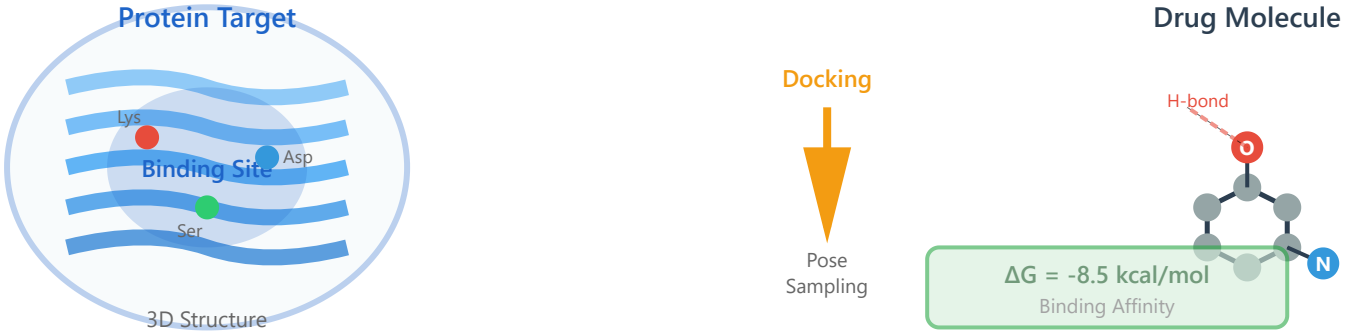
# Docking Simulation




Scoring: vdW + Electrostatic + H-bonds + Solvation + Entropy

## Protein preparation

Structure optimization

## Binding site detection

Active site identification

## Conformational sampling

Exploring binding modes

## Scoring functions

Binding affinity estimation

## Induced fit

Protein flexibility modeling