Package 'hmdbQuery'

April 17, 2025

Title utilities for exploration of human metabolome database

Description Define utilities for exploration of human metabolome database, including functions to retrieve specific metabolite entries and data snapshots with pairwise associations (metabolite-gene,-protein,-disease).

Version 1.29.0

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Suggests knitr, annotate, gwascat, testthat, rmarkdown

Depends R (>= 3.5), XML

Imports S4Vectors, methods, utils

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Contents

biospecimens,HmdbEntry-method 2
diseases,HmdbEntry-method 2
hmdb1 3
HmdbEntry 3
HmdbEntry-class 4
hmdb_disease 4
hmdb_gene 5
hmdb_omim 5

hmdb_protein 6
store,HmdbEntry-method 6
tissues,HmdbEntry-method 7

Index **8**

`biospecimens,HmdbEntry-method`
extract biospecimen associations

Description

extract biospecimen associations

Usage

```
## S4 method for signature 'HmdbEntry'
biospecimens(x)
```

Arguments

x	HmdbEntry instance

Value

character vector

Examples

```
data(hmdb1)
biospecimens(hmdb1)
```

`diseases,HmdbEntry-method`
extract disease associations

Description

extract disease associations

Usage

```
## S4 method for signature 'HmdbEntry'
diseases(x)
```

Arguments

x	HmdbEntry instance

Value

DataFrame

Examples

```
data(hmdb1)
diseases(hmdb1)
```

`hmdb1` *hmdb1: demonstration HMDB entry*

Description

hmdb1: demonstration HMDB entry

Usage

```
hmdb1
```

Format

HmdbEntry instance

Source

www.hmdb.ca

`HmdbEntry` *Constructor for HmdbEntry instance*

Description

Constructor for HmdbEntry instance

Usage

```
HmdbEntry(
  prefix = "http://www.hmdb.ca/metabolites/",
  id = "HMDB0000001",
  keepFull = TRUE
)
```

Arguments

`prefix`	character(1) URL of HMDB source accepting queries for XML documents
`id`	character(1) HMDB identifier tag
`keepFull`	logical(1) indicating that entire parsed XML will be retained

Value

instance of HmdbEntry, or a list

Note

The XML returned by hmdb.ca can have different structures for different metabolites. If the mapping form XML to list is not as anticipated for a given metabolite, the xmlToList result is returned with a warning. Such entries should be reported to the hmdbQuery maintainer for map revision.

Examples

```
HmdbEntry()
```

`HmdbEntry-class` *basic container for an HMDB metabolite entry*

Description

basic container for an HMDB metabolite entry

Slots

`metabolite` character(1) institutional name of metabolite

`id` HMDB identifier

`diseases` S4Vectors DataFrame instance listing associated diseases

`biospecimens` S4Vectors DataFrame instance listing associated biospecimens

`tissues` S4Vectors DataFrame instance listing associated tissues

`store` contains parsed XML

Note

Ontological tagging of diseases and other associated elements should be considered.

`hmdb_disease` *hmdb_disease: Sept 2017 extract from hmdb.ca of direct disease associations*

Description

hmdb_disease: Sept 2017 extract from hmdb.ca of direct disease associations

Usage

```
hmdb_disease
```

Format

S4Vectors DataFrame

Note

This table also includes a column of metabolite name.

Source

www.hmdb.ca xml

hmdb_gene *hmdb_gene: Sept 2017 extract from hmdb.ca of direct gene associations*

Description

hmdb_gene: Sept 2017 extract from hmdb.ca of direct gene associations

Usage

```
hmdb_gene
```

Format

S4Vectors DataFrame

Source

www.hmdb.ca xml

hmdb_omim *hmdb_omim: Sept 2017 extract from hmdb.ca of direct omim associations*

Description

hmdb_omim: Sept 2017 extract from hmdb.ca of direct omim associations

Usage

```
hmdb_omim
```

Format

S4Vectors DataFrame

Source

www.hmdb.ca xml

hmdb_protein *hmdb_protein: Sept 2017 extract from hmdb.ca of direct protein associations*

Description

hmdb_protein: Sept 2017 extract from hmdb.ca of direct protein associations

Usage

```
hmdb_protein
```

Format

S4Vectors DataFrame

Source

www.hmdb.ca xml

store,HmdbEntry-method *extract general association metadata in store slot*

Description

extract general association metadata in store slot

Usage

```
## S4 method for signature 'HmdbEntry'
store(x)
```

Arguments

x	HmdbEntry instance

Value

list

Examples

```
data(hmdb1)
names(store(hmdb1))
```

`tissues,HmdbEntry-method` *extract tissue associations*

Description

extract tissue associations

Usage

```
## S4 method for signature 'HmdbEntry'
tissues(x)
```

Arguments

`x`	HmdbEntry instance

Value

character vector

Examples

```
data(hmdb1)
tissues(hmdb1)
```

Index

∗ **datasets**
hmdb1, 3
hmdb_disease, 4
hmdb_gene, 5
hmdb_omim, 5
hmdb_protein, 6

biospecimens
(biospecimens,HmdbEntry-method), 2
biospecimens,HmdbEntry-method, 2

diseases (diseases,HmdbEntry-method), 2
diseases,HmdbEntry-method, 2

hmdb1, 3
hmdb_disease, 4
hmdb_gene, 5
hmdb_omim, 5
hmdb_protein, 6
HmdbEntry, 3
HmdbEntry-class, 4

store (store,HmdbEntry-method), 6
store,HmdbEntry-method, 6

tissues (tissues,HmdbEntry-method), 7
tissues,HmdbEntry-method, 7