Package 'rmelting'

April 2, 2018

Title R Interface to MELTING 5

Version 0.0.0.9000

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

Depends R (>= 3.4.3), rJava (>= 0.5-0)

Imports rJava, melting5jars

License GPL-2 | GPL-3

Encoding UTF-8

LazyData true

RoxygenNote 6.0.1

Remotes github::hrbrmstr/melting5jars

RdMacros Rdpack

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

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

R topics documented:

`melting` *melting*

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

```
\begin{alltt}
 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, self = FALSE, correction.factor,
         method.approx = c("ahs01", "che93", "che93corr",
                           "marschdot", "owe69", "san98",
                           "wetdna91", "wetrna91", "wetdnarna91"),
         method.nn = c("all97", "bre86", "san04", "san96", "sug96",
                       "tan04", "fre86", "xia98", "sug95", "tur06"),
         method.GU = c("tur99"),
         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.Na = c("ahs01", "kam71", "marschdot",
                           "owc1904", "owc2004", "owc2104", "owc2204",
                           "san96", "san04", "schlif",
                           "tanna06", "tanna07", "wet91"),
         correction.Mg = c("oxcmg08", "tanmg06", "tanmg07"),
         correction.NaMg = c("oxcmix08", "tanmix07"),
         method.Naeq = c("ahs01", "mit96", "pey00"),
         correction.DMSO = c("ahs01", "cul76", "esc80", "mus80"),
         correction.formamide = c("bla96", "lincorr")) \end{alltt}
```

Arguments

`sequence`	Sequence (5' to 3') of one strand of the nucleic acid duplex as a character string.
`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 ($molL^{-1}$) 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 numeric value (see **Ion and agent concentrations**).

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

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

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

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

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

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

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

`self` logical. Specifies 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 sequences of length lesser than `size.threshold`. Either `"all97"`, `"bre86"`, `"san04"`, `"san96"`, `"sug96"`, `"tan04"`, `"fre86"`, `"xia98"`, `"sug95"` or `"tur06"` (see **Nearest neighbor models**).

`method.GU` Specify the nearest neighbor model to compute the contribution of GU base pairs to the thermodynamic of helix-coil transition. Available method is `"tur99"` (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"` or `"zno08"` (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 pecific 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.Na`
: Specify the correction method for Na ions. Either `"ahs01"`, `"kam71"`, `"owc1904"`, `"owc2004"`, `"owc2104"`, `"owc2204"`, `"san96"`, `"san04"`, `"schlif"`, `"tanna06"`, `"wetdna91"`, `"tanna07"`, `"wetrna91"` or `"wetdnarna91"` (see **Sodium corrections**).

`correction.Mg`
: Specify the correction method for Mg ions. Either `"owcmg08"`, `"tanmg06"` or `"tanmg07"` (see **Magnesium corrections**).

`correction.NaMg`
: Specify the correction method for mixed Na and Mg ions. Either `"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**).

Mandatory arguments

The following are the arguments which are mandatory for computation.

- sequence
- 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
- 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.
- hybridisation.type

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

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+ concentration 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 specified by the argument self.

Correction factor for nucleic acid concentration

For self complementary sequences (Auto detected or specified in 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

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

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 et al., 1962
che93corr	DNA	No mismatch; Na=0, Mg=0.0015, Tris=0.01, K=0.05	Marmur et al., 1962
marschdot	DNA	No mismatch	Wetmur 1991; Marmur et al., 196
owe69	DNA	No mismatch	Owen et al., 1969; Blake 1996; Bl
san98	DNA	No mismatch	SantaLucia 1998; von Ahsen et al
wetdna91*	DNA		Wetmur 1991
wetrna91*	RNA		Wetmur 1991
wetdnarna91*	DNA/RNA		Wetmur 1991

Nearest neighbor models

Model	Type	Limits/Remarks
all97*	DNA	
bre86	DNA	
san04	DNA	
san96	DNA	
sug96	DNA	
tan04	DNA	
fre86	RNA	
xia98*	RNA	
sug95*	DNA/RNA	
tur06*	DNA	A sodium correction (san04) is automatically applied to convert the entropy (Na = 0.1M) into the

GU wobble base pairs effect

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

Single mismatch effect

Model	Type	Limits/Remarks	Reference
allsanpey*	DNA		Allawi et al., 1997; Allawi et al., 1998a; Allawi et al., 1998b
tur06	RNA		Lu et al., 2006
zno07*	RNA		Davis et al., 2007
zno08	RNA	At least one adjacent GU base pair.	Davis et al., 2008

Tandem mismatches effect

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

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	NA	Bommarito e
sugdna02	DNA	Only terminal poly A self complementary sequences.	Ohmichi et a
sugrna02	RNA	Only terminal poly A self complementary sequences.	Ohmichi et a
ser08*	RNA	Only 3' UA, GU and UG terminal base pairs only 5' UG and GU terminal base pairs.	Miller et al.,

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., 200
sugrna02	RNA	Only terminal poly A self complementary sequences.	Ohmichi et al., 200
ser05	RNA	Depends on the available thermodynamic parameters for single dangling end.	O'Toole et al., 200
ser06*	RNA		O'Toole et al., 200

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

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		Davis et al., 2007

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 et al., 2004

ser07	RNA	Less reliable results. Some missing parameters.	Blose, Manni, Klapec, Stranger-Jones, Zyra, Sim, Gr
tur06*	RNA		Lu et al., 2006

Internal 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 et al., 2004
tur06*	RNA	Not tested with experimental results.	Lu et 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. 2 to 7 CNG repeats.	Broda et al., 2005

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 Norman E. et al., 2005
zno07*	RNA	Only IU base pairs.	Wright et al., 2007

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

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

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

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

Sodium corrections

Correcion	Type	Limits/Remarks	Reference
ahs01	DNA	Na>0.	von Ahsen et a
kam71	DNA	Na>0; Na>=0.069; Na<=1.02.	Frank-Kamene
marschdot	DNA	Na>=0.069; Na<=1.02.	Marmur et al.,
owc1904	DNA	Na>0.	Owczarzy et al
owc2004	DNA	Na>0.	Owczarzy et al
owc2104	DNA	Na>0.	Owczarzy et al
owc2204*	DNA	Na>0.	Owczarzy et al
san96	DNA	Na>=0.1.	SantaLucia et a
san04	DNA	Na>=0.05; Na<=1.1; Oligonucleotides inferior to 16 bases.	SantaLucia et a
schlif	DNA	Na>=0.07; Na<=0.12.	Schildkraut et a
tanna06	DNA	Na>=0.001; Na<=1.	Tan et al., 2006
tanna07*	RNA	Na>=0.003; Na<=1.	Tan et al., 2007
wet91	RNA, DNA and RNA/DNA	Na>0.	Wetmur 1991

Magnesium corrections

Correcion	Type	Limits/Remarks	Reference
oxcmg08*	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 et al., 2006
tanmg07*	RNA	Mg>=0.1; Mg<=0.3.	Tan et al., 2007

Mixed Sodium and Magnesium corrections

Correcion	Type	Limits/Remarks	Reference
oxcmix08*	DNA	Mg>=0.0005; Mg<=0.6; Na+K+Tris/2>0.	Owczarzy et al., 2008
tanmix07	DNA and RNA	Mg>=0.1; Mg<=0.3; Na+K+Tris/2>=0.1; Na+K+Tris/2<=0.3.	Tan et al., 2007

Sodium equivalent concentration methods

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

DMSO corrections

Correcion	Type	Limits/Remarks	Reference

ahs01	DNA	Not tested with experimental results.	von Ahsen et al., 2001
cul76	DNA	Not tested with experimental results.	Cullen et al., 1976
esc80	DNA	Not tested with experimental results.	Escara et al., 1980
mus80	DNA	Not tested with experimental results.	Musielski et al., 1981

Formamide corrections

Correcion	Type	Limits/Remarks	Reference
bla96	DNA	With formamide concentration in mol/L.	Blake 1996
lincorr	DNA	With formamide concentration in %.	McConaughy et al., 1969; Record 1967; Hutton 1977

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