

Descriptor MAE ↓

2D composition

All

NumAromaticRings

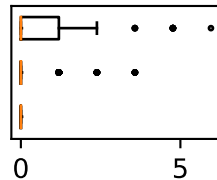
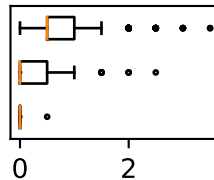
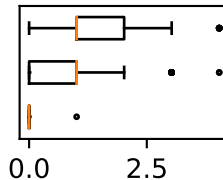
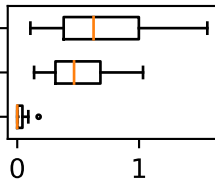
NOCCount

fr_halogen

Random emb + random noise

Template emb + random noise

Reconstruction



3D shape

All

Asphericity

PBF

RadiusOfGyration

Random emb + random noise

Template emb + random noise

Reconstruction

