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Coarse-grained simulations of the C-terminus of ATG2A in a buckled bilayer

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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 C-terminal region of the lipid transport protein ATG2A on a buckled POPC bilayer.

Generation of buckled membrane

1 Make a POPC bilayer using the *insane* method.

1.1 Solvate with 150 mM NaCl.

2 Run a 10 ns simulation to compress the membrane into a buckled shape.

2.1 Use the Berendsen barostat anisotropically coupled to the *Y* and *Z* directions. Set the compressibility to 3×10^{-4} bar^{-1} in these dimensions, and to 0 in all others. Set the pressure to 12 bar in *Y* and 1 bar in *Z*.

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

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

2.4 Set the relative dielectric constant to 15.

Docking of ATG2A C-terminus to buckled membrane

3 Place the buckled membrane in a simulation box. Place the C-terminus of ATG2A at a random position of the same simulation box. Add Martini 3 water and solvate with 150 mM NaCl.

4 Run a 1 µs membrane simulation.

4.1 To fix the lateral axes, couple the Parrinello-Rahman barostat only to the *Z* dimension with a compressibility of 3×10^{-4} bar^{-1} and a coupling constant of 1 ps. Set the compressibility to 0 in all other dimensions.

Simulation of ATG2A C-terminus bound to the buckled membrane

5 Use the membrane-bound configuration as a starting point for 10 independent replicas.

5.1 Draw initial velocities according to the Maxwell-Boltzmann distribution at 310 K.

6 Run all simulations for 1 μs with the lateral axes fixed as described in the previous section.