**Assignment 10**
Due: *In Lecture*, Wednesday, February 22

In this Assignment, you will develop a spreadsheet or program that converts raw GPC data into $\overline{M_n}$, $\overline{M_w}$ and PDI values for your polymer. One way you might do this is to use functions in Microsoft Excel to convert your columns of intensity data into other values. Alternately, you might write a computer program to convert each data value. Regardless of how you do this, your method should be robust enough for you to use repeatedly throughout the course.

For this Assignment, turn in:

- Graphs of your GPC data, including both the polystyrene standards and your synthesized polymer, in which you've plotted refractive index detector response (h_i) against elution volume (V_e). Remember that the data you obtain from the GPC instrument relates detector response to "scan number"; you will have to convert this to elution volume given the detector acquisition rate and the GPC flow rate. Make sure that your data has a baseline detector response very near zero. (The "autozero" function of the detector should have done this at the beginning of your run.)

- A calibration graph, based on the instrument calibration run, in which $\log(M_x)$ for each of the five calibrant peaks is plotted against its observed V_e. Fit your five data points to a function (either a line or a polynomial) that allows you to mathematically transform V_e into M_x for every point in your sample runs.

- One page of the spreadsheet in which you have converted V_e into M_x for all of your data points and used this data to calculate $\overline{M_n}$, $\overline{M_w}$ and PDI ($\overline{M_w}/\overline{M_n}$) for your polymer sample. One irreverent description of how you might do this can be found at Paul Russo's GPC page, http://macro.lsu.edu/howto/gpc.doc. Russo shows how M_x can be evaluated for each data point from the calibration curve by hand, one by one. I recommend that, instead, you use your spreadsheet skills to transform V_e into M_x for all data points, and then determine $\overline{M_n}$, $\overline{M_w}$ and PDI. The relationship between $\overline{M_n}$ and your instrument response data is given in equation 3.3 in the lab instructions; you should derive the relationship for $\overline{M_w}$ yourself. Noise in the high-mass region of the GPC trace can bias your $\overline{M_w}$ value significantly; as a result, you may have to take data from the region of the peak only. You can do this by setting a threshold of, say, 5% above baseline to count data. Graphically:

use only this data

5% threshold
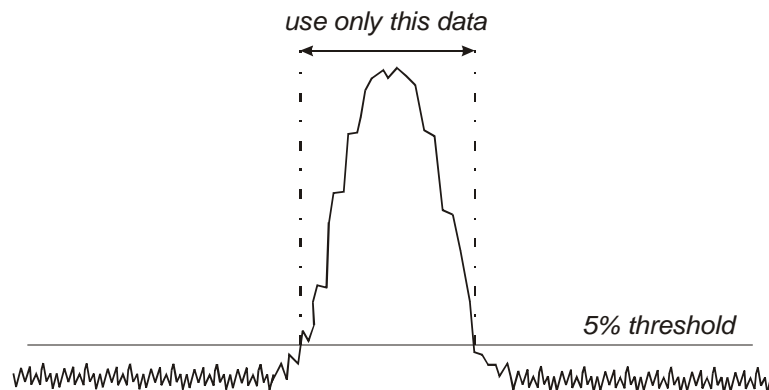
You will have to exercise your spreadsheet math skills to do these calculations—but once you do, you will be able to use this spreadsheet to determine molecular weight information for any polymer you make. So, you might want to make this spreadsheet work well, because you will be cutting and pasting all of your future GPC data into it. Make the page that you submit contain some data from a peak in your GPC—don't just turn in a chart of baseline data.

Once you have calculated $\overline{M_n}$, take a look at how it compares to the GPC trace of the standards. Does your GPC peak occur at roughly the same elution volume (V_e) as the standard peak with the closest M_x? Do your calculations make at least qualitative sense? If not, you should troubleshoot your spreadsheet calculations.

Once this Assignment has been graded and returned to you, post your original GPC data file as well as the $\overline{M_n}$, $\overline{M_w}$ and PDI values you calculated on the WebCT Discussion Board. Put your values in the message, and attach your original GPC data file(s) using the "Attach file" function of the Discussion Board. (Please don't post your calculation spreadsheet; everyone should develop their own tool for calculating $\overline{M_n}$, $\overline{M_w}$ and PDI.) In this way, your classmates can take your GPC data and paste it into their own spreadsheet.