

Supplementary Material
Intrinsic Curvature Properties of Photosynthetic Proteins in Chromatophores

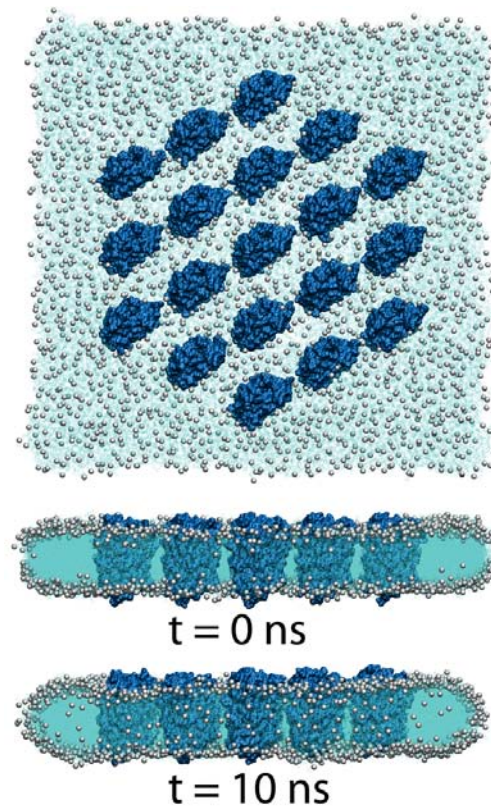


Figure 9: Simulation of 19 rhodopsins placed in the same membrane patch as used in the 7-LH2 simulations. This simulation was performed as a control for the LH2 simulations, to ensure that the curvature seen in the LH2 simulations is not an artifact produced by the water-exposed membrane edges. The 19 rhodopsins were arranged hexagonally so that the area covered by the rhodopsins was comparable to that covered by seven LH2s. This rhodopsin system was equilibrated for 10 ns (the amount of time needed for the formation of curvature in the LH2 systems). No curvature was seen to develop. The absence of curvature in this control simulation suggests that the curvature seen in the LH2 simulations is not a simulation artifact and instead, is due to interactions specific to LH2.

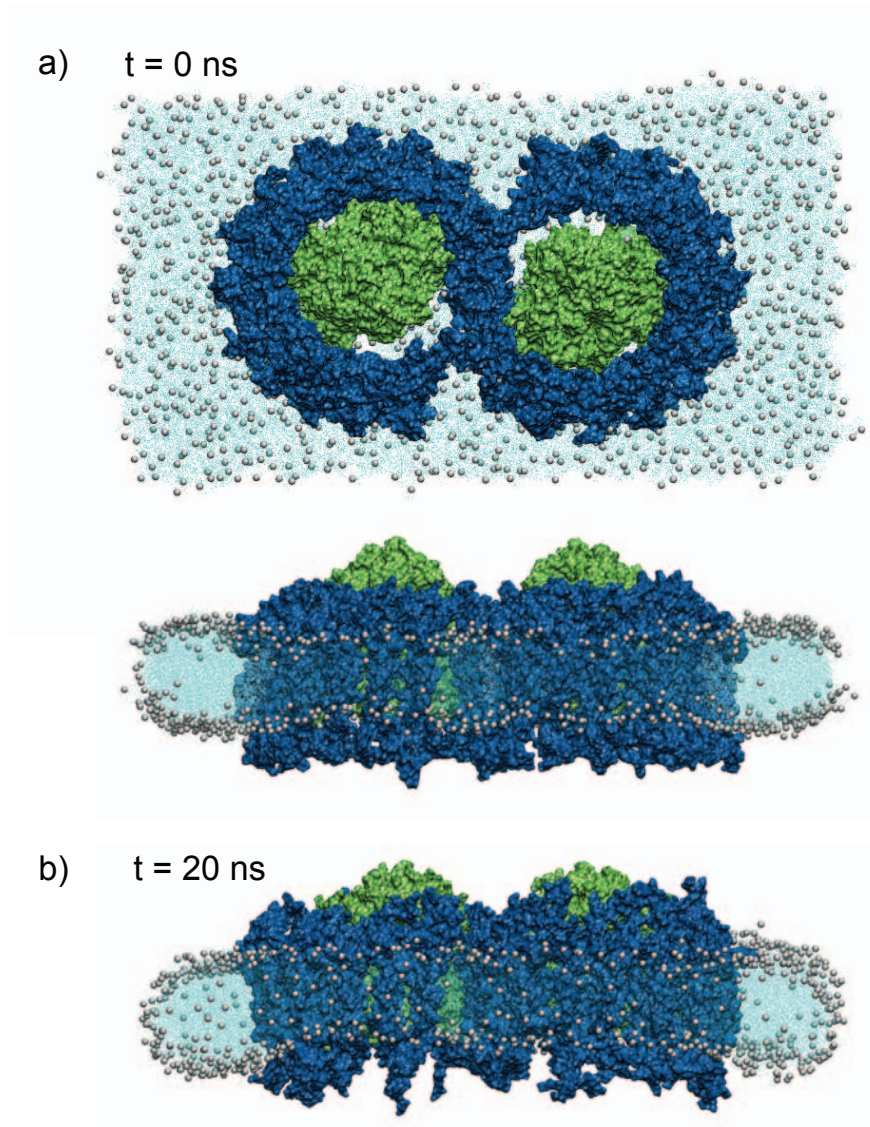


Figure 11: Simulation of the LH1-RC dimer without the PufX polypeptide. LH1 colored in blue and the RCs in green. a) Snapshots at the beginning of the simulation, viewed from the cytoplasm (top), and a view parallel to the plane of the membrane (bottom). b) Snapshot of the simulated system at the end of the 20 ns equilibration. The LH1-RC dimer exhibits a slight bend at the dimerizing junction.

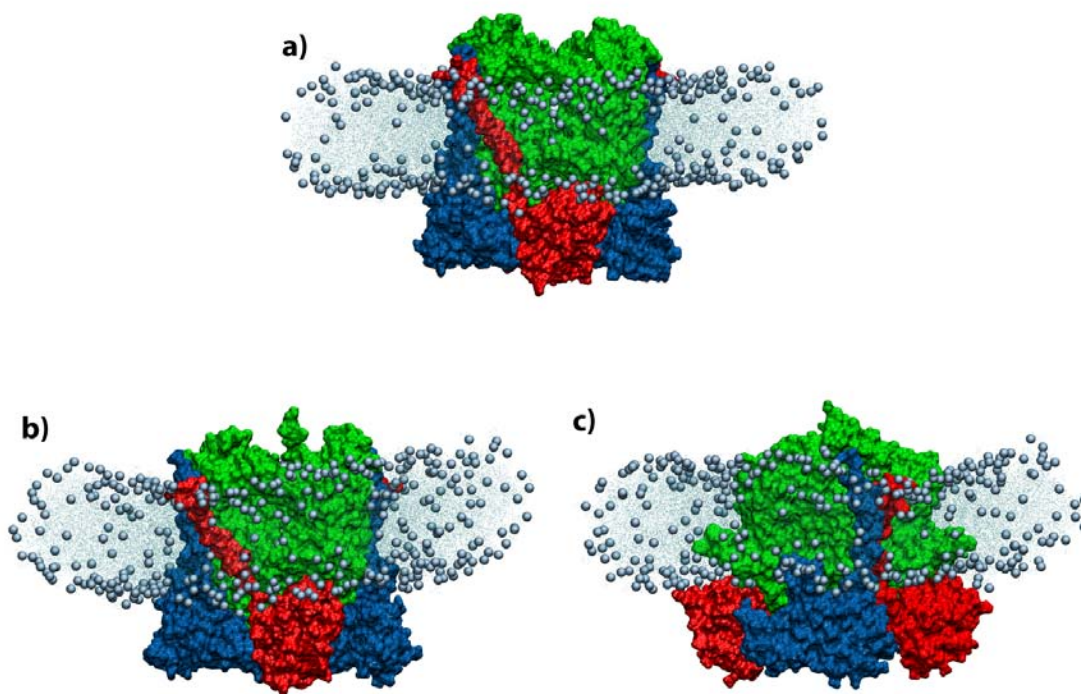


Figure 12: Simulation result of single bc_1 -dimer resulting in a negatively curved lipid bilayer after 5 ns of equilibration. These simulations demonstrated the potential for the bc_1 -dimer to occupy a curved as well as flat lipid bilayer. This lipid curvature was observed to occur subsequent to the elevation of an intramembrane helix on the surface of cytochrome b residing at the polar-nonpolar interface of the lipid bilayer. Dislocation of this helix into the nonpolar region exposed polar residues of cytochrome b which was subsequently solvated by waters passing into the polar region of the bilayer. This is believed to have elevated selected regions of the lipid bilayer and subsequently resulted in membrane curvature. a.) Snapshot of the simulation, along the ISP axis, after minimization and before equilibration ($t = 0$ ns). b.) Snapshot of the simulated system at $t = 5$ ns, viewed along the ISP axis. Symmetric negative curvature of the lipid bilayer was observed, suggesting bc_1 can accommodate areas of negative bilayer curvature in the chromatophores such as the neck of *Rb. sphaeroides* chromatophores. c.) Snapshot of the simulated system at $t = 5$ ns, viewed along the Cyt- c_1 axis. Asymmetric curvature of the lipid bilayer was observed. As seen on the right, the lipid bilayer is elevated to a negative curvature and is displaced from the top of the ISP subunit. On the left, the bilayer exhibits a radius of curvature of 0 and is not displaced but instead rests upon the top of the ISP subunit.