KP05

Multi-stage docking simulation… Fast Poisson-Boltzmann solver and re-ranking methods

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Multi-stage docking simulation is a compromise between cost and accuracy to find novel ligand molecules for target proteins. Conventional docking software such as Dock, FlexX, Adam&Eve, Gold, etc represents the first stage, and the full-atom simulations by Amber etc represent the last stage. As a mid-stage, we adopted implicit solvent model with solvation effect incorporated with Poisson Boltzmann (PB) methods. Because PB solver is very CPU intensive, we have developed a fast PB solver without recourse to the generalized Born approximation. To supplement some deficiency in PB methods, we have also developed an efficient Re-scoring method. Multi-stage simulation result obtained for DNA gyrase inhibitors and randomly selected compounds is promising.