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MODELLING MODIFIERS OF ENZYME ACTIVITY

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Modification of enzyme activity can be rationalized through a few simple assumptions: Each enzyme has a specific turnover rate (k_{cat1}) and affinity for its substrate (K_{M1}); When an enzyme is bound by a modifier, its specific turnover rate and/or affinity for its substrate are altered resulting in new values (k_{cat2}, K_{M2}).When looking at a population of enzymes experimentally (E), the observed enzymatic turnover rate and/or affinity of the enzyme for its substrate relies on the fraction of the total population associated with the modifier (X). For example, if [E]tot=[E] the enzyme population express k_{cat1} and K_{M1}, if [E]tot=[EX] the enzyme population express the modifier induced k_{cat2} and K_{M2} and if there is a mixture such as [E]tot= 50%[E] + 50%[EX] then the enzyme population would express a turnover rate and/or affinity for its substrate halfway between the two states (i.e. K_{M1}-(50%(K_{M1}-K_{M2}) or Vmax1-(50%(V_{max1}-V_{max2})). In this case, Vmax replaces kcat as in the Michaelis-Menten equation Vmax is the product of enzyme concentration and kcat. By relating the fraction of the enzyme population bound by the modifier to the modifiers binding constant (K_x) a simple expression that can describe activation or inhibition is defined.

$$v = \frac{[S]}{[S] + K_{M1} - (K_{M1} - K_{M2})\frac{[X]}{[X] + K_x}} V_{max1} - (V_{max1} - V_{max2})\frac{[X]}{[X] + K_x}$$

Here the utility of this expression will be examined by globally fitting the equation to real and simulated data and its ability to model data will be compared to more traditional methods of modeling modifiers of enzymatic activity.

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