How the Mathematics Behind Molecular Interactions Could Help Streamline Pharmaceutical Development

Science and mathematics are inextricably linked. Often, expertise in one requires experience in the other.

In the case of pharmaceutical development, fundamental mathematical equations underlie even the most complex molecular interactions. By studying the mathematical basis of the relationships between molecules, researchers can predict how changes might affect different reactions between molecules.

Binding Sites

Many pharmaceutical advancements rely on molecular

interactions at binding sites. Macromolecules, such as the proteins that make up much of the human molecular catalog, have binding sites which allow the protein to attach to and interact with another molecule. Molecular binding creates a change within the protein that can cause it—and the cell—to function differently.

In some situations, proteins and other molecules don't bind as they should. This can occur for a number of reasons, but continued binding issues can inhibit normal protein and cell function, leading to disease. For example, if the brain's proteins don't bind correctly with serotonin, neurotransmitters cannot function correctly, often resulting in anxiety and depression. This is just one example; protein binding happens constantly and is a key aspect of many diseases such as cancer and **neurodegenerative disease**.

Remedying Flawed Molecular Interactions

Medications and medicine rely on the binding process to do their job. Therefore, they are tasked with binding to proteins at specific binding sites that lack natural binding opportunities.

Of course, there are many disease mechanisms, but all hinge on faulty molecular interactions.

There are three main criteria for all molecular binding interactions, including:

- Bond strength
- Link rigidity
- Size of linkage array

If one of the above is compromised, it can lead to diseased or disordered cell processes. Luckily, scientists have uncovered ways to change or manipulate these factors to control what occurs between two molecules or predict how **molecular interactions** will change with altered binding.

Experimenting With Binding Properties

Historically, experiments to see how medications bind to a protein were performed primarily in a lab setting. This meant trying different families of chemical compounds until one could properly bind to the protein and then identifying which of several analogous compounds most effectively addressed the disease or disorder at hand.

Now, scientists at the University of Minnesota have developed a computational model that takes some of the guesswork—and time—out of this process. Rather than running back-to-back experiments on hundreds or thousands of compounds, scientists can use a mathematical framework to predict how the molecules might interact. This streamlines the testing process, allowing scientists to make model predictions and then test valid candidates in real-time lab experiments. Though this framework does not eliminate the need for lab experiments by any means, it does allow researchers to change test parameters and develop a better understanding of which molecules will bind effectively to the desired binding sites.

Moving Forward

Researchers hope to use new computational models and mathematical frameworks to create a web-based app accessible to the scientific community. Researchers around the world could utilize these frameworks to test and develop pharmaceutical medications and other types of therapies for many diseases. This could provide huge breakthroughs in treatments for a wide range of conditions such as cancer, autoimmune disease, and neurological diseases.

Sources:

https://www.news-medical.net/news/20200103/Novel-study-on-molecular-interactions-could-make-it-easier-to-develop-new-medicines.aspx (Jan 2020)