A Computational Framework for Simulating Protein Organization in Thylakoid Membranes

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In the grana membranes of plants, the efficiency of photosynthetic light harvesting and electron transport depends on the spatial arrangement of proteins, collectively referred to as the "protein landscape." This landscape is tightly regulated to ensure optimal photosynthetic efficiency. Therefore, a robust modeling tool is essential for understanding and potentially engineering photosynthetic regulation. In this study, we present a novel computational model to simulate the organization of different types of proteins in thylakoid membranes. Using Monte Carlo sampling, we simulate membranes of various sizes and protein densities. The model exploits the precise atomic structures of proteins and enforces volume exclusion to capture realistic protein packing on the 100 nm length scale. As a proof of concept, we applied our Monte Carlo membrane model to the protein landscape of the grana membrane in *Arabidopsis thaliana*. We performed Monte Carlo simulations on the particle maps measured by freeze-fracture cryo-electron tomography and revealed protein identities and orientations. We also demonstrated that when only accounting for volume exclusion, the simulated membrane packing at biological protein densities the model is capable for describing the overall protein landscape for real-world membranes. Looking forward, this model is adaptable and will provide a quantitative platform for comparing experimental data with theoretical models of thylakoid membranes of different sizes and with various protein densities.