Maynor_Black_Masthead.pdf

Solving Enzyme Kinetics using the Lambert (W) Function

Senior Project

In partial fulfillment of the requirements for

The Esther G. Maynor Honors College

University of North Carolina at Pembroke

By

Virginia L. Collins

Criminal Justice

04/28/2023



­­­­­­­­­­­­­\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ \_\_04/28/2023\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_



Virginia Collins Date

Honors College Scholar

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Dr. Siva Mandjiny Date

Faculty Mentor

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Joshua Kalin Busman, Ph.D. Date

Senior Project Coordinator

Acknowledgements

First, I would like to thank Dr. Siva Mandjiny for his support, guidance, and creativity that made this project possible. He gave me a great challenge and it was really interesting to learning new things with this project. I would also like to thank Dr. Joshua Busman and the Honors College for the support and guidance which allowed me to do something outside of my degree that I wanted to learn about. Lastly, I would like like to show my deepest gratitude to Antoinette Collins, because without her support, proofreading, and code-checking, I don’t think I could have done this project, and it wouldn’t have turned out as good as it has.

Abstract

For this project, a computer program was written in C# uses the Lambert W function to calculate enzyme kinetics. The program takes experimental data on enzyme activity and substrate concentration, and outputs the Michaelis-Menten constant and other relevant parameters. This program produces results that can be compared to results obtained using traditional experimental methods. This program provides a fast and accurate alternative to traditional methods for calculating enzyme kinetics and has the potential to be a valuable tool for researchers in biochemistry and related fields.

Solving Enzyme Kinetics using the Lambert (W) Function

In Biochemistry, the field of enzyme kinetics investigates the rates of enzyme-catalyzed reactions as a function of substrate concentration. The Michaelis-Menten equation is one of the most widely used models for calculating enzyme kinetics and how it relates the speed of the reaction to substrate concentration, maximum reaction rate, and Michaelis constant. The Michaelis-Menten equation is:

In this equation, v is the reaction velocity, Vmax is the maximum velocity reached once the enzyme is saturated, Km is the concentration of the substrate once it has reached half its maximum velocity, and [S] is the concentration of the substrate. This formula can be rearranged to be put in the Lambert W Function and find the Km and the Vmax of the substrate concentration and reaction velocity that is entered.

I took on this project because I wanted to learn a little bit about programming because that is what my mother does for a living. I took on a big task doing this project because before this, I had never coded anything more complex than having a robot make a few turns and I knew virtually nothing about C#. I had also learned very little about the Lambert W function, so I didn’t know what I was getting into. It took over a month just for me to learn the basics of programming in C#, and even then, just writing the base code for the program proved very challenging and I made many mistakes. The original program didn’t even run because I didn’t realize I also had to program a place for the code to be executed. I learned about creating front-ends and back-ends which take the main code and tell it what to do.

Programming is a lot more complicated than I was lead to believe while learning C# for over a month. Having a teacher walk you through everything step-by-step makes it seem a lot easier than it is. When I actually sat down, after over a month of spending at least 25 hours a week just learning to code in one programming language, I still felt extremely lost. I started by doing just the math necessary to actually create the program, but then actually turning the math into a program seemed way harder than it needed to be.

I eventually got what I thought was all I needed to create the program after struggling to write this small section of code, I then discovered I needed to code a place for the program to be executed in and instructions to tell the code how to run. This took way longer than I thought I would need to spend on this project, but it was all worth it.

In this program, you put in a file with your numbers for your substrate concentrations and your initial velocities. You must have at least two points for each at different concentrations for the program to run. When you run the program with those numbers, it will give you your Vmax and Km values. It is very easy to run and works almost like an online calculator. It will give you a new file that will open in Excel with all the values. This way, if you later want to do more with the data the program calculated, you can because it’s already in an Excel file and you don’t have to move the data again.

The main code is the math behind the project. It is the main part of the project that tells the program what to do. This is built in the source code section of the program.Text

Description automatically generated

Figure : Main Code- SeniorProject.cs

Text

Description automatically generated

Figure : Second half of the main code-SeniorProject.cs

The second part of the code is written on a separate window where the interface for the program was built. The purpose of this window is to create a place for the user to interact with. The way I did this was to create text boxes and put words in some, but leave some blank for the user to enter their own information. This was one of the quickest sections to do but getting the interface to look exactly like you want it can be hard.

Graphical user interface, application

Description automatically generated

Figure : MainWindow.xaml

The next part of the code is the code which is behind the main window which the user interacts with. This code is used to work together with the main code in SeniorProject.cs and provide support for the MainWindow.xaml section of the code. Having all these sections makes the code more readable and manageable for the average programmer.

Text

Description automatically generated

Figure : MainWindow.xaml.cs

Text

Description automatically generated

Figure : Second half of MainWindow.xaml.cs

This project was really fun in some ways but also really frustrating in others. Some of the most frustrating parts came from trying to understand what the Lambert W function was and how to use it because I am not very good at math and the Lambert W function is fairly complex math. I eventually came to understand the Lambert W function and what it is used for but it took me a few hours of doing some practice problems and watching some videos to understand what it was for. I also spent quite a few hours in Dr. Mandjiny’s office asking about the Lambert W function and how it worked. Another part of frustration came from the code itself because it took many attempts to get this code to properly work. It would throw up error codes at every turn and everything had to be precisely punctuated and capitalized or it would not execute properly. This really frustrated me and lead me to realize that while programming is a very interesting topic it is not something I want to further explore past this project. I did enjoy learning something new and now have a new skillset, if ever I need to know how to program in C#.

References

1. Golicnik, M. Explicit reformulations of time-dependent solution for a Michalis-Menten enzyme reaction model. Analytical Biochemistry 2010, 406, 94-96.
2. Microsoft. (n.d.). C# Fundamentals for Absolute Beginners. Microsoft Learn. https://learn.microsoft.com/en-us/shows/csharp-fundamentals-for-absolute-beginners/
3. Her, Cheenou; Alonzo, Aaron P.; Vang, Justin Y.; Torres, Ernesto; Krishnan, V.V. Real-Time Enzyme Kinetics by Quantitative NMR Spectroscopy and Determination of the Michalis-Menten Constant Using the Lambert-W Function. *J. Chem. Educ.* 2015, 92, 1943 – 1948.
4. Gouge, Melissa, "Using the Lambert Function to Map Enzyme Kinetics" (2021). ONU Student Research Colloquium. 19. https://digitalcommons.onu.edu/student\_research\_colloquium/2021/posters/19
5. Michaelis-Menten and the Lambert W function. Michaelis-menten and the Lambert W function. (n.d.). Retrieved April 28, 2023, from https://cran.r-project.org/web/packages/renz/vignettes/Lambert.html
6. Goličnik, M. (2012). On the Lambert W function and its utility in biochemical kinetics. Biochemical engineering journal, 63, 116-123.
7. Mandjiny, S. (2021, September 27). Lambert W Function.