Term Information

Effective Term	Spring 2018

General Information

Course Bulletin Listing/Subject Area	Chemistry
Fiscal Unit/Academic Org	Chemistry - D0628
College/Academic Group	Arts and Sciences
Level/Career	Graduate, Undergraduate
Course Number/Catalog	5240
Course Title	Introduction to Protein Modeling
Transcript Abbreviation	Intr Protein Model
Course Description	This course provides a practical introduction to the theory and methods of molecular modeling and computational chemistry as it pertains to modeling large biological molecules such as proteins. Hands-on experience will be obtained by all attendees in doing molecular mechanics and modeling dynamic systems (molecular dynamics).
Semester Credit Hours/Units	Fixed: 3

Offering Information

Length Of Course	14 Week
Flexibly Scheduled Course	Never
Does any section of this course have a distance education component?	No
Grading Basis	Letter Grade
Repeatable	No
Course Components	Lecture
Grade Roster Component	Lecture
Credit Available by Exam	No
Admission Condition Course	No
Off Campus	Never
Campus of Offering	Columbus

Prerequisites and Exclusions

Prerequisites/Corequisites	Prereq: Successful completion of Organic Chemistry II (CHEM 2520 or 2620 or 2920H).
Exclusions	
Electronically Enforced	Yes

Cross-Listings

Cross-Listings	

Subject/CIP Code

Subject/CIP Code	40.0501
Subsidy Level	Doctoral Course
Intended Rank	Senior, Masters, Doctoral

Requirement/Elective Designation

The course is an elective (for this or other units) or is a service course for other units

Course Details

Course goals or learning objectives/outcomes

- Apply fundamental physicochemical principles and concepts which underlie molecular modeling
- Appraise recent applications of molecular modeling which successfully address important biological questions
- Evaluate the scope of applicability of molecular modeling including its advantages and limitations
- Develop the practical skills necessary to perform molecular modeling studies
- Perform their own molecular dynamics study and analyze its results

Content Topic List

- Introduction, Basic amino acid & protein structure
- DNA & RNA structure, Visualizing protein structures: PyMol et al
- Alignment of structures (protein-protein), Molecular Modeling
- Molecular Modeling
- Modeling small molecules, PDB structures pharmacophore modeling
- Homology modeling
- loop modeling – fixing poor structure & structure validation
- Molecular Dynamics & Solvation
- Normal mode analysis
- Protein-protein , Protein-ligand docking
- Glycoproteins & membranes
- Modeling trans-membrane proteins
- Enzymes & QM/MM

Sought Concurrence

No

Attachments

- CHEM Curricular Map - Version 1.pdf: Curriculum Map

  (Other Supporting Documentation. Owner: Sutherland,Laura Nicolle Romrell)
- 5240 Syllabus 2018 (091917).docx: Updated Syllabus

  (Syllabus. Owner: Sutherland,Laura Nicolle Romrell)
- Chemistry 5240 Curricular Mapping Justification.docx: Justification for course mapping

  (Other Supporting Documentation. Owner: Sutherland,Laura Nicolle Romrell)

Comments

- Uploaded revised syllabus and justification for why course is believed to be operating at the advanced level for all six CHEM major program goals. *(by Sutherland,Laura Nicolle Romrell on 09/19/2017 12:54 PM)*
- See 9-14-17 email to T Gustafson and L Sutherland *(by Vankeerbergen,Bernadette Chantal on 09/14/2017 12:54 PM)*

Workflow Information

Status	User(s)	Date/Time	Step
Submitted	Sutherland,Laura Nicolle Romre	06/07/2017 08:16 AM	Submitted for Approval
Approved	Gustafson,Terry Lee	06/07/2017 08:37 AM	Unit Approval
Approved	Haddad,Deborah Moore	06/07/2017 08:53 AM	College Approval
Revision Requested	Vankeerbergen,Bernadette Chantal	09/14/2017 12:55 PM	ASCCAO Approval
Submitted	Sutherland,Laura Nicolle Romre	09/19/2017 12:54 PM	Submitted for Approval
Approved	Gustafson,Terry Lee	09/19/2017 12:57 PM	Unit Approval
Approved	Haddad,Deborah Moore	09/19/2017 03:54 PM	College Approval
Pending Approval	Nolen,Dawn Vankeerbergen,Bernadette Chantal Oldroyd,Shelby Quinn Hanlin,Deborah Kay Jenkins,Mary Ellen Bigler	09/19/2017 03:54 PM	ASCCAO Approval

THE OHIO STATE UNIVERSITY

CHEMISTRY 5240 – Spring 2018

Introduction to Protein Modeling

Lecture: MWF, 1:50-2:45, MP0008 (3 credit hours)

Instructor:	Dr. Richard Spinney
Email:	Spinney.2@osu.edu
Office:	120A Celeste Lab
Office Hours:	Drop-in or by appointment
Textbooks:	***Introduction to Protein Architecture: The Structural Biology of Proteins***, Lesk, Arthur M., Oxford University Press, 2001. Or ***Proteins Structure and Function***, Whitford, David, Wiley, 2005. Or any biochemistry textbook. ***Molecular Modeling: Basic Principles and Applications***, 3rd Ed. Hans-Dieter Holtje, Wolfgang Sippl, Didier Rognan & Gerd Folkers, Wiley-VCH 2008, or Jensen or Cramer if you already have one of those.
Other Materials:	*Molecular Modeling and Simulations,* Tamar Schilk, Springer 2002. *Introduction to Computational Chemistry,* Frank Jensen, 2007. *Molecular Modeling: Principles and Applications,* Andrew Leach, 2001. *Structural Bioinformatics, 2nd Ed.* Gu & Bourne 2009. *Understanding Bioinformatics,* Marketa Zvelebil & Jeremy O. Braum 2008. *Biophysics an Introduction,* Rodney Cotterill, 2002. Introduction to Protein Structure. C. Branden & J. Tooze, Garland Publishing, 2002. *Molecular Modeling of Proteins 2nd Ed.* Andreas Kudol 2015.

Required Prerequisites: Successful completion of Chemistry 2520 (Organic Chemistry II) with a C or better; or graduate standing; or permission of the instructor.

Recommended pre/co-requisites: Biochemistry 4511 suggested but not required.

Course Description & Goals: To provide a practical introduction to the theory and methods of molecular modeling and computational chemistry as it pertains to modeling large biological molecules such as proteins. Hands-on experience will be obtained by all attendees in doing molecular mechanics and modeling dynamic systems (molecular dynamics).

My intention in this class is to provide students with the basic background for critical analysis of computational methodologies and their applications. I do not stress memorization of specific details of various topics that are covered in the course; rather, the emphasis is on the understanding and critical thinking. Therefore, the course is designed to use Monday and Friday classes to discuss basic concepts and, from time to time, mathematical derivations and in class exercises. Wednesdays will be used for software training and discussing assignments. The class runs like a workshop with a significant number of in-class exercises, as such **attendance is mandatory**. Any missed exercises due to an absence without prior permission will be counts as a zero unless it is a recognized University excuse (medical, family emergency etc.) in which case the student will have one week to make-up the missing assignment.

Software: All students will be provided access to modern molecular modeling software such as Molecular Operating Environment (MOE)* and Yasara, as well as a number of open source web-based applications in order to practice protein modeling. The software runs on PCs in the Computational Chemistry Instructional Facility (MP0008). Access to MP0008 requires a chemistry computer account and Buck ID for door access.

Course Objectives:
By the end of the course the student should be able to:
- Apply fundamental physicochemical principles and concepts which underlie molecular modeling
- Appraise recent applications of molecular modeling which successfully address important biological questions
- Evaluate the scope of applicability of molecular modeling including its advantages and limitations
- Develop the practical skills necessary to perform molecular modeling studies
- Perform their own molecular dynamics study and analyze its results

Student Responsibility: Each student receives this syllabus in the first week of the term. It is your responsibility to read this material and be familiar with the course content, procedures, and grading. You are also responsible for any announcements made in class and on Carmen concerning course procedures. (If you are absent, you are expected to get notes, announcements, etc. from another student in the class.)

Carmen | carmen.osu.edu: Carmen is the Learning Management System (LMS) used at Ohio State. It utilizes an LMS engine called Canvas. Log in to Carmen on your device to access your course materials, complete assignments, turn in select assignments, view your grades, and track your progress throughout the semester. A Canvas app is also free to download for both Android and iOS, making it easy to log in to your course from anywhere.

Grading: Your performance in the course will be evaluated based on the components below. Any concerns about your grades or performance should be addressed with your instructor promptly.

Component	%	Notes, Dates & Coverage
Weekly assignments & in class exercises	60%	Short reports
Individual projects	10%	Short formal reports - ~5 pages
exam	30%	Scheduled by the Registrar

Note: For all assignments and projects you must complete the computational work for a grade greater than zero.

Attendance Policy: Due to the nature of the material and limitations of any textbook, as well as the software training required, attendance is expected at every lecture. Failure to do so will have negative consequences for your final grade in the course. Unexcused absences will result in a 1% loss to your overall grade.

Exercises: There are a number of in class exercises, they count the same as homework.

Homework Assignments: Problem sets will be handed out in class, usually on Wednesdays, and will be due one week later by the start of class. For consistency, there will be no extensions on due dates.

For the homework, exercises, projects (and exam), you **MUST** do all of the work yourself. You are welcome to discuss issues of how to do the calculations (i.e. use the software) with other students or your instructor. However, you must do all of the calculations yourself, and submit the required written report or data files. If there is any doubt, you will be asked to produce the output files for any calculation performed. It would be advisable to keep all of your work until the end of the semester.

Homework and exercises address specific topics / issues in protein modeling and you are only required to answer the specific questions and perform specific calculations.

Individual Project: The course is meant to be a practical introduction to protein modeling, so besides attending lectures and doing the problem sets, each student is expected to work on a small “research” style project. The project is open, hopefully based on a suggestion from the student.

If you have difficulties coming up with a problem of interest, please discuss the matter with me, there are a number of continuing projects you may work on. You should start the project by the ninth week of classes to be sure of completing it on time (by the end of the eighth week of classes you must have a project and basic methodology completed). The final written report (~ 5 pages long) is due by the last Friday of classes. You will be asked in the seventh week of the course for a short abstract detailing the nature of your project.

The individual project is a short formal report. They need to include: An introduction, a brief (~1/2 page) introduction to the nature of the experiment and why it is important.

- A procedure, detailing the software used and level of theory of the calculation, in sufficient detail so I can reproduce your experiment exactly as you did it.
- A data section, well formatted and organized, making use of tables and figures as appropriate.
- Finally a discussion / conclusion section where you discuss your experimental findings, and address any questions from the problem set.
- **ALL** sources **MUST** be properly referenced!

The style is complete sentences and paragraphs (point form is not appropriate), all figures and tables need to be properly labeled and titled (Tables at the top, Figures at the bottom, sequentially numbered), proper references for any source is required. Again the reports are individual projects you should not discuss or share your report with anyone as this is considered Academic Misconduct and will be treated as such. If you have any questions about the report ask your instructor. More information is available in Carmen.

Exams: The exam is a scheduled part of this course and attendance is required. The exam is comprehensive and will take place during the university scheduled time. Sixty days after final grades are posted, your grade in Carmen is considered final and all other records are destroyed.

Tentative Course Schedule:

Week	Topics	Assignments
Jan. 8 (3)	Introduction, Basic amino acid & protein structure	Ex1, Ex2
Jan. 15 (2)	DNA & RNA structure, Visualizing protein structures: PyMol et al	Ex3
Jan. 22 (3)	Alignment of structures (protein-protein), Molecular Modeling	HW1
Jan. 29 (3)	Molecular Modeling	HW2
Feb. 5 (3)	Modeling small molecules, PDB structures pharmacophore modeling	HW3
Feb. 12 (3)	Homology modeling	HW4
Feb. 19 (3)	loop modeling – fixing poor structure & structure validation	HW5
Feb. 26 (3)	Molecular Dynamics & Solvation	HW6
Mar. 5 (3)	Normal mode analysis	HW7
Mar. 12	Spring Break	
Mar. 19 (3)	Protein-protein , Protein-ligand docking	HW8
Mar. 26 (3)	Glycoproteins & membranes	HW9
Apr. 2 (3)	Modeling trans-membrane proteins	HW10
Apr. 9 (3)	Enzymes & QM/MM	HW11, Exam
Apr. 16 (3)	Projects	
Apr. 23 (1)		Project due
Apr. 25	Final exam (comprehensive)	

Disability Services: The University strives to make all learning experiences as accessible as possible. If you anticipate or experience academic barriers based on your disability (including mental health, chronic or temporary medical conditions), please let me know immediately so that we can privately discuss options. To establish reasonable accommodations, I may request that you register with Student Life Disability Services. After registration, make arrangements with me as soon as possible to discuss your accommodations so that they may be implemented in a timely fashion. **SLDS contact information:** slds@osu.edu; 614-292-3307; slds.osu.edu; 098 Baker Hall, 113 W. 12th Avenue.

Commitment to Diversity: The Department of Chemistry and Biochemistry promotes a welcoming and inclusive environment for all students and staff, regardless of race, gender, ethnicity, national origin, disability or sexual orientation. There is no tolerance for hateful speech or actions. All violations of this policy should be reported to the OSU Bias Assessment and Response Team (BART, studentaffairs.osu.edu/bias). The Department encourages diversity at all levels, particularly among the next generation of scientists. Students are encouraged to participate in organizations that provide support specifically for science and engineering students who are African-American, Asian, disabled, Hispanic, LGBTQ or women. These organizations are listed on the Colleges of Arts and Sciences (artsandsciences.osu.edu/stem-organizations) and Engineering (engineering.osu.edu/studentorgs) websites.

STANDARDS OF ACADEMIC CONDUCT

Violations of academic standards in General Chemistry will be referred to the University Committee of Academic Misconduct (COAM) as required by Faculty Rules. It is the responsibility of COAM to investigate all reported cases of student academic misconduct; illustrated by, but not limited to, cases of plagiarism and any dishonest practices in connection with examinations, quizzes, and graded assignments. Instructors shall report all instances of alleged academic misconduct to the committee (Faculty Rule 3335-5-487). For additional information see the Code of Student Conduct: **http://studentaffairs.osu.edu/pdfs/csc_12-31-07.pdf**

Student Responsibilities: *Any graded material submitted in this course must represent your own work.* This includes exams, quizzes, homework, and computational assignments, which are to be an individual effort. Unauthorized group efforts by students, use of another student's course materials, or assistance from individuals who already have taken the course, could place you in jeopardy of violation of the standards for this course. In some courses, group work is acceptable on certain activities (as explicitly stated by your instructor). In these cases, it is important that you know and understand where authorized collaboration (working in a group) ends and collusion (working together in an unauthorized manner) begins. Identical answers indicate copying or unacceptable group efforts - always answer questions in your own unique words. It is important that you consult with your instructor for clarification on whether or not collaboration is appropriate on an activity.

You should not assist others in violating academic standards. Students supplying materials for others to "look at" may be charged with academic misconduct. Never allow another student access to your assignments – even after completion of the course. "I didn't know they were going to copy my work" is not an acceptable excuse.

Exams/Quizzes/Homework: Examinations are a crucial part of university courses, and the integrity of these assessments is taken very seriously. During exams and quizzes, staff will monitor for violations of academic integrity. Video recordings or photos may be taken by department staff during exams or quizzes. Any violation, or appearance of a violation, on exams and quizzes will be immediately reported to COAM with a recommended **minimum** penalty a failing grade for the course. Below is a non-exhaustive list of examples of Academic Misconduct on exams and quizzes:

- Viewing or copying others' answers, use of crib material (e.g. a "cheat sheet"), or use of stored constants and formulas in calculators on quizzes, activities, midterm examinations, or the final exam. This kind of behavior is regarded as a severe violation of academic standards, no matter how small the action.
- Students should take care to preventatively avoid appearances of academic misconduct during testing. Best practices for avoiding the appearance of academic misconduct include focusing on one's own exam, making efforts to conceal one's own answer sheet and written work on exam pages both during and after the exam, not allowing one's own eyes to "wander the room," avoiding writing answers in the margins to be seen by other students, clearly ceasing working when time is called, and not speaking with other students at any point during the exam, including when in line to turn in the exam. It is the students' responsibility to inform the instructor ahead of time of any medical conditions that may result in the exhibition of these behaviors, so that appropriate arrangements can be made.
- Unauthorized removal of any exam materials from the exam room will be treated as Academic Misconduct.

Computational Laboratory: Computer laboratory work is the essence of this course in chemistry. All laboratory work in this course is to be an individual effort, unless explicitly stated by your instructor. Evidence of copying or unauthorized "working together" on computer laboratory course work will be submitted to COAM. You are expected to perform all parts of the experiments yourself. The accumulation of data, calculations derived from that data, and any conclusions or answers to questions associated with that experiment are to be your own work. Academic misconduct involving computer lab work includes but is not limited to the following:

- Computer lab data may not be altered or "made up". Violations of these laboratory guidelines will be prosecuted with the minimum recommended penalty of a zero for the entire course.
- Plagiarism or the submission of work based on old material is considered to be academic misconduct no matter how small the infraction. Possession of another student's lab report(s) will raise immediate concerns about academic misconduct.
- Individuals retaking the course must complete all work for the course during the current semester and may not submit any parts of any assignments that were performed in a previous semester (see item #6 in "Ten Suggestions for Preserving Academic Integrity", http://oaa.osu.edu/coamtensuggestions.html).

*I would like to thank the Chemical Computing Group (www.chemcomp.com) for kindly providing free teaching licenses for the Molecular Operating Environment (MOE). Without their assistance you would not have the learning experience

Curricular Map Justification for CHEM 5240

When this course was originally reviewed by the CBC UG Instructional Assessment committee, it was deemed to be operating at the Advanced level for all six of our program goals. Our undergraduate students are expected to perform at a very high level in this course, suitable for a senior thesis or graduate research project.

Based on feedback from the ASCCAO committee, this course was re-evaluated by Dr. Terry Gustafson (Vice Chair of Undergraduate Studies), Dr. Dick Swenson (Program Director and Chair of the CBC UG Assessment Committee), Dr. Rick Spinney (Proposed instructor for this course), and Ms. Laura Sutherland (Program Manager). During this re-evaluation, however, it was determined that the original mapping numbers (advanced level for all six program goals) was correct. Below is additional justification for why we believe that this course is operating at the Advanced Level for all six of our program goals:

PG1: "Students develop knowledge within a historical perspective of the chemical principles and theories, both factual and conceptual"

The course develops the theories and concepts applicable to protein modeling by examining them from a developmental (historical) perspective, how the theories developed, change and improve over time and what the current state of the art is.

PG2: "Working both individually and in groups, students solve both classical and contemporary chemistry problems which exemplify the current integrated nature of science disciplinary and interdisciplinary principles"

This is the idea behind the implementation of the course. The students do 12 exercises and 11 homework problems addressing current issues in protein modeling using state of the art software. The course is problem solving intensive, they learn how to use the software to solve problems. Many of the problems relate to biological/medical issues.

PG3: "Perform experimental laboratory procedures in a safe and ethical manner, collect and properly evaluate scientific data"

The students perform 23 exercises & homework sets and one formal research project. They are required to analyze the data and evaluate the significance of their findings for all of their work.

PG4: "Students develop effective skills in oral and written communication of scientific knowledge, formulate logical explanations and conclusions, and construct effective arguments."

The student write a number of short reports and one research style paper and are required to do an oral presentation of their research to the other students.

PG5: "Students retrieve information from the literature, and become proficient in online database searching including the evaluation of the quality and validity of both the source and content of such searches."

The starting point for most of the exercises and homework problems is the retrieval and evaluation of data from public data banks. They are then required to “repair” faulty data if present and proceed with the rest of the project.

PG6: “Students recognize social, historical, and philosophical implications of scientific discoveries, and understand the potential of science and technology to address problems of the contemporary world.”

The exercises and homework are drawn from the literature and represent common problems faced in protein modeling. The students make use of state of the art software licensed to the department and a number of open access software platforms running on the web. Many of the proteins we study are of biological/medicinal interest in fighting disease and cancer.

CHEM Curricular Map - Version 1

	KEY					Students develop knowledge within a historical perspective of the chemical principles and theories, both factual and conceptual	Working both individually and in groups, students solve both classical and contemporary chemistry problems which exemplify the current integrated nature of science disciplinary and interdisciplinary principles	Perform experimental laboratory procedures in a safe and ethical manner, collect and properly evaluate scientific data	Students develop effective skills in oral and written communication of scientific knowledge, formulate logical explanations and conclusions, and construct effective arguments.	Students retrieve information from the literature, and become proficient in online database searching including the evaluation of the quality and validity of both the source and content of such searches.	Students recognize social, historical, and philosophical implications of scientific discoveries, and understand the potential of science and technology to address problems of the contemporary world.
0 =	*Not in course*										
1 =	*Beginning Level*										
2 =	*Intermediate Level*										
3 =	*Advanced Level*										
	Name	**Elective**	**BA**	**BS**	**Lec/Lab**	**PG1- Foundational Knowledge**	**PG2- Problem Solving**	**PG3- Laboratory Finesse**	**PG4- Scientific Communication**	**PG5- Information Acquisition**	**PG6- Real World Implications**
CHEM 1210	Gen Chem 1		x	x	both	1	0	1	0	0	0
CHEM 1220	Gen Chem 2		x	x	both	1	0	1	0	0	0
CHEM 1610	Majrs Gen Chem 1		x	x	both	1	0	1	0	0	0
CHEM 1620	Majrs Gen Chem 2		x	x	both	1	1	1	1	0	1
CHEM 1910H	Hnrs Gen Chem 1		x	x	both	1	0	1	0	0	0
CHEM 1920H	Hnrs Gen Chem 2		x	x	both	1	1	1	1	0	1
CHEM 1612	PLTL Chem 1		x	x	Workshop	1	1	0	0	0	0
CHEM 1622*	**PLTL Chem 2**		x	x	Workshop	1	1	0	0	0	0
CHEM 2510	Org Lec 1		x	x	Lec	2	1	0	1	0	1
CHEM 2520	Org Lec 2		x	x	Lec	2	2	0	2	0	1
CHEM 2610	Mjrs Org Lec 1		x	x	Lec	2	1	0	1	0	1
CHEM 2620	Mjrs Org Lec 2		x	x	Lec	2	2	0	2	0	1
CHEM 2910H	Hnrs Org Lec 1		x	x	Lec	2	1	0	1	0	1
CHEM 2920H	Hnrs Org Lec 2		x	x	Lec	2	2	0	2	0	1
CHEM 2540	Org Lab 1		x	x	Lab	1	1	2	1	1	1
CHEM 2550	Org Lab 2		x	x	Lab	2	2	2	2	1	1
CHEM 5420	Org Spectroscopy	x			Lec	2	3	0	2	0	1
CHEM 5430	Carbohydrates	x			Lec	3	3	0	2	2	1
CHEM 52XX*	**Neurotransmitters**	x			Lec	3	3	0	2	2	2
CHEM 2210	Anal Chem 1		x	x	both	2	2	2	2	1	2
CHEM 2210H	Hnrs Anal Chem 1		x	x	both	2	2	2	2	2	2
CHEM 4870	Anal Chem 2			x	both	3	3	3	0	0	3
CHEM 4880	Instr. Analysis			x	Lab	0	3	3	3	2	3
CHEM 2990*	**Prof Dev**	x			Lec	0	0	0	3	3	0
CHEM 4300	P Chem 1			x	Lec	3	3	0	0	0	2
CHEM 4310	P Chem 2			x	Lec	3	3	0	0	0	2
CHEM 4410	P Chem Lab		x	x	Lab	0	3	3	3	3	2
BIOCHEM 5721	P Biochem 1		x		Lec	3	3	0	0	0	2
BIOCHEM 5722	P Biochem 2		x		Lec	3	3	0	0	0	2
BIOCHEM 4511	Intro Biochem	x			Lec	3	2	0	2	1	0
BIOCHEM 5621	Biochem Lab	x			Lab	3	3	3	3	2	1
CHEM 3510	Inorg Chem			x	Lec	3	2	0	0	0	3
CHEM 4550	Inorg Lab	x			Lab	3	3	3	3	0	3
CHEM 4998/98H	Research	x			Lab	3	3	3	2	3	3
CHEM 4999/99H	Thesis Research	x			Lab	3	3	3	3	3	3
CHEM 5440	Computational	x			Lec	3	3	3	3	3	3
CHEM 5520	Nanochemistry	x			Lec	3	3	0	3	3	3
CHEM 5240*	**Protein Modeling**	x			Lec	3	3	3	3	3	3

**Courses in red are the new courses we were hoping to get approved by Spring 2018*