# metaboliteIDmapping

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`metaboliteIDmapping` *metaboliteIDmapping package*

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

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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

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metabolitesMapping
```

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