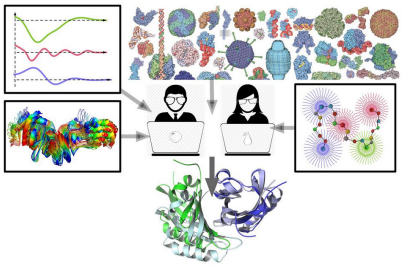

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Assembly of membrane protein complexes with encapsulated lipids

Recent breakthroughs in X-ray crystallography, Cryo-EM and complementary approaches resulted in elucidation of many new structures of membrane proteins (MPs) and their complexes. Several classes of MPs, such as microbial rhodopsins, rotary ATPase subunits c, or light harvesting complexes 2, form ring-like assemblies with several lipid molecules trapped inside. Whereas the proteins are usually well resolved in experimental structures, the lipids are more disordered and cannot be readily modeled; the number and nature of the trapped molecules is also often not clear. This is problematic, because the trapped lipids cannot exchange with the pool of the surrounding membrane lipids in simulations, and the errors in the starting models can not correct themselves, as often happens in normal molecular dynamics simulations of soluble and membrane proteins. To address this problem, we simulated the process of the assembly of the MP-lipid complex explicitly, and then removed the excess lipids to achieve a very good fit to the noisy experimental densities that are available [1]. The presented approach is expected to be generalizable to all MP complexes with encapsulated lipid patches. Besides producing molecular models of MP-lipid complexes, the approach also highlights intriguing adaptations of ring-forming MPs that promote efficient assembly.

1. Novitskaia, O.; Buslaev, P.; Gushchin, I. Assembly of Spinach Chloroplast ATP Synthase Rotor Ring Protein-Lipid Complex. *Front. Mol. Biosci.* 2019, 6.

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