

**MOLECULAR MODELLING AND DRUG DESIGNING**

**UNIT I**

Concepts of molecular modelling – coordinate systems, molecular graphics and visualization tools - RASMOL, CHIME, MOLMOL.

**UNIT II**

Molecular mechanics - Newton's laws of motion, Introduction to force fields, Components and characteristics of force fields. Integration algorithms

**UNIT III**

Quantum Mechanics - Introduction and concepts - Semi empirical approaches - Basis sets and Quantum mechanical force fields.

**UNIT IV**

Introduction to drugs - Classification of drugs - Drug receptor interactions – Study on different kinds of receptors- Applications of molecular modelling in drug discovery.

**UNIT V**

Quantitative structure activity relationships - Applications in drug discovery - Software tools for QSAR - An overview of common descriptors- Interpretation of results.

**Reference books:**

1. *Molecular modelling* - Principles and applications by Andrews R Leech, Academic press, 2001.
2. *Molecular mechanics*, Comba and Hambly, Wiley VCH publishers, 1998