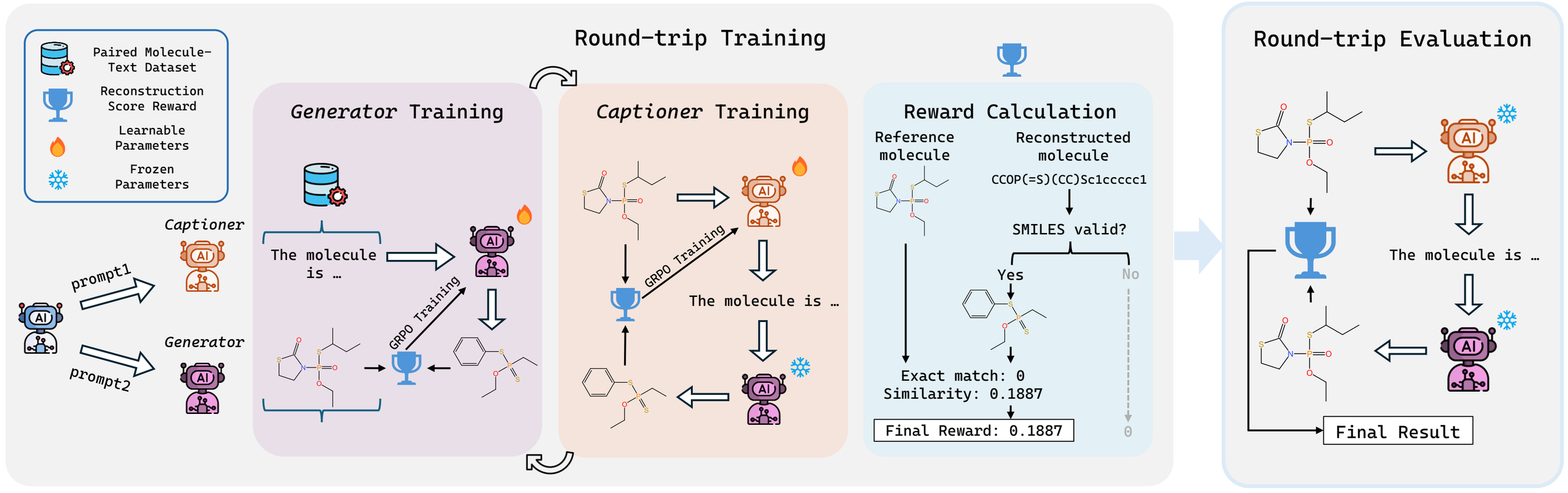
Paired Molecule–Text Dataset
Reconstruction Score Reward
Learnable Parameters
Frozen Parameters
Captioner
Generator
prompt1
prompt2
Round-trip Training
Generator Training
The molecule is …
GRPO Training
Captioner Training
GRPO Training
The molecule is …
Reward Calculation
Reference molecule
Reconstructed molecule
CCOP(=S)(CC)Sc1ccccc1
SMILES valid?
Yes
No
Exact match: 0
Similarity: 0.1887
Final Reward: 0.1887
0
Round-trip Evaluation
The molecule is …
Final Result