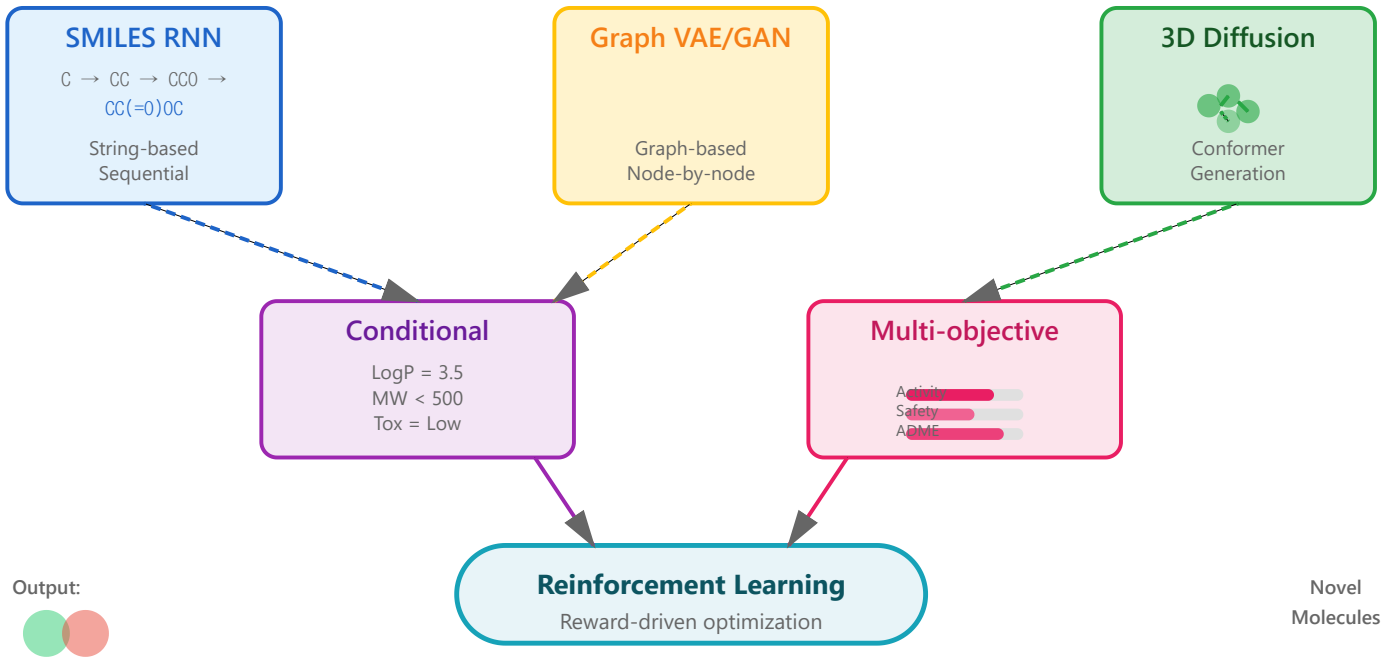
Generative Models



Principles & Mechanisms

SMILES RNN

Principle: Sequential character-level generation using recurrent neural networks (LSTM/GRU)

Mechanism:

Graph VAE/GAN

Principle: Direct graph representation with variational autoencoder or generative adversarial network

Mechanism:

3D Diffusion Models

Principle: Denoising diffusion process in 3D coordinate space

Mechanism:

- Generates 3D conformers directly

- Treats molecules as text strings
- Learns syntax rules of SMILES notation
- Generates one character at a time
- Fast and simple, but may produce invalid structures

- Operates on molecular graphs directly
- Adds nodes and edges iteratively
- Learns continuous latent space
- Better chemical validity guarantees

- Gradually denoises random coordinates
- Captures geometric constraints
- Produces physically realistic structures