

# PHSC-523: Molecular Modeling

The course includes 4 units teachings on computational chemistry, molecular modeling, elements of chemoinformatics, and drug design and discovery. Unit 1 focuses on experimental aspects and computer models of molecules and their behavior in gas and condensed phases; quantum and molecular mechanics etc. Unit 2 focuses on molecular modeling which includes ligand-based Drug Design, Quantitative structure-activity relationships (QSAR)- Introduction of Molecular Descriptors (1D,2D and 3D), Statistical analysis- Linear and Nonlinear Methods etc. Unit 3 focuses on history of chemoinformatics, definition of chemoinformatics, chemical structure representation as well as introduction to chemical structure file formats etc. Lastly, Unit 4 focuses on drug design and discovery of contour of Drugs -Development of New Drugs - molecular recognition in drug design- Introduction to molecular diversity etc.

**Credits:** 3

**Program:** Pharmaceutical Science