

# Data fusion for drug-target interaction prediction in drug repositioning

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## Contact person

Daniele Parisi

## Organisation

**Name of the organisation** Katholieke Universiteit Leuven (KUL)

**Department** ESAT

**Country** Belgium

**Geographical Area** Flemish Region

## Partners and collaborations

Biotech/TU-Dresden, Max-Planck-Institut für Informatik Saarbrücken

## SCOPE OF THE METHOD

<b>The Method relates to</b>	Human health
<b>The Method is situated in</b>	Translational - Applied Research
<b>Type of method</b>	In silico

## DESCRIPTION

### Method keywords

Bioinformatics

drug screening

computational models

Machine learning

IC50

### **Scientific area keywords**

pharmaceutical screening

pharmacology

### **Method description**

Identifying drug-target interactions is a crucial step in drug repositioning, the process of suggesting new indications for known drugs. There are about 9000 FDA-approved and experimental small molecule drugs and more than 500.000 protein records available. Performing *in vitro* experiments would be too expensive and time-consuming to check all the putative drug-target couples, therefore computational techniques might help to predict compound biological activity (IC50) and suggest new putative medical indications for existing drugs. Bayesian Matrix Factorization and deep neural network can integrate structural information of drugs, proteins and their binding to better predict the affinity of their interaction (IC50) and suggest new drug-target targets, with a big impact on the drug discovery process. Different kind of side information can be used to help the prediction process, such as chemical structures of the drugs, 3D structures of the protein targets or phenotypic effect of drug-target interactions. In my thesis, I analyse the contribution brought by structural information in the prediction process, taking into account the difficulties related to the usage of those kind of data.

### **Method status**

Still in development

## **PROS, CONS & FUTURE POTENTIAL**

### **Advantages**

Virtual screening can suggest candidates to test *in vitro* and on animal models excluding non-active compounds, saving considerable amount of time and money.

### **Challenges**

The amount and quality of data available are a bottleneck for the method. Deep

learning approaches need big dataset to make accurate predictions.

## **Modifications**

The accurate selection of the right side information and the integration of negative data might improve the accuracy of prediction.

## **Future & Other applications**

A reliable strategy for computational drug-target interaction prediction can be used for virtual screening and drug repositioning, representing an important occasion for pharmacological research in rare diseases.

## **REFERENCES, ASSOCIATED DOCUMENTS AND OTHER INFORMATION**

### **References**

PhD thesis under development. Soon available for publication and sharing.

*Coordinated by*



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