Course Syllabus – CHEM 4503 "Biocomputing in Drug Design I"

Instructor:	Ghislain Deslongchamps	**Class Day(s):**	MWF
Email:	ghislain[at]unb.ca	**Time:**	MWF: 11:30-12:20 (lectures) W: 2:30-5:20 (lab)
Phone:		**Location:**	MWF lectures: Toole 303 W lab: ITD-414
Office Location:	Toole 237	**Office Hours:**	See below

We recognize and respectfully acknowledge that all UNB course interactions take place on unsurrendered and unceded traditional lands of the Wolastoqiyik.

About the Course

Course Description:
6 ch (3C, 3L) Description: Introduction to computer-assisted drug design. Course topics include intermolecular interactions, conformational analysis, molecular mechanics, molecular dynamics, docking, pharmacophores, protein modeling, QSAR, and cheminformatics. Course includes lectures and a weekly computer laboratory component.

Course Prerequisites:
Prerequisite: CHEM 3523 or permission of the instructor.

Textbook(s):
Optional reference textbook:
Introduction to Computational Chemistry, 3rd Ed., Frank Jensen, Wiley, 2017. ISBN 9781118825990 https://www.amazon.ca/Frank-Jensen/dp/1118825993/

Course Topics:
Course topics will be selected from the following list:

- Molecular mechanics
- Conformational searching
- Electrostatics
- Solvation
- Cheminformatics
- Monte Carlo/Metropolis methods
- Molecular dynamics
- QSAR
- Flexible alignment
- Docking/virtual screening
- Homology modeling
- Scaffold replacement

Learning outcomes:
Upon completion of this course, you should be able to:

- understand the fundamentals of various molecular modeling methods.
- understand the mathematical methods behind molecular mechanics and molecular dynamics simulations and carry out simple calculations based on the underlying equations.

- understand the fundamental concepts behind drug docking, pharmacophore perception, QSAR, homology modeling of proteins, cheminformatics, and other topics.
- carry out basic molecular modeling simulations using commercial drug discovery software (MOE, chemcomp.com), including:
    - molecular mechanics calculations
    - conformational analyses (systematic and stochastic methods)
    - molecular dynamics simulations
    - drug docking
    - flexible alignment
    - pharmacophore modeling
    - quantitative structure-activity relationships (QSAR)
    - homology modeling of proteins

Successfully achieving all the course outcomes and expectations requires that you honour the course policies, attend regular classes and labs, and complete all coursework in good faith and on time.

In-person lectures (MWF, 11:30-12:20)

- All lectures are to be held in person in Toole 303 every MWF 11:30-12:20.

In-person computer labs (W, 2:30-5:30)

- All computer labs will be held in person every Wednesday 2:30-5:20 in ITD-414 (Information Technology Centre, D floor, lab 414). Lab experiment details will be made available on D2L prior to each lab time. During the labs, both your instructor and a T.A. will be available to help you throughout the afternoon.
- To use the computers in ITD-414 all students must first set their FCS (Faculty of Computer Science) password to match their UNB password either by following the login screen instructions in the lab or by using this link: https://www.cs.unb.ca/pwreset
- You will be submitting hand-written (or electronic) lab reports after each lab. Instructions on lab report submission will be provided prior to each lab session.
- Lab challenges: An optional molecular modeling challenge will be provided at the end of each week's lab. Participation and performance will be assessed at the end of the term to assign bonus marks (up to 5/100 points) to individuals at the discretion of the instructor.
- Remote access: Students will be able to access the computer lab remotely *outside of normal lab hours* at https://remotelab.cs.unb.ca. Full instructions on how to access the remote lab: https://www.cs.unb.ca/help/remote-lab-gui-access.shtml.

Office hours

- Dr. Deslongchamps will be available in person every Monday from 1:30-3:30 in his office (Toole-237). For a Teams meeting, please email *ghislain@unb.ca* to arrange a time slot. If you cannot attend regular office hours, please email him to arrange an alternate time.

- If you have comments or questions of any other nature (other courses, academic advising, or anything else), please email *ghislain@unb.ca* anytime. You can expect an email response within a day.
- Although D2L Brightspace will be used to provide course materials and other information, please do not contact him through any of the D2L communication features (chat, discussion...); they will not be monitored.
- Likewise, please do not contact him through the Teams class chat outside of normal lecture/lab hours and office hours; it will not be monitored.

Online Materials

All online course materials can be found in D2L Brightspace, UNB's online Learning Management System. You can access it through the MyUNB portal for single login to all UNB services (https://my.unb.ca/Pages/default.aspx) or directly at https://lms.unb.ca/.

Online components in D2L Brightspace may include:

- Class information
- PowerPoint lectures (pdf)
- Lecture videos (linked from Teams)
- Computer lab files
- Articles (pdf)
- Links

Course Evaluation, Grading, and Course Policies

Course Evaluation Scheme*

Item	Value	Date Due	Details
Lab reports	30%	every Wednesday	Individual reports to be submitted by the end of each lab afternoon. Instructions will be given on the first lab period.
Midterm exam	30%	Oct. 16, 2024 2:30-5:20	3-hour exam in ITD-414. Covers lectures and labs up to Oct. 14, inclusive. Comprises a section on lecture materials as well as a section that requires the use of MOE.**
Final exam	40%	Final exam period, TBA	3-hour period in ITD-414. Covers all lectures and labs. Comprises a section on lecture materials as well as a section that requires the use of MOE.**

* Discretionary bonus points for lab challenges will be added to total course score.
** During the midterm and final exam, students will have access to MOE as well as its built-in "Help" menu. Access to any other resources, printed or online, is strictly forbidden.

Grading Scale:

A+: 90%, **A**: 85%, **A-**: 80%, **B+**: 74%, **B**: 68%, **B-**: 62%, **C+**: 56%, **C**: 50%, **D**: 40%, **F**: <40%,

Course Policies:

Expectations for participation and attendance:

- It is expected that students will attend all lectures. Lectures may include course material not available on D2L. Students are expected to participate and to contribute to classroom discussions (UNB policy). Wednesday afternoon computer labs are compulsory.

Extensions or penalties for late work, missed exams, late for test/exam:

- There will be no make-up opportunity for the in-class midterm exam. If missed, the value of the midterm will be automatically transferred to that of the final exam (i.e., 70% of final grade). UNB policy.
- If any lab is missed because of acceptable exceptions, it will be the student's responsibility to complete the lab on his/her/their own time and to submit a lab report prior to the next lab session. If more than one lab is missed, only the first lab report will be graded.
- Time extensions for completing labs and submitting lab reports may be granted at the discretion of the instructor.

Policy on extra credit:

- Students may not receive extra credit for any component of this course.
- The final course grade will be strictly calculated based on accumulated lab report, midterm, and final exam scores, as well as lab challenge bonus points.

Class Recording and Copyright:

- Anyone who wishes to video or audio record lecture presentations or distribute course notes or other similar materials must obtain written consent at the instructor's discretion beforehand. Otherwise, all such reproduction is an infringement of copyright and is absolutely prohibited and subject to academic penalties (see Academic Offences below). In the case of private use by students with documented disabilities, the instructor's consent will not be unreasonably withheld.
- Any course content shared by your instructor is for your personal use for course purposes, is subject to copyright and cannot be shared without the explicit permission of the copyright owner, which may include but not be limited to the course instructor, their colleagues, textbook publishers, and multimedia vendors.
- Sharing of any personal information, including but not limited to personal views and opinions with others, other than for course purposes, is not permitted and may violate UNB's Policy for the Protection of Personal Information and Privacy.

Email Etiquette:

Please view this short video on email etiquette:
https://www.youtube.com/watch?v=r_jL94Q66E4&feature=youtu.be

Key Technologies

Molecular Operating Environment (MOE)
MOE is a leading drug discovery software platform from the Chemical Computing Group ULC (CCG, www.chemcomp.com) that is currently used in the pharmaceutical industry worldwide. All labs will be based on the usage of MOE to carry out a wide range of computer-aided molecular design experiments. MOE can run under Windows or Linux in the lab. A basic understanding of either operating system to open/save files and folders is recommended.

Students have access MOE off-campus. Once your FCS password has been reset at the start of term (https://www.cs.unb.ca/pwreset), you may go to https://www.cs.unb.ca/help/remote-lab-gui-access.shtml to run MOE remotely from your FCS account.

Desire2Learn Brightspace (D2L)
UNB's learning management system is D2L Brightspace. Information about using D2L:
https://www.unb.ca/fredericton/cetl/tls/educational/d2l/student-resources.html
For D2L technical support, contact: d2l@unb.ca

M365/Microsoft Office
As a UNB student you are entitled to install Microsoft 365 (M365) on your personal computer: Web-based Office products (Word, Excel, PowerPoint, and more); cloud-based services (SharePoint, Teams, OneDrive); tools and services for productivity and collaboration
https://unbcloud.sharepoint.com/sites/M365/SitePages/O365-at-UNB.aspx

You are also entitled to download and install the full Microsoft Office suite (Word, Excel, PowerPoint, etc.) on your personal computer:
https://unbcloud.sharepoint.com/sites/ITServices/SitePages/Software.aspx

Teams is the messaging app for real-time collaboration and communication, meetings, file and app sharing at UNB. It requires a computer with a webcam and a microphone or a tablet/cellphone that can run the Teams app. Unless speaking during a group session, please mute your audio. If you have connectivity issues, turning off your webcam may improve performance.
https://unbcloud.sharepoint.com/sites/M365/SitePages/Studying-Remotely.aspx#microsoft-teams

General Technical Support

For general technical support, please contact Information Technology Services (ITS) Help Desk at helpdesk@unb.ca or by phone (UNBF: 457-2222, UNBSJ: 657-2222 or visit in person at the Harriet Irving Library Learning Commons.
Important: ITS does not provide technical support related to the installation and usage of MOE on your personal computer, please email your instructor for any MOE related questions.

Equity, Diversity, and Inclusion

UNB embraces the idea of an intellectual community enriched by diversity along a number of dimensions, including gender, gender identity, sexual orientation, age, culture, ability, race, ethnicity, language, religion, and nationality. It is my intent that all students be well served by this course, that students' learning needs be addressed both in and out of class, and that the diversity students bring to this class be viewed as a resource, strength, and benefit. Your instructor intends to provide materials and activities that are respectful of diversity. In addition, if any of our class meetings conflict with your religious holidays, please let your instructor know so that arrangements can be made for you.

- Location of gender-neutral washrooms on campus (scroll down): https://www.unb.ca/humanrights/resources/index.html
- Office of Human Rights and Positive Environment: https://www.unb.ca/humanrights/index.html

Services for Students with Disabilities

If you are a student with a disability of any type (physical, mental, learning, medical, chronic health, sensory; visible or invisible) you are strongly encouraged to register with the UNBF Student Accessibility Centre (SAC) (https://www.unb.ca/fredericton/studentservices/academic-success/accessibility-centre/) so that you may receive appropriate services and accommodations. Once you are registered with SAC, the instructor will be notified via the UNBF SAC Accommodation Letter of your specific accommodations. If you would like to discuss your particular needs with the instructor, please book a time for a confidential appointment.

Plagiarism and Academic Offences

The university has carefully defined what it considers plagiarism, and these regulations are found in the UNB Undergraduate Calendar, University Wide Academic Regulations, Regulation VIII, which pertains to plagiarism and other academic offences.

Plagiarism is not difficult to spot; web sources can be quickly traced through a variety of specialty search engines. Professors are required to follow the disciplinary procedures.

For more information, please see the Undergraduate Calendar, University Wide Academic Regulations, Regulation VIII, or visit: http://go.unb.ca/tlsPb0XX5 . **It is the student's responsibility to know the regulations.**