Drug Repurposing Guidebook

Building Block I440

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	*In silico* models for screening for drug repurposing candidates
References	https://www.frontiersin.org/articles/10.3389/fchem.2020.00343/full https://www.frontiersin.org/articles/10.3389/fchem.2020.00093/full https://pubmed.ncbi.nlm.nih.gov/30205360/ https://www.imi.europa.eu/projects-results/project-factsheets/etox
Description	One of the developments that has shown quite some promise for drug repurposing is the development of *in silico* models. Over the last decades, the use and efficacy of computational, or *in silico,* models in drug development has significantly grown. Thanks to the availability of increasing amounts of data, and growing numbers and possibilities of data analysis strategies, in silico models have gained in usability and therefore traction in drug repurposing. There are different *in silico* models, for example, working on drug: target interactions using molecular dynamics, or in silico prediction of toxicities. These in silico approaches are demonstrating their ability to generate reliable predictions as well as new knowledge on the mode of action of drugs and the mechanisms underlying their side effects.
Category	Compound and network databases and tools to use them
Type of BB	Development practice
Geographical scope	International

ITEM	DESCRIPTION
Availability	Open Access (code and repository). For both rare and non-rare diseases. For both drug repurposing and de novo drug development.
Scope of use	To combine different types and kinds of data, and extract most available information from this.
Stakeholders involved	Preclinical researchers from academia and industry
Enablers/ Requirements	NA
Output	A list of drug repurposing candidates for a specific disorder that can be tested in further wet-lab studies. New knowledge based on existing datasets.
Best time to apply and time window	Discovery of drug repurposing candidates
Expert tips	If you do intend to use *in silico* models, make sure you have several robust data sets, including different data sources Pro: Allows you to systematically discover new correlations that you might have missed otherwise. Con: Sufficient (freely accessible) data is needed if you want to be able to find new information