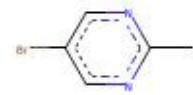


OR

Simpler deep learning method on QSPR properties
 (see GPR, MLP, etc.)

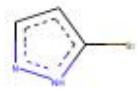
Starting blocks



logP: -2.74

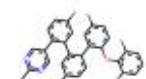


logP: -2.50



logP: -3.30

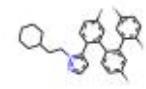
REACTOR



logP: 8.63



logP: 8.98



logP: 8.15

MolDQN



logP: -0.51

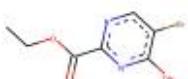


logP: 14.89

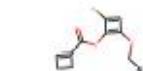


logP: 15.39

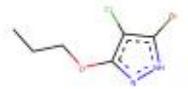
GCPN



logP: -1.57

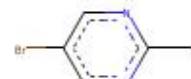


logP: -0.95



logP: -0.41

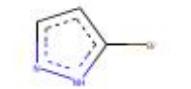
Starting blocks



QED: 0.59

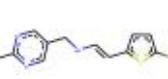


QED: 0.50



QED: 0.58

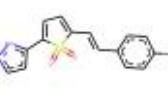
REACTOR



QED: 0.94

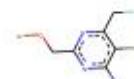


QED: 0.93

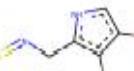


QED: 0.91

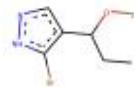
MolDQN



QED: 0.93

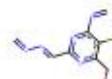


QED: 0.93



QED: 0.64

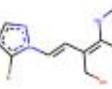
GCPN



QED: 0.66



QED: 0.57

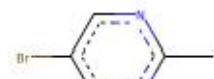


QED: 0.64

(a) Samples for cLogP objective

(b) Samples for QED objective

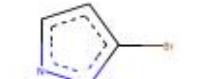
Starting blocks



DRD2: 0



DRD2: 0



DRD2: 0

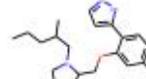
REACTOR



DRD2: 1



DRD2: 1

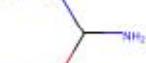


DRD2: 1

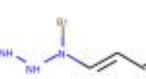
MolDQN



DRD2: 1

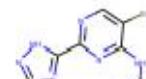


DRD2: 1



DRD2: 1

GCPN



DRD2: 0



DRD2: 0



DRD2: 0

(c) Samples for DRD2 objective

Realistic big data

Created polymer in Unity \rightarrow geomol-like network for accurate angles

MPNN

MLP for properties

Big data ideal:

CAN DO BY HAND OR IGNORE

Monomer

MPNN

embeddings for bonding locations

geomol-like model for bond angles

\rightarrow similar RL-based architecture as low-data but check for impossible conformations