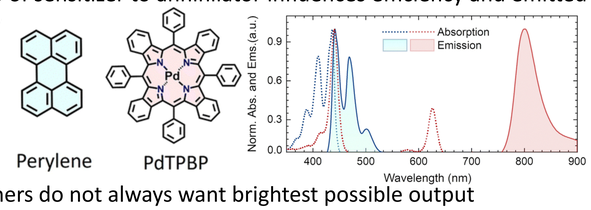
Modeling Annihilator to Sensitizer Ratios for Optimal Light Intensity in TTA Upconversion

Aishani Ghosh
Advisors: Dr. Shupei Yu, Dr. Kevin Crowthers

Background

- TTA-UC converts low-energy light → higher-energy light
- Sensitizer absorbs low-energy photon; transfers energy to annihilator
- Annihilator emits higher-energy photon (shorter wavelength) than the sensitizer originally absorbed (Naimovičius et al., 2023).
- Sensitizers and annihilators are dissolved in a solvent (commonly THF)
- The ratio of sensitizer to annihilator influences efficiency and emitted light intensity



Purpose:

- Researchers do not always want brightest possible output
- In biological applications, high-intensity light can damage cells with prolonged exposure (Dou et al., 2017).
- Sensitizers and annihilators are expensive, so reducing their ratio can lower material costs.
- Understanding the effect of ratio on light intensity can better design experiments

Goal

Test a variety of ratios for sensitizer-annihilator pairings and model it on a graph to better understand the effect of ratio on light intensity. Based on the results, design a mathematical trend to predict the light intensity from a given ratio.

Aim 1: Test 5 different ratios and observe the light intensity

Aim 2: Model the data collected on a graph and find trends/formula

Aim 3: Using the created graph, confirm accuracy by experimenting whether a new ratio matches the light intensity predicted

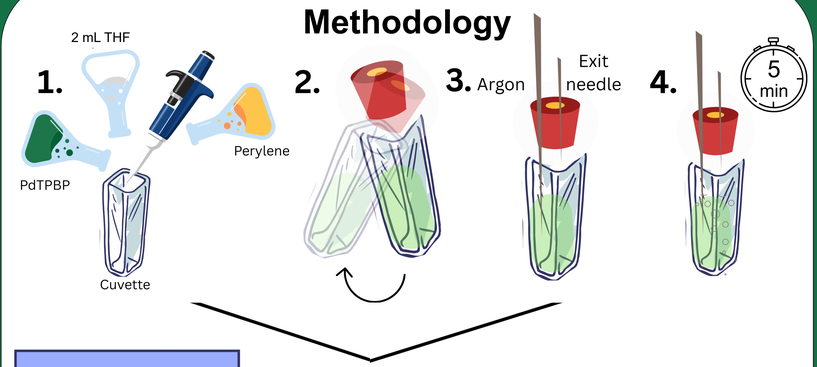
The relationship between the ratio of PdTPBP to Perylene and light intensity can be modeled with a quartic function.

Research Question

Q: How does the ratio between annihilator and sensitizer in a TTA-UC system affect the peak light intensity produced?

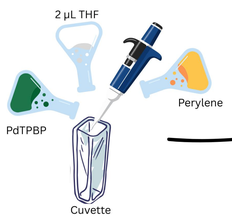
H: Modeling various annihilator-to-sensitizer ratios in a TTA-UC system utilizing Perylene and PdTPBP demonstrates an increasing light intensity as the ratio increases until the optimal ratio is reached, and light intensity begins to decrease due to self-quenching.

Methodology

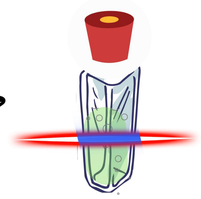


Ratios Tested (Sensitizer: Annihilator)	
1:0, 0:1	1:150
1:50	1:175
1:100	1:200

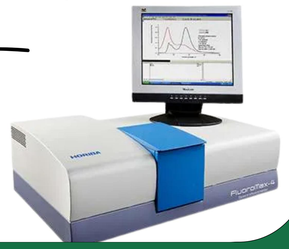
Create TTA-UC systems



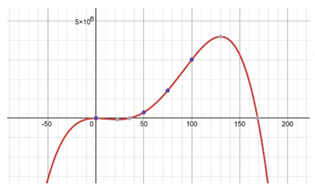
Observe final sample under red laser



Measure sample using spectrofluormeter



Develop a formula to define the relationship



Retest & Refine

Results

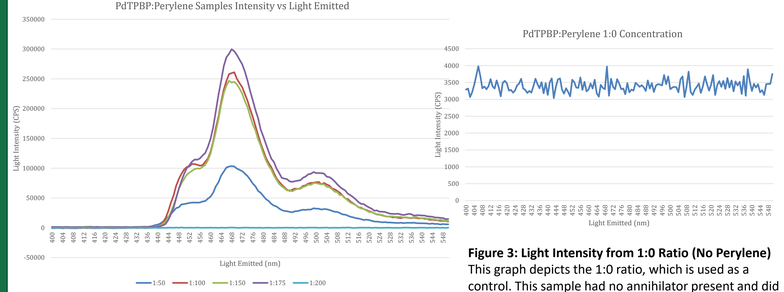


Figure 1: Light Intensity from Ratios of PdTPBP to Perylene
Ratios tested include 1:50, 1:100, 1:150, 1:175, and 1:200. They peak at 106860, 264410, 248440, 303040, and 3980 nm, respectively. Paired T-test between two trials of 1:100 was conducted (p-value=5.83*10^-20).

Figure 3: Light Intensity from 1:0 Ratio (No Perylene)
This graph depicts the 1:0 ratio, which is used as a control. This sample had no annihilator present and did not emit any light. The light intensity fluctuates around a mean of 3396.49 nm.

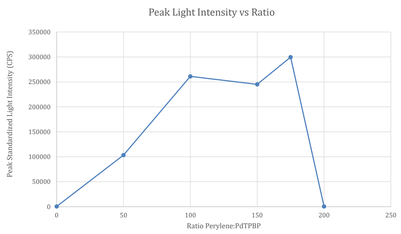


Figure 2: Peak Light Intensity from Each Ratio of Perylene to PdTPBP
This graph depicts the peak light intensity recorded for each ratio against the ratio tested in Perylene:PdTPBP form. Regression analysis was performed to find a function to model it (R^2=0.9031).

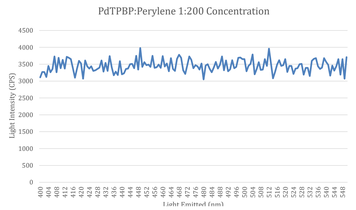


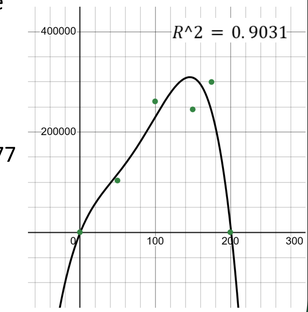
Figure 4: Light Intensity from 1:200 of PdTPBP to Perylene
This graph depicts the 1:200 ratio. This sample had 200 times the amount of annihilator than sensitizer present and did not emit any light. The light intensity fluctuates around a mean of 3448.742 nm.

Analysis

- As seen in the peak between the 1:50 and 1:100 graphs, the 1:100 ratio has a **2.52 times increase** in light intensity from the 1:50 ratio, though the annihilator has only doubled from 10.4 to 20.9 µL.
- Each ratio trial was significantly different, as found with an **ANOVA** test **(p-value=3.8*10^(-46)).**
- Trials of the same ratio were significantly similar. **Paired t-test** found **p-value = 5.83*10^(-20).**

Conclusions

- Evident that the concentration of annihilator in a TTA-UC sample plays a large role in the light intensity.
- Data most closely matches the quartic function:
  $y = -0.002x^4 + 0.5742x^3 - 51.2x^2 + 3738.3x - 1677$
- Rapidly decreasing after hitting its peak at 1:175.
- The model predicts the peak at 1:146.21, slightly off.



Further Research

- Replicate the experiment with different TTA-UC pairings
- Study the effect of concentration on light intensity
- Continue collecting data to strengthen the model's precision
- Use the model in designing TTA-UC experiments; Note its utility