Kinetics Proposal 1

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All work must be **very neat** and **organized**. If you need to collect your thoughts, please use a separate sheet of paper. Proposals are a **group effort**. Please submit the completed document as a PDF to the **Kinetics Proposal 1** D2L DropBox folder <u>before</u> the scheduled end of lab.

1. In a complete, well-written sentence, summarize in your own words the overall goal(s) for the Kinetics Project.

Overall goal is to determine the shelf life of two drugs in an alkaline based solution at room temperature by finding out the rate order and observed rate constant. This information will help us decide how to best preserve the drug so that it does not degrade through changing the concentration of the alkaline solution and the concentration of the drugs used.

Do drugs

2. In your own words, the goal for this first session of the Kinetics Project is...

Goals for the first session are to find the NaOH concentration and volume ratio of Phenolax/NaOH and Pyoctanin/NaOH that give initial absorbance values between 1-1.1 and degrades over a period of 150-250 seconds to an absorbance value of 0.2-0.1. Then from the results, determine a proposal to find the rate order, observed rate constant, and shelf life.

3. **Semi-Quantitative Exploration Results**. **Clearly summarize** the **key results** from your systematic semi-quantitative exploration of 1) at least 3 different *volume ratios of the* Phenolax *and* NaOH *solutions/dilutions* on the Phenolax degradation rate, and 2) at least 3 different *volume ratios of the* Pyoctanin *and* NaOH *solutions/dilutions* on the Pyoctanin degradation rate. Be sure to specify the diluted NaOH concentrations indicating the volumes used to prepare the NaOH dilutions - there should be at least two (2) different NaOH dilutions explored for Pyoctanin and Phenolax. Hint: What happens with the observed color intensity over time for different ratios and NaOH dilutions? What volume of Pyoctanin and Phenolax in relation to the NaOH concentration and volume are within the appropriate absorbance range to collect your data?

Table 1: Phenolax and Pyoctanin NaOH Degradation Semi-Quantitative Exploration Data and Observations.

NaOH Concentration	Volume of NaOH	Volume of NanoPure	Volume of Phenolax	Volume of Pyoctanin	Color at time = 0 seconds	Color at time = 250 seconds
1.0M	3.00 mL	0.00 mL	29	64	Pheno:Bright pink magenta color Pyoc: Dark Indigo purple blue	Color is gone clear once like it was before the adding of the drug

	1	T	T			T
						Color was
						gone at
						around
						180-190
						seconds
					Pheno:Bright pink	Color fully
0.75M	2.25 mL	0.75 mL	29	64	magenta color	cleared out
0.75101					Pyoc: Dark Indigo	around 190
					purple blue	seconds
					Pheno:Bright pink	For Pheno
					magenta color	at 0.5 M
					Pyoc: Dark Indigo	there was
					purple blue	still color
					rr.	after the
						250
						seconds we
						observed
						for.
						Pyoc all
						Colored
						cleared out
						before the
						250
						seconds
0.5M	1.50 mL	1.50 ml	29	64		ended fully
0.51	1.50 III.	1.30 1111	23	04		gone
						around
						180seconds.
						The 0.5
						molarity
						ratio took
						the longest
						for color to
						disappear
						especially
						when we
						looked at
						color
						change for
						pheno

To calculate the volume of Phenolax needed:

Phenolax =
$$\frac{0.75}{5.02 \times 10^4 \text{cm}^{-1} \text{M}^{-1} \times 1.00 \text{ cm}} = 1.49 \times 10^{-5} \text{M} = \frac{1.49 \times 10^{-5} \text{M} \times 3 \text{mL}}{1.57 \times 10^{-3} \text{M}} = 0.02847 \text{ mL} \times 1000$$

= 28.47 μ L

To calculate the volume of Pyoctanin:

Pycotanin =
$$\frac{0.75}{8.65 \times 10^{5} \text{cm}^{-1} \text{M}^{-1} \text{x} 1.00 \text{ cm}} = 8.6705 \times 10^{-7} \text{M} = \frac{8.6705 \times 10^{-7} \text{M} \times 3 \text{mL}}{4.08 \times 10^{-5} \text{M}} = 0.06375 \text{ mL} \times 1000$$
$$= 63.75 \mu \text{L}$$

4. **Proposal 1.** Based on your semi-quantitative exploration, **propose a plan**, and **justify each step** to experimentally determine n, k_{obs} and t_{90} at room temperature for **PHENOLAX**, where the condition [NaOH] >> [Phenolax] exists as described in the Kinetics Guide. **Please NUMBER your procedural steps.**

Procedural Step

- 1) Fill a 20 ml vial with NaOH
- 2) Gather 3, 10 ml vials.
- Choose 3 Molarity ratios, e.x. 1.0 M, 0.75 M, 0.5 M.
- Calculate the appropriate volumes of the systems for a total volume of 3ml using C1*V1=C2*V2
- 5) For Phenolax, set aside three vials and fill it with the three different molarity ratios.
- 6) Use Beer's Law to calculate the molarity of Phenolax solutions based on the chosen absorbance levels
- 7) Use the molarity of the Phenolax to calculate the volume of the respective solutions using the following formula: $C_dV_d=C_sV_s$
- 8) Take the molarity in step 5, times that by the total volume of the NaOH and Nanopure solution and divide it by the molar mass of the respective solutions.
- 9) In the three vials from step3 containing the NaOH and Nanopure mixture, add in the determined volume of Phenolax in Step 8.
- 10) Add the solution to a cuvette and place it in the spectrometer, recording data for absorbance vs. time. Set a stopwatch for 250 seconds, observing any changes in color.
- 11) Using the observed absorbance value as it degrades over time, we can then calculate the rate order, the K_c values, and the shelf life.

- Justification based on data/observations, or technical instructions, or conceptual understanding
- Gathering an appropriate amount of NaOH for the upcoming experiment
- These vials are used to create our 3ml systems in which we will place our drug (phenolax) in 3 different molarity ratios
- In order to examine how different ratios of phenolax to NaOH affect different the degradation of the drug
- 4) You are to determine the exact volumes for each corresponding ratio so that your ratios have a small margin of error, and readings will be accurate
- 5) Clearly separating the ratio systems from each other ensureing not to have them mixed up
- 6) Beer's Law gives us the exact molarity of our pheno solution at a specific absorbance level
- 7) Using the formula of: $C_dV_d = C_sV_s$ you can determine the exact volume of Phenolax.
- 8) This will give us the volume in milliliters, multiply by 1000 to get the volume in microliters.
- 9) This will allow us to observe color changes as it will provide a visualization of Phenolax degrading over time.
- 10) This will allow us to record the absorbance value from the instant Phenolax is placed into the NaOH solution. It needs to happen instantly as Phenolax can degrade fairly quickly. 250 seconds should be ample time to fully see the Phenolax in the NaOH solution degrade.
- 11) The rate order, K_c values and the shelf life are the values we are looking for and the absorbance level from the spectrometer can help us determine it. We will use the following equations:

$$t_{90} = \frac{[X]_0}{10k_{\text{obs}}}$$
$$t_{90} = -\frac{\ln(0.9)}{k_{\text{obs}}}$$

0.111
$t_{90} = \frac{0.111}{k_{obs}[X]_0}$
The three equations will give us three different graphs
that we can use to find the R^2 value. This value will
help us determine which formula is applicable as we
can see which R^2 value is closest to 1.