

Drug Repurposing Guidebook

Building Block I436

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	Chemical Compound Databases
References	https://ecbd.eu/ https://www.ebi.ac.uk/chebi Global Substance Registration System (GSRS) National Center for Advancing Translational Sciences (nih.gov)
Description	Several chemical compound databases exist, which include collections of small molecules. Examples are the Chemical Entities of Biological Interest (ChEBI), which is a freely available dictionary of molecular entities focused on 'small' chemical compounds. The term 'molecular entity' refers to any constitutionally or isotopically distinct atom, molecule, ion, ion pair, radical, radical ion, complex, conformer, etc., identifiable as a separately distinguishable entity. The molecular entities in question are either products of nature or synthetic products used to intervene in the processes of living organisms.
Category	Pre-clinical development
Type of BB	Development resource
Geographical scope	Accessible from all over the world
Availability	Open-source
Scope of use	The cope of use is to find a molecule that modulates the previous found drug target or signaling pathway.

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Stakeholders involved	<p>The experts supporting the databases: ChEBI merges data from different sources: IntEnz, KEGG COMPOUND, PDBeChem, and ChEMBL to eliminate redundancy.</p> <p>The repurposing developer</p>
Enablers/ Requirements	<p>Quick availability of known molecules with known mode of action. The signaling pathway or drug target should be identified.</p>
Output	<p>Shortcut to existing molecules to target a drug target or pathway. Data on the different molecular structures can be downloaded.</p>
Best time to apply and time window	<p>In the early phases of development, once the disease and molecular target are identified.</p>
Expert tips	<p>When a drug target or pathway is identified it is a “must-to-do” to check whether already known/approved drugs for the target or pathway exist.</p>