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Molecular Dynamics Simulations of F1-ATPase Using GPU Supercomputer[1] MATTHEW ANDERSON[2], SNDOR VOLKN-KACS[3], Azusa Pacific University — Single-molecule imaging has produced many videos of biomolecular events, including the binding and release of ADP and inorganic phosphate (Pi) from ATPase. However, the poor video quality of single-molecule imaging makes it inadequate for robust research. Recently, molecular dynamics simulations have become able to access the microsecond timescales associated with the release of ADP and Pi. Using MD simulations, we have developed a method of describing large domain motion of F1-ATPase subunits with large trajectory files. These large trajectories obtained from unbiased MD simulations contain the collective coordinates associated with the bending and torsional motion of subunits. These all-atom simulations produced three distinct trajectories using an X-ray crystallography structure with all three active subunits occupied by nucleotides. Our hypothesis suggested that, under these conditions, an ADP should be released within a few microseconds. Early simulations showed that one trajectory resulted in the release of an Pi. However, it was not found that the ADP was released in this during the microsecond time frame. This project optimized our simulations to capture the release of Pi and ADP. Biased techniques such as steered MD and metadynamics may be used to improve sampling later.

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