Package 'rmelting'

January 15, 2019

Title R Interface to MELTING 5

Version 0.99.1	
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 (>= 3.5.0), rJava (>= 0.5-0)	
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BugReports https://github.com/aravind-j/rmelting/issues VignetteBuilder knitr	
R topics documented:	
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Description

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

Usage

```
melting(sequence, comp.sequence = NULL,
       nucleic.acid.conc,
       Na.conc, Mg.conc, Tris.conc, K.conc,
       dNTP.conc, DMSO.conc, formamide.conc,
       size.threshold = 60, force.self = FALSE, correction.factor,
       method.singleMM = c("allsanpey", "tur06", "zno07", "zno08"),
       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("mct04"),
       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", "mus80"),
       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 locked nucleic acids (AL, GL, TL and CL) to the thermodynamic of helix-coil transition. Available method is "mct04" (see Locked nucleic acids 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 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 [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
al197*	DNA		Allawi and SantaLucia, 1997
tur06*	2'-O-MeRNA/	A sodium correction	Kierzek et al., 2006
	RNA	(san04) is	
		automatically applied to	
		convert the entropy (Na =	
		0.1M) into the entropy (Na =	
		1M).	
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/		SantaLucia et al., 1996
	RNA		

^{*} 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	Davis and Znosko, 2008
		pair.	

^{*} 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	Allawi and SantaLucia, 1997;
		mismatches.	Allawi and SantaLucia, 1998;
			Allawi and SantaLucia, 1998;
			Allawi and SantaLucia, 1998;
			Peyret et al., 1999
tur99*	RNA	No adjacent GU or UG base	Mathews et al., 1999; Lu et
		pairs.	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	Ohmichi et al., 2002
		complementary sequences.	
sugrna02	RNA	Only terminal poly A self	Ohmichi et al., 2002
		complementary sequences.	
ser08*	RNA	Only 3' UA, GU and UG	O'Toole et al., 2006; Miller
		terminal base pairs only 5'	et al., 2008
		UG and GU terminal base	
		pairs.	

^{*} 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	Ohmichi et al., 2002

		complementary sequences.	
sugrna02	RNA	Only terminal poly A self	Ohmichi et al., 2002
		complementary sequences.	
ser05	RNA	Depends on the available	O'Toole et al., 2005
		thermodynamic parameters for	
		single dangling end.	
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	Ohmichi et al., 2002
		complementary sequences.	
sugrna02*	RNA	Only terminal poly A self	Ohmichi et al., 2002
		complementary sequences.	

^{*} 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.	SantaLucia and Hicks, 2004
		Not tested with experimental	
		results.	
tur06	RNA	Not tested with experimental	Lu et al., 2006
		results.	
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	Blose et al., 2007
		missing parameters.	
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	Mathews et al., 1999; Lu et
		results.	al., 2006

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.	Broda et al., 2005
		2 to 7 CNG repeats.	

^{*} 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	Watkins and SantaLucia, 2005
		base pairs containing inosine	
		bases.	
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'	Kawakami et al., 2001
		contexts.	

^{*} 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	Asanuma et al., 2005
		the number of cis azobenzene	
		increases.	

^{*} 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.

Locked nucleic acids effect:

Model	Type	Limits/Remarks	Reference
mct04*	DNA		McTigue et al., 2004

^{*} Default model for computation.

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

^{*} Default model for computation.

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	Na>=0.003; Na<=1.	Tan and Chen, 2007
	or		
	2'-O-MeRNA/RNA		
wet91	RNA,	Na>0.	Wetmur, 1991
	DNA		
	and		
	RNA/DNA		
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;	SantaLucia and Hicks, 2004;
		Oligonucleotides inferior to	SantaLucia, 1998
		16 bases.	

^{*} 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	Tan and Chen, 2006
		length superior to 6 base	
		pairs.	
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;	Owczarzy et al., 2008
		Na+K+Tris/2>0.	
tanmix07	DNA,	Mg>=0.1; Mg<=0.3;	Tan and Chen, 2007
	RNA	Na+K+Tris/2>=0.1;	
	or	Na+K+Tris/2<=0.3.	
	2'-O-MeRNA/RNA		

^{*} 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
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	Blake, 1996
		in mol/L.	
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.

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See Also

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

Examples

print.melting 17

```
## Not run:
browseVignettes(package = 'rmelting')
## End(Not run)
```

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

See Also

melting

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