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Atomistic molecular dynamics simulation of ATG13-ATG101-WIPI3/ATG13-ATG101-WIPI3-WIPI2 complex on a membrane bilayer

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Protocol status: Working
We use this protocol and it's working

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Abstract

This protocol details molecular dynamics simulations of the ATG13-ATG101-WIPI3/ATG13-ATG101-WIPI3-WIPI2 complex on a membrane bilayer and analysis of the stability of the protein-protein interfaces.

Model Preparation

1 Begin with the AlphaFold2-predicted model of the ATG13-ATG101-WIPI3/ ATG13-ATG101-WIPI3-WIPI2 complex as the initial structure for the simulation.

2 Put this protein complex on a membrane bilayer and remove some lipids near the protein segments that insert into the membrane.

Membrane Composition

3 Consider the following membrane composition: 65% DOPC, 20% DOPE, 10% DOPS, and 5% PI(3)P.

Simulation Runs

4 Perform 1 μs production run of the simulation system. Perform minimization and equilibration before carrying out the production run.

5 Maintain system pressure at 1 Bar and temperature at 303 K using Parrinello-Rahman barostat and Nose-Hoover thermostat.

Electrostatic Interactions

6 Treat long-range electrostatic interactions using the particle mesh Ewald method.

Analysis

7 Monitor the time evolution of the distance between ATG13 D217 and WIPI3 K42/K44, along with the RMSD of the ATG13 DHF motif and its interacting WIPI3 residues, as well as the ATG13-WIPI2 interface.