

Investigations of takeout proteins' ligand binding and release mechanism using molecular dynamics simulation

Xu-Ri Huang and **Xi Zhao**
Jilin University, P R China

Takeout (To) proteins exist in a diverse range of insect species and are involved in many important processes of insect physiology and behaviours. As ligand carriers, To proteins can also transport the small molecule to the target tissues. However, ligand release mechanism of To proteins is unclear. In this contribution, the process and pathway of the ligand binding and release are revealed by conventional molecular dynamics simulation, steered molecular dynamics simulation and umbrella sampling methods. Our results show that the α 4-side of the protein is the unique gate for the ligand binding and release. The structural analysis confirms that the internal cavity of the protein has high rigidity, which is in accordance with the recent experimental results. By using the potential of mean force (PMF) calculations in combination with residue cross correlation calculation, we concluded that the binding between the ligand and To proteins is a process of conformational selection. Furthermore, the conformational changes of To proteins and the hydrophobic interactions between ligand and protein internal cavity can both be key factors for ligand binding and release.

Biography

Xu-Ri Huang has completed his PhD in 1991 from Jilin University. Now, he is a Professor of Institute of Theoretical Chemistry, Jilin University. His research focuses on theoretical chemistry, such as catalysis reaction mechanism and biomolecular simulation. He has published more than 150 papers in reputed journals.

huangxr@jlu.edu.cn

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