Computational Chemistry (CHEM 395, CHEM 435)
Fall 2015
Mo, Wedn 7:00 to 8:15 PM, CC - 103

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Computer modeling are frequently used to correlate enzyme structure and function, and to guide the design of new drugs. Yet, this usefulness has been mostly based on the use of the computer as a visualization tool rather than a source of accurate quantitative predictions of the catalytic activity or inhibition. However, after half-century in the making, computer simulations are poised for major breakthrough. This special-topics course will cover important developments in our understanding of chemistry of biomolecules on the atomic level.

Course Layout and Objectives

The course will be a combination of theoretical lectures, assigned reading, and tutorials and hands-on practice with computer program MOE (http://www.chemcomp.com)

The course will cover material in the following areas

- Structure-function relationships, solvation free energies
- Writing research article and research publication process
- Molecular mechanics, building small molecules, calculating total molecular energy, measuring molecular geometry
- Applied quantum mechanics, QSAR, flexible alignment of molecules
- Protein sequence analysis and homology modeling
- Drug design I: small molecule docking
- Drug design II: pharmacophore modeling
- Molecular dynamics

Grading: Your grade will be calculated using your scores from ten homeworks, two writing assignments and final exam. Each homework will contribute 5 points, each writing assignment 10 points and final exam 30 points. Grades will be assigned using the following scale:

Total Points	Letter Grade	Total Percent Score	Letter Grade
> 90	A	54 – 48	C
90 – 80	A-	48 – 40	C-
80 – 72	B+	40 – 35	D+
72 – 66	B	35 – 30	D
66 – 60	B-	30 or less	F
60 – 54	C+		

Ethical Considerations:

Students will not collaborate on any exams. Students may collaborate on general solution strategy for homework problems but each student must present his own solution. Only those materials permitted by the instructor may be used to assist in examinations. Students will not represent the work of others as their own. Identical homeworks will receive zero points. Any student caught cheating during an exam will be reported to the Deans office and will receive zero points for the given exam.

Homework Policy: Homework will be assigned at Mo or Wedn class. To receive full credit, a student's homework has to be submitted in person at the beginning of the next Mo class and the student must be able to explain the logical and numerical steps that he made to arrive to his/her answer.

Examinations: Excused students who cannot attend an exam will be given a replacement exam. Medical or personal reasons for missing exams must be communicated to the instructor prior to the exam, and their proof will be required. Missed unexcused exams will receive zero points.

Recommended books:

A. R. Leach, Molecular Modelling: Principles and Applications, 2nd ed, Prentice Hall, 2001.
A. Fersht, Structure and Mechanism in Protein Science: A Guide to Enzyme Catalysis and Protein Folding, W. H Freeman and Company, New York, 1999.
A. Warshel, Computer Modeling of Chemical Reactions in Enzymes and Solutions, John Wiley & Sons, New York, 1991