# Package 'metabolighteR'

March 25, 2021

```
Type Package
Title Interface to the 'Metabolights' RESTful API
Version 0.1.2
Date 2021-03-25
Description
      Access to the 'Metabolights' RESTful API <a href="https://www.ebi.ac.uk/metabolights/index">https://www.ebi.ac.uk/metabolights/index</a>. Re-
      trieve 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
```

2 download\_study\_file

## **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

### 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)
```

4 get\_study\_contacts

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')
```

get\_study\_desc 5

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)
```

get\_study\_meta 7

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)
```

8 get\_study\_pubs

### 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')
```

get\_study\_samples 9

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()
```

10 get\_webservice

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)
```

# **Index**

```
download_study_file, 2
get_isa_investigation, 3
get_private_studies, 3
get_studies, 4
{\tt get\_study\_contacts}, {\tt 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
\verb"get_study_samples", 9
{\tt get\_study\_tech}, \textcolor{red}{9}
get_study_title, 10
get_webservice, 10
mtbls_key, 11
```