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## The Preference for Membrane Curvature of Neutral Lipids and the Role in Lipid Droplet Formation

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Lipid droplets (LDs) are organelles responsible for lipid storage and metabolism, consisting of an oily core containing various types of neutral lipids (NLs), bounded by a monolayer of phospholipids and proteins. LDs form within the endoplasmic reticulum (ER) membrane, which possesses regions with different degrees of curvature. Previous work has shown that LDs form in the curved regions of ER membrane, i.e., the ER tubular region, and that membrane curvature promotes the nucleation of LDs in vitro. Interestingly, this same work suggests that free NLs, in this case, triolein (TO), prefer to localise in the flat regions of the ER membrane. Using molecular dynamics simulations (MD), we construct buckled membranes, which possess both flat and highly curved regions, containing a small concentration of free TO, below the critical concentration required for LD nucleation. We find, conversely to the experimental work, that free TO in these simulations prefers to localise in the curved regions of our buckled membranes. This finding opens many questions, such as the difference in free TO localisation in the presence of an LD, the preference of different NLs for curved vs flat membrane regions, and the origin of the differences between simulation and experimental results.

## Session

Computational methods

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