

Package: metabolighteR (via r-universe)

June 9, 2026

Type Package

Title Interface to the 'Metabolights' REST API

Version 0.1.5

Date 2026-05-19

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, 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

Roxygen list(markdown = TRUE)

VignetteBuilder knitr

biocViews RepositoryData, Metabolomics, MassSpectrometryData

Config/pak/sysreqs libicu-dev libxml2-dev libssl-dev

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

Date/Publication 2026-06-09 10:25:09 UTC

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

RemoteRef HEAD

RemoteSha 50b53af8217ec92b45e4d51ab0fee965fdd6c409

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	8
get_study_descriptors	8
get_study_factors	9
get_study_files	9
get_study_meta	10
get_study_org	11
get_study_protocols	11
get_study_pubs	12
get_study_samples	12
get_study_tech	13
get_study_title	13
get_user_studies	14
get_webservice	14
mtbls_key	15
read.MAF	15
search_metabolite	16
write.MAF	16
Index	18

all_get_methods	<i>All Public GET Methods</i>
-----------------	-------------------------------

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	<i>Create a dataframe representing a MAF file</i>
------------	---

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	<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	<i>Get Studies</i>
-------------	--------------------

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	<i>Get Study Assay File</i>
----------------------	-----------------------------

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)
```

<code>get_study_meta</code>	<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

```
## 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	<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

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

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

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

get_user_studies	<i>Get Studies for User</i>
------------------	-----------------------------

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	<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

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

mtbls_key	<i>Set API Token</i>
-----------	----------------------

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	<i>Read MAF file to dataframe</i>
----------	-----------------------------------

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	<i>Search Metabolite</i>
-------------------	--------------------------

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	<i>Write a dataframe to a MAF file</i>
-----------	--

Description

Write a suitably formatted data frame to a MAF file.

Usage

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

Arguments

<code>maf</code>	MAF data frame to write
<code>file</code>	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](#), 8

[get_study_descriptors](#), 8

[get_study_factors](#), 9

[get_study_files](#), 9

[get_study_meta](#), 10

[get_study_org](#), 11

[get_study_protocols](#), 11

[get_study_pubs](#), 12

[get_study_samples](#), 12

[get_study_tech](#), 13

[get_study_title](#), 13

[get_user_studies](#), 14

[get_webservice](#), 14

[mtbls_key](#), 15

[read.MAF](#), 15

[search_metabolite](#), 16

[write.MAF](#), 16