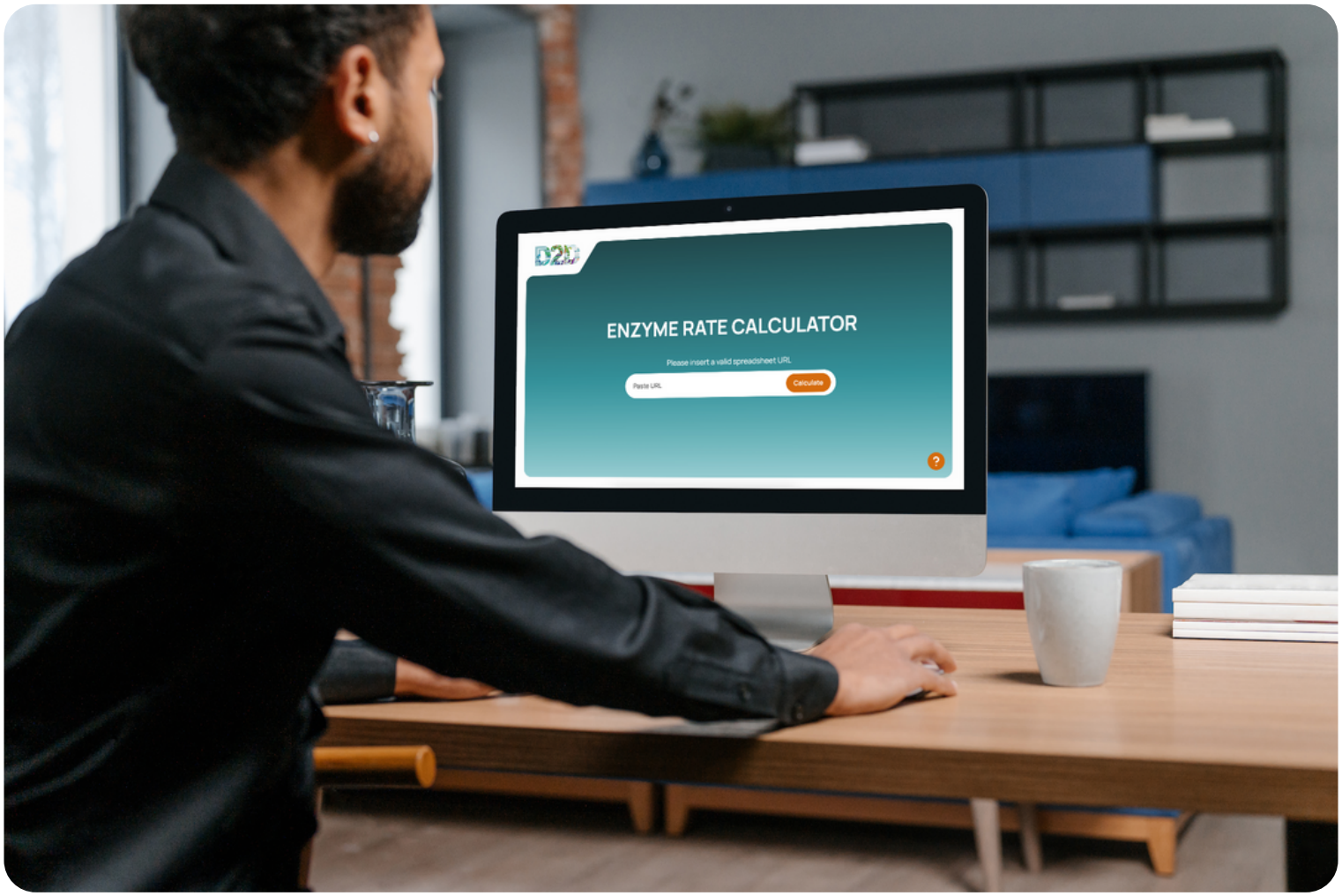


USER MANUAL

Enzyme Rate Calculator

INDEX

INTRODUCTION

The **D2D initiative seeks** to improve enzyme research by acquiring accurate kinetic and thermal stability data for previously unexamined mutant enzymes. The challenge lies in researchers manually calculating enzyme activity rates, particularly when spectrophotometers lack specialized software.

The underlying scientific goal of D2D is to facilitate academic crowd-sourcing to rapidly address protein design questions that would normally take isolated labs decades to answer.

CALCULATIONS

RATE CALCULATIONS

In each substrate trial, a comprehensive set of 18 data points is gathered, captured at one-minute intervals ranging from 0 to 17 minutes. The determination of the maximal rate involves the analysis of three consecutive data points, wherein the slope is derived through the application of the **least squares regression.**

To illustrate, consider a trial conducted for a specific substrate, and let's walk through the procedural steps involved in this process.

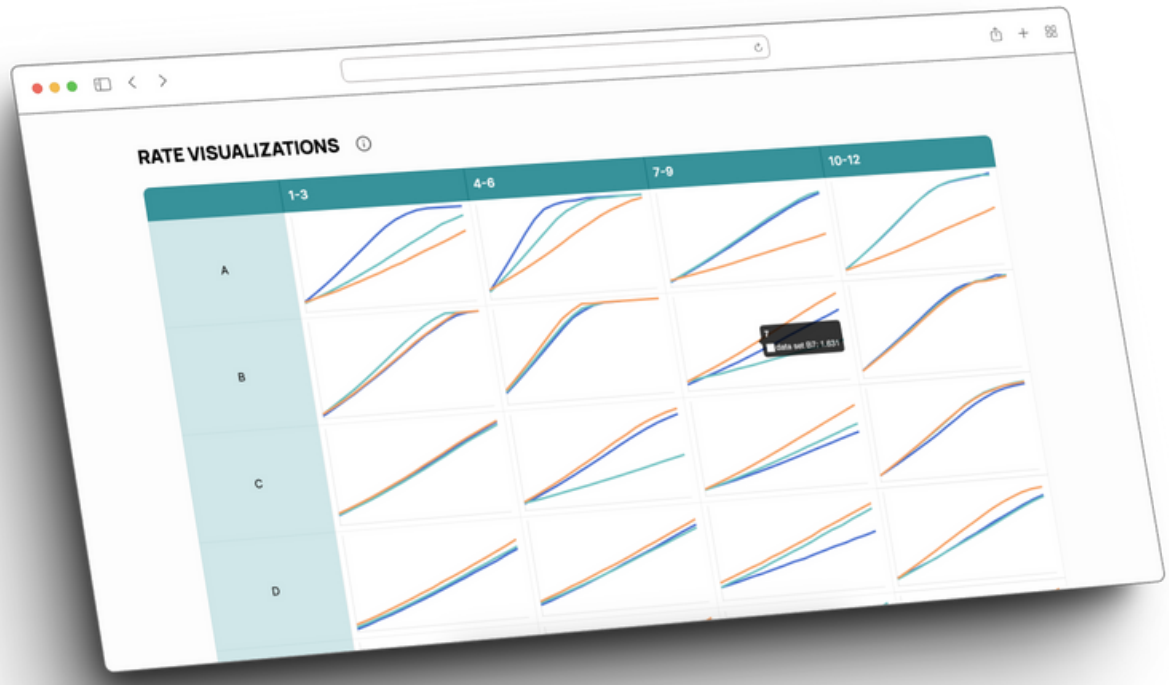
Fig	A1
0:00:00	0.049
0:01:00	0.05
0:02:00	0.05
0:03:00	0.051
0:04:00	0.052
0:05:00	0.052
0:06:00	0.053
0:07:00	0.054
0:08:00	0.055
0:09:00	0.056
0:10:00	0.057
0:11:00	0.058
0:12:00	0.059
0:13:00	0.06
0:14:00	0.061
0:15:00	0.062
0:16:00	0.063
0:17:00	0.064

- The initial set of three data points consists of timestamps [0 minutes, 1 minute, 2 minutes], and the slope is determined from the coordinates [(0, 0.049), (1, 0.05), (2, 0.05)], where x represents the minutes, and y signifies the substrate quantity.

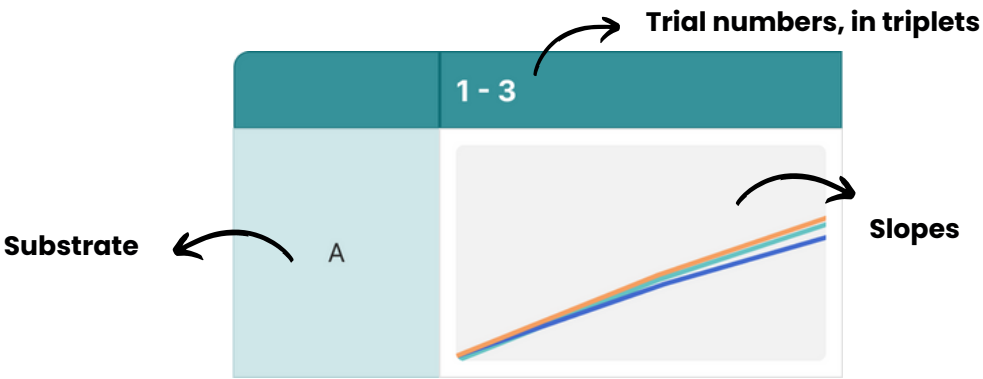
- Subsequently, the analysis continues with the next three consecutive data points [(1, 0.05), (2, 0.05), (3, 0.051)], and this sequential process repeats. The same methodology is applied until the slope is computed for the final set of three consecutive points [(15, 0.062), (16, 0.063), (17, 0.063)].

- The highest calculated slope throughout these iterations is identified as the maximal rate and is then documented and presented in the reaction rate data table.

RATE GRAPHS

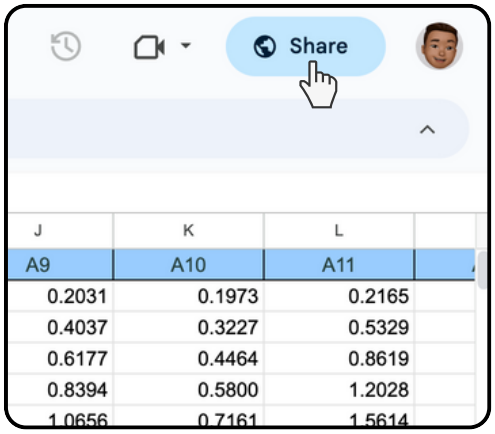


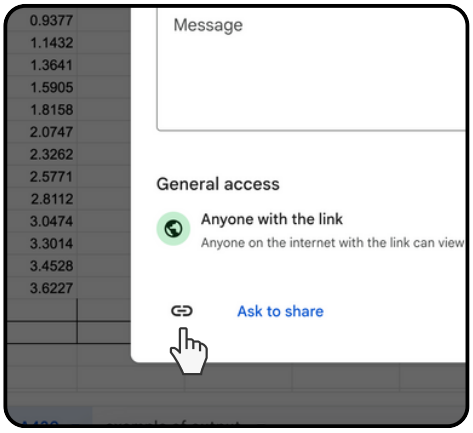
Every graph showcases data from three trials conducted on the same substrate, each identified by its corresponding row and column. Each graph is a standalone React component created using the Charts.js package, and these components are encapsulated within a table component.



TUTORIAL

Finding the URL



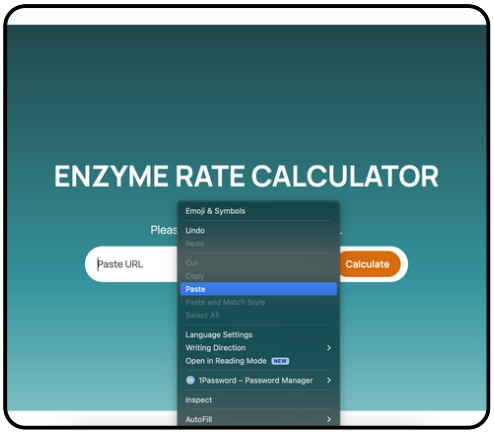


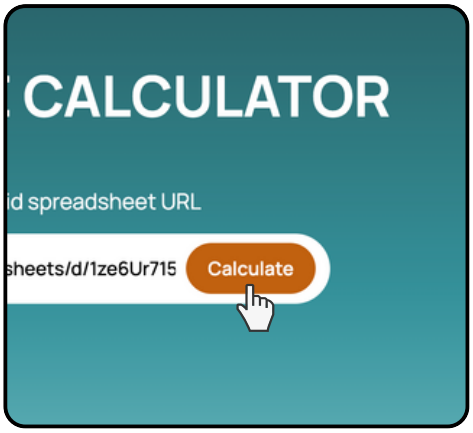
Step 1 – Open the file and click Share.

Step 2 – Click Copy link/ link icon

⚠ Adjust the Access settings to "people with the link" before copying the link

Calculating the rates

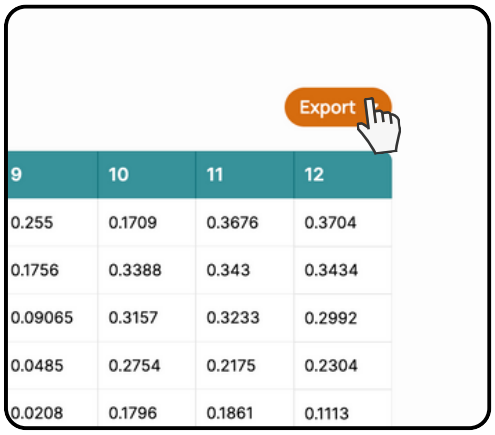


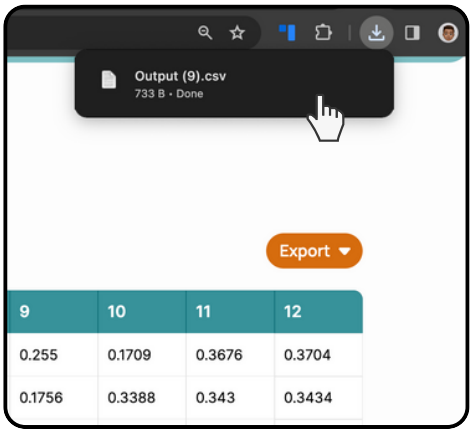


Step 1 – Paste the Copied URL

Step 2 – Click Calculate

Export rate table

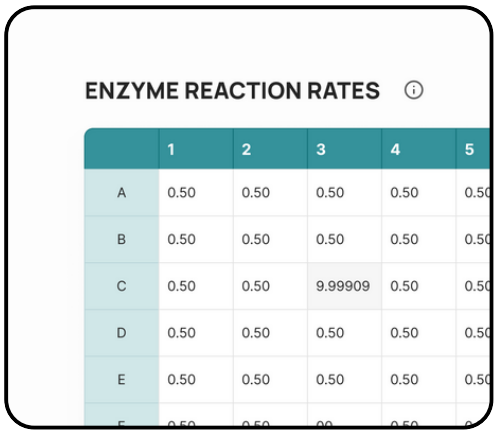


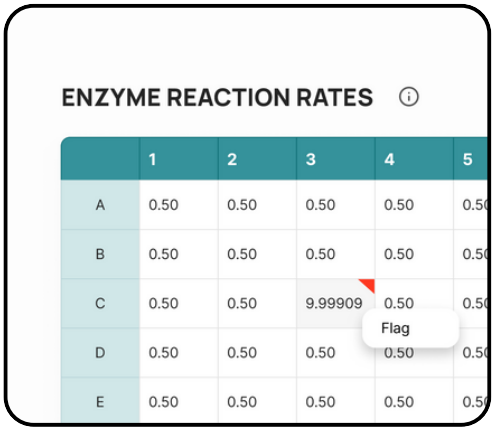


Step 1 – Click the export button to export the calculated rate table .

Step 2 – A .csv file should have downloaded.

Flag Data

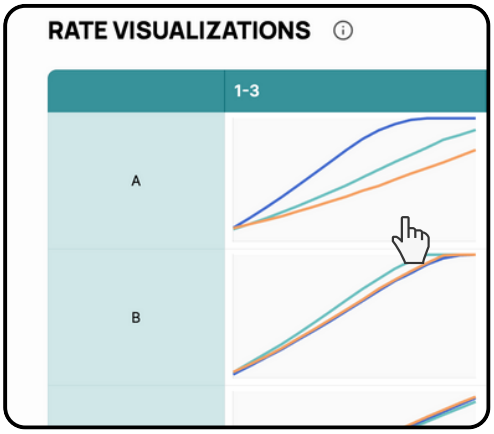




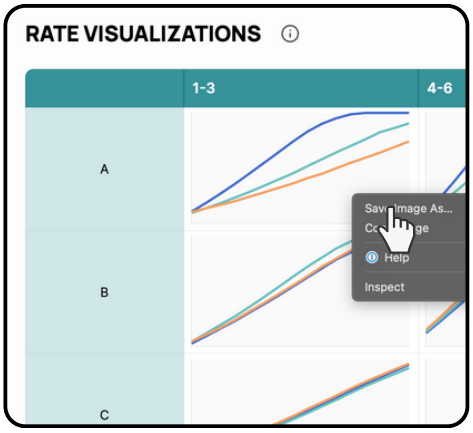
Step 1 – Right click on any outlier data on the Reaction rate Table

Step 2 – Click on Flag. *This will mark/flag the data that you selected*

Export Graph



Step 1 – Right click on any graph on the RATE VISUALIZATION Table



Step 2 – Click on *Save Image as,* This will download the individul graph

ABOUT THE TEAM

About the Team

CodeLab is a software and design agency at UC Davis, working on real-world projects in an industry-like environment.

The Aim of this project was to develop an application that automates the calculation of enzyme activity rates & user-friendly options for visualizing readings through graphs to streamline data analysis experience. Learn more about the journey here

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