School of Physical and Chemical Sciences

UNIVERSITY OF CANTERBURY
Te Whare Wānanga o Waitaha
CHRISTCHURCH NEW ZEALAND

General Course Information | Ngā Whakamārama

CHEM 347
Drug Discovery and Development

0.125 EFTS 15 Points
Second Semester 2022

Description | Whakamahuki
This course covers the drug discovery and development process, all the way from lead generation, to structure optimisation, synthetic production, and the protection and development of intellectual property. Topics to be covered include:

- lead generation
- chemical approaches to molecular diversity
- computers in drug discovery and development
- clinical trials and regulatory hurdles
- patenting and intellectual property protection and development
- process chemistry
- the development and use of native flora and fauna as part of the drug discovery process including, ethical, legal and intellectual property issues around indigenous knowledge in such cases will be discussed, both with respect to New Zealand and in a wider global context
- obligations under the Treaty of Waitangi, and associated Treaty Claims
- the un-resolved treaty claim Wai262 will be discussed.

A key aspect of this **Capstone Course** is a mock drug discovery exercise which will require students to apply all of the knowledge and understanding they have acquired in the previous parts of the Medicinal Chemistry program. Therefore, during the second part of the course students will be assigned to a small team, who together will represent a start-up pharmaceutical company. Each student will actively participate in an interactive drug discovery and development process, mimicking all aspects the real-world situation.

Timetable | Wātaka
Lectures and tutorials: Four contact hours per week (weeks 1-2 and 5-6); two contact hours in weeks 3 and 4. Details to be confirmed on 'My Timetable' and the Web.
Computer labs: Two hours in weeks 3 and 4. Details to be confirmed on 'My Timetable' and the Web.
Group sessions: Two hours per week (weeks 7-12). 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
Professor Antony Fairbanks, Room West 801 ext 92517, ***antony.fairbanks@canterbury.ac.nz***

Assessment | Aromatawai

Assignments:	60%
Oral presentation:	10%
Exam:	30%

Examination and Formal Tests | Ngā Whakamātautau Ōkawa
End of year Exam: Two hours, with questions from Rudi Marquez, Tim Allison, and Antony Fairbanks

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: CHEM246, CHEM346
R: None

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 (Ako)* as soon as possible.

Goal of the Course
Students who follow this course will develop a complete understanding of the drug discovery and development process. This is a capstone course of the Medicinal Chemistry program, that will require students to use knowledge and understanding that have developed in earlier Medicinal Chemistry courses (CHEM246, CHEM346), and to assimilate this with new information presented here. At the conclusion of the course students should have a complete appreciation of the drug discovery process, all the way from initial molecular lead generation, through molecular optimisation and synthetic production, to clinical approval and therapeutic administration. The course will also introduce students to important ethical, legal and regulatory processes encountered along the drug discovery pathway.

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

- appraise how lead compounds may be identified from screening processes
- investigate how modern synthetic chemistry approaches lead to the creation of molecular diversity
- demonstrate the principles and practicalities of solid-supported synthesis
- investigate the use of state-of-the-art computer software for the manipulation of protein crystal structures and molecular docking processes
- critique the different types of intellectual property, and how they may be protected and exploited, both globally and with respect to Mātauranga Māori
- demonstrate obligations under the Treaty of Waitangi
- respect and value Treaty Claims and the Treaty Claims process
- appraise other ethical issues relating to drug development and their commercial exploitation
- critique regulatory hurdles and the clinical trial process
- synthesise all aspects of material covered in the Medicinal Chemistry program to a mock drug development exercise

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
- planning
- creativity
- teamworking and cooperation
- working effectively and professionally with diverse communities
- bicultural competence
- innovation
- entrepreneurship
- written communication
- oral communication, including answering questions posed by a panel of assessors

Summary of the Course Content

The topics coved by this course are:

LEAD GENERATION AND DIVERSITY ORIENTATED SYNTHESIS **(8 lectures)**
This part of the course will consider how the medicinal chemistry process begins. We will consider how compounds with desired biological activity are first identified. This may be either from screening libraries of synthetic compounds or natural products. The production of synthetic compound libraries for screening will be discussed using diversity orientated synthesis, including an introduction to solid-supported chemical synthesis. Some pitfalls and limitations of the production of simple compound libraries will be discussed, alongside next generation approaches to exploration of diverse of 3D molecular structures.
Lecturer: Professor Rudi Marquez, ext 90162, *rudi.marquez@canterbury.ac.nz*

COMPUTER AIDED DRUG DESIGN **(2 lectures plus 2 computer labs)**
The use of computer modelling is now considered to be an integral part of the drug discovery process. This part of the course will consider how computers may aid drug design and optimisation in cases where 3-D information is available for the molecular target. This will include hands-on experience of the use and manipulation of protein crystal structures and simple molecular docking software.
Lecturer: Dr Timothy Allison, ext *93034, timothy.allison@canterbury.ac.nz*

LEGAL AND ETHICAL ISSUES: INDIGENOUS KNOWLEDGE AND THE TREATY OF WAITANG **(2 lectures)**
The development and use of native flora and fauna as part of the drug discovery process will be considered as an example of the importance of the consideration of the rights of indigenous peoples, both in NZ and globally. Ethical, legal and intellectual property issues around indigenous knowledge in such cases will be discussed, both with respect to New Zealand and in a wider global context. In an NZ-context obligations arising from the Treaty of Waitangi will be discussed, including associated Treaty Claims, such as the un-resolved treaty claim Wai262.
Lecturers: Dr Abby Suszko, ext 95819, abby.suszko@canterbury.ac.nz
Dr David Jefferson, ext 90820, david.jefferson@canterbury.ac.nz

LEGAL AND REGULATORY PROCESSES: INTELLECTUAL PROPERTY PROTECTION AND DEVELOPMENT AND CLINICAL TRIALS **(6 lectures)**
This part of the course will provide an overview of the regulatory, legal, clinical and business aspects of the drug development process, and the practicalities of the pharmaceutical business world. It will include a discussion of Intellectual property protection, development, and exploitation, including the PCT process. Progression of a drug through toxicology screening and clinical trials – Phase I, II and III – and the final processes and hurdles encountered before entering the clinic will be discussed. The process of regulatory approval will be discussed, including the requirement to adhere codes of Good Manufacturing Practice and Good Laboratory Practice. Process chemistry will be introduced, highlighting the very different issues that need to be considered when synthesis is scaled up. Finally the business world will be introduced; funding drug development; corporate structure and roles.
Lecturer: Professor Antony Fairbanks, ext 92517, *antony.fairbanks@canterbury.ac.nz*

MOCK DRUG DISCOVERY EXCERISE **(6 x 2hr weekly interactive sessions, split into groups of 4/5)**
This section of the course will be highly interactive, and will comprise group and individual activities as a mock drug development process is undertaken. Students will be split into small groups to work together, and each will be charged with the establishment of a small 'Pharmaceutical Company' the main goal of which will be the development of a new drug against a specific therapeutic target. Each week the teams will be given data on four lead molecular structures what have been tested against a specific drug-target; their group task for the following week will be to suggest four new compounds for testing in order to improve their drug candidates' properties. Each week feedback will be given to the groups on predicted *in vitro* biological activities of their four compounds, together with key toxicological and pharmacokinetic properties of the molecules identified. There will be four iterations of this process altogether, after which each group must identify their lead development compound.

During the drug development process each group member will also be assigned a specific role within the company role. They will be required to perform a specific role-related task during the program, and write a final report on their activities within this role.

This part of the course will be assessed by two written reports from each group member (one on their specific task, and one on their group's drug development program) and oral presentations by each group member to a panel of assessors.

Lecturers: Professor Steven Bull, Erskine Visitor, University of Bath, UK
Professor Antony Fairbanks, ext 92517, *antony.fairbanks@canterbury.ac.nz*

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 ('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 | 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.
- ***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 | Ngā Pairuri Motuhake*:** 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 | Tononga Wā Āpiti: 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 | 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: 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 | 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, 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 | 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
2022