**Parameters that I Examine**

Baseline Variation

There are three options for the intercept and slope values if we choose whether or not to add or subtract the standard errors calculated with the diagonal elements of the covariance matrix. The three possible variations for each value are:

* 1. Nominal (directly from fitting function)
  2. Nominal – standard error
  3. Nominal + standard erros

Each of these can vary independently, so there are a total of 9 possible ways for these two parameters to change with each other. I looked at each of these, used them as the baseline intercept and slope, and found which version of baseline produced the min and max QY.

Diode Correction Choices

There are only two options for varying the method of diode correction: use the actual data or take the average signal value and use that for the correction. The latter method is justified because the variance of diode signal is several orders of magnitude below the mean signal value.

Look-up Table Interpolation

Each look up table has four options for interpolation with the scipy.interpolate.interp1d function, for a total of 16 different interpolation combinations:

1. Linear
2. Linear spline
3. Quadratic spline
4. Cubic spline

Look-up Table Splitting

Here, we want to judge the look up tables based on whether their effect changes when we take only even or only odd values. For each look up table, we may use all the values, even values, or odd values – a total of 3 options per. Hence, there are 9 possible ways to split the LUT together.

LUT Wavelength Shifting

An additional source of uncertainty comes from the PTI system itself. We do not have a clear way to find out whether the light coming out of the excitation monochromator is actually at the excitation wavelength that we specified. If we assume that the output monochromator and the data recorded by Felix are the same, then we can use the secondary transmission peak to check the wavelength of light incident on the sample. Theoretically, if we excite at λ, then the secondary peak should appear at 2λ. Therefore, the difference between the peaks will be equal to λ., the true wavelength. With this is mind and taking the corrected data, we fit each peak to a Gaussian function and use the difference in their means to get the true excitation wavelength. This allows us to judge whether the incoming wavelength differs from that specified by Felix.

From each of these five parameters, we can have a total of 9 \* 2 \* 16 \* 9 \* 2 = 5184 possible variations. I first examine how varying each individually affects the final quantum yield measurement. Then, I look at all the variations and the QY results that they give.

**The Method Itself**

Conditions for the calculation of nominal quantum yields:

1. Baseline parameter values (slope and intercept) are used unmodified
2. The diode correction is taken from the actual data given in the acquisition file
3. Look-up tables are interpolated using a cubic spline method
4. All values of the LUT are used for the interpolation
5. The LUTs are not shifted, i.e. the value at 350 nm in a LUT is applied to the acquisition value at 350 nm

Determining the effect of each parameter individually

To determine how accurate the nominal quantum yield value is, I varied these parameters one at a time, leaving all other parameters equal to their nominal values (those conditions listed above).

Combining parameters

We may also iterate over the 5184 possible parameter variations in order to determine how