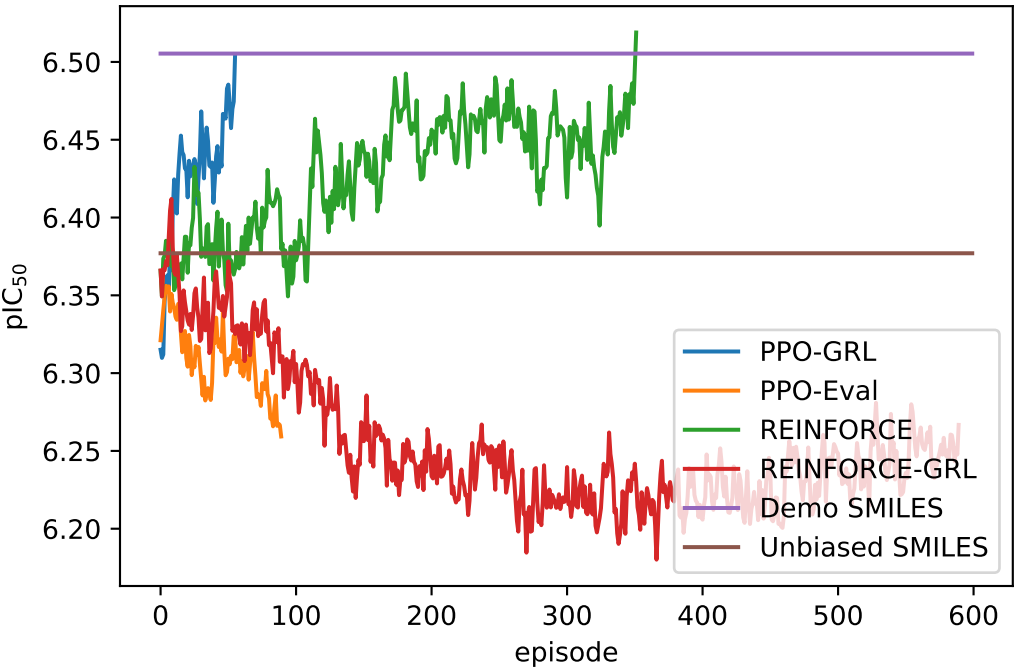
6.50
6.45
6.40
6.35
6.30
6.25
6.20
pIC50
0
100
200
300
400
500
600
episode
PPO-GRL
PPO-Eval
REINFORCE
REINFORCE-GRL
Demo SMILES
Unbiased SMILES