



# CHEM3801

## Medicinal Chemistry

Session 1, Weekday attendance, North Ryde 2020

*Department of Molecular Sciences*

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## General Information

### Unit convenor and teaching staff

Unit Convenor

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Fiday 2-6 PM

Lecturer

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Have an open door policy, but students are encouraged to arrange a meeting via email

Lecturer/Demonstrator

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4WW 334

Have an open door policy, but students are encouraged to arrange a meeting via email

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

### 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.

## Assessment Tasks

### Coronavirus (COVID-19) Update

Assessment details are no longer provided here as a result of changes due to the Coronavirus (COVID-19) pandemic.

Students should consult [iLearn](#) for revised unit information.

[Find out more about the Coronavirus \(COVID-19\) and potential impacts on staff and students](#)

## General Assessment Information

### Spectroscopy Training

Due: **April 7**

Weighting: **0%**

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

1. Please start this task in week 1 and make a plan to complete all modules by the end of week 6.

<https://www.khanacademy.org/science/organic-chemistry/spectroscopy-jay>.

### Provisional Patent Application

Due: Week 1, Week 7, Week 14

Weighting: **25%**

The practical work (synthesis and antibacterial structure activity relationship of sulfonamides) will be conducted in groups, with ~6 people per group.

1. You will prepare a group report in the style of a PATENT application by **midday Week 14, Tuesday June 10 (5% group mark and 5% individual mark)**. This will also require submission of every group member's labbook as well as the FINAL patent application.
2. By the end of **Week 1**, each group will develop a written justification of their choice of final target compounds (2 compounds per student) and possible synthetic procedures (this contributes to your participation mark under point 3).
3. By the end of **week 7**, individual laboratory notebooks (hardcopy) will be submitted for marking **AND** each group will submit a formal write up of the experimental procedure ("Examples" section of the patent) for the synthesis of **ONE** of your sulfonamide final products for EACH student, including spectral data, written out in a chemistry Journal

format. So if you have 6 group member, 6 examples are required (**5% individual mark, no group mark**). The Examples sections needs to be provided as one group document though marks will be allocated to individuals for their contribution. In addition, each group will submit the "Technical Field", "Background of the Invention" and "Object of the Invention" sections as hard-copy (not through turn-it-in) of their group's patent, written in patent format (**5% group mark**).

4. By **midday week 14, Tuesday June 11**, individual laboratory notebooks will be submitted for marking (**5% individual mark**). General safety and participation in the laboratory will also be considered in the mark. ,

Full details on what is expected for assessment of the practical component is provided in the laboratory manual and on the web site (see under "Laboratory Notes").

## Mid-semester test

Due: **April 28**

Weighting: **15%**

There will be a 50 minute test (**15%**) in **Week 8, Tuesday May 28, 8 AM in the lecture session**. This will cover up to the end of prodrugs. This is designed to give you specific feedback on your understanding of the topics up to this stage to assist you in your further study of the unit.

## Quizzes

Due: in lectures and online

Weighting: **5%**

Short quizzes (**5%**) may be conducted at any time. Quizzes will also be conducted online. They are to 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. Quizzes may contain questions from the spectroscopy workshop.

## Pharmaceutical Agent Presentation

Due: **May 12**

Weighting: **5%**

You will present a short oral on a clinically used pharmaceutical agent, providing information on its structure and function at a molecular level. Peer feedback will be provided. This will be conducted in the **week 10 May 12** lecture/tutorial class session (**8-10 AM**). This will help in your consolidation of the medicinal chemistry concepts taught. The format is 3 minutes and 3

powerpoint slides including references.

## Final exam

Due: week 15 (to be confirmed)

Weighting: **50%**

The final exam (/50%) will be 3 hours in length with 10 minutes reading time. It is designed to 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.

## Delivery and Resources

### Coronavirus (COVID-19) Update

Any references to on-campus delivery below may no longer be relevant due to COVID-19.

Please check here for updated delivery information: [https://ask.mq.edu.au/account/pub/display/unit\\_status](https://ask.mq.edu.au/account/pub/display/unit_status)

## Unit Web Page

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

Just login and follow the prompts to CHEM3801/6801 Medicinal Chemistry.

You can use any web browser such as Firefox, Internet Explorer or Safari to login.

iLearn is the name for Macquarie University's Learning Management System (LMS). The iLearn online learning environment enables learning, teaching, communication and collaboration. It is used to make lecture notes, laboratory notes, discussion forums, digital lecture recordings and other learning resources available to students online.

## General

CHEM3801 is a 10 credit point unit and will require an average of 10 hours of work (contact and self study time) per week over the 15 weeks. For students with weak chemistry backgrounds, more time per week will probably be necessary to perform satisfactorily in this unit. CHEM3801 is run with three hours of lectures/tutorials per week, along with 4 hour blocks of laboratories/workshops. Students are expected to attend all lectures, tutorials and laboratory classes. Active participation by the students in all of these fora is encouraged.

- Lectures will be presented as a combination of formal lectures and interactive tutorial sessions. Some lecture material will be available on the unit web site, while other material will be provided in the lecture class. 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 other questions, 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.

- Quizzes and a mid session test will also be run in the lecture session. The in class quizzes will cover any material prior to that day's lecture, therefore all students are expected to keep up to date with lecture material through revision each week. Online quizzes are also provided, with accompanying resources. The quizzes and mid session test are designed to allow you to continuously learn and to identify what you understand and the areas that you need to spend more time on, with minimal assessment penalty.
- All laboratory experiments will be conducted in groups. These have a highly collaborative and investigative approach, where you will be designing and synthesising a series of sulfonamides and subsequently testing them for antibacterial activity to determine the important features for their antibacterial activity. This laboratory work is designed to give real life experiences in research by involving students in the design of the experiments, using literature procedures as a guide, and trouble-shooting to identify the best experimental conditions. It will emphasise the importance of being well prepared, efficient and being fully aware of all safety procedures, proper recording and reporting of all data and interpreting of all results, and having an analytical and inquisitive approach. There will be 6 wet labs run in two streams (A and B) starting in Weeks 2/3. There will be 7 dry labs. The first one is in the 1000-level labs in week 1 (Friday 2-6PM) for the whole class where the semester's lab work will be planned for your group. Bring your laptop. Another 6 dry labs to write up results and draft the patent will be held in the 2000/3000-level writeup room starting in weeks 3/2.

Further information on technology used: You are expected to access the unit web site frequently. This contains important information including notes on the topics to be covered; the laboratory manual; What You Need to Know Sheets; your marks for practicals, quizzes and the mid-session exam; and past exam papers, including with answers. Additionally, the web site will also be used to post important messages and links to internet facilities and sites of relevance to the course, downloadable software, and lots of other interesting material.

All students are required to undertake the Kahn Academy course on spectroscopy before the end of the mid-semester break <https://www.khanacademy.org/science/organic-chemistry/spectroscopy-jay>. There are also resources in the library (PDF file in special reserve to help you with this).

If you do not have your own computer you may wish to access the Medicinal Chemistry web resources on campus using the PC computers in the Library or in the computer laboratories in 17 Wally's Walk. To view notes on all the topics and past exams on the unit web site, you will

require Adobe Acrobat Reader Version 10 or later to be installed on your computer. Acrobat Reader can be downloaded from the Adobe web site <https://get.adobe.com/reader/?loc=uk>. If you are using the computers in the library, then Acrobat has already been installed. Please note information will also be sent by email to your student email account so please look at your email account on a frequent basis.

You are expected to access SciFinder Scholar and Reaxys to assist in searching the literature. These are available through the library web site.

Hand-held calculators will be occasionally used in tutorials and practicals, for tests and in the final examination. Note that text-retrieval calculators are not allowed in the in-semester tests or final examination.

## Unit Schedule

### Coronavirus (COVID-19) Update

The unit schedule/topics and any references to on-campus delivery below may no longer be relevant due to COVID-19. Please consult [iLearn](#) for latest details, and check here for updated delivery information: [https://ask.mq.edu.au/account/pub/display/unit\\_status](https://ask.mq.edu.au/account/pub/display/unit_status)

### Topics Lecturer

### Lect/Tut

- |   |         |       |
|---|---------|-------|
| • Overview of Medicinal Chemistry                                       | wk 1-2  | PK/JJ |
| ◦ Cellular targets of bioactive compounds                               |         |       |
| ◦ Binding of drugs to their targets                                     |         |       |
| ◦ Agonists and antagonists  |         |       |
| • Protein structure and function  | wk 2-3  | JJ    |
| ◦ Enzyme kinetics   |         |       |
| ◦ Interaction of enzymes with inhibitors (competitive, non-competitive) |         |       |
| • Nucleic acids   | wk 4    | JJ    |
| • Drug discovery from nature  | wk 5-8  | JJ    |
| ◦ Drugs from synthesis  |         |       |
| ◦ Optimisation of lead compound, structure-activity relationships       |         |       |
| ◦ Physicochemical properties of drugs                                   |         |       |
| ◦ Drug absorption, distribution, metabolism and excretion               |         |       |
| ◦ Prodrugs  |         |       |
| • Mid-semester test   | wk 8    | JJ    |
| • Quantitative structure-activity relationships                         | wk 9-10 | PK    |
| ◦ Case Study 1 (G-coupled protein receptor agonists and antagonists)    |         |       |
| • 3 minute Pharmaceutical agent presentations                           | wk 10   | PK/JJ |



- Combinatorial Chemistry wk 11 PK
  - Case Study 2 (Combinatorial discovery of non-peptide binding elements to Src SH3 domains)
  - Case Study 3 (antiviral prodrugs; the Case Study of Wuhan Coronavirus)
- Antibacterial agents wk 12-13 AP
  - Case Study 4 (betalactam antibiotics)
  - Case Study 5 (antifungals)

## Policies and Procedures

Macquarie University policies and procedures are accessible from [Policy Central \(https://staff.mq.edu.au/work/strategy-planning-and-governance/university-policies-and-procedures/policy-central\)](https://staff.mq.edu.au/work/strategy-planning-and-governance/university-policies-and-procedures/policy-central). 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](#)
- [Grade Appeal Policy](#)
- [Complaint Management Procedure for Students and Members of the Public](#)
- [Special Consideration Policy](#) (**Note:** *The Special Consideration Policy is effective from 4 December 2017 and replaces the Disruption to Studies Policy.*)

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

If you would like to see all the policies relevant to Learning and Teaching visit [Policy Central \(https://staff.mq.edu.au/work/strategy-planning-and-governance/university-policies-and-procedures/policy-central\)](https://staff.mq.edu.au/work/strategy-planning-and-governance/university-policies-and-procedures/policy-central).

## Student Code of Conduct

Macquarie University students have a responsibility to be familiar with the Student Code of Conduct: <https://students.mq.edu.au/study/getting-started/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)

## Student Support

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

### Learning Skills

Learning Skills ([mq.edu.au/learningskills](http://mq.edu.au/learningskills)) provides academic writing resources and study strategies to help you improve your marks and take control of your study.

- [Getting help with your assignment](#)
- [Workshops](#)
- [StudyWise](#)
- [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

Students with a disability are encouraged to contact the [Disability Service](#) who can provide appropriate help with any issues that arise during their studies.

## Student Enquiries

For all student enquiries, visit Student Connect at [ask.mq.edu.au](http://ask.mq.edu.au)

If you are a Global MBA student contact [globalmba.support@mq.edu.au](mailto:globalmba.support@mq.edu.au)

## 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

Wet labs are now on every second week with students doing labs in two streams, one doing wet labs in even weeks and the other doing wet labs in odd weeks. Students not doing wet labs will be workshopping their lab report/patent application.

mid-semester test has been moved to an earlier date (April 28, the first day back after Easter break)

new topic on antiviral prodrugs has been added

The in-lecture discussions of the lab reports has ben replaced with new lectures from AP