Package: rtemisbio (via r-universe)

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Description Bio-informatics utilities

License GPL (>= 3)

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Contents

`rtemisbio-package` **rtemisbio***: Bioinformatics ops*

Description

Bioinformatics utilities

Author(s)

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`a3` *Create an* `a3` *object*

Description

Creates an `a3` object given amino acid sequence and annotations.

Usage

```
a3(
  seq,
  site = NULL,
  region = NULL,
  ptm = NULL,
  clv = NULL,
  variant = NULL,
  uniprotid = NULL,
  description = NULL,
  reference = NULL
)
```

Arguments

seq	Character: Amino acid sequence.
site	Named list of vectors of integer indices of sites, e.g. `list("N-terminal repeat" = c(46, 47, 52), "Microtubule binding domain" = c(244, 245, 246))`
region	Named list of integer indices, e.g. `list("Phosphodegron" = c(46, 47, 48, 49, 50, 51), "KXGS" = c(259, 260, 261, 262))` or character vectors with index range of regions in format `start:end`, e.g. `list(Phosphodegron = c("46:51", "149:154"), KXGS = c("259:262", "290:293"))`
ptm	Named list of vectors with indices of post-translational modifications, e.g. `list("Phosphorylation" = c(17, 18, 29, 30), "Acetylation" = c(148, 150, 163))`
clv	Named list of cleavage sites, e.g. `list(CTSL = c(54, 244, 319), CTSD = c(340, 391, 426))`
variant	List of lists with variant information. Each list must contain a `Position` element
uniprotid	Character: Uniprot ID.
description	Character: Description of the data / experiment.
reference	Character: Link to reference (journal publication, preprint, etc.)

Details

We choose to keep NULL elements as empty lists in JSON, since we want users to be able to easily add annotations, whether programmaticaly, using a web app, or manually.

Value

`a3` object

Author(s)

EDG

---

aa_sub *Perform amino acid substitutions*

Description

Perform amino acid substitutions

Usage

```
aa_sub(x, substitutions, verbosity = 1)
```

Arguments

x	Character or charactr vector: Amino acid sequence. e.g. "ARND" or c("A", "R", "N", "D")
substitutions	Character vector: Substitutions to perform in the format "OriginalPositionNew", e.g. c("C291A", "C322A")

Value

Character vector with substitutions performed.

Author(s)

EDG

---

aggregate.xt *Aggregate method for* xt *object*

Description

Aggregate method for xt object

Usage

```
## S3 method for class 'xt'
aggregate(
  x,
  groupname,
  fn = mean,
  backend = getOption("rt.backend", "base"),
  ...
)
```

Arguments

x	xt object.
fn	Function: Function to apply to each group.
backend	Character: "base", "data.table", or "dplyr"; backend to use for aggregation.
...	Additional arguments passed to fn.
group	Character: Grouping variable.

Author(s)

EDG

as.a3 *as.a3*

Description

as.a3

Usage

```
as.a3(x)
```

Arguments

x	Object to convert to a3.

Value

a3 object.

Author(s)

EDG

as.a3.default *as.a3*

Description

as.a3

Usage

```
## Default S3 method:
as.a3(x)
```

Arguments

x	Object to convert to a3.

Value

a3 object.

Author(s)

EDG

as.a3.list *as.a3.list method*

Description

as.a3.list method

Usage

```
## S3 method for class 'list'
as.a3(x)
```

Arguments

x	List: Named list with elements Sequence, Annotations, UniprotID. Annotations is a named list with possible elements Site, Region, PTM, Cleavage_site, Variant, Description, Reference.

Value

a3 object.

Author(s)

EDG

as.xt *as.xt*

Description

as.xt

Usage

```
as.xt(x)
```

Arguments

x	Object to convert to xt.

Value

xt object.

Author(s)

EDG

as.xt.default *as.xt*

Description

as.xt

Usage

```
## Default S3 method:
as.xt(x)
```

Arguments

x	Object to convert to xt.

Value

xt object.

Author(s)

EDG

as.xt.list *as.xt.list method*

Description

as.xt.list method

Usage

```
## S3 method for class 'list'
as.xt(x)
```

Arguments

x	List: Named list with elements x, y, y2, xunits, yunits, y2units, Description, Reference.

Value

xt object.

Author(s)

EDG

gene2sequence *Get the sequence of a gene*

Description

Get the sequence of a gene

Usage

```
gene2sequence(
  gene,
  organism = "hsapiens",
  biomart = "ensembl",
  host = "https://www.ensembl.org",
  seq_type = "coding",
  verbosity = 1
)
```

Arguments

gene	Character: Gene name.
organism	Character: Organism name.
biomart	Character: Biomart name.
host	Character: Host address.

Value

data.frame with columns "gene", "ensembl_transcript_id" and "sequence".

Author(s)

EDG

int2range *Convert integer range to character with colon separator*

Description

Convert integer range to character with colon separator

Usage

```
int2range(x)
```

Arguments

x	Integer vector. Must be consecutive integers from lowest to highest.

Value

Character with colon separator.

Author(s)

EDG

Examples

```
## Not run:
x <- 34:42
int2range(x)
int2range(28:34)
int2range(c(3, 4, 5, 6))
# This will throw an error:
int2range(c(3, 4, 5, 6, 8))

## End(Not run)
```

---

light_dark_ratio *Calculate light/dark ratio for* xt *object*

Description

Calculates light/dark ratio for each y and y2 timeseries in an xt object.

Usage

```
light_dark_ratio(
  x,
  groupname = "Lights",
  fn = mean,
  backend = getOption("rt.backend", "data.table"),
  ...
)
```

Arguments

x	xt object.
fn	Function: Function to apply to each group.
backend	Character: "base", "data.table", or "dplyr"; backend to use for aggregation.
...	Additional arguments passed to fn.

Value

data.frame with columns for group and summary statistic.

Author(s)

EDG

---

plot.a3 *Plot method for* a3 *object*

Description

Plot method for a3 object

Usage

```
## S3 method for class 'a3'
plot(x, ...)
```

Arguments

x	a3 object.
...	Additional arguments passed to rtemis::dplot3_protein.

Author(s)

EDG

---

plot.xt *Plot method for* xt *object*

Description

Plot method for xt object

Usage

```
## S3 method for class 'xt'
plot(x, ...)
```

Arguments

x	xt object.
...	Additional arguments passed to rtemis::dplot3_xt.

Author(s)

EDG

print.a3 *Print method for* a3 *object*

Description

Print method for a3 object

Usage

```
## S3 method for class 'a3'
print(x, head.n = 10, ...)
```

Arguments

x	a3 object.
...	Not used.

Author(s)

EDG

print.xt *Print method for* xt *object*

Description

Print method for xt object

Usage

```
## S3 method for class 'xt'
print(x, head.n = 10, ...)
```

Arguments

x	xt object.
...	Not used.

Author(s)

EDG

read.a3json *Read* a3 *object from JSON file*

Description

Read a3 object from JSON file

Usage

```
read.a3json(filepath, verbosity = 0L)
```

Arguments

filepath	Character: Path to JSON file.
verbosity	Integer: if greater than 0, print messages.

Value

a3 object.

Author(s)

EDG

read.xtjson *Read* xt *object from JSON file*

Description

Read xt object from JSON file

Usage

```
read.xtjson(filepath, verbosity = 0L)
```

Arguments

filepath	Character: Path to JSON file.
verbosity	Integer: if greater than 0, print messages.

Details

Note that factors saved under group are written as character by write.xtjson and when they are read back in, they are converted back to factors using factor. This means that the levels will be set alphabetically. If needed, reorder them after reading in the JSON file using factor.

Value

xt object.

Author(s)

EDG

---

summary.a3 *Summary method for* a3 *object*

Description

Summary method for a3 object

Usage

```
## S3 method for class 'a3'
summary(object, ...)
```

Arguments

object	a3 object.

Author(s)

EDG

---

toxt *Create an* xt *object*

Description

Creates an xt object from time series data.

Usage

```
toxt(
  x,
  y,
  x2 = NULL,
  y2 = NULL,
  zt = NULL,
  shade = NULL,
  group = NULL,
  xunits = NULL,
```

```
  yunits = NULL,
  y2units = NULL,
  description = NULL,
  reference = NULL
)
```

Arguments

x	Named list of datetime vectors.
y	Named list of numeric vectors: When plotted, these will correspond to the left y-axis.
x2	Named list of datetime vectors: When plotted, these will correspond to the right x-axis. If not provided, x will be used for both y and y2.
y2	Named list of numeric vectors: When plotted, these will correspond to the right y-axis.
zt	Numeric vector: Zeitgeber time. If provided, this will be used to label x-axis ticks. Assumes a single datetime vector in x. Elements in zt must correspond to elements in x.
shade	Binary vector: 0 indicates no shading, 1 indicates shading. If provided, this will be used to shade the plot.
group	Named list of factors: Grouping variable(s).
xunits	Character: Units for x.
yunits	Character: Units for y.
y2units	Character: Units for y2.
description	Character: Description of the data / experiment.
reference	Character: Link to reference (journal publication, preprint, etc.)

Value

xt object

Author(s)

EDG

---

uniprot_get *Get protein sequence from UniProt*

Description

Get protein sequence from UniProt

Usage

```
uniprot_get(
  accession,
  baseURL = "https://rest.uniprot.org/uniprotkb",
  verbosity = 1
)
```

Arguments

accession	Character: UniProt Accession number - e.g. "Q9UMX9"
baseURL	Character: UniProt rest API base URL. Default = "https://rest.uniprot.org/uniprotkb"
verbose	Logical: If TRUE, print messages to console

Value

List with two elements: Annotation & Sequence

Author(s)

E.D. Gennatas

Examples

```
## Not run:
mapt <- uniprot_get("Q9UMX9")

## End(Not run)
```

---

write.a3json *Write* a3 *object to JSON file*

Description

Write a3 object to JSON file

Usage

```
write.a3json(x, filepath, overwrite = FALSE)
```

Arguments

x	a3 object, as created by as.a3().
filepath	Character: Path to save JSON file.

Author(s)

EDG

`write.xtjson` *Write* `xt` *object to JSON file*

Description

Write `xt` object to JSON file

Usage

```
write.xtjson(x, filepath, overwrite = FALSE)
```

Arguments

`x`	`xt` object, as created by toxt or as.xt.
`filepath`	Character: Path to save JSON file.

Author(s)

EDG

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