CHEM 436 / CHEM 630: Molecular Modelling of Proteins
Syllabus for Winter 2018 Term

GENERAL INFORMATION

This 3-credit course offers a hands-on introduction to the computer tools used to predict the structure of a protein from its amino acid sequence, and to get insight into its function. The student will learn modelling techniques such as sequence alignment, homology modelling, computer visualization, molecular dynamics, and molecular docking.

Instructor: **Dr. Guillaume Lamoureux**
Office: SP-201.09
Office Hours: Fridays from 10:00 to 11:00 (or by appointment)
Email: guillaume.lamoureux@concordia.ca
(Please put "CHEM 436/630" in the subject of your email.)
Website: http://faculty.concordia.ca/glamoure/teaching.html

Tutorials: Wednesdays from 18:00 to 22:00
Location: CC-203

FORMAT

Sessions will typically consist of a lecture introducing the topic and related concepts, followed by a computer tutorial/laboratory.

EVALUATION

The final grade for the course is composed as follows: 5% for the pre-lab reports and preparation, 55% for the lab reports, and 40% for the written exam. Pre-lab reports are worth 1% each. Lab reports are worth 10% each except lab report #2, which is worth 15%. The minimum passing grade for the course is 50% but **of these 50 points at least 30 should come from the lab and pre-lab reports and at least 20 should come from the written exam**.

The material is the same for both CHEM 436 and CHEM 630 courses, but students registered to CHEM 630 will be held to higher standards for the lab reports and will have to answer more questions at the written exam.

PRE-LABORATORY REPORTS

Pre-lab reports should be submitted electronically (to guillaume.lamoureux@concordia.ca) before the tutorial. Any pre-lab report received after 6 PM the day it is due will be given the mark "0".

LABORATORY REPORTS

The reports should present all the information needed for the reader to assess the validity and significance of the results. They should (probably) be organized as follows:
- Introduction (background and motivation)
- Methods, Results, and Discussion
- Summary/Conclusion
- References
- Appendix (screen shots, longer tables, etc.)

Students are responsible for keeping track of all the information needed to write the reports—either by emailing it to themselves or by transferring it to an online storage services such as Dropbox (https://www.dropbox.com) or Google Drive (https://drive.google.com).

SUBMITTING THE REPORTS

All lab reports should be submitted both as a hard copy (directly to the instructor) and in electronic form (to guillaume.lamoureux@concordia.ca). **The electronic copy should be in Portable Document Format (PDF).** Unless specific agreement with the instructor is obtained prior to the due date, the grade for late lab reports will be reduced by 10% per day late.

PLAGIARISM AND OTHER FORMS OF ACADEMIC DISHONESTY

The academic code of conduct can be found in the Undergraduate Calendar at http://www.concordia.ca/academics/undergraduate/calendar/current/17-10.html, and in the Graduate Calendar at http://www.concordia.ca/academics/graduate/calendar/current/policies-procedures.html. Any form of unauthorized collaboration, cheating, copying or plagiarism found in this course will be reported and the appropriate sanctions applied. Ignorance of these regulations is no excuse and will not result in a reduced sanction in any case where academic misconduct is observed. Students can find more resources at http://www.concordia.ca/students/academic-integrity.html.

CALENDAR

Please note that this calendar may change as the semester proceeds.

Date		Topics
Jan 10	Lecture	Introduction to the course and the online resources
Jan 17	**Due date**	**Pre-Lab #1**
	Tutorial 1a	Protein sequence alignment
Jan 24	Tutorial 1b	Comparison/validation of alignments
Jan 31	Tutorial 1c	Protein visualization
Feb 7	**Due date**	**Lab Report #1 (version 1) and Pre-Lab #2**
	Tutorial 2a	Homology modelling 1
Feb 14	Tutorial 2b	Homology modelling 2
Feb 28	**Due date**	**Lab Report #1 (version 2)**
	Tutorial 2c	Comparison/validation of models
Mar 7	**Due date**	**Lab Report #2 and Pre-Lab #3**
	Tutorial 3a	Empirical force fields
Mar 14	Tutorial 3b	Molecular dynamics: Simple systems
Mar 21	**Due date**	**Lab Report #3 and Pre-Lab #4**
	Tutorial 4a	Molecular dynamics: Setup
Mar 28	Tutorial 4b	Molecular dynamics: Analysis
Apr 4	**Due date**	**Lab Report #4 and Pre-Lab #5**
	Tutorial 5	Molecular docking
Apr 11	Tutorial 5	Molecular docking (continued)
Apr 18	**Due date**	**Lab Report #5**
TBA		**Written exam**

REQUIRED READING

Specific reading material will be provided with each Tutorial. Some will be identified as "**Reference material**", to be consulted in preparation for the tutorials and during the tutorials, if need be. Some will be identified simply as "**Reading**", which should be considered study material for the reports and in preparation to the final exam. Some will be identified as "**Required pre-lab reading**", and will be specifically required as part of the pre-lab preparation. Those will usually be scientific articles describing the techniques used in the tutorial or reporting research done using those techniques.

BIBLIOGRAPHY

There is no textbook for the course, but the following books have been put at the Reserve of the Vanier Library. It is strongly recommend that the are consulted throughout the course.

- **Anna Tramontano, *Introduction to Bioinformatics* (2007).**
  Nice, concise introduction to sequence alignment and homology modelling.
- **Marketa Zvelebil and Jeremy O. Baum, *Understanding Bioinformatics* (2008).**
  Well-organized, fairly complete treatment of the topic. Discusses many practical/technical issues in detail.
- **Andrew R. Leach, *Molecular Modelling: Principles and Applications,* 2nd Edition (2001).**
  Covers a lot of material. Of particular interest for the course are Chapter 4 (empirical force fields), Chapter 7 (molecular dynamics methods), Chapter 10 (protein structure prediction) and Chapter 12 (molecular docking and drug design).