School of Physical and Chemical Sciences

UNIVERSITY OF CANTERBURY
Te Whare Wānanga o Waitaha
CHRISTCHURCH NEW ZEALAND

General Course Information | Ngā Whakamārama

CHEM 246
Introduction to Medicinal Chemistry

0.125 EFTS 15 Points
Second Semester 2022

Description | Whakamahuki
This course is an introduction to the basic concepts of Medicinal Chemistry, which forms the first course that is specific to the major in Medicinal Chemistry. The course will begin with a consideration of how many drugs/pharmaceuticals work. We will then undertake a structural survey of the biological macromolecules that drug molecules bind to in order to produce their desired effects. The possibilities and opportunities from 'drugging' biological macromolecules such as enzymes, nucleic acids and receptors will be discussed. The concept of pharmacokinetics, i.e. how the body affects a drug molecule after its administration, through various metabolic processes will be discussed. This introductory course will then close with a consideration of how Medicinal Chemists can optimise the molecular properties of a potential drug molecule to try and produce compounds that display enhanced desired biological effects in living organisms (*in vivo*).

Timetable | Wātaka
Lectures/Tutorials: Three contact hours of lectures/tutorials per week. Details to be confirmed on 'My Timetable' and the Web.

Students should note that in the Science Faculty that the average student is responsible for approximately 4.5 hours of additional study for each hour of lecture at the 300-level.

Course Coordinator | Kairuruku Akoranga
Dr Daniel Foley, *daniel.foley@canterbury.ac.nz*

Assessment | Aromatawai
Test 1 (TA Block): **30%**
Test 2 (JJ Block): **30%**
Exam (DF Block, and overarching concepts from the entire course): **40%**

Examination and Formal Tests | Ngā Whakamātautau Ōkawa
End of year Exam: Three hours, with questions from Daniel Foley, Jodie Johnston and Timothy Alison

Textbooks | Tuhinga
An Introduction to Medicinal Chemistry, Graham L. Patrick, Oxford University Press, Sixth Edition, 2017 Copies are available on reserve in the Engineering and Physical Sciences Library

Prerequisites
P: 15 points from CHEM212 or BCHM212.

Web-based resources
Various learning resources (lecture material, reference links, quizzes, discussion forums etc.) for this course are available via the University of Canterbury's *Learn (Ako)* web site -- http://learn.canterbury.ac.nz/. This site will also be used regularly as a means of communication and information distribution for all of your Canterbury courses. You should familiarise yourself with *Learn* as soon as possible.

Goal of the Course
This course aims to give students a broad introduction to the field of medicinal chemistry. The overall objective is give students an appreciation of how many drugs/pharmaceuticals work at a molecular level, and how molecular structure affects biological activity, both *in vitro* and *in vivo*. Specifically drug interactions with enzymes, nucleic acids and receptors will be dissected, and how biological activity can be assessed discussed. The course will also act as an introduction to pharmacokinetics, i.e. how the body affects a drug molecule after its administration. Molecular structure of drug molecules will be correlated with pharmacokinetic properties, and structural modifications to increase in vivo biological activity discussed.

Learning Outcomes
As a student in this course I will develop the ability to:

- analyse the macromolecular structures of enzymes, nucleic acids and some receptors
- evaluate how small molecules may bind to enzymes, nucleic acids or receptors
- evaluate the various biological effects that may arise from this binding
- conjecture structural modifications that may be made to a molecular structure to increase its binding affinity
- evaluate the uses and limitations of *in vitro* assays for biological activity
- contrast the range metabolic processes that a drug molecule may undergo when administered to a whole organism
- evaluate the origins and basis of Lipinski's rules of five
- identify functional groups and structural features of a molecule that make it incompatible with drug development
- identify structural modifications that may be made to a molecular structure to increase its likely effectiveness as a drug molecule *in vivo*
- synthesise a holistic understanding of how initial *in vitro* bioactivity may be translated into potentially beneficial *in vivo* biological effects

Transferable Skill Register
As a student in this course I will develop the following skills:

- analytical critical thinking and problem solving
- pattern spotting and logical analysis
- digital literacy
- working effectively and professionally with diverse communities written communication

Summary of the Course Content

The topics coved by this course are:

AN INTRODUCTION TO DRUGS AND DRUG TARGETS **(12 lectures/problem solving sessions)**

This part of the course will introduce you to drug molecules, and explain what they interact with in biological systems, and unravel the molecular basis of different types of binding interactions. The structure and functions of several important biological macromolecules (enzymes, receptors and nucleic acids) which are common targets for drug action will be summarised.

Lecturer: ***Dr Timothy Allison, timothy.allison@canterbury.ac.nz***

THE MOLECULAR BASIS OF BIOLOGICAL DRUG TARGETS **(12 lectures/problem solving sessions)**

This part of the course will consider the interactions of small molecule drugs with a range of biological targets. Small molecule drug interactions with enzymes, receptors and nucleic acids will be covered in detail, highlighting the molecular basis of these interactions and the biological effects that can result from drug action, including the different modes of enzyme inhibition, and agonism and antagonism of receptors.

Lecturer: ***Dr Jodie Johnston, jodie.johnston@canterbury.ac.nz***

PHARMACOKINETICS AND OPTIMISING DRUG ACTION **(12 lectures/problem solving sessions)**

Pharmacokinetics is the subject that describes how the body affects drug molecules after their administration, through absorption, distribution and metabolism. Often a drug molecule will display desired biological activity (for example as an enzyme inhibitor) when tested against an isolated biological target macromolecule in a test tube (*in vitro*), but little or none of the desired biological effects are observed when given to a whole organism (*in vivo*)! This part of the course will discuss how the molecular structure and properties of a drug molecule affect its pharmacokinetics and therefore govern its suitability for clinical development. Lipinski's rules of five will be discussed and their utility as a guide for drug development assessed. Methods for molecular structure optimisation to enhance desired *in vivo* biological activity and to improve drug pharmacokinetics will also be discussed.

Lecturer: Dr Daniel Foley, daniel.foley@canterbury.ac.nz

GENERAL INFORMATION 2022

Policy on 'Dishonest Practice'

The University has strict guidelines regarding 'dishonest practice' and 'breach of instructions' in relation to the completion and submission of examinable material. In cases where dishonest practice is involved in tests or other work submitted for credit a department may choose to not mark such work ('Academic Integrity and Breach of Instruction Regulations').

The School of Physical and Chemical Sciences upholds this policy. It considers plagiarism, collusion, copying, and ghost writing to be unacceptable and dishonest practices:

- ***Plagiarism*** is the presentation of any material (text, data or figures, on any medium including computer files) from any other source without clear and adequate acknowledgement of the source.
- ***Collusion*** is the presentation of work performed in whole, or in part, in conjunction with another person or persons, but submitted as if it has been completed by the named author alone. This interpretation is not intended to discourage students from having discussions about how to approach an assigned task and incorporating general ideas that come from those discussions into their own individual submissions, but acknowledgement is necessary.
- ***Copying*** is the use of material (in any medium, including computer files) produced by another person or persons with or without their knowledge and approval. **This includes copying of the lab reports (raw data may be shared within the group if permitted or required by the experiment) - data analysis and interpretation of obtained results MUST be performed individually.**
- ***Ghost writing*** is the use of other person(s) (with, or without payment) to prepare all or part of an item of work submitted for assessment.

Additional Information

Special consideration of assessment*:** If you feel that illness, injury, bereavement or any other critical extenuating circumstance beyond your control has prevented you from completing an item of assessment or affected your performance in that assessment, you may apply for special consideration. Special consideration is not available for items worth less than 10% of the course. Applications for special consideration should be made **within five days** of the due date for the work or examination. In the case of illness or injury, medical consultation should normally have taken place shortly before, or within 24 hours after, the due date for the required work or the date of the test or examination. For details on special consideration, or to make an application, refer to the Examinations Office website http://www.canterbury.ac.nz/exams/. ***You have the right to appeal any decision.

Extensions of deadlines: Where an extension may be granted for an assessment item, this will be decided by application to the course co-ordinator.

Late withdrawal from the course: If you are prevented by extenuating circumstances from completing the course after the final date for withdrawing from the course, you may apply for special consideration for late discontinuation. For details on special consideration, or to make an application, refer to the Examinations Office website

http://www.canterbury.ac.nz/exams/. Applications must be submitted ***within five days*** of the end of the main examination period for the semester.

Missing of tests**:** In rare cases a student will not be able to sit a test. In such cases, the student should consult with the course co-ordinator to arrange alternative procedures. **This must be done well in advance of the set date for the test.**

Past tests and exams: these can be found on our website using the link below:
www.chem.canterbury.ac.nz/for/undergraduate.shtml

Submission of reports and assignments**: Reports (including lab reports) and assignments should be handed in on time.** Extensions will be granted only in exceptional circumstances (such as illness or bereavement). If an extension is required, as early as possible you should request it from the lecturer concerned.
Note: If you do not submit an assignment for assessment, you will be allotted zero marks, which will affect your final result. You should ensure that you pick up marked assignments and keep them until the end of the course as evidence that the work was completed and marked in the case that either is disputed. To guard against accidental loss, it would be prudent to keep photocopies or electronic copies of anything submitted.

Late Work: Acceptance of late work will be at the discretion of the course coordinator. Please contact the coordinator if your assessment is likely to be late.

Marks and Grades: The following numbers should be considered as a guide to the expected grades under normal circumstances. The School reserves the right to adjust mark/grade conversions, if necessary.

Please note that for all invigilated assessments (tests and exams) worth 33% and above, failure to obtain a mark of at least 40% will result in a final grade no higher than an R at 100 and 200 level, and a C- at 300 level.

Grade:	**A+**	**A**	**A−**	**B+**	**B**	**B−**	**C+**	**C**	**C-**	**D**	**E**
Minimum mark %:	**90**	**85**	**80**	**75**	**70**	**65**	**60**	**55**	**50**	**40**	**0**

Reconsideration of Grades: Students should, in the first instance, speak to the course co-ordinator about their marks. If they cannot reach an agreeable solution, or have questions about their grade in a course, students should then speak to the Director of Undergraduate Studies, Assoc Prof Greg Russell (phone 3694228). Students can appeal any decision made on their final grade. You can apply at the Registry for reconsideration of the final grade within four weeks of the date of publication of final results. Be aware that there are time limits for each step of the appeals process.

Students with Disabilities: Students with disabilities should speak with someone at Equity and Disability Service, phone: 369 3334 (or ext. 93334), email: eds@canterbury.ac.nz).

Academic Advice**:** Assoc Prof Greg Russell is the coordinator of undergraduate chemistry courses. His interest is in the academic performance and well-being of all such students. Anyone experiencing problems with their chemistry courses or requiring guidance about their B.Sc. in Chemistry should get in contact with Greg.

Staff-Class Rep Liaison**:** Assoc Prof Greg Russell is in charge of liaison with students in chemistry courses. Your class will appoint a student representative to the liaison committee at the start of the semester. Please feel free to talk to the Academic Liaison or the student rep about any problems or concerns that you might have.

Greg Russell (greg.russell@canterbury.ac.nz, tel. 369 5129)
Director of Undergraduate Studies
School of Physical and Chemical Sciences
2022