Dynamic Light Scattering Graphic User Interface Manual

Self-Assembly of Soft Materials Laboratory
University of California, Los Angeles

Table of Contents

Dynamic Light Scattering Graphic User Interface Overview

The Dynamic Light Scattering (DLS) Graphic User Interface (GUI) is designed for the analysis of DLS data. This application is meant to be complimentary to DLS machines in order to provide the user with the flexibility to choose different parameters to analyze the data. The application is available for downloads for Windows 10 and Mac operating systems here.

Loading Data

1. Data Preparation

The application takes in a .txt file that contains two columns with the first column containing the delay time and the second column containing the raw intensity time correlation data. An example of an acceptable data file is shown below.

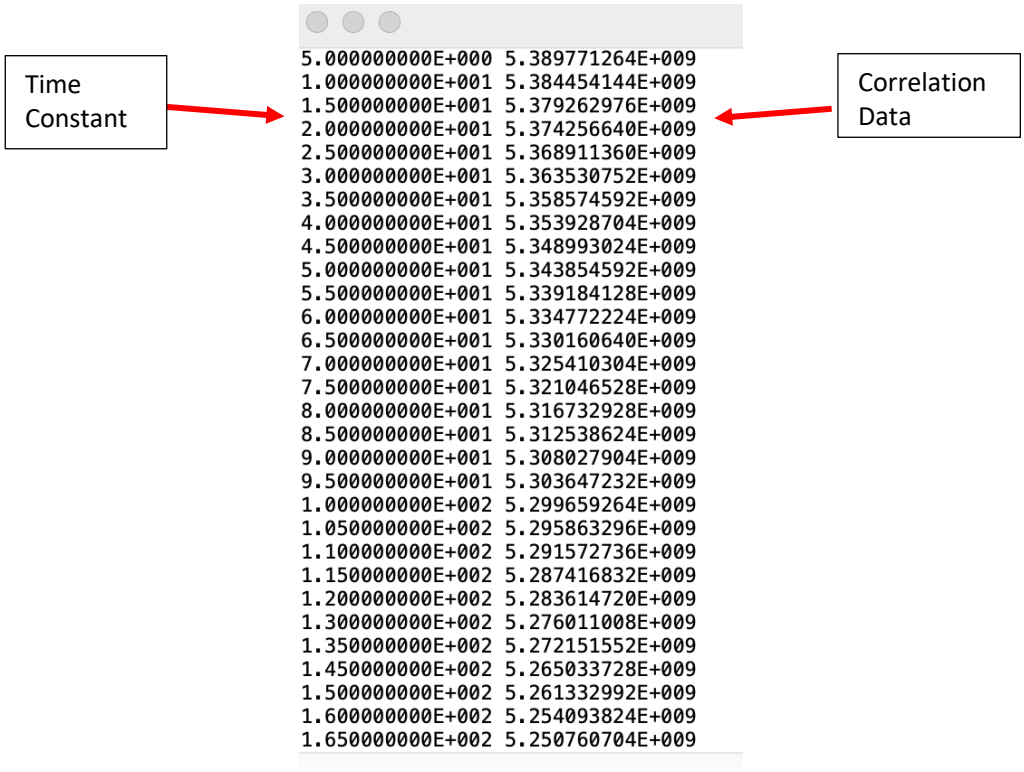

Figure 1. Example of acceptable data file

2. Loading Data

To load a .txt file, click on the Load Data on the top left of the GUI. This should launch a File Explorer (for PC) or a Finder window (Mac) and select your desired file. The name of the file will be displayed on the right of the Load Data button.

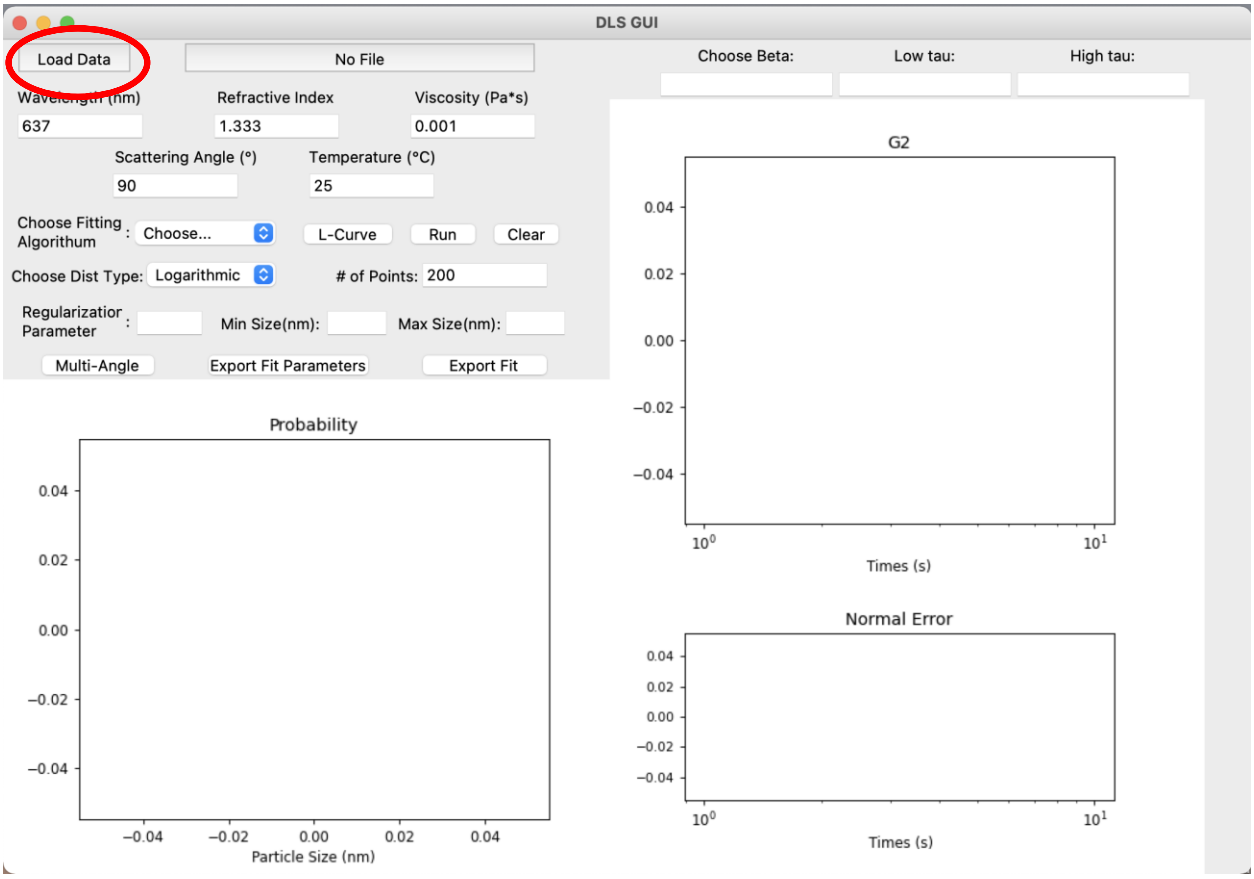

Figure 2. The Load Data button highlighted at the top right corner of the GUI.

Adjusting Parameters

1. Adjusting Beta and Baseline Values

Once an acceptable file has been loaded, a plot of the data points will appear on the plot labeled G2. Here the user can adjust the beta parameter by typing in the *Choose Beta* entry box. The baseline is calculated by averaging the value of points within a desired range. The upper bounds and lower bounds of such range can be set by changing the values in the *high* tau and *low tau* entry boxes, respectively.

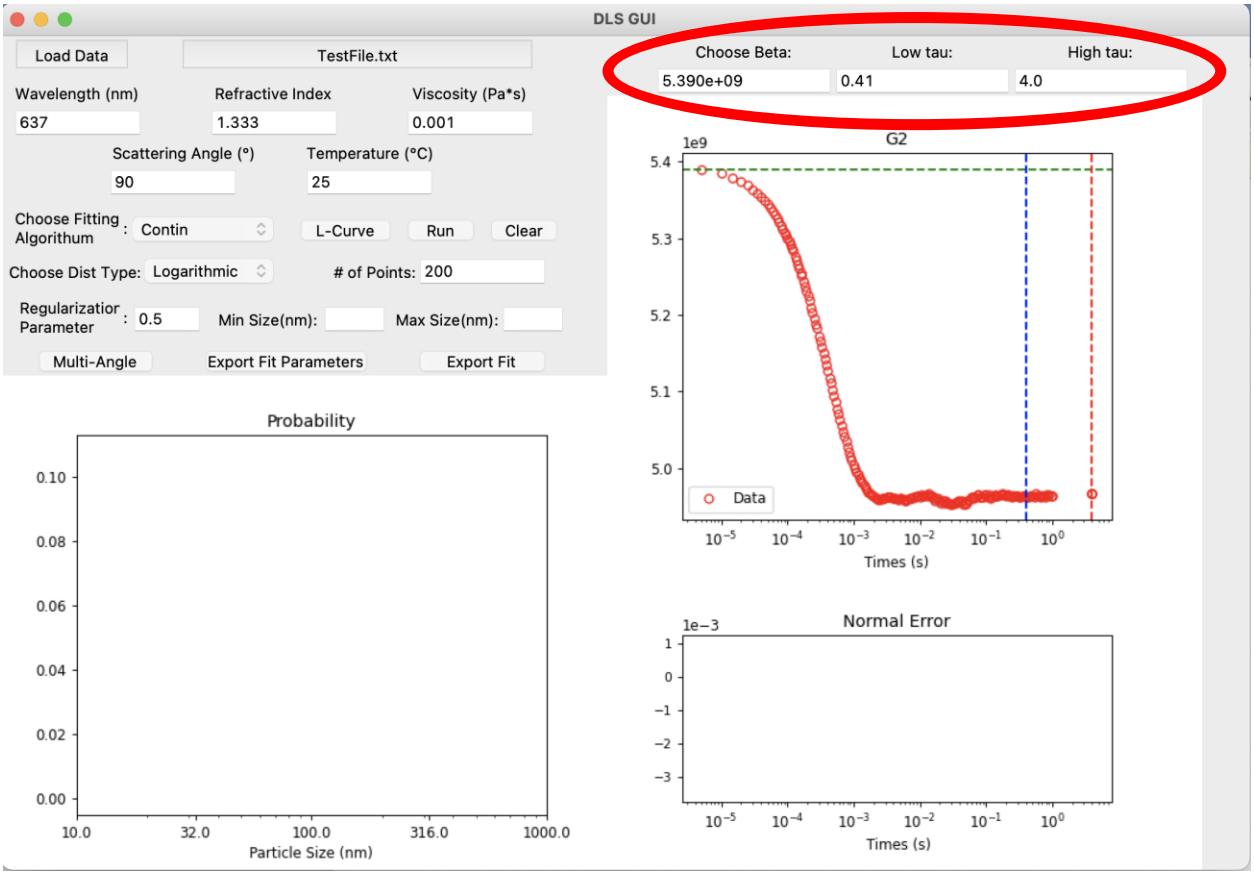

Figure 3. The red circles represent the data from the file. The green dashed line represents the value used as the beta for the fit calculations. The lower limit of the baseline is marked by the red dashed line and the upper limit of the baseline is marked by the blue dashed line. The plot will automatically update when the values of the entry boxes are changed.

2. Adjusting Experimental Parameters

The user is able to adjust the parameters of the experiment such as the Wavelength of the laser (in nanometers), Refractive Index and Viscosity (in pascal-seconds) of the solvent, Scattering Angle (in degrees) of the detector, and Temperature (in degrees Celsius) by editing the values in the perspective entry boxes.

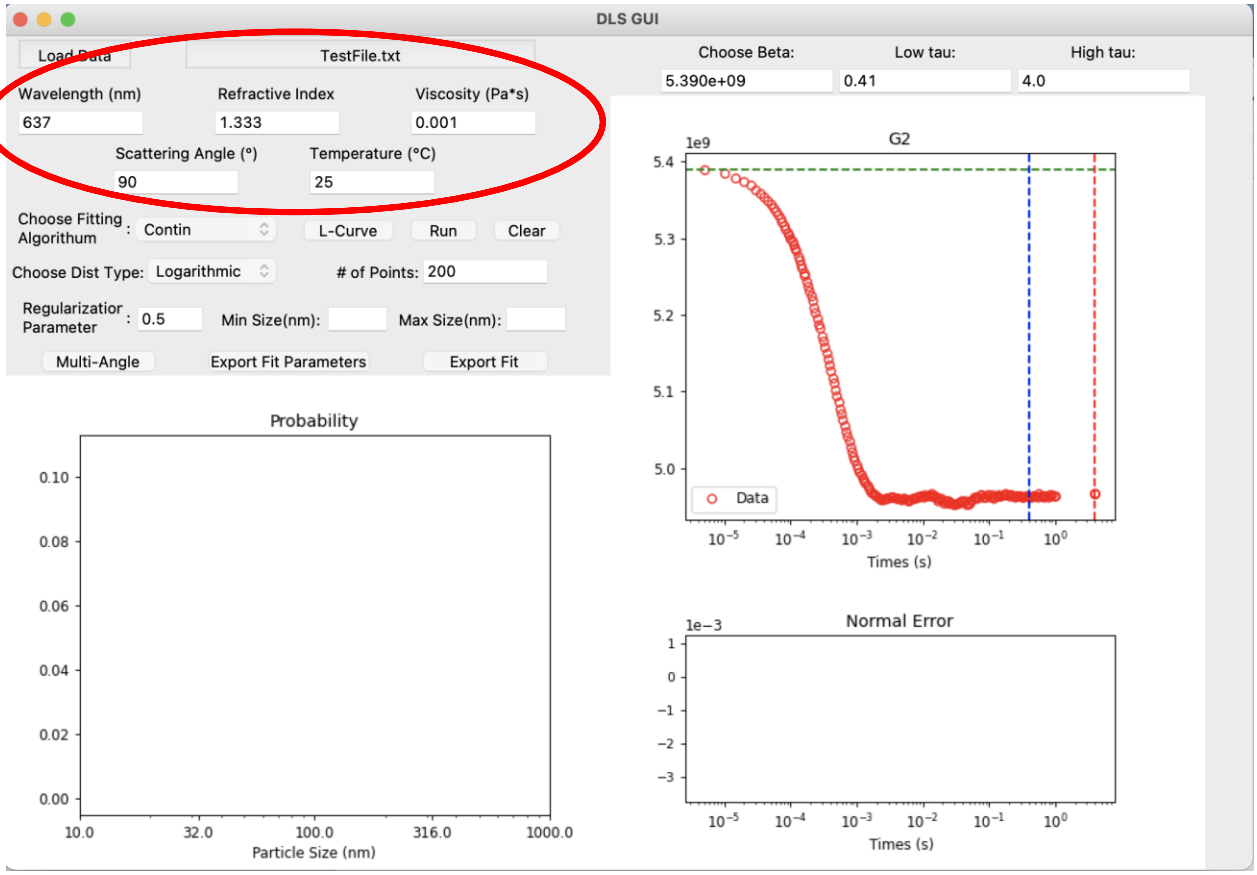

Figure 4. The experimental parameters shown are typical values for experiments where the particles are dispersed in water. When any of the entry boxes are edited, the GUI will automatically clear any fit data.

3. Choosing a Fitting Algorithm

The user can choose a fitting algorithm by clicking the drop-down menu and can choose from 8 different algorithms. Linear Fit, Quad Fit, Cubic Fit and Quartic Fit are cumulant expansion algorithms. NNLS, CONTIN, REPES and DYNALS are regularization methods.

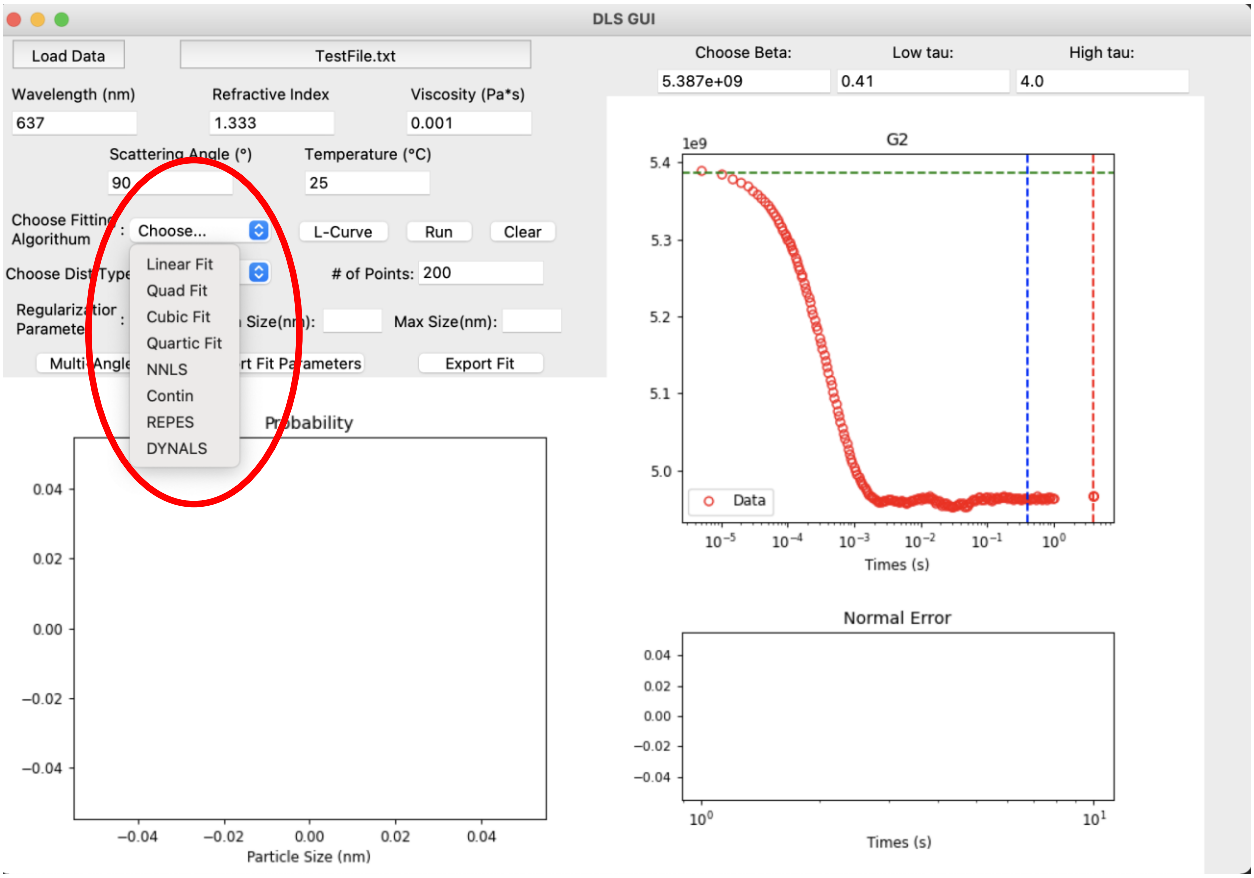

Figure 5. The GUI allows for the picking of one of eight fitting algorithms by clicking the drop-down menu highlighted above. The user can change the fitting algorithm at any point.

i) Regularization Methods

If a regularization algorithm is selected, the Min Size, Max Size, and Regularization parameter are auto filled and can be adjusted by editing the value in the appropriate entry boxes.

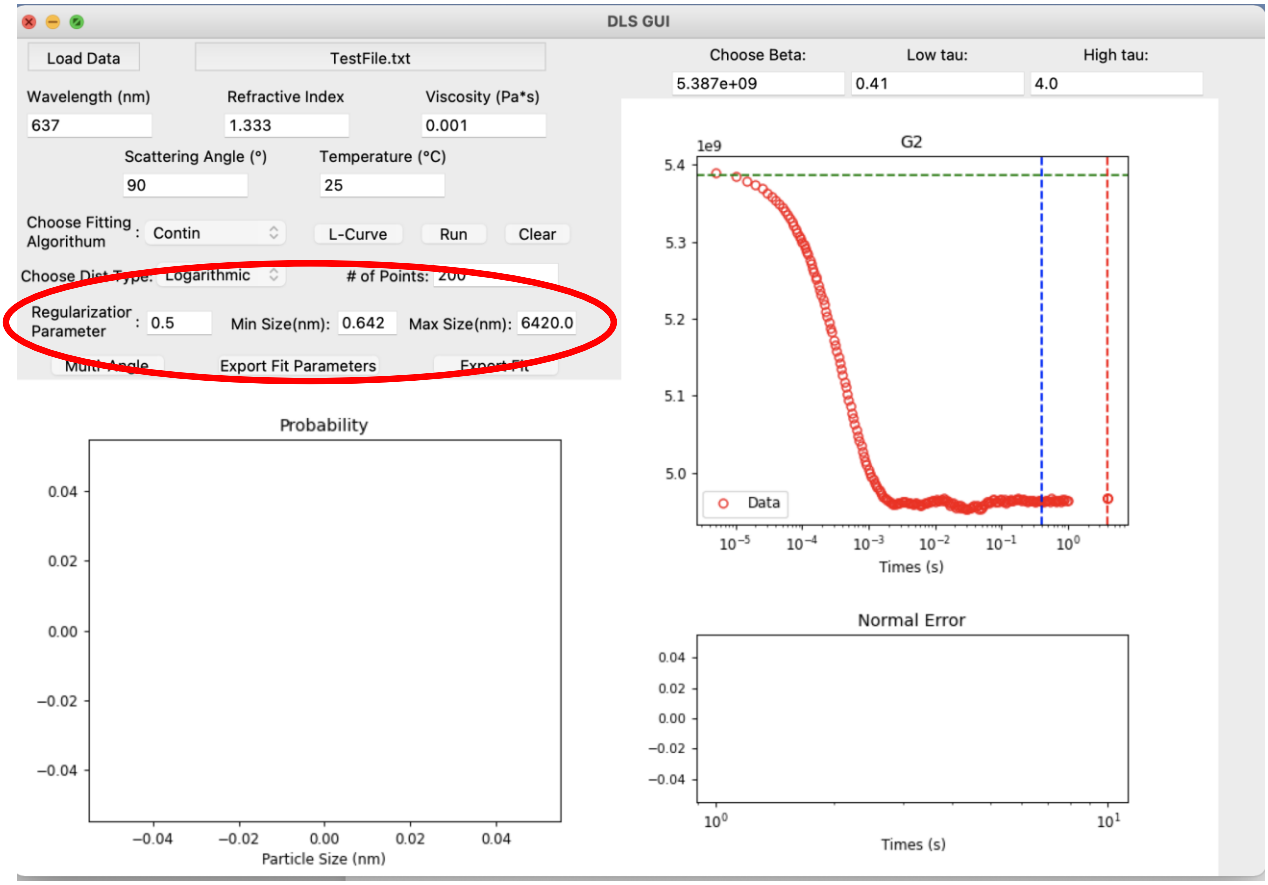

Figure 6. The Regularization parameter, Min, and Max size entries are highlighted above. These can be pre-set for the cumulant expansion; however, it is not necessary to do so. The Min and Max size are used to set the ranges for the calculation of the particles size distribution.

ii) L-Curve Function

The CONTIN and DYNALS algorithms depend on the regularization parameter. To help select a regularization parameter, an L-Curve function was developed. To launch the algorithm, click the L-Curve button. A pop-up should appear asking if you wish to continue. (Note: This program may take over ten minutes to run).

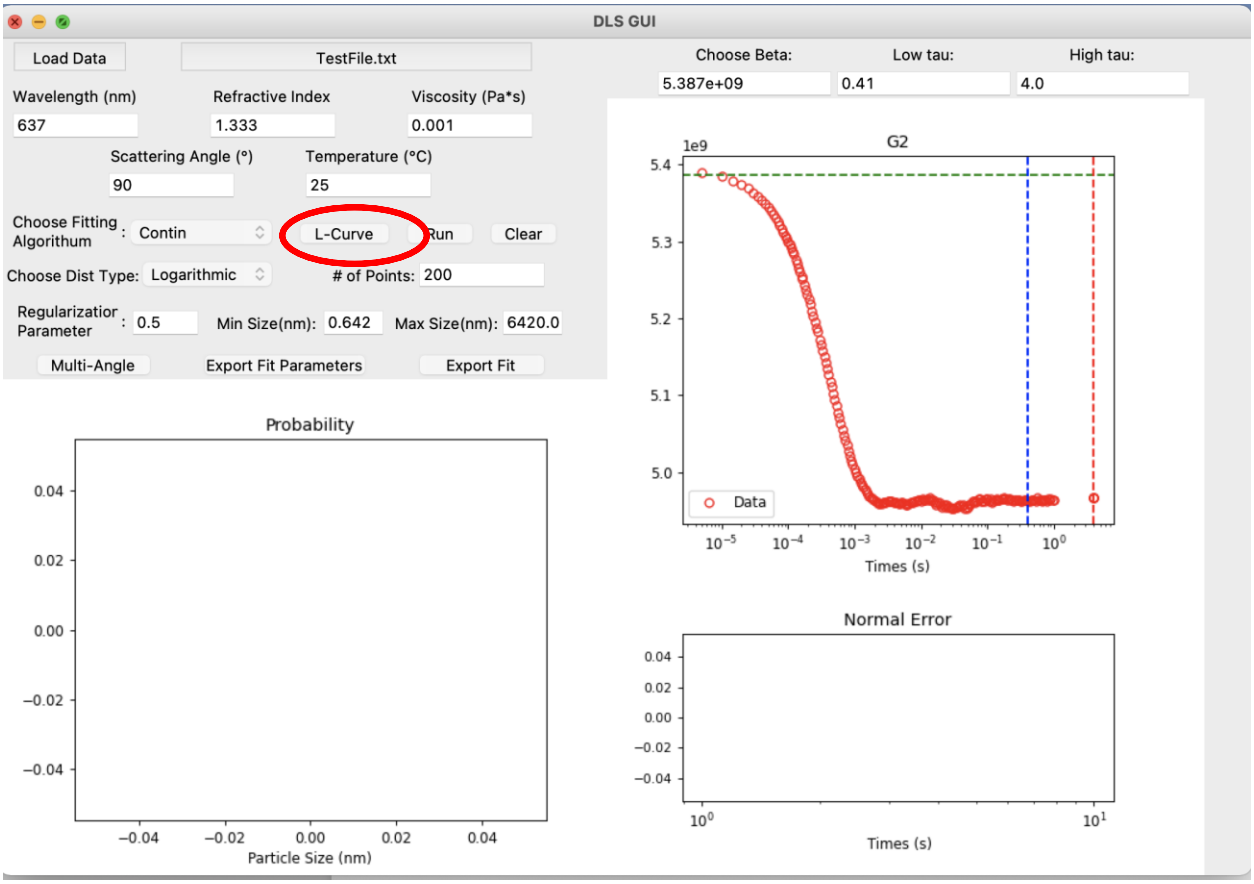

Figure 7. The L-Curve Button is highlighted. A pop-up window should appear automatically. If the pop-up does not appear it is probable that the pop-up is behind the GUI.

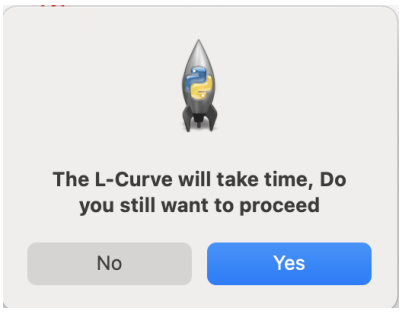

Figure 8. The L-Curve pop-up. If *NO* is selected, the window disappears and the GUI will function normally. If *Yes,* the pop-up will close and the function will proceed. At this time the GUI cannot be updated until the operation is finished or the GUI is closed via Task Manger (Windows) or Activity Monitor (Mac).

iii) L-Curve Results

Once the function is finished, another window will pop-up with the computed optimal value, the L-Curve plot, and the Residuals plot. The optimal point is filled in in both graphs. In addition, a .txt file with the L-curve data will appear in the same folder the data file is located in. The file will have the name *filename_L_Curve.txt*.

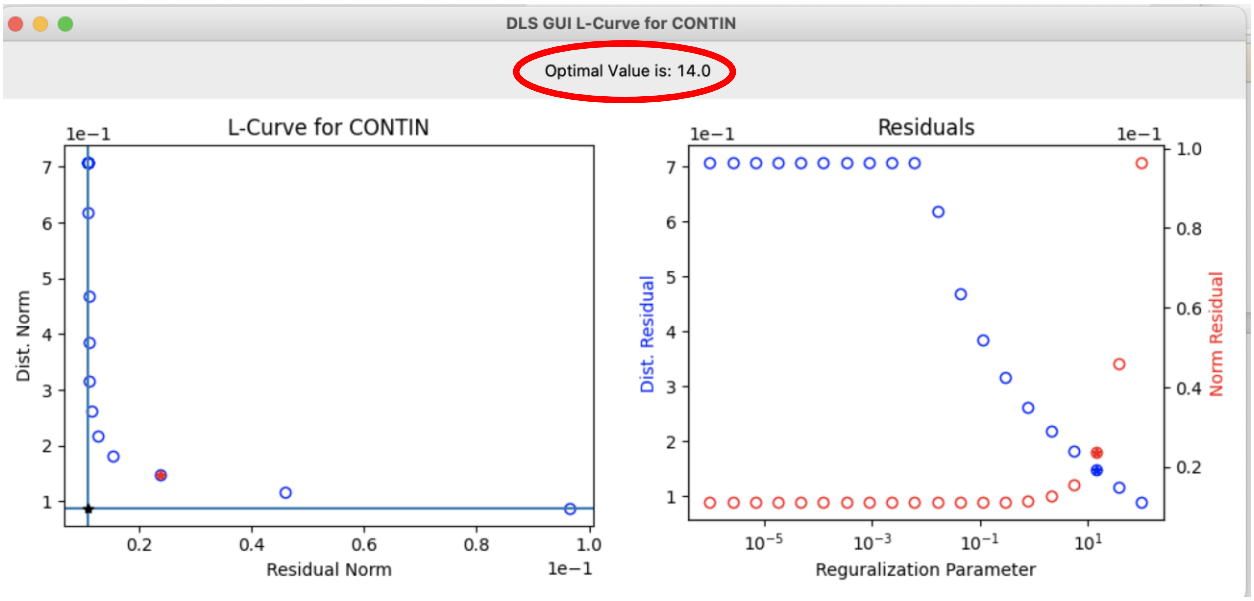

Figure 9. The L-Curve output pop-up window. The optimal value found by the L-curve function will appear in the center of the pop-up and is highlighted above. The L-curve plots the distribution norm vs the residual norm. The lines in the L-Curve plot represent the optimal value used for the algorithm for each category and the intersecting point is represented by the black star. The Residuals plot shows the distribution norm vs the regularization parameter and the residual norm vs the regularization parameter. The values at the optimal value are filled in with a star.

TestFile_L_Curve.txt

```
|Reg. Param |Residual |Dist. Norm||

|1e-06      |0.01106   |0.7072     |
|2.637e-06  |0.01106   |0.7072     |
|6.952e-06  |0.01106   |0.7072     |
|1.833e-05  |0.01106   |0.7072     |
|4.833e-05  |0.01106   |0.7072     |
|0.0001274  |0.01106   |0.7072     |
|0.000336   |0.01106   |0.7072     |
```

Figure 10. Above is an example of the .txt file the L-curve function produces when it is running. The file will contain three columns: Regularization Parameter, the residual norm, and the distribution norm deliberated by '|'.

4. Fitting Type and Number of Points

The GUI allows for two types of size distributions: linear and logarithmic. This dictates the spacing between points for the fitting. The number of points can also be adjusted by changing the value in the respective entry box.

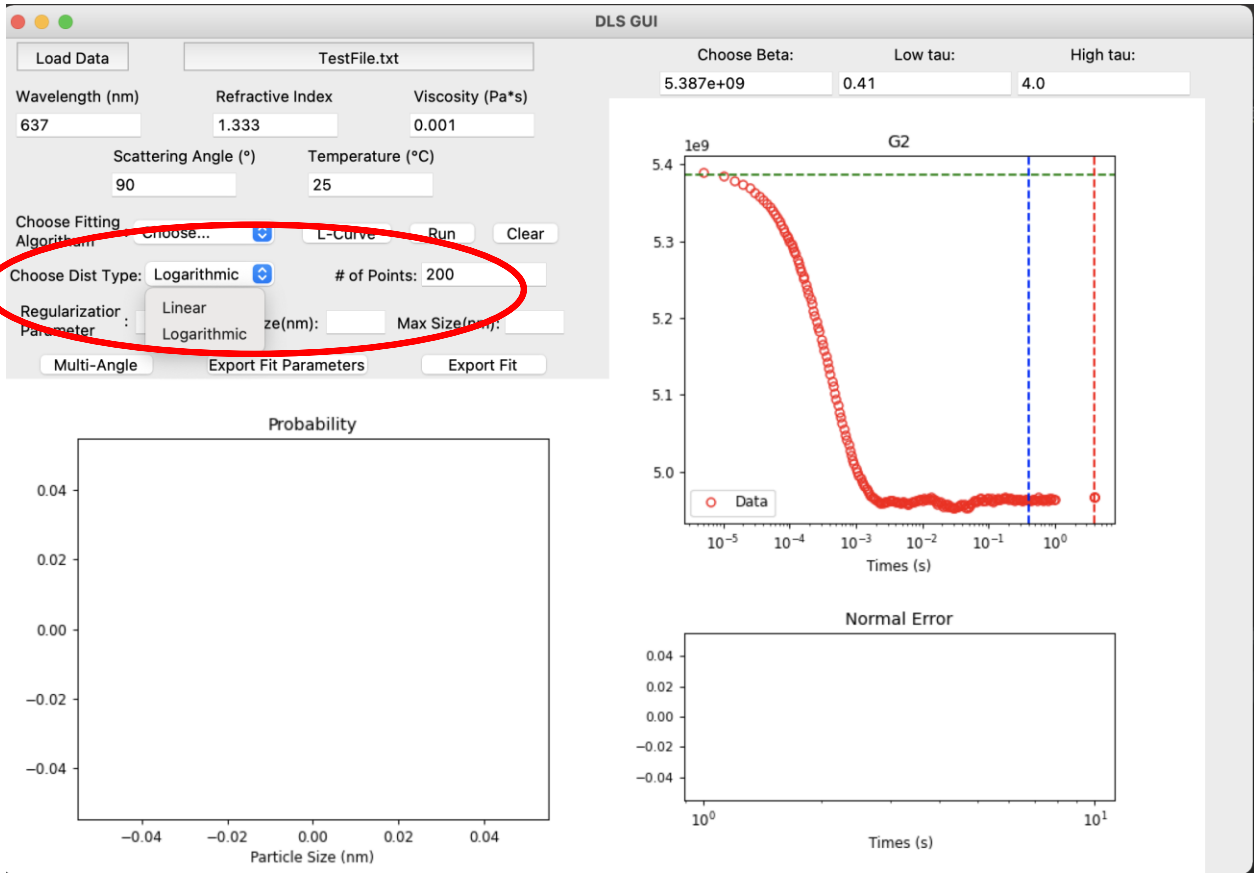

Figure 10. The drop-down menu that allows for the changing of the distribution type and the entry box for the number of points are highlighted above.

Analyzing the Data

Once satisfied with the parameters, click the run button and the GUI will analyze the data. The GUI will plot the G2 fit (Top Right), the normalized error (bottom right), and the size distribution (bottom left).

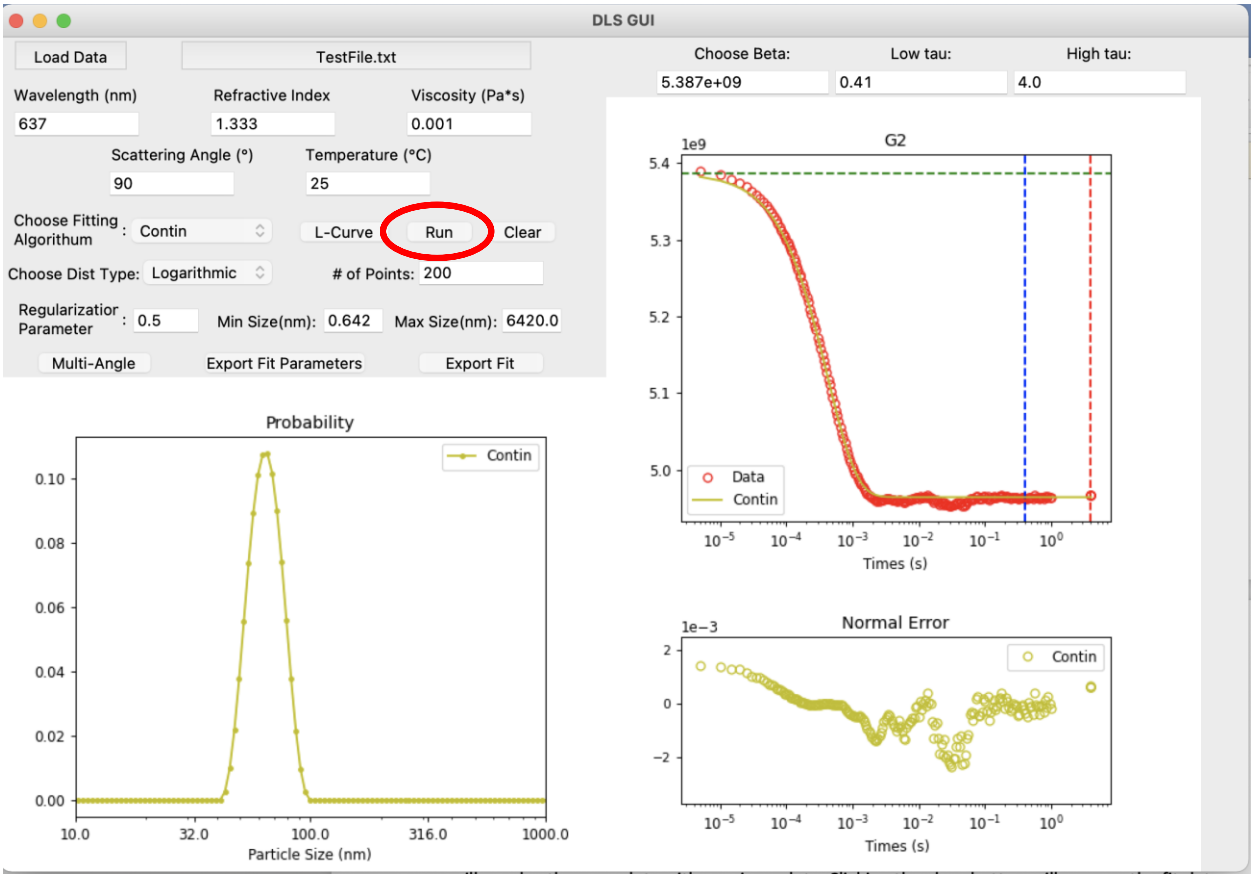

Figure 11. The Run button is highlighted above and the results of clicking the *Run*. The CONTIN algorithm was used to produce the analysis with a regularization parameter of 0.5.

Comparing Different Algorithms

Multiple fits can be conducted by changing the fitting parameters and then clicking run. This will overlay the new plots with the previous ones. Clicking the clear button will remove the fit data from all the plots while leaving only the data points on the G2 plot.

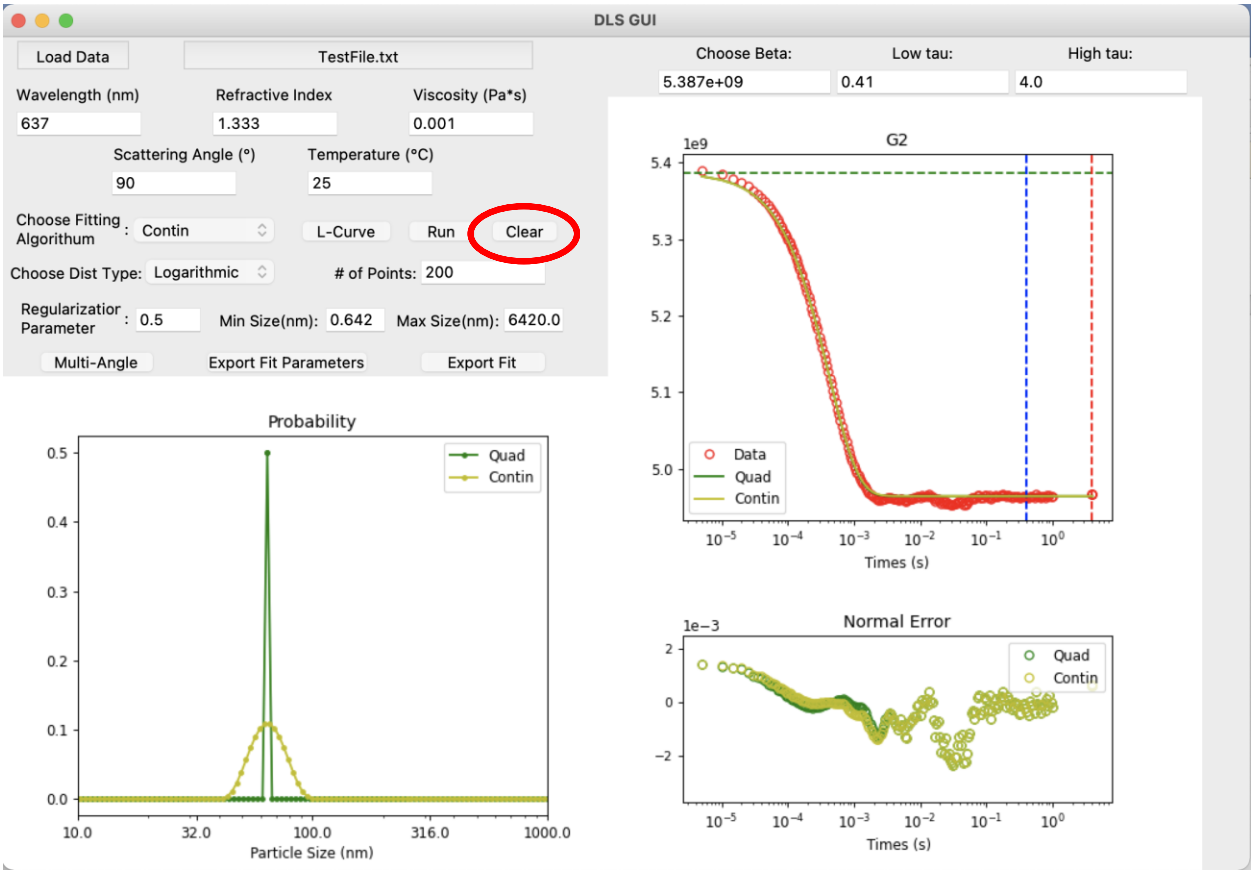

Figure 12. When multiple fittings are run on the same data set and experimental parameters, the plots will be updated. The different fitting algorithms will have a different color that will be labeled in the legend. The *Clear* button is highlighted, and when it is pressed the GUI will clear all fit data; the GUI will appear revert to looking similar to Figure 3.

Exporting Information

1) Exporting Fit Data

To export the fit data information, click the Export Fit button. This will generate a .txt file labeled *filename_FitData.txt* in the folder with the data.

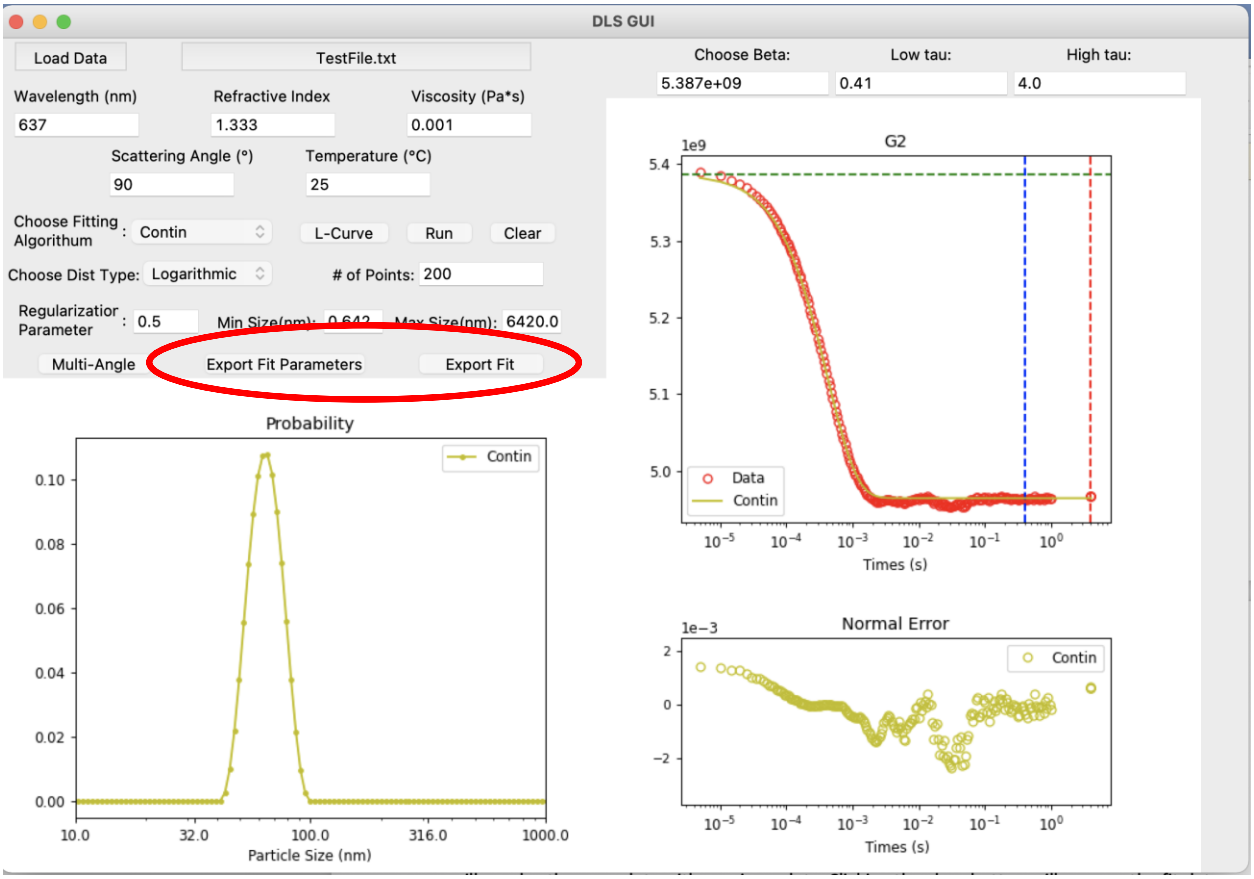

Figure 13. The *Export Fit Parameters* and *Export Fit* buttons are highlighted above.

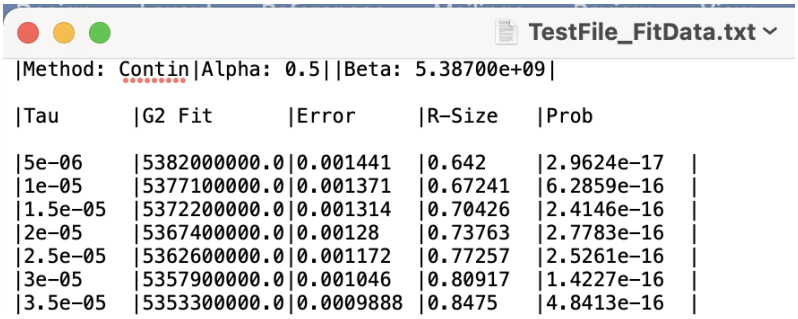

Figure 14. An example of the file generated by *Export Fit* button. The file contains 5 columns: time delay value, G2 Fit value, normalized error, particle size, and probability all delaminated by '|'

2) Exporting Fit Parameters (Cumulant Methods Only)

If a cumulant expansion algorithm was selected, the values for the gamma modified gaussian distribution can be exported by clicking the Export Fit button. A file with the parameters will be in the same folder with the name *filename_FitParam.txt.*

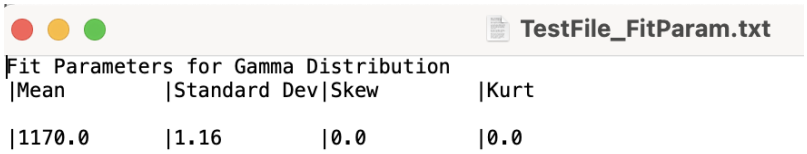

Figure 15. An example of the file generated by the *Export Fit Parameters* button. These values are used for a modified Gaussian distribution function for the gamma distribution.

Multi-Angle Analysis

To analyze data from a multi-angle DLS experiment or quickly analyze a large amount of data the Multi-Angle function can be used. When the Multi-Angle button is clicked, a second window will pop up.

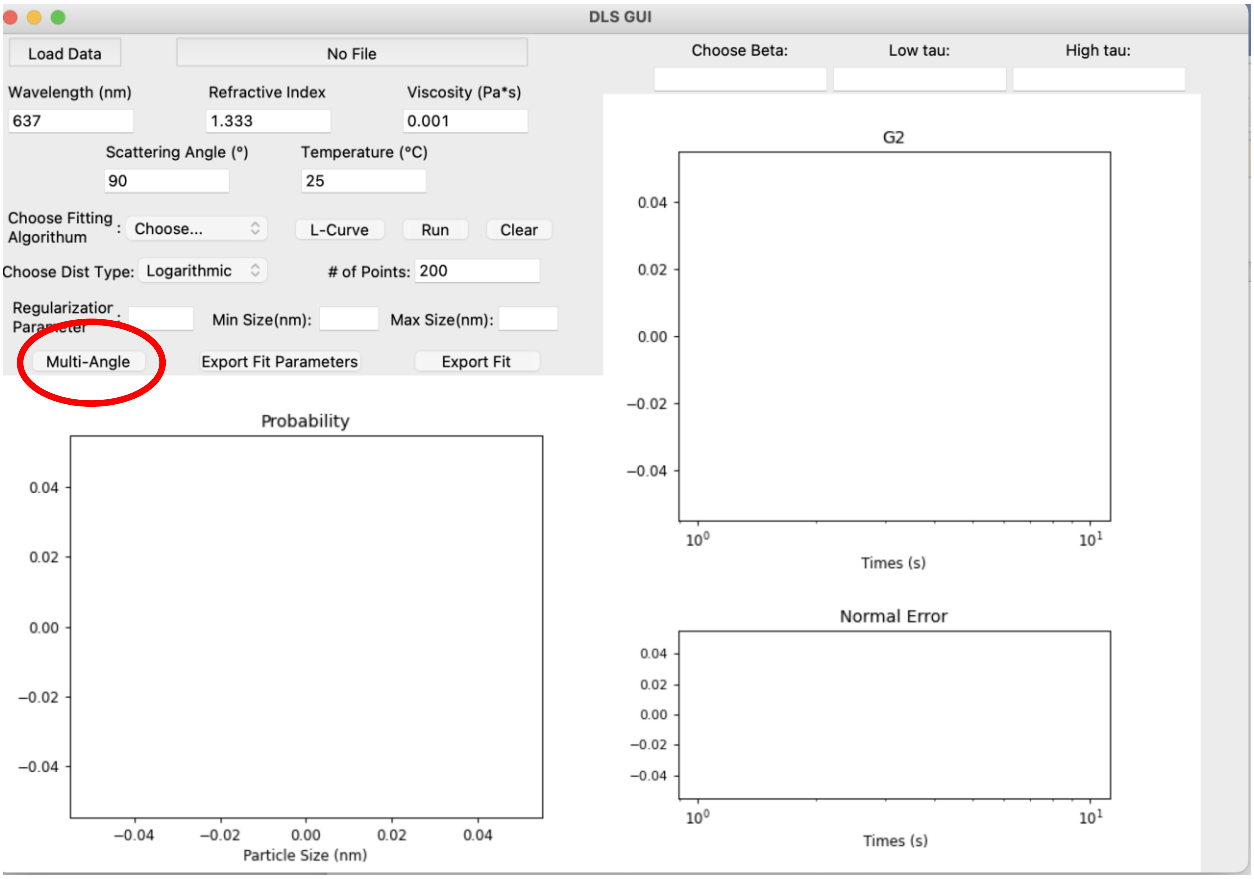

Figure 16. The *Multi-Angle* button is highlighted above. Once pressed, a second window should appear in front of the GUI.

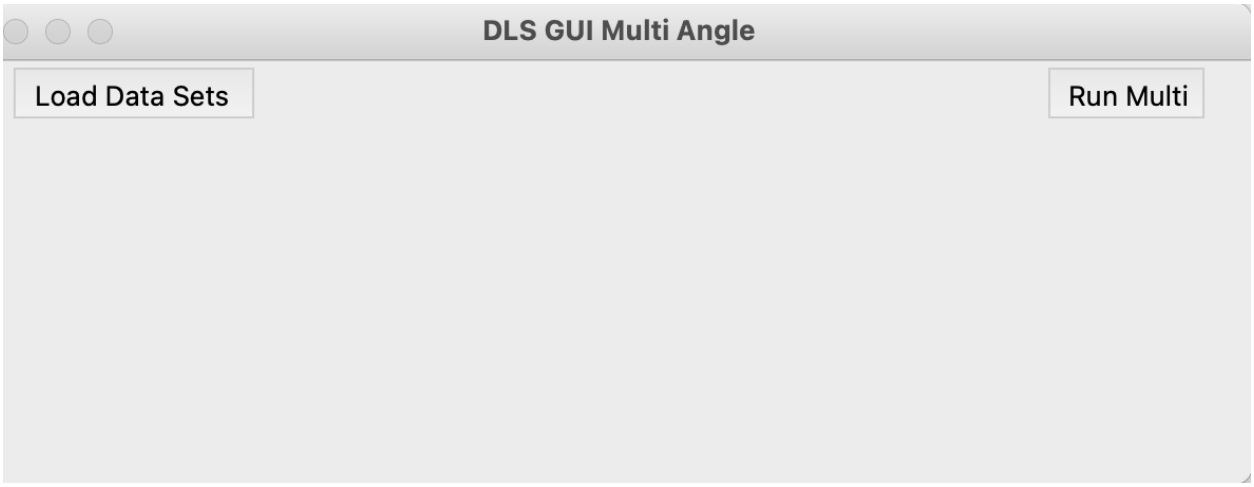

Figure 17. The second window that will pop-up once the *Multi-Angle* button is pressed. If it does not pop-up it is most likely behind the main GUI window.

1) Loading the Multi-Angle Data

To load the data, click the *Load Data Sets* button. A File Explorer (Windows) or a Finder window (Mac) will pop-up. Select the folder containing the Multi-Angle Data. If the folder is valid, the data will be plotted on the main GUI window and the names of the files will be listed in the Multi Angle window. **Important:** This function requires the folder to only contain acceptable data files (Reference Section A for data file format).

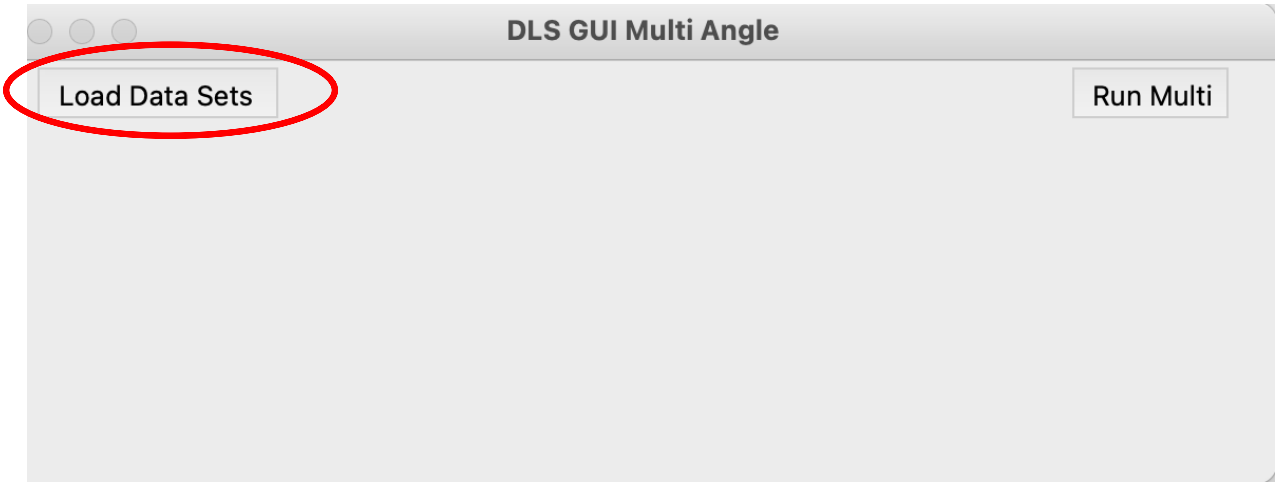

Figure 18. The *Load Data Sets* button is highlighted above.

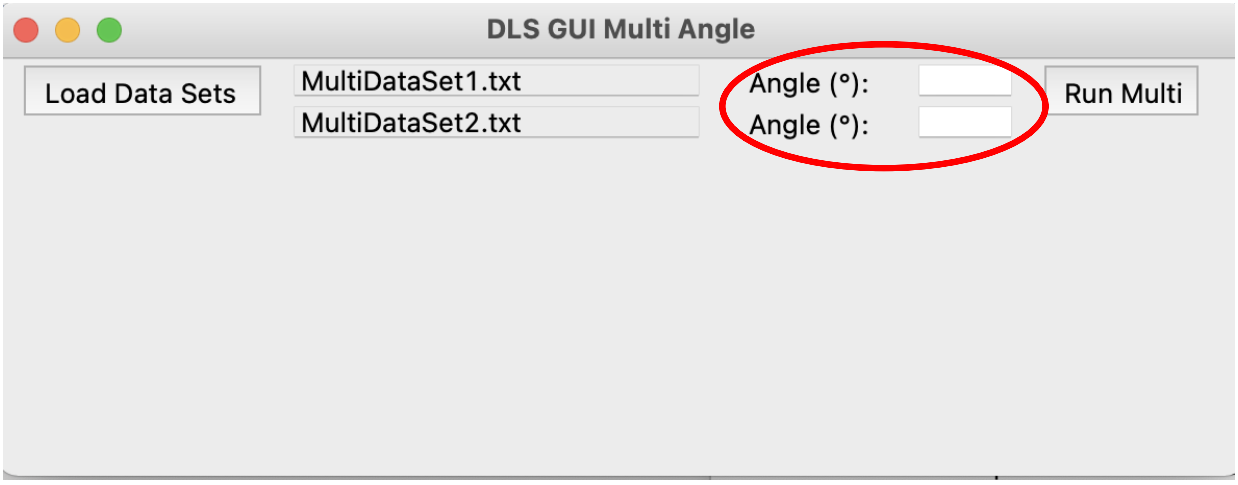

Figure 19. A list of the data files should appear in the *DLS GUI Multi Angle Window.* The user can enter the scattering corresponding to the data set by entering the value in the entry boxes highlighted above.

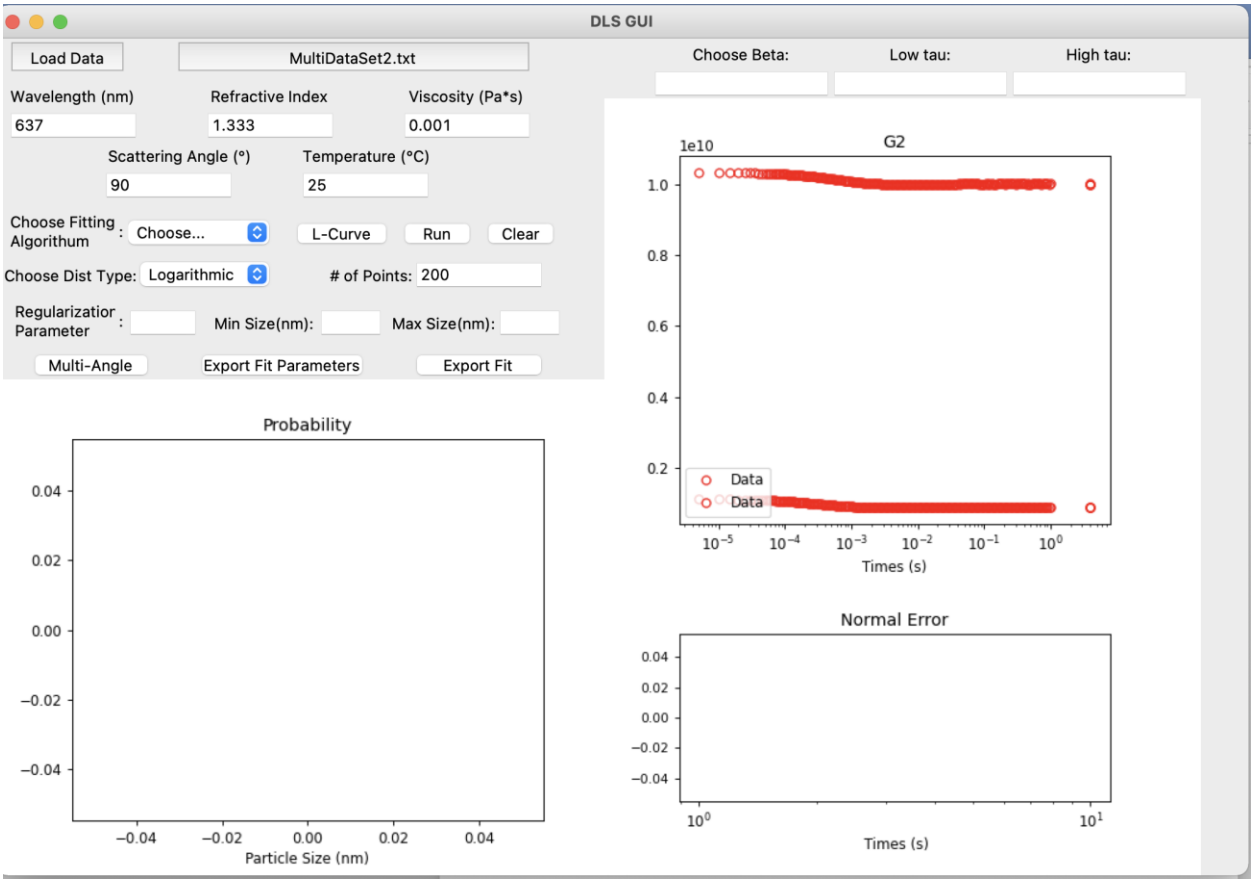

Figure 20. If the loading of the data files worked properly the G2 graph will contain plots of the data. All the experimental parameters (except for the angle which is set individually in the *Multi Angle* window) and fitting parameters can be set in main GUI window.

2) Preparing Data Sets

The multi-angle algorithm will use the parameters set in the main DLS GUI window for the analysis of all the files. To select a fitting algorithm, use the drop-down menu shown in Figure 5. If no fitting algorithm is chosen, the default fitting algorithm is the CONTIN algorithm with a regularization parameter of 0.5. The angle for the experiments must be filled out in the second window. **Note**: The multi-angle will use the predicted baseline range and beta for each data file.

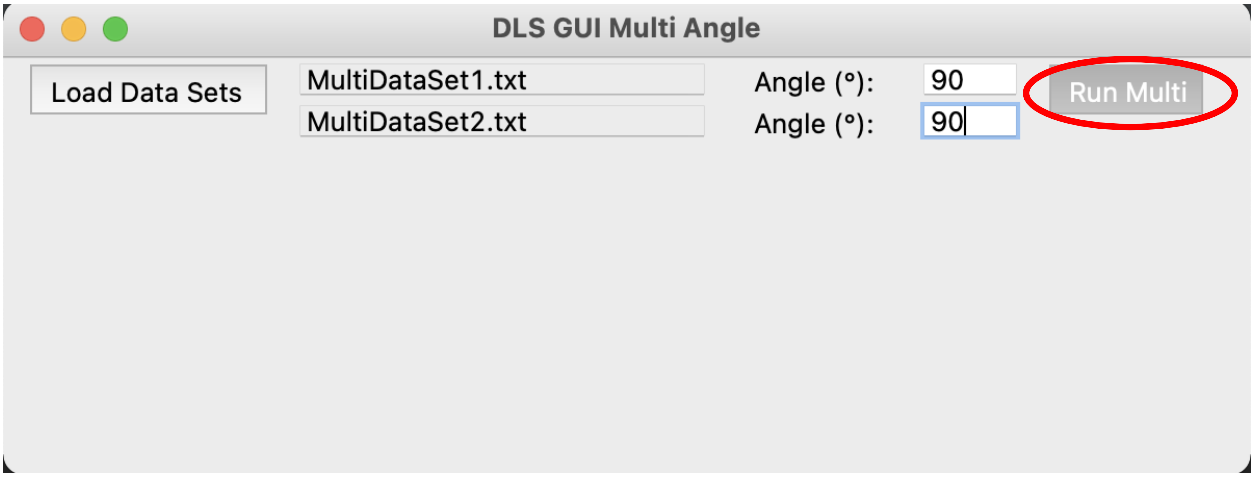

Figure 21. Once satisfied with the experimental parameters and fitting parameters. Click Run Multi to execute the program.

3) Analyzing Multi Angle Data

Once the multi angle function has finished, the Multi Angle window will close and the GUI will plot the G2 fit, Particle Size Distribution and Normalized error of the fits overlaid in their respective plots. In the folder containing the data files, a file will be generated for each data set that will be named *FileName_Fit_Data.txt*. This file will contain the fitting information. The structure of the file will be the same as Figure 14.

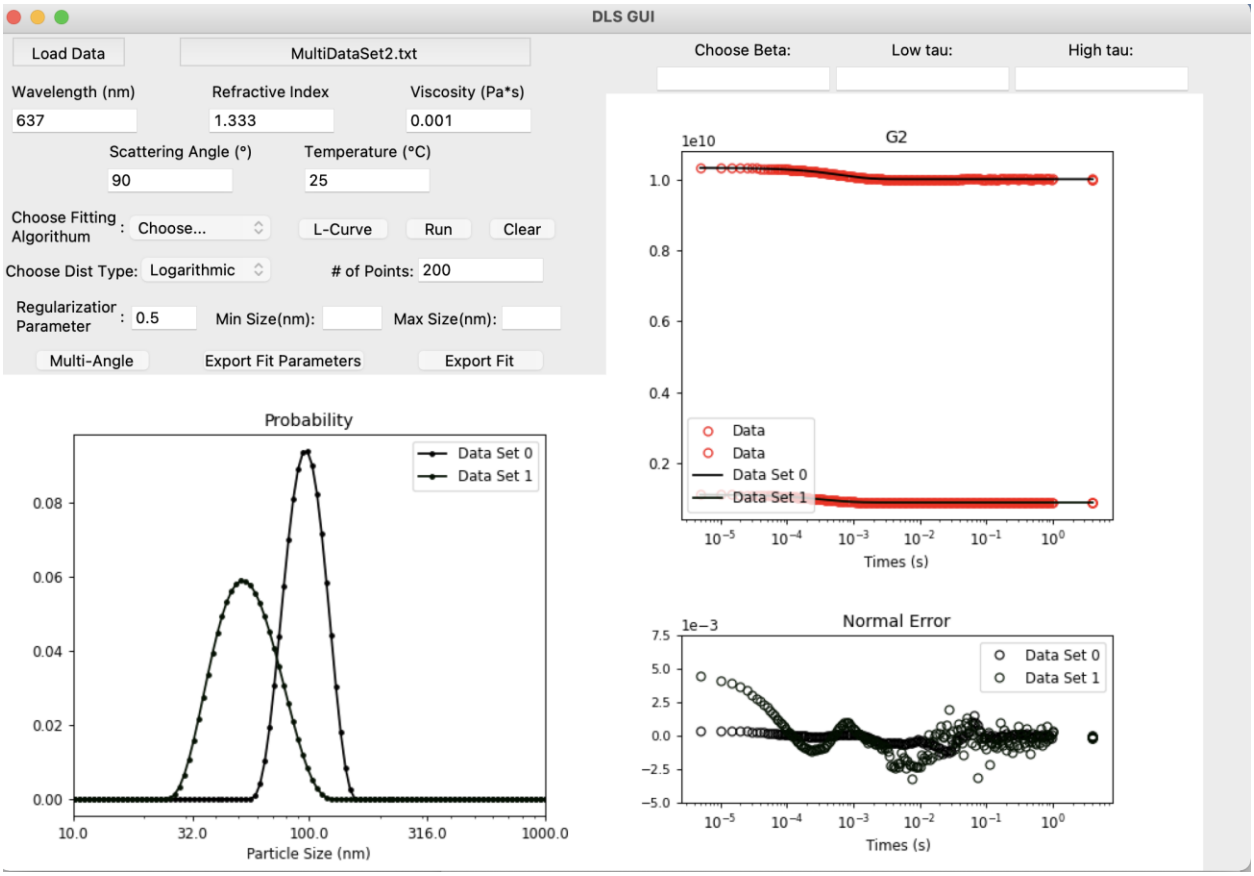

Figure 22. Sample output when the Multi Angle function has completed. The plots will be overlaid onto the same figure. The default algorithm was used to conduct this analysis.

Contact Information

For any questions, feedback and bug reports please email:
DLS.GUI.UCLA@gmail.com