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Molecular Level Insight into Non-bilayer Structure Formation in Thylakoid Membranes

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Thylakoid membranes, integral to photosynthesis, possess a unique lipid composition dominated by monogalactosyl diacylglycerols (MGDGs), which play essential roles in supporting protein function and modulating photoprotective processes. In this study, we employed all atom and coarse-grained molecular dynamics simulations to explore how varying MGDG concentrations influence the structural and dynamic properties of lipid bilayers characteristic of higher plant thylakoid membranes. Our findings reveal that MGDG promotes increased membrane fluidity and dynamic fluctuations in membrane thickness without affecting curvature. Under high hydration conditions, MGDG-rich bilayers spontaneously formed stable inverted hexagonal phases, suggesting a hydration-dependent stability for these non-bilayer structures. Notably, while MGDG clustering was observed within the membrane stacks, a substantial amount of MGDG was enough for non-bilayer formation. We also observed a decrease in lipid mobility in these inverted hexagonal structures, suggesting a regulatory role for non-bilayer phases in thylakoid membrane dynamics. These insights advance our understanding of plant membrane organization, with broader implications for non-bilayer forming organelles and the structural adaptations required for photosynthetic efficiency and resilience under fluctuating environmental conditions.