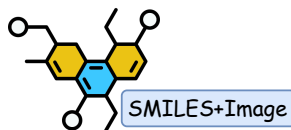
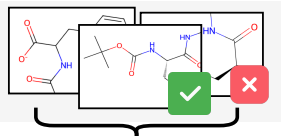
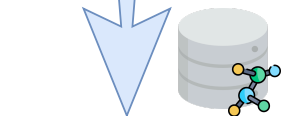


Prompt Design



Fingerprint Similarity



Few-shot Example



User

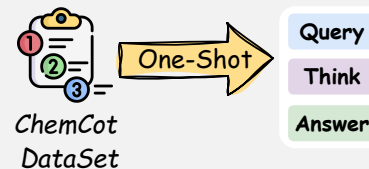
[Role] Chemist Expert
[Task] bace/bbbp...

Stage1: Cold-start SFT

Expert Knowledge



Reasoning Template



User

[Role] Chemist Expert [Example] Similar Molecules
[Task] bace/bbbp... [input Mol] SMILES + Image

Assistant

<think> 1. Comparison
..... 2. Consistency
</think> 3. Analysis

Reject Sampling



MPPReasoner

RLPGR

Foundation Layer



Reasoning Layer



Chemistry Layer



Dynamic Sample



Reasoning Model

Stage2: Principle-guided RL