Membranes with branched lipids are more disrupted by solvents

Background

- Lignocellulosic biomass offers a renewable, carbon-neutral route to sustainable fuels and chemicals.
- Solvent and product toxicity limit microbial biofuel yields.
- Solvents weaken membranes, but how lipid structure affects tolerance is not fully understood.

Approach

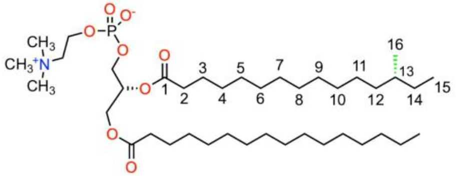
We performed all-atom molecular dynamics simulations of branched (APPC) and straight-chain (DPPC) lipid bilayers using the GROMACS simulation software and CHARMM36 force field to examine how varying butanol concentrations affect membrane structure and dynamics, including thickness, lipid packing, diffusion, and interleaflet coupling.

Results

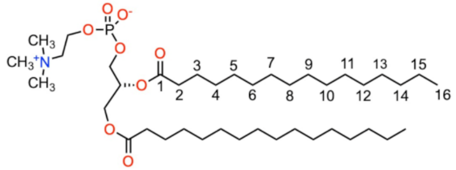
- MD simulations show that branched-chain membranes become disordered and permeable under butanol stress, while straight-chain membranes remain more stable and resistant.
- A single methyl branch dramatically changes how membranes respond to solvent stress..

Significance/Impacts

Balancing branched and straight lipids may optimize membrane fluidity and solvent tolerance for microbial production of biofuel.

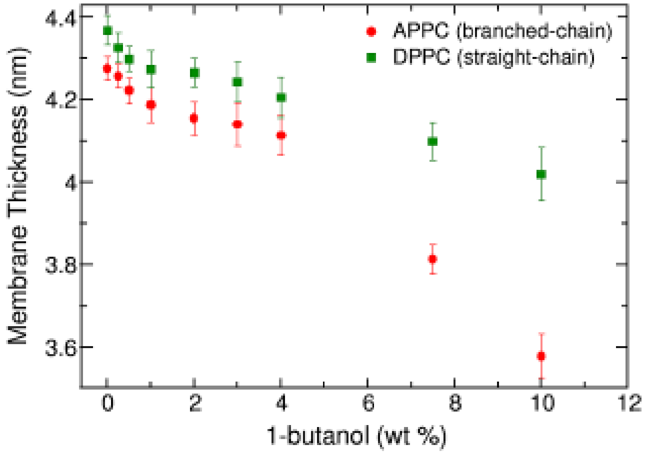


A

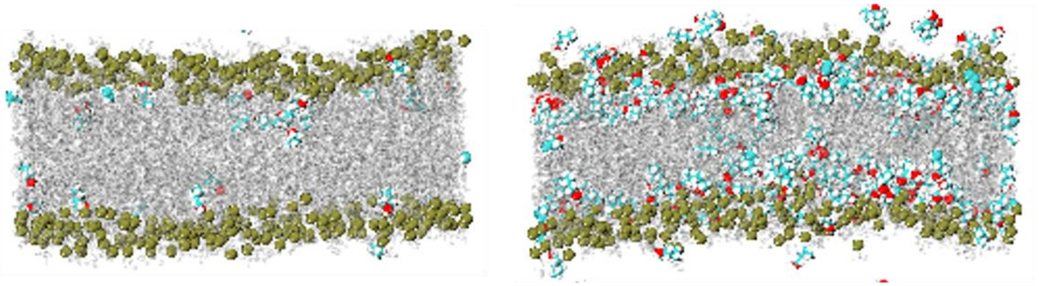


B

Phospholipids used in this study: (A) branched with a methyl (green) at C13, 1-anteiso-palmitoyl-2-palmitoyl-*sn*-glycero-3-phosphocholine (APPC) and (B) linear, 1,2-dipalmitoyl-*sn*-glycero-3-phosphocholine (DPPC).



Calculated membrane thickness decreases with increasing butanol.



MD snapshots illustrate the increasing disorder of an APCC membrane at 0.5% (left) to 4% (right).

Aggrey *et al.* (2025). Divergent Responses of Branched and straight-chain lipid membranes to butanol stress revealed by molecular dynamics simulation. *Biophys J*. DOI: 10.1016/j.bpj.2025.10.015