**Department of Chemistry Syllabus**

This syllabi is advisory only. For details on a particular instructor's syllabus (including books), consult the instructor's course page. For a list of what courses are being taught each quarter, refer to the Courses page. *Every instructor has prerogative to teach the course as they see fit and ultimately the instructor's syllabus supersedes all others.*

***CHE 130B: Pharmaceutical Chemistry 2 (i.e. Computational Drug Design)***

Approved: Prerequisite of 130A, however contact the instructor for exceptions.

Suggested Textbook: (actual textbook varies by instructor; check your instructor)

There is no required text. Software used is provided and is primarily free online tools, PyMol, and the OpenEye Suite.

Suggested Schedule:

Week 1: Molecular Visualization of Protein-Small Molecule Interactions

Week 2: Prediction of critical binding interactions and organismal differences

Week 3: Geometry optimization of small molecules

Week 4: Property screen of small molecule library

Week 5: Ligand based virtual screen

Week 6: Docking lead molecule into COX2 active site

Week 7: Design of Bioisosteres

Week 8: Protein Structure Homology Modeling

Week 9– 10: Drug Design Project

Additional Notes: This is a computational course which is graded on weekly labs (~50%) and a quarter long design project (~50%). There are no midterms or quizzes.

Learning Goals: Students will be able to use modern computational tools to analyze and design targeted molecular interactions between small molecules and proteins.