Medc 319: Computer-Aided Drug Design

BIOMOLECULAR SCIENCES

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
- Pre-Requisite: 24 Earned Hours

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