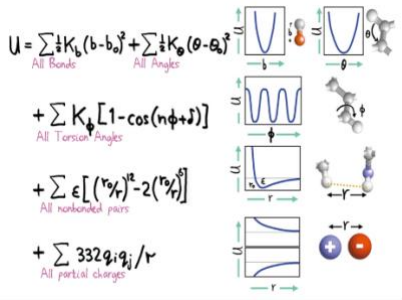
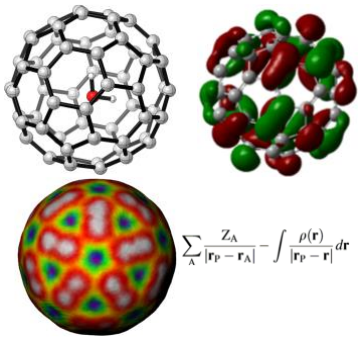


Computational Biochemistry CHEM.5670/201 Fall 2025

Time/Location:
MW 5:00–6:15 p.m.
Location: Olsen 104



Instructor: **Dr. Valeri Barsegov and Dr. Lawrence Wolf**
Office: Olney Hall 501C and Olney Hall 409 (Department of Chemistry)
Office hours: Mon and Wed: by appointment.
Email: Valeri_Barsegov@uml.edu; Lawrence_Wolf@uml.edu

Accessing course: Lectures and office hours as shown above

Course description: Covers basic physical and chemical principles and provides applications for Computational Drug Discovery: 1) Quantum Chemistry calculations; 2) Molecular Dynamics simulations; 3) Machine Learning; and 4) Molecular Docking. 3 credits.

Required textbook: None; access lecture notes or Power Point presentations available online at https://faculty.uml.edu/vbarsegov/teaching/lectures.html

Supplemental Material: "Computational Chemistry" by E. G. Lewars; Essentials of Computational Chemistry by C. J. Cramer; Introduction to Statistical Learning by G. James, D. Witten, T. Hastie and R. Tibshirani

Comp. equipment: Access to computer in computer lab (or notebook).

The following topics and chapters will be covered. You will be expected to take your own notes during the lectures. Unless informed otherwise, you are responsible for all material in the lectures.

Module 1	Quantum Chemistry calculations	Assignement 1
Module 2	Classical MD simulations	Term Project
Module 3	Statistical Learning	Assignment 2
Module 4	Molecular Docking	Assignment 3

Homework: Hard copies for each Assignment and for each Module and Term Project to be submitted before the due dates (TBA). Your grade for that assignment will be based solely on the Assignments 1-3, and Term Project.

Exams: None.

Grade: Your course grade will be based on the following:
Assignment 1 20%, Assignment 2 20%, Assignment 3 20%, and Term Project 40%

Grading scale: 30–49 D, 50–70 C, 71–89 B, 90–100 A.

ELO: This course meets the Essential Learning Outcome (ELO) of *Quantitative Literacy* as defined under the Core Curriculum requirements. As such, the course will strengthen the students' competency and comfort in working with numerical data for computational drug discovery.

Course Learning Outcomes: Quantum Chemistry: 1) Apply force field methods to predict structures of molecules; 2) Learn foundations of quantum chemistry and the fundamentals of quantitative molecular orbital theory; 3) Apply modern quantum chemistry methods including Hartree-Fock and DFT to predict electronic structure of molecules including various properties; Classical Simulations: 4) Learn basics underlying numerical algorithms used in Molecular Dynamics simulations; 5) Use Molecular Dynamics simulations for predicting and interpreting molecular structure; Statistical Learning: 6) Learn statistical modeling approaches employed in supervised/unsupervised machine learning, including regression, classification, resampling, unsupervised learning; 7) Apply Machine Learning approaches to computational drug discovery; Molecular Docking: 8) Learn physical principles used in Molecular Docking; 9) Apply these approaches to predict structures of complexes of proteins with short peptides.

Teaching Methods:

Class meetings will entail a mixture of power point slides, board notes, and computer lab. Students will be expected to follow along with slides and take notes as needed. Students are encouraged to participate by asking questions and responding to questions posed during lectures. All lecture slides, (lab) assignments, and additional course content will become available online.

Student Mental Health and Well-being:

Your personal health and well-being are important to all of us at the university. I'm available to talk about your stresses or concerns related to your coursework in my class.
Here are some resources to support your well-being:

Service/Office	Description	Contact Info
Counseling Services	Provides crisis intervention, assessment, referrals, short term individual counseling and group therapy.	(978) 934-6800
UMatter2	University-wide initiative to support students and promote mental health. Includes access to Togetherall peer-to-peer platform.	(978) 934-6671

CLASS Advising	Provides advising services including goal setting, course selection, SIS functions, changing majors/minors and course deletions.	(978) 934-2936 Advisement@uml.edu
Office of Student Life & Wellbeing	Advances holistic student success through health-promoting actions and collaboration into campus culture.	(978) 934-4342 Wellbeing@uml.edu

Disability accommodation:

If you have a documented disability that will require classroom or testing accommodations, please notify me as soon as possible after the first class meeting so that I can make appropriate arrangements. Please email or speak to me either during office hours or privately after class as I respect and want to protect your privacy. For further information, visit the Student Disability Services webpage at http://www.uml.edu/student-services/disability/default.aspx. In addition, Student Disability Services supports literacy software (available to all students) that allows you to read on-screen text aloud, research and check written work, and create study guides. You can download the software from https://www.uml.edu/accessibility/assistive-technology.aspx.

Attendance and Participation:

You are expected to attend the class regularly, as this is one of the most important contributors to student success. However, you may occasionally need to miss class due to illness, emergency, or caring for a sick family member. Do not come to class if you are ill. In such cases, you are responsible for making up any missed work. You must communicate your requests to me regularly and with as much advance notice as possible. If an instructor becomes ill or needs to miss class or office hours, the instructor will communicate with you as soon as possible via email.

If the campus is closed due to weather or other unforeseen circumstances, please check email and blackboard for information on how to proceed. Class may be cancelled, held virtually, or course material may be presented in a different way in order to stay on schedule.

Academic integrity:

Academic honesty is essential to maintaining trust in the learning environment and ensuring that all students are evaluated fairly. Students are responsible for the honest completion and representation of their work, and academic dishonesty in any form will not be tolerated. Acts such as plagiarism, cheating, fabrication, or facilitating dishonesty undermine the integrity of the academic community and may result in disciplinary action, up to and including failure of the assignment or course, and referral to the provost's office and suspension or dismissal in the case of multiple infractions.

Students are responsible for the honest completion and representation of their work and are held to the highest standards of integrity. If you choose to remain in this course, you must agree that

you will neither give nor receive any unauthorized help on your assignments, term project, or other work. Please review UMass Lowell's policy regarding academic integrity on this website: https://www.uml.edu/catalog/undergraduate/policies/academic-policies/academic-integrity.aspx

AI and Academic integrity: The purpose of this course is to give you a quantitative understanding of physical and biochemical principles underlying computational drug discovery. It is the UML policy to prioritize academic integrity and the authentic demonstration of students' knowledge and skills. Consequently, **the use of Artificial Intelligence (AI) tools, including but not limited to generative technologies and similar platforms, is strictly prohibited in completing any assignments or exams in this course.**

Violations of this policy will be considered academic misconduct and will be subject to disciplinary actions in line with the university's academic integrity procedures. This approach is taken to maintain a fair and equitable learning environment and to encourage the development of skills required for academic and professional work in chemistry without reliance on AI-generated content.

University Privacy Statement:

UMass Lowell recognizes the importance of mutual trust between students and faculty. Massachusetts is a two-party consent state, which means it is illegal to record someone without their permission. Recordings of classroom lectures are the intellectual property of the instructor. Instructors have the right to prohibit audio and video recording of their lectures, unless the requesting student is registered with Disabilities Services and recording of class sessions is an approved accommodation. In addition, sharing or selling recordings of classroom activities, discussions or lectures with any other person or medium without permission of the instructor is prohibited, and may result in sanctions for academic dishonesty or referral to the dean's or provost's office.

Diversity and inclusion:

UMass Lowell—and your professor—values the many forms of human experiences and backgrounds. Enrich yourself by practicing respect in your interactions, and enrich one another by sharing your point of view, knowing that differences will be respected, appreciated, and recognized as a source of strength. The Office of Multicultural Affairs (OMA) supports and advocates for students while leading programs, workshops, and events that foster understanding, equity, and belonging across campus. Students are encouraged to connect with OMA staff for support, to learn about cultural and identity-based student organizations, and to participate in community-building opportunities. Contact (978) 934-4336 or Multicultural_Affairs@uml.edu

Classroom community standards:

UMass Lowell values human diversity in all its forms, whether expressed through race and ethnicity, culture, political and social views, religious and spiritual beliefs, language and geographic characteristics, gender, gender identities and sexual orientations, learning and physical abilities, age, and social or economic classes. Diversity and individual differences are respected, appreciated, and recognized as a source of strength in this class. Please interact respectfully with one another.

Course Outline:

Quantum Chemistry Module (8-9 lectures):
1) Potential Energy Surfaces; 2) Matrix Algebra; 3) Foundations of Quantum Chemistry; 4) Semi-empirical Molecular Orbital Theory; 5) Hartree-Fock model; 6) Basis Sets; 7) Density Functional Theory; 8) Combined Quantum/Classical methods (QM/MM)

Classical Molecular Dynamics Module (8-9 lectures):
1) Fundamentals of Molecular Mechanics of biomolecules; 2) Force Fields (GROMACS, AMBER, CHARMM, OPLS) for computer simulations of biomolecules (RNA, DNA and proteins); 3) Nonbonded interactions (electrostatics, van der Waals interactions); 4) Molecular Dynamics (MD) simulations; running MD simulations; 5) Algorithms used in MD simulations: MD integrators, etc.; 6) Langevin Dynamics simulations.

Statistical Learning Module (8 lectures):
1) Linear models; simple and multivariate linear regression; 2) Classification problems; logistic regression, linear discriminant analysis; 3) Resampling methods: cross-validation, bootstrap; 4) Model selection and regularization methods: subset selection, shrinkage methods, dimensional reduction; 5) Nonlinear models: polynomial regression, regression splines, generalize additive models; 6) Tree-based methods: bagging, random forests; 7) Support Vector Machines (SVMs): support vector classifiers; 8) Unsupervised Learning: principal component analysis, clustering methods.

Molecular Docking Module (4 lectures):
1) Introduction to Molecular Docking (motivation, applications, terminology); 2) Preparing proteins (or other target molecules) and ligands (peptides) for docking simulations; 3) Docking algorithms (search problem, sampling, scoring functions, search space); 4) Analysis and interpretation of docking results, including validation strategies and other approaches beyond docking.