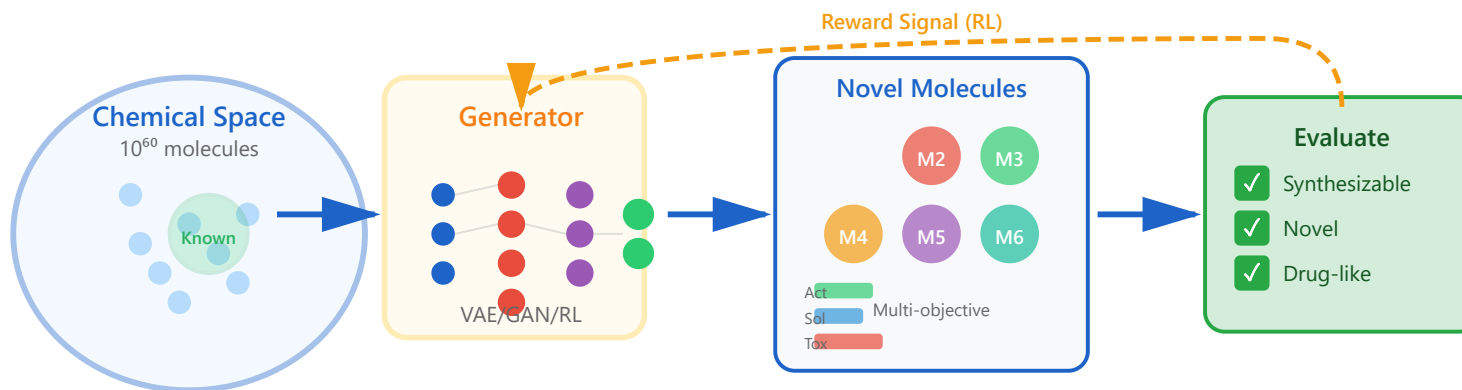


De Novo Design



Chemical space exploration

Novel compound generation

Reinforcement learning

Goal-directed optimization

VAE/GAN approaches

Generative architectures

Synthesizability

Chemical feasibility assessment

Diversity metrics

Novelty quantification