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

Direction for each can be found in the Lab Manual

• *Proposal:* your choice of a "drug family"; 50 points

• *Literature Report:* background on your "drug family" (~5 pages); your choice of a "drug family"; 150 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_cittation.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!