

OpenEye

Sayan's Project

Data

NEW! 3D & Analyze

Molecule Search

Floe

System

← [back to Jobs](#)

JOB

JOB PARAMETERS

Details

Name

ML Build: Graph convolution Model on pregenerated Features for Small Molecules

Status

Success

Duration

58m 19s

Created

6/24/2025, 3:57:06 PM

Source

[ML Build: Graph convolution Model on pregenerated Features for Small Molecules](#)

Floe

[Small Molecules](#)

Source Floe Version

0.12.1.a158

Tags

[+ Add a tag](#)

Job Id

281847

Cost

\$0.68 (USD)

Email me if this job cost exceeds

\$5.00 (USD)

Terminate this job if the cost exceeds

\$6.00 (USD)

Log Stream

DOWNLOAD

VIEW

Generate Debugging Data

GENERATE

Results (2 of 2)

VIEW IN PROJECT DATA

▼

Reports (1)

▼

FLOE

FLOE REPORT

[gcnn_report 3.index](#)

Pearson coeff

Tau

R2

MAE Test

MSE Test

Pval

0.9

0.74

0.72

0.68

0.78

0.000E+0

GCNN hyperparameters used to train the prediction model

#Params

Batch size

Epochs

Type

Loss

GraphDir

47973

8192

100

Reg

L2

256

Model status: Possible Overfit

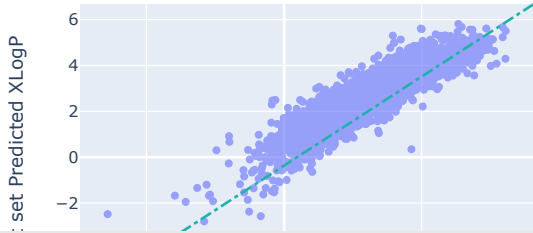
"

Ratio of #Model_Parameter(47973) to #Input(37264): 0.777

Too many model parameters with respect to input size. Decrease Graph Convolutional layers.

Regression Loss for GCNN L2 on Validation Set

set Predicted XLogP



DELETE JOB

RE-RUN JOB

