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Description

The melting temperature of nucleic acid sequences can be calculated in three method, the Wallace rule (Thein & Wallace (1986) <doi:10.1016/S0140-6736(86)90739-7>), empirical formulas based on G and C content (Marmur J. (1962) <doi:10.1016/S0022-2836(62)80066-7>, Schildkraut C. (2010) <doi:10.1002/bip.360030207>, Wetmur J G (1991) <10.3109/10409239109114069>, Untergasser,A. (2012) <doi:10.1093/nar/gks596>, von Ahsen N (2001) <PMID:11673362>) and nearest neighbor thermodynamics (Breslauer K J (1986) <doi:10.1073/pnas.83.11.3746>, Sugimoto N (1996) <doi:10.1093/nar/24.22.4501>, Allawi H (1998) <doi:10.1093/nar/26.11.2694>, SantaLucia J (2004) <doi:10.1146/annurev.biophys.32.110601.141800>, Freier S (1986) <doi:10.1073/pnas.83.24.9373>, Xia T (19 marito S (2000) <doi:10.1093/nar/28.9.1929>, Turner D H (2010) <doi:10.1093/nar/gkp892>, Sugimoto N (1995) <doi:10.1016/S0048-9697(98)00088-6>, Allawi H T (1997) <doi:10.1021/bi962590c>, Santalucia N (2005) <doi:10.1093/nar/gki918>), and it can also be corrected with salt ions and chemical compound (SantaLucia J (1996) <doi:10.1021/bi951907q>, SantaLucia J(1998) <doi:10.1073/pnas.95.4.1460>, Owczarzy R (2004) <doi:10.1021/bi034621r>, Owczarzy R (2008) <doi:10.102

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`TmCalculator-package` *Melting Temperature of Nucleic Acid Sequences*

Description

The melting temperature of nucleic acid sequences can be calculated in three method, the Wallace rule, empirical formulas based on G and C content and nearest neighbor thermodynamics, and it can also be corrected with salt ions and chemical compound.

Details

Package:	TmCalculator
Type:	Package
Version:	1.0.0
Date:	2019-01-25
License:	GPL (>= 2)

Author(s)

Author: Junhui Li Maintainer: Junhui Li <junhuili@cau.edu.cn>

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urner D H , Mathews D H . NNDB, et al. the nearest neighbor parameter database for predicting stability of nucleic acid secondary structure[J]. Nucleic Acids Research, 2010, 38(Database issue):D280-D282.

Breslauer K J , Frank R , Blocker H , et al. Predicting DNA duplex stability from the base sequence.[J]. Proceedings of the National Academy of Sciences, 1986, 83(11):3746-3750.

Sugimoto N , Nakano S , Yoneyama M , et al. Improved Thermodynamic Parameters and Helix Initiation Factor to Predict Stability of DNA Duplexes[J]. Nucleic Acids Research, 1996, 24(22):4501-5.

Allawi, H. Thermodynamics of internal C.T mismatches in DNA[J]. Nucleic Acids Research, 1998, 26(11):2694-2701.

Hicks L D , Santalucia J . The thermodynamics of DNA structural motifs.[J]. Annual Review of Biophysics & Biomolecular Structure, 2004, 33(1):415-440.

Freier S M , Kierzek R , Jaeger J A , et al. Improved free-energy parameters for predictions of RNA duplex stability.[J]. Proceedings of the National Academy of Sciences, 1986, 83(24):9373-9377.

Xia T , Santalucia , J , Burkard M E , et al. Thermodynamic Parameters for an Expanded Nearest-Neighbor Model for Formation of RNA Duplexes with Watson-Crick Base Pairs,[J]. Biochemistry, 1998, 37(42):14719-14735.

Chen J L , Dishler A L , Kennedy S D , et al. Testing the Nearest Neighbor Model for Canonical RNA Base Pairs: Revision of GU Parameters[J]. Biochemistry, 2012, 51(16):3508-3522.

Bommarito S, Peyret N, Jr S L. Thermodynamic parameters for DNA sequences with dangling ends[J]. Nucleic Acids Research, 2000, 28(9):1929-1934.

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Sugimoto N , Nakano S I , Katoh M , et al. Thermodynamic Parameters To Predict Stability of RNA/DNA Hybrid Duplexes[J]. Biochemistry, 1995, 34(35):11211-11216.

Allawi H, SantaLucia J: Thermodynamics and NMR of internal G-T mismatches in DNA. Biochemistry 1997, 36:10581-10594.

Santalucia N E W J . Nearest-neighbor thermodynamics of deoxyinosine pairs in DNA duplexes[J]. Nucleic Acids Research, 2005, 33(19):6258-67.

Peyret N , Seneviratne P A , Allawi H T , et al. Nearest-Neighbor Thermodynamics and NMR of DNA Sequences with Internal A-A, C-C, G-G, and T-T Mismatches, [J]. Biochemistry, 1999, 38(12):3468-3477.

c2s *convert a vector of characters into a string*

Description

Simply convert a vector of characters such as c("H","e","l","l","o","W","o","r","l","d") into a single string such as "HelloWorld".

Usage

```
c2s(characters)
```

Arguments

characters	A vector of characters

Value

Retrun a strings

Author(s)

Junhui Li

References

```
citation("TmCalculator")
```

See Also

s2c

Examples

```
c2s(c("H","e","l","l","o","W","o","r","l","d"))
```

check_filter *Check and filter valid base of nucleotide sequences*

Description

In general, whitespaces and non-base characters are removed and characters are converted to uppercase in given method.

Usage

```
check_filter(ntseq, method)
```

Arguments

ntseq	The primer/probe sequence as string or vector of characters
method	TM_Wallace: check and return "A","B","C","D","G","H","I","K","M","N","R","S","T","V","W" and "Y" TM_GC: check and return "A","B","C","D","G","H","I","K","M","N","R","S","T","V","W", "X" and "Y" TM_NN: check and return "A","C","G","I" and "T"

Value

Return a sequence which fullfils the requirements of the given method.

Author(s)

Junhui Li

Examples

```
ntseq <- c("ATCGBDHKMNRVYWSqq")
check_filter(ntseq,method='Tm_Wallace')
check_filter(ntseq,method='Tm_NN')
```

chem_correction *Correct melting temperature with chemical substances*

Description

Correct a given melting temperature with DMSO and formamide, and these corrections are rough approximations.

Usage

```
chem_correction(Tm, DMSO = 0, fmd = 0, DMSOfactor = 0.75,
fmdfactor = 0.65, fmdmethod = "concentration", ptGC = NULL)
```

Arguments

Tm	Melting temperature
DMSO	Percent DMSO
fmd	Formamide concentration in percentage (fmdmethod="concentration") or molar (fmdmethod="molar").
DMSOfactor	Coeffecient of Tm decreases per percent DMSO. Default=0.75 von Ahsen N (2001) <PMID:11673362>. Other published values are 0.5, 0.6 and 0.675.
fmdfactor	Coeffecient of Tm decrease per percent formamide. Default=0.65. Several papers report factors between 0.6 and 0.72.
fmdmethod	"concentration" method for formamide concentration in percentage and "molar" for formamide concentration in molar.
ptGC	Content of GC

Details

fmdmethod = "concentration" Tm = Tm - factor*percentage_of_formamide

fmdmethod = "molar" Tm = Tm + (0.453(f(GC)) - 2.88) x [formamide]

Author(s)

Junhui Li

References

von Ahsen N, Wittwer CT, Schutz E , et al. Oligonucleotide melting temperatures under PCR conditions: deoxynucleotide Triphosphate and Dimethyl sulfoxide concentrations with comparison to alternative empirical formulas. Clin Chem 2001, 47:1956-C1961.

Examples

```
chem_correction(70, DMSO=3) #67.75
chem_correction(70, fmd=5) #66.75
chem_correction(70, fmdmethod="molar", fmd=1.25,ptGC=50) #66.68
```

`complement` *reverse complement and complement base of nucleotide sequences*

Description

get reverse complement and complement nucleotide sequences

Usage

```
complement(ntseq, reverse = FALSE)
```

Arguments

`ntseq`	The primer/probe sequence as string or vector of characters
`reverse`	Get reverse complemet sequence or not

Value

nucleotide sequences

Author(s)

Junhui Li

Examples

```
complement("ATCGYCGYsWwsaVv")
complement("ATCGYCGYsWwsaVv",reverse=TRUE)
```

`GC` *Calculate G and C content of nucleotide sequences*

Description

Calculate G and C content of nucleotide sequences.The number of G and C in sequence is divided by length of sequence(when totalnt is TRUE) or the number of all A,T,C,G and ambiguous base.

Usage

```
GC(ntseq, ambiguous = FALSE, totalnt = FALSE)
```

Arguments

ntseq	The primer/probe sequence as string or vector of characters
ambiguous	Ambiguous bases are taken into account to compute the G and C content when ambiguous is TRUE.
totalnt	Sum of 'G' and 'C' bases divided by the length of the sequence when totalnt is TRUE

Value

Content of G and C(range from 0 to 100)

Author(s)

Junhui Li

Examples

```
GC(c("a","t","c","t","g","g","g","c","c","a","g","t","a"))#53.84615
GC("GCATSWSYK",ambiguous = TRUE)#55.55556
```

---

s2c *convert a string into a vector of characters*

Description

Simply convert a single string such as "HelloWorld" into a vector of characters such as c("H","e","l","l","o","W","o","r","l","d

Usage

```
s2c(strings)
```

Arguments

strings	A single string such as "HelloWorld"

Value

Retrun a vector of characters

Author(s)

Junhui Li

References

```
citation("TmCalculator")
```

See Also

c2s

Examples

```
s2c(c("HelloWorld"))
```

`salt_correction` *Calculate the corrected melting temperature with salt ions*

Description

It will correct melting temperature or entropy based different operations

Usage

```
salt_correction(Na = 0, K = 0, Tris = 0, Mg = 0, dNTPs = 0,
method = 1, ntseq = NULL, ambiguous = FALSE)
```

Arguments

`Na`	Millimolar concentration of Na
`K`	Millimolar concentration of K
`Tris`	Millimolar concentration of Tris
`Mg`	Millimolar concentration of Mg
`dNTPs`	Millimolar concentration of dNTPs
`method`	Which method to be applied. Methods 1-4 correct Tm, method 5 corrects deltaS, methods 6 and 7 correct 1/Tm.
`ntseq`	The primer/probe sequence as string or vector of characters
`ambiguous`	Ambiguous bases are taken into account to compute the G and C content when ambiguous is TRUE.

Details

methods 1-4: Tm(new) = Tm(old) + corr

method 5: deltaS(new) = deltaS(old) + corr

methods 6+7: Tm(new) = 1/(1/Tm(old) + corr)

The methods are:

1 Schildkraut C (2010) <doi:10.1002/bip.360030207>

2 Wetmur J G (1991) <doi:10.3109/10409239109114069>

3 SantaLucia J (1996) <doi:10.1021/bi951907q>

4 SantaLucia J (1998) <doi:10.1073/pnas.95.4.1460>

5 SantaLucia J (1998) <doi:10.1073/pnas.95.4.1460>

6 Owczarzy R (2004) <doi:10.1021/bi034621r>

7 Owczarzy R (2008) <doi:10.1021/bi702363u>

Author(s)

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Owczarzy R , Moreira B G , You Y , et al. Predicting Stability of DNA Duplexes in Solutions Containing Magnesium and Monovalent Cations[J]. Biochemistry, 2008, 47(19):5336-5353.

Examples

```
ntseq <- c("acgtTGCAATGCCGTAWSDBSYXX")
salt_correction(Na=390, K=20, Tris=0, Mg=10, dNTPs=25, method=7, ntseq)
mySeq <- c("A", "C", "G", "T", "T", "G", "C", "A", "A", "T", "G",
"C", "C", "G", "T", "A", "W", "S", "D", "B","S", "Y", "X", "X")
salt_correction(Na=390, K=20, Tris=0, Mg=10, dNTPs=25, method=7, mySeq)
```

Tm_GC — *Calculate the melting temperature using empirical formulas based on GC content*

Description

Calculate the melting temperature using empirical formulas based on GC content with differenct rules

Usage

```
Tm_GC(ntseq, ambiguous = FALSE, userset = NULL, variant = "Primer3Plus",
Na = 50, K = 0, Tris = 0, Mg = 0, dNTPs = 0, saltcorr = 0, mismatch = TRUE)
```

Arguments

ntseq	The primer/probe sequence as string or vector of characters
ambiguous	Ambiguous bases are taken into account to compute the G and C content when ambiguous is TRUE.
userset	A vector of fou coefficientr values. Usersets override valuesets.
variant	Empirical constants coefficient with 8 variant: Chester1993, QuikChange, Schildkraut1965, Wetmur1991_MELTING, Wetmur1991_RNA, Wetmur1991_RNA/DNA, Primer3Plus and vonAhsen2001
Na	Millimolar concentration of Na
K	Millimolar concentration of K
Tris	Millimolar concentration of Tris
Mg	Millimolar concentration of Mg
dNTPs	Millimolar concentration of dNTPs
saltcorr	Type of salt correction. Default=5.
mismatch	If 'True' (default) every 'X' in the sequence is counted as mismatch

Details

Empirical constants coefficient with 8 variant: Chester1993: Tm = 69.3 + 0.41(Percentage_GC) - 650/N

QuikChange: Tm = 81.5 + 0.41(Percentage_GC) - 675/N - Percentage_mismatch

Schildkraut1965: Tm = 81.5 + 0.41(Percentage_GC) - 675/N + 16.6 x log[Na+]

Wetmur1991_MELTING: Tm = 81.5 + 0.41(Percentage_GC) - 500/N + 16.6 x log([Na+]/(1.0 + 0.7 x [Na+])) - Percentage_mismatch

Wetmur1991_RNA: Tm = 78 + 0.7(Percentage_GC) - 500/N + 16.6 x log([Na+]/(1.0 + 0.7 x [Na+])) - Percentage_mismatch

Wetmur1991_RNA/DNA: Tm = 67 + 0.8(Percentage_GC) - 500/N + 16.6 x log([Na+]/(1.0 + 0.7 x [Na+])) - Percentage_mismatch

Primer3Plus: Tm = 81.5 + 0.41(Percentage_GC) - 600/N + 16.6 x log[Na+]

vonAhsen2001: Tm = 77.1 + 0.41(Percentage_GC) - 528/N + 11.7 x log[Na+]

Author(s)

Junhui Li

References

Marmur J , Doty P . Determination of the base composition of deoxyribonucleic acid from its thermal denaturation temperature.[J]. Journal of Molecular Biology, 1962, 5(1):109-118.

Schildkraut C . Dependence of the melting temperature of DNA on salt concentration[J]. Biopolymers, 2010, 3(2):195-208.

Wetmur J G . DNA Probes: Applications of the Principles of Nucleic Acid Hybridization[J]. CRC Critical Reviews in Biochemistry, 1991, 26(3-4):33.

Untergasser A , Cutcutache I , Koressaar T , et al. Primer3–new capabilities and interfaces[J]. Nucleic Acids Research, 2012, 40(15):e115-e115.

von Ahsen N, Wittwer CT, Schutz E , et al. Oligonucleotide melting temperatures under PCR conditions: deoxynucleotide Triphosphate and Dimethyl sulfoxide concentrations with comparison to alternative empirical formulas. Clin Chem 2001, 47:1956-1961.

Examples

```
ambiguous=TRUE
userset=NULL
variant="Primer3Plus"
Na=50
K=0
Tris=0
Mg=0
dNTPs=0
saltcorr=0
mismatch=TRUE
ntseq <- c("ATCGTGCGTAGCAGTACGATCAGTAG")
Tm_GC(ntseq,ambiguous,userset,variant,Na, K,Tris, Mg, dNTPs, saltcorr, mismatch)
```

`Tm_NN` *Calculate melting temperature using nearest neighbor thermodynamics*

Description

Calculate melting temperature using nearest neighbor thermodynamics

Usage

```
Tm_NN(ntseq, ambiguous = FALSE, comSeq = NULL, shift = 0, nn_table = "DNA_NN4",
tmm_table = "DNA_TMM1", imm_table = "DNA_IMM1",de_table = "DNA_DE1", dnac1 = 25,
dnac2 = 25, selfcomp = FALSE, Na = 50, K = 0, Tris = 0, Mg = 0, dNTPs = 0, saltcorr = 5)
```

Arguments

`ntseq`	The primer/probe sequence as string or vector of characters
`ambiguous`	Ambiguous bases are taken into account to compute the G and C content when ambiguous is TRUE.
`comSeq`	Complementary sequence. The sequence of the template/target in 3'->5' direction
`shift`	Shift of the primer/probe sequence on the template/target sequence, default=0. for example: when shift=0, the first nucleotide base at 5‘ end of primer align to first one at 3‘ end of template. When shift=-1, the secound nucleotide base at 5‘ end of primer align to first one at 3‘ end of template. When shift=1, the first nucleotide base at 5‘ end of primer align to secound one at 3‘ end of template. The shift parameter is necessary to align primer/probe and template/target if they have different lengths or if they should have dangling ends.

nn_table	Thermodynamic NN values, eight tables are implemented. For DNA/DNA hybridizations: DNA_NN1,DNA_NN2,DNA_NN3,DNA_NN4 For RNA/RNA hybridizations: RNA_NN1,RNA_NN2,RNA_NN3 For RNA/DNA hybridizations: R_DNA_NN1
tmm_table	Thermodynamic values for terminal mismatches. Default: DNA_TMM1
imm_table	Thermodynamic values for internal mismatches, may include insosine mismatches. Default: DNA_IMM1
de_table	Thermodynamic values for dangling ends: DNA_DE1(default),RNA_DE1
dnac1	Concentration of the higher concentrated strand [nM]. Typically this will be the primer (for PCR) or the probe. Default=25.
dnac2	Concentration of the lower concentrated strand [nM].
selfcomp	Sequence self-complementary, default=False. If 'True' the primer is thought binding to itself, thus dnac2 is not considered.
Na	Millimolar concentration of Na
K	Millimolar concentration of K
Tris	Millimolar concentration of Tris
Mg	Millimolar concentration of Mg
dNTPs	Millimolar concentration of dNTPs
saltcorr	Type of salt correction. Default=5.

Details

DNA_NN1: Breslauer K J (1986) <doi:10.1073/pnas.83.11.3746>

DNA_NN2: Sugimoto N (1996) <doi:10.1093/nar/24.22.4501>

DNA_NN3: Allawi H (1998) <doi:10.1093/nar/26.11.2694>

DNA_NN4: SantaLucia J (2004) <doi:10.1146/annurev.biophys.32.110601.141800>

RNA_NN1: Freier S (1986) <doi:10.1073/pnas.83.24.9373>

RNA_NN2: Xia T (1998) <doi:10.1021/bi9809425>

RNA_NN3: Chen JL (2012) <doi:10.1021/bi3002709>

R_DNA_NN1: Sugimoto N (1995)<doi:10.1016/S0048-9697(98)00088-6>

DNA_TMM1: Bommarito S (2000) <doi:10.1093/nar/28.9.1929>

DNA_IMM1: Peyret N (1999) <doi:10.1021/bi9825091> & Allawi H T (1997) <doi:10.1021/bi962590c> & Santalucia N (2005) <doi:10.1093/nar/gki918>

DNA_DE1: Bommarito S (2000) <doi:10.1093/nar/28.9.1929>

RNA_DE1: Turner D H (2010) <doi:10.1093/nar/gkp892>

Author(s)

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References

Breslauer K J , Frank R , Blocker H , et al. Predicting DNA duplex stability from the base sequence.[J]. Proceedings of the National Academy of Sciences, 1986, 83(11):3746-3750.

Sugimoto N , Nakano S , Yoneyama M , et al. Improved Thermodynamic Parameters and Helix Initiation Factor to Predict Stability of DNA Duplexes[J]. Nucleic Acids Research, 1996, 24(22):4501-5.

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Hicks L D , Santalucia J . The thermodynamics of DNA structural motifs.[J]. Annual Review of Biophysics & Biomolecular Structure, 2004, 33(1):415-440.

Freier S M , Kierzek R , Jaeger J A , et al. Improved free-energy parameters for predictions of RNA duplex stability.[J]. Proceedings of the National Academy of Sciences, 1986, 83(24):9373-9377.

Xia T , Santalucia , J , Burkard M E , et al. Thermodynamic Parameters for an Expanded Nearest-Neighbor Model for Formation of RNA Duplexes with Watson-Crick Base Pairs,[J]. Biochemistry, 1998, 37(42):14719-14735.

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Bommarito S, Peyret N, Jr S L. Thermodynamic parameters for DNA sequences with dangling ends[J]. Nucleic Acids Research, 2000, 28(9):1929-1934.

Turner D H , Mathews D H . NNDB: the nearest neighbor parameter database for predicting stability of nucleic acid secondary structure[J]. Nucleic Acids Research, 2010, 38(Database issue):D280-D282.

Sugimoto N , Nakano S I , Katoh M , et al. Thermodynamic Parameters To Predict Stability of RNA/DNA Hybrid Duplexes[J]. Biochemistry, 1995, 34(35):11211-11216.

Allawi H, SantaLucia J: Thermodynamics and NMR of internal G-T mismatches in DNA. Biochemistry 1997, 36:10581-10594.

Santalucia N E W J . Nearest-neighbor thermodynamics of deoxyinosine pairs in DNA duplexes[J]. Nucleic Acids Research, 2005, 33(19):6258-67.

Peyret N , Seneviratne P A , Allawi H T , et al. Nearest-Neighbor Thermodynamics and NMR of DNA Sequences with Internal A-A, C-C, G-G, and T-T Mismatches, [J]. Biochemistry, 1999, 38(12):3468-3477.

Examples

```
ntseq <- c("AAAATTTTTTTCCCCCCCCCCCCCCGGGGGGGGGGGGGTGTGCGCTGC")
Tm_NN(ntseq, ambiguous = FALSE, comSeq = NULL, shift = 0, nn_table = "DNA_NN4",
tmm_table = "DNA_TMM1", imm_table = "DNA_IMM1",de_table = "DNA_DE1", dnac1 = 25,
dnac2 = 25, selfcomp = FALSE, Na = 50, K = 0, Tris = 0, Mg = 0, dNTPs = 0, saltcorr = 5)
```

Tm_Wallace *Calculate the melting temperature using the 'Wallace rule'*

Description

The Wallace rule is often used as rule of thumb for approximate melting temperature calculations for primers with 14 to 20 nt length.

Usage

```
Tm_Wallace(ntseq, ambiguous = FALSE)
```

Arguments

ntseq	The primer/probe sequence as string or vector of characters
ambiguous	Ambiguous bases are taken into account to compute the G and C content when ambiguous is TRUE.

Value

a numeric melting temperature

Author(s)

Junhui Li

References

Thein S L , Lynch J R , Weatherall D J , et al. DIRECT DETECTION OF HAEMOGLOBIN E WITH SYNTHETIC OLIGONUCLEOTIDES[J]. The Lancet, 1986, 327(8472):93.

Examples

```
ntseq = c('acgtTGCAATGCCGTAWSDBSY') #for wallace rule
Tm_Wallace(ntseq,ambiguous = TRUE)
Tm_Wallace(ntseq,ambiguous = FALSE)
```

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