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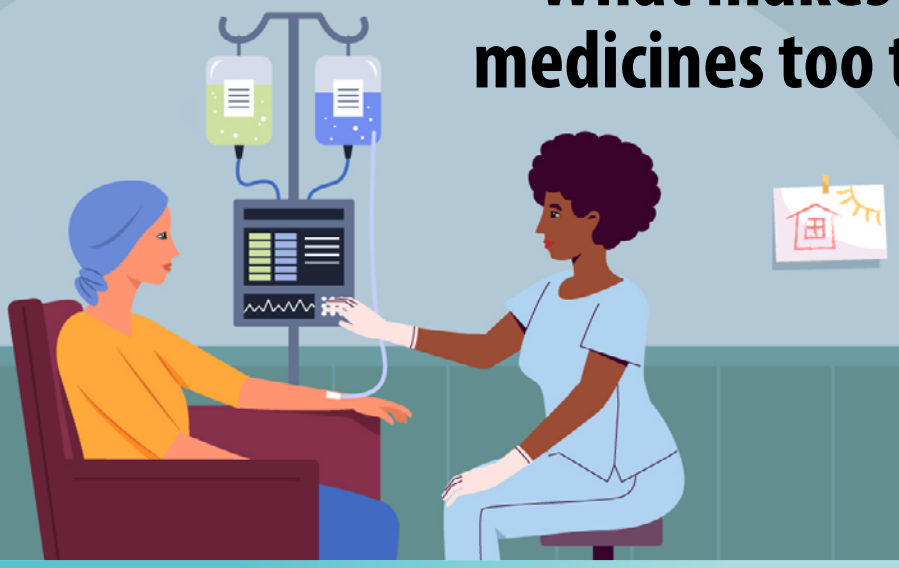
What makes some medicines too thick?



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Abstract

A lot of thought goes into the creation of a medicine. One important consideration is how the medicine is given. Some medicines can be given in pills or sprays. Others need to be injected using a syringe. Some even require procedures in a medical center. The physical properties of the medicine will determine how it can be given. So, what if we could change those physical properties on demand?

We wanted to investigate the physical properties of medicines containing monoclonal antibodies. They are used to treat cancer and autoimmune diseases. They often have to be given intravenously at a medical center because these medicines can get very viscous (thick). We wanted to know why. So we developed several models and ran computer simulations to see what was happening. We found that interactions between the antibodies and charged particles in the solution created temporary clusters. We can use this information to modify medicines and make them more accessible.

Introduction

Have you ever had to take medicine when you were sick? Designing new medicines is complex. There are many things to consider. The **solution** needs to be stable so it can be stored. It also needs to be produced at a large scale. Then, researchers need to figure out how to give the medicine to patients.

Sometimes medicines need to be given in high concentrations. But concentrated solutions can have high **viscosity** (Fig. 1). Highly viscous medicines are given to patients **intravenously**. This can only happen in a

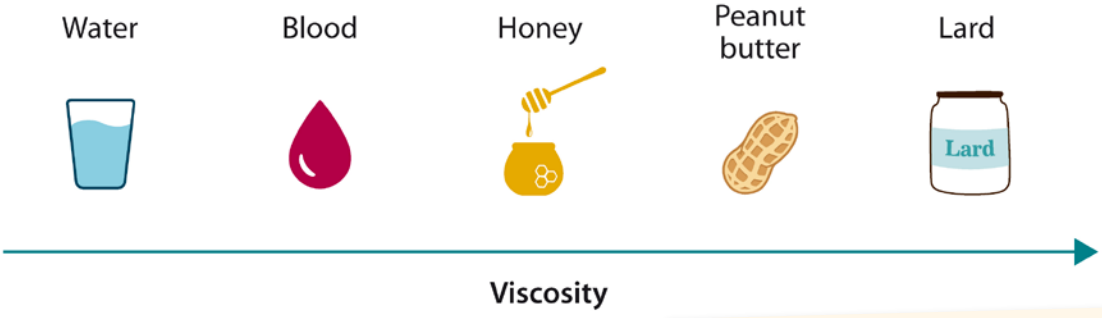


Figure 1: Examples of liquids with different viscosities.

doctor's office or hospital. The process is inconvenient and expensive. If these medicines were less viscous, people could take them at home using syringes. This could save money. It would also ensure that more people had access to treatment.

Understanding why some medicines become viscous isn't easy. To study this, scientists would ideally look at every atom in a medicine. But that's far too complex when millions of molecules interact! Instead, researchers use **coarse-grained models**, which simplify the molecules by grouping several atoms into simple "beads". These simplified models make it possible to study how several molecules behave at once while still capturing the most important properties of the solutions. One important property to consider is **electrostatic interactions** between charged parts of the molecules.

We wanted to develop a new model to look at the viscosity of medicines. In particular, we wanted to look at medicines containing **monoclonal antibodies**. These concentrated and highly viscous medicines are used to treat cancer and **autoimmune diseases**. **Antibodies** are a natural part of the immune system. They recognize foreign intruders in the body so that other cells can destroy them. And monoclonal antibodies can be modified to recognize any type of cell. This is what makes them so effective!

Methods

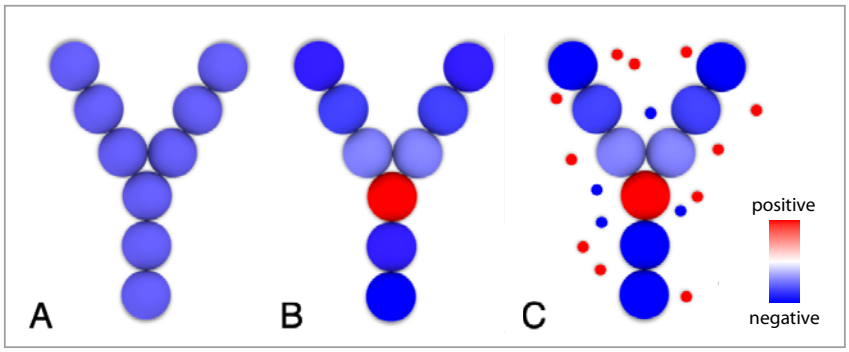
We used computer simulations to develop three coarse-grained models (Fig. 2). Each model is represented by 9 beads. We based our models on a specific antibody that can identify viruses in the body.

Antibodies are chains of molecules called **amino acids**. Amino acids can have positive or negative charges. Or they can be neutral. These electrostatic properties help antibodies interact with foreign cells. They can also help antibodies interact with **ions** in solutions.

Model A - Simple model with a uniform charge across the antibody. This means that the total charge of the amino acids is spread equally over the 9 beads.

Model B - Simple model with uneven charges across the antibody. We mapped the charges of the original amino acids onto our model. For each bead in our model, we averaged the charges on the amino acids that were nearby.

Model C - Complex model with uneven charges across the antibody AND ions in the solution. This is very similar to Model B but with positive and negative ions in the solution.



For each model we looked at different antibody concentrations. We compared our results to previous laboratory values. We also calculated other parameters that help describe interactions between molecules.

Figure 2: Our three antibody models. Each bead represents a part of the antibody and the average charge for the amino acids in that area. For Model C, the small red and blue dots around the antibody represent charged ions in the solution.

Results

We found that the viscosity increased as the antibody concentration increased (see Fig. 3 on p.3). We also discovered that Model C matched our laboratory evidence the best.

We saw that at high concentrations, antibodies formed temporary clusters. This was because of two things:

1. Areas on the antibodies that had opposite charges interacted with each other.
2. Areas on the antibodies interacted with ions in the solutions. This stabilized the antibodies and allowed them to stay clustered for longer, even if they had the same charge.

How would you describe the relationship between antibody concentration and viscosity?

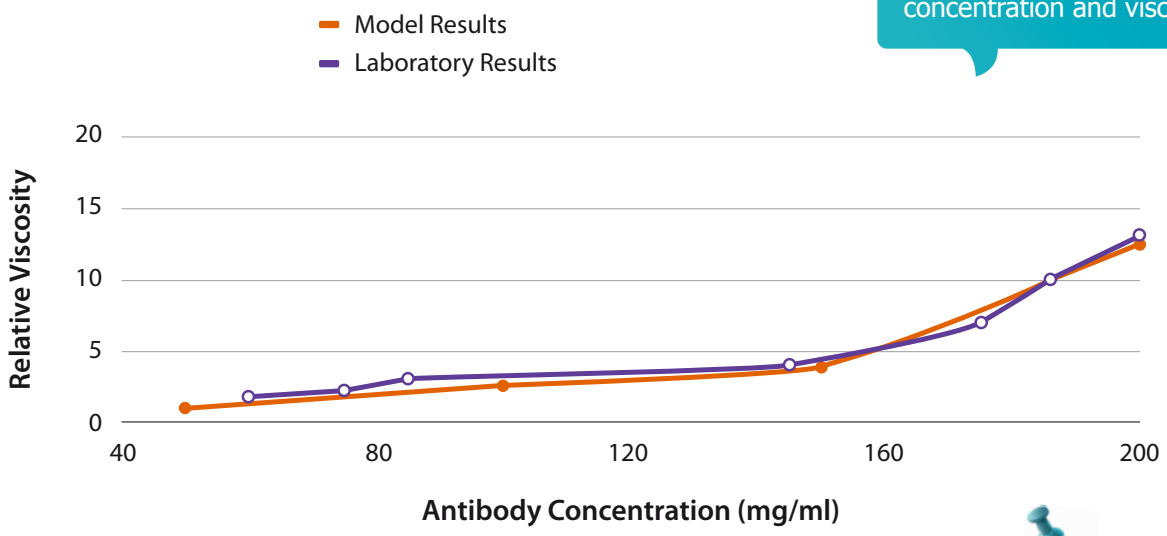


Figure 3: The relationship between antibody concentration and viscosity for Model C compared to laboratory results.

Discussion

We found that we needed to include ions in the solution to make a realistic model. When antibodies form temporary clusters, it can increase viscosity. This happens when areas on the antibodies interact with each other. Our results suggest they do this because of electrostatic interactions with each other and with ions in the solution. Future models should make sure to include both of these interactions.

It is important to continue developing models that align with experiments in the laboratory. This gives scientists a basic framework of the medicine's molecular properties. Then they can add or remove things from the model to see if it changes the viscosity. For example, different interactions or how internally flexible the model is. Only by combining computer simulations and laboratory experiments can researchers understand how medicines behave. Then they can make new ones. Our results suggest that antibody concentrations can change viscosity. Adding other molecules to reduce clustering and using new **solvents** could also make a difference.

If scientists can reduce the viscosity of monoclonal antibody medicines, it will make them cheaper and more accessible. They could be given by syringe instead of intravenously. This means that patients could take the medicine themselves at home. Our molecular model could help scientists figure out how to make this happen. Then more patients could get the life-saving treatments they need.

Conclusion

It is really hard to investigate things that are too small to see. Technological advances like the microscope have let us see into a microscopic world. Computer simulations and models can help us see processes that are too small even for a microscope.

You interact with technology every day. What are some ways that it can help you investigate things you are interested in? How can it help you solve problems in a different way? Just because you can't see something doesn't mean that it has to stay a mystery!

Glossary of Key Terms

Amino acid - building blocks of proteins. There are 22 amino acids that are incorporated into proteins. They each have a different functional group with different binding and electrical properties.

Antibody - a Y-shaped protein produced by white blood cells. They are essential in the immune response. They bind to specific foreign particles to stop them from functioning or for other immune cells to destroy.

Autoimmune disease - a condition where the body's immune system accidentally attacks and destroys its own cells. Examples of autoimmune diseases are arthritis, type 1 diabetes, and lupus.

Coarse-grained model - a simplified model used to simulate a complex system. These types of models are widely used to examine small molecules that are represented by balls or small beads.

Electrostatic interaction - the forces of attraction or repulsion between particles that are electrically charged. These interactions are responsible for helping molecules bond, stay stable, and interact with each other.

Intravenous - administering liquids, nutrients, or medication directly into a person's vein.

Ion - a charged atom or molecule.

Monoclonal antibody - protein made in a lab that mimics a natural antibody. They can be modified to target certain cells, block signals, and attack harmful cells. They are commonly used to treat cancer and autoimmune diseases.

Solution - a liquid containing multiple substances.

Solvent - the major component of a solution that other substances (solutes) are dissolved into.

Viscosity - the resistance of molecules in a fluid to movement. It is caused by friction between layers of fluid molecules when they are moving. It is a property of the fluid as a whole and cannot be applied to individual molecules. Think of it as how sticky a fluid is to itself. For example, water pours very easily and has a lower viscosity than honey, which is highly viscous.

REFERENCES

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World Pharmaceutical Frontiers: The viscosity problem
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Check your understanding

1 What are three things that researchers need to consider when they are designing medicines?

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2 What are antibodies? Why are they important? What makes monoclonal antibodies unique?

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3 Describe the differences among the three models we used. What makes Model C more complex? Why is this an important thing to include in a more realistic model?

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4 A pharmaceutical company is trying to design a lower viscosity formulation of a common cancer treatment. Based on the results of this study, give three recommendations that might help reduce the viscosity of their medicine.

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5 Using computer simulations and models can be powerful tools to study molecular interactions. But they do come with some limitations. Talk with the person next to you. What are three limitations that might come with using computer simulations and models?
