

# POPG vs SQDG: The tale of two lipids in LH1RC

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From cyanobacteria to higher plants photosynthetic membranes contain galactolipids such as mono- and digalactosyldiacylglycerol (MGDG and DGDG), as well as negatively charged lipids, such as sulfoquinovosyldiacylglycerol (SQDG) and phosphatidylglycerol (PG). Often, plants and algae struggle to survive without nutrients, leading to the development of nutrient-saving mechanisms. Under phosphate starvation, PG is replaced by SQDG in some photosynthetic membranes, while under sulfur deprivation, the opposite will occur. Biological data strongly support a complementarity between SQDG and PG and indicate the importance of maintaining the total amount of anionic lipids in photosynthetic membranes. Photosynthetic purple bacteria can capture and convert sunlight with a remarkable nearly 100% quantum efficiency. A key component of this process is the light-harvesting complex1 - reaction center (LH1-RC), which is responsible for light harvesting and charge separation. The LH1-RC membrane complex has a highly conserved local lipid composition that is dominated by anionic lipids, which may establish specific interactions with the protein. Characterization of these functionally important lipid-protein interactions with experimental techniques is however still prohibitively challenging. With the Martini force field, we present coarse-grained molecular dynamics simulations of monomeric and dimeric LH1RC, in PG and SQDG rich membranes. Physical properties of SQDG and PG membrane are similar despite their different chemical headgroups. Results show that LH1-RC prefers anionic over neutral lipids. Additionally, anionic lipids in the inner leaflet of the membrane promote energy transfer from LH1 to RC by interacting with basic amino acids. The results presented here establish that SQDG and PG are good substitutes for each other in nutrient starvation conditions to maintain the LH1RC functional organization and its photosynthesis activity.