result in both the partial loss of α-helical structure, as well as differences in peptide positioning with respect to the lipids.

1469-Pos
Antimicrobial Peptides in Toroidal and Cylindrical Pores
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Antimicrobial peptides (AMPs) are small, usually cationic peptides, which permeabilize biological membranes. Understanding their mechanism of action might help design better antibiotics. Using molecular dynamics (MD) simulations, we investigate the preference of alamethicin and melittin for pores of different shapes. In the simulations, an alamethicin hexamer initially embedded in a pre-formed cylindrical pore preserves the pore shape or closes the pore if glutamines in the N-terminus are not located within the pore. On the other hand, when a melittin tetramer is embedded in a toroidal pore or in a cylindrical pore, at the end of the simulations the pore is lined both with peptides and lipid headgroups, and, thus, can be classified as a toroidal pore. These observations agree with the prevailing views that alamethicin forms barrel-stave pores whereas melittin forms toroidal pores. The melittin tetramer interacts more strongly with lipids in the toroidal pore than in the cylindrical one, due to more favorable electrostatic interactions. Using an implicit membrane model, modified to include pores of different shapes, we show that melittin is better solvated in toroidal pores than in cylindrical ones.

Membrane Structure I

1470-Pos
Hybrid Lipids as a Biological Line-Active Component
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The lipid raft hypothesis posits that certain cellular functions are mediated by small (nanometric to tens of nanometers) domains rich in sphingolipids and cholesterol. These sphingolipids have two completely saturated hydrocarbon tails that show good orientational order in the membrane. The surrounding phase consists mostly of lipids with at least one unsaturated bond in the hydrocarbon tails which forces a "kink" in the chain and inhibits ordering. In vitro, this phase separation can be replicated; however, the finite domains coarsen into macroscopic domains with time. We have extended a model for the interactions of lipids in the membrane, motivated by the work in (Elliott et al., PRL 2006 and Garbes Putzel and Schick, Biophys. J. 2008), which depends entirely on the local ordering of hydrocarbon tails. We generalize this model to INCLUDE an additional species THAT IS LINE ACTIVE and identify a biologically relevant component, a hybrid lipid with one fully saturated hydrocarbon chain and one chain with at least one unsaturated bond, that may serve as a line-active component. we show that in some cases, the hybrid is capable of reducing the line tension between the saturated and unsaturated domains to zero, thus stabilizing finite sized domains in equilibrium. We then present simple packing arguments that predict the expected size of such domains as a function of the molecular volume and area per headgroup of the composing lipids which is dictated by parameters such as cholesterol concentration, chain length and degree of unsaturation.

1471-Pos
Characterization of Horizontal Lipid Bilayers as a Model System to Study Lipid Phase Separation
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Black lipid membranes are widely used as a model system to study ion channel activity with electrophysiological techniques. In this study we characterize the properties of the bilayer system with respect to its dynamics of lipid phase separation using single molecule fluorescence fluctuation and electrophysiological techniques. On the nanosecond time scale we determined the rotational motions of fluorescently labeled lipids using confocal time resolved anisotropy to probe the microscopic viscosity of the membrane. Simultaneously long range mobility was investigated by the lateral diffusion of the lipids through the laser focus with fluorescence correlation spectroscopy. Depending on the solvent used for membrane preparation, lateral diffusion coefficients between $D_{lat} = 10 - 25$ $\mu m^2/s$ and rotational diffusion coefficients of $D_{rot} = 2.8 \cdot 10^7 \ s^{-1} - 1.4 \cdot 10^7 \ s^{-1}$ were measured in pure liquid disordered (Ld) membranes. In ternary mixtures containing saturated, unsaturated phospholipids and cholesterol, liquid ordered (Lo) domains segregated from the Ld phase at 23°C. The lateral mobility of lipids in Lo domains was ~8-fold lower compared to the Ld phase while the rotational mobility decreased by a factor of 1.5. Burst integrated steady state

anisotropy histograms as well as anisotropy imaging were used to visualize the rotational mobility of lipid probes in phase separated bilayers. The electrical conductance of pure Ld and ternary bilayers was linearly dependent on the temperature. No discrete current fluctuations were found near the phase transition between coexisting Ld and Lo domains. Our results demonstrate that horizontal bilayers can be used as an alternative model system for lipid phase separation (taking solvent partitioning into account) favorably when electrical properties of the membrane want to be studied in parallel

1472-Pos
Phase-Field Modeling and Simulations of Lipid Membranes Coupling Composition with Membrane Mechanical Properties
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The plasma membrane, a lipid bilayer membrane surrounding all mammalian cells, is not homogeneous, but rather contains domains termed 'rafts,' defined as regions enriched with cholesterol and saturated lipids. Understanding how and why these rafts form is of great importance to cell biologists and immunologists, since they are involved in many important cell functions and processes including endocytosis, cell adhesion, signaling, protein organization, lipid regulation, and infection by pathogens. These raft structures also show great potential for technological applications, especially in connection with biosensors and drug delivery systems. We examine the formation and evolution of lipid raft-like domains in multicomponent lipid membrane vesicles using a continuum-level simulation method. Our objective is to investigate how various physical parameters input into the model, such as spontaneous curvature, bending rigidity, and phase fraction, affect the dynamics and equilibrium morphological phases formed in two-phase lipid membrane systems. This model is applied to membranes with spherical background geometries, simulating the compositional and shape evolution of lipid vesicles, coupled using a modified Helfrich free energy. The compositional evolution is modeled using a phase-field method and is described by a Cahn-Hilliard-type equation, while the shape changes are described by relaxation dynamics in which the vesicle surface area is conserved. We find that the compositional and morphological evolution are significantly altered when the mechanical coupling is present by comparing the results with those of systems where this coupling is absent. More specifically, we find that the evolution is significantly slowed when the phases have equal and opposite spontaneous curvatures and are present in roughly equal amounts. We also investigate equilibrium shapes formed by completely phase-separated vesicles as a function of spontaneous curvature, bending rigidity, and phase fraction.

1473-Pos
Computation of Lipid Headgroup Interactions
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The equilibrium structure of lipid aggregates is determined by the balance of numerous forces between hydrophobic acyl chains, hydrophilic lipid headgroups, and the lipid's environment. Among these forces, lipid headgroup interactions are both important to the stability of lipid structures and responsible for many of the interactions between biological membranes and aqueous solutes including ions and soluble peptides. In order to model these headgroup interactions, we consider the electrical properties of the headgroup molecules via the multipole expansion. While common lipid headgroups such as phosphatidylcholine are electrically neutral, they are characterized by non-zero higher order terms in the multipole expansion. Making a dipole approximation, we employ a two dimensional lattice of classical dipoles to model the headgroup networks of lipid aggregates. Restrictions to each dipole's position and orientation are imposed to account for the effect of hydrocarbon chains which are not included in the model. A Monte Carlo algorithm is used to calculate headgroup-headgroup interactions and network energies in both dipole and point-charge approximations.

1474-Pos
X-Ray Scattering from Gold Labeled Supported Membranes
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