



# CBMS842

## Advanced Medicinal Chemistry

S2 Day 2019

*Dept of Molecular Sciences*

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#### **Disclaimer**

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## General Information

Unit convenor and teaching staff

Lecturer and co-convenor

Joanne Jamie

[joanne.jamie@mq.edu.au](mailto:joanne.jamie@mq.edu.au)

Contact via 98508283

4 Wally's Walk room 231

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

Lecturer and Co-convenor

Peter Karuso

[peter.karuso@mq.edu.au](mailto:peter.karuso@mq.edu.au)

Contact via 9850 8290

4WW 232

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

Lecturer and tutor

Vaughan Moon

[vaughan.moon@mq.edu.au](mailto:vaughan.moon@mq.edu.au)

Contact via 9850 8309

4 Wally's Walk room 204

Credit points

4

Prerequisites

(Admission to MBiotech or MBioBus or MLabQAMgt or MRadiopharmSc or MSc or GradCertLabQAMgt or GradDipLabQAMgt or MScInnovation) and permission by special approval

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:

By the end of this unit, you should be able to apply the principles of rational drug design for the creation of drug libraries

By the end of this unit, you should be able to exploit structure activity relationships (SAR) and quantitative structure activity relationships (QSAR) principles to understand drug modes of action

By the end of this unit, you should be able to design the structure of small molecules by combining the principles of drug design to create potential new drugs

By the end of this unit, you should 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

By the end of the unit, you should be able to research and communicate a contemporary topic in medicinal chemistry through oral and online discussion.

## General Assessment Information

The final exam is a 3 hr written exam.

Assignments are based on the previous 2 weeks work.

The report is a major work that you will start preparing in week 5 and complete in week 13. It involves a written report.

The oral presentation will be a 5 - 10 minute talk on a contemporary topic related to medicinal chemistry with an online discussion component.

The weekly classes are a participation hurdle and failure to participate in at least 10 of the 13

weekly classes will result in you failing CBMS842. Participation includes active engagement with the weekly tasks and in class objectives.

If you are unable to attend a class, please contact Peter Karuso (peter.karuso@mq.edu.au) or Joanne Jamie (joanne.jamie@mq.edu.au) immediately. In addition, you must submit a Special Consideration request at ask.mq.edu.au to justify your absence.

Your marks will be placed on the CBMS842 iLearn site.

Your final grade will be based on the mark from the aggregation of the individual assessments, **with 50% or greater needed overall for a pass.**

**Medical certificates or other official documents must be lodged as part of a Special Consideration request at ask.mq.edu.au as soon as possible if you are absent for any of the weekly classes or miss the due date for any of the assessment tasks.** If your reason is regarded as valid for missing an assignment you will be given an average of the other assignments. If you miss the final exam for a valid reason, a supplementary exam will be provided. Any assessment tasks not submitted on time that does not get approval through the Special Consideration request will get a 10% deduction of marks for every weekday late.

**Final Examination Details:** The examination timetable will be available in Draft form approximately eight weeks before the commencement of the examinations and in final form approximately four weeks before the commencement of the examinations. You are expected to present yourself for examination at the time and place designated by the University in the Examination Timetable. This could be any day after the final week of semester and up until the final day of the official examination period. It is Macquarie University policy to **not set early examinations** for individuals or groups of students. All students are expected to ensure that they are available until the final day of the official examination period.

The only exception to sitting an examination at the designated time is because of documented illness or unavoidable disruption. Absence from the final exam will result in a grade of F except in the case of a genuine medical emergency or misadventure as defined by the University (see below). In these circumstances you should apply for a Supplementary Exam at ask.mq.edu.au.

**NOTE: If you apply for a Supplementary Examination, you must make yourself available for the Supplementary Exam times in early December - specific examination dates and times will be determined at a later date. If you are not available at that time, there is no guarantee an additional examination time will be offered.**

## Assessment Tasks

Name	Weighting	Hurdle	Due
<u>Final Exam</u>	50%	No	Examination period
<u>Research Report</u>	20%	No	Week 13
<u>Five Assignments</u>	15%	No	Weeks 4, 6, 8, 10, 12

Name	Weighting	Hurdle	Due
<u>Oral Presentation</u>	10%	No	Weeks 4 - 13
<u>Class participation</u>	5%	Yes	weeks 1-13

## Final Exam

Due: **Examination period**

Weighting: **50%**

This is a 3 hr final exam

On successful completion you will be able to:

- By the end of this unit, you should be able to apply the principles of rational drug design for the creation of drug libraries
- By the end of this unit, you should be able to exploit structure activity relationships (SAR) and quantitative structure activity relationships (QSAR) principles to understand drug modes of action
- By the end of this unit, you should be able to design the structure of small molecules by combining the principles of drug design to create potential new drugs
- By the end of this unit, you should 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 Report

Due: **Week 13**

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:

- By the end of this unit, you should be able to apply the principles of rational drug design for the creation of drug libraries
- By the end of this unit, you should be able to exploit structure activity relationships (SAR) and quantitative structure activity relationships (QSAR) principles to understand drug modes of action
- By the end of this unit, you should be able to design the structure of small molecules by

combining the principles of drug design to create potential new drugs

- By the end of this unit, you should 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

## Five Assignments

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:

- By the end of this unit, you should be able to apply the principles of rational drug design for the creation of drug libraries
- By the end of this unit, you should be able to exploit structure activity relationships (SAR) and quantitative structure activity relationships (QSAR) principles to understand drug modes of action
- By the end of this unit, you should be able to design the structure of small molecules by combining the principles of drug design to create potential new drugs

## Oral Presentation

Due: **Weeks 4 - 13**

Weighting: **10%**

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

On successful completion you will be able to:

- By the end of this unit, you should 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
- By the end of the unit, you should be able to research and communicate a contemporary topic in medicinal chemistry through oral and online discussion.

## Class participation

Due: **weeks 1-13**

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:

- By the end of this unit, you should be able to apply the principles of rational drug design for the creation of drug libraries
- By the end of this unit, you should be able to exploit structure activity relationships (SAR) and quantitative structure activity relationships (QSAR) principles to understand drug modes of action
- By the end of this unit, you should be able to design the structure of small molecules by combining the principles of drug design to create potential new drugs
- By the end of this unit, you should 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
- By the end of the unit, you should be able to research and communicate a contemporary topic in medicinal chemistry through oral and online discussion.

## Delivery and Resources

This is a self taught unit using the "molecular conceptual" and 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 CBMS606 Medicinal Chemistry is assumed knowledge.

## 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 \(https://staff.mq.edu.au/work/strategy-planning-and-governance/university-policies-and-procedures/policy-central\)](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.*)

Undergraduate 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](https://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 improve your marks and take control of your study.

- [Workshops](#)
- [StudyWise](#)
- [Academic Integrity Module for Students](#)
- [Ask a Learning Adviser](#)

## 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.

## Graduate Capabilities

### PG - Capable of Professional and Personal Judgment and Initiative

Our postgraduates will demonstrate a high standard of discernment and common sense in their professional and personal judgment. They will have the ability to make informed choices and decisions that reflect both the nature of their professional work and their personal perspectives.

This graduate capability is supported by:

### Learning outcomes

- By the end of this unit, you should be able to apply the principles of rational drug design for the creation of drug libraries
- By the end of this unit, you should be able to exploit structure activity relationships (SAR)

and quantitative structure activity relationships (QSAR) principles to understand drug modes of action

- By the end of this unit, you should be able to design the structure of small molecules by combining the principles of drug design to create potential new drugs
- By the end of this unit, you should 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
- By the end of the unit, you should be able to research and communicate a contemporary topic in medicinal chemistry through oral and online discussion.

## **Assessment tasks**

- Research Report
- Class participation

## **PG - Discipline Knowledge and Skills**

Our postgraduates will be able to demonstrate a significantly enhanced depth and breadth of knowledge, scholarly understanding, and specific subject content knowledge in their chosen fields.

This graduate capability is supported by:

## **Learning outcomes**

- By the end of this unit, you should be able to apply the principles of rational drug design for the creation of drug libraries
- By the end of this unit, you should be able to exploit structure activity relationships (SAR) and quantitative structure activity relationships (QSAR) principles to understand drug modes of action
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- By the end of the unit, you should be able to research and communicate a contemporary topic in medicinal chemistry through oral and online discussion.

## **Assessment tasks**

- Final Exam
- Research Report
- Five Assignments

- Oral Presentation
- Class participation

## PG - Critical, Analytical and Integrative Thinking

Our postgraduates will be capable of utilising and reflecting on prior knowledge and experience, of applying higher level critical thinking skills, and of integrating and synthesising learning and knowledge from a range of sources and environments. A characteristic of this form of thinking is the generation of new, professionally oriented knowledge through personal or group-based critique of practice and theory.

This graduate capability is supported by:

### Learning outcomes

- By the end of this unit, you should be able to apply the principles of rational drug design for the creation of drug libraries
- By the end of this unit, you should be able to exploit structure activity relationships (SAR) and quantitative structure activity relationships (QSAR) principles to understand drug modes of action
- By the end of this unit, you should be able to design the structure of small molecules by combining the principles of drug design to create potential new drugs
- By the end of this unit, you should 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
- By the end of the unit, you should be able to research and communicate a contemporary topic in medicinal chemistry through oral and online discussion.

### Assessment tasks

- Final Exam
- Research Report
- Five Assignments
- Oral Presentation
- Class participation

## PG - Research and Problem Solving Capability

Our postgraduates will be capable of systematic enquiry; able to use research skills to create new knowledge that can be applied to real world issues, or contribute to a field of study or practice to enhance society. They will be capable of creative questioning, problem finding and problem solving.

This graduate capability is supported by:

## Learning outcomes

- By the end of this unit, you should be able to apply the principles of rational drug design for the creation of drug libraries
- By the end of this unit, you should be able to exploit structure activity relationships (SAR) and quantitative structure activity relationships (QSAR) principles to understand drug modes of action
- By the end of this unit, you should be able to design the structure of small molecules by combining the principles of drug design to create potential new drugs
- By the end of this unit, you should 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
- By the end of the unit, you should be able to research and communicate a contemporary topic in medicinal chemistry through oral and online discussion.

## Assessment tasks

- Final Exam
- Research Report
- Five Assignments
- Oral Presentation
- Class participation

## PG - Effective Communication

Our postgraduates will be able to communicate effectively and convey their views to different social, cultural, and professional audiences. They will be able to use a variety of technologically supported media to communicate with empathy using a range of written, spoken or visual formats.

This graduate capability is supported by:

## Learning outcomes

- By the end of this unit, you should 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
- By the end of the unit, you should be able to research and communicate a contemporary topic in medicinal chemistry through oral and online discussion.

## Assessment tasks

- Final Exam

- Research Report
- Five Assignments
- Oral Presentation
- Class participation

## PG - Engaged and Responsible, Active and Ethical Citizens

Our postgraduates will be ethically aware and capable of confident transformative action in relation to their professional responsibilities and the wider community. They will have a sense of connectedness with others and country and have a sense of mutual obligation. They will be able to appreciate the impact of their professional roles for social justice and inclusion related to national and global issues

This graduate capability is supported by:

### Learning outcomes

- By the end of this unit, you should 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
- By the end of the unit, you should be able to research and communicate a contemporary topic in medicinal chemistry through oral and online discussion.

### Assessment tasks

- Research Report
- Class participation

## Changes from Previous Offering

There have been minor changes to the order of topics and assessment structure. The classes have been expanded to 4 hour sessions to allow the majority of sessions using the programs MOE and Molecular Conceptor to be done during class time.