

# Package ‘metabolomicsWorkbenchR’

March 30, 2021

**Type** Package

**Title** Metabolomics Workbench in R

**Version** 1.0.0

**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.

**License** GPL-3

**Encoding** UTF-8

**RoxygenNote** 7.1.1

**Collate** 'parse\_fcns.R' 'generics.R' 'class\_def.R' 'constants.R'  
'metabolomicsWorkbenchR.R'

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

**Suggests** BiocStyle, covr, knitr, rmarkdown, testthat

**VignetteBuilder** knitr

**biocViews** Software, Metabolomics

**Depends** R (>= 4.0)

**git\_url** <https://git.bioconductor.org/packages/metabolomicsWorkbenchR>

**git\_branch** RELEASE\_3\_12

**git\_last\_commit** 7c8fe4c

**git\_last\_commit\_date** 2020-10-27

**Date/Publication** 2021-03-29

**Author** Gavin Rhys Lloyd [aut, cre],  
Ralf Johannes Maria Weber [aut]

**Maintainer** Gavin Rhys Lloyd <g.r.lloyd@bham.ac.uk>

## R topics documented:

check_pattern . . . . .	2
check_puts . . . . .	2
context . . . . .	3

do_query . . . . .	3
input_item . . . . .	5
is_valid . . . . .	6
metabolomicsWorkbenchR . . . . .	7
output_item . . . . .	7
\$.mw_base-method . . . . .	8

## Index 9

---

check_pattern	<i>Check input against acceptable input pattern</i>
---------------	---

---

### 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	<i>Check inputs/outputs match</i>
------------	-----------------------------------

---

### 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	<i>Contexts</i>
---------	-----------------

---

**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
```

---

do_query	<i>Query the Metabolomics Workbench database</i>
----------	--

---

**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_item	<i>Input items</i>
------------	--------------------

---

### 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	<i>Check validity of context and inputs/outputs</i>
----------	---

---

### 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.

## See Also

- `do_query` for a simple example.
- `browseVignettes("metabolomicsWorkbenchR")` for more info.
- Visit [https://www.metabolomicsworkbench.org/tools/mw\\_rest.php](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
```



# Index

## \* datasets

context, 3  
input\_item, 5  
output\_item, 7  
\$, mw\_base-method, 8

check\_pattern, 2  
check\_pattern, mw\_input\_item-method  
(check\_pattern), 2  
check\_puts, 2  
check\_puts, mw\_input\_item-method  
(check\_puts), 2  
context, 3

do\_query, 3, 7  
do\_query, character, character, character, character-method  
(do\_query), 3  
do\_query, character, character, character, missing-method  
(do\_query), 3  
do\_query, mw\_context, mw\_input\_item, character, mw\_DE\_item-method  
(do\_query), 3  
do\_query, mw\_context, mw\_input\_item, character, mw\_MAE\_item-method  
(do\_query), 3  
do\_query, mw\_context, mw\_input\_item, character, mw\_output\_item-method  
(do\_query), 3  
do\_query, mw\_context, mw\_input\_item, character, mw\_SE\_item-method  
(do\_query), 3  
do\_query, mw\_context, mw\_input\_item, character, mw\_untarg\_DE\_item-method  
(do\_query), 3  
do\_query, mw\_context, mw\_input\_item, character, mw\_untarg\_SE\_item-method  
(do\_query), 3  
do\_query, mw\_exactmass\_context, character, character, missing-method  
(do\_query), 3  
do\_query, mw\_exactmass\_context, list, character, character-method  
(do\_query), 3  
do\_query, mw\_exactmass\_context, list, character, missing-method  
(do\_query), 3  
do\_query, mw\_exactmass\_context, list, character, mw\_output\_item-method  
(do\_query), 3  
do\_query, mw\_moverz\_context, character, character, missing-method  
(do\_query), 3  
do\_query, mw\_moverz\_context, list, character, character-method  
(do\_query), 3

do\_query, mw\_moverz\_context, list, character, missing-method  
(do\_query), 3  
do\_query, mw\_moverz\_context, list, character, mw\_output\_item-method  
(do\_query), 3

input\_item, 5  
is\_valid, 6  
is\_valid, mw\_context, character, character, character-method  
(is\_valid), 6  
is\_valid, mw\_exactmass\_context, character, character, missing-method  
(is\_valid), 6  
is\_valid, mw\_moverz\_context, character, character, missing-method  
(is\_valid), 6

metabolomicsWorkbenchR, 7

output\_item, 7