WideDTA:
deep drug-target binding affinity prediction

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1 INTRODUCTION

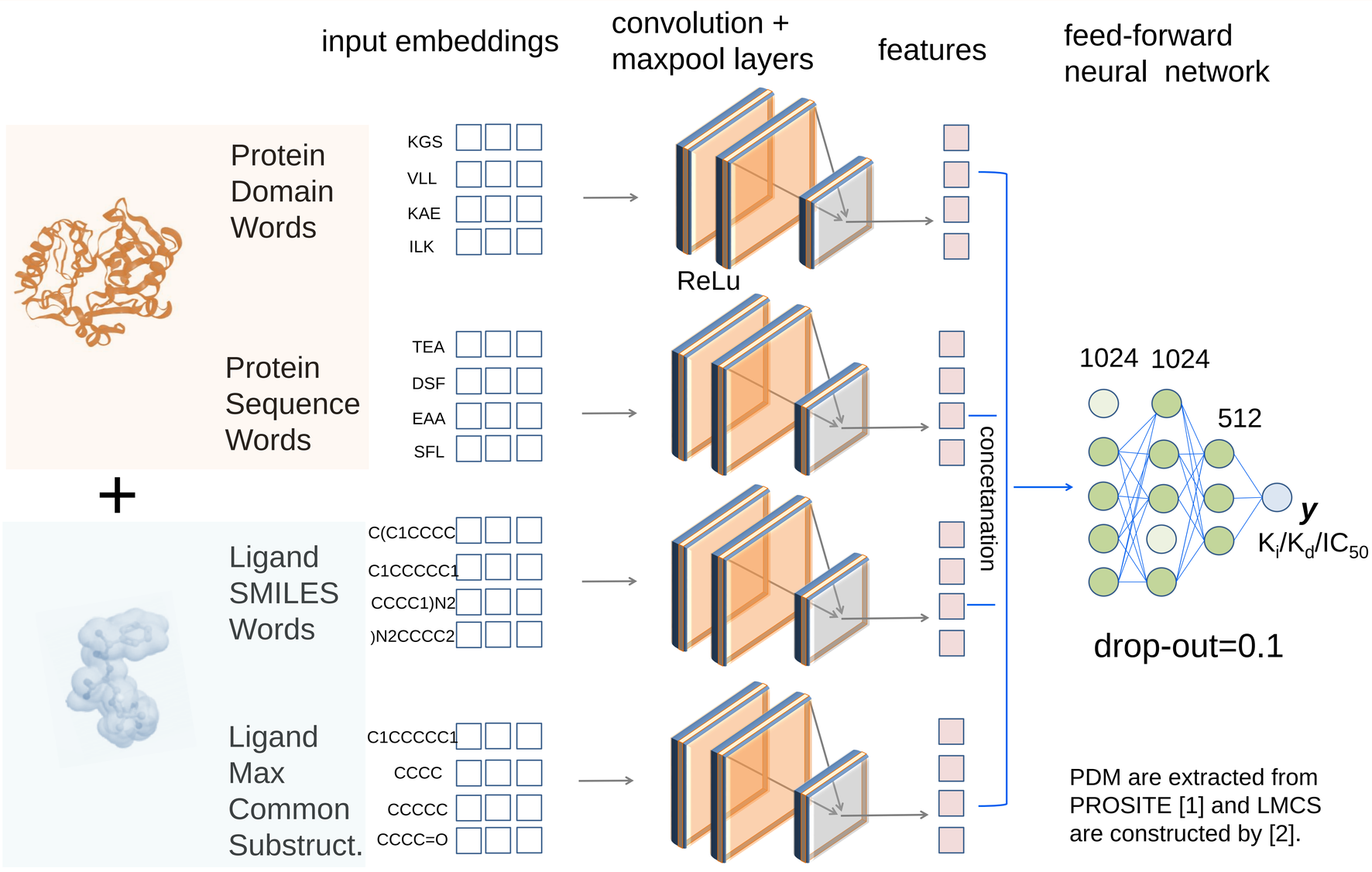
Prediction of the interaction affinity between proteins and compounds is a major challenge in the drug discovery process.

WideDTA is a deep-learning based prediction model that employs four text-based information sources:

- protein sequence (**PS**),
- ligand SMILES (**LS**),
- protein domains and motifs (**PDM**),
- maximum common substructure (**LMCS**) words

to predict binding affinity.

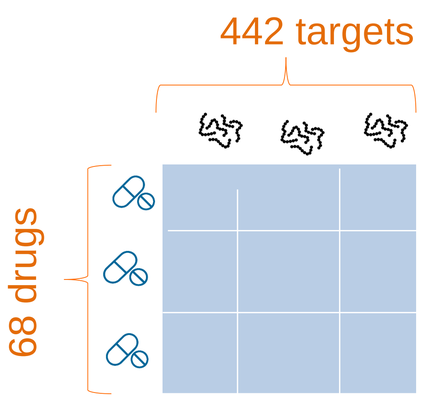
2 WideDTA Architecture



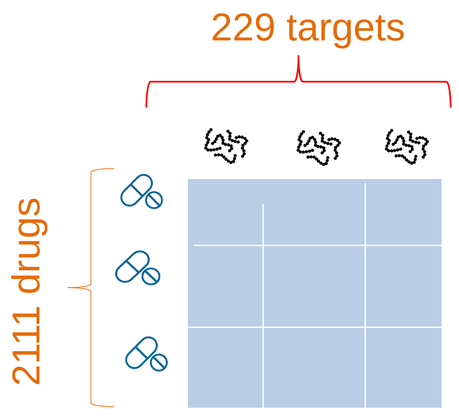
3 EXPERIMENTS & RESULTS

DATASETS

Davis Kinase (pK_d) [3]

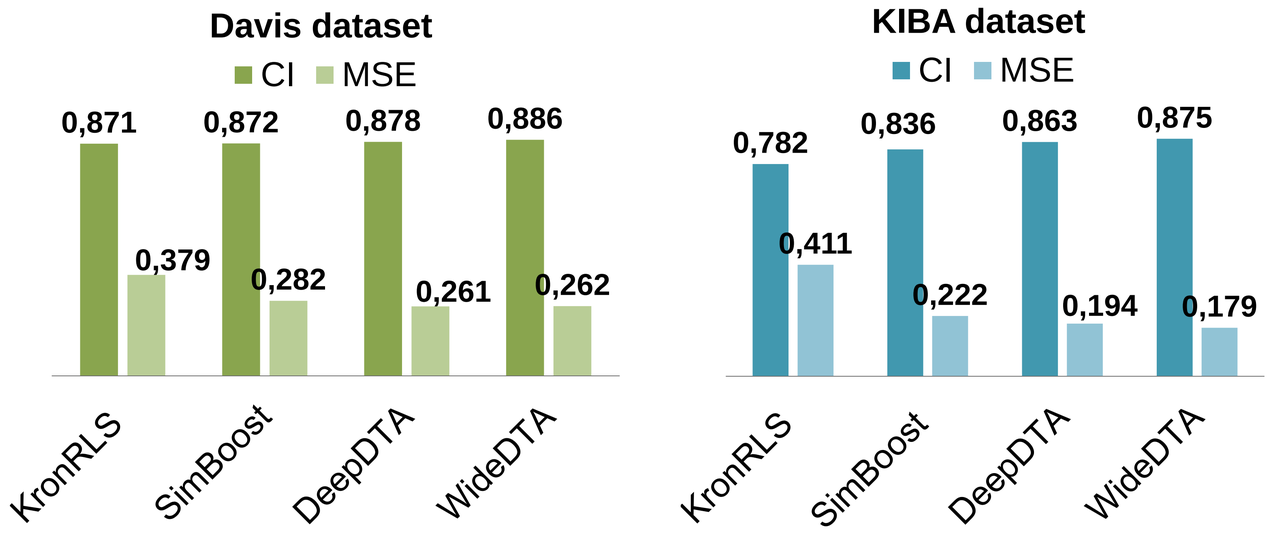


KIBA Kinase (KIBA score) [4]



We compared the performance of WideDTA with a state-of-art deep learning based approach, DeepDTA [5] and two traditional machine learning based models in drug-target that we refer to as KronRLS [6] and SimBoost [7].

SMILES sequences are represented in **DeepSMILES** [8] which yielded better performance in terms of evaluation metrics.



WideDTA model that combined all textual sources protein PS + PDM + LS + LMCS achieved better performance than other possible combinations.

4 CONCLUSION

- We proposed a deep-learning based approach to predict drug-target binding affinity, WideDTA, that combines four different textual pieces of information related to proteins and ligands.
- The protein sequence, domains and motifs were all represented as a set of 3-residue words, whereas for ligands, 8-character chemical words and maximum common substructure (MCS) words were extracted from the complete SMILES strings.
- DeepDTA is a character based approach, whereas WideDTA uses word representations. Our results suggest that the word based approach can be an alternatve to the character based approach.

References

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