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ISSN: 2167-7956
Journal of
Biomolecular Research
& Therapeutics

Perspective

Molecular Dynamics and its Protein Synthesis in Phospholipids

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DESCRIPTION

Photosynthesis is controlled by a dynamic interaction of protein, enzymes, pigments, hydrocarbons and cofactors on a vast spatiotemporal scale. Molecular Dynamics (MD) simulations provide a powerful toolkit for investigating dynamic processes. As a result MD is well adapted to solve a wide range of issues that arise in photosynthesis. The photosynthesis membranes or thylakoid is a continuous membrane system formed of a lipid bilayer mostly composed of valuable activities and phospholipids with embedded protein complexes and cofactors. The thylakoid divides the chloroplast's aqueous phase into two domains the lumen (the inner section) and the stroma (the outer portion). The first phases of photosynthesis collectively known as the light reactions occur in this membrane. Electrons are taken from water and transported across the membrane through these processes, while protons are pushed into the lumen, resulting in a proton gradient across the membrane.

The proton gradient and electrons are employed to supply Adenosine Triphosphate (ATP) and Nicotinamide Adenine Dinucleotide Phosphate (NADPH) to the downstream. In terms of structures, organisation, composition and functioning the thylakoid is a highly dynamic system the transport mechanisms engaged in light reactions are merely a subset of the "dynamic processes" that occur in the thylakoid. Indeed because the quality or quantity of daily sunshine can fluctuate abruptly and irregularly, photosynthetic organisms must adjust to these changes through short-term and long-term conditioning techniques. To prevent photooxidation these systems optimize the use of light and balance the amount of excitation in the thylakoid. As a result, photosynthesis structure and composition are dynamically adjusted in response to variations in light circumstances. Understanding the molecular mechanics of light reactions requires the employment of a tool that can rebuild the ensemble of potential conformations, reorganisations, interactions and motions within the thylakoid. X-ray diffraction and cryo-electron microscopy have been used to generate high-resolution structures of the key photosynthetic complexes active in the earliest steps of photosynthesis. MD simulations are used in biomechanics to simulate small-scale biochemical pathways as an ensemble of classical particles and to follow their dynamics within a simulation box. It can be accomplished by examining the trajectory (coordinates and velocities) produced by the motion of each particle in the simulation box beginning with a known set of initial positions such as the protein exact location from a high-resolution crystal structure.

Significantly, further time is required to equilibrate the system's other features. For example in MD simulations with lipid membranes the membrane should achieve stable values of thickness, area per lipid, hydration and so on that are expected for the lipids used. Depending on the size of the membrane patch, this equilibration normally takes hundreds of nanoseconds. Improved sampling approaches offer an alternate method for capturing significant states or processes that occur beyond the conventional time scale of atomistic or MD simulations in a tolerable processing period. The purpose is often to sample portions of the potential energy surface that have more energy and thus less frequently visited during a regular MD simulation. When experimental tools are unavailable, protein modeling may be the only option to gather structural information. Molecular Dynamics (MD) simulation is a method for simulating protein mobility in given settings using classical molecular dynamics. MD simulation could be widely employed in protein design when accurate modeling of target protein dynamics and descriptions of the relationship between conformational changes and protein function at the atomic level are required.

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Received: 03-Feb-2023, Manuscript No. BOM-23-20103; **Editor assigned:** 06-Feb-2023, Pre QC No. BOM-23-20103(PQ); **Reviewed:** 21-Feb-2023, QC No. BOM-23-20103; **Revised:** 28-Feb-2023, Manuscript No. BOM-23-20103 (R); **Published:** 07-Mar-2023, DOI: 10.35248/2167-7956.23.12.264.

Citation: Hailee L (2023) Molecular Dynamics and its Protein Synthesis in Phospholipids. J Biol Res Ther. 12:264.