

Final Report - Codes

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

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Supercomputing Challenge

Final Report

April 1st, 2026

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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 ($0.1 * \text{concentration}$).

Python Code – in Raspberry Pi

```
import RPi.GPIO as GPIO
import time
s2 = 22
s3 = 23
out = 24
GPIO.setmode(GPIO.BCM)
GPIO.setup(s2,GPIO.OUT)
GPIO.setup(s3,GPIO.OUT)
GPIO.setup(21,GPIO.OUT)#redled
GPIO.setup(out,GPIO.IN)
def frequency():
    start = time.time()
    count = 0
    while time.time()-start<0.1:
        if GPIO.input(out) == 0:
            while GPIO.input(out) == 0:
                pass
            while GPIO.input(out) == 1:
                pass
            count = count + 1
    return count
def detectcolor():
    GPIO.output(s2,False)
    GPIO.output(s3,False)
    red = frequency()

    GPIO.output(s2,True)
    GPIO.output(s3,True)
    green = frequency()

    GPIO.output(s2,False)
    GPIO.output(s3,True)
    blue = frequency()

    return red,green,blue
while True:
    r,g,b = detectcolor()
    if r > 1.3*g and r > 1.1*b:
        if b > 0.6*r:
            print("PS detected")
            GPIO.output(21,True)

    else:
```

```
    print("red detected")
    GPIO.output(21,True)
else:
    print("not red")
    GPIO.output(21,False)
time.sleep(1)
GPIO.cleanup()
```