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

Instruction Type(s)
• Lecture/Lab: Lecture/Lab for Medc 319

Subject Areas
• Pharmaceutical Sciences

Related Areas
• 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