A chance to work with Dr. Rupar's Data
(Connects to Figure 2A, 2C, 3A&B, and 3C)

Dr. Rupar has provided the raw data for Figures S2, S3, S7 and S10 (supplementary information), which connects to Figures 2A, 2C, 3A&B, and 3C from the article. In order to perform statistical length analysis on the micelles, approximately 300 - 400 cylinders were carefully traced by hand to determine the contour length. Histograms of the length distribution were constructed.

From this data, values for the standard deviation of the length distribution, σ, were determined. In addition, values of L_n and L_w of each sample were was calculated based on the equations below (The L_n and L_w values were calculated using equations based on M_n and M_w polymer molecular weights):

$$L_n = \frac{\sum_{i=1}^{n} N_i L_i}{\sum_{i=1}^{n} N_i} \qquad L_w = \frac{\sum_{i=1}^{n} N_i L_i^2}{\sum_{i=1}^{n} N_i L_i}$$

Where:
L_n = number average length (arithmetic mean)
L_w = weight average length (weighted arithmetic mean)
Σ = sum
i = counting unit
L_i = length of micelle
N_i = number of micelles

Students will have the opportunity to calculate the polydispersity of the micelle samples by using the following equation:

$$PDI = L_w/L_n$$

A "narrow" PDI is anything ≤ 1.10.

This activity will have students:

- Take data, normalize it, and then construct length distribution histograms
- Observe how changes in PDI can influence the shape of the length distribution histogram
- Calculate
    1. Number Average
    2. Weighted Average
    3. Polydispersity (PDI)
    4. Standard deviation (Stdev)
    5. Standard deviation/L_n

Instructions:

1. Fill in all items colored red in excel sheet.
    - Length^2 (**This value is needed to calculate L_w**)
    - Normalized Frequency (**This value is necessary for the histogram**)
        - = Frequency/ Sum of Frequency column
2. Construct length distribution histograms. (**The distribution is going to be used to draw correlations regarding PDI and distribution shape later on in this activity**)
    - The column labeled as "Bin" will be the x-axis (label as Length) and the column labeled as "normalized frequency" which you just calculated will be on the y-axis.
        - Bin is in reference to "binning", which is done to construct the histogram. For example on the first excel spreadsheet (labeled as Figure 2A): Bin 0 has a value of 0 because there are 0 micelles with a length between 0-20nm. Bin 100 has a value of 81 because there are 81 micelles with a length between 100-120nm. Bin 200 has a value of 9 because there are 9 micelles with a length between 200-220nm.
3. Calculate L_n
    - Take the average of the Length column.
4. Solve for L_w
    - =Sum of the Length^2 column / Sum of the Length column.

After calculating L_n and L_w:

5. Calculate PDI

6. Generate some observations correlating PDI and distribution shape. For example
    - As the PDI increases, does the distribution broaden, narrow, or stay the same?
    - Will a "narrow" PDI give a narrow distribution?

Useful excel commands:

- =SUM(*insert cell range here*)
- =AVERAGE(*insert cell range here*)
- =STDEV(*insert cell range here*)
- = *insert cell here*/*insert cell here*

For more information on polydispersity calculations see:
http://www.pslc.ws/macrog/weight.htm
http://www.pslc.ws/macrog/average.htm