



# CHEM3801

## Medicinal Chemistry

Session 1, In person-scheduled-weekday, North Ryde 2022

*School of Natural Sciences*

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## General Information

Unit convenor and teaching staff

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Credit points

10

Prerequisites

(CHEM2601 or CBMS203 or CBMS204) and 10cp in CBMS or BMOL or CHEM units at 2000 level or above

Corequisites

Co-badged status

CHEM6801 Medicinal Chemistry

### Unit description

Medicinal chemistry is the application of chemistry to the discovery, design and synthesis of new drugs. This unit is of value to all molecular sciences and medical sciences students. The central core of the unit is the description of methods used for the discovery of new drugs, how these are modified to produce more active compounds, transportation to and from their points of action and how they are cleared from the body. Topics include: the structure and function of biological targets (proteins and DNA); sources of new drugs from nature; and lead generation and methods of lead modification to make more active, selective or less toxic drugs. This is followed by a study of structure-activity relationship methods; pharmacokinetics, drug metabolism and prodrugs, and chemical genetics. Case studies are also provided, including antibacterial and anticancer agents, and nucleic acid therapies. The theory is complemented by a discovery-based laboratory project incorporating synthetic chemistry, spectroscopic methods, bioassays and computational chemistry to elucidate the essential structural features necessary for the sulfonamide class of antibacterial agents.

## Important Academic Dates

Information about important academic dates including deadlines for withdrawing from units are available at <https://www.mq.edu.au/study/calendar-of-dates>

## Learning Outcomes

On successful completion of this unit, you will be able to:

**ULO1:** Describe the structure and function of biological targets and the interaction of drugs or drug leads with these targets at a molecular level; methods of drug discovery and development; qualitative and quantitative structure-activity relationship methods; pharmacokinetics; the design of more active, selective or less toxic drugs; drug metabolism and prodrugs; and the mechanism of action of specific classes of drugs.

**ULO2:** Analyse data and solve problems using medicinal chemistry principles.

**ULO3:** Use the primary literature and scientific databases (SciFinder and Reaxys) to plan and execute the synthesis of druglike molecules and undertake literature reviews.

**ULO4:** Execute laboratory skills (synthesis, purification and instrumental and spectral analysis) in a safe manner, accurately record laboratory observations in an appropriate scientific manner, and analyse experimental results to solve related problems.

**ULO5:** Work with peers to conduct group work in an efficient, collaborative and equitable fashion.

**ULO6:** Communicate medicinal chemistry concepts competently in oral presentations and in written format in exams, tests and laboratory reports and communicate conclusions based on experiments in the form of written reports.

## General Assessment Information

**NOTE: Late submissions will be accepted (with penalties) ONLY for assessment tasks related to "Practical Work".**

### General Faculty Policy on assessment submission deadlines and late submissions:

Online quizzes, in-class activities, or scheduled tests and exams must be undertaken at the time indicated in the unit guide. Should these activities be missed due to illness or misadventure, students may apply for Special Consideration.

All other assessments must be submitted by 5:00 pm on their due date. Should these assessments be missed due to illness or misadventure, students should apply for Special Consideration.

Assessments not submitted by the due date will receive a mark of zero **unless** late submissions are specifically allowed as indicated in the unit guide or on iLearn.

If late submissions are permitted as indicated in the unit guide or on iLearn a consistent penalty will be applied for late submissions as follows:

A 12-hour grace period will be given after which the following deductions will be applied to the awarded assessment mark: 12 to 24 hours late = 10% deduction; for each day thereafter, an additional 10% per day or part thereof will be applied until five days beyond the due date. After this time, a mark of zero (0) will be given. For example, an assessment worth 20% is due 5 pm on 1 January. Student A submits the assessment at 1 pm, 3 January. The assessment received a mark of 15/20. A 20% deduction is then applied to the mark of 15, resulting in the loss of three (3) marks. Student A is then awarded a final mark of 12/20.

## Assessment Tasks

Name	Weighting	Hurdle	Due
<a href="#"><u>Spectroscopy Training</u></a>	0%	No	1 April
<a href="#"><u>Quizzes</u></a>	5%	No	Weeks 3,5,7,9,11 (see due dates in iLearn)
<a href="#"><u>Mid-semester test</u></a>	15%	No	Week 7
<a href="#"><u>Pharmaceutical agent presentation</u></a>	5%	No	Week 11
<a href="#"><u>Practical work</u></a>	25%	No	3 June
<a href="#"><u>Final Examination</u></a>	50%	No	Formal Examination Period

## Spectroscopy Training

Assessment Type <sup>1</sup>: Participatory task

Indicative Time on Task <sup>2</sup>: 7 hours

Due: **1 April**

Weighting: **0%**

All students are required to undertake the Kahn Academy course on spectroscopy before week 7.

On successful completion you will be able to:

- Execute laboratory skills (synthesis, purification and instrumental and spectral analysis) in a safe manner, accurately record laboratory observations in an appropriate scientific manner, and analyse experimental results to solve related problems.

## Quizzes

Assessment Type <sup>1</sup>: Quiz/Test

Indicative Time on Task <sup>2</sup>: 5 hours

Due: **Weeks 3,5,7,9,11 (see due dates in iLearn)**

Weighting: **5%**

Quizzes allow identification of any deficiency in knowledge and understanding and to encourage continuous learning of the lecture material without the stress of a significant assessment component.

On successful completion you will be able to:

- Describe the structure and function of biological targets and the interaction of drugs or drug leads with these targets at a molecular level; methods of drug discovery and development; qualitative and quantitative structure–activity relationship methods; pharmacokinetics; the design of more active, selective or less toxic drugs; drug metabolism and prodrugs; and the mechanism of action of specific classes of drugs.
- Communicate medicinal chemistry concepts competently in oral presentations and in written format in exams, tests and laboratory reports and communicate conclusions based on experiments in the form of written reports.

## Mid-semester test

Assessment Type <sup>1</sup>: Quiz/Test

Indicative Time on Task <sup>2</sup>: 10 hours

Due: **Week 7**

Weighting: **15%**

Mid-semester Test will cover unit content up to and including week 7.

On successful completion you will be able to:

- Describe the structure and function of biological targets and the interaction of drugs or drug leads with these targets at a molecular level; methods of drug discovery and development; qualitative and quantitative structure–activity relationship methods; pharmacokinetics; the design of more active, selective or less toxic drugs; drug metabolism and prodrugs; and the mechanism of action of specific classes of drugs.
- Analyse data and solve problems using medicinal chemistry principles.

## Pharmaceutical agent presentation

Assessment Type <sup>1</sup>: Presentation

Indicative Time on Task <sup>2</sup>: 5 hours

Due: **Week 11**

Weighting: **5%**

Students will deliver an oral presentation on a clinically used pharmaceutical agent, providing information on its structure and function at a molecular level. Peer feedback will be provided.

On successful completion you will be able to:

- Describe the structure and function of biological targets and the interaction of drugs or drug leads with these targets at a molecular level; methods of drug discovery and development; qualitative and quantitative structure–activity relationship methods; pharmacokinetics; the design of more active, selective or less toxic drugs; drug metabolism and prodrugs; and the mechanism of action of specific classes of drugs.
- Use the primary literature and scientific databases (SciFinder and Reaxys) to plan and execute the synthesis of druglike molecules and undertake literature reviews.
- Work with peers to conduct group work in an efficient, collaborative and equitable

fashion.

- Communicate medicinal chemistry concepts competently in oral presentations and in written format in exams, tests and laboratory reports and communicate conclusions based on experiments in the form of written reports.

## Practical work

Assessment Type <sup>1</sup>: Lab report

Indicative Time on Task <sup>2</sup>: 20 hours

Due: **3 June**

Weighting: **25%**

The practical work (synthesis and antibacterial structure activity relationship of sulfonamides) will be conducted in small groups. Students will be required to maintain good laboratory notes, perform risk assessments and have safe laboratory practices. Each group will develop a written justification of their choice of final target compounds and possible synthetic procedures, will submit a short introductory report, formal write up of an experimental procedure, and a final group report. This assessment item counts 25%, of which 15% is for individual performance and 10% for group performance.

On successful completion you will be able to:

- Describe the structure and function of biological targets and the interaction of drugs or drug leads with these targets at a molecular level; methods of drug discovery and development; qualitative and quantitative structure–activity relationship methods; pharmacokinetics; the design of more active, selective or less toxic drugs; drug metabolism and prodrugs; and the mechanism of action of specific classes of drugs.
- Analyse data and solve problems using medicinal chemistry principles.
- Use the primary literature and scientific databases (SciFinder and Reaxys) to plan and execute the synthesis of druglike molecules and undertake literature reviews.
- Execute laboratory skills (synthesis, purification and instrumental and spectral analysis) in a safe manner, accurately record laboratory observations in an appropriate scientific manner, and analyse experimental results to solve related problems.
- Work with peers to conduct group work in an efficient, collaborative and equitable fashion.
- Communicate medicinal chemistry concepts competently in oral presentations and in written format in exams, tests and laboratory reports and communicate conclusions based on experiments in the form of written reports.

## Final Examination

Assessment Type <sup>1</sup>: Examination

Indicative Time on Task <sup>2</sup>: 20 hours

Due: **Formal Examination Period**

Weighting: **50%**

The final examination will be in the regular university examination period. This will assess specific understanding and holistic concepts of all the topics presented within the course and an opportunity for you to show what knowledge you have obtained and how you can apply this in new situations to solve complex problems.

On successful completion you will be able to:

- Describe the structure and function of biological targets and the interaction of drugs or drug leads with these targets at a molecular level; methods of drug discovery and development; qualitative and quantitative structure–activity relationship methods; pharmacokinetics; the design of more active, selective or less toxic drugs; drug metabolism and prodrugs; and the mechanism of action of specific classes of drugs.
- Communicate medicinal chemistry concepts competently in oral presentations and in written format in exams, tests and laboratory reports and communicate conclusions based on experiments in the form of written reports.

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<sup>1</sup> If you need help with your assignment, please contact:

- the academic teaching staff in your unit for guidance in understanding or completing this type of assessment
- the [Writing Centre](#) for academic skills support.

<sup>2</sup> Indicative time-on-task is an estimate of the time required for completion of the assessment task and is subject to individual variation

## Delivery and Resources

CHEM3801 Medicinal Chemistry is a 10 credit point unit requiring 150 hours of work over the semester (formal contact hours and self study time). This is an average of 10 hours of work per week over each of the 15 weeks of semester. Formal contact hours for CHEM3801 consist of 2 hours of lectures and a 1-hour interactive tutorial (SGTA) per week, along with 7 x 4-hour laboratory classes throughout semester. Students are expected to participate in all lectures, tutorials and laboratory classes. Active participation by students in all of these activities will be essential for success in the unit.



## Lectures

The unit will cover 2 hours of lecture material each week. Some lecture material will be available on the unit web site, while other material will be provided during the lecture classes. You should use these lectures as a starting point and supplement their content with material from the text book, the scientific literature and from other online sources. Much of the unit content builds on content covered in previous weeks, so it will be essential to keep up to date with the lecture material throughout the semester.

## Interactive Tutorials (SGTAs)

A 1-hour interactive tutorial (SGTA) will be held each week. This is your opportunity to interact directly with the teaching staff, to ask lots of pertinent questions and to identify any weaknesses or clarify misconceptions you may have. Learning is an active process, and as such, you must engage with the material. This means reading the textbook (and beyond) before and after lectures, attempting the assignment questions and discussing the concepts with your classmates and lecturers. Do not be afraid to ask questions – everyone benefits from a robust and open discussion of the topics. Five short quizzes (each worth 1% of the unit total) will also be run throughout semester. The quizzes may include any material that has been covered in the unit up to that point, so you are expected to keep up to date with lectures and to revise course material each week. The quizzes are designed to help you to learn continuously and to identify what you understand and the areas that you need to spend more time on, with minimal assessment penalty.

## Laboratory Classes

Laboratory classes will be conducted in small teams and require a highly collaborative and investigative approach. You will be designing and synthesising a series of sulfonamide antibiotics and subsequently testing them for antibacterial activity to determine the important features for their antibacterial activity. This laboratory work is designed to give real-world experience in research by involving you in the design of the experiments, using literature procedures as a guide, and troubleshooting to identify the best experimental conditions. The classes will emphasise the importance of teamwork and being well prepared and efficient. You will need to be fully aware of safety procedures, proper recording and reporting of raw data and interpretation of results. This will require an analytical and inquisitive approach. The first (dry) laboratory class starts in Week 1, where you will meet your fellow team members, plan your synthetic routes and complete risk assessments. There will then be a series of wet labs sessions run throughout semester. Please refer to the iLearn site for a detailed schedule. The final (dry) laboratory class will bring all the teams back together to discuss their results and to finalise the laboratory reports. To maximise the amount of wet lab time available to complete the experiments, you will need to be highly organised and to have prepared thoroughly BEFORE entering the laboratory. If you are not able to "hit the ground running" each laboratory class, you risk running out of time by the end of semester.

## Unit Web Page

The web page for this unit can be found at [ilearn.mq.edu.au](https://ilearn.mq.edu.au).

Login with your MQ student ID number and password, then follow the prompts to "CHEM3801 Medicinal Chemistry."

During semester, the CHEM3801 iLearn site will be used to communicate important information to you. It is your responsibility to regularly check the iLearn site for important announcements and updates.

## Unit Text Book

"An Introduction to Medicinal Chemistry" by Graham L. Patrick, Sixth Edition, Oxford University Press 2017.

The text book may be purchased from [www.booktopia.com.au](http://www.booktopia.com.au) or other book shops. Limited copies of the text book are also available in the MQ Library.

## Off-shore students

Off-shore students **must** email the convenor as soon as possible to discuss study options.

## COVID Information and on-campus classes

On-campus teaching continues to be scheduled for Session 1, 2022. Masks are compulsory for all classes in indoor spaces and social distancing will be implemented wherever possible. Students will also be required to sanitise surfaces before and after use.

Students are requested to minimise the risk of spreading COVID to themselves and others in accordance with the university and NSW Health guidelines: <https://www.mq.edu.au/about/corona-virus-faqs> and <https://www.nsw.gov.au/covid-19/stay-safe>.

Any further requirements or changes to units in relation to COVID will be communicated to students via iLearn.

## Policies and Procedures

Macquarie University policies and procedures are accessible from [Policy Central \(https://policies.mq.edu.au\)](https://policies.mq.edu.au). Students should be aware of the following policies in particular with regard to Learning and Teaching:

- [Academic Appeals Policy](#)
- [Academic Integrity Policy](#)
- [Academic Progression Policy](#)

- [Assessment Policy](#)
- [Fitness to Practice Procedure](#)
- [Assessment Procedure](#)
- [Complaints Resolution Procedure for Students and Members of the Public](#)
- [Special Consideration Policy](#)

Students seeking more policy resources can visit [Student Policies](https://students.mq.edu.au/support/study/policies) (<https://students.mq.edu.au/support/study/policies>). It is your one-stop-shop for the key policies you need to know about throughout your undergraduate student journey.

To find other policies relating to Teaching and Learning, visit [Policy Central](https://policies.mq.edu.au) (<https://policies.mq.edu.au>) and use the [search tool](#).

## Student Code of Conduct

Macquarie University students have a responsibility to be familiar with the Student Code of Conduct: <https://students.mq.edu.au/admin/other-resources/student-conduct>

## Results

Results published on platform other than [eStudent](#), (eg. iLearn, Coursera etc.) or released directly by your Unit Convenor, are not confirmed as they are subject to final approval by the University. Once approved, final results will be sent to your student email address and will be made available in [eStudent](#). For more information visit [ask.mq.edu.au](http://ask.mq.edu.au) or if you are a Global MBA student contact [globalmba.support@mq.edu.au](mailto:globalmba.support@mq.edu.au)

## Academic Integrity

At Macquarie, we believe [academic integrity](#) – honesty, respect, trust, responsibility, fairness and courage – is at the core of learning, teaching and research. We recognise that meeting the expectations required to complete your assessments can be challenging. So, we offer you a range of resources and services to help you reach your potential, including free [online writing and maths support](#), [academic skills development](#) and [wellbeing consultations](#).

## Student Support

Macquarie University provides a range of support services for students. For details, visit <http://students.mq.edu.au/support/>

## The Writing Centre

[The Writing Centre](#) provides resources to develop your English language proficiency, academic writing, and communication skills.

- [Workshops](#)
- [Chat with a WriteWISE peer writing leader](#)
- [Access StudyWISE](#)
- [Upload an assignment to Studiosity](#)
- [Complete the Academic Integrity Module](#)

The Library provides online and face to face support to help you find and use relevant information resources.

- [Subject and Research Guides](#)
- [Ask a Librarian](#)

## Student Services and Support

Macquarie University offers a range of [Student Support Services](#) including:

- [IT Support](#)
- [Accessibility and disability support](#) with study
- Mental health [support](#)
- [Safety support](#) to respond to bullying, harassment, sexual harassment and sexual assault
- [Social support including information about finances, tenancy and legal issues](#)

## Student Enquiries

Got a question? Ask us via [AskMQ](#), or contact [Service Connect](#).

## IT Help

For help with University computer systems and technology, visit [http://www.mq.edu.au/about\\_us/offices\\_and\\_units/information\\_technology/help/](http://www.mq.edu.au/about_us/offices_and_units/information_technology/help/).

When using the University's IT, you must adhere to the [Acceptable Use of IT Resources Policy](#). The policy applies to all who connect to the MQ network including students.

## Changes from Previous Offering

Prof. Peter Karuso will no longer be teaching in this unit. A/Prof. Koushik Venkatesan will teach a new section on metals in medicine.