Predicting the drug and micro-/nano-plastic interactions inside the body using molecular dynamics modeling and machine learning

Ahana Koushik

Supercomputing Challenge

Final Report

April 2nd, 2025

Albuquerque Academy

Team members:

None

Executive Summary

The purpose of this project is to predict by using computer simulation software and molecular modeling to match the interaction between thousands of drugs with the most common types of micro- /nano-plastics in our body (e.g. polyethylene).

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?

Description of the method

I am using simple kinetic 1 model as the base to simulate interaction between polystyrene (PS) and polyvinyl chloride (PVC) – which are two very common source of plastics .

I built a model based on pseudo-first order reaction by first simulating a reaction where one reactant is in large excess, effectively making the reaction appear first-order with respect to the other reactant in Netlogo Software. Next, I used the data described in Liu et al., that describe rate constants for reactants and products for Ciprofloxacin (Cipro) which is an antibiotic that helps will bacteria and sickness, and polystyrene (PS) or polyvinyl chloride (PVC) – which are two very common source of plastics. In this study, the authors have provided rate constants and kinetic fitting parameters for PS and PVC to the Cipro based on real experiments which is shown below. I used k1 which is the rate constants for pristine (not aged) PVC and PS values in 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.

```
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., 2019. Similarly, **0.288 is the rate constant for PVC and Cipro interaction.**

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 that I used for the pseudo first-order reaction came from a validated experimental dataset from Liu et al, 2019.

Results

Figure 1: The figure 1 shows the Netlogo layout

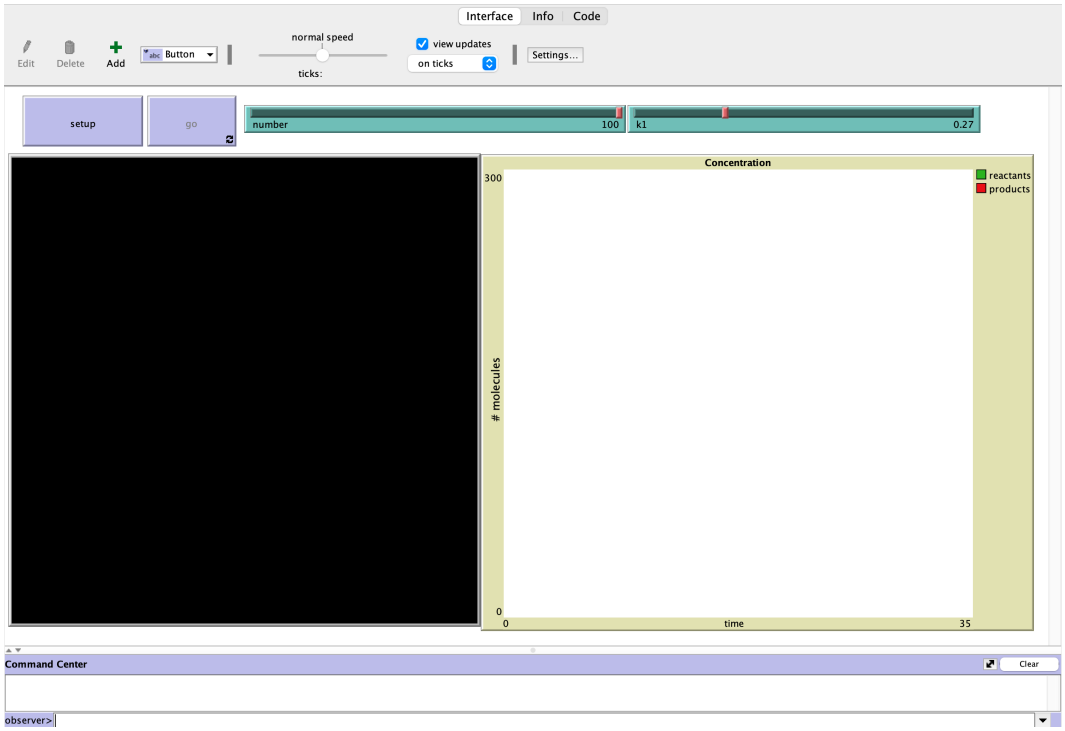


Figure 2: The figure 2 shows the PS – Cipro simulation over time in Netlogo

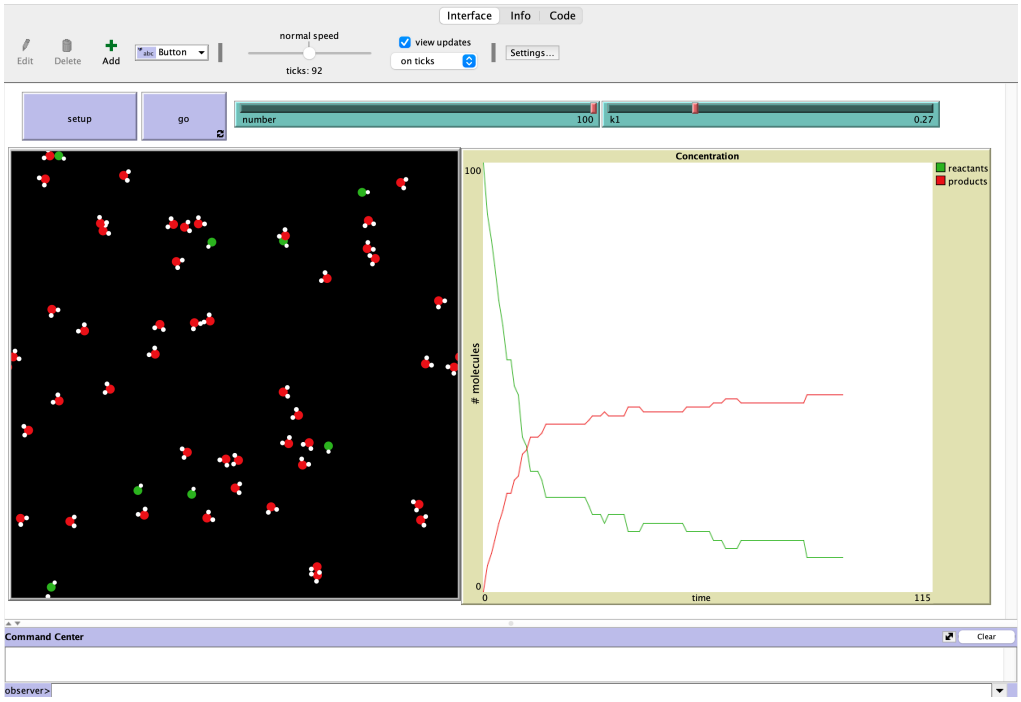
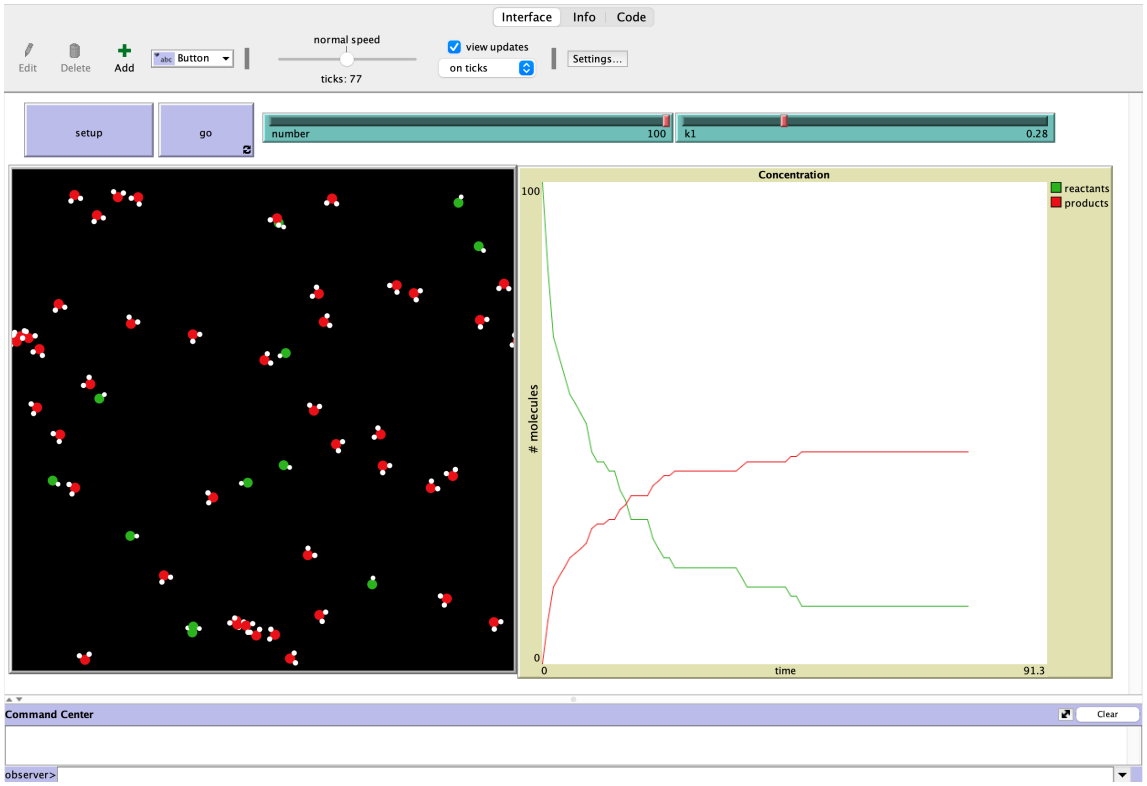


Figure 3: The figure 3 shows the PVC – Cipro simulation over time in Netlogo



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.

Software, references, tables, and other products

Netlogo, Liu et al (2019) datasets, and Pseudo first-order reaction formula

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 useful tool 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.