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Conformational transitions of uracil transporter-UraA from *Escherichia coli*: A molecular simulation study

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The nucleobase:cation symporter 2 (NCS2) family proteins affects several crucial processes such as the uptake of nucleobases and transport of vitamin C in most living organisms on Earth. uracil transporter (UraA) from the *Escherichia coli*, known as the representative NCS2 protein, catalyzes symport of a uracil and an H+ ion via an alternating access mechanism. The experimental results shows that protonation state changes of some key amino acid residues can regulate conformational changes of UraA, but the details and process of conformational transitions are unknown during uracil transport. We studied the different effects of protonation states of Glu241, Glu290 and His245 on UraA conformational transitions using molecular simulations. We observed that, inward-open conformation reverts to the outward-open conformation of UraA in DDP+L (Glu241 and Glu290 deprotonation, His245 protonation, substrate exits) and DDP-L (Glu241 and Glu290 deprotonation, His245 protonation, no substrate exits). The results show that the presence of proton in the His245 directly restricts the motion of gate domain and further changes motion modes between core domain and gate domain. Therefore, we propose a new transport model for UraA.

Biography

Xi Zhao obtained his PhD in 2007 from Jilin University and was a Visiting Scholar from University of California Irvine, Department of Chemistry. Now he is Associate Professor at Institute of Theoretical Chemistry, Jilin University. His research focuses on biomolecular simulation. He has published more than 25 papers in reputed journals.

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