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FREE ENERGY CALCULATION FOR GRAMICIDIN A (GA) CHANNEL WITH NO EQUILIBRIUM REQUIREMENT

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Abstract: Today, the most important reason of the work with molecular dynamics simulation method of biomolecular systems is to ensure understanding physical mechanism and dynamic properties that is not readily accessible to experimental methods. Gramicidin channels (Figure 1) are bacterial channels with radius of approximately 2 Å. The channel is a simple test system for controlling the accuracy of the method of free energy and force field because of the simple structure. In addition, theoretical calculations of free energy that called Crooks fluctuation theorem for non-equilibrium systems are available at literature. In this study, primarily, free energy calculation methods that do not require equilibrium state were developed for complex systems and compared with the free energy simulation work in equilibrium condition. Finally the validity of the method was tested for the GA channels.

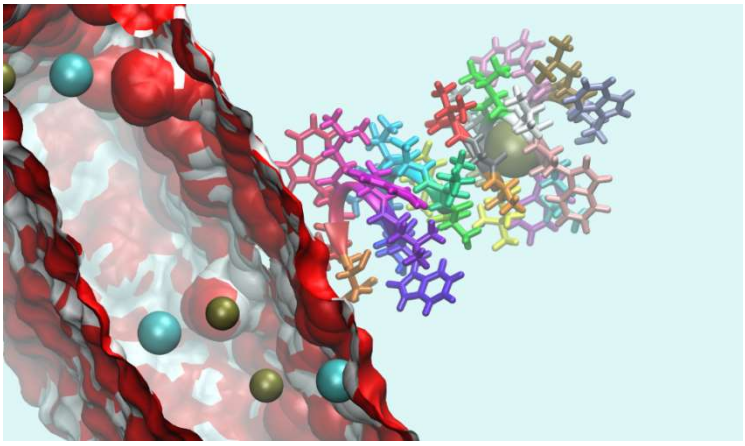

Figure 1: Gramicidin A Channel

Keywords: *Gramicidin A Channel; Crooks Fluctuation Theorem; Non-equilibrium Systems*

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