Review of Available Deep Learning Tools for Protein-Ligand Interactions Prediction

Architecture of large projects in bioinformatics 23/24L

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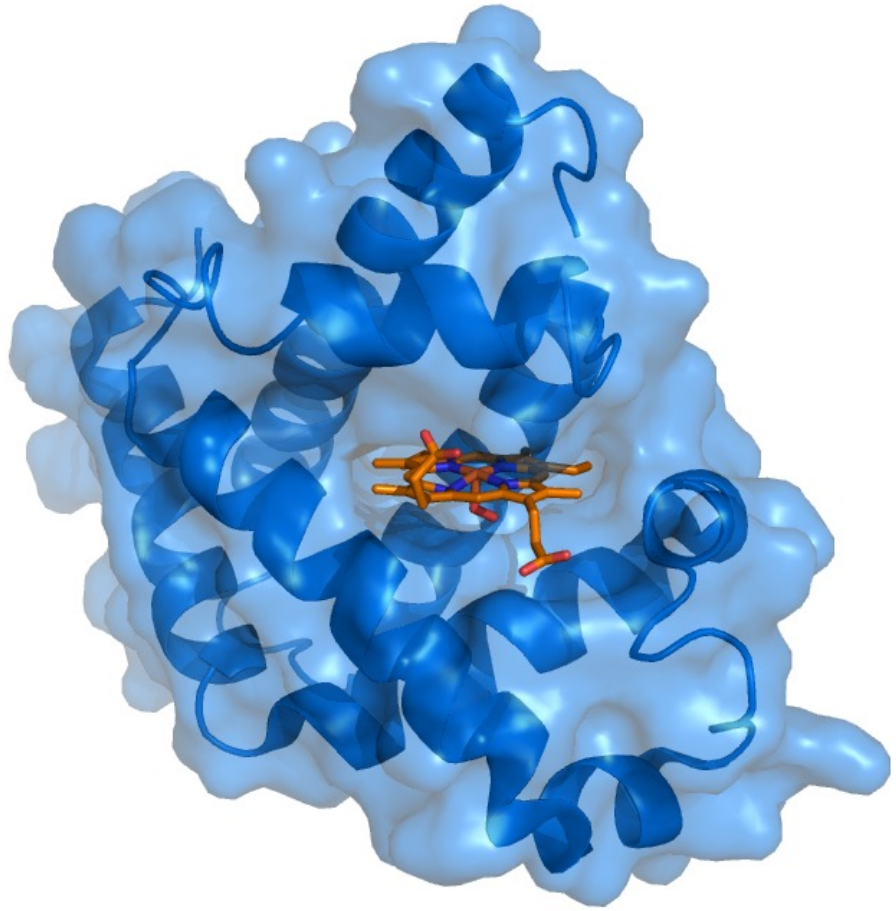
Introduction: problem definition

Protein-ligand interactions prediction can encompass manifold tasks, including estimating:

- whether a ligand binds to a protein or not (**binary classification**)
- chemical values describing the quality of binding (**regression task**)
- location of the binding site in a protein (**segmentation task**)
- ligand pose in binding pocket (**pose estimation**)
- etc…

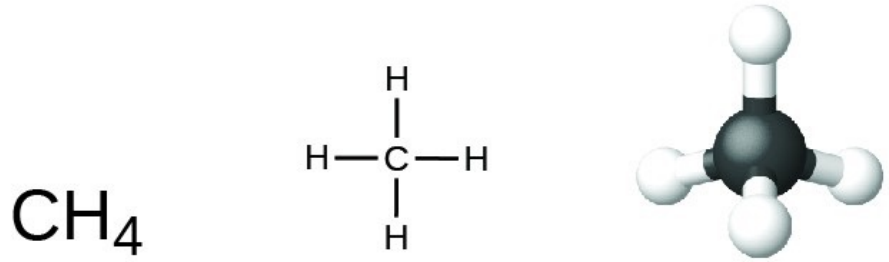


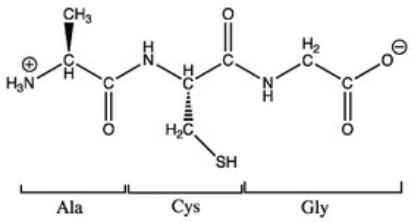
Myoglobin with its ligand heme bound. Based on PDB: 1MBO

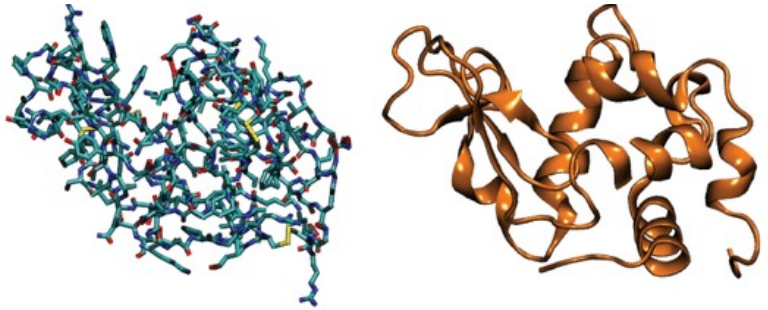
Introduction: data representation

Ligands, being mostly small chemical compounds, can be represented in various ways, including:

- 2D or 3D spatial graphs
- text formulas (like SMILES)







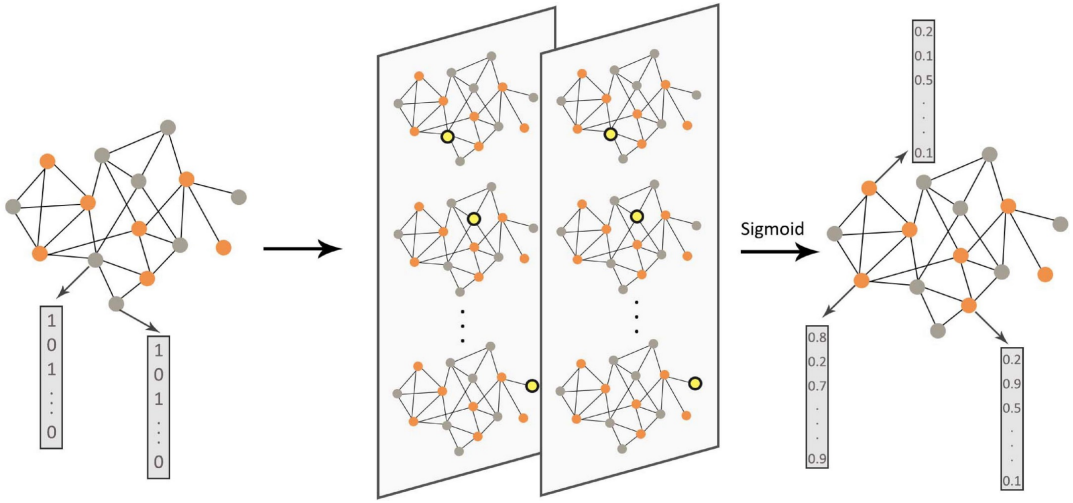
Proteins, depending on the task, can be represented as:

- 3D objects
- text amino acid sequences
- only binding pockets (like 3D objects or spatial graphs)

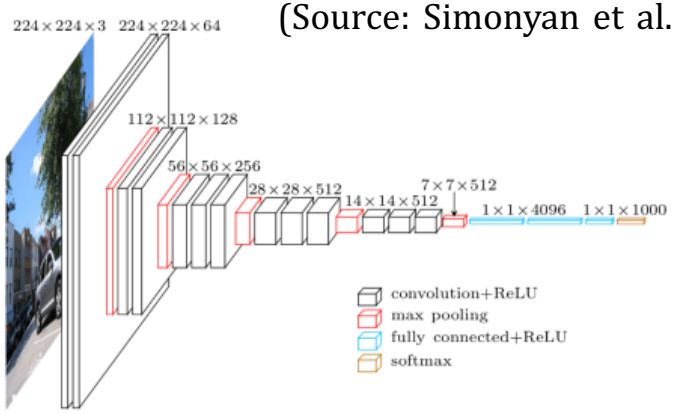
Introduction: DL approaches

Depending on the input data representation and desired task to complete, one can use a magnitude of different neural network architectures, including:

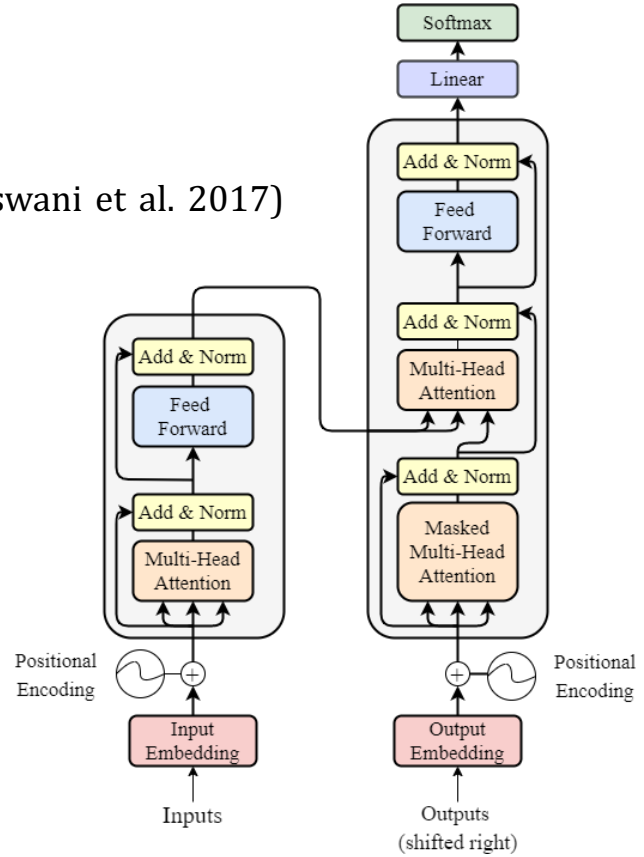
- Convolutional networks
- Graph networks
- Language models (RNNs or Transformers)
- Combinations of the above



(Source: Zhang et al. 2021)



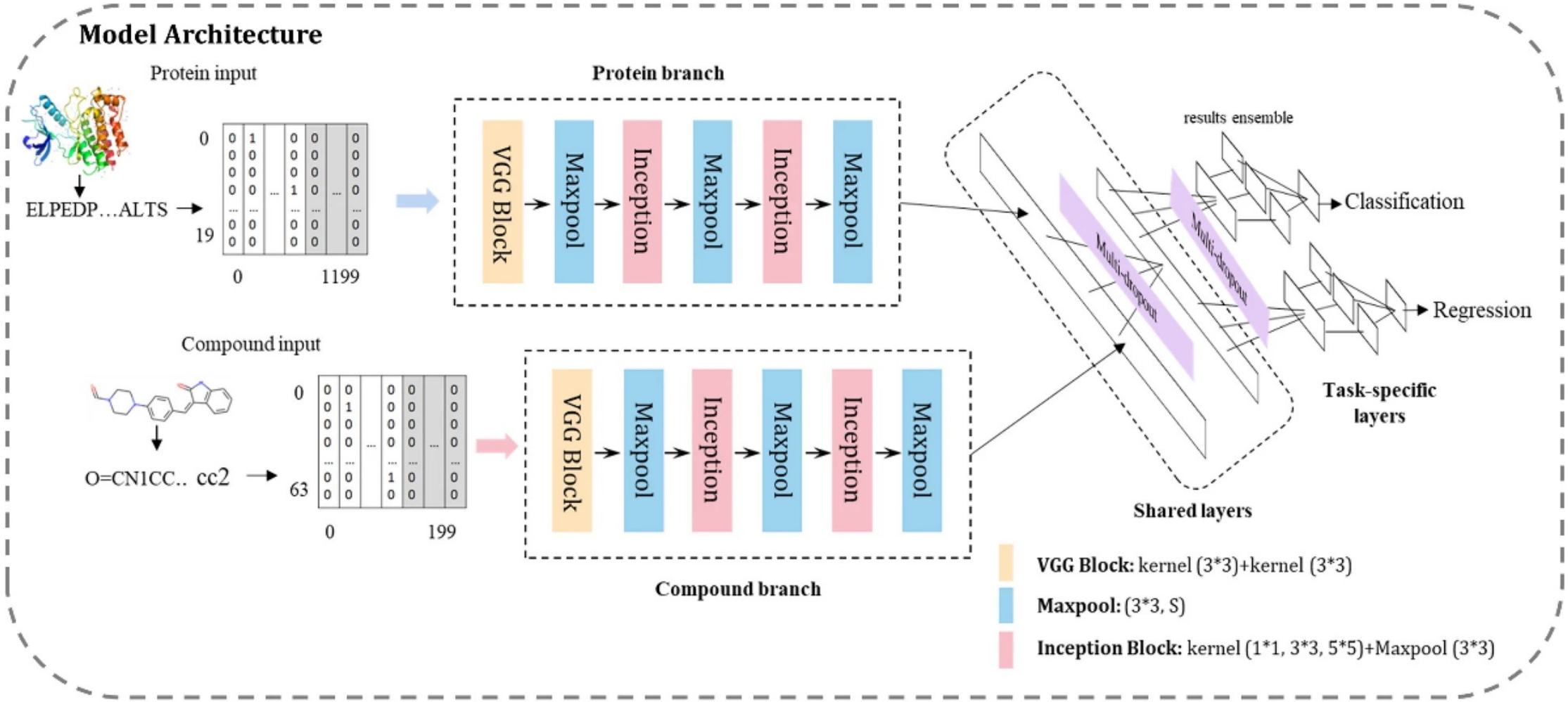
(Source: Simonyan et al. 2015)



(Source: Vaswani et al. 2017)

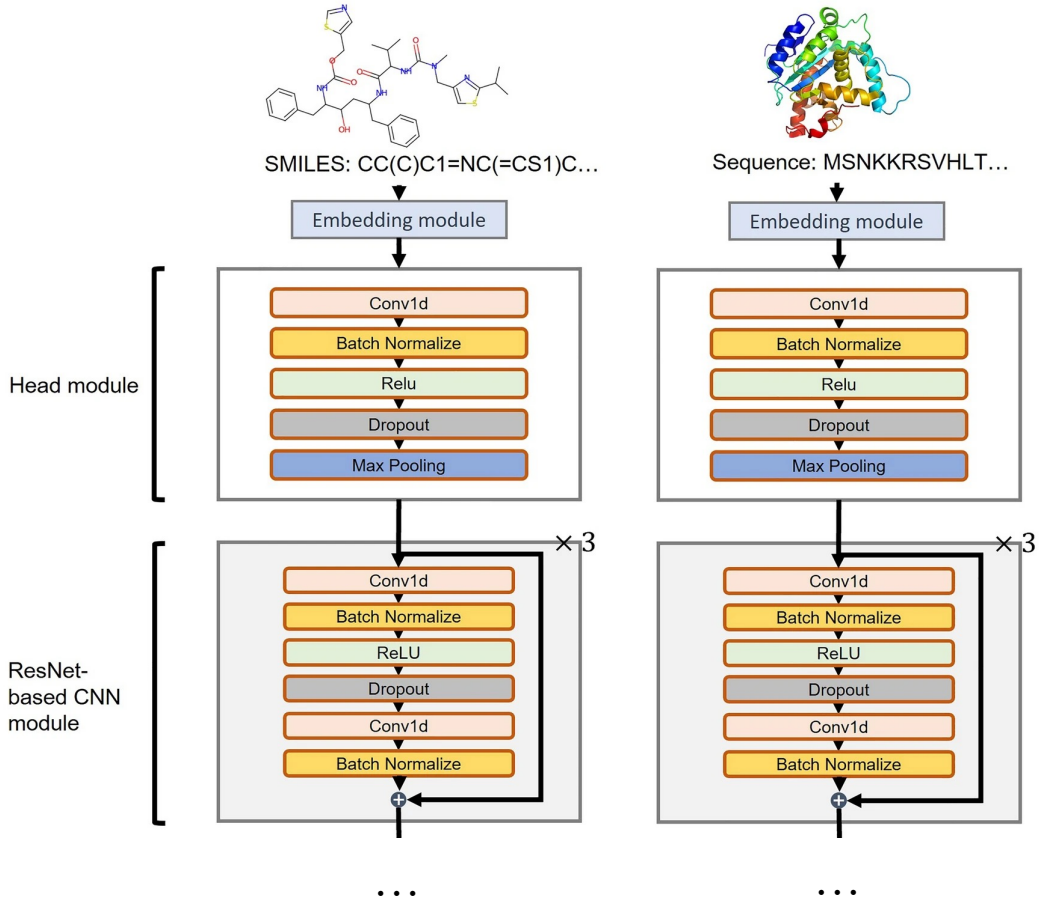
Multi-PLI: interpretable multi-task deep learning model for unifying protein–ligand interaction datasets

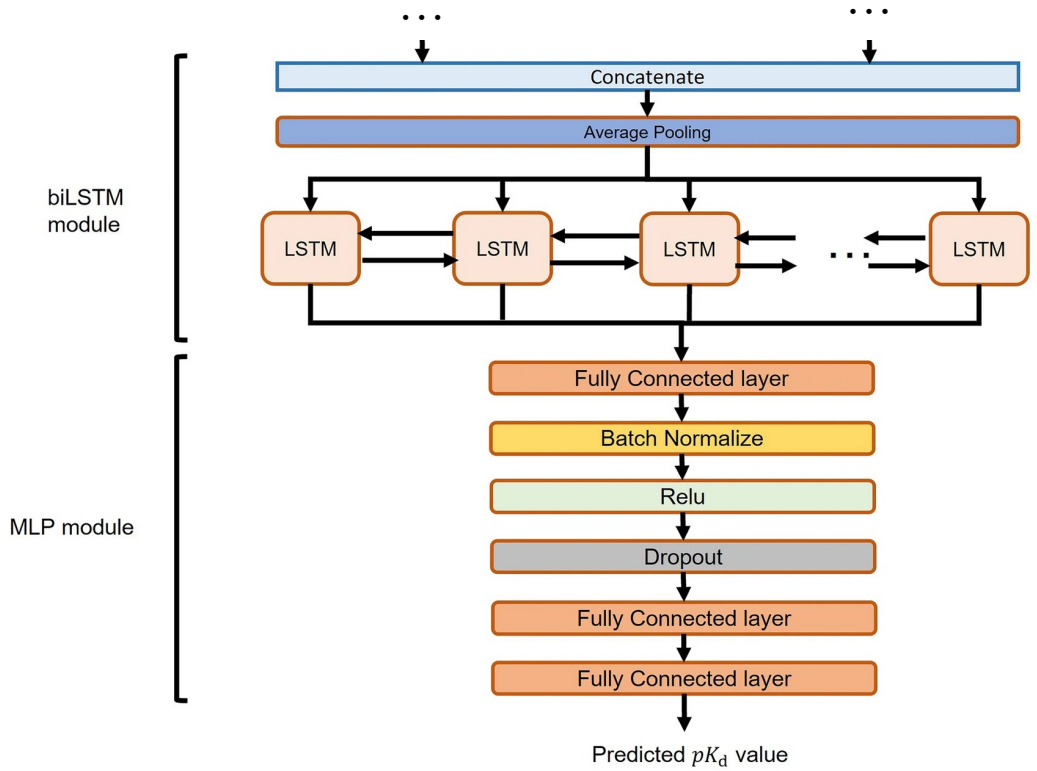
Fan Hu, Jiaxin Jiang, Dongqi Wang, Muchun Zhu and Peng Yin (2021)



DeepLPI: a novel deep learning-based model for protein–ligand interaction prediction for drug repurposing

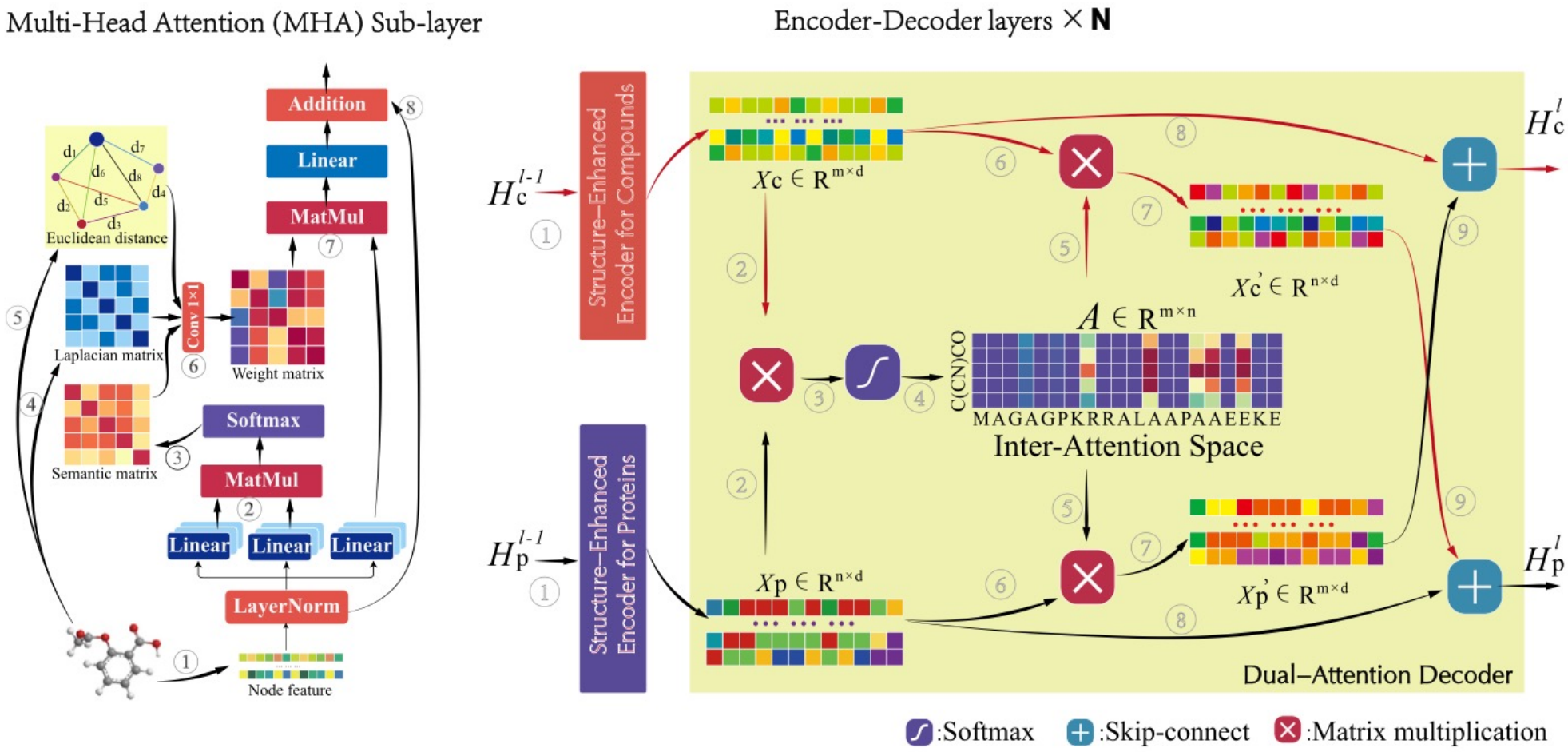
Bomin Wei, Yue Zhang & Xiang Gong (2022)





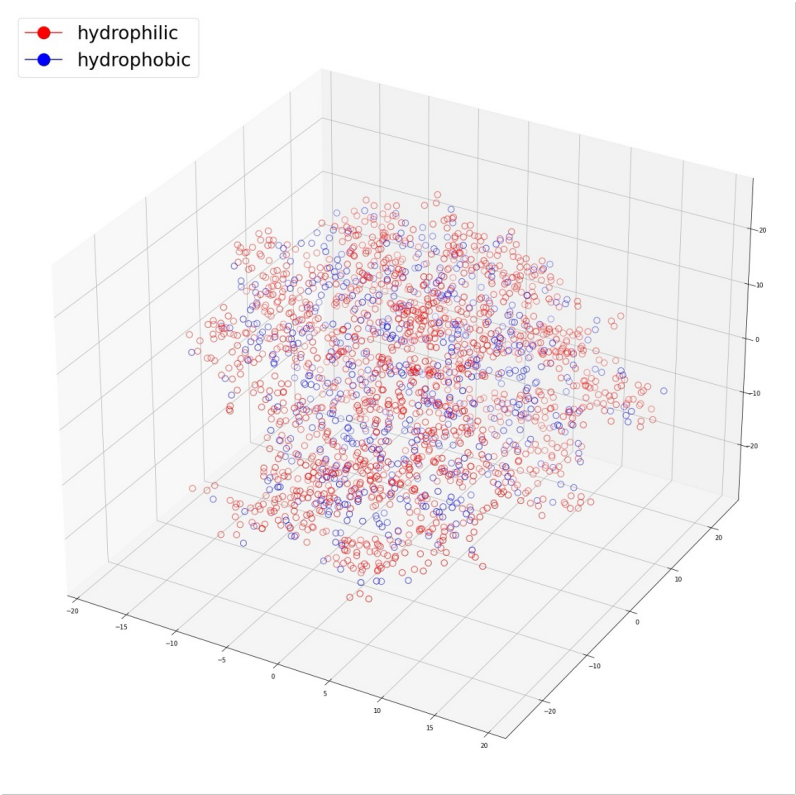
GraphsformerCPI: Graph Transformer for Compound–Protein Interaction Prediction

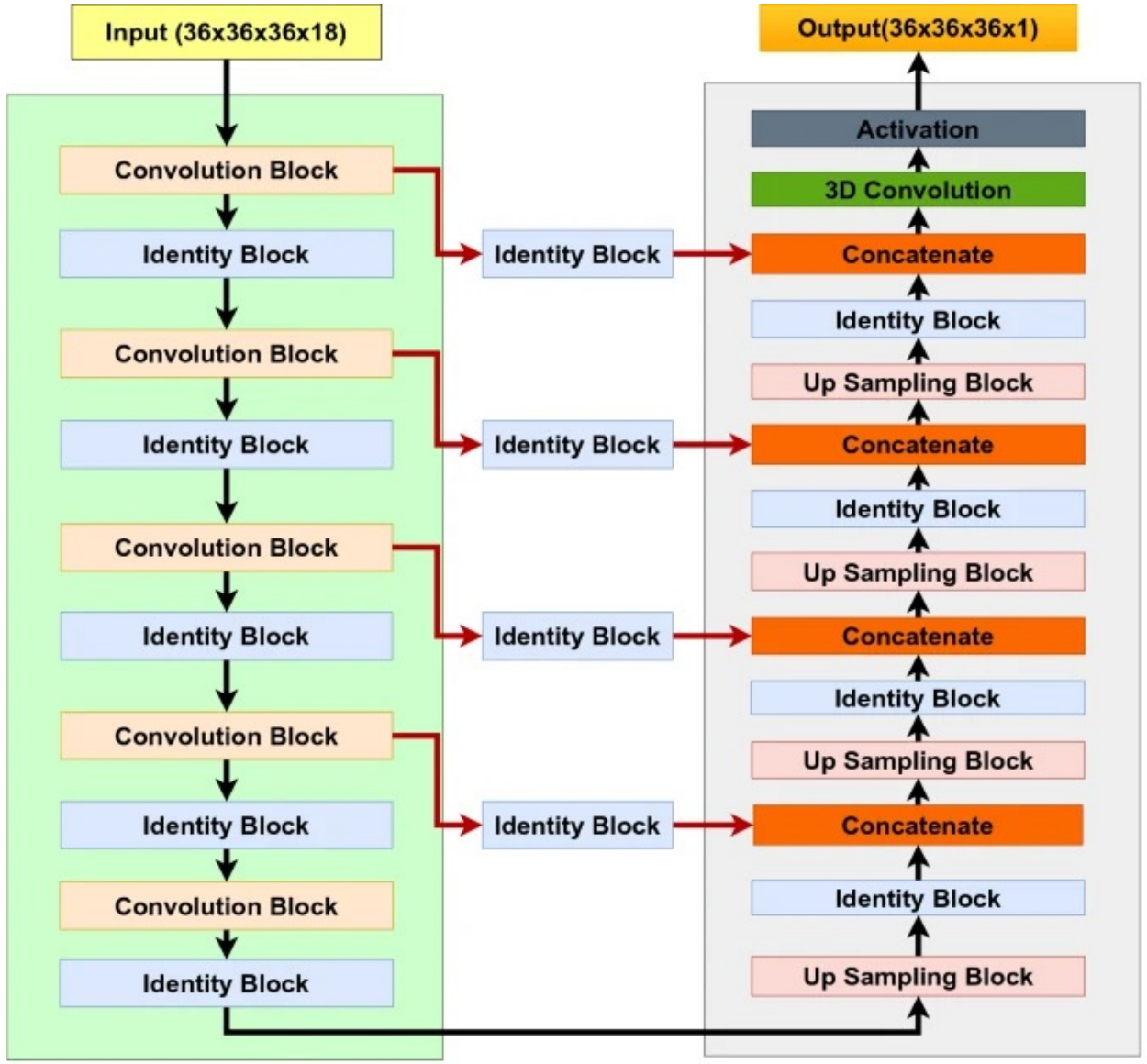
Jun Ma, Zhili Zhao, Tongfeng Li, Yunwu Liu, Jun Ma & Ruisheng Zhang (2024)



PUResNet: prediction of protein-ligand binding sites using deep residual neural network

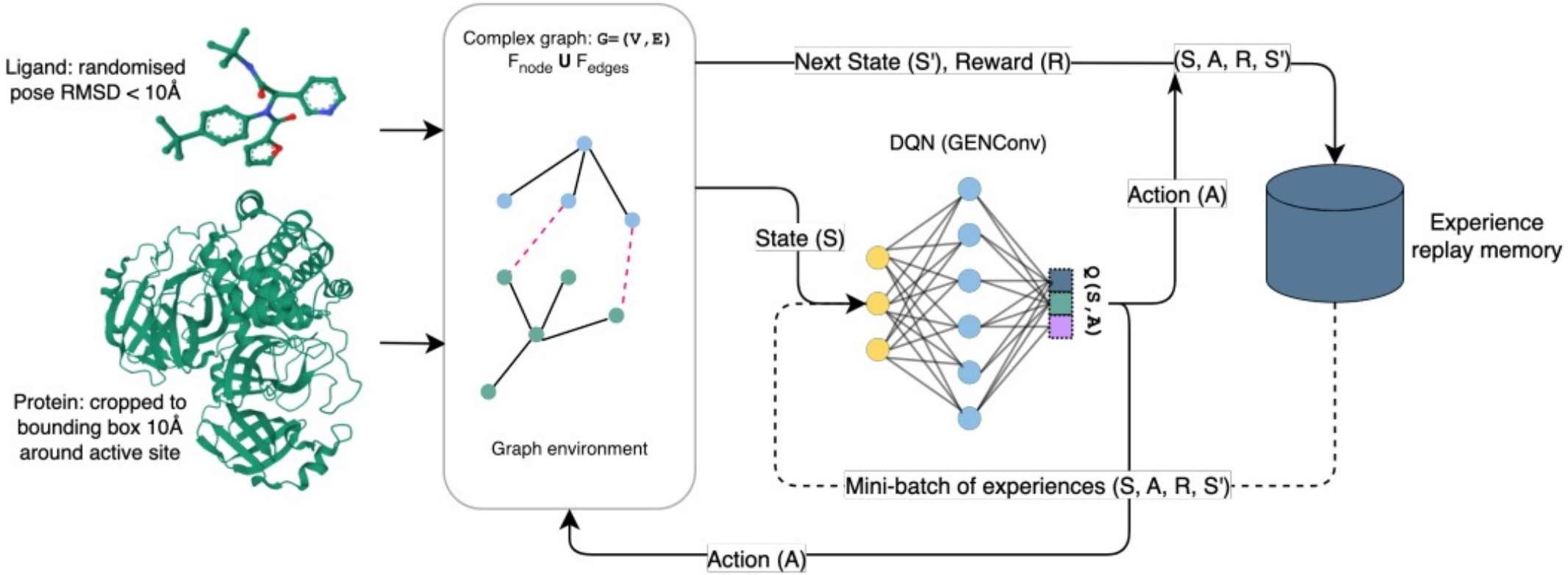
Jeevan Kandel, Hilal Tayara & Kil To Chong (2021)





PandoraRLO: Unveiling Protein-Ligand Interactions with Reinforcement Learning for Optimized Pose Prediction

Justin Jose; Ujjaini Alam, Divye Singh, Pooja Arora (2023)



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Thank you for attention.