## Package 'rmelting'

March 18, 2025

```
Title R Interface to MELTING 5
Version 1.22.0
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.
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```

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| meltingBatch   | <br> |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| print.melting. | <br> |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
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melting

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Compute melting temperature of a nucleic acid duplex

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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,
        "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 ap-

proach 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 calcu-

lation 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)

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,<br>Tris=0.01, K=0.05 | Marmur and Doty, 1962       |
| che93corr    | DNA     | No mismatch; Na=0, Mg=0.0015,<br>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                |

<sup>\*</sup> 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/ | 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  |                         |

<sup>\*</sup> 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    |

<sup>\*</sup> 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.                         |                              |

<sup>\*</sup> 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                    |

<sup>\*</sup> 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 |

<sup>\*</sup> 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 |

<sup>\*</sup> 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.  |                      |

<sup>\*</sup> 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       |

<sup>\*</sup> 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            |

<sup>\*</sup> 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                   |

<sup>\*</sup> 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. | Broda et al., 2005 |
|        |      | 2 to 7 CNG repeats.           |                    |

<sup>\*</sup> 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          |

<sup>\*</sup> 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.                      |                       |

<sup>\*</sup> 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                    |                      |

<sup>\*</sup> 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               |

<sup>\*</sup> 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 |

<sup>\*</sup> 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 |

<sup>\*</sup> 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  | Na>=0.003; Na<=1.   | Tan and Chen, 2007           |
| wet91      | or<br>2'-O-MeRNA/RNA<br>RNA,<br>DNA<br>and | Na>0.               | Wetmur, 1991                 |

|           | 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.                    |   |

<sup>\*</sup> 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    |

<sup>\*</sup> 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 |                      |                       |

<sup>\*</sup> 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<sup>+</sup>] 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           |

<sup>\*</sup> 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  |

<sup>\*</sup> 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 |

<sup>\*</sup> 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**

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,
   ...
)
```

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#### **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). A character vector of 3' to 5' complementary sequences of the nucleic acid comp.sequence 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. logical. If TRUE, gives the details about the options (default or user specified) options.out 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**

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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.

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## Examples

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

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

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

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