Syllabus - Fall 2016

Computational Chemistry [CHEM-UA 752]

Instructor:

Professor Yingkai Zhang, 1166D Waverly Building,, 212-998-7882,*yz22@nyu.edu*
TAs: Ms. Yuwei Yang (yy1274@nyu.edu) , 1166 Waverly Building
Mr. Haotian Li (haotian.li@nyu.edu), 1166 Waverly Building

Lecture/lab Time and Place:

Wednesday, 2:00 PM - 3:15 PM at LSTC_MACLB (Lecture)
Friday, 12:30 PM - 3:00 PM at LSTC_MACLB (Lab)

Office Hour Time and Place:

Tuesday, 4:00 PM – 5:00 PM , 1166 Waverly Building

Course website: Class

Course Goal:

- This course is a full-scale introduction to computational chemistry and biomolecular modeling, including special topics on computational-aided drug design..
- to assist you in developing a practical understanding of computational methods (strengths, limitations, applicability)
- to assist you in developing competence in applying these computational methods to molecular modeling.

Reference books

- Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems, by David Young, 2004, John Wiley & Sons. (dx.doi.org/10.1002/0471220655)
- Molecular Modeling: Principles and Applications, second edition by Andrew R. Leach (Pearson Education EMA, January 2001)
- Essentials of Computational Chemistry, by Christopher J. Cramer, Second Edition, John Wiley & Sons, 2004.

Grading

Lab	(30%)
Exam	(40%)
Final project	(30%)

Late lab report/Final Project policy: each late day deducts 20% of total points. It will not be graded if it is more than 5 days past the due date.

Tentative Schedule

Week 1:
Sep. 7 Introduction to molecular structure modeling, visualization, databases.
Sep. 9 Exploration of PDB database, Linux tutorial, and Hands on exercises.
Week 2:
Sep. 14 Protein structure
Sep. 16 Biomolecular visualization: Chimera and Hands-on exercises
Week 3:
Sep. 21 Introduction to Computational Quantum Chemistry
Sep. 23 High performance computing, Gaussian and Hands-on exercises
Week 4:
Sep. 28 MM force field.
Sep. 30 High performance computing, Amber and Hands-on exercises
Week 5:
Oct. 5 Energy Minimization Techniques and conformation analysis
Oct. 7 Biomolecular modeling I: Amber and Hands-on exercises
Week 6:
Oct. 12 Computational analysis of binding interfaces
Oct. 14 Hands-on binding pocket analysis exercise
Week 7
Oct. 19 **EXAM 1**
Oct 21 Biomolecular modeling II: simulation, analysis and hands-on exercises
Week 8
Oct. 26 Molecular dynamics simulations
Oct. 28 Biomolecular Modeling III: simulation, analysis and hands-on exercises
Week 9
Nov. 2 Introduction to Statistical Mechanics
Nov. 4 Biomolecular Modeling IV: simulation, analysis and hands-on exercise
Week 10
Nov. 9 Solvation modeling: explicit vs. implicit
Nov, 11 Biomolecular Modeling V: : Modeling solvation effects
Week 11
Nov. 16 Free energy calculations: biomolecular recognition
Nov. 18 Biomolecular Modeling VI: Ligand docking

Week 12
Nov. 23 No class Thanks giving
Week 13
Nov. 30 Exam II
Dec. 2 Course project discussion and course projects
Week 14
Dec. 7 Course project
Dec. 9 Course project
Week 15
Dec. 14 Course project
Dec. 16 Course project presentation
Dec. 19 Course project report will be due on Dec. 19.