Package 'disprose'

October 13, 2022

Type Package
Title Discriminating Probes Selection
Version 0.1.6
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Description Set of tools for molecular probes selection and design of a microarray, e.g. the assessment of physical and chemical properties, blast performance, selection according to sensitivity and selectivity. Methods used in package are described in: Lorenz R., Stephan H.B., Höner zu Siederdissen C. et al. (2011) <doi:10.1186 1748-7188-6-26="">; Camacho C., Coulouris G., Avagyan V. et al. (2009) <doi:10.1186 1471-2105-10-421="">.</doi:10.1186></doi:10.1186>
License GPL-3
Encoding UTF-8
Language en-us
LazyData true
Suggests BBmisc, biomartr, curl, DBI, dplyr, rentrez, reutils, RSQLite, stats, stringr, seqinr, TmCalculator, utils, XML
Depends R (>= $3.5.0$)
RoxygenNote 7.1.2
NeedsCompilation no
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Repository CRAN
Date/Publication 2022-03-18 23:30:02 UTC
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add_adapters

Add adapters to probes

Description

Add set of adapters to oligonucleotide probes

Usage

```
add_adapters(
  probe.id.var,
  probe.var,
  ad.len,
  ad.nucl = "t",
  end = c(3, 5),
  mc.cores = 1,
  digits = 4,
  return = "dataframe",
  data,
  data.probe.id.var,
```

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```
count.mfe = FALSE,
RNAfold.path,
temperature = 40,
trim.mfe = FALSE,
MFEmin = 0,
MFE.files.dir = NULL,
delete.MFE.files = FALSE,
verbose = TRUE
)
```

Arguments

probe.id.var vector of probes' identification numbers

probe.var character; character; vector of nucleotide probes

ad.len integer; vector of adapter length

ad.nucl character; vector of adapter nucleotides

end integer; probe's end for adapter attachment. Possible values are 3 and 5.

mc.cores integer; number of processors for parallel computation (not supported on Win-

dows)

digits integer; number of decimal places to round the result (MFE)

return character; returned object; possible values are: "vector" (vector of nucleotide

probes with added adapters), "dataframe" (data frame with probes, adapters and their characteristics), "add" (user's data frame with added data of probes,

adapters and their characteristics)

data, data.probe.id.var

user's data frame and it's variable with probes identification numbers (used if

return = "add")

count.mfe logical; count minimum folding energy for probes with adapters

RNAfold.path, temperature, trim.mfe, MFEmin, MFE.files.dir, delete.MFE.files

used if count.mfe = TRUE; see count_MFE[disprose] for details

verbose logical; show messages

Details

ad.len parameter indicates number of ad.nucl repeats. For example, with ad.len =5 for ad.nucl = "t" adapter will be "ttttt" and for ad.nucl = "ac" adapter will be "acacacacac".

ad.len, ad.nucl and end might be vectors of any length. All possible variants of adapters will be added to probes and tested.

For MFE counting ViennaRNA Package (UNIX or Windows) must be installed. see count_MFE[disprose] for details

Value

Vector of nucleotide probes with added adapters, or data frame with probes, adapters and their characteristics, or user's data frame with added data of probes, adapters and their characteristics.

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Author(s)

Elena N. Filatova

Examples

ann.data

Chlamydia pneumoniae genome annotation.

Description

A dataset containing Chlamydia pneumoniae TW-183 (complete sequence, NC_005043.1.) genome annotation

Usage

ann.data

Format

```
A data frame with 2218 rows and 9 variables:
```

```
seqid sequence identification number source source database name type type of annotated region start region's start position end region's end position score score strand strand phase phase attribute region description
```

Source

```
https://www.ncbi.nlm.nih.gov/
```

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annotate_probes

Annotate probes

Description

Get genome annotation for oligonucleotide sequence

Usage

```
annotate_probes(
  source = "data.frame",
  ann.data = NULL,
 gff.path = NULL,
 org.name,
  db = "refseq",
  refs = TRUE,
  probe.id.var,
  probe.start.var,
  probe.stop.var,
  file.annot = NULL,
  save.format = "txt",
  sep = ";",
  return = "add.resume",
  priority = c("CDS", "gene", "region"),
  data.probe.id.var,
  delete.downloads = FALSE,
  verbose = TRUE
)
```

Arguments

source

```
character; genome annotation source. Possible values are: "data.frame" (from
                  data frame), "giff" (from GIFF file), "load" (download from NCBI with get-
                  GFF function)
ann.data
                  genome annotation data frame
                  character; .gff file name and path
gff.path
                  character; the scientific name of the organism of interest
org.name
db
                  character; database from which the genome shall be retrieved; possible values
                  are "refseq", "genbank", "ensembl"
                  logical; download genome if it isn't marked in the database as either a reference
refs
                  or a representative genome
                  vector of probes' identification numbers
probe.id.var
probe.start.var, probe.stop.var
                  integer; vector of probes' start and end coordinates
```

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character; resulting annotation file name and path file.annot save.format character; format of resulting annotation file; possible values are "txt", "csv" character; field separator string sep character; returned object; possible values are: "annotation" (annotation data return frame), "resume" (annotation attributes only), "add.resume" (user's data frame with added annotation attributes) priority character; vector of sequence ontology types that should be returned in resume in the first place data, data.probe.id.var users data frame and probes' identification variable in it (used if return = "add.resume") delete.downloads logical; delete files that were downloaded from NCBI

verbose logical; show messages

Details

This function uses boimartr genome annotation retrieval instruments. See getGFF for details. If retrieval is not available, GFF file may be used.

This function creates annotation ".txt" or ".csv" file. By default file is created in working directory. Optionally function returns annotation resume, i.e. annotation attribute for specified sequence ontology (SO). Priorities of SOs are set by user in priopity parameter. For example, if priopity = c("CDS", "gene", "region"), the function returns resume for "CDS" SO, if there are none for "gene" CO etc. If there are several attributes meet priority, the first annotation attribute is returned. If none of priority COs found, the first annotation attribute is returned.

Number of found annotations are indicated in returned data ("ann.n" column).

Value

Annotation data frame, or annotation attributes, or user's data frame with added annotation attributes. Also annotation file is created.

Author(s)

Elena N. Filatova

Examples

```
path<-tempdir()</pre>
dir.create(path) # create temporal directory
data(ann.data) # load genome annotation data frame
annotation<-annotate_probes(source = "data.frame", ann.data = ann.data,</pre>
                probe.id.var = 1:5,
                probe.start.var = c(1, 100, 200, 300, 400),
                probe.stop.var = c (99, 199, 299, 399, 499),
                file.annot = paste0(path, "/annotation.txt"), save.format = "txt",
                return = "resume")
file.remove(paste0(path, "/annotation.txt")) # delete files
unlink(path, recursive = TRUE)
```

blast.fill 7

blast.fill

Local BLAST results with added content.

Description

Result of BLAST of 5 probes against local database of target nucleotide sequences of Chlamydia pneumoniae. Local BLAST was performed with blast_local () function. Subjects' Genbank Identifiers are added with fill_blast_result () function.

Usage

blast.fill

Format

A data frame with 72 rows and 19 variables:

probe probe sequence

probe.length probe sequence's length

Qid query identification number

Qstart query start position

Qend query end position

Rgi subject GenInfo Identifier number

Racc subject NCBI accession number

Rtitle subject title

Rtaxid subject taxon identificator

Rstart subject start position

Rend subject end position

alig.length length of alignment

mismatch amount of mismatches

gaps amount of gaps

ident.number amount of identical positions

score alignment score

bitscore alignment bitscore

Evalue alignment e-value

Qcover query coverage, %

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blast.raw

Local BLAST results.

Description

Result of BLAST of 5 probes against local database of target nucleotide sequences of Chlamydia pneumoniae. Local BLAST was performed with blast_local () function.

Usage

blast.raw

Format

A data frame with 72 rows and 19 variables:

probe probe sequence

probe.length probe sequence's length

Qid query identification number

Qstart query start position

Qend query end position

Rgi subject GenInfo Identifier number

Racc subject NCBI accession number

Rtitle subject title

Rtaxid subject taxon identificator

Rstart subject start position

Rend subject end position

alig.length length of alignment

mismatch amount of mismatches

gaps amount of gaps

ident.number amount of identical positions

score alignment score

bitscore alignment bitscore

Evalue alignment e-value

Qcover query coverage, %

blast_local 9

blast_local

Local BLAST

Description

Perform nucleotide BLAST with local database

Usage

```
blast_local(
  probe.var,
 probe.id.var = NULL,
  fasta.way = NULL,
 blastn.way = NULL,
 db.way = NULL,
 out.way = NULL,
 mc.cores = 1,
 add.query.info = FALSE,
  temp.db = NULL,
 delete.files = FALSE,
  eval = 1000,
 ws = 7,
  reward = 1,
 penalty = -3,
  gapopen = 5,
 gapextend = 2,
 maxtargetseqs = 500,
  verbose = TRUE
)
```

Arguments

probe.var	character; query - vector of nucleotide sequences
probe.id.var	vector of identification numbers for query sequences
fasta.way	character; name and path to FASTA file
blastn.way	character; name and path to blastn executable file
db.way	character; name and path to local BLAST database
out.way	character; name and path to blastn output file
mc.cores	integer; number of processors for parallel computation (not supported on Windows)
${\it add.} {\it query.} \\ {\it info}$	logical; add query nucleotide sequence and its length to result
temp.db	character; temporal SQLite database name and path
delete.files	logical; delete created FASTA and output files
eval	integer; expect value for saving hits

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ws integer; length of initial exact match
reward integer; reward for a nucleotide match
penalty integer; penalty for a nucleotide mismatch

gapopen integer; cost to open a gap gapextend integer; cost to extend a gap

maxtargetseqs integer; number of aligned sequences to keep

verbose logical; show messages

Details

For this function BLAST+ executables (blastn) must be installed and local nucleotide database must be created.

While working, the function creates blastn input FASTA file and output file. If files exist already, they will be overwritten. Those files could be deleted by delete.files = TRUE parameter.

If no probe.id.var is provided, query sequences are numbered in order, starting with 1.

Query cover is query coverage per HSP (as a percentage)

If add.query.info = TRUE function saves data in temporal SQLite database. Function will stop if same database already exists, so deleting temporal database (by setting delete.files = TRUE) is highly recommended.

"no lines available in input" error is returned when there are no BLAST results matching the specified parameters. Adjust BLAST parameters.

Value

Data frame with BLAST alignments: query sequence id, start and end of alignment in query, subject GI, accession, title and taxon id, start and end of alignment in subject, length of alignment, number of mismatches and gaps, number of identical matches, raw score, bit score, expect value and query cover. If add.result.info = TRUE, query sequence and its length are also added to data frame.

Author(s)

Elena N. Filatova

References

Camacho C., Coulouris G., Avagyan V. et al. (2009). BLAST+: architecture and applications. BMC Bioinformatics 10, 421. https://bmcbioinformatics.biomedcentral.com/articles/10.1186/1471-2105-10-421.

Examples

```
## Not run:
# This function is using BLAST applications. BLAST+ should be installed.
# Local nucleotide database should be created
# Local database of target sequences of Chlamydia pneumoniae was created
# in temporal directory previously (see make_blast_DB () function)
path <- tempdir()</pre>
```

count_PhCh

Calculate physical and chemical properties

Description

Calculates GC-content, detects several nucleotides in a row, calculates minimum folding energy and melting temperature for oligonucleotide probes.

Usage

```
count_PhCh(
  probe.var,
  trim = FALSE,
  data,
  digits = 4,
 mc.cores = 1,
 MFE.files.dir = NULL,
  delete.MFE.files = FALSE,
  GCmin = 40,
  GCmax = 60,
  nucl.pattern = c("a", "t", "g", "c"),
  n.crit = 5,
  RNAfold.path,
  temperature = 40,
  MFEmin = -3,
  TD.params = NULL,
  TMmin = 55,
  TMmax = 60,
  verbose = TRUE,
  Na = 50,
  K = 0,
  Tris = 0,
  Mg = 0,
```

```
dNTPs = 0
count_GC(
  probe.var,
  trim.gc = FALSE,
 GCmin = 40,
 GCmax = 60,
 mc.cores = 1,
  add.to.data = FALSE,
 data,
  digits = 4
count_REP(
  probe.var,
  trim.rep = FALSE,
 nucl.pattern = c("a", "t", "g", "c"),
 n.crit = 5,
 mc.cores = 1,
 add.to.data = FALSE,
 data
)
count_MFE(
  probe.var,
 RNAfold.path,
  temperature = 40,
  trim.mfe = FALSE,
 MFEmin = -3,
  add.to.data = FALSE,
  data,
 MFE.files.dir = NULL,
  delete.MFE.files = FALSE,
 mc.cores = 1,
 digits = 4,
  verbose = TRUE
)
count_TM(
  probe.var,
 TD.params = NULL,
  trim.tm = FALSE,
  TMmin = 55,
  TMmax = 60,
  add.to.data = FALSE,
  data,
  digits = 4,
```

```
mc.cores = 1,
verbose = TRUE,
Na = 50,
K = 0,
Tris = 0,
Mg = 0,
dNTPs = 0
)
```

Arguments

probe.var character; vector of nucleotide probes trim, trim.gc, trim.rep, trim.mfe, trim.tm

logical; whether to select results that meet the criterion

digits integer; number of decimal places to round the result

mc.cores integer; number of processors for parallel computation (not supported on Win-

dows)

MFE. files.dir character; directory for RNAfold input and output files

delete.MFE.files

logical; delete RNAfold input and output files

GCmin, GCmax numeric; minimum and maximum value of GC-content (percent, used if trim =

TRUE)

nucl.pattern character; vector of nucleotide pattern

n.crit integer; minimal amount of nucleotide pattern's repeats in a row to detect

RNAfold.path character; name and path to RNAfold executable file

temperature numeric; folding design temperature

MFEmin numeric; maximum value of folding energy (used if trim = TRUE)

TD. params character; vector of length 4, contains designation for four tables with thermo-

dynamic values (nn_table - thermodynamic NN values, tmm_table - thermodynamic values for terminal mismatches, imm_table - thermodynamic values for internal mismatches, de_table - thermodynamic values for dangling ends). See

Tm_NN for details.

TMmin, TMmax numeric; minimum and maximum value of melting temperature (used if trim =

TRUE)

verbose logical; show messages

Na numeric; millimolar concentration of Na, default is 50 (used for count_TM func-

tion)

K numeric; millimolar concentration of K, default is 0 (used for count_TM func-

tion)

Tris numeric; millimolar concentration of Tris, default is 0 (used for count_TM func-

tion)

Mg numeric; millimolar concentration of Mg, default is 0 (used for count_TM func-

tion)

dNTPs numeric; millimolar concentration of dNTPs, default is 0 (used for count_TM function)

add.to.data, data

logical; add result vector to specified data frame (used unconditionally if trim = TRUE)

Details

GC-content trimming selects results that are between GCmin and GCmax (inclusive). Nucleotides' amount trimming deletes probes that contain n.crit or more of same nucleotides (pattern) in a row. Minimum folding energy trimming selects results that are equal or more than MFEmin. Melting temperature trimming selects results that are between TMmin and TMmax (inclusive).

This function is using ViennaRNA service to count minimum folding energy. ViennaRNA Package (UNIX or Windows) must be installed. While counting MFE, working directory is set to MFE.files.dir and input and output files for ViennaRNA ("seq_in" and "seq_out") are created in the working directory. Afterwards the working directory is changed back to user's setting. If no MFE.files.dir exists it is created and is not deleted even if delete. MFE.files = TRUE.

Melting temperature is counted with Tm_NN function. Indication of thermodynamic values must be provided. By default they are: nn_table = "DNA_NN4", tmm_table = "DNA_TMM1", imm_table = "DNA_IMM1", de_table = "DNA_DE1".

Value

If trim = FALSE, count_PhCh function returns data frame with GC-count (GC.percent), nucleotide repeats (repeats, TRUE/FALSE), minimum folding energy (MFE) and melting temperature (TM) columns. If trim = TRUE, count_PhCh function returns provided data frame with attached four columns and rows selected according to values GCmin, GCmax, n.crit, MFEmin, TMmin, TMmax.

If trim.gc=FALSE, count_GC function returns GC.percent vector or data with attached GC.percent column (when add.to.data = TRUE). If trim.gc = TRUE, count_GC function returns provided data frame with attached GC.percent column and rows selected according to GCmin, GCmax values.

If trim.rep = FALSE, count_REP function returns repeats vector (logical; TRUE/FALSE - there are/there are no nucleotide repeats) or data with attached repeats column (when add.to.data = TRUE). If trim.rep = TRUE, count_REP function returns provided data frame with attached repeats column and rows selected according to n.crit value.

If trim.mfe = FALSE, count_MFE function returns MFE vector or data with attached MFE column (when add.to.data = TRUE). If trim.mfe = TRUE, count_MFE function returns provided data frame with attached MFE column and rows selected according to MFEmin value.

If trim.tm = FALSE, count_TM function returns TM vector or data with attached TM column (when add.to.data = TRUE). If trim.tm = TRUE, count_TM function returns provided data frame with attached TM column and rows selected according to TMmin, TMmax values.

Functions

- count_PhCh: Calculates GC.percent, detects several nucleotides in a row, calculates minimum folding energy and melting temperature
- count_GC: Calculates GC-content (percent)
- count_REP: Detects several nucleotides in a row

- count_MFE: Calculates minimum folding energy
- count_TM: Calculates melting temperature

Author(s)

Elena N. Filatova

References

Lorenz R., Stephan H.B., Höner zu Siederdissen C. et al. (2011). ViennaRNA Package 2.0. Algorithms for Molecular Biology, 6, 1. https://almob.biomedcentral.com/articles/10.1186/1748-7188-6-26.

Examples

```
probes <- data.frame (ids = 1:3, probes = c ("acacacacacaca", "aaaaagggggtttttcccc",</pre>
                                               "atgcgctagctcagc"))
probes <- count_GC (probe.var = probes$probes, trim.gc = FALSE, GCmin = 40, GCmax = 60,</pre>
                   add.to.data = TRUE, data = probes)
probes <- count_REP (probe.var = probes$probes, trim.rep = FALSE, n.crit = 5,</pre>
                     add.to.data = TRUE, data = probes)
## Not run:
# This function is using ViennaRNA service. ViennaRNA Package must be installed.
MFE.files.dir <- tempdir()</pre>
probes <- count_MFE (probe.var = probes$probes, RNAfold.path = "D:/Vienna/RNAfold.exe",</pre>
                     temperature = 40, trim.mfe = FALSE, MFEmin = 0,
                    MFE.files.dir = MFE.files.dir, delete.MFE.files = TRUE,
                     add.to.data = TRUE, data = probes, mc.cores = 1)
unlink (MFE.files.dir, recursive = TRUE)
## End(Not run)
probes <- count_TM (probe.var = probes$probes, TD.params = NULL, trim.tm = FALSE,</pre>
                   TMmin = 55, TMmax = 60, add.to.data = TRUE, data = probes,
                   digits = 4, mc.cores = 1)
# All in one command
## Not run:
# This function is using ViennaRNA service. ViennaRNA Package must be installed.
MFE.files.dir <- tempdir()</pre>
probes2 <- count_PhCh (probe.var = probes$probes, trim = FALSE,</pre>
                      nucl.pattern = c ("a", "t", "g", "c"), n.crit = 5,
                      MFE.files.dir = MFE.files.dir, delete.MFE.files = TRUE,
                       RNAfold.path = "D:/Vienna/RNAfold.exe", temperature = 40,
                       TD.params = NULL, digits = 3, mc.cores = 1,
                       data = probes)
unlink (MFE.files.dir, recursive = TRUE)
## End(Not run)
```

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cut_probes

Cut probes

Description

Generate probes from nucleotide reference sequences

Usage

```
cut_probes(
  ref.seq.from.file = FALSE,
  ref.seq.id,
  ref.seq.db,
  fasta.file = NULL,
  delete.fasta = FALSE,
  start = 1,
  stop = NULL,
  start.correction = FALSE,
  size = 24:32,
  delete.incomplete = FALSE,
  delete.identical = FALSE,
  give.probes.id = FALSE,
 mc.cores = 1,
  verbose = TRUE
)
```

Arguments

```
ref.seq.from.file
                  logical; read reference sequences from file (TRUE) or download them from NCBI
                  data base (FALSE).
ref.seq.id
                  identification number of reference nucleotide sequences. Only used when ref.seq.from.file
                  = FALSE. GenBank accession numbers, GenInfo identifiers (GI) or Entrez unique
                  identifiers (UID) may be used.
                  character; NCBI database for search. See entrez_dbs for possible values. Only
ref.seq.db
                  used when ref.seq.from.file = FALSE.
fasta.file
                  character; FASTA file name and path, only used when ref.seq.from.file =
                  TRUE.
delete.fasta
                  logical; delete FASTA file.
start, stop
                  integer; number of first and last nucleotide of the reference sequence's segment
                  that should be cut into probes. All sequence is used by default.
start.correction
                  logical; count probes' start and stop nucleotides relatively to the specified seg-
                  ment (FALSE) or to the whole sequence (TRUE). Only used if start>1.
size
                  integer; vector of probe size
```

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Details

This function takes nucleotide sequences and cut them on segments (probes) of given size. Sequences might be downloaded from given FASTA file or from NCBI data bases. In the latter case, FASTA file is created. If desired, FASTA file can be deleted after.

Not all sequence must be cut on probes, you may define needed segment by start and stop parameters. Note that in this case probes' start and stop nucleotides would be counted relatively to the specified segment (start.correction = FALSE) or to the whole sequence (start.correction = TRUE).

Undeciphered nucleotides are the one that are indicated by "rywsmkhbvdn" symbols.

Probes' identification numbers are created by adding numeric indexes to reference sequence's identification number.

See cut_string, delete_duplicates_DF and make_ids for details.

Value

Data frame with probe id (optionally), sequence id, probe size, start and stop nucleotide, sequence.

Author(s)

Elena N. Filatova

Examples

cut_string

Cut string into segments

Description

Cuts character string into segments of given size.

Usage

```
cut_string(string, size)
```

Arguments

string character string; vector of length 1
size integral; vector of length of segments

Details

This function works with one string only. Segments are cut from start to end of a string. size might be a vector of any length, all possible variants will be cut.

Value

Data frame with segment size, start and end point, segment string.

Author(s)

Elena N. Filatova

Examples

```
cut_string (string = "aaatttttttccgc", size = 12:14)
```

Description

Delete data frame rows if they contain duplicated values.

Usage

```
delete_duplicates_DF(
  data,
  duplicated.var,
  exact = FALSE,
  stay = "first",
  choose.var,
  choose.stay.val,
  pattern,
  mc.cores = 1,
  verbose = TRUE
)
```

Arguments

data data frame; duplicated.var variable that contains duplicated values exact logical; values are to be matched as is character; which row with duplicated values will stay; possible values are "first" stay (first of rows), "choose" (depending of the value of other variable) and "none" (rows with values that contain pattern will be removed) choose.var, choose.stay.val vector of additional variable to choose the preferred row and it's preferred value (used if stay = "choose") pattern deleted pattern (used if stay = "none") integer; number of processors for parallel computation (not supported on Winmc.cores logical; show messages verbose

Details

This function checks if there are repeated values in the data frame (in the duplicated.var). If repeated values are found, the first row with duplicated value stays, others are deleted (if stay = "first"). If stay = "choose" the first row with duplicated values and choose.var = choose.stay.val will stay. If there are no rows with choose.var = choose.stay.val, the first row will stay.

If stay = "none" all rows with values that contain pattern will be removed.

Value

Data frame without rows that contain duplicates in duplicated.var

Author(s)

Elena N. Filatova

20 fill_blast_result

Examples

fill_blast_result

Complement BLAST result

Description

Provides subjects' GenInfo Identifiers if BLAST alignment result does not contain one.

Usage

```
fill_blast_results(
  blast.result,
  AcNum.column.name = "Racc",
 GI.column.name = "Rgi",
  delete.version = FALSE,
  version.sep = ".",
  add.gi = "DB",
  add.gi.df,
  temp.db = NULL,
  delete.temp = FALSE,
  add.gi.db = NULL,
  add.gi.table = NULL,
  add.gi.ac.column.name = "AC",
  add.gi.gi.column.name = "GI",
 mc.cores = 1,
  verbose = TRUE
)
delete_AcNum_version(ac.num.var, version.sep = ".", mc.cores = 1)
```

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Arguments

blast.result data frame; BLAST alignment result

AcNum.column.name, GI.column.name

character; name of column with subject accession numbers and GenInfo Identi-

fier numbers from BLAST result data frame

delete.version logical; remove version suffix from subject accession number

version.sep character; accession number and version suffix separator (a dot for NCBI acces-

sion numbers)

add.gi character; table with linked accession and GI numbers is taken from SQLite

database ("DB") or data frame ("DF")

add.gi.df data frame with table (used if add.gi = "DF")

temp.db character; temporal SQLite database name and path
delete.temp logical; delete created temporal SQLite database

add.gi.db, add.gi.table, add.gi.ac.column.name, add.gi.gi.column.name

SQLite database name and path, table name and name of columns with accession

and GI numbers (used if add.gi = "DB")

mc.cores integer; number of processors for parallel computation (not supported on Win-

dows)

verbose logical; show messages ac.num.var vector of accession numbers

Details

BLAST alignment, performed with local database, may not contain subject GI information. Also subject accession may contain version suffix. This can make it difficult to analyze the results further. This function adds subject GI and removes subject accession version suffix.

To add GI GenInfo Identifiers table with them linked to accession numbers must be provided as data frame or SQLite database table. add.gi.df must be a data frame with column one - accession numbers, column two - GenInfo Identifier numbers. If add.gi = "DF" temporal SQLite database is created.

SQLite database table with accession and GI numbers should not contain duplicated rows. It is also highly recommended to index accession numbers' variable in database.

delete.version executes in the first step, so if you use this option accession numbers in add.gi table must not contain version suffix.

AcNum.column.name, GI.column.name, add.gi.ac.column.name and dd.gi.gi.column.name must be column names exactly as in data frame.

Value

blast.result data frame with added GI and deleted accession version suffix.

Functions

- fill_blast_results: Provides subjects' Genbank Identifiers if BALST alignment result does not contain one
- delete_AcNum_version: Remove accession version suffix

get_GA_files

Author(s)

Elena N. Filatova

Examples

get_GA_files

Read GISAID sequence file

Description

Get metadata and nucleotide sequence from GISAID files

Usage

```
get_GA_files(
   dir.path,
   return = "both",
   seq.return = "data.frame",
   fasta.file = NULL,
   verbose = TRUE
)
```

Arguments

dir.path	character; directory name and path
return	character; type of returned object; possible values are: "info" (sequence metadata), "seq" (nucleotide sequences), "both" (both of them).
seq.return	character; sequence returned object; possible values are "vector", "data.frame" and "fasta"
fasta.file	character; FASTA file name and path, only used if return = "fasta"
verbose	logical; show messages

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Details

This function works with downloaded from GISAID "Input for the Augur pipeline" archives (with "metadata.tsv" and "sequences.fasta" files). Archives must be unzipped before usage. All extracted from GISAID archive files must be in one directory.

If return = "seq", serial numbers are used as sequence identification numbers.

Metadata is transformed into data frame of the same format as get_seq_info function does. Sequences are transformed into data type of the same format as get_seq_for_DB function does.

Value

List of length two, where first is metadata and second is nucleotide sequence. If return = "info" or return = "seq" only first or second element is returned.

Author(s)

Elena N. Filatova

Examples

```
## Not run:
# First download some sequences' archives from GISAID (https://www.gisaid.org/)
# unzip them and put into "gisaidfiles" directory

res <- get_GA_files (dir.path = "gisaidfiles", return = "info")
res <- get_GA_files (dir.path = "gisaidfiles", return = "seq", seq.return = "data.frame")
res <- get_GA_files (dir.path = "gisaidfiles", return = "both", seq.return = "fasta")

## End(Not run)</pre>
```

get_GIs

Get GenInfo Identifier numbers

Description

Retrieves NCBI sequence identifiers (GIs) for given organism name or taxon identifier.

Usage

```
get_GIs(
  org.name,
  db,
  n.start = 1,
  n.stop = NULL,
  step = 99999,
  return.vector = TRUE,
  check.result = FALSE,
```

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```
term = NULL,
  temp.dir = NULL,
  delete.temp = FALSE,
  verbose = TRUE
)
get_GIs_fix(
  gis.list,
 org.name,
  db,
  n.start = 1,
  n.stop = NULL,
  step = 99999,
  term = NULL,
  temp.dir = NULL,
  delete.temp = FALSE,
  verbose = TRUE
)
```

Arguments

org.name

	ganism/taxon.
db	character; NCBI database for search. See entrez_dbs() for possible values.
n.start	integer; download starting value. Default is 1.
n.stop	integer; download finishing value. Default is NULL, which provides retrieval of all available GIs.
step	integer; download increment value.
return.vector	logical; whether to return GI numbers as character vector (another variant is list of vectors).
check.result	logical; check if download was done correctly.
term	character; search query.
temp.dir	character; name and path of directory for downloaded temporary files (only for "Windows" OS)
delete.temp	logical; delete downloaded files (only for "Windows" OS, does not delete directory).
verbose	logical; show messages
gis.list	list of previously downloaded GIs vectors.

character; scientific name or taxon identifier (written as "txid0000") of the or-

Details

This function sends the query to NCBI database and returns sequence identifiers according to the query. By default the query is organism, so the function returns GI numbers for all sequences that are associated with the requested organism. For example, if org.name = "Homo sapiens" the function will download GI numbers for all sequences that answer the query "Homo sapiens[Organism]". For any other query use parameter term.

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The function downloads GI numbers by piecemeal, by several pieces in one block. The size of the block is defined by parameter step. It is useful if by any reason the download was interrupted, so later it is possible to reload only the missing blocks without the need to reload the entire amount of data. By default, all available GI numbers are downloaded, but you may also choose start and finish notes by specifying the parameters n. start and n. stop. The numeration starts with 1, not 0. At the end the resulting list of blocks (list of character vectors) is unlisted into one character vector. You may prevent this by setting return.vector = FALSE. Also, regardless of return.vector settings, the list of blocks is returned if the download was somehow compromised.

If download was corrupted you may use get_GIs_fix() function to reload the missing block. The corrupted list of blocks should be set in gis.list parameter. You may also check and reload data when get_GIs() function is running by specifying check.result = TRUE.

The function checks for user's OS type. For Windows temporal files are created while downloading, so temp.dir and delete.temp parameters should be set. This helps to solve the "routines:SSL23_GET_SERVER_HELLO:tlsv1 alert protocol version" problem by using curl instead of RCurl. However it slows down the function. If there is no temp.dir directory, it will be created and will not be removed (only temporal files will be deleted if delete.temp = TRUE).

In progress the functions turn off and on scientific notation.

Value

get_GIs() returns character vector of GI numbers. If return.vector = FALSE or there are missing data, list of character vectors is returned.

get_GIs_fix() returns list of character vectors.

Functions

- get_GIs: Retrieves NCBI sequence identifiers (GIs) for given organism name or taxon identifier.
- get_GIs_fix: Checks the downloads and tries to retrieve the compromised data.

Author(s)

Elena N. Filatova

Examples

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Description

Retrieves nucleotide sequences from NCBI for given identification numbers.

Usage

```
get_seq_for_DB(
   ids,
   db,
   check.result = FALSE,
   return = "data.frame",
   fasta.file = NULL,
   exclude.from.download = FALSE,
   exclude.var,
   exclude.pattern,
   exclude.fixed = TRUE,
   verbose = TRUE
)
```

Arguments

ids vector of NCBI sequences' identification numbers: GenBank accession num-

bers, GenInfo identifiers (GI) or Entrez unique identifiers (UID)

db character; NCBI database for search. See entrez_dbs() for possible values

check.result logical; check if download was done correctly

return character; sequence returned object; possible values are "vector", "data.frame"

and "fasta"

fasta.file character; FASTA file name and path, only used if return = "fasta"

exclude.from.download

logical; ignore some sequences while downloading

exclude.var vector that is used to define which sequences should be ignored, only used if

exclude.from.download = TRUE.

exclude.pattern

value that matches to exclude.var and marks unwanted sequences, only used

if exclude.from.download = TRUE

exclude.fixed logical; match exclude.pattern as is, only used if exclude.from.download

= TRUE.

verbose logical; show messages

res.data data.frame; data frame of nucleotide ids and previously downloaded sequences

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Details

Master records (for example, in WGS-project) do not contain any nucleotide. They might be excluded from download with exclude.from.download parameters. However this has no affect and such ids do not have to be excluded when loading.

If writing FASTA to existing FASTA file, sequences are appended.

Value

If return = "vector" function returns vector of nucleotide sequences, return = "data.frame" - data frame with nucleotide ids and nucleotide sequences, return = "fasta" - writes FASTA file, no data returned.

Functions

- get_seq_for_DB: Retrieves NCBI nucleotide sequences for given identification numbers.
- get_seq_for_DB_fix: Checks the downloads and tries to retrieve the compromised data.

Author(s)

Elena N. Filatova

Examples

get_seq_info

Get NCBI sequence record

Description

Retrieves information about sequences from NCBI records for given organism name or taxon identifier.

Usage

```
get_seq_info(
  org.name,
  db,
  n.start = 1,
  n.stop = NULL,
  step = 500,
  return.dataframe = FALSE,
```

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```
check.result = FALSE,
  term = NULL,
  verbose = TRUE
)
get_seq_info_fix(
  info.list,
 web.history = NULL,
 org.name = NULL,
  db,
  n.start = 1,
  n.stop = NULL,
  step = 500,
  term = NULL,
  verbose = TRUE
)
info_listtodata(info.list, unlist = TRUE, verbose = TRUE)
```

Arguments

org.name	character; scientific name	or taxon identifier (written as	"txid0000") of the or-
----------	----------------------------	---------------------------------	------------------------

ganism/taxon.

db character; NCBI database for search. See entrez_dbs() for possible values.

n.start integer; download starting value. Default is 1.

n. stop integer; download finishing value. Default is NULL, which provides retrieval of

all available GIs.

step integer; download increment value. Maximum is 500.

return.dataframe

integer; whether to return information as structured data frame (another variant

is list of lists).

check.result logical; check if download was done correctly.

term character; search query. verbose logical; show messages

info.list list of previously downloaded records.

web.history previously saved web_history object for use in calls to the NCBI. New web.history

is created if none is provided.

unlist logical; unlist result before transforming (only recommended if step > 1).

Details

This function sends the query to NCBI database and returns sequence records according to the query. By default the query is organism, so the function returns data of all sequences that are associated with the requested organism. For example, if org.name = "Homo sapiens" the function will download data for all records that answer the query "Homo sapiens[Organism]". For any other query use parameter term.

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The function downloads records by piecemeal, by several pieces in one block. The size of the block is defined by parameter step. It is useful if by any reason the download was interrupted, so later it is possible to reload only the missing blocks without the need to reload the entire amount of data. By default, all available records are downloaded, but you may also choose start and finish points by specifying the parameters n.start and n.stop. The numeration starts with 1, not 0. At the end the resulting list of blocks (list of lists if step > 1) is unlisted into one data frame that contains information about record GI, UID, caption, source database, organism, strain etc. You may prevent this by setting return.dataframe = FALSE. Also, regardless of return.dataframe settings, the list of blocks is returned if the download was somehow compromised. Optionally, you can turn the resulting list into data frame later using the function info_listtodata(). Note that in this case, if parameter info.list was inherited from get_seq_info() function, the result must be unlisted first (use unlist = TRUE).

If download was corrupted you may use get_seq_info() function to reload the missing block. The corrupted list of blocks should be set in info.list parameter. You may also check and reload data when get_seq_infos() function is running by specifying check.result = TRUE.

In progress the functions turn off and on scientific notation.

Value

get_seq_info() returns data frame that contains most of sequence information from NCBI records. If return.dataframer = FALSE or there are missing data, list of lists is returned. List contains full information from NCBI records.

```
get_seq_info_fix() returns list of lists.
info_listtodata() returns data frame.
```

Functions

- get_seq_info: Retrieves NCBI sequence records for given organism name or taxon identifier.
- get_seq_info_fix: Checks the downloads and tries to retrieve the compromised data.
- info_listtodata: Transforms downloaded list into data frame.

Author(s)

Elena N. Filatova

Examples

30 make_blast_DB

make_blast_DB

Builds local database for BLAST

Description

Builds a BLAST database with local sequences using FASTA file.

Usage

```
make_blast_DB(
  makeblastdb.way,
  fasta.way,
  db.way,
  db.type = "nucl",
  db.title,
  delete.fasta = FALSE,
  verbose = TRUE
)
```

Arguments

makeblastdb.way

character; name and path to makeblastdb executable file

fasta.way character; name and path to FASTA file

db.way character; name and path to local BLAST database

db.type character; type of BLAST database db.title character; BLAST data base title

delete.fasta logical; delete FASTA file verbose logical; show messages

Details

This function is using BLAST applications. BLAST+ (UNIX or Windows) should be installed.

Value

The function creates local BLAST data base. No additional data is returned.

Author(s)

Elena N. Filatova

References

```
Camacho C., Coulouris G., Avagyan V. et al. (2009). BLAST+: architecture and applications. BMC Bioinformatics 10, 421. https://bmcbioinformatics.biomedcentral.com/articles/10.1186/1471-2105-10-421.
```

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Examples

```
## Not run:
# This function is using BLAST applications. BLAST+ should be installed.
# FASTA file with sequences for local data base should be downloaded first (see get_seq_for_DB ())
path <- tempdir()</pre>
dir.create (path)
# load metadata for target sequences of Chlamydia pneumoniae
(meta.target)
# load sequences, it will take about 3 minutes
get_seq_for_DB (ids = meta.target$gi, db = "nucleotide", check.result = TRUE,
              return="fasta", fasta.file = paste0 (path, "/seq.fasta"), verbose = TRUE)
# create local data base, it will take 0.235217 seconds
make_blast_DB (makeblastdb.way = "D:/Blast/blast-2.11.0+/bin/makeblastdb.exe",
              fasta.way = paste0 (path, "/seq.fasta"), db.title = "Cl_pneumoniae",
              db.way = paste0 (path, "/DB"), db.type = "nucl", delete.fasta = FALSE)
# delete FASTA file (also can set delete.fasta = TRUE)
file.remove (paste0 (path, "/seq.fasta"))
## End(Not run)
```

make_ids

Create unique identification values

Description

Creates unique identification values by adding numbers to identical values.

Usage

```
make_ids(var, sep = "_")
```

Arguments

var vector of values

sep character; string to separate the terms

Details

This function takes vector with same values and adds numbers to create unique values.

Value

Character vector of var with attached numbers.

Author(s)

Elena N. Filatova

32 meta.all

Examples

```
var<-c("one", "two", "three", "one", "two", "three", "one")
make_ids(var)</pre>
```

meta.all

Metadata of all available Chlamydia pneumoniae's sequences.

Description

A dataset containing metadata of all Chlamydia pneumoniae's nucleotide sequences that were downloaded from NCBI Nucleotide database (November, 2021)

Usage

meta.all

Format

```
A data frame with 9062 rows and 21 variables:
uid sequence identification number
gi sequence identification number
GB_AcNum sequence identification number
createdate date of note's creation
updatedate date of last note's update
source_db database
organism organism name
title sequence title
strain strain
taxid taxon identificator
length sequence length
biomol biomolecule
moltype molecular type
genome genome type
complete sequence completness
geneticcode type of genetic and codon codes
strand strand
host host
country country
isolation_source isolation material
collection_date collection date
```

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Source

```
https://www.ncbi.nlm.nih.gov/
```

meta.target

Metadata of target Chlamydia pneumoniae's sequences.

Description

A dataset containing target nucleotide sequences of Chlamydia pneumoniae that were downloaded from NCBI Nucleotide database (November, 2021). Target sequences are chosen from all available sequences as targets for discriminating probes.

Usage

meta.target

Format

A data frame with 183 rows and 21 variables:

uid sequence identification numbergi sequence identification number

GB_AcNum sequence identification number

createdate date of note's creation

updatedate date of last note's update

source_db database

organism organism name

title sequence title

strain strain

taxid taxon identificator

length sequence length

biomol biomolecule

moltype molecular type

genome genome type

complete sequence completness

geneticcode type of genetic and codon codes

strand strand

host host

country country

isolation_source isolation material **collection date** collection date

Source

```
https://www.ncbi.nlm.nih.gov/
```

34 normalize_DF

normalize_DF

Normalize variable

Description

Normalize variable in a data frame

Usage

```
normalize_DF(
  data,
  var.name,
  method = "mean",
  norm.number,
  return = "add.end",
  digits = 2
)
```

Arguments

data frame with numeric variable that should be normalized

var.name character; data frame column name with numeric variable that should be nor-

malized

method character; normalization method; possible values are: "mean" (normalize to

mean), "median" (normalize to median), "number" (normalize to given num-

ber)

norm.number numeric; a value to normalize to (if method = "number")

return character; return object; possible values are: "vector" (return a vector of nor-

malized values), "replace" (replace var.name values with normalized values in data frame), "add.near" (add normalized values next to var.name values in data frame), "add.end" (add normalized values as the latter column in data

frame)

digits integer; number of decimal places to round the normalized value

Details

This function scales variable to a range of (0-1), where 1 get values that are the most close to mean, median or given number. See normalize for details.

var.name must be exact column name as in data frame.

Value

Vector or data frame with normalized values.

Author(s)

Elena N. Filatova

rate_DF

Examples

rate_DF

Rate variables

Description

Count data frame's row rate according to several variables

Usage

```
rate_DF(
  data,
  rate.var,
  weights,
  return = "add",
  as.percent = FALSE,
  percent.var,
  digits = 2
)
```

Arguments

data	data frame with rated variables
rate.var	character; vector of data frame column names with numeric variables of range (0-1) that should be used for rating
weights	numeric; vector of variables' weights (their sum must be 1)
return	character; return object; possible values are: "vector" (return a vector of rate values), "add" (add rated values as the latter column in data frame)
as.percent	logical; if some rated variables are percentages
percent.var	character; vector of data frame column names with rated variables that are percentages
digits	integer; number of decimal places to round the rate value

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Details

This function counts rate as rate = var1*weight1 + var2*weight2 + var3*weight3 + . . . etc. All variables must be in range (0-1) and sum of weights must be 1. If you use percentages as rating variable, use as percent = TRUE. Those variables would be divided by 100 before rating and then would be multiplicated by 100 after rating.

rate.var and percent.var must be exact column names as in data frame.

Value

Vector or data frame with rate values.

Author(s)

Elena N. Filatova

Examples

```
data <- data.frame (N = 1:5, percent = c(12, 15, 18, 20, 94), number = c(0.1, 0.5, 0.6, 0.8, 0.9))
rate_DF (data = data, rate.var = c("percent", "number"), weights = c(0.4, 0.6), return = "add",
as.percent = TRUE, percent.var = "percent")
```

```
read_and_unite_files Read and unite files
```

Description

Read a bunch of table files and unite them in one data frame

Usage

```
read_and_unite_files(
  path,
  pattern,
  sep = ";",
  header = TRUE,
  add.file.id = FALSE,
  file.id = NULL,
  unique = FALSE
)
```

Arguments

```
path character; directory path
pattern character; file names pattern
sep character; the field separator character
```

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header	logical; files contain the names of the variables as its first line
add.file.id	logical; add file identification columns
file.id	data frame with file identification values
unique	logical; delete repeated rows

Details

All files must be tables of same type. All files must be in one directory.

File identification columns might be added. There might be any number of such columns. They are added at the beginning of result data frame. File identification values are set as file.id data frame, where each column contains possible identification values and column names are names of identificator. If no file.id provided file names are set by default.

Value

data frame with united files' content.

Author(s)

Elena N. Filatova

Examples

```
read_from_table_file Read table file
```

Description

Read table file and selects the required rows and columns.

38 read_from_table_file

Usage

```
read_from_table_file(
   file,
   choose.columns = FALSE,
   column.names,
   select = FALSE,
   select.column.name,
   select.val,
   unique = FALSE,
   sep = ";",
   header = TRUE
)
```

Arguments

file character; file name and path choose.columns logical; return chosen columns only character; vector of name of columns that are chosen to be returned column.names select logical; return only rows that contain selected values in one column select.column.name character; name of column that contains selected values select.val vector of values that define rows that should be returned unique logical; delete duplicated rows character; the field separator character sep header logical; files contain the names of the variables as its first line

Details

This function reads table files and returns data frame with selected rows (only rows with specified values) and columns. Also duplicated rows may be deleted.

column.names and select.column.name must be exact column names as in data frame.

Value

Data frame with file content, optionally trimmed.

Author(s)

Elena N. Filatova

Examples

store_in_DB 39

store_in_DB

Store data in SQLite database

Description

Write, read and delete tables from SQLite database.

Usage

```
list_DB(database)
write_to_DB(
  database,
  data,
  table,
 overwrite = FALSE,
 append = FALSE,
  verbose = TRUE
)
index_DB(database, table, index.unique, index.column.name, verbose = TRUE)
read_from_DB(
  database,
  table,
  choose.columns = FALSE,
  column.names,
  select = FALSE,
  select.column.name,
  select.val,
  unique = FALSE
)
delete_from_DB(database, table, verbose = TRUE)
```

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Arguments

database character; SQLite database name and path.

data frame that should be stored as database table.

table character; table name.

overwrite logical; use overwrite = TRUE if you want to overwrite a table that already ex-

ists in database

append logical; append rows to table verbose logical; show messages

index.unique logical; vector of indicators to create unique or not unique indexes

index.column.name

vector of indexed columns' names

choose.columns logical; return chosen columns only

column. names character; vector of name of columns that are chosen to be returned select logical; return only rows that contain selected values in one column

select.column.name

character; name of column that contains selected values

select.val vector of values that define rows that should be returned

unique logical; delete duplicated rows

Details

This functions help to store big data frames in SQLite database which makes it faster to save and read the data.

This function creates SQLlite connection to database, fulfills the task and then disconnects. If no database has been created yet, creates one.

Do not use overwrite = TRUE if table does not exists. Do not use append = TRUE and overwrite = TRUE at the same time, no append is possible while overwriting.

If multiple indexes are created in one table, they are unrelated.

Do not use dots in data frame character variables, use underscore.

Parameters choose.columns=FALSE, column.names, select, select.column.name, select.val, unique are only used with linkread_from_DB function. Those parameters define rows and columns that will be returned.

Value

list_DB returns character vector of names of database tables.

read_from_DB returns a data frame with the content of SQLite table.

Functions

- list_DB: Lists all tables from SQLite database
- write_to_DB: Writes data frame into SQLite database table
- index_DB: Creates SQLite indexes in database table
- read_from_DB: Reads table from SQLite database and writes it into data frame.
- delete_from_DB: Deletes table from SQLite database.

Author(s)

Elena N. Filatova

Examples

```
mydata <- as.data.frame (matrix(1:10, 2, 5))</pre>
database <- tempfile()</pre>
write_to_DB (database, data = mydata, table = "table1", overwrite = FALSE)
list_DB (database)
mydata2 <- as.data.frame (matrix(11:20, 2, 5))</pre>
write_to_DB (database, data = mydata2, table = "table1", overwrite = TRUE)
mydata3 <- read_from_DB (database, table = "table1")</pre>
delete_from_DB (database, table = "table1")
file.remove (database)
# example with reading table with restricted columns and rows.
mydata \leftarrow data.frame(ids = c(1:6), titles = c("A", "B", "C", "D", "E", "E"),
                     other = rep("other", 6))
database <- tempfile()</pre>
write_to_DB (database, data = mydata, table = "table1", overwrite = FALSE)
read_from_DB(database, "table1", choose.columns = TRUE, column.names = c("ids", "titles", "other"),
            select = TRUE, select.column.name = "ids", select.val = 3:6, unique = TRUE)
read_from_DB(database, "table1", choose.columns = TRUE, column.names = c("titles", "other"),
            select = TRUE, select.column.name = "ids", select.val = 3:6, unique = TRUE)
file.remove (database)
```

summarize_blast_result

Summarize BLAST result

Description

Summarize aligned, not aligned and undesirably aligned sequences

Usage

```
summarize_blast_result(
   sum.aligned = "sp",
   blast.probe.id.var,
   blast.res.id.var,
   blast.res.title.var,
   reference.id.var,
   reference.title.var,
   titles = FALSE,
   add.blast.info = FALSE,
   data.blast.info,
   check.blast.for.source = FALSE,
```

```
source = NULL,
      switch.ids = FALSE,
      switch.table,
      mc.cores = 1,
      digits = 2,
      sep = ";",
      temp.db = NULL,
      delete.temp.db = TRUE,
      return = "summary",
      write.alignment = "DB",
      alignment.db = NULL,
      alignment.table.sp.aligned = NULL,
      alignment.table.sp.not.aligned = NULL,
      alignment.table.nonsp = NULL,
      change.colnames.dots = TRUE,
      file.sp.aligned = NULL,
      file.sp.not.aligned = NULL,
      file.nonsp = NULL,
      verbose = TRUE
    )
Arguments
    sum.aligned
                     character; summarize specific or not specific alignments; possible values are
                     "sp" (aligned and not aligned specific subjects) and "nonsp" (aligned non spe-
                     cific subjects)
    blast.probe.id.var
                     vector of query identification numbers from BLAST result data
    blast.res.id.var, blast.res.title.var
                     vector of subject identification numbers and titles from BLAST result data
    reference.id.var, reference.title.var
                     vector of identification numbers and titles of specific sequences that should be
                     or might be aligned
    titles
                     logical; include titles in alignment reports
```

add.blast.info logical; add other BLAST results

data.blast.info

data frame; additional BLAST result from BLAST result data

check.blast.for.source

logical; delete queries that are not aligned with one obligatory sequence

source identification number of obligatory sequence for alignment

switch.ids logical; use different identification numbers for BLAST result's subjects

switch.table data frame; table of old and new identification numbers (and new titles) linked

by row

mc.cores integer; number of processors for parallel computation (not supported on Win-

dows)

digits integer; number of decimal places to round the result

character; the field separator character sep character; temporal SQLite database name and path temp.db delete.temp.db logical; delete temporal SQLite database afterwards character; returned object; possible values are "list" (list of data frames with return alignment summary and report for each probe) and "summary" (data frame with summary for all probes is returned and alignment reports are written into files or SQLite database tables) write.alignment character; write alignment reports into files ("file") or SQLite database tables ("DB"; used if (return = "summary")) alignment.db, alignment.table.sp.aligned, alignment.table.sp.not.aligned, alignment.table.nonsp character; SQLite database name and path, tables names (used if write.alignment = "DB") change.colnames.dots logical; change dots to underscore in data frame column names (used if write.alignment = "DB") file.sp.aligned, file.sp.not.aligned, file.nonsp character; file names and path (used if write.alignment = "file") logical; show messages verbose

Details

This function works with data frame created by blast_local function. It takes BLAST results, divides aligned subjects on specific (that should be aligned) and non specific (that should not be aligned) according to reference) values. Function summarizes amount of aligned and not aligned specific subjects and amount of aligned non specific subjects.

When sum.aligned = "sp" aligned and not aligned specific subjects are summarized and reference.id.var and reference.title.var should contain sequences that it is necessary to align with. When sum.aligned = "nonsp" aligned non specific subjects are summarized and reference.id.var should contain sequences that may be aligned (that are not considered as non specific), no titles needed.

When return = "summary", function returns summary (amount of aligned and not aligned subjects) and writes sorted alignments (alignment report) in file (write.alignment = "file") or SQLite database (write.alignment = "DB"). Usually only subjects' ids and (optionally) titles are returned, but you may add as many BLAST results as you like with add.blast.info and data.blast.info parameters. If you add some BLAST results, all alignments will present in alignment report, if not - duplicated subjects will be deleted.

By default result tables in database (if write.alignment = "DB") are "sp_aligned", "sp_not_aligned" and "nonsp", Results are written by appending, so if files or tables already exist, data will be added into them.

If subjects identification numbers in BLAST result data differ from those in reference.id.var you may use switch.ids = TRUE to change BLAST ids into new according to switch.table. switch.table must be a data frame with column one - old ids, column two - new ids and (optionally) column three - new titles. Do not use dots in column names.

When check.blast.for.source = TRUE probes that are non blasted for one special subject (usually the sequence that was cut for probes) are deleted. No check.blast.for.source is performed

if sum.aligned = "nonsp". Check for source is performed after the possible id. switch, so source should be identification number of same type as reference.

Probe identification number must be character variable.

If alignment report is written into database, probe identification variable is indexed in all tables. Also it is highly recommended to set change.colnames.dots = TRUE to change possible dots to underscore within result data frame's column names and avoid further mistakes.

While working function saves data in temporal SQLite database. Function will stop if same database already exists, so deleting temporal database is highly recommended.

Value

List of data frames with alignment summary and report for each probe or data frame with summary for all probes (alignment reports are written into files or SQLite database tables).

Author(s)

Elena N. Filatova

Examples

```
path <- tempdir()</pre>
dir.create (path)
# load blast results with subject accession numbers
data(blast.fill)
#load metadata of all Chlamydia pneumoniae sequences - they are subjects that
# do not count as nonspecific and may be aligned
data(meta.all)
# load metadata with target Chlamydia pneumoniae sequences - they are specific subjects
# that must be aligned
# make new accession numbers to count all WGS sequences as one (see unite_NCBI_ac.nums ())
meta.target.new.ids <- unite_NCBI_ac.nums (data = meta.target,</pre>
                                           ac.num.var = meta.target$GB_AcNum,
                                           title.var = meta.target$title,
                                           db.var = meta.target$source_db,
                                           type = "shotgun", order = TRUE,
                                           new.titles = TRUE)
# summarize blast results, count aligned specific subjects with "switch ids" option
# (WGS sequences are counted as one). Add query cover information.
blast.sum.sp <- summarize_blast_result (sum.aligned = "sp",</pre>
                                        blast.probe.id.var = blast.fill$Qid,
                                        blast.res.id.var = blast.fill$Racc,
                                        blast.res.title.var = blast.fill$Rtitle,
                                        reference.id.var = meta.target.new.ids$new.id,
                                     reference.title.var = meta.target.new.ids$new.title,
                                        titles = TRUE,
                                        add.blast.info = TRUE,
                                data.blast.info = data.frame(Qcover = blast.fill$Qcover),
                                   switch.ids = TRUE, switch.table = meta.target.new.ids,
                               temp.db = paste0 (path, "/temp.db"), delete.temp.db = TRUE,
                                        return = "summary", write.alignment = "DB",
                                        alignment.db = paste0 (path, "/alig.db"))
```

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```
# summarize nonspecific alignments (that are not in meta.all dataframe)
blast.sum.nonsp <- summarize_blast_result (sum.aligned = "nonsp",</pre>
                                           blast.probe.id.var = blast.fill$Qid,
                                           blast.res.id.var = blast.fill$Racc,
                                           blast.res.title.var = blast.fill$Rtitle,
                                           reference.id.var = meta.all$GB_AcNum,
                                           reference.title.var = meta.all$title,
                                           titles = TRUE, switch.ids = FALSE,
                                           add.blast.info = TRUE,
                                data.blast.info = data.frame(Qcover = blast.fill$Qcover),
                                           temp.db = paste0 (path, "/temp.db"),
                                           delete.temp.db = TRUE,
                                           return = "summary", write.alignment = "DB",
                                           alignment.db = paste0 (path, "/alig.db"))
# all specific targets are aligned
sp.aligned <- read_from_DB(database = paste0 (path, "/alig.db"), table = "sp_aligned")</pre>
# no targets that are not aligned
sp.not.aligned <- read_from_DB(database = paste0 (path, "/alig.db"), table = "sp_not_aligned")
# No nonspecific alignments
nonsp <- read_from_DB(database = paste0 (path, "/alig.db"), table = "nonsp")</pre>
file.remove (paste0 (path, "/alig.db"))
```

trim DF

Trim data frame

Description

If the numeric value of the data frame variable does not meet the specified conditions, the function deletes the entire row.

Usage

```
trim_DF(data, trim.var.name, trim.action, trim.thresh)
```

Arguments

data frame

trim.var.name character; vector of data frame column names with numeric variables that should be tested for conditions

trim.action character; vector of test conditions; possible values are: "more", "eqmore" (more or equal), "less", "eqless" (less or equal).

trim.thresh numeric; vector of condition threshold values

Details

This function takes the vector of data frame variables and for each of them test if they satisfy the specified conditions. Not satisfying values are deleted with the entire data frame row. You may set as many conditions for as many variables as you like.

trim. values must be exact column names as in data frame.

Value

data frame without rows with values that do not satisfy the specified conditions.

Author(s)

Elena N. Filatova

Examples

unite_NCBI_ac.nums

Assigns master record's id to all project records

Description

The function assigns the project master record's NCBI access number to all records that belong to the project.

Usage

```
unite_NCBI_ac.nums(
  data,
  ac.num.var,
  title.var,
  db.var,
  type = "shotgun",
  order = TRUE,
  new.titles = FALSE
)
```

Arguments

data frame; contains information about sequence records.

ac.num.var character; data frame variable that contains sequence accession numbers.

title.var character; data frame variable that contains sequence titles.

db.var character; data frame variable that contains source data base names.

type character; type of the project which records should be united with one accession

number. At the moment "shotgun" is the only possible value which corresponds to the whole genome shotgun sequencing project with shotgun technol-

ogy.

order logical; rearrange a data frame in alphabetical order of accession numbers (highly

recommended).

new.titles logical; add new titles according to new access numbers.

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Details

The function looks through all records in a data frame. If the record belongs to the project (for example, WGS-project), the function assigns the project master record's NCBI access number to this record. If the record is not related to any project, it retains its own accession number.

It is highly recommended to arrange the data in alphabetical order of accession numbers, since the first record among similar ones is determined as master record.

Value

```
If new.titles = FALSE data frame with old and new access numbers is returned.

If new.titles = TRUE data frame with old and new access numbers and new titles is returned.
```

Author(s)

Elena N. Filatova

Examples

unite_two_DF

Combine two data frames

Description

Combine two data frames according to shared variable

Usage

```
unite_two_DF(
  data1,
  data1.shared.var,
  data1.shared.column.num = 1,
  data2,
  data2.shared.var,
  data2.shared.column.num = 1,
  delete.not.shared = FALSE,
  not.shared = "all",
  verbose = TRUE
)
```

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Arguments

Details

This function combines columns of two data frames according to shared.var which acts like rows' identification number. If shared.var value from one data frame do not present in other data frame, NAs are produced. Those absent rows are deleted when delete.not.shared = TRUE.

data1.shared.var and data2.shared.var must contain unique values within its own data frame.

Order of rows in resulting data frame is according to data1. data2. shared.var is removed from resulting data frame.

Value

Combined data frame.

Author(s)

Elena N. Filatova

Examples

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