Molecular Modeling and virtual screening techniques

What is Molecular Modeling?



- Molecular modeling is the use of computer-based techniques to represent and study the structures, properties, and behaviors of molecules.
- It helps scientists visualize how a drug interacts with the target in the body (usually a protein or enzyme) at the atomic level.
- **Molecular modeling can predict:**
  - Shape and size of molecules
  - How molecules bind to each other (like a drug binding to a protein)
  - Stability and flexibility of molecules
  - Energy associated with different structures
- To do this, two main approaches are used:
  1. **Molecular Mechanics**
  2. **Quantum Mechanics**

Introduction Molecular Mechanics (MM)

What is it?

- Molecular Mechanics is a classical approach.
- It treats atoms as small balls and chemical bonds as springs, like a ball-and-stick model.
- It does not consider electrons directly, so it's not based on quantum theory.
- It uses force fields to calculate the energy of a molecule based on its structure.

What are Force Fields?

- Force fields are sets of mathematical equations and parameters used to describe the energy of a molecular system.

- **The total energy is calculated as a sum of:**
  - Bond stretching energy (how far a bond is from its ideal length)
  - Angle bending energy (how far bond angles are from their ideal values)
  - Torsional energy (energy due to rotation around bonds)
  - Non-bonded interactions:
    - Van der Waals forces (weak attractions or repulsions between atoms)
    - Electrostatic interactions (charges attracting or repelling each other)

Why use Molecular Mechanics?

- Fast and efficient for large molecules like proteins and DNA
- Useful for geometry optimization and conformational studies
- Works well for modeling molecular dynamics (motion over time)

Advantages of MM:

- Very fast and can be used for large molecules like proteins and DNA.
- Good for geometry optimization (finding stable shapes).
- Doesn't require heavy computation.

Limitations:

- Cannot simulate chemical reactions (bond breaking/forming)
- Depends heavily on the quality of the force field
- Does not handle electronic effects like charge transfer or polarization accurately

Introduction Quantum Mechanics (QM)

What is it?

- Quantum Mechanics is a more detailed and accurate method.
- It is based on the principles of quantum physics and considers electrons explicitly.
- It solves mathematical equations (like Schrödinger's equation) to determine the behavior of electrons in a molecule.

Key Concepts:

- Electrons behave both like particles and waves
- The total energy of a molecule is derived from solving equations about how electrons move and interact
- It gives information about:
  - Electron density

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