meltR.A usage and output

2022-09-08

```
library(MeltR)
library(tidyverse)
```

```
## -- Attaching packages --------------------------------------- tidyverse 1.3.1 --
```

```
## v ggplot2 3.4.0      v purrr   0.3.4
## v tibble  3.1.8      v dplyr   1.0.9
## v tidyr   1.2.0      v stringr 1.4.0
## v readr   2.1.2      v forcats 0.5.1
```

```
## -- Conflicts ------------------------------------------ tidyverse_conflicts() --
## x dplyr::filter() masks stats::filter()
## x dplyr::lag()    masks stats::lag()
```

```
devtools::load_all()
```

```
## i Loading meltR.A.paper
```

```
df = df.absorbance %>% filter(Experiment == "CROWD DP1")
meltR.A(df,
        NucAcid = c("RNA", "CGCGCG"),
        Mmodel = "Homoduplex.2State",
        concT = 80,
        fitTs = c(15, 70),
        wavelength = 280)
```

```
## [1] "Individual curves"
## [1] "dH and dG are in kcal/mol and dS is in cal/mol/K. Tms are in deg Celsius"
##   Sample       Ct     dH      dS    dG    Tm
## 9     12 1.55e-05 -56.16 -156.83 -7.52 40.86
## 6      8 2.10e-05 -52.79 -145.06 -7.80 44.00
## 3      4 3.13e-05 -54.56 -150.10 -8.01 46.45
## 8     11 6.85e-05 -53.23 -147.90 -7.36 45.66
## 5      7 9.66e-05 -55.50 -154.06 -7.72 48.72
## 2      3 1.57e-04 -54.44 -150.32 -7.81 51.39
## 7     10 2.34e-04 -55.57 -154.58 -7.62 51.44
## 4      6 3.95e-04 -55.71 -154.16 -7.89 55.05
## 1      2 6.89e-04 -56.61 -157.03 -7.91 56.97
## [1] "Summary"
## [1] "dH and dG are in kcal/mol and dS is in cal/mol/K. Tms are in deg Celsius"
##              Method    dH SE.dH      dS SE.dS    dG SE.dG Tm_at_0.1mM
## 1 1 Individual fits -54.95  1.30 -152.23  4.11 -7.74  0.21       49.09
## 2 2 Tm versus ln[Ct] -53.16  4.64 -146.69 14.42 -7.66  0.19       49.04
## 3         3 Global fit -55.38  0.17 -153.41  0.52 -7.80  0.01       49.37
##   SE.Tm_at_0.1mM
## 1           3.81
## 2           0.42
## 3           0.04
## [1] "Maximum %error across methods"
##    dH  dS  dG
## 1 4.1 4.5 1.8
```