BROMOCEA code: An Improved Grand Canonical Monte Carlo/Brownian Dynamics Algorithm Including Explicit Atoms

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All-atom molecular dynamics (MD) simulations have a long history of applications studying ion and substrate permeation across biological and artificial pores. While offering unprecedented insights into the underpinning transport processes, MD simulations are limited in time-scales and ability to simulate physiological membrane potentials or asymmetric salt solutions and require substantial computational power. While several approaches to circumvent all of these limitations were developed, Brownian dynamics (BD) simulations remain an attractive option to the field. The main limitation, however, is an apparent lack of protein flexibility important for the accurate description of permeation events. In the present contribution, we report an extension of the BD scheme which includes conformational dynamics. To achieve this goal, the dynamics of amino-acid residues was incorporated into the many-body potential of mean force and into the Langevin equations of motion. The developed software solution, called BROMOCEA, was applied to ion transport and substrate translocation through the OmpC porin. The present tests strongly indicate that the inclusion of pore flexibility enhances permeation properties.

References

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