

## Computer-aided drug design methods

### Structure-based drug design methods

Homology modeling / de novo structure prediction

Molecular dynamics simulations

Ligand Docking

Machine learning

### Ligand-based drug design methods

QSAR modeling

Pharmacophore modeling

Similarity search

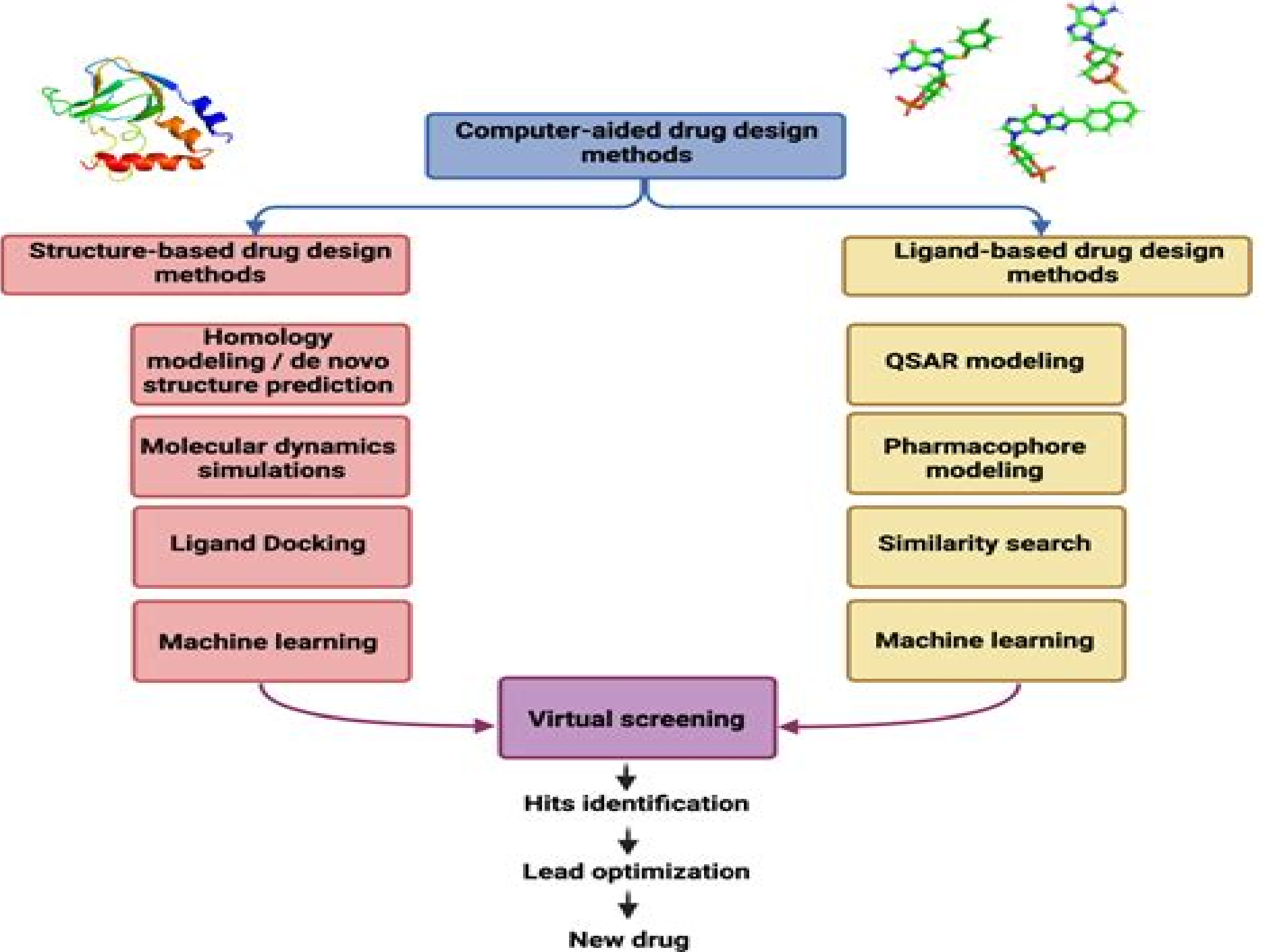
Machine learning

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Hits identification

Lead optimization

New drug



# Receptor Based Drug Design

**L Darling-Hammond**



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