

Kinetics Summary and Proposal 2

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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 2** D2L DropBox folder before the scheduled end of lab.*

1. In your own words, the **goal for this second session** of the *Kinetics Project* is...

Implementing Proposal 1 for Phenolax to determine the rate order (n), half life (t_{90}), and observed rate constant (k) at room temperature

2. **Observations and Results from Implementing Proposal 1.** Using the numbered steps from your **Proposal 1** (submitted last session), report your results/observations for each procedural step in the left column. In the right column, explain what these results/observations indicate (use the step number to connect the explanations/indications to the observations/results).

Observation	Explanation or Indication
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<p>When we implemented our proposed procedure, we observed the following:</p> <p>1) Fill a 20 ml vial with NaOH</p> <p>(part of the logistics of my experiment)</p> <p>2) Gather 3, 10 ml vials.</p> <p>(part of the logistics of my experiment)</p> <p>3) Choose 3 Molarity ratios, e.x. 1.0 M, 0.75 M, 0.5 M. We observed the molarity ratio of 0.5 to be the best as it was the ratio in which drug decay was slowest.</p> <p>4) Calculate the appropriate volumes of the systems for a total volume of 3 ml using $C_1 \cdot V_1 = C_2 \cdot V_2$</p> <p>(part of the logistics of my experiment)</p> <p>used to transfer the calculations of the molarity of a 10ml system to a 3ml system</p> <p>5) For Phenolax, set aside a vials and fill it with the 0.5 molarity ratio.</p> <p>(part of the logistics of my experiment)</p> <p>6) Use Beer's Law to calculate the molarity of Phenolax solutions based on the chosen absorbance levels</p> <p>7) Use the molarity of the Phenolax to calculate the volume of the respective solutions using the following formula: $C_d V_d = C_s V_s$</p> <p>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</p>	<p>Based on these results/observations, we concluded:</p> <p>1)(part of the logistics of my experiment)</p> <p>2)(part of the logistics of my experiment)</p> <p>3) We concluded that the solution that had the slowest decay value would provide the best results as the experiment is tested for 300s and the other ratios had to quick of a decay rate</p> <p>4) we concluded that our volume of our system was 1.5ml of NaOH and 1.5 ml of nanopure</p> <p>5) (part of the logistics of my experiment)</p> <p>6) Using beers law we concluded that our concentration over time ranged from 1.345E-05 to 8.688E-07 from 1s to 300s</p> <p>7)(part of the logistics of my experiment)</p> <p>8)(part of the logistics of my experiment)</p> <p>9) We concluded that to ensure best results the drug system needs to be shaken in order to properly gather the data out of the spectrometer</p> <p>10) In our graph of absorbance v time we concluded that the decay of the drug was a lot faster at the earlier times in the reaction</p> <p>11)(part of the logistics of my experiment)</p> <p>12) (part of the logistics of my experiment)</p>
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<p>respective solutions.</p> <p>9) In the vials from step 3 containing the NaOH and Nanopure mixture, add in the determined volume of Phenolax in Step 8 and shake. we observed that without a proper mix of the drug into our system the drug will sit in only one part of the system and decay there.</p> <p>10) The spectrometer calibrates the machine so the graph is looking at absorbance vs time. Changing the spectrometer parameters measuring the absorbance at 550 nm for 300 seconds.</p> <p>11) Add the solution to a cuvette and place it in the spectrometer, recording data for absorbance vs. time. Observe any changes in color.</p> <p>11) Using the observed absorbance value as it degrades over time, we can then transfer the data into excel and using the graphs of the data in excel we can determine the order of the reaction.</p> <p>12) In excel take your absorbance values and divide it by the epsilon value (5.02×10^4) to get the concentration for your experiment.</p> <p>13) Once you have the concentration you can graph for time v concentration using time and concentration will help you to determine the order of your experiment.</p> <p>14) In order to get a order value for your reaction you need to mess with the parameters of the concentration</p>	<p>13) We concluded that the experiment could not have been 0th order as the graph of concentration over time did not fit a linear trend line</p> <p>14) We concluded that the reaction was 1st order by comparing the graphs of time v $\ln(\text{concentration})$ and time v $1/\text{concentration}$. The graph with the best linear trendline fit was time v $\ln(\text{concentration})$</p>
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values (to calculate for 1st order you use the Ln(concentration) and to test for 2nd order you use 1/concentration)	
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3. **Proposal 2.** Given your **Proposal 1** findings reported above, propose, and justify a plan to experimentally determine n , k_{obs} and t_{90} at room temperature for **PYOCTANIN**, where the condition $[NaOH] \gg [Pyoctanin]$ exists as described in the *Kinetics Guide*.

Please NUMBER your procedural steps.

Procedural Step	Justification
<ol style="list-style-type: none"> 1) Fill a 20 ml vial with NaOH 2) Gather 3, 10 ml vials. 3) Choose one of 3 Molarity ratios, e.x. 1.0 M, 0.75 M, 0.5 M. 4) Calculate the appropriate volumes of the systems for a total volume of 3ml using $C_1 \cdot V_1 = C_2 \cdot V_2$ 5) For Pyoctanin, set aside a vial and fill it with the chosen molarity ratio. 6) Use Beer's Law to calculate the molarity of Pyoctanin solutions based on the chosen absorbance levels 7) Use the molarity of the Pyoctanin to calculate the volume of the respective solutions using the following formula: $C_d V_d = C_s V_s$ 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) Set up the spectrometer. First, calibrate using a blank cuvette, then change the axis from Absorbance vs λ to Concentration vs Time. Select 550 nm as the wavelength. Then under the Experiment tab, set the time range for 0 seconds – 300 seconds. 10) In the vial from step3 containing the NaOH and Nanopure mixture, add in the determined volume of Pyoctanin in Step 8. Shake. 11) Add the solution to a cuvette and place it in the spectrometer, recording data for concentration (M) vs. time (seconds). 12) Using the observed Concentration value as it degrades over time, we can then calculate the rate order, the K_c values, and the shelf life. 	<ol style="list-style-type: none"> 1) Gathering an appropriate amount of NaOH for the upcoming experiment 2) These vials are used to create our 3ml systems in which we will place our drug (Pyocatnin) in our chosen molarity ratio. 3) In order to examine how different ratios of NanoPure to NaOH affect the degradation of the drug (Pyoctanin). 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 ensuring not to have them mixed up. 6) Beer's Law gives us the exact molarity of our Pyoctanin solution at a specific absorbance level. 7) Using the formula of: $C_d V_d = C_s V_s$ you can determine the exact volume of Pyoctanin. 8) This will give us the volume in milliliters, multiply by 1000 to get the volume in microliters. 9) These settings for the spectrometer will allow us to measure the Concentration vs Time instead of the Absorbance vs Wavelength. The data obtained from the Concentration vs Time graph/table will give us data to calculate 0th, 1st, and 2nd order through the equations listed below: $0^{th}Order = [Pyc]$ $1^{st}Order = \ln[Pyc]$ $2^{nd}Order = \frac{1}{[Pyc]}$ 10) This will allow us to observe color changes as it will provide a visualization of Pyoctanin degrading over time. Shaking will ensure that the solution is thoroughly mixed. 11) This will allow us to record the absorbance value from the instant Pyoctanin is placed into the NaOH solution. It needs to happen instantly as Pyoctanin can degrade fairly quickly. 300

seconds should be ample time to fully see the Pyoctanin in the NaOH solution degrade.

- 12) The rate order, K_c values and the shelf life are the values we are looking for and the Concentration level from the spectrometer can help us determine it. Once we have obtained these values, we will then plot them in Excel, plotting Concentration vs Time graphs for each order. Then, plot a trend line to obtain a linear equation for each graph, as well as a R^2 value to help identify the observed rate constant as the graph with the R^2 value that is closest to 1 will be the rate order. We will use the following equations to help us determine the rate order, observed rate constant (k value) and thus the shelf-life:

$$0^{\text{th}}\text{Order} = [\text{Pyc}]$$

$$1^{\text{st}}\text{Order} = \ln[\text{Pyc}]$$

$$2^{\text{nd}}\text{Order} = \frac{1}{[\text{Pyc}]}$$

$$t_{90} = \frac{[\text{Pyc}]_0}{10k_{obs}}$$

$$t_{90} = -\frac{\ln(0.9)}{k_{obs}}$$

$$t_{90} = \frac{0.111}{k_{obs}[\text{Pyc}]_0}$$

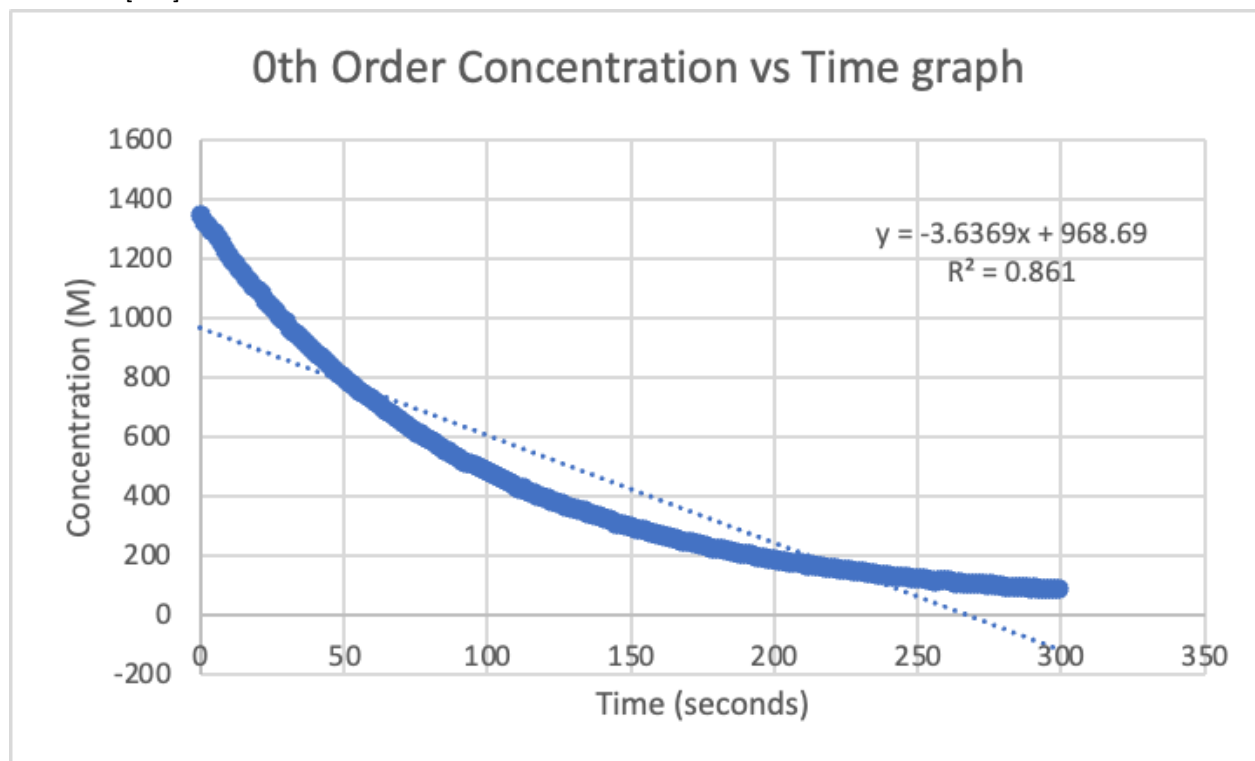
Technical Skill Evaluation

Graphical Determination of the Rate Order n and Observed Rate Constant, k_{obs} . Using EXCEL prepare three plots ($[Phx]$ vs. t , $\ln[Phx]$ vs. t , and $1/[Phx]$ vs. t) to enable determination of the order n (the rate order with respect to the molar concentration of Phenolax) and the observed rate constant, k_{obs} , for the base-mediated Phenolax degradation. Carefully reproduce (draw) or paste in the three graphs giving the linear equation with R^2 value (from EXCEL). Clearly explain how you derived the values of n and k_{obs} using the plots.

From the three graphs below, we determined that the 1st order Concentration vs Time graph had the R^2 value that was closest to 1. This helped us to identify the n value (rate order). By plotting a trendline and using the equation function in Excel, we were able to come up with a linear equation and an R^2 value. Our linear equation then gave us the observed rate constant (k) which was equal to 0.0094. Knowing the k value and the rate order, we are able to calculate the t_{90} by using the following formula:

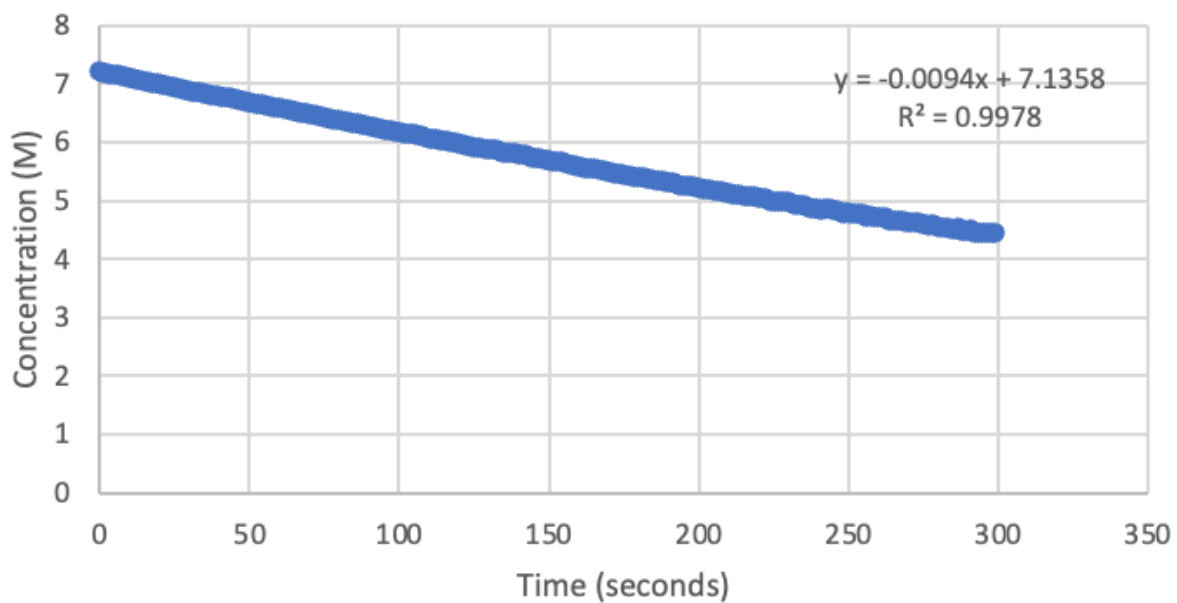
$$t_{90} = -\frac{\ln(0.9)}{k_{obs}} = -\frac{\ln(0.9)}{0.0094} = 11.209 \text{ seconds}$$

0th order: $[Phx]$ vs Time

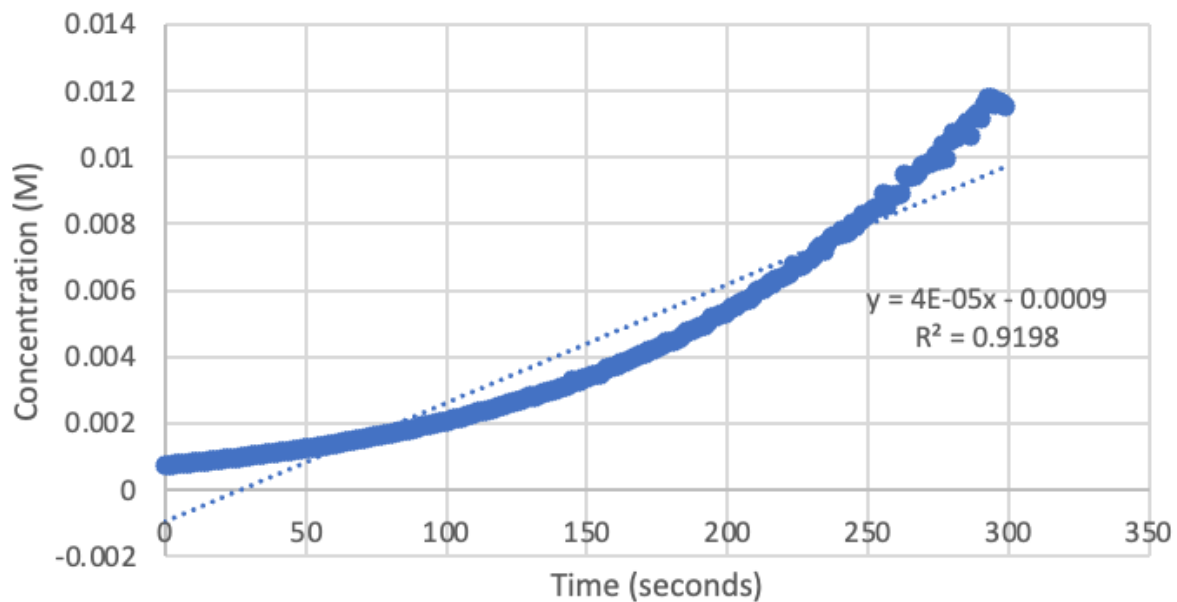


1st order: $\ln[Phx]$ vs Time

1st Order Concentration vs Time graph

2nd Order: $1/[Phx]$ vs Time

2nd Order Concentration vs Time graph



Phenolax Shelf-life Calculation. Based on your experimentally determined order n (the rate order with respect to the molar concentration of Phenolax) and rate constant, k_{obs} , (both from above) calculate the t_{90} (shelf-life). Show all work.

$$t_{90} = -\frac{\ln(0.9)}{k_{obs}} = -\frac{\ln(0.9)}{0.0094} = 11.209 \text{ seconds}$$