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Data Article

Calculation of statistic estimates of kinetic parameters from substrate uncompetitive inhibition equation using the median method

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ABSTRACT

We provide initial rate data from enzymatic reaction experiments and tis processing to estimate the kinetic parameters from the substrate uncompetitive inhibition equation using the median method published by Eisenthal and Cornish-Bowden (Cornish-Bowden and Eisenthal, 1974; Eisenthal and Cornish-Bowden, 1974). The method was denominated the direct linear plot and consists in the calculation of the median from a dataset of kinetic parameters V_{max} and K_m from the Michaelis–Menten equation. In this opportunity we present the procedure to applicate the direct linear plot to the substrate uncompetitive inhibition equation; a three-parameter equation. The median method is characterized for its robustness and its insensibility to outlier. The calculations are presented in an Excel datasheet and a computational algorithm was developed in the free software Python. The kinetic parameters of the substrate uncompetitive inhibition equation V_{max}, K_m and K_s were calculated using three experimental points from the dataset formed by 13 experimental points. All the 286 combinations were calculated. The dataset of kinetic parameters resulting from this combinatorial was used to calculate the

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median which corresponds to the statistic estimator of the real kinetic parameters. A comparative statistical analyses between the median method and the least squares was published in Valencia et al. [3].

Specifications Table

Subject area	*Biochemistry*
More specific subject area	*Enzyme kinetics*
Type of data	*Tables, text file, graph, figure*
How data was acquired	*Simulated data of initial reaction rate*
Data format	*Raw and analyzed output data*
Experimental factors	
Experimental features	*Initial reaction rates were generated using the substrate uncompetitive inhibition equation with real values $V_{max} = 1$, $K_m = 1$ and $K_s = 100$ and relative error from a normal distribution with standard deviation of 0.5*
Data source location	
Data accessibility	*Data is with this article*

Value of the data

- The data and calculations involved in the application of the direct linear plot to a three-parameter equation were described.
- The data arisen from this application was explicitly exposed and procedures explained.
- The data allows to visualize the advantages of the direct linear plot when applied to complex equations.
- Datasheets and algorithms can be used to generate new data and analysis to compare the direct linear plot with other estimation methods.

1. Data description

The raw data consists in initial rates from enzymatic reaction considering the substrate uncompetitive inhibition equation. This data was generated through simulation of the initial rate calculated from the substrate uncompetitive inhibition equation adding a relative error from a normal distribution with standard deviation 0.5. The analyzed data was a list of kinetic parameters V_{max}, K_m and K_s obtained using the direct linear plot method [1,2]. The resulting data was the statistic estimators of V_{max}, K_m and K_s calculated from the median of the previous list.