Syllabus - Spring 2017

SP TOCS: Computational Chemistry [CHEM-GA 2672 (001)]

Instructor:

Professor Yingkai Zhang, 1166D Waverly Building,, 212-998-7882,*yz22@nyu.edu*

Lecture/lab Time and Place:

Tuesday/Thursday, 9:30 AM - 10:45 AM at LSTC_MACLB

Office Hour Time and Place:

Monday, 4:00 PM – 5:00 PM , 1166D 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

- 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

Homework	(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:
Jan. 24 Introduction to molecular modeling, visualizations.
Jan. 26 Exploration of PDB structural database, CSD and PubChem databases.
Week 2:
Jan. 31 Biomolecular structure introduction, homology modeling
Feb. 2 Biomolecular visualization: Chimera and Hands-on exercises
Week 3:
Feb. 7 Introduction to Computational Quantum Chemistry
Feb. 9 High performance computing, Gaussian and Hands-on exercises
Week 4:
Feb. 14 MM force field.
Feb. 16 High performance computing, Amber and Hands-on exercises
Week 5:
Feb. 21 Energy Minimization Techniques and conformation analysis
Feb. 23 Biomolecular modeling I: Amber and Hands-on exercises
Week 6:
Feb. 28 Molecular dynamics simulations
Mar. 2 Biomolecular modeling II: simulation, analysis and hands-on exercises
Week 7
Mar. 7 **EXAM 1**
Mar. 9 Introduction to Statistical Mechanics
Week 8
Mar. 14 Spring Break, No class.
Mar. 16 Spring Break, No class
Week 9
Mar. 21 Solvation modeling: explicit vs. implicit
Mar. 23 Biomolecular Modeling III: : Modeling solvation effects
Week 10
Mar. 28 Free energy calculations: biomolecular recognition
Mar. 30 Biomolecular Modeling IV: modeling biomolecular recognition
Week 11
April. 4 Ligand docking
April. 6 Biomolecular Modeling V: Ligand Docking with Vina
Week 12
April. 11 Computational analysis of binding interfaces
April 13 Hands-on binding pocket analysis exercise
Week 13
April. 18 Biomolecular modeling literature discussion
April . 20 Biomolecular modeling literature discussion and course project discussion
Week 14

April 25 Exam II
April 27 Course project
Week 15
May 2 Course project
May 4 Course project
Week 16
May 9 Course project presentation
May 15 Course project report due