

BLtrimmer usage and output

2022-09-09

```
library(MeltR)
library(tidyverse)

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

## v ggplot2 3.3.6      v purrr  0.3.4
## v tibble  3.1.7      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.fit = meltR.A(df,
  NucAcid = c("RNA", "ACCGGU"),
  Mmodel = "Homoduplex.2State",
  concT = 80,
  fitTs = c(20, 65))

## [1] "Individual curves"
##   Sample      Ct      H      S      G      Tm
## 1      14 5.259360e-04 -55.61 -0.1570 -6.92 50.19
## 2      15 7.161730e-05 -55.68 -0.1574 -6.87 42.62
## 3      16 1.518661e-05 -59.44 -0.1685 -7.18 38.77
## 4      18 3.077518e-04 -44.85 -0.1238 -6.45 47.45
## 5      19 4.351600e-05 -53.15 -0.1492 -6.86 40.95
## 6      20 9.795616e-06 -69.96 -0.2029 -7.02 36.61
## 7      22 1.509123e-04 -58.39 -0.1664 -6.79 44.41
## 8      23 2.289100e-05 -51.80 -0.1446 -6.95 39.23
## 9      24 6.984597e-06 -57.50 -0.1639 -6.67 33.54
## [1] "Summary"
##           Method      H SE.H      S SE.S      G SE.G Tm_at_0.1mM
## 1 1 individual fits -56.26 6.75 -159.30 21.34 -6.86 0.21      43.62
## 2 2 Tm versus ln[Ct] -58.24 3.50 -165.42 11.12 -6.93 0.07      43.85
## 3 3 Global fit -53.58 0.48 -150.78 1.50 -6.82 0.02      43.74
## SE.Tm_at_0.1mM
## 1      7.85
## 2      3.95
## 3      0.59
## [1] "fractional error between methods"
##           H      S      G
## 1 0.08317468 0.09236593 0.01601164
## [1] "dH and dG are in kcal/mol and dS is in cal/mol/K. Tms are in deg Celsius"

Trimmed = BLTrimmer(meltR.A.fit,
  n.ranges.float = 5,
  range.step.float = 5,
  n.combinations = 1000)

## [1] "You are trying to test 1000 baseline combinations"
```

```
## [1] "Do you think this is possible?"
## [1] "Fitting 1000 combinations of 5 different baselines per sample"
## |
```

Trimmed\$Ensemble.energies

##	Method	H	CI95.H	S	CI95.S	G
## 1	1 individual fits	-56.47 -58.55 to	-54.11 -159.96	-166.61 to	-152.42	-6.86
## 2	2 Tm versus ln[Ct]	-57.10 -58.87 to	-54.83 -161.94	-167.61 to	-154.74	-6.87
## 3	3 Global fit	-56.80 -60.54 to	-53.53 -160.82	-173.1 to	-150.59	-6.92
##	CI95.G Tm_at_0.1mM	CI95.Tm_at_0.1mM				
## 1	-6.91 to -6.81	43.64	43.33 to 43.97			
## 2	-6.91 to -6.82	43.63	43.43 to 43.87			
## 3	-7.06 to -6.8	43.97	43.2 to 44.53			