

# Package ‘hmdbQuery’

September 18, 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** 1.25.0

**Author** Vince Carey <stvjc@channing.harvard.edu>

**Suggests** knitr, annotate, gwascat, testthat, rmarkdown

**Depends** R (>= 3.5), XML

**Imports** S4Vectors, methods, utils

**Maintainer** VJ Carey <stvjc@channing.harvard.edu>

**License** Artistic-2.0

**LazyLoad** yes

**biocViews** Metabolomics, Infrastructure

**VignetteBuilder** knitr

**RoxygenNote** 7.1.2

**Encoding** UTF-8

**git\_url** <https://git.bioconductor.org/packages/hmdbQuery>

**git\_branch** devel

**git\_last\_commit** 78b8b80

**git\_last\_commit\_date** 2024-04-30

**Repository** Bioconductor 3.20

**Date/Publication** 2024-09-17

## 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	<i>hmdb1: demonstration HMDB entry</i>
-------	--

---

**Description**

hmdb1: demonstration HMDB entry

**Usage**

```
hmdb1
```

**Format**

HmdbEntry instance

**Source**

[www.hmdb.ca](http://www.hmdb.ca)

---

HmdbEntry	<i>Constructor for HmdbEntry instance</i>
-----------	---

---

**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 from 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	<i>basic container for an HMDB metabolite entry</i>
-----------------	---

---

**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	<i>hmdb_disease: Sept 2017 extract from hmdb.ca of direct disease associations</i>
--------------	--

---

**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	<i>hmdb_gene: Sept 2017 extract from hmdb.ca of direct gene associations</i>
-----------	--

---

**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	<i>hmdb_omim: Sept 2017 extract from hmdb.ca of direct omim associations</i>
-----------	--

---

**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	<i>hmdb_protein: Sept 2017 extract from hmdb.ca of direct protein associations</i>
--------------	--

---

**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	<i>extract general association metadata in store slot</i>
------------------------	---

---

**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](#)