RexPo 22
THE 1st INTERNATIONAL CONFERENCE
ON DRUG REPURPOSING
MAASTRICHT 2ND-3RD SEP 2022

NeDRex - an integrative and interactive network medicine platform for drug repurposing

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Abstract

Traditional drug discovery faces a severe efficacy crisis. Repurposing of registered drugs provides an alternative with lower costs, reduced risk, and faster clinical application. The underlying mechanisms of complex diseases are best described by disease modules. These modules represent disease-relevant pathways and contain potential drug targets which can be identified in silico with network-based methods. The data necessary for the identification of disease modules and network-based drug repurposing are scattered across independent databases, moreover, existing studies have been limited to predictions for specific diseases or non-translational algorithmic approaches. Hence, there is an unmet need for adaptable tools allowing biomedical researchers to employ network-based drug repurposing approaches for their specific use cases. We close this gap with NeDRex[1], an integrative and interactive platform for network-based drug repurposing (available at https://nedrex.net). NeDRex integrates different data sources covering genes, proteins, drugs, drug targets, disease annotations, and their relationships, resulting in a network with 350,142 nodes and 14,127,004 edges. NeDRex allows for constructing heterogeneous biological

networks and mining them. It provides users with a variety of network-based methods (available via NeDRexApp and the web application NeDRex-Web https://web.nedrex.net/) to derive disease modules associated with diseases under study, prioritize drugs targeting disease mechanisms, and statistical validation. Benefiting from the expert-in-the-loop paradigm, researchers from biomedical sciences can leverage their domain knowledge at different points of the workflow. The approach used in NeDRex is also adapted for COVID-19 drug repurposing and available via the web tool CoVex[2] (https://exbio.wzw.tum.de/covex/).

Keywords

Drug repurposing, Network medicine, Disease module identification, Data integration, Heterogeneous networks, Network pharmacology, COVID-19 drug candidates

References

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The REPO-TRIAL project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 777111. This reflects only the author's view and the European Commission is not responsible for any use that may be made of the information it contains.