Package: metabolighteR (via r-universe)

May 26, 2026

Type Package

Title Interface to the 'Metabolights' REST API

Version 0.1.4

Date 2025-02-19

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

License GPL (>= 3)

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

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

RoxygenNote 7.2.3

Encoding UTF-8

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

Roxygen list(markdown = TRUE)

VignetteBuilder knitr

biocViews RepositoryData, Metabolomics, MassSpectrometryData

Config/pak/sysreqs libicu-dev libssl-dev

Repository https://aberhrml.r-universe.dev

Date/Publication 2025-04-11 09:03:55 UTC

RemoteUrl https://github.com/aberHRML/metabolighteR

RemoteRef HEAD

RemoteSha 62ad800132f8a707038d5e9f900f2678115851c2

Contents

all_get_methods 2
create.MAF 3
download_study_file 3
get_isa_investigation 4
get_private_studies 4
get_studies 5
get_study_assay_file 5
get_study_assay_list 6
get_study_audit 6
get_study_contacts 7
get_study_desc 7
get_study_descriptors 8
get_study_factors 8
get_study_files 9
get_study_meta 9
get_study_org 10
get_study_protocols 10
get_study_pubs 11
get_study_samples 11
get_study_tech 12
get_study_title 12
get_user_studies 13
get_webservice 13
mtbls_key 14
read.MAF 14
write.MAF 15

Index **16**

`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

```
get_studies()
```

`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

```
get_study_assay_file('MTBLS375')
```

`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

```
get_study_assay_list('MTBLS375')
```

`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

```
get_user_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` *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

Examples

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

`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

Examples

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

`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

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

```
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

Examples

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

`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

```
get_study_tech()
```

`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_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

```
get_user_studies
```

`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

```
get_webservice()
```

`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)
```

`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())
```

Index

all_get_methods, 2

create.MAF, 3

download_study_file, 3

get_isa_investigation, 4
get_private_studies, 4
get_studies, 5
get_study_assay_file, 5
get_study_assay_list, 6
get_study_audit, 6
get_study_contacts, 7
get_study_desc, 7
get_study_descriptors, 8
get_study_factors, 8
get_study_files, 9
get_study_meta, 9
get_study_org, 10
get_study_protocols, 10
get_study_pubs, 11
get_study_samples, 11
get_study_tech, 12
get_study_title, 12
get_user_studies, 13
get_webservice, 13

mtbls_key, 14

read.MAF, 14

write.MAF, 15