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MASTER'S DEGREE IN SECURITY ENGINEERING AND ARTIFICAL INTELLIGENCE (MESIIA)

MASTER'S Thesis FINAL PROJECT

Directed by Prof. Francesc Serratosa

Prediction of drug–protein binding affinity using existing graph convolutional neural network models on URV In-house dataset

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1 Introduction

A virus encodes one or more proteases which are enzymes that spur the formation of new protein products, thus play crucial roles in virus replication , and are important targets for the design and development of potent antiviral agents or drugs. Binding affinity is the strength of the binding interaction between a single biomolecule (e.g., a virus protein) to its ligand or binding partner (e.g., a drug). it is a key to appreciating the intermolecular interactions driving biological processes and measured as part of the drug discovery process to help design drugs that bind their targets selectively and specifically.

References

[1] [Thin et al.] Thin Nguyen; Hang Le; Thomas P. Quinn; Tri Nguyen; Thuc Duy Le; and Svetha Venkatesh, "GraphDTA: predicting drug–target binding affinity with graph neural networks", Journal Bioinformatics, Volume 37, Issue 8, March 2021, Pages 1140–1147 Available at https://academic.oup.com/bioinformatics/article/37/8/1140/5942970.

[2] Related data, pre-trained models and source code in [1] are publicly available at https://github.com/thinng/GraphDTA.

[3] the repository forked from [2] to perform operations in this thesis available at https://github.com/YoussefEzz/GraphDTA_forked.