

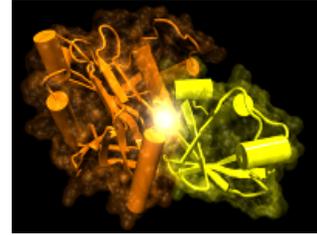
Computational Biology: From sequence to structure to function
BIOL 7800

Spring Semester 2019

Term: January 9 – April 27
Class Times: TTh 9:00am – 10:20am
Location: 213 Tureaud Hall

Instructor: Michal Brylinski
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Office 1: 407 Choppin Hall
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Office hours: Tue 3pm – 5pm (Office 1)
Thu 3pm – 5pm (Office 1)
or by appointment



Course Objectives: Current methods in biology for the modeling of protein structure and molecular function from genomic data. Main focus will be on the application of various computational techniques to support experimental efforts and to help design better experiments. The strengths and limitations of diverse molecular modeling strategies will be discussed. Students are expected to be able to apply many of the covered modeling techniques to their research. Progress will be assessed through homework assignments, in-class presentations and discussions, and exams.

Homework: Simple modeling tasks will be assigned, collected and graded. You may discuss homework assignments with your classmates and use free online resources to accomplish them. Homework is due in no later than 5pm on the due date.

Grading Policy: Projects 33%
Presentations 33%
Final 34%

Tentative schedule:

Classical bioinformatics

- **Week 1:** Protein sequence alignments, database searches

Protein threading and meta-threading

- **Week 2:** Modeling in the “twilight zone” of sequence similarity

Protein secondary structure

- **Week 3:** Assignment from structure, prediction from sequence, [HW1](#)

Protein tertiary structure

- **Week 4:** Structure comparison and alignment, structural classification
- **Week 5:** Template-based modeling
- **Week 6:** Template free modeling (protein folding)

Protein function prediction

- **Week 7:** Homology-based methods, [HW2](#)
- **Week 8:** Structure-based methods

Cheminformatics

- **Week 9:** Ligand docking, binding affinity prediction and virtual screening
- **Week 10:** 2D molecular fingerprints, 3D chemical matching
- **Week 11:** Drug cross-reactivity, drug repositioning, [HW3](#)

Protein-protein interactions

- **Week 12:** Protein rigid body docking, refinement of modeled associations

Molecular mechanics and dynamics

- **Week 13:** Principles and bio applications of MM/MD

High-performance computing

- **Week 14:** Computational biology and high-performance computing, prep for Final Exam

Students with disabilities: If any student feels that he/she has a disability and needs special accommodations of any nature whatsoever, the instructor will work with you to provide reasonable accommodations to ensure that you have a fair opportunity to perform in this class. Please advise the instructor of such disability and the desired accommodations at some point before, during or immediately after the first scheduled class period.