Molecular Modeling & Molecular Simulation Summer 2016

- **Instructor**
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- **Web Site**
  https://mulan.swmed.edu/mmms

- **Objectives**
  1. To provide an introduction to some current methods in molecular modeling
  2. To provide hands-on experience with various molecular modeling software packages
  3. To provide some background on the theoretical and computational methods use in molecular modeling
  4. To provide some understanding of the capabilities, limitations and reliability of various molecular modeling methods

- **Books**
  1. Molecular Modelling. Principles and Applications. A. R. Leach, Addison Wesley Longman Limited,1996
  2. Essentials of Computational Chemistry - Theories and Models, 2nd Edition, Christopher J. Cramer
  3. Molecular Modeling and Simulation: an interdisciplinary guide, 2nd Edition, Tamar Schlick
  4. Exploring Chemistry with Electronic Structure Methods, 2nd Edition, James B. Foresman and Aeleen Frisch
  5. Computer Simulation of Liquids, M. P. Allen & D. J. Tildesley, 1987

Grade Info

Grade: 40% assignment, 30% reading assignment and 30% project presentation

Projects (all the calculations will be performed on BioHPC)

1. To identify novel drug leads through virtual high-throughput screening for a protein target
2. To explore the dynamics of a protein system
3. To calculate the binding free energies of a set of inhibitors binding to a protein target

Teaching Style

1. Lecture section (about 70 to 90 minutes)
2. Lab section (about 30 to 50 minutes)

Schedules

Lecture 1 (July 5) *Introduction to molecular modeling & molecular simulations*
Lecture 2 (July 7) *Computer-aided drug design*
Lecture 3 (July 12) *Introduction to quantum mechanics*

Lecture 4 (July 14) *Introduction to Molecular mechanics*
Lecture 5 (July 19) *Introduction to Molecular dynamics simulations*
Lecture 6 (July 21) *Solvent effect, free energy calculations*
Lecture 7 (July 26) *QM/MM, Normal model analysis, elastic network model*
Lecture 8 (July 28) *Protein modeling & project presentation (10 minutes)*