



MCB*4050 Protein and Nucleic Acid Structure

Fall 2018
Section(s): C01

Department of Molecular and Cellular Biology
Credit Weight: 0.50
Version 1.00 - August 24, 2018

1 Course Details

1.1 Calendar Description

This course explores the relationship between the functions and the three dimensional structures of DNA, RNA and proteins. Topics covered include how these structures are determined, the principles governing their folding and architecture, why some proteins don't fold at all, and the use of these structures to guide drug discovery. Practical skills are emphasized, including the use of bioinformatics and visualisation tools to analyse sequences and structures.

Pre-Requisite(s): BIOC*3560

1.2 Timetable

Lectures: Tues. & Thurs. 2:30 – 3:50 p.m.

Room: MACS 209

1.3 Final Exam

Exam time and location is subject to change. Please see WebAdvisor for the latest information.

Friday, Dec. 14, 2018

19:00 - 21:00 (7:00 PM - 9:00 PM)

2 Instructional Support

2.1 Instructor(s)

Steffen Graether

Email: graether@uoguelph.ca
Telephone: +519-824-4120 x56457
Office: SSC 2255
Office Hours: By appointment. Scheduled office hours will be listed before the

3 Learning Resources

There is no textbook assigned for this course.

3.1 Required Resource(s)

Courselink (Website)

<https://courselink.uoguelph.ca>

Courselink will be used as the primary repository for course materials.

Assignments and tutorials will be posted on Courselink; completed assignments need to be submitted on Courselink.

4 Learning Outcomes

4.1 Course Learning Outcomes

By the end of this course, you should be able to:

1. Describe the energetic basis of protein folding and function.
 2. Describe the levels of protein structural organization.
 3. Describe how proteins fold, including the role of chaperones, and the roles of proteins that do not fold spontaneously into well-ordered structures.
 4. Analyse a protein's sequence and structure with a variety of bioinformatics and visualization tools.
 5. Describe how novel protein structures are determined experimentally.
 6. Describe the organization of nucleic acid structures, and the ways they interact with their cognate protein partners.
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5 Teaching and Learning Activities

5.1 Course Content

Topics	Details
1. Amino acids and protein energetics	The amino acids, electrostatic forces, dipoles, van der Waals interactions, H-bonds, properties of water as solvent, hydrophobic interactions
2. Secondary structure	Dihedral angles, helices and β -strands, loops and turns, Ramachandran plots
3. Tertiary structure	Organization of secondary structure elements into folds, packing patterns and domain organization
4. Quaternary	The formation of protein oligomers, the role of symmetry,

Topics	Details
structure	organization of fibers and virus shells, and the functioning of large, supermolecular machines
5. Protein Folding	Energetics and mechanisms of the protein folding, barriers to protein folding and how cells overcome the folding obstacles
6. Sequence bioinformatics	Single and multiple sequence alignments, blast searches, predicting secondary structure, molecular evolution and phylogeny
7 Structural bioinformatics	The pdb file format, structure superposition and similarity searches, mapping sequence conservation onto structures, structural and sequence correlates of binding and catalysis
8 Computational structural biology	Force fields, molecular dynamics, <i>ab initio</i> protein folding, homology modeling, docking and covariance approaches to structure
9. Structure determination methods	The methodology, theoretical underpinnings, uses and limitations of x-ray crystallography, NMR spectroscopy electron microscopy for determining experimental structures
10. Nucleic acid structure	Forces and interactions that govern nucleic acid structure, DNA double helices, non-canonical nucleic acid structures, RNA based machines, and DNA recognition by DNA binding proteins
11. Intrinsically disordered proteins	Proteins that do not form a well-defined hydrophobic core and proteins that fold only upon binding, the functional roles of IUPs, bioinformatics means of detecting unstructured regions of proteins
12. Drug discovery (time permitting)	The process of drug discovery, the structural basis of drug action, virtual screening, computational chemistry and structure guided drug discovery

5.2 Lecture Format

Lectures will be presented primarily using Powerpoint presentations. Lecture materials will be provided before the lecture and will be usually bundled by topic.

5.3 Important Dates

First day of class	2018/09/06
PyMOL Assignment	2018/09/21
Midterm	2018/10/18
Last Day to Drop	2018/11/02
Structure Analysis	2018/11/16
Last Lecture	2018/11/29
Final Examination	2018/12/14

6 Assessments

6.1 Marking Schemes & Distributions

Name	Scheme A (%)
PyMOL Assignment	0
Midterm	30
Structure Analysis Assignment	25
Final Examination	45
Total	100

6.2 Assessment Details

PyMOL Assignment (0%)

Date: Fri, Sep 21, 5:00 PM

PyMOL is a program that interprets and displays pdb (protein database) files to produce dynamic, interactive three-dimensional representations of molecular structures. You will be downloading and then using this program throughout this course for both exploring the course material and completing the structure annotation assignment. Therefore, you are asked to complete a tutorial (available on CourseLink) teaching you how to use this program. A short assignment will give you the opportunity to practice your skills by replicating a series of figures from recent publications. **Completion of the assignment is due on Friday, Sept. 21 at 5:00 pm and is ungraded requirement for the course.** Note that you will need access to a computer with an internet connection in order to complete the Pymol assignment and the structure analysis assignment.

Midterm (30%)

Date: Thu, Oct 18, 2:30 PM - 3:50 PM

Midterm: The in-class midterm covers topics 1 through 5, and is worth **30% of the final grade.**

Structure Analysis Assignment (25%)

Date: Fri, Nov 16, 5:00 PM

The Protein Structure Analysis Project: Students will be asked to analyse aspects an experimental structure deposited in the main structural archive (the pdb) but for which there is no published analysis (i.e. no paper). The assignment is then to complete some basic analyses and documentation of the structure and associated sequence. This assignment will require using a variety of bioinformatics tools to make useful inferences as to what the function of the protein is, and how it might function. Students will also be required to submit publication quality figures generated in PyMol and other tools.

The Protein Structure Analysis Assignment is due on Fri., Nov. 16 at 5:00 pm and is worth 25% of the final grade.

Final Examination (45%)

Date: Fri, Dec 14, 7:00 PM - 9:00 PM

Location TBA.

Exam will cover topics 6 - 12 inclusive, but students are expected to know all concepts from topics 1-5 as well.

7 Course Statements

7.1 Grading

Assignments will be submitted to Courselink. Penalties for late submission are 10% of the assignment grade per day late or less, up to a maximum of 50%. Assignments more than five days late will be assigned a mark of zero.

8 Department of Molecular and Cellular Biology Statements

8.1 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](#)

8.2 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>

8.3 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.uoguelph.ca/~ksomers/>
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9 University Statements

9.1 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.

9.2 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 regulations and procedures for [Academic Consideration](#) are detailed in the Undergraduate Calendar.

9.3 Drop Date

Courses that are one semester long must be dropped by the end of the fortieth class day; two-semester courses must be dropped by the last day of the add period in the second semester. The regulations and procedures for [Dropping Courses](#) are available in the Undergraduate Calendar.

9.4 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.

9.5 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.

More information: www.uoguelph.ca/sas

9.6 Academic Misconduct

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 discourages misconduct. 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.

The [Academic Misconduct Policy](#) is detailed in the Undergraduate Calendar.

9.7 Recording of Materials

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

9.8 Resources

The [Academic Calendars](#) are the source of information about the University of Guelph's procedures, policies and regulations which apply to undergraduate, graduate and diploma programs.
