💻 HANDS-ON

RDKit and DeepChem

Molecule manipulation

Loading, parsing, and modifying molecular structures

Descriptor calculation

Computing physicochemical properties and fingerprints

Model training

Building predictive models with DeepChem framework

Scaffold splitting

Creating train/test splits based on molecular scaffolds

Performance evaluation

Assessing model accuracy using appropriate metrics

```
# Example: RDKit & DeepChem workflow
from rdkit import Chem
import deepchem as dc

# Load molecules and compute descriptors
featurizer = dc.feat.CircularFingerprint()
loader = dc.data.CSVLoader(tasks=['activity'], featurizer=featurizer)
```