

Package ‘rmzqc’

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Title Creation, Reading and Validation of 'mzqc' Files

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Description Reads, writes and validates 'mzQC' files. The 'mzQC' format is a standardized file format for the exchange, transmission, and archiving of quality metrics derived from biological mass spectrometry data, as defined by the HUPO-PSI (Human Proteome Organisation - Proteomics Standards Initiative) Quality Control working group.
See <<https://hupo-psi.github.io/mzQC/>> for details.

Imports jsonlite, jsonvalidate, knitr, methods, ontologyIndex,
rmarkdown, R6, R6P, testthat, tools

VignetteBuilder knitr

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URL <https://github.com/MS-Quality-hub/rmzqc>

BugReports <https://github.com/MS-Quality-hub/rmzqc/issues>

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Author Chris Bielow [aut, cre] (ORCID:
<<https://orcid.org/0000-0001-5756-3988>>),
David Jimenez-Morales [rev, ctb] (ORCID:
<<https://orcid.org/0000-0003-4356-6461>>),
Jeremi Maciejewski [ctb]

Maintainer Chris Bielow <chris.bielow@bsc.fu-berlin.de>

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check_type	<i>Checks the value's class type, which should match at least of the types given in any_expected_class_types.</i>
------------	---

Description

Checks the value's class type, which should match at least of the types given in any_expected_class_types.

Usage

check_type(value, any_expected_class_types, expected_length = 0)

Arguments

- value A certain value (e.g. a single value, data.frame etc)
- any_expected_class_types A vector of valid class types, any of which the @p value should have
- expected_length The expected length of value (usually to check if its a single value); 0 (default) indicates that length can be ignored

Examples

```
check_type(1, "numeric", 1) # TRUE
check_type("1", "numeric", 1) # FALSE
check_type(1, "numeric", 2) # FALSE
check_type("ABC", "character", 1) # TRUE
check_type("ABC", "character") # TRUE
check_type("ABC", "character", 2) # FALSE
check_type(c("ABC", "DEF"), "character", 2) # TRUE
check_type(1.1, c("numeric", "double")) # TRUE
check_type(1.1, c("numeric", "double"), 1) # TRUE
check_type(matrix(1:9, nrow=3), "matrix") # TRUE
check_type(data.frame(a=1:3, b=4:6), c("something", "data.frame")) # TRUE
```

CV_	CV_
-----	-----

Description

Define a Singleton class which can hold a CV dictionary (so we do not have to load the .obo files over and over again)

Details

Get the full data by calling the 'getData()' function (which returns a list containing a 'CV', 'URI' and 'version'), or 'getCV()' which is a shorthand for 'getData()\$CV'. You can set your own custom CV by calling 'setData()'. By default, the latest release of the PSI-MS-CV (see [getCVDictionary](#)). Wherever you need this data, simply re-grab the singleton using 'CV_\$new()' (or use the convenience function getCVSingleton() from outside the package)

Super class

```
R6P::Singleton -> CV_
```

Methods

Public methods:

- [CV_\\$ensureHasData\(\)](#)
- [CV_\\$byID\(\)](#)
- [CV_\\$setData\(\)](#)
- [CV_\\$getData\(\)](#)
- [CV_\\$getCV\(\)](#)

Method ensureHasData(): Make sure that the CV data is loaded

Usage:

```
CV_$ensureHasData()
```

Method byID(): A function to retrieve a CV entry using its ID

Usage:

```
CV_$byID(id)
```

Arguments:

id A CV accession, e.g. 'MS:1000560'

Returns: A CV term, or NULL if the ID is unknown

Method setData(): Set a user-defined object (= a list of 'CV', 'URI' and 'version'), as obtained from [getCVDictionary](#)

Usage:

```
CV_$setData(cv_data)
```

Arguments:

cv_data The result of a call to [getCVDictionary](#)

Method getData(): Gets the underlying data (CV, URI and version)

Usage:

```
CV_$getData()
```

Method getCV(): A shorthand for 'getData()\$CV', i.e. the CV data.frame.

Usage:

```
CV_$getCV()
```

Examples

```
## Not run:
cv_dict = CV$new() ## uses 'getCVDictionary()' to populate the singleton
cv_2 = CV$new() ## uses the same data without parsing again
cv_2$setData(getCVDictionary("custom", "https://my.com/custom.obo"))

## End(Not run)
```

filenameToCV	<i>For a given filename (e.g. "test.mzML"), check the suffix and translate it to an PSI-MS CV term, e.g. 'MS:1000584'</i>
--------------	---

Description

The following mapping is currently known: .raw : MS:1000563 ! Thermo RAW format .mzML : MS:1000584 ! mzML format .mzData : MS:1000564 ! PSI mzData format .wiff : MS:1000562 ! ABI WIFF format .pkl : MS:1000565 ! Micromass PKL format .mzXML : MS:1000566 ! ISB mzXML format .yep : MS:1000567 ! Bruker/Agilent YEP format .dta : MS:1000613 ! Sequest DTA format .mzMLb : MS:1002838 ! mzMLb format

Usage

```
filenameToCV(filepath)
```

Arguments

filepath A filename (with optional path)

Details

Falls back to 'MS:1000560 ! mass spectrometer file format' if no match could be found.

Upper/lowercase is ignored, i.e. "mzML == mzml".

Value

A CV term accession as string, e.g. 'MS:1000584'

Examples

```
filenameToCV("test.mzML") # MS:1000584
filenameToCV("test.raw") # MS:1000563
filenameToCV(c("test.raw", "bla.mzML"))
```

fromDatatoMzQC	<i>Allow conversion of plain named lists of R objects (from JSON) to mzQC objects</i>
----------------	---

Description

Allow conversion of plain named lists of R objects (from JSON) to mzQC objects

Usage

```
fromDatatoMzQC(mzqc_class, data, context = NULL)
```

Arguments

mzqc_class	Prototype of the class to convert 'data' into
data	A list of: A datastructure of R lists/arrays as obtained by 'jsonlite::fromJSON()'
context	A trace through the mzQC object tree to aid users in case of errors

Examples

```
data = rmzqc::MzQCcvParameter$new("acc", "myName", "value")
data_recovered = rmzqc::fromDatatoMzQC(rmzqc::MzQCcvParameter,
  list(jsonlite::fromJSON(jsonlite::toJSON(data))))
```

fromDatatoMzQCobj	<i>Allow conversion of a plain R object (obtained from JSON) to an mzQC object</i>
-------------------	--

Description

If you have a list of elements, call fromDatatoMzQC.

Usage

```
fromDatatoMzQCobj(mzqc_class, data, context = NULL)
```

Arguments

mzqc_class	Prototype of the class to convert 'data' into
data	A datastructure of R lists/arrays as obtained by 'jsonlite::fromJSON()'
context	A trace through the mzQC object tree to aid users in case of errors

Examples

```
data = MzQCcvParameter$new("acc", "myName", "value")
data_recovered = fromDatatoMzQCobj(MzQCcvParameter, jsonlite::fromJSON(jsonlite::toJSON(data)))
data_recovered
```

getCVDictionary	<i>Fetch and parse the 'psi-ms.obo' and some metadata from the usual sources to use as ontology.</i>
-----------------	--

Description

If `use_local_fallback` is `TRUE`, this function will never fail. Otherwise, it may fail if the internet connection is flawed or internal URLs related to GitHubs API become stale.

Usage

```
getCVDictionary(
  source = c("latest", "local", "custom"),
  custom_uri = NULL,
  use_local_fallback = TRUE
)
```

Arguments

<code>source</code>	Where to get the PSI-MS CV from: - 'latest' will download 'psi-ms.obo' from https://api.github.com/repos/HUPO-PSI/psi-ms-CV/releases/latest - 'local' will use <code>rmzqc/cv/psi-ms.obo</code> (which might be outdated, if you need the latest terms) - 'custom' uses a user-defined URI in <code>custom_uri</code>
<code>custom_uri</code>	Used when 'source' is set to 'custom'. The URI can be local or remote, e.g. <code>'c:/obo/my.obo'</code> or <code>'https://www.abc.com/my.obo'</code>
<code>use_local_fallback</code>	When downloading a file from a URI fails, should we fall back to the local <code>psi-ms.obo</code> shipped with <code>rmzqc</code> ?

Details

A `'pato.obo'`, and `'uo.obo'` from the `'rmzqc/cv/'` folder are automatically merged into the result. See `CV_` class to use this function efficiently.

Value

A list with `'CV'`, `'URI'` and `'version'`, where `'CV'` is a `data.frame` with columns `'id'`, `'name'`, `'def'`, `'parents'`, `'children'` (and many more) which contains the CV entries

getCVInfo	Returns an MzQCcontrolledVocabulary for the currently used CV (see getCVSingleton) using <code>getCVSingleton()\$getData()\$URI</code> and <code>\$version</code> .
-----------	--

Description

Returns an [MzQCcontrolledVocabulary](#) for the currently used CV (see [getCVSingleton](#)) using `getCVSingleton()$getData()$URI` and `$version`.

Usage

```
getCVInfo()
```

getCVSingleton	Returns the CV singleton. See CV_ .
----------------	---

Description

Returns the CV singleton. See [CV_](#).

Usage

```
getCVSingleton()
```

getCVTemplate	Fills a MzQCcvParameter object with <code>id(accession)</code> and <code>name</code> . The value (if any) needs to be set afterwards.
---------------	---

Description

Fills a [MzQCcvParameter](#) object with `id(accession)` and `name`. The value (if any) needs to be set afterwards.

Usage

```
getCVTemplate(accession, CV = getCVSingleton())
```

Arguments

<code>accession</code>	The ID (=accession) of the term in the CV
<code>CV</code>	A CV dictionary, as obtained by <code>getCVDictionary()</code> ; defaults to the global singleton, which is populated automatically

Value

An instance of [MzQCcvParameter](#)

getDefaultCV	Returns an MzQCcontrolledVocabulary for the currently used CV (see getCVSingleton)
--------------	---

Description

Returns an MzQCcontrolledVocabulary for the currently used CV (see [getCVSingleton](#))

Usage

```
getDefaultCV()
```

Note

This function will be deprecated soon. Use [getCVInfo](#) instead.

getLatest_PSICV_URL	Get the latest PSI-MS CV release URL
---------------------	--------------------------------------

Description

This may fail (e.g. if no internet connection is available, or URLs became invalid) then 'NULL' will be returned instead of an URL. A warning may be emitted, if the URL is out of date (i.e. the GitHub API changed).

Usage

```
getLatest_PSICV_URL()
```

getLocal_CV_Version	Obtains the 'data-version' from a local (i.e. non-url) PSI-MS-CV
---------------------	--

Description

Obtains the 'data-version' from a local (i.e. non-url) PSI-MS-CV

Usage

```
getLocal_CV_Version(local_PSIMS_obo_file)
```

Arguments

local_PSIMS_obo_file

A path to a local file, e.g. 'c:/temp/my.obo'

Examples

```
getLocal_CV_Version(system.file("./cv/psi-ms.obo", package="rmzqc")) # "4.1.95"
```

```
getQualityMetricTemplate
```

Fills a MzQCqualityMetric object with id(accession) and name. The value (if any) and unit (if any) need to be set afterwards.

Description

The accession must be valid (or allow_unknown_id must be TRUE)

Usage

```
getQualityMetricTemplate(
  accession,
  CV = getCVSingleton(),
  allow_unknown_id = FALSE
)
```

Arguments

accession	The ID (=accession) of the term in the CV
CV	A CV dictionary, as obtained by getCVDictionary(); defaults to the global singleton, which is populated automatically
allow_unknown_id	Allows invalid accession; if 'FALSE' this function errors if accession is unknown

Value

An instance of MzQCqualityMetric

```
getSyntaxValidator      Get a syntax validator for mzQC
```

Description

Get a syntax validator for mzQC

Usage

```
getSyntaxValidator()
```

hasFileSuffix	<i>Checks if filepath ends in suffix (ignoring lower/upper case differences). If suffix does not start with a '.' it is prepended automatically.</i>
---------------	--

Description

Checks if filepath ends in suffix (ignoring lower/upper case differences). If suffix does not start with a '.' it is prepended automatically.

Usage

```
hasFileSuffix(filepath, suffix)
```

Arguments

filepath	A relative or absolute path to a file, whose suffix is checked
suffix	This is the suffix we expect (the '.' is prepended internally if missing)

Value

TRUE if yes, FALSE otherwise

Examples

```
hasFileSuffix("bla.txt", "txt") # TRUE
hasFileSuffix("bla.txt", ".txt") # TRUE
hasFileSuffix("bla.txt", ".TXT") # TRUE
hasFileSuffix("foo", "") # TRUE
hasFileSuffix("", "") # TRUE
hasFileSuffix("bla.txt", "doc") # FALSE
hasFileSuffix("bla.txt", ".doc") # FALSE
hasFileSuffix("fo", ".doc") # FALSE
hasFileSuffix("", ".doc") # FALSE
```

isUndefined	<i>Tell if a variable's value is undefined (NA or NULL); If yes, and it is required by the mzQC standard, we can raise an error.</i>
-------------	--

Description

You can pass multiple variable, which are all checked. If **any** of them is undefined, the function returns TRUE

Usage

```
isUndefined(s, ..., verbose = TRUE, context = NULL)
```

Arguments

s	A variable to be checked for NA/NULL
...	More variable to be checked
verbose	If TRUE and 's' is NULL/NA, will print the name of the variable which was passed in
context	An optional string will be using within a warning message, to ease tracking of where in the mzQC structure the undefined value occurs

Examples

```

isUndefined(NA)      ## TRUE
isUndefined(NULL)    ## TRUE
isUndefined(NA, NULL) ## TRUE
isUndefined("")      ## FALSE
isUndefined(list(1,2,3)) ## FALSE
isUndefined("", NA)  ## TRUE
isUndefined(NA, "")  ## TRUE
isUndefined(1)       ## FALSE
myVar = NA
isUndefined(myVar)    ## TRUE, with warning "Variable 'myVar' is NA/NULL!"

```

isValidMzQC	<i>Checks validity (= completeness) of mzQC objects - or lists (JSON arrays) thereof</i>
-------------	--

Description

Note: Returns TRUE for empty lists!

Usage

```
isValidMzQC(x, parent_context = NULL)
```

Arguments

x	An mzQC R6 class (or list of them), which will be subjected to validation
parent_context	Internal parameter used to track the path in nested validations

Details

This function checks if an mzQC object or a list of mzQC objects is valid. For lists, all elements need to be valid for the function to return TRUE. The function provides detailed error messages that include the path to the invalid field, making it easier to identify validation issues in complex nested structures.

Examples

```

isValidMzQC(MzQCcvParameter$new("MS:4000059"))          # FALSE
isValidMzQC(MzQCcvParameter$new("MS:4000059", "Number of MS1 spectra")) # TRUE
isValidMzQC(list(MzQCcvParameter$new("MS:4000059")))    # FALSE
isValidMzQC(list(MzQCcvParameter$new("MS:4000059", "Number of MS1 spectra"))) # TRUE

```

localFileToURI	<i>Convert a local filename, e.g. <code>"/myData/test.mzML"</code> to a proper URI (e.g. <code>"file:///user/bielow/myData/test.mzML"</code>)</i>
----------------	---

Description

Relative filenames are made absolute. Backslashes as path separators are replaced by forward slashes (as commonly seen on Windows).

Usage

```
localFileToURI(local_filename, must_exist = TRUE)
```

Arguments

local_filename Path to a file (can be relative to current getwd(); or absolute)
 must_exist Require the file to exist

Value

A URI starting with "file://" followed by an absolute path

MzQCanalysisSoftware	<i>Details of the software used to create the QC metrics</i>
----------------------	--

Description

Details of the software used to create the QC metrics
 Details of the software used to create the QC metrics

Public fields

accession Accession number identifying the term within its controlled vocabulary.
 name Name of the controlled vocabulary term describing the software tool.
 version Version number of the software tool.
 uri Publicly accessible URI of the software tool or documentation.
 description (optional) Definition of the controlled vocabulary term.
 value (optional) Name of the software tool.

Methods

Public methods:

- [MzQCanalysisSoftware\\$new\(\)](#)
- [MzQCanalysisSoftware\\$isValid\(\)](#)
- [MzQCanalysisSoftware\\$toJSON\(\)](#)
- [MzQCanalysisSoftware\\$fromData\(\)](#)
- [MzQCanalysisSoftware\\$clone\(\)](#)

Method `new()`: Constructor

Usage:

```
MzQCanalysisSoftware$new(
  accession = NA_character_,
  name = NA_character_,
  version = NA_character_,
  uri = NA_character_,
  description = NA_character_,
  value = NA_character_
)
```

Arguments:

accession String value for initialization of field accession
 name String value for initialization of field name
 version String value for initialization of field version
 uri Optional string value for initialization of field uri
 description Optional string value for initialization of field description
 value Optional string value for initialization of field value

Method `isValid()`: Verifies validity of the object

Usage:

```
MzQCanalysisSoftware$isValid(context = "MzQCanalysisSoftware")
```

Arguments:

context Optional string describing location in mzQC structure that is used for more informative warning texts.

Method `toJSON()`: Creates JSON file from this object.

Usage:

```
MzQCanalysisSoftware$toJSON(...)
```

Arguments:

... Optional parameters for `jsonlite::asJSON()`

Method `fromData()`: Sets data for this object from plain named lists of R objects

Usage:

```
MzQCanalysisSoftware$fromData(data, context = "MzQCanalysisSoftware")
```

Arguments:

data A datastructure of R lists/arrays as obtained by 'jsonlite::fromJSON()'
context Optional string describing location in mzQC structure that is used for more informative warning texts.

Method clone(): The objects of this class are cloneable with this method.

Usage:

MzQCanalysisSoftware\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

MzQCbaseQuality

Base class of runQuality/setQuality

Description

Base class of runQuality/setQuality

Base class of runQuality/setQuality

Public fields

metadata The metadata for this run/setQuality

qualityMetrics Array of MzQCqualityMetric objects

Methods

Public methods:

- `MzQCbaseQuality$new()`
- `MzQCbaseQuality$isValid()`
- `MzQCbaseQuality$getMetric()`
- `MzQCbaseQuality$toJSON()`
- `MzQCbaseQuality$fromData()`
- `MzQCbaseQuality$clone()`

Method new(): Constructor

Usage:

MzQCbaseQuality\$new(metadata = MzQCmetadata\$new(), qualityMetrics = list())

Arguments:

metadata Optional MzQCmetadata value for initialization of field metadata

qualityMetrics Optional list value for initialization of field qualityMetrics

Method isValid(): Verifies validity of the object

Usage:

MzQCbaseQuality\$isValid(context = "MzQCbaseQuality")

Arguments:

context Optional string describing location in mzQC structure that is used for more informative warning texts.

Method getMetric(): Fetches metrics which match specified accession or name from the object.

Usage:

```
MzQCbaseQuality$getMetric(accession = NULL, name = NULL)
```

Arguments:

accession Search by accession
name Search by name

Method toJSON(): Creates JSON file from this object.

Usage:

```
MzQCbaseQuality$toJSON(...)
```

Arguments:

... Optional parameters for jsonlite::asJSON()

Method fromData(): Sets data for this object from plain named lists of R objects

Usage:

```
MzQCbaseQuality$fromData(mdata, context = "MzQCbaseQuality")
```

Arguments:

mdata A datastructure of R lists/arrays as obtained by 'jsonlite::fromJSON()'
context Optional string describing location in mzQC structure that is used for more informative warning texts.

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
MzQCbaseQuality$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

MzQCbaseQuality_getMetric

Extract a certain metric from a runQuality's list of MzQCqualityMetric

Description

You must provide either the accession or the name of the metric, but not both.

Arguments

accession	Accession of the MzQCqualityMetric
name	Name of the MzQCqualityMetric (less stable than accession)

Details

Usually there should be only one MzQCqualityMetric which matches, however, this function will return all matches.

Note: this function will stop() if not results are found

Value

A list of MzQCqualityMetric's which match.

MzQCcontrolledVocabulary

A controlled vocabulary document, usually pointing to an .obo file

Description

A controlled vocabulary document, usually pointing to an .obo file

A controlled vocabulary document, usually pointing to an .obo file

Public fields

name Full name of the controlled vocabulary.

uri Publicly accessible URI of the controlled vocabulary.

version (optional) Version of the controlled vocabulary.

Methods**Public methods:**

- `MzQCcontrolledVocabulary$new()`
- `MzQCcontrolledVocabulary$isValid()`
- `MzQCcontrolledVocabulary$toJSON()`
- `MzQCcontrolledVocabulary$fromData()`
- `MzQCcontrolledVocabulary$clone()`

Method new(): Constructor

Usage:

```
MzQCcontrolledVocabulary$new(  
  name = NA_character_,  
  uri = NA_character_,  
  version = NA_character_  
)
```

Arguments:

name String value for initialization of field name

uri String value for initialization of field uri

version Optional string value for initialization of field version

Method isValid(): Verifies validity of the object

Usage:

```
MzQCcontrolledVocabulary$isValid(context = "MzQCcontrolledVocabulary")
```

Arguments:

context Optional string describing location in mzQC structure that is used for more informative warning texts.

Method toJSON(): Creates JSON file from this object.

Usage:

```
MzQCcontrolledVocabulary$toJSON(...)
```

Arguments:

... Optional parameters for jsonlite::asJSON()

Method fromData(): Sets data for this object from plain named lists of R objects

Usage:

```
MzQCcontrolledVocabulary$fromData(data, context = "MzQCcontrolledVocabulary")
```

Arguments:

data A datastructure of R lists/arrays as obtained by 'jsonlite::fromJSON()'

context Optional string describing location in mzQC structure that is used for more informative warning texts.

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
MzQCcontrolledVocabulary$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```
MzQCcontrolledVocabulary$new(
  "Proteomics Standards Initiative Quality Control Ontology",
  "https://github.com/HUPO-PSI/psi-ms-CV/releases/download/v4.1.129/psi-ms.obo",
  "4.1.129")
```

MzQCcvParameter	<i>A controlled vocabulary parameter, as detailed in the OBO file</i>
-----------------	---

Description

A controlled vocabulary parameter, as detailed in the OBO file

A controlled vocabulary parameter, as detailed in the OBO file

Public fields

accession Accession number identifying the term within its controlled vocabulary.

name Name of the controlled vocabulary term describing the parameter.

value (optional) Value of the parameter.

description (optional) Definition of the controlled vocabulary term.

Methods

Public methods:

- [MzQCcvParameter\\$new\(\)](#)
- [MzQCcvParameter\\$isValid\(\)](#)
- [MzQCcvParameter\\$toJSON\(\)](#)
- [MzQCcvParameter\\$fromData\(\)](#)
- [MzQCcvParameter\\$clone\(\)](#)

Method new(): Constructor

Usage:

```
MzQCcvParameter$new(  
  accession = NA_character_,  
  name = NA_character_,  
  value = NA,  
  description = NA_character_  
)
```

Arguments:

accession String value for initialization of field accession

name String value for initialization of field name

value Optional value for initialization of field value

description Optional string value for initialization of field description

Method isValid(): Verifies validity of the object

Usage:

```
MzQCcvParameter$isValid(context = "MzQCcvParameter")
```

Arguments:

context Optional string describing location in mzQC structure that is used for more informative warning texts.

Method toJSON(): Creates JSON file from this object.

Usage:

```
MzQCcvParameter$toJSON(...)
```

Arguments:

... Optional parameters for jsonlite::asJSON()

Method fromData(): Sets data for this object from plain named lists of R objects

Usage:

```
MzQCcvParameter$fromData(data, context = "MzQCcvParameter")
```

Arguments:

data A datastructure of R lists/arrays as obtained by 'jsonlite::fromJSON()'

context Optional string describing location in mzQC structure that is used for more informative warning texts.

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
MzQCcvParameter$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```
MzQCcvParameter$new("MS:4000070",
                    "retention time acquisition range",
                    c(0.2959, 5969.8172))
isValidMzQC(MzQCcvParameter$new("MS:0000000"))
```

MzQCDateTime

An mzQC-formatted date+time in ISO8601 format, as required by the mzQC spec doc.

Description

An mzQC-formatted date+time in ISO8601 format, as required by the mzQC spec doc.

An mzQC-formatted date+time in ISO8601 format, as required by the mzQC spec doc.

Details

The format is "%Y-%m-%dT%H:%M:%S".

Public fields

`datetime` A correctly formatted date time (use as read-only)

Methods**Public methods:**

- `MzQCDateTime$new()`
- `MzQCDateTime$set()`
- `MzQCDateTime$isValid()`
- `MzQCDateTime$toJSON()`
- `MzQCDateTime$fromData()`
- `MzQCDateTime$clone()`

Method `new()`: Constructor

Usage:

```
MzQCDateTime$new(date = as.character(Sys.time()))
```

Arguments:

`date` Optional POSIXct value for initialization of field `datetime`. Defaults to `Sys.time()`

Method `set()`: Sets `datetime` value

Usage:

```
MzQCDateTime$set(date)
```

Arguments:

`date` New date-time

Method `isValid()`: Verifies validity of the object

Usage:

```
MzQCDateTime$isValid(context = "MzQCDateTime")
```

Arguments:

`context` Optional string describing location in `mzQC` structure that is used for more informative warning texts.

Method `toJSON()`: Creates JSON file from this object.

Usage:

```
MzQCDateTime$toJSON(...)
```

Arguments:

`...` Optional parameters for `jsonlite::asJSON()`

Method `fromData()`: Sets data for this object from plain named lists of R objects

Usage:

```
MzQCDateTime$fromData(data, context = "MzQCDateTime")
```

Arguments:

`data` A datastructure of R lists/arrays as obtained by `'jsonlite::fromJSON()'`

context Optional string describing location in mzQC structure that is used for more informative warning texts.

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
MzQCDateTime$new(clone(deep = FALSE))
```

Arguments:

deep Whether to make a deep clone.

Examples

```
dt1 = MzQCDateTime$new("1900-01-01") ## yields "1900-01-01T00:00:00Z"
dt2 = MzQCDateTime$new(Sys.time())
## test faulty input
## errors with 'character string is not in a standard unambiguous format'
try(MzQCDateTime$new('lala'), silent=TRUE)
## test roundtrip conversion from/to JSON
dt2$fromData(jsonlite::fromJSON(jsonlite::toJSON(dt1)))
```

MzQCinputFile

An inputfile within metadata for a run/setQuality

Description

An inputfile within metadata for a run/setQuality

An inputfile within metadata for a run/setQuality

Public fields

name The name MUST uniquely match to a location (specified below) listed in the mzQC file.

location Unique file location, REQUIRED to be specified as a URI. The file URI is RECOMMENDED to be publicly accessible.

fileFormat An MzQCcvParameter with 'accession' and 'name'.

fileProperties An array of MzQCcvParameter, usually with 'accession', 'name' and 'value'. Recommended are at least two entries: a) Completion time of the input file (MS:1000747) and b) Checksum of the input file (any child of: MS:1000561 ! data file checksum type).

Methods

Public methods:

- `MzQCinputFile$new()`
- `MzQCinputFile$isValid()`
- `MzQCinputFile$toJSON()`
- `MzQCinputFile$fromData()`

- `MzQCinputFile$clone()`

Method `new()`: Constructor

Usage:

```
MzQCinputFile$new(  
  name = NA_character_,  
  location = NA_character_,  
  fileFormat = MzQCcvParameter$new(),  
  fileProperties = list()  
)
```

Arguments:

name String value for initialization of field name

location String value for initialization of field location

fileFormat Optional MzQCcvParameter value for initialization of field fileFormat

fileProperties Optional list value for initialization of field fileProperties

Method `isValid()`: Verifies validity of the object

Usage:

```
MzQCinputFile$isValid(context = "MzQCinputFile")
```

Arguments:

context Optional string describing location in mzQC structure that is used for more informative warning texts.

Method `toJSON()`: Creates JSON file from this object.

Usage:

```
MzQCinputFile$toJSON(...)
```

Arguments:

... Optional parameters for `jsonlite::asJSON()`

Method `fromData()`: Sets data for this object from plain named lists of R objects

Usage:

```
MzQCinputFile$fromData(data, context = "MzQCinputFile")
```

Arguments:

data A datastructure of R lists/arrays as obtained by `'jsonlite::fromJSON()'`

context Optional string describing location in mzQC structure that is used for more informative warning texts.

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
MzQCinputFile$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

MzQCmetadata

*The metadata for a run/setQuality***Description**

The metadata for a run/setQuality

The metadata for a run/setQuality

Public fields

label Unique name for the run (for runQuality) or set (for setQuality).

inputFiles Array/list of MzQCinputFile objects

analysisSoftware Array/list of MzQCanalysisSoftware objects

cvParameters (optional) Array of cvParameters objects

Methods**Public methods:**

- [MzQCmetadata\\$new\(\)](#)
- [MzQCmetadata\\$isValid\(\)](#)
- [MzQCmetadata\\$toJSON\(\)](#)
- [MzQCmetadata\\$fromData\(\)](#)
- [MzQCmetadata\\$clone\(\)](#)

Method new(): Constructor

Usage:

```
MzQCmetadata$new(
  label = NA_character_,
  inputFiles = list(),
  analysisSoftware = list(),
  cvParameters = list()
)
```

Arguments:

label String value for initialization of field label

inputFiles Optional list value for initialization of field inputFiles

analysisSoftware Optional list value for initialization of field analysisSoftware

cvParameters Optional list value for initialization of field cvParameters

Method isValid(): Verifies validity of the object

Usage:

```
MzQCmetadata$isValid(context = "MzQCmetadata")
```

Arguments:

context Optional string describing location in mzQC structure that is used for more informative warning texts.

Method toJSON(): Creates JSON file from this object.

Usage:

MzQCmetadata\$.toJSON(...)

Arguments:

... Optional parameters for jsonlite::asJSON()

Method fromData(): Sets data for this object from plain named lists of R objects

Usage:

MzQCmetadata\$.fromData(data, context = "MzQCmetadata")

Arguments:

data A datastructure of R lists/arrays as obtained by 'jsonlite::fromJSON()'

context Optional string describing location in mzQC structure that is used for more informative warning texts.

Method clone(): The objects of this class are cloneable with this method.

Usage:

MzQCmetadata\$.clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

MzQCmzQC

Root element of an mzQC document

Description

Root element of an mzQC document

Root element of an mzQC document

Details

At least one of runQualities or setQualities MUST be present.

Public fields

version Version of the mzQC format.

creationDate Creation date of the mzQC file.

contactName Name of the operator/creator of this mzQC file.

contactAddress Contact address (mail/e-mail or phone)

description Description and comments about the mzQC file contents.

runQualities Array of MzQCrunQuality;

setQualities Array of MzQCsetQuality

controlledVocabularies Array of CV domains used (obo files)

Methods

Public methods:

- [MzQCmzQC\\$new\(\)](#)
- [MzQCmzQC\\$isValid\(\)](#)
- [MzQCmzQC\\$toJSON\(\)](#)
- [MzQCmzQC\\$fromData\(\)](#)
- [MzQCmzQC\\$clone\(\)](#)

Method `new()`: Constructor

Usage:

```
MzQCmzQC$new(
  version = NA_character_,
  creationDate = MzQCDateTime$new(),
  contactName = NA_character_,
  contactAddress = NA_character_,
  description = NA_character_,
  runQualities = list(),
  setQualities = list(),
  controlledVocabularies = list()
)
```

Arguments:

version String value for initialization of field version
 creationDate MzQCDateTime value for initialization of field creationDate
 contactName Optional string value for initialization of field contactName
 contactAddress Optional string value for initialization of field contactAddress
 description Optional string value for initialization of field description
 runQualities Optional list value for initialization of field runQualities
 setQualities Optional list value for initialization of field setQualities
 controlledVocabularies Optional list value for initialization of field controlledVocabularies

Method `isValid()`: Verifies validity of the object

Usage:

```
MzQCmzQC$isValid(context = "MzQCmzQC")
```

Arguments:

context Optional string describing location in mzQC structure that is used for more informative warning texts.

Method `toJSON()`: Creates JSON file from this object.

Usage:

```
MzQCmzQC$toJSON(...)
```

Arguments:

... Optional parameters for `jsonlite::asJSON()`

Method `fromData()`: Sets data for this object from plain named lists of R objects

Usage:

```
MzQCmzQC$fromData(data, context = "MzQCmzQC")
```

Arguments:

data A datastructure of R lists/arrays as obtained by 'jsonlite::fromJSON()'

context Optional string describing location in mzQC structure that is used for more informative warning texts.

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
MzQCmzQC$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

MzQCQualityMetric	<i>The central class to store QC information</i>
-------------------	--

Description

The central class to store QC information

The central class to store QC information

Public fields

accession Accession number identifying the term within its controlled vocabulary.

name Name of the controlled vocabulary element describing the metric.

description (optional) Definition of the controlled vocabulary term.

value (optional) Value of the metric (single value, n-tuple, table, matrix). The structure is not checked by our mzQC implementation and must be handled by the caller, see [toQCMetric](#).

unit (optional) Array of unit(s), stored as MzQcvParameter

Methods**Public methods:**

- [MzQCQualityMetric\\$new\(\)](#)
- [MzQCQualityMetric\\$isValid\(\)](#)
- [MzQCQualityMetric\\$toJSON\(\)](#)
- [MzQCQualityMetric\\$fromData\(\)](#)
- [MzQCQualityMetric\\$clone\(\)](#)

Method `new()`: Constructor

Usage:

```
MzQCqualityMetric$new(
  accession = NA_character_,
  name = NA_character_,
  description = NA_character_,
  value = NA,
  unit = list()
)
```

Arguments:

accession String value for initialization of field accession

name String value for initialization of field name

description Optional string value for initialization of field description

value Optional value for initialization of field value

unit Optional unit value for initialization of field unit

Method isValid(): Verifies validity of the object

Usage:

```
MzQCqualityMetric$isValid(context = "MzQCqualityMetric")
```

Arguments:

context Optional string describing location in mzQC structure that is used for more informative warning texts.

Method toJSON(): Creates JSON file from this object.

Usage:

```
MzQCqualityMetric$toJSON(...)
```

Arguments:

... Optional parameters for jsonlite::asJSON()

Method fromData(): Sets data for this object from plain named lists of R objects

Usage:

```
MzQCqualityMetric$fromData(data, context = "MzQCqualityMetric")
```

Arguments:

data A datastructure of R lists/arrays as obtained by 'jsonlite::fromJSON()'

context Optional string describing location in mzQC structure that is used for more informative warning texts.

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
MzQCqualityMetric$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

MzQCrunQuality	<i>A runQuality object. Use to report metrics for individual runs which are independent of other runs.</i>
----------------	--

Description

The object is an alias for MzQCbaseQuality.

Super class

```
rmzqc:MzQCbaseQuality -> MzQCrunQuality
```

Methods**Public methods:**

- `MzQCrunQuality$clone()`

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
MzQCrunQuality$clone(deep = FALSE)
```

Arguments:

`deep` Whether to make a deep clone.

MzQCsetQuality	<i>A setQuality object. Use it for metrics which are specific to sets, i.e. only for values which only make sense in the set context and cannot be stored as runQuality (see mzQC spec doc).</i>
----------------	--

Description

The object is an alias for MzQCbaseQuality.

Super class

```
rmzqc:MzQCbaseQuality -> MzQCsetQuality
```

Methods**Public methods:**

- `MzQCsetQuality$clone()`

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
MzQCsetQuality$clone(deep = FALSE)
```

Arguments:

`deep` Whether to make a deep clone.

NULL_to_charNA	<i>Converts a NULL to NA_character_; or returns the argument unchanged otherwise</i>
----------------	--

Description

This is useful for missing list elements (which returns NULL), but when the missing element in refClass should be NA_character_ (and NULL would return an error)

Usage

```
NULL_to_charNA(char_or_NULL)
```

Arguments

char_or_NULL A string or NULL

Examples

```
NULL_to_charNA(NA)     ## NA
NULL_to_charNA(NULL) ## NA_character_
NULL_to_charNA("hi") ## "hi"
```

NULL_to_NA	<i>Converts a NULL to NA; or returns the argument unchanged otherwise</i>
------------	---

Description

This is useful for missing list elements (which returns NULL), but when the missing element in refClass should be NA (and NULL would return an error)

Usage

```
NULL_to_NA(var_or_NULL)
```

Arguments

var_or_NULL A variable of any kind or NULL

Examples

```
NULL_to_NA(NA)     ## NA
NULL_to_NA(NULL) ## NA
NULL_to_NA("hi") ## "hi"
```

parseOBO	<i>Get the information of each CV term from an obo file.</i>
----------	--

Description

Get the information of each CV term from an obo file.

Usage

```
parseOBO(cv_obo_file)
```

Arguments

cv_obo_file A local path to an .obo file

Value

A data.frame containing CV term information

readMZQC	<i>Read a JSON file in mzQC format into an MzQCmzQC root object</i>
----------	---

Description

Read a JSON file in mzQC format into an MzQCmzQC root object

Usage

```
readMZQC(filepath)
```

Arguments

filepath A filename (with path) to read from.

Value

An MzQCmzQC root object from which all the data can be extracted/manipulated

readMZQCFromJSON	<i>Read a JSON object in mzQC format into an MzQCmzQC root object</i>
------------------	---

Description

Read a JSON object in mzQC format into an MzQCmzQC root object

Usage

```
readMZQCFromJSON(json_obj)
```

Arguments

json_obj A generic R object (list of lists...)

Value

An MzQCmzQC root object from which all the data can be extracted/manipulated

removeFileSuffix	<i>Removes the last suffix (including the last dot) from a filename. If no dot exists, the full string is returned.</i>
------------------	---

Description

Removes the last suffix (including the last dot) from a filename. If no dot exists, the full string is returned.

Usage

```
removeFileSuffix(filepath)
```

Arguments

filepath A filename (with optional path – which is retained)

Value

The input with removed suffix

Examples

```
removeFileSuffix("test.tar.gz") # --> 'test.tar'
removeFileSuffix("test.mzML") # --> 'test'
removeFileSuffix("/path/to/test.mzML") # --> '/path/to/test'
removeFileSuffix("test_no_dot") # --> 'test_no_dot'
```

removeIfExists	<i>Remove a file, if it exists (useful for temporary files which may or may not have been created)</i>
----------------	--

Description

Remove a file, if it exists (useful for temporary files which may or may not have been created)

Usage

```
removeIfExists(tmp_filename)
```

Arguments

tmp_filename A path to a local file

Value

NULL if file is missing, otherwise TRUE/FALSE depening on successful removal

toAnalysisSoftware	<i>From an ID, e.g. "MS:1003162" (for PTX-QC), and some additional information, create an 'analysisSoftware' node for mzQC</i>
--------------------	--

Description

From an ID, e.g. "MS:1003162" (for PTX-QC), and some additional information, create an 'analysisSoftware' node for mzQC

Usage

```
toAnalysisSoftware(id, version = "unknown", uri = NULL, value = NA_character_)
```

Arguments

id	The CV accession
version	The version of the tool which created the metric/mzQC
uri	URI to the homepage, or if NULL (default), will be extracted from the definition in the PSI MS-CV (if possible)
value	An optional name for the software (if different from the CV's name)

Value

An MzQCanalysisSoftware object

Examples

```
# use 'version = packageVersion("PTXQC")' if the package is installed
toAnalysisSoftware(id = "MS:1003162", version = "1.0.12")
```

toQCMetric

Create an 'MzQCQualityMetric' object from two inputs (id and value).

Description

Create an 'MzQCQualityMetric' object from two inputs (id and value).

Usage

```
toQCMetric(
  id,
  value,
  on_violation = c("error", "warn"),
  allow_unknown_id = FALSE
)
```

Arguments

id	The CV accession
value	The data, as computed by some QC software in the required format.
on_violation	What to do when 'value' is not of the correct type (according to the given 'id')? Default: "error"; or "warn"
allow_unknown_id	Allows invalid accession, and also does not check the value type; if 'FALSE' this function errors

Details

The inputs are:

- an ID of a QC metric, e.g. "MS:4000059" (number of MS1 spectra)
- a value

The value must be in the correct format depending on the metric. The value type (see below) is checked (a warning/error is given if mismatching): The following requirements for values apply:

- single value: R single value; the unit is deduced from the CVs 'has_units'
- n-tuple: an R vector, e.g. using c(1,2,3), i.e. all values have the same type; the unit is deduced from the CVs 'has_units'
- table: an R list(); all columns defined using CVs 'has_column' must be present (a warning/error is given otherwise)

- matrix: an R matrix, i.e. all values have the same type; the unit is deduced from the CVs 'has_units'

Upon violation of the value type (e.g. data.frame instead of single value), an error or a warning is emitted (see @p on_violation):

```
toQCMetric(id = "MS:4000059", value = data.frame(n = 1)) # errors: wrong value format
```

Value

An MzQCanalysisSoftware object

Examples

```
## single value
toQCMetric(id = "MS:4000059", value = 13405) # number of MS1 spectra

## n-tuple
toQCMetric(id = "MS:4000051", value = c(31.3, 35.99, 38.44)) # XIC-FWHM quantiles

## table
toQCMetric(id = "MS:4000063", # MS2 known precursor charges fractions
  value = list("MS:1000041" = 1:3,
    "U0:0000191" = c(0.7, 0.6, 0.8)))

## test an invalid CV accession/id
toQCMetric(id = "MS:0000", value = "ID_is_not_valid", allow_unknown_id = TRUE)

## matrix (MS:4000006): there is no example in the CV yet, so this cannot be tested)
#toQCMetric(id = "MS:400000?", value = matrix(1:12, nrow = 3, ncol = 4)) # ???

# does not work since the 'id' is not derived from a valid value type
#toQCMetric(id = "MS:0000000", value = "ID_is_not_valid")

# does not work, since the ID is unknown and 'allow_unknown_id' is FALSE by default
#toQCMetric(id = "MS:0000", value = "ID_is_not_valid")
```

validateFromFile

Syntactically validates an mzQC document which is present as a file.

Description

The returned TRUE/FALSE has additional attributes in case of errors. Use attributes(result) to access them.

Usage

```
validateFromFile(filepath, verbose = TRUE)
```

Arguments

filepath	A path to a file (e.g. "c:/my.mzQC", or "test.mzQC")
verbose	Show extra information if validation fails

Value

TRUE/FALSE if validation was successful/failed

validateFromObj	<i>Syntactically validates an mzQC document which is already in memory as mzQC root object, as obtained by, e.g. readMZQC().</i>
-----------------	--

Description

This method is less performant than validateFromString, because it needs to convert the R object to a JSON string first.

Usage

```
validateFromObj(mzqc_root, verbose = TRUE)
```

Arguments

mzqc_root	An mzQC root object
verbose	Show extra information if validation fails

Details

The returned TRUE/FALSE has additional attributes in case of errors. Use attributes(result) to access them.

Value

TRUE/FALSE if validation was successful/failed

validateFromString	<i>Syntactically validates an mzQC document which is already in memory as JSON string. e.g. the string "{ mzQC : {} }"</i>
--------------------	--

Description

If the string object passed into this function contains multiple elements (length > 1). then they will be concatenated using '\n' before validation.

Usage

```
validateFromString(JSON_string, verbose = TRUE)
```

Arguments

JSON_string	A string which contains JSON (multiple lines allowed)
verbose	Show extra information if validation fails

Details

The returned TRUE/FALSE has additional attributes in case of errors. Use attributes(result) to access them.

Value

TRUE/FALSE if validation was successful/failed

writeMZQC	<i>Writes a full mzQC object to disk.</i>
-----------	---

Description

You can in theory also provide any mzQC subelement, but the resulting mzQC file will not validate since its incomplete.

Usage

```
writeMZQC(filepath, mzqc_obj)
```

Arguments

filepath	A filename (with optional path) to write to.
mzqc_obj	An MzQCmzQC root object, which is serialized to JSON and then written to disk

Details

The filename should have '.mzQC' (case sensitive) as suffix. There will be a warning otherwise.

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