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)

Grading

<table>
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<tr>
<th>Component</th>
<th>Percentage</th>
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<tbody>
<tr>
<td>Homework</td>
<td>(30%)</td>
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<tr>
<td>Exam</td>
<td>(40%)</td>
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<tr>
<td>Final project</td>
<td>(30%)</td>
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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.

#### 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
<table>
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<tr>
<th>Date</th>
<th>Event</th>
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<tbody>
<tr>
<td>April 25</td>
<td>Exam II</td>
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<td>April 27</td>
<td>Course project</td>
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<td><strong>Week 15</strong></td>
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<td>May 2</td>
<td>Course project</td>
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<td>May 4</td>
<td>Course project</td>
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<td><strong>Week 16</strong></td>
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<td>May 9</td>
<td>Course project presentation</td>
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<td>May 15</td>
<td>Course project report due</td>
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