

## Computational Chemistry Related to Drug Design

This course will provide hands-on experience with modern computational methods used in the drug design process. A variety of different computational methods will be described and applied using real-life drugs and related molecules.

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### Recommended Texts

- *“Molecules and Medicine”* E. J. Corey, Barbara Czako, Laszlo Kurti Wiley, 2007
- *“The Organic Chemistry of Drug Design and Drug Action”*, Richard B. Silverman Elsevier/Academic Press

### Our Expectations

- *This course is not about memorization. It is about developing analytical thinking and problem-solving skills.*
- We will utilize and expand upon undergraduate Organic Chemistry.

### Course Overview

Lab 1: Visualizing and Interacting with Protein Structures

Lab 2: Structural Conservation in Proteins

Lab 3: Geometry optimization of small molecules

Lab 4: Property screen of small molecule library

Lab 5: Ligand based virtual screen

Lab 6: Docking lead molecule into a protein's active site

Lab 7: Design of Bioisosteres

### Course Requirements

Mini lab reports: 450 points (50 – 95 each)

Drug Design Project: 550 points (3 parts)

Total: 1000 points

### Drug Design Project

Directions for each can be found in the Lab Manual

- *Proposal:* your choice of a “drug family”; 25 points
- *Literature Report:* background on your “drug family” (~5 pages); your choice of a “drug family”; 100 points
- *Presentation:* brief presentation to the class on your “drug family” and designs; 75 points
- *Final Project:* computations and report on your “drug family”; 350 points

- Examples of “A” level final projects:

<https://www.biorxiv.org/content/10.1101/772137v1.full.pdf>

<https://www.biorxiv.org/content/10.1101/2023.02.25.529947v1.full>

<https://www.biorxiv.org/content/10.1101/2022.04.06.487400v1.full>

<https://www.biorxiv.org/content/10.1101/2022.04.27.489637v1.full>

<https://www.biorxiv.org/content/10.1101/2022.10.10.511679v1.full>

- **Citations:** All citation has to be done **ACS style** (please visit see ACS\_citation.pdf to see how you cite). Must also include in-text citation. An example of writing with in-text style citation can be found here: <https://www.biorxiv.org/content/10.1101/772137v1.full.pdf>

### **Policies**

- **assignments:** All late assignments will be assessed a penalty that is proportional to how late the assignment is. No exceptions will be made.
- **mutual respect:** We are all adults and should treat each other as such. Cheating of any kind (including plagiarism!) will not be tolerated.

### **Strategies for Success**

- **don't wait:** The drug design project is a lot of work, so start as early as possible!