Package 'metabolighteR'

February 9, 2022

Type Package
Title Interface to the 'Metabolights' RESTful API
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Description Access to the 'Metabolights' RESTful API https://www.ebi.ac.uk/metabolights/ index>. Retrieve elements of publically available 'Metabolights' studies.
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R topics documented:
download_study_file

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 ${\tt download_study_file} \quad \quad \textit{Download Study File Contents}$

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 3

```
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)</pre>
```

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

```
## Not run:
get_private_studies()
## End(Not run)
```

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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

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

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get_study_desc

Get Study Description

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 Get Study Descriptors
```

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

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

get_study_files

get_study_factors

Get Study Factors

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

Get Study Files

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

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

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get_study_meta

Get Study Meta

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

Get Study Organisms

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

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

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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

Get Study Publications

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

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

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get_study_samples

Get Study Samples

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

Get Study Technology

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

```
get_study_tech()
```

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get_study_title

Get Study Title

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

Get Web-service details

Description

Retrieve details about the Metabolights RESTful WebService

Usage

```
get_webservice()
```

Value

a list of the MTBLS webservice information

```
get_webservice()
```

mtbls_key

mtbls_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

```
mtbls_key(API_KEY = NULL)
```

Arguments

API_KEY

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

```
## Not run:
# If API Token is set in `.Renviron`
mtbls_key()
# If API Token is not set in `.Renviron`
mtbls_key('XXXX-0000-XXXX-0000')
## End(Not run)
```

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