

Package: uncleR (via r-universe)

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Title an R package for parsing UNcle data

Version 0.1

Depends R (>= 4.1.0)

Description UNcleR is an R package for parsing data exported from Unchained Labs UNcle instruments for the purpose of downstream analysis of biologics stability data.

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Encoding UTF-8

LazyData true

RoxygenNote 7.1.1

Imports magrittr, tibble, purrr, tidyr, dplyr (>= 1.0.0), readxl, stringr, readr, tidyselect, rlang

Repository <https://eric-hunt.r-universe.dev>

RemoteUrl <https://github.com/eric-hunt/uncleR>

RemoteRef HEAD

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add_meta	<i>Join user-defined metadata from 'uncleR::get_meta' function to imported Uncle data</i>
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Description

add_meta

Usage

```
add_meta(data, meta)
```

Arguments

data	a dataframe to assign metadata to
meta	a named list of tibbles containing metadata for experiments imported from 'uncleR::get_meta' function defaults to c("well")

Value

a dataframe with metadata added as new variables, matched according to well

consolidate_experiments	<i>Consolidates Uncle Experiments</i>
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Description

This function consolidates experiments for a protein based on directory hierarchy. The hierarchy should be as follows from within the working directory where these functions will be executed:

Usage

```
consolidate_experiments(  
  prot_dir,  
  join_vars = NULL,  
  legacy = FALSE,  
  SLShheader = TRUE,  
  DLShheader = FALSE  
)
```

Arguments

prot_dir	a character string identical to subdirectory name of working directory where the experiment "Exports" folder is located for the protein being analyzed
legacy	a boolean value, TRUE if individual SLS/DLS spectra files were exported, FALSE if SLS/DLS "bundle" files were exported; default is FALSE
SLShheader	sets header argument for uncler: : import_SLSSum; defaults to TRUE
DLShheader	sets header argument for uncler: : import_DLSSum; defaults to FALSE

Details

<wd>/ <prot_dir>/ "Exports"/ "General Screen" "pH Screen" ...

The prot_dir argument should match the name of the protein subdirectory within the working directory. This is deliberate as it forces the user to make a coherent choice about which data to process. Exported summary and spectra should be contained within named subdirectories of a directory named "Exports" located within the prot_dir directory.

consolidate_experiments

Value

a named list of dataframes containing the consolidated data for each experiment

get_meta

Get metadata from unified Excel document

Description

get_meta

Usage

get_meta(path)

Arguments

path	a character string path to an Excel document containing metadata for each experiment in separate worksheets defaults to c("well")
------	---

Value

a named list of tibbles containing metadata for experiments

import_DLSSpec	<i>Import Uncle DLS spectra into R</i>
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Description

import_DLSSpec

Usage

```
import_DLSSpec(
  directory_path,
  pattern = NULL,
  type = NA,
  header = TRUE,
  combine = TRUE
)
```

Arguments

directory_path	a path to a directory containing the exported .xlsx files
pattern	a regex pattern for further selecting files in the directory; defaults to NULL to force user input that discriminates intensity from mass DLS files
type	a character string, "C", "I", or "M", to signify if the data is correlation function, intensity, or mass distribution DLS spectra
header	if TRUE skips first 3 rows of .xlsx file to remove Uncle header; default is TRUE
combine	if TRUE, returns all imported data merged into one unified dataframe with an "origin" column listing the original file path, FALSE will return a list of dataframes; default is TRUE

Value

a named (with filename) list of dataframes or a single merged dataframe

import_DLSSum	<i>Import Uncle Tm/Tagg DLS summary into R</i>
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Description

import_DLSSum

Usage

```
import_DLSSum(  
  directory_path,  
  pattern = "DLS Sum",  
  sheet = NULL,  
  temp_cutoff = 25,  
  header = FALSE,  
  combine = TRUE  
)
```

Arguments

directory_path	a path to a directory containing the exported .xlsx files
pattern	a regex pattern for further selecting files in the directory, defaults to "DLS Sum"
sheet	character string to specify sheet if multi-sheet workbook is exported
temp_cutoff	numeric value, excluding all DLS data obtained at temperatures above this value, default is 100 (°C)
header	if TRUE skips first 4 rows of .xlsx file to remove Uncle header, default is FALSE
combine	if TRUE, returns all imported data merged into one unified dataframe with an "origin" column listing the original file path, FALSE will return a list of dataframes; default is TRUE

Value

a named (with filename) list of dataframes or a single merged dataframe

import_dynamicBundle *Import dynamic Uncle spectra (DLS) into R*

Description

import_dynamicBundle

Usage

```
import_dynamicBundle(  
  directory_path,  
  pattern = "DLS Bundle",  
  skip = 2,  
  combine = TRUE  
)
```

Arguments

directory_path	a path to a directory containing the exported .xlsx files
pattern	a regex for narrowing selection of files in the 'directory_path'; defaults to "DLS Bundle"
skip	number of rows of embedded run metadata in the .xlsx file to remove; default is 2
combine	if TRUE, returns all imported data merged into one unified dataframe with an "origin" column listing the original file path, FALSE will return a list of dataframes; default is TRUE

Details

Note: This import function will only import DLS spectra performed at the beginning of the temperature ramp, i.e. the lowest temperature.

Value

a named (with filename) list of dataframes or a single merged dataframe

import_FLUORspec	<i>Import Uncle fluorescence spectra into R</i>
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Description

import_FLUORspec

Usage

```
import_FLUORspec(
  directory_path,
  pattern = "Tm Spec",
  header = TRUE,
  combine = TRUE
)
```

Arguments

directory_path	a path to a directory containing the exported .xlsx files
pattern	a regex pattern for further selecting files in the directory; defaults to "Tm Spec"
header	if TRUE skips first 3 rows of .xlsx file to remove Uncle header; default is TRUE
combine	if TRUE, returns all imported data merged into one unified dataframe with an "origin" column listing the original file path, FALSE will return a list of dataframes; default is TRUE

Value

a named (with filename) list of dataframes or a single merged dataframe

import_SLSpec	<i>Import Uncle Tagg spectra into R</i>
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Description

import_SLSpec

Usage

```
import_SLSpec(  
  directory_path,  
  pattern = "SLS Spec",  
  lambda = 266,  
  header = TRUE,  
  combine = TRUE  
)
```

Arguments

`directory_path` a path to a directory containing the exported .xlsx files

`pattern` a regex pattern for further selecting files in the directory; defaults to SLS Spec

`lambda` a number value representing wavelength for Tagg spectra, typically 266nm for small aggregates and 473nm for large aggregates; default is 266nm

`header` if TRUE skips first 1 rows of .xlsx file to remove Uncle header; default is TRUE

`combine` if TRUE, returns all imported data merged into one unified dataframe with an "origin" column listing the original file path, FALSE will return a list of dataframes; default is TRUE

Value

a named (with filename) list of dataframes or a single merged dataframe

import_SLSSum	<i>Import Uncle Tm/Tagg SLS summary into R</i>
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Description

import_SLSSum

Usage

```
import_SLSSum(
  directory_path,
  pattern = "SLS Sum",
  sheet = NULL,
  header = FALSE,
  combine = TRUE
)
```

Arguments

`directory_path` a path to a directory containing the exported .xlsx files

`pattern` a regex pattern for further selecting files in the directory; defaults to "SLS Sum"

`sheet` character string to specify sheet if multi-sheet workbook is exported

`header` if TRUE skips first 4 rows of .xlsx file to remove Uncle header; default is FALSE

`combine` if TRUE, returns all imported data merged into one unified dataframe with an "origin" column listing the original file path, FALSE will return a list of dataframes; default is TRUE

Value

a named (with filename) list of dataframes or a single merged dataframe

`import_staticBundle` *Import static Uncle spectra (nanoDSF and SLS) into R*

Description

`import_staticBundle`

Usage

```
import_staticBundle(
  directory_path,
  pattern = "SLS Bundle",
  skip = 3,
  combine = TRUE
)
```

Arguments

`directory_path` a path to a directory containing the exported .xlsx files

`pattern` a regex for narrowing selection of files in the 'directory_path'; defaults to "SLS Bundle"

skip	number of rows of embedded run metadata in the .xlsx file to remove; default is 3
combine	if TRUE, returns all imported data merged into one unified dataframe with an "origin" column listing the original file path, FALSE will return a list of dataframes; default is TRUE

Value

a named (with filename) list of dataframes or a single merged dataframe

join_SLS_DLS	<i>Joins imported and parsed DLS and Tm/Tagg SLS summary dataframes from the same experiment</i>
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Description

join_SLS_DLS

Usage

```
join_SLS_DLS(SLS_data, DLS_data, .by = c("well", "sample_num", "prot_conc"))
```

Arguments

SLS_data	a dataframe object containing SLS data
DLS_data	a dataframe object containing DLS data
.by	a character vector of variable names by which to join tables; defaults to c("well", "sample_num", "prot_conc")

Value

a dataframe

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