

Modeling of enzymatic organophosphate hydrolysis: towards design of new biocatalysts

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Some organophosphate pesticides tend to accumulate in aquatic environment and their decontamination belongs now to urgent research tasks. Enzymatic biodegradation seems to be one of the most promising options, but none of known enzymes existing in nature are sufficiently useful for this purpose, so new mutated variants started to be subject patent applications [1] and even theoretical design [2]. However, the catalytic activity of recently designed enzyme [2] could be considerably improved via directed evolution and the role of additional mutations is not completely understood. In order to explore the catalytic activity detailed molecular mechanism of diethyl-7-hydroxycoumarynyl phosphate hydrolysis by modified adenosine deaminase [2] has been modeled within ONIOM approach. Reactant interactions with active site residues have been analyzed using ab initio and atomic multipole approximation in order to interpret observed catalytic activity changes resulting from aminoacid mutations. In addition the utility of atomic multipole expansion in exploring relative stabilities of interacting biomolecules will be also discussed [3]

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Literature

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