

Course Syllabus – CHEM 4503 “Biocomputing in Drug Design”

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: ADM
Office Location:	Toole 237	Office Hours:	See below

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

About the Course

Course Description:

5 ch (3C, 3L) Description: Introduction to biocomputing in the pharmaceutical industry. Topics include molecular modeling, rational drug design, high throughput screening and combinatorial chemistry, protein modeling and 3D bioinformatics. Course includes lectures and a computer laboratory component.

NOTE: For the lab component of this course, students must have access to a PC/Mac computer (or laptop) with administrator privileges to install course specific software. A 3-button scroll-wheel mouse is required.

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	Molecular dynamics
Conformational searching	QSAR
Electrostatics	Flexible alignment
Solvation	Docking/virtual screen
Cheminformatics	Homology modelling
Monte Carlo/Metropolis methods	Scaffold replacement

Learning outcomes:

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

- Understand the fundamentals of molecular mechanics and the Newtonian basis of molecular modelling.
- Understand the mathematics 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 modelling of proteins, cheminformatics, and other topics.
- Understand the use and scope of molecular modelling in drug design.
- Work with MOE in a Mac/Win environment of your choice.
- Be able to carry out basic molecular modelling simulations using MOE, including:
 - molecular mechanics calculations
 - conformational analyses (systematic and stochastic methods)
 - molecular dynamics simulations
 - drug docking
 - flexible alignment
 - quantitative structure-activity relationships (QSAR)
 - homology modelling 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.

Live lectures (MWF, 11:30-12:20)

- Unless covid restrictions change, all lectures will be held in-person in Toole 303 every MWF 11:30-12:20.
- For students with covid-related accommodation, lectures will be simulcast over MS Teams, recorded (audio/video), and will be made available on D2L within one day for review and notes consolidation. If those individuals have questions/comments during lectures, they are asked to please unmute their microphone, communicate with the instructor and wait for a response. Questions may also be submitted via chat but video is much preferred.

Online computer labs (W, 2:30-5:30)

- All online computer labs will be live and moderated on Teams every Wednesday 2:30-5:20. Lab experiments will be made available on D2L prior to lab time. During the lab periods, myself and your T.A. (Amir Ayati, amir.ayati@unb.ca) will be available to help you throughout the afternoon. You may call me or Amir via Teams anytime for one-on-one help. Once again, queries may also be submitted via chat but video is preferred. You will also be able to share your screen with either of us so we can more easily work out solutions to any problems. If answers or clarifications are of benefit to the whole class, they will normally be communicated via Teams video/chat.
- Lab sessions will not be recorded on Teams.

- You will have to submit lab reports by the end of each Wednesday afternoon using Crowdmark. Instructions on lab report submission will be provided before the first lab session.

Virtual office hours

- **I will be available live every Monday and Friday from 1:30-2:30 on Teams.** Please contact me on Teams video if you have any course-related questions. If you cannot attend this regular time, please email me to arrange an alternate time.
- If you have comments or questions of any other nature (other courses, academic advising, or anything else), please email me anytime. You can expect an email response within a day. We can also arrange a time to meet individually through Teams if your query cannot be efficiently addressed by email response.
- Desire2Learn (D2L) will be used to provide course materials and other information. However, please do not contact me through any of the D2L communication features (chat, discussion...); they will not be monitored.
- Likewise, please do not contact me through the Teams class chat outside of normal lecture/lab hours and office hours; it will not be monitored.

Online Materials

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

Key Technologies

Microsoft 365

As a UNB student you are entitled to install Microsoft 365 (M365), a suite of programs that includes Word (word processor), Excel (spreadsheets), PowerPoint (presentations), Teams (communication), OneNote (notes), Stream (video sharing), Sway (presentations), and others. Teams is what you and your instructor will use to take part in online classes and labs.

M365 is free and can be accessed through your MyUNB portal (my.unb.ca, UNB login required).

Note: M365 can be run as cloud-based apps from within web browsers or as standalone applications that can be downloaded and installed to your computer (PC/Mac). Some of these are available as simpler apps for mobile platforms (iOS/Android) but it is recommended that you use the full versions of M365 because the mobile apps may not support all the available features.

More information is available at:

<https://unbcloud.sharepoint.com/sites/UNBO365/SitePages/Studying-Remotely.aspx>

(UNB login required)

MS Teams

For off-campus participation to lectures and labs using MS Teams, your computer should have a webcam, and a microphone. Unless speaking during a session, please mute your audio. If you have connectivity issues, turning off your webcam may improve performance. Finally, you should participate in a quiet space free of noise and distraction (participating in a coffee shop, for example, is not recommended).

- Teams Student Startup Guide: <https://www.unb.ca/fredericton/cetl/student-startup-guide.pptx>

Desire2Learn Brightspace (D2L)

UNB's learning management system is D2L Brightspace. Information about using D2L is available here:

<https://www.unb.ca/fredericton/cetl/tls/educational/d2l/student-resources.html>

For D2L technical support, contact: d2l@unb.ca

Molecular Operating Environment (MOE)

MOE is a leading drug discovery software platform from the Chemical Computing Group (CCG, www.chemcomp.com) that will be used for the computer labs in this course. Because of the alternative delivery requirements, all students must download and install MOE to their home computer. MOE runs on Windows, MacOS and requires a 3-button scroll-wheel mouse. Students will be allowed to use MOE on their personal computers strictly for CHEM4503 course purposes. Distribution of MOE by any means is strictly prohibited and a severe violation of UNB's software license agreement.

Instructions on how to obtain and install MOE will be provided in class and on D2L.

CrowdMark

This is an online grading software that you may be using for you to submit lab reports or exams. Information about using CrowdMark is available here:

[https://www.unbtl.ca/itl/pdfs/Crowdmark Student QuickStart Guide.pdf](https://www.unbtl.ca/itl/pdfs/Crowdmark%20Student%20QuickStart%20Guide.pdf)

Technical Requirements

Technical Preparation and Requirements

This course will be delivered via live lectures broadcasted synchronously and by live instructor-moderated online labs. Please note that you are responsible for ensuring that the technical requirements are met so that you can fully participate in all course learning activities, especially the MOE labs.

All students must have following:

System/Software	Essential Requirements
Hardware	PC or Mac, minimum of 4GB RAM and 3.0 GHz single processor 3-button scroll-wheel mouse (for MOE)
Operating System	PC: minimum Windows 10 Mac: minimum Mac OSX 10.12 or later
Internet Speed	High speed Internet is recommended.
Internet Browser	Updated version of a web browser that supports HTML5 including, Internet Explorer, Edge, Firefox, Google Chrome, or Safari. To verify your browser, go to https://www.whatismybrowser.com/ and ensure that a green checkmark displays with the text "Your web browser is up to date".
Software	<ul style="list-style-type: none"> - MOE 2020. Instructions on how to obtain and install MOE will be provided during the first week of classes by email and D2L. - VPN client. To run, MOE must first communicate with UNB via Forticlient, UNB's virtual private network. Please login to my.unb.ca and navigate to "I want to..." , "Download free software", "Students - Browse Software" then download and install "Forticlient VPN Client" for your operating system. - Adobe Acrobat Reader (https://www.adobe.com)

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.

Course Evaluation, Grading, and Course Policies

Course Evaluation Scheme

Item	Value	Date Due	Details
Lab reports	30%	every Wednesday	Individual reports to be submitted online by the end of each lab afternoon via Crowdmark. Instructions will be given on the first lab period.

Item	Value	Date Due	Details
Midterm	30%	Oct. 20, 2021 2:30-5:20 ADM	3-hour period. Covers lectures and labs up to Oct. 19. Requires MOE access on student computer.*
Final exam	40%	Exam period TBA	3-hour period. Covers all lectures and labs. Requires MOE access on student computer.*

* During midterm and final exam, students have access to the MOE "Help" menu. Access to any other resources, printed or online, is strictly forbidden.

Grading Scale:

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

Course Policies:

Expectations for participation and attendance:

It is expected that students will attend all the live lectures. These may include course material not available on D2L. Students are expected to participate and to contribute to classroom discussions ([UNB policy](#)). All lectures will be recorded on Teams and be made available for later review on D2L.

Computer labs are compulsory and must be completed during live Wednesday afternoon sessions. Lab sessions will be moderated over Teams but will not be recorded.

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

There will be no make-up opportunity for the in-class midterm examination. 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, it will be the student's responsibility to complete the lab on his or her own time and without assistance from a lab TA. If more than one lab is missed, only the first lab report, if received within 5 days of the original lab date, will be considered for grading.

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.

Class Recording and Copyright:

Anyone who wishes to video or audio record lecture presentations or distribute course notes or other similar materials provided by instructors must obtain the instructor's written consent 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.

Privacy Statement for Online Course Recordings:

- The content shared by your instructor 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.
- Any recordings of online classes provided by your instructor are for your personal use for course purposes only and not to be shared with others.
- 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.
- Personal opinions, views, and commentary provided in the course of online delivery may be considered personal information, which requires the consent of the person who provided it in order to share it ethically and legally. Course videos are to be used only to help you learn the course material.

Email Etiquette:

Please view this short video on email etiquette:

https://www.youtube.com/watch?v=r_jL94Q66E4&feature=youtu.be

Getting organized for online academic success

Your Academic Work is Your Full-Time Job

Treat your studies at UNB as a full-time job, if you are enrolled full-time. Every lecture hour of a course takes on average 3 hours of work outside of that, preparing, reviewing, studying, and working on assignments. Set aside about 40 hours of time per week for your academic work and use this rule-of-thumb as a guide to setting expectations for the others with whom you share your living space, which will most likely also be your learning and study space. If you have a job while studying at UNB, try to keep it to no more than 15 hours per week.

Create Your Learning and Study Space

This brings us to the first and very important consideration: your learning and study space. These may be two different spaces because you will need to spend time on a computer in live online classes and meetings. You'll also need a web camera with a microphone, and speakers or headphones to participate. This may be problematic if you share a computer while living at

home. You will need to schedule this time, and perhaps negotiate it with the others you live with, especially if they work at home or are also taking online courses.

The study space may also require access to a computer most of the time, and certainly a quiet place organized with the things you need to work, such as desk space, a comfortable chair, room to lay out paper and books, good lighting, and a water bottle. A study timer may be useful, and if you don't have a desk, a lap desk may do. You need a way to upload copies of handwritten work, whether by scanning or photographing documents. You may need to repurpose a room or part of one in your house or apartment, or your bedroom.

Manage Your Time

Since your academic work is your full-time job, likely to take 40 hours per week, you need to set an academic work schedule on a weekly basis. To get set up to do this, look at the key academic dates for the entire term and note the important ones:

<https://www.unb.ca/secretariat/students/undergraduatedatesmain.html>

Student Resources for Studying Remotely:

<https://unbcloud.sharepoint.com/sites/UNBO365/SitePages/Studying-Remotely.aspx>

Library information

UNB Libraries (www.lib.unb.ca) supports your learning and academic success. Librarians will help you navigate academic resources and guide you through your research and information needs. Examples of this support include finding reliable sources for your assignments, searching the scholarly databases, and offering advice on the quality of your research. A vast collection of resources is available to you online and in print at lib.unb.ca. Research help is available by phone, e-mail, chat, and in-person.

The Harriet Irving Library (HIL) is the main library at UNBF. The UNBSJ library is located in the Hans W. Klohn Commons.

The libraries offer quiet and group study space. Book a Group Study Room online at http://www.lib.unb.ca/services/group_study.php

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. I intend to provide materials and activities that are respectful of diversity. Your suggestions are encouraged and appreciated. In addition, if any of our class meetings conflict with your religious holidays, please let me know so that we can make arrangements 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)

(<http://www.unb.ca/fredericton/studentservices/academics/accessibility/>) 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 calendar section B.19 IX Academic Offences:

Plagiarism includes:

1. quoting verbatim or almost verbatim from any source, regardless of format, without acknowledgement;
2. adopting someone else's line of thought, argument, arrangement, or supporting evidence (such as, statistics, bibliographies, etc.) without indicating such dependence;
3. submitting someone else's work, in whatever form (essay, film, workbook, artwork, computer materials, etc.) without acknowledgement;
4. knowingly representing as one's own work any idea of another.

NOTE: In courses which include group work, a penalty may be imposed on all members of the group unless an act of plagiarism is identified clearly with an individual student or students.

Please note that 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 outlined in the calendar (B.17. IX. A. 1-2).

OTHER ACADEMIC OFFENCES you need to be aware of include:

1. Cheating on examination, tests, assignments or reports, including but not limited to:
Impersonating a candidate at an examination or test or in connection with any assignment in a course or availing oneself of the results of impersonation.
Obtaining, through theft, bribery, collusion, purchase, or other improper manner,
 1. an examination or test paper prior to the date and time for writing the examination or test;
 2. academic materials belonging to another person, e.g. laboratory reports, assignments, papers, computer materials, datasets.

2. Falsifying or knowingly submitting false assignments or credentials, records, transcripts, or other academic documents.
3. Submitting a false health or other certificate.
4. Submitting identical or substantially similar work for one course or program of study, which has been or is being submitted for another course or program of study, without the prior express knowledge and approval of the instructors.
5. Interfering with the right of other students to pursue their studies.
6. Knowingly aiding or abetting any of the above offences.
7. Tampering with, or altering, in any deceptive way, work subsequently presented for a review of the grade awarded.

Penalties for plagiarism and other academic offences range from a minimum of F (zero) in the assignment, exam or test to a maximum of suspension or expulsion from the University, plus a notation of the academic offence on the student's transcript.

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