

Medc 319: Computer-Aided Drug Design

MEDICINAL CHEMISTRY

The student will learn to utilize state-of-the-art commercial software to conduct Computer-Aided Structure Based Drug Design (CADD). De novo design will be conducted after database screening (aka database mining, virtual screening) as a method to invent small molecules that bind to the active site(s) of protein X-ray structures. The course will involve discussion of protein molecules, X-ray crystallography produced structures of proteins or protein-ligand complexes, molecular interactions that are either attractive or repulsive in nature, and computer software for visualization, manipulation, and energy calculations.

2 Credits

Prerequisites

- Pre-requisite: Pharmacy PY1 or PY2

Instruction Type(s)

- Lecture/Lab: Lecture/Lab for Medc 319

Subject Areas

- [Pharmaceutical Sciences](#)

Related Areas

- [Clinical and Industrial Drug Development \(MS, PhD\)](#)
- [Industrial and Physical Pharmacy and Cosmetic Sciences \(MS, PhD\)](#)
- [Medicinal and Pharmaceutical Chemistry](#)
- [Natural Products Chemistry and Pharmacognosy \(MS, PhD\)](#)
- [Pharmaceutical Marketing and Management](#)
- [Pharmaceutics and Drug Design \(MS, PhD\)](#)
- [Pharmacoeconomics/Pharmaceutical Economics \(MS, PhD\)](#)
- [Pharmacy \(PharmD - USA - PharmD, BS/BPharm - Canada\)](#)
- [Pharmacy Administration and Pharmacy Policy and Regulatory Affairs \(MS, PhD\)](#)
- [Pharmacy, Pharmaceutical Sciences, and Administration, Other](#)

