MeltShiny

https://github.com/oss-slu/MeltWin2.0

Problem

Researchers are currently using an old program called MeltWin to analyze DNA absorbance data. This program was designed over 20 years ago, requires older computer systems, and lacks newer features. Furthermore, a lack of source code makes modification impossible. As such there is a need for a newer program that both includes the functions of MeltWin, runs on modern systems, and introduces newer "automatic" features.

Collaborators

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Clients

The program has been designed based on consultation with SLU chemistry department researchers, including the faculty lead and graduate and undergraduate student researchers.

However, the program has been designed to be applicable for all researchers who are interested in analyzing absorbance data for DNA/RNA.

Why is this research relevant?

Molecules absorb light differently. This property yields data that can mathematically be translated into the strengths of the bonds formed by the strands of DNA or RNA molecules being tested. Knowing the strength is important for determining the shape and stability of the whole molecule. In biological applications, knowing the structure allows for the understanding of function.

MeltWin vs. MeltR vs. MeltShiny

- MeltWin
  - Developed in the 80's
  - No source code
  - Only runs on older windows systems
  - Features a graphical interface
  - Has necessary functions required for absorbance data analysis
- MeltR
  - A R package, written by Jacob Sieg- Penn State University chemistry faculty
  - Written in the R programming language
  - Possesses same functions as MeltWin, but includes newer features
  - No graphical interface, so the user has to interact with it via the command line
- MeltShiny
  - Written in R with the RShiny package
  - The front end code includes a graphical user interface
  - The underlying functions come from the integration of MeltR's source code

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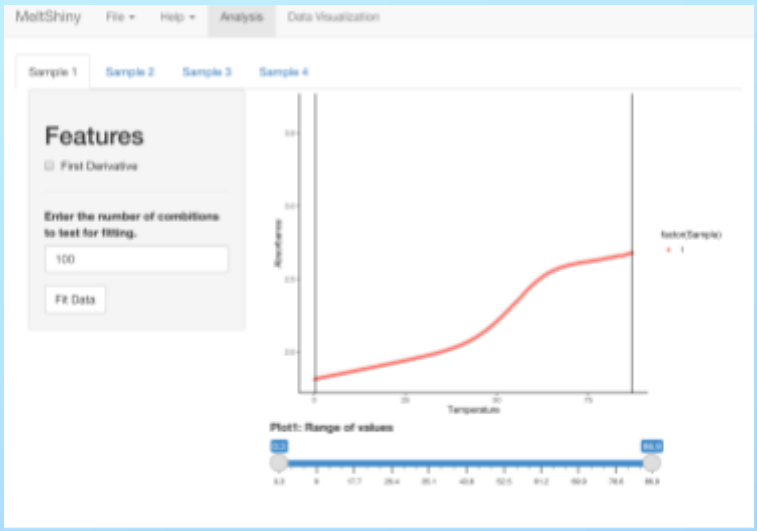
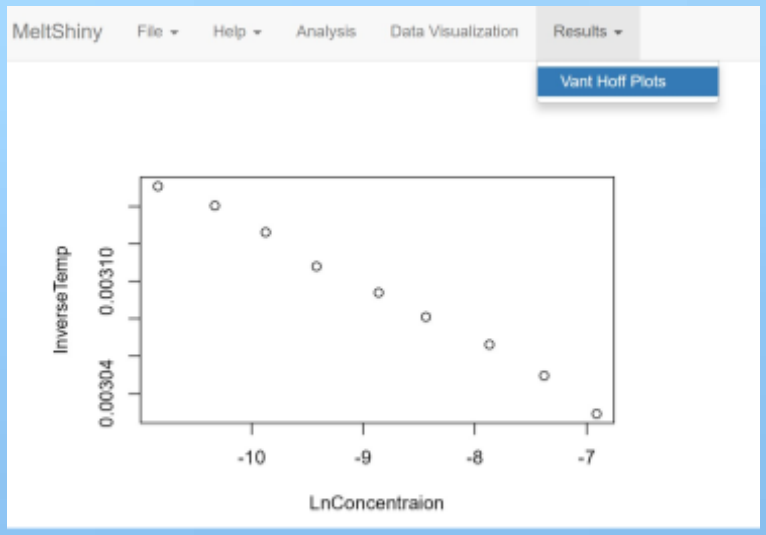
Features

- ☑ Upload and automatically format multiple CSV files from the research machine output into a form that MeltR can interpret
- ☑ Include parameters during file upload
  - ☑ Molecular state, pathlength, blanks, nucleic acid + sequence, wavelength
- ☑ View each sample as its own temperature vs. absorbance graph for analysis
- ☑ Show a baseline best fit line for each graph prior to re-fitting
- ☑ Option to display the first derivative and/ or best fit line on each graph
- ☑ Manual fit performed by using an iteration value of one and moving boundary bars
- ☐ Input the number of iterations for the automatic blt trimmer (MeltR's best fit line tool)
- ☑ View the Van't Hoff plot, 1/temp vs ln(concentration), after fitting data
- ☑ View the results table
  - ☑ Show the thermodynamic parameters for each sample
  - ☑ Show the averages of those parameters with fractional error for the overall dataset
- ☐ Automatically or manually remove outliers from either the Van't Hoff plot or the data table
- ☐ Save either or both of the Van't Hoff plot and data table into one pdf file
- ☐ Help page for instructions on how to use MeltShiny



Example of Analysis Page



Example of a Van't Hoff Plot