Molecular Dynamics

Chemspace Virtual Screening Services

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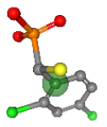
INPUT

What do we expect as Input?

PDB code of a protein

RCSB PDB PROTEIN DATA BANK

Structure file in sdf, mol2, pdb, cif, xyz formates



Sequence

....IVEGSDAEIGMSPWQVMLFRKSPQELLCG
ASLISDRWVLTAAHCLLYPPWDKNFTENDLLV
RIGKHSRT...

We can make structure modeling of the protein of interest

PIPELINE

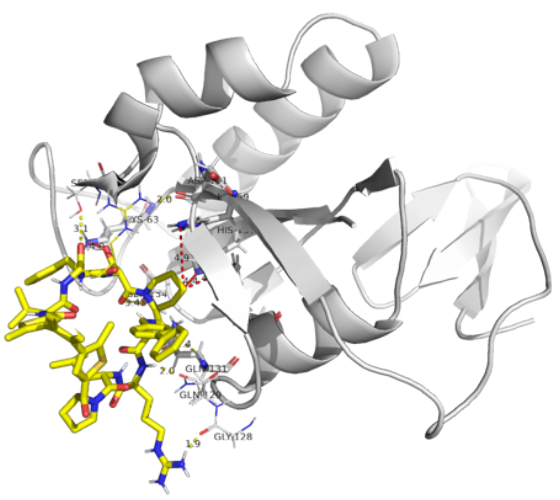
Molecular Dynamics Pipeline

- **INPUT** Structure coordinate file (pdb, sdf, mol, etc.)
- **System preparation** Solvation, adding ions and energy minimization
- **System equilibration** Temperature and pressure equilibration
- **Simulation** Run simulation $r(t_0+\Delta t)$
- **Analysis**

OUTPUT

RESULTS

- Molecular dynamics simulation of protein-ligand complexes, single ligand, receptor in the membrane, etc.
- Analysis of the trajectory
- Comprehensive study of protein-ligand interactions
- Calculation of the free binding energy



MISSION OF MOLECULAR DYNAMICS

- Demonstration of the evolution of the biological system in time
- Investigation target-drug interaction in depth
- Validation of ligands selected during virtual screening
- Estimation of protein-ligand binding energy