metaboliteIDmapping

February 28, 2024

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 (Comp-tox), 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

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