# BIOL 4005/5005-008 - Contemporary Topics in Biology

## Computational Molecular Modeling: From Classical Methods to AI

**Instructor**: Yanxiao Han, PhD **Email**: Yanxiao.Han@unt.edu

**Office**: SRB 236 **Office hour**: Wed 9-10 AM, Friday 11-12 AM.

**Course Level:** Undergraduate / Graduate
**Time**: Tuesday/Thursday from 11:00 a.m. - 12:20 p.m
**Format:** Lecture + Hands-on examples

**Room: Lang 319**

---

**Course Description**

This course introduces the principles and applications of molecular modeling, with a focus on examine biomolecules and drug discovery. Students will learn classical modeling methods, molecular dynamics simulations, docking, and free energy calculations, as well as modern AI-driven approaches. Hands-on experience will be included.

---

**Learning Outcomes**

By the end of the course, students will be able to:

1. Explain fundamental principles of molecular modeling and simulation.
2. Apply classical force fields and/or quantum mechanical methods to study biomolecules.
3. Perform ligand docking and binding affinity estimation.
4. Use molecular visualization and analysis tools.
5. Run and analyze molecular dynamics (MD) simulations.
6. Understand the role of AI/ML in protein modeling and drug discovery.
7. Critically evaluate molecular modeling studies in literature.

---

**Topics by Week**

**Week 1:** Introduction to Molecular Modeling and the role of AI
**Week 2:** Molecular Structure & Force Fields – atoms, bonds, potentials
**Week 3:** Energy Functions & Conformational Search
**Week 4:** Molecular Dynamics Simulations – principles and algorithms
**Week 5:** Predicting Structures of Proteins and Other Biomolecules

**Week 6:** Protein design
**Week 7:** Fourier transforms and convolution. Or Free Energy Calculations – MM/PBSA, FEP, thermodynamic cycles
**Week 8:** Image-analysis
**Week 9:** Midterm Exam + Student Project Proposal Due
**Week 10:** Microscopy
**Week 11:** Diffusion and cellular-level simulation
**Week 12:** Ligand docking and virtual screening
**Week 13:** X-ray crystallography
**Week 14:** Cryogenic Electron Microscopy
**Week 15:** Review, Student Project Presentations
**Week 16**: Future Trends in Molecular Modeling + Final Exam

| | | Topic | Quiz | Assignment (A) | Student project |
|---|---|---|---|---|---|
| Jan 13, 15 | Week 1 | Introduction simulation and AI | | Post A1 on Jan13 | |
| Jan 20, 22 | Week 2 | Molecular Structure & Force Fields | | | |
| Jan 27, 29 | Week 3 | Energy Functions & Conformational Search | Quiz 1 | | |
| Feb 3, 5 | Week 4 | Molecular Dynamics Simulations | | A1 due on Feb 5, Post A2 on Feb 3 | |
| Feb 10, 12 | Week 5 | Predicting structures | | | |
| Feb 17, 19 | Week 6 | Protein design | Quiz 2 | | |
| Feb 24, 26 | Week 7 | Fourier transforms convolution | | | Project proposal due on Feb 26 |
| Mar 3, 5 | Week 8 | Review and midterm exam | | A2 due on Mar 5, Post A3 on Mar 3 | |
| Mar 10, 12 | Spring break | | | | |
| Mar 17, 19 | Week 9 | Image-analysis | | | |
| Mar 24, 26 | Week 10 | Microscopy | Quiz 3 | | |
| Mar 31, April 2 | Week 11 | Diffusion and cellular-level simulation | | | |
| April 7, 9 | Week 12 | Ligand docking and virtual screening | | | |
| April 14, 16 | Week 13 | X-ray crystallography | Quiz 4 | A3 due on April 16 | |

| | | | | | |
|---|---|---|---|---|---|
| April 21, 23 | Week 14 | Cryogenic Electron Microscopy | | | |
| April 28, 30 | Week 15 | Review and Student Project Presentations | | | Student Project Presentations |
| May 5, 8 | Final week | | | | |

---

**Software and Tools**

- **MD Simulations:**

  **CHARMM-GUI – http://www.charmm-gui.org/**

  **MDWeb (IRB Barcelona) – http://mmb.irbbarcelona.org/MDWeb/**

  **PlayMolecule – https://playmolecule.com/**

  GROMACS, NAMD, AMBER

- **Docking:**

  **SwissDock** – http://www.swissdock.ch/

  **DockThor** – http://www.dockthor.lncc.br/

  **CB-Dock2** – http://cao.labshare.cn/cb-dock2/

  AutoDock, Schrödinger Glide (if available)

- **QM Calculations:** Gaussian, ORCA
- **Visualization:** VMD, PyMOL
- **AI tools:** Google Colab notebooks, AlphaFold

---

**Assessment**

- Hands-on Lab Assignments – 20%
- Quiz – 10%
- Midterm Exam – 20%
- Final Project (simulation or analysis with report + presentation) – 20%
- Final Exam – 20%
- Participation – 10%

**Prerequisites**

- Physical Chemistry or Biochemistry (recommended)
- Basic programming (Python) helpful but not required

B107 / C+ in {[(BIOL 1710 / B101 ) AND (BIOL 1720 / B102 ) AND (BIOL 1750 / BIOL 1760 / BI03)] AND [(BIOL 2041+2 / 2140 / 2241 / 2251 / 2302 +2312) / B104] AND [(CHEM 2370 + CHEM 3210) / B106] AND [MATH 1650/ MATH 1680]} 2.5 GPA average in these courses.

**Academic Misconduct:**
Students are expected to abide by the Student Code of Conduct as it appears in the UNT catalog. Academic misconduct will not be tolerated. No cheating will be tolerated. Anyone cheating (all forms) or exhibiting behaviors consistent with cheating, including, but not limited to, assisting other students with cheating: talking during a testing event, accepting credit for another's work, etc., will receive as a minimum punishment a grade of zero for the graded item. More severe punishment will be taken depending on the circumstances. Any incidents of academic dishonesty will be reported to the appropriate authorities.
The following scenarios are examples of forms of cheating:
• Copying a fellow student's work or copying a previous student's work.
• Accessing or taking a quiz or exam outside of our classroom without permission
• Notes written on body parts, clothing, cheat sheets, etc., during a test.
• Listening to headphones (regardless of what is being played) during an exam
• Any form of communication with your neighbor during a test.
• Talking to anyone but the instructor or proctor during a quiz or examination.
• Communicating via cell phones with other people during a test.
• Notes or books are open during in-class exams and quizzes.
• Disclosing or soliciting examination questions to those who may have been absent from an exam.
• Plagiarism (copying entirely or whole phrases from books or websites).
• Any two students handing in assignments with word-for-word responses

**SPOT Evaluations:**
SPOT (Student Perception of Teaching) evaluations for the course will be available during course weeks 12-15 and can be accessed via a link provided through email or the course Blackboard home page. I will provide time during the class period to complete the SPOT (via laptop or smart device) and encourage your feedback on course content, teaching methods, resources utilized, exam structure, PBLs, etc. Please let me know what worked for you and what didn't, and why. Your opinions are valuable to me and will help me adapt the course for future semesters.

**Disability Accommodations.**
The University of North Texas makes reasonable academic accommodations for students with disabilities. Students seeking accommodation must first register with the Office of Disability Accommodation (ODA) to verify their eligibility. If a disability is verified, the ODA will provide you with an accommodation letter to be delivered to the faculty to begin a private discussion regarding your specific needs in a course. You may request accommodations at any time; however, ODA notices of

accommodation should be provided as early as possible in the semester to avoid any delay in implementation. Note that students must obtain a new letter of accommodation for every semester and must meet with each faculty member prior to implementation in each class. For additional information, see the Office of Disability Accommodation website at http://www.unt.edu/oda . You may also contact them by phone at 940.565.4323.