

Package ‘metaboliteIDmapping’

December 10, 2025

Title Mapping of Metabolite IDs from Different Sources

Version 0.99.11

Description The package provides a comprehensive mapping table of nine different Metabolite ID formats and their common name. The data has been collected and merged from four publicly available source, including HMDB, Comptox Dashboard, ChEBI, and the graphite Bioconductor R package.

License GPL-3

Depends R (>= 4.0.0)

Imports AnnotationHub

Suggests BiocStyle, magrittr, graphite, dplyr, tidyr, tibble, rappdirs, XML, readxl, stringr, utils, knitr, sets, R.utils, readr, conflicted, rmarkdown

biocViews AnnotationHub, CustomDBSchema, FunctionalAnnotation

VignetteBuilder knitr

URL <https://github.com/yigbt/metaboliteIDmapping>

Encoding UTF-8

LazyData true

RoxygenNote 7.0.2

git_url <https://git.bioconductor.org/packages/metaboliteIDmapping>

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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	<i>ID Mapping table of nine different metabolite ID formats</i>
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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

`metabolitesMapping`

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