Package: cascade (via r-universe)

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Title Contextualizing untargeted Annotation with Semi-quantitative Charged Aerosol Detection for pertinent characterization of natural Extracts

Version 0.0.0.9000

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Description This package provides the infrastructure to perform Automated Composition Assessment of Natural Extracts.

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URL https://github.com/adafede/cascade, https://adafede.github.io/cascade

BugReports https://github.com/adafede/cascade/issues

Depends R (>= 4.3.0)

Imports baseline (>= 1.3.5), caTools (>= 1.18.3), data.table (>= 1.15.4), dplyr (>= 1.1.4), forcats (>= 1.0.0), furrr (>= 0.3.1), ggplot2 (>= 3.5.1), gt (>= 0.11.1), htmltools (>= 0.5.8.1), MSnbase (>= 2.28.1), mzR (>= 2.36.0), plotly (>= 4.10.4), progressr (>= 0.15.0), purrr (>= 1.0.2), R.utils, tibble (>= 3.2.1), tidytable (>= 0.11.1), tima (>= 2.11.0), utils, WikidataQueryServiceR (>= 1.0.0)

Remotes taxonomicallyinformedannotation/tima

Suggests BiocManager, knitr, lifecycle, testthat (>= 3.0.0)

Config/testthat/edition 3

Encoding UTF-8

LazyData true

ByteCompile true

Roxygen list(markdown = TRUE)

RoxygenNote 7.3.2

Collate 'normalize_chromatograms_list.R' 'add_chromato_line.R' 'baseline_chromatogram.R' 'cascade-package.R' 'change_intensity_name.R' 'check_chromatograms.R'

'load_chromatograms.R' 'deriv.R' 'middle_pts.R' 'second_der.R'
'signal_sharpening.R' 'filter_fft.R' 'improve_signal.R'
'extract_chromatogram.R' 'check_chromatograms_alignment.R'
'check_export_dir.R' 'prepare_rt.R' 'prepare_peaks.R'
'prepare_mz.R' 'get_peaks.R' 'peaks_progress.R'
'normalize_chromato.R' 'join_peaks.R' 'preprocess_peaks.R'
'improve_signals_progress.R' 'preprocess_chromatograms.R'
'prepare_features.R' 'plot_peak_detection.R' 'load_name.R'
'load_features.R' 'check_peaks_integration.R' 'colors.R'
'compare_peaks.R' 'correct_acn.R' 'extract_ms_peak.R'
'extract_ms_progress.R' 'format_gt.R' 'wiki_progress.R'
'treemaps_progress.R' 'taxon_name_to_qid.R' 'tables_progress.R'
'queries_progress.R' 'prepare_plot.R' 'prepare_hierarchy.R'
'plot_histograms.R' 'make_no_stereo.R'
'make_chromatographiable.R' 'hierarchies_grouped_progress.R'
'hierarchies_progress.R' 'generate_ids.R'
'prepare_comparison.R' 'no_other.R' 'make_other.R'
'plot_results.R' 'make_confident.R' 'y_as_na.R'
'keep_best_candidates.R' 'generate_pseudochromatograms.R'
'molinfo.R' 'load_features_informed.R' 'load_annotations.R'
'generate_tables.R' 'histograms_progress.R'
'load_features_not_informed.R' 'load_ms_data.R'
'plot_chromatogram.R' 'prehistograms_progress.R'
'transform_ms.R' 'process_compare_peaks.R'
'save_histograms_progress.R' 'save_treemaps_progress.R'

VignetteBuilder knitr

biocViews metabolite annotation, charged aerosol detector, semi-quantitative, natural products, computational metabolomics, specialized metabolome

X-schema.org-keywords metabolite annotation, charged aerosol detector, semi-quantitative, natural products, computational metabolomics, specialized metabolome

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Repository https://adafede.r-universe.dev

RemoteUrl https://github.com/adafede/cascade

RemoteRef main

RemoteSha ea17a73f41cf13d4aa7ddf54ac217b0403f4a3c6

Contents

`add_chromato_line` *Add chromato line*

Description

Add chromato line

Usage

```
add_chromato_line(
  plot,
  chromato,
  shift = 0,
  normalize_time,
  name,
  color,
  polarity = "pos"
)
```

Arguments

plot	Plot
chromato	Chromato
shift	Shift
normalize_time	Normalize time
name	Name
color	Color
polarity	Polarity

Value

A plot with added chromato line

Examples

```
NULL
```

---

baseline_chromatogram *Baseline chromatogram*

Description

Baseline chromatogram

Usage

```
baseline_chromatogram(df)
```

Arguments

df	Dataframe

Value

A dataframe with baselined chromatogram

Examples

```
NULL
```

change_intensity_name *Change intensity name*

Description

Change intensity name

Usage

```
change_intensity_name(df, name)
```

Arguments

df	Dataframe
name	Name

Value

A dataframe with changed intensity name

Examples

```
NULL
```

check_chromatograms *Check chromatograms*

Description

Check chromatograms

Usage

```
check_chromatograms(
  chromatograms = c("bpi_pos", "cad_pos", "pda_pos"),
  normalize_time = FALSE,
  shift_cad = 0,
  shift_pda = 0,
  type = "improved"
)
```

Arguments

chromatograms	Chromatograms
normalize_time	Normalized time
shift_cad	Shift CAD
shift_pda	Shift PDA
type	Type

Value

A plot

Examples

```
NULL
```

---

check_chromatograms_alignment
Check chromatograms alignment

Description

Check chromatograms alignment

Usage

```
check_chromatograms_alignment(
  file_negative = NULL,
  file_positive = NULL,
  time_min = 0.5,
  time_max = 32.5,
  cad_shift = 0.05,
  pda_shift = 0.1,
  fourier_components = 0.01,
  frequency = 1,
  resample = 1,
  chromatograms = c("bpi_pos", "cad_pos", "pda_pos"),
  type = "baselined",
  normalize_intensity = TRUE,
  normalize_time = FALSE,
  show_example = FALSE
)
```

Arguments

file_negative	Negative file path
file_positive	Positive file path
time_min	Minimum time
time_max	Maximum time
cad_shift	CAD shift
pda_shift	PDA shift
fourier_components	Fourier components
frequency	Frequency
resample	Resample
chromatograms	Chromatograms to plot
type	Type. "baselined" or "improved"
normalize_intensity	Normalize intensity? Default to TRUE
normalize_time	Normalize time? Default to FALSE
show_example	Show example? Default to FALSE

Value

A plot with (non-)aligned chromatograms

Examples

```
## Not run:
check_chromatograms_alignment(show_example = TRUE)

## End(Not run)
```

---

check_export_dir *Check export dir*

Description

Check export dir

Usage

```
check_export_dir(dir)
```

Arguments

dir	Dir

Value

A log of checked dir

Examples

```
NULL
```

`check_peaks_integration` *Check chromatograms alignment*

Description

Check chromatograms alignment

Usage

```
check_peaks_integration(
  file = NULL,
  features = NULL,
  detector = "cad",
  chromatogram = "baselined",
  min_area = 0.005,
  min_intensity = 10000,
  shift = 0.05,
  show_example = FALSE,
  fourier_components = 0.01,
  time_min = 0.5,
  time_max = 32.5,
  frequency = 1,
  resample = 1
)
```

Arguments

`file`	File path
`features`	Features path
`detector`	Detector
`chromatogram`	Chromatogram
`min_area`	Minimum area
`min_intensity`	Minimum intensity
`shift`	shift
`show_example`	Show example? Default to FALSE
`fourier_components`	Fourier components

time_min	Time min
time_max	Time max
frequency	Frequency
resample	Resample

Value

A plot with (non-)aligned chromatograms

Examples

```
## Not run:
check_peaks_integration(show_example = TRUE)

## End(Not run)
```

---

compare_peaks *Compare peaks*

Description

Compare peaks

Usage

```
compare_peaks(x, list_ms_peaks, peaks_prelist)
```

Arguments

x	X
list_ms_peaks	list_ms_peaks
peaks_prelist	peaks_prelist

Value

A comparison score

Examples

```
NULL
```

deriv *Deriv*

Description

Deriv

Usage

```
deriv(x, y)
```

Arguments

x	X
y	Y

Value

The derivative

Examples

```
NULL
```

extract_chromatogram *Extract chromatogram*

Description

Extract chromatogram

Usage

```
extract_chromatogram(list, type)
```

Arguments

list	List
type	Type

Value

An extracted chromatogram

Examples

```
NULL
```

extract_ms_peak *Extract MS peak*

Description

Extract MS peak

Usage

```
extract_ms_peak(x)
```

Arguments

x	X

Value

A peak

Examples

```
NULL
```

extract_ms_progress *Extract MS progress*

Description

Extract MS progress

Usage

```
extract_ms_progress(xs, ms_data, peaks_prelist)
```

Arguments

xs	XS
ms_data	MS Data
peaks_prelist	Peaks prelist

Value

A list of extracted MS peaks

Examples

```
NULL
```

filter_fft *Filter FFT*

Description

Filter FFT

Usage

```
filter_fft(x, components)
```

Arguments

x	X
components	Components

Value

The fourier filtered x

Examples

```
NULL
```

format_gt *Temp GT function*

Description

Temp GT function

Usage

```
format_gt(table, title = "", subtitle = "")
```

Arguments

table	Table
title	Title
subtitle	Subtitle

Value

A formatted GT table

Examples

```
NULL
```

generate_ids *Generate IDs*

Description

Generate IDs

Usage

```
generate_ids(
  taxa = c("Swertia", "Kopsia", "Ginkgo"),
  comparison = c("Swertia", "Kopsia"),
  no_stereo = TRUE,
  filter_ms_conditions = TRUE,
  start = "0",
  end = "9999",
  limit = "1000000"
)
```

Arguments

taxa	Taxa
comparison	Comparison
no_stereo	No stereo
filter_ms_conditions	Filter MS conditions
start	Start
end	End
limit	Limit

Value

IDs

Examples

```
## Not run:
generate_ids()

## End(Not run)
```

`generate_pseudochromatograms` *Generate pseudochromatograms*

Description

Generate pseudochromatograms

Usage

```
generate_pseudochromatograms(
  annotations = NULL,
  features_informed = NULL,
  features_not_informed = NULL,
  file = NULL,
  detector = "cad",
  show_example = FALSE,
  min_confidence = 0.4,
  min_similarity_prefilter = 0.6,
  min_similarity_filter = 0.8,
  mode = "pos",
  organism = "Swertia chirayita",
  fourier_components = 0.01,
  frequency = 1,
  resample = 1,
  shift = 0.05,
  time_min = 0.5,
  time_max = 32.5
)
```

Arguments

`annotations`	Annotations
`features_informed`	Features informed
`features_not_informed`	Features not informed
`file`	File
`detector`	Detector
`show_example`	Show example? Default to FALSE
`min_confidence`	Min confidence
`min_similarity_prefilter`	Min similarity pre filter
`min_similarity_filter`	Min similarity filter

mode	Mode
organism	Organism
fourier_components	Fourier components
frequency	Frequency
resample	Resample
shift	Shift
time_min	Time min
time_max	Time max

Value

A list of plots

Examples

```
## Not run:
generate_pseudochromatograms(show_example = TRUE)

## End(Not run)
```

---

generate_tables *Generate IDs*

Description

Generate IDs

Usage

```
generate_tables(
  annotations = NULL,
  file_negative = NULL,
  file_positive = NULL,
  min_confidence = 0.4,
  show_example = FALSE,
  export_csv = TRUE,
  export_html = TRUE,
  export_dir = "data/processed",
  export_name = "cascade_table"
)
```

Arguments

annotations	Annotations
file_negative	File negative
file_positive	File positive
min_confidence	Min confidence
show_example	Show example? Default to FALSE
export_csv	Export CSV
export_html	Export HTML
export_dir	Export Dir
export_name	Export name

Value

Tables

Examples

```
## Not run:
generate_tables()

## End(Not run)
```

---

get_peaks *Get peaks*

Description

Get peaks

Usage

```
get_peaks(
  chrom_list,
  lambdas,
  fit = c("egh", "gaussian", "raw"),
  sd.max = 50,
  max.iter = 100,
  time.units = c("min", "s", "ms"),
  estimate_purity = FALSE,
  noise_threshold = 0.001,
  collapse = FALSE,
  ...
)
```

Arguments

chrom_list	Chrom list
lambdas	Lambdas
fit	Fit
sd.max	Sd max
max.iter	Max iter
time.units	Time units
estimate_purity	Estimate purity
noise_threshold	Noise Threshold
collapse	Collapse
...	...

Value

Peaks

Note

This was imported from {chromatographR} package and parallelization was removed as it was causing issues on Windows.

Author(s)

Ethan Bass

Source

https://github.com/ethanbass/chromatographR

Examples

```
NULL
```

---

hierarchies_grouped_progress

Hierarchies grouped progress

Description

Hierarchies grouped progress

Usage

```
hierarchies_grouped_progress(xs)
```

Arguments

xs	XS

Value

A list of grouped hierarchies

Examples

```
NULL
```

---

hierarchies_progress *Hierarchies Progress*

Description

Hierarchies Progress

Usage

```
hierarchies_progress(xs)
```

Arguments

xs	XS

Value

A list of hierarchies

Examples

```
NULL
```

histograms_progress *Histograms progress*

Description

Histograms progress

Usage

```
histograms_progress(xs)
```

Arguments

xs	XS

Value

A list of histograms

Examples

```
NULL
```

improve_signal *Improve signal*

Description

Improve signal

Usage

```
improve_signal(
  df,
  fourier_components = 0.01,
  frequency = 2,
  resample = 1,
  time_min = 0,
  time_max = Inf
)
```

Arguments

df	Dataframe
fourier_components	Fourier components
frequency	Frequency
resample	Resample
time_min	Time min
time_max	Time max

Value

A dataframe with improved signal

Examples

```
NULL
```

---

improve_signals_progress *Improve signals progress*

Description

Improve signals progress

Usage

```
improve_signals_progress(
  xs,
  fourier_components = 0.01,
  frequency = 2,
  resample = 1,
  time_min = 0,
  time_max = Inf
)
```

Arguments

xs	XS
fourier_components	Fourier components
frequency	Frequency
resample	Resample
time_min	Time min
time_max	Time max

Value

A list of data frames with improved signals

Examples

```
NULL
```

`join_peaks` *Join peaks*

Description

Join peaks

Usage

```
join_peaks(chromatograms, peaks, min_area)
```

Arguments

`chromatograms`	Chromatograms
`peaks`	Peaks
`min_area`	Min area

Value

A dataframe with joined peaks

Examples

```
NULL
```

`keep_best_candidates` *Keep best candidates*

Description

Keep best candidates

Usage

```
keep_best_candidates(df)
```

Arguments

`df`	Dataframe

Value

A dataframe containing the best candidates only

Examples

```
NULL
```

---

load_annotations *Load annotations*

Description

Load annotations

Usage

```
load_annotations(file = NULL, show_example = FALSE, mode = "pos")
```

Arguments

file	File
show_example	Show example? Default to FALSE
mode	Mode

Value

A table of annotations

Examples

```
NULL
```

---

load_chromatograms *Load chromatograms*

Description

Load chromatograms

Usage

```
load_chromatograms(file = NULL, show_example = FALSE, example_polarity = "pos")
```

Arguments

file	File
show_example	Show example? Default to FALSE
example_polarity	Example polarity

Value

A list of chromatograms

Examples

```
NULL
```

---

load_features *Load features*

Description

Load features

Usage

```
load_features(file = NULL, show_example = FALSE)
```

Arguments

file	File
show_example	Show example? Default to FALSE

Value

A table of features

Examples

```
NULL
```

load_features_informed *Load features informed*

Description

Load features informed

Usage

```
load_features_informed(file = NULL, show_example = FALSE)
```

Arguments

file	File
show_example	Show example? Default to FALSE

Value

A table of informed features

Examples

```
NULL
```

load_features_not_informed *Load features not informed*

Description

Load features not informed

Usage

```
load_features_not_informed(file = NULL, show_example = FALSE)
```

Arguments

file	File
show_example	Show example? Default to FALSE

Value

A table of non informed features

Examples

```
NULL
```

`load_ms_data` *Load MS data*

Description

Load MS data

Usage

```
load_ms_data(file = NULL, show_example = FALSE)
```

Arguments

`file`	File
`show_example`	Show example? Default to FALSE

Value

MS data

Examples

```
NULL
```

`load_name` *Load name*

Description

Load name

Usage

```
load_name(
  file = NULL,
  default = "210619_AR_06_V_03_2_01.mzML",
  show_example = FALSE
)
```

Arguments

`file`	File
`default`	Default
`show_example`	Show example? Default to FALSE

Value

A name

Examples

```
NULL
```

`make_chromatographiable` *Make chromatographiable*

Description

Make chromatographiable

Usage

```
make_chromatographiable(
  df,
  mass_min = 50,
  mass_max = 1500,
  logp_min = -1,
  logp_max = 6
)
```

Arguments

`df`	Dataframe
`mass_min`	Mass min
`mass_max`	Mass max
`logp_min`	Log P min
`logp_max`	Log P max

Value

A dataframe containing chromatographiable compounds

Examples

```
NULL
```

make_confident *Make confident*

Description

Make confident

Usage

```
make_confident(df, score)
```

Arguments

df	Dataframe
score	Score

Value

A dataframe containing annotations with scores above the confidence threshold set

Examples

```
NULL
```

make_no_stereo *Make no stereo*

Description

Make no stereo

Usage

```
make_no_stereo(df)
```

Arguments

df	Dataframe

Value

A dataframe with no stereo structures

Examples

```
NULL
```

make_other *Make other*

Description

Make other

Usage

```
make_other(dataframe, value = "peak_area")
```

Arguments

dataframe	Dataframe
value	Value

Value

A dataframe with harmonized "other" subcategories

Examples

```
NULL
```

middle_pts *Middle pts*

Description

Middle pts

Usage

```
middle_pts(x)
```

Arguments

x	X

Value

Middle pts

Examples

```
NULL
```

molinfo *Molinfo*

Description

Molinfo

Usage

```
molinfo(x)
```

Arguments

x	X

Value

A mol image

Examples

```
NULL
```

normalize_chromato *Normalize chromato*

Description

Normalize chromato

Usage

```
normalize_chromato(x, df_xy)
```

Arguments

x	X
df_xy	Df X Y

Value

A normalized chromato

Examples

```
NULL
```

normalize_chromatograms_list *Normalize chromatograms list*

Description

Normalize chromatograms list

Usage

```
normalize_chromatograms_list(
  list,
  shift = 0,
  normalize_intensity = TRUE,
  normalize_time = FALSE
)
```

Arguments

list	List
shift	Shift
normalize_intensity	Normalize time
normalize_time	Normalize intensity

Value

A dataframe with normalized chromatograms

Examples

```
NULL
```

no_other *No other*

Description

No other

Usage

```
no_other(dataframe)
```

Arguments

dataframe	Dataframe

Value

A dataframe with no other

Examples

```
NULL
```

---

peaks_progress *Peaks progress*

Description

Peaks progress

Usage

```
peaks_progress(df_xy)
```

Arguments

df_xy	Df X Y

Value

A list of peaks

Examples

```
NULL
```

plot_chromatogram *Plot chromatogram*

Description

Plot chromatogram

Usage

```
plot_chromatogram(df, text)
```

Arguments

df	Dataframe
text	Text

Value

A plot of a chromatogram

Examples

```
NULL
```

plot_histograms *Plot histograms*

Description

Plot histograms

Usage

```
plot_histograms(dataframe, chromatogram, label, y = "values", xlab = TRUE)
```

Arguments

dataframe	Dataframe
chromatogram	Chromatogram
label	Label
y	Y
xlab	Xlab

Value

A plot of histograms

Examples

```
NULL
```

`plot_histograms_confident` *Plot histograms confident*

Description

Plot histograms confident

Usage

```
plot_histograms_confident(
  dataframe,
  chromatogram,
  level = "max",
  time_min,
  time_max
)
```

Arguments

`dataframe`	Dataframe
`chromatogram`	Chromatogram
`level`	Level
`time_min`	Time min
`time_max`	Time max

Value

A plot of confident histograms

Examples

```
NULL
```

plot_histograms_litt *Plot histograms litt*

Description

Plot histograms litt

Usage

```
plot_histograms_litt(dataframe, label, y = "values", xlab = TRUE)
```

Arguments

dataframe	Dataframe
label	Label
y	Y
xlab	Xlab

Value

A plot of literature histograms

Examples

```
NULL
```

plot_histograms_taxo *Plot histograms taxo*

Description

Plot histograms taxo

Usage

```
plot_histograms_taxo(
  dataframe,
  chromatogram,
  level = "max",
  mode = "pos",
  time_min,
  time_max
)
```

Arguments

dataframe	Dataframe
chromatogram	Chromatogram
level	Level
mode	Mode
time_min	Time min
time_max	Time max

Value

A plot of taxo histograms

Examples

```
NULL
```

---

plot_peak_detection *Plot peak detection*

Description

Plot peak detection

Usage

```
plot_peak_detection(df1, df2, fun)
```

Arguments

df1	DF 1 containing chromatogram
df2	DF 2 containing peaks
fun	Fun

Value

A plot with (non-)detected peaks

Examples

```
NULL
```

plot_results_1 *Plot results 1*

Description

Plot results 1

Usage

```
plot_results_1(list, chromatogram, mode = "pos", time_min, time_max)
```

Arguments

list	List
chromatogram	Chromatogram
mode	Mode
time_min	Time min
time_max	Time max

Value

A list of plots

Examples

```
NULL
```

plot_results_2 *Plot results 2*

Description

Plot results 2

Usage

```
plot_results_2(list)
```

Arguments

list	List

Value

A list of plots

Examples

```
NULL
```

`predict_response` *Predict response*

Description

Predict response

Usage

```
predict_response(
  acn = 100,
  peak_area,
  p1q1 = 1e-05,
  p1q2 = -6e-04,
  p1q3 = -0.0778,
  p2q1 = 2e-05,
  p2q2 = -0.00022,
  p2q3 = 0.05499,
  p3q1 = -0.00017,
  p3q2 = 0.0209,
  p3q3 = 1.4041
)
```

Arguments

`acn`	ACN
`peak_area`	Peak area
`p1q1`	P1Q1
`p1q2`	P1Q2
`p1q3`	P1Q3
`p2q1`	P2Q1
`p2q2`	P2Q2
`p2q3`	P2Q3
`p3q1`	P3Q1
`p3q2`	P3Q2
`p3q3`	P3Q3

Value

The concentration

Examples

```
NULL
```

prehistograms_progress *Prehistograms progress*

Description

Prehistograms progress

Usage

```
prehistograms_progress(xs)
```

Arguments

xs	XS

Value

A list of prehistograms

Examples

```
NULL
```

prepare_comparison *Prepare comparison*

Description

Prepare comparison

Usage

```
prepare_comparison(
  features_informed = NULL,
  features_not_informed = NULL,
  candidates_confident,
  min_similarity_prefilter = 0.6,
  min_similarity_filter = 0.8,
  mode = "pos",
  show_example = FALSE
)
```

Arguments

features_informed	Features informed
features_not_informed	Features not informed
candidates_confident	Candidates confident
min_similarity_prefilter	Min similarity pre filter
min_similarity_filter	Min similarity filter
mode	Mode
show_example	Show example? Default to FALSE

Value

A list of peaks

Examples

```
NULL
```

---

prepare_features *Prepare features*

Description

Prepare features

Usage

```
prepare_features(df, min_intensity, name)
```

Arguments

df	Df
min_intensity	Min intensity
name	Name

Value

A dataframe of prepared features

Examples

```
NULL
```

prepare_hierarchy *Prepare hierarchy*

Description

Prepare hierarchy

Usage

```
prepare_hierarchy(
  dataframe,
  type = "analysis",
  detector = "ms",
  rescale = FALSE
)
```

Arguments

dataframe	Dataframe
type	Type
detector	Detector
rescale	Rescale

Value

A dataframe with prepared hierarchy

Examples

```
NULL
```

prepare_mz *Prepare mz*

Description

Prepare mz

Usage

```
prepare_mz(x)
```

Arguments

x	X

Value

A list of prepared mz's

Examples

```
NULL
```

---

prepare_peaks *Prepare peaks*

Description

Prepare peaks

Usage

```
prepare_peaks(x)
```

Arguments

x	X

Value

Prepared peaks

Examples

```
NULL
```

---

prepare_plot *Prepare plot*

Description

Prepare plot

Usage

```
prepare_plot(dataframe, organism = "species")
```

Arguments

dataframe	Dataframe
organism	Organism

Value

A dataframe prepared for plots

Examples

```
NULL
```

---

prepare_plot_2 *Prepare plot 2*

Description

Prepare plot 2

Usage

```
prepare_plot_2(dataframe)
```

Arguments

dataframe	Dataframe

Value

A dataframe prepared for plots

Examples

```
NULL
```

---

prepare_rt *Prepare rt*

Description

Prepare rt

Usage

```
prepare_rt(x, shift = 0)
```

Arguments

x	X
shift	Shift

Value

Prepared RTs

Examples

```
NULL
```

`preprocess_chromatograms` *Preprocess chromatograms*

Description

Preprocess chromatograms

Usage

```
preprocess_chromatograms(
  detector = "cad",
  fourier_components = 0.01,
  frequency = 2,
  list,
  name,
  resample = 1,
  shift = 0,
  signal_name = "UV.1_CAD_1_0",
  time_min = 0,
  time_max = Inf
)
```

Arguments

`detector`	Detector
`fourier_components`	Fourier components
`frequency`	Frequency
`list`	List
`name`	Name
`resample`	Resample
`shift`	Shift
`signal_name`	Signal name
`time_min`	Time min
`time_max`	Time max

Value

A list of preprocessed chromatograms

Examples

```
NULL
```

`preprocess_peaks` *Preprocess peaks*

Description

Preprocess peaks

Usage

```
preprocess_peaks(
  detector = "cad",
  df_features,
  df_long,
  df_xy,
  name,
  shift = 0,
  min_area = 0
)
```

Arguments

`detector`	Detector
`df_features`	DF features
`df_long`	DF long
`df_xy`	DF X Y
`name`	Name
`shift`	shift
`min_area`	Minimum area

Value

A list of lists and dataframe with preprocessed peaks

Examples

```
NULL
```

`process_compare_peaks` *Process compare peaks*

Description

Process compare peaks

Usage

```
process_compare_peaks(
  file = NULL,
  features = NULL,
  type = "baselined",
  detector = "cad",
  export_dir = "data/interim/peaks",
  show_example = FALSE,
  fourier_components = 0.01,
  frequency = 1,
  min_area = 0.005,
  min_intensity = 10000,
  resample = 1,
  shift = 0.05,
  time_min = 0.5,
  time_max = 32.5
)
```

Arguments

`file`	File path
`features`	Features path
`type`	Type. "original", "baselined" or "improved"
`detector`	Detector
`export_dir`	Export directory
`show_example`	Show example? Default to FALSE
`fourier_components`	Fourier components
`frequency`	Frequency
`min_area`	Min area
`min_intensity`	Min intensity
`resample`	Resample
`shift`	Shift
`time_min`	Time min
`time_max`	Time max

Value

A plot with (non-)aligned chromatograms

Examples

```
## Not run:
check_chromatograms_alignment(show_example = TRUE)

## End(Not run)
```

---

p_acn_i *P ACN I*

Description

P ACN I

Usage

```
p_acn_i(acn_eluent, q1, q2, q3)
```

Arguments

acn_eluent	ACN eluent
q1	Q1
q2	Q2
q3	Q3

Value

P ACN I

Examples

```
NULL
```

queries_progress *Queries progress*

Description

Queries progress

Usage

```
queries_progress(
  xs,
  start = "0",
  end = "9999",
  limit = "1000000",
  query_part_1,
  query_part_2,
  query_part_3,
  query_part_4
)
```

Arguments

xs	XS
start	Start
end	End
limit	Limit
query_part_1	query_part_1
query_part_2	query_part_2
query_part_3	query_part_3
query_part_4	query_part_4

Value

A list of queries

Examples

```
NULL
```

save_histograms_progress *Save histograms progress*

Description

Save histograms progress

Usage

```
save_histograms_progress(xs)
```

Arguments

xs	XS

Value

Saved histograms

Examples

```
NULL
```

save_treemaps_progress *Save treemaps progress*

Description

Save treemaps progress

Usage

```
save_treemaps_progress(xs, type = "treemap")
```

Arguments

xs	XS
type	Type

Value

Saved treemaps

Examples

```
NULL
```

second_der *Second der*

Description

Second der

Usage

```
second_der(x, y)
```

Arguments

x	X
y	Y

Value

The second derivative

Examples

```
NULL
```

signal_sharpening *Signal sharpening*

Description

Signal sharpening

Usage

```
signal_sharpening(
  time,
  intensity,
  k2 = 250,
  k4 = 1250000,
  sigma = 0.05,
  Smoothing_width = 8,
  Baseline_adjust = 0
)
```

Arguments

time	time
intensity	intensity
k2	K2
k4	K4
sigma	Sigma
Smoothing_width	Smoothing width
Baseline_adjust	Baseline adjust

Value

A sharpened signal

Examples

```
NULL
```

---

tables_progress *Tables progress*

Description

Tables progress

Usage

```
tables_progress(xs, structures_classified)
```

Arguments

xs	XS
structures_classified	structures classified

Value

A list of tables

Examples

```
NULL
```

taxon_name_to_qid *Taxon name to QID*

Description

Taxon name to QID

Usage

```
taxon_name_to_qid(taxon_name)
```

Arguments

taxon_name	Taxon name

Value

A QID

Examples

```
## Not run:
taxon_name_to_qid(taxon_name = "Gentiana lutea")

## End(Not run)
```

transform_ms *Transform MS*

Description

Transform MS

Usage

```
transform_ms(x)
```

Arguments

x	X

Value

A list with transformed MS

Examples

```
NULL
```

`treemaps_progress` *Treemaps progress*

Description

Treemaps progress

Usage

```
treemaps_progress(xs, type = "treemap", hierarchies)
```

Arguments

`xs`	XS
`type`	Type
`hierarchies`	Hierarchies

Value

A list of treemaps

Examples

```
NULL
```

`treemaps_progress_no_title` *Treemaps progress no title*

Description

Treemaps progress no title

Usage

```
treemaps_progress_no_title(xs, type = "treemap", hierarchies)
```

Arguments

`xs`	XS
`type`	Type
`hierarchies`	Hierarchies

Value

A list of treemaps with no title

Examples

```
NULL
```

`wiki_progress` *Wiki progress*

Description

Wiki progress

Usage

```
wiki_progress(xs)
```

Arguments

xs	XS

Value

A list of results of Wikidata queries

Examples

```
NULL
```

`y_as_na` *Y as NA*

Description

Y as NA

Usage

```
y_as_na(x, y)
```

Arguments

x	x
y	y

Value

Y's replaced as NA's in X

Examples

```
NULL
```

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