

Package ‘metabolighteR’

December 11, 2020

Type Package

Title Interface to the 'Metabolights' RESTful API

Version 0.1.1

Date 2020-12-11

Description

Access to the 'Metabolights' RESTful API <<https://www.ebi.ac.uk/metabolights/index>>. Retrieve elements of publically available 'Metabolights' studies.

Depends magrittr

Imports httr, dplyr, purrr, crayon

License GPL (>= 3)

LazyData true

URL <https://github.com/aberHRML/metabolighteR>

BugReports <https://github.com/aberHRML/metabolighteR/issues>

RoxygenNote 7.1.0

Encoding UTF-8

Suggests covr, testthat, tibble, knitr, rmarkdown, tidyr

Roxygen list(markdown = TRUE)

VignetteBuilder knitr

NeedsCompilation no

Author Tom Wilson [aut, cre] (<<https://orcid.org/0000-0003-3112-4682>>)

Maintainer Tom Wilson <tpw2@aber.ac.uk>

R topics documented:

download_study_file	2
get_isa_investigation	3
get_private_studies	3
get_studies	4
get_study_contacts	4

get_study_desc	5
get_study_descriptors	5
get_study_factors	6
get_study_files	6
get_study_meta	7
get_study_org	7
get_study_protocols	8
get_study_pubs	8
get_study_samples	9
get_study_tech	9
get_study_title	10
get_webservice	10
mtbls_key	11
Index	12

download_study_file	<i>Download Study File Contents</i>
---------------------	-------------------------------------

Description

Download the contents of a specified file from a public study

Usage

download_study_file(study_id, filename)

Arguments

- study_id a character string of a valid MTBLS study id
- filename a character of the full filename and extension to download

Value

a tibble of file contents

get_isa_investigation *Get ISA Investigation File*

Description

Retrieve the ISA Investigation for a specified Metabolights Study

Usage

```
get_isa_investigation(study_id)
```

Arguments

study_id A character string of a valid MTBLS study id

Value

the ISA-tab Investigation output

Examples

```
## Not run:
ISA <- get_isa_investigation('MTBLS375')
writeLines(isa_investigation_parse, con = paste0('outpath/ISA.txt'))

## End(Not run)
```

get_private_studies *Get Private Studies*

Description

Retrieve all private studies which belong to your user account

Usage

```
get_private_studies()
```

Value

a tibble of your private Study IDs

Examples

```
## Not run:
get_private_studies()

## End(Not run)
```

`get_studies`*Get Studies*

Description

Retrieve a list of all publically available Metabolights studies

Usage

```
get_studies()
```

Value

a tibble of Study IDs

Examples

```
get_studies()
```

`get_study_contacts`*Get Study Contacts*

Description

Retrieve the contact details for a specified public study '

Usage

```
get_study_contacts(study_id)
```

Arguments

`study_id` a character string of a valid MTBLS study id

Value

a tibble of study contacts

Examples

```
get_study_contacts('MTBLS375')
```

get_study_desc	<i>Get Study Description</i>
----------------	------------------------------

Description

Retrieve the abstract based description of a public study

Usage

```
get_study_desc(study_id)
```

Arguments

study_id	A character string of a valid MTBLS study id
----------	--

Value

a character string of the study description

Examples

```
get_study_desc('MTBLS375')
```

get_study_descriptors	<i>Get Study Descriptors</i>
-----------------------	------------------------------

Description

Retrieve the study descriptors and annotation values for a publically available study

Usage

```
get_study_descriptors(study_id)
```

Arguments

study_id	A character string of a valid MTBLS study id
----------	--

Value

a tibble of study descriptors

Examples

```
get_study_descriptors('MTBLS375')
```

get_study_factors	<i>Get Study Factors</i>
-------------------	--------------------------

Description

Retrieve the study factors and annotation values for a publically available study

Usage

```
get_study_factors(study_id)
```

Arguments

study_id	A character string of a valid MTBLS study id
----------	--

Value

a tibble of study factors

Examples

```
get_study_factors('MTBLS375')
```

get_study_files	<i>Get Study Files</i>
-----------------	------------------------

Description

Retrieve the names and type of all files that have been deposited with the public study. If raw_data is TRUE then details of raw data files(ie, .mzML) are also returned.

Usage

```
get_study_files(study_id, raw_data = FALSE)
```

Arguments

study_id	A character string of a valid MTBLS study id
raw_data	logical; if TRUE then raw data file info is also returned. (Default is FALSE)

Value

a tibble of file info

Examples

```
get_study_files('MTBLS375', raw_data = FALSE)
```

get_study_meta	<i>Get Study Meta</i>
----------------	-----------------------

Description

Retrieve the meta data for a publically available study

Usage

```
get_study_meta(study_id)
```

Arguments

study_id	A character string of a valid MTBLS study id
----------	--

Value

a tibble of study meta data

Examples

```
get_study_meta('MTBLS375')
```

get_study_org	<i>Get Study Organisms</i>
---------------	----------------------------

Description

Retrieve the organisms used within a study

Usage

```
get_study_org(study_id)
```

Arguments

study_id	A character string of a valid MTBLS study id
----------	--

Value

a tibble of study organism data

Examples

```
## Not run:  
get_study_org('MTBLS375')  
  
## End(Not run)
```

get_study_protocols	<i>Get Study Protocols</i>
---------------------	----------------------------

Description

Retrieve the protocol information that has been deposited for a public study

Usage

```
get_study_protocols(study_id)
```

Arguments

study_id	A character string of a valid MTBLS study id
----------	--

Value

a tibble of study protocols

Examples

```
get_study_protocols('MTBLS375')
```

get_study_pubs	<i>Get Study Publications</i>
----------------	-------------------------------

Description

Retrieve details on any publications that have been associated with the study

Usage

```
get_study_pubs(study_id)
```

Arguments

study_id	A character string of a valid MTBLS study id
----------	--

Value

a tibble of study publications

Examples

```
get_study_pubs('MTBLS375')
```

get_study_samples	<i>Get Study Samples</i>
-------------------	--------------------------

Description

Get a list of all sample names mapped to files within the study

Usage

```
get_study_samples(study_id)
```

Arguments

study_id	A character string of a valid MTBLS study id
----------	--

Value

a tibble of filename sample name and reliability score. 1.0 indicates a perfect match

Examples

```
## Not run:  
get_study_samples('MTBLS375')  
  
## End(Not run)
```

get_study_tech	<i>Get Study Technology</i>
----------------	-----------------------------

Description

Retrieve a tibble of all Study IDs and the analytical technology used in the study

Usage

```
get_study_tech()
```

Value

a tibble of study id and technology

Examples

```
get_study_tech()
```

get_study_title	<i>Get Study Title</i>
-----------------	------------------------

Description

Retrieve the full title of the study

Usage

```
get_study_title(study_id)
```

Arguments

study_id	A character string of a valid MTBLS study id
----------	--

Value

a character string of the study title

Examples

```
get_study_title('MTBLS375')
```

get_webservice	<i>Get Web-service details</i>
----------------	--------------------------------

Description

Retrieve details about the Metabolights RESTful Webservice

Usage

```
get_webservice()
```

Value

a list of the MTBLS webservice information

Examples

```
get_webservice()
```

`mtbbs_key`*Set API Token*

Description

Set your Metabolights API Token as global option. If MTBLS_API_KEY is set in `.Renviron` then this variable will be passed directly to the MTBLS_API_KEY option. If no MTBLS_API_KEY is set in `.Renviron`, then the API Token must be passed as an input in the `set_api_token` function

Usage

```
mtbbs_key(API_KEY = NULL)
```

Arguments

API_KEY a character string of your Metabolights API Token (Default is NULL)

Examples

```
## Not run:

# If API Token is set in `.Renviron`

mtbbs_key()

# If API Token is not set in `.Renviron`

mtbbs_key('XXXX-0000-XXXX-0000')

## End(Not run)
```

Index

`download_study_file`, [2](#)

`get_isa_investigation`, [3](#)
`get_private_studies`, [3](#)
`get_studies`, [4](#)
`get_study_contacts`, [4](#)
`get_study_desc`, [5](#)
`get_study_descriptors`, [5](#)
`get_study_factors`, [6](#)
`get_study_files`, [6](#)
`get_study_meta`, [7](#)
`get_study_org`, [7](#)
`get_study_protocols`, [8](#)
`get_study_pubs`, [8](#)
`get_study_samples`, [9](#)
`get_study_tech`, [9](#)
`get_study_title`, [10](#)
`get_webservice`, [10](#)

`mtbls_key`, [11](#)