

# Package ‘rmelting’

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**Title** R Interface to MELTING 5

**Version** 1.21.0

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

**Depends** R (>= 3.6)

**Imports** Rdpack, rJava (>= 0.9-8)

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

**SystemRequirements** Java

**biocViews** BiomedicalInformatics, Cheminformatics,

**License** GPL-2 | GPL-3

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**LazyData** true

**RoxygenNote** 7.2.1

**RdMacros** Rdpack

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

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

**VignetteBuilder** knitr

**git\_url** <https://git.bioconductor.org/packages/rmelting>

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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 ( <b>Note:</b> 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 <sup>-1</sup> ) in excess as a numeric value.  |
| hybridisation.type | The hybridisation type. Either "dnadna", "rnarna", "dnarna", "rnadna", "mrnarna" or "rnamrna" (see <b>Hybridisation type options</b> ).                   |
| Na.conc            | Concentration of Na ions (M) as a positive numeric value (see <b>Ion and agent concentrations</b> ).  |
| Mg.conc            | Concentration of Mg ions (M) as a positive numeric value (see <b>Ion and agent concentrations</b> ).  |
| Tris.conc          | Concentration of Tris ions (M) as a positive numeric value (see <b>Ion and agent concentrations</b> ).  |
| K.conc             | Concentration of K ions (M) as a positive numeric value (see <b>Ion and agent concentrations</b> ).   |
| dNTP.conc          | Concentration of dNTP (M) as a positive numeric value (see <b>Ion and agent concentrations</b> ).   |
| DMSO.conc          | Concentration of DMSO (%) as a positive numeric value (see <b>Ion and agent concentrations</b> ).   |
| formamide.conc     | Concentration of formamide (M or % depending on correction method) as a positive numeric value (see <b>Ion and agent concentrations</b> ).                |
| 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 <b>Self complementary sequences</b> ). 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 <b>Correction factor for nucleic acid concentration</b> ).   |
| <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 <b>Approximative formulas</b> ).                  |
| <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 <b>Perfectly matching sequences</b> ). |
| <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 <b>GU wobble base pairs effect</b> ).  |
| <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 <b>Single mismatch effect</b> ).   |
| <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 <b>Tandem mismatches effect</b> ).   |
| <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 <b>Single dangling end effect</b> ).   |
| <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 <b>Double dangling end effect</b> ).   |
| <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 <b>Long dangling end effect</b> ).   |
| <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 <b>Internal loop effect</b> ).  |
| <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 <b>Single bulge loop effect</b> ).   |

- 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 |
|----------------------|----------------|------------------------|
| <code>dnadna</code>  | DNA            | DNA                    |
| <code>rnarna</code>  | RNA            | RNA                    |
| <code>dnarna</code>  | DNA            | RNA                    |
| <code>rnadna</code>  | RNA            | DNA                    |
| <code>mrnarna</code> | 2-o-methyl RNA | RNA                    |
| <code>rnamrna</code> | 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                |
|------------------------|------|---|--------------------------|
| <code>ahs01</code>     | DNA  | No mismatch                                     | von Ahsen et al., 2001   |
| <code>che93</code>     | DNA  | No mismatch; Na=0, Mg=0.0015, Tris=0.01, K=0.05 | Marmur and Doty, 1962    |
| <code>che93corr</code> | DNA  | No mismatch; Na=0, Mg=0.0015, Tris=0.01, K=0.05 | Marmur and Doty, 1962    |
| <code>schdot</code>    | 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/<br>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/<br>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;<br>Allawi and SantaLucia, 1998;<br>Allawi and SantaLucia, 1998;<br>Allawi and SantaLucia, 1998;<br>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;<br>Allawi and SantaLucia, 1998;<br>Allawi and SantaLucia, 1998;<br>Allawi and SantaLucia, 1998;<br>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:**

| <b>Model</b> | <b>Type</b> | <b>Limits/Remarks</b>  | <b>Reference</b>     |
|--------------|-------------|--|----------------------|
| 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:**

| <b>Model</b> | <b>Type</b> | <b>Limits/Remarks</b>                              | <b>Reference</b>     |
|--------------|-------------|--|----------------------|
| 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:**

| <b>Model</b> | <b>Type</b> | <b>Limits/Remarks</b>  | <b>Reference</b>           |
|--------------|-------------|--|----------------------------|
| 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:**

| <b>Model</b> | <b>Type</b> | <b>Limits/Remarks</b>                           | <b>Reference</b>           |
|--------------|-------------|---|----------------------------|
| 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<br>2'-O-MeRNA/RNA          |   |   |
| wet91      | RNA,<br>DNA<br>and<br>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;<br>Oligonucleotides inferior to<br>16 bases. | SantaLucia and Hicks, 2004;<br>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<br>length superior to 6 base<br>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;<br>Na+K+Tris/2>0.                      | Owczarzy et al., 2008 |
| tanmix07   | DNA,<br>RNA<br>or<br>2'-O-MeRNA/RNA | Mg>=0.1; Mg<=0.3;<br>Na+K+Tris/2>=0.1;<br>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;<br>Record, 1967; Casey and<br>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

```
# 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 ( <b>Note:</b> 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 <a href="#">melting</a> ).  |

### 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", "GACUACCUG", "GACGAUCUG")

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

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

```

---

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

---

**Description**

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

**Usage**

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

**Arguments**

|                  |   |
|------------------|---|
| <code>x</code>   | An object of class <code>melting</code> . |
| <code>...</code> | 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
```

# Index

\* **internal**

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