Package ‘hmdbQuery’

May 29, 2024

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 1.24.0

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Suggests knitr, annotate, gwascat, testthat, rmarkdown

Depends R (>= 3.5), XML

Imports S4Vectors, methods, utils

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**biospecimens, HmdbEntry-method**

`extract biospecimen associations`

**Description**

extract biospecimen associations

**Usage**

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

**Arguments**

- `x` HmdbEntry instance

**Value**

character vector

**Examples**

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

---

**diseases, HmdbEntry-method**

`extract disease associations`

**Description**

extract disease associations

**Usage**

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

- x: HmdbEntry instance

**Value**

DataFrame

**Examples**

data(hmdb1)
diseases(hmdb1)

**Description**

hmdb1: demonstration HMDB entry

**Usage**

hmdb1

**Format**

HmdbEntry instance

**Source**

www.hmdb.ca

**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()
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: 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

**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

**Description**

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

**Usage**

hmdb_protein

**Format**

S4Vectors DataFrame

**Source**

www.hmdb.ca xml
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

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