

Package: geosalz.phreeqc (via r-universe)

October 1, 2026

Title R Package for Preparing Lab Samples as PHREEQC Input for Project GeoSalz

Version 0.1.0

Description R Package for Preparing Lab Samples as PHREEQC input for project GeoSalz.

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URL <https://github.com/KWB-R/geosalz.phreeqc>

BugReports <https://github.com/KWB-R/geosalz.phreeqc/issues>

Imports dplyr, janitor, kwb.base, kwb.utils, magrittr, readr, rlang, stringr, tibble, tidyr, tidyselect

Suggests covr, knitr, openxlsx, phreeqc, rmarkdown

VignetteBuilder knitr

Remotes cran/phreeqc, kwb-r/kwb.base, kwb-r/kwb.utils

Encoding UTF-8

LazyData true

Roxygen list(markdown = TRUE)

RoxygenNote 7.2.1

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

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add_solution_id	<i>Add solution id</i>
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Description

Add solution id

Usage

add_solution_id(samples)

Arguments

samples	data.frame with samples in wide format, i.e. parameters are columns and each row is one samole
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Value

add "solution_id"

convert_simulations_to_list	<i>Convert Simulation Results to list</i>
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Description

Convert Simulation Results to list

Usage

convert_simulations_to_list(simulations)

Arguments

simulations	tibble with simulation results as rewtrieved by read_simulations
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Value

list with simulation results in structure for export to EXCEL

`convert_to_numeric_lab_values`*Convert to numeric Laboratory Values*

Description

Convert to numeric Laboratory Values

Usage

```
convert_to_numeric_lab_values(  
  samples_tidy,  
  country = "en",  
  detLimFactorBelow = 0.5,  
  ...  
)
```

Arguments

<code>samples_tidy</code>	data.frame with samples in tidy format, i.e. parameters are columns and each row is one value
<code>country</code>	"en" if value is given in English format (decimal point ".", thousands separator ",") or "de" if value is given in German format (decimal point ",", thousands separator ".").
<code>detLimFactorBelow</code>	actor by which detection limit is multiplied in order to get a valid value when the value was below the detection limit. Default value: 0.5
<code>...</code>	additional arguments passed to hsLabValToVal

Value

data.frame with additional columns "outOfLimit" (with "<" or ">" sign) and "numericValue"

`package_file`*Path to File Stored in Package*

Description

Path to File Stored in Package

Usage

```
package_file(...)
```

Arguments

... segments of path to file, in the simplest form just a file name

Value

full path to file within "extdata" folder of the installed package

```
prepare_solutions_input
```

Prepare PHREEQC Solutions Input File

Description

Prepare PHREEQC Solutions Input File

Usage

```
prepare_solutions_input(samples_tidy, title = "", min_spaces = 3)
```

Arguments

<code>samples_tidy</code>	data.frame with samples in tidy format, i.e. parameters are columns and each row is one value
<code>title</code>	user defined title (default: "")
<code>min_spaces</code>	minimum spaces after parameter name based on longest parameter name (default: 3 spaces)

Value

input text to be used as PHREEQC input

Examples

```
file_samples <- system.file("extdata/phreeqc-input.csv",
  package = "geosalz.phreeqc")
samples <- read.csv2(file_samples)
samples_tidy <- geosalz.phreeqc::tidy_samples(samples) %>%
  geosalz.phreeqc::convert_to_numeric_lab_values()
prepare_solutions_input(samples_tidy)
```

read_output_file	<i>Read phreeqc output text file into a nested list structure</i>
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Description

Read phreeqc output text file into a nested list structure

Usage

```
read_output_file(file)
```

Arguments

file	full path to phreeqc output file. Template: <code>system.file("extdata/phreeqc_output.txt", package = "geosalz.phreeqc")</code>
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read_simulations	<i>Read Simulations</i>
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Description

Read Simulations

Usage

```
read_simulations(phreeqc_output)
```

Arguments

phreeqc_output vector with lines of PHREEQC output file

Value

returns list with elements "end_of_simulations_seconds", input and output

remove_missing_samples

Remove Missing Parameters

Description

Remove Missing Parameters

Usage

```
remove_missing_samples(
  samples_tidy,
  pattern_missing = "n\\.\\.s?a\\.|-",
  col_value = "value"
)
```

Arguments

samples_tidy	data.frame with samples in tidy format, i.e. parameters are columns and each row is one value
pattern_missing	remove samples marked "n. a." or "- "
col_value	value column (default: "value")

Value

data.frame without missing samples

tidy_samples

Tidy Samples

Description

Tidy Samples

Usage

```
tidy_samples(samples)
```

Arguments

samples	data.frame with samples in wide format, i.e. parameters are columns and each row is one sample. Coerce samples data.frame to as.character to address potential input format error
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Value

data.frame with samples in tidy format, i.e. parameters are columns and each row is one value

trim_vector

*Remove Empty Elements at the Start or End of a Vector***Description**

Remove Empty Elements at the Start or End of a Vector

Usage

```
trim_vector(x)
```

Arguments

x vector of character

Value

x with empty elements at the beginning and end of x being removed

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