Enzyme Kinetics

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1 Background Biology

Enzymes are biological molecules responsible for increasing reaction rates in living organisms as well as in other applications(such as washing powders). Enzymes require a substrate molecule that will bind forming an enzyme-substrate complex (from here referred to as a complex). This complex can result in a product if a particular reaction takes place. However not all complexes formed will result in product formation, sometimes the substrate will disassociate allowing it to bind to another free enzyme. We can write this as a series of three reactions.

$$S + E \xrightarrow{k_1} C$$
$$C \xrightarrow{k_{-1}} S + E$$
$$C \xrightarrow{k_2} P + E$$

Here S is the substrate, E enzyme, C complex and P represents product. The values k_1, k_{-1} and k_2 represent the rate at which each reaction occurs. The first equation represent the formation of a enzyme-substrate complex. The second describes the disassociation of a complex whilst the third the product formation. In our example we are assuming that the enzyme is reusable after product formation.

The file *"Enzyme Kinetics.py"* runs what is known as a Gillespie simulation for the above reaction, a method you may use in your project(the theory behind this simulation is something you might cover later). Essentially we assign each reaction a probability constructed from the rate of a given reaction, divided by the total sum of all rates. Then using a randomly generated number between 0 and 1 pick the reaction that is occurring. This adds an element of randomness to the simulation known as a stochastic simulation.

Currently the code given runs a single simulation for the initial population $(1000, 100, 0, 0) = (S, E, C, P)$ but here are a few small tasks that could be undertaken by adapting the code.

1. Adjust the code to run four simulations instead of a single one.
2. For each molecule, plot the result of these simulations on one figure against time t.
3. Change the initial population and see how the figures are altered.
4. Run a higher number simulations (100+) and plot the mean values.