

# Package ‘MSA2dist’

December 5, 2025

**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** 1.15.0

**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. DNASTringSet alignments can be analysed as codon alignments to look for synonymous and nonsynonymous substitutions (dN/dS) in a parallelised fashion using a variety of substitution models. Non-aligned coding sequences can be directly used to construct pairwise codon alignments (global/local) and calculate dN/dS without any external dependencies.

**License** GPL-3 + file LICENSE

**Encoding** UTF-8

**LazyData** false

**biocViews** Alignment, Sequencing, Genetics, GO

**Depends** R (>= 4.4.0)

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

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

**LinkingTo** Rcpp, RcppThread

**VignetteBuilder** knitr

**NeedsCompilation** yes

**SystemRequirements** C++11

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

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

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---

|              |                     |
|--------------|---------------------|
| aa2selfscore | <i>aa2selfscore</i> |
|--------------|---------------------|

---

**Description**

This function return the selfscore from an AAStringSet.

**Usage**

```
aa2selfscore(aa, scorematrix = "BLOSUM62")
```

**Arguments**

|             |                                         |
|-------------|-----------------------------------------|
| aa          | AAStringSet [mandatory]                 |
| scorematrix | score matrix to use [default: BLOSUM62] |

**Value**

data.frame

**Author(s)**

Kristian K Ullrich

**See Also**

[XStringSet-class](#), [substitution\\_matrices](#)

**Examples**

```
data(woodmouse, package="ape")
#cds2aa(dnabin2dnastring(woodmouse), shorten=TRUE,
#genetic.code=Biostrings::getGeneticCode("2"))
woodmouse |> dnabin2dnastring() |> cds2aa(shorten=TRUE,
genetic.code=Biostrings::getGeneticCode("2")) |> aa2selfscore()
```

---

aabin2aastring

*aabin2aastring*


---

**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 an `AAStringSet` into an ape `AAbin`.

**Usage**

```
aastring2aabin(aa)
```

**Arguments**

`aa` `AAStringSet` [mandatory]

**Value**

An object of class `AAbin`

**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,
  symmetric = TRUE,
  score = NULL,
  mask = NULL,
  region = NULL
)
```

**Arguments**

|           |                                                                                                              |
|-----------|--------------------------------------------------------------------------------------------------------------|
| aa        | AAStringSet [mandatory]                                                                                      |
| threads   | number of parallel threads [default: 1]                                                                      |
| symmetric | symmetric score matrix [default: TRUE]                                                                       |
| 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")
#astring2dist(cds2aa(hiv), score=granthamMatrix())
hiv |> cds2aa() |> astring2dist(score=granthamMatrix())
## create mask
mask1 <- IRanges::IRanges(start=c(11,41,71), end=c(20,50,80))
## use mask
hiv |> cds2aa() |> astring2dist(score=granthamMatrix(), mask=mask1)
## use region
region1 <- IRanges::IRanges(start=c(1,75), end=c(45,85))
hiv |> cds2aa() |> astring2dist(score=granthamMatrix(), region=region1)
## use mask and region
hiv |> cds2aa() |> astring2dist(score=granthamMatrix(),
  mask=mask1, region=region1)
## use asymmetric score matrix
myscore <- granthamMatrix()
myscore[5, 6] <- 0
h <- hiv |> cds2aa() |> astring2dist(score=myscore, symmetric=FALSE)
h$distSTRING[1:2, 1:2]
```

---

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     | DNAStrngSet 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 DNAStrngSet 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()
## mixing 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 | <i>addpos2string</i> |
|---------------|----------------------|

---

## 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   | DNASTringSet or AAStringSet [mandatory] |
| chrom | chromosome name [mandatory]             |
| start | start position [mandatory]              |
| end   | end position [mandatory]                |

## Value

An object of class DNASTringSet 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 | <i>addregion2string</i> |
|------------------|-------------------------|

---

### Description

This function adds region 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

```
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*cds2aa*

---

## Description

This function translates a DNAStringSet into an AAStringSet.

## Usage

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

## 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] |
| return.cds   | return shorten cds instead of aa [default: FALSE]                                             |

## 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,
#genetic.code=Biostrings::getGeneticCode("2"))
woodmouse |> dnabin2dnastring() |> cds2aa(shorten=TRUE,
genetic.code=Biostrings::getGeneticCode("2"))
woodmouse |> dnabin2dnastring() |> cds2aa(shorten=TRUE, return.cds=TRUE) |>
cds2aa(genetic.code=Biostrings::getGeneticCode("2"))
```

cds2codonaln

*cds2codonaln*

## 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 <a href="#">pairwiseAlignment</a> ) [default: global]                                                                 |
| substitutionMatrix | substitution matrix representing the fixed substitution scores for an alignment (see <a href="#">pairwiseAlignment</a> ) [default: BLOSUM62] |
| gapOpening         | the cost for opening a gap in the alignment (see <a href="#">pairwiseAlignment</a> ) [default: 10]                                           |
| gapExtension       | the incremental cost incurred along the length of the gap in the alignment (see <a href="#">pairwiseAlignment</a> ) [default: 0.5]           |

`remove.gaps`      specify if gaps in the codon alignment should be removed [default: FALSE]  
`...`                other cds2aa parameters

**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)
```

---

|                                 |                           |
|---------------------------------|---------------------------|
| <code>cdsstring2codonaln</code> | <i>cdsstring2codonaln</i> |
|---------------------------------|---------------------------|

---

**Description**

This function takes two sequences as `DNAStringSet`, and their corresponding `AAStringSet`, calculates a global alignment and converts this alignment back into a codon alignment.

**Usage**

```
cdsstring2codonaln(
  cds,
  aa,
  type = "global",
  substitutionMatrix = "BLOSUM62",
  gapOpening = 10,
  gapExtension = 0.5,
  remove.gaps = FALSE
)
```

**Arguments**

|                                 |                                                                                                                                              |
|---------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------|
| <code>cds</code>                | two sequences DNASTringSet [mandatory]                                                                                                       |
| <code>aa</code>                 | two sequences AAStringSet [mandatory]                                                                                                        |
| <code>type</code>               | type of alignment (see <a href="#">pairwiseAlignment</a> ) [default: global]                                                                 |
| <code>substitutionMatrix</code> | substitution matrix representing the fixed substitution scores for an alignment (see <a href="#">pairwiseAlignment</a> ) [default: BLOSUM62] |
| <code>gapOpening</code>         | the cost for opening a gap in the alignment (see <a href="#">pairwiseAlignment</a> ) [default: 10]                                           |
| <code>gapExtension</code>       | the incremental cost incurred along the length of the gap in the alignment (see <a href="#">pairwiseAlignment</a> ) [default: 0.5]           |
| <code>remove.gaps</code>        | 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
cds <- Biostrings::DNASTringSet(c("ATGCAACATTGC", "ATGCATTGC"))
names(cds) <- c("cds1", "cds2")
## get protein alignment
aa <- MSA2dist::cds2aa(cds)
cdsstring2codonaln(cds, aa)
```

---

|                   |                          |
|-------------------|--------------------------|
| 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  
 dn ds 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 <a href="#">dnastring2codonmat</a> [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 | <i>compareCodons</i> |
|---------------|----------------------|

---

### 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 | <i>dnastring2aln</i> |
|---------------|----------------------|

---

**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 | <i>dnastring2codonmat</i> |
|--------------------|---------------------------|

---

**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

*dnastring2dist*

---

**Description**

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

**Usage**

```
dnastring2dist(
  dna,
  model = "IUPAC",
  threads = 1,
  symmetric = TRUE,
  score = NULL,
```

```

    mask = NULL,
    region = NULL,
    ...
)

```

### Arguments

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

### 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)
## use asymmetric score matrix
myscore <- iupacMatrix()
myscore[1, 4] <- 0.5
(hiv |> dnastring2dist(score=myscore, symmetric=FALSE))$distSTRING[1:2, 1:2]

```

---

|                  |                         |
|------------------|-------------------------|
| dnastring2dnabin | <i>dnastring2dnabin</i> |
|------------------|-------------------------|

---

## Description

This function converts a DNASTringSet into an ape DNABin.

## Usage

```
dnastring2dnabin(dna)
```

## Arguments

dna                      DNASTringSet [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 | <i>GENETIC_CODE_TCAG</i> |
|-------------------|--------------------------|

---

## 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)
```

---

|                  |                         |
|------------------|-------------------------|
| globalDeletionAA | <i>globalDeletionAA</i> |
|------------------|-------------------------|

---

**Description**

This function returns an AAStringSet reduced by all sites containing any gaps ("-", "+", ".") or missing ("X") sites.

**Usage**

```
globalDeletionAA(aa)
```

**Arguments**

aa                    AAStringSet [mandatory]

**Value**

AAStringSet

**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))
#globalDeletionAA(cds2aa(cds1.cds2.aln))
cds1.cds2.aln |> cds2aa() |> globalDeletionAA()
```

---

granthamMatrix

*granthamMatrix*

---

**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 | <i>hiv-data</i> |
|----------|-----------------|

---

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")
```

---

|              |                     |
|--------------|---------------------|
| indices2kaks | <i>indices2kaks</i> |
|--------------|---------------------|

---

Description

This function calculates Ka/Ks (pN/pS) for all combinations given in an indices list 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**

```
indices2kaks(
  cds,
  indices,
  model = "Li",
  threads = 1,
  isMSA = TRUE,
  sgc = "1",
  verbose = FALSE,
  ...
)
```

**Arguments**

|         |                                                                                                                                                                                                                    |
|---------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| cds     | DNAStringSet coding sequence alignment [mandatory]                                                                                                                                                                 |
| indices | list list of indices to calculate Ks/Ks [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")
## create indices
idx <- list(c(2, 3), c(5,7,9))
#indices2kaks(hiv, idx, model="Li")
hiv |> indices2kaks(idx, model="Li")
#indices2kaks(hiv, idx, model="NG86")
hiv |> indices2kaks(idx, model="NG86")
#indices2kaks(hiv, idx, model="NG86", threads=2)
hiv |> indices2kaks(idx, 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")
## create indices
idx <- list(c(1, 2), c(1,3))
## set isMSA to FALSE to automatically create pairwise codon alignments
#indices2kaks(cds_sequences, idx, model="Li", isMSA=FALSE)
cds_sequences |> indices2kaks(idx, model="Li", isMSA=FALSE)
```

---

*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 | <i>makePostalignedSeqs</i> |
|---------------------|----------------------------|

---

## 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(pwalign::pairwiseAlignment(
  cds2aa(Biostrings::DNAStringSet(cds1)),
  cds2aa(Biostrings::DNAStringSet(cds2))))
```

---

|         |                |
|---------|----------------|
| pal2nal | <i>pal2nal</i> |
|---------|----------------|

---

## Description

This function takes an `AAStringSet` alignment and its corresponding coding sequences `DNAStrngSet` and converts the protein alignment into a codon alignment.

## Usage

```
pal2nal(pal, nal, remove.gaps = FALSE)
```

## Arguments

|                          |                                                                                         |
|--------------------------|-----------------------------------------------------------------------------------------|
| <code>pal</code>         | <code>AAStringSet</code> [mandatory]                                                    |
| <code>nal</code>         | <code>DNAStrngSet</code> [mandatory]                                                    |
| <code>remove.gaps</code> | specify if gaps in the codon alignment should be removed [default: <code>FALSE</code> ] |

## Value

codon alignment as `DNAStrngSet`

## 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
cds <- Biostrings::DNAStrngSet(c("ATGCAACATTGC", "ATGCATTGC"))
names(cds) <- c("cds1", "cds2")
## get protein alignment
aa <- MSA2dist::cds2aa(cds)
msa <- makePostalignedSeqs(pwalign::pairwiseAlignment(aa[1], aa[2]))[[1L]]
names(msa) <- names(aa)
## get codon alignment
nal <- MSA2dist::pal2nal(pal=msa, nal=cds)
nal
```

popinteger

*popinteger*

---

**Description**

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

**Usage**

```
popinteger(seq)
```

**Arguments**

seq                      DNASTringSet 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 DNASTringSet or an AAStringSet metadata information.

## Usage

```
popnames(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(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(dnavector, scoreMatrix, ncores = 1L, symmetric = 1L)
```

**Arguments**

|             |                                     |
|-------------|-------------------------------------|
| dnavector   | StringVector [mandatory]            |
| scoreMatrix | NumericMatrix [mandatory]           |
| ncores      | number of cores [default: 1]        |
| symmetric   | symmetric score matrix [default: 1] |

**Value**

list

**Author(s)**

Kristian K Ullrich

**Examples**

```
## load example sequence data
data("hiv", package="MSA2dist")
rcpp_distSTRING(dnavector=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, symmetric = 1L)
```

**Arguments**

|           |                                     |
|-----------|-------------------------------------|
| aavector  | StringVector [mandatory]            |
| ncores    | number of cores [default: 1]        |
| symmetric | symmetric score matrix [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, symmetric = 1L)
```

**Arguments**

|           |                                     |
|-----------|-------------------------------------|
| dnavector | StringVector [mandatory]            |
| ncores    | number of cores [default: 1]        |
| symmetric | symmetric score matrix [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)
```

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