

Package ‘rmelting’

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Title R Interface to MELTING 5

Version 1.20.0

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)

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RdMacros Rdpack

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

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melting	<i>Compute melting temperature of a nucleic acid duplex</i>
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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.

<code>force.self</code>	logical. Enforces that sequence is self complementary and complementary sequence is not required (seed Self complementary sequences). Default is FALSE.
<code>correction.factor</code>	Correction factor to be used to modulate the effect of the nucleic acid concentration (<code>nucleic.acid.conc</code>) in the computation of melting temperature (see Correction factor for nucleic acid concentration).
<code>method.approx</code>	Specify the approximative formula to be used for melting temperature calculation for sequences of length greater than <code>size.threshold</code> . Either "ahs01", "che93", "che93corr", "schdot", "owe69", "san98", "wetdna91", "wetrna91" or "wetdnarna91" (see Approximative formulas).
<code>method.nn</code>	Specify the nearest neighbor model to be used for melting temperature calculation for perfectly matching sequences of length lesser than <code>size.threshold</code> . Either "all97", "bre86", "san04", "san96", "sug96", "tan04", "fre86", "xia98", "sug95" or "tur06" (see Perfectly matching sequences).
<code>method.GU</code>	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).
<code>method.singleMM</code>	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).
<code>method.tandemMM</code>	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).
<code>method.single.dangle</code>	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).
<code>method.double.dangle</code>	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).
<code>method.long.dangle</code>	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).
<code>method.internal.loop</code>	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).
<code>method.single.bulge.loop</code>	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**)
- 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 the thermodynamic stability of nucleic acid duplexes. Their concentration limits depend 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

owe69	DNA	No mismatch	Doty, 1962; Chester and Marshak, 1993; Schildkraut and Lifson, 1965; Wahl et al., 1987; Britten et al., 1974; Hall et al., 1980; 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
all197*	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	$Na \geq 0.07$; $Na \leq 0.12$.	Schildkraut and Lifson, 1965
tanna06	DNA	$Na \geq 0.001$; $Na \leq 1$.	Tan and Chen, 2006
tanna07*	RNA	$Na \geq 0.003$; $Na \leq 1$.	Tan and Chen, 2007
	or 2'-O-MeRNA/RNA		
wet91	RNA, DNA and RNA/DNA	$Na > 0$.	Wetmur, 1991
kam71	DNA	$Na > 0$; $Na \geq 0.069$; $Na \leq 1.02$.	Frank-Kamenetskii, 1971
marschdot	DNA	$Na \geq 0.069$; $Na \leq 1.02$.	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 $\frac{[Mg^{2+}]^{0.5}}{[Mon^+]}$ ratio, where $[Mon^+] = [Na^+] + [Tris^+] + [K^+]$.

If,

$[Mon^+] = 0$ 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 $[Tris^+]$ 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
cu176	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

- Marmur J, Doty P (1962). "Determination of the base composition of deoxyribonucleic acid from its thermal denaturation temperature." *Journal of Molecular Biology*, **5**(1), 109–118.
- Schildkraut C, Lifson S (1965). "Dependence of the melting temperature of DNA on salt concentration." *Biopolymers*, **3**(2), 195–208.

- Record MT (1967). "Electrostatic effects on polynucleotide transitions. I. Behavior at neutral pH." *Biopolymers*, **5**(10), 975–992.
- McConaughy BL, Laird C, McCarthy BJ (1969). "Nucleic acid reassociation in formamide." *Biochemistry*, **8**(8), 3289–3295.
- Owen RJ, Hill LR, Lapage SP (1969). "Determination of DNA base compositions from melting profiles in dilute buffers." *Biopolymers*, **7**(4), 503–516.
- Frank-Kamenetskii MD (1971). "Simplification of the empirical relationship between melting temperature of DNA, its GC content and concentration of sodium ions in solution." *Biopolymers*, **10**(12), 2623–2624.
- Britten RJ, Graham DE, Neufeld BR (1974). "Analysis of repeating DNA sequences by reassociation." *Methods in Enzymology*, **29**, 363–418.
- Cullen BR, Bick MD (1976). "Thermal denaturation of DNA from bromodeoxyuridine substituted cells." *Nucleic Acids Research*, **3**(1), 49–62.
- Hutton JR (1977). "Renaturation kinetics and thermal stability of DNA in aqueous solutions of formamide and urea." *Nucleic Acids Research*, **4**(10), 3537–3555.
- Casey J, Davidson N (1977). "Rates of formation and thermal stabilities of RNA:DNA and DNA:DNA duplexes at high concentrations of formamide." *Nucleic Acids Research*, **4**(5), 1539–1552.
- Hall TJ, Grula JW, Davidson EH, Britten RJ (1980). "Evolution of sea urchin non-repetitive DNA." *Journal of Molecular Evolution*, **16**(2), 95–110.
- Escara JF, Hutton JR (1980). "Thermal stability and renaturation of DNA in dimethyl sulfoxide solutions: Acceleration of the renaturation rate." *Biopolymers*, **19**(7), 1315–1327.
- Musielski H, Mann W, Laue R, Michel S (1981). "Influence of dimethylsulfoxide on transcription by bacteriophage T3-induced RNA polymerase." *Zeitschrift für allgemeine Mikrobiologie*, **21**(6), 447–456.
- Freier SM, Kierzek R, Jaeger JA, Sugimoto N, Caruthers MH, Neilson T, Turner DH (1986). "Improved free-energy parameters for predictions of RNA duplex stability." *Proceedings of the National Academy of Sciences*, **83**(24), 9373.
- Breslauer KJ, Frank R, Blocker H, Marky LA (1986). "Predicting DNA duplex stability from the base sequence." *Proceedings of the National Academy of Sciences*, **83**(11), 3746.
- Wahl GM, Barger SL, Kimmel AR (1987). "Molecular hybridization of immobilized nucleic acids: Theoretical concepts and practical considerations." *Methods in Enzymology*, **152**, 399–407.
- Wetmur JG (1991). "DNA probes: Applications of the principles of nucleic acid hybridization." *Critical Reviews in Biochemistry and Molecular Biology*, **26**(3-4), 227–259.
- Chester N, Marshak DR (1993). "Dimethyl sulfoxide-mediated primer T_m reduction: A method for analyzing the role of renaturation temperature in the polymerase chain reaction." *Analytical Biochemistry*, **209**(2), 284–290.
- Sugimoto N, Katoh M, Nakano S, Ohmichi T, Sasaki M (1994). "RNA/DNA hybrid duplexes with identical nearest-neighbor base-pairs have identical stability." *FEBS Letters*, **354**(1), 74–78.
- Sugimoto N, Nakano S, Katoh M, Matsumura A, Nakamuta H, Ohmichi T, Yoneyama M, Sasaki M (1995). "Thermodynamic parameters to predict stability of RNA/DNA hybrid duplexes." *Biochemistry*, **34**(35), 11211–11216.
- SantaLucia J, Allawi HT, Seneviratne PA (1996). "Improved nearest-neighbor parameters for predicting DNA duplex stability." *Biochemistry*, **35**(11), 3555–3562.

- Sugimoto N, Nakano S, Yoneyama M, Honda K (1996). "Improved thermodynamic parameters and helix initiation factor to predict stability of DNA duplexes." *Nucleic Acids Research*, **24**(22), 4501–4505.
- Blake RD, Delcourt SG (1996). "Thermodynamic effects of formamide on DNA stability." *Nucleic Acids Research*, **24**(11), 2095–2103.
- Blake RD (1996). "Denaturation of DNA." In Meyers RA (ed.), *Encyclopedia of molecular biology and molecular medicine*, volume 2, 1–19. VCH Verlagsgesellschaft, Weinheim, Germany.
- Mitsuhashi M (1996). "Technical report: Part 1. Basic requirements for designing optimal oligonucleotide probe sequences." *Journal of Clinical Laboratory Analysis*, **10**(5), 277–284.
- Allawi HT, SantaLucia J (1997). "Thermodynamics and NMR of internal G·T mismatches in dna." *Biochemistry*, **36**(34), 10581–10594.
- SantaLucia J (1998). "A unified view of polymer, dumbbell, and oligonucleotide DNA nearest-neighbor thermodynamics." *Proceedings of the National Academy of Sciences*, **95**(4), 1460.
- Xia T, SantaLucia J, Burkard ME, Kierzek R, Schroeder SJ, Jiao X, Cox C, Turner DH (1998). "Thermodynamic parameters for an expanded nearest-neighbor model for formation of RNA duplexes with Watson-Crick base pairs." *Biochemistry*, **37**(42), 14719–14735.
- Allawi HT, SantaLucia J (1998). "Thermodynamics of internal C·T mismatches in DNA." *Nucleic Acids Research*, **26**(11), 2694–2701.
- Blake RD, Delcourt SG (1998). "Thermal stability of DNA." *Nucleic Acids Research*, **26**(14), 3323–3332.
- Allawi HT, SantaLucia J (1998). "Nearest neighbor thermodynamic parameters for internal G·A mismatches in DNA." *Biochemistry*, **37**(8), 2170–2179.
- Allawi HT, SantaLucia J (1998). "Nearest-neighbor thermodynamics of internal A·C mismatches in dna: sequence dependence and pH effects." *Biochemistry*, **37**(26), 9435–9444.
- Mathews DH, Sabina J, Zuker M, Turner DH (1999). "Expanded sequence dependence of thermodynamic parameters improves prediction of RNA secondary structure." *Journal of Molecular Biology*, **288**(5), 911–940.
- Peyret N, Seneviratne PA, Allawi HT, SantaLucia J (1999). "Nearest-Neighbor Thermodynamics and NMR of DNA Sequences with Internal A·A, C·C, G·G, and T·T Mismatches." *Biochemistry*, **38**(12), 3468–3477.
- Peyret N (2000). *Prediction of nucleic acid hybridization: Parameters and algorithms*. Ph.D. Thesis, Wayne State University, Detroit, MI.
- Bommarito S, Peyret N, SantaLucia J (2000). "Thermodynamic parameters for DNA sequences with dangling ends." *Nucleic Acids Research*, **28**(9), 1929–1934.
- Kawakami J, Kamiya H, Yasuda K, Fujiki H, Kasai H, Sugimoto N (2001). "Thermodynamic stability of base pairs between 2-hydroxyadenine and incoming nucleotides as a determinant of nucleotide incorporation specificity during replication." *Nucleic Acids Research*, **29**(16), 3289–3296.
- von Ahsen N, Wittwer CT, Schutz E (2001). "Oligonucleotide melting temperatures under PCR conditions: Nearest-neighbor corrections for Mg²⁺, deoxynucleotide triphosphate, and dimethyl sulfoxide concentrations with comparison to alternative empirical formulas." *Clinical Chemistry*, **47**(11), 1956–1961.

- Le Novere N (2001). "MELTING, computing the melting temperature of nucleic acid duplex." *Bioinformatics*, **17**(12), 1226–1227.
- Ohmichi T, Nakano S, Miyoshi D, Sugimoto N (2002). "Long RNA dangling end has large energetic contribution to duplex stability." *Journal of the American Chemical Society*, **124**(35), 10367–10372.
- SantaLucia J, Hicks D (2004). "The thermodynamics of DNA structural motifs." *Annual Review of Biophysics and Biomolecular Structure*, **33**(1), 415–440.
- Tanaka F, Kameda A, Yamamoto M, Ohuchi A (2004). "Thermodynamic parameters based on a nearest-neighbor model for DNA sequences with a single-bulge loop." *Biochemistry*, **43**(22), 7143–7150.
- McTigue PM, Peterson RJ, Kahn JD (2004). "Sequence-dependent thermodynamic parameters for locked nucleic acid (LNA)-DNA duplex formation." *Biochemistry*, **43**(18), 5388–5405.
- Owczarzy R, You Y, Groth CL, Tataurov AV (2011). "Stability and mismatch discrimination of locked nucleic acid-DNA duplexes." *Biochemistry*, **50**(43), 9352–9367.
- Owczarzy R, You Y, Moreira BG, Manthey JA, Huang L, Behlke MA, Walder JA (2004). "Effects of sodium ions on DNA duplex oligomers: Improved predictions of melting temperatures." *Biochemistry*, **43**(12), 3537–3554.
- Broda M, Kierzek E, Gdaniec Z, Kulinski T, Kierzek R (2005). "Thermodynamic stability of RNA structures formed by CNG trinucleotide repeats. Implication for prediction of RNA structure." *Biochemistry*, **44**(32), 10873–10882.
- Watkins NE, SantaLucia J (2005). "Nearest-neighbor thermodynamics of deoxyinosine pairs in DNA duplexes." *Nucleic Acids Research*, **33**(19), 6258–6267.
- Asanuma H, Matsunaga D, Komiyama M (2005). "Clear-cut photo-regulation of the formation and dissociation of the DNA duplex by modified oligonucleotide involving multiple azobenzenes." *Nucleic Acids Symposium Series*, 35–36. <http://www.ncbi.nlm.nih.gov/pubmed/17150620>.
- O'Toole AS, Miller S, Serra MJ (2005). "Stability of 3' double nucleotide overhangs that model the 3' ends of siRNA." *RNA*, **11**(4), 512–516. <http://www.ncbi.nlm.nih.gov/pubmed/15769878>.
- Lu ZJ, Turner DH, Mathews DH (2006). "A set of nearest neighbor parameters for predicting the enthalpy change of RNA secondary structure formation." *Nucleic Acids Research*, **34**(17), 4912–4924.
- Kierzek E, Mathews DH, Ciesielska A, Turner DH, Kierzek R (2006). "Nearest neighbor parameters for Watson-Crick complementary heteroduplexes formed between 2'-O-methyl RNA and RNA oligonucleotides." *Nucleic Acids Research*, **34**(13), 3609–3614.
- Tan Z, Chen S (2006). "Nucleic acid helix stability: Effects of salt concentration, cation valence and size, and chain length." *Biophysical Journal*, **90**(4), 1175–1190.
- O'Toole AS, Miller S, Haines N, Zink MC, Serra MJ (2006). "Comprehensive thermodynamic analysis of 3' double-nucleotide overhangs neighboring Watson-Crick terminal base pairs." *Nucleic Acids Research*, **34**(11), 3338–3344.
- Tan Z, Chen S (2007). "RNA helix stability in mixed Na(+)/Mg(2+) solution." *Biophysical Journal*, **92**(10), 3615–3632.
- Wright DJ, Rice JL, Yanker DM, Znosko BM (2007). "Nearest neighbor parameters for inosine-uridine pairs in RNA duplexes." *Biochemistry*, **46**(15), 4625–4634.

Davis AR, Znosko BM (2007). “Thermodynamic characterization of single mismatches found in naturally occurring RNA.” *Biochemistry*, **46**(46), 13425–13436.

Blose JM, Manni ML, Klapac KA, Stranger-Jones Y, Zyra AC, Sim V, Griffith CA, Long JD, Serra MJ (2007). “Non-nearest-neighbor dependence of stability for RNA bulge loops based on the complete set of group I single nucleotide bulge loops.” *Biochemistry*, **46**(51), 15123–15135.

Badhwar J, Karri S, Cass CK, Wunderlich EL, Znosko BM (2007). “Thermodynamic characterization of RNA duplexes containing naturally occurring 1 * 2 nucleotide internal loops.” *Biochemistry*, **46**(50), 14715–14724.

Davis AR, Znosko BM (2008). “Thermodynamic characterization of naturally occurring RNA single mismatches with G-U nearest neighbors.” *Biochemistry*, **47**(38), 10178–10187.

Miller S, Jones LE, Giovannitti K, Piper D, Serra MJ (2008). “Thermodynamic analysis of 5’ and 3’ single- and 3’ double-nucleotide overhangs neighboring wobble terminal base pairs.” *Nucleic Acids Research*, **36**(17), 5652–5659.

Owczarzy R, Moreira BG, You Y, Behlke MA, Walder JA (2008). “Predicting stability of DNA duplexes in solutions containing magnesium and monovalent cations.” *Biochemistry*, **47**(19), 5336–5353.

Watkins NE, Kennelly WJ, Tsay MJ, Tuin A, Swenson L, Lee H, Morosyuk S, Hicks DA, SantaLucia J (2011). “Thermodynamic contributions of single internal rA·dA, rC·dC, rG·dG and rU·dT mismatches in RNA/DNA duplexes.” *Nucleic Acids Research*, **39**(5), 1894–1902.

Chen JL, Dishler AL, Kennedy SD, Yildirim I, Liu B, Turner DH, Serra MJ (2012). “Testing the nearest neighbor model for canonical rna base pairs: Revision of GU parameters.” *Biochemistry*, **51**(16), 3508–3522.

Dumousseau M, Rodriguez N, Juty N, Le Novere N (2012). “MELTING, a flexible platform to predict the melting temperatures of nucleic acids.” *BMC Bioinformatics*, **13**, 101.

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	<i>Compute melting temperature of multiple nucleic acid duplexes in batch</i>
--------------	---

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", "AAAAAAA",
             "CAACTTGATATTATTA", "CAAATAAAG", "GCGAGC", "GGGACC",
             "CAAAGAAAG", "CTGACAAGTGC", "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", "GACUACCU", "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	<i>Evaluate expression and capture all warnings and errors if any along with results</i>
--------	--

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 Error Returns NA as the value along with the error message.

Examples

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

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

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

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