

Drug Repurposing Guidebook

Building Block I453

This document defines the content of the FACT SHEET to be created for each identified tool, incentives, initiative or practice (the Building Block) introduced by public bodies or used by developers to expedite drug repurposing in Rare Diseases (RDs).

ITEM	DESCRIPTION
Building Block (BB) Title	Drug databases
References	<p>The Drug Repurposing Hub: https://clue.io/repurposing</p> <p>DrugBank: https://go.drugbank.com/</p> <p>DrugRepurposing Online: https://drugrepurposing.info</p> <p>PROMISCUOUS 2.0 from Charité: Promiscuous 2.0 (charite.de); PROMISCUOUS: a database for network-based drug-repositioning - PMC (nih.gov)</p> <p>OpenTargets: https://platform.opentargets.org/ doi: 10.1093/nar/gkaa1027</p> <p>Pubmed Yosef Masoudi-Sobhanzadeh, et al. Drug databases and their contributions to drug repurposing, Genomics, Vol 112, Issue 2, 2020, p. 1087-1095, https://doi.org/10.1016/j.vgeno.2019.06.021</p>
Description	<p>The Drug Repurposing Hub is a curated and annotated collection of FDA-approved drugs, clinical trial drugs, and pre-clinical tool compounds with a companion information resource.</p> <p>Together with the website, the platform offers a drug repurposing library available as assay-ready plates at single concentration per compound or with 4-point dilution format for each compound. The screening of this library plates might be performed yourself or in collaboration with the Broad Institute's Center for the Development of _____ Therapeutics; https://www.broadinstitute.org/center-development-therapeutics-cdot.</p>

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	<p>DrugBank is a free-to-access, online database containing information on drugs and drug targets. It combines detailed drug data (i.e. chemical, pharmacological and pharmaceutical) with comprehensive drug target (i.e. sequence, structure, and pathway) information.</p> <p>The latest release of this database (version 5.1.9, released 2022-01-03) contains 14,747 drug entries including 2,721 approved small molecule drugs, 1,535 approved biologics (proteins, peptides, vaccines, and allergenics), 132 nutraceuticals and over 6,696 experimental (discovery-phase) drugs.</p> <p>PROMISCUOUS 2.0 database provides a uniform data-set for drug repositioning where the search can be performed from drug or target side.</p> <p>Drug repurposing online is a proprietary database, created by Numedius.</p> <p>The article from Pubmed lists many databases related to drug repurposing.</p>
Category	Supporting tools
Type of BB	Development resource
Geographical scope	International
Availability	<p>Open access for the web versions. Use and re-distribution of the content requires a license.</p> <p>For all stakeholders involved in the search for new indications or uses for existing drugs.</p> <p>Some databases such as Drug repurposing online have various levels of access, free (restricted) and premium; the latter is available either by paying or by contributing.</p>
Scope of use	To perform drug prioritization analysis and explore novel druggable targets for developed drugs
Stakeholders involved	Preclinical researchers from academia and industry

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	Chemists to re-design new drugs
Enablers/ Requirements	<p>Internet access to resources and information.</p> <p>Expertise in bioinformatics for advanced resources</p>
Output	<p>A tool to explore new indications for approved drugs or compounds in early stage research and clinical trials, susceptible to be re-purposed</p> <p>New knowledge for new target for a drug or for new treatment for a disease</p>
Best time to apply and time window	In the early stages of the drug repurposing process
Expert tips	<p>PROS:</p> <ul style="list-style-type: none"> • Web interfaces of the tools are open access • Datasets can be download or access through an API. • Datasets cover drugs in early stage research, clinical trials and approval. <p>CONS:</p> <ul style="list-style-type: none"> • Use of the datasets to advanced functions (e.g. repurposing, build predictive machine learning model) may require expertise in bioinformatics skills. • A paid license is required for non-academic users