

ChEMBL csv file

Transformed into

Ligands

Erlotinib

pIC50

pKi

pKd

SMILES:
c1cc1nc...

MorganFingerprint featurizer

Sequence:
GSGWWQL...

OneHotSequence featurizer

y = pIC50

x and y are
ML-ready values

kinoml.ml

File

Data Acquisition

Featurization

ML

1

2

3