computer simulations, these moduli can be determined by fitting power spectra of fluctuating fields to the predictions of those continuum theories. This data analysis involves numerous choices, such as how to define a membrane surface or how to determine the fitting range, which significantly affect the observables of interest. Here, we examine in detail the systematic trends resulting from these choices, on the basis of atomistic simulation trajectories of 13 different lipid model membranes created by Venable *et al*. [CPL **192**, 60 (2015)]. We in particular discuss systematic effects connected with: (1) interpolation of height and directional fields; (2) normalization and averaging of lipid directors; (3) determining small-scale cutoffs. Additionally, we discuss statistical aspects such as correcting for time correlations in the power spectra, getting uncertainties on the parameters, and simultaneously fitting different spectra. The systematic shifts in the moduli arising from equally plausible choices are often larger than the statistical uncertainties. We propose a tentative set of criteria based on which the relative merits of such choices could be evaluated.

1573-Pos
Lipid Chain Upturns and Orientational Potential in Membrane Liquid Crystals
Abhinav Ramkumar[1,2], Michael F. Brown[3], Horia I. Petrache[2].
[1]Department of Physics, University of Pennsylvania, Philadelphia, PA, USA, [2]Department of Physics, Indiana University-Purdue University Indianapolis, Indianapolis, IN, USA, [3]Department of Chemistry and Department of Physics, University of Arizona, Tucson, AZ, USA.
Lipid bilayers in the fluid state are characterized by significant disorder of the acyl chains. Experimentally this can be seen by the low order parameters measured by 2H NMR spectroscopy [1, 2] and by other methods such as x-ray scattering that measures a reduced membrane thickness compared to ordered phases. In addition, IR and EPR spectroscopy that each measure a characteristic order parameter. All-atom Molecular Dynamics (MD) simulations of lipid bilayers show that acyl chain disorder can be described analytically using a mean-field orientational potential (potential of mean-torque) acting at the level of carbon segments [3]. The simplest approximation is a first-order term in which the alignment potential is quantified by a $\varepsilon 1$ that we call a torque-strength. As shown by us and others, this approximation is sufficient for the calculation of geometric quantities such as the membrane thickness and cross-sectional area per lipid. However, there are other physical parameters of interest in the biophysics of membranes. One important parameter that contributes to the membrane free energy is the orientational entropy. Here we show that the first order mean-torque approximation needs to include an extra term (with an additional parameter $\varepsilon 1'$) to account for chain upturns. We find that upturned carbon segments experience a stronger alignment field because upturns necessarily place the remaining carbon segments higher on the membrane normal, i.e. close to the headgroups. Such statistical models of lipid membrane structure can better account for the contributions to membrane free energy that governs biological functions such as cellular signaling by ion channels.
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1574-Pos
Recent Updates to the Charmm Lipid Force Fields
Yalun Yu[1], Jeffery B. Klauda[2], Alexander D. MacKerell[3], Benoit Roux[4], Richard W. Pastor[5].
[1]Biophysics Program, University of Maryland, College Park, MD, USA, [2]Dept Chemistry and Biomolecular Engineering, Univ Maryland, College Park, MD, USA, [3]Dept Pharmaceutical Sciences, Univ of Maryland Baltimore, Baltimore, MD, USA, [4]Dept Biochemistry and Molecular Biology, Univ Chicago, Chicago, IL, USA, [5]Lab of Computational Biology, NHLBI NIH, Bethesda, MD, USA.
Since its release in the early 1990s, the CHARMM lipid force field (FF) has been updated frequently to agree with experimental data and to work with state-of-art simulation protocols. The most recent all-atom version, C36, has been heavily used due to the diversity of lipids it covers and the well-designed parameters, but it is not suitable for monolayer simulations due to the inconsistency of surface tension with experiment. To fix this problem, we introduced the long-range Lennard-Jones (LJ) interactions using the LJ Particle Mesh Ewald (LJ-PME) method and optimized the C36 parameter set to work with LJ-PME. The new force field, called C36/LJ-PME, achieved excellent agreement with a wide range of experimental data for a variety of lipid types, currently including phosphatidylcholines, phosphatidylethanolamines, phosphatidylglycerols, ether lipids and lipids with (poly)unsaturated tails. Besides the additive, CHARMM also has a polarizable lipid force field, DRUDE. While the polarizable model can provide a more realistic representation of the lipid, parameters for the DRUDE lipid force field were not optimized to the optimum, leading to unsatisfactory membrane compressibilities. Here we also report our most recent work on the DRUDE lipid force field toward a better modeling of lipid.

1575-Pos
Using Molecular Dynamics Simulations to Elucidate a Role for Bacterial Ceramides
Anushriya Subedy[1], Liam M. Sharp[1], Eric A. Klein[2], Grace H. Brannigan[3].
[1]Center for Computational and Integrative Biology, Rutgers Univ, Camden, NJ, USA, [2]Dept of Biology, Rutgers Univ, Camden, NJ, USA, [3]Dept Physics, Rutgers Univ, Camden, NJ, USA.
Sphingolipids synthesis was thought to be rare in Gram-negative bacteria, previously only found in a handful of taxa. We recently discovered ceramides in Caulobacter crescentus and demonstrated that these lipids play an important role in antibiotic and phage sensitivity. However, the mechanism by which ceramides affect resistance to antimicrobials, as well as their effects on the integrity of the cell membrane are not yet clear. In this study, a coarse-grained molecular dynamics simulation of a prototypical bacterial outer membrane is used to observe changes in the conformation of the outer membrane lipids in the presence of ceramides. The outer membrane of a Gram-negative bacteria is asymmetric with an outer leaflet dominated by lipopolysaccharide (LPS). LPS is composed of three domains that extend from the outer membrane: a membrane-embedded lipid A, the attached core polysaccharide chain, and the O-antigen polysaccharide chain. Rough LPS consists of lipid A and core oligosaccharides only, while smooth LPS contains lipid A, core sugars, and O-antigen chains. Membranes were simulated with a one to one ratio of rough to smooth LPS, with ceramide concentrations ranging from ten to forty percent of total lipids. In order to understand the role of ceramide in outer membrane structure and function, this study considers their effects on the flexibility of O-antigen as well as the clustering and packing of LPS and membrane lipids.

1576-Pos
Interaction between Biomimetic Lipid Membranes and Trodusquemine: An Atomic Force Microscopy Study
Davide Odino[1], Silvia Errico[2], Claudio Canale[1], Riccardo Ferrando[1], Fabrizio Chiti[2], Annalisa Relini[3].
[1]Department of Physics, University of Genoa, Genoa, Italy, [2]Department of Experimental and Clinical Biomedical Sciences, University of Florence, Florence, Italy, [3]Department of Chemistry and Industrial Chemistry, University of Genoa, Genoa, Italy.
Trodusquemine is an aminosterol which has been proposed as a potential drug against Parkinson's and Alzheimer's diseases. It has been shown to reduce the toxicity of α-synuclein and Aβ oligomers in neuroblastoma cells. To further elucidate its mechanism of action, we have studied the effects of trodusquemine on biomimetic membranes. In particular, we have used atomic force microscopy to investigate the morphological and mechanical properties of supported lipid bilayers, mimicking neuronal membranes, in the absence and in the presence of trodusquemine. These membranes exhibit a phase separation between a fluid matrix (L_α), more disordered at the molecular level, and ordered domains (L_β) with larger thickness. Various quantitative information is obtained through the AFM images, in particular we have found that at low concentretions of trodusquemine (1-15 μM) the coexistence of the ordered and the disordered phases was preserved. This suggests that the typical trodusquemine concentrations found to be pharmacologically effective do not alter the membrane morphology essential for its biological function. Furthermore, we have performed force spectroscopy measurements on the membrane again using AFM. The analysis of force curves allowed us to obtain the bilayer breakthrough force, which is the maximum force that the bilayer can withstand before rupture, and the Young modulus, which represents the elasticity of the lipid layer. Compared to the absence of trodusquemine, in the presence of 5 μM trodusquemine an increase of the breakthrough force is observed, corresponding to an increase in the mechanical strength of the bilayer. This growth in resistance to indentation could contribute to increased resistance of the membranes to the toxic action of misfolded protein oligomers. Force spectroscopy measurements are in progress to determine the bilayer elastic modulus as a function of trodusquemine concentration.

1577-Pos
The Saponins Affect the Electrical Properties of the Lipid Bilayers
Svetlana S. Efimova, Olga S. Ostroumova.
Institute of Cytology of Russian Academy of Sciences, St Petersburg, Russian Federation.