

General Course Information | Ngā Whakamārama

CHEM 246

Introduction to Medicinal Chemistry

0.125 EFTS 15 Points
Second Semester 2023

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, + general concepts spanning 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 | Tuhiinga

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 covered 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 | TE KIMI MŌHIOHIO 2023

Policy on 'Dishonest Practice' | Ngā Takahitanga me ngā Tinihanga

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 – see the online guidelines in relation to '[Academic Integrity](#)'.

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

- **Plagiarism | Tārua Whānako** 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. Note that the use of **AI generative tools such as ChatGPT** for assessment work is *strictly forbidden*, except where the lecturer concerned has specifically granted approval.
- **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) (whether with or without payment) to prepare all or part of an item of work submitted for assessment.

Special consideration of assessment | Ngā Pairuri Motuhake

'[Special Consideration](#)' (previously termed 'Aegrotat Application') for an item of assessment is for students who have covered the work involved but have been prevented from demonstrating their knowledge or skills at the time of the assessment due to unforeseen circumstances, whether illness, injury, bereavement, car crash or any other extenuating circumstance *beyond one's control*. Special Consideration for a test/exam may be because a student has not sat it or has done so with impaired performance. Applications can be submitted via the above link and must be made **no later than five working days after the assessment due date**. Note that special consideration is **not available for items worth less than 10% of the overall course mark**. In the case of illness or injury, medical consultation should normally have taken place either shortly before or within 24 hours after the due date for the required work or test/examination.

Note that you may be required to sit a special exam or your grade may not be changed if there is insufficient evidence of your performance from other invigilated assessment items in the course. **You have the right to appeal any decision.**

It is important to understand that Special Consideration is only available *where course work has been covered*, and the inability to demonstrate this fully is both *no longer possible* AND is due to *unexpected circumstances beyond one's control*. Thus Special Consideration is **NOT available for:**

- essays, assignments or quizzes where an extension of time is available to complete the assessment item (see below for the process to involved);
- missed lectures during the semester;
- experiencing examination anxiety;
- having several examinations or assessments close together;
- known impairment, such as chronic illness (medical or psychological), injury or disability unless medical evidence confirms that the circumstances were exacerbated, despite appropriate management, at the time of assessment;
- mistaking the date or time of an examination (this is a circumstance one can control!);
- failing to turn up to an examination or test because of sleeping in (a circumstance as above!);
- where applications are repeatedly made for the same or similar reason, then the application may be declined on the grounds that the reason is not unexpected;
- where the application is made at the time of the assessment but the supporting documentation is received significantly after this date or after the date results are released; or
- the application is made following the release of results (unless under exceptional circumstances).

Extensions of deadlines | Tononga Wā Āpiti

Where an extension may be granted for an assessment item, this will be decided by application to the course co-ordinator and/or the lecturer concerned.

Late withdrawal from a 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 | Te Matangaro i ngā Whakamātautau

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

Past tests can be found on our [Chemistry Undergraduate](#) website. Past exams can be found on the [Library website](#).

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 for assessment will be at the discretion of the course coordinator and/or the lecturer concerned. If your assessment is likely to be late, please contact the relevant of these people **before the assessment is due**. Never assume that an extension will be automatically granted – some courses have the policy of no late work being accepted. A commonly exercised policy is to deduct 10% of the total marks for each day that the work is late, where weekends and public holidays also count as such days.

Marks and Grades | Taumata Ako

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; in general this requirement will not be applied at 300 level, but if it is then the course coordinator will inform the class and it will result in a final grade no higher than a C–.

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](#). 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 | Te Whaikaha

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

2023