💻 HANDS-ON

Molecular Generation

SMILES RNN

Recurrent neural networks for sequential generation

Graph VAE

Variational autoencoders for graph-based generation

Reinforcement learning

Policy-based optimization for desired properties

Property optimization

Guiding generation toward specific target profiles

Diversity analysis

Measuring chemical diversity in generated libraries

```
# Example: Generative model workflow
from rdkit import Chem
import torch

# Load pre-trained generative model
model = MolecularRNN.load('pretrained_model.pt')
generated_smiles = model.sample(n_molecules=100)
```