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In silico Model of Transamination Reaction Mechanism

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Abstract : w-Transaminase (w-TA) is broadly used for synthesizing chiral amines with a high enantiopurity. However, the reaction mechanism of w-TA has been not well studied, contrary to a-transaminase (a-TA) such as AspTA. Here, we propose in silico model on the reaction mechanism of w-TA. Based on the modeling results which showed large free energy gaps between external aldimine and quinonoid on deamination (or ketimine and quinonoid on amination), withdrawal of Ca-H seemed as a critical step which determines the reaction rate on both amination and deamination reactions, which is consistent with previous researches. Hyperconjugation was also observed in both external aldimine and ketimine which weakens Ca-H bond to elevate Ca-H abstraction.

Keywords : computational modeling, reaction intermediates, w-transaminase, in silico model
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