Package: metabolighteR (via r-universe)

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Type Package

Title Interface to the 'Metabolights' REST API

Version 0.1.5

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Description Access to the 'Metabolights' REST API <`https://www.ebi.ac.uk/metabolights/index`>. Retrieve elements of publicly available 'Metabolights' studies.

Depends magrittr

Imports httr, dplyr, purrr, crayon, jsonlite, stringr, rvest, glue, tibble

License GPL (>= 3)

URL `https://github.com/aberHRML/metabolighteR`

BugReports `https://github.com/aberHRML/metabolighteR/issues`

RoxygenNote 7.3.2

Encoding UTF-8

Suggests covr, testthat, knitr, rmarkdown, tidyr, dbplyr

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VignetteBuilder knitr

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Contents

`all_get_methods` *All Public GET Methods*

Description

Retrieve a list of all the available public `GET` methods

Usage

```
all_get_methods()
```

Value

a `tbl_df` of API `GET` methods

`create.MAF` *Create a dataframe representing a MAF file*

Description

MAF files combine the metabolite abundance matrix, the spectral data like m/z and retention time, and the metabolite names, structures and database identifiers.

Usage

```
create.MAF(assaytype = "LCMS", nrow = NULL, abundances = NULL)
```

Arguments

`assaytype`	Currently unused, but would be used for different MAF files for NMR and MS
`nrow`	Create the MAF with nrow empty rows.
`abundances`	is a data frame or matrix with the metabolite abundances, intensities or concentrations.

Details

If an abundance matrix is given, the the generated MAF will have as many (empty) spectral and identification metadata rows as abundance rows, joined to the provided abundance matrix.

nrow and abundances should be mutually exclusive, but that is not yet tested.

Examples

```
maf <- create.MAF(nrow=17)
```

`download_study_file` *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` *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

```
## Not run:
get_studies()

## End(Not run)
```

`get_study_assay_file` *Get Study Assay File*

Description

Retrieve the filename details for available assays of a public study

Usage

```
get_study_assay_file(study_id)
```

Arguments

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

Value

a character string of the study assay filename

Examples

```
## Not run:
get_study_assay_file('MTBLS375')

## End(Not run)
```

`get_study_assay_list` *Get Study Description*

Description

Retrieve the abstract based description of a public study

Usage

```
get_study_assay_list(study_id)
```

Arguments

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

Value

a list off the study assays and associated details

Examples

```
## Not run:
get_study_assay_list('MTBLS375')

## End(Not run)
```

`get_study_audit` *Get Study Audit*

Description

Retrieve a list of available audit folders for a study

Usage

```
get_study_audit(study_id)
```

Arguments

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

Value

a `list` of available audit folders

Examples

```
## Not run:
get_study_audit('MTBLS375')

## End(Not run)
```

`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

```
## Not run:
get_study_contacts('MTBLS375')

## End(Not run)
```

`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

```
## Not run:
get_study_desc('MTBLS375')

## End(Not run)
```

`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

Examples

```
## Not run:
get_study_descriptors('MTBLS375')

## End(Not run)
```

`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

```
## Not run:
get_study_factors('MTBLS375')

## End(Not run)
```

`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

Examples

```
## Not run:
get_study_files('MTBLS375', raw_data = FALSE)

## End(Not run)
```

`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

```
## Not run:
get_study_meta('MTBLS375')

## End(Not run)
```

`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

Examples

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

## End(Not run)
```

`get_study_protocols` *Get Study Protocols*

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

```
## Not run:
get_study_protocols('MTBLS375')

## End(Not run)
```

`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

Examples

```
## Not run:
get_study_pubs('MTBLS375')

## End(Not run)
```

`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

Examples

```
## Not run:
get_study_tech()

## End(Not run)
```

`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

```
## Not run:
get_study_title('MTBLS375')

## End(Not run)
```

`get_user_studies` *Get Studies for User*

Description

Retrieve a list of studies for a user

Usage

```
get_user_studies()
```

Value

a `list` of user owned studies

Examples

```
## Not run:
get_user_studies()

## End(Not run)
```

`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

Examples

```
## Not run:
get_webservice()

## End(Not run)
```

`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`)

Examples

```
## 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)
```

`read.MAF` *Read MAF file to dataframe*

Description

Read the MAF file as data frame.

Usage

```
read.MAF(file)
```

Arguments

`file`	A filename to a MAF file

Value

a data frame. Row and column names are NOT "fixed" via `make.names`

Examples

```
file <- system.file("examples/m_MTBLS1968_LC-MS_positive_reverse-phase_metabolite_profiling_v2_maf.tsv",
                    package = "metabolighteR")
maf <- read.MAF(file)
```

`search_metabolite` *Search Metabolite*

Description

Search Metabolite

Usage

```
search_metabolite(search_name)
```

Arguments

`search_name`	A character string of a chemical name to search for

Examples

```
## Not run:
search_metabolite('proline')

## End(Not run)
```

`write.MAF` *Write a dataframe to a MAF file*

Description

Write a suitably formatted data frame to a MAF file.

Usage

```
write.MAF(maf, file = "")
```

Arguments

`maf`	MAF data frame to write
`file`	either a character string naming a file or a connection open for writing. "" indicates output to the console.

Examples

```
maf <- create.MAF(nrow=17)
write.MAF(maf, file=tempfile())
```

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