EVB simulations of the reaction catalyzed by cytidine deaminase

Popular science summary

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Enzymes are functional units of cells. Many reactions occur very slowly without any catalysis. Enzymes increase the rate of these reactions to make sure they happen with an appreciable rate in the cells. Regarding the vital role of enzymes in biological processes, having an in depth information about their catalytic mechanism at atomic level is important. Unfortunately, not all of this information can be acquired via experimental approaches due to the practical limitations. Therefore, theoretical and computational methods are applied to the questions that could not directly be answered by experiments. In these approaches the enzymes are described either by classical mechanics or quantum mechanics and through computer simulations the catalytic mechanism and the role of different functional groups is determined. This information further could be used for drug discovery, enzyme optimization and many other purposes.

In this project we tried to create such a model of cytidine deaminase from *E.coli* which catalyzes the hydrolytic deamination of cytidine. This enzyme plays a major role in pyridine salvaging. Moreover, cytidine deaminase is extremely interesting in term of understanding the thermodynamic basis of catalysis due to large body of available experiential data. To simulate the reaction, the empirical valence bond method was used in which the system is described using classical mechanics definition and the simulation is parametrized to quantum mechanics calculations. We were able to reproduce the experimental information with an acceptable error.

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