

meltR.A usage and output

2022-09-08

```

library(MeltR)
library(tidyverse)

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

## v ggplot2 3.3.6      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 DP5")

meltR.A(df,
  NucAcid = c("RNA", "ACCGGU"),
  Mmodel = "Homoduplex.2State",
  concT = 80,
  fitTs = c(20, 65))

## [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
## 1      24 6.98e-06 -57.50 -163.89 -6.67 33.54
## 2      20 9.79e-06 -69.96 -202.94 -7.02 36.61
## 3      16 1.52e-05 -59.44 -168.51 -7.18 38.77
## 4      23 2.29e-05 -51.80 -144.59 -6.95 39.23
## 5      19 4.35e-05 -53.15 -149.24 -6.86 40.95
## 6      15 7.17e-05 -55.68 -157.35 -6.87 42.62
## 7      22 1.51e-04 -58.39 -166.38 -6.79 44.41
## 8      18 3.07e-04 -44.84 -123.81 -6.45 47.45
## 9      14 5.25e-04 -55.61 -156.99 -6.92 50.19
## [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 -56.26  6.75 -159.30 21.35 -6.86  0.21      43.64
## 2 2 Tm versus ln[Ct] -58.22  3.50 -165.37 11.11 -6.93  0.07      43.84
## 3 3 Global fit -53.58  0.48 -150.79  1.50 -6.82  0.02      43.75
## SE.Tm_at_0.1mM
## 1      2.68
## 2      0.32
## 3      0.05
## [1] "%error between methods"
##    dH  dS  dG
## 1 8.3 9.2 1.6

```