

# USER MANUAL

## Enzyme Rate Calculator

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# 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

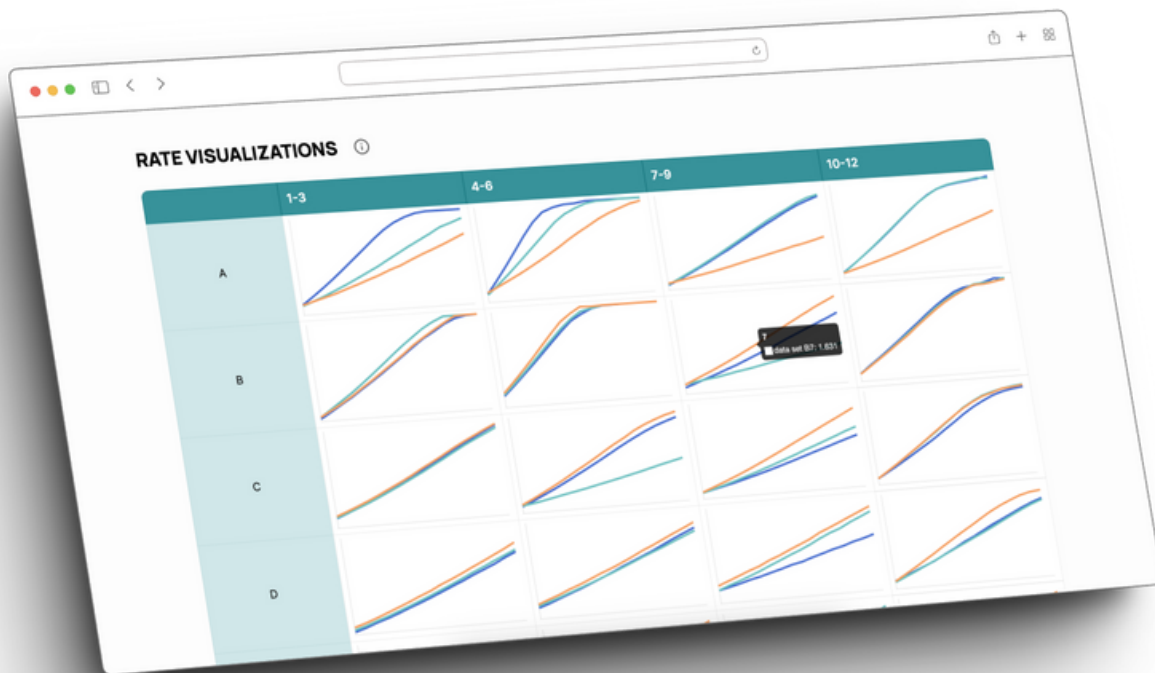
In each substrate trial, a comprehensive set of 18 data points is gathered, captured at one-minute intervals ranging from 0 to 17 minutes. The determination of the maximal rate involves the analysis of three consecutive data points, wherein the slope is derived through the application of the **least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

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

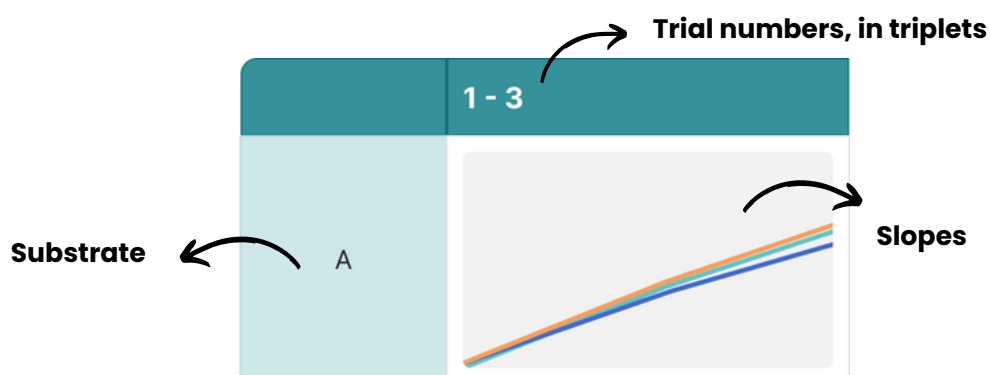
Fig	A1
0:00:00	0.049
0:01:00	0.05
0:02:00	0.05
0:03:00	0.051
0:04:00	0.052
0:05:00	0.052
0:06:00	0.053
0:07:00	0.054
0:08:00	0.055
0:09:00	0.056
0:10:00	0.057
0:11:00	0.058
0:12:00	0.059
0:13:00	0.06
0:14:00	0.061
0:15:00	0.062
0:16:00	0.063
0:17:00	0.064

- 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.

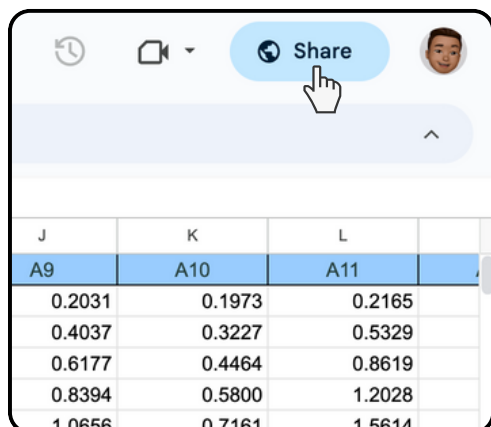


# TUTORIAL

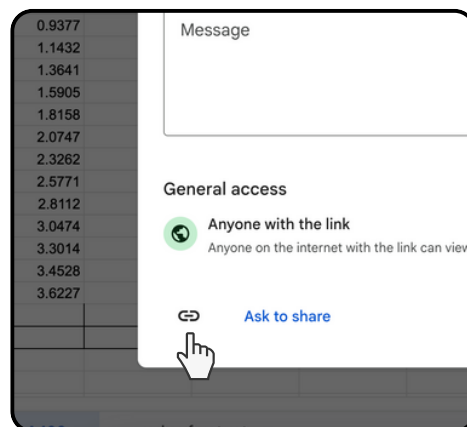




# Finding the URL



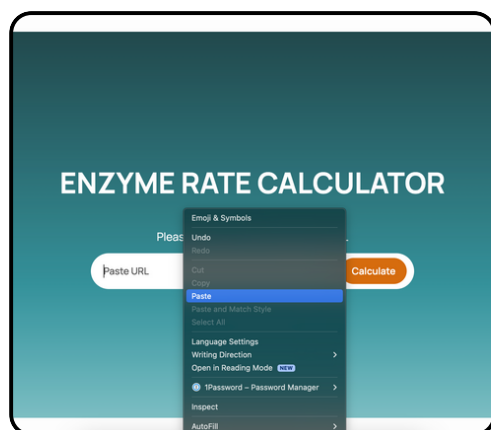
**Step 1** - Open the file and click Share.



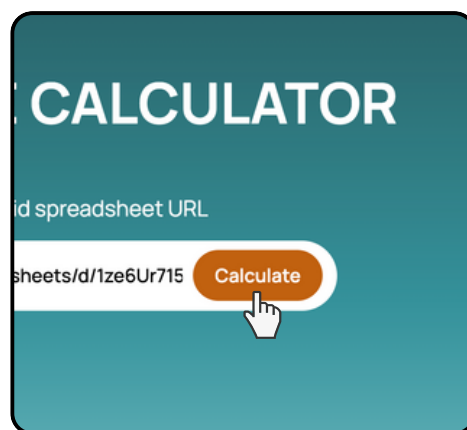
**Step 2** - Click Copy link/ link icon

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

# Calculating the rates

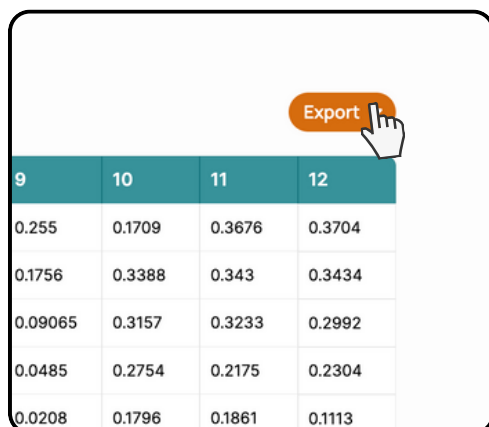


**Step 1** - Paste the Copied URL



**Step 2** - Click Calculate

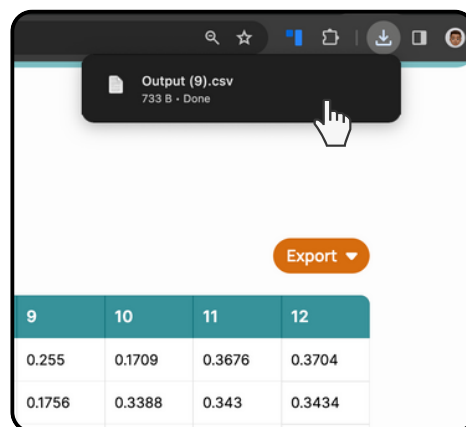
# Export rate table



A screenshot of a web application showing a table with 4 columns (9, 10, 11, 12) and 6 rows of numerical data. An orange 'Export' button is located at the top right of the table, and a hand cursor is clicking on it.

9	10	11	12
0.255	0.1709	0.3676	0.3704
0.1756	0.3388	0.343	0.3434
0.09065	0.3157	0.3233	0.2992
0.0485	0.2754	0.2175	0.2304
0.0208	0.1796	0.1861	0.1113

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

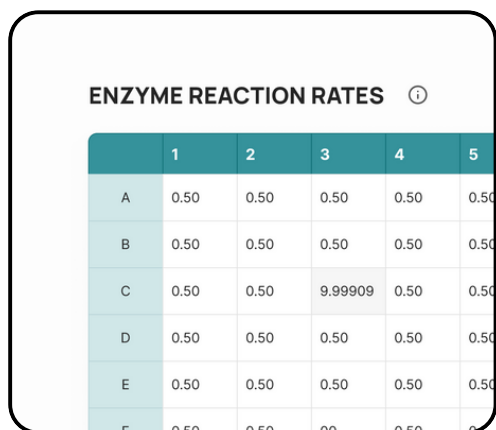


A screenshot of a web browser window. A dark notification box at the top says 'Output (9).csv' and '733 B · Done'. Below the table, an orange 'Export' button with a dropdown arrow is visible. The table data is partially visible.

9	10	11	12
0.255	0.1709	0.3676	0.3704
0.1756	0.3388	0.343	0.3434

**Step 2** – A .csv file should have downloaded.

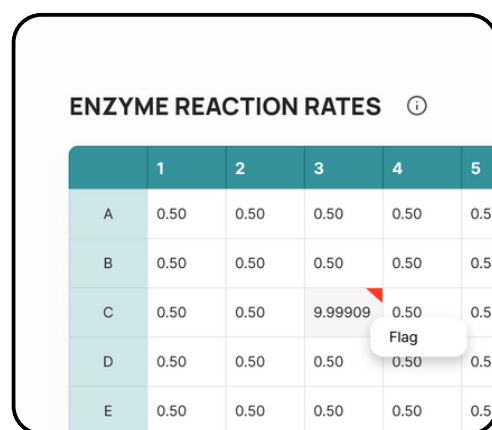
# Flag Data



A screenshot of a web application showing a table titled 'ENZYME REACTION RATES'. The table has 6 rows (A-F) and 6 columns (1-5). A hand cursor is hovering over the cell containing '9.99909' in row C, column 3.

	1	2	3	4	5
A	0.50	0.50	0.50	0.50	0.50
B	0.50	0.50	0.50	0.50	0.50
C	0.50	0.50	9.99909	0.50	0.50
D	0.50	0.50	0.50	0.50	0.50
E	0.50	0.50	0.50	0.50	0.50
F	0.50	0.50	0.50	0.50	0.50

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

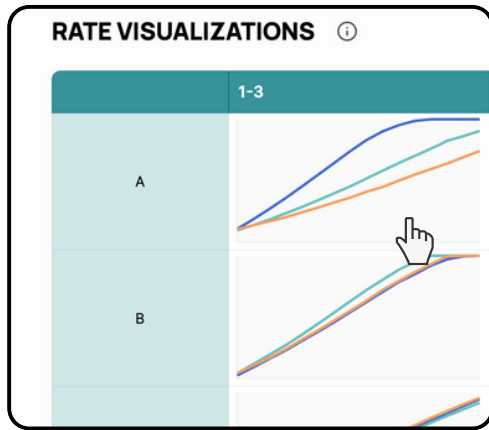


A screenshot of the same web application showing the 'ENZYME REACTION RATES' table. A red tooltip with the word 'Flag' is now visible over the cell containing '9.99909' in row C, column 3.

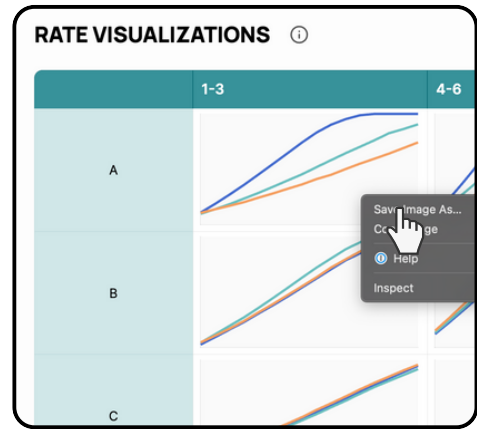
	1	2	3	4	5
A	0.50	0.50	0.50	0.50	0.50
B	0.50	0.50	0.50	0.50	0.50
C	0.50	0.50	9.99909	0.50	0.50
D	0.50	0.50	0.50	0.50	0.50
E	0.50	0.50	0.50	0.50	0.50
F	0.50	0.50	0.50	0.50	0.50

**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 individual graph

# ABOUT THE TEAM

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# 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](#)

# CONTACT



# Contact us

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