

Recent Announcements

AI Chemistry and Biochemistry 001

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Chemistry 4640/5640 Artificial Intelligence in Chemistry and Biochemistry

University of Colorado, Denver, College of Liberal Arts and Sciences, Department of Chemistry

Syllabus, Spring 2026

Instructor	Woonghee Lee, Ph.D.
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Office Hours	T 8:30 AM – 9:30 AM or upon appointment

Course Dates/Times T/Th 9:30 PM – 11:45 AM

Course Location NC 1313

Course Description, Semester Hours: 3

Artificial Intelligence (AI) changes every aspect of our lives. In this course, we explore AI and its applications from the perspective of a chemist/biochemist. The role of AI and the latest trends in modern chemistry and biochemistry will be taught. Students will learn how to connect modern AI techniques to their own research projects, using both experimental and computational data. Prereq: CHEM 2031, CHEM 2061 and CHEM 3411 with a C- or higher. Pre/Coreq: CHEM 3810/4810/5810 and CHEM 4630/5630. Term offered: spring. Max hours: 3 Credits.

A student who successfully completes the Artificial Intelligence in Chemistry and Biochemistry course will be able to do the following:

1. Technical Knowledge: Student demonstrates knowledge of the fundamental principles and the practical applications of modern artificial intelligence methods to the chemistry and biochemistry problems.
2. Critical Thinking: Student demonstrates knowledge and understanding of the advantages and limitations in using the artificial intelligence methods to the chemistry and biochemistry problems.
3. Information Literacy: Student will have the ability to know when there is a need for information, to be able to identify, locate, and evaluate developed artificial intelligence methods from journal articles and code repositories.
4. Presentation: Students will have the ability to present their project in the conference talk format. The oral presentation will be followed by a short QnA with audience.
5. Teamwork: Student demonstrates the ability to work with peers in a constructive and supportive manner.

Topics covered include:

Advancing research through artificial intelligence

Supervised learning methods and chemical shift assignment problems

Unsupervised learning and allosteric communication networks in proteins

Simulated annealing/Monte Carlo simulation and protein 3D structures

Neural networks and learned representations for the protein dihedral angle prediction

Applying machine learning models for the chemical shift prediction

Deep learning methods for the non-uniform sampling data reconstruction

Computer vision techniques to enhance NMR spectra

Linear models, kernels, and trees

Representations of atomistic systems

Generative AI

Software tools used:

Computational exercises will complement the learning objectives of the course and will provide a deeper understanding of artificial intelligence applications in chemistry and biochemistry. Notes on introduction to Python, Jupyter Notebooks / Google Colab, Virtual Machine, POKY, and other software packages will be provided. Every computational task will include a step-by-step guide that will help you complete the assignment.

Required Texts and Materials:

No textbook needs to be purchased.

A laptop is required for this course. A student has two options: 1. Use one's own, and 2. Free rent from the chemistry department office for the semester with no cost.

Evaluation:

This course will consist of six AI topics, with four different assessments: quizzes, topic leads, the shark tank, and the final project presentation.

Assignments:

<u>Grading Area</u>	<u>% of Total Grade</u>
Topic Lead	20
Quiz	10
Shark Tank	20
Final Project Presentation	50

Letter grades:

<u>Percentage</u>	<u>Letter Grade</u>
94 – 100	A
90 – 93	A-
87 – 89	B+
84 – 86	B
80 – 83	B-

77 – 79	C+
74 – 76	C
60 – 73	C-
54 – 59	D+
50 – 53	D
44 – 49	D-
0 – 43	F

Graduate students:

Graduate students will be required to include in their final project an operational AI implementation posted to Github with step-by-step instruction in the README file or the Jupyter Notebook file. Issues and Pull Requests tabs in Github will be used to provide feedback among grad students. For graduate students, this assignment will be worth 20% of the Final Project points. Graduate students will present the first and last literature weeks.

Schedule:

Before spring break.

- Tuesdays – Dr. Lee provides lectures and hands-on practices.
- Thursdays – Two student presents recent and/or milestone subjects from literature.
- Shark Tank – Students propose and sell their project. Sharks give feedback.

After spring break.

- Each week students sits down and discuss with Dr. Lee for their project until the presentation day.

Week of 1/18/2022: AI in Chemistry and Biochemistry

- Recommended literature:

De novo designed proteins neutralize lethal snake venom toxins

<https://www.nature.com/articles/s41586-024-08393-x>  (<https://www.nature.com/articles/s41586-024-08393-x>).

Week of 1/25/2022: Programming for Chemistry and Biochemistry

- SciPy 1.0: fundamental algorithms for scientific computing in Python, <https://doi.org/10.1038/s41592-019-0686-2> , <https://doi.org/10.1038/s41592-020-0772-5> 
- Biopython: freely available Python tools for computational molecular biology and bioinformatics, <https://doi.org/10.1093/bioinformatics/btp163> 

Week of 2/1/2022: Unsupervised Learning

- Unsupervised Learning Methods for Molecular Simulation Data, <https://doi.org/10.1021/acs.chemrev.0c01195> 
- Multivariate Analysis in Metabolomics, <https://doi.org/10.2174/2213235x11301010092> 

Week of 2/8/2022: Supervised Learning

- Supervised learning of a chemistry functional with damped dispersion, <https://doi.org/10.1038/s43588-022-00371-5> 
- Combining Machine Learning and Computational Chemistry for Predictive Insights Into Chemical Systems, <https://doi.org/10.1021/acs.chemrev.1c00107> 

Week of 2/15/2022: (Deep) Neural Networks

- Accurate structure prediction of biomolecular interactions with AlphaFold 3, <https://doi.org/10.1038/s41586-024-07487-w> 
- Using Deep Neural Networks to Reconstruct Non-uniformly Sampled NMR Spectra, <https://doi.org/10.1007/s10858-019-00265-1> 

Week of 2/22/2022: Computer Vision

- Image Quality Assessment: From Error Visibility to Structural Similarity, <https://doi.org/10.1109/TIP.2003.819861> 

- CryoDRGN2: Ab Initio Neural Reconstruction of 3D Protein Structures From Real Cryo-EM Images, <https://doi.org/10.1109/ICCV48922.2021.00403>  (<https://doi.org/10.1109/ICCV48922.2021.00403>)

Week of 3/1/2022: Simulated Annealing/Monte Carlo Simulation

- Peer Reviewed: Learning Optimization From Nature: Genetic Algorithms and Simulated Annealing, <https://doi.org/10.1038/346343a0>  (<https://doi.org/10.1038/346343a0>)
- Crystallography & NMR system: A new software suite for macromolecular structure determination, <https://onlinelibrary.wiley.com/doi/epdf/10.1107/S0907444998003254>  (<https://onlinelibrary.wiley.com/doi/epdf/10.1107/S0907444998003254>)
- FuncFetch: an LLM-assisted workflow enables mining thousands of enzyme–substrate interactions from published manuscripts, <https://doi.org/10.1093/bioinformatics/btae756>  (<https://doi.org/10.1093/bioinformatics/btae756>)

Week of 3/15/2022: Shark Tank

Week of 3/22/2022: Spring Break. No classes.

Week of 3/29/2022: Project Work

Week of 4/5/2022: Project Work.

Week of 4/12/2022: Project Work.

Week of 4/19/2022 Project Work.

Week of 4/26/2022: Final Project Presentation

Policy

If students miss a session for a valid reason, students will need to provide a proof. Students can review the University of Colorado Denver administrative policy on student attendance and absences at

Curve Policy: Basically, there is no curve applied to either individual assessments or the final grade. However, depending on FCQ participation (over 80%) and students' accomplishment, the instructor will consider.

Late Work Policy: Late work completion will receive a grade of zero.

Extra Credit Policy: Throughout the semester there may be extra credit opportunities, via the attendance and analysis of select UCD Chemistry Department Seminars. Extra credit is granted upon the submission of a summary of the seminar through the course's Canvas course shell. Students are allowed to submit up to three extra credit assignments; to receive credit students must submit the assignment for each respective seminar within one week of the seminar.

Grades of "Incomplete": Incomplete grades are given only in a situation where unexpected emergencies prevent a student from completing the course and the remaining work can be completed the next semester. The instructor is the final authority on whether the student qualifies for an incomplete. Incomplete work must be finished by the end of the subsequent semester or the "I" will automatically be recorded as an "F" on the student's transcript.

Course Policies: Technology and Media

Canvas: The course webpage is available through the Canvas course shell. Login at <https://canvas.cuonline.edu>. Students who are registered (or on the waitlist) for CHEM 4640/5640, are automatically registered for access to the Canvas course webpage. Students that have any problems with logging in or using Canvas, please contact help@cuonline.edu or call 1 (303) 315-3700. The course grades, syllabus, lecture notes, any additional materials, and important announcements will be posted on the course shell.

Students are responsible for checking the course webpage at least once per week for important announcements, updates, and content. Students are required to check grades and correct any clerical errors with the instructor within one week of grades being posted.

E-mail: This course requires that students maintain an e-mail address in Canvas. Students should log into Canvas and check their e-mail address under “Settings”. If a student would like to change their e-mail preference, within Canvas under “Settings” select “Add Email Address” and register the preferred e-mail address. The instructor will communicate with students through Canvas or through the e-mail address maintained in Canvas. When students need to communicate or schedule an office hour appointment with the instructor, the TA is the first person to contact if not urgent.

Mobile Device Usage: The general use of mobile devices is prohibited during lecture, and they must be on silent or vibrate mode during this time.

Course Policies: Student Expectations

Civility: Students and the instructor each have the responsibility for maintaining an appropriate learning environment. Those who fail to adhere to such behavioral standards may be subject to discipline. Professional courtesy and sensitivity are especially important with respect to individuals and topics dealing with differences of race, culture, religion, politics, sexual orientation, gender, gender variance, and nationalities. Class rosters are provided to the instructor with the student's legal name. The instructor will gladly honor the student's request to address him/her by an alternate name or gender pronoun. Please advise the instructor of this preference early in the semester so that the appropriate changes to the instructor's records can be made.

Quantitative Chemistry: This course requires the use of a device for performing AI development/analysis in and out of class, including but not limited to quizzes and exams. Students are responsible for providing their own laptop that meets the needs of the course.

Reading: Students are expected to read relevant material(s), as described the course schedule shown above, before coming to the lecture.

Diversity and Inclusion: I will work to make this class as healthy and positive a learning environment as possible for every student. CU Denver has a wonderfully diverse student population, and I celebrate the cross-section of future scientists, health care professionals, and other contributors to society that is represented in our class. Thus, I encourage and welcome contributions from all of you regardless of background, experiences, socioeconomic status, sexual orientation, gender identity, religious/spiritual inclination, cultural background, age, race, ethnicity, ability or disability. I hope this course will help to produce a scientific and medical workforce that better reflects the diversity of our society, although there is

a long way to go toward this goal. On the other hand, the scientific enterprise today is already highly international, and I encourage all students to pursue international and cross-cultural experiences as part of their training. In this course, I strive to create an environment in which everyone is included; one in which everyone's perspective is respected, taken into consideration, and valued; one in which prejudices of any kind are discouraged. We all have unconscious or implicit biases which can only be overcome through thoughtful awareness. I am working to recognize and acknowledge my own and minimize their impact on my teaching, and I welcome your constructive feedback.

Military Duty: If you are a student in the military with the potential of being called to military service or training during the semester, you are encouraged to contact your school or college Associate Dean or Advising Office immediately.

Religious Observances: Students who want to observe their religious holidays at times when academic requirements conflict with those observances must make a request for a reasonable accommodation for the observance within a timely manner, at least two weeks prior to the holiday; the request is to be in writing.

Student Grievances: Student complaints about this course or instructor should be communicated directly to the instructor in a face-to-face meeting (unless this course is an online course). If the issues cannot be resolved, students should meet with the chairperson of the Chemistry Department. Contact 303-315-7650 to arrange a meeting. If meeting with chairperson does not resolve the issues, students may appeal to the Associate Dean of Student Success in the Office of the CLAS Dean (NC 5014, 303-315-7000). The decision of the Associate Dean is final. Students may also meet with the CU Denver Ombudsman to ask for assistance. For additional information, please see the CLAS policy "Procedures for Student Grievances about Courses or Faculty" available from the Office of the CLAS Dean.

Early Action Statement

Succeeding at college does not mean that you don't struggle in a class or classes or during particular semesters. My goal as your instructor and our goal at CU Denver is to do all we can to support every student and facilitate their success. Early Action (Course Progress Report: CPR) is one of the ways we try to support our students. It's a process by which individual courses can link you to campus supports and it's a time for your instructors to let you know what changes you can make toward success in the course and engage in a learning partnership with you. This is a way to open up the conversation between you and your instructor so that together you can work out how to achieve your goals in the course.

Getting an Early Action is not an indication that you will not succeed in the course. It is a call to action. You might get an email or phone call. Please engage this process. Students who have taken advantage of resources offered them are able to move forward and succeed in the course.

University Policies

Disability Access: The University of Colorado Denver is committed to ensuring the full participation of all students in its programs, including students with disabilities. If a student has a disability or thinks they have a disability and needs accommodations to succeed in this course, the instructor encourages the student to contact Disability Resources and Services (DRS) and/or speak with the instructor as soon as they can. DRS office is located in Student Commons Room 2116 and can be contacted via e-mail at disabilityresources@ucdenver.edu (<mailto:disabilityresources@ucdenver.edu>). The instructor is committed to providing equal access as required by federal law, and the instructor is interested in developing strategies for student success in this course.

DRS requires students to provide current and adequate documentation of their disabilities. Once a student has registered with DRS, DRS will review the documentation and assess the student's request for academic accommodations in light of the documentation. DRS will then provide the student with a letter indicating which academic accommodations have been approved. Students who provide a copy of a DRS letter to their instructor will be provided with approved accommodations in their respective course(s).

Link to university policy on service animals: <http://equity.ucdenver.edu/wp-content/uploads/2017/02/Service-Animal-Policy- FINAL-DRAFT-2016-11-30.pdf>

Discussing Grades over Email: According to the University's interpretation of the Family Education Rights and Privacy Act (FERPA), your instructors are not allowed to discuss grades via email, as it is not considered a secure means of communication. However, I am able to discuss your grades via email if you include the following disclaimer (or some similar statement) in your email to me: "I understand that email is not a secure means of communication and give you permission to discuss my grade via email."

Academic Dishonesty: Students are expected to know, understand, and comply with the ethical standards of the University. A university's reputation is built on a standing tradition of excellence and scholastic integrity. As members of the University of Colorado Denver academic community, faculty and students accept the responsibility to maintain the highest standards of intellectual honesty and ethical conduct.

Academic dishonesty is defined as a student's use of unauthorized assistance with intent to deceive an instructor or other such person who may be assigned to evaluate the student's work in meeting course and degree requirements.

Examples of academic dishonesty include, but are not limited to, the following:

1. **Plagiarism:** Plagiarism is the use of another person's distinctive words or ideas without acknowledgment. Examples include:

1. Word-for-word copying of another person's ideas or words;
2. The mosaic (the interspersing of one's own words here and there while, in essence, copying another's work);
3. The paraphrase (the rewriting of another's work, yet still using their fundamental idea or theory);
4. Fabrication of references (inventing or counterfeiting sources);
5. Submission of another's work as one's own;
6. Neglecting quotation marks on material that is otherwise acknowledged.

Acknowledgment is not necessary when the material used is common knowledge.

1. **Cheating:** Cheating involves the possession, communication, or use of information, materials, notes, study aids or other devices not authorized by the instructor in an academic exercise, or communication with another person during such an exercise. Examples include:

1. Copying from another's paper or receiving unauthorized assistance from another during an academic exercise or in the submission of academic material;
2. Using a calculator when its use has been disallowed;
3. Collaborating with another student or students during an academic exercise without the consent of the instructor.

1. **Fabrication and Falsification:** Fabrication involves inventing or counterfeiting information, i.e., creating results not obtained in a study or lecture experiment. Falsification, on the other hand, involves the deliberate alteration of results to suit one's needs in an experiment or other academic exercise.

1. **Multiple Submissions:** This is the submission of academic work for which academic credit has already been earned, when such submission is made without instructor authorization.
2. **Misuse of Academic Materials:** The misuse of academic materials includes, but is not limited to, the following:
 1. Stealing or destroying library or reference materials or computer programs;
 2. Stealing or destroying another student's notes or materials, or having such materials in one's possession without the owner's permission;
 3. Receiving assistance in locating or using sources of information in an assignment when such assistance has been forbidden by the instructor;
 4. Illegitimate possession, disposition, or use of examinations or answer keys to examinations;
 5. Unauthorized alteration, forgery, or falsification;
 6. Unauthorized sale or purchase of examinations, papers, or assignments.
1. **Complicity in Academic Dishonesty:** Complicity involves knowingly contributing to another's acts of academic dishonesty. Examples include:
 1. Knowingly aiding another in any act of academic dishonesty;
 2. Allowing another to copy from one's paper for an assignment or exam;
 3. Distributing test questions or information about the materials to be tested before the scheduled exercise;
 4. Taking an exam or test for someone else;
 5. Signing another's name on attendance roster or on an academic exercise.

Students who fail to comply with the UC Denver CLAS Academic Ethics Policy are subject to disciplinary action as set forth by the College policy. For more information regarding the Academic Ethics Committee policies and procedures, please refer to <https://clas.ucdenver.edu/faculty-staff/policies-procedures/handling-academic-dishonesty>  (<https://clas.ucdenver.edu/faculty-staff/policies-procedures/handling-academic-dishonesty>).

Course Summary:

Date	Details	Due
Thu Feb 12, 2026	 <u>Quiz 2</u> (https://ucdenver.instructure.com/courses/573253/assignments/2096231)	due by 11:59pm
Thu Feb 19, 2026	 <u>Quiz 3</u> (https://ucdenver.instructure.com/courses/573253/assignments/2096232)	due by 11:59pm
Thu Feb 26, 2026	 <u>Quiz 4</u> (https://ucdenver.instructure.com/courses/573253/assignments/2096234)	due by 11:59pm
Thu Mar 5, 2026	 <u>Quiz 5</u> (https://ucdenver.instructure.com/courses/573253/assignments/2096235)	due by 11:59pm
Thu Mar 12, 2026	 <u>Quiz 6</u> (https://ucdenver.instructure.com/courses/573253/assignments/2096236)	due by 11:59pm
Sat Mar 21, 2026	 <u>Shark Tank</u> (https://ucdenver.instructure.com/courses/573253/assignments/2096242)	due by 11:59pm
Fri Apr 3, 2026	 <u>Progress Report</u> (https://ucdenver.instructure.com/courses/573253/assignments/2096221)	due by 11:59pm
Fri Apr 10, 2026	 <u>Progress Report</u> (https://ucdenver.instructure.com/courses/573253/assignments/2096222)	due by 11:59pm
Thu Apr 16, 2026	 <u>Progress Report</u> (https://ucdenver.instructure.com/courses/573253/assignments/2096227)	due by 11:59pm
Fri Apr 17, 2026	 <u>Progress Report</u> (https://ucdenver.instructure.com/courses/573253/assignments/2096224)	due by 11:59pm
Fri Apr 24, 2026	 <u>Progress Report</u> (https://ucdenver.instructure.com/courses/573253/assignments/2096225)	due by 11:59pm
Tue Apr 28, 2026	 <u>Progress Report</u> (https://ucdenver.instructure.com/courses/573253/assignments/2096228)	due by 11:59pm
Thu Apr 30, 2026	 <u>Final Project Presentation</u> (https://ucdenver.instructure.com/courses/573253/assignments/2096217)	due by 11:59pm
Fri May 1, 2026	 <u>Final Project Feedback</u> (https://ucdenver.instructure.com/courses/573253/assignments/2096215)	due by 11:59pm

Date	Details	Due
Wed May 6, 2026	 <u>Seminar Summary 1</u> (https://ucdenver.instructure.com/courses/573253/assignments/2096238)	due by 11:59pm
	 <u>Seminar Summary 2</u> (https://ucdenver.instructure.com/courses/573253/assignments/2096239)	due by 11:59pm
	 <u>Seminar Summary 3</u> (https://ucdenver.instructure.com/courses/573253/assignments/2096241)	due by 11:59pm
	 <u>Presentation 1</u> (https://ucdenver.instructure.com/courses/573253/assignments/2096218)	
	 <u>Presentation 2</u> (https://ucdenver.instructure.com/courses/573253/assignments/2096219)	
	 <u>Presentation 2</u> (https://ucdenver.instructure.com/courses/573253/assignments/2101659)	
	 <u>Quiz</u> (https://ucdenver.instructure.com/courses/573253/assignments/2096230)	