

A DATASETS

DrugBank
(13183)

BIOSNAP
(7341)

BindingDB
(3804)

DAVIS
(379)

Yamanishi E
(1109)

Yamanishi IC
(414)

Yamanishi GPCR
(318)

Yamanishi NR
(80)

Origin

- Affinity experiments
- Manually curated
- Text mining + manually curated

B MODELS

Transductive Inductive

DTINet

2017

Compact feature

DDR

2018

Path-category-based

DTiGEMS+

2020

node2vec

DTi2Vec

2021

node2vec

NeoDTI

2019

MPNN

Moltrans

2020

Transformers

EEG-DTI

2021

GCN

Hyper-Attention-DTI

2021

Transformers

C EVALUATION

Naive classifier based on node2vec

Optimal comparison of models

Input
Network

node2vec

Generated
Embeddings

Neural
Network

Link
Prediction

AUC

