

How cells control their borders

March 30 2022



Permeability of solutes as a function of their lipophilicity. A Overview of experimental assay. Kinetic data obtained with the calcein self-quenching assay using vesicles composed of DOPC mixed with buffer (gray) or osmotically shocked with 52.5 mM KCl (cyan), 50 mM sodium formate (red), 50 mM sodium L-lactate (blue) or 120 mM glycerol (orange) at 20 °C. B Schematic description of the permeation process, x(t), through a lipid membrane with an example free energy profile, $\Delta G(x)$ (lipid tails, gray; glycerol moiety, purple;



phosphate moiety, ochre; and choline moiety, blue; water molecules are not shown). C Selected free energy profiles from simulations of solutes with varying hydrophobicity levels (I most hydrophilic, IX most hydrophobic) permeating through a DOPC lipid membrane as a function of the distance from the bilayer center along the membrane. Only one half of the whole symmetric permeation profile is shown. D Solvent accessibility profiles of the permeating solutes along the permeation pathway. Solutes interact with solvent molecules even deep in the membrane tail region (x

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