



# **BIOC\*4050 Protein and Nucleic Acid Structure**

Fall 2023

Section(s): C01

Department of Molecular and Cellular Biology

Credit Weight: 0.50

Version 1.00 - August 22, 2023

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## **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-Requisites:** BIOC\*3560

**Equates:** MCB\*4050

### **1.2 Course 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.

### **1.3 Timetable**

Lecture time: Tuesday/Thursday, 2:30-3:50 pm. Room: ANNU 156

Format: In person classroom teaching.

Time and format is subject to change. Please see WebAdvisor for the latest information.

### **1.4 Final Exam**

A final exam will be held in person Monday, December 11th, 2023 from 8:30 - 10:30 a.m.

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## 2 Instructional Support

### 2.1 Instructional Support Team

<b>Instructor:</b>	Matthew Kimber
<b>Email:</b>	mkimber@uoguelph.ca
<b>Telephone:</b>	+1-519-824-4120 x52568
<b>Office:</b>	SCI 2254
<b>Office Hours:</b>	Office hours will be held before the midterm, final and structure assignment. At all other times, meetings are available by prior email arrangement

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## 3 Learning Resources

There is no textbook assigned for this course.

### 3.1 Required Resources

#### 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.

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## 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 move, how they fold, 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 predicted computationally and 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. <b>Amino acids and protein energetics</b>	The amino acids, electrostatic forces, dipoles, van der Waals interactions, H-bonds, properties of water as solvent, hydrophobic interactions
2. <b>Secondary structure</b>	Dihedral angles, helices and $\beta$ -strands, loops and turns, Ramachandran plots
3 <b>Tertiary structure</b>	Organization of secondary structure elements into folds, packing patterns and domain organization
4. <b>Quaternary structure</b>	The formation of protein oligomers, the role of symmetry, organization of fibers and virus shells, and the functioning of large, super-molecular machines
5. <b>Protein dynamics, folding and disorder</b>	Protein motion, the energetics and mechanisms of the protein folding, proteins which never fold or only fold in certain contexts
6. <b>Protein Function</b>	Protein modifications, protein binding and catalysis
7. <b>Sequence bioinformatics</b>	Single and multiple sequence alignments, blast searches, predicting secondary structure, molecular evolution and phylogeny
8. <b>Structural bioinformatics</b>	The pdb file format, structure superposition and similarity searches, mapping sequence conservation onto structures, structural and sequence correlates of binding and catalysis
9. <b>Computational structural biology</b>	Force fields, molecular dynamics, <i>ab initio</i> protein folding, homology modeling, docking and AlphaFold
10. <b>Structure determination methods</b>	The methodology, theoretical underpinnings, uses and limitations of x-ray crystallography, NMR spectroscopy electron microscopy for determining experimental structures

<b>Topics</b>	<b>Details</b>
<b>11. Nucleic acid structure</b>	Forces and interactions that govern nucleic acid structure, DNA double helices, non- canonical nucleic acid structures, RNA based machines, and DNA recognition by binding proteins
<b>12. Drug discovery</b>	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 bundled by topic.

## 5.3 Important Dates

<b>First day of class</b>	<b>2023/09/07</b>
<b>PyMOL Assignment</b>	<b>2023/09/25</b>
<b>Fall break (no class)</b>	<b>2023/10/10</b>
<b>Midterm</b>	<b>2023/10/19</b>
<b>Structure Analysis Assignment</b>	<b>2023/11/20</b>
<b>Last Lecture</b>	<b>2023/11/30</b>
<b>Final Examination</b>	<b>2023/12/11</b>

## 6 Assessments

### 6.1 Marking Schemes & Distributions

Name	Scheme A (%)
PyMOL Assignment	5
Midterm	30
Structure Analysis Assignment	20
Final Examination	45
Total	100

## 6.2 Assessment Details

### PyMOL Assignment (5%)

**Date:** Mon, Sep 25, 5:00 PM

**Learning Outcome:** 4

**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 Monday, Sept 25th at 5:00 pm.** 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 19, 2:30 PM - 3:50 PM, ANNU 156

**Learning Outcome:** 1, 2, 3

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

### Structure Analysis Assignment (20%)

**Date:** Mon, Nov 20, 5:00 PM

**Learning Outcome:** 4

**The Protein Structure Analysis Project:** Students will be asked to analyse aspects a predicted AlphaFold structure which has not been previously analyzed in the literature. The assignment is then to complete 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 Mon., Nov. 20 at 5:00 pm and is worth 20% of the final grade.**

### Final Examination (45%)

**Date:** Mon, Dec 11, 8:30 AM - 10:30 AM, TBA

**Learning Outcome:** 4, 5, 6

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

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## 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.selfregulationskills.ca/>

## 8.4 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>)

## 8.5 Course Offering Information Disclaimer

Please note that course delivery format (face-to-face vs online) is subject to change up to the first-class day depending on requirements placed on the University and its employees by public health bodies, and local, provincial and federal governments. Any changes to course format prior to the first class will be posted on WebAdvisor/Student Planning as they become available.

# 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 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>

### 9.3 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>

### 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 make a booking at least 14 days in advance, and no later than November 1 (fall), March 1 (winter) or July 1 (summer). Similarly, new or changed accommodations for online quizzes, tests and exams must be approved at least a week ahead of time.

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>



## 9.6 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>

## 9.7 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.

## 9.8 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>

## 9.9 Disclaimer

Please note that the ongoing COVID-19 pandemic may necessitate a revision of the format of course offerings, changes in classroom protocols, and academic schedules. Any such changes will be announced via CourseLink and/or class email.

This includes on-campus scheduling during the semester, mid-terms and final examination

schedules. All University-wide decisions will be posted on the COVID-19 website (<https://news.uoguelph.ca/2019-novel-coronavirus-information/>) and circulated by email.

## 9.10 Illness

Medical notes will not normally be required for singular instances of academic consideration, although students may be required to provide supporting documentation for multiple missed assessments or when involving a large part of a course (e.g.. final exam or major assignment).

## 9.11 Covid-19 Safety Protocols

For information on current safety protocols, follow these links:

- <https://news.uoguelph.ca/return-to-campusess/how-u-of-g-is-preparing-for-your-safe-return/>
- <https://news.uoguelph.ca/return-to-campusess/spaces/#ClassroomSpaces>

Please note, these guidelines may be updated as required in response to evolving University, Public Health or government directives.

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