan	27-Jan	3-Feb	10-Feb	17-Feb	24-Feb	2-Mar	9-Mar	16-Mar	23-Mar	30-Mar
Week no.		1	2	3	4	5	6	7	8	9	10	11	12
CH313 - Physical Chemistry													
Mon	9am	Phases		Mol. Interact.	Spect.	Kinetics	Electrochem.		Macromol.	Surface	Quantum	Quantum	Tut.
Dillon		*DL*		*HC*	*AR*	*HC*	*DL*		*DC*	*DC*	*AR*	*AR*	*TBA*
CH307 - Inorganic Chemistry													
Tue	10am	Lab. Intro.	Organomet. Chem.		Comp. Chem./Kinetics		Test 1		Coord. Chem.		***Bank***	Nucl. Chem.	Tut.
Dillon		*LR*	*CP*		*AE*				*PF*		***Holiday***	*LR*	*AE*
CH313 - Physical Chemistry													
Tue	11am	Phases	Mol. Interact.		Spect.	Kinetics	Electrochem.	Macromol.		Surface	***Bank***	Tut.	Tut.
Dillon		*DL*	*HC*		*AR*	*HC*	*DL*	*DC*		*DC*	***Holiday***	*TBA*	*TBA*
CH313 - Physical Chemistry													
Wed	10am	Phases	Mol. Interact.	Spect.		Kinetics	Electrochem.	Macromol.	Surface		Quantum	Tut.	Tut.
Dillon		*DL*	*HC*	*AR*		*HC*	*DL*	*DC*	*DC*		*AR*	*TBA*	*TBA*
CH307 - Inorganic Chemistry													
Wed	11am	Lab. Intro.	Organomet. Chem.		Comp. Chem./Kinetics		Coord. Chem.			Nucl. Chem.		Test 2	Tut.
Dillon		*LR*	*CP*		*AE*		*PF*			*LR*			*PF*
CH313 - Physical Chemistry													
Fri	10am	Phases	Mol. Interact.	Spect.		Kinetics	Electrochem.	Macromol.	Surface		Quantum	Tut.	Tut.
Dillon		*DL*	*HC*	*AR*		*HC*	*DL*	*DC*	*DC*		*AR*	*TBA*	*TBA*
CH307 - Inorganic Chemistry													
Fri	11am	Organomet. Chem			Comp. Chem./Kinetics		Coord. Chem.			Nucl. Chem.		Tut.	Tut.
Dillon		*CP*			*AE*		*PF*			*LR*		*CP*	*LR*
Practicals													
Tue or Wed or Thu	2pm	**CH334 Labs**											
		Inorganic Practicals					*Orals*	*Physical Chemistry Practicals - **Bank Holiday 17/03/2020***					*Orals*

Third Year Chemistry 2018/19 - Semester II (cont.)

Week beginning		13-Jan	20-Jan	27-Jan	3-Feb	10-Feb	17-Feb	24-Feb	2-Mar	9-Mar	16-Mar	23-Mar	30-Mar
Week no.		1	2	3	4	5	6	7	8	9	10	11	12
CH3103 - Validation in the Pharmaceutical and Medical Devices Industry													
Wed	**9am**	Validation				Med. Dev.	Reach						
Dillon		*CP*				*MC*	*MH*						
CH3103 - Validation in the Pharmaceutical and Medical Devices Industry													
Thu	**9am**	Validation				Med. Dev.	Reach		Project Presentations				
Dillon		*CP*				*MC*	*MH*		5 & 12 March, 9am-noon				
CH3103 - Validation in the Pharmaceutical and Medical Devices Industry													
Thu	**11am**	Validation			Med. Dev.		Validation						
AC216		*CP*			*MC*		*CP*						
CH3101 - Computers in Chemical Research													
Mon	**2pm**		Mol. Graph.	Excel		Spartan '10		e-Searching	PDB	VMD	Project	Project	
Finnegan PC Suite			*POL*	*HC*		*DC*		*POL*	*PC*	*DC*	Report	Presentation	
Fri	**2pm**	Introduction	Report Writing	Technical Writing	Plagiarism	Referencing	Presentations		Posters	Project Report		Project	
Finnegan PC Suite		*PF*	*AE*	*EM*	*PF*	*PF*	*PC*		*CP*			Presentation	