

metaboliteIDmapping

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metaboliteIDmapping *metaboliteIDmapping package*

Description

This package loads an ID mapping table of 9 highly used metabolite ID formats, including Pubchem, Comptox Chemical Dashboard, KEGG, HMDB, Drugbank, ChEBI, and CAS. Metabolites can also be addressed by their common name. The mapping table contains more than 1.1 million metabolite entries.

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metabolitesMapping *ID Mapping table of nine different metabolite ID formats*

Description

Four different sources of annotated metabolites, i.e., HMDB, ChEBI, CompTox, and the graphite R package, have been retrieved to compile a comprehensive mapping of available metabolite IDs. ID formats that are represented in the mapping table are: DTXCID (Comptox), DTXSID (Comptox), CAS-number, CID (Pubchem), SID (Pubchem), HMDB, ChEBI, KEGG, Drugbank, and their common name.

Usage

metabolitesMapping

Format

A tibble with 9 variables and over 1.1 million metabolites:

DTXCID DSSTox structure identifier, character
DTXSID DSSTox substance identifier, character
CAS CAS registry number, character
CID Pubchem compound identifier, character
CID Pubchem substance identifier, character
HMDB Human Metabolome Database identifier (new format), character
ChEBI Chemical Entities of Biological Interest identifier, character
KEGG KEGG Compound identifier, character
Drugbank Drugbank identifier, character
Name Metabolite common name, character

Examples

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