

# Package ‘seqinr’

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**Title** Biological Sequences Retrieval and Analysis

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## BugReports

<http://lists.r-forge.r-project.org/cgi-bin/mailman/listinfo/seqinr-forum>

**Imports** ade4,segmented

**Depends** R (>= 2.10.0)

**Description** Exploratory data analysis and data visualization for biological sequence (DNA and protein) data. Seqinr includes utilities for sequence data management under the ACNUC system described in Gouy, M. et al. (1984) Nucleic Acids Res. 12:121-127 <doi:10.1093/nar/12.1Part1.121>.

**License** GPL (>= 2)

**SystemRequirements** zlib headers and library.

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seqinr-package*Biological Sequences Retrieval and Analysis*

---

**Description**

Exploratory data analysis and data visualization for biological sequence (DNA and protein) data. Include also utilities for sequence data management under the ACNUC system.

**Author(s)**

Delphine Charif [aut], Olivier Clerc [ctb], Carolin Frank [ctb], Jean R. Lobry [aut], Anamaria Necşulea [ctb], Leonor Palmeira [ctb], Simon Penel [cre], Guy Perrière [ctb]

**References**

citation('seqinr')

---

a*Converts amino-acid three-letter code into the one-letter one*

---

**Description**

This is a vectorized function to convert three-letters amino-acid code into the one-letter one, for instance "Ala" into "A".

**Usage**

a(aa)

**Arguments**

aa                    A vector of string. All strings are 3 chars long.

**Details**

Allowed character values for aa are given by aaa(). All other values will generate a warning and return NA. Called without arguments, a() returns the list of all possible output values.

**Value**

A vector of single characters.

**Author(s)**

D. Charif, J.R. Lobry

## References

The IUPAC one-letter code for aminoacids is described at: <http://www.chem.qmul.ac.uk/iupac/AminoAcid/>  
`citation("seqinr")`

## See Also

[aaa](#), [translate](#)

## Examples

```
#  
# Show all possible input values:  
#  
aaa()  
  
#  
# Convert them in one letter-code:  
#  
a(aaa())  
  
#  
# Check consistency of results:  
#  
stopifnot( aaa(a(aaa())) == aaa())  
  
#  
# Show what happens with non-allowed values:  
#  
a("SOS") # should be NA and a warning is generated
```

---

aaa

*Converts amino-acid one-letter code into the three-letter one*

---

## Description

This is a vectorized function to convert one-letter amino-acid code into the three-letter one, for instance "A" into "Ala".

## Usage

```
aaa(aa)
```

## Arguments

aa                    A vector of single characters.

## Details

Allowed character values for aa are given by `a()`. All other values will generate a warning and return NA. Called without arguments, `aaa()` returns the list of all possible output values.

## Value

A vector of char string. All strings are 3 chars long.

## Author(s)

J.R. Lobry

## References

The IUPAC one-letter code for aminoacids is described at: <http://www.chem.qmul.ac.uk/iupac/AminoAcid/> citation("seqinr")

## See Also

[a](#), [translate](#)

## Examples

```
#
# Show all possible input values:
#

a()

#
# Convert them in one letter-code:
#

aaa(a())

#
# Check consistency of results:
#

stopifnot(a(aaa(a()))) == a())

#
# Show what happens with non-allowed values:
#

aaa("Z") # should be NA and a warning is generated
```

aacost

*Aerobic cost of amino-acids in Escherichia coli and G+C classes***Description**

The metabolic cost of amino-acid biosynthesis in *E. coli* under aerobic conditions from table 1 in Akashi and Gojobori (2002). The G+C classes are from Lobry (1997).

**Usage**

```
data(aacost)
```

**Format**

A data frame with 20 rows for the amino-acids and the following 7 columns:

**aaa** amino-acid (three-letters code).

**a** amino-acid (one-letter code).

**prec** precursor metabolites (see details).

**p** number of high-energy phosphate bonds contained in ATP and GTP molecules.

**h** number of available hydrogen atoms carried in NADH, NADPH, and FADH<sub>2</sub> molecules.

**tot** total metabolic cost assuming 2 high-energy phosphate bonds per hydrogen atom.

**gc** an ordered factor (l<m<h) for the G+C class of the amino-acid (see details)

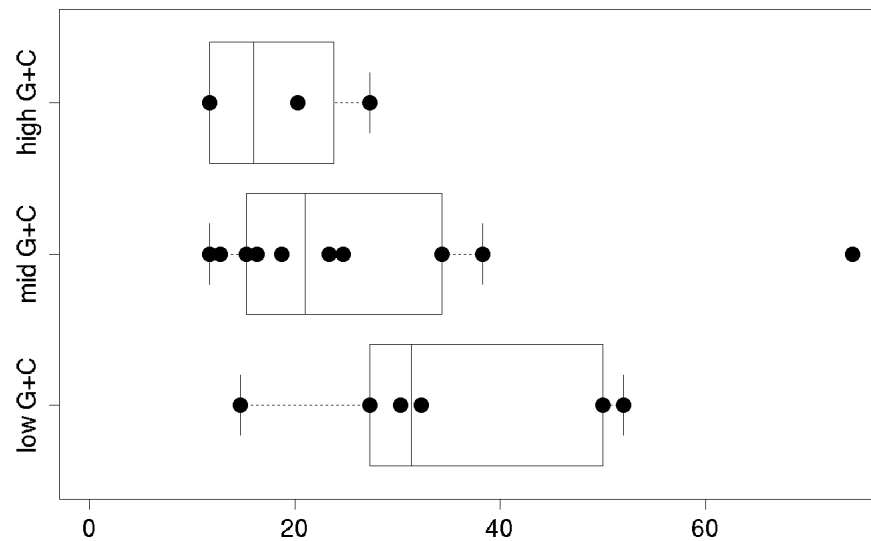
**Details**

Precursor metabolites are: penP, ribose 5-phosphate; PRPP, 5-phosphoribosyl pyrophosphate; eryP, erythrose 4-phosphate; 3pg, 3-phosphoglycerate; pep, phosphoenolpyruvate; pyr, pyruvate; acCoA, acetyl-CoA; akg, alpha-ketoglutarate; oaa, oxaloacetate. Negative signs on precursor metabolites indicate chemicals *gained* through biosynthetic pathways. Costs of precursors reflect averages for growth on glucose, acetate, and malate (see Table 6 in the supporting information from Akashi and Gojobori 2002).

The levels l<m<h for the gc ordered factor stand for Low G+C, Middle G+C, High G+C amino-acid, respectively. The frequencies of Low G+C amino-acids monotonously decrease with G+C content. The frequencies of High G+C amino-acids monotonously increase with G+C content. The frequencies of Middle G+C amino-acids first increase and then decrease with G+C content. These G+C classes are from Lobry (1997).

example(aacost) reproduces figure 2 from Lobry (2004).





### Source

Akashi, H, Gojobori, T. (2002) Metabolic efficiency and amino acid composition in the proteomes of *Escherichia coli* and *Bacillus subtilis*. *Proceedings of the National Academy of Sciences of the United States of America*, **99**:3695-3700.

Lobry, J.R. (1997) Influence of genomic G+C content on average amino-acid composition of proteins from 59 bacterial species. *Gene*, **205**:309-316.

Lobry, J.R. (2004) Life history traits and genome structure: aerobiosis and G+C content in bacteria. *Lecture Notes in Computer Sciences*, **3039**:679-686.

### References

```
citation("seqinr")
```

### Examples

```
data(aacost)
levels(aacost$gc) <- c("low G+C", "mid G+C", "high G+C")
stripchart(aacost$tot~aacost$gc, pch = 19, ylim = c(0.5,3.5),
  xlim = c(0, max(aacost$tot)),
  xlab = "Metabolic cost (high-energy phosphate bonds equivalent)",
  main = "Metabolic cost of the 20 amino-acids\nas function of their G+C class" )
boxplot(aacost$tot~aacost$gc, horizontal = TRUE, add = TRUE)
```

aaindex

*List of 544 physicochemical and biological properties for the 20 amino-acids*

## Description

Data were imported from release 9.1 (AUG 2006) of the aaindex1 database. See the reference section to cite this database in a publication.

## Usage

```
data(aaindex)
```

## Format

A named list with 544 elements having each the following components:

**H** String: Accession number in the aaindex database.

**D** String: Data description.

**R** String: LITDB entry number.

**A** String: Author(s).

**T** String: Title of the article.

**J** String: Journal reference and comments.

**C** String: Accession numbers of similar entries with the correlation coefficients of 0.8 (-0.8) or more (less). Notice: The correlation coefficient is calculated with zeros filled for missing values.

**I** Numeric named vector: amino acid index data.

## Details

A short description of each entry is available under the D component:

alpha-CH chemical shifts (Andersen et al., 1992)

Hydrophobicity index (Argos et al., 1982)

Signal sequence helical potential (Argos et al., 1982)

Membrane-buried preference parameters (Argos et al., 1982)

Conformational parameter of inner helix (Beghin-Dirkx, 1975)

Conformational parameter of beta-structure (Beghin-Dirkx, 1975)

Conformational parameter of beta-turn (Beghin-Dirkx, 1975)

Average flexibility indices (Bhaskaran-Ponnuswamy, 1988)

Residue volume (Bigelow, 1967)

Information value for accessibility; average fraction 35 Information value for accessibility; average fraction 23 Retention coefficient in TFA (Browne et al., 1982)

Retention coefficient in HFBA (Browne et al., 1982)

Transfer free energy to surface (Bull-Breese, 1974)

Apparent partial specific volume (Bull-Breese, 1974)  
alpha-NH chemical shifts (Bundi-Wuthrich, 1979)  
alpha-CH chemical shifts (Bundi-Wuthrich, 1979)  
Spin-spin coupling constants  $3J_{\text{H}\alpha\text{NH}}$  (Bundi-Wuthrich, 1979)  
Normalized frequency of alpha-helix (Burgess et al., 1974)  
Normalized frequency of extended structure (Burgess et al., 1974)  
Steric parameter (Charton, 1981)  
Polarizability parameter (Charton-Charton, 1982)  
Free energy of solution in water, kcal/mole (Charton-Charton, 1982)  
The Chou-Fasman parameter of the coil conformation (Charton-Charton, 1983)  
A parameter defined from the residuals obtained from the best correlation of the Chou-Fasman parameter of beta-sheet (Charton-Charton, 1983)  
The number of atoms in the side chain labelled 1+1 (Charton-Charton, 1983)  
The number of atoms in the side chain labelled 2+1 (Charton-Charton, 1983)  
The number of atoms in the side chain labelled 3+1 (Charton-Charton, 1983)  
The number of bonds in the longest chain (Charton-Charton, 1983)  
A parameter of charge transfer capability (Charton-Charton, 1983)  
A parameter of charge transfer donor capability (Charton-Charton, 1983)  
Average volume of buried residue (Chothia, 1975)  
Residue accessible surface area in tripeptide (Chothia, 1976)  
Residue accessible surface area in folded protein (Chothia, 1976)  
Proportion of residues 95 Proportion of residues 100 Normalized frequency of beta-turn (Chou-Fasman, 1978a)  
Normalized frequency of alpha-helix (Chou-Fasman, 1978b)  
Normalized frequency of beta-sheet (Chou-Fasman, 1978b)  
Normalized frequency of beta-turn (Chou-Fasman, 1978b)  
Normalized frequency of N-terminal helix (Chou-Fasman, 1978b)  
Normalized frequency of C-terminal helix (Chou-Fasman, 1978b)  
Normalized frequency of N-terminal non helical region (Chou-Fasman, 1978b)  
Normalized frequency of C-terminal non helical region (Chou-Fasman, 1978b)  
Normalized frequency of N-terminal beta-sheet (Chou-Fasman, 1978b)  
Normalized frequency of C-terminal beta-sheet (Chou-Fasman, 1978b)  
Normalized frequency of N-terminal non beta region (Chou-Fasman, 1978b)  
Normalized frequency of C-terminal non beta region (Chou-Fasman, 1978b)  
Frequency of the 1st residue in turn (Chou-Fasman, 1978b)  
Frequency of the 2nd residue in turn (Chou-Fasman, 1978b)  
Frequency of the 3rd residue in turn (Chou-Fasman, 1978b)  
Frequency of the 4th residue in turn (Chou-Fasman, 1978b)  
Normalized frequency of the 2nd and 3rd residues in turn (Chou-Fasman, 1978b)  
Normalized hydrophobicity scales for alpha-proteins (Cid et al., 1992)  
Normalized hydrophobicity scales for beta-proteins (Cid et al., 1992)  
Normalized hydrophobicity scales for alpha+beta-proteins (Cid et al., 1992)  
Normalized hydrophobicity scales for alpha/beta-proteins (Cid et al., 1992)  
Normalized average hydrophobicity scales (Cid et al., 1992)  
Partial specific volume (Cohn-Edsall, 1943)  
Normalized frequency of middle helix (Crawford et al., 1973)  
Normalized frequency of beta-sheet (Crawford et al., 1973)  
Normalized frequency of turn (Crawford et al., 1973)

Size (Dawson, 1972)  
Amino acid composition (Dayhoff et al., 1978a)  
Relative mutability (Dayhoff et al., 1978b)  
Membrane preference for cytochrome b: MPH89 (Degli Esposti et al., 1990)  
Average membrane preference: AMP07 (Degli Esposti et al., 1990)  
Consensus normalized hydrophobicity scale (Eisenberg, 1984)  
Solvation free energy (Eisenberg-McLachlan, 1986)  
Atom-based hydrophobic moment (Eisenberg-McLachlan, 1986)  
Direction of hydrophobic moment (Eisenberg-McLachlan, 1986)  
Molecular weight (Fasman, 1976)  
Melting point (Fasman, 1976)  
Optical rotation (Fasman, 1976)  
pK-N (Fasman, 1976)  
pK-C (Fasman, 1976)  
Hydrophobic parameter  $\pi$  (Fauchere-Pliska, 1983)  
Graph shape index (Fauchere et al., 1988)  
Smoothed upsilon steric parameter (Fauchere et al., 1988)  
Normalized van der Waals volume (Fauchere et al., 1988)  
STERIMOL length of the side chain (Fauchere et al., 1988)  
STERIMOL minimum width of the side chain (Fauchere et al., 1988)  
STERIMOL maximum width of the side chain (Fauchere et al., 1988)  
N.m.r. chemical shift of alpha-carbon (Fauchere et al., 1988)  
Localized electrical effect (Fauchere et al., 1988)  
Number of hydrogen bond donors (Fauchere et al., 1988)  
Number of full nonbonding orbitals (Fauchere et al., 1988)  
Positive charge (Fauchere et al., 1988)  
Negative charge (Fauchere et al., 1988)  
pK-a(RCOOH) (Fauchere et al., 1988)  
Helix-coil equilibrium constant (Finkelstein-Ptitsyn, 1977)  
Helix initiation parameter at position  $i-1$  (Finkelstein et al., 1991)  
Helix initiation parameter at position  $i,i+1,i+2$  (Finkelstein et al., 1991)  
Helix termination parameter at position  $j-2,j-1,j$  (Finkelstein et al., 1991)  
Helix termination parameter at position  $j+1$  (Finkelstein et al., 1991)  
Partition coefficient (Garel et al., 1973)  
Alpha-helix indices (Geisow-Roberts, 1980)  
Alpha-helix indices for alpha-proteins (Geisow-Roberts, 1980)  
Alpha-helix indices for beta-proteins (Geisow-Roberts, 1980)  
Alpha-helix indices for alpha/beta-proteins (Geisow-Roberts, 1980)  
Beta-strand indices (Geisow-Roberts, 1980)  
Beta-strand indices for beta-proteins (Geisow-Roberts, 1980)  
Beta-strand indices for alpha/beta-proteins (Geisow-Roberts, 1980)  
Aperiodic indices (Geisow-Roberts, 1980)  
Aperiodic indices for alpha-proteins (Geisow-Roberts, 1980)  
Aperiodic indices for beta-proteins (Geisow-Roberts, 1980)  
Aperiodic indices for alpha/beta-proteins (Geisow-Roberts, 1980)  
Hydrophobicity factor (Goldsack-Chalifoux, 1973)  
Residue volume (Goldsack-Chalifoux, 1973)  
Composition (Grantham, 1974)

Polarity (Grantham, 1974)  
Volume (Grantham, 1974)  
Partition energy (Guy, 1985)  
Hydration number (Hopfinger, 1971), Cited by Charton-Charton (1982)  
Hydrophilicity value (Hopp-Woods, 1981)  
Heat capacity (Hutchens, 1970)  
Absolute entropy (Hutchens, 1970)  
Entropy of formation (Hutchens, 1970)  
Normalized relative frequency of alpha-helix (Isogai et al., 1980)  
Normalized relative frequency of extended structure (Isogai et al., 1980)  
Normalized relative frequency of bend (Isogai et al., 1980)  
Normalized relative frequency of bend R (Isogai et al., 1980)  
Normalized relative frequency of bend S (Isogai et al., 1980)  
Normalized relative frequency of helix end (Isogai et al., 1980)  
Normalized relative frequency of double bend (Isogai et al., 1980)  
Normalized relative frequency of coil (Isogai et al., 1980)  
Average accessible surface area (Janin et al., 1978)  
Percentage of buried residues (Janin et al., 1978)  
Percentage of exposed residues (Janin et al., 1978)  
Ratio of buried and accessible molar fractions (Janin, 1979)  
Transfer free energy (Janin, 1979)  
Hydrophobicity (Jones, 1975)  
pK (-COOH) (Jones, 1975)  
Relative frequency of occurrence (Jones et al., 1992)  
Relative mutability (Jones et al., 1992)  
Amino acid distribution (Jukes et al., 1975)  
Sequence frequency (Jungck, 1978)  
Average relative probability of helix (Kanehisa-Tsong, 1980)  
Average relative probability of beta-sheet (Kanehisa-Tsong, 1980)  
Average relative probability of inner helix (Kanehisa-Tsong, 1980)  
Average relative probability of inner beta-sheet (Kanehisa-Tsong, 1980)  
Flexibility parameter for no rigid neighbors (Karplus-Schulz, 1985)  
Flexibility parameter for one rigid neighbor (Karplus-Schulz, 1985)  
Flexibility parameter for two rigid neighbors (Karplus-Schulz, 1985)  
The Kerr-constant increments (Khanarian-Moore, 1980)  
Net charge (Klein et al., 1984)  
Side chain interaction parameter (Krigbaum-Rubin, 1971)  
Side chain interaction parameter (Krigbaum-Komoriya, 1979)  
Fraction of site occupied by water (Krigbaum-Komoriya, 1979)  
Side chain volume (Krigbaum-Komoriya, 1979)  
Hydropathy index (Kyte-Doolittle, 1982)  
Transfer free energy, CHP/water (Lawson et al., 1984)  
Hydrophobic parameter (Levitt, 1976)  
Distance between C-alpha and centroid of side chain (Levitt, 1976)  
Side chain angle theta(AAR) (Levitt, 1976)  
Side chain torsion angle phi(AAAR) (Levitt, 1976)  
Radius of gyration of side chain (Levitt, 1976)  
van der Waals parameter R0 (Levitt, 1976)

van der Waals parameter epsilon (Levitt, 1976)  
Normalized frequency of alpha-helix, with weights (Levitt, 1978)  
Normalized frequency of beta-sheet, with weights (Levitt, 1978)  
Normalized frequency of reverse turn, with weights (Levitt, 1978)  
Normalized frequency of alpha-helix, unweighted (Levitt, 1978)  
Normalized frequency of beta-sheet, unweighted (Levitt, 1978)  
Normalized frequency of reverse turn, unweighted (Levitt, 1978)  
Frequency of occurrence in beta-bends (Lewis et al., 1971)  
Conformational preference for all beta-strands (Lifson-Sander, 1979)  
Conformational preference for parallel beta-strands (Lifson-Sander, 1979)  
Conformational preference for antiparallel beta-strands (Lifson-Sander, 1979)  
Average surrounding hydrophobicity (Manavalan-Ponnuswamy, 1978)  
Normalized frequency of alpha-helix (Maxfield-Scheraga, 1976)  
Normalized frequency of extended structure (Maxfield-Scheraga, 1976)  
Normalized frequency of zeta R (Maxfield-Scheraga, 1976)  
Normalized frequency of left-handed alpha-helix (Maxfield-Scheraga, 1976)  
Normalized frequency of zeta L (Maxfield-Scheraga, 1976)  
Normalized frequency of alpha region (Maxfield-Scheraga, 1976)  
Refractivity (McMeekin et al., 1964), Cited by Jones (1975)  
Retention coefficient in HPLC, pH7.4 (Meek, 1980)  
Retention coefficient in HPLC, pH2.1 (Meek, 1980)  
Retention coefficient in NaClO<sub>4</sub> (Meek-Rossetti, 1981)  
Retention coefficient in NaH<sub>2</sub>PO<sub>4</sub> (Meek-Rossetti, 1981)  
Average reduced distance for C-alpha (Meirovitch et al., 1980)  
Average reduced distance for side chain (Meirovitch et al., 1980)  
Average side chain orientation angle (Meirovitch et al., 1980)  
Effective partition energy (Miyazawa-Jernigan, 1985)  
Normalized frequency of alpha-helix (Nagano, 1973)  
Normalized frequency of beta-structure (Nagano, 1973)  
Normalized frequency of coil (Nagano, 1973)  
AA composition of total proteins (Nakashima et al., 1990)  
SD of AA composition of total proteins (Nakashima et al., 1990)  
AA composition of mt-proteins (Nakashima et al., 1990)  
Normalized composition of mt-proteins (Nakashima et al., 1990)  
AA composition of mt-proteins from animal (Nakashima et al., 1990)  
Normalized composition from animal (Nakashima et al., 1990)  
AA composition of mt-proteins from fungi and plant (Nakashima et al., 1990)  
Normalized composition from fungi and plant (Nakashima et al., 1990)  
AA composition of membrane proteins (Nakashima et al., 1990)  
Normalized composition of membrane proteins (Nakashima et al., 1990)  
Transmembrane regions of non-mt-proteins (Nakashima et al., 1990)  
Transmembrane regions of mt-proteins (Nakashima et al., 1990)  
Ratio of average and computed composition (Nakashima et al., 1990)  
AA composition of CYT of single-spanning proteins (Nakashima-Nishikawa, 1992)  
AA composition of CYT2 of single-spanning proteins (Nakashima-Nishikawa, 1992)  
AA composition of EXT of single-spanning proteins (Nakashima-Nishikawa, 1992)  
AA composition of EXT2 of single-spanning proteins (Nakashima-Nishikawa, 1992)  
AA composition of MEM of single-spanning proteins (Nakashima-Nishikawa, 1992)

AA composition of CYT of multi-spanning proteins (Nakashima-Nishikawa, 1992)  
AA composition of EXT of multi-spanning proteins (Nakashima-Nishikawa, 1992)  
AA composition of MEM of multi-spanning proteins (Nakashima-Nishikawa, 1992)  
8 A contact number (Nishikawa-Ooi, 1980)  
14 A contact number (Nishikawa-Ooi, 1986)  
Transfer energy, organic solvent/water (Nozaki-Tanford, 1971)  
Average non-bonded energy per atom (Oobatake-Ooi, 1977)  
Short and medium range non-bonded energy per atom (Oobatake-Ooi, 1977)  
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Weights for coil at the window position of -1 (Qian-Sejnowski, 1988)  
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Normalized positional residue frequency at helix termini N5 (Aurora-Rose, 1998)  
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Normalized positional residue frequency at helix termini C4 (Aurora-Rose, 1998)  
Normalized positional residue frequency at helix termini C3 (Aurora-Rose, 1998)  
Normalized positional residue frequency at helix termini C2 (Aurora-Rose, 1998)  
Normalized positional residue frequency at helix termini C1 (Aurora-Rose, 1998)  
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Surface composition of amino acids in intracellular proteins of mesophiles (percent) (Fukuchi-Nishikawa, 2001)

Surface composition of amino acids in extracellular proteins of mesophiles (percent) (Fukuchi-Nishikawa, 2001)

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Interior composition of amino acids in intracellular proteins of thermophiles (percent) (Fukuchi-Nishikawa, 2001)

Interior composition of amino acids in intracellular proteins of mesophiles (percent) (Fukuchi-Nishikawa, 2001)

Interior composition of amino acids in extracellular proteins of mesophiles (percent) (Fukuchi-Nishikawa, 2001)

Interior composition of amino acids in nuclear proteins (percent) (Fukuchi-Nishikawa, 2001)

Entire chain composition of amino acids in intracellular proteins of thermophiles (percent) (Fukuchi-Nishikawa, 2001)

Entire chain composition of amino acids in intracellular proteins of mesophiles (percent) (Fukuchi-Nishikawa, 2001)

Entire chain composition of amino acids in extracellular proteins of mesophiles (percent) (Fukuchi-Nishikawa, 2001)

Entire chain composition of amino acids in nuclear proteins (percent) (Fukuchi-Nishikawa, 2001)

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Slopes tripeptide FDPB VFF all (Avbelj, 2000)

Slopes tripeptide FDPB PARSE neutral (Avbelj, 2000)

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 Hydrophobicity index (Engelman et al., 1986)  
 Hydrophobicity index (Fasman, 1989)

## Source

<http://www.genome.jp/aaindex>

## References

From the original aaindex documentation:

Please cite the following references when making use of the database:

Kawashima, S. and Kanehisa, M. (2000) AAindex: amino acid index database. *Nucleic Acids Res.*, **28**:374.

Tomii, K. and Kanehisa, M. (1996) Analysis of amino acid indices and mutation matrices for sequence comparison and structure prediction of proteins. *Protein Eng.*, **9**:27-36.

Nakai, K., Kidera, A., and Kanehisa, M. (1988) Cluster analysis of amino acid indices for prediction of protein structure and function. *Protein Eng.* **2**:93-100.

## Examples

```

#
# Load data:
#

data(aaindex)
```

```
#
# Suppose that we need the Kyte & Doolittle Hydrophaty index. We first look
# at the entries with Kyte as author:
#

which(apply(aaindex, function(x) length(grep("Kyte", x$A)) != 0))

#
# This should return that entry number 151 named KYTJ820101 is the only
# one that fit our request. We can access to it by position or by name,
# for instance:
#

aaindex[[151]]$I
aaindex[["KYTJ820101"]]$I
aaindex$KYTJ820101$I
```

---

AAstat

*To Get Some Protein Statistics*


---

### Description

Returns simple protein sequence information including the number of residues, the percentage physico-chemical classes and the theoretical isoelectric point.

### Usage

```
AAstat(seq, plot = TRUE)
```

### Arguments

seq	a protein sequence as a vector of upper-case chars
plot	if TRUE, plots the presence of residues splitted by physico-chemical classes along the sequence.

### Value

A list with the three following components:

Compo	A factor giving the amino acid counts.
Prop	A list giving the percentage of each physico-chemical classes (Tiny, Small, Aliphatic, Aromatic, Non-polar, Polar, Charged, Positive, Negative).
Pi	The theoretical isoelectric point

### Author(s)

D. Charif, J.R. Lobry

**References**

`citation("seqinr")`

**See Also**

[computePI](#), [SEQINR.UTIL](#), [SeqFastaAA](#)

**Examples**

```
seqAA <- read.fasta(file = system.file("sequences/seqAA.fasta", package = "seqinr"),
  seqtype = "AA")
AAstat(seqAA[[1]])
```

---

acnucopen

*open and close a remote access to an ACNUC database*

---

**Description**

These are low level functions to start and stop a remote access to an ACNUC database.

**Usage**

```
acnucopen(db, socket, challenge = NA)
acnucclose(socket)
clientid(id = paste("seqinr_",
  packageDescription("seqinr")$Version, sep = ""),
  socket, verbose = FALSE)
quitacnuc(socket)
```

**Arguments**

db	the remote ACNUC database name
socket	an object of class sockconn connecting to an ACNUC server
challenge	unimplemented yet
id	client ID definition defaulting to seqinr + package version number
verbose	logical, if TRUE mode verbose is on

**Details**

these low level functions are usually not used directly by the user. Use [choosebank](#) to open a remote ACNUC database and [closebank](#) to close it.

**Value**

For openacnuc a list with the following components: type : the type of database that was opened. totseqs, totspec, totkey : total number of seqs, species, keywords in opened database. ACC\\_LENGTH, LA\\_MNEMO, WIDTH\\_KW, WIDTH\\_SP, WIDTH\\_SMJ, WIDTH\\_AUT, WIDTH\\_BIB, lrtxt, SUBINLNG: max lengths of record keys in database.



**Author(s)**

J.R. Lobry

**References**

citation("seqinr")

**See Also**[choosebank](#), [closebank](#)**Examples**

```
## Not run: # Need internet connection
mysocket <- socketConnection( host = "pbil.univ-lyon1.fr",
  port = 5558, server = FALSE, blocking = TRUE)
readLines(mysocket, n = 1) # OK acnuc socket started
acnucopen("emblTP", socket = mysocket) -> res
expected <- c("EMBL", "14138095", "236401", "1186228", "8",
  "16", "40", "40", "20", "20", "40", "60", "504")
stopifnot(all(unlist(res) == expected))
tryalreadypopen <- try(acnucopen("emblTP", socket = mysocket))
stopifnot(inherits(tryalreadypopen, "try-error"))
# Need a fresh socket because acnucopen() close it if error:
mysocket <- socketConnection( host = "pbil.univ-lyon1.fr",
  port = 5558, server = FALSE, blocking = TRUE)
tryoff <- try(acnucopen("off", socket = mysocket))
stopifnot(inherits(tryoff, "try-error"))

mysocket <- socketConnection( host = "pbil.univ-lyon1.fr",
  port = 5558, server = FALSE, blocking = TRUE)
tryinexistent <- try(acnucopen("tagadatagadatsointsoin", socket = mysocket))
stopifnot(inherits(tryinexistent, "try-error"))

mysocket <- socketConnection( host = "pbil.univ-lyon1.fr",
  port = 5558, server = FALSE, blocking = TRUE)
trycloseunopened <- try(acnucclose(mysocket))
stopifnot(inherits(trycloseunopened, "try-error"))

## End(Not run)
```

## Description

Conventions used to name forensic microsatellite alleles (STR) are described in Bar *et al.* (1994). The name "9.3" means for instance that there are 9 repetitions of the complete base oligomer and an incomplete repeat with 3 bp.

## Usage

```
al2bp(allele.name, repeat.bp = 4, offLadderChars = "><", split = "\\.")
```

## Arguments

allele.name	The name of the allele, coerced to a string type.
repeat.bp	The length in bp of the microsatellite base repeat, most of them are tetranucleotides so that it defaults to 4. Do not forget to change this to 5 for loci based on pentanucleotides such as Penta D or Penta E.
offLadderChars	NA is returned when at least one of these characters are found in the allele name. Off ladder alleles are typically reported as "<8" or ">19"
split	The convention is to use a dot, as in "9.3", between the number of repeats and the number of bases in the incomplete repeat. On some locales where the decimal separator is a comma this could be a source of problem, try to use "," instead for this argument which is forwarded to <a href="#">strsplit</a> .

## Details

Warnings generated by faulty numeric conversions are suppressed here.

## Value

A single numeric value corresponding to the size in bp of the allele, or NA when characters spotting off ladder alleles are encountered or when numeric conversion is impossible (*e.g.* with "X" or "Y" allele names at Amelogenin locus).

## Author(s)

J.R. Lobry

## References

Bar, W. and Brinkmann, B. and Lincoln, P. and Mayr, W.R. and Rossi, U. (1994) DNA recommendations. 1994 report concerning further recommendations of the DNA Commission of the ISFH regarding PCR-based polymorphisms in STR (short tandem repeat) systems. *Int. J. Leg. Med.*, **107**:159-160.

```
citation("seqinR")
```

## See Also

[identifiler](#) for forensic microsatellite allele name examples.

## Examples

```
#
# Quality check and examples:
#
stopifnot( al2bp("9") == 36 ) # 9 repeats of a tetranucleotide is 36 bp
stopifnot( al2bp(9) == 36 )   # also OK with numerical argument
stopifnot( al2bp(9, 5) == 45 ) # 9 repeats of a pentanucleotide is 45 bp
stopifnot( al2bp("9.3") == 39 ) # microvariant case
stopifnot( is.na(al2bp("<8")) ) # off ladder case
stopifnot( is.na(al2bp(">19")) ) # off ladder case
stopifnot( is.na(al2bp("X")) ) # non STR case
#
# Application to the alleles names in the identifiler data set where all loci are
# tetranucleotide repeats:
#
data(identifiler)
al.names <- unlist(identifiler)
al.length <- sapply(al.names, al2bp)
loc.names <- unlist(lapply(identifiler, names))
loc.nall <- unlist(lapply(identifiler, function(x) lapply(x,length)))
loc.fac <- factor(rep(loc.names, loc.nall))
par(lend = "butt", mar = c(5,6,4,1)+0.1)
boxplot(al.length~loc.fac, las = 1, col = "lightblue",
        horizontal = TRUE, main = "Range of allele lengths at forensic loci",
        xlab = "Length (bp)", ylim = c(0, max(al.length, na.rm = TRUE)))
```

---

alllistranks

*To get the count of existing lists and all their ranks on server*


---

## Description

This is a low level function to get the total number of list and all their ranks in an opened database.

## Usage

```
alllistranks(socket = autosocket(), verbose = FALSE)
alr(socket = autosocket(), verbose = FALSE)
```

## Arguments

socket	an object of class sockconn connecting to a remote ACNUC database (default is a socket to the last opened database).
verbose	if TRUE, verbose mode is on

## Details

This low level function is usually not used directly by the user.

**Value**

A list with two components:

count	count of existing lists
rank	their rank

**Author(s)**

J.R. Lobry

**References**

`citation("seqinr")`

**See Also**

[choosebank](#), [query](#)

**Examples**

```
## Not run: # Need internet connection
choosebank("emblTP")
tmp1 <- query("tmp1", "sp=Borrelia burgdorferi", virtual = TRUE)
tmp2 <- query("tmp2", "sp=Borrelia burgdorferi", virtual = TRUE)
tmp3 <- query("tmp3", "sp=Borrelia burgdorferi", virtual = TRUE)
(result <- allistranks())
stopifnot(result$count == 3) # Three ACNUC lists
stopifnot(result$ranks == 2:4) # Starting at rank 2
#
# Summay of current lists defined on the ACNUC server:
#
sapply(result$ranks, getliststate)
closebank()

## End(Not run)
```

---

amb

---

*Expansion of IUPAC nucleotide symbols*


---

**Description**

This function returns the list of nucleotide matching a given IUPAC nucleotide symbol, for instance `c("c", "g")` for "s".

**Usage**

```
amb(base, forceToLower = TRUE, checkBase = TRUE,
    IUPAC = s2c("acgturymkswbdhvn"), u2t = TRUE)
```

**Arguments**

base	an IUPAC symbol for a nucleotide as a single character
forceToLower	if TRUE the base is forced to lower case
checkBase	if TRUE the character is checked to belong to the allowed IUPAC symbol list
IUPAC	the list of allowed IUPAC symbols
u2t	if TRUE "u" for uracil in RNA are changed into "t" for thymine in DNA

**Details**

Non ambiguous bases are returned unchanged (except for "u" when u2t is TRUE).

**Value**

When base is missing, the list of IUPAC symbols is returned, otherwise a vector with expanded symbols.

**Author(s)**

J.R. Lobry

**References**

The nomenclature for incompletely specified bases in nucleic acid sequences at: <http://www.chem.qmul.ac.uk/iubmb/misc/naseq.html>  
citation("seqinr")

**See Also**

See [bma](#) for the reverse operation. Use [tolower](#) to change upper case letters into lower case letters.

**Examples**

```
#  
# The list of IUPAC symbols:  
#  
  
amb()  
  
#  
# And their expansion:  
#  
  
sapply(amb(), amb)
```

---

**AnoukResult***Expected numeric results for Ka and Ks computation*

---

**Description**

This data set is what should be obtained when running `kaks()` on the test file `Anouk.fasta` in the `sequences` directory of the `seqinR` package.

**Usage**

```
data(AnoukResult)
```

**Format**

A list with 4 components of class `dist`.

**ka** Ka

**ks** Ks

**vka** variance for Ka

**vks** variance for Ks

**Details**

See the example in [kaks](#).

**Source**

The fasta test file was provided by Anamaria Necşulea.

**References**

```
citation("seqinr")
```

---

**as.alignment***Constructor for class alignment*

---

**Description**

Returns an object of (S3) class `alignment`.

**Usage**

```
as.alignment(nb = NULL, nam = NULL, seq = NULL, com = NULL)
```

**Arguments**

nb	integer. The number of sequences in the alignment.
nam	vector of nb character strings. The sequence names.
seq	vector of nb character strings. The aligned sequences.
com	vector of nb character strings. The comments about sequences.

**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)**

D. Charif, J.R. Lobry

**References**

citation("seqinr")

**See Also**

[read.alignment](#), [as.matrix.alignment](#), [read.fasta](#), [write.fasta](#), [reverse.align](#), [dist.alignment](#).

**Examples**

```
as.alignment(nb = 2, nam = c("one", "two"),
  seq = c("-ACGT", "GACG-"), com = c("un", "deux"))
```

---

as.matrix.alignment      *as.matrix.alignment*

---

**Description**

Converts an alignment into a matrix of characters

**Usage**

```
## S3 method for class 'alignment'
as.matrix(x, ...)
```

**Arguments**

`x` an object of the class alignment.  
`...` additional arguments to be passed to or from methods.

**Value**

A matrix of characters.

**Author(s)**

J.R. Lobry

**See Also**

[read.alignment](#)

**Examples**

```
phylip <- read.alignment(file = system.file("sequences/test.phylip",  
  package = "seqinr"), format = "phylip")  
as.matrix(phylip)
```

---

autosocket

*Returns a socket to the last opened database*

---

**Description**

This is a low level function that is mainly used to select automatically the last opened ACNUC database for functions using sockets.

**Usage**

```
autosocket()
```

**Value**

An object of class sockconn.

**Author(s)**

J.R. Lobry

**References**

<http://doua.prabi.fr/databases/acnuc.html>  
`citation("seqinr")`



**See Also**

[choosebank](#), [connections](#).

**Examples**

```
## Not run: #Need internet connection
choosebank("emblTP")
autosocket()
closebank()

## End(Not run)
```

---

baselineabif

*Estimation of baseline value*

---

**Description**

This function tries to estimate the baseline value for RFU data from capillary electrophoresis with the heuristic that the most common value is the baseline.

**Usage**

```
baselineabif(rfu, maxrfu = 1000)
```

**Arguments**

rfu	a numeric vector of signal value
maxrfu	signal values greater or equal to maxrfu are forced to NA

**Value**

A single numeric value for the estimated baseline.

**Author(s)**

J.R. Lobry

**See Also**

[JL0](#) for a dataset example, [plotabif](#) to plot this kind of data, [peakabif](#) to estimate peak parameters.

## Examples

```
data(JL0)
rfu <- JL0$Data$DATA.1
bl <- baselineabif(rfu)
plot(1:length(rfu), rfu, type = "l",
     xlab = "Time [datapoint units]",
     ylab = "Signal [RFU]",
     main = "Example of baseline estimates")
abline(h = bl, col="red", lty = 2)
legend("topright", inset = 0.02, "Baseline estimate", lty = 2, col = "red")
```

bma

*Computing an IUPAC nucleotide symbol*

## Description

This function returns the IUPAC symbol for a nucleotide sequence, for instance `c("c", "c", "g")` is coded by "s".

## Usage

```
bma(nucl, warn.non.IUPAC = TRUE, type = c("DNA", "RNA"))
```

## Arguments

<code>nucl</code>	a nucleotide sequence as a vector of single chars
<code>warn.non.IUPAC</code>	if TRUE warns when no IUPAC symbol is possible
<code>type</code>	whether this is a DNA or a RNA sequence

## Details

The sequence is forced in lower case letters and ambiguous bases are expanded before trying to find an IUPAC symbol.

## Value

A single IUPAC symbol in lower case, or NA when this is not possible.

## Author(s)

J.R. Lobry

## References

The nomenclature for incompletely specified bases in nucleic acid sequences at: <http://www.chem.qmul.ac.uk/iubmb/misc/naseq.html>  
`citation("seqinr")`

**See Also**

See [amb](#) for the reverse operation. Use [toupper](#) to change lower case letters into upper case letters.

**Examples**

```
stopifnot(bma(s2c("atatattttata")) == "w")
stopifnot(bma(s2c("gcggcgcgcggc")) == "s")
stopifnot(bma(s2c("ACGT")) == "n")
stopifnot(is.na(bma(s2c("atatattt---tatat")))) # a warning is issued
```

---

c2s

*conversion of a vector of chars into a string*


---

**Description**

This is a simple utility function to convert a vector of chars such as `c("m", "e", "r", "g", "e", "d")` into a single string such as "merged".

**Usage**

```
c2s(chars = c("m", "e", "r", "g", "e", "d"))
```

**Arguments**

chars                      a vector of chars

**Value**

a string

**Author(s)**

J.R. Lobry

**References**

`citation("seqinr")`

**See Also**

[s2c](#)

**Examples**

```
c2s( c("m", "e", "r", "g", "e", "d") )
```

---

cai*Codon Adaptation Index*

---

**Description**

The Codon Adaptation Index (Sharp and Li 1987) is the most popular index of gene expressivity with about 1000 citations 20 years after its publication. Its values range from 0 (low) to 1 (high). The implementation here is intended to work exactly as in the program codonW written by John Peden during his PhD thesis under the supervision of P.M. Sharp.

**Usage**

```
cai(seq, w, numcode = 1, zero.threshold = 0.0001, zero.to = 0.01)
```

**Arguments**

seq	a coding sequence as a vector of single characters
w	a vector for the relative adaptiveness of each codon
numcode	the genetic code number as in <a href="#">translate</a>
zero.threshold	a value in w below this threshold is considered as zero
zero.to	a value considered as zero in w is forced to this value. The default is from Bulmer (1988).

**Details**

Adapted from the documentation of the CAI function in the program codonW written by John Peden: CAI is a measurement of the relative adaptiveness of the codon usage of a gene towards the codon usage of highly expressed genes. The relative adaptiveness (w) of each codon is the ratio of the usage of each codon, to that of the most abundant codon for the same amino acid. The CAI index is defined as the geometric mean of these relative adaptiveness values. Non-synonymous codons and termination codons (genetic code dependent) are excluded. To aid computation, the CAI is calculated as using a natural log summation. To prevent a codon having a relative adaptiveness value of zero, which could result in a CAI of zero; these codons have fitness of zero (<.0001) are adjusted to 0.01.

**Value**

A single numerical value for the CAI.

**Author(s)**

J.R. Lobry

## References

Sharp, P.M., Li, W.-H. (1987) The codon adaptation index - a measure of directional synonymous codon usage bias, and its potential applications. *Nucleic Acids Research*, **15**:1281-1295.

Bulmer, M. (1988). Are codon usage patterns in unicellular organisms determined by selection-mutation balance. *Journal of Evolutionary Biology*, **1**:15-26.

Peden, J.F. (1999) Analysis of codon usage. PhD Thesis, University of Nottingham, UK.

The program codonW used here for comparison is available at <http://codonw.sourceforge.net/> under a GPL licence.

```
citation("seqinr").
```

## See Also

[caitab](#) for some w values from codonW. [uco](#) for codon usage tabulation.

## Examples

```
#
# How to reproduce the results obtained with the C program codonW
# version 1.4.4 written by John Peden. We use here the "input.dat"
# test file from codonW (Saccharomyces cerevisiae).
#
inputdatfile <- system.file("sequences/input.dat", package = "seqinr")
input <- read.fasta(file = inputdatfile) # read the FASTA file
#
# Import results obtained with codonW
#
scucofile <- system.file("sequences/scuco.txt", package = "seqinr")
scuco.res <- read.table(scucofile, header = TRUE) # read codonW result file
#
# Use w for Saccharomyces cerevisiae
#
data(caitab)
w <- caitab$sc
#
# Compute CAI and compare results:
#
cai.res <- sapply(input, cai, w = w)
plot(cai.res, scuco.res$CAI,
     main = "Comparison of seqinR and codonW results",
     xlab = "CAI from seqinR",
     ylab = "CAI from codonW",
     las = 1)
abline(c(0,1))
```

caitab

Codon Adaptation Index (CAI) w tables

**Description**

Information about a preferred set of codons for highly expressed genes in three species.

**Usage**

```
data(caitab)
```

**Format**

A data frame with 64 rows for the codons and the following 3 columns:

**ec** *Escherichia coli*

**bs** *Bacillus subtilis*

**sc** *Saccharomyces cerevisiae*

**Details**

Codons are given by `row.names(caitab)`.

**Source**

The data were hard-encoded in the C program codonW version 1.4.4 written by John Peden available at <http://codonw.sourceforge.net/>. The data are from the file codonW.h. According to this source file, there were no reference for *Escherichia coli* and *Bacillus subtilis* and the reference for *Saccharomyces cerevisiae* was Sharp and Cowe (1991).

It turns out that the data for *Escherichia coli* and *Saccharomyces cerevisiae* are identical to table 1 in Sharp and Li (1987) where the missing values for the stop codons are represented here by zeros. All codons were documented by at least one count in both datasets.

The data for *Bacillus subtilis* are from table 2 in Shields and Sharp (1987). Missing values for stops codons are represented as previously by zeros, missing values for single-box amino-acids are represented by 1 here. Note that some codons were undocumented in this dataset and that a 0.5 value in absolute frequencies was already forced to avoid zeros. It is therefore impossible to use directly these data to obtain the exact expected CAI values as documented in `cai` because of overlapping with documented codons.

**References**

Sharp, P.M., Li, W.-H. (1987) The codon adaptation index - a measure of directional synonymous codon usage bias, and its potential applications. *Nucleic Acids Research*, **15**:1281-1295.

Shields, D.C., Sharp, P.M. (1987) Synonymous codon usage in *Bacillus subtilis* reflects both traditional selection and mutational biases. *Nucleic Acids Research*, **15**:8023-8040.

Sharp, P. M., Cowe, E. (1991). Synonymous codon usage in *Saccharomyces cerevisiae*. *Yeast*, 7:657-678.

Peden, J.F. (1999) Analysis of codon usage. PhD Thesis, University of Nottingham, UK.

`citation("seqinr")`

### See Also

[cai](#) for an example using this dataset to compute CAI values.

### Examples

```
data(caitab)
```

---

chargaff

*Base composition in ssDNA for 7 bacterial DNA*

---

### Description

Long before the genomic era, it was possible to get some data for the global composition of single-stranded DNA chromosomes by direct chemical analyses. These data are from Chargaff's lab and give the base composition of the L (Ligth) strand for 7 bacterial chromosomes.

### Usage

```
data(chargaff)
```

### Format

A data frame with 7 observations on the following 4 variables.

[A ] frequencies of A bases in percent

[G ] frequencies of G bases in percent

[C ] frequencies of C bases in percent

[T ] frequencies of T bases in percent

### Details

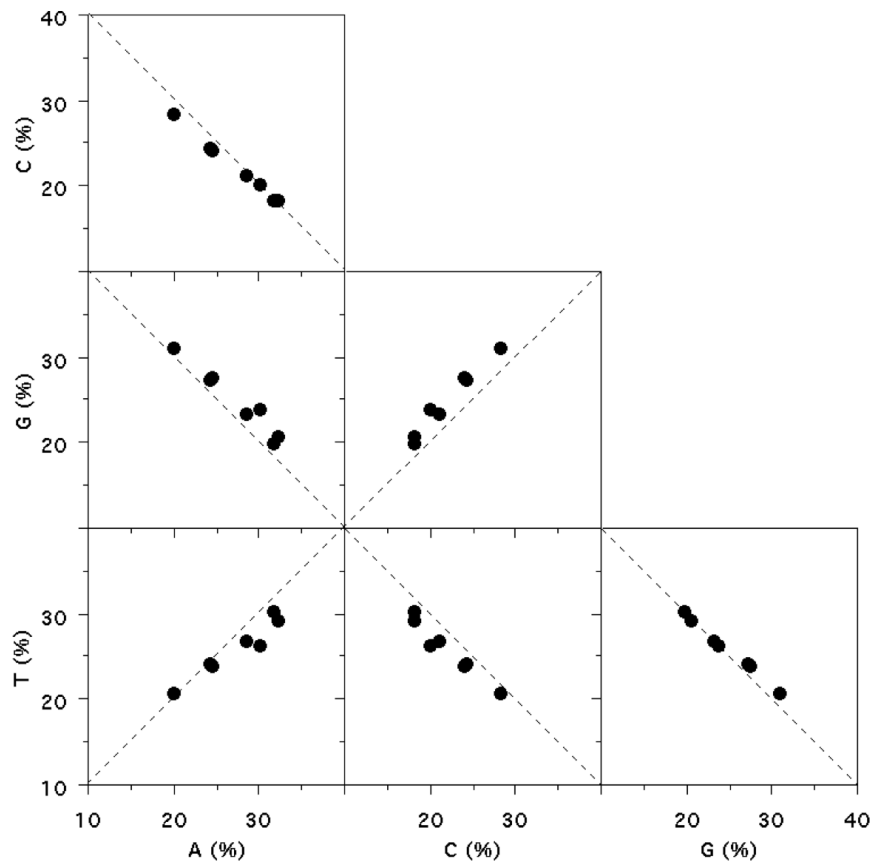
Data are from Table 2 in Rudner *et al.* (1969) for the L-strand. Data for *Bacillus subtilis* were taken from a previous paper: Rudner *et al.* (1968). This is in fact the average value observed for two different strains of *B. subtilis*: strain W23 and strain Mu8u5u16.

Denaturated chromosomes can be separated by a technique of intermitent gradient elution from a column of methylated albumin kieselguhr (MAK), into two fractions, designated, by virtue of their buoyant densities, as L (light) and H (heavy). The fractions can be hydrolyzed and subjected to chromatography to determined their global base composition.

The surprising result is that we have almost exactly A=T and C=G in single stranded-DNAs. The second paragraph page 157 in Rudner *et al.* (1969) says: "Our previous work on the complementary strands of *B. subtilis* DNA suggested an additional, entirely unexpected regularity, namely, the

equality in either strand of 6-amino and 6-keto nucleotides ( $A + C = G + T$ ). This relationship, which would normally have been regarded merely as the consequence of base-pairing in DNA duplex and would not have been predicted as a likely property of a single strand, is shown here to apply to all strand specimens isolated from denaturated DNA of the AT type (Table 2, preps. 1-4). It cannot yet be said to be established for the DNA specimens from the equimolar and GC types (nos. 5-7)."

Try `example(chargaff)` to mimic figure page 17 in Lobry (2000) :



Note that `example(chargaff)` gives more details: the red areas correspond to non-allowed values because the sum of the four bases frequencies cannot exceed 100%. The white areas correspond to possible values (more exactly to the projection from  $R^4$  to the corresponding  $R^2$  planes of the region of allowed values). The blue lines correspond to the very small subset of allowed values for which we have in addition PR2 state, that is  $[A]=[T]$  and  $[C]=[G]$ . Remember, these data are for ssDNA!

### Source

Rudner, R., Karkas, J.D., Chargaff, E. (1968) Separation of *B. subtilis* DNA into complementary strands, III. Direct Analysis. *Proceedings of the National Academy of Sciences of the United States of America*, **60**:921-922.

Rudner, R., Karkas, J.D., Chargaff, E. (1969) Separation of microbial deoxyribonucleic acids into



complementary strands. *Proceedings of the National Academy of Sciences of the United States of America*, **63**:152-159.

## References

Lobry, J.R. (2000) The black hole of symmetric molecular evolution. Habilitation thesis, Université Claude Bernard - Lyon 1. <https://pbil.univ-lyon1.fr/members/lobry/articles/HDR.pdf>.

`citation("seqinr")`

## Examples

```
data(chargaff)
op <- par(no.readonly = TRUE)
par(mfrow = c(4,4), mai = rep(0,4), xaxs = "i", yaxs = "i")
xlim <- ylim <- c(0, 100)

for( i in 1:4 )
{
  for( j in 1:4 )
  {
    if( i == j )
    {
      plot(chargaff[,i], chargaff[,j], t = "n", xlim = xlim, ylim = ylim,
           xlab = "", ylab = "", xaxt = "n", yaxt = "n")
      polygon(x = c(0, 0, 100, 100), y = c(0, 100, 100, 0), col = "lightgrey")
      for( k in seq(from = 0, to = 100, by = 10) )
      {
        lseg <- 3
        segments(k, 0, k, lseg)
        segments(k, 100 - lseg, k, 100)
        segments(0, k, lseg, k)
        segments(100 - lseg, k, 100, k)
      }
      string <- paste(names(chargaff)[i], "\n\n", xlim[1], "% -", xlim[2], "%")
      text(x=mean(xlim), y=mean(ylim), string, cex = 1.5)
    }
    else
    {
      plot(chargaff[,i], chargaff[,j], pch = 1, xlim = xlim, ylim = ylim,
           xlab = "", ylab = "", xaxt = "n", yaxt = "n", cex = 2)
      iname <- names(chargaff)[i]
      jname <- names(chargaff)[j]
      direct <- function() segments(0, 0, 50, 50, col="blue")
      invers <- function() segments(0, 50, 50, 0, col="blue")
      PR2 <- function()
      {
        if( iname == "[A]" & jname == "[T]" ) { direct(); return() }
        if( iname == "[T]" & jname == "[A]" ) { direct(); return() }
        if( iname == "[C]" & jname == "[G]" ) { direct(); return() }
        if( iname == "[G]" & jname == "[C]" ) { direct(); return() }
        invers()
      }
    }
  }
}
```

```

    }
    PR2()
    polygon(x = c(0, 100, 100), y = c(100, 100, 0), col = "pink4")
    polygon(x = c(0, 0, 100), y = c(0, 100, 0))
  }
}
# Clean up
par(op)

```

---

choosebank

*To select a database structured under ACNUC and located on the web*


---

## Description

This function allows to select one of the databases structured under ACNUC and located on the web. Called without arguments, `choosebank()`, will return the list of available databases. Then, you can use [query](#) to make your query and get a list of sequence names. Remote access to ACNUC databases works by opening a socket connection on a port (for example on port number 5558 at `pbil.univ-lyon1.fr`) and by communicating on this socket following the protocol described in the section references.

## Usage

```

choosebank(bank = NA, host = "pbil.univ-lyon1.fr", port = 5558, server = FALSE,
           blocking = TRUE, open = "a+", encoding = "", verbose = FALSE,
           timeout = 5, infobank = FALSE, tagbank = NA)

```

## Arguments

bank	string. The name of the bank. If NA, choosebank will return the names of all database known by the server.
host	string. Host name for port (see <a href="#">socketConnection</a> )
port	integer. The TCP port number (see <a href="#">socketConnection</a> )
server	logical. Should the socket be a client or a server? (see <a href="#">socketConnection</a> )
blocking	logical. (see <a href="#">socketConnection</a> )
open	string. A description of how to open the connection (see <a href="#">socketConnection</a> )
encoding	string. The name of the encoding to be used. (see <a href="#">socketConnection</a> )
verbose	logical. If TRUE, verbose mode is on
timeout	integer. The timeout in seconds for <code>socketConnection</code> . Default 5 seconds.
infobank	logical. If <code>infobank</code> is TRUE and <code>bank</code> is NA, a data.frame with all database informations will be returned
tagbank	string. If <code>bank</code> is NA and <code>tagbank</code> is documented, the names of special purposes databases are returned. Current allowed values are TP for frozen databases (TP is an acronym for "travaux pratiques" which means practicals in french, these databases are useful mainly for teaching so as to have stable results), TEST for test databases, and DEV for databases under development (unstable).

## Details

When called without arguments, `choosebank()` returns a list of all the databases names known by the server, as a vector of string. When called with `choosebank(Infobank = TRUE)`, a `data.frame` with more information is returned.

## Value

When called with a regular bank name, an (invisible) list with 6 components:

<code>socket</code>	an object of class <code>socket</code>
<code>bankname</code>	the name of the bank
<code>banktype</code>	the type of the bank (GENBANK, EMBL, SWISSPROT, NBRF)
<code>totseqs</code>	the total number of sequences present in the opened database
<code>totspecs</code>	the total number of species present in the opened database
<code>totkeys</code>	the total number of keywords present in the opened database

When called with `bank = NA`:

A vector of all available bank names.

When called with `bank = NA` and `Infobank = TRUE`, a `data.frame` with three columns:

<code>bank</code>	The name of the bank.
<code>status</code>	The bank status (on/of).
<code>info</code>	Short description of bank with last release date.

## Note

The invisible list returned when a database is opened is stored in the variable `banknameSocket` in the global environment.

## Author(s)

D. Charif, J.R. Lobry

## References

For more information about the socket communication protocol with ACNUC please get at [http://doua.prabi.fr/databases/acnuc/remote\\_acnuc.html](http://doua.prabi.fr/databases/acnuc/remote_acnuc.html). To get the release date and content of all the databases located at the pbil, please look at the following url: <http://doua.prabi.fr/search/releases>

Gouy, M., Milleret, F., Mugnier, C., Jacobzone, M., Gautier, C. (1984) ACNUC: a nucleic acid sequence data base and analysis system. *Nucl. Acids Res.*, **12**:121-127.

Gouy, M., Gautier, C., Attimonelli, M., Lanave, C., Di Paola, G. (1985) ACNUC - a portable retrieval system for nucleic acid sequence databases: logical and physical designs and usage. *Comput. Appl. Biosci.*, **3**:167-172.

Gouy, M., Gautier, C., Milleret, F. (1985) System analysis and nucleic acid sequence banks. *Biochimie*,

67:433-436.

```
citation("seqinr")
```

### See Also

[where.is.this.acc](#) if you have a sequence accession number but you don't know which database to open, [query](#) to make a query when a database is opened, [connection](#), [socketConnection](#)

### Examples

```
## Not run: # Need internet connection
# Show available databases:
choosebank()
# Show frozen databases:
choosebank(tag = "TP")
# Select a database:
choosebank("emblTP", tag = "TP")
# Do something with the database:
myseq <- gfrag("LMFLCHR36", start = 1, length = 30)
stopifnot(myseq == "cgcgctgctggcggcaatgaagcgttcgatg")
# Close the database:
closebank()
## End(Not run)
```

---

circle

*Draws a circle*

---

### Description

Draws a circle or an arc-circle on the current graphic device

### Usage

```
circle(x = 0, y = 0, r = 1, theta = c(0, 360), n = 100, ...)
```

### Arguments

x	x coordinate for the center of the circle
y	y coordinate for the center of the circle
r	radius of the circle
theta	start and stop angle
n	number of points for polygon object
...	arguments passed to <a href="#">polygon</a>

### Value

none

**Author(s)**

J.R. Lobry

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

```

par(mfrow = c(2, 2), mar = c(0,0,2,0))
setup <- function(){
  plot.new()
  plot.window(xlim = c(-1,1), ylim = c(-1,1), asp = 1)
}

setup()
circle(col = "lightblue")
title(main = "theta = c(0, 360)")

setup()
circle(col = "lightblue", theta = c(0, 270))
title(main = "theta = c(0, 270)")

setup()
circle(col = "lightblue", theta = c(-90, 180))
title(main = "theta = c(-90, 180)")

setup()
n <- 20
for(i in seq(0, 360, length = n)){
  circle(col = "lightblue", theta = c(i, i+360/(2*n)))
}
title(main = "many thetas")

```

closebank

*To close a remote ACNUC database***Description**

This function tries to close a remote ACNUC database.

**Usage**

```
closebank(socket = autosocket(), verbose = FALSE)
```

**Arguments**

socket	an object of class sockconn connecting to a remote ACNUC database (default is a socket to the last opened database).
verbose	Logical. If TRUE, verbose mode is on

**Author(s)**

J.R. Lobry

**References**

`citation("seqinr")`

**See Also**

[choosebank](#)

**Examples**

```
## Not run: # Need internet connection
choosebank("emblTP")
closebank()

## End(Not run)
```

---

clustal

*Example of results obtained after a call to read.alignment*

---

**Description**

This data set gives an example of a protein alignment obtained after a call to the function `read.alignment` on an alignment file in "clustal" format.

**Usage**

```
clustal
```

**Format**

A List of class alignment

**Source**

<http://www.clustal.org/>

**References**

Thompson, J.D., Higgins D.G., Gibson T.J. (1994) *CLUSTAL W: improving the sensitivity of progressive multiple sequence alignment through sequence weighting, position specific gap penalties and weight matrix choice*. Nucleic Acids Res. 22(22):4673-80.

col2alpha

*To use a standard color with an alpha transparency channel***Description**

Takes as input a standard R color and an alpha value to return its rgb coding.

**Usage**

```
col2alpha(color, alpha = 0.5)
```

**Arguments**

color	A standard R color as in <a href="#">colors</a> .
alpha	An alpha transparency value in the interval [0,1].

**Value**

same as in [rgb](#).

**Author(s)**

J.R. Lobry

**See Also**

[colors](#), [col2rgb](#), [rgb](#).

**Examples**

```
#
# Need alpha transparency channel
#
par(mar = c(0, 0, 2, 2)+0.1, oma = c(0, 0, 2, 0), mfrow = c(3,2))
for(testcol in c("blue", "red", "green", "yellow", "purple", "darkgreen")){
  plot(0,0, type="n", xlim=0:1, ylim = 0:1, axes = FALSE, xlab = "", ylab = "", main = testcol)
  n <- 11
  for(i in seq(0, 1, length = n)){
    col <- col2alpha(testcol, i)
    rect(i, 0, i + 1/n, 1, col = col, border = "black", xpd = NA)
    text(i+0.5/n, 0.5, round(i,2), xpd = NA)
  }
}
mtext("Effect of alpha on some colors\nNote: need alpha transparency channel",
      side = 3, outer = TRUE)
#
# The subtractive color scheme:
#
par(mar = c(0,0,3,0))
```

```

plot.new()
plot.window(xlim = c(-1.5, 1.5), ylim = c(-1,1.75), asp = 1)
n <- 10
alpha <- 1/n
for(i in 1:(2*n)){
  circle(x = -0.5, y = 0, col = col2alpha("yellow", alpha))
  circle(x = 0.5, y = 0, col = col2alpha("cyan", alpha))
  circle(x = 0, y = 3/4, col = col2alpha("magenta", alpha))
}
title("Subtractive color scheme\nNote: need alpha transparency channel")

```

comp

*complements a nucleic acid sequence***Description**

Complements a sequence, for instance if the sequence is "a", "c", "g", "t" it returns "t", "g", "c", "a". This is not the reverse complementary strand. This function can handle ambiguous bases if required.

**Usage**

```
comp(seq, forceToLower = TRUE, ambiguous = FALSE)
```

**Arguments**

seq	a DNA sequence as a vector of single chars
forceToLower	if TRUE characters in seq are forced to lower case
ambiguous	if TRUE ambiguous bases in seq are handled

**Value**

a vector of characters which is the complement of the sequence, not the reverse complementary strand. Undefined values are returned as NA.

**Author(s)**

D. Charif, J.R. Lobry

**References**

```
citation("seqinr")
```

**See Also**

Because ssDNA sequences are always written in the 5'→3' direction, use `rev(comp(seq))` to get the reverse complementary strand (see [rev](#)).



**Examples**

```
##
## Show that comp() does *not* return the reverse complementary strand:
##

c2s(comp(s2c("aaaattttggggcccc")))

##
## Show how to get the reverse complementary strand:
##

c2s(rev(comp(s2c("aaaattttggggcccc"))))

##
## Show what happens with non allowed values:
##

c2s(rev(comp(s2c("aaaaXttttYggggZcccc"))))

##
## Show what happens with ambiguous bases:
##

allbases <- s2c("abcdghkmstvn")
comp(allbases) # NA are produced
comp(allbases, ambiguous = TRUE) # No more NA

##
## Routine sanity checks:
##

stopifnot(identical(comp(allbases, ambiguous = TRUE), s2c("tvghcdmksabwn")))
stopifnot(identical(comp(c("A", "C", "G", "T"), forceToLower = FALSE), c("T", "G", "C", "A")))
```

---

computePI

---

*To Compute the Theoretical Isoelectric Point*


---

**Description**

This function calculates the theoretical isoelectric point of a protein. Isoelectric point is the pH at which the protein has a neutral charge. This estimate does not account for the post-translational modifications.

**Usage**

```
computePI(seq)
```

**Arguments**

```
seq          Protein sequence as a vector of single chars in upper case
```

**Value**

The theoretical isoelectric point (pI) as a numerical vector of length one.

**Note**

Protein pI is calculated using pK values of amino acids described in Bjellqvist et al. See also SEQINR.UTIL for more details.

**Author(s)**

D. Charif, J.R. Lobry

**References**

The algorithm is the same as the one which is implemented at the following url: [http://www.expasy.org/tools/pi\\_tool-doc.html](http://www.expasy.org/tools/pi_tool-doc.html) but with many trials in case of convergence failure of the non-linear regression procedure. citation("seqinr")

**See Also**

[SEQINR.UTIL](#)

**Examples**

```
#
# Simple sanity check with all 20 amino-acids in one-letter code alphabetical order:
#
prot <- s2c("ACDEFGHIKLMNPQRSTVWY")
stopifnot(all.equal(computePI(prot), 6.78454))
#
# Read a protein sequence in a FASTA file and then compute its pI :
#
myProts <- read.fasta(file = system.file("sequences/seqAA.fasta",
  package = "seqinr"), seqtype = "AA")
computePI(myProts[[1]]) # Should be 8.534902
```

---

consensus

*Consensus and profiles for sequence alignments*

---

**Description**

This function returns a consensus using various methods (see details) or a profile from a sequence alignment.

**Usage**

```
consensus(matali, method = c("majority", "threshold", "IUPAC", "profile"),
  threshold = 0.60, warn.non.IUPAC = FALSE, type = c("DNA", "RNA"))
con(matali, method = c("majority", "threshold", "IUPAC", "profile"),
  threshold = 0.60, warn.non.IUPAC = FALSE, type = c("DNA", "RNA"))
```

**Arguments**

<code>matali</code>	an object of class <code>alignment</code> as returned by <code>read.alignment</code> , or a matrix of characters.
<code>method</code>	select the method to use, see details.
<code>threshold</code>	for the <code>threshold</code> method, a numeric value between 0 and 1 indicating the minimum relative frequency for a character to be returned as the consensus character. If none, NA is returned.
<code>warn.non.IUPAC</code>	for the IUPAC method this argument is passed to <code>bma</code> with a default value set to FALSE to avoid warnings due to gap characters in the alignment.
<code>type</code>	for the IUPAC method this argument is passed to <code>bma</code> .

**Details**

**"majority"** The character with the higher frequency is returned as the consensus character.

**"threshold"** As above but in addition the character relative frequency must be higher than the value controlled by the `threshold` argument. If none, NA is returned.

**"IUPAC"** Make sense only for nucleic acid sequences (DNA or RNA). The consensus character is defined if possible by an IUPAC symbol by function `bma`. If this is not possible, when there is a gap character for instance, NA is returned.

**"profile"** With this method a matrix with the count of each possible character at each position is returned.

`con` is a short form for `consensus`.

**Value**

Either a vector of single characters with possible NA or a matrix with the method profile.

**Author(s)**

J.R. Lobry

**References**

`citation("seqinr")`

**See Also**

See `read.alignment` to import alignment from files.

**Examples**

```
#
# Read 5 aligned DNA sequences at 42 sites:
#
phylip <- read.alignment(file = system.file("sequences/test.phylip",
  package = "seqinr"), format = "phylip")
#
```

```

# Show data in a matrix form:
#
# (matali <- as.matrix(phylip))
#
# With the majority rule:
#
# res <- consensus(phylip)
# stopifnot(c2s(res) == "aaaccctggccgttcagggtaaaccgtggccgggcagggtat")
#
# With a threshold:
#
# res.thr <- consensus(phylip, method = "threshold")
# res.thr[is.na(res.thr)] <- "." # change NA into dots
# stopifnot(c2s(res.thr) == "aa.c..t.gc.gtt..g..t.a.cc..ggccg.....ta.")
# stopifnot(c2s(res.thr) == "aa.cc.tggccgttcagggtaaacc.tggccgg.cagggtat")
#
# With an IUPAC summary:
#
# res.iup <- consensus(phylip, method = "IUPAC")
# stopifnot(c2s(res.iup) == "amvsbnkkgcmkkmmgsktrmrssndkgcmrkdmvskyaw")
# replace 3 and 4-fold symbols by dots:
# res.iup[match(res.iup, s2c("bdhvn"), nomatch = 0) > 0] <- "."
# stopifnot(c2s(res.iup) == "am.s..kkgcmkkmmgsktrmrss..kgcmrk.mm.skyaw")
#
# With a profile method:
#
# (res <- consensus(phylip, method = "profile"))
#
# Show the connection between the profile and some consensus:
#
# bxc <- barplot(res, col = c("green", "blue", "orange", "white", "red"), border = NA,
#   space = 0, las = 2, ylab = "Base count",
#   main = "Profile of a DNA sequence alignment",
#   xlab = "sequence position", xaxs = "i")
#
# text(x = bxc, y = par("usr")[4], lab = res.thr, pos = 3, xpd = NA)
# text(x = bxc, y = par("usr")[1], lab = res.iup, pos = 1, xpd = NA)

```

count

*Composition of dimer/trimer/etc oligomers***Description**

Counts the number of times dimer/trimer/etc oligomers occur in a sequence. Note that the oligomers are overlapping by default.

**Usage**

```

count(seq, wordsize, start = 0, by = 1,
      freq = FALSE, alphabet = s2c("acgt"), frame = start)

```

**Arguments**

seq	a vector of single characters.
wordsize	an integer giving the size of word (n-mer) to count.
start	an integer (0, 1, 2,...) giving the starting position to consider in the sequence. The default value 0 means that we start at the first nucleotide in the sequence.
by	an integer defaulting to 1 for the window step.
freq	if TRUE, word relative frequencies (summing to 1) are returned instead of counts
alphabet	a vector of single characters used to build the oligomer set.
frame	synonymous for start

**Details**

count counts the occurrence of all words by moving a window of length word. The window step is controlled by the argument by. start controls the starting position in the sequence for the count.

**Value**

This function returns a [table](#) whose [dimnames](#) are all the possible oligomers. All oligomers are returned, even if absent from the sequence.

**Author(s)**

D. Charif, J.R. Lobry with suggestions from Gabriel Valiente, Stefanie Hartmann and Christian Gautier

**References**

`citation("seqinr")`

**See Also**

[table](#) for the class of the returned objet. See [rho](#) and [zscore](#) for dinucleotide statistics.

**Examples**

```
a <- s2c("acgggtacggtcccatcgaa")
##
## To count dinucleotide occurrences in sequence a:
##
count(a, word = 2)
##
## To count trinucleotide occurrences in sequence a, with start = 2:
##
count(a, word = 3, start = 2)
##
## To count dinucleotide relative frequencies in sequence a:
##
count(a, word = 2, freq = TRUE)
##
```

```
## To count dinucleotides in codon positions III-I in a coding sequence:
##
alldinuclIIIPi <- s2c("NNaaNatNttNtgNgtNtcNctNtaNagNggNgcNcgNgaNacNccNcaNN")
resIIIPi <- count(alldinuclIIIPi, word = 2, start = 2, by = 3)
stopifnot(all( resIIIPi == 1))
##
## Simple sanity check:
##
#alldinucl <- "aattgtctaggcgacca"
#stopifnot(all(count(s2c(alldinucl), 2) == 1))
#alldiaa <- "aaxxzxbxvxyxwxtxsxpxfxmxkxlixhxgxexqxcxdxnrxazzbzbvzyzwztzszpzfzmzkzlxizhzgzezqzczdznz
#rzabbvbybwbtsbpbfbmbkblbibhbgbqcbdbnrbavvyvwtvsvpfvmkvlvivhvgvevqvcvdcvncrvayywytytyspyfyfymyky
#lyiyhygyeyqcydynryyawtwswpwwfwmmkwliwhwgwewqwcwdwnwrwattstptftmtktltithtgtetqtctdnttrtasspsfsmsks
#lsishsgsesqscdsnsrsappfpmpkplpiphpgpepqpdpnpnpaffmfkflfifhfgfefqfcfdfnfrfamkmmlmimhgmegmqmcmdmnm
#rmakklkikhkgkekqkckdknkrkallilhlglelqlclldlnrlaiihigieiqicidiniriahhghehqhchdhnhrhaggegqgcgdgngrgae
#eqecedenereaqqcqdnqrqaccdncrcaddndrdannrnarra"
#stopifnot(all(count(s2c(alldiaa), 2, alphabet = s2c("arndcqe ghilkmfpstwyvbx")) == 1))
##
## Example with dinucleotide count in the complete Human mitochondrion genome:
##
humanMito <- read.fasta(file = system.file("sequences/humanMito.fasta", package = "seqinr"))
##
## Get the dinucleotide count:
##
dinu <- count(humanMito[[1]], 2)
##
## Put the results in a 4 X 4 array:
##
dinu2 <- dinu
dim(dinu2) <- c(4, 4)
nucl <- s2c("ACGT")
dimnames(dinu2) <- list(paste(nucl, "-3'", sep = ""), paste("5'-", nucl, sep = ""))
##
## Show that CpG and GpT dinucleotides are depleted:
##
mosaicplot(t(dinu2), shade = TRUE,
  main = "Dinucleotide XpY frequencies in the Human\mitochondrion complete genome",
  xlab = "First nucleotide: Xp",
  ylab = "Second nucleotide: pY", las = 1, cex = 1)
mtext("Note the depletion in CpG and GpT dinucleotides", side = 1, line = 3)
```

countfreelists

*The number of free lists available and annotation lines in an ACNUC server*

## Description

Returns the number of free lists available list of names of annotation lines in the opened ACNUC database.

**Usage**

```
countfreelists(socket = autosocket())  
cfl(socket = autosocket())
```

**Arguments**

socket	an object of class sockconn connecting to a remote ACNUC database (default is a socket to the last opened database).
--------	--

**Value**

a list with the following 2 components:

free	numeric. The number of free lists
annotlines	vector of strings. Names of annotation lines

**Author(s)**

J.R. Lobry

**References**

<http://doua.prabi.fr/databases/acnuc.html>

citation("seqinr")

**See Also**

[choosebank](#), [query](#)

**Examples**

```
## Not run: # Need internet connection  
choosebank("emblTP")  
(rescountfreelists <- countfreelists())  
stopifnot(all(rescountfreelists$annotlines ==  
  c("ALL", "AC", "PR", "DT", "KW", "OS", "OC",  
    "OG", "RN", "RC", "RP", "RX", "RG", "RA", "RT", "RL", "DR",  
    "CC", "AH", "AS", "FH", "FT", "CO", "SQ", "SEQ")))  
closebank()  
  
## End(Not run)
```

---

countsubseqs	<i>Number of subsequences in an ACNUC list</i>
--------------	--

---

### Description

Returns the number of subsequences in the ACNUC list of rank lrank.

### Usage

```
countsubseqs(lrank, socket = autosocket())
css(lrank, socket = autosocket())
```

### Arguments

lrank	the rank of the ACNUC list to consider.
socket	an object of class sockconn connecting to a remote ACNUC database (default is a socket to the last opened database).

### Value

Numeric.

### Author(s)

J.R. Lobry

### References

<http://doua.prabi.fr/databases/acnuc.html>  
 citation("seqinr")

### See Also

[choosebank](#), [query](#), [glr](#) to get a list rank from its name.

### Examples

```
## Not run: # Need internet connection
choosebank("emblTP")
mylist<-query("mylist", "N=@", virtual = TRUE) # select all (seqs + subseqs)
mylist$nelem # 14138094 seqs + subseqs
stopifnot(mylist$nelem == 14138094)
css(glr("mylist")) # 1604500 subsequences only
stopifnot(css(glr("mylist")) == 1604500)
closebank()

## End(Not run)
```



---

crelistfromclientdata *To create on server an ACNUC list from data lines sent by client*

---

## Description

This function is usefull if you have a local file with sequence names (sequence ID), or sequence accession numbers, or species names, or keywords. This allows you to create on the server a list with the corresponding items.

## Usage

```
crelistfromclientdata(listname, file, type,
  socket = autosocket(), invisible = TRUE,
  verbose = FALSE, virtual = FALSE)
clfcd(listname, file, type, socket = autosocket(),
  invisible = TRUE, verbose = FALSE, virtual = FALSE)
```

## Arguments

listname	The name of the list as a quoted string of chars
file	The local file name
type	Could be one of "SQ", "AC", "SP", "KW", see examples
socket	an object of class sockconn connecting to a remote ACNUC database (default is a socket to the last opened database).
invisible	if FALSE, the result is returned visibly.
verbose	if TRUE, verbose mode is on
virtual	if TRUE, no attempt is made to retrieve the information about all the elements of the list. In this case, the req component of the list is set to NA.

## Details

clfcd is a shortcut for crelistfromclientdata.

## Value

The result is directly assigned to the object listname in the user workspace. This is an objet of class qaw, a list with the following 6 components:

call	the original call
name	the ACNUC list name
nelem	the number of elements (for instance sequences) in the ACNUC list
typelist	the type of the elements of the list. Could be SQ for a list of sequence names, KW for a list of keywords, SP for a list of species names.
req	a list of sequence names that fit the required criteria or NA when called with parameter virtual is TRUE
socket	the socket connection that was used

**Author(s)**

J.R. Lobry

**References**

`citation("seqinr")`

**See Also**

[choosebank](#), [query](#), [savelist](#) for the reverse operation with an ACNUC list of sequences.

**Examples**

```
## Not run: # Need internet connection
choosebank("emblTP")
#
# Example with a file that contains sequence names:
#
fileSQ <- system.file("sequences/bb.mne", package = "seqinr")
listSQ <- crelistfromclientdata("listSQ", file = fileSQ, type = "SQ")
sapply(listSQ$req, getName)
#
# Example with a file that contains sequence accession numbers:
#
fileAC <- system.file("sequences/bb.acc", package = "seqinr")
listAC <- crelistfromclientdata("listAC", file = fileAC, type = "AC")
sapply(listAC$req, getName)
#
# Example with a file that contains species names:
#
fileSP <- system.file("sequences/bb.sp", package = "seqinr")
listSP <- crelistfromclientdata("listSP", file = fileSP, type = "SP")
sapply(listSP$req, getName)
#
# Example with a file that contains keywords:
#
fileKW <- system.file("sequences/bb.kwd", package = "seqinr")
listKW <- crelistfromclientdata("listKW", file = fileKW, type = "KW")
sapply(listKW$req, getName)
#
# Summary of ACNUC lists:
#
sapply(alr())$rank, getliststate)
closebank()

## End(Not run)
```

dia.bactgensize

*Distribution of bacterial genome size from GOLD***Description**

This function tries to download the last update of the GOLD (Genomes OnLine Database) to extract bacterial genomes sizes when available. The histogram and the default density() output is produced. Optionally, a maximum likelihood estimate of a superposition of two or three normal distributions is also represented.

**Usage**

```
dia.bactgensize(fit = 2, p = 0.5, m1 = 2000, sd1 = 600, m2 = 4500,
               sd2 = 1000, p3 = 0.05, m3 = 9000, sd3 = 1000, maxgensize = 20000,
               source = c("ftp://pbil.univ-lyon1.fr/pub/seqinr/data/goldtable15Dec07.txt",
                          "http://www.genomesonline.org/DBs/goldtable.txt"))
```

**Arguments**

fit	integer value. If fit == 0 no normal fit is produced, if fit == 2 try to fit a superposition of two normal distributions, if fit == 3 try to fit a superposition of three normal distributions.
p	initial guess for the proportion of the first population.
m1	initial guess for the mean of the first population.
sd1	initial guess for the standard deviation of the first population.
m2	initial guess for the mean of the second population.
sd2	initial guess for the standard deviation of the second population.
p3	initial guess for the proportion of the third population.
m3	initial guess for the mean of the third population.
sd3	initial guess for the standard deviation of the third population.
maxgensize	maximum admissible value in bp for a bacterial genome size: only value less or equal to this threshold are considered.
source	the file with raw data. By default a local (outdated) copy is used.

**Value**

An invisible dataframe with three components:

genus	genus name
species	species names
gs	genome size in Kb

**Author(s)**

J.R. Lobry

## References

Please cite the following references when using data from GOLD:

Kyrpides, N.C. (1999) Genomes OnLine Database (GOLD 1.0): a monitor of complete and ongoing genome projects world-wide. *Bioinformatics*, **15**:773-774.

Bernal, A., Ear, U., Kyrpides, N. (2001) Genomes OnLine Database (GOLD): a monitor of genome projects world-wide. *Nucleic Acids Research*, **29**:126-127.

Liolios, K., Tavernarakis, N., Hugenholtz, P., Kyrpides, N.C. (2006) The Genomes On Line Database (GOLD) v.2: a monitor of genome projects worldwide. *Nucleic Acids Research*, **34**:D332-D334.

Liolios, K., Mavrommatis, K., Tavernarakis, N., Kyrpides, N.C. (2008) The Genomes On Line Database (GOLD) in 2007: status of genomic and metagenomic projects and their associated meta-data. *Nucleic Acids Research*, **in press**:D000-D000.

```
citation("seqinr")
```

## See Also

[density](#)

## Examples

```
## Not run: # Need internet connection
#
# With a local outdated copy from GOLD:
#
#   dia.bactgensize()
#
# With last GOLD data:
#
# The URL is no more accessible.
# dia.bactgensize(source = "http://www.genomesonline.org/DBs/goldtable.txt")

## End(Not run)
```

---

dinucl

*Mean zscore on 242 complete bacterial chromosomes*

---

## Description

This dataset contains the mean zscores as computed on all intergenic sequences (intergenic) and on all CDS (coding) from 242 complete bacterial chromosomes (as retrieved from Genome Reviews database on June 16, 2005).

**Usage**

```
data(dinucl)
```

**Format**

List of two dataframes of 242 chromosomes and 16 dinucleotides: one for intergenic, one for coding sequences.

**intergenic** the mean of zscore computed with the base model on each intergenic sequence

**coding** the mean of zscore computed with the codon model on each coding sequence

**References**

Palmeira, L., Guéguen, L. and Lobry JR. (2006) UV-targeted dinucleotides are not depleted in light-exposed Prokaryotic genomes. *Molecular Biology and Evolution*, **23**:2214-2219.

<http://mbe.oxfordjournals.org/cgi/reprint/23/11/2214>

```
citation("seqinr")
```

**See Also**

[zscore](#)

**Examples**

```
data(dinucl)
par(mfrow = c(2, 2), mar = c(4,4,0.5,0.5)+0.1)
myplot <- function(x){
  plot(dinucl$intergenic[, x], dinucl$coding[, x],
       xlab = "intergenic", ylab = "coding",
       las = 1, ylim = c(-6, 4),
       xlim = c(-3, 3), cex = 0)
  rect(-10,-10,-1.96,10,col="yellow", border = "yellow")
  rect(1.96,-10,10,10,col="yellow", border = "yellow")
  rect(-10,-10,10,-1.96,col="yellow", border = "yellow")
  rect(-10,1.96,10,10,col="yellow", border = "yellow")
  abline(v=0,lty=3)
  abline(h=0,lty=3)
  abline(h=-1.96,lty=2)
  abline(h=+1.96,lty=2)
  abline(v=-1.96,lty=2)
  abline(v=+1.96,lty=2)
  points(dinucl$intergenic[, x], dinucl$coding[, x], pch = 21,
         col = rgb(.1,.1,.1,.5), bg = rgb(.5,.5,.5,.5))
  legend("bottomright", inset = 0.02,
        legend = paste(substr(x,1,1), "p",
                          substr(x,2,2), " bias", sep = ""), cex = 1.25, bg = "white")
  box()
}
myplot("CT")
```

```
myplot("TC")
myplot("CC")
myplot("TT")
```

---

dinucleotides	<i>Statistical over- and under- representation of dinucleotides in a sequence</i>
---------------	---

---

## Description

These two functions compute two different types of statistics for the measure of statistical dinucleotide over- and under-representation : the rho statistic, and the z-score, each computed for all 16 dinucleotides.

## Usage

```
rho(sequence, wordsize = 2, alphabet = s2c("acgt"))
zscore(sequence, simulations = NULL, modele, exact = FALSE, alphabet = s2c("acgt"), ... )
```

## Arguments

sequence	a vector of single characters.
wordsize	an integer giving the size of word (n-mer) to consider.
simulations	If NULL, analytical solution is computed when available (models base and codon). Otherwise, it should be the number of permutations for the z-score computation
modele	A string of characters describing the model chosen for the random generation
exact	Whether exact analytical calculation or an approximation should be used
alphabet	A vector of single characters.
...	Optional parameters for specific model permutations are passed on to <a href="#">permutation</a> function.

## Details

The rho statistic, as presented in Karlin S., Cardon LR. (1994), can be computed on each of the 16 dinucleotides. It is the frequency of dinucleotide  $xy$  divided by the product of frequencies of nucleotide  $x$  and nucleotide  $y$ . It is equal to 1.00 when dinucleotide  $xy$  is formed by pure chance, and it is superior (respectively inferior) to 1.00 when dinucleotide  $xy$  is over- (respectively under-) represented. Note that if you want to reproduce Karlin's results you have to compute the statistic from the sequence concatenated with its inverted complement that is with something like `rho(c(myseq, rev(comp(myseq))))`.

The zscore statistic, as presented in Palmeira, L., Guéguen, L. and Lobry JR. (2006). The statistic is the normalization of the rho statistic by its expectation and variance according to a given random sequence generation model, and follows the standard normal distribution. This statistic can be computed with several models (cf. [permutation](#) for the description of each of the models). We provide analytical calculus for two of them: the base permutations model and the codon permutations model.

The base model allows for random sequence generation by shuffling (with/without replacement) of all bases in the sequence. Analytical computations are available for this model: either as an approximation for large sequences (cf. Palmeira, L., Guéguen, L. and Lobry JR. (2006)), either as the exact analytical formulae (cf. Schbath, S. (1995)).

The position model allows for random sequence generation by shuffling (with/without replacement) of bases within their position in the codon (bases in position I, II or III stay in position I, II or III in the new sequence).

The codon model allows for random sequence generation by shuffling (with/without replacement) of codons. Analytical computation is available for this model (Gautier, C., Gouy, M. and Louail, S. (1985)).

The syncodon model allows for random sequence generation by shuffling (with/without replacement) of synonymous codons.

### Value

a table containing the computed statistic for each dinucleotide

### Author(s)

L. Palmeira, J.R. Lobry with suggestions from A. Coghlan.

### References

Gautier, C., Gouy, M. and Louail, S. (1985) Non-parametric statistics for nucleic acid sequence study. *Biochimie*, **67**:449-453.

Karlin S. and Cardon LR. (1994) Computational DNA sequence analysis. *Annu Rev Microbiol*, **48**:619-654.

Schbath, S. (1995) Étude asymptotique du nombre d'occurrences d'un mot dans une chaîne de Markov et application à la recherche de mots de fréquence exceptionnelle dans les séquences d'ADN. *Thèse de l'Université René Descartes, Paris V*

Palmeira, L., Guéguen, L. and Lobry, J.R. (2006) UV-targeted dinucleotides are not depleted in light-exposed Prokaryotic genomes. *Molecular Biology and Evolution*, **23**:2214-2219. <http://mbe.oxfordjournals.org/cgi/reprint/23/11/2214>

citation("seqinr")

### See Also

[permutation](#)

### Examples

```
## Not run:
sequence <- sample(x = s2c("acgt"), size = 6000, replace = TRUE)
rho(sequence)
zscore(sequence, modele = "base")
zscore(sequence, modele = "base", exact = TRUE)
zscore(sequence, modele = "codon")
zscore(sequence, simulations = 1000, modele = "syncodon")
```

```
## End(Not run)
```

---

dist.alignment

---

*Pairwise Distances from Aligned Protein or DNA/RNA Sequences*


---

## Description

These functions compute a matrix of pairwise distances from aligned sequences using similarity (Fitch matrix, for protein sequences only) or identity matrix (for protein and DNA sequences). The resulting matrix contains the squared root of the pairwise distances. For example, if identity between 2 sequences is 80 the squared root of (1.0 - 0.8) i.e. 0.4472136.

## Usage

```
dist.alignment(x, matrix = c("similarity", "identity"), gap)
```

## Arguments

x	an object of class alignment, as returned by read.alignment for instance
matrix	the matrix distance to be used, partial matching allowed
gap	-optional- with nucleotides, if set to 1, gaps will be counted in the identity measure

## Value

The distance matrix, object of class dist, computed by using the specified distance measure.

## Author(s)

D. Charif, J.R. Lobry

## References

The reference for the similarity matrix is :  
 Fitch, W.M. (1966) An improved method of testing for evolutionary homology. *J. Mol. Biol.*, **16**:9-16.

```
citation("seqinr")
```

## See Also

[read.alignment](#)



## Examples

```
myseqs <- read.alignment(file = system.file("sequences/test.mase",
package = "seqinr"), format = "mase")
dist.alignment(myseqs, matrix = "identity" )
as.matrix(dist.alignment(myseqs, matrix = "identity" ))
```

---

dotchart.uco

*Cleveland plot for codon usage tables*


---

## Description

Draw a Cleveland dot plot for codon usage tables

## Usage

```
dotchart.uco(x, numcode = 1, aa3 = TRUE, pt.cex = 0.7, alphabet =
  s2c("tcag"), pch = 21, gpch = 20, bg = par("bg"), cex
  = 0.7, color = "black", gcolor = "black", lcolor =
  grey(0.9), xlim, ...)
```

## Arguments

x	table of codon usage as computed by uco.
numcode	the number of the code to be used by translate.
aa3	logical. If TRUE use the three-letter code for amino- acids. If FALSE use the one-letter code for amino-acids.
pt.cex	the character size to be used for points.
alphabet	character for codons labels
pch	the plotting character or symbol to be used.
gpch	the plotting character or symbol to be used for group values.
bg	the background color to be used.
cex	the character expansion size passed to <a href="#">dotchart</a> .
color	the color(s) to be used for points an labels.
gcolor	the single color to be used for group labels and values.
lcolor	the color(s) to be used for the horizontal lines.
xlim	horizontal range for the plot
...	graphical parameters can also be specified as arguments

Value

An invisible list with components:

x	table of codon usage
labels	codon names
groups	amino acid factor
gdata	sums by amino acid
ypg	the y-axis coordinates for amino acids
ypi	the y-axis coordinates for codons

Author(s)

J.R. Lobry

References

Cleveland, W. S. (1985) The Elements of Graphing Data. Monterey, CA: Wadsworth. `citation("seqinr")`

See Also

[dotchart](#), [uco](#), [aaa](#), [translate](#)

Examples

```
# Load dataset:
data(ec999)
# Compute codon usage for all coding sequences:
ec999.uco <- lapply(ec999, uco, index="eff")
# Put it in a dataframe:
df <- as.data.frame(lapply(ec999.uco, as.vector))
# Add codon names:
row.names(df) <- names(ec999.uco[[1]])
# Compute global codon usage:
global <- rowSums(df)
# Choose a title for the graph:
title <- "Codon usage in 999 E. coli coding sequences"
# Plot data:
dotchart.uco(global, main = title)
```

---

dotPlot	<i>Dot Plot Comparison of two sequences</i>
---------	---

---

Description

Dot plots are most likely the oldest visual representation used to compare two sequences (see Maizel and Lenk 1981 and references therein). In its simplest form, a dot is produced at position (i,j) iff character number i in the first sequence is the same as character number j in the second sequence. More elaborated forms use sliding windows and a threshold value for two windows to be considered as matched.

**Usage**

```
dotPlot(seq1, seq2, wsize = 1, wstep = 1, nmatch = 1, col = c("white", "black"),
        xlab = deparse(substitute(seq1)), ylab = deparse(substitute(seq2)), ...)
```

**Arguments**

seq1	the first sequence (x-axis) as a vector of single chars.
seq2	the second sequence (y-axis) as a vector of single char.
wsize	the size in chars of the moving window.
wstep	the size in chars for the steps of the moving window. Use wstep == wsize for non-overlapping windows.
nmatch	if the number of match per window is greater than or equal to nmatch then a dot is produced.
col	color of points passed to image.
xlab	label of x-axis passed to image.
ylab	label of y-axis passed to image.
...	further arguments passed to image.

**Value**

NULL.

**Author(s)**

J.R. Lobry

**References**

Maizel, J.V. and Lenk, R.P. (1981) Enhanced Graphic Matrix Analysis of Nucleic Acid and Protein Sequences. *Proceedings of the National Academy of Science USA*, **78**:7665-7669.

```
citation("seqinr")
```

**See Also**

[image](#)

**Examples**

```
#
# Identity is on the main diagonal:
#
dotPlot(letters, letters, main = "Direct repeat")
#
# Internal repeats are off the main diagonal:
#
dotPlot(rep(letters, 2), rep(letters, 2), main = "Internal repeats")
```

```

#
# Inversions are orthogonal to the main diagonal:
#
dotPlot(letters, rev(letters), main = "Inversion")
#
# Insertion in the second sequence yields a vertical jump:
#
dotPlot(letters, c(letters[1:10], s2c("insertion"), letters[11:26]),
  main = "Insertion in the second sequence", asp = 1)
#
# Insertion in the first sequence yields an horizontal jump:
#
dotPlot(c(letters[1:10], s2c("insertion")), letters[11:26]), letters,
  main = "Insertion in the first sequence", asp = 1)
#
# Protein sequences have usually a good signal/noise ratio because there
# are 20 possible amino-acids:
#
aafile <- system.file("sequences/seqAA.fasta", package = "seqinr")
protein <- read.fasta(aafile)[[1]]
dotPlot(protein, protein, main = "Dot plot of a protein\n", wsize = 1, wstep = 1, nmatch = 1)
#
# Nucleic acid sequences have usually a poor signal/noise ratio because
# there are only 4 different bases:
#
dnafile <- system.file("sequences/malM.fasta", package = "seqinr")
dna <- protein <- read.fasta(dnafile)[[1]]
dotPlot(dna[1:200], dna[1:200],
  main = "Dot plot of a nucleic acid sequence\n", wsize = 1, wstep = 1, nmatch = 1)
#
# Play with the wsize, wstep and nmatch arguments to increase the
# signal/noise ratio:
#
dotPlot(dna[1:200], dna[1:200], wsize = 3, wstep = 3, nmatch = 3,
  main = "Dot plot of a nucleic acid sequence\n", wsize = 3, wstep = 3, nmatch = 3)

```

---

draw.oriloc

*Graphical representation for nucleotide skews in prokaryotic chromosomes.*


---

## Description

Graphical representation for nucleotide skews in prokaryotic chromosomes.

## Usage

```

draw.oriloc(ori, main = "Title",
  xlab = "Map position in Kb",
  ylab = "Cumulated combined skew in Kb", las = 1, las.right = 3,
  ta.mtext = "Cumul. T-A skew", ta.col = "pink", ta.lwd = 1,

```

```
cg.mtext = "Cumul. C-G skew", cg.col = "lightblue", cg.lwd = 1,
cds.mtext = "Cumul. CDS skew", cds.col = "lightgreen", cds.lwd = 1,
sk.col = "black", sk.lwd = 2,
add.grid = TRUE, ...)
```

### Arguments

<code>ori</code>	A data frame obtained with the <code>oriloc</code> function.
<code>main</code>	The main title of the plot.
<code>xlab</code>	The x-axis title.
<code>ylab</code>	The y-axis title.
<code>las</code>	The style of axis labels for the bottom and left axes.
<code>las.right</code>	The style of axis labels for the right axis.
<code>ta.mtext</code>	The marginal legend for the TA skew.
<code>ta.col</code>	The color for the TA skew.
<code>ta.lwd</code>	The line width for the TA skew.
<code>cg.mtext</code>	The marginal legend for the CG skew.
<code>cg.col</code>	The color for the CG skew.
<code>cg.lwd</code>	The line width for the CG skew.
<code>cds.mtext</code>	The marginal legend for the CDS skew.
<code>cds.col</code>	The color for the CDS skew.
<code>cds.lwd</code>	The line width for the CDS skew.
<code>sk.col</code>	The color for the cumulated combined skew.
<code>sk.lwd</code>	The line width for the cumulated combined skew.
<code>add.grid</code>	Logical, if TRUE a vertical grid is added to the plot.
<code>...</code>	Further arguments are passed to the function <code>plot</code> .

### Author(s)

J.R. Lobry

### References

`citation("seqinr")`

### See Also

[oriloc](#), [rearranged.oriloc](#), [extract.breakpoints](#)

## Examples

```
## Not run: # need internet connection
#
# Example with Chlamydia trachomatis complete genome
#
ori <- oriloc()
draw.oriloc(ori)
#
# The same, using more options from function draw.oriloc()
#
draw.oriloc(ori,
  main = expression(italic(Chlamydia~~trachomatis)~~complete~~genome),
  ta.mtext = "TA skew", ta.col = "red",
  cg.mtext = "CG skew", cg.col = "blue",
  cds.mtext = "CDS skew", cds.col = "seagreen",
  add.grid = FALSE)

## End(Not run)
```

---

draw.rearranged.oriloc

*Graphical representation for rearranged nucleotide skews in prokaryotic chromosomes.*

---

## Description

Graphical representation for rearranged nucleotide skews in prokaryotic chromosomes.

## Usage

```
draw.rearranged.oriloc(rearr.ori, breaks.gcfw = NA,
  breaks.gcrev = NA, breaks.atfw = NA, breaks.atrev = NA)
```

## Arguments

rearr.ori	A data frame obtained with the rearranged.oriloc function.
breaks.gcfw	The coordinates of the breakpoints in the GC-skew, for forward transcribed protein coding sequences. These coordinates can be obtained with the extract.breakpoints function.
breaks.gcrev	The coordinates of the breakpoints in the GC-skew, for reverse transcribed protein coding sequences. These coordinates can be obtained with the extract.breakpoints function.
breaks.atfw	The coordinates of the breakpoints in the AT-skew, for forward transcribed protein coding sequences. These coordinates can be obtained with the extract.breakpoints function.
breaks.atrev	The coordinates of the breakpoints in the AT-skew, for reverse transcribed protein coding sequences. These coordinates can be obtained with the extract.breakpoints function.

**Author(s)**

J.R. Lobry, A. Necşulea

**References**

Necşulea, A. and Lobry, J.R. (2007) A New Method for Assessing the Effect of Replication on DNA Base Composition Asymmetry. *Molecular Biology and Evolution*, **24**:2169-2179.

**See Also**

[rearranged.oriloc](#), [extract.breakpoints](#)

**Examples**

```
## Not run:
### Example for Chlamydia trachomatis ###

### Rearrange the chromosome and compute the nucleotide skews ###

#r.ori <- rearranged.oriloc(seq.fasta = system.file("sequences/ct.fasta.gz", package = "seqinr"),
#  g2.coord = system.file("sequences/ct.coord", package = "seqinr"))

r.ori <- rearranged.oriloc(seq.fasta = system.file("sequences/ct.fasta.gz", package = "seqinr"),
  g2.coord = system.file("sequences/ct.coord", package = "seqinr"))

### Extract the breakpoints for the rearranged nucleotide skews ###

breaks <- extract.breakpoints(r.ori, type = c("gcfw", "gcrev"),
  nbreaks = c(2, 2), gridsize = 50, it.max = 100)

### Draw the rearranged nucleotide skews and ###
### place the position of the breakpoints on the graphics ###

draw.rearranged.oriloc(r.ori, breaks.gcfw = breaks$gcfw$breaks,
  breaks.gcrev = breaks$gcrev$breaks)
## End(Not run)
```

---

draw.recstat

*Graphical representation of a recstat analysis.*


---

**Description**

This function displays the results returned by recstat with two plots. The first one shows the factor scores of a CA computed on the codon composition of a DNA sequence. The second one shows the locations of all Start and Stop codons in this sequence.

**Usage**

```
draw.recstat(rec, fac = 1, direct = TRUE, xlim = c(1, seqsize),
  col = c("red", "blue", "purple"))
```

**Arguments**

rec	list of elements returned by recstat function.
fac	axis of the CA to use for display ( $4 \geq \text{fac} \geq 1$ ).
direct	a logical for the choice of direct or reverse strand.
xlim	starting and ending positions in the sequence for the plot.
col	vector of colour codes for the three frames of the sequence.

**Details**

The first plot shows the factor scores of the sliding windows, this for the three possible frames of the strand selected by the user. The second shows the Start (filled grey triangles pointing up) and Stop (solid black triangles pointing down) codons positions. Note that the standard genetic code is used for that purpose. Visual detection of putative CDS is performed through the simultaneous use of these two graphics. If a CDS is located within the sequence, the factor scores for the windows located in the corresponding reading frame will be significantly separated from the two others. Moreover, the region where this separation is seen should be located between a Start and a Stop codon.

**Author(s)**

O. Clerc, G. Perrière

**See Also**

[test.li.recstat](#), [test.co.recstat](#)

**Examples**

```
ff <- system.file("sequences/ECOUNC.fsa", package = "seqinr")
seq <- read.fasta(ff)
rec <- recstat(seq[[1]], seqname = getName(seq))
draw.recstat(rec)
```

---

ec999

*999 coding sequences from E. coli*

---

**Description**

This dataset contains 999 coding sequences from the Escherichia coli chromosome



**Usage**

```
data(ec999)
```

**Format**

List of 999 vectors of characters, one for each coding sequence.

```
ECFOLE.FOLE chr [1:672] "A" "T" "G" "C" ...
```

```
ECMSBAG.MSBA chr [1:1749] "A" "T" "G" "C" ...
```

```
ECNARZYW-C.NARV chr [1:681] "A" "T" "G" "A" ...
```

```
... ... TRUNCATED ...
```

```
XYLEECOM.MALK chr [1:1116] "A" "T" "G" "G" ...
```

```
XYLEECOM.LAMB chr [1:1341] "A" "T" "G" "A" ...
```

```
XYLEECOM.MALM chr [1:921] "A" "T" "G" "A" ...
```

**References**

Lobry, J.R., Gautier, C. (1994) Hydrophobicity, expressivity and aromaticity are the major trends of amino-acid usage in 999 *Escherichia coli* chromosome-encode genes. *Nucleic Acids Research*, **22**:3174-3180.

```
citation("seqinr")
```

**Examples**

```
data(ec999)
#
# How to export sequences in a FASTA file:
#
write.fasta(ec999, names(ec999), file = "ec999.ffn")
```

---

ECH

---

*Forensic Genetic Profile Allelic Ladder Raw Data*


---

**Description**

This is an example of allelic ladder raw data for a human STR genetic profile at 16 loci (*viz.* D8S1179, D21S11, D7S820, CSF1PO, D3S1358, TH01, D13S317, D16S539, D2S1338, D19S433, vWA, TPOX, D18S51, Amelogenin, D5S818, FGA) which are commonly used in forensic sciences for individual identifications.

**Usage**

```
data(ECH)
```

**Format**

A list with 3 components as in [JL0](#)

**Author(s)**

J.R. Lobry

**Source**

Data were kindly provided by the INPS (Institut National de Police Scientifique) which is the national forensic sciences institute in France. Experiments were done at the LPS (Laboratoire de Police Scientifique de Lyon) in 2008.

**References**

```
citation("seqinr")
```

Anonymous (2006) Applied Biosystem Genetic Analysis Data File Format. Available at [http://www.appliedbiosystems.com/support/software\\_community/ABIF\\_File\\_Format.pdf](http://www.appliedbiosystems.com/support/software_community/ABIF_File_Format.pdf). Last visited on 03-NOV-2008.

**See Also**

function [read.abif](#) to import files in ABIF format, data [gs500liz](#) for internal size standards, data [identifiler](#) for allele names in the allelic ladder, data [JL0](#) for an example of an individual sample file.

**Examples**

```
data(JL0)
```

---

EXP

*Vectors of coefficients to compute linear forms.*

---

**Description**

This dataset is used to compute linear forms on codon frequencies: if `codfreq` is a vector of codon frequencies then `drop(freq %*% EXP$CG3)` will return for instance the G+C content in third codon positions. Base order is the lexical order: a, c, g, t (or u).

**Usage**

```
data(EXP)
```

**Format**

List of 24 vectors of coefficients

```

A num [1:4] 1 0 0 0
A3 num [1:64] 1 0 0 0 1 0 0 0 1 0 ...
AGZ num [1:64] 0 0 0 0 0 0 0 0 1 0 ...
ARG num [1:64] 0 0 0 0 0 0 0 0 1 0 ...
AU3 num [1:64] 1 0 0 1 1 0 0 1 1 0 ...
BC num [1:64] 0 1 0 0 0 0 0 0 0 0 ...
C num [1:4] 0 1 0 0
C3 num [1:64] 0 1 0 0 0 1 0 0 0 1 ...
CAI num [1:64] 0.00 0.00 -1.37 -2.98 -2.58 ...
CG num [1:4] 0 1 1 0
CG1 num [1:64] 0 0 0 0 0 0 0 0 0 0 ...
CG12 num [1:64] 0 0 0 0 0.5 0.5 0.5 0.5 0.5 0.5 ...
CG2 num [1:64] 0 0 0 0 1 1 1 1 1 1 ...
CG3 num [1:64] 0 1 1 0 0 1 1 0 0 1 ...
CGN num [1:64] 0 0 0 0 0 0 0 0 0 0 ...
F1 num [1:64] 1.026 0.239 1.026 0.239 -0.097 ...
G num [1:4] 0 0 1 0
G3 num [1:64] 0 0 1 0 0 0 1 0 0 0 ...
KD num [1:64] -3.9 -3.5 -3.9 -3.5 -0.7 -0.7 -0.7 -0.7 -4.5 -0.8 ...
Q num [1:64] 0 0 0 0 1 1 1 1 0 0 ...
QA3 num [1:64] 0 0 0 0 1 0 0 0 0 0 ...
QC3 num [1:64] 0 0 0 0 0 1 0 0 0 0 ...
U num [1:4] 0 0 0 1
U3 num [1:64] 0 0 0 1 0 0 0 1 0 0 ...

```

**Details**

It's better to work directly at the amino-acid level when computing linear forms on amino-acid frequencies so as to have a single coefficient vector. For instance EXP\$KD to compute the Kyte and Doolittle hydrophaty index from codon frequencies is valid only for the standard genetic code.

An alternative for `drop(freq %%% EXP$CG3)` is `sum( freq * EXP$CG3 )`, but this is less efficient in terms of CPU time. The advantage of the latter, however, is that thanks to recycling rules you can use either `sum( freq * EXP$A )` or `sum( freq * EXP$A3 )`. To do the same with the `%%%` operator you have to explicit the recycling rule as in `drop( freq %%% rep(EXP$A, 16))`.

**Source**

ANALSEQ EXPFILES for command EXP.

<http://pbil.univ-lyon1.fr/software/doclogi/docanals/manuel.html>

## References

citation("seqinr")

**A** content in A nucleotide

**A3** content in A nucleotide in third position of codon

**AGZ** Arg content (aga and agg codons)

**ARG** Arg content

**AU3** content in A and U nucleotides in third position of codon

**BC** Good choice (Bon choix). Gouy M., Gautier C. (1982) codon usage in bacteria : Correlation with gene expressivity. *Nucleic Acids Research*,**10(22)**:7055-7074.

**C** content in C nucleotides

**C3** content in A nucleotides in third position of codon

**CAI** Codon adaptation index for E. coli. Sharp, P.M., Li, W.-H. (1987) The codon adaptation index - a measure of directionam synonymous codon usage bias, and its potential applications. *Nucleic Acids Research*,**15**:1281-1295.

**CG** content in G + C nucleotides

**CG1** content in G + C nucleotides in first position of codon

**CG12** content in G + C nucleotides in first and second position of codon

**CG2** content in G + C nucleotides in second position of codon

**CG3** content in G + C nucleotides in third position of codon

**CGN** content in CGA + CGU + CGA + CGG

**F1** From Table 2 in Lobry, J.R., Gautier, C. (1994) Hydrophobicity, expressivity and aromaticity are the major trends of amino-acid usage in 999 *Escherichia coli* chromosome-encode genes. *Nucleic Acids Research*,**22**:3174-3180.

**G3** content in G nucleotides in third position of codon

**KD** Kyte, J., Doolittle, R.F. (1982) A simple method for displaying the hydropathic character of a protein. *J. Mol. Biol.*,**157** :105-132.

**Q** content in quartet

**QA3** content in quartet with the A nucleotide in third position

**QC3** content in quartet with the A nucleotide in third position

**U** content in U nucleotide

**U3** content in U nucleotides in third position of codon

## Examples

data(EXP)

---

extract.breakpoints	<i>Extraction of breakpoint positions on the rearranged nucleotide skews.</i>
---------------------	---

---

## Description

Extraction of breakpoint positions on the rearranged nucleotide skews.

## Usage

```
extract.breakpoints(rearr.ori,
  type = c("atfw", "atrev", "gcfw", "gcrev"),
  nbreaks, gridsize = 100, it.max = 500)
```

## Arguments

rearr.ori	A data frame obtained with the rearranged.oriloc function.
type	The type of skew for which to extract the breakpoints; must be a subset of c("atfw", "atrev", "gcfw", "gcrev").
nbreaks	The number of breakpoints to extract for each type of skew. Provide a vector of the same length as type.
gridsize	To make sure that the best breakpoints are found, and to avoid finding only a local extremum of the likelihood and residual sum of square functions, a grid search is performed. The search for breakpoints is repeated gridsize times, with different starting values for the breakpoints.
it.max	The maximum number of iterations to be performed when searching for the breakpoints. This argument corresponds to the it.max argument in segmented.

## Details

This method uses the segmented function in the segmented package to extract the breakpoints positions in the rearranged nucleotide skews obtained with the rearranged.oriloc function. To make sure that the best breakpoints are found, and to avoid finding only a local extremum of the likelihood and residual sum of square functions, a grid search is performed. The search for breakpoints is repeated gridsize times, with different starting values for the breakpoints.

## Value

This function returns a list, with as many elements as the type argument (for example \$gcfw will contain the results for the rearranged GC-skew, for forward-encoded genes). Each element of this list is also a list, containing the following information: in \$breaks the position of the breakpoints on the rearranged chromosome; in \$slopes.left the slopes of the segments on the left side of each breakpoint; in \$slopes.right the slopes of the segments on the right side of each breakpoint; in \$real.coord, the coordinates of the breakpoints on the real chromosome (before rearrangement).

## Author(s)

A. Necşulea

## References

`citation("segmented")`

Necşulea, A. and Lobry, J.R. (in prep) A novel method for assessing the effect of replication on DNA base composition asymmetry. *Molecular Biology and Evolution*, **24**:2169-2179.

## See Also

[oriloc](#), [draw.rearranged.oriloc](#), [rearranged.oriloc](#)

## Examples

```
### Example for Chlamydia trachomatis ###

### Rearrange the chromosome and compute the nucleotide skews ###

## Not run: r.ori <- rearranged.oriloc(seq.fasta = system.file("sequences/ct.fasta.gz", package = "seqinr"),
  g2.coord = system.file("sequences/ct.coord", package = "seqinr"))
## End(Not run)

### Extract the breakpoints for the rearranged nucleotide skews ###

## Not run: breaks <- extract.breakpoints(r.ori, type = c("gcfw", "gcrev"),
  nbreaks = c(2, 2), gridsize = 50, it.max = 100)
## End(Not run)

### Draw the rearranged nucleotide skews and ###
### place the position of the breakpoints on the graphics ###

## Not run: draw.rearranged.oriloc(r.ori, breaks.gcfw = breaks$gcfw$breaks,
  breaks.gcrev = breaks$gcrev$breaks)
## End(Not run)
```

---

extractseqs

*To extract the sequences information of a sequence or a list of sequence in different formats*

---

## Description

The function allows to extract large amount of data as whole genome sequences, using different output formats and types of extraction. This function is not yet available for windows in zlib mode.

## Usage

```
extractseqs(listname,socket = autosocket(), format="fasta",
operation="simple",feature="xx", bounds="xx", minbounds="xx",
verbose = FALSE, nzlines=1000, zlib = FALSE)
exseq(listname,socket = autosocket(),
format="fasta",operation="simple", feature="xx",
bounds="xx", minbounds="xx", verbose = FALSE, nzlines=1000, zlib = FALSE)
```

## Arguments

<code>listname</code>	the name of list on server (may be a virtual list)
<code>socket</code>	an object of class <code>sockconn</code> connecting to a remote ACNUC database (default is a socket to the last opened database).
<code>format</code>	the format of output.Can be <code>acnuc</code> , <code>fasta</code> , <code>flat</code> or <code>coordinates</code>
<code>operation</code>	the type of extraction. Can be <code>simple</code> , <code>translate</code> , <code>fragment</code> , <code>feature</code> or <code>region</code>
<code>feature</code>	-optional- the feature to be extracted (for operations "feature" or "region"): a feature table item (CDS, mRNA,...)
<code>bounds</code>	-optional- the bounds for extraction (for operations "fragment" or "region")
<code>minbounds</code>	-optional- the minimal bounds for extraction (for operations "fragment" or "region")
<code>verbose</code>	if TRUE, verbose mode is on
<code>nzlines</code>	number of line in zlib mode
<code>zlib</code>	logical. If TRUE sequences are download in zlib compress mode.

## Details

To extract a list of sequences (`lrank` argument) or a single sequence (`seqnum` argument) using different output formats and types of extraction. All formats except "coordinates" extract sequence data. Format "coordinates" extract coordinate data; `start > end` indicates the complementary strand.

**listname** sequence list name.

**socket** a socket of class `connection` and `sockconn` returned by `choosebank`. Default value (auto) means that the socket will be set to to the socket component of the `banknameSocket` variable.

**format** `acnuc`, `fasta`, `flat` or `coordinates`

**operation** `simple`, `translate`, `fragment`, `feature` or `region`

**feature** (for operations "feature" or "region") a feature table item (CDS, mRNA,...).

***simple*** each sequence or subsequence is extracted.

***translate*** meaningful only for protein-coding (sub)sequences that are extracted as protein sequences. Nothing is extracted for non-protein coding sequences.

***fragment*** Allows to extract any part of the sequence(s) in list. Such part is specified by the `bounds` and `minbounds` arguments according to the syntax suggested by these examples:

132,1600	to extract from nucl. 132 to nucl 1600 of the sequence. If applied to a subsequence, coordinates are in the parentheses
-10,10	to extract from 10 nucl. BEFORE the 5' end of the sequence to nucl. 10 of it. Useful only for subsequences, and not for the whole sequence
e-20,e+10	to extract from 20 nucl. BEFORE the 3' end of the sequence to 10 nucl. AFTER its 3' end. Useful only for subsequences, and not for the whole sequence
-20,e+5	to extract from 20 nucl. BEFORE the 5' end of the sequence to 5 nucl. AFTER its 3' end.

**bounds** (for operations "fragment" or "region") see syntax above.

**minbounds** same syntax as bounds. When the sequence data is too short for this quantity to be extracted, nothing is extracted. When the sequence data is between minbounds and bounds, extracted sequence data is extended by N's to the desired length.

### Value

Sequence data.

### Author(s)

S. Penel

### References

`citation("seqinr")`

### See Also

[choosebank](#), [query](#) [getlistrank](#)

### Examples

```
## Not run: # Need internet connection
choosebank("emblTP")
mylist <- query("mylist", "k=globin", virtual = TRUE)
mylist.fasta <- exseq("mylist", verbose = TRUE)
# 103 lines of FASTA
stopifnot(length(mylist.fasta) == 103)
closebank()

## End(Not run)
```

---

fasta

*Example of results obtained after a call to read.alignment*

---

### Description

This data set gives an example of a amino acids alignment obtained after a call to the function `read.alignment` on an alignment file in "fasta" format.

### Usage

fasta

### Format

A List of class alignment



## Source

<https://pbil.univ-lyon1.fr/help/formats.html/>

## References

Pearson W.R. and Lipman D.J. (1988) *Improved tools for biological sequence comparison..Proc Natl Acad Sci U S A.* 85(8):2444-8.

---

fastacc

*Fast Allele in Common Count*

---

## Description

The purpose of this function is to compute as fast as possible the number of allele in common between a target (typically the genetic profile observed at a crime scene, possibly a mixture with dropouts) and a database reference (typically genetic profile of individuals). Both are assumed to be pre-encoded at the bit level in a consistent way.

## Usage

```
fastacc(target, database)
```

## Arguments

target	the <a href="#">raw</a> encoding of the target, typically 40 octets for a core-CODIS profile in 2009
database	the <a href="#">raw</a> encoding of the database. If there are n entries in the database, then the database must n times longer than the target.

## Details

This function is an RFC state. Comments are welcome.

Genetic profiles are encoded at the bit level. One bit represents one allele. Count is based on a logical AND at bit level. Bit count is encoded at C level using the precomputed approach: one indirection with an auxiliary table of size 256 called `bits_in_char` which is pre-computed at R level and passed at C level.

## Value

A vector of [integer](#) giving for each entry in the database how many alleles are in common between the entry and the target.

## Warning

Experimental, first release scheduled for seqnr 2.0-6 by the end of 2009

**Author(s)**

J.R. Lobry

**References**

citation("seqinr")

**See Also**

FIXME

**Examples**

```

#
# NOTE:
#
# This example section is a proof-of-concept stuff. Most code should be
# embeded in documented functions to avoid verbosity. But at the RFC stage
# this is perhaps not a too bad idea to show how powerfull R is.
#

#
# Let's start from the 16 loci available in the AmpFLSTR kit:
#

path <- system.file("abif/AmpFLSTR_Bins_v1.txt", package = "seqinr")
resbin <- readBins(path)
codis <- resbin[["Identifiler_CODIS_v1"]]
names(codis)

#
# We count how many different alleles are present per locus:
#

na <- unlist(lapply(codis, function(x) length(x[[1]])))
na

#
# The number of octets required to encode a genetic for each locus is then:
#

ceiling(na/8)

#
# We need then a total of 40 octets to code these profiles:
#

sum(ceiling(na/8))

#
# Let's definene a function to encode a profile at a given locus, and vice versa :
#

```

```

prof2raw <- function(profile, alleles) {
  if (!is.ordered(alleles)) stop("ordered factor expected for alleles")
  if (!is.character(profile)) stop("vector of character expected for profile")
  noctets <- ceiling(length(alleles)/8)
  res.b <- rawToBits(raw(noctets))
  for (i in 1:length(profile)) {
    res.b[which(profile[i] == alleles)] <- as.raw(1)
  }
  return(packBits(res.b, type = "raw"))
}

raw2prof <- function(rawdata, alleles) {
  if (!is.ordered(alleles)) stop("ordered factor expected for alleles")
  if (!is.raw(rawdata)) stop("vector of raw expected for rawdata")
  res <- as.character(alleles)[as.logical(rawToBits(rawdata))]
  return(paste(res, collapse = ", "))
}

#
# Let now code all alleles present in codis as ordered factors:
#

allalleles <- lapply(codis, function(x) factor(x[, 1], levels = x[, 1], ordered = TRUE))

#
# Let's play with our encoding/decoding utilities with first locus:
#

allalleles[[1]] # <8 8 9 10 11 12 13 14 15 16 17 18 19 >19
res <- prof2raw(c("8", "9", "13", "14", ">19"), allalleles[[1]])
res # c6 20
rawToBits(res) # 00 01 01 00 00 00 01 01 00 00 00 00 01 00 00
raw2prof(res, allalleles[[1]]) # "8, 9, 13, 14, >19"

#
# Let define a profile with all possible alleles:
#

ladder <- unlist(lapply(allalleles, function(x) prof2raw(as.character(x),x)))
names(ladder) <- NULL
stopifnot(identical(as.integer(ladder),
  c(255L, 63L, 255L, 255L, 255L, 63L, 255L, 63L, 255L, 31L, 255L,
    63L, 255L, 255L, 7L, 255L, 3L, 255L, 63L, 255L, 255L, 255L, 255L,
    15L, 255L, 127L, 255L, 3L, 255L, 255L, 255L, 255L, 3L, 3L, 255L,
    15L, 255L, 255L, 255L, 7L))) # simple sanity check

#
# Let's make a simulated database. Here we use a random sampling
# with a uniform distribution between all possible profile possible
# at a given locus. A more realist sampling for an individual database
# would be to sample only two alleles at each locus according to
# observed frequencies in populations.

```

```

#

n <- 10^5 # the number of records in the database
DB <- sapply(ladder, function(x) as.raw(sample(0:as.integer(x), size = n, replace = TRUE)))

#
# Now we make sure that the target is in the database:
#

target <- DB[666, ]
DB <- as.vector(t(DB)) # put DB as a flat database (is it useful?)

#
# Now we compute the number of alleles in common between the
# target and all the entries in the DB:
#

system.time(res <- fastacc(target,DB)) # Fast, isn't it ?
stopifnot(which.max(res) == 666) # sanity check

#
# Don't run : too tedious for routine check. We check here that complexity is
# linear in time up to a 10 10^6 database size (roughly the size of individual
# profiles at the EU level)
#

## Not run:
maxn <- 10^7
DB <- sapply(ladder, function(x) as.raw(sample(0:as.integer(x),
  size = maxn, replace = T)))
target <- DB[666, ]
DB <- as.vector(t(DB))

np <- 10
nseq <- seq(from = 10^5, to = maxn, length = np)
res <- numeric(np)
i <- 1
for (n in nseq) {
  print(i)
  res[i] <- system.time(tmp <- fastacc(target, DB[1:n]))[1]
  stopifnot(which.max(tmp) == 666)
  i <- i + 1
}
dbse <- data.frame(list(nseq = nseq, res = res))

x <- dbse$nseq
y <- dbse$res
plot(x, y, type = "b", xlab = "Number of entries in DB", ylab = "One query time [s]",
  las = 1, xlim = c(0, maxn), ylim = c(0, max(y)), main = "Data base size effect on query time")
lm1 <- lm(y ~ x - 1)
abline(lm1, col = "red")
legend("topleft", inset = 0.01, legend = paste("y =", formatC(lm1$coef[1],
  digits = 3), "x"), col = "red", lty = 1)

```

```
#
# On my laptop the slope is 2.51e-08, that is a 1/4 of second to scan a database
# with 10 10^6 entries.
#

## End(Not run)

## end
```

---

G+C Content

*Calculates the fractional G+C content of nucleic acid sequences.*

---

### Description

Calculates the fraction of G+C bases of the input nucleic acid sequence(s). It reads in nucleic acid sequences, sums the number of 'g' and 'c' bases and writes out the result as the fraction (in the interval 0.0 to 1.0) to the total number of 'a', 'c', 'g' and 't' bases. Global G+C content GC, G+C in the first position of the codon bases GC1, G+C in the second position of the codon bases GC2, and G+C in the third position of the codon bases GC3 can be computed. All functions can take ambiguous bases into account when requested.

### Usage

```
GC(seq, forceToLower = TRUE, exact = FALSE, NA.GC = NA, oldGC = FALSE)
GC1(seq, frame = 0, ...)
GC2(seq, frame = 0, ...)
GC3(seq, frame = 0, ...)
GCpos(seq, pos, frame = 0, ...)
```

### Arguments

seq	a nucleic acid sequence as a vector of single characters
frame	for coding sequences, an integer (0, 1, 2) giving the frame
forceToLower	logical. if TRUE force sequence characters in lower-case. Turn this to FALSE to save time if your sequence is already in lower-case (cpu time is approximately divided by 3 when turned off)
exact	logical: if TRUE ambiguous bases are taken into account when computing the G+C content (see details). Turn this to FALSE to save time if your you can neglect ambiguous bases in your sequence (cpu time is approximately divided by 3 when turned off)
NA.GC	what should be returned when the GC is impossible to compute from data, for instance with NNNNNNN. This behaviour could be different when argument exact is TRUE, for instance the G+C content of WWSS is NA by default, but is 0.5 when exact is set to TRUE
...	arguments passed to the function GC

<code>pos</code>	for coding sequences, the codon position (1, 2, 3) that should be taken into account to compute the G+C content
<code>oldGC</code>	logical defaulting to FALSE: should the GC content computed as in <code>seqinR &lt;= 1.0-6</code> , that is as the sum of 'g' and 'c' bases divided by the length of the sequence. As from <code>seqinR &gt;= 1.1-3</code> , this argument is deprecated and a warning is issued.

## Details

When `exact` is set to TRUE the G+C content is estimated with ambiguous bases taken into account. Note that this is time expensive. A first pass is made on non-ambiguous bases to estimate the probabilities of the four bases in the sequence. They are then used to weight the contributions of ambiguous bases to the G+C content. Let `nx` be the total number of base 'x' in the sequence. For instance suppose that there are `nb` bases 'b'. 'b' stands for "not a", that is for 'c', 'g' or 't'. The contribution of 'b' bases to the GC base count will be:

$$nb * (nc + ng) / (nc + ng + nt)$$

The contribution of 'b' bases to the AT base count will be:

$$nb * nt / (nc + ng + nt)$$

All ambiguous bases contributions to the AT and GC counts are weighted in similar way and then the G+C content is computed as `ngc / (nat + ngc)`.

## Value

`GC` returns the fraction of G+C (in [0,1]) as a numeric vector of length one. `GCpos` returns GC at position `pos`. `GC1`, `GC2`, `GC3` are wrappers for `GCpos` with the argument `pos` set to 1, 2, and 3, respectively. NA is returned when `seq` is NA. NA.GC defaulting to NA is returned when the G+C content can not be computed from data.

## Author(s)

D. Charif, L. Palmeira, J.R. Lobry

## References

`citation("seqinR")`.

The program `codonW` used here for comparison is available at <http://codonw.sourceforge.net/>.

## See Also

You can use [s2c](#) to convert a string into a vector of single character and [tolower](#) to convert upper-case characters into lower-case characters. Do not confuse with [gc](#) for garbage collection.

**Examples**

```

mysequence <- s2c("agtctggggggccccccttttaagtagatagatagctagtcgta")
GC(mysequence) # 0.4761905
GC1(mysequence) # 0.6428571
GC2(mysequence) # 0.3571429
GC3(mysequence) # 0.4285714
#
# With upper-case characters:
#
myUCsequence <- s2c("GGGGGGGGGA")
GC(myUCsequence) # 0.9
#
# With ambiguous bases:
#
GC(s2c("acgt")) # 0.5
GC(s2c("acgtssss")) # 0.5
GC(s2c("acgtssss"), exact = TRUE) # 0.75
#
# Missing data:
#
stopifnot(is.na(GC(s2c("NNNN"))))
stopifnot(is.na(GC(s2c("NNNN"), exact = TRUE)))
stopifnot(is.na(GC(s2c("WWSS"))))
stopifnot(GC(s2c("WWSS"), exact = TRUE) == 0.5)
#
# Coding sequences tests:
#
cdstest <- s2c("ATGATG")
stopifnot(GC3(cdstest) == 1)
stopifnot(GC2(cdstest) == 0)
stopifnot(GC1(cdstest) == 0)
#
# How to reproduce the results obtained with the C program codonW
# version 1.4.4 written by John Peden. We use here the "input.dat"
# test file from codonW (there are no ambiguous base in these
# sequences).
#
inputdatfile <- system.file("sequences/input.dat", package = "seqinr")
input <- read.fasta(file = inputdatfile) # read the FASTA file
inputoutfile <- system.file("sequences/input.out", package = "seqinr")
input.res <- read.table(inputoutfile, header = TRUE) # read codonW result file
#
# remove stop codon before computing G+C content (as in codonW)
#
GC.codonW <- function(dnaseq, ...){
  GC(dnaseq[seq_len(length(dnaseq) - 3)], ...)
}
input.gc <- sapply(input, GC.codonW, forceToLower = FALSE)
max(abs(input.gc - input.res$GC)) # 0.0004946237

plot(x = input.gc, y = input.res$GC, las = 1,
     xlab = "Results with GC()", ylab = "Results from codonW",

```

```

main = "Comparison of G+C content results")
abline(c(0, 1), col = "red")
legend("topleft", inset = 0.01, legend = "y = x", lty = 1, col = "red")
## Not run:
# Too long for routine check
# This is a benchmark to compare the effect of various parameter
# setting on computation time
n <- 10
from <- 10^4
to <- 10^5
size <- seq(from = from, to = to, length = n)
res <- data.frame(matrix(NA, nrow = n, ncol = 5))
colnames(res) <- c("size", "FF", "FT", "TF", "TT")
res[, "size"] <- size

for(i in seq_len(n)){
  myseq <- sample(x = s2c("acgtws"), size = size[i], replace = TRUE)
  res[i, "FF"] <- system.time(GC(myseq, forceToLower = FALSE, exact = FALSE))[3]
  res[i, "FT"] <- system.time(GC(myseq, forceToLower = FALSE, exact = TRUE))[3]
  res[i, "TF"] <- system.time(GC(myseq, forceToLower = TRUE, exact = FALSE))[3]
  res[i, "TT"] <- system.time(GC(myseq, forceToLower = TRUE, exact = TRUE))[3]
}

par(oma = c(0,0,2.5,0), mar = c(4,5,0,2) + 0.1, mfrow = c(2, 1))
plot(res$size, res$TT, las = 1,
xlab = "Sequence size [bp]",
ylim = c(0, max(res$TT)), xlim = c(0, max(res$size)), ylab = "")
title(ylab = "Observed time [s]", line = 4)
abline(lm(res$TT~res$size))
points(res$size, res$FT, col = "red")
abline(lm(res$FT~res$size), col = "red", lty = 3)
points(res$size, res$TF, pch = 2)
abline(lm(res$TF~res$size))
points(res$size, res$FF, pch = 2, col = "red")
abline(lm(res$FF~res$size), lty = 3, col = "red")

legend("topleft", inset = 0.01,
  legend = c("forceToLower = TRUE", "forceToLower = FALSE"),
  col = c("black", "red"), lty = c(1,3))
legend("bottomright", inset = 0.01, legend = c("exact = TRUE", "exact = FALSE"),
pch = c(1,2))

mincpu <- lm(res$FF~res$size)$coef[2]

barplot(
c(lm(res$FF~res$size)$coef[2]/mincpu,
  lm(res$TF~res$size)$coef[2]/mincpu,
  lm(res$FT~res$size)$coef[2]/mincpu,
  lm(res$TT~res$size)$coef[2]/mincpu),
horiz = TRUE, xlab = "Increase of CPU time",
col = c("red", "black", "red", "black"),
names.arg = c("(F,F)", "(T,F)", "(F,T)", "(T,T)"), las = 1)

```



```
title(ylab = "forceToLower,exact", line = 4)

mtext("CPU time as function of options", outer = TRUE, line = 1, cex = 1.5)

## End(Not run)
```

---

**gb2fasta***Conversion of GenBank file into fasta file*

---

**Description**

Converts a single entry in GenBank format into a fasta file.

**Usage**

```
gb2fasta(source.file, destination.file)
```

**Arguments**

source.file	GenBank file
destination.file	Fasta file

**Details**

Multiple entries in GenBank file are not supported.

**Value**

none

**Author(s)**

J.R. Lobry

**References**

```
citation("seqinr")
```

**See Also**

[oriloc](#)

## Examples

```
myGenBankFile <- system.file("sequences/ct.gbk.gz", package = "seqinr")
myFastaFileName <- "Acinetobacter_ADPI_uid61597.fasta"
gb2fasta(myGenBankFile, myFastaFileName)
readLines(myFastaFileName)[1:5]
#
# Should be :
#
# [1] ">CHLTCG 1042519 bp"
# [2] "gcggccgcccgggaaattgctaaaagatgggagcaaagagttagagatctacaagataaa"
# [3] "ggtgctgcacgaaaattattaaatgatcctttaggccgacgaacacctaattatcagagc"
# [4] "aaaaatccaggtgagtatactgtagggaattccatgtttacgatggctctcaggtagcg"
# [5] "aatctccagaacgtcgacactggtttttgctggacatgagcaatctctcagacgttgta"
#
```

---

gbk2g2

---

*Conversion of a GenBank format file into a glimmer-like one*


---

## Description

This function reads a file in GenBank format and converts the features corresponding to CDS (Coding Sequences) into a format similar to glimmer program output.

## Usage

```
gbk2g2(gbkfile = "ftp://pbil.univ-lyon1.fr/pub/seqinr/data/ct.gbk",
g2.coord = "g2.coord")
```

## Arguments

gbkfile	The name of the GenBank file
g2.coord	The name of the output file in glimmer-like format

## Details

Partial CDS (either 5' or 3') and join in features are discarded.

## Value

The input file is returned invisibly.

## Author(s)

J.R. Lobry

## References

citation("seqinr")

**See Also**

[oriloc](#) which uses glimmer-like files, [gbk2g2.euk](#) for eukaryotic sequences with introns.

**Examples**

```
## Not run: # need internet connection
suppressWarnings(gbk2g2(g2.coord = "gbk2g2.test"))
res <- read.table("gbk2g2.test")
head(res)
stopifnot(nrow(res) == 892)

## End(Not run)
```

---

gbk2g2.euk

---

*Conversion of a GenBank format file into a glimmer-like one. Eukaryotic version.*


---

**Description**

This function reads a file in GenBank format and converts the features corresponding to CDS (Coding Sequences) into a format similar to glimmer program output. This function is specifically made for eukaryotic sequences, i.e. with introns.

**Usage**

```
gbk2g2.euk(gbkfile = system.file("sequences/ame1.gbk", package = "seqinr"),
g2.coord = "g2.coord")
```

**Arguments**

gbkfile	The name of the GenBank file
g2.coord	The name of the output file

**Details**

This function returns the coordinates of the exons annotated in the GenBank format file.

**Value**

A data frame with three columns will be written to the g2.coord file. The first column corresponds to the name of the gene, given in the GenBank file through the /gene feature. The second and third column contain the start and the stop position of the exon.

**Author(s)**

J.R. Lobry, A. Necşulea

**References**

```
citation("seqinr")
```

**See Also**

```
oriloc, gbk2g2
```

**Examples**

```
## Not run: gbk2g2.euk()
```

---

gcO2

*GC content and aerobiosis in bacteria*


---

**Description**

This data set was used in Naya *et al.* (2002) to study the relationship between the genomic G+C content of bacteria and whether they are (strictly) aerobes or anaerobes.

**Format**

gcO2 is a data frame.

**Source**

Naya, H., Romero, H., Zavala, A., Alvarez, B. and Musto, H. (2002) Aerobiosis increases the Genomic Guanine Plus Cytosine Content (GC

Data imported into seqinr by J.R. Lobry on 09-OCT-2016. Original source location given in the article was <http://oeg.fcien.edu.uy/GCprok/> but is no more active. Data were copied at <http://pbil.univ-lyon1.fr/R/donnees/gcO2.txt> (cf. section 2.1 in Lobry, J.R (2004) Life history traits and genome structure: aerobiosis and G+C content in bacteria. *Lecture Notes in Computer Sciences*, **3039**:679-686). Import was from this last resource. There are 130 aerobic genera in this data set while fig. 1 in Naya *et al.* (2002) gives 126. There is no way to track down the reason for this difference because the original data set was lost (Héctor Musto pers. comm.). The number of anaerobic genera (n = 69) is consistent between the present data set and fig. 1 in Naya *et al.* (2002).

**References**

```
citation("seqinr")
```

**Examples**

```
data(gcO2)
```

gcT

*GC content and temperature in bacteria***Description**

This data set was used in Galtier and Lobry (1997) to study the relationship between the optimal growth temperature of bacteria and their G+C content at the genomic level and locally where selection is active to maintain secondary structures in the stems of RNAs.

**Format**

gcT is a list containing the 9 following components:

**species** is a data frame containing the optimal growth temperature and genomic G+C content for 772 bacterial species. Detailed explanations for this table and the following are available in the README component.

**genus** is a data frame containing the optimal growth temperature and genomic G+C content for 224 bacterial genus.

**details** is a data frame with more information, see README.

**gc16S** is a data frame containing the optimal growth temperature and stems G+C content for 16S RNA from 165 bacterial genus.

**gctRNA** is a data frame containing the optimal growth temperature and stems G+C content for tRNA from 51 bacterial genus.

**gc23S** is a data frame containing the optimal growth temperature and stems G+C content for 23S RNA from 38 bacterial genus.

**gc5S** is a data frame containing the optimal growth temperature and stems G+C content for 5S RNA from 71 bacterial genus.

**README** is the original README file from <ftp://biom3.univ-lyon1.fr/pub/datasets/JME97/> last updated 13-MAY-2002.

**importgcT** is the R script used to import data.

**Source**

Galtier, N. & Lobry, J.R. (1997). Relationships between genomic G+C content, RNA secondary structures, and optimal growth temperature in prokaryotes. *Journal of Molecular Evolution* **44**:632-636.

Data imported into seqinr with the R script given in the last component of the dataset by J.R. Lobry on 09-OCT-2016.

**References**

```
citation("seqinr")
```

**Examples**

```
data(gcT)
```

---

get.db.growth

*Get the exponential growth of nucleic acid database content*


---

### Description

Connects to the embl database to read the last release note about the number of nucleotides in the DDBJ/EMBL/Genbank database content. A log-linear fit is represented by dia.bd.growth() with an estimate of the doubling time in months.

### Usage

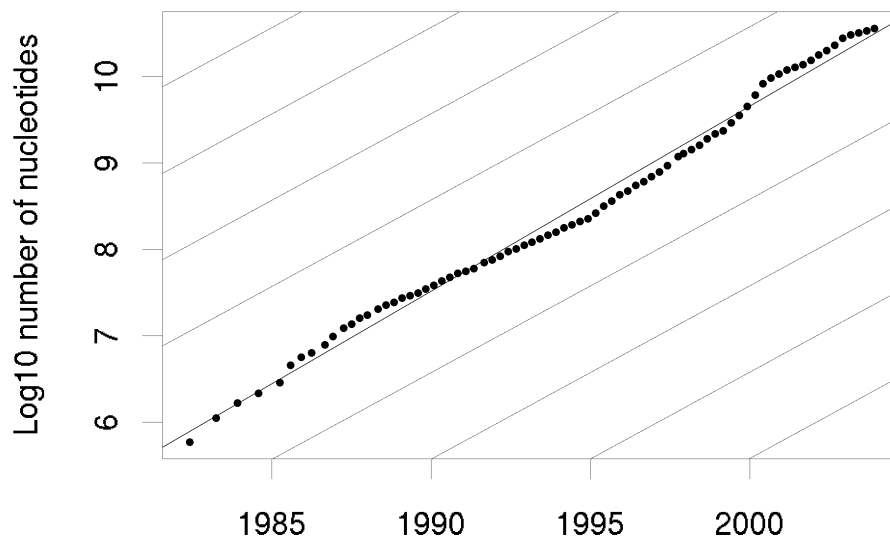
```
get.db.growth(
  where = "ftp://ftp.ebi.ac.uk/pub/databases/embl/doc/relnotes.txt")
dia.db.growth( get.db.growth.out = get.db.growth(), Moore = TRUE, ... )
```

### Arguments

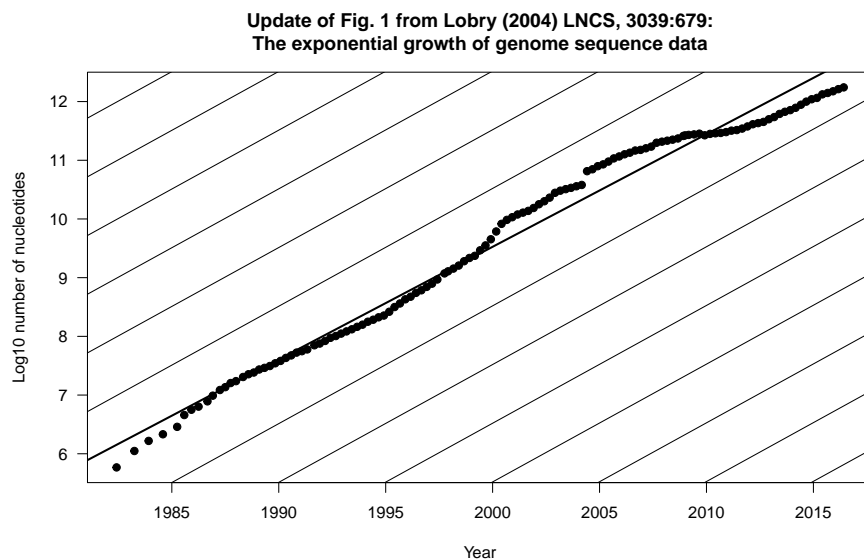
where	the file containig the database growth table.
get.db.growth.out	the output from get.db.growth()
Moore	logical, if TRUE add lines corresponding to an exponential growth rate with a doubling time of 18 months, that is Moore's law.
...	further arguments to plot

### Details

This is a screenshot from fig. 1 in Lobry (2004):



At that time the doubling time was 16.9 months. This is an update in 2016 from release 3.1-5 of the seqinr tutorial [http://seqinr.r-forge.r-project.org/seqinr\\_3\\_1-5.pdf](http://seqinr.r-forge.r-project.org/seqinr_3_1-5.pdf):



The doubling time was 18.8 months in this update. The fit to Moore's law is still striking over such a long period.

### Value

A dataframe with the statistics from the embl site.

### Author(s)

J.R. Lobry

### References

[http://www.ebi.ac.uk/embl/Documentation/Release\\_notes/current/relnotes.txt](http://www.ebi.ac.uk/embl/Documentation/Release_notes/current/relnotes.txt)

Lobry, J.R. (2004) Life History Traits and Genome Structure: Aerobiosis and G+C Content in Bacteria. *Lectures Notes in Computer Sciences*, **3039**:679-686.

`citation("seqinr")`

### Examples

```
## Not run:
### Need internet connection
data <- get.db.growth()
dia.db.growth(data)

## End(Not run)
```

---

`get.ncbi`*Bacterial complete genome data from ncbi ftp site*

---

**Description**

Try to connect to ncbi ftp site to get a list of complete bacterial genomes.

**Usage**

```
get.ncbi(repository = "ftp://ftp.ncbi.nih.gov/genomes/Bacteria/")
```

**Arguments**

<code>repository</code>	Where to look for data. The default value is the location of the complete bacterial genome sequences at ncbi ftp repository.
-------------------------	--

**Value**

Returns a data frame which contains the following columns:

<code>species</code>	The species name as given by the corresponding folder name in the repository (e.g. <i>Yersinia\_pestis\_KIM</i> ).
<code>accession</code>	The accession number as given by the common prefix of file names in the repository (e.g. <i>NC\_004088</i> ).
<code>size.bp</code>	The size of the sequence in bp (e.g. <i>4600755</i> ).
<code>type</code>	A factor with two levels (plasmid or chromosome) tentatively deduced from the description of the sequence.

**WARNING**

This function is highly dependant on ncbi ftp site conventions for which we have no control. The ftp connection apparently does not work when there is a proxy, this problem is circumvented here in a rather crude way.

**Author(s)**

J.R. Lobry

**References**

```
citation("seqinr")
```

**Examples**

```
## Not run: bacteria <- get.ncbi()
## Not run: summary(bacteria)
```



---

`getAnnot`*Generic Function to get sequence annotations*

---

### Description

Annotations are taken from the Annot attribute for sequences imported from a FASTA file and retrieved from an ACNUC server for objects of the SeqAcnucWeb class.

### Usage

```
getAnnot(object, ...)  
## S3 method for class 'SeqAcnucWeb'  
getAnnot(object, ..., nbl = 100, socket = autosocket())
```

### Arguments

<code>object</code>	an object of the class SeqAcnucWeb or SeqFastadna, or SeqFastaAA or a list of these objects
<code>nbl</code>	the maximum number of line of annotation to read. Reading of lines stops when nbl lines have been transmitted or at the last annotation line of the sequence (SQ or ORIGIN line).
<code>socket</code>	an object of class sockconn connecting to a remote ACNUC database (default is a socket to the last opened database).
<code>...</code>	further arguments passed to or from other methods

### Value

getAnnot returns a vector of string of characters containing the annotations for the sequences.

### Author(s)

D. Charif, J.R. Lobry, L. Palmeira

### References

`citation("seqinr")`

### See Also

[query](#), [SeqAcnucWeb](#), [c2s](#), [translate](#) and [prepgetannots](#) to select the annotation lines.

## Examples

```
#
# List all available methods for getAnnot generic function:
#
  methods(getAnnot)
#
# SeqAcnucWeb class example:
#
  ## Not run:
  # Need internet connection
  choosebank("emblTP")
  fc<-query("fc", "sp=felis catus et t=cds et O=mitochondrion et Y>2001 et no k=partial")
  # get the first 5 lines annotating the first sequence:
  annots <- getAnnot(fc$req[[1]], nbl = 5)
  cat(annots, sep = "\n")
  # or use the list method to get them all at once:
  annots <- getAnnot(fc$req, nbl = 5)
  cat(annots, sep = "\n")
  closebank()

## End(Not run)
#
# SeqFastaAA class example:
#
  aafile <- system.file("sequences/seqAA.fasta", package = "seqinr")
  sfaa <- read.fasta(aafile, seqtype = "AA")
  getAnnot(sfaa[[1]])
#
# SeqFastadna class example:
#
  dnafile <- system.file("sequences/ma1M.fasta", package = "seqinr")
  sfdna <- read.fasta(file = dnafile)
  getAnnot(sfdna[[1]])
#
# Example with a FASTA file with multiple entries:
#
  ff <- system.file("sequences/someORF.fsa", package = "seqinr")
  fs <- read.fasta(ff)
  getAnnot(fs) # the list method is used here to get them all at once
#
# Default getAnnot method example. An error is produced because
# there are no annotations by default:
#
  result <- try(getAnnot(letters))
  stopifnot(!inherits("result", "try-error"))
```

## Description

getFrag is used to extract the sequence fragment starting at the begin position and ending at the end position.

## Usage

```
getFrag(object, begin, end, ...)
## S3 method for class 'SeqAcnucWeb'
getFrag(object, begin, end, ..., socket = autosocket(), name = getName(object))
## S3 method for class 'SeqFastadna'
getFrag(object, begin, end, ..., name = getName(object))
## S3 method for class 'SeqFastaAA'
getFrag(object, begin, end, ..., name = getName(object))
## S3 method for class 'SeqFrag'
getFrag(object, begin, end, ..., name = getName(object))
```

## Arguments

object	an object of the class <a href="#">SeqAcnucWeb</a> or <a href="#">SeqFastadna</a> , or <a href="#">SeqFastaAA</a> or <a href="#">SeqFrag</a> or a list of these objects
begin	First position of the fragment to extract. This position is included. Numerotation starts at 1.
end	Last position of the fragment to extract. This position is included.
socket	an object of class sockconn connecting to a remote ACNUC database (default is a socket to the last opened database by <a href="#">choosebank</a> ).
name	the sequence name
...	further arguments passed to or from other methods

## Value

getFrag returns an object of class [SeqFrag](#).

## Author(s)

D. Charif, J.R. Lobry, L. Palmeira

## References

`citation("seqinr")`

## See Also

[SeqAcnucWeb](#), [SeqFastadna](#), [SeqFastaAA](#), [SeqFrag](#)

**Examples**

```
#
# List all available methods for getFrag generic function:
#
#   methods(getFrag)
#
# Example with a DNA sequence from a FASTA file:
#
dnafile <- system.file("sequences/malM.fasta", package = "seqinr")
sfdna <- read.fasta(file = dnafile)
myfrag <- getFrag(sfdna[[1]], begin = 1, end = 10)
stopifnot(getSequence(myfrag, as.string = TRUE) == "atgaaaatga")
```

---

getKeyword

*Generic function to get keywords associated to sequences*


---

**Description**

Get keywords from an ACNUC server.

**Usage**

```
getKeyword(object, ...)
## S3 method for class 'SeqAcnucWeb'
getKeyword(object, ..., socket = autosocket())
```

**Arguments**

object	an object of the class <a href="#">SeqAcnucWeb</a> , or a list of them, or the object resulting from <a href="#">query</a>
socket	an object of class sockconn connecting to a remote ACNUC database (default is a socket to the last opened database by <a href="#">choosebank</a> ).
...	further arguments passed to or from other methods

**Value**

getKeyword returns a vector of strings containing the keyword(s) associated to a sequence.

**Author(s)**

D. Charif, J.R. Lobry, L. Palmeira

**References**

`citation("seqinr")`

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

```
#
# List all available methods for getKeyword generic function:
#
#   methods(getKeyword)
#
# Example of keyword extraction from an ACNUC server:
#
## Not run:
# Need internet connection
choosebank("emblTP")
fc<-query("fc", "sp=felis catus et t=cds et o=mitochondrion")
getKeyword(fc$req[[1]])
# Should be:
# [1] "DIVISION ORG" "RELEASE 62" "CYTOCHROME B" "SOURCE" "CDS"
closebank()

## End(Not run)
```

getLength

*Generic function to get the length of sequences***Description**

getLength returns the total number of bases or amino-acids in a sequence.

**Usage**

```
getLength(object, ...)
```

**Arguments**

object	an object of the class <a href="#">SeqAcnucWeb</a> or <a href="#">SeqFastadna</a> , or <a href="#">SeqFastaAA</a> or <a href="#">SeqFrag</a> or a list of these objects
...	further arguments passed to or from other methods

**Value**

getLength returns a numeric vector giving the length of the sequences.

**Author(s)**

D. Charif, J.R. Lobry, L. Palmeira

## References

`citation("seqinr")`

## See Also

[SeqAcnucWeb](#), [SeqFastadna](#), [SeqFastaAA](#), [SeqFrag](#)

## Examples

```
#
# List all available methods for getLength generic function:
#
  methods(getLength)
#
# Example with seven DNA sequences from a FASTA file:
#
ff <- system.file("sequences/someORF.fsa", package = "seqinr")
fs <- read.fasta(file = ff)
stopifnot(all(getLength(fs) == c(5573, 5825, 2987, 3929, 2648, 2597, 2780)))
#
# Example with 49 sequences from an ACNUC server:
#
## Not run:
# Need internet connection
choosebank("emblTP")
fc <- query("fc", "sp=felis catus et t=cds et o=mitochondrion")
getLength(fc)
closebank()

## End(Not run)
```

---

getlistrank

*To get the rank of a list from its name*

---

## Description

This is a low level function to get the rank of a list on server from its name.

## Usage

```
getlistrank(listname, socket = autosocket(), verbose = FALSE)
glr(listname, socket = autosocket(), verbose = FALSE)
```

## Arguments

listname	the name of list on server
socket	an object of class sockconn connecting to a remote ACNUC database (default is a socket to the last opened database).
verbose	if TRUE, verbose mode is on

**Details**

This low level function is usually not used directly by the user.

**Value**

The rank of list named listname on server, or 0 if no list with this name exists.

**Author(s)**

J.R. Lobry

**References**

`citation("seqinr")`

**See Also**

[choosebank](#), [query](#)

**Examples**

```
## Not run:
# Need internet connection
choosebank("emblTP")
MyListName <- query("MyListName", "sp=Borrelia burgdorferi", virtual = TRUE)
(result <- getlistrank("MyListName"))
stopifnot(result == 2)
closebank()

## End(Not run)
```

---

getliststate

*Asks for information about an ACNUC list of specified rank*

---

**Description**

Reply gives the type of list, its name, the number of elements it contains, and, for sequence lists, says whether the list contains only parent seqs (locus=T).

**Usage**

```
getliststate(lrank, socket = autosocket())
gls(lrank, socket = autosocket())
gln(lrank, ...)
```

**Arguments**

lrank	the name of the ACNUC list to modify
socket	an object of class sockconn connecting to a remote ACNUC database (default is a socket to the last opened database).
...	arguments passed to getliststate

**Value**

NA in case of problem and an warning is issued. When there is no problem a list with the following 4 components:

type	string. Type of ACNUC list (SQ, KW, SP)
name	string. ACNUC list name
count	numeric. Number of elements in ACNUC list
locus	logical. For ACNUC sequence lists TRUE means that the list contains only parent sequences. NA otherwise.

gln is a shortcut for `getliststate(lrank, ...)$name`

**Author(s)**

J.R. Lobry

**References**

<http://doua.prabi.fr/databases/acnuc.html>  
 citation("seqinr")

**See Also**

[choosebank](#), [query](#), [alr](#), [glr](#)

**Examples**

```
## Not run:
### Need internet connection
choosebank("emblTP")
mylist <- query("mylist", "sp=felis catus et t=cds", virtual=TRUE)
getliststate(glr("mylist")) # SQ, MYLIST, 603, FALSE
gln(glr("mylist")) # MYLIST (upper case letters on server)
closebank()

## End(Not run)
```



---

getLocation	<i>Generic function to get the location of subsequences on the parent sequence</i>
-------------	--

---

## Description

This function works only with subsequences from an ACNUC server.

## Usage

```
getLocation(object, ...)  
## S3 method for class 'SeqAcnucWeb'  
getLocation(object, ..., socket = autosocket())
```

## Arguments

object	an object of the class <a href="#">SeqAcnucWeb</a> , or a list of them, or an object created by <a href="#">query</a>
socket	an object of class sockconn connecting to a remote ACNUC database (default is a socket to the last opened database by <a href="#">choosebank</a> ).
...	further arguments passed to or from other methods

## Value

A list giving the positions of the sequence on the parent sequence. If the sequence is a subsequence (e.g. coding sequence), the function returns the position of each exon on the parent sequence. NA is returned for parent sequences and a warning is issued.

## Author(s)

D. Charif, J.R. Lobry, L. Palmeira

## References

`citation("seqinr")`

## See Also

[SeqAcnucWeb](#)

## Examples

```
#  
# List all available methods for getLocation generic function:  
#  
  methods(getLocation)  
#  
# Example with a subsequence from an ACNUC server:
```

```
#
## Not run:
# Need internet connection
choosebank("emblTP")
fc <- query("fc", "sp=felis catus et t=cds et o=mitochondrion")
getLocation(fc$req[[5]])
closebank()

## End(Not run)
```

---

getName

*Generic function to get the names of sequences*


---

## Description

GetName returns the sequence names.

## Usage

```
getName(object, ...)
```

## Arguments

object	an object of the class <a href="#">SeqAcnucWeb</a> or <a href="#">SeqFastadna</a> , or <a href="#">SeqFastaAA</a> or <a href="#">SeqFrag</a> or a list of these objects
...	further arguments passed to or from other methods

## Value

an object of class character containing the names of the sequences

## Author(s)

D. Charif, J.R. Lobry, L. Palmeira

## References

```
citation("seqinr")
```

## See Also

[SeqAcnucWeb](#), [SeqFastadna](#), [SeqFastaAA](#), [SeqFrag](#)

## Examples

```
#
# List all available methods for getName generic function:
#
#   methods(getName)
#
# Example with seven DNA sequences from a FASTA file:
#
ff <- system.file("sequences/someORF.fsa", package = "seqinr")
fs <- read.fasta(file = ff)
stopifnot(all(getName(fs) == c("YAL001C", "YAL002W", "YAL003W",
  "YAL005C", "YAL007C", "YAL008W", "YAL009W")))
#
# Example with 49 sequences from an ACNUC server:
#
## Not run:
# Need internet connection
choosebank("emblTP")
fc <- query("fc", "sp=felis catus et t=cds et o=mitochondrion")
getName(fc)
closebank()

## End(Not run)
```

---

getSequence

*Generic function to get sequence data*


---

## Description

getSequence returns the sequence either as vector of single characters or as a single string of multiple characters.

## Usage

```
getSequence(object, as.string = FALSE, ...)
## S3 method for class 'SeqAcnucWeb'
getSequence(object, as.string = FALSE, ..., socket = autosocket())
```

## Arguments

object	an object of the class <a href="#">SeqAcnucWeb</a> or <a href="#">SeqFastadna</a> , or <a href="#">SeqFastaAA</a> or <a href="#">SeqFrag</a> or a list of these objects, or an object of class qaw created by <a href="#">query</a>
as.string	if TRUE sequences are returned as strings of multiple characters instead of a vector of single characters
socket	an object of class sockconn connecting to a remote ACNUC database (default is a socket to the last opened database).
...	further arguments passed to or from other methods

**Value**

For a single sequence an object of class character containing the characters of the sequence, either of length 1 when `as.string` is `TRUE`, or of the length of the sequence when `as.string` is `FALSE`. For many sequences, a list of these.

**Author(s)**

D. Charif, J.R. Lobry, L. Palmeira

**References**

`citation("seqinr")`

**See Also**

[SeqAcnucWeb](#), [SeqFastadna](#), [SeqFastaAA](#), [SeqFrag](#)

**Examples**

```
#
# List all available methods for getSequence generic function:
#
  methods(getSequence)
#
# SeqAcnucWeb class example:
#
  ## Not run: # Need internet connection
  choosebank("emblTP")
  fc <- query("fc", "sp=felis catus et t=cds et o=mitochondrion")
  getSequence(fc$req[[1]])
  getSequence(fc$req[[1]], as.string = TRUE)
  closebank()

## End(Not run)
#
# SeqFastaAA class example:
#
  aafile <- system.file("sequences/seqAA.fasta", package = "seqinr")
  sfaa <- read.fasta(aafile, seqtype = "AA")
  getSequence(sfaa[[1]])
  getSequence(sfaa[[1]], as.string = TRUE)
#
# SeqFastadna class example:
#
  dnafile <- system.file("sequences/someORF.fsa", package = "seqinr")
  sfdna <- read.fasta(file = dnafile)
  getSequence(sfdna[[1]])
  getSequence(sfdna[[1]], as.string = TRUE)
#
# SeqFrag class example:
#
  sfrag <- getFrag(object = sfdna[[1]], begin = 1, end = 10)
```

```
getSequence(sfrag)
getSequence(sfrag, as.string = TRUE)
```

---

getTrans

*Generic function to translate coding sequences into proteins*


---

## Description

This function translates nucleic acid sequences into the corresponding peptide sequence. It can translate in any of the 3 forward or three reverse sense frames. In the case of reverse sense, the reverse-complement of the sequence is taken. It can translate using the standard (universal) genetic code and also with non-standard codes. Ambiguous bases can also be handled.

## Usage

```
getTrans(object, sens = "F", NAstring = "X", ambiguous = FALSE, ...)
## S3 method for class 'SeqAcnucWeb'
getTrans(object, sens = "F", NAstring = "X", ambiguous = FALSE, ...,
  frame = "auto", numcode = "auto")
## S3 method for class 'SeqFastadna'
getTrans(object, sens = "F", NAstring = "X", ambiguous = FALSE, ...,
  frame = 0, numcode = 1)
## S3 method for class 'SeqFrag'
getTrans(object, sens = "F", NAstring = "X", ambiguous = FALSE, ...,
  frame = 0, numcode = 1)
```

## Arguments

object	an object of the class <a href="#">SeqAcnucWeb</a> or <a href="#">SeqFastadna</a> , or <a href="#">SeqFrag</a> or a list of these objects, or an object of class qaw created by <a href="#">query</a>
numcode	The ncbi genetic code number for translation. By default the standard genetic code is used, and for sequences coming from an ACNUC server the relevant genetic code is used by default.
NAstring	How to translate amino-acids when there are ambiguous bases in codons.
ambiguous	If TRUE, ambiguous bases are taken into account so that for instance GGN is translated to Gly in the standard genetic code.
frame	Frame(s) (0,1,2) to translate. By default the frame 0 is used.
sens	Direction for translation: F for the direct strand e and R for the reverse complementary strand.
...	further arguments passed to or from other methods

**Details**

The following genetic codes are described here. The number preceding each code corresponds to numcode.

- 1 standard
- 2 vertebrate.mitochondrial
- 3 yeast.mitochondrial
- 4 protozoan.mitochondrial+mycoplasma
- 5 invertebrate.mitochondrial
- 6 ciliate+dasycladaceal
- 9 echinoderm+flatworm.mitochondrial
- 10 euplotid
- 11 bacterial+plantplastid
- 12 alternativeyeast
- 13 ascidian.mitochondrial
- 14 alternativeflatworm.mitochondrial
- 15 blepharism
- 16 chlorophycean.mitochondrial
- 21 trematode.mitochondrial
- 22 scenedesmus.mitochondrial
- 23 hraustochytrium.mitochondria

**Value**

For a single sequence an object of class character containing the characters of the sequence, either of length 1 when `as.string` is TRUE, or of the length of the sequence when `as.string` is FALSE. For many sequences, a list of these.

**Author(s)**

D. Charif, J.R. Lobry, L. Palmeira

**References**

`citation("seqinr")`

**See Also**

[SeqAcnucWeb](#), [SeqFastadna](#), [SeqFrag](#)

The genetic codes are given in the object `SEQINR.UTIL`, a more human readable form is given by the function `tablecode`. Use `aaa` to get the three-letter code for amino-acids.

## Examples

```
#
# List all available methods for getTrans generic function:
#
  methods(getTrans)
#
# Toy CDS example invented by Leonor Palmeira:
#
  toycds <- s2c("tctgagcaaataaatcgg")
  getTrans(toycds) # should be c("S", "E", "Q", "I", "N", "R")
#
# Toy CDS example with ambiguous bases:
#
  toycds2 <- s2c("tcngarcarathaaycgn")
  getTrans(toycds2) # should be c("X", "X", "X", "X", "X", "X")
  getTrans(toycds2, ambiguous = TRUE) # should be c("S", "E", "Q", "I", "N", "R")
  getTrans(toycds2, ambiguous = TRUE, numcode = 2) # should be c("S", "E", "Q", "X", "N", "R")
#
# Real CDS example:
#
  realcds <- read.fasta(file = system.file("sequences/malM.fasta", package = "seqinr"))[[1]]
  getTrans(realcds)
# Biologically correct, only one stop codon at the end
  getTrans(realcds, frame = 3, sens = "R", numcode = 6)
# Biologically meaningless, note the in-frame stop codons

#
# Complex transsplicing operations, the correct frame and the correct
# genetic code are automatically used for translation into protein for
# sequences coming from an ACNUC server:
#
## Not run:
# Need internet connection.
# Translation of the following EMBL entry:
#
# FT    CDS                join(complement(153944..154157),complement(153727..153866),
# FT                                complement(152185..153037),138523..138735,138795..138955)
# FT                                /codon_start=1
  choosebank("emblTP")
  trans <- query("trans", "N=AE003734.PE35")
  getTrans(trans$req[[1]])

## End(Not run)
```

---

getType

*To get available subsequence types in an opened ACNUC database*

---

## Description

This function returns all subsequence types (e.g. CDS, TRNA) present in an opened ACNUC database, using default database if no socket is provided.

**Usage**

```
getType(socket = autosocket())
```

**Arguments**

socket            an object of class sockconn connecting to a remote ACNUC database (default is a socket to the last opened database).

**Value**

a list containing a short description for each subsequence type.

**Author(s)**

D. Charif, J.R. Lobry

**References**

```
citation("seqinr")
```

**See Also**

[choosebank](#), [query](#)

**Examples**

```
## Not run:  
# Need internet connection  
choosebank("emblTP")  
getType()  
## End(Not run)
```

---

gfrag	<i>Extract sequence identified by name or by number from an ACNUC server</i>
-------	--

---

**Description**

Get length characters from sequence identified by name or by number starting from position start (counted from 1).

**Usage**

```
gfrag(what, start, length, idby = c("name", "number"), socket = autosocket())
```



**Arguments**

what	A sequence name or number
start	Start position from 1
length	Number of requested characters (answer may be shorter)
idby	Is the sequence identified by name or number? Default to name
socket	an object of class sockconn connecting to a remote ACNUC database (default is a socket to the last opened database).

**Value**

A string of characters with at most length characters (may be shorter than asked for). NA is returned and a warning is issued in case of problem (non existent sequence for instance).

**Author(s)**

J.R. Lobry

**References**

<http://doua.prabi.fr/databases/acnuc.html>

`citation("seqinr")`

**See Also**

[choosebank](#), [query](#)

**Examples**

```
## Not run: # Need internet connection
choosebank("emblTP")
gfrag("LMFLCHR36", start = 1, length = 3529852) -> myseq
stopifnot(nchar(myseq) == 3529852)
closebank()

## End(Not run)
```

---

ghelp

*Get help from an ACNUC server*

---

**Description**

Reads one item of information in specified help file from an ACNUC server. There are differences between ACNUC clients so that this help could be confusing. However, the query language is common to all clients so that the most recent documentation is most likely here.

**Usage**

```
ghelp(item = c("GENERAL", "SELECT", "SPECIES", "KEYWORD"),  
      file = c("HELP", "HELP_WIN"), socket = autosocket(), catresult = TRUE)
```

**Arguments**

item	the name of the desired help item
file	the name of the help file on server side.
socket	an object of class sockconn connecting to a remote ACNUC database (default is a socket to the last opened database).
catresult	logical. If TRUE output is redirected to the console.

**Value**

A vector of string which is returned invisibly and "cated" to the console by default.

**Author(s)**

J.R. Lobry

**References**

<http://doua.prabi.fr/databases/acnuc.html>  
citation("seqinr")

**See Also**

[choosebank](#), [query](#)

**Examples**

```
## Not run:  
### Need internet connection  
choosebank("emblTP")  
ghelp()  
ghelp("SELECT")  
# To get info about current database:  
ghelp("CONT")  
  
## End(Not run)
```

gs500liz

*GS500LIZ size standards***Description**

GS500LIZ is an internal size standard often used in capillary electrophoresis. It contains 16 fragments ranging in size from 35 to 500 bp. Note that they are not all used for calibration : fragments at 250 and 340 bp may migrate anomalously (most likely because of secondary structure formation).

**Usage**

```
data(gs500liz)
```

**Format**

A list with 3 components.

**liz** a vector of 16 values for the fragment sizes in bp.

**mask1** a vector of 16 logicals to remove fragments whose migration may be anomalous (250 and 340 bp).

**mask2** a vector of 16 logicals to remove extreme fragments (35, 50, 490, 500 bp) so that the resulting fragments are in the 75-450 bp range.

**Examples**

```
data(gs500liz)
op <- par(no.readonly = TRUE)
par(lend = "butt", mar = c(5,0,4,0)+0.1)
x <- gs500liz$liz
n <- length(x)
y <- rep(1, n)
plot(x, y, type = "h", yaxt = "n", xlab = "Fragment size [bp]",
     main = "GS500LIZ size standard", lwd = 2)
x1 <- x[!gs500liz$mask1]
segments(x1, 0, x1, 1, col = "red", lwd = 2)
x2 <- x[!gs500liz$mask2]
segments(x2, 0, x2, 1, col = "blue", lwd = 2)
col <- rep("black", n)
col[!gs500liz$mask1] <- "red"
col[!gs500liz$mask2] <- "blue"
text(x, 1.05, paste(x, "bp"), srt = 90, col = col)
legend("top", inset = 0.1, legend = c("regular", "imprecise (mask1)", "extreme (mask2)"),
     lwd = 2, col = c("black", "red", "blue"))
par(op)
```

---

identifiler	<i>Identifiler allele names</i>
-------------	---------------------------------

---

**Description**

Names of the alleles in the Applied Biosystem identifiler allelic ladder.

**Usage**

```
data(identifiler)
```

**Format**

A list with 4 components for the four fluorochromes.

**FAM** a list of 4 loci

**VIC** a list of 5 loci

**NED** a list of 4 loci

**PET** a list of 3 loci

**Examples**

```
data(identifiler)
op <- par(no.readonly = TRUE)
par(mar = c(3,8,4,2)+0.1)
allcount <- unlist(lapply(identifiler, function(x) lapply(x, length)))
barplot(allcount[order(allcount)], horiz = TRUE, las = 1,
main = "Allele count per locus", col = "lightblue")
par(op)
```

---

isenum	<i>Get the ACNUC number of a sequence from its name or accession number</i>
--------	---

---

**Description**

Gives the ACNUC number of a sequence in the number element of the returned list. More informations are returned for subsequences corresponding to coding sequences.

**Usage**

```
isenum(what, idby = c("name", "access"), socket = autosocket())
isn(what, ...)
getNumber.socket(socket, name)
getAttributesocket(socket, name)
```

**Arguments**

what	a sequence name or a sequence accession number
idby	is the sequence identified by name or by accession number? Default to name
socket	an object of class <code>sockconn</code> connecting to a remote ACNUC database (default is a socket to the last opened database).
...	arguments passed to <code>isenum</code> .
name	a sequence name.

**Value**

A list with the following 6 components:

number	numeric. The ACNUC number of the sequence.
length	numeric. The length of the sequence.
frame	numeric. The reading frame (0, 1, or 2) of the sequence for CDS.
gencode	numeric. ACNUC's genetic code (0 means universal) of the sequence for CDS.
ncbigc	numeric. NCBI's genetic code (0 means universal) of the sequence for CDS.
otheraccessmatches	logical. If TRUE it means that several sequences are attached to the given accession number, and that only the ACNUC number of the first attached sequence is returned in the number component of the list.

`isn(what, ...)` is a shortcut for `isenum(what, ...) $number`.

As from `seqinR` 1.1-3 `getNumber.socket` and `getAttributesocket` are deprecated (a warning is issued).

**Author(s)**

J.R. Lobry

**References**

<http://doua.prabi.fr/databases/acnuc.html>

`citation("seqinr")`

**See Also**

[choosebank](#), [query](#)

## Examples

```
## Not run:
### Need internet connection
choosebank("emblTP")
isenum("LMFLCHR36")
isn("LMFLCHR36")
stopifnot(isn("LMFLCHR36") == 13682678)
# Example with CDS:
isenum("AB004237")

## End(Not run)
```

---

JLO

*Forensic Genetic Profile Raw Data*


---

## Description

This is an example of raw data for a human STR genetic profile at 16 loci (*viz.* D8S1179, D21S11, D7S820, CSF1PO, D3S1358, TH01, D13S317, D16S539, D2S1338, D19S433, vWA, TPOX, D18S51, Amelogenin, D5S818, FGA) which are commonly used in forensic sciences for individual identifications.

## Usage

```
data(JLO)
```

## Format

A list with 3 components.

**Header** a list corresponding to the header in the ABIF file

**Directory** a data.frame corresponding to the Directory in the ABIF file

**Data** a list with all raw data in the ABIF file.

## Details

This dataset is the expected result when reading the file `2_FAC321_0000205983_B02_004.fsa` with the function [read.abif](#). This dataset is used for the quality check of this function.

## Author(s)

J.R. Lobry

## Source

The DNA source is from the author so that there are no privacy concern. Data were kindly provided by the INPS (Institut National de Police Scientifique) which is the national forensic sciences institute in France. Experiments were done at the LPS (Laboratoire de Police Scientifique de Lyon) in 2008.

## References

```
citation("seqinr")
```

Anonymous (2006) Applied Biosystem Genetic Analysis Data File Format. Available at [http://www.appliedbiosystems.com/support/software\\_community/ABIF\\_File\\_Format.pdf](http://www.appliedbiosystems.com/support/software_community/ABIF_File_Format.pdf). Last visited on 03-NOV-2008.

## See Also

function `read.abif` to import files in ABIF format, data `gs500liz` for internal size standards, data `ECH` for the corresponding allelic ladder, data `identifiler` for allele names in the allelic ladder.

## Examples

```
data(JL0)
```

---

kaks

*Ka and Ks, also known as dn and ds, computation*

---

## Description

Ks and Ka are, respectively, the number of substitutions per synonymous site and per non-synonymous site between two protein-coding genes. They are also denoted as ds and dn in the literature. The ratio of nonsynonymous (Ka) to synonymous (Ks) nucleotide substitution rates is an indicator of selective pressures on genes. A ratio significantly greater than 1 indicates positive selective pressure. A ratio around 1 indicates either neutral evolution at the protein level or an averaging of sites under positive and negative selective pressures. A ratio less than 1 indicates pressures to conserve protein sequence (*i.e.* purifying selection). This function estimates the Ka and Ks values for a set of aligned sequences using the method published by Li (1993) and gives the associated variance matrix.

## Usage

```
kaks(x, verbose = FALSE, debug = FALSE, forceUpperCase = TRUE, rmgap = TRUE)
```

## Arguments

x	An object of class <code>alignment</code> , obtained for instance by importing into R the data from an alignment file with the <code>read.alignment</code> function. This is typically a set of coding sequences aligned at the protein level, see <code>reverse.align</code> .
verbose	If TRUE add to the results the value of L0, L2, L4 (respectively the frequency of non-synonymous sites, of 2-fold synonymous sites, of 4-fold synonymous sites), A0, A2, A4 (respectively the number of transitional changes at non-synonymous, 2-fold, and 4-fold synonymous sites ) and B0, B2, B4 (respectively the number of transversional changes at non-synonymous, 2-fold, and 4-fold synonymous sites).
debug	If TRUE turns debug mode on.

forceUpperCase	If TRUE, the default value, all character in sequences are forced to the upper case if at least one 'a', 'c', 'g', or 't' is found in the sequences. Turning it to FALSE if the sequences are already in upper case will save time.
rmgap	If TRUE all positions with at least one gap are removed. If FALSE only positions with nothing else than gaps are removed.

### Value

ks	matrix of Ks values
ka	matrix of Ka values
vks	variance matrix of Ks
vka	variance matrix of Ka

### Note

Computing Ka and Ks makes sense for coding sequences that have been aligned at the amino-acid level before retro-translating the alignment at the nucleic acid level to ensure that sequences are compared on a codon-by-codon basis. Function [reverse.align](#) may help for this.

As from seqinR 2.0-3, when there is at least one non ACGT base in a codon, this codon is considered as a gap-codon (---). This makes the computation more robust with respect to alignments with out-of-frame gaps, see example section.

Gap-codons (---) are not used for computations.

When the alignment does not contain enough information (*i.e.* close to saturation), the Ka and Ks values are forced to 10 (more exactly to 9.999999).

Negative values indicate that Ka and Ks can not be computed.

According to Li (1993) and Pamilo and Bianchi (1993), the rate of synonymous substitutions Ks is computed as:  $Ks = (L2.A2 + L4.A4) / (L2 + L4) + B4$

and the rate of non-synonymous substitutions Ka is computed as:  $Ka = A0 + (L0.B0 + L2.B2) / (L0 + L2)$

### Author(s)

D. Charif, J.R. Lobry

### References

Li, W.-H., Wu, C.-I., Luo, C.-C. (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**:150-174

Li, W.-H. (1993) Unbiased estimation of the rates of synonymous and nonsynonymous substitution. *J. Mol. Evol.*, **36**:96-99.

Pamilo, P., Bianchi, N.O. (1993) Evolution of the *Zfx* and *Zfy* genes: Rates and interdependence between genes. *Mol. Biol. Evol.*, **10**:271-281



Hurst, L.D. (2002) The Ka/Ks ratio: diagnosing the form of sequence evolution. *Trends Genet.*, **18**:486-486.

The C program implementing this method was provided by Manolo Gouy. More info is needed here to trace back the original C source so as to credit correct source. The original FORTRAN-77 code by Chung-I Wu modified by Ken Wolfe was available here <http://wolfe.gen.tcd.ie/lab/pub/li93/> but this is no more true as 2017-07-01.

For a more recent discussion about the estimation of Ka and Ks see:

Tzeng, Y.H., Pan, R., Li, W.-H. (2004) Comparison of three methods for estimating rates of synonymous and nonsynonymous nucleotide substitutions. *Mol. Biol. Evol.*, **21**:2290-2298.

The method implemented here is noted LWL85 in the above paper.

The cite this package in a publication, as any R package, try something as `citation("seqinr")` at your R prompt.

### See Also

[read.alignment](#) to import alignments from files, [reverse.align](#) to align CDS at the aa level, [kaksTorture](#) for test on one-codon CDS.

### Examples

```
#
# Simple Toy example:
#
s <- read.alignment(file = system.file("sequences/test.phylip", package = "seqinr"),
  format = "phylip")
kaks(s)
#
# Check numeric results on an simple test example:
#
data(AnoukResult)
Anouk <- read.alignment(file = system.file("sequences/Anouk.fasta", package = "seqinr"),
  format = "fasta")
if( ! all.equal(kaks(Anouk), AnoukResult) ) {
  warning("Poor numeric results with respect to AnoukResult standard")
} else {
  print("Results are consistent with AnoukResult standard")
}
#
# As from seqinR 2.0-3 the following alignment with out-of-frame gaps
# should return a zero Ka value.
#
# >Reference
# ATGTGGTCGAGATATCGAAAGCTAGGGATATCGATTATATATAGCAAGATCGATAGAGGA
# TCGATGATCGATCGGGATCGACAGCTG
```

```

# >With out-of-frame gaps
# AT-TGGTCCAGGTATCGTAAGCTAGGGATATCGATTATATATAGCAAGATCGATAGGGGA
# TCGATGATCGATCGGGA--GACAGCTG
#
# This test example provided by Darren Obbard is now used as a routine check:
#
Darren <- read.alignment(file = system.file("sequences/DarrenObbard.fasta", package = "seqinr"),
  format = "fasta")
stopifnot( all.equal(kaks(Darren)$ka[1], 0) )
#
# As from seqinR 3.4-0, non-finite values should never be returned for
# Ka and Ks even for small sequences. The following test checks that this
# is true for an alignment of the 64 codons, so that we compute Ka and
# Ks for all possible pairs of codons.
#
wrds <- as.alignment(nb = 64, nam = words(), seq = words())
res <- kaks(wrds)
if(any(!is.finite(res$ka))) stop("Non finite value returned for Ka")
if(any(!is.finite(res$ks))) stop("Non finite value returned for Ks")

```

---

kaksTorture

---

*Expected numeric results for Ka and Ks in extreme cases*


---

## Description

This data set is what should be obtained when running `kaks()` on the test file `kaks-torture.fasta` in the `sequences` directory of the `seqinR` package.

## Usage

```
data(kaksTorture)
```

## Format

A list with 4 components of class `dist`.

**ka** Ka

**ks** Ks

**vka** variance for Ka

**vks** variance for Ks

## Source

See comments in `kaks-torture.fasta` for R code used to produce it.

## References

```
citation("seqinr")
```

**Examples**

```
data(kaksTorture)
kaks.torture <- read.alignment(file = system.file("sequences/kaks-torture.fasta",
  package = "seqinr"), format = "fasta")
#
# Failed on windows :
#
# stopifnot(identical(kaksTorture, kaks(kaks.torture)))
# stopifnot(identical(kaksTorture, kaks(kaks.torture, rmgap = FALSE)))
```

---

knowndbs	<i>Description of databases known by an ACNUC server</i>
----------	--

---

**Description**

Returns, for each database known by the server, its name (a valid value for the bank argument of [choosebank](#)), availability (off means temporarily unavailable), and description.

**Usage**

```
knowndbs(tag = c(NA, "TP", "TEST", "DEV"), socket = autosocket())
kdb(tag = c(NA, "TP", "TEST", "DEV"), socket = autosocket())
```

**Arguments**

tag	default to NA, see details
socket	an object of class sockconn connecting to a remote ACNUC database (default is a socket to the last opened database).

**Details**

When the optional tag argument is used, only databases tagged with the given string are listed; when this argument is NA (by default), only untagged databases are listed. The tag argument thus allows to identify series of special purpose (tagged) databases, in addition to default (untagged) ones.

**Value**

A dataframe with 3 columns:

bank	string. Valid bank values known by the ACNUC server
status	string. "on" means available, "off" means temporarily unavailable
info	string. short description of the database

**Author(s)**

J.R. Lobry

## References

<http://doua.prabi.fr/databases/acnuc.html>

`citation("seqinr")`

The full list of untagged and tagged databases is here : [http://doua.prabi.fr/databases/acnuc/banques\\_raa.php](http://doua.prabi.fr/databases/acnuc/banques_raa.php).

## See Also

`choosebank` when called without arguments.

## Examples

```
## Not run:  
### Need internet connection  
choosebank("emblTP")  
kdb()  
closebank()  
  
## End(Not run)
```

---

lseqinr

*To see what's inside the package seqinr*

---

## Description

This is just a shortcut for `ls("package:seqinr")`

## Usage

```
lseqinr()
```

## Value

The list of objects in the package seqinr

## Note

Use `library(help=seqinr)` to have a summary of the functions available in the package.

## Author(s)

J.R. Lobry

## References

`citation("seqinr")`

## Examples

```
lseqinr()
```

---

m16j

*Fragment of the E. coli chromosome*

---

## Description

A fragment of the *E. coli* chromosome that was used in Lobry (1996) to show the change in GC skew at the origin of replication (*i.e.* the chirochore structure of bacterial chromosomes)

## Usage

```
data(m16j)
```

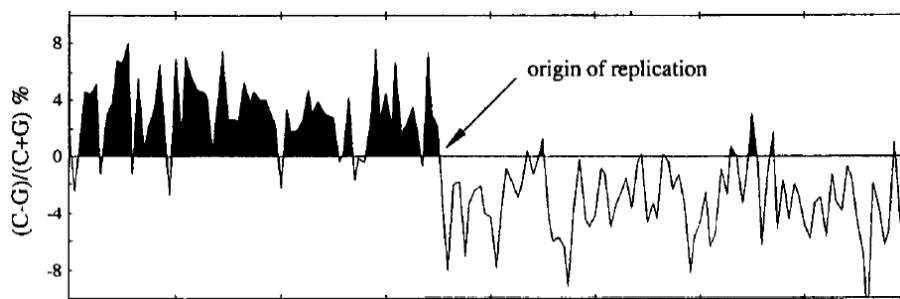
## Format

A string of 1,616,539 characters

## Details

The sequence used in Lobry (1996) was a 1,616,174 bp fragment obtained from the concatenation of nine overlapping sequences (U18997, U00039, L10328, M87049, L19201, U00006, U14003, D10483, D26562). Ambiguities have been resolved since then and it was a chimeric sequence from K-12 strains MG1655 and W3110, the sequence used here is from strain MG1655 only (Blattner *et al.* 1997).

The chirochore structure of bacterial genomes is illustrated below by a screenshot of a part of figure 1 from Lobry (1996). See the example section to reproduce this figure.



## Source

*Escherichia coli* K-12 strain MG1655. Fragment from U00096 from the EBI Genome Reviews. Acnuc Release 7. Last Updated: Feb 26, 2007. XX DT 18-FEB-2004 (Rel. .1, Created) DT 09-JAN-2007 (Rel. 65, Last updated, Version 70) XX

## References

Lobry, J.R. (1996) Asymmetric substitution patterns in the two DNA strands of bacteria. *Molecular Biology and Evolution*, **13**:660-665.

F.R. Blattner, G. Plunkett III, C.A. Bloch, N.T. Perna, V. Burland, M. Riley, J. Collado-Vides, J.D. Glasner, C.K. Rode, G.F. Mayhew, J. Gregor, N.W. Davis, H.A. Kirkpatrick, M.A. Goeden, D.J. Rose, B. Mau, and Y. Shao. (1997) The complete genome sequence of *Escherichia coli* K-12. *Science*, **277**:1453-1462

```
citation("seqinr")
```

## Examples

```
#
# Load data:
#
data(m16j)
#
# Define a function to compute the GC skew:
#
gcskew <- function(x) {
  if (!is.character(x) || length(x) > 1)
    stop("single string expected")
  tmp <- tolower(s2c(x))
  nC <- sum(tmp == "c")
  nG <- sum(tmp == "g")
  if (nC + nG == 0)
    return(NA)
  return(100 * (nC - nG)/(nC + nG))
}
#
# Moving window along the sequence:
#
step <- 10000
wsize <- 10000
starts <- seq(from = 1, to = nchar(m16j), by = step)
starts <- starts[-length(starts)]
n <- length(starts)
result <- numeric(n)
for (i in seq_len(n)) {
  result[i] <- gcskew(substr(m16j, starts[i], starts[i] + wsize - 1))
}
#
# Plot the result:
#
xx <- starts/1000
yy <- result
n <- length(result)
hline <- 0
plot(yy ~ xx, type = "n", axes = FALSE, ann = FALSE, ylim = c(-10, 10))
polygon(c(xx[1], xx, xx[n]), c(min(yy), yy, min(yy)), col = "black", border = NA)
```

```
usr <- par("usr")
rect(usr[1], usr[3], usr[2], hline, col = "white", border = NA)
lines(xx, yy)
abline(h = hline)
box()
axis(1, at = seq(0, 1600, by = 200))
axis(2, las = 1)
title(xlab = "position (Kbp)", ylab = "(C-G)/(C+G) [percent]",
      main = expression(paste("GC skew in ", italic(Escherichia~coli))))
arrows(860, 5.5, 720, 0.5, length = 0.1, lwd = 2)
text(860, 5.5, "origin of replication", pos = 4)
```

---

mase

---

*Example of results obtained after a call to read.alignment*


---

## Description

This data set gives an example of a protein alignment obtained after a call to the function `read.alignment` on an alignment file in "mase" format.

## Usage

```
mase
```

## Format

A List of class alignment

## Source

<http://www.clustal.org/>

## References

Faullcner,D.V. and Jurka,J. (1988) *Multiple sequences alignment editor(MASE)*. Trends Biochem. Sa., 13, 321-322.

---

modifylist

---

*Modification of an ACNUC list*


---

## Description

This function modifies a previously existing ACNUC list by selecting sequences either by length, either by date, either for the presence of a given string in annotations.

**Usage**

```
modifylist(listname, modlistname = listname, operation,
  type = c("length", "date", "scan"), socket = autosocket(),
  virtual = FALSE, verbose = FALSE)
```

**Arguments**

listname	the name of the ACNUC list to modify
modlistname	the name of the modified ACNUC list. Default is to use the same list name so that previous list is lost.
operation	a string of character describing the operation to be done, see details.
type	the type of operation, could be one of "length", "date", "scan". Default is "length"
socket	an object of class sockconn connecting to a remote ACNUC database (default is a socket to the last opened database).
virtual	if TRUE, no attempt is made to retrieve the information about all the elements of the list. In this case, the req component of the list is set to NA.
verbose	logical, if TRUE mode verbose is on

**Details**

Example of possible values for the argument operation:

**length** as in "> 10000" or "< 500"

**date** as in "> 1/jul/2001" or "< 30/AUG/98"

**scan** specify the string to be searched for

Character < is to be understood as <= and > likewise.

**Value**

The result is directly assigned to the object modlistname in the user workspace. This is an object of class qaw, a list with the following 6 components:

call	the original call
name	the ACNUC list name
nelem	the number of elements (for instance sequences) in the ACNUC list
typelist	the type of the elements of the list. Could be SQ for a list of sequence names, KW for a list of keywords, SP for a list of species names.
req	a list of sequence names that fit the required criteria or NA when called with parameter virtual is TRUE
socket	the socket connection that was used

**Author(s)**

J.R. Lobry



## References

<http://doua.prabi.fr/databases/acnuc.html>

`citation("seqinr")`

## See Also

[choosebank](#), [query](#) and [prepgetannots](#) to select the annotation lines for scan.

## Examples

```
## Not run: # Need internet connection
choosebank("emblTP")
mylist <- query("mylist", "sp=felis catus et t=cds", virtual=TRUE)
mylist$nelem # 603 sequences
stopifnot(mylist$nelem == 603)

# select sequences with at least 1000 bp:
mylist <- modifylist("mylist", operation = ">1000", virtual = TRUE)
mylist$nelem # now, only 132 sequences
stopifnot(mylist$nelem == 132)

# scan for "felis" in annotations:
mylist <- modifylist("mylist", op = "felis", type = "scan", virtual = TRUE)
mylist$nelem # now, only 33 sequences
stopifnot(mylist$nelem == 33)

# modify by date:
mylist <- modifylist("mylist", op = "> 1/jul/2001", type = "date", virtual = TRUE)
mylist$nelem # now, only 15 sequences
stopifnot(mylist$nelem == 15)

# Summary of current ACNUC lists, one list called MYLIST on sever:
sapply(alr()$rank, getliststate)
closebank()

## End(Not run)
```

---

move

*Rename an R object*

---

## Description

Rename object from into to.

## Usage

```
move(from, to)
mv(from, to)
```

**Arguments**

from	an R object name
to	the new R object name

**Value**

none.

**Author(s)**

J.R. Lobry

**References**

`citation("seqinr")`

**See Also**

[swap](#)

**Examples**

```
#
# Example in a new empty environment:
#
local({
  zefplock <- pi
  print(ls())
  print(zefplock)
  mv(zefplock, toto)
  print(ls())
  print(toto)
  stopifnot(identical(toto, pi)) # Sanity check
})
#
# Check that self-affectation is possible:
#
mv(mv, mv) # force self-affectation for the function itself
mv(mv, mv) # OK, function mv() still exists
```

---

msf

*Example of results obtained after a call to read.alignment*

---

**Description**

This data set gives an example of a protein alignment obtained after a call to the function `read.alignment` on an alignment file in "msf" format.

**Usage**

```
msf
```

**Format**

A List of class alignment

**Source**

<http://www.ebi.ac.uk/2can/tutorials/formats.html#MSF/>

---

n2s	<i>function to convert the numeric encoding of a DNA sequence into a vector of characters</i>
-----	---

---

**Description**

By default, if no 'levels' arguments is provided, this function will just transform your vector of integer into a DNA sequence according to the lexical order: 0 -> "a", 1 -> "c", 2 -> "g", 3 -> "t", others -> NA.

**Usage**

```
n2s(nseq, levels = c("a", "c", "g", "t"), base4 = TRUE)
```

**Arguments**

nseq	A vector of integers
levels	the translation vector
base4	when this logical is true, the numerical encoding of levels starts at 0, when it is false the numerical encoding of levels starts at 1.

**Value**

a vector of characters

**Author(s)**

J.R. Lobry

**References**

`citation("seqinr")`

**See Also**

[s2n](#)

Examples

```
##example of the default behaviour:
nseq <- sample(x = 0:3, size = 100, replace = TRUE)
n2s(nseq)
# Show what happens with out-of-range and NA values:
nseq[1] <- NA
nseq[2] <- 777
n2s(nseq)[1:10]
# How to get an RNA instead:
n2s(nseq, levels = c("a", "c", "g", "u"))
```

---

oriloc	<i>Prediction of origin and terminus of replication in bacteria.</i>
--------	--

---

Description

This program finds the putative origin and terminus of replication in procaryotic genomes. The program discriminates between codon positions.

Usage

```
oriloc(seq.fasta = system.file("sequences/ct.fasta.gz", package = "seqinr"),
      g2.coord = system.file("sequences/ct.predict", package = "seqinr"),
      glimmer.version = 3,
      oldoriloc = FALSE, gbk = NULL, clean.tmp.files = TRUE, rot = 0)
```

Arguments

seq.fasta	Character: the name of a file which contains the DNA sequence of a bacterial chromosome in fasta format. The default value, <code>system.file("sequences/ct.fasta.gz", package = "seqinr")</code> is the fasta file <code>ct.fasta.gz</code> . This is the file for the complete genome sequence of <i>Chlamydia trachomatis</i> that was used in Frank and Lobry (2000). You can replace this by something like <code>seq.fasta = "myseq.fasta"</code> to work with your own data if the file <code>myseq.fasta</code> is present in the current working directory (see <a href="#">getwd</a> ), or give a full path access to the sequence file (see <a href="#">file.choose</a> ).
g2.coord	Character: the name of file which contains the output of glimmer program ( <code>*.predict</code> in glimmer version 3)
glimmer.version	Numeric: glimmer version used, could be 2 or 3
oldoriloc	Logical: to be set at TRUE to reproduce the (deprecated) outputs of previous (publication date: 2000) version of the oriloc program.
gbk	Character: the URL of a file in GenBank format. When provided oriloc use as input a single GenBank file instead of the <code>seq.fasta</code> and the <code>g2.coord</code> . A local temporary copy of the GenBank file is made with <a href="#">download.file</a> if <code>gbk</code> starts with <code>http://</code> or <code>ftp://</code> or <code>file://</code> and with <a href="#">file.copy</a> otherwise. The local copy is then used as input for <a href="#">gb2fasta</a> and <a href="#">gbk2g2</a> to produce a fasta file and a glimmer-like (version 2) file, respectively, to be used by oriloc instead of <code>seq.fasta</code> and <code>g2.coord</code> .

<code>clean.tmp.files</code>	Logical: if TRUE temporary files generated when working with a GenBank file are removed.
<code>rot</code>	Integer, with zero default value, used to permute circularly the genome.

### Details

The method builds on the fact that there are compositional asymmetries between the leading and the lagging strand for replication. The programs works only with third codon positions so as to increase the signal/noise ratio. To discriminate between codon positions, the program use as input either an annotated genbank file, either a fasta file and a glimmer2.0 (or glimmer3.0) output file.

### Value

A data.frame with seven columns: `g2num` for the CDS number in the `g2.coord` file, `start.kb` for the start position of CDS expressed in Kb (this is the position of the first occurrence of a nucleotide in a CDS *regardless* of its orientation), `end.kb` for the last position of a CDS, `CDS.excess` for the DNA walk for gene orientation (+1 for a CDS in the direct strand, -1 for a CDS in the reverse strand) cumulated over genes, `skew` for the cumulated composite skew in third codon positions, `x` for the cumulated T - A skew in third codon position, `y` for the cumulated C - G skew in third codon positions.

### Note

The method works only for genomes having a single origin of replication from which the replication is bidirectional. To detect the composition changes, a DNA-walk is performed. In a 2-dimensional DNA walk, a C in the sequence corresponds to the movement in the positive y-direction and G to a movement in the negative y-direction. T and A are mapped by analogous steps along the x-axis. When there is a strand asymmetry, this will form a trajectory that turns at the origin and terminus of replication. Each step is the sum of nucleotides in a gene in third codon positions. Then orthogonal regression is used to find a line through this trajectory. Each point in the trajectory will have a corresponding point on the line, and the coordinates of each are calculated. Thereafter, the distances from each of these points to the origin (of the plane), are calculated. These distances will represent a form of cumulative skew. This permits us to make a plot with the gene position (gene number, start or end position) on the x-axis and the cumulative skew (distance) at the y-axis. Depending on where the sequence starts, such a plot will display one or two peaks. Positive peak means origin, and negative means terminus. In the case of only one peak, the sequence starts at the origin or terminus site.

### Author(s)

J.R. Lobry, A.C. Frank

### References

More illustrated explanations to help understand oriloc outputs are available there: <https://pbil.univ-lyon1.fr/software/Oriloc/howto.html>.

Examples of oriloc outputs on real sequence data are there: <https://pbil.univ-lyon1.fr/software/Oriloc/index.html>.

The original paper for oriloc:

Frank, A.C., Lobry, J.R. (2000) Oriloc: prediction of replication boundaries in unannotated bacterial chromosomes. *Bioinformatics*, **16**:566-567.  
<https://doi.org/10.1093/bioinformatics/16.6.560>

A simple informal introduction to DNA-walks:

Lobry, J.R. (1999) Genomic landscapes. *Microbiology Today*, **26**:164-165.  
[http://seqinr.r-forge.r-project.org/MicrTod\\_1999\\_26\\_164.pdf](http://seqinr.r-forge.r-project.org/MicrTod_1999_26_164.pdf)

An early and somewhat historical application of DNA-walks:

Lobry, J.R. (1996) A simple vectorial representation of DNA sequences for the detection of replication origins in bacteria. *Biochimie*, **78**:323-326.

Glimmer, a very efficient open source software for the prediction of CDS from scratch in prokaryotic genome, is described at <http://www.cbcb.umd.edu/software/glimmer/>.

For a description of Glimmer 1.0 and 2.0 see:

Delcher, A.L., Harmon, D., Kasif, S., White, O., Salzberg, S.L. (1999) Improved microbial gene identification with GLIMMER, *Nucleic Acids Research*, **27**:4636-4641.

Salzberg, S., Delcher, A., Kasif, S., White, O. (1998) Microbial gene identification using interpolated Markov models, *Nucleic Acids Research*, **26**:544-548.

`citation("seqinr")`

## See Also

[draw.oriloc](#), [rearranged.oriloc](#)

## Examples

```
## Not run:
#
# A little bit too long for routine checks because oriloc() is already
# called in draw.oriloc.Rd documentation file. Try example(draw.oriloc)
# instead, or copy/paste the following code:
#
out <- oriloc()
plot(out$st, out$sk, type = "l", xlab = "Map position in Kb",
      ylab = "Cumulated composite skew",
      main = expression(italic(Chlamydia~~trachomatis)~~complete~~genome))
#
# Example with a single GenBank file:
```

```
#
out2 <- oriloc(gbk="ftp://pbil.univ-lyon1.fr/pub/seqinr/data/ct.gbk")
draw.oriloc(out2)
#
# (some warnings are generated because of join in features and a gene that
# wrap around the genome)
#

## End(Not run)
```

---

parser.socket

*Utility function to parse answers from an ACNUC server*

---

## Description

Answers from server looks like : "code=0&lrank=2&count=150513&type=SQ&locus=F".

## Usage

```
parser.socket(onlinefromserver, verbose = FALSE)
```

## Arguments

onlinefromserver	a string
verbose	logical, if TRUE mode verbose is on

## Value

A vector of mode character or NULL if onlinefromserver is NULL or if its length is 0.

## Author(s)

J.R. Lobry

## References

citation("seqinr")

## See Also

[choosebank](#), [query](#)

## Examples

```
stopifnot(all(parser.socket("code=0&lrank=2&count=150513&type=SQ&locus=F")
== c("0", "2", "150513", "SQ", "F")))
```

peakabif

*Extraction of Peak locations, Heights and Surfaces from ABIF data***Description**

Simple peak location for data imported with the [read.abif](#) function using cubic spline interpolation.

**Usage**

```
peakabif(abifdata,
  chanel,
  npeak,
  thres = 400/yscale,
  fig = TRUE,
  chanel.names = c(1:4,105),
  DATA = paste("DATA", chanel.names[chanel], sep = "."),
  tmin = 1/tscale,
  tmax = abifdata$Data[["SCAN.1"]]/tscale,
  tscale = 1000,
  yscale = 1000,
  irange = (tmin*tscale):(tmax*tscale),
  y = abifdata$Data[[DATA]][irange]/yscale,
  method = "monoH.FC",
  maxrfu = 1000,
  ...)
```

**Arguments**

abifdata	the result returned by <a href="#">read.abif</a>
chanel	the dye number
npeak	the expected number of peaks
thres	scaled threshold value
fig	logical: should localized peaks be plotted
chanel.names	numbers extensions used for the DATA
DATA	names of the DATA components
tmin	scaled starting time for the time axis
tmax	scaled ending time for the time axis
tscale	scale factor for the time axis
yscale	scale factor for the y-axis (RFU)
irange	indices of data to be plotted
y	values used for the y-axis
method	method to be used by <a href="#">splinefun</a>
maxrfu	argument passed to <a href="#">baselineabif</a>
...	arguments forwarded to <a href="#">plot</a>



**Value**

Returns invisibly a list with the unscaled values for the locations of peaks, heights of peaks and surfaces of peaks and baseline estimate. The peak location are in datapoint units, that is an integer starting at 1 for the first experimental point, 2 for the second experimental point, etc. However, due to interpolation between points the estimated peak location is usually not an integer.

**Author(s)**

J.R. Lobry

**References**

`citation("seqnr")`

**See Also**

function [read.abif](#) to import files in ABIF format, [plotabif](#) to plot them, data [gs500liz](#) for internal size standards, data [identifiler](#) for allele names in the allelic ladder, data [JLO](#) for an example of an individual sample file, data [ECH](#) for an example of an allelic ladder.

**Examples**

```
data(JLO)
JLO$maxis <- peakabif(JLO, 5, npeak = 14, tmin = 2.7, thres = 0.1)$maxis
```

---

permutation

---

*Sequence permutation according to several different models*


---

**Description**

Generates a random permutation of a given sequence, according to a given model. Available models are : base, position, codon, syncodon.

**Usage**

```
permutation(sequence, modele='base', frame=0,
  replace=FALSE, prot=FALSE, numcode=1, ucweight = NULL)
```

**Arguments**

sequence	A nucleic acids sequence
modele	A string of characters describing the model chosen for the random generation
frame	Only active for the position, codon, syncodon models: starting position of CDS as in <code>splitseq</code>
replace	This option is not active for the syncodon model: if TRUE, sampling is done with replacement

prot	Only available for the codon model: if TRUE, the first and last codons are preserved, and only intern codons are shuffled
numcode	Only available for the syncodon model: the genetic code number as in translate.
ucoweight	A list of weights containing the desired codon usage bias as generated by ucoweight. If none is specified, the codon usage of the given sequence is used.

### Details

The base model allows for random sequence generation by shuffling (with/without replacement) of all bases in the sequence.

The position model allows for random sequence generation by shuffling (with/without replacement) of bases within their position in the codon (bases in position I, II or III stay in position I, II or III in the new sequence).

The codon model allows for random sequence generation by shuffling (with/without replacement) of codons.

The syncodon model allows for random sequence generation by shuffling (with/without replacement) of synonymous codons.

### Value

a sequence generated from the original one by a given model

### Author(s)

L. Palmeira

### References

`citation("seqinr")`

### See Also

[synsequence](#)

### Examples

```
data(ec999)
sequence=ec999[1][[1]]

new=permutation(sequence,model='base')
identical(all.equal(count(new,1),count(sequence,1)),TRUE)

new=permutation(sequence,model='position')
identical(all.equal(GC(new),GC(sequence)),TRUE)
identical(all.equal(GC2(new),GC2(sequence)),TRUE)
identical(all.equal(GC3(new),GC3(sequence)),TRUE)

new=permutation(sequence,model='codon')
identical(all.equal(uco(new),uco(sequence)),TRUE)
```

```
new=permutation(sequence,model='syncodon',numcode=1)
identical(all.equal(translate(new),translate(sequence)),TRUE)
```

---

phylip

*Example of results obtained after a call to read.alignment*

---

### Description

This data set gives an example of a amino acids alignment obtained after a call to the function read.alignment on an alignment file in "phylip" format.

### Usage

phylip

### Format

A List of class alignment

### Source

<http://evolution.genetics.washington.edu/phylip.html>

### References

<http://evolution.genetics.washington.edu/phylip.html>

---

pK

*pK values for the side chain of charged amino acids from various sources*

---

### Description

This compilation of pK values is from Joanna Kiraga (2008).

### Usage

data(pK)

### Format

A data frame with the seven charged amino-acid in row and six sources in column. The rownames are the one-letter code for amino-acids.

## Source

Table 2 in Kiraga (2008).

## References

- Kiraga, J. (2008) Analysis and computer simulations of variability of isoelectric point of proteins in the proteomes. PhD thesis, University of Wroclaw, Poland.
- Bjellqvist, B., Hughes, G.J., Pasquali, Ch., Paquet, N., Ravier, F., Sanchez, J.Ch., Frutiger S., Hochstrasser D. (1993) The focusing positions of polypeptides in immobilized pH gradients can be predicted from their amino acid sequences. *Electrophoresis*, **14**:1023-1031.
- EMBOSS data were from release 5.0 and were still the same in release 6.6 <http://emboss.sourceforge.net/apps/release/6.6/emboss/apps/iep.html> last visited 2016-06-03.
- Murray, R.K., Granner, D.K., Rodwell, V.W. (2006) *Harper's illustrated Biochemistry*. 27th edition. Published by The McGraw-Hill Companies.
- Sillero, A., Maldonado, A. (2006) Isoelectric point determination of proteins and other macromolecules: oscillating method. *Comput Biol Med.*, **36**:157-166.
- Solomon, T.W.G. (1998) *Fundamentals of Organic Chemistry*, 5th edition. Published by Wiley.
- Stryer L. (1999) *Biochemia*. czwarta edycja. Wydawnictwo Naukowe PWN.
- citation("seqinr")

## Examples

```
data(pK)
data(SEQINR.UTIL) # for N and C terminal pK values
prot <- s2c("ACDEFGHIKLMNPQRSTVWY")
compoAA <- table(factor(prot, levels = LETTERS))
nTermR <- which(LETTERS == prot[1])
cTermR <- which(LETTERS == prot[length(seq)])

computeCharge <- function(pH, compoAA, pK, nTermResidue, cTermResidue){
  cter <- 10^(-SEQINR.UTIL$pk[cTermResidue,1]) /
    (10^(-SEQINR.UTIL$pk[cTermResidue,1]) + 10^(-pH))
  nter <- 10^(-pH) / (10^(-SEQINR.UTIL$pk[nTermResidue,2]) + 10^(-pH))
  carg <- as.vector(compoAA['R'] * 10^(-pH) / (10^(-pK['R']) + 10^(-pH)))
  chis <- as.vector(compoAA['H'] * 10^(-pH) / (10^(-pK['H']) + 10^(-pH)))
  clys <- as.vector(compoAA['K'] * 10^(-pH) / (10^(-pK['K']) + 10^(-pH)))
  casp <- as.vector(compoAA['D'] * 10^(-pK['D']) / (10^(-pK['D']) + 10^(-pH)))
  cglu <- as.vector(compoAA['E'] * 10^(-pK['E']) / (10^(-pK['E']) + 10^(-pH)))
  ccys <- as.vector(compoAA['C'] * 10^(-pK['C']) / (10^(-pK['C']) + 10^(-pH)))
  ctyr <- as.vector(compoAA['Y'] * 10^(-pK['Y']) / (10^(-pK['Y']) + 10^(-pH)))
  charge <- carg + clys + chis + nter - (casp + cglu + ctyr + ccys + cter)
  return(charge)
}

pHseq <- seq(from = 0, to = 14, by = 0.1)
Bje <- pK$Bjellqvist
names(Bje) <- rownames(pK)
res <- computeCharge(pHseq, compoAA, Bje, nTermR, cTermR)
```

```

plot(pHseq, res, type = "l", ylab = "Charge", las = 1,
     main = paste("Charge of protein\n", c2s(prot)),
     xlab = "pH")
for(j in 2:ncol(pK)){
  src <- pK[,j]
  names(src) <- rownames(pK)
  res <- computeCharge(pHseq, compoAA, src, nTermR, cTermR)
  lines(pHseq, res, lty = j, col = rainbow(5)[j])
}

abline(h=0)
abline(v=computePI(prot))
legend("bottomleft", inset = 0.01, colnames(pK), lty = 1:6, col = c("black", rainbow(5)))

```

plot.SeqAcnucWeb

*To Plot Subsequences on the Parent Sequence***Description**

This function plots all the type of subsequences on a parent sequence. Subsequences are represented by colored rectangle on the parent sequence. For example, types could be CDS, TRNA, RRNA .... In order to get all the types that are available for the selected database, use `getType`.

**Usage**

```

## S3 method for class 'SeqAcnucWeb'
plot(x, types = getType()$sname, socket = autosocket(), ...)

```

**Arguments**

<code>x</code>	A sequence of class <code>SeqAcnucWeb</code>
<code>types</code>	The type of subsequences to plot. Default value is to consider all possible sub-sequence types.
<code>socket</code>	an object of class <code>sockconn</code> connecting to a remote ACNUC database (default is a socket to the last opened database).
<code>...</code>	not currently used

**Value**

An invisible list giving, for each subsequence, its position on the parent sequence.

**Author(s)**

D. Charif, J.R. Lobry

**References**

<http://doua.prabi.fr/databases/acnuc.html>  
 citation("seqinr")

**See Also**[getType](#), [query](#)**Examples**

```
## Not run:
### Need internet connection
choosebank("emblTP")
mylist <- query("mylist", "AC=AB078009")
plot(mylist$req[[1]])

## End(Not run)
```

plotabif

*Electrophoregram plot for ABIF data***Description**

Simple chromatogram plot for data imported with the [read.abif](#) function.

**Usage**

```
plotabif(abifdata,
  chanel = 1,
  tmin = 1/tscale,
  tmax = abifdata$Data[["SCAN.1"]]/tscale,
  tscale = 1000,
  yscale = 1000, type = "l", las = 1,
  xlab = paste("Time", tscale, sep = "/"),
  ylab = paste("RFU", yscale, sep = "/"),
  irange = (tmin*tscale):(tmax*tscale),
  x = irange/tscale,
  xlim = c(tmin, tmax),
  chanel.names = c(1:4,105),
  DATA = paste("DATA", chanel.names[chanel], sep = "."),
  y = abifdata$Data[[DATA]][irange]/yscale,
  ylim = c(min(y), max(y)),
  dyn = abifdata$Data[[paste("DyeN", chanel, sep = ".")]],
  main = paste(deparse(substitute(abifdata)), chanel, dyn, sep = " ; "),
  calibr = NULL,
  ladder.bp = NULL,
  allele.names = "identifiler",
  ladder.lab = TRUE,
  ...)
```

**Arguments**

abifdata	the result returned by <a href="#">read.abif</a>
chanel	the dye number
tmin	scaled starting time for the time axis
tmax	scaled ending time for the time axis
tscale	scale factor for the time axis
yscale	scale factor for the y-axis (RFU)
type	type of line drawing forwarded to <a href="#">plot</a>
las	orientation of axis labels forwarded to <a href="#">plot</a>
xlab	x-axis label forwarded to <a href="#">plot</a>
ylab	y-axis label forwarded to <a href="#">plot</a>
irange	indices of data to be plotted
x	values used for the x-axis
xlim	limits for the x-axis forwarded to <a href="#">plot</a>
chanel.names	numbers extensions used for the DATA
DATA	names of the DATA components
y	values used for the y-axis
ylim	limits for the y-axis forwarded to <a href="#">plot</a>
dyn	dye name
main	title for the plot forwarded to <a href="#">plot</a>
calibr	an optional calibration function to convert time into bp
ladder.bp	an optional ladder scale in bp (calibr must be provided)
allele.names	name of the dataset with allele names
ladder.lab	logical: should allele names be added on plot
...	arguments forwarded to <a href="#">plot</a>

**Value**

Returns invisibly its local graphical parameter settings.

**Author(s)**

J.R. Lobry

**References**

`citation("seqinr")`

**See Also**

function [read.abif](#) to import files in ABIF format, data [gs500liz](#) for internal size standards, data [identifiler](#) for allele names in the allelic ladder, data [JLO](#) for an example of an individual sample file, data [ECH](#) for an example of an allelic ladder.

## Examples

```
data(ECH)
plotabif(ECH,channel = 1, tmin = 3.2, tmax = 6.1)
```

---

plotladder

*Simple plot of an allelic ladder from ABIF data*

---

## Description

Simple representation of an observed allelic ladder.

## Usage

```
plotladder(abifdata, channel, calibr, allele.names = "identifiler", npeak = NULL, ...)
```

## Arguments

abifdata	the result returned by <a href="#">read.abif</a>
channel	the dye number
calibr	a mandatory calibration function to convert time into bp
allele.names	name of the dataset which contains allele names as in <code>link{identifiler}</code>
npeak	expected number of peaks, deduced from <code>allele.names</code> by default
...	arguments forwarded to <a href="#">peakabif</a>

## Value

Returns invisibly the location of peaks in bp.

## Author(s)

J.R. Lobry

## References

`citation("seqinr")`

## See Also

function [read.abif](#) to import files in ABIF format, [plotabif](#) to plot them, data [gs500liz](#) for internal size standards, data [identifiler](#) for allele names in the allelic ladder, data [JLO](#) for an example of an individual sample file, data [ECH](#) for an example of an allelic ladder.



**Examples**

```

#
# load an example of allelic ladder results from an ABIF (*.fsa) file:
#
data(ECH)
#
# Extract from internal size standard channel number 5 the location
# of 14 peaks:
#
ECH.maxis <- peakabif(ECH, 5, npeak = 14, tmin = 2.7, thres = 0.1, fig = FALSE)$maxis
#
# Load data about the expected size of peaks in bp for calibration:
#
data(gs500liz)
lizbp <- gs500liz$liz # All peaks size in bp
lizbp[!gs500liz$mask1 | !gs500liz$mask2] <- NA # Mark useless peaks
lizbp <- lizbp[-c(1,2)] # The first two peaks are not extracted from ECH
ECH.calibr <- splinefun(ECH.maxis[!is.na(lizbp)], lizbp[!is.na(lizbp)])
#
# Show the allelic ladder for the 4 dyes:
#
plotladder(ECH, 1, ECH.calibr, tmin = 3.1, thres = 0.3, fig = FALSE)
plotladder(ECH, 2, ECH.calibr, tmin = 3.1, thres = 0.35, fig = FALSE)
plotladder(ECH, 3, ECH.calibr, tmin = 3.1, thres = 0.2, fig = FALSE)
plotladder(ECH, 4, ECH.calibr, tmin = 3.1, thres = 0.2, fig = FALSE)

```

plotPanels

*Representation of Amplicon Size Ranges of a STR kit.***Description**

Plot amplicon size ranges grouped by dye color.

**Usage**

```
plotPanels(kitname, data, xlim = NULL, cex = 0.75, alpha = 0.5)
```

**Arguments**

kitname	string of characters for the kit name.
data	an output from the <a href="#">readPanels</a> function.
xlim	x-axis range.
cex	character expansion factor.
alpha	alpha transparency channel for colors.

**Value**

none

**Author(s)**

J.R. Lobry

**See Also**

[readPanels](#).

**Examples**

```
path1 <- system.file("abif/AmpFLSTR_Panels_v1.txt", package = "seqinr")
res1 <- readPanels(path1)

par(mfrow = c(2,1))
plotPanels("Identifiler_v1", res1)
plotPanels("SEfiler_v1", res1)
```

---

pmw	<i>Protein Molecular Weight</i>
-----	---------------------------------

---

**Description**

With default parameter values, returns the apparent molecular weight of one mole (6.0221415 e+23) of the input protein expressed in gram at sea level on Earth with terrestrial isotopic composition.

**Usage**

```
pmw(seqaa, Ar = c(C = 12.0107, H = 1.00794, O = 15.9994,
N = 14.0067, P = 30.973762, S = 32.065), gravity = 9.81,
unit = "gram", checkseqaa = TRUE)
```

**Arguments**

seqaa	a protein sequence as a vector of single chars. Allowed values are "*ACDE-FGHIKLMNPQRSTVWY", non allowed values are ignored.
Ar	a named vector for the mean relative atomic masses of CHONPS atoms. Defaults values are from the natural terrestrial sources according to the 43rd IUPAC General Assembly in Beijing, China in August 2005 (See <a href="http://iupac.org/category/recent-releases/">http://iupac.org/category/recent-releases/</a> for updates).
gravity	gravitational field constant in standard units. Defaults to 9.81 m/s2, that is to the average value at sea level on Earth. Negative values are not allowed.
unit	a string that could be "gram" to get the result in grams (1 g = 0.001 kg) or "N" to get the result in Newton units (1 N = 1 kg.m/s2).
checkseqaa	if TRUE pmw() warns if a non-allowed character in seqaa is found.

## Details

**Algorithm** Computing the molecular mass of a protein is close to a linear form on amino-acid frequencies, but not exactly since we have to remove  $n - 1$  water molecules for peptidic bound formation.

**Cysteine** All cysteines are supposed to be in reduced (-SH) form.

**Methionine** All methionines are supposed to be not oxidized.

**Modifications** No post-traductional modifications (such as phosphorylations) are taken into account.

**Rare** Rare amino-acids (pyrolysine and selenocysteine) are not handled.

**Warning** Do not use defaults values for Ar to compute the molecular mass of alien's proteins: the isotopic composition for CHONPS atoms could be different from terrestrial data in a xenobiotic context. Some aliens are easily offended, make sure not to initiate one more galactic war by reporting wrong results.

## Value

The protein molecular weight as a single numeric value.

## Author(s)

J.R. Lobry

## References

`citation("seqinr")`

## See Also

[s2c](#), [c2s](#), [aaa](#), [a](#)

## Examples

```
allowed <- s2c("*ACDEFGHIKLMNPQRSTVWY") # All allowed chars in a protein
pmw(allowed)
all.equal(pmw(allowed), 2395.71366) # Should be true on most platforms
#
# Compute the apparent molecular weight on Moon surface:
#
pmw(allowed, g = 1.6)
#
# Compute the apparent molecular weight in absence of gravity:
#
pmw(allowed, g = 0) # should be zero
#
# Reports results in Newton units:
#
pmw(allowed, unit = "N")
#
# Compute the mass in kg of one mol of this protein:
```

```
#
pmw(allowed)/10^3
#
# Compute the mass for all amino-acids:
#
sapply(allowed[-1], pmw) -> aamw
names(aamw) <- aaa(names(aamw))
aamw
```

---

prepgetannots

*Select annotation lines in an ACNUC database*


---

## Description

This function is called before using [getAnnot](#) or [modifylist](#) with a scan type operation to select the annotation lines to be returned or scanned.

## Usage

```
prepgetannots(what = "all", setfor = c("scan", "getannots"),
              socket = autosocket(), verbose = FALSE)
pga(what = "all", setfor = c("scan", "getannots"),
    socket = autosocket(), verbose = FALSE)
```

## Arguments

what	the default "all" means that all annotation lines are selected. This can be more specific, see details.
setfor	this is used when what has its default "all" value. The behaviour is different for <a href="#">getAnnot</a> and <a href="#">modifylist</a> with a scan type operation: annotations but not sequences are scanned, but sequences can be returned by <a href="#">getAnnot</a> . The default value is "scan".
socket	an object of class sockconn connecting to an ACNUC server
verbose	logical, if TRUE mode verbose is on

## Details

The names of annotation lines in the opened ACNUC database is returned by [countfreelists](#), they are forced to upper case letters by prepgetannots when supplied with the what argument.

For the EMBL/SWISSPROT format, keys are: ALL, AC, DT, KW, OS, OC, OG, OH, RN, RC, RP, RX, RA, RG, RT, RL, DR, AH, AS, CC, FH, FT, SQ, SEQ.

For GenBank: ALL, ACCESSION, VERSION, KEYWORDS, SOURCE, ORGANISM, REFERENCE, AUTHORS, CONSRTM, TITLE, JOURNAL, PUBMED, REMARK, COMMENT, FEATURES, ORIGIN, SEQUENCE.

For FT (embl, swissprot) and FEATURES (GenBank), one or more specific feature keys can be specified using lines with only uppercase and such as

**FEATURES|CDS FT|TRNA**

Keys ALL and SEQ/SEQUENCE stand for all annotation and sequence lines, respectively. For the scan operation, key ALL stand for the DE/DEFINITION lines, and SEQ/SEQUENCE cannot be used (annotations but not sequence are scanned).

**Value**

The function returns invisibly the annotation lines names.

**Author(s)**

J.R. Lobry

**References**

`citation("seqinr")`

**See Also**

`getAnnot`, `modifylist`, `countfreelists`

**Examples**

```
## Not run: # Need internet connection
choosebank("genbank")
mylist <- query("mylist", "n=AQF16SRRN")
pga() # We want to scan all annotations, including FEATURES
mylist <- modifylist("mylist", operation = "strain", type = "scan")
mylist$nelem # should be 1

## End(Not run)
```

---

prettyseq

*Text representation of a sequence from an ACNUC server*

---

**Description**

To get a text representation of sequence of rank num and of its subsequences, with bpl bases per line (default = 60), and with optional translation of protein-coding subsequences

**Usage**

```
prettyseq(num, bpl = 60, translate = TRUE, socket = autosocket())
```

**Arguments**

num	rank of the sequence in the ACNUC database
bpl	number of base per line
translate	should coding sequences be translated?
socket	an object of class sockconn connecting to a remote ACNUC database (default is a socket to the last opened database).

**Value**

An invisible vector of string. The output is redirected to the console.

**Author(s)**

J.R. Lobry

**References**

<http://doua.prabi.fr/databases/acnuc.html>  
citation("seqinr")

**See Also**

[choosebank](#), [query](#)

**Examples**

```
## Not run:  
### Need internet connection  
choosebank("emblTP")  
prettyseq(111)  
  
## End(Not run)
```

---

print.qaw

*Print method for objects from class qaw*

---

**Description**

Print the number of elements, their type and the corresponding query.

**Usage**

```
## S3 method for class 'qaw'  
print(x, ...)
```

**Arguments**

x	A objet of class qaw
...	not used

**Value**

None.

**Author(s)**

J.R. Lobry

**References**

citation("seqinr")

**See Also**

[print](#)

**Examples**

```
## Not run:
### Need internet connection
choosebank("emblTP")
list1 <- query("sp=felis catus")
list1
# 4732 SQ for sp=felis catus

## End(Not run)
```

---

print.SeqAcnucWeb	<i>Print method for objects from class SeqAcnucWeb</i>
-------------------	--

---

**Description**

Print the name, length, frame and genetic code number.

**Usage**

```
## S3 method for class 'SeqAcnucWeb'
print(x, ...)
```

**Arguments**

x	A sequence of class SeqAcnucWeb
...	Arguments passed to print

**Value**

None.

**Author(s)**

J.R. Lobry

**References**

`citation("seqinr")`

**See Also**

`print`

**Examples**

```
## Not run:
### Need internet connection
choosebank("emblTP")
mylist <- query("mylist", "sp=felis catus")
mylist$req[[1]]
#      name      length      frame      ncbicg
# "A06937"      "34"      "0"      "1"

## End(Not run)
```

---

prochlo	<i>Zscore on three strains of Prochlorococcus marinus</i>
---------	---

---

**Description**

This dataset contains the zscores computed with the codon model on all CDS from 3 strains of Prochlorococcus marinus (as retrieved from Genome Reviews database on June 16, 2005)

**Usage**

`data(prochlo)`

**Format**

List of three dataframes of the zscore of each of the 16 dinucleotides on each CDS retrieved from the specific strain.

**BX548174** strain adapted to living at a depth of 5 meters (high levels of UV exposure) base model on each intergenic sequence

**AE017126** strain adapted to living at a depth of 120 meters (low levels of UV exposure)

**BX548175** strain adapted to living at a depth of 135 meters (low levels of UV exposure)



## References

Palmeira, L., Guéguen, L. and Lobry JR. (2006) UV-targeted dinucleotides are not depleted in light-exposed Prokaryotic genomes. *Molecular Biology and Evolution*, **23**:2214-2219.  
<http://mbe.oxfordjournals.org/cgi/reprint/23/11/2214>

```
citation("seqinr")
```

## See Also

[zscore](#)

## Examples

```
#
# Show the four YpY for the three ecotypes:
#
data(prochlo)
oneplot <- function(x){
  plot(density(prochlo$BX548174[, x]),
       ylim = c(0,0.4), xlim = c(-4,4), lty=3,
       main = paste(substr(x,1,1), "p", substr(x,2,2), " bias", sep = ""),
       xlab="",ylab="",las=1, type = "n")
  rect(-10,-1,-1.96,10, col = "yellow", border = "yellow")
  rect(1.96,-1,10,10, col = "yellow", border = "yellow")
  lines(density(prochlo$BX548174[, x]),lty=3)
  lines(density(prochlo$AE017126[, x]),lty=2)
  lines(density(prochlo$BX548175[, x]),lty=1)
  abline(v=c(-1.96,1.96),lty=5)
  box()
}
par(mfrow=c(2,2),mar=c(2,3,2,0.5) + 0.1)
oneplot("CT")
oneplot("TC")
oneplot("CC")
oneplot("TT")
#
# Show YpY biases with respect to light exposure
#
curdev <- getOption("device")
OK <- FALSE
devlist <- c("X11", "windows", "quartz") # interactive with width and height in inches
for(i in devlist){
  if(exists(i) && identical(get(i), curdev)){
    OK <- TRUE
    break
  }
}
if(OK){
  curdev(width = 18, height = 11)
  par(oma = c(0, 0, 3, 0), mfrow = c(1, 2), mar = c(5, 4, 0, 0), cex = 1.5)
```

```

example(waterabs, ask = FALSE) #left figure

par(mar = c(5, 0, 0, 2))
plot(seq(-5, 3, by = 1), seq(0, 150, length = 9), col = "white",
     ann = FALSE, axes = FALSE, xaxs = "i", yaxs = "i")
axis(1, at = c(-1.96, 0, 1.96), labels = c(-1.96, 0, 1.96))
lines(rep(-1.96, 2), c(0, 150), lty=2)
lines(rep(1.96, 2), c(0, 150), lty=2)
title(xlab = "zscore distribution", cex = 1.5, adj = 0.65)

selcol <- c(6, 8, 14, 16)
z5 <- prochlo$BX548174[, selcol]
z120 <- prochlo$AE017126[, selcol]
z135 <- prochlo$BX548175[, selcol]

todo <- function(who, xx, col = "black", bottom, loupe){
  dst <- density(who[, xx])
  sel <- which(dst$x >= -3)
  lines(dst$x[sel], dst$y[sel]*loupe + (bottom), col = col)
}

todo2 <- function(who, bottom, loupe){
  todo(who, "CC", "blue", bottom, loupe)
  todo(who, "CT", "red", bottom, loupe)
  todo(who, "TC", "green", bottom, loupe)
  todo(who, "TT", "black", bottom, loupe)
}

todo3 <- function(bottom, who, leg, loupe = 90){
  lines(c(-5,-3), c(150 - leg, bottom + 20))
  rect(-3,bottom,3,bottom+40)
  text(-2.6,bottom+38, paste(leg, "m"))
  todo2(who, bottom, loupe)
}

todo3(bottom = 110, who = z5, leg = 5)
todo3(bottom = 50, who = z120, leg = 120)
todo3(bottom = 5, who = z135, leg = 135)

legend(-4.5,110,c('CpC', 'CpT', 'TpC', 'TpT'),lty=1,pt.cex=cex,
      col=c('blue', 'red', 'green', 'black'))

mtext(expression(paste("Dinucleotide composition for three ",
  italic("Prochlorococcus marinus"), " ecotypes")), outer = TRUE, cex = 2, line = 1)
}

```

---

query

---

*To get a list of sequence names from an ACNUC data base located on the web*


---

## Description

This is a major command of the package. It executes all sequence retrievals using any selection criteria the data base allows. The sequences are coming from ACNUC data base located on the web

and they are transferred by socket. The command produces the list of all sequence names that fit the required criteria. The sequence names belong to the class of sequence SeqAcnucWeb.

### Usage

```
query(listname, query, socket = autosocket(),
invisible = TRUE, verbose = FALSE, virtual = FALSE)
```

### Arguments

listname	The name of the list as a quoted string of chars
query	A quoted string of chars containing the request with the syntax given in the details section
socket	an object of class sockconn connecting to a remote ACNuc database (default is a socket to the last opened database).
invisible	if FALSE, the result is returned visibly.
verbose	if TRUE, verbose mode is on
virtual	if TRUE, no attempt is made to retrieve the information about all the elements of the list. In this case, the req component of the list is set to NA.

### Details

The query language defines several selection criteria and operations between lists of elements matching criteria. It creates mainly lists of sequences, but also lists of species (or, more generally, taxa) and of keywords. See <http://doua.prabi.fr/databases/acnuc/cfonctions.html#QUERYLANGUAGE> for the last update of the description of the query language.

Selection criteria (no space before the = sign) are:

**SP=taxon** seqs attached to taxon or any other below in tree; @ wildcard possible

**TID=id** seqs attached to given numerical NCBI's taxon id

**K=keyword** seqs attached to keyword or any other below in tree; @ wildcard possible

**T=type** seqs of specified type

**J=journalname** seqs published in journal specified using defined journal code

**R=refcode** seqs from reference specified such as in jcode/volume/page (e.g., JMB/13/5432)

**AU=name** seqs from references having specified author (only last name, no initial)

**AC=accessionno** seqs attached to specified accession number

**N=seqname** seqs of given name (ID or LOCUS); @ wildcard possible

**Y=year** seqs published in specified year; > and < can be used instead of =

**O=organelle** seqs from specified organelle named following defined code (e.g., chloroplast)

**M=molecule** seqs from specified molecule as named in ID or LOCUS annotation records

**ST=status** seqs from specified data class (EMBL) or review level (UniProt)

**F=filename** seqs whose names are in given file, one name per line (unimplemented use [clfcd](#) instead)

**FA=filename** seqs attached to accession numbers in given file, one number per line (unimplemented use **clfcd** instead)

**FK=filename** produces the list of keywords named in given file, one keyword per line (unimplemented use **clfcd** instead)

**FS=filename** produces the list of species named in given file, one species per line (unimplemented use **clfcd** instead)

**listname** the named list that must have been previously constructed

Operators (always followed and preceded by blanks or parentheses) are:

**AND** intersection of the 2 list operands

**OR** union of the 2 list operands

**NOT** complementation of the single list operand

**PAR** compute the list of parent seqs of members of the single list operand

**SUB** add subsequences of members of the single list operand

**PS** project to species: list of species attached to member sequences of the operand list

**PK** project to keywords: list of keywords attached to member sequences of the operand list

**UN** unproject: list of seqs attached to members of the species or keywords list operand

**SD** compute the list of species placed in the tree below the members of the species list operand

**KD** compute the list of keywords placed in the tree below the members of the keywords list operand

The query language is case insensitive. Three operators (AND, OR, NOT) can be ambiguous because they can also occur within valid criterion values. Such ambiguities can be solved by encapsulating elementary selection criteria between escaped double quotes.

## Value

The result is directly assigned to the object `listname` in the user workspace. This is an object of class `qaw`, a list with the following 6 components:

<code>call</code>	the original call
<code>name</code>	the ACNUC list name
<code>nelem</code>	the number of elements (for instance sequences) in the ACNUC list
<code>typelist</code>	the type of the elements of the list. Could be <code>SQ</code> for a list of sequence names, <code>KW</code> for a list of keywords, <code>SP</code> for a list of species names.
<code>req</code>	a list of sequence names that fit the required criteria or <code>NA</code> when called with parameter <code>virtual</code> is <code>TRUE</code>
<code>socket</code>	the socket connection that was used

## Note

Most of the documentation was imported from ACNUC help files written by Manolo Gouy

## Author(s)

J.R. Lobry, D. Charif

## References

To get the release date and content of all the databases located at the pbi, please look at the following url: <http://doua.prabi.fr/search/releases>

Gouy, M., Milleret, F., Mugnier, C., Jacobzone, M., Gautier, C. (1984) ACNUC: a nucleic acid sequence data base and analysis system. *Nucl. Acids Res.*, **12**:121-127.

Gouy, M., Gautier, C., Attimonelli, M., Lanave, C., Di Paola, G. (1985) ACNUC - a portable retrieval system for nucleic acid sequence databases: logical and physical designs and usage. *Comput. Appl. Biosci.*, **3**:167-172.

Gouy, M., Gautier, C., Milleret, F. (1985) System analysis and nucleic acid sequence banks. *Biochimie*, **67**:433-436.

```
citation("seqinr")
```

## See Also

[choosebank](#), [getSequence](#), [getName](#), [crelistfromclientdata](#)

## Examples

```
## Not run:
# Need internet connection
choosebank("genbank")
bb <- query("bb", "sp=Borrelia burgdorferi")
# To get the names of the 4 first sequences:
sapply(bb$req[1:4], getName)
# To get the 4 first sequences:
sapply(bb$req[1:4], getSequence, as.string = TRUE)

## End(Not run)
```

---

read.abif

---

*Read ABIF formatted files*


---

## Description

ABIF stands for Applied Biosystem Inc. Format, a binary format modeled after TIFF format. Corresponding files usually have an \*.ab1 or \*.fsa extension.

## Usage

```
read.abif(filename, max.bytes.in.file = file.info(filename)$size,
  pied.de.pilote = 1.2, verbose = FALSE)
```

## Arguments

filename            The name of the file.  
 max.bytes.in.file        The size in bytes of the file, defaulting to what is returned by `file.info`  
 pied.de.pilote    Safety factor: the argument `n` to `readBin` is set as `pied.de.pilote*max.bytes.in.file`.  
 verbose            logical [FALSE]. If TRUE verbose mode is on.

## Details

All data are imported into memory, there is no attempt to read items on the fly.

## Value

A list with three components: Header which is a list that contains various low-level information, among which `numelements` is the number of elements in the directory and `dataoffset` the offset to find the location of the directory. Directory is a data.frame for the directory of the file with the number of row being the number of elements in the directory and the 7 columns describing various low-level information about the elements. Data is a list with the number of components equal to the number of elements in the directory.

## Author(s)

J.R. Lobry

## References

`citation("seqinR")`

Anonymous (2006) Applied Biosystem Genetic Analysis Data File Format. Available at [http://www.appliedbiosystems.com/support/software\\_community/ABIF\\_File\\_Format.pdf](http://www.appliedbiosystems.com/support/software_community/ABIF_File_Format.pdf). Last visited on 03-NOV-2008.

The figure in the example section is an attempt to reproduce figure 1A from:

Krawczyk, J., Goesmann, A., Nolte, R., Werber, M., Weisshaar, B. (2009) Trace2PS and FSA2PS: two software toolkits for converting trace and fsa files to PostScript format. *Source Code for Biology and Medicine*, 4:4.

## See Also

`readBin` which is used here to import the binary file and `file.info` to get the size of the file. See `JL0` for the files used in quality check.

## Examples

```
#
# Quality check:
#

data(JL0)
JL0.check <- read.abif(system.file("abif/2_FAC321_0000205983_B02_004.fsa",
```

```

    package = "seqinr"))
stopifnot(identical(JL0, JL0.check))

#
# Try to reproduce figure 1A from Krawczyk et al. 2009:
#

Krawczyk <- read.abif(system.file("abif/samplefsa2ps.fsa",
    package = "seqinr"))$Data
x <- 1:length(Krawczyk[["DATA.1"]])
par(mar = c(2,4,2,0)+0.1, cex = 0.5)
plot(x, Krawczyk[["DATA.1"]], type = "l", col = "blue",
     ylab = "", xlab = "",
     ylim = c(-2000, 10000), cex = 0.5,
     main = "Figure 1A from Krawczyk et al. 2009",
     xaxs = "i", yaxs = "i",
     xaxt = "n", yaxt = "n")
axis(1, at = seq(2000, 24000, by = 2000))
axis(2, at = seq(-1000, 10000, by = 1000), las = 1)
lines(x, Krawczyk[["DATA.2"]], col = "green")
lines(x, Krawczyk[["DATA.3"]], col = "black")
lines(x, Krawczyk[["DATA.4"]], col = "red")

```

---

read.alignment	<i>Read aligned sequence files in mase, clustal, phylip, fasta or msf format</i>
----------------	--

---

## Description

Read a file in mase, clustal, phylip, fasta or msf format. These formats are used to store nucleotide or protein multiple alignments.

## Usage

```
read.alignment(file, format, forceToLower = TRUE)
```

## Arguments

file	the name of the file which the aligned sequences are to be read from. If it does not contain an absolute or relative path, the file name is relative to the current working directory, <a href="#">getwd</a> .
format	a character string specifying the format of the file : mase, clustal, phylip, fasta or msf
forceToLower	a logical defaulting to TRUE stating whether the returned characters in the sequence should be in lower case (introduced in seqinR release 1.1-3).

## Details

**"mase"** The mase format is used to store nucleotide or protein multiple alignments. The beginning of the file must contain a header containing at least one line (but the content of this header may be empty). The header lines must begin by ; ; . The body of the file has the following structure: First, each entry must begin by one (or more) commentary line. Commentary lines begin by the character ; . Again, this commentary line may be empty. After the commentaries, the name of the sequence is written on a separate line. At last, the sequence itself is written on the following lines.

**"clustal"** The CLUSTAL format (\*.aln) is the format of the ClustalW multialignment tool output. It can be described as follows. The word CLUSTAL is on the first line of the file. The alignment is displayed in blocks of a fixed length, each line in the block corresponding to one sequence. Each line of each block starts with the sequence name (maximum of 10 characters), followed by at least one space character. The sequence is then displayed in upper or lower cases, '-' denotes gaps. The residue number may be displayed at the end of the first line of each block.

**"msf"** MSF is the multiple sequence alignment format of the GCG sequence analysis package. It begins with the line (all uppercase) !!NA\\_MULTIPLE\\_ALIGNMENT 1.0 for nucleic acid sequences or !!AA\\_MULTIPLE\\_ALIGNMENT 1.0 for amino acid sequences. Do not edit or delete the file type if its present.(optional). A description line which contains informative text describing what is in the file. You can add this information to the top of the MSF file using a text editor.(optional) A dividing line which contains the number of bases or residues in the sequence, when the file was created, and importantly, two dots (..) which act as a divider between the descriptive information and the following sequence information.(required) msf files contain some other information: the Name/Weight, a Separating Line which must include two slashes (//) to divide the name/weight information from the sequence alignment.(required) and the multiple sequence alignment.

**"phylip"** PHYLIP is a tree construction program. The format is as follows: the number of sequences and their length (in characters) is on the first line of the file. The alignment is displayed in an interleaved or sequential format. The sequence names are limited to 10 characters and may contain blanks.

**"fasta"** Sequence in fasta format begins with a single-line description (distinguished by a greater-than (>) symbol), followed by sequence data on the next line.

## 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)

D. Charif, J.R. Lobry



## References

`citation("seqinr")`

## See Also

To read aligned sequences in NEXUS format, see the function `read.nexus` that was available in the `CompPairWise` package (not sure it is still maintained as of 09/09/09). The NEXUS format was mainly used by the non-GPL commercial PAUP software.

Related functions: [as.matrix.alignment](#), [read.fasta](#), [write.fasta](#), [reverse.align](#), [dist.alignment](#).

## Examples

```
mase.res <- read.alignment(file = system.file("sequences/test.mase", package = "seqinr"),
  format = "mase")
clustal.res <- read.alignment(file = system.file("sequences/test.aln", package = "seqinr"),
  format="clustal")
phylip.res <- read.alignment(file = system.file("sequences/test.phylip", package = "seqinr"),
  format = "phylip")
msf.res <- read.alignment(file = system.file("sequences/test.msf", package = "seqinr"),
  format = "msf")
fasta.res <- read.alignment(file = system.file("sequences/Anouk.fasta", package = "seqinr"),
  format = "fasta")

#
# Quality control routine sanity checks:
#

data(mase); stopifnot(identical(mase, mase.res))
data(clustal); stopifnot(identical(clustal, clustal.res))
data(phylip); stopifnot(identical(phylip, phylip.res))
data(msf); stopifnot(identical(msf, msf.res))
data(fasta); stopifnot(identical(fasta, fasta.res))
```

---

<code>read.fasta</code>	<i>read FASTA formatted files</i>
-------------------------	-----------------------------------

---

## Description

Read nucleic or amino-acid sequences from a file in FASTA format.

## Usage

```
read.fasta(file = system.file("sequences/ct.fasta.gz", package = "seqinr"),
  seqtype = c("DNA", "AA"), as.string = FALSE, forceDNAtolower = TRUE,
  set.attributes = TRUE, legacy.mode = TRUE, seqonly = FALSE, strip.desc = FALSE,
  bfa = FALSE, sizeof.longlong = .Machine$sizeof.longlong,
  endian = .Platform$endian, apply.mask = TRUE)
```

## Arguments

file	The name of the file which the sequences in fasta format are to be read from. If it does not contain an absolute or relative path, the file name is relative to the current working directory, <a href="#">getwd</a> . The default here is to read the <code>ct.fasta.gz</code> file which is present in the <code>sequences</code> folder of the <code>seqinR</code> package.
seqtype	the nature of the sequence: DNA or AA, defaulting to DNA
as.string	if TRUE sequences are returned as a string instead of a vector of single characters
forcedNAtolower	whether sequences with <code>seqtype == "DNA"</code> should be returned as lower case letters
set.attributes	whether sequence attributes should be set
legacy.mode	if TRUE lines starting with a semicolon ';' are ignored
seqonly	if TRUE, only sequences are returned without attempt to modify them or to get their names and annotations (execution time is divided approximately by a factor 3)
strip.desc	if TRUE the '>' at the beginning of the description lines is removed in the annotations of the sequences
bfa	logical. If TRUE the fasta file is in MAQ binary format (see details). Only for DNA sequences.
sizeof.longlong	the number of bytes in a C long long type. Only relevant for <code>bfa = TRUE</code> . See <a href="#">.Machine</a>
endian	character string, "big" or "little", giving the endianness of the processor in use. Only relevant for <code>bfa = TRUE</code> . See <a href="#">.Platform</a>
apply.mask	logical defaulting to TRUE. Only relevant for <code>bfa = TRUE</code> . When this flag is TRUE the mask in the MAQ binary format is used to replace non acgt characters in the sequence by the <code>n</code> character. For pure acgt sequences (without gaps or ambiguous bases) turning this to FALSE will save time.

## Details

FASTA is a widely used format in biology, some FASTA files are distributed with the `seqinR` package, see the examples section below. Sequence in FASTA format begins with a single-line description (distinguished by a greater-than '>' symbol), followed by sequence data on the next lines. Lines starting by a semicolon ';' are ignored, as in the original FASTA program (Pearson and Lipman 1988). The sequence name is just after the '>' up to the next space ' ' character, trailing infos are ignored for the name but saved in the annotations.

There is no standard file extension name for a FASTA file. Commonly found values are `.fasta`, `.fas`, `.fa` and `.seq` for generic FASTA files. More specific file extension names are also used for fasta sequence alignment (`.fsa`), fasta nucleic acid (`.fna`), fasta functional nucleotide (`.ffn`), fasta amino acid (`.faa`), multiple protein fasta (`.mpfa`), fasta RNA non-coding (`.frn`).

The MAQ fasta binary format was introduced in `seqinR` 1.1-7 and has not been extensively tested. This format is used in the MAQ (Mapping and Assembly with Qualities) software (<http://maq.sourceforge.net/>). In this format the four nucleotides are coded with two bits and the sequence

is stored as a vector of C unsigned long long. There is in addition a mask to locate non-acgt characters.

### Value

By default read.fasta return a list of vector of chars. Each element is a sequence object of the class SeqFastadna or SeqFastaAA.

### Note

The old argument File that was deprecated since seqinR >= 1.1-3 is no more valid since seqinR >= 2.0-6. Just use file instead.

### Author(s)

D. Charif, J.R. Lobry

### References

Pearson, W.R. and Lipman, D.J. (1988) Improved tools for biological sequence comparison. *Proceedings of the National Academy of Sciences of the United States of America*, **85**:2444-2448

According to MAQ's FAQ page <http://maq.sourceforge.net/faq.shtml> last consulted 2016-06-07 the MAQ manuscript has not been published.

citation("seqinr")

### See Also

[write.fasta](#) to write sequences in a FASTA file, [gb2fasta](#) to convert a GenBank file into a FASTA file, [read.alignment](#) to read aligned sequences, [reverse.align](#) to get an alignment at the nucleic level from the one at the amino-acid level

### Examples

```
#
# Simple sanity check with a small FASTA file:
#
smallFastaFile <- system.file("sequences/smallAA.fasta", package = "seqinr")
mySmallProtein <- read.fasta(file = smallFastaFile, as.string = TRUE, seqtype = "AA")[[1]]
stopifnot(mySmallProtein == "SEQINRSEQINRSEQINRSEQINR*")
#
# Simple sanity check with the gzipped version of the same small FASTA file:
#
smallFastaFile <- system.file("sequences/smallAA.fasta.gz", package = "seqinr")
mySmallProtein <- read.fasta(file = smallFastaFile, as.string = TRUE, seqtype = "AA")[[1]]
stopifnot(mySmallProtein == "SEQINRSEQINRSEQINRSEQINR*")
#
# Example of a DNA file in FASTA format:
#
dnafile <- system.file("sequences/malM.fasta", package = "seqinr")
#
# Read with defaults arguments, looks like:
```

```

#
# $XYLEECOM.MALM
# [1] "a" "t" "g" "a" "a" "a" "a" "t" "g" "a" "a" "t" "a" "a" "a" "a" "g" "t"
# ...
read.fasta(file = dnafile)
#
# The same but do not turn the sequence into a vector of single characters, looks like:
#
# $XYLEECOM.MALM
# [1] "atgaaaatgaataaaaagtctcatcgtcctctgtttatcagcagggttactggcaagcgc
# ...
read.fasta(file = dnafile, as.string = TRUE)
#
# The same but do not force lower case letters, looks like:
#
# $XYLEECOM.MALM
# [1] "ATGAAAATGAATAAAAAGTCTCATCGTCCTCTGTTTATCAGCAGGGTTACTGGCAAGC
# ...
read.fasta(file = dnafile, as.string = TRUE, forceDNAtolower = FALSE)
#
# Example of a protein file in FASTA format:
#
aafile <- system.file("sequences/seqAA.fasta", package = "seqinr")
#
# Read the protein sequence file, looks like:
#
# $A06852
# [1] "M" "P" "R" "L" "F" "S" "Y" "L" "L" "G" "V" "W" "L" "L" "L" "S" "Q" "L"
# ...
read.fasta(aafile, seqtype = "AA")
#
# The same, but as string and without attributes, looks like:
#
# $A06852
# [1] "MPRLFSYLLGVWLLLSQLPREIPGQSTNDFIKACGRELVRLWVEICGSVSWGRTALSLEEP
# QLETGPPAETMPSSITKDAEILKMMLEFVPNLPQELKATLSERQPSLRELQQSASKDSNLNFEFEK
# KIILNRQNEAEDKSLLLEKLNGLDKHSRKKRLFRMTLSEKCCQVGCIRKDIARLC*"
#
read.fasta(aafile, seqtype = "AA", as.string = TRUE, set.attributes = FALSE)
#
# Example with a FASTA file that contains comment lines starting with
# a semicolon character ';'
#
legacyfile <- system.file("sequences/legacy.fasta", package = "seqinr")
legacyseq <- read.fasta(file = legacyfile, as.string = TRUE)
stopifnot( nchar(legacyseq) == 921 )
#
# Example of a MAQ binary fasta file produced with maq fasta2bfa ct.fasta ct.bfa
# on a platform where .Platform$endian == "little" and .Machine$sizeof.longlong == 8
#
fastafile <- system.file("sequences/ct.fasta.gz", package = "seqinr")
bfafile <- system.file("sequences/ct.bfa", package = "seqinr")

```

```

original <- read.fasta(fastafile, as.string = TRUE, set.att = FALSE)
bfavers <- read.fasta(bfafile, as.string = TRUE, set.att = FALSE, bfa = TRUE,
  endian = "little", sizeof.longlong = 8)
if(!identical(original, bfavers)){
  warning(paste("trouble reading bfa file on a platform with endian =",
    .Platform$endian, "and sizeof.longlong =", .Machine$sizeof.longlong))
}

```

---

readBins

---

*Import GenMapper Bins configuration file*


---

## Description

In a Bins configuration file there is a description for a given identification kit of the expected allele sizes for all the markers available in the kit.

## Usage

```

readBins(file,
  colnames = c("allele.name", "size.bp", "minus.bp", "plus.bp"))

```

## Arguments

file	The name of the Bins configuration file.
colnames	The names to be used for the columns of the data.frames.

## Details

The expected allele sizes are typically plus or minus 0.5 bp.

## Value

A list whose first element is the file header info and following elements are lists, one for each kit encountered in the file. For each kit we have a list of data.frames, one per marker.

## Author(s)

J.R. Lobry

## References

citation("seqinR")

## See Also

[readPanels.](#)

## Examples

```
#
# Check that we can read the 2 exemple files in the seqinR package:
#
path1 <- system.file("abif/AmpFLSTR_Bins_v1.txt", package = "seqinr")
resbin1 <- readBins(path1)
path2 <- system.file("abif/Promega_Bins_v1.txt", package = "seqinr")
resbin2 <- readBins(path2)
#
# Show the kits described in resbin1:
#
names(resbin1)
#
# Show the markers in a given kit:
#
names(resbin1[["Identifiler_v1"]])
#
# Show alleles expected sizes for a given marker:
#
resbin1[["Identifiler_v1"]][["D8S1179"]]
#
# Simple quality check since seqinr 2.0-4 with a configuration file
# containing trailing tabulations:
#
path3 <- system.file("abif/Prototype_PowerPlex_EP01_Bins.txt", package = "seqinr")
resbin3 <- readBins(path3)
ncols <- sapply(resbin3[[2]], ncol)
stopifnot(all(ncols == 4))
```

---

readfirstrec	<i>Low level function to get the record count of the specified ACNUC index file</i>
--------------	---

---

## Description

Called without arguments, the list of available values for argument type is returned.

## Usage

```
readfirstrec(socket = autosocket(), type)
```

## Arguments

socket	an object of class sockconn connecting to a remote ACNUC database (default is a socket to the last opened database).
type	the ACNUC index file

## Details

Available index files are:

**AUT** AUTHOR one record for each author name (last name only, no initials)

**BIB** BIBLIO one record for each reference

**ACC** ACCESS one record for each accession number

**SMJ** SMJYT one record for each status, molecule, journal, year, type, organelle, division, and db structure information

**SUB** SUBSEQ one record for each parent or sub-sequence

**LOC** LOCUS one record for each parent sequence

**KEY** KEYWORDS one record for each keyword

**SPEC** SPECIES one record for each taxon

**SHRT** SHORTL mostly, one record for each element of a short list

**LNG** LONGL one record for each group of SUBINLNG elements of a long list

**EXT** EXTRACT (for nucleotide databases only) one record for each exon of each subsequence

**TXT** TEXT one lrtxt-character record for each label of a species, keyword, or SMJYT

## Value

The record count of ACNUC index file, or NA if missing (typically when asking for type = EXT on a protein database).

## Author(s)

J.R. Lobry

## References

See ACNUC physical structure at <http://doua.prabi.fr/databases/acnuc/structure.html>.

`citation("seqinr")`

## See Also

[choosebank](#)

## Examples

```
## Not run:
# Need internet connection
choosebank("genbank")
allowedtype <- readfirstrec()
sapply(allowedtype, function(x) readfirstrec(type = x))

## End(Not run)
```

---

`readPanels`*Import GenMapper Panels configuration file*

---

### Description

In a Panel configuration file there is a description for a given identification kit of the marker names, their dye label color, expected size range, expected positive control genotypes, number of bases in core repeat, stutter percentages, and allele names.

### Usage

```
readPanels(file,  
  colnames = c("marker", "dye.col", "min.bp", "max.bp", "exp.pcg", "repeat.bp",  
    "stutter.pc", "uknw", "allele names"))
```

### Arguments

<code>file</code>	The name of the Panel configuration file.
<code>colnames</code>	The names to be used for the columns of the data.frames.

### Details

Number of bases in core repeat is set to 9 for Amelogenin locus.

### Value

A list whose first element is the file header info and following elements data.frames, one for each kit encountered in the file.

### Author(s)

J.R. Lobry

### References

`citation("seqinR")`

### See Also

[readBins](#), [plotPanels](#).



## Examples

```
#
# Check that we can read the 2 example files in the seqinR package:
#
path1 <- system.file("abif/AmpFLSTR_Panels_v1.txt", package = "seqinr")
res1 <- readPanels(path1)
path2 <- system.file("abif/Promega_Panels_v1.txt", package = "seqinr")
res2 <- readPanels(path2)
#
# Show the kits described in res1:
#
names(res1)
#
# Show some data for a given kit:
#
res1[["Identifiler_v1"]][, 1:7]
#
# Plot a simple summary of two kits:
#
par(mfrow = c(2,1))
plotPanels("Identifiler_v1", res1)
plotPanels("PowerPlex_16_v1", res2)

#
# Simple quality check since seqinR 2.0-4 with a file which containing
# a non constant number of tabulations as separator:
#
path3 <- system.file("abif/Prototype_PowerPlex_EP01_Pa.txt", package = "seqinr")
res3 <- readPanels(path3)
```

---

readsmj

*Low level function to read ACNUC SMJYT index files*


---

## Description

Extract informations from the SMJYT index file for status, molecule, journal, year, type, organelle, division, and db structure information.

## Usage

```
readsmj(socket = autosocket(), num = 2, nl = 10, recnum.add = FALSE, nature.add = TRUE,
plong.add = FALSE, libel.add = FALSE, sname.add = FALSE, all.add = FALSE)
```

## Arguments

socket	an object of class sockconn connecting to a remote ACNUC database (default is a socket to the last opened database).
num	rank number of first record.

<code>n1</code>	number of records to read.
<code>recnum.add</code>	to extract record numbers.
<code>nature.add</code>	to extract as a factor with human understandable levels the nature of the name. Unordered levels are: status, molecule, journal, year, type, organelle, division and dbstrucinfo.
<code>plong.add</code>	to extract the plong.
<code>libel.add</code>	to extract the label of the name.
<code>sname.add</code>	to extract the short version of the name, that is without the first two characters.
<code>all.add</code>	to extract all (all flags set to TRUE).

**Value**

A data.frame with requested columns.

**Author(s)**

J.R. Lobry

**References**

See ACNUC physical structure at: <http://doua.prabi.fr/databases/acnuc/structure.html>.

`citation("seqinr")`

**See Also**

[choosebank](#) to start a session and [readfirstrec](#) to get the total number of records.

---

rearranged.oriloc	<i>Detection of replication-associated effects on base composition asymmetry in prokaryotic chromosomes.</i>
-------------------	--

---

**Description**

Detection of replication-associated effects on base composition asymmetry in prokaryotic chromosomes.

**Usage**

```
rearranged.oriloc(seq.fasta = system.file("sequences/ct.fasta.gz", package = "seqinr"),
  g2.coord = system.file("sequences/ct.predict", package = "seqinr"))
```

## Arguments

<code>seq.fasta</code>	The path of the file containing a FASTA-format sequence. Default value: the FASTA sequence of the <i>Chlamydia trachomatis</i> chromosome.
<code>g2.coord</code>	The path of the file containing the coordinates of the protein coding genes found on this chromosome. This file can be obtained using the function <code>gbk2g2</code> . The format of the file is similar to the output of the Glimmer2 program. The first column contains the index or the name of the gene, the second one contains the start position and the third column contains the end position. For reverse transcribed genes, the start position is greater than the end position.

## Details

The purpose of this method is to decouple replication-related and coding sequence-related effects on base composition asymmetry. In order to do so, the analyzed chromosome is artificially rearranged to obtain a perfect gene orientation bias - all forward transcribed genes on the first half of the chromosome, and all reverse transcribed genes on the other half. This rearrangement conserves the relative order of genes within each of the two groups - both forward-encoded and reverse-encoded genes are placed on the rearranged chromosome in increasing order of their coordinates on the real chromosome. If the replication mechanism has a significant effect on base composition asymmetry, this should be seen as a change of slope in the nucleotide skews computed on the rearranged chromosome; the change of slope should take place at the origin or the terminus of replication. Use `extract.breakpoints` to detect the position of the changes in slope on the rearranged nucleotide skews.

## Value

A data.frame with six columns: `meancoord.rearr` contains the gene index on the rearranged chromosome; `gcskew.rearr` contains the normalized GC-skew  $((G-C)/(G+C))$  computed on the third codon positions of protein coding genes, still on the rearranged chromosome; `atskew.rearr` contains the normalized AT-skew  $((A-T)/(A+T))$  computed on the third codon positions of protein coding genes; `strand.rearr` contains the transcription strand of the gene (either "forward" or "reverse"); `order` contains the permutation that was used to obtain a perfect gene orientation bias; `meancoord.real` contains the mid-coordinate of the genes on the real chromosome (before the rearrangement).

## Author(s)

A. Necşulea

## References

Necşulea, A. and Lobry, J.R. (2007) A New Method for Assessing the Effect of Replication on DNA Base Composition Asymmetry. *Molecular Biology and Evolution*, **24**:2169-2179.

## See Also

[oriloc](#), [draw.rearranged.oriloc](#), [extract.breakpoints](#)

## Examples

```
### Example for Chlamydia trachomatis ###

### Rearrange the chromosome and compute the nucleotide skews ###

## Not run: r.ori <- rearranged.oriloc(seq.fasta =
  system.file("sequences/ct.fasta.gz", package = "seqinr"),
  g2.coord = system.file("sequences/ct.predict", package = "seqinr"))
## End(Not run)

### Extract the breakpoints for the rearranged nucleotide skews ###

## Not run: breaks <- extract.breakpoints(r.ori, type = c("gcfw", "gcrev"),
  nbreaks = c(2, 2), gridsize = 50, it.max = 100)
## End(Not run)

### Draw the rearranged nucleotide skews and place the position of the breakpoints ###
### on the graphics ###

## Not run: draw.rearranged.oriloc(r.ori, breaks.gcfw = breaks$gcfw$breaks,
  breaks.gcrev = breaks$gcrev$breaks)
## End(Not run)
```

---

recstat

*Prediction of Coding DNA Sequences.*

---

## Description

This function aims at predicting the position of Coding DNA Sequences (CDS) through the use of a Correspondence Analysis (CA) computed on codon composition, this for the three reading frames of a DNA strand.

## Usage

```
recstat(seq, sizewin = 90, shift = 30, seqname = "no name")
```

## Arguments

seq	a nucleic acid sequence as a vector of characters
sizewin	an integer, multiple of 3, giving the length of the sliding window
shift	an integer, multiple of 3, giving the length of the steps between two windows
seqname	the name of the sequence

## Details

The method is built on the hypothesis that the codon composition of a CDS is biased while it is not the case outside these regions. In order to detect such bias, a CA on codon frequencies is computed on the six possible reading frames of a DNA sequence (three from the direct strand and three from the reverse strand). When there is a CDS in one of the reading frame, it is expected that the CA factor scores observed in this frame (for both rows and columns) will be significantly different from those in the two others.

## Value

This function returns a list containing the following components:

<code>seq</code>	a single DNA sequence as a vector of characters
<code>sizewin</code>	length of the sliding window
<code>shift</code>	length of the steps between windows
<code>seqsize</code>	length of the sequence
<code>seqname</code>	name of the sequence
<code>vdep</code>	a vector containing the positions of windows starts
<code>vind</code>	a vector containing the reading frame of each window
<code>vstopd</code>	a vector of stop codons positions in direct strand
<code>vstopr</code>	a vector of stop codons positions in reverse strand
<code>vinitd</code>	a vector of start codons positions in direct strand
<code>vinitr</code>	a vector of start codons positions in reverse strand
<code>resd</code>	a matrix containing codons frequencies for all the windows in the three frames of the direct strand
<code>resr</code>	a matrix containing codons frequencies for all the windows in the three frames of the reverse strand
<code>resd.coa</code>	list of class <code>coa</code> and <code>dudi</code> containing the result of the CA computed on the codons frequencies in the direct strand
<code>resr.coa</code>	list of class <code>coa</code> and <code>dudi</code> containing the result of the CA computed on the codons frequencies in the reverse strand

## Note

This method works only with DNA sequences long enough to obtain a sufficient number of windows. As the optimal windows length has been estimated to be 90 bp by Fichant and Gautier (1987), the minimal sequence length is around 500 bp. The method can be used on prokaryotic and eukaryotic sequences. Also, only the four first factors of the CA are kept. Indeed, most of the time, only the first factor is relevant in order to detect CDS.

## Author(s)

O. Clerc, G. Perrière

## References

The original paper describing recstat is:

Fichant, G., Gautier, C. (1987) Statistical method for predicting protein coding regions in nucleic acid sequences. *Comput. Appl. Biosci.*, **3**, 287–295.

<http://bioinformatics.oxfordjournals.org/content/3/4/287.abstract>

## See Also

[draw.recstat](#), [test.li.recstat](#), [test.co.recstat](#)

## Examples

```
ff <- system.file("sequences/ECOUNC.fsa", package = "seqinr")
seq <- read.fasta(ff)
rec <- recstat(seq[[1]], seqname = getName(seq))
```

---

residuecount	<i>Total number of residues in an ACNUC list</i>
--------------	--

---

## Description

Computes the total number of residues (nucleotides or aminoacids) in all sequences of the list of specified rank.

## Usage

```
residuecount(lrank, socket = autosocket())
```

## Arguments

lrank	the list rank on the ACNUC server
socket	an object of class sockconn connecting to a remote ACNUC database (default is a socket to the last opened database).

## Value

A single numeric value corresponding to the total number of residues or NA in case of problem.

## Author(s)

J.R. Lobry

## References

<http://doua.prabi.fr/databases/acnuc.html>

`citation("seqinr")`

**See Also**

[choosebank](#), [query](#), [glr](#)

**Examples**

```
## Not run:
### Need internet connection
choosebank("emblTP")
mylist <- query("mylist", "t=CDS", virtual = TRUE)
stopifnot(residuecount(glr("mylist")) == 1611439240)
stopifnot(is.na(residuecount(glr("unknowlist")))) # A warning is issued

## End(Not run)
```

---

revaligntest

*Three aligned nucleic acid sequences*

---

**Description**

This dataset is used as a sanity check in [reverse.align](#).

**Usage**

```
data(revaligntest)
```

**Format**

An object of class alignment with 3 sequences.

**References**

```
citation("seqinr")
```

**See Also**

[reverse.align](#)

**Examples**

```
data(revaligntest)
```

---

reverse.align	<i>Reverse alignment - from protein sequence alignment to nucleic sequence alignment</i>
---------------	--

---

## Description

This function produces an alignment of nucleic protein-coding sequences, using as a guide the alignment of the corresponding protein sequences.

## Usage

```
reverse.align(nucl.file, protaln.file, input.format = 'fasta', out.file,
             output.format = 'fasta', align.prot = FALSE, numcode = 1,
             clustal.path = NULL, forceDNAtolower = TRUE, forceAAtolower = FALSE)
```

## Arguments

nucl.file	A character string specifying the name of the FASTA format file containing the nucleotide sequences.
protaIn.file	A character string specifying the name of the file containing the aligned protein sequences. This argument must be provided if align.prot is set to FALSE.
input.format	A character string specifying the format of the protein alignment file : 'mase', 'clustal', 'phylip', 'fasta' or 'msf'.
out.file	A character string specifying the name of the output file.
output.format	A character string specifying the format of the output file. Currently the only implemented format is 'fasta'.
align.prot	Boolean. If TRUE, the nucleic sequences are translated and then the protein sequences are aligned with the ClustalW program. The path of the ClustalW binary must also be given (clustal.path)
numcode	The NCBI genetic code number for the translation of the nucleic sequences. By default the standard genetic code is used.
clustal.path	The path of the ClustalW binary. This argument only needs to be set if align.prot is TRUE.
forceDNAtolower	logical passed to <a href="#">read.fasta</a> for reading the nucleic acid file.
forceAAtolower	logical passed to <a href="#">read.alignment</a> for reading the aligned protein sequence file.

## Details

This function an alignment of nucleic protein-coding sequences using as a guide the alignment of the corresponding protein sequences. The file containing the nucleic sequences is given in the compulsory argument 'nucl.file'; this file must be written in the FASTA format.

The alignment of the protein sequences can either be provided directly, through the 'protaIn.file' parameter, or reconstructed with ClustalW, if the parameter 'align.prot' is set to TRUE. In the latter case, the pathway of the ClustalW binary must be given in the 'clustal.path' argument.



The protein and nucleic sequences must have the same name in the files `nucl.file` and `protaln.file`.

The reverse-aligned nucleotide sequences are written to the file specified in the compulsory `'out.file'` argument. For now, the only output format implemented is FASTA.

Warning: the `'align.prot=TRUE'` option has only been tested on LINUX operating systems. ClustalW must be installed on your system in order for this to work.

**Value**

NULL

**Author(s)**

A. Necşulea

**References**

`citation('seqinr')`

**See Also**

[read.alignment](#), [read.fasta](#), [write.fasta](#)

**Examples**

```
#
# Read example 'bordetella.fasta': a triplet of orthologous genes from
# three bacterial species (Bordetella pertussis, B. parapertussis and
# B. bronchiseptica):
#

nucl.file <- system.file('sequences/bordetella.fasta', package = 'seqinr')
triplet <- read.fasta(nucl.file)

#
# For this example, 'bordetella.pep.aln' contains the aligned protein
# sequences, in the Clustal format:
#

protaln.file <- system.file('sequences/bordetella.pep.aln', package = 'seqinr')
triplet.pep<- read.alignment(protaln.file, format = 'clustal')

#
# Call reverse.align for this example:
#

reverse.align(nucl.file = nucl.file, protaln.file = protaln.file,
              input.format = 'clustal', out.file = 'test.revalign')

#
# Simple sanity check against expected result:
```

```
#

res.new <- read.alignment("test.realign", format = "fasta")
data(revaligntest)
stopifnot(identical(res.new, revaligntest))

#
# Alternatively, we can use ClustalW to align the translated nucleic
# sequences. Here the ClustalW program is accessible simply by the
# 'clustalw' name.
#

## Not run:
reverse.align(nucl.file = nucl.file, out.file = 'test.realign.clustal',
  align.prot = TRUE, clustal.path = 'clustalw')
## End(Not run)
```

---

rot13

*Ergheaf gur EBG-13 pvcurevat bs n fgevat*

---

## Description

rot13 applied to the above title returns the string "Returns the ROT-13 ciphering of a string".

## Usage

```
rot13(string)
```

## Arguments

string            a string of characters.

## Value

a string of characters.

## Author(s)

J.R. Lobry

## References

```
citation("seqinr")
```

## See Also

[chartr](#)

**Examples**

```
##
## Simple ciphering of a string:
##
message <- "Hello, world!"
rot13(message) # "Uryyb, jbeyq!"
##
## Routine sanity check:
##
stopifnot(identical(rot13(rot13(message)), message))
```

s2c

*conversion of a string into a vector of chars***Description**

This is a simple utility function to convert a single string such as "BigBang" into a vector of chars such as c("B", "i", "g", "B", "a", "n", "g").

**Usage**

```
s2c(string)
```

**Arguments**

string            a string of chars

**Value**

a vector of chars. If supplied argument is not a single string, a warning is issued and NA returned.

**Author(s)**

J.R. Lobry

**References**

citation("seqinr")

**See Also**

[c2s](#)

**Examples**

```
stopifnot(all(s2c("BigBang") == c("B", "i", "g", "B", "a", "n", "g")))
```

---

`s2n`*simple numerical encoding of a DNA sequence.*

---

**Description**

By default, if no `levels` arguments is provided, this function will just code your DNA sequence in integer values following the lexical order (`a > c > g > t`), that is 0 for "a", 1 for "c", 2 for "g", 3 for "t" and NA for ambiguous bases.

**Usage**

```
s2n(seq, levels = s2c("acgt"), base4 = TRUE, forceToLower = TRUE)
```

**Arguments**

<code>seq</code>	the sequence as a vector of single chars
<code>levels</code>	allowed char values, by default a, c, g and t
<code>base4</code>	if TRUE the numerical encoding will start at 0, if FALSE at 1
<code>forceToLower</code>	if TRUE the sequence is forced to lower case characters

**Value**

a vector of integers

**Note**

The idea of starting numbering at 0 by default is that it enforces a kind of isomorphism between the paste operator on DNA chars and the + operator on integer coding for DNA chars. By this way, you can work either in the char set, either in the integer set, depending on what is more convenient for your purpose, and then switch from one set to the other one as you like.

**Author(s)**

J.R. Lobry

**References**

`citation("seqinr")`

**See Also**

[n2s](#), [factor](#), [unclass](#)

## Examples

```
##
## Example of default behaviour:
##
urndna <- s2c("acgt")
seq <- sample( urndna, 100, replace = TRUE ) ; seq
s2n(seq)
##
## How to deal with RNA:
##
urnrna <- s2c("acgt")
seq <- sample( urnrna, 100, replace = TRUE ) ; seq
s2n(seq)
##
## what happens with unknown characters:
##
urnmess <- c(urndna,"n")
seq <- sample( urnmess, 100, replace = TRUE ) ; seq
s2n(seq)
##
## How to change the encoding for unknown characters:
##
tmp <- s2n(seq) ; tmp[is.na(tmp)] <- -1; tmp
##
## Simple sanity check:
##
stopifnot(all(s2n(s2c("acgt")) == 0:3))
```

---

savelist

---

*Save sequence names or accession numbers into a file*


---

## Description

This function retrieves all sequence names or all accession number from an ACNUC list and saves them into a file.

## Usage

```
savelist(lrank, type = c("N", "A"),
         filename = paste(gln(lrank), ifelse(type == "N", "mne", "acc"),
                           sep = "."), socket = autosocket(), warnme = TRUE)
```

## Arguments

lrank	the rank of the ACNUC list to consider.
type	use "N" for sequence names (mnemonics) and "A" for accession numbers. Default is "N".
filename	a string of character giving the name of the file to save results.

socket	an object of class sockconn connecting to a remote ACNUC database (default is a socket to the last opened database).
warnme	if TRUE a message is issued on the console when complete.

**Value**

none.

**Author(s)**

J.R. Lobry

**References**

<http://doua.prabi.fr/databases/acnuc.html>  
 citation("seqinr")

**See Also**

[choosebank](#), [query](#), [glr](#) to get a list rank from its name, [clfcd](#) for the inverse operation of [savelist](#)

**Examples**

```
## Not run:
### Need internet connection
choosebank("emblTP")
mylist <- query("mylist", "sp=felis catus et t=cds", virtual=TRUE)
savelist(glr("mylist"))
# 603 sequence mnemonics written into file: MYLIST.mne
savelist(glr("mylist"), type = "A")
# 603 sequence accession numbers written into file: MYLIST.acc

## End(Not run)
```

---

SeqAcnucWeb

---

*Sequence coming from a remote ACNUC data base*


---

**Description**

`as.SeqAcnucWeb` is called by many functions, for instance by `query`, and should not be directly called by the user. It creates an object of class `SeqAcnucWeb`. `is.SeqAcnucWeb` returns TRUE if the object is of class `SeqAcnucWeb`.

**Usage**

```
as.SeqAcnucWeb(object, length, frame, ncbigc)
is.SeqAcnucWeb(object)
```

**Arguments**

object	a string giving the name of a sequence present in the data base
length	a string giving the length of the sequence present in the data base
frame	a string giving the frame of the sequence present in the data base
ncbigc	a string giving the ncbi genetic code of the sequence present in the data base

**Value**

as.SeqAcnucWeb returns an object sequence of class SeqAcnucWeb. Note that as from seqinR 1.1-3 the slot socket has been deleted to save space for long lists.

**Author(s)**

D. Charif, J.R. Lobry

**References**

citation("seqinr")

**Examples**

```
## Not run: # Need internet connection
choosebank("emblTP")
mylist <- query("mylist", "sp=felis catus et t=cds et o=mitochondrion")
stopifnot(is.SeqAcnucWeb(mylist$req[[1]]))
closebank()

## End(Not run)
```

---

SeqFastaAA

*AA sequence in Fasta Format*


---

**Description**

as.SeqFastaAA is called by the function as.read.fasta. It creates an object of class SeqFastaAA. is.SeqFastaAA returns TRUE if the object is of class SeqFastaAA. summary.SeqFastaAA gives the AA composition of an object of class SeqFastaAA.

**Usage**

```
as.SeqFastaAA(object, name = NULL, Annot = NULL)
is.SeqFastaAA(object)
## S3 method for class 'SeqFastaAA'
summary(object,...)
```

**Arguments**

object	a vector of chars representing a biological sequence
name	NULL a character string specifying a name for the sequence
Annot	NULL a character string specifying some annotations for the sequence
...	additional arguments affecting the summary produced

**Value**

as.SeqFastaAA returns an object sequence of class SeqFastaAA. summary.SeqFastaAA returns a list which the following components:

composition	the AA counting of the sequence
AA.Property	the percentage of each group of amino acid in the sequence. By example, the groups are small, tiny, aliphatic, aromatic ...

**Author(s)**

D. Charif

**References**

citation("seqinr")

**Examples**

```
s <- read.fasta(file = system.file("sequences/seqAA.fasta", package = "seqinr"), seqtype="AA")
is.SeqFastaAA(s[[1]])
summary(s[[1]])
myseq <- s2c("MSPTAYRRGSPAFLV*")
as.SeqFastaAA(myseq, name = "myseq", Annot = "blablabla")
myseq
```

---

SeqFastadna

---

*Class for DNA sequence in Fasta Format*


---

**Description**

as.SeqFastadna is called by many functions as read.fasta. It creates an object of class SeqFastadna. is.SeqFastadna returns TRUE if the object is of class SeqFastadna. summary.SeqFastadna gives the base composition of an object of class SeqFastadna.

**Usage**

```
as.SeqFastadna(object, name = NULL, Annot = NULL)
is.SeqFastadna(object)
## S3 method for class 'SeqFastadna'
summary(object, alphabet = s2c("acgt"), ...)
```



Arguments

object	a vector of chars representing a biological sequence
name	NULL a character string specifying a name for the sequence
Annot	NULL a character string specifying some annotations for the sequence
...	additional arguments affecting the summary produced
alphabet	a vector of single characters

Value

as.SeqFastadna returns an object sequence of class SeqFastadna. summary.SeqFastadna returns a list which the following components:

length	the legth of the sequence
compo	the base counting of the sequence
GC	the percentage of G+C in the sequence

Author(s)

D. Charif

References

citation("seqinr")

Examples

```
s <- read.fasta(system.file("sequences/malM.fasta",package="seqinr"))
is.SeqFastadna(s[[1]])
summary(s[[1]])
myseq <- s2c("acgttgatgctagctagcatcgat")
as.SeqFastadna(myseq, name = "myseq", Annot = "blablabla")
myseq
```

---

SeqFrag	<i>Class for sub-sequences</i>
---------	--------------------------------

---

Description

as.SeqFrag is called by all methods of [getFrag](#), but not directly by the users. It creates an object sequence of class SeqFrag.

Usage

```
as.SeqFrag(object, begin, end, name)
is.SeqFrag(object)
```

Arguments

object	an object sequence of class seqFastadna, seqFastaAA, seqAcnucWeb or seqFrag
begin	the first base of the fragment to get
end	the last base of the fragment to get
name	the name of the sequence

Value

as.SeqFrag returns a biological sequence with the following attributes:

seqMother	the name of the sequence from which the sequence comes
begin	the position of the first base of the fragment on the mother sequence
end	the position of the last base of the fragment on the mother sequence
class	SeqFrag which is the classfor sub-sequence

is.SeqFrag returns TRUE if the object is of class Seqfrag.

Author(s)

D. Charif, J.R. Lobry

References

citation("seqinr")

See Also

[getFrag](#), [getLength](#), [getName](#), [getSequence](#), [getTrans](#)

Examples

```
s <- read.fasta(file = system.file("sequences/malM.fasta", package = "seqinr"))
getFrag(s[[1]], 1, 10)
```

---

SEQINR.UTIL	<i>utility data for seqinr</i>
-------------	--------------------------------

---

Description

This data set gives the genetics code, the name of each codon, the IUPAC one-letter code for aminoacids and the physico-chemical class of amino acid and the pK values of amino acids described in Bjellqvist *et al.* (1993).

**Format**

SEQINR.UTIL is a list containing the 4 following objects:

**CODES.NCBI** is a data frame containing the genetics code : The standard ('Universal') genetic code with a selection of non-standard codes.

**CODON.AA** is a three columns data frame. The first column is a factor containing the codon. The second column is a factor giving the aminoacids names for each codon. The last column is a factor giving the IUPAC one-letter code for aminoacids

**AA.PROPERTY** is a list giving the physico-chemical class of amino acid. The different classes are the following one : Tiny, Small, Aliphatic, Aromatic, Non.polar, Polar, Charged, Basic, Acidic

**pK** is a data frame. It gives the pK values of amino acids described in Bjellqvist *et al.* (1993) , which were defined by examining polypeptide migration between pH 4.5 to 7.3 in an immobilised pH gradient gel environment with 9.2M and 9.8M urea at 15 degree or 25 degree

**Source**

Data prepared by D. Charif.

The genetic codes have been taken from the ncbi database: <https://www.ncbi.nlm.nih.gov/Taxonomy/Utils/wprintgc.cgi>. Last visited on 2016-10-05 corresponding to last update of the Genetic Codes: April 30, 2013.

The IUPAC one-letter code for aminoacids is described at: <http://www.chem.qmul.ac.uk/iupac/AminoAcid/>. pK values of amino acids were taken from Bjellqvist et al.

Bjellqvist, B., Hughes, G.J., Pasquali, Ch., Paquet, N., Ravier, F., Sanchez, J.-Ch., Frutiger, S. & Hochstrasser, D.F.(1993) The focusing positions of polypeptides in immobilized pH gradients can be predicted from their amino acid sequences. *Electrophoresis*, **14**, 1023-1031.

**References**

`citation("seqinr")`

**Examples**

```
data(SEQINR.UTIL)
```

---

setlistname

*Sets the name of an ACNUC list identified by its rank*

---

**Description**

This is a low level function to set the name of a list from an ACNUC server. It should not be used directly by end users.

**Usage**

```
setlistname(lrank, name = "list1", socket = autosocket())
```

**Arguments**

lrank	the list rank on the ACNUC server
name	the name to use for this list
socket	an object of class sockconn connecting to a remote ACNUC database (default is a socket to the last opened database).

**Value**

A single numeric value corresponding to:

NA	Empty answer from server.
0	OK.
3	if another list with that name already existed and was deleted.
4	no list of rank lrank exists.

**Author(s)**

J.R. Lobry

**References**

<http://doua.prabi.fr/databases/acnuc.html>  
 citation("seqinr")

**See Also**

[choosebank](#), [query](#), [glr](#)

**Examples**

```
## Not run:
### Need internet connection
choosebank("emblTP")
mylist <- query("mylist", "sp=felis catus et t=CDS", virtual = TRUE)
# Change list name on server:
setlistname(lrank = glr("mylist"), name = "feliscatus") # 0, OK.
glr("mylist") # 0, list doesn't exist no more.
glr("feliscatus") # 2, this list exists.
# Note the danger here: the object mylist is still present in the user workspace
# while the corresponding list was deleted from server.

## End(Not run)
```

---

splitseq	<i>split a sequence into sub-sequences</i>
----------	--

---

**Description**

Split a sequence into sub-sequences of 3 (the default size) with no overlap between the sub-sequences.

**Usage**

```
splitseq(seq, frame = 0, word = 3)
```

**Arguments**

seq	a vector of chars
frame	an integer (0, 1, 2) giving the starting position to split the sequence
word	an integer giving the size of the sub-sequences

**Value**

This function returns a vector which contains the sub-sequences.

**Author(s)**

J.R. Lobry

**References**

`citation("seqinr")`

**See Also**

[split](#)

**Examples**

```
cds <- s2c("aacgttcaggtcgtcgctacgtactgttt")
#
# To obtain the codon sequence in frame 0:
#
stopifnot(identical(splitseq(cds),
  c("aac", "gtt", "gca", "ggt", "cgc", "tcg", "cta", "cgt", "agc", "tac", "tgt")))
#
# Show the effect of frame and word with a ten char sequence:
#
(tenchar <- s2c("1234567890"))
splitseq(tenchar, frame = 0)
splitseq(tenchar, frame = 1)
```

```
splitseq(tenchar, frame = 2)
splitseq(tenchar, frame = 0, word = 2)
splitseq(tenchar, frame = 0, word = 1)
```

---

**stresc***Utility function to escape LaTeX special characters present in a string*

---

## Description

This function returns a vector of strings in which LaTeX special characters are escaped, this was useful in conjunction with xtable.

## Usage

```
stresc(strings)
```

## Arguments

strings            A vector of strings to deal with.

## Value

Returns a vector of strings with escaped characters within each string.

## Author(s)

J.R. Lobry

## References

```
citation("seqinr")
```

## See Also

[s2c](#)

## Examples

```
stresc("MISC_RNA")
stresc(c("BB_0001", "BB_0002"))
```

---

stutterabif	<i>Stutter ratio estimation</i>
-------------	---------------------------------

---

## Description

This function tries to estimate the stutter ratio, either in terms of peak height ratios or peak surface ratio.

## Usage

```
stutterabif(abifdata, chanel, poswild, datapointbefore = 70,
  datapointafter = 20, datapointsigma = 3.5,
  chanel.names = c(1:4, 105), DATA = paste("DATA", chanel.names[chanel], sep = "."),
  maxrfu = 1000, method = "monoH.FC", pms = 6, fig = FALSE)
```

## Arguments

abifdata	the result returned by <a href="#">read.abif</a>
chanel	the dye number
poswild	the position in datapoint units of the allele at the origin of the stutter product, typically obtained after a call to <a href="#">peakabif</a>
datapointbefore	how many datapoints before poswild to be include in analysis
datapointafter	how many datapoints after poswild to be include in analysis
datapointsigma	initial guess for the standard deviation of a peak
chanel.names	numbers extensions used for the DATA
DATA	names of the DATA components
maxrfu	argument passed to <a href="#">baselineabif</a>
method	method to be used by <a href="#">splinefun</a>
pms	how many standard deviations (after gaussian fit) before and after the mean peak values should be considered for spline function interpolation
fig	should a summary plot be produced?

## Details

FIXME, See R code for now

## Value

A list with the following components:

rh	Stutter ratio computed as the height of the stutter divided by the height of its corresponding allele
rs	Stutter ratio computed as the surface of the stutter divided by the surface of its corresponding allele

h1	The height of the stutter with baseline at 0
h2	The height of the allele with baseline at 0
s1	The surface of the stutter
s2	The surface of the allele
p	A list of additional parameter that could be usesfull, see example

**Author(s)**

J.R. Lobry

**See Also**

[JL0](#) for a dataset example, [peakabif](#) to get an estimate of peak location.

**Examples**

```
#
# Load pre-defined dataset, same as what would be obtained with read.abif:
#

data(JL0)

#
# Get peak locations in the blue channel:
#

maxis <- peakabif(JL0, 1, npeak = 6, tmin = 3, fig = FALSE)$maxis

#
# Compute stutter ratio for first peak and ask for a figure:
#

tmp <- stutterabif(JL0, 1, maxis[1], fig = TRUE)

#
# Show in addition the normal approximation used at the stutter peak:
#

xx <- seq(tmp$p$mu1 - 6*tmp$p$sd1, tmp$p$mu1 + 6*tmp$p$sd1, le = 100)
lines(xx, tmp$p$p1*dnorm(xx, tmp$p$mu1, tmp$p$sd1), col = "darkgreen")

#
# Show in addition the normal approximation used at allele peak:
#

xx <- seq(tmp$p$mu2 - 6*tmp$p$sd2, tmp$p$mu2 + 6*tmp$p$sd2, le = 100)
lines(xx, tmp$p$p2*dnorm(xx, tmp$p$mu2, tmp$p$sd2), col = "darkgreen")
```



---

`swap`*Exchange two R objects*

---

**Description**

Exchange object `x` with object `y`.

**Usage**

```
swap(x, y)
```

**Arguments**

<code>x</code>	an R object
<code>y</code>	an R object

**Value**

none.

**Author(s)**

J.R. Lobry

**References**

```
citation("seqinr")
```

**See Also**

[move](#)

**Examples**

```
#
# Example in a new empty environment:
#
local({
  x <- 0:9
  y <- 10:19
  print(x)
  print(y)
  swap(x[1], y[2])
  print(x)
  print(y)
})
#
# Sanity check with a bubble sort:
#
```

```
bubble.sort <- function(tab, n = length(tab)){
  i <- 1
  while(i < n){
    if(tab[i + 1] < tab[i]){
      swap(tab[i], tab[i+1])
      i <- 1
    } else {
      i <- i+1
    }
  }
  return(tab)
}
set.seed(1)
x <- rnorm(10)
stopifnot(identical(sort(x), bubble.sort(x)))
```

---

syncodons	<i>Synonymous codons</i>
-----------	--------------------------

---

**Description**

Returns all synonymous codons for each codon given

**Usage**

```
syncodons(codons, numcode = 1)
```

**Arguments**

- codons           A sequence of codons as generated by splitseq
- numcode         The genetic code number as in translate

**Value**

a list containing, for each codon given (list tags), all synonymous codons (including the original one)

**Author(s)**

L. Palmeira, J.R. Lobry

**References**

```
citation("seqinr")
```

**See Also**

[synsequence](#)

**Examples**

```

#
# The four synonymous codons for Alanine in the standard genetic code:
#
syncodons("ggg")
#
# With a sequence:
#
toy cds <- s2c("tctgagcaaataaatcgg")
syncodons(splitseq(toy cds))
#
# Sanity check with the standard genetic code:
#
stdgencode <- structure(list(
  ttt = c("ttc", "ttt"),
  ttc = c("ttc", "ttt"),
  tta = c("cta", "ctc", "ctg", "ctt", "tta", "ttg"),
  ttg = c("cta", "ctc", "ctg", "ctt", "tta", "ttg"),
  tct = c("agc", "agt", "tca", "tcc", "tcg", "tct"),
  tcc = c("agc", "agt", "tca", "tcc", "tcg", "tct"),
  tca = c("agc", "agt", "tca", "tcc", "tcg", "tct"),
  tcg = c("agc", "agt", "tca", "tcc", "tcg", "tct"),
  tat = c("tac", "tat"),
  tac = c("tac", "tat"),
  taa = c("taa", "tag", "tga"),
  tag = c("taa", "tag", "tga"),
  tgt = c("tgc", "tgt"),
  tgc = c("tgc", "tgt"),
  tga = c("taa", "tag", "tga"),
  tgg = "tgg",
  ctt = c("cta", "ctc", "ctg", "ctt", "tta", "ttg"),
  ctc = c("cta", "ctc", "ctg", "ctt", "tta", "ttg"),
  cta = c("cta", "ctc", "ctg", "ctt", "tta", "ttg"),
  ctg = c("cta", "ctc", "ctg", "ctt", "tta", "ttg"),
  cct = c("cca", "ccc", "ccg", "cct"),
  ccc = c("cca", "ccc", "ccg", "cct"),
  cca = c("cca", "ccc", "ccg", "cct"),
  ccg = c("cca", "ccc", "ccg", "cct"),
  cat = c("cac", "cat"),
  cac = c("cac", "cat"),
  caa = c("caa", "cag"),
  cag = c("caa", "cag"),
  cgt = c("aga", "agg", "cga", "cgc", "cgg", "cgt"),
  cgc = c("aga", "agg", "cga", "cgc", "cgg", "cgt"),
  cga = c("aga", "agg", "cga", "cgc", "cgg", "cgt"),
  cgg = c("aga", "agg", "cga", "cgc", "cgg", "cgt"),
  att = c("ata", "atc", "att"),
  atc = c("ata", "atc", "att"),
  ata = c("ata", "atc", "att"),
  atg = "atg",
  act = c("aca", "acc", "acg", "act"),
  acc = c("aca", "acc", "acg", "act"),

```

```

aca = c("aca", "acc", "acg", "act"),
acg = c("aca", "acc", "acg", "act"),
aat = c("aac", "aat"),
aac = c("aac", "aat"),
aaa = c("aaa", "aag"),
aag = c("aaa", "aag"),
agt = c("agc", "agt", "tca", "tcc", "tcg", "tct"),
agc = c("agc", "agt", "tca", "tcc", "tcg", "tct"),
aga = c("aga", "agg", "cga", "cgc", "cgg", "cgt"),
agg = c("aga", "agg", "cga", "cgc", "cgg", "cgt"),
gtt = c("gta", "gtc", "gtg", "gtt"),
gtc = c("gta", "gtc", "gtg", "gtt"),
gta = c("gta", "gtc", "gtg", "gtt"),
gtg = c("gta", "gtc", "gtg", "gtt"),
gct = c("gca", "gcc", "gcg", "gct"),
gcc = c("gca", "gcc", "gcg", "gct"),
gca = c("gca", "gcc", "gcg", "gct"),
gcg = c("gca", "gcc", "gcg", "gct"),
gat = c("gac", "gat"),
gac = c("gac", "gat"),
gaa = c("gaa", "gag"),
gag = c("gaa", "gag"),
ggt = c("gga", "ggc", "ggg", "ggg"),
ggc = c("gga", "ggc", "ggg", "ggg"),
gga = c("gga", "ggc", "ggg", "ggg"),
ggg = c("gga", "ggc", "ggg", "ggg"),

.Names = c("ttt", "ttc", "tta", "ttg", "tct", "tcc", "tca", "tcg", "tat", "tac",
"taa", "tag", "tgt", "tgc", "tga", "tgg", "ctt", "ctc", "cta",
"ctg", "cct", "ccc", "cca", "ccg", "cat", "cac", "caa", "cag",
"cgt", "cgc", "cga", "cgg", "att", "atc", "ata", "atg", "act",
"acc", "aca", "acg", "aat", "aac", "aaa", "aag", "agt", "agc",
"aga", "agg", "gtt", "gtc", "gta", "gtg", "gct", "gcc", "gca",
"gcg", "gat", "gac", "gaa", "gag", "ggt", "ggc", "gga", "ggg"))
#
# Now the check:
#
currentresult <- syncodons(words(alphabet = s2c("tcag")))
stopifnot(identical(stdgencode, currentresult))

```

---

synsequence

*Random synonymous coding sequence generation*


---

## Description

Generates a random synonymous coding sequence, according to a certain codon usage bias

## Usage

```
synsequence(sequence, numcode = 1, ucoweight = NULL)
```

**Arguments**

sequence	A nucleic acids sequence
numcode	The genetic code number as in translate
ucoweight	A list of weights containing the desired codon usage bias as generated by ucoweight

**Value**

a sequence translating to the same protein sequence as the original one (cf. translate), but containing synonymous codons

**Author(s)**

L. Palmeira

**References**

`citation("seqinr")`

**See Also**

[ucoweight](#)

**Examples**

```
data(ec999)
sequence=ec999[1][[1]]
synsequence(sequence,1,ucoweight(sequence))
```

---

tablecode

*to plot genetic code as in textbooks*

---

**Description**

This function plots a genetic code table as in textbooks, that is following the order T > C > A > G so that synonymous codons are almost always in the same boxes.

**Usage**

```
tablecode(numcode = 1, urn.rna = s2c("TCAG"), dia = FALSE, latexfile = NULL,
label = latexfile, size = "normalsize", caption = NULL,
preaa = rep("", 64), postaa = rep("", 64),
precodon = preaa, postcodon = postaa)
```

**Arguments**

numcode	The genetic code number as in <code>translate</code>
urn.rna	The letters to display codons, use <code>s2c("UCAG")</code> if you want the code in terms of RNA sequence
latexfile	The name of a LaTeX file if you want to redirect the output
label	The label for the LaTeX table
size	The LaTeX size of characters for the LaTeX table
preaa	A string to insert before the amino-acid in the LaTeX table
postaa	A string to insert after the amino-acid in the LaTeX table
precodon	A string to insert before the codon in the LaTeX table
postcodon	A string to insert after the codon in the LaTeX table
caption	The caption of the LaTeX table
dia	to produce a yellow/blue plot for slides

**Details**

The codon order for `preaa`, `postaa`, `precodon`, and `postcodon` should be the same as in `paste(paste(rep(s2c("tcag"), e`

**Author(s)**

J.R. Lobry

**References**

`citation("seqinr")`

**See Also**

[translate](#), [syncodons](#)

**Examples**

```
#
# Show me the standard genetic code:
#

tablecode()
```

---

test.co.recstat	<i>Tests if regions located between Stop codons contain putative CDSs.</i>
-----------------	--

---

### Description

This test uses columns (codons) factor scores computed by recstat in order to determine if the regions located between two Stop codons correspond to putative CDSs.

### Usage

```
test.co.recstat(rec, fac = 1, length.min = 150, stop.max = 0.2, win.lim = 0.8,  
  direct = TRUE, level = 0.01)
```

### Arguments

rec	list of elements returned by recstat function.
fac	axis of the CA to use for test ( $4 \geq \text{fac} \geq 1$ ).
length.min	minimal length between two Stop codons.
stop.max	threshold for Stop codons relative position in a window to determine if this window can be used for test computation.
win.lim	minimum proportion of windows inside a region showing a p-value below the threshold for Kruskal-Wallis test.
direct	a logical for the choice of direct or reverse strand.
level	p-value threshold for Kruskal-Wallis test.

### Details

The test is computed for all windows located between two Stop codons separated by at least length.min nucleotides. For each window inside a region considered, a Kruskal-Wallis test is computed on the factor scores of the codons found in this window, this for the three possible reading frames. If a proportion of at least win.lim windows in the region reject the null hypothesis of means equality between the reading frames, then, there is a good probability that a CDS is located in the region.

Inside the first and the last windows of a region submitted to the test, the relative position of the two Stop codons is used to determine if those windows can be used in the analysis. If the first Stop is located within the stop.max fraction of the 5' end of the window, then this window is kept in the analysis. In the same way, if the second Stop is located within the stop.max fraction of the 3' end of the window, this window is also kept in the analysis.

### Value

The result is returned as a list containing three matrices (one for each reading frame). All matrices have the same structure, with rows corresponding to the regions between two Stop codons. Columns Start and End give the location of starting and ending positions of the region; and CDS is a binary indicator equal to 1 if a putative CDS is predicted, and to 0 if not.

Author(s)

O. Clerc, G. Perrière

See Also

[test.li.recstat](#)

Examples

```
ff <- system.file("sequences/ECOUNC.fsa", package = "seqinr")
seq <- read.fasta(ff)
rec <- recstat(seq[[1]], seqname = getName(seq))
test.co.recstat(rec)
```

---

test.li.recstat	<i>Tests if regions located between Stop codons contain putative CDSs.</i>
-----------------	--

---

Description

This test uses rows (windows) factor scores computed by recstat in order to determine if the regions located between two Stop codons correspond to putative CDSs.

Usage

```
test.li.recstat(rec, fac = 1, length.min = 150, stop.max = 0.2,
  direct = TRUE, level = 0.05)
```

Arguments

rec	list of elements returned by recstat function.
fac	axis of the CA to use for test ( $4 \geq \text{fac} \geq 1$ ).
length.min	minimal length between two Stop codons.
stop.max	threshold for Stop codons relative position in a window to determine if this window can be used for test computation.
direct	a logical for the choice of direct or reverse strand.
level	p-value threshold for t-test.

Details

The test is computed for all regions between two Stop codons separated by at least length.min nucleotides, this for the three possible reading frames of a DNA strand. For each region considered, two t-tests are computed for comparing the mean of the factor scores of the windows from the reading frame in which the region is located with the means of the factor scores from the corresponding windows in the two other reading frames. If both t-tests reject the null hypothesis of means equality, then there is a good probability that a CDS is located in the region.



Inside the first and the last windows of a region submitted to the test, the relative position of the two Stop codons is used to determine if those windows can be used in the analysis. If the first Stop is located within the `stop.max` fraction of the 5' end of the window, then this window is kept in the analysis. In the same way, if the second Stop is located within the `stop.max` fraction of the 3' end of the window, this window is also kept in the analysis.

### Value

The result is returned as a list containing three matrices (one for each reading frame). All matrices have the same structure, with rows corresponding to the regions between two Stop codons. Columns `Start` and `End` give the location of starting and ending positions of the region; `Mean_i` gives the mean of the factor scores for the windows located in the region, this for reading frame `i`; `t(i,j)` gives the p-value of the t-test computed between the means from reading frames `i` and `j`; and `CDS` is a binary indicator equal to 1 if a putative CDS is predicted, and to 0 if not.

### Author(s)

O. Clerc, G. Perrière

### See Also

[test.co.recstat](#)

### Examples

```
ff <- system.file("sequences/ECOUNC.fsa", package = "seqinr")
seq <- read.fasta(ff)
rec <- recstat(seq[[1]], seqname = getName(seq))
test.li.recstat(rec)
```

---

toyaa

*A toy example of amino-acid counts in three proteins*

---

### Description

This is a toy data set to illustrate the importance of metric choice.

### Usage

```
data(toyaa)
```

### Format

A data frame with 3 observations on the following 3 variables:

**Ala** Alanine counts

**Val** Valine counts

**Cys** Cysteine counts

**Source**

This toy example was inspired by Gautier, C: Analyses statistiques et évolution des séquences d'acides nucléiques. PhD thesis (1987), Université Claude Bernard - Lyon I.

**References**

```
citation("seqinr")
```

**Examples**

```
data(toyaa)
```

---

toycodon	<i>A toy example of codon counts in three coding sequences</i>
----------	--

---

**Description**

This is a toy data set to illustrate synonymous and non-synonymous codon usage analyses.

**Usage**

```
data(toyaa)
```

**Format**

A data frame with 3 observations (coding sequences) for 10 codons.

**Source**

Created for release 1.0-4 of seqinr's vignette.

**References**

```
citation("seqinr")
```

**Examples**

```
data(toycodon)
```

---

translate

---

*Translate nucleic acid sequences into proteins*


---

### Description

This function translates nucleic acid sequences into the corresponding peptide sequence. It can translate in any of the 3 forward or three reverse sense frames. In the case of reverse sense, the reverse-complement of the sequence is taken. It can translate using the standard (universal) genetic code and also with non-standard codes. Ambiguous bases can also be handled.

### Usage

```
translate(seq, frame = 0, sens = "F", numcode = 1, NAstring = "X", ambiguous = FALSE)
```

### Arguments

seq	the sequence to translate as a vector of single characters in lower case letters.
frame	Frame(s) (0,1,2) to translate. By default the frame 0 is used.
sens	Sense to translate: F for forward sense and R for reverse sense.
numcode	The ncbi genetic code number for translation. By default the standard genetic code is used.
NAstring	How to translate amino-acids when there are ambiguous bases in codons.
ambiguous	If TRUE, ambiguous bases are taken into account so that for instance GGN is translated to Gly in the standard genetic code.

### Details

The following genetic codes are described here. The number preceding each code corresponds to numcode.

- 1** standard
- 2** vertebrate.mitochondrial
- 3** yeast.mitochondrial
- 4** protozoan.mitochondrial+mycoplasma
- 5** invertebrate.mitochondrial
- 6** ciliate+dasycladaceal
- 9** echinoderm+flatworm.mitochondrial
- 10** euplotid
- 11** bacterial+plantplastid
- 12** alternativeyeast
- 13** ascidian.mitochondrial
- 14** alternativeflatworm.mitochondrial

- 15 blepharism
- 16 chlorophycean.mitochondrial
- 21 trematode.mitochondrial
- 22 scenedesmus.mitochondrial
- 23 thraustochytrium.mitochondria
- 24 Pterobranchia.mitochondrial
- 25 CandidateDivision.SR1+Gracilibacteria
- 26 Pachysolen.tannophilus

## Value

translate returns a vector of single characters containing the peptide sequence in the standard one-letter IUPAC code. Termination (STOP) codons are translated by the character '\*'.

## Author(s)

D. Charif, J.R. Lobry

## References

The genetic codes have been taken from the ncbi taxonomy database: <https://www.ncbi.nlm.nih.gov/Taxonomy/Utils/wprintgc.cgi>. Last update October 05, 2000.

The IUPAC one-letter code for aminoacids is described at: <http://www.chem.qmul.ac.uk/iupac/AminoAcid/>

citation("seqinr")

## See Also

Use `tolower` to change upper case letters into lower case letters. For coding sequences obtained from an ACNUC server with `query` it's better to use the function `getTrans` so that the relevant genetic code and the relevant frame are automatically used. The genetic codes are given in the object `SEQINR.UTIL`, a more human readable form is given by the function `tablecode`. Use `aaa` to get the three-letter code for amino-acids.

## Examples

```
##
## Toy CDS example invented by Leonor Palmeira:
##
toycds <- s2c("tctgagcaaataaatcgg")
translate(seq = toycds) # should be c("S", "E", "Q", "I", "N", "R")
##
## Toy CDS example with ambiguous bases:
##
toycds2 <- s2c("tcngarcarathaaycgn")
translate(toycds2) # should be c("X", "X", "X", "X", "X", "X")
translate(toycds2, ambiguous = TRUE) # should be c("S", "E", "Q", "I", "N", "R")
translate(toycds2, ambiguous = TRUE, numcode = 2) # should be c("S", "E", "Q", "X", "N", "R")
```

```
##
## Real CDS example:
##
realcds <- read.fasta(file = system.file("sequences/malM.fasta", package = "seqinr"))[[1]]
translate(seq = realcds)
# Biologically correct, only one stop codon at the end
translate(seq = realcds, frame = 3, sens = "R", numcode = 6)
# Biologically meaningless, note the in-frame stop codons

## Not run:
## Need internet connection.
## Translation of the following EMBL entry:
##
## FT      CDS                join(complement(153944..154157),complement(153727..153866),
## FT                                complement(152185..153037),138523..138735,138795..138955)
## FT                                /codon_start=1
## FT                                /db_xref="FLYBASE:FBgn0002781"
## FT                                /db_xref="GOA:Q86B86"
## FT                                /db_xref="TrEMBL:Q86B86"
## FT                                /note="mod(mdg4) gene product from transcript CG32491-RZ;
## FT                                trans splicing"
## FT                                /gene="mod(mdg4)"
## FT                                /product="CG32491-PZ"
## FT                                /locus_tag="CG32491"
## FT                                /protein_id="AA041581.1"
## FT                                /translation="MADDEQFSLCWNFNFTNLSAGFHESLCRGDLVDVSLAAEGQIVKA
## FT                                HRLVLSVCSPFFRKMFTQMPSTHAIIVFLNNVSHSALKDLIQFMYCGEVNVKQDALPAF
## FT                                ISTAESLQIKGLTDNDPAPQPPQESSPPPAAPHVQQQIPARVQRQQPRASARYKIET
## FT                                VDDGLGDEKQSTTQIVIQTAAAPQATIVQQQPQQAQQIQSQQLQTGTTTTATLVSTN
## FT                                KRSAQRSSLTPASSAGVKRSKTSTSANVMDPLDSTTETGATTTAQLVPQQITVQTSVV
## FT                                SAAEAKLHQSPQQVRQEEAEYIDLPMELPTKSEPDPYSEDHGDAAGDAEGTYVEDDTYG
## FT                                DMRYDDSYFTENEDAGNQTAANTSGGGVTATTSKAVVKQQSQNYSESSFVDTSGDQGNT
## FT                                EAQVTQHVRNCGPQMFLISRKGGTLLTINNFBVYRSNLKFFGKSNNILYWEVCQNRSVKC
## FT                                RSRLKTIGDDLVTNDVHNHMGDNKRIEAAKAAGMLIHKKLSSLTAADKIQGSWKMDTE
## FT                                GNPDHLPKM"
choosebank("emblTP")
trans <- query("trans", "N=AE003734.PE35")
getTrans(trans$req[[1]])
## Complex transsplicing operations, the correct frame and the correct
## genetic code are automatically used for translation into protein.

## End(Not run)
```

---

trimSpace

*Trim leading and/or trailing spaces in strings*


---

## Description

This function removes from a character vector the longest successive run of space characters starting at the beginning of the strings (leading space), or the longest successive run of space characters at the end of the strings (trailing space), or both (and this is the default behaviour).

**Usage**

```
trimSpace(x, leading = TRUE, trailing = TRUE, space = "[:space:]")
```

**Arguments**

x	a character vector
leading	logical defaulting to TRUE: should leading spaces be trimmed off?
trailing	logical defaulting to TRUE: should trailing spaces be trimmed off?
space	an extended regular expression defining space characters

**Details**

The default value for the space character definition is large: in addition to the usual space, other character such as the tabulation and newline character are considered as space characters. See extended regular expression for a complete list.

**Value**

a character vector with the same length as x.

**Author(s)**

J.R. Lobry

**References**

`citation("seqinr")`.

**See Also**

Extended regular expressions are described in [regular expression](#) (aka [regexp](#)).

**Examples**

```
#
# Simple use:
#
stopifnot( trimSpace("  seqinR  ") == "seqinR" )

#
# Basic use, remove space at both ends:
#
testspace <- c("  with leading space", "with trailing space  ", "  with both  ")
stopifnot(all( trimSpace(testspace) == c("with leading space",
                                         "with trailing space",
                                         "with both")))

#
# Remove only leading space:
#
```

```

stopifnot(all( trimSpace(testspace, trailing = FALSE) == c("with leading space",
                                                         "with trailing space  ",
                                                         "with both  ")))

#
# Remove only trailing space:
#
stopifnot(all( trimSpace(testspace, leading = FALSE) == c("  with leading space",
                                                         "with trailing space",
                                                         "  with both"))))

#
# This should do nothing:
#
stopifnot(all( trimSpace(testspace, leading = FALSE, trailing = FALSE) == testspace))

#
# How to use alternative space characters:
#
allspaces <- "\t\n\f\r seqinR \t\n\f\r"
stopifnot(trimSpace(allspaces) == "seqinR")
stopifnot(trimSpace(allspaces, space = "\t\n") == "\f\r seqinR \t\n\f\r")

```

uco

*Codon usage indices*

## Description

uco calculates some codon usage indices: the codon counts *eff*, the relative frequencies *freq* or the Relative Synonymous Codon Usage *rscu*.

## Usage

```
uco(seq, frame = 0, index = c("eff", "freq", "rscu"), as.data.frame = FALSE,
    NA.rscu = NA)
```

## Arguments

<code>seq</code>	a coding sequence as a vector of chars
<code>frame</code>	an integer (0, 1, 2) giving the frame of the coding sequence
<code>index</code>	codon usage index choice, partial matching is allowed. <i>eff</i> for codon counts, <i>freq</i> for codon relative frequencies, and <i>rscu</i> the RSCU index
<code>as.data.frame</code>	logical. If TRUE: all indices are returned into a data frame.
<code>NA.rscu</code>	when an amino-acid is missing, RSCU are no more defined and reported as missing values (NA). You can force them to another value (typically 0 or 1) with this argument.

## Details

Codons with ambiguous bases are ignored.

RSCU is a simple measure of non-uniform usage of synonymous codons in a coding sequence (Sharp *et al.* 1986). RSCU values are the number of times a particular codon is observed, relative to the number of times that the codon would be observed for a uniform synonymous codon usage (i.e. all the codons for a given amino-acid have the same probability). In the absence of any codon usage bias, the RSCU values would be 1.00 (this is the case for sequence cds in the exemple thereafter). A codon that is used less frequently than expected will have an RSCU value of less than 1.00 and vice versa for a codon that is used more frequently than expected.

Do not use correspondence analysis on RSCU tables as this is a source of artifacts (Perrière and Thioulouse 2002, Suzuki *et al.* 2008). Within-aminoacid correspondence analysis is a simple way to study synonymous codon usage (Charif *et al.* 2005). For an introduction to correspondence analysis and within-aminoacid correspondence analysis see the chapter titled *Multivariate analyses* in the seqinR manual that ships with the seqinR package in the **doc** folder. You can also use internal correspondence analysis if you want to analyze simultaneously a row-block structure such as the within and between species variability (Lobry and Chessel 2003).

If `as.data.frame` is FALSE, uco returns one of these:

**eff** a table of codon counts

**freq** a table of codon relative frequencies

**rscu** a numeric vector of relative synonymous codon usage values

If `as.data.frame` is TRUE, uco returns a data frame with five columns:

**aa** a vector containing the name of amino-acid

**codon** a vector containing the corresponding codon

**eff** a numeric vector of codon counts

**freq** a numeric vector of codon relative frequencies

**rscu** a numeric vector of RSCU index

## Value

If `as.data.frame` is FALSE, the default, a table for `eff` and `freq` and a numeric vector for `rscu`.  
If `as.data.frame` is TRUE, a data frame with all indices is returned.

## Author(s)

D. Charif, J.R. Lobry, G. Perrière



## References

```
citation("seqinr")
```

Sharp, P.M., Tuohy, T.M.F., Mosurski, K.R. (1986) Codon usage in yeast: cluster analysis clearly differentiates highly and lowly expressed genes. *Nucl. Acids. Res.*, **14**:5125-5143.

Perrière, G., Thioulouse, J. (2002) Use and misuse of correspondence analysis in codon usage studies. *Nucl. Acids. Res.*, **30**:4548-4555.

Lobry, J.R., Chessel, D. (2003) Internal correspondence analysis of codon and amino-acid usage in thermophilic bacteria. *Journal of Applied Genetics*, **44**:235-261. [http://jag.igr.poznan.pl/2003-Volume-44/2/pdf/2003\\_Volume\\_44\\_2-235-261.pdf](http://jag.igr.poznan.pl/2003-Volume-44/2/pdf/2003_Volume_44_2-235-261.pdf).

Charif, D., Thioulouse, J., Lobry, J.R., Perrière, G. (2005) Online Synonymous Codon Usage Analyses with the ade4 and seqinR packages. *Bioinformatics*, **21**:545-547. <https://pbil.univ-lyon1.fr/members/lobry/repro/bioinfo04/>.

Suzuki, H., Brown, C.J., Forney, L.J., Top, E. (2008) Comparison of Correspondence Analysis Methods for Synonymous Codon Usage in Bacteria. *DNA Research*, **15**:357-365. <http://dnaresearch.oxfordjournals.org/cgi/reprint/15/6/357>.

## Examples

```
## Show all possible codons:
words()

## Make a coding sequence from this:
(cds <- s2c(paste(words(), collapse = "")))

## Get codon counts:
uco(cds, index = "eff")

## Get codon relative frequencies:
uco(cds, index = "freq")

## Get RSCU values:
uco(cds, index = "rscu")

## Show what happens with ambiguous bases:
uco(s2c("aaannnttt"))

## Use a real coding sequence:
rcds <- read.fasta(file = system.file("sequences/ma1M.fasta", package = "seqinr"))[[1]]
uco( rcds, index = "freq")
uco( rcds, index = "eff")
uco( rcds, index = "rscu")
uco( rcds, as.data.frame = TRUE)
```

```
## Show what happens with RSCU when an amino-acid is missing:
ecolicgpe5 <- read.fasta(file = system.file("sequences/ecolicgpe5.fasta",package="seqinr"))[[1]]
uco(ecolicgpe5, index = "rscu")

## Force NA to zero:
uco(ecolicgpe5, index = "rscu", NA.rscu = 0)
```

---

ucoweight	<i>Weight of each synonymous codon</i>
-----------	--

---

**Description**

Returns a list containing, for each of the 20 amino acids + STOP codon, the codon usage bias of each of the synonymous codon according to a given codon sequence.

**Usage**

```
ucoweight(sequence, numcode = 1)
```

**Arguments**

sequence	A nucleic acids sequence
numcode	The genetic code number as in translate

**Value**

a list containing, for each of the 20 amino acids and STOP codon (list tags), the weight of each synonymous codon (including the original one).

**Author(s)**

L. Palmeira

**References**

```
citation("seqinr")
```

**See Also**

[synsequence](#)

**Examples**

```
data(ec999)
ucoweight(ec999[1][[1]])
```

---

waterabs*Light absorption by the water column*

---

## Description

The absorption of light by water is highly dependent on the wavelength, this dataset gives the absorption coefficients from 200 to 700 nm.

## Usage

```
data(waterabs)
```

## Format

A data.frame with 2 columns:

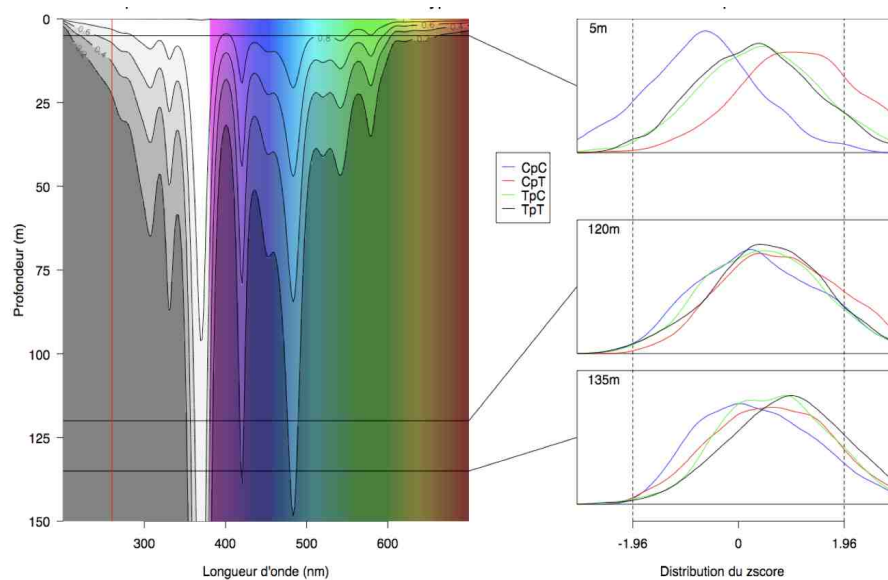
**lambda** wavelength in nm

**abs** absorption coefficient in 1/cm

## Source

Data were compiled by Palmeira (2007) from the cited references.

The example section allows to reproduce the left part of figure 2.7 from Palmeira (2007):



## References

Palmeira, L. (2007) *Analyse et modélisation des dépendances entre sites voisins dans l'évolution des séquences d'ADN*, PhD thesis, Université Claude Bernard - Lyon I.

Litjens R. A., Quickenden T. I. and Freeman C. G. (1999). Visible and near-ultraviolet absorption spectrum of liquid water. *Applied Optics*, **38**:1216-1223.

Quickenden T. I. & Irvin J. A. (1980). The ultraviolet absorption spectrum of liquid water. *The Journal of Chemical Physics*, **72**:4416-4428.

```
citation("seqinr")
```

## Examples

```
data(waterabs)

d <- 100*seq(from = 0, to = 150, by = 1) # depth in cm
lambda <- waterabs$lambda                # wavelength in nm
abs <- waterabs$absorption                # absorption coefficient cm-1
#
# Smooth signal with cubic splines
#
tmp <- spline(lambda, abs, n = 255)
lambda <- tmp$x
abs <- tmp$y

zun <- sapply(abs,function(x) 10^(-x*d))
z <- sapply(nrow(zun):1, function(x) zun[x,])
#
# Set up world coordinates:
#
plot.new()
plot.window(xlim = range(lambda), ylim = range(d), xaxs = "i", yaxs = "i")
#
# Annotate:
#
title(ylab = 'Depth under water surface (m)', xlab = "Wavelength (nm)",
main = "Light absorption by the water column")
axis(2 , at = seq(0, 15000, l = 7),
      labels = rev(c("0","25","50","75","100","125","150")), las = 1)
axis(1,at=(3:6)*100,labels= TRUE)
#
# Show me rainbow colors:
#
alpha <- 1
coul=c(rep(rgb(1,1,1, alpha = alpha), 181),
      rev(hsv(h=seq(0,5/6,l=320),alpha = alpha)))
rect(seq(200,699), 0, seq(201,700), 15000 , col = coul, border = coul)
#
# Grey scale:
```

```
#
  ngris <- 5
  image(x = lambda, y = d, z = z, col = rgb(1:ngris, 1:ngris, 1:ngris, alpha = 0.7*(ngris:1),
    max = ngris),
    axes = F, add = TRUE,
    breaks = seq(from = min(z), to = max(z), length = ngris + 1))

#
# Contour lines:
#
  contour(x = lambda, y = d, z = z, add = TRUE, drawlabels = TRUE, labcex = 0.75,
    col = 'black',
    levels = seq(from = min(z), to = max(z), length = ngris + 1))
  box()
```

---

where.is.this.acc	<i>Scans databases for a given sequence accession number</i>
-------------------	--

---

## Description

This function loops over all available ACNUC databases to look for a given sequence accession number. This is useful when you have a sequence accession number and you don't know in which database it is present.

## Usage

```
where.is.this.acc(acc, stopAtFirst = TRUE, ...)
```

## Arguments

acc	An accession number as a string of characters such as "NC_001416".
stopAtFirst	Logical. If TRUE, the default, the function stops at the first database where the accession number is found.
...	Arguments passed to the function <a href="#">choosebank</a> .

## Value

The function returns invisibly a vector of strings of characters for the names of the ACNUC databases in which the accession number was found.

## Author(s)

J.R. Lobry

## References

`citation("seqinr")`

**See Also**

[choosebank](#) to open a given ACNUC database.

**Examples**

```
## Not run: # Need internet connection
where.is.this.acc("NC_001416") # first found in phever2dna bank (2016-06-01)

## End(Not run)
```

---

words	<i>To get all words from an alphabet.</i>
-------	---

---

**Description**

Generates a vectors of all the words from a given alphabet, with right positions varying faster, for instance if the alphabet is `c("0", "1")` and the length is 2 you will obtain `c("00", "01", "10", "11")`

**Usage**

```
words(length = 3, alphabet = s2c("acgt"))
```

**Arguments**

- |          |                                       |
|----------|---------------------------------------|
| length   | the number of characters in the words |
| alphabet | a vector of characters                |

**Value**

A vector of string whith length characters.

**Author(s)**

J.R. Lobry

**References**

```
citation("seqinr")
```

**See Also**

[kronecker](#), [outer](#)

## Examples

```
#
# Get all 64 codons:
#
stopifnot(all(words() ==
c("aaa", "aac", "aag", "aat", "aca", "acc", "acg", "act", "aga", "agc", "agg",
  "agt", "ata", "atc", "atg", "att", "caa", "cac", "cag", "cat", "cca", "ccc",
  "ccg", "cct", "cga", "cgc", "cgg", "cgt", "cta", "ctc", "ctg", "ctt", "gaa",
  "gac", "gag", "gat", "gca", "gcc", "gcg", "gct", "gga", "ggc", "ggg", "ggg",
  "gta", "gtc", "gtg", "gtt", "taa", "tac", "tag", "tat", "tca", "tcc", "tcg",
  "tct", "tga", "tgc", "tgg", "tgt", "tta", "ttc", "ttg", "ttt")))
#
# Get all codons with u c a g for bases:
#
words(alphabet = s2c("ucag"))
#
# Get all tetranucleotides:
#
words(length = 4)
#
# Get all dipeptides:
#
words(length = 2, alphabet = a()[-1])
```

words.pos

*Positions of possibly degenerated motifs within sequences*

## Description

word.pos searches all the occurrences of the motif pattern within the sequence text and returns their positions. This function is based on regexp allowing thus for complex motif searches. The main difference with [gregexpr](#) is that non disjoint matches are reported here.

## Usage

```
words.pos(pattern, text, ignore.case = FALSE,
          perl = TRUE, fixed = FALSE, useBytes = TRUE, ...)
```

## Arguments

pattern	character string containing a <a href="#">regular expression</a> (or character string for fixed = TRUE) to be matched in the given character vector.
text	a character vector where matches are sought.
ignore.case	if FALSE, the pattern matching is case sensitive and if TRUE, case is ignored during matching.
perl	logical. Should perl-compatible regexps be used if available? Has priority over extended.

fixed	logical. If TRUE, pattern is a string to be matched as is. Overrides all conflicting arguments.
useBytes	logical. If TRUE the matching is done byte-by-byte rather than character-by-character.
...	arguments passed to <a href="#">regexpr</a> .

### Details

Default parameter values have been tuned for speed when working biological sequences.

### Value

a vector of positions for which the motif pattern was found in the sequence text.

### Author(s)

J.R. Lobry

### References

`citation("seqinr")`

### See Also

[regexpr](#)

### Examples

```
myseq <- "tatagaga"
words.pos("t", myseq) # Should be 1 3
words.pos("tag", myseq) # Should be 3
words.pos("ga", myseq) # Should be 5 7
# How to specify ambiguous base ? Look for YpR motifs by
words.pos("[ct][ag]", myseq) # Should be 1 3
#
# Show the difference with gregexpr:
#
words.pos("toto", "totototo") # 1 3 5 (three overlapping matches)
unlist(gregexpr("toto", "totototo")) # 1 5 (two disjoint matches)
```

---

write.fasta

*Write sequence(s) into a file in fasta format*

---

### Description

Writes one or more sequences into a file in FASTA format.



**Usage**

```
write.fasta(sequences, names, file.out, open = "w", nbchar = 60, as.string = FALSE)
```

**Arguments**

sequences	A DNA or protein sequence (in the form of a vector of single characters by default) or a list of such sequences.
as.string	FALSE. When set to TRUE sequences are in the form of strings instead of vectors of single characters.
names	The name(s) of the sequences.
nbchar	The number of characters per line (default: 60)
file.out	The name of the output file.
open	Mode to open the output file, use "w" to write into a new file, use "a" to append at the end of an already existing file.

**Value**

none.

**Author(s)**

A. Necşulea

**References**

`citation("seqinr")`

**See Also**

[read.fasta](#)

**Examples**

```
## Read 3 sequences from a FASTA file:
ortho <- read.fasta(file = system.file("sequences/ortho.fasta", package =
"seqinr"))

## Select only third codon positions:
ortho3 <- lapply(ortho, function(x) x[seq(from = 3, to = length(x), by = 3)])

## Write the 3 modified sequences to a file:
write.fasta(sequences = ortho3, names = names(ortho3), nbchar = 80, file.out = "ortho3.fasta")

## Read them again from the same file and check that sequences are preserved:
ortho3bis <- read.fasta("ortho3.fasta", set.attributes = FALSE)
stopifnot(identical(ortho3bis, ortho3))
```

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