

Package ‘MSA2dist’

April 10, 2023

Type Package

Title MSA2dist calculates pairwise distances between all sequences of a DNASTringSet or a AAStringSet using a custom score matrix and conducts codon based analysis

Version 1.2.0

Description MSA2dist calculates pairwise distances between all sequences of a DNASTringSet or a AAStringSet using a custom score matrix and conducts codon based analysis. It uses scoring matrices to be used in these pairwise distance calculations which can be adapted to any scoring for DNA or AA characters. E.g. by using literal distances MSA2dist calculates pairwise IUPAC distances.

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Encoding UTF-8

LazyData false

biocViews Alignment, Sequencing, Genetics, GO

Depends R (>= 4.2.0)

Imports Rcpp, Biostrings, GenomicRanges, IRanges, ape, doParallel, dplyr, foreach, methods, parallel, rlang, seqinr, stringr, tibble, tidyr, stats, stringi

Suggests rmarkdown, knitr, devtools, testthat, ggplot2, BiocStyle

LinkingTo Rcpp, RcppThread

VignetteBuilder knitr

NeedsCompilation yes

SystemRequirements C++11

URL <https://gitlab.gwdg.de/mpievolbio-it/MSA2dist>,
<https://mpievolbio-it.pages.gwdg.de/MSA2dist/>

BugReports <https://gitlab.gwdg.de/mpievolbio-it/MSA2dist/issues>

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Author Kristian K Ullrich [aut, cre] (<<https://orcid.org/0000-0003-4308-9626>>)

Maintainer Kristian K Ullrich <ullrich@evolbio.mpg.de>

R topics documented:

aabin2aastring	3
AAMatrix-data	4
aastring2aabin	4
aastring2aln	5
aastring2dist	6
addmask2string	7
addpop2string	8
addpos2string	9
addregion2string	10
aln2aastring	12
aln2dnastring	13
cds2aa	14
cds2codonaln	15
codon2numberAMBIG	16
codon2numberTCAG	17
codonmat2pnps	17
codonmat2xy	19
compareCodons	20
dnabin2dnastring	21
dnastring2aln	22
dnastring2codonmat	23
dnastring2dist	24
dnastring2dnabin	25
dnastring2kaks	26
GENETIC_CODE_TCAG	28
getmask	29
getpos	30
globalDeletion	31
granthamMatrix	31
hiv-data	32
iupac-data	33
iupacMatrix	33
makePostalignedSeqs	34
popinteger	35
popnames	36
rcpp_distSTRING	37
rcpp_KaKs	37

<i>aabin2aastring</i>	3
rcpp_pairwiseDeletionAA	38
rcpp_pairwiseDeletionDNA	39
region	40
regionused	41
string2region	42
subString	43
upriidx	44
Index	45

<i>aabin2aastring</i>	<i>aabin2aastring</i>
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Description

This function converts an ape AAbin into AAStringSet.

Usage

```
aabin2aastring(aabin)
```

Arguments

aabin ape AAbin [mandatory]

Value

An object of class AAStringSet

Author(s)

Kristian K Ullrich

See Also

[as.alignment](#) [as.DNAbin.alignment](#) [AAStringSet](#)

Examples

```
data(woodmouse, package="ape")
## convert into AAStringSet
#aabin2aastring(ape::trans(woodmouse, 2))
ape::trans(woodmouse, 2) |> aabin2aastring()
```

AAMatrix-data

AAMatrix-data

Description

getAAMatrix() from the alakazam package.

Usage

```
data(AAMatrix)
```

Format

an object of class matrix

Value

score matrix

References

Gupta N, Vander Heiden J, Uduman M, Gadala-Maria D, Yaari G, Kleinstein S (2015) Change-O: a toolkit for analyzing large-scale B cell immunoglobulin repertoire sequencing data. *Bioinformatics*. **31(20)**, 3356-3358.

Examples

```
data("AAMatrix", package="MSA2dist")
```

aastring2aabin

aastring2aabin

Description

This function converts a AAStringSet into an ape DNABin.

Usage

```
aastring2aabin(aa)
```

Arguments

aa AAStringSet [mandatory]

Value

An object of class DNABin

Author(s)

Kristian K Ullrich

See Also[as.alignment](#) [as.DNABin.alignment](#)**Examples**

```
## define two cds sequences
cds1 <- Biostrings::DNASTring("ATGCAACATTGC")
cds2 <- Biostrings::DNASTring("ATG---CATTGC")
cds1.cds2.aln <- c(Biostrings::DNASTringSet(cds1),
  Biostrings::DNASTringSet(cds2))
## convert into AAbin
#aastring2aabin(cds2aa(cds1.cds2.aln))
cds1.cds2.aln |> cds2aa() |> aastring2aabin()
```

`aastring2aln``aastring2aln`

Description

This function converts a AAStringSet into an seqinr alignment.

Usage

```
aastring2aln(aa)
```

Arguments

`aa` AAStringSet [mandatory]

Value

An object of class alignment which is a list with the following components:

`nb` the number of aligned sequences

`nam` a vector of strings containing the names of the aligned sequences

`seq` a vector of strings containing the aligned sequences

`com` a vector of strings containing the commentaries for each sequence or NA if there are no comments

Author(s)

Kristian K Ullrich

See Also[as.alignment](#)

Examples

```
## define two cds sequences
cds1 <- Biostrings::DNAString("ATGCAACATTGC")
cds2 <- Biostrings::DNAString("ATG---CATTGC")
cds1.cds2.aln <- c(Biostrings::DNAStringSet(cds1),
  Biostrings::DNAStringSet(cds2))
#aastring2aln(cds2aa(cds1.cds2.aln))
cds1.cds2.aln |> cds2aa() |> aastring2aln()
```

aastring2dist

aastring2dist

Description

This function calculates pairwise distances for all combinations of a AAStringSet.

Usage

```
aastring2dist(aa, threads = 1, score = NULL, mask = NULL, region = NULL)
```

Arguments

aa	AAStringSet [mandatory]
threads	number of parallel threads [default: 1]
score	score matrix use a score matrix to calculate distances [mandatory]
mask	IRanges object indicating masked sites [default: NULL]
region	IRanges object indicating region to use for dist calculation (by default all sites are used) [default: NULL]

Value

A data.frame of pairwise distance values `distSTRING`, sites used `sitesUsed` and region used `regionUsed`

Author(s)

Kristian K Ullrich

See Also

[dnastring2dist](#)

Examples

```
## load example sequence data
data("hiv", package="MSA2dist")
#aastring2dist(cds2aa(hiv), score=granthamMatrix())
hiv |> cds2aa() |> aastring2dist(score=granthamMatrix())
## create mask
mask1 <- IRanges::IRanges(start=c(11,41,71), end=c(20,50,80))
## use mask
hiv |> cds2aa() |> aastring2dist(score=granthamMatrix(), mask=mask1)
## use region
region1 <- IRanges::IRanges(start=c(1,75), end=c(45,85))
hiv |> cds2aa() |> aastring2dist(score=granthamMatrix(), region=region1)
## use mask and region
hiv |> cds2aa() |> aastring2dist(score=granthamMatrix(),
  mask=mask1, region=region1)
```

addmask2string

addmask2string

Description

This function adds mask information as an IRanges object, START and END information, to a DNASTringSet or an AAStringSet and puts them into the metadata information. This information can be used to restrict the distance calculation to specific regions of the DNASTringSet or the AAStringSet.

Usage

```
addmask2string(seq, mask = NULL, append = TRUE)
```

Arguments

seq	DNASTringSet or AAStringSet [mandatory]
mask	IRanges object [mandatory]
append	indicate if mask should be appended or overwritten [default: TRUE]

Value

An object of class DNASTringSet or AAStringSet

Author(s)

Kristian K Ullrich

See Also

[addregion2string](#), [addpop2string](#), [addpos2string](#)

Examples

```

## load example sequence data
data(iupac, package="MSA2dist")
iupac.aa <- iupac |> cds2aa(shorten = TRUE)
## create mask
mask1 <- IRanges::IRanges(start=c(1,41), end=c(20,50))
## add mask
iupac.aa <- iupac.aa |> addmask2string(mask=mask1)
#(iupac.aa |> slot("metadata"))$mask
iupac.aa |> getmask()
## append mask
mask2 <- IRanges::IRanges(start=c(21), end=c(30))
iupac.aa <- iupac.aa |> addmask2string(mask=mask2)
#(iupac.aa |> slot("metadata"))$mask
iupac.aa |> getmask()
## overwrite mask
iupac.aa <- iupac.aa |> addmask2string(mask=mask2, append=FALSE)
#(iupac.aa |> slot("metadata"))$mask
iupac.aa |> getmask()
## reduce by mask
#iupac.aa.region <- iupac.aa |> string2region(mask=
#   (iupac.aa |> slot("metadata"))$mask)
iupac.aa.region <- iupac.aa |> string2region(mask=
  getmask(iupac.aa))
#iupac.aa.region |> slot("metadata")
iupac.aa.region |> getmask()

```

addpop2string

addpop2string

Description

This function adds population information to a DNAStringSet or an AAStringSet and puts them into the metadata information.

__Note__: All unassigned sequences will be put into pop "unassigned"!

Do not use "unassigned" as a population name!

__Note__: Names in a population in the poplist must match sequence names!

__Note__: Duplicated assignments are allowed!

Usage

```
addpop2string(seq, poplist)
```

Arguments

seq	DNAStringSet or AAStringSet [mandatory]
poplist	named list of populations either as index or names per population (do not mix index and names in one population) [mandatory]

Value

An object of class DNASTringSet or AAStringSet

Author(s)

Kristian K Ullrich

See Also

[addmask2string](#), [addregion2string](#), [addpos2string](#)

Examples

```
## load example sequence data
data(iupac, package="MSA2dist")
iupac.aa <- iupac |> cds2aa(shorten = TRUE)
## create poplist
poplist <- list(FRA = grep("Mmd.FRA", names(iupac)),
               GER = grep("Mmd.GER", names(iupac)),
               IRA = grep("Mmd.IRA", names(iupac)),
               AFG = grep("Mmm.AFG", names(iupac)))
iupac.aa <- iupac.aa |> addpop2string(poplist)
#(iupac.aa |> slot("metadata"))$pop.integer
iupac.aa |> popinteger()
#(iupac.aa |> slot("metadata"))$pop.names
iupac.aa |> popnames()
## mxixing index and names
poplist <- list(FRA = names(iupac)[grep("Mmd.FRA", names(iupac))],
               GER = grep("Mmd.GER", names(iupac)),
               IRA = names(iupac)[grep("Mmd.IRA", names(iupac))],
               AFG = grep("Mmm.AFG", names(iupac)))
iupac.aa <- iupac.aa |> addpop2string(poplist)
iupac.aa |> popinteger()
iupac.aa |> popnames()
## leaving out some sequences which will be assigned as "unassigned"
poplist <- list(FRA = names(iupac)[grep("Mmd.FRA", names(iupac))],
               GER = grep("Mmd.GER", names(iupac)),
               IRA = names(iupac)[grep("Mmd.IRA", names(iupac))])
iupac.aa <- iupac.aa |> addpop2string(poplist)
iupac.aa |> popinteger()
iupac.aa |> popnames()
```

addpos2string

addpos2string

Description

This function adds GenomicRanges information, CHROM, START and END to a DNASTringSet or an AAStringSet and puts them into the metadata information. This information can be used to find overlaps with a chromosome wide mask.

Usage

```
addpos2string(seq, chrom = NULL, start = NULL, end = NULL)
```

Arguments

seq	DNAStrngSet or AAStringSet [mandatory]
chrom	chromosome name [mandatory]
start	start position [mandatory]
end	end position [mandatory]

Value

An object of class DNAStrngSet or AAStringSet

Author(s)

Kristian K Ullrich

See Also

[addmask2string](#), [addregion2string](#), [addpop2string](#)

Examples

```
## load example sequence data
data(iupac, package="MSA2dist")
## add position
iupac <- iupac |> addpos2string(chrom="chr1", start=1, end=1000)
#(iupac |> slot("metadata"))$GRanges
iupac |> getpos()
```

addregion2string *addregion2string*

Description

This function adds region information as an IRanges object, START and END information, to a DNAStrngSet or an AAStringSet and puts them into the metadata information. This information can be used to restrict the distance calculation to specific regions of the DNAStrngSet or the AAStringSet.

Usage

```
addregion2string(seq, region = NULL, append = TRUE)
```

Arguments

seq	DNASTringSet or AAStringSet [mandatory]
region	IRanges object [mandatory]
append	indicate if region should be appended or overwritten [default: TRUE]

Value

An object of class DNASTringSet or AAStringSet

Author(s)

Kristian K Ullrich

See Also

[addmask2string](#), [addpop2string](#), [addpos2string](#)

Examples

```
## load example sequence data
data(iupac, package="MSA2dist")
iupac.aa <- iupac |> cds2aa(shorten = TRUE)
## create region
region1 <- IRanges::IRanges(start=c(1,41), end=c(20,50))
## add region
iupac.aa <- iupac.aa |> addregion2string(region=region1)
#(iupac.aa |> slot("metadata"))$region
iupac.aa |> region()
## append region
region2 <- IRanges::IRanges(start=c(21), end=c(30))
iupac.aa <- iupac.aa |> addregion2string(region=region2)
#(iupac.aa |> slot("metadata"))$region
iupac.aa |> region()
## overwrite region
iupac.aa <- iupac.aa |> addregion2string(region=region2, append=FALSE)
#(iupac.aa |> slot("metadata"))$region
iupac.aa |> region()
## reduce by region
#iupac.aa.region <- iupac.aa |> string2region(region=
# (iupac.aa |> slot("metadata"))$region)
iupac.aa.region <- iupac.aa |> string2region(region=
  region(iupac.aa))
#iupac.aa.region |> slot("metadata")
iupac.aa.region |> region()
```

aln2aastring *aln2aastring*

Description

This function converts a seqinr alignment into an AAStringSet.

Usage

```
aln2aastring(aln)
```

Arguments

aln seqinr alignment [mandatory]

Value

An object of class AAStringSet

Author(s)

Kristian K Ullrich

See Also

[as.alignment AAStringSet](#)

Examples

```
## define two cds sequences
cds1 <- Biostrings::DNASTring("ATGCAACATTGC")
cds2 <- Biostrings::DNASTring("ATG---CATTGC")
cds1.cds2.aln <- c(Biostrings::DNASTringSet(cds1),
  Biostrings::DNASTringSet(cds2))
#aastring2aln(cds2aa(cds1.cds2.aln))
cds1.cds2.aln |> cds2aa() |> aastring2aln() |> aln2aastring()
```

aln2dnastring	<i>aln2dnastring</i>
---------------	----------------------

Description

This function converts a seqinr alignment into an DNASTringSet.

Usage

```
aln2dnastring(aln)
```

Arguments

aln seqinr alignment [mandatory]

Value

An object of class DNASTringSet

Author(s)

Kristian K Ullrich

See Also

[as.alignment DNASTringSet](#)

Examples

```
## define two cds sequences
cds1 <- Biostrings::DNASTring("ATGCAACATTGC")
cds2 <- Biostrings::DNASTring("ATG---CATTGC")
cds1.cds2.aln <- c(Biostrings::DNASTringSet(cds1),
  Biostrings::DNASTringSet(cds2))
## convert into alignment
#dnastring2aln(cds1.cds2.aln)
cds1.cds2.aln |> dnastring2aln()
## convert back into DNASTringSet
#aln2dnastring(dnastring2aln(cds1.cds2.aln))
cds1.cds2.aln |> dnastring2aln() |> aln2dnastring()
```

cds2aa	<i>cds2aa</i>
--------	---------------

Description

This function translates a DNASTringSet into an AAStringSet.

Usage

```
cds2aa(cds, shorten = FALSE, frame = 1, framelist = NULL, genetic.code = NULL)
```

Arguments

cds	DNASTringSet [mandatory]
shorten	shorten all sequences to multiple of three [default: FALSE]
frame	indicates the first base of a the first codon [default: 1]
framelist	supply vector of frames for each entry [default: NULL]
genetic.code	The genetic code to use for the translation of codons into Amino Acid letters [default: NULL]

Value

AAStringSet

Author(s)

Kristian K Ullrich

See Also

[XStringSet-class](#), [translate](#)

Examples

```
## define two cds sequences
cds1 <- Biostrings::DNASTring("ATGCAACATTGC")
cds2 <- Biostrings::DNASTring("ATG---CATTGC")
cds1.cds2.aln <- c(Biostrings::DNASTringSet(cds1),
  Biostrings::DNASTringSet(cds2))
#cds2aa(cds1.cds2.aln)
cds1.cds2.aln |> cds2aa()
## alternative genetic code
data(woodmouse, package="ape")
#cds2aa(dnabin2dnastring(woodmouse), shorten=TRUE)
woodmouse |> dnabin2dnastring() |> cds2aa(shorten=TRUE)
#cds2aa(dnabin2dnastring(woodmouse), shorten=TRUE,
woodmouse |> dnabin2dnastring() |> cds2aa(shorten=TRUE,
genetic.code=Biostrings::getGeneticCode("2"))
```

cds2codonaln	<i>cds2codonaln</i>
--------------	---------------------

Description

This function takes two single sequence DNASTring's or two single sequence DNASTringSet's, converts them into aa, calculates a global alignment and converts this alignment back into a codon alignment.

Usage

```
cds2codonaln(  
  cds1,  
  cds2,  
  type = "global",  
  substitutionMatrix = "BLOSUM62",  
  gapOpening = 10,  
  gapExtension = 0.5,  
  remove.gaps = FALSE  
)
```

Arguments

cds1	single sequence DNASTringSet or DNASTring [mandatory]
cds2	single sequence DNASTringSet or DNASTring [mandatory]
type	type of alignment (see pairwiseAlignment) [default: global]
substitutionMatrix	substitution matrix representing the fixed substitution scores for an alignment (see pairwiseAlignment) [default: BLOSUM62]
gapOpening	the cost for opening a gap in the alignment (see pairwiseAlignment) [default: 10]
gapExtension	the incremental cost incurred along the length of the gap in the alignment (see pairwiseAlignment) [default: 0.5]
remove.gaps	specify if gaps in the codon alignment should be removed [default: FALSE]

Value

codon alignment as DNASTringSet

Author(s)

Kristian K Ullrich

References

Pagès, H et al. (2014) Biostrings: Efficient manipulation of biological strings. *R package version, 2(0)*.

See Also

[pairwiseAlignment](#)

Examples

```
## define two cds sequences
cds1 <- Biostrings::DNASTring("ATGCAACATTGC")
cds2 <- Biostrings::DNASTring("ATGCATTGC")
cds2codonaln(cds1, cds2)
```

codon2numberAMBIG	<i>codon2numberAMBIG</i>
-------------------	--------------------------

Description

This function converts a codon into a number, but accept N and -.

Usage

```
codon2numberAMBIG(codon)
```

Arguments

codon [mandatory]

Value

An object of class `numeric`

Author(s)

Kristian K Ullrich

See Also

[GENETIC_CODE](#)

Examples

```
#unlist(lapply(names(Biostrings::GENETIC_CODE), codon2numberAMBIG))
names(Biostrings::GENETIC_CODE) |> codon2numberAMBIG()
```

codon2numberTCAG	<i>codon2numberTCAG</i>
------------------	-------------------------

Description

This function converts a codon into a number.

Usage

```
codon2numberTCAG(codon)
```

Arguments

codon [mandatory]

Value

An object of class numeric

Author(s)

Kristian K Ullrich

See Also

[GENETIC_CODE](#)

Examples

```
#unlist(lapply(names(Biostrings::GENETIC_CODE), codon2numberTCAG))
names(Biostrings::GENETIC_CODE) |> codon2numberTCAG()
```

codonmat2pnps	<i>codonmat2pnps</i>
---------------	----------------------

Description

This function calculates pn/ps according to *Nei and Gojobori (1986)*.

Usage

```
codonmat2pnps(codonmat)
```

Arguments

codonmat codon matrix of two columns to be compared [mandatory]

Value

An object of class pnps which is a list with the following components:

seq1 sequence1 name
 seq2 sequence2 name
 Codons sequence2 name
 Compared sequence2 name
 Ambiguous sequence2 name
 Indels sequence2 name
 Ns sequence2 name
 Sd sequence2 name
 Sn sequence2 name
 S sequence2 name
 N sequence2 name
 ps sequence2 name
 pn sequence2 name
 pnps sequence2 name
 ds sequence2 name
 dn sequence2 name
 dnps sequence2 name

Author(s)

Kristian K Ullrich

References

Nei and Gojobori. (1986) Simple methods for estimating the numbers of synonymous and nonsynonymous nucleotide substitutions. *Mol. Biol. Evol.*, **3(5)**, 418-426.

Ganeshan et al. (1997) Human immunodeficiency virus type 1 genetic evolution in children with different rates of development of disease. *J. Virology*. **71(1)**, 663-677.

Yang et al. (2000) Codon-substitution models for heterogeneous selection pressure at amino acid sites. *Genetics*. **155(1)**, 431-449.

See Also

[kaks](#)

Examples

```
## load example sequence data
data("hiv", package="MSA2dist")
#codonmat2pnps(dnastring2codonmat(hiv)[,c(1, 2)])
(hiv |> dnastring2codonmat())[,c(1, 2)] |> codonmat2pnps()
```

codonmat2xy

codonmat2xy

Description

This function calculates average behavior of each codon for all pairwise comparisons for indels, syn, and nonsyn mutations according to *Nei and Gojobori (1986)*.

Usage

```
codonmat2xy(codonmat, threads = 1)
```

Arguments

codonmat	codon matrix obtained via <code>dnastring2codonmat</code> [mandatory]
threads	number of parallel threads [default: 1]

Value

A data.frame object with the following components:

Codon Codon index

n number of comparison

SynSum Sum of syn

NonSynSum Sum of nonsyn

IndelSum Sum of indels

SynMean average syn per codon

NonSynMean average nonsyn per codon

IndelMean average indels per codon

CumSumSynMean cumulative average syn per codon

CumSumNonSynMean cumulative average nonsyn per codon

CumSumIndelMean cumulative indels per codon

Author(s)

Kristian K Ullrich

References

Nei and Gojobori. (1986) Simple methods for estimating the numbers of synonymous and nonsynonymous nucleotide substitutions. *Mol. Biol. Evol.*, **3(5)**, 418-426.

Ganeshan et al. (1997) Human immunodeficiency virus type 1 genetic evolution in children with different rates of development of disease. *J. Virology*. **71(1)**, 663-677.

Yang et al. (2000) Codon-substitution models for heterogeneous selection pressure at amino acid sites. *Genetics*. **155(1)**, 431-449.

See Also

[dnastring2codonmat](#) [codonmat2pnps](#) [dnastring2kaks](#) [kaks](#)

Examples

```
## load example sequence data
data("hiv", package="MSA2dist")
#codonmat2xy(dnastring2codonmat(hiv))
hiv |> dnastring2codonmat() |> codonmat2xy()
#codonmat2xy(dnastring2codonmat(hiv), threads=2)
hiv |> dnastring2codonmat() |> codonmat2xy(threads=2)
```

compareCodons

compareCodons

Description

This function compares two codons and returns the number of syn and non-syn sites according to *Nei and Gojobori (1986)*.

Usage

```
compareCodons(codA, codB)
```

Arguments

codA	codon A [mandatory]
codB	codon B [mandatory]

Value

vector of syn and non-syn sites

Author(s)

Kristian K Ullrich

References

- Nei and Gojobori. (1986) Simple methods for estimating the numbers of synonymous and nonsynonymous nucleotide substitutions. *Mol. Biol. Evol.*, **3(5)**, 418-426.
- Ganeshan et al. (1997) Human immunodeficiency virus type 1 genetic evolution in children with different rates of development of disease. *J. Virology*. **71(1)**, 663-677.
- Yang et al. (2000) Codon-substitution models for heterogeneous selection pressure at amino acid sites. *Genetics*. **155(1)**, 431-449.

See Also[kaks](#)**Examples**

```
compareCodons("AAA", "TTA")
compareCodons("AAA", "TAT")
compareCodons("AAA", "ATT")
compareCodons("AAA", "TTT")
## load example sequence data
data("hiv", package="MSA2dist")
compareCodons(dnastring2codonmat(hiv)[1,1], dnastring2codonmat(hiv)[1,2])
```

dnabin2dnastring	<i>dnabin2dnastring</i>
------------------	-------------------------

Description

This function converts an ape DNABin into a DNASTringSet.

Usage

```
dnabin2dnastring(dnabin)
```

Arguments

dnabin ape DNABin [mandatory]

Value

An object of class DNASTringSet

Author(s)

Kristian K Ullrich

See Also

[as.alignment](#) [as.DNABin.alignment](#) [DNASTringSet](#)

Examples

```
data(woodmouse, package="ape")
## convert into DNASTringSet
#dnabin2dnastring(woodmouse)
woodmouse |> dnabin2dnastring()
```

`dnastring2aln`*dnastring2aln*

Description

This function converts a DNASTringSet into an seqinr alignment.

Usage

```
dnastring2aln(dna)
```

Arguments

`dna` DNASTringSet [mandatory]

Value

An object of class alignment which is a list with the following components:

`nb` the number of aligned sequences

`nam` a vector of strings containing the names of the aligned sequences

`seq` a vector of strings containing the aligned sequences

`com` a vector of strings containing the commentaries for each sequence or NA if there are no comments

Author(s)

Kristian K Ullrich

See Also

[as.alignment](#)

Examples

```
## define two cds sequences
cds1 <- Biostrings::DNASTring("ATGCAACATTGC")
cds2 <- Biostrings::DNASTring("ATG---CATTGC")
cds1.cds2.aln <- c(Biostrings::DNASTringSet(cds1),
  Biostrings::DNASTringSet(cds2))
## convert into alignment
#dnastring2aln(cds1.cds2.aln)
cds1.cds2.aln |> dnastring2aln()
```

dnastring2codonmat *dnastring2codonmat*

Description

This function converts a DNASTringSet into a codon matrix.

Usage

```
dnastring2codonmat(cds, shorten = FALSE, frame = 1, framelist = NULL)
```

Arguments

cds	DNASTringSet [mandatory]
shorten	shorten all sequences to multiple of three [default: FALSE]
frame	indicates the first base of a the first codon [default: 1]
framelist	supply vector of frames for each entry [default: NULL]

Value

An object of class alignment which is a list with the following components:

nb the number of aligned sequences

nam a vector of strings containing the names of the aligned sequences

seq a vector of strings containing the aligned sequences

com a vector of strings containing the commentaries for each sequence or NA if there are no comments

Author(s)

Kristian K Ullrich

See Also

[as.alignment](#)

Examples

```
## define two cds sequences
cds1 <- Biostrings::DNASTring("ATGCAACATTGC")
cds2 <- Biostrings::DNASTring("ATG---CATTGC")
cds1.cds2.aln <- c(Biostrings::DNASTringSet(cds1),
  Biostrings::DNASTringSet(cds2))
## convert into alignment
#dnastring2codonmat(cds1.cds2.aln)
cds1.cds2.aln |> dnastring2codonmat()
## use frame 2 and shorten to circumvent multiple of three error
cds1 <- Biostrings::DNASTring("-ATGCAACATTGC-")
cds2 <- Biostrings::DNASTring("-ATG---CATTGC-")
```

```

cds1.cds2.aln <- c(Biostrings::DNASTringSet(cds1),
  Biostrings::DNASTringSet(cds2))
cds1.cds2.aln |> dnastring2codonmat(frame=2, shorten=TRUE)

```

dnastring2dist	<i>dnastring2dist</i>
----------------	-----------------------

Description

This function calculates pairwise distances for all combinations of a DNASTringSet.

Usage

```

dnastring2dist(
  dna,
  model = "IUPAC",
  threads = 1,
  score = NULL,
  mask = NULL,
  region = NULL,
  ...
)

```

Arguments

dna	DNASTringSet [mandatory]
model	specify model either "IUPAC" or any model from <code>ape::dist.dna</code> [default: IUPAC]
threads	number of parallel threads [default: 1]
score	score matrix use score matrix to calculate distances [default: NULL]
mask	IRanges object indicating masked sites [default: NULL]
region	IRanges object indicating region to use for dist calculation. Default is null, meaning all sites are used [default: NULL]
...	other <code>ape::dist.dna</code> parameters (see dist.dna)

Value

A data.frame of pairwise distance values `distSTRING` and sites used `sitesUsed`

Author(s)

Kristian K Ullrich

See Also

[dist.dna](#)

Examples

```
## load example sequence data
data("hiv", package="MSA2dist")
#dnastring2dist(hiv, model="IUPAC")
hiv |> dnastring2dist(model="IUPAC")
#dnastring2dist(hiv, model="K80")
hiv |> dnastring2dist(model="K80")
data("woodmouse", package="ape")
#dnastring2dist(dnabin2dnastring(woodmouse), score=iupacMatrix())
woodmouse |> dnabin2dnastring() |> dnastring2dist()
#dnastring2dist(hiv, model = "IUPAC", threads = 2)
hiv |> dnastring2dist(model = "IUPAC", threads = 2)
## create mask
mask1 <- IRanges::IRanges(start=c(1,61,121), end=c(30,90,150))
## use mask
hiv |> dnastring2dist(model="IUPAC", mask=mask1)
## use region
region1 <- IRanges::IRanges(start=c(1,139), end=c(75,225))
hiv |> dnastring2dist(model="IUPAC", region=region1)
## use mask and region
hiv |> dnastring2dist(model="IUPAC", mask=mask1, region=region1)
```

dnastring2dnabin *dnastring2dnabin*

Description

This function converts a DNAStrngSet into an ape DNABin.

Usage

```
dnastring2dnabin(dna)
```

Arguments

dna DNAStrngSet [mandatory]

Value

An object of class DNABin

Author(s)

Kristian K Ullrich

See Also

[as.alignment](#) [as.DNABin.alignment](#)

Examples

```
## define two cds sequences
cds1 <- Biostrings::DNASTring("ATGCAACATTGC")
cds2 <- Biostrings::DNASTring("ATG---CATTGC")
cds1.cds2.aln <- c(Biostrings::DNASTringSet(cds1),
  Biostrings::DNASTringSet(cds2))
## convert into DNABin
#dnastring2dnabin(cds1.cds2.aln)
cds1.cds2.aln |> dnastring2dnabin()
```

dnastring2kaks	<i>dnastring2kaks</i>
----------------	-----------------------

Description

This function calculates Ka/Ks (pN/pS) for all combinations of a DNASTringSet. If the sequences in the DNASTringSet are not a multiple-sequence alignment, pairwise codon alignments can be calculated on the fly. Models used and implemented according to *Li (1993)* (using seqinr) or *Nei and Gojobori (1986)* (own implementation) or models from KaKs_Calculator2 ported to MSA2dist with Rcpp.

Usage

```
dnastring2kaks(
  cds,
  model = "Li",
  threads = 1,
  isMSA = TRUE,
  sgc = "1",
  verbose = FALSE,
  ...
)
```

Arguments

cds	DNASTringSet coding sequence alignment [mandatory]
model	specify codon model either "Li" or "NG86" or one of KaKs_Calculator2 model "NG", "LWL", "LPB", "MLWL", "MLPB", "GY", "YN", "MYN", "MS", "MA", "GNG", "GLWL", "GLPB", "GMLWL", "GMLPB", "GYN", "GMYN" [default: Li]
threads	number of parallel threads [default: 1]
isMSA	cds DNASTringSet represents MSA [default: TRUE]
sgc	standard genetic code (for KaKs Calculator models) [default: 1]
verbose	verbosity (for KaKs Calculator models) [default: FALSE]
...	other codon alignment parameters

Value

A data.frame of KaKs values

Author(s)

Kristian K Ullrich

References

- "MS/MA/GNG/GLWL/GLPB/GMLWL/GMLPB/GYN:" Wang et al. (2010) KaKs_Calculator 2.0: a toolkit incorporating gamma-series methods and sliding window strategies. *Genomics, proteomics & bioinformatics*. **8(1)**, 77-80.
- "Li/LWL:" Li et al. (1985) A new method for estimating synonymous and nonsynonymous rates of nucleotide substitution considering the relative likelihood of nucleotide and codon changes. *Mol. Biol. Evol.*, **2(2)**, 150-174.
- "Li/LPB:" Li (1993). Unbiased estimation of the rates of synonymous and nonsynonymous substitution. *Journal of molecular evolution*, 36(1), pp.96-99.
- "NG86/NG:" Nei and Gojobori. (1986) Simple methods for estimating the numbers of synonymous and nonsynonymous nucleotide substitutions. *Mol. Biol. Evol.*, **3(5)**, 418-426.
- "LPB:" Pamilo and Bianchi. (1993) Evolution of the Zfx and Zfy genes: Rates and interdependence between genes. *Mol. Biol. Evol.*, **10**, 271-281.
- "MLWL/MLPB:" Tzeng et al. (2004). Comparison of three methods for estimating rates of synonymous and nonsynonymous nucleotide substitutions. *Mol. Biol. Evol.*, **21(12)**, 2290-2298.
- "GY:" Goldman and Yang (1994). A codon-based model of nucleotide substitution for protein-coding DNA sequences. *Mol. Biol. Evol.*, **11(5)** 725-736.
- "YN:" Yang et al. (2000) Codon-substitution models for heterogeneous selection pressure at amino acid sites. *Genetics*. **155(1)**, 431-449.
- "MYN:" Zhang et al. (2006). Computing Ka and Ks with a consideration of unequal transitional substitutions. *BMC evolutionary biology*, **6(1)**, 1-10.
- "data(hiv):" Ganeshan et al. (1997) Human immunodeficiency virus type 1 genetic evolution in children with different rates of development of disease. *J. Virology*. **71(1)**, 663-677.
- Wang et al. (2009). gamma-MYN: a new algorithm for estimating Ka and Ks with consideration of variable substitution rates. *Biology Direct*, **4(1)**, 1-18.

See Also

[kaks](#)

Examples

```
## load example sequence data
data("hiv", package="MSA2dist")
#dnastring2kaks(hiv, model="Li")
hiv |> dnastring2kaks(model="Li")
#dnastring2kaks(hiv, model="NG86")
hiv |> dnastring2kaks(model="NG86")
```

```
#dnastring2kaks(hiv, model="NG86", threads=2)
hiv |> dnastring2kaks(model="NG86", threads=2)

## define three unaligned cds sequences
cds1 <- Biostrings::DNASTring("ATGCAACATTGC")
cds2 <- Biostrings::DNASTring("ATGCATTGC")
cds3 <- Biostrings::DNASTring("ATGCAATGC")
cds_sequences <- Biostrings::DNASTringSet(list(cds1, cds2, cds3))
names(cds_sequences) <- c("cds1", "cds2", "cds3")
## set isMSA to FALSE to automatically create pairwise codon alignments
#dnastring2kaks(cds_sequences, model="Li", isMSA=FALSE)
cds_sequences |> dnastring2kaks(model="Li", isMSA=FALSE)
```

GENETIC_CODE_TCAG *GENETIC_CODE_TCAG*

Description

GENETIC_CODE from Biostrings extended by codon number and number of syn sites.

Usage

```
codon2number(codon)
```

Arguments

codon codon [mandatory]

Value

An object of class `numeric`

Author(s)

Kristian K Ullrich

See Also

[GENETIC_CODE](#)

Examples

```
GENETIC_CODE_TCAG
```

getmask	<i>getmask</i>
---------	----------------

Description

This function shows the mask slot from a DNASTringSet or an AAStringSet metadata information.

Usage

```
getmask(seq)
```

Arguments

seq DNASTringSet or AAStringSet [mandatory]

Value

IRanges information from metadata

Author(s)

Kristian K Ullrich

See Also

[addpop2string](#)

Examples

```
## load example sequence data
data(iupac, package="MSA2dist")
iupac.aa <- iupac |> cds2aa(shorten = TRUE)
## create mask
mask1 <- IRanges::IRanges(start=c(1,41), end=c(20,50))
## add mask
iupac.aa <- iupac.aa |> addmask2string(mask=mask1)
#(iupac.aa |> slot("metadata"))$mask
iupac.aa |> getmask()
```

getpos	<i>getpos</i>
--------	---------------

Description

This function shows the position slot from a DNASTringSet or an AAStringSet metadata information.

Usage

```
getpos(seq)
```

Arguments

seq DNASTringSet or AAStringSet [mandatory]

Value

GenomicRanges information from metadata

Author(s)

Kristian K Ullrich

See Also

[addpop2string](#)

Examples

```
## load example sequence data
data(iupac, package="MSA2dist")
## add position
iupac <- iupac |> addpos2string(chrom="chr1", start=1, end=1000)
#(iupac |> slot("metadata"))$GRanges
iupac |> getpos()
```

globalDeletion	<i>globalDeletion</i>
----------------	-----------------------

Description

This function returns a DNASTringSet reduced by all sites containing any gaps ("-", "+", ".") or missing ("N") sites.

Usage

```
globalDeletion(dna)
```

Arguments

dna DNASTringSet [mandatory]

Value

DNASTringSet

Author(s)

Kristian K Ullrich

Examples

```
## define two cds sequences
cds1 <- Biostrings::DNASTring("ATGCAACATTGC")
cds2 <- Biostrings::DNASTring("ATG---CATTGC")
cds1.cds2.aln <- c(Biostrings::DNASTringSet(cds1),
  Biostrings::DNASTringSet(cds2))
globalDeletion(cds1.cds2.aln)
```

granthamMatrix	<i>granthamMatrix</i>
----------------	-----------------------

Description

This function creates a granthamMatrix object to be used with the rcpp_distSTRING function. By default, the grantham matrix is defined as from Grantham 1974. (see <https://link.springer.com/article/10.1007/s00335-017-9704-9>)

Usage

```
granthamMatrix()
```

Value

matrix

Author(s)

Kristian K Ullrich

References

Grantham R. (1974). Amino Acid Difference Formula to Help Explain Protein Evolution. *Science*, **185**(4154), 862-864.

See Also

[aastring2dist](#), [dist.dna](#)

Examples

```
granthamMatrix()
```

hiv-data

hiv-data

Description

Example cds sequences from HIV-1 sample 136 patient 1 from Sweden envelope glycoprotein (env) gene, V3 region as DNASTringSet.

Usage

```
data(hiv)
```

Format

an object of class DNASTringSet see [XStringSet-class](#)

References

Yang et al. (2000) Codon-substitution models for heterogeneous selection pressure at amino acid sites. *Genetics*. **155**(1), 431-449.

Examples

```
data("hiv", package="MSA2dist")
```

`iupac-data`*iupac-data*

Description

Example IUPAC sequences created with `angsd` from different house mouse (*Mus musculus*) sub-populations from Harr et al. (2016) `DNAStringSet`.

Usage

```
data(iupac)
```

Format

an object of class `DNAStringSet` see [XStringSet-class](#)

References

Harr et al. (2016) Genomic resources for wild populations of the house mouse, *Mus musculus* and its close relative *Mus spretus*. *Scientific data*. **3(1)**, 1-14.

Examples

```
data("iupac", package="MSA2dist")
```

`iupacMatrix`*iupacMatrix*

Description

This function creates a `iupacMatrix` object to be used with the `rcpp_distSTRING` function. By default, the `iupac matrix` is defined as literal distance obtained from Chang et al. 2017. (see <https://link.springer.com/article/10.1007/s00335-017-9704-9>)

Usage

```
iupacMatrix()
```

Value

score matrix

Author(s)

Kristian K Ullrich

References

Chang,P. L.,Kopania,E.,Keeble,S.,Sarver,B. A.,Larson, E.,Orth,A,... & Dean,M. D. (2017). Whole exome sequencing of wild-derived inbred strains of mice improves power to link phenotype and genotype. *Mammalian genome*,**28(9-10)**,416-425.

See Also

[dnastring2dist,dist.dna](#)

Examples

```
iupacMatrix()
```

makePostalignedSeqs *makePostalignedSeqs*

Description

This function is a fork from an internal function from Biostrings

Usage

```
makePostalignedSeqs(x)
```

Arguments

x x

Value

get internal function makePostalignedSeqs

Author(s)

Kristian K Ullrich

See Also

[pairwiseAlignment, cds2codonaln](#)

Examples

```
## define two cds sequences
cds1 <- Biostrings::DNASTring("ATGCAACATTGC")
cds2 <- Biostrings::DNASTring("ATGCATTGC")
makePostalignedSeqs(Biostrings::pairwiseAlignment(
  cds2aa(Biostrings::DNASTringSet(cds1)),
  cds2aa(Biostrings::DNASTringSet(cds2))))
```

popinteger

popinteger

Description

This function shows the population integer slot from a DNAStrngSet or an AAStringSet metadata information.

Usage

```
popinteger(seq)
```

Arguments

seq DNAStrngSet or AAStringSet [mandatory]

Value

population integer from metadata

Author(s)

Kristian K Ullrich

See Also

[addpop2string](#)

Examples

```
## load example sequence data
data(iupac, package="MSA2dist")
iupac.aa <- iupac |> cds2aa(shorten = TRUE)
## create poplist
poplist <- list(FRA = grep("Mmd.FRA", names(iupac)),
               GER = grep("Mmd.GER", names(iupac)),
               IRA = grep("Mmd.IRA", names(iupac)),
               AFG = grep("Mmm.AFG", names(iupac)))
iupac.aa <- iupac.aa |> addpop2string(poplist)
popinteger(iupac.aa)
```

popnames	<i>popnames</i>
----------	-----------------

Description

This function shows the population names slot from a DNAStrngSet or an AAStringSet metadata information.

Usage

```
popnames(seq)
```

Arguments

```
seq          DNAStrngSet or AAStringSet [mandatory]
```

Value

population names from metadata

Author(s)

Kristian K Ullrich

See Also

[addpop2string](#)

Examples

```
## load example sequence data
data(iupac, package="MSA2dist")
iupac.aa <- iupac |> cds2aa(shorten = TRUE)
## create poplist
poplist <- list(FRA = grep("Mmd.FRA", names(iupac)),
               GER = grep("Mmd.GER", names(iupac)),
               IRA = grep("Mmd.IRA", names(iupac)),
               AFG = grep("Mmm.AFG", names(iupac)))
iupac.aa <- iupac.aa |> addpop2string(poplist)
popnames(iupac.aa)
```

rcpp_distSTRING	<i>rcpp_distSTRING</i>
-----------------	------------------------

Description

calculates pairwise distances using a score matrix

Usage

```
rcpp_distSTRING(dnvector, scoreMatrix, ncores = 1L)
```

Arguments

dnvector	StringVector [mandatory]
scoreMatrix	NumericMatrix [mandatory]
ncores	number of cores [default: 1]

Value

list

Author(s)

Kristian K Ullrich

Examples

```
## load example sequence data
data("hiv", package="MSA2dist")
rcpp_distSTRING(dnvector=as.character(hiv), scoreMatrix=iupacMatrix())
```

rcpp_KaKs	<i>rcpp_KaKs</i>
-----------	------------------

Description

calculates KaKs as implemented in KaKs Calculator 2.0 MSA2dist with Rcpp.

Usage

```
rcpp_KaKs(cdsstr, sgc = "1", method = "YN", verbose = FALSE)
```

Arguments

cdsstr	StringVector [mandatory]
sgc	standard genetic code to use [default: 1]
method	KaKs Calculator 2.0 codon model [default: YN]
verbose	specify if verbose output [default: FALSE]

Value

list

Author(s)

Kristian K Ullrich

References

Wang et al. (2010) KaKs_Calculator 2.0: a toolkit incorporating gamma-series methods and sliding window strategies. *Genomics, proteomics & bioinformatics*. **8(1)**, 77-80.

Examples

```
## load example sequence data
data("hiv", package="MSA2dist")
rcpp_KaKs(cdsstr=as.character(hiv[1:3]))
```

rcpp_pairwiseDeletionAA

rcpp_pairwiseDeletionAA

Description

returns number of AA sites used

Usage

```
rcpp_pairwiseDeletionAA(aavector, ncores = 1L)
```

Arguments

aavector	StringVector [mandatory]
ncores	number of cores [default: 1]

Value

list

Author(s)

Kristian K Ullrich

Examples

```
## load example sequence data
data("hiv", package="MSA2dist")
h <- hiv |> cds2aa() |> as.character()
rcpp_pairwiseDeletionAA(aavector=h, ncores=1)
```

```
rcpp_pairwiseDeletionDNA
      rcpp_pairwiseDeletionDNA
```

Description

returns number of DNA sites used

Usage

```
rcpp_pairwiseDeletionDNA(dnavector, ncores = 1L)
```

Arguments

dnavector	StringVector [mandatory]
ncores	number of cores [default: 1]

Value

list

Author(s)

Kristian K Ullrich

Examples

```
## load example sequence data
data("woodmouse", package="ape")
w <- woodmouse |> dnabin2dnastring() |> as.character()
rcpp_pairwiseDeletionDNA(dnavector=w, ncores=1)
```

region	<i>region</i>
--------	---------------

Description

This function shows the region slot from a DNASTringSet or an AAStringSet metadata information.

Usage

```
region(seq)
```

Arguments

seq DNASTringSet or AAStringSet [mandatory]

Value

region IRanges object from metadata

Author(s)

Kristian K Ullrich

See Also

[addpop2string](#)

Examples

```
## load example sequence data
data(iupac, package="MSA2dist")
iupac.aa <- iupac |> cds2aa(shorten = TRUE)
## create region
region1 <- IRanges::IRanges(start=c(1,41), end=c(20,50))
## add region
iupac.aa <- iupac.aa |> addregion2string(region=region1)
iupac.aa |> region()
```

regionused	<i>regionused</i>
------------	-------------------

Description

This function shows the region used slot from a DNASTringSet or an AAStringSet metadata information.

Usage

```
regionused(seq)
```

Arguments

seq DNASTringSet or AAStringSet [mandatory]

Value

population names from metadata

Author(s)

Kristian K Ullrich

See Also

[addpop2string](#)

Examples

```
## load example sequence data
data("hiv", package="MSA2dist")
## create mask
mask1 <- IRanges::IRanges(start=c(11,41,71), end=c(20,50,80))
## use mask
hiv.region <- hiv |> cds2aa() |> string2region(mask=mask1)
#(hiv.region |> slot("metadata"))$regionUsed
hiv.region |> regionused()
```

string2region	<i>string2region</i>
---------------	----------------------

Description

This function subsets a DNASTringSet or an AAStringSet by a mask and region given one or both options as IRanges.

Usage

```
string2region(seq, mask = NULL, region = NULL, add = TRUE)
```

Arguments

seq	DNASTringSet or AAStringSet [mandatory]
mask	IRanges object indicating masked sites [default: NULL]
region	IRanges object indicating region to use for dist calculation (by default all sites are used) [default: NULL]
add	indicate if mask and region should be added to metadata [default: TRUE]

Value

A list object with the following components:
 DNASTringSet or AAStringSet
 regionUsed

Author(s)

Kristian K Ullrich

See Also

[dnastring2dist](#)

Examples

```
## load example sequence data
data("hiv", package="MSA2dist")
## create mask
mask1 <- IRanges::IRanges(start=c(11,41,71), end=c(20,50,80))
## use mask
hiv.region <- hiv |> cds2aa() |> string2region(mask=mask1)
#(hiv.region |> slot("metadata"))$regionUsed
hiv.region |> regionused()
## use region
region1 <- IRanges::IRanges(start=c(1,75), end=c(45,85))
hiv.region <- hiv |> cds2aa() |> string2region(region=region1)
```

```
 #(hiv.region |> slot("metadata"))$regionUsed
 hiv.region |> regionused()
 ## use mask and region
 hiv.region <- hiv |> cds2aa() |> string2region(mask=mask1, region=region1)
 #(hiv.region |> slot("metadata"))$regionUsed
 hiv.region |> regionused()
```

subString

subString

Description

This function gets a subsequence from a DNASTring, RNASTring, AAString, BString, DNASTringSet, RNASTringSet, AAStringSet, BStringSet object from the Biostrings package.

Usage

```
subString(x, s, e)
```

Arguments

x	DNASTringSet, RNASTring, AAString, BString, DNASTringSet, RNASTringSet, AAStringSet, BStringSet [mandatory]
s	start vector [mandatory]
e	end vector [mandatory]

Value

subsequence of an Biostrings object

Author(s)

Kristian K Ullrich

See Also

[subseq](#)

Examples

```
## define two cds sequences
cds1 <- Biostrings::DNASTring("ATGCAACATTGC")
cds2 <- Biostrings::DNASTring("ATG---CATTGC")
cds1.cds2.aln <- c(Biostrings::DNASTringSet(cds1),
  Biostrings::DNASTringSet(cds2))
subString(cds1.cds2.aln, c(1,7), c(3,12))
```

uptriidx	<i>uptriidx</i>
----------	-----------------

Description

This function returns upper tri index for usage with `pivot_long` reduction.

Usage

```
uptriidx(n, diag = FALSE)
```

Arguments

n	dimension of initial matrix [mandatory]
diag	indicate if diag should be retained [default: FALSE]

Value

list of positions

Author(s)

Kristian K Ullrich

Examples

```
uptriidx(10)
```

Index

* datasets

- AAMatrix-data, 4
- hiv-data, 32
- iupac-data, 33

- aabin2aastriing, 3
- AAMatrix (AAMatrix-data), 4
- AAMatrix-data, 4
- aastriing2aabin, 4
- aastriing2aln, 5
- aastriing2dist, 6, 32
- AAStriiingSet, 3, 12
- addmask2striing, 7, 9–11
- addpop2striing, 7, 8, 10, 11, 29, 30, 35, 36, 40, 41
- addpos2striing, 7, 9, 9, 11
- addrregion2striing, 7, 9, 10, 10
- aln2aastriing, 12
- aln2dnastriing, 13
- as.alignment, 3, 5, 12, 13, 21–23, 25
- as.DNABin.alignment, 3, 5, 21, 25

- cds2aa, 14
- cds2codonaln, 15, 34
- codon2number (GENETIC_CODE_TCAG), 28
- codon2numberAMBIG, 16
- codon2numberTCAG, 17
- codonmat2pnps, 17, 20
- codonmat2xy, 19
- compareCodons, 20

- dist.dna, 24, 32, 34
- dnabin2dnastriing, 21
- dnastriing2aln, 22
- dnastriing2codonmat, 19, 20, 23
- dnastriing2dist, 6, 24, 34, 42
- dnastriing2dnabin, 25
- dnastriing2kaks, 20, 26
- DNAStriiingSet, 13, 21

- GENETIC_CODE, 16, 17, 28

- GENETIC_CODE_TCAG, 28
- getmask, 29
- getpos, 30
- globalDeletion, 31
- granthamMatrix, 31

- hiv (hiv-data), 32
- hiv-data, 32

- iupac (iupac-data), 33
- iupac-data, 33
- iupacMatrix, 33

- kaks, 18, 20, 21, 27

- makePostalignedSeqs, 34

- pairwiseAlignment, 15, 16, 34
- popinteger, 35
- popnames, 36

- rcpp_distSTRING, 37
- rcpp_KaKs, 37
- rcpp_pairwiseDeletionAA, 38
- rcpp_pairwiseDeletionDNA, 39
- region, 40
- regionused, 41

- striing2region, 42
- subseq, 43
- subStriiing, 43

- translate, 14

- uptriidx, 44