Package ‘metabolomicsWorkbenchR’

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Type Package

Title Metabolomics Workbench in R

Version 1.23.0

Description This package provides functions for interfacing with the Metabolomics Workbench RESTful API. Study, compound, protein and gene information can be searched for using the API. Methods to obtain study data in common Bioconductor formats such as SummarizedExperiment and MultiAssayExperiment are also included.

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Encoding UTF-8

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Collate 'parse_fcns.R' 'generics.R' 'class_def.R' 'constants.R' 'helper_fcns.R' 'metabolomicsWorkbenchR.R'

Imports data.table, httr, jsonlite, methods, MultiAssayExperiment, struct, SummarizedExperiment, utils

Suggests BiocStyle, covr, knitr, HDF5Array, httptest, rmarkdown, structToolbox, testthat, pmp, grid, png

VignetteBuilder knitr

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Contents

`check_pattern` *Check input against acceptable input pattern*

Description

Checks an input_value against a regex pattern to determine if the input_value is valid. This method is used internally and not for intended for general use.

Usage

```
check_pattern(I, input_value, match)

## S4 method for signature 'mw_input_item'
check_pattern(I, input_value, match)
```

Arguments

`I`	An mw_input_item.
`input_value`	The value for the input item (character).
`match`	The type of match. One of "exact" or "partial".

Value

TRUE if input matches the pattern, or throws an error.

Examples

```
check_pattern(input_item$study_id,'ST000001','exact')
```

`check_puts` *Check inputs/outputs match*

Description

Checks that the provided inputs and output are compatible. This method is used internally and not for intended for general use.

Usage

```
check_puts(input_item, output_item)

## S4 method for signature 'mw_input_item'
check_puts(input_item, output_item)
```

Arguments

`input_item`	An mw_input_item.
`output_item`	An mw_output_item.

Value

TRUE if the items are compatible or throws an error if not.

Examples

```
check_puts(input_item$study_id,output_item$summary)
```

`context` *Contexts*

Description

A predefined list of mw_context objects. The context have been created to mirror the metabolomics workbench API documentation contexts as closely as possible.

Usage

```
context
```

Format

An object of class `list` of length 7.

Examples

```
# list available contexts
names(context)

# get the context 'study'
context$study
```

`context_inputs` *Valid inputs*

Description

Get a list of valid input_items for a context.

Usage

```
context_inputs(context)
```

Arguments

`context`	The name of a valid context (character)

Value

A list of input item names for a context

Examples

```
# list of input items for the "study" context
context_inputs("study")
```

`context_outputs` *Valid outputs*

Description

Get a list of valid output_items for a context.

Usage

```
context_outputs(context)
```

Arguments

`context`	The name of a valid context (character)

Value

A list of output item names for a context

Examples

```
# list of output items for the "study" context
context_outputs("study")
```

`do_query` *Query the Metabolomics Workbench database*

Description

Sends a query to the metabolomics database and returns the result. Note that while objects derived from mw_base can be used the recommended approach is to use character inputs.

Usage

```
do_query(context, input_item, input_value, output_item)

## S4 method for signature 'character,character,character,character'
do_query(context, input_item, input_value, output_item)

## S4 method for signature 'mw_moverz_context,list,character,mw_output_item'
do_query(context, input_item, input_value, output_item)

## S4 method for signature 'mw_moverz_context,list,character,character'
do_query(context, input_item, input_value, output_item)

## S4 method for signature 'mw_moverz_context,list,character,missing'
do_query(context, input_item, input_value, output_item)

## S4 method for signature 'mw_moverz_context,character,character,missing'
do_query(context, input_item, input_value, output_item)

## S4 method for signature 'character,character,character,missing'
do_query(context, input_item, input_value, output_item)

## S4 method for signature 'mw_exactmass_context,list,character,mw_output_item'
do_query(context, input_item, input_value, output_item)

## S4 method for signature 'mw_exactmass_context,list,character,character'
do_query(context, input_item, input_value, output_item)

## S4 method for signature 'mw_exactmass_context,list,character,missing'
do_query(context, input_item, input_value, output_item)

## S4 method for signature 'mw_exactmass_context,character,character,missing'
do_query(context, input_item, input_value, output_item)

## S4 method for signature 'character,character,character,missing'
do_query(context, input_item, input_value, output_item)

## S4 method for signature 'mw_context,mw_input_item,character,mw_output_item'
do_query(context, input_item, input_value, output_item)

## S4 method for signature 'mw_context,mw_input_item,character,mw_SE_item'
do_query(context, input_item, input_value, output_item)
```

```
## S4 method for signature
## 'mw_context,mw_input_item,character,mw_untarg_SE_item'
do_query(context, input_item, input_value, output_item)

## S4 method for signature 'mw_context,mw_input_item,character,mw_DE_item'
do_query(context, input_item, input_value, output_item)

## S4 method for signature
## 'mw_context,mw_input_item,character,mw_untarg_DE_item'
do_query(context, input_item, input_value, output_item)

## S4 method for signature 'mw_context,mw_input_item,character,mw_MAE_item'
do_query(context, input_item, input_value, output_item)
```

Arguments

`context`	A valid context name (character)
`input_item`	A valid input_item name (character)
`input_value`	The value for the input item (character).
`output_item`	A valid output_item (character).

Value

A data.frame, or other output appropriate to the output_item.

Examples

```
# Get a summary of all studies with "diabetes" in the title

df = do_query(
  context = 'study',
  input_item = 'study_title',
  input_value = 'diabetes',
  output_item = 'summary'
)
```

`input_example` *Valid input_value for input_item*

Description

Displays a valid input_value for an input_item and returns an example that matches the required input pattern.

Usage

```
input_example(input_item)
```

Arguments

`input_item`	The name of a valid input_item (character)

Value

An example input value matching the pattern required for the chosen input item.

Examples

```
# example input_value for input item "study_id"
input_example('study_id')
```

`input_item` *Input items*

Description

A predefined list of mw_input_item objects. The items have been created to mirror the Metabolomics Workbench API documentation input items as closely as possible.

Usage

```
input_item
```

Format

An object of class `list` of length 41.

Examples

```
# list available input_items
names(input_item)

# get the input item 'study_id'
input_item$study_id
```

`is_valid` *Check validity of context and inputs/outputs*

Description

Compares the input and output items to the expected values for a context and returns TRUE if the inputs/puts are valid for the provided context or an error if not. This method is used internally and not for intended for general use.

Usage

```
is_valid(context, input_item, input_value, output_item)

## S4 method for signature 'mw_context,character,character,character'
is_valid(context, input_item, input_value, output_item)

## S4 method for signature 'mw_moverz_context,character,character,missing'
is_valid(context, input_item, input_value)

## S4 method for signature 'mw_exactmass_context,character,character,missing'
is_valid(context, input_item, input_value)
```

Arguments

`context`	An mw_context object.
`input_item`	An mw_input_item object, or the name of one.
`input_value`	The value for the input item (character).
`output_item`	An mw_output_item, or the name of one.

Value

TRUE or an error.

Examples

```
is_valid(context$study,
  input_item$study_id$name,
  'ST000001',
  output_item$summary$name
)
```

`metabolomicsWorkbenchR` *metabolomicsWorkbenchR*

Description

This package provides an interface to the Metabolomics Workbench API. It can be used to query the Metabolomics Workbench for study, compound, protein, gene information and more. All endpoints of the API are available via a simple `do_query` method. A number of convenience functions are included to import study data as `SummarizedExperiment` objects to facilitate use within R and the Bioconductor community.

Author(s)

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See Also

- `do_query` for a simple example.
- `browseVignettes("metabolomicsWorkbenchR")` for more info.
- Visit `https://www.metabolomicsworkbench.org/tools/mw_rest.php` for details of the API.

`output_item` *Output items*

Description

A predefined list of mw_output_item objects. The items have been created to mirror the Metabolomics Workbench API documentation output items as closely as possible.

Usage

```
output_item
```

Format

An object of class `list` of length 31.

Examples

```
# list available output_items
names(output_item)

# get the output item 'summary'
output_item$summary
```

`$,mw_base-method` *Get slot value from mw_base objects*

Description

Gets the value of a slot from mw_base objects, provided they are not listed as ’private’.

Usage

```
## S4 method for signature 'mw_base'
x$name
```

Arguments

`x`	An object derived from mw_base.
`name`	The name of the slot to access.

Value

The assigned to the slot.

Examples

```
# an object derived from mw_base object
C = context$study
# access the name slot
C$name
```

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