

## AI in Drug Design

- Drug-protein interaction prediction
- Protein- protein interaction prediction
- Target protein structure prediction
- AI in *De novo* drug design

## AI in Drug Repurposing

- To identify therapeutic target
- Insight into diseases treatment
- Evaluation of new therapeutic
- Use of existing drug

## AI in Drug Discovery

## AI in Drug Screening

- Bioactivity prediction
- Toxicity prediction
- Physiochemical property prediction
- To identify and classify target protein

## AI in Chemical synthesis

- Synthetic routes design
- Determine reaction mechanism
- To determine reaction yield
- Retrosynthesis pathways prediction