



MOLS8851

Advanced Medicinal Chemistry

Session 2, Weekday attendance, North Ryde 2021

Archive (Pre-2022) - Department of Molecular Sciences

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Session 2 Learning and Teaching Update

The decision has been made to conduct study online for the remainder of Session 2 for all units WITHOUT mandatory on-campus learning activities. Exams for Session 2 will also be online where possible to do so.

This is due to the extension of the lockdown orders and to provide certainty around arrangements for the remainder of Session 2. We hope to return to campus beyond Session 2 as soon as it is safe and appropriate to do so.

Some classes/teaching activities cannot be moved online and must be taught on campus. You should already know if you are in one of these classes/teaching activities and your unit convenor will provide you with more information via iLearn. If you want to confirm, see the list of [units with mandatory on-campus classes/teaching activities](#).

Visit the [MQ COVID-19 information page](#) for more detail.

General Information

Unit convenor and teaching staff

Peter Karuso

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Credit points

10

Prerequisites

Admission to GradDipBiotech or GradCertLabAQMgt or GradDipLabAQMgt or MBiotech or MBioBus or MLabAQMgt or MRadiopharmSc or MSc or MScInnovationChemBiomolecularSc and (CHEM6801 or CBMS606)

Corequisites

Co-badged status

Unit description

This unit builds on the fundamentals of medicinal chemistry, including the discovery, design and development of new medicines. The aim of the unit is to integrate chemical biology and organic chemistry to reveal how these are used in medicinal chemistry to design and synthesise new drugs and to understand their mode of action. The unique aspect of this unit is the focus on computational chemistry in the field of drug design and development. This includes aspects of molecular modelling, molecular dynamics, docking, pharmacophore modelling and QSAR as they relate to the understanding of drug action and design of new drugs.

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: Apply the principles of rational drug design for the creation of drug libraries.

ULO2: Exploit structure activity relationships (SAR) and quantitative structure activity relationships (QSAR) principles to determine drug modes of action.

ULO3: Design the structure of small molecules by combining the principles of drug design to create potential new drugs.

ULO4: Communicate the above advanced medicinal chemistry concepts competently in

oral presentations and in written format in the form of a report and a final exam.

ULO5: Research and communicate a contemporary topic in medicinal chemistry through oral and online discussion.

Assessment Tasks

Name	Weighting	Hurdle	Due
<u>Class participation</u>	5%	Yes	continuous
<u>Five Assignments</u>	15%	No	Weeks 4, 6, 8, 10, 12
<u>Research Report</u>	20%	No	27/9/2021, 8/11/2021
<u>Oral Presentation</u>	10%	No	Week 12
<u>Final Exam</u>	50%	No	Week 15

Class participation

Assessment Type ¹: Participatory task

Indicative Time on Task ²: 13 hours

Due: **continuous**

Weighting: **5%**

This is a hurdle assessment task (see [assessment policy](#) for more information on hurdle assessment tasks)

Participation in the weekly classes is a hurdle and you are expected to attend all classes. In the event of illness or misadventure, you can justify your absence from a class by submitting a Special Consideration request.

On successful completion you will be able to:

- Apply the principles of rational drug design for the creation of drug libraries.
- Exploit structure activity relationships (SAR) and quantitative structure activity relationships (QSAR) principles to determine drug modes of action.
- Design the structure of small molecules by combining the principles of drug design to create potential new drugs.
- Communicate the above advanced medicinal chemistry concepts competently in oral presentations and in written format in the form of a report and a final exam.
- Research and communicate a contemporary topic in medicinal chemistry through oral

and online discussion.

Five Assignments

Assessment Type ¹: Quiz/Test

Indicative Time on Task ²: 25 hours

Due: **Weeks 4, 6, 8, 10, 12**

Weighting: **15%**

5 assignments, each worth 3% - short assignments based on previous 2 weeks of classes.

On successful completion you will be able to:

- Apply the principles of rational drug design for the creation of drug libraries.
- Exploit structure activity relationships (SAR) and quantitative structure activity relationships (QSAR) principles to determine drug modes of action.
- Design the structure of small molecules by combining the principles of drug design to create potential new drugs.

Research Report

Assessment Type ¹: Report

Indicative Time on Task ²: 18 hours

Due: **27/9/2021, 8/11/2021**

Weighting: **20%**

Using what you have learnt, pick a drug target, research what is known about this target and summarise the relevant literature and design your own compounds to test. Present this review in a written report.

On successful completion you will be able to:

- Apply the principles of rational drug design for the creation of drug libraries.
- Exploit structure activity relationships (SAR) and quantitative structure activity relationships (QSAR) principles to determine drug modes of action.
- Design the structure of small molecules by combining the principles of drug design to create potential new drugs.
- Communicate the above advanced medicinal chemistry concepts competently in oral presentations and in written format in the form of a report and a final exam.

Oral Presentation

Assessment Type ¹: Presentation

Indicative Time on Task ²: 12 hours

Due: **Week 12**

Weighting: **10%**

An oral presentation and class discussion (including online) on a contemporary medicinal chemistry topic.

On successful completion you will be able to:

- Communicate the above advanced medicinal chemistry concepts competently in oral presentations and in written format in the form of a report and a final exam.
- Research and communicate a contemporary topic in medicinal chemistry through oral and online discussion.

Final Exam

Assessment Type ¹: Examination

Indicative Time on Task ²: 30 hours

Due: **Week 15**

Weighting: **50%**

This is a 3 hr final exam

On successful completion you will be able to:

- Apply the principles of rational drug design for the creation of drug libraries.
- Exploit structure activity relationships (SAR) and quantitative structure activity relationships (QSAR) principles to determine drug modes of action.
- Design the structure of small molecules by combining the principles of drug design to create potential new drugs.
- Communicate the above advanced medicinal chemistry concepts competently in oral presentations and in written format in the form of a report and a final exam.

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

This is a self taught unit using the "molecular concepthor" and ChemComp (MOE) software. Each week a set number of tasks are assigned and assessed. There is no text book set for this unit but the material covered in CHEM6801/CBMS606 (Medicinal Chemistry) and at least 2000-level Organic Chemistry is assumed knowledge. The text books for this assumed knowledge at Patrick ["an introduction to medicinal chemistry"](#) and McMurry ["Organic Chemistry"](#)

Unit Schedule

WEEK 1

- Introduction to Drug Discovery
- Principles of Rational Drug Design

WEEK 2

- Structure Activity Relationships (SAR)
- Bioisosterism

WEEK 3

- Bioinformatics
- Protein Structure

WEEK 4

- Library Design
- Molecular Graphics

WEEK 5

- Molecular Geometry
- Molecular Energies
- Conformational Analysis

WEEK 6

- Protein Ligand Binding
- Principles of Structure Based Design

WEEK 7

- Molecular Docking: Principles and Methods

WEEK 8

- Case Studies - Structure Based Design
- Case Studies - Docking in Drug Discovery
- Analysis of Protein Ligand Complexes

WEEK 9

- Principles in Pharmacophore elucidation
- Ligand based Approaches

WEEK 10

- Examples of Pharmacophores
- Case Studies - Ligand Design

WEEK 11

- QSAR: Principles and Methods
- Case Studies - QSAR and 3D-QSAR

WEEK 12

- Project Completion

WEEK 13

- Project submission
- Review

MOE WORKSHOPS

1. Introduction to MOE
2. Building Molecules
3. 3D Visualisations
4. Structure based design
5. Docking
6. Ligand based design
7. Protein Ligand Interaction footprints

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](#)
- [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) (<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 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.