Package 'seqinr'

May 19, 2022

Encoding UTF-8

Version 4.2-16

Date 2022-05-19

Title Biological Sequences Retrieval and Analysis

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BugReports
https://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.

URL https://seqinr.r-forge.r-project.org/

NeedsCompilation yes

Repository CRAN

Repository/R-Forge/Project seqinr

Repository/R-Forge/Revision 2145

Repository/R-Forge/DateTimeStamp 2022-05-19 11:26:14

Date/Publication 2022-05-19 21:00:02 UTC

R topics documented:

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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: https://www.bioinformatics.org/sms/iupac.html
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: https://www.bioinformatics.org/sms/iupac.html 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 FADH2 molcules.

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

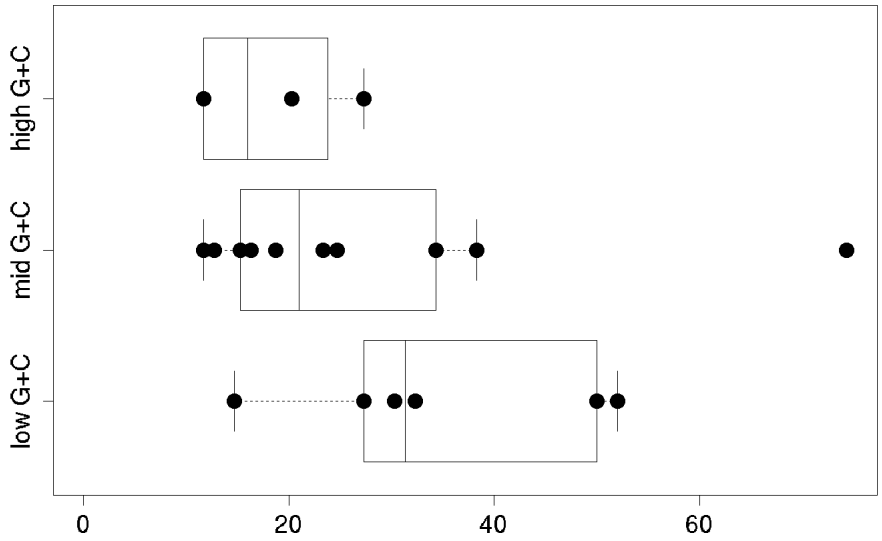
gc an ordered factor (l<m<h) for the G+C class of the amino-acid (see details)

Details

Precursor metabolites are: penP, ribose 5-phosphate; PRPP, 5-phosphoribosyl pyrophosphate; eryP, erythrose 4-phosphate; 3pg, 3-phosphoglycerate; pep, phospho*enol*pyruvate; 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 3JHalpha-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 posision i-1 (Finkelstein et al., 1991)
Helix initiation parameter at posision i,i+1,i+2 (Finkelstein et al., 1991)
Helix termination parameter at posision j-2,j-1,j (Finkelstein et al., 1991)
Helix termination parameter at posision 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)
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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 NaClO4 (Meek-Rossetti, 1981)
Retention coefficient in NaH2PO4 (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 bata-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)
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AA composition of CYT of multi-spanning proteins (Nakashima-Nishikawa, 1992)
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14 A contact number (Nishikawa-Ooi, 1986)
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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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HPLC parameter (Parker et al., 1986)
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Surrounding hydrophobicity in alpha-helix (Ponnuswamy et al., 1980)
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Hydrophobicity (Prabhakaran, 1990)
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Weights for alpha-helix at the window position of -4 (Qian-Sejnowski, 1988)
Weights for alpha-helix at the window position of -3 (Qian-Sejnowski, 1988)
Weights for alpha-helix at the window position of -2 (Qian-Sejnowski, 1988)
Weights for alpha-helix at the window position of -1 (Qian-Sejnowski, 1988)
Weights for alpha-helix at the window position of 0 (Qian-Sejnowski, 1988)
Weights for alpha-helix at the window position of 1 (Qian-Sejnowski, 1988)
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Weights for beta-sheet at the window position of -1 (Qian-Sejnowski, 1988)
Weights for beta-sheet at the window position of 0 (Qian-Sejnowski, 1988)
Weights for beta-sheet at the window position of 1 (Qian-Sejnowski, 1988)
Weights for beta-sheet at the window position of 2 (Qian-Sejnowski, 1988)
Weights for beta-sheet at the window position of 3 (Qian-Sejnowski, 1988)
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Weights for coil at the window position of -3 (Qian-Sejnowski, 1988)
Weights for coil at the window position of -2 (Qian-Sejnowski, 1988)
Weights for coil at the window position of -1 (Qian-Sejnowski, 1988)
Weights for coil at the window position of 0 (Qian-Sejnowski, 1988)
Weights for coil at the window position of 1 (Qian-Sejnowski, 1988)
Weights for coil at the window position of 2 (Qian-Sejnowski, 1988)
Weights for coil at the window position of 3 (Qian-Sejnowski, 1988)
Weights for coil at the window position of 4 (Qian-Sejnowski, 1988)
Weights for coil at the window position of 5 (Qian-Sejnowski, 1988)
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Average relative fractional occurrence in A0(i) (Rackovsky-Scheraga, 1982)
Average relative fractional occurrence in AR(i) (Rackovsky-Scheraga, 1982)
Average relative fractional occurrence in AL(i) (Rackovsky-Scheraga, 1982)

Average relative fractional occurrence in EL(i) (Rackovsky-Scheraga, 1982)
Average relative fractional occurrence in E0(i) (Rackovsky-Scheraga, 1982)
Average relative fractional occurrence in ER(i) (Rackovsky-Scheraga, 1982)
Average relative fractional occurrence in A0(i-1) (Rackovsky-Scheraga, 1982)
Average relative fractional occurrence in AR(i-1) (Rackovsky-Scheraga, 1982)
Average relative fractional occurrence in AL(i-1) (Rackovsky-Scheraga, 1982)
Average relative fractional occurrence in EL(i-1) (Rackovsky-Scheraga, 1982)
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Relative preference value at N’ (Richardson-Richardson, 1988)
Relative preference value at N-cap (Richardson-Richardson, 1988)
Relative preference value at N1 (Richardson-Richardson, 1988)
Relative preference value at N2 (Richardson-Richardson, 1988)
Relative preference value at N3 (Richardson-Richardson, 1988)
Relative preference value at N4 (Richardson-Richardson, 1988)
Relative preference value at N5 (Richardson-Richardson, 1988)
Relative preference value at Mid (Richardson-Richardson, 1988)
Relative preference value at C5 (Richardson-Richardson, 1988)
Relative preference value at C4 (Richardson-Richardson, 1988)
Relative preference value at C3 (Richardson-Richardson, 1988)
Relative preference value at C2 (Richardson-Richardson, 1988)
Relative preference value at C1 (Richardson-Richardson, 1988)
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Information measure for N-terminal helix (Robson-Suzuki, 1976)
Information measure for middle helix (Robson-Suzuki, 1976)
Information measure for C-terminal helix (Robson-Suzuki, 1976)
Information measure for extended (Robson-Suzuki, 1976)
Information measure for pleated-sheet (Robson-Suzuki, 1976)
Information measure for extended without H-bond (Robson-Suzuki, 1976)
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Information measure for N-terminal turn (Robson-Suzuki, 1976)
Information measure for middle turn (Robson-Suzuki, 1976)
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Mean fractional area loss (Rose et al., 1985)
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Side chain hydropathy, corrected for solvation (Roseman, 1988)
Loss of Side chain hydropathy by helix formation (Roseman, 1988)
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Principal component I (Sneath, 1966)
Principal component II (Sneath, 1966)
Principal component III (Sneath, 1966)
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Zimm-Bragg parameter sigma x 1.0E4 (Sueki et al., 1984)
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Unfolding Gibbs energy in water, pH9.0 (Yutani et al., 1987)
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Normalized positional residue frequency at helix termini N2 (Aurora-Rose, 1998)
Normalized positional residue frequency at helix termini N3 (Aurora-Rose, 1998)
Normalized positional residue frequency at helix termini N4 (Aurora-Rose, 1998)
Normalized positional residue frequency at helix termini N5 (Aurora-Rose, 1998)
Normalized positional residue frequency at helix termini C5 (Aurora-Rose, 1998)
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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Interior composition of amino acids in intracellular proteins of mesophiles (percent) (Fukuchi-Nishikawa, 2001)
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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)
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Knowledge-based membrane-propensity scale from 1D_Helix in MPtopo databases (Punta-Maritan, 2003)
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PRILS index (Cornette et al., 1987)
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Optimized relative partition energies - method D (Miyazawa-Jernigan, 1999)
Hydrophobicity index (Engelman et al., 1986)
Hydrophobicity index (Fasman, 1989)

Source

https://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)
```

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

which(sapply(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. The functions ignore ambiguous amino acids (e.g. "B", "Z", "X", "J").

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 splited 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, L_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))
 tryalreadyopen <- try(acnucopen("emblTP", socket = mysocket))
 stopifnot(inherits(tryalreadyopen, "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)
```

al2bp *To Convert a forensic microsatellite allele name into its length in base pairs*

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 strsplit.

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 spoting off ladder alleles are encountedred 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 <- alllistranks())
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: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC341218/

```
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 runing `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 whith 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

JLO for a dataset example, plotabif to plot this kind of data, peakabif to estimate peak parameters.

Examples

```
data(JLO)
rfu <- JLO$Data$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

`nucl`	a nucleotide sequence as a vector of single chars
`warn.non.IUPAC`	if TRUE warns when no IUPAC symbol is possible
`type`	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: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC341218/

```
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("atatttt---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 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 translate
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 writen 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 writen 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 writen 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

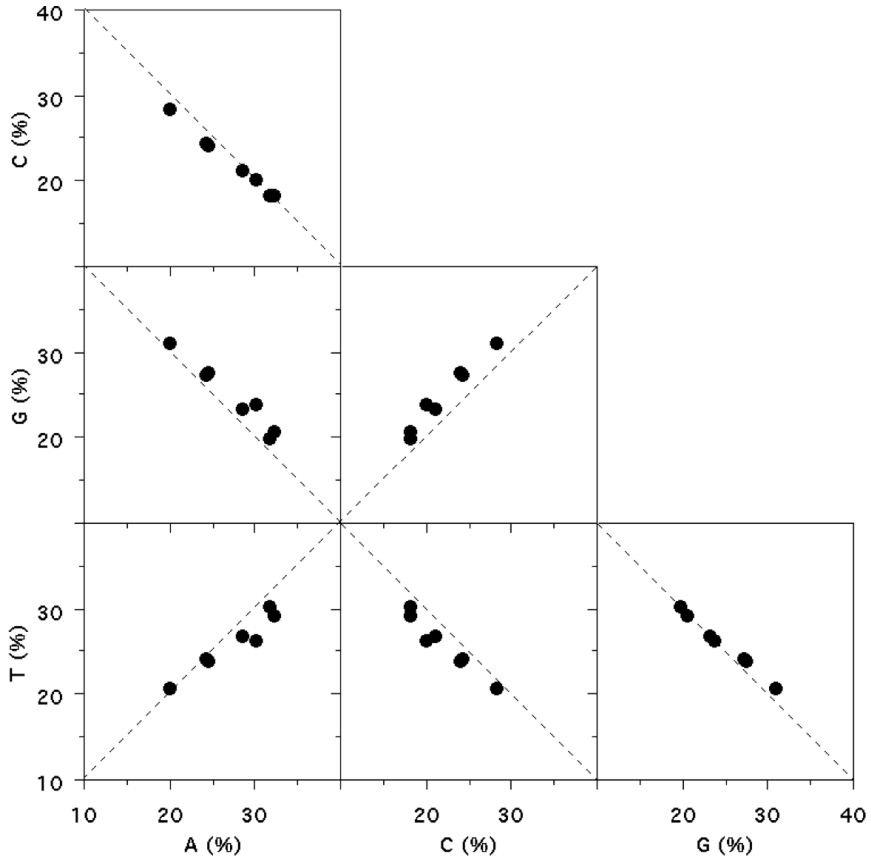
[T] frequencies of T bases in percent

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 beause 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 `socketConnection`)
`port`	integer. The TCP port number (see `socketConnection`)
`server`	logical. Should the socket be a client or a server? (see `socketConnection`)
`blocking`	logical. (see `socketConnection`)
`open`	string. A description of how to open the connection (see `socketConnection`)
`encoding`	string. The name of the encoding to be used. (see `socketConnection`)
`verbose`	logical. If TRUE, verbose mode is on
`timeout`	integer. The timeout in seconds for `socketConnection`. Default 5 seconds.
`infobank`	logical. If `infobank` is TRUE and `bank` is `NA`, a data.frame with all database informations will be returned
`tagbank`	string. If `bank` is `NA` and `tagbank` 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:

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

When called with bank = NA:

`names`	A vector of all available bank names.

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

`bank`	The name of the bank.
`status`	The bank status (on/of).
`info`	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. 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 == "cgcgtgctggcggcaatgaagcgttcgatg")
# 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 polygon

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

```
data(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 chanel*

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 colors.
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 substractive 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("Substractive 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 reverve 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("abcdghkmstvwn")
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: https://web.expasy.org/compute_pi/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 variuous 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

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

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 controled by the threshold argument. If none, NA id 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) == "amvsbnkkgcmkkkmmgsktrmrssndkgcmrkdmmvskyaw")
  # replace 3 and 4-fold symbols by dots:
  res.iup[match(res.iup, s2c("bdhvn"), nomatch = 0) > 0] <- "."
  stopifnot(c2s(res.iup) == "am.s..kkgcmkkkmmgsktrmrss..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 occurence 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 <- "aaxxzxbxvxyxwxtxsxpxfxmxkxlxixhxgxexqxcxdxnxrxazzbzvzyzwztzszpzfzmzkzlzizhzgzezqzczdznz
#rzabbvbybwbtbsbpbfbmbkblbibhbgbebqbcbdbnbrbavvyvwvtvsvpvfvmvkvlvivhvgvevqvcvdvnvrvayywytysypyfymyky
#lyiyhygyeyqycydynyryawwtwswpwfwmwkwlwiwhwgwewqwcwdwnwrwattstptftmtktltithtgtetqtctdtntrtasspsfsmsks
#lsishsgsesqscsdsnsrsappfpmpkplpiphpgpepqpcpdpnprpaffmfkflfifhfgfefqfcfdfnfrfammkmlmimhmgmemqmcmdmnm
#rmakklkikhkgkekqkckdknkrkallilhlglelqlcldlnlrlaiihigieiqicidiniriahhghehqhchdhnhrhaggegqgcgdgngrgae
#eqecedenereaqqcqdqnqrqaccdcncrcaddndrdannrnarra"
#stopifnot(all(count(s2c(alldiaa), 2, alphabet = s2c("arndcqeghilkmfpstwyvbzx")) == 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\nmitochondrion 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 *Number of subsequences in an ACNUC list*

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("https://pbil.univ-lyon1.fr/datasets/seqinr/data/goldtable15Dec07.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 admissive value in bp for a bacterial genome size: only value less or equal to this threshold are considrered.
`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 metadata. *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.
https://academic.oup.com/mbe/article/23/11/2214/1335460

```
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` *Statistical over- and under- representation of dinucleotides in a sequence*

Description

These two functions compute two different types of statistics for the measure of statistical dinculeotide 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 `permutation` 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 frequence 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(mysed))))`.

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. https://academic.oup.com/mbe/article/23/11/2214/1335460

```
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. Note: seqinr::dist.alignment is the square root version of ape::dist.gene (and not ape::dist.dna).

Usage

```
dist.alignment(x, matrix = c("identity", "similarity"),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- logical, with identity matrix, if set to `TRUE`, 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, offset = 0.4, ...)
```

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 `dotchart`.
`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
`offset`	offset in inches of ylab and labels; was hardwired to 0.4 before R 4.0.0
`...`	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 *Dot Plot Comparison of two sequences*

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 eleborated 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\nwsize = 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\nwsize = 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\nwsize = 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

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

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 ($4 \geq$ fac ≥ 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:
#
fname <- tempfile(pattern = "ecc999", tmpdir = tempdir(), fileext = "ffn")
tempdir(check = FALSE)
write.fasta(ec999, names(ec999), file = fname)
```

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 JLO

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 https://www.thermofisher.com/at/en/home/brands/applied-biosystems.html. 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 JLO for an example of an individual sample file.

Examples

```
data(JLO)
```

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` *Extraction of breakpoint positions on the rearranged nucleotide skews.*

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

listname	the name of list on server (may be a virtual list)
socket	an object of class sockconn connecting to a remote ACNUC database (default is a socket to the last opened database).
format	the format of output.Can be acnuc, fasta,flat or coordinates
operation	the type of extraction. Can be simple, translate, fragment, feature or region
feature	-optional- the feature to be extracted (for operations "feature" or "region"): a feature table item (CDS, mRNA,...)
bounds	-optional- the bounds for extraction (for operations "fragment" or "region")
minbounds	-optional- the minimal bounds for extraction (for operations "fragment" or "region")
verbose	if TRUE, verbose mode is on
nzlines	number of line in zlib mode
zlib	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 pare
-10,10	to extract from 10 nucl. BEFORE the 5' end of the sequence to nucl. 10 of it. Useful only for subsequences, a
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 su
-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

```
data(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 `raw` encoding of the target, typically 40 octets for a core-CODIS profile in 2009
`database`	the `raw` 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 schedulded for seqinr 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
# enbeded 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 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 usefull?)

#
# 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,
alphabet = s2c("acgtswmkryvhdb"))
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
pos	for coding sequences, the codon position (1, 2, 3) that should be taken into account to compute the G+C content
oldGC	logical defaulting to FALSE: should the GC content computed as in seqinR <= 1.0-6, that is as the sum of 'g' and 'c' bases divided by the length of the sequence. As from seqinR >= 1.1-3, this argument is deprecated and a warning is issued.
alphabet	alphabet used. This allows you to choose ambiguous bases used during GC calculation.

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 note nx 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 is 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 vetor 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("agtctgggggcccctttaagtagatagatagctagtcgta")
   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 writen 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_ADP1_uid61597.fasta"
myFastaFileName <-tempfile(pattern = "Acinetobacter_ADP1_uid61597",
 tmpdir = tempdir(), fileext = "fasta")
tempdir(check = FALSE)
gb2fasta(myGenBankFile, myFastaFileName)
readLines(myFastaFileName)[1:5]
#
# Should be :
#
# [1] ">CHLTCG 1042519 bp"
# [2] "gcggccgcccgggaaattgctaaaagatgggagcaaagagttagagatctacaagataaa"
# [3] "ggtgctgcacgaaaattattaaatgatcctttaggccgacgaacacctaattatcagagc"
# [4] "aaaaatccaggtgagtatactgtagggaattccatgttttacgatggtcctcaggtagcg"
# [5] "aatctccagaacgtcgacactggtttttggctggacatgagcaatctctcagacgttgta"
#
```

---

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 =  "https://pbil.univ-lyon1.fr/datasets/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 (stricly) 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 ressource. 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 were 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. Detailled 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.gowth() with an estimate of the doubling time in months.

Usage

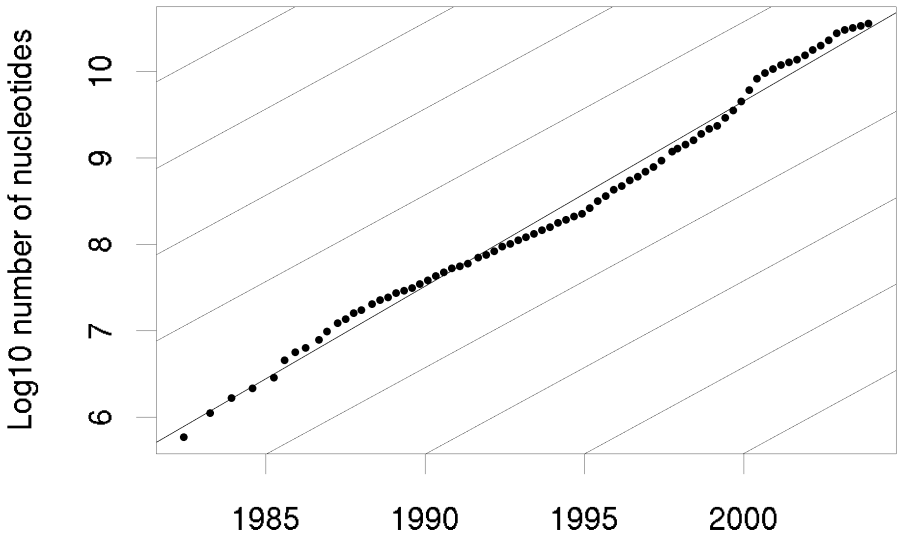
```
get.db.growth(
where = "ftp://ftp.ebi.ac.uk/pub/databases/embl/doc/relnotes.txt")
dia.db.growth( get.db.growth.out = get.db.growth(), Moore = TRUE, ... )
```

Arguments

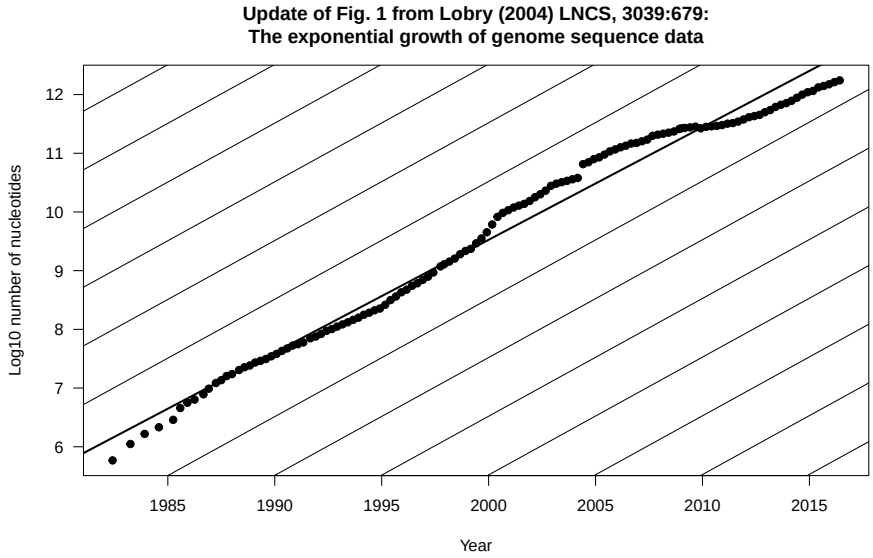
`where`	the file containig the database growth table.
`get.db.growth.out`	the output from get.db.growth()
`Moore`	logical, if TRUE add lines corresponding to an exponential growth rate with a doubling time of 18 months, that is Moore's law.
`...`	further arguments to plot

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 https://seqinr.r-forge.r-project.org/seqinr_3_1-5.pdf:



The doubling time was 18.8 monts 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

https://www.ebi.ac.uk/ena/browser

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)
```

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

object	an object of the class SeqAcnucWeb or SeqFastadna, or SeqFastaAA or a list of these objects
nbl	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).
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

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/malM.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"))
```

---

getFrag *Generic function to extract sequence fragments*

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 SeqAcnucWeb or SeqFastadna, or SeqFastaAA or SeqFrag 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 choosebank).
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 SeqAcnucWeb, or a list of them, or the object resulting from query
socket	an object of class sockconn connecting to a remote ACNUC database (default is a socket to the last opened database by choosebank).
...	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 SeqAcnucWeb or SeqFastadna, or SeqFastaAA or SeqFrag 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 *Generic function to get the location of subsequences on the parent sequence*

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 SeqAcnucWeb, or a list of them, or an object created by query
socket	an object of class sockconn connecting to a remote ACNUC database (default is a socket to the last opened database by choosebank).
...	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 isued.

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 SeqAcnucWeb or SeqFastadna, or SeqFastaAA or SeqFrag 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 chararacters 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 `SeqAcnucWeb` or `SeqFastadna`, or `SeqFastaAA` or `SeqFrag` or a list of these objects, or an object of class qaw created by `query`
`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 SeqAcnucWeb or SeqFastadna, or SeqFrag or a list of these objects, or an object of class qaw created by query
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

# Read from an alignment as suggested by Dr. H. Suzuki
fasta.res   <- read.alignment(file = system.file("sequences/Anouk.fasta", package = "seqinr"),
 format = "fasta")

AA1 <- seqinr::getTrans(s2c(fasta.res$seq[[1]]))
AA2 <- seqinr::translate(s2c(fasta.res$seq[[1]]))
identical(AA1, AA2)

AA1 <- lapply(fasta.res$seq, function(x) seqinr::getTrans(s2c(x)))
AA2 <- lapply(fasta.res$seq, function(x) seqinr::translate(s2c(x)))
identical(AA1, AA2)

#
# 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 *Extract sequence identified by name or by number from an ACNUC server*

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. The 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 likey 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` *Identifiler allele names*

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` *Get the ACNUC number of a sequence from its name or accession number*

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)
getAttributsocket(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 `sockconn` connecting to a remote ACNUC database (default is a socket to the last opened database).
`...`	arguments passed to `isenum`.
`name`	a sequence name.

Value

A list whith 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 nunmber, 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 `getAttributsocket` 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 https://www.thermofisher.com/at/en/home/brands/applied-biosystems.html. 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(JLO)
```

---

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 alignment, obtained for instance by importing into R the data from an alignment file with the read.alignment function. This is typically a set of coding sequences aligned at the protein level, see reverse.align.
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 alignement 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 programm 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)$ka[1], 0) )
#
# As from seqinR 3.4-0, non-finite values should never be returned for
# Ka and Ks even for small sequences. The following test checks that this
# is true for an alignement of the 64 codons, so that we compute Ka and
# Ks for all possible pairs of codons.
#
wrd <- as.alignment(nb = 64, nam = words(), seq = words())
res <- kaks(wrd)
if(any(!is.finite(res$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 runing `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 *Description of databases known by an ACNUC server*

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.

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 functionc 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)
```

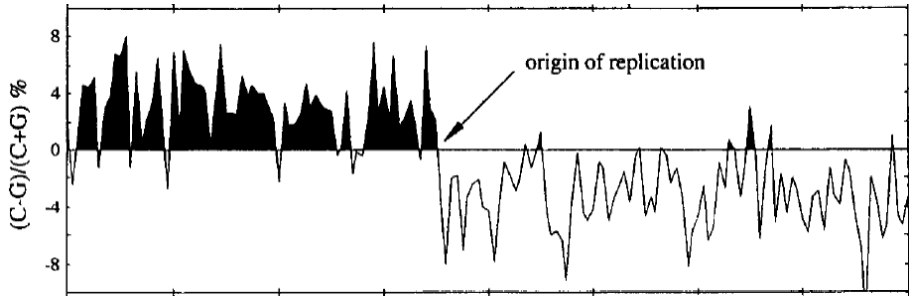
Format

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 its 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. Rilley, 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

```
data(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 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

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

```
data(msf)
```

Format

A List of class alignment

Source

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

n2s *function to convert the numeric encoding of a DNA sequence into a vector of characters*

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 *Prediction of origin and terminus of replication in bacteria.*

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, system.file("sequences/ct.fasta.gz", package ="seqinr") is the fasta file ct.fasta.gz. This is the file for the complete genome sequence of *Chlamydia trachomatis* that was used in Frank and Lobry (2000). You can replace this by something like seq.fasta = "myseq.fasta" to work with your own data if the file myseq.fasta is present in the current working directory (see getwd), or give a full path access to the sequence file (see file.choose).
g2.coord	Character: the name of file which contains the output of glimmer program (*.predict 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 seq.fasta and the g2.coord. A local temporary copy of the GenBank file is made with download.file if gbk starts with http:// or ftp:// or file:// and whith file.copy otherwise. The local copy is then used as input for gb2fasta and gbk2g2 to produce a fasta file and a glimmer-like (version 2) file, respectively, to be used by oriloc instead of seq.fasta and g2.coord .
clean.tmp.files	Logical: if TRUE temporary files generated when working with a GenBank file are removed.
rot	Integer, with zero default value, used to permute circurlarly 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 occurence 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) cummulated over genes, `skew` for the cummulated composite skew in third codon positions, `x` for the cummulated T - A skew in third codon position, `y` for the cummulated 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 permets 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.

doi:10.1093/bioinformatics/16.6.560

A simple informal introduction to DNA-walks:
Lobry, J.R. (1999) Genomic landscapes. *Microbiology Today*, **26**:164-165.
https://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 decribed at http://ccb.jhu.edu/software/glimmer/index.shtml.
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="https://pbil.univ-lyon1.fr/datasets/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(onelinefromserver, verbose = FALSE)
```

Arguments

`onelinefromserver`	a string
`verbose`	logical, if TRUE mode verbose is on

Value

A vector of mode character or NULL if `onelinefromserver` 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 read.abif
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 splinefun
maxrfu	argument passed to baselineabif
...	arguments forwarded to plot

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("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 lader.

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,ucoweight = 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 `splitseq`
`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,modele='base')
identical(all.equal(count(new,1),count(sequence,1)),TRUE)

new=permutation(sequence,modele='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,modele='codon')
identical(all.equal(uco(new),uco(sequence)),TRUE)
```

```
new=permutation(sequence,modele='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

```
data(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., Frutige,r 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

`x`	A sequence of class `SeqAcnucWeb`
`types`	The type of subsequences to plot. Default value is to consider all possible subsequence types.
`socket`	an object of class `sockconn` connecting to a remote ACNUC database (default is a socket to the last opened database).
`...`	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 read.abif
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 plot
las	orientation of axis labels forwarded to plot
xlab	x-axis label forwarded to plot
ylab	y-axis label forwarded to plot
irange	indices of data to be plotted
x	values used for the x-axis
xlim	limits for the x-axis forwarded to plot
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 plot
dyn	dye name
main	title for the plot forwarded to plot
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 plot

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 lader.

Examples

```
data(ECH)
plotabif(ECH,chanel = 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, chanel, calibr, allele.names = "identifiler", npeak = NULL, ...)
```

Arguments

`abifdata`	the result returned by `read.abif`
`chanel`	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 `link{identifiler}`
`npeak`	expected number of peaks, deduced from `allele.names` by default
`...`	arguments forwarded to `peakabif`

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 lader.

Examples

```
  #
  # load an example of allelic ladder results from an ABIF (*.fsa) file:
  #
data(ECH)
  #
  # Extract from internal size standard chanel 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 readPanels function.
xlim	x-axis range.
cex	character expansion factor.
alpha	alpha transparency chanel 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 *Protein Molecular Weight*

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 see 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 "*ACDEFGHIKLMNPQRSTVWY", non allowed values are ignored.
Ar	a named vector for the mean relative atomic masses of CHONPS atoms. Defaults values are from to the natural terrestrial sources according to the 43rd IUPAC General Assembly in Beijing, China in August 2005 (See https://iupac.org/category/recent-releases/ for updates).
gravity	gravitational field constant in standard units. Defaults to 9.81 m/s2, that is to the average value at see 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 repporting 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 getAnnot and modifylist with a scan type operation: annotations but not sequences are scanned, but sequences can be returned by getAnnot. 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 *Print method for objects from class SeqAcnucWeb*

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   ncbigc
  # "A06937"     "34"      "0"      "1"

## End(Not run)
```

---

prochlo *Zscore on three strains of Prochlorococcus marinus*

Description

This dataset contains the zscores computed with the codon model on all CDS from 3 strains of Procholorococcus 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.
https://academic.oup.com/mbe/article/23/11/2214/1335460

```
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 transfered 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 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

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 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

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 fromat 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 https://www.thermofisher.com/at/en/home/brands/applied-biosystems.html. 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 JLO for the files used in quality check.

Examples

```
#
# Quality check:
#

data(JLO)
JLO.check <- read.abif(system.file("abif/2_FAC321_0000205983_B02_004.fsa",
```

```
  package = "seqinr"))
stopifnot(identical(JLO, JLO.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` *Read aligned sequence files in mase, clustal, phylip, fasta or msf format*

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, `getwd`.
`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).
`...`	For the `fasta` format, extra arguments are passed to the `read.fasta` function.

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))

#
# Example of using extra arguments from the read.fasta function, here to keep
# whole headers for sequences names.
#

whole.header.test <-
 read.alignment(file = system.file("sequences/LTPs128_SSU_aligned_First_Two.fasta",
 package = "seqinr"), format = "fasta", whole.header = TRUE)
whole.header.test$nam

# Sould be:
#
# [1] "D50541\t1\t1411\t1411bp\trna\tAbiotrophia defectiva\tAerococcaceae"
# [2] "KP233895\t1\t1520\t1520bp\trna\tAbyssivirga alkaniphila\tLachnospiraceae"
#
```

read.fasta *read FASTA formatted files*

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,
  whole.header = 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, getwd. The default here is to read the ct.fasta.gz file which is present in the sequences folder of the seqinR 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 seqtype == "DNA" 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 as 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
whole.header	if TRUE the whole header line, except the first '>' character, is kept for sequence name. If FALSE, the default, the name is truncated at the first space (" ") character.
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 bfa = TRUE. See .Machine

endian	character string, "big" or "little", giving the endianness of the processor in use. Only relevant for bfa = TRUE. See .Platform
apply.mask	logical defaulting to TRUE. Only relevant for bfa = TRUE. When this flag is TRUE the mask in the MAQ binary format is used to replace non acgt characters in the sequence by the n 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, trailling 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 alignement (.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] "atgaaaatgaataaaagtctcatcgtcctctgtttatcagcagggttactggcaagcgc
# ...
  read.fasta(file = dnafile, as.string = TRUE)
#
# The same but do not force lower case letters, looks like:
#
# $XYLEECOM.MALM
# [1] "ATGAAAATGAATAAAAGTCTCATCGTCCTCTGTTTATCAGCAGGGTTACTGGCAAGC
# ...
  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:
#
# $A06852
# [1] "MPRLFSYLLGVWLLLSQLPREIPGQSTNDFIKACGRELVRLWVEICGSVSWGRTALSLEEP
# QLETGPPAETMPSSITKDAEILKMMLEFVPNLPQELKATLSERQPSLRELQQSASKDSNLNFEEFK
# KIILNRQNEAEDKSLLELKNLGLDKHSRKKRLFRMTLSEKCCQVGCIRKDIARLC*"
#
  read.fasta(aafile, seqtype = "AA", as.string = TRUE, set.attributes = FALSE)
#
# Example with a FASTA file that contains comment lines starting with
# a semicolon character ';'
#
  legacyfile <- system.file("sequences/legacy.fasta", package = "seqinr")
  legacyseq <- read.fasta(file = legacyfile, as.string = TRUE)
  stopifnot( nchar(legacyseq) == 921 )
#
# Example of a MAQ binary fasta file produced with maq fasta2bfa ct.fasta ct.bfa
# on a platform where .Platform$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 trailling 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` *Low level function to get the record count of the specified ACNUC index file*

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

file	The name of the Panel configuration file.
colnames	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 exemple 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.
nl	number of records to read.
recnum.add	to extract record numbers.
nature.add	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.
plong.add	to extract the plong.
libel.add	to extract the label of the name.
sname.add	to extract the short version of the name, that is without the first two characters.
all.add	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 *Detection of replication-associated effects on base composition asymmetry in prokaryotic chromosomes.*

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

seq.fasta	The path of the file containing a FASTA-format sequence. Default value: the FASTA sequence of the Chlamydia trachomatis chromosome.
g2.coord	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 gbk2g2. 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 (fot both rows and columns) will be significantly different from those in the two others.

Value

This function returns a list containing the following components:

seq	a single DNA sequence as a vector of characters
sizewin	length of the sliding window
shift	length of the steps between windows
seqsize	length of the sequence
seqname	name of the sequence
vdep	a vector containing the positions of windows starts
vind	a vector containing the reading frame of each window
vstopd	a vector of stop codons positions in direct strand
vstopr	a vector of stop codons positions in reverse strand
vinitd	a vector of start codons positions in direct strand

vinitr	a vector of start codons positions in reverse strand
resd	a matrix containing codons frequencies for all the windows in the three frames of the direct strand
resr	a matrix containing codons frequencies for all the windows in the three frames of the reverse strand
resd.coa	list of class coa and dudi containing the result of the CA computed on the codons frequencies in the direct strand
resr.coa	list of class coa and dudi 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.
https://academic.oup.com/bioinformatics/article-abstract/3/4/287/218186

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 *Total number of residues in an ACNUC list*

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 *Reverse alignment - from protein sequence alignment to nucleic sequence alignment*

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.
protaln.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 setif align.prot is TRUE.
forceDNAtolower	logical passed to read.fasta for reading the nucleic acid file.
forceAAtolower	logical passed to read.alignment 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, trough the 'protaln.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:
#
myOutFileName <-tempfile(pattern = "test", tmpdir = tempdir(), fileext = "revalign")
tempdir(check = FALSE)

#reverse.align(nucl.file = nucl.file, protaln.file = protaln.file,
#                     input.format = 'clustal', out.file = 'test.revalign')

reverse.align(nucl.file = nucl.file, protaln.file = protaln.file,
                     input.format = 'clustal', out.file = myOutFileName)

#
# Simple sanity check against expected result:
#

#res.new <- read.alignment("test.revalign", format = "fasta")

res.new <- read.alignment(myOutFileName, 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.revalign.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

`seq`	the sequence as a vector of single chars
`levels`	allowed char values, by default a, c, g and t
`base4`	if TRUE the numerical encoding will start at O, if FALSE at 1
`forceToLower`	if TRUE the sequence is forced to lower case caracters

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 *Class for sub-sequences*

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 *utility data for seqinr*

Description

This data set gives the genetics code, the name of each codon, the IUPAC one-letter code for amino acids 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 differents 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 descibed at: https://www.bioinformatics.org/sms/iupac.html. 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 *split a sequence into sub-sequences*

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("aacgttgcaggtcgctcgctacgtagctactgttt")
#
# 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` *Stutter ratio estimation*

Description

This function tries to estimate the stutter ratio, either in terms of peak heigth 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 `read.abif`
`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 `peakabif`
`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 `baselineabif`
`method`	method to be used by `splinefun`
`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

JLO 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(JLO)

  #
  # Get peak locations in the blue channel:
  #

maxis <- peakabif(JLO, 1, npeak = 6, tmin = 3, fig = FALSE)$maxis

  #
  # Compute stutter ratio for first peak and ask for a figure:
  #

tmp <- stutterabif(JLO, 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

x	an R object
y	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 *Synonymous codons*

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:
#
toycds <- s2c("tctgagcaaataaatcgg")
syncodons(splitseq(toycds))
#
# 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", "ggt"),
  ggc = c("gga", "ggc", "ggg", "ggt"),
  gga = c("gga", "ggc", "ggg", "ggt"),
  ggg = c("gga", "ggc", "ggg", "ggt")),

.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 translate
urn.rna	The letters to display codons, use s2c("UCAG") 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"), each =16), s2c("tcag"), sep = ""), rep(s2c("tcag"), each = 4), sep = "")

Author(s)

J.R. Lobry

References

citation("seqinr")

See Also

translate, syncodons

Examples

```
#
# Show me the standard genetic code:
#

 tablecode()
```

`test.co.recstat` *Tests if regions located between Stop codons contain putative CDSs.*

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 ($4 \geq$ `fac` ≥ 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

```
## Not run: # CPU time  is too long with windows
ff <- system.file("sequences/ECOUNC.fsa", package = "seqinr")
seq <- read.fasta(ff)
rec <- recstat(seq[[1]], seqname = getName(seq))
test.co.recstat(rec)

## End(Not run)
```

---

test.li.recstat *Tests if regions located between Stop codons contain putative CDSs.*

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 ($4 \geq$ `fac` ≥ 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 *A toy example of codon counts in three coding sequences*

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: https://www.bioinformatics.org/sms/iupac.html

```
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

# Read from an alignment as suggested by Dr. H. Suzuki
fasta.res   <- read.alignment(file = system.file("sequences/Anouk.fasta", package = "seqinr"),
 format = "fasta")

AA1 <- seqinr::getTrans(s2c(fasta.res$seq[[1]]))
AA2 <- seqinr::translate(s2c(fasta.res$seq[[1]]))
identical(AA1, AA2)

AA1 <- lapply(fasta.res$seq, function(x) seqinr::getTrans(s2c(x)))
AA2 <- lapply(fasta.res$seq, function(x) seqinr::translate(s2c(x)))
identical(AA1, AA2)

## 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="AAO41581.1"
## FT                   /translation="MADDEQFSLCWNNFNTNLSAGFHESLCRGDLVDVSLAAEGQIVKA
## FT                   HRLVLSVCSPFFRKMFTQMPSNTHAIVFLNNVSHSALKDLIQFMYCGEVNVKQDALPAF
## FT                   ISTAESLQIKGLTDNDPAPQPPQESSPPPAAPHVQQQQIPAQRVQRQQPRASARYKIET
## FT                   VDDGLGDEKQSTTQIVIQTTAAPQATIVQQQQPQQAAQQIQSQQLQTGTTTTATLVSTN
## FT                   KRSAQRSSLTPASSSAGVKRSKTSTSANVMDPLDSTTETGATTTAQLVPQQITVQTSVV
## FT                   SAAEAKLHQQSPQQVRQEEAEYIDLPMELPTKSEPDYSEDHGDAAGDAEGTYVEDDTYG
## FT                   DMRYDDSYFTENEDAGNQTAANTSGGGVTATTSKAVVKQQSQNYSESSFVDTSGDQGNT
## FT                   EAQVTQHVRNCGPQMFLISRKGGTLLTINNFVYRSNLKFFGKSNNILYWECVQNRSVKC
## FT                   RSRLKTIGDDLYVTNDVHNHMGDNKRIEAAKAAGMLIHKKLSSLTAADKIQGSWKMDTE
## FT                   GNPDHLPKM"
choosebank("emblTP")
trans <- query("trans", "N=AE003734.PE35")
trans1 <- getTrans(trans$req[[1]])
## Complex transsplicing operations, the correct frame and the correct
## genetic code are automatically used for translation into protein.
seq <- getSequence(trans$req[[1]])
```

```
identical(translate(seq),trans1)
#default frame and genetic code are correct
trans <- query("trans", "N=AB004237")
trans1 <- getTrans(trans$req[[1]])
## Complex transsplicing operations, the correct frame and the correct
## genetic code are automatically used for translation into protein.
seq <- getSequence(trans$req[[1]])
identical(translate(seq),trans1)
#default  genetic code is not correct
identical(translate(seq,numcode=2),trans1)
#genetic code is 2

## 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 begining 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 trimed off?
`trailing`	logical defaulting to `TRUE`: should trailing spaces be trimed 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 expressionsare 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

seq	a coding sequence as a vector of chars
frame	an integer (0, 1, 2) giving the frame of the coding sequence
index	codon usage index choice, partial matching is allowed. eff for codon counts, freq for codon relative frequencies, and rscu the RSCU index. "eff", "freq", and "rscu" correspond to "R0", "R1", and "R3", respectively, in Suzuki et al. (2005) "2.2 Normalization of codon usage data". "eff" and "rscu" correspond to "AF" and "RSCU", respectively, in Suzuki et al. (2008) "2.2. Definitions of codon usage data".
as.data.frame	logical. If TRUE: all indices are returned into a data frame.
NA.rscu	when an amino-acid is missing, RSCU are no more defined and repported 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.

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., Saito, R. Tomita, R. (2005) A problem in multivariate analysis of codon usage data and a possible solution. *FEBS Lett.*, **579**:6499-504. https://febs.onlinelibrary.wiley.com/doi/full/10.1016/j.febslet.2005.10.032.

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. https://academic.oup.com/dnaresearch/article/15/6/357/513030.

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/malM.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 *Weight of each synonymous codon*

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:

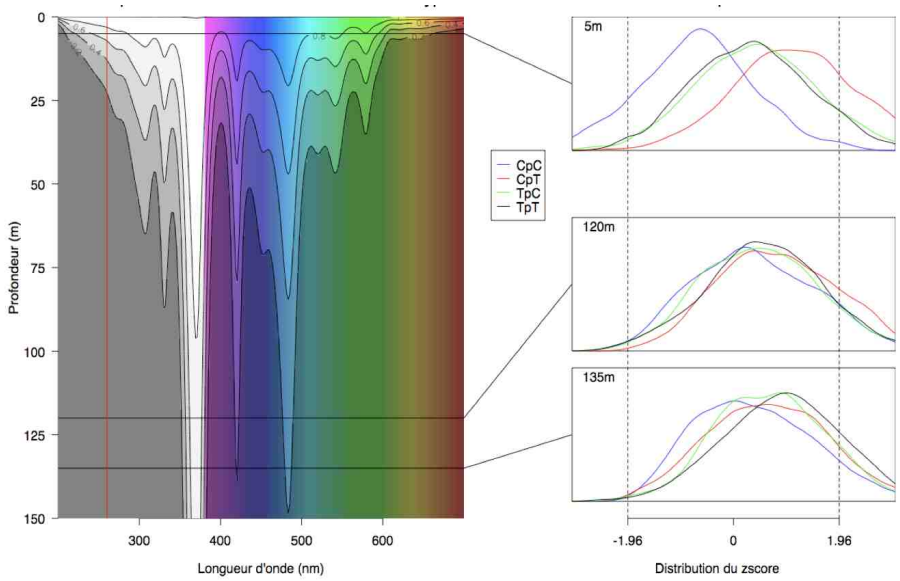
lambda wavelength in nm

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` *Scans databases for a given sequence accession number*

Description

This function loops over all availabale 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 choosebank.

Value

The function resturns 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 *To get all words from an alphabet.*

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", "ggt",
   "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 occurences 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 regular expression (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 regexpr.

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)

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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:
fname <- tempfile(pattern = "ortho3", tmpdir = tempdir(), fileext = "fasta")
#write.fasta(sequences = ortho3, names = names(ortho3), nbchar = 80, file.out = "ortho3.fasta")
write.fasta(sequences = ortho3, names = names(ortho3), nbchar = 80, file.out = fname)

## Read them again from the same file and check that sequences are preserved:
ortho3bis <- read.fasta(fname, set.attributes = FALSE)
stopifnot(identical(ortho3bis, ortho3))
```

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