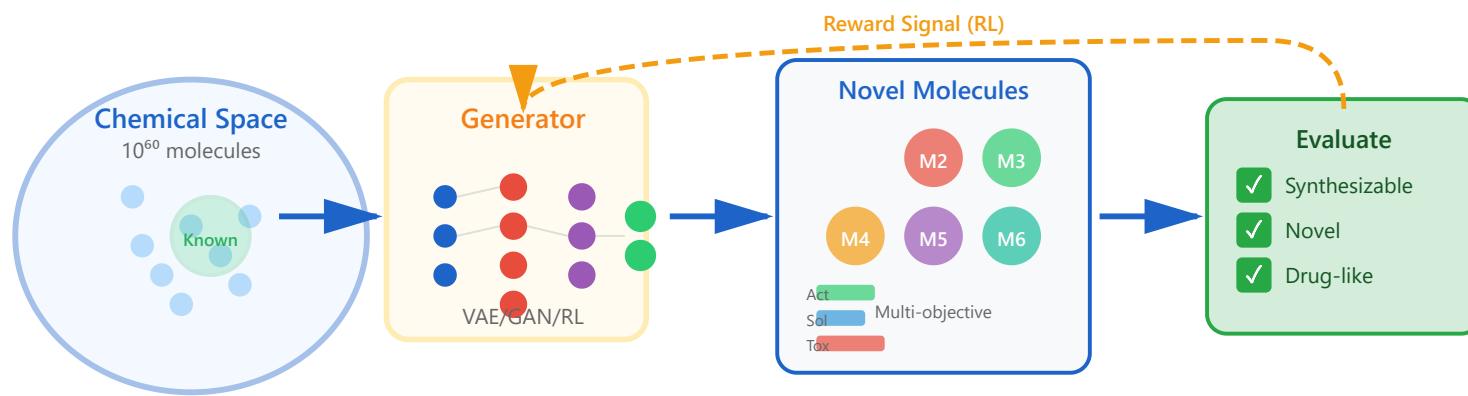


De Novo Design



Chemical space exploration

Novel compound generation

VAE/GAN approaches

Generative architectures

Diversity metrics

Novelty quantification

Reinforcement learning

Goal-directed optimization

Synthesizability

Chemical feasibility assessment