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Coarse-grained MD simulations of ATG2A and ATG2A-ATG9A with initially dispersed lipids

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We use this protocol and it's working

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Abstract

This protocol details coarse-grained molecular dynamics simulations of the lipid transport protein ATG2A, alone and in complex with ATG9A, with initially dispersed POPC lipids.

Model preparation

1 Generate structures of Atg2 and the Atg2-Atg9 complex using AlfaFold 3. Optionally include 50 molecules of oleic acid in the model prediction to induce displacement of the N-terminal helices.

2 Map the atomistic models to CG resolution using *Martinize2*.

2.1 Add an elastic network with a force constant of 500 kJ mol^{-1} nm^{-2} and lower and upper cutoffs of 0.5 and 0.9 nm. Manually remove elastic network constraints from disordered regions of the protein.

3 Place CG proteins in a simulation box using *gmx insert-molecules*.

4 Randomly place POPC lipids in the simulation box.

5 Fill the rest of the simulation box with water (using the Martini 3 water model).

6 Replace water molecules with 150 mM NaCl, include neutralising ions.

Energy minimisation

7 Minimise the potential energy of the system using the steepest descend algorithm for 50000 steps.

MD simulation

8 Simulate for 400ns using GROMACS 2022.4 and Martini 3.

8.1 Run simulation in the NPT ensemble. Keep temperature (310 K) and pressure (1 bar) constant using the Berendsen thermostat and barostat, respectively.

8.2 Use the Verlet cutoff scheme with cut-off distance of 1.418 nm for the short-range neighbor list. Update this list every 20 steps.

8.3 Cut-off Coulomb and van-der Waals interactions at 1.2 nm.

8.4 Use a dielectric constant of 15.