Final Report

Low-Cost Raspberry Pi & Molecular Simulations for Microplastic-Drug Classification via LFA

Ahana Koushik
Supercomputing Challenge
Final Report
April 1st, 2026

Albuquerque Academy

Team members:
None

Executive Summary:
The purpose of this project is to predict the possible binding between nano/micro-plastics (styrene) with a pharmaceutical drug (ciprofloxin or 'cipro' – a broad spectrum antibiotic). Using computer simulation software's, molecular modeling, and the development of a Raspberry Pi colored sensor, we can detect the interaction between cipro with the most common type of micro- /nano-plastics in our body- polystyrene.

Statement of the problem:
Every tissue in our body is flooded with microplastics. Surprisingly, the brain acts like a sponge and takes up the most micro- and nano-plastics compared to other tissues in our body. The majority of us are also on medications for several types of diseases, and in some cases multiple medications per day. However, we don't know if micro- and nano-plastics in the tissues/circulations would bind with these medications and either prevent their effectiveness or make them into a different compound altogether?

Materials
Software, references, tables, and other products
NetLogo, Liu et al (2019) datasets, and Pseudo first-order reaction formula
Molecular Operating Environment (MOE) – Demo version – permission from
Pristine polystyrene (PS) plastic (200nm in diameter) – from Alpha Nanotech
Common medicines (Ciprofloxin/'CIP')–research grade.
Filters (0.4 and 0.2 micrometers)

Pipette and tips
Syringe, Gloves, Plastic forceps

TCS3200 Color Sensor Module from Amazon for Raspberry Pi:

- Equipped with the TCS3200 chip, it can achieve higher-precision color recognition and greater performance stability.
- Active light source control system: White LED light can be controlled to turn on and off, supports detection of the true color of non-luminous objects, and expands application scenarios (such as industrial sorting, printed product detection)
- Strong anti-light interference ability: Built-in optical filtering technology effectively suppresses ambient light interference and can still maintain color detection accuracy under complex lighting conditions
- Wide voltage compatible design: 3-5V wide voltage power supply, seamlessly adapts to mainstream control systems such as Arduino and STM32, without additional circuit adaptation
- Macro precision detection: Optimized optical structure design, 1cm optimal detection distance to achieve high-resolution color capture, suitable for precision instruments and small space scenes.

Description of the method:
As a continuation of last year's project, I used the 'Simple Kinetics Model 1' in NetLogo to simulate only the interaction between polystyrene (PS) and Ciprofloxin (cipro). I built a model based on a pseudo-first-order reaction by first simulating a reaction in which one reactant is in large excess, effectively making the reaction appear first-order with respect to the other reactant in NetLogo. Next, I used the data described in Liu et al., which report rate constants for reactants and products of Ciprofloxacin (Cipro), an antibiotic that helps with bacterial infections and sickness, and polystyrene (PS), a very common plastic. In this study, the authors have provided rate constants and kinetic fitting parameters for PS to Cipro based on experimental data, as shown below. I used k_1, the rate constant for pristine (not aged) PS values in a pseudo-first-order reaction, in NetLogo.

Table S1 Kinetic fitting parameters of the pristine and aged microplastics, including pseudo-first and pseudo-second order dynamics.

Adsorbent	Pseudo-first order			Pseudo-second order		
	k_1	q	R^2	k_2	q	R^2
PS	0.273	2.580	0.951	0.041	3.170	0.948
PVC	0.288	2.790	0.972	0.037	3.410	0.976
Aged PS	0.598	4.860	0.684	0.061	5.480	0.840

Aged PVC	1.570	3.070	0.642	0.296	3.280	0.854

Liu et al, Environmental Pollutions 246 (2019) 26-33

I used the following code in Netlogo. I used the Simple Kinetic 1 model in Netlogo and replaced the code which simulates simple kinetics with the pseudo first-order reaction.

NetLogo® Code

```
to react-forward
  if (any? other reactants-here) and
    ;; multiply k1 rate constant by the initial concentration of rate-limiting reactant - either PS or CIP - which is adjustable
    random-float 1 < (0.273 * number)
   [ ask one-of other reactants-here
      [ die ]
     set breed products
     set color red ]
end
```

The above code simulates a reaction where red turtles (reactants) have a 10% chance of turning green (products) in each time step, based on their concentration. **0.273 is the rate constant for PS and Cipro interaction** from Liu et al.,

The random-float 1 < (0.273 * number) line checks if a random-float number between 0 and 1 is less than the reaction rate (0.1 * concentration).

Discussion on model verification/validation:

I'm still in the early stages of testing interactions between microplastics and drugs. However, the rate constants I used for the pseudo-first-order reaction were taken from a validated experimental dataset by Liu et al. (2019).

Results:

Figure 2: Figure 1 shows the NetLogo layout

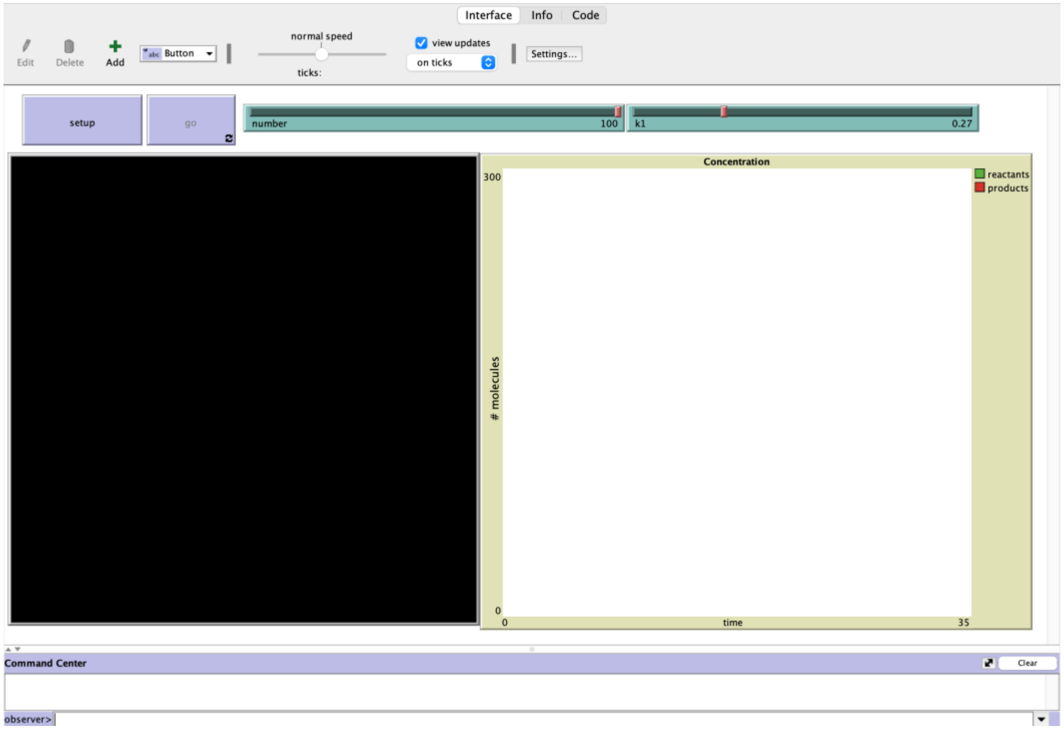
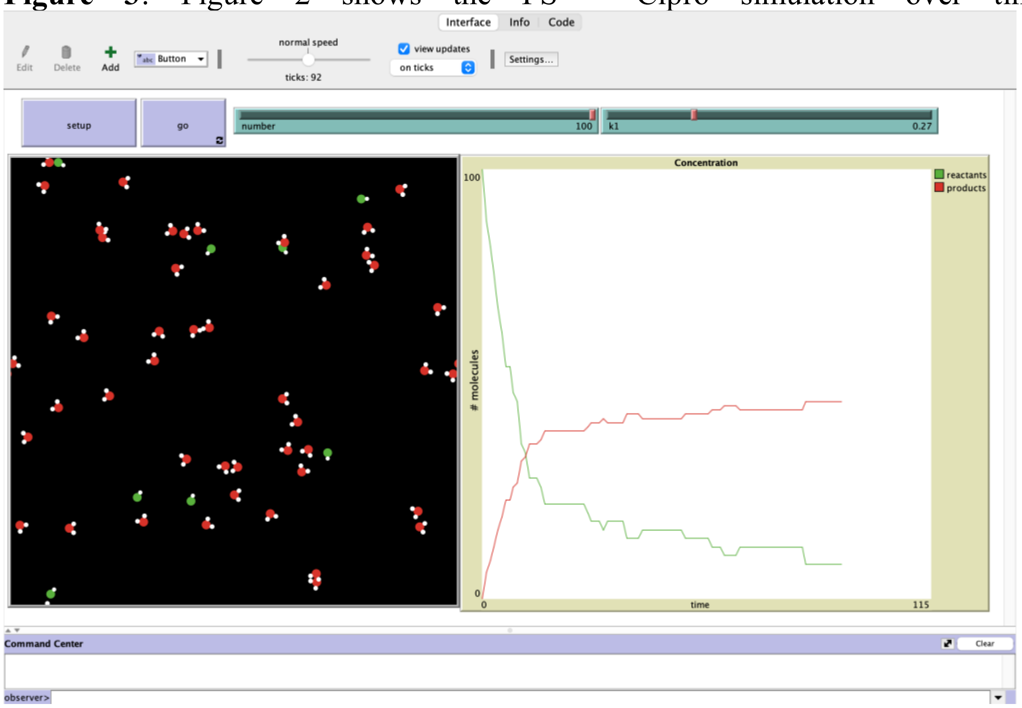


Figure 3: Figure 2 shows the PS – Cipro simulation over time in NetLogo



Molecular Operating Environment (MOE) Simulation (Results):

The second computational modeling I used was the molecular operating environment software, which demonstrates a 3D molecular structure and binding of styrene and cipro. Below demonstrates the procedure of the docking procedure and images from the environment:

1. Download - Ciprofloxacin and Styrene 3D structures (as SDF files) from PubChem

2. Load these structures into the ‘Molecular Operating Environment’ (MOE) Software
3. Select Compute ”Protonate 3D”
4. Select Compute “Energy Minimize”
5. Shown are the interaction structures after protonating 3D and energy minimization

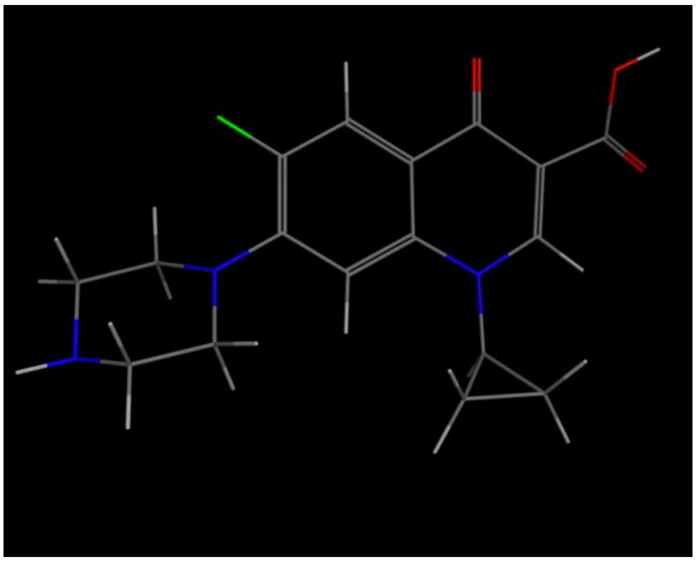


Figure 4. Molecular structure of cipro

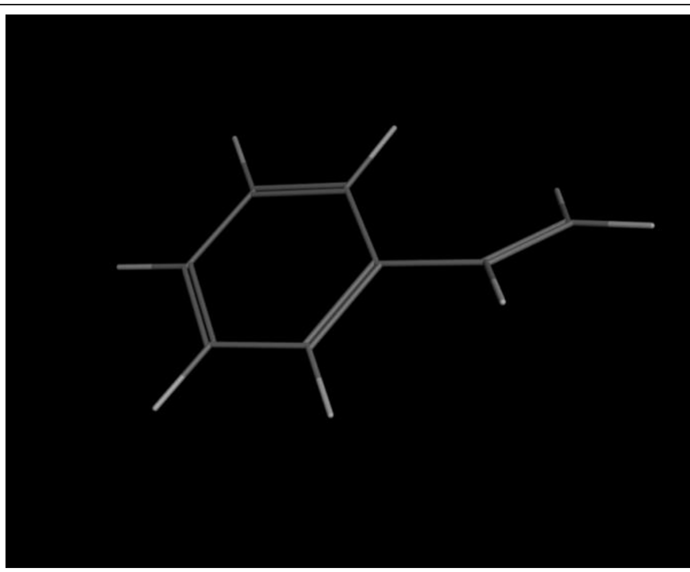


Figure 5. Molecular structure of styrene monomer

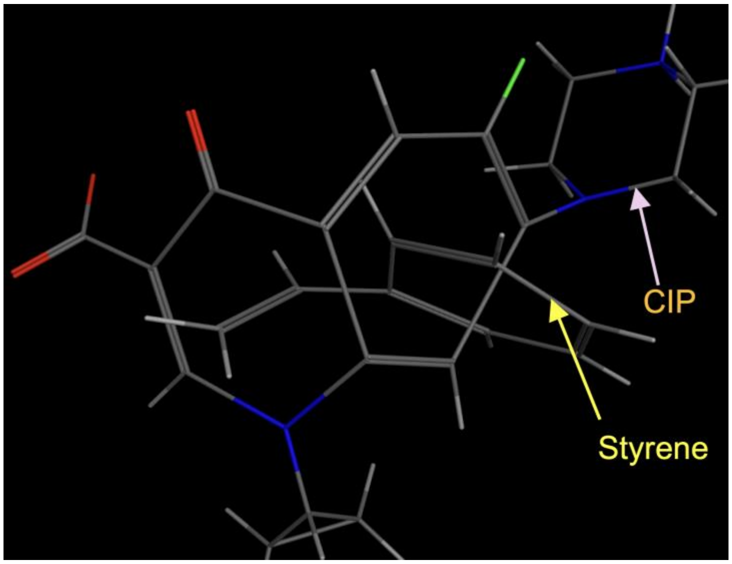


Figure 6. Molecular docking of Ciprofloxacin and Styrene: (after Protonate 3D and energy minimization in MOE)

Validation of PS + Cipro Interactions (Experiment):

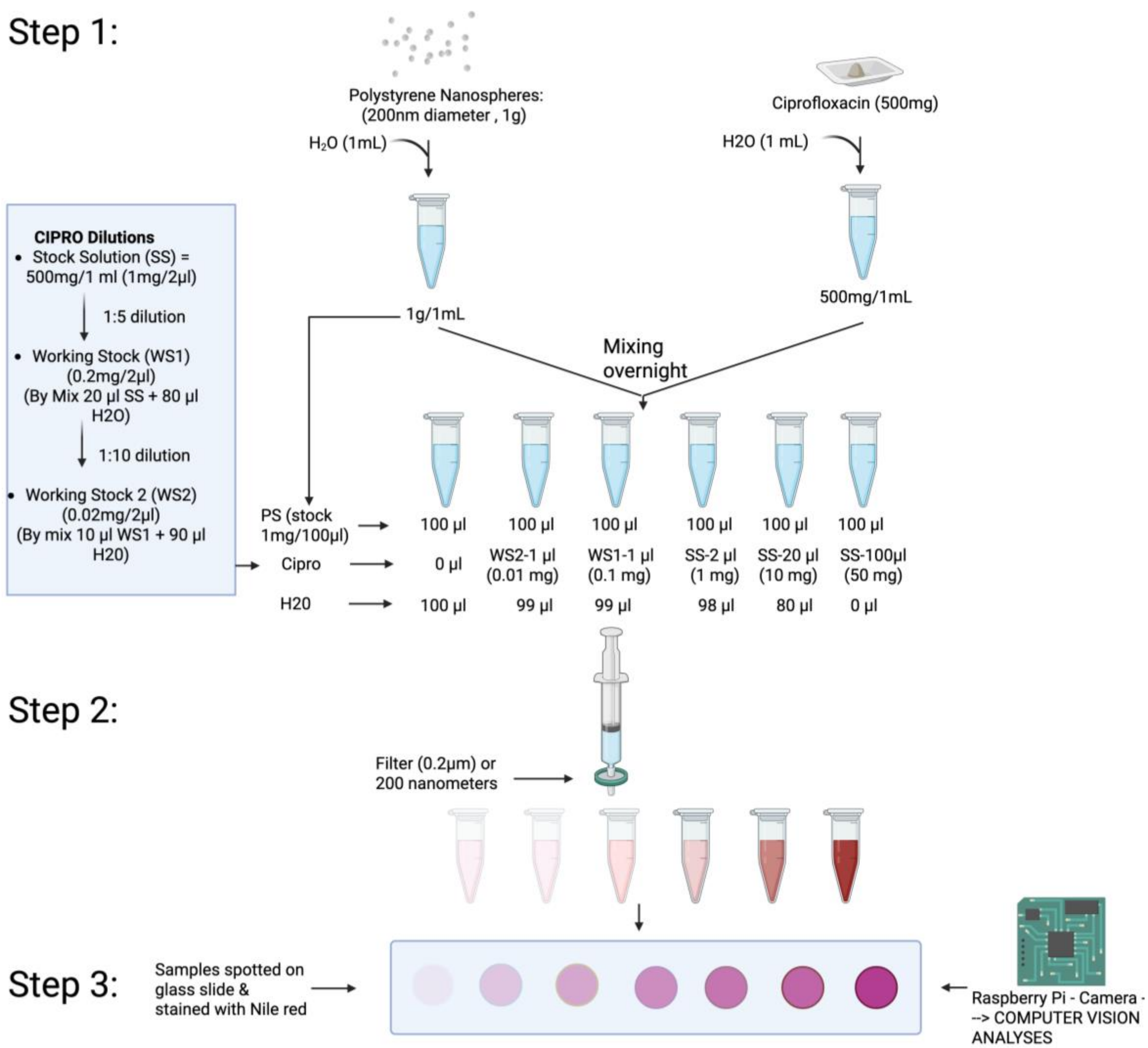


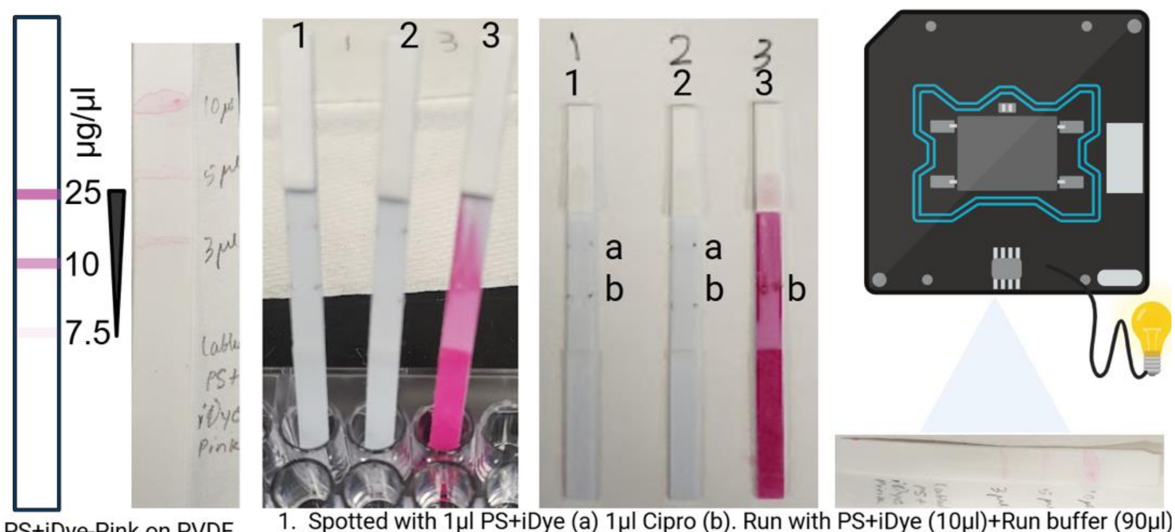
Figure 7: Validation of PS + Cipro interaction using size-based filtration method. PS concentration was kept constant (1mg/100ml) and mixed with different Cipro concentrations (0mg, 10mg, 100mg, 1mg, 10mg, and 50mg) of Cipro. 💡IDEA – as the concentration of Cipro increases, it leads to more binding with PS, and the PS + Cipro stays stuck in the 0.2mm filter. Small PS can pass through and be detected in the collection tube. Total volume made up to 200 ul with H20. Controls – Only Cipro, no PS; and only PS, no Cipro. **Graphics created by the student using BioRender, 2026.*

Cipro Con→	0 mg	10 mg	100 mg	1 mg	10 mg	50 mg
Vol. Recovered (ml)→	156	121	98	40	2	1

Table 1: Volume recovered from step 2 (Table) shows reduced PS in the flow through after filtering.

Raspberry Pi Sensor Detection of LFA Strips:

Lateral Flow Assay (LFA) is a rapid paper-based tool for detecting specific analytes. In this project, I first spotted cipro onto the LFA strip with stained polystyrene in the well. Through capillary action- the ability of a liquid to flow through narrow spaces against gravity. The iDye pink-stained polystyrene bound cipro and showed a labeled spot on the LFA strip. Lastly, a Raspberry Pi sensor was used to detect this spot as an 'interaction' between the polystyrene and cipro interaction on the LFA strip (***Figure 8)***. Python code was written on a Raspberry Pi to capture the output of this polystyrene-cipro interaction as an LED signal. That is using a color sensor camera attached to the Raspberry Pi,



1. Spotted with 1µl PS+iDye (a) 1µl Cipro (b). Run with PS+iDye (10µl)+Run buffer (90µl)
2. Spotted with 1µl PS+iDye (a & b). Run with Cipro (10µl)+Run buffer (90µl)
3. Spotted with 1µl Cipro (b). Run with PS+iDye (50µl)+Run buffer (50µl)

Figure 8: Spotted LFA-based analyses of PS+Cipro. Only 50µl of the iDye-Pink-stained polystyrene beads in the well (along with the LFA run buffer – the dark pink strip and condition 3 above) showed a clear spot 'b' on the LFA strip, indicating that the PS-iDye pick retained in the area of the strip where the cipro was spotted.

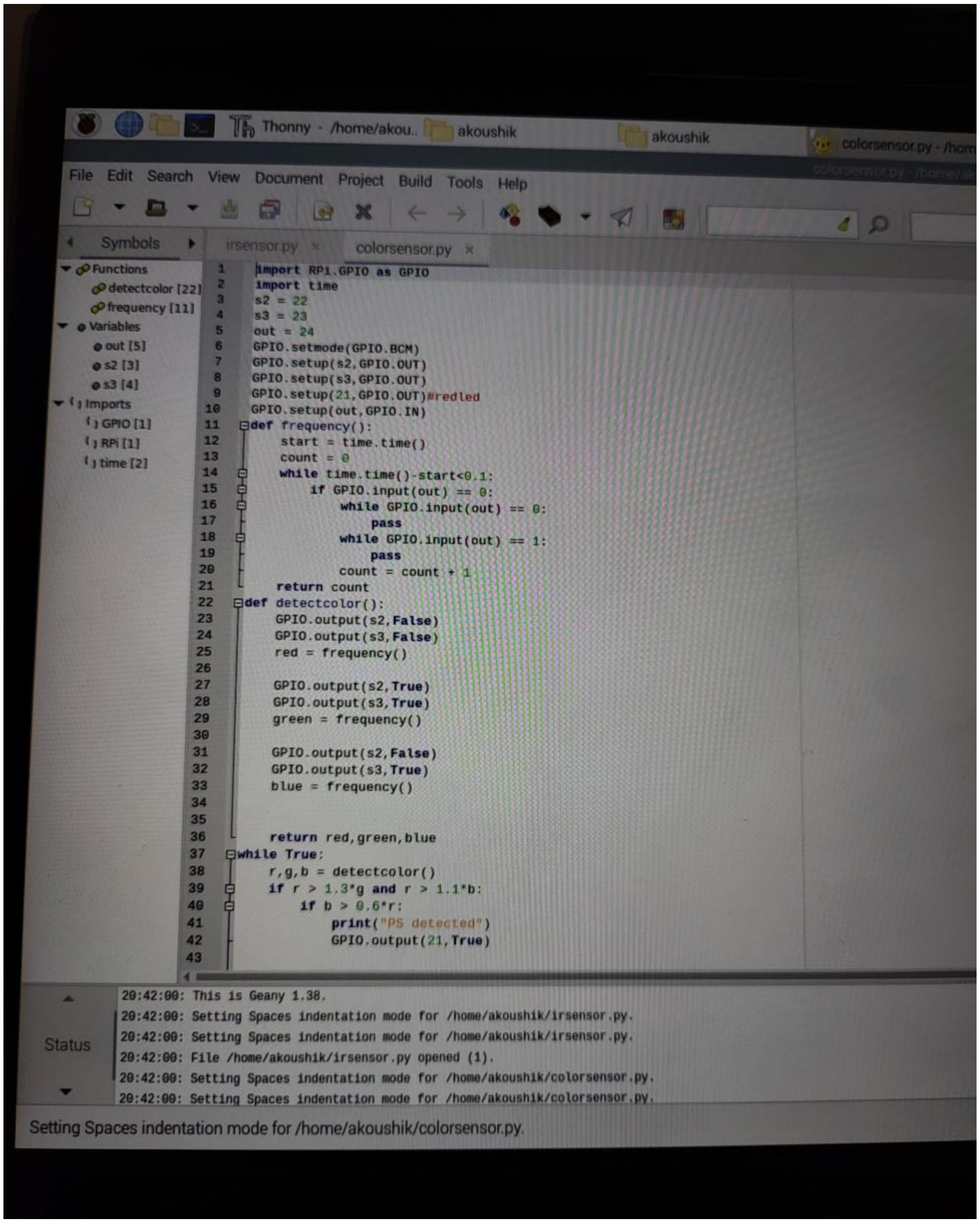


Figure 9: Python Code to program Raspberry Pi to activate the color sensor camera and giving an output as a LED turn on signal upon detecting the cipro-+PS-iDye-pink stained bank on the LFA strip.

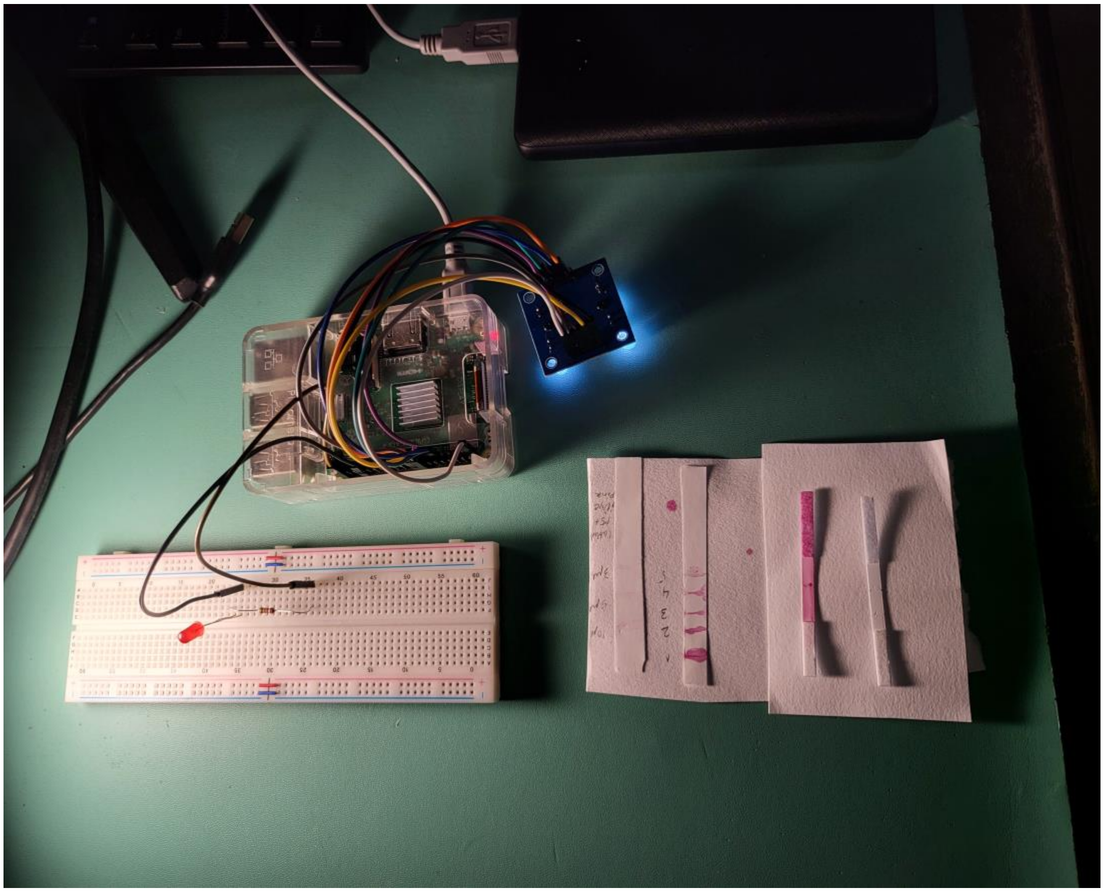
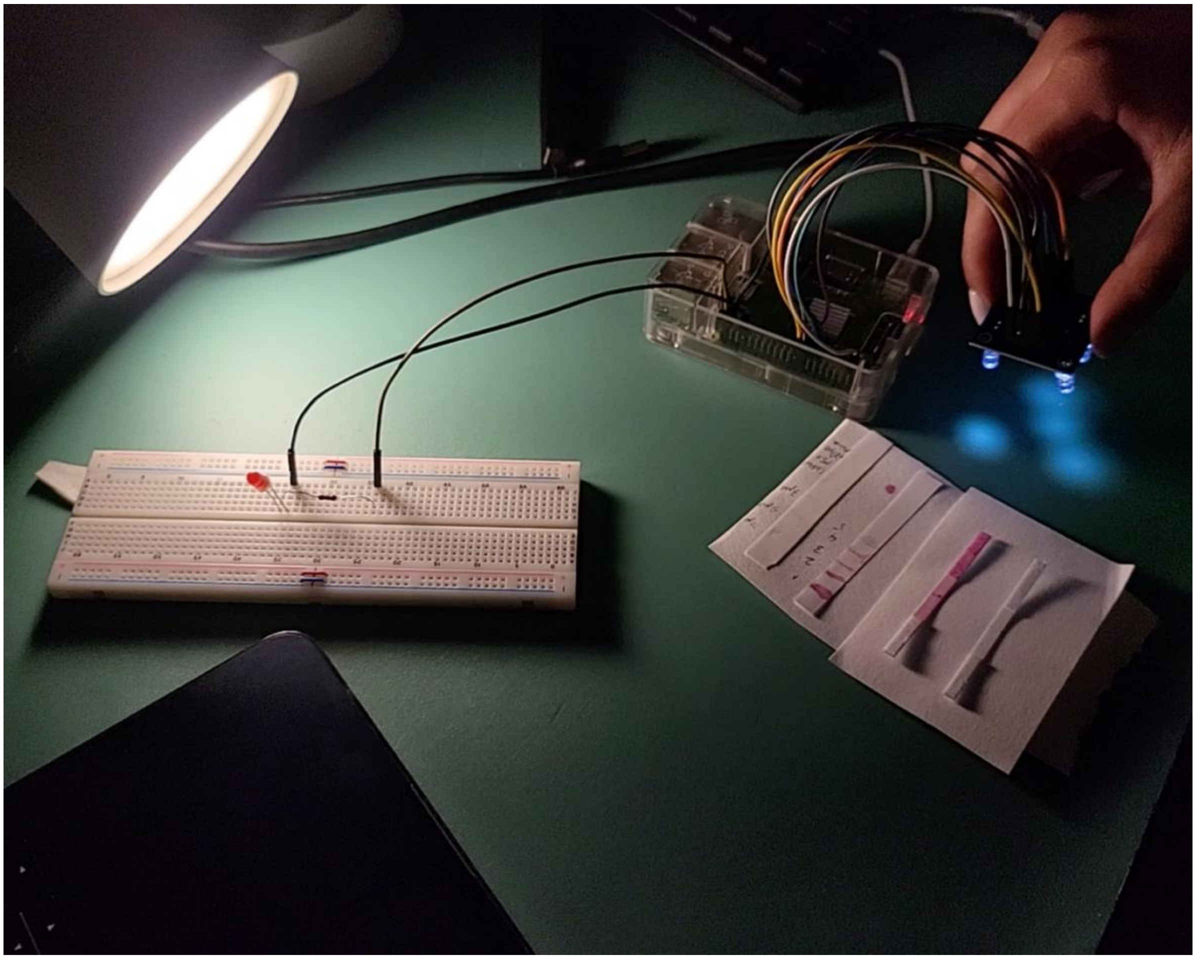


Figure 10: Picture of Raspberry Pi setup with color sensor camera.



Movie 1: Raspberry Pi and color sensor camera detecting the cipro-polystyrene-iDye pink-stained spot and turning the LED light on (Double click for the movie).

Conclusions:

In conclusion, NetLogo can be used to simulate the interaction between PS/PVC and Cipro. If I can find rate constants for other drugs and microplastics, NetLogo can be used to simulate such interactions as well.

Future Plans:

In the future, hopefully I can make it a more portable device and change the program to which the color light can change to the intensity of the concentration. Additionally, I might use this tool for other nano/micro-plastic and pharmaceutical drug interactions as well as ameliorating the raspberry pi in which it can detect various concentrations of different plastics and drugs.

Most significant achievement on the project

Microplastics are in every organ of our body, and it is important to understand how they might interact with pharmaceuticals, drugs, and their metabolites. NetLogo can be a useful tool to understand these interactions.

Acknowledgements
I would like to thank my parents and my computer science teacher in helping me with this project.

References

Guangzhou Liu, Zhilin Zhu, Yuxin Yang, Yiran Sun, Fei Yu, Jie Ma, Sorption behavior and mechanism of hydrophilic organic chemicals to virgin and aged microplastics in freshwater and seawate., Environmental Pollution, Volume 246, 2019, Pages 26-33, ISSN 0269-7491, https://doi.org/10.1016/j.envpol.2018.11.100.