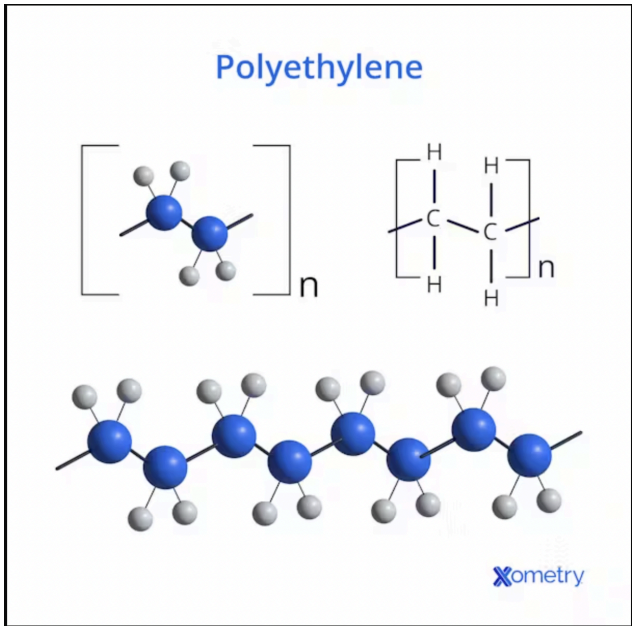
Sowmya Sankaran
Ahana Koushik
Albuquerque Academy Team 2

Interim Report: Predicting the Drug-Microplastic Interactions in the Body Using Machine Learning Modeling

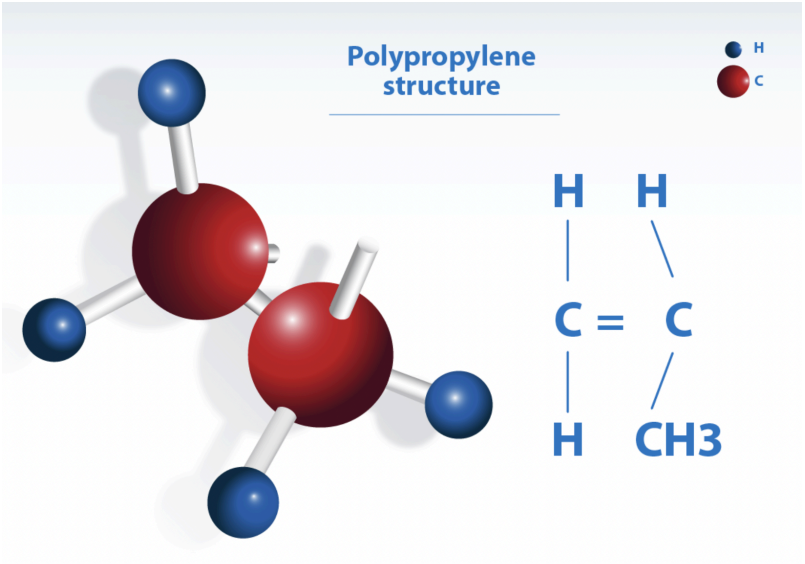
It is clear from past research that every tissue in our body is flooded with microplastics. Surprisingly, the brain acts like a sponge and takes up the most micro- and nano-plastics compared to other tissues in our body. Additionally, the majority of people are also on medications for several types of diseases and, in some cases, multiple medications per day. However, there has been no research on whether micro- and nano-plastics in tissues or circulations would bind with these medications. If this happened, it could either prevent the medicine's effectiveness or make them into a different compound altogether. 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).

First, we chose several microplastics and common medicines, learning about the molecular structure of them all. In order to simulate the interaction between these molecules, we have to pick the most accurate representation of these molecular structures, accounting for different types of microplastics and medicines and their behaviors. As the complexity of drug-microplastic interactions is significant, we selected a few different medicines and microplastics to use as an initial representative sample for our simulations. We chose two microplastics- Polyethylene and Polypropylene- to use for the simulations. Polyethylene is formed from the monomer ethylene. It is made up of several "chains" of methylene, which all come together to form a *backbone*. An image of this structure is included below.



https://www.xometry.com/resources/materials/polyethylene/

Meanwhile, Polypropylene is a type of double-bonded hydrocarbon. When the bonds are broken and then rejoined, they form polypropylene, a polymer chain. An image of polypropylene's molecular structure is below.



https://www.petrocuyo.com/en/technology/polypropylene

Additionally, we will use a representative sample of drugs. The ones we will start with are Ibuprofen and Tylenol, using them combined with the two microplastics listed above to create a basic simulation. We will then expand on this small sample, using a broad variety of different microplastics and common drugs, to make our simulation broader and more accurate.

As our simulations may require substantial computational resources, we are using online applications that provide us with cheap, accessible GPU power, such as Google Colab and Jupyter. Using these, we have significant power to simulate our interactions without using very expensive resources. We also will consider strategies that help us optimize these simulations to be more computationally efficient. Additionally, based on the final size and computational power needed for our simulation, we may also leverage parallel computing techniques to make our simulations faster. These include the pre-built parallel computing application in a Jupyter notebook, an IPython cluster.

In this project, we are not able to do an in vitro or in vivo study to experimentally validate our simulations. This is because of several health considerations, especially considering unqualified minors working in a potentially dangerous environment. However, the research developed in this project can be used to validate data by scientists that involve these experimental approaches, such as studying the interactions of the simulated drugs and microplastics in a lab rat or an insect. This will help us learn more about the experimental results and possible interference of microplastics in the effectiveness of these drugs.

Using a free and open-source software suite for high-performance molecular dynamics and output analysis like GROMACS or Jupyter, Python programs to simulate our molecular interactions, and large language models, we are predicting the interactions of different types of microplastics with common drugs. There have not been many studies on these kinds of interactions, and this project is the first to try and develop this knowledge using simulations. Using these simulations, accurate experimental data can be produced that can validate the observations made about these interactions. This would involve collaborating with experts in

other fields, as they can do a more experimental study whereas our project is fully focused on simulations.

Microplastics in the human body can have devastating and immediate effects. These include an increased chance of respiratory disorders, cardiovascular disease, cell and DNA damage, and the infiltration of brain tissue. If we do not know what drugs can mitigate these effects and which ones could possibly make these impacts stronger, there is no way that we can even begin to solve the problem that is microplastics in the human body. The research developed in this project can play a crucial role in these first steps using accurate simulations of drug-microplastics interactions, helping pave the way for a solution to the effects of microplastics in our bodies.

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