



# MCB\*6370 Protein Structural Biology and Bioinformatics

Winter 2021

Section(s): C01

Department of Molecular and Cellular Biology

Credit Weight: 0.50

Version 1.00 - March 02, 2021

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## 1 Course Details

### 1.1 Calendar Description

This course explores structural biology from three perspectives: 1) the fundamental concepts in structural biology; 2) the methods used to determine structures (including x-ray crystallography, NMR, electron microscopy, and computational modeling); 3) the bioinformatic concepts and tools used to compare, contrast and assign biochemical function to protein structures and sequences. The course emphasizes building a conceptual and practical skill set that will be applicable to any structure related problem.

### 1.2 Course Description

#### **Course synopsis:**

This course will explore the relationship between protein sequence and three-dimensional structure. Students will gain experience with critical assessment of recent protein structure journal articles and the tools and methodology required for modeling, docking, and designing protein structure.

#### **Objectives:**

Mastery of PyMOL for analysing structures and generating figures

Understanding and applying homology modelling

Understanding of the process of scientific dissemination

Writing proficiency

Mastery of scientific manuscript formatting/style

Multipanel figure generation

Critical analysis of contemporary primary literature

Mastery of oral presentation skills

**Recommended background:** The course is designed for students who have met the requirements for entry to the M.Sc. or Ph.D. programs of the Department of Molecular and Cellular Biology, having completed an honours (science) B.Sc. degree or the equivalent. It is expected that students have a good working knowledge of basic biochemistry, including a familiarity with the main concepts of protein structures.

**Assignment groups:** The mini-assignments (PyMOL images and homology modelling exercise) may be done individually. The journal club presenters and the structural annotation

projects may be done in groups of two. Students can suggest groupings and the instructors will help to match unpaired students. Grouping number will depend on the final enrollment.

### 1.3 Timetable

Mondays 1:30 to 4:30 p.m.

Class meetings will be conducted over online tools. Microsoft Teams, which allows for better multi-person meetings will be used. Note classes are synchronous, and attendance is required.

### 1.4 Final Exam

There is no final exam for this course.

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## 2 Instructional Support

### 2.1 Instructional Support Team

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|----------------------|---------------------------------------|
| <b>Instructor:</b>   | Matthew Kimber                        |
| <b>Email:</b>        | mkimber@uoguelph.ca                   |
| <b>Telephone:</b>    | +1-519-824-4120 x52568                |
| <b>Office:</b>       | SSC 2254                              |
| <b>Office Hours:</b> | By appointment, over videoconference. |

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## 3 Learning Resources

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## 4 Learning Outcomes

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## 5 Teaching and Learning Activities

### 5.1 Lecture

|                | <b>Week</b> | <b>Topics</b>   | <b>Tutorials</b>                                  | <b>Assignment Due</b> |
|----------------|-------------|---|---|-----------------------|
| <b>Topics:</b> | 1           | Review of the Course; writing, oral presentations   | PyMOL tutorial Advanced features<br>Superposition |                       |
|                | 2           | Review of Protein Structure Fundamentals  |   | PyMOL image #1        |
|                |             | Sequences<br><br>Sequence alignments  |   |                       |
|                | 3           | BLAST and other sequence search tools/ Sequence databases/ MSA / Phylogenetic trees / file types<br><br>Annotation, names, ontology |   | PyMOL image #2        |
|                |             |   | Bioinformatics Tutorial<br>(complete on your own) |                       |
|                | 4           | Structural Bioinformatics<br><br>CONSURF, PISA –  |   | PyMOL image #3        |

| <b>Week</b> | <b>Topics</b>   | <b>Tutorials</b> | <b>Assignment Due</b>                                   |
|-------------|---|------------------|---|
|             | oligomeric states   |                  |   |
|             | Functional Assignment   |                  |   |
| 5           | BRENDA<br>String database<br>Microarray datasets<br>Literature searches |                  | Journal Club<br><br>PyMOL<br>image #4                   |
| 6           | X-ray crystallography   |                  | Journal Club<br><br>PyMOL<br>image #5                   |
|             | <b>Reading Week</b>   |                  |   |
| 7           | Electron microscopy   |                  | Journal Club<br><br>Homology<br>modelling               |
| 8           | NMR   |                  | Journal Club  |
| 9           | No Class  |                  |   |
| 10          | Computational<br>Methods<br>(Protein modeling,<br>molecular dynamics)   |                  | Journal Club  |
| 11          |   |                  | Presentations<br>Structural<br>Annotation<br>Assignment |

| <b>Week</b> | <b>Topics</b> | <b>Tutorials</b> | <b>Assignment Due</b>                                   |
|-------------|---------------|------------------|---|
| 12          |               |                  | Presentations<br>Structural<br>Annotation<br>Assignment |

\*Schedule is subject to change depending on the final enrollment numbers.

## 6 Assessments

### **PyMOL Tutorial, PyMOL Image and Homology Modelling:**

Protein structure visualization is an extremely important skill in structural biology. The purpose of the tutorial is to familiarize students with the use of the very powerful, general-purpose macromolecular structure viewing, analysis and documenting program called PyMOL.

The Image assignments are designed to assess your mastery of PyMOL as well as some ancillary programs and concepts. The value of these assignments will be measured in your improved presentations for your proposals and thesis defences and the quality of the figures you submit for your publications.

The homology modelling assignment will introduce you to the techniques used to take a sequence with similarity to a known structure and create a plausible structural model. PyMOL will be used to show the new structure and how it relates to its template, and a pseudo-energy function will be used to show what problem areas may exist in the model structure.

### **Journal Club Presentations:**

Each student will present a research paper which focuses on some particular structure-function relations problem, with all students participating in a discussion of the work. One student will be assigned to lead the discussion, and should be deeply familiar with the paper, have done any additional reading required to understand the material being analysed, and should be looking to stimulate a meaningful discussion with their peers. The primary focus should be on this discussion; the leader may optionally use PowerPoint or PyMOL to show figures from the paper, the whiteboard, etc. if they feel that it helps foster the discussion, but these materials will not be the focus of the evaluation. All students are expected to be able to intelligently discuss the content of the paper, and therefore need to be familiar with its content and have done some further reading into the background to the problem. Students are expected to have informed opinions about the methodology, its applicability to the problem, the quality of the results obtained and the appropriateness of the interpretation.

**Structure Annotation Paper:**

The final assignment for the course is a structure annotation assignment. Students will be assigned a recently deposited structure in the protein data bank. This structure, determined as part of a structural genomics effort, will have minimal analysis completed, and no associated paper published. Students will then analyse the structure and sequence using sequence and structure based bioinformatics tools (including, but not limited to, those discussed in class), searches of the relevant literature and functional databases. This analysis will be centered on documenting the structure (using PyMOL and other tools to produce publication quality figures), and to objectively evaluate the existing evidence for various candidate functions for the protein. The results of this analysis will be presented as a scientific manuscript, and presented in-class using standard scientific presentation methods.

**Turnitin:**

In this course, your instructor will be using Turnitin, integrated with the Courselink Dropbox tool, to detect possible plagiarism, unauthorized collaboration or copying as part of the ongoing efforts to maintain academic integrity at the University of Guelph. All submitted assignments will be included as source documents in the Turnitin.com reference database solely for the purpose of detecting plagiarism of such papers. Use of the Turnitin.com service is subject to the Usage Policy posted on the Turnitin.com site.

**6.1 Marking Schemes & Distributions****Grade Assessment**

Mini assignments:

PyMOL images: 10%

Modelling exercise: 5%

Journal Club:

Presentation: 20%

Participation: 10%

Structural Annotation:

Written 40%

Oral Presentation 15%

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## 7 Department of Molecular and Cellular Biology Statements

### 7.1 Academic Advisors

If you are concerned about any aspect of your academic program:

- Make an appointment with a program counsellor in your degree program. [B.Sc. Academic Advising](#) or [Program Counsellors](#)

### 7.2 Academic Support

If you are struggling to succeed academically:

- Learning Commons: There are numerous academic resources offered by the Learning Commons including, Supported Learning Groups for a variety of courses, workshops related to time management, taking multiple choice exams, and general study skills. You can also set up individualized appointments with a learning specialist. <http://www.learningcommons.uoguelph.ca/>
- Science Commons: Located in the library, the Science Commons provides support for physics, mathematic/statistics, and chemistry. Details on their hours of operations can be found at: <http://www.lib.uoguelph.ca/get-assistance/studying/chemistry-physics-help> and <http://www.lib.uoguelph.ca/get-assistance/studying/math-stats-help>

### 7.3 Wellness

If you are struggling with personal or health issues:



- Counselling services offers individualized appointments to help students work through personal struggles that may be impacting their academic performance. <https://www.uoguelph.ca/counselling/>
- Student Health Services is located on campus and is available to provide medical attention. <https://www.uoguelph.ca/studenthealthservices/clinic>
- For support related to stress and anxiety, besides Health Services and Counselling Services, Kathy Somers runs training workshops and one-on-one sessions related to stress management and high performance situations. <http://www.selfregulationskills.ca/>

## 7.4 Personal information

Personal information is collected under the authority of the University of Guelph Act (1964), and in accordance with Ontario's Freedom of Information and Protection of Privacy Act (FIPPA) <http://www.e-laws.gov.on.ca/index.html>. This information is used by University officials in order to carry out their authorized academic and administrative responsibilities and also to establish a relationship for alumni and development purposes.

For more information regarding the Collection, Use and Disclosure of Personal Information policies please see the Undergraduate Calendar. (<https://www.uoguelph.ca/registrar/calendars/undergraduate/current/intro/index.shtml>)

# 8 University Statements

## 8.1 Email Communication

As per university regulations, all students are required to check their e-mail account regularly: e-mail is the official route of communication between the University and its students.

## 8.2 When You Cannot Meet a Course Requirement

When you find yourself unable to meet an in-course requirement because of illness or compassionate reasons please advise the course instructor (or designated person, such as a teaching assistant) in writing, with your name, id#, and e-mail contact. The grounds for Academic Consideration are detailed in the Undergraduate and Graduate Calendars.

Undergraduate Calendar - Academic Consideration and Appeals  
<https://www.uoguelph.ca/registrar/calendars/undergraduate/current/c08/c08-ac.shtml>

Graduate Calendar - Grounds for Academic Consideration  
<https://www.uoguelph.ca/registrar/calendars/graduate/current/genreg/index.shtml>

Associate Diploma Calendar - Academic Consideration, Appeals and Petitions  
<https://www.uoguelph.ca/registrar/calendars/diploma/current/index.shtml>

### 8.3 Drop Date

Students will have until the last day of classes to drop courses without academic penalty. The deadline to drop two-semester courses will be the last day of classes in the second semester. This applies to all students (undergraduate, graduate and diploma) except for Doctor of Veterinary Medicine and Associate Diploma in Veterinary Technology (conventional and alternative delivery) students. The regulations and procedures for course registration are available in their respective Academic Calendars.

Undergraduate Calendar - Dropping Courses

<https://www.uoguelph.ca/registrar/calendars/undergraduate/current/c08/c08-drop.shtml>

Graduate Calendar - Registration Changes

<https://www.uoguelph.ca/registrar/calendars/graduate/current/genreg/genreg-reg-regchg.shtml>

Associate Diploma Calendar - Dropping Courses

<https://www.uoguelph.ca/registrar/calendars/diploma/current/c08/c08-drop.shtml>

### 8.4 Copies of Out-of-class Assignments

Keep paper and/or other reliable back-up copies of all out-of-class assignments: you may be asked to resubmit work at any time.

### 8.5 Accessibility

The University promotes the full participation of students who experience disabilities in their academic programs. To that end, the provision of academic accommodation is a shared responsibility between the University and the student.

When accommodations are needed, the student is required to first register with Student Accessibility Services (SAS). Documentation to substantiate the existence of a disability is required; however, interim accommodations may be possible while that process is underway.

Accommodations are available for both permanent and temporary disabilities. It should be noted that common illnesses such as a cold or the flu do not constitute a disability.

Use of the SAS Exam Centre requires students to book their exams at least 7 days in advance and not later than the 40th Class Day.

For Guelph students, information can be found on the SAS website

<https://www.uoguelph.ca/sas>

For Ridgetown students, information can be found on the Ridgetown SAS website

<https://www.ridgetownc.com/services/accessibilityservices.cfm>

### 8.6 Academic Integrity

The University of Guelph is committed to upholding the highest standards of academic integrity, and it is the responsibility of all members of the University community-faculty, staff, and students-to be aware of what constitutes academic misconduct and to do as much as possible to prevent academic offences from occurring. University of Guelph students have the responsibility of abiding by the University's policy on academic misconduct regardless of their location of study; faculty, staff, and students have the responsibility of supporting an environment that encourages academic integrity. Students need to remain aware that instructors have access to and the right to use electronic and other means of detection.

Please note: Whether or not a student intended to commit academic misconduct is not relevant for a finding of guilt. Hurried or careless submission of assignments does not excuse students from responsibility for verifying the academic integrity of their work before submitting it. Students who are in any doubt as to whether an action on their part could be construed as an academic offence should consult with a faculty member or faculty advisor.

Undergraduate Calendar - Academic Misconduct

<https://www.uoguelph.ca/registrar/calendars/undergraduate/current/c08/c08-amisconduct.shtml>

Graduate Calendar - Academic Misconduct

<https://www.uoguelph.ca/registrar/calendars/graduate/current/genreg/index.shtml>

## 8.7 Recording of Materials

Presentations that are made in relation to course work - including lectures - cannot be recorded or copied without the permission of the presenter, whether the instructor, a student, or guest lecturer. Material recorded with permission is restricted to use for that course unless further permission is granted.

## 8.8 Resources

The Academic Calendars are the source of information about the University of Guelph's procedures, policies, and regulations that apply to undergraduate, graduate, and diploma programs.

Academic Calendars

<https://www.uoguelph.ca/academics/calendars>

## 8.9 Disclaimer

Please note that the ongoing COVID-19 pandemic may necessitate a revision of the format of course offerings and academic schedules. Any such changes will be announced via CourseLink and/or class email. All University-wide decisions will be posted on the COVID-19 website (<https://news.uoguelph.ca/2019-novel-coronavirus-information/>) and circulated by email.

## 8.10 Illness

The University will not normally require verification of illness (doctor's notes) for fall 2020 or

winter 2021 semester courses. However, requests for Academic Consideration may still require medical documentation as appropriate.

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