



Molecular Informatics

CBE 5734

Credit Hours:

3.00 - 3.00

Course Levels:

Undergraduate (1000-5000 level)

Graduate (5000-8000 level)

Course Components:

Lecture

Course Description:

Overview of molecular informatics, with emphasis on its use in modern drug discovery and exploration of chemical structure-property relationships.

Prerequisites and Co-requisites:

Prereq: Sr or Grad standing in Engineering, or permission of instructor.

Course Goals / Objectives:

- Understand the basic concepts of chemical and biomolecular informatics, with emphasis on how these impact areas relevant to chemical and biomolecular engineers
 - Understand recently-developed high-throughput experimental techniques commonly used in chemical and biochemical processes, and how these require new and improved ways of analyzing the vast quantities of data generated by these methods
 - Become familiar with public databases for chemical and biological data, and methods for extracting information from these. Emphasis on internet resources for engineers interested in informatics
 - Introduce common statistical methods used in informatics, including sequence analysis, multivariate regression, pattern analysis, hierarchical organization of data, recursive partitioning
 - Explore a specific case study to learn how informatics techniques are used to explore chemical toxicity
-

Course Topics:

- Overview of databases for chemical information. Representation of the chemical structures of molecules (SDF and MOL files, SMILES code, graph theory approaches, etc.)
 - Methods for evaluating the similarity between chemical compounds: substructure representation, cluster analysis, recursive partitioning, and other methods
 - Use of molecular descriptors and physicochemical properties in chemoinformatics
 - Nucleic acids, genes and genomes; amino acids, proteins and proteomes; classifying amino acids based on their chemical properties; overview of gene and protein databases
 - Sequence analysis: alignment of gene and protein sequences (dot matrix plots, scoring matrices, gap penalties, FASTA and BLAST algorithms)
 - Markov chain analysis of single sequences, brief introduction to hidden Markov models (HMM)
 - Overview of high throughput screening experiments and data analysis: microarray experiments to determine gene expression profiles and HTS chemical toxicity studies
-

Designation:

Elective