Title: Study of the macromolecular crowding effect on enzymatic reaction

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In a prokaryote cell-like E. Coli, we can find many macromolecular types that occupy approximately 40 % of total volume acting as a hindrance between two elements that react, these elements are substrate and enzyme. The rate constant value for the reaction expected can be calculated previously, but after terminated the reaction inside a period, we can see that there is a considerable deviation between the rate constant calculated and previously predicted.

This is the experimental subject carried on this project, we can reproduce something similar to an intracellular environment with a computer program, using a Monte Carlo method to gather all useful data used sadistically to calculate the rate constant for the reaction.

In this program, we put all the elements involved in these simulations in special mention the hindrance, that will be the main protagonist almost in all simulations, to verify the "crowding effect". This effect is attributed due to the hindrance that collides with substrate and enzymes before reacting to each other, at naked eye we can think that a hindrance between these two elements makes the rate constant for the reaction decrease but the simulation results says completely the opposite.

All simulations performed in this project are done by a computer program performed with "Fortran 90" a better version than "Fortran 77", and the posterior rate constant fitting through all results recollected with Python (another computer language).