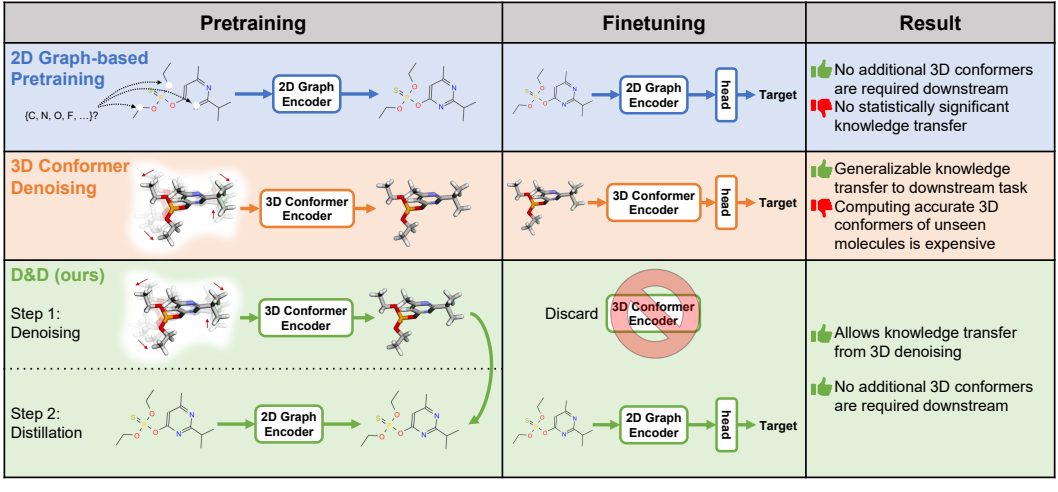

Pretraining
Finetuning
Result
2D Graph-based Pretraining
{C, N, O, F, ...}?
2D Graph Encoder
2D Graph Encoder
head
Target
No additional 3D conformers are required downstream
No statistically significant knowledge transfer
3D Conformer Denoising
3D Conformer Encoder
3D Conformer Encoder
head
Target
Generalizable knowledge transfer to downstream task
Computing accurate 3D conformers of unseen molecules is expensive
D&D (ours)
Step 1: Denoising
3D Conformer Encoder
Discard
3D Conformer Encoder
Step 2: Distillation
2D Graph Encoder
2D Graph Encoder
head
Target
Allows knowledge transfer from 3D denoising
No additional 3D conformers are required downstream