metaboliteIDmapping

November 6, 2026

`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.

Author(s)

Sebastian Canzler <sebastian.canzler@ufz.de>

`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

```
metabolitesMapping
```

Index

∗ **datasets**
metabolitesMapping, 1
∗ **package**
metaboliteIDmapping, 1

metaboliteIDmapping, 1
metabolitesMapping, 1