Package ‘rmelting’

April 18, 2024

Title R Interface to MELTING 5

Version 1.19.0

Description R interface to the MELTING 5 program (https://www.ebi.ac.uk/biomodels/tools/melting/) to compute melting temperatures of nucleic acid duplexes along with other thermodynamic parameters.

Depends R (>= 3.6)

Imports Rdpack, rJava (>= 0.9-8)

Suggests readxl, knitr, rmarkdown, reshape2, pander, testthat

SystemRequirements Java

biocViews BiomedicalInformatics, Cheminformatics,

License GPL-2 | GPL-3

Encoding UTF-8

LazyData true

RoxygenNote 7.2.1

RdMacros Rdpack

URL https://github.com/aravind-j/rmelting, https://aravind-j.github.io/rmelting/

BugReports https://github.com/aravind-j/rmelting/issues

VignetteBuilder knitr

git_url https://git.bioconductor.org/packages/rmelting

git_branch devel

git_last_commit aad86c8

git_last_commit_date 2023-10-24

Repository Bioconductor 3.19

Date/Publication 2024-04-17

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`melting` *Compute melting temperature of a nucleic acid duplex*

Description

Compute the enthalpy and entropy of helix-coil transition, and then the melting temperature of a nucleic acid duplex with the MELTING 5 software (Le Novère, 2001; Dumousseau et al., 2012).

Usage

```
melting(sequence, comp.sequence = NULL,
        nucleic.acid.conc,
        hybridisation.type = c("dnadna", "rnarna", "dnarna",
                               "rnadna", "mrnarna", "rnamrna"),
        Na.conc, Mg.conc, Tris.conc, K.conc,
        dNTP.conc, DMSO.conc, formamide.conc,
        size.threshold = 60, force.self = FALSE, correction.factor,
        method.approx = c("ahs01", "che93", "che93corr",
                          "schdot", "owe69", "san98",
                          "wetdna91", "wetrna91", "wetdnarna91"),
        method.nn = c("all97", "bre86", "san04", "san96", "sug96",
                      "tan04", "fre86", "xia98", "sug95", "tur06"),
        method.GU = c("tur99", "ser12"),
        method.singleMM = c("allsanpey", "tur06", "zno07", "zno08", "wat11"),
        method.tandemMM = c("allsanpey", "tur99"),
        method.single.dangle = c("bom00", "sugdna02", "sugrna02", "ser08"),
        method.double.dangle = c("sugdna02", "sugrna02", "ser05", "ser06"),
        method.long.dangle = c("sugdna02", "sugrna02"),
        method.internal.loop = c("san04", "tur06", "zno07"),
        method.single.bulge.loop = c("tan04", "san04", "ser07" ,"tur06"),
```

```
        method.long.bulge.loop = c("san04", "tur06"),
        method.CNG = c("bro05"),
        method.inosine = c("san05", "zno07"),
        method.hydroxyadenine = c("sug01"),
        method.azobenzenes = c("asa05"),
        method.locked = c("owc11", "mct04"),
        method.consecutive.locked = c("owc11"),
        method.consecutive.locked.singleMM = c("owc11"),
        correction.ion = c("ahs01", "kam71", "marschdot",
                           "owc1904", "owc2004", "owc2104",
                           "owc2204", "san96", "san04", "schlif",
                           "tanna06", "tanna07", "wet91",
                           "owcmg08", "tanmg06", "tanmg07",
                           "owcmix08", "tanmix07"),
        method.Naeq = c("ahs01", "mit96", "pey00"),
        correction.DMSO = c("ahs01", "cul76", "esc80", "mus81"),
        correction.formamide = c("bla96", "lincorr"))
```

Arguments

`sequence` Sequence (5' to 3') of one strand of the nucleic acid duplex as a character string (**Note:** Uridine and thymidine are not considered as identical).

`comp.sequence` Complementary sequence (3' to 5') of the nucleic acid duplex as a character string.

`nucleic.acid.conc` Concentration of the nucleic acid strand (M or mol L^{-1}) in excess as a numeric value.

`hybridisation.type` The hybridisation type. Either `"dnadna"`, `"rnarna"`, `"dnarna"`, `"rnadna"`, `"mrnarna"` or `"rnamrna"` (see **Hybridisation type options**).

`Na.conc` Concentration of Na ions (M) as a positive numeric value (see **Ion and agent concentrations**).

`Mg.conc` Concentration of Mg ions (M) as a positive numeric value (see **Ion and agent concentrations**).

`Tris.conc` Concentration of Tris ions (M) as a positive numeric value (see **Ion and agent concentrations**).

`K.conc` Concentration of K ions (M) as a positive numeric value (see **Ion and agent concentrations**).

`dNTP.conc` Concentration of dNTP (M) as a positive numeric value (see **Ion and agent concentrations**).

`DMSO.conc` Concentration of DMSO (%) as a positive numeric value (see **Ion and agent concentrations**).

`formamide.conc` Concentration of formamide (M or % depending on correction method) as a positive numeric value (see **Ion and agent concentrations**).

`size.threshold` Sequence length threshold to decide approximative or nearest-neighbour approach for computation. Default is 60.

`force.self` logical. Enforces that `sequence` is self complementary and `complementary sequence` is not required (seed **Self complementary sequences**). Default is `FALSE`.

`correction.factor`
Correction factor to be used to modulate the effect of the nucleic acid concentration (`nucleic.acid.conc`) in the computation of melting temperature (see **Correction factor for nucleic acid concentration**).

`method.approx` Specify the approximative formula to be used for melting temperature calculation for sequences of length greater than `size.threshold`. Either `"ahs01"`, `"che93"`, `"che93corr"`, `"schdot"`, `"owe69"`, `"san98"`, `"wetdna91"`, `"wetrna91"` or `"wetdnarna91"` (see **Approximative formulas**).

`method.nn` Specify the nearest neighbor model to be used for melting temperature calculation for perfectly matching sequences of length lesser than `size.threshold`. Either `"all97"`, `"bre86"`, `"san04"`, `"san96"`, `"sug96"`, `"tan04"`, `"fre86"`, `"xia98"`, `"sug95"` or `"tur06"` (see **Perfectly matching sequences**).

`method.GU` Specify the nearest neighbor model to compute the contribution of GU base pairs to the thermodynamic of helix-coil transition. Either `"tur99"` or `"ser12"` (see **GU wobble base pairs effect**).

`method.singleMM`
Specify the nearest neighbor model to compute the contribution of single mismatch to the thermodynamic of helix-coil transition. Either `"allsanpey"`, `"tur06"`, `"zno07"` `"zno08"` or `"wat11"` (see **Single mismatch effect**).

`method.tandemMM`
Specify the nearest neighbor model to compute the contribution of tandem mismatches to the thermodynamic of helix-coil transition. Either `"allsanpey"` or `"tur99"` (see **Tandem mismatches effect**).

`method.single.dangle`
Specify the nearest neighbor model to compute the contribution of single dangling end to the thermodynamic of helix-coil transition. Either `"bom00"`, `"sugdna02"`, `"sugrna02"` or `"ser08"` (see **Single dangling end effect**).

`method.double.dangle`
Specify the nearest neighbor model to compute the contribution of double dangling end to the thermodynamic of helix-coil transition. Either `"sugdna02"`, `"sugrna02"`, `"ser05"` or `"ser06"` (see **Double dangling end effect**).

`method.long.dangle`
Specify the nearest neighbor model to compute the contribution of long dangling end to the thermodynamic of helix-coil transition. Either `"sugdna02"` or `"sugrna02"` (see **Long dangling end effect**).

`method.internal.loop`
Specify the nearest neighbor model to compute the contribution of internal loop to the thermodynamic of helix-coil transition. Either `"san04"`, `"tur06"` or `"zno07"` (see **Internal loop effect**).

`method.single.bulge.loop`
Specify the nearest neighbor model to compute the contribution of single bulge loop to the thermodynamic of helix-coil transition. Either `"san04"`, `"tan04"`, `"ser07"` or `"tur06"` (see **Single bulge loop effect**).

`method.long.bulge.loop`
: Specify the nearest neighbor model to compute the contribution of long bulge loop to the thermodynamic of helix-coil transition. Either `"san04"` or `"tur06"` (see **Long bulge loop effect**).

`method.CNG`
: Specify the nearest neighbor model to compute the contribution of CNG repeats to the thermodynamic of helix-coil transition. Available method is `"bro05"` (see **CNG repeats effect**).

`method.inosine`
: Specify the specific nearest neighbor model to compute the contribution of inosine bases (I) to the thermodynamic of helix-coil transition. Either `"san05"` or `"zno07"` (see **Inosine bases effect**).

`method.hydroxyadenine`
: Specify the nearest neighbor model to compute the contribution of hydroxyadenine bases (A*) to the thermodynamic of helix-coil transition. Available method is `"sug01"` (see **Hydroxyadenine bases effect**).

`method.azobenzenes`
: Specify the nearest neighbor model to compute the contribution of azobenzenes (X_T for trans azobenzenes and X_C for cis azobenzenes) to the thermodynamic of helix-coil transition. Available method is `"asa05"` (see **Azobenzenes effect**).

`method.locked`
: Specify the nearest neighbor model to compute the contribution of single locked nucleic acids (AL, GL, TL and CL) to the thermodynamic of helix-coil transition. Either `"owc11"` or `"mct04"` (see **Single locked nucleic acids effect**).

`method.consecutive.locked`
: Specify the nearest neighbor model to compute the contribution of consecutive locked nucleic acids (AL, GL, TL and CL) to the thermodynamic of helix-coil transition. Available method is `"owc11"` (see **Consecutive locked nucleic acids effect**).

`method.consecutive.locked.singleMM`
: Specify the nearest neighbor model to compute the contribution of consecutive locked nucleic acids (AL, GL, TL and CL) with a single mismatch to the thermodynamic of helix-coil transition. Available method is `"owc11"` (see **Consecutive locked nucleic acids with single mismatch effect**).

`correction.ion`
: Specify the correction method for ions. Either one of the following:

- Na corrections`"ahs01"`, `"kam71"`, `"owc1904"`, `"owc2004"`, `"owc2104"`, `"owc2204"`, `"san96"`, `"san04"`, `"schlif"`, `"tanna06"`, `"wetdna91"`, `"tanna07"`, `"wetrna91"` or `"wetdnarna91"` (see **Sodium corrections**)
- Mg corrections`"owcmg08"`, `"tanmg06"` or `"tanmg07"` (see **Magnesium corrections**)
- Mixed Na Mg corrections`"owcmix08"`, `"tanmix07"` or `"tanmix07"` (see **Mixed Sodium and Magnesium corrections**)

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`method.Naeq`
: Specify the ion correction which gives a sodium equivalent concentration if other cations are present. Either `"ahs01"`, `"mit96"` or `"pey00"` (see **Sodium equivalent concentration methods**).

`correction.DMSO`
: Specify the correction method for DMSO. Specify the correction method for DMSO. Either `"ahs01"`, `"mus81"`, `"cul76"` or `"esc80"` (see **DMSO corrections**).

`correction.formamide`
: Specify the correction method for formamide. Specify the correction method for formamide Either `"bla96"` or `"lincorr"` (see **Formamide corrections**).

Value

A list with the following components:

`Environment` A list with details about the melting temperature computation environment.

`Options` A list with details about the options (default or user specified) used for melting temperature computation.

`Results` A list with the results of the melting temperature computation including the enthalpy and entropy in case of nearest neighbour methods.

`Message` Error and/or Warning messages, if any.

Mandatory arguments

The following are the arguments which are mandatory for computation.

`sequence` 5' to 3' sequence of one strand of the nucleic acid duplex as a character string. Recognises A, C, G, T, U, I, X_C, X_T, A*, AL, TL, GL and CL. U and T are not considered identical (see **Recognized nucleotides**).

`comp.sequence` Mandatory if there are mismatches, inosine(s) or hydroxyadenine(s) between the two strands. If not specified, it is computed as the complement of `sequence`. Self-complementarity in `sequence` is detected even though there may be (are) dangling end(s) and `comp.sequence` is computed (see **Self complementary sequences**).

`nucleic.acid.conc` See **Correction factor for nucleic acid concentration.**

`Na.conc, Mg.conc, Tris.conc, K.conc` At least one cation (Na, Mg, Tris, K) concentration is mandatory, the other agents(dNTP, DMSO, formamide) are optional (see **Ion and agent concentrations**).

`hybridisation.type` See **Hybridisation type options.**

Recognized nucleotides

Code	Type
A	Adenine
C	Cytosine
G	Guanine
T	Thymine
U	Uracil
I	Inosine
X_C	Trans azobenzenes
X_T	Cis azobenzenes
A*	Hydroxyadenine
AL	Locked nucleic acid
TL	"
GL	"

CL "

U and T are not considered identical.

Hybridisation type options

The details of the possible options for hybridisation type specified in the argument `hybridisation.type` are as follows:

Option	Sequence	Complementary sequence
dnadna	DNA	DNA
rnarna	RNA	RNA
dnarna	DNA	RNA
rnadna	RNA	DNA
mrnarna	2-o-methyl RNA	RNA
rnamrna	RNA	2-o-methyl RNA

This parameter determines the nature of the sequences in the arguments `sequence` and `comp.sequence`.

Ion and agent concentrations

Ion concentrations are specified by the arguments `Na.conc`, `Mg.conc`, `Tris.conc` and `K.conc`, while agent concentrations are specified by the arguments `dNTP.conc`, `DMSO.conc` and `formamide.conc`.

These values are used for different correction functions which approximately adjusts for effects of these ions (Na, Mg, Tris, K) and/or agents (dNTP, DMSO, formamide) on on thermodynamic stability of nucleic acid duplexes. Their concentration limits depends on the correction method used. All the concentrations must be in M, except for the DMSO (%) and formamide (% or M depending on the correction method). Note that $[\text{Tris}^+]$ is about half of the total tris buffer concentration.

Self complementary sequences

Self complementarity for perfect matching sequences or sequences with dangling ends is detected automatically. However it can be enforced by the argument `force.self = TRUE`.

Correction factor for nucleic acid concentration

For self complementary sequences (Auto detected or specified by `force.self`) it is 1. Otherwise it is 4 if the both strands are present in equivalent amount and 1 if one strand is in excess.

Approximative estimation formulas

Formula	Type	Limits/Remarks	Reference
ahs01	DNA	No mismatch	von Ahsen et al., 2001
che93	DNA	No mismatch; Na=0, Mg=0.0015, Tris=0.01, K=0.05	Marmur and Doty, 1962
che93corr	DNA	No mismatch; Na=0, Mg=0.0015, Tris=0.01, K=0.05	Marmur and Doty, 1962
schdot	DNA	No mismatch	Wetmur, 1991; Marmur and

			Doty, 1962; Chester and Marshak, 1993; Schildkraut and Lifson, 1965; Wahl et al., 1987; Britten et al., 1974; Hall et al., 1980
owe69	DNA	No mismatch	Owen et al., 1969; Frank-Kamenetskii, 1971; Blake, 1996; Blake and Delcourt, 1998
san98	DNA	No mismatch	SantaLucia, 1998; von Ahsen et al., 2001
wetdna91*	DNA		Wetmur, 1991
wetrna91*	RNA		Wetmur, 1991
wetdnarna91*	DNA/RNA		Wetmur, 1991

* Default formula for computation.

Note that calculation is increasingly incorrect when the length of the duplex decreases. Further, it does not take into account nucleic acid concentration.

Nearest neighbor models

Perfectly matching sequences:

Model	Type	Limits/Remarks	Reference
all97*	DNA		Allawi and SantaLucia, 1997
tur06*	2'-O-MeRNA/RNA	A sodium correction (san04) is automatically applied to convert the entropy (Na = 0.1M) into the entropy (Na = 1M).	Kierzek et al., 2006
bre86	DNA		Breslauer et al., 1986
san04	DNA		SantaLucia and Hicks, 2004
san96	DNA		SantaLucia et al., 1996
sug96	DNA		Sugimoto et al., 1996
tan04	DNA		Tanaka et al., 2004
fre86	RNA		Freier et al., 1986
xia98*	RNA		Xia et al., 1998
sug95*	DNA/RNA		SantaLucia et al., 1996

* Default model for computation.

GU wobble base pairs effect:

Model	Type	Limits/Remarks	Reference
tur99	RNA		Mathews et al., 1999
ser12*	RNA		Chen et al., 2012

* Default model for computation.

GU base pairs are not taken into account by the approximative mode.

Single mismatch effect:

Model	Type	Limits.Remarks	Reference
`allsanpey*`	DNA		Allawi and SantaLucia, 1997; Allawi and SantaLucia, 1998; Allawi and SantaLucia, 1998; Allawi and SantaLucia, 1998; Peyret et al., 1999
`wat11*`	DNA/RNA		Watkins et al., 2011
`tur06`	RNA		Lu et al., 2006
`zno07*`	RNA		Davis and Znosko, 2007
`zno08`	RNA	At least one adjacent GU base pair.	Davis and Znosko, 2008

* Default model for computation.

Single mismatches are not taken into account by the approximative mode.

Tandem mismatches effect:

Model	Type	Limits.Remarks	Reference
`allsanpey*`	DNA	Only GT mismatches and TA/TG mismatches.	Allawi and SantaLucia, 1997; Allawi and SantaLucia, 1998; Allawi and SantaLucia, 1998; Allawi and SantaLucia, 1998; Peyret et al., 1999
`tur99*`	RNA	No adjacent GU or UG base pairs.	Mathews et al., 1999; Lu et al., 2006

* Default model for computation.

Tandem mismatches are not taken into account by the approximative mode. Note that not all the mismatched Crick's pairs have been investigated.

Single dangling end effect:

Model	Type	Limits.Remarks	Reference
`bom00*`	DNA		Bommarito et al., 2000
`sugdna02`	DNA	Only terminal poly A self complementary sequences.	Ohmichi et al., 2002
`sugrna02`	RNA	Only terminal poly A self complementary sequences.	Ohmichi et al., 2002
`ser08*`	RNA	Only 3' UA, GU and UG terminal base pairs only 5' UG and GU terminal base pairs.	O'Toole et al., 2006; Miller et al., 2008

* Default model for computation.

Single dangling ends are not taken into account by the approximative mode.

Double dangling end effect:

Model	Type	Limits/Remarks	Reference
`sugdna02*`	DNA	Only terminal poly A self complementary sequences.	Ohmichi et al., 2002
`sugrna02`	RNA	Only terminal poly A self complementary sequences.	Ohmichi et al., 2002
`ser05`	RNA	Depends on the available thermodynamic parameters for single dangling end.	O'Toole et al., 2005
`ser06*`	RNA		O'Toole et al., 2006

* Default model for computation.
Double dangling ends are not taken into account by the approximative mode.

Long dangling end effect:

Model	Type	Limits/Remarks	Reference
`sugdna02*`	DNA	Only terminal poly A self complementary sequences.	Ohmichi et al., 2002
`sugrna02*`	RNA	Only terminal poly A self complementary sequences.	Ohmichi et al., 2002

* Default model for computation.
Long dangling ends are not taken into account by the approximative mode.

Internal loop effect:

Model	Type	Limits.Remarks	Reference
`san04*`	DNA	Missing asymmetry penalty. Not tested with experimental results.	SantaLucia and Hicks, 2004
`tur06`	RNA	Not tested with experimental results.	Lu et al., 2006
`zno07*`	RNA	Only for 1x2 loop.	Badhwar et al., 2007

* Default model for computation.
Internal loops are not taken into account by the approximative mode.

Single bulge loop effect:

Model	Type	Limits/Remarks	Reference
`tan04*`	DNA		Tan and Chen, 2007
`san04`	DNA	Missing closing AT penalty.	SantaLucia and Hicks, 2004
`ser07`	RNA	Less reliable results. Some missing parameters.	Blose et al., 2007
`tur06*`	RNA		Lu et al., 2006

* Default model for computation.
Single bulge loops are not taken into account by the approximative mode.

Long bulge loop effect:

Model	Type	Limits.Remarks	Reference
`san04*`	DNA	Missing closing AT penalty.	SantaLucia and Hicks, 2004
`tur06*`	RNA	Not tested with experimental results.	Mathews et al., 1999; Lu et al., 2006

* Default model for computation.
Long bulge loops are not taken into account by the approximative mode.

CNG repeats effect:

Model	Type	Limits/Remarks	Reference
`bro05*`	RNA	Self complementary sequences. 2 to 7 CNG repeats.	Broda et al., 2005

* Default model for computation.
CNG repeats are not taken into account by the approximative mode. The contribution of CNG repeats to the thermodynamic of helix-coil transition can be computed only for 2 to 7 CNG repeats. N represents a single mismatch of type N/N.

Inosine bases effect:

Model	Type	Limits/Remarks	Reference
`san05*`	DNA	Missing parameters for tandem base pairs containing inosine bases.	Watkins and SantaLucia, 2005
`zno07*`	RNA	Only IU base pairs.	Wright et al., 2007

* Default model for computation.
Inosine bases (I) are not taken into account by the approximative mode.

Hydroxyadenine bases effect:

Model	Type	Limits/Remarks	Reference
`sug01*`	DNA	Only 5' GA*C 3'and 5' TA*A 3' contexts.	Kawakami et al., 2001

* Default model for computation.
Hydroxyadenine bases (A*) are not taken into account by the approximative mode.

Azobenzenes effect effect:

Model	Type	Limits/Remarks	Reference
`asa05*`	DNA	Less reliable results when the number of cis azobenzene increases.	Asanuma et al., 2005

* Default model for computation.
Azobenzenes (X_T for trans azobenzenes and X_C for cis azobenzenes) are not taken into account by the approximative mode.

Single locked nucleic acids effect:

Model	Type	Limits.Remarks	Reference
mct04	DNA		McTigue, Peterson, and Kahn, 2004
owc11*	DNA		Owczarzy, You, Groth, and Tataurov, 2011

* Default model for computation.
Locked nucleic acids (AL, GL, TL and CL) are not taken into account by the approximative mode.

Consecutive locked nucleic acids effect:

Model	Type	Limits.Remarks	Reference
owc11*	DNA		Owczarzy et al., 2011

* Default model for computation.
Locked nucleic acids (AL, GL, TL and CL) are not taken into account by the approximative mode.

Consecutive locked nucleic acids with single mismatch effect:

Model	Type	Limits.Remarks	Reference
owc11*	DNA		Owczarzy et al., 2011

* Default model for computation.
Locked nucleic acids (AL, GL, TL and CL) are not taken into account by the approximative mode.

Ion corrections

Sodium corrections:

Correction	Type	Limits.Remarks	Reference
ahs01	DNA	Na>0.	von Ahsen et al., 2001
schlif	DNA	Na>=0.07; Na<=0.12.	Schildkraut and Lifson, 1965
tanna06	DNA	Na>=0.001; Na<=1.	Tan and Chen, 2006
tanna07*	RNA or 2'-O-MeRNA/RNA	Na>=0.003; Na<=1.	Tan and Chen, 2007
wet91	RNA, DNA and RNA/DNA	Na>0.	Wetmur, 1991
kam71	DNA	Na>0; Na>=0.069; Na<=1.02.	Frank-Kamenetskii, 1971
marschdot	DNA	Na>=0.069; Na<=1.02.	Marmur and Doty, 1962; Blake and Delcourt, 1998
owc1904	DNA	Na>0. (equation 19)	Owczarzy et al., 2004
owc2004	DNA	Na>0. (equation 20)	Owczarzy et al., 2004
owc2104	DNA	Na>0. (equation 21)	Owczarzy et al., 2004

owc2204*	DNA	Na>0. (equation 22)	Owczarzy et al., 2004
san96	DNA	Na>=0.1.	SantaLucia et al., 1996
san04	DNA	Na>=0.05; Na<=1.1; Oligonucleotides inferior to 16 bases.	SantaLucia and Hicks, 2004; SantaLucia, 1998

* Default correction method for computation.

Magnesium corrections:

Correction	Type	Limits/Remarks	Reference
owcmg08*	DNA	Mg>=0.0005; Mg<=0.6.	Owczarzy et al., 2008
tanmg06	DNA	Mg>=0.0001; Mg<=1; Oligomer length superior to 6 base pairs.	Tan and Chen, 2006
tanmg07*	RNA	Mg>=0.1; Mg<=0.3.	Tan and Chen, 2007

* Default correction method for computation.

Mixed Sodium and Magnesium corrections:

Correction	Type	Limits.Remarks	Reference
owcmix08*	DNA	Mg>=0.0005; Mg<=0.6; Na+K+Tris/2>0.	Owczarzy et al., 2008
tanmix07	DNA, RNA or 2'-O-MeRNA/RNA	Mg>=0.1; Mg<=0.3; Na+K+Tris/2>=0.1; Na+K+Tris/2<=0.3.	Tan and Chen, 2007

* Default correction method for computation.

The ion correction by Owczarzy et al. (2008) is used by default according to the $\frac{[\mathrm{Mg}^{2+}]^{0.5}}{[\mathrm{Mon}^{+}]}$ ratio, where $[\mathrm{Mon}^{+}] = [\mathrm{Na}^{+}] + [\mathrm{Tris}^{+}] + [\mathrm{K}^{+}]$.

If,

$[\mathrm{Mon}^{+}]$ **= 0** Default sodium correction is used.

Ratio < 0.22, Default sodium correction is used.

0.22 <= Ratio < 6 Default mixed Na and Mg correction is used.

Ratio >= 6 Default magnesium correction is used.

Note that $[\mathrm{Tris}^{+}]$ is about half of the total tris buffer concentration.

Sodium equivalent concentration methods:

Correction	Type	Limits/Remarks	Reference
ahs01*	DNA		von Ahsen et al., 2001
mit96	DNA		Mitsuhashi, 1996
pey00	DNA		Peyret, 2000

* Default correction method for computation.

For the other types of hybridization, the DNA default correction is used. If there are other cations when an approximative approach is used, a sodium equivalence is automatically computed. In case of nearest neighbor approach, the sodium equivalence will be used only if a sodium correction is specified by the argument `correction.ion`.

Denaturing agent corrections

DMSO corrections:

Correction	Type	Limits/Remarks	Reference
`ahs01*`	DNA	Not tested with experimental results.	von Ahsen et al., 2001
`cul76`	DNA	Not tested with experimental results.	Cullen and Bick, 1976
`esc80`	DNA	Not tested with experimental results.	Escara and Hutton, 1980
`mus81`	DNA	Not tested with experimental results.	Musielski et al., 1981

* Default correction method for computation.

For the other types of hybridization, the DNA default correction is used. If there is DMSO when an approximative approach is used, a DMSO correction is automatically computed. In case of nearest neighbor approach and approximative approach, the DMSO correction will be used only if a sodium correction is specified by the argument `correction.ion`.

Formamide corrections:

Correction	Type	Limits/Remarks	Reference
`bla96*`	DNA	With formamide concentration in mol/L.	Blake, 1996
`lincorr`	DNA	With a formamide volume.	McConaughy et al., 1969; Record, 1967; Casey and Davidson, 1977; Hutton, 1977

* Default correction method for computation.

For the other types of hybridization, the DNA default correction is used. If there is formamide when an approximative approach is used, a formamide correction is automatically computed. In case of nearest neighbor approach and approximative approach, the formamide correction will be used only if a sodium correction is specified by the argument `correction.ion`.

References

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See Also

For more details about algorithm, formulae and methods, see the documentation for MELTING 5.

Examples

```
# Basic usage
melting(sequence = "CAGTGAGACAGCAATGGTCG", nucleic.acid.conc = 2e-06,
        hybridisation.type = "dnadna", Na.conc = 1)

# For more detailed examples refer the vignette.
## Not run:

browseVignettes(package = 'rmelting')

## End(Not run)
```

meltingBatch *Compute melting temperature of multiple nucleic acid duplexes in batch*

Description

Compute the enthalpy and entropy of helix-coil transition, and then the melting temperature of multiple nucleic acid duplexes in batch.

Usage

```
meltingBatch(
  sequence,
  comp.sequence = NULL,
  environment.out = TRUE,
  options.out = TRUE,
  message.out = TRUE,
  ...
)
```

Arguments

`sequence`	A character vector of 5' to 3' sequences of one strand of the nucleic acid duplex (**Note:** Uridine and thymidine are not considered as identical).
`comp.sequence`	A character vector of 3' to 5' complementary sequences of the nucleic acid duplex. Complementary sequences are computed by default, but need to be specified in case of mismatches, inosine(s) or hydroxyadenine(s) between the two strands.
`environment.out`	logical. If `TRUE`, gives the melting temperature computation environment details in the output. Default is `TRUE`.
`options.out`	logical. If `TRUE`, gives the details about the options (default or user specified) used for melting temperature computation in the output. Default is `TRUE`.
`message.out`	logical. If `TRUE`, gives the error and/or warning messages, if any in the output. Default is `TRUE`.
`...`	Arguments for melting temperature computation (See `melting`).

Value

A data frame of the melting temperature computation results along with the details of environment, options and messages if specified by the arguments `environment.out`, `options.out` and `message.out` respectively.

See Also

`melting`

Examples

```
sequence <- c("CAAAAAG", "CAAAAAAG", "TTTTATAATAAA", "CCATCGCTACC",
              "CAAACAAAG", "CCATTGCTACC", "CAAAAAAAG", "GTGAAC", "AAAAAAAA",
              "CAACTTGATATTATTA", "CAAATAAAG", "GCGAGC", "GGGACC",
              "CAAAGAAAG", "CTGACAAGTGTC", "GCGAAAAGCG")

meltingBatch(sequence, nucleic.acid.conc = 0.0004,
             hybridisation.type = "dnadna", Na.conc = 1)

seq <- c("GCAUACG", "CAGUAGGUC", "CGCUCGC", "GAGUGGAG", "GACAGGCUG",
         "CAGUACGUC", "GACAUCCUG", "GACCACCUG", "CAGAAUGUC", "GCGUCGC",
         "CGUCCGG", "GACUCUCUG", "CAGCUGGUC", "GACUAGCUG", "CUCUGCUC",
         "GCGUCCG", "GUCCGCG", "CGAUCAC", "GACUACCUG", "GACGAUCUG")

comp.seq <- c("CGUUUGC", "GUCGGCCAG", "GCGUGCG", "CUCUUCUC", "CUGUGCGAC",
              "GUCGGGCAG", "CUGUUGGAC", "CUGGGGGAC", "GUCUGGCAG", "CGCUGCG",
              "GCUGGCC", "CUGAUAGAC", "GUCGUUCAG", "CUGAGCGAC", "GAGUUGAG",
              "CGCUGGC", "CUGGCGC", "GCUUGUG", "CUGAGGGAC", "CUGCCAGAC")

meltingBatch(sequence = seq, comp.seq = comp.seq, nucleic.acid.conc = 0.0004,
             hybridisation.type = "rnarna", Na.conc = 1,
             method.singleMM = "tur06")
```

`print.melting` *Prints melting temperature from a* `melting` *object*

Description

`print.melting` prints to console the melting temperature value from an object of class `melting`.

Usage

```
## S3 method for class 'melting'
print(x, ...)
```

Arguments

`x`	An object of class `melting`.
`...`	Unused

Value

The melting temperature value (degree Celsius) in the console.

See Also

`melting`

withWE *Evaluate expression and capture all warnings and errors if any along with results*

Description

Not exported. Strictly internal

Usage

```
withWE(expr)
```

Arguments

expr	The expression to be evaluated.

Value

- In cas of Warning(s)Returns the value along with the warning message(s).
- In cas of ErrorReturns NA as the value along with the error message.

Examples

```
foo <- function(){
  warning("oops")
  1}

foo <- function(){
  warning("oops")
  warning("again oops")
  1}

foo <- function(){
  warning("oops")
  log("a")}
```

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