CHEM3801

Medicinal Chemistry

Session 1, Weekday attendance, North Ryde 2021

Archive (Pre-2022) - Department of Molecular Sciences

Contents

Notice

As part of Phase 3 of our return to campus plan, most units will now run tutorials, seminars and other small group activities on campus, and most will keep an online version available to those students unable to return or those who choose to continue their studies online.

To check the availability of face-to-face activities for your unit, please go to timetable viewer. To check detailed information on unit assessments visit your unit's iLearn space or consult your unit convenor.

General Information

Unit convenor and teaching staff
Convenor, Lecturer
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Lecturer
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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

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

If you are unable to complete an assessment item due to illness or misadventure, you must submit a request for Special Consideration. Late assessment items will not be accepted without Special Consideration being approved.

Further details on applying for Special Consideration can be found here: students.mq.edu.au/study/my-study-program/special-consideration

Assessment Tasks

Name	Weighting	Hurdle	Due
Spectroscopy Training	0%	No	18 April
Quizzes	5%	No	Weeks 3,5,7,9,11
Mid-semester test	15%	No	27 April
Pharmaceutical agent presentation	5%	No	11 May
Practical work	25%	No	2 April (Draft), 4 June (Final)
Final Examination	50%	No	Formal examination period

Spectroscopy Training

Assessment Type [1]: Participatory task
Indicative Time on Task [2]: 7 hours
Due: **18 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 [1]: Quiz/Test
Indicative Time on Task [2]: 5 hours

Due: **Weeks 3,5,7,9,11**
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 [1]: Quiz/Test
Indicative Time on Task [2]: 10 hours
Due: **27 April**
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 [1]: Presentation

Indicative Time on Task [2]: 5 hours
Due: **11 May**
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 [1]: Lab report
Indicative Time on Task [2]: 20 hours
Due: **2 April (Draft), 4 June (Final)**
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 [1]: Examination
Indicative Time on Task [2]: 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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[1] 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.

[2] 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 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. For students with weaker chemistry backgrounds, more time per week will likely be needed to perform satisfactorily in this unit. 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. This will consist of a mixture of pre-recorded lectures and interactive (live) lectures. 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. A 1-hour mid-semester test (worth 15%) will be run in Week 8 during the allocated lecture time. This test will cover all course material up to and including Week 7.

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 5 wet labs sessions run in two streams (Group A and Group B) on alternating weeks, starting in Weeks 2/3. The final (dry) laboratory class in Week 13 will bring all the team 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 will almost certainly run 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.

Login with your MQ student ID number and password, then follow the prompts to "CHEM3801/6801 Medicinal Chemistry."

During semester, the CHEM3801/6801 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 or other book shops. Limited copies of the text book are also available in the MQ Library.

Unit Schedule

Week	Topic	Lecturer
1	Introduction to Medicinal Chemistry; Introduction to Structure-Activity Relationships	Joanne Jamie
2	Protein Structure and Function; Interaction of Proteins with Drugs; Developing Agonists and Antagonists	Joanne Jamie
3	Enzyme Kinetics; Enzyme Inhibitors as Drugs	Joanne Jamie
4	Nucleic Acids Structure and Function; Drugs Interacting with DNA & RNA	Joanne Jamie
5	Drug Discovery; Lead Optimisation; Structure-Activity Relationships	Joanne Jamie
6	Physicochemical Properties; Absorption, Distribution, Metabolism and Excretion	Joanne Jamie
7	Prodrugs	Joanne Jamie
8	Mid-Semester Test	
9	Quantitative Structure-Activity Relationships	Peter Karuso
10	Combinatorial Chemistry	Peter Karuso
11	G-protein-coupled Receptors	Peter Karuso
12	Antibacterial Agents	Andrew Piggott
13	Antifungal Agents	Andrew Piggott

Policies and Procedures

Macquarie University policies and procedures are accessible from Policy Central (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
- Grade Appeal Policy
- Complaint Management 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). 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) 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 or if you are a Global MBA student contact 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) 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

If you are a Global MBA student contact 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/.

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

The Unit Convenor has changed from Prof. Peter Karuso to A/Prof. Andrew Piggott.

Three lectures per week have changed to two lectures and one SGTA per week.