ML4Science Hackathon

Harpriya and Anirvinya

Descriptors explored

Morgan fingerprints

Speculative handpicked descriptors.

Failed attempt at incorporating mol2vec along w/ the above descriptors.

Methods tried

Simple CNN (2 fully connected layers) w/ morgan fingerprints

Kernel ridge regression (polynomial kernel) (better than CNN)

XGBoostRegressor (worked the best)