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Molecular Simulations in Biomedicine – The Value of Free Runs

Nishizawa K*
School of Medical Technology, Teikyo University, Japan

Editorial

In the era of the coronavirus pandemic, many supercomputing resources are devoted to simulations targeted for drug development as well as characterization of virus particle dynamics. Such a situation would remind many computational biochemists of the question of how to prioritize the computational tasks in biomedicine. For academic institutions with relatively low economic resources, cloud computing may help to reduce the cost. Nonetheless, the cost of electricity for computation should be of universal concern.

On the other hand, there seems to be a growing need for computational analyses among experimental biophysicists and biochemists eager to know the atomistic basis for physiological phenomena. However, collaborations which initially look promising often turn out to be too costly after some consideration. The cost in this context seems to connote the overall contribution integrating the economic cost and the insights obtainable from the simulations. In this sense, this is a biomedical issue.

Recent improvements in force fields have made atomistic molecular dynamic (MD) simulations a useful tool in biomedicine. Protein-ligand interactions are of particular importance in this area, and innovative methods for enhanced sampling and meta-dynamics-based derivation of free energy profile have made such analyses much easier than ever before. However, slow diffusion of molecules often imposes a burden. For the systems containing a biomembrane, viscosity of lipids further slows sampling, often hampering meaningful simulations of ion channels or membrane receptors and their ligands. How can we proceed with such slow systems?

My honest view is that accuracy and precision required in biomedicine-oriented computational studies may not be the same as those required in typical physicochemical studies, in which the derivation of the free energy profiles is prioritized for rigorous discussion. From our experience, free MD runs (or metadynamics runs with a simple biasing potential) to search stable configurations/conformations often benefit. An ensemble of free runs with different initial positions and structures, even those less intensive (10-20%) relative to free energy computations, can provide insights into the dynamics of protein-ligand interactions and help us design (and simplify) subsequent free energy computations. Given the limited computational resources, making the most of free runs may become a new standard.

***Corresponding author:** Kazuhisa Nishizawa, MD PhD, School of Medical Technology, Teikyo University, Itabashi, Tokyo, Japan; kazunet@med.teikyo-u.ac.jp

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