Data fusion for drug-target interaction prediction in drug repositioning

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Organisation

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Partners and collaborations

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

SCOPE OF THE METHOD

The Method relates to	Human health
The Method is situated in	Translational - Applied Research
Type of method	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 prediciton 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.

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