P-2.181

Exploring F-atpase Dynamics Via Mc/md Simulations

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FOF1 ATPase is a molecular motor that synthesizes ATP by utilizing the proton gradient across the membrane, playing a central role in cellular energy production. It consists of FO motor, which rotates in response to proton transport, and F1 motor, which uses this rotational motion to synthesize ATP. Here, we developed a hybrid Monte Carlo (MC) and Molecular Dynamics (MD) simulation system focusing on proton translocation within FO motor, a process that is difficult to observe directly in experiments. Using this system, we thoroughly analyzed the relationship between proton transport and rotational motion of FO motor and elucidated the theoretical conditions necessary to sustain continuous rotation. Additionally, we provided a generalized solution regarding the rotational symmetry differences observed in FO motors across various species.

Our findings offer new insights into the mechanism of ATPase and contribute to a broader understanding of molecular motor function. These insights also have potential applications in bioenergetic conversion technologies, paving the way for innovations in energy efficiency and molecular design. Through multiscale simulations, we have successfully bridged the gap between molecular-level processes and larger mechanical function of the motor, providing frameworks for future studies on the dynamic coupling between proton transport and ATP synthesis.