Bilayers at the ILL

Contribution ID: **60** Type: **Poster**

Comparing molecular dynamics force fields in bacteria membranemModels

Wednesday, 11 December 2019 18:00 (15 minutes)

The cell membrane is a universal component found in both prokaryotic and eukaryotic cells, which is composed mainly of a series of lipid mixtures that act as a physical barrier against various pathogens, in addition to other functions that remain unknown. There is a large difference in the lipid composition of bacterial and mammalians cytoplasmic membranes, a fact that can be used to obtain antimicrobial selectivity. One of the most exciting advances in the scope of Molecular Dynamics (MD) simulations of bacterial membranes in the last years has been the development of molecular-level models that incorporate the heterogeneity of the non-protein constituents, and now frequently a mixture of phospholipids is used in simulation studies.[1,2] While MD simulations can provide invaluable detailed structural and dynamical information about the studied system, the crucial issue of the reliability of such simulations is the quality of the force field. Whereas much effort has been dedicated to parametrize and optimize the force fields for biomembrane modelling, most of the comparisons have been done for homogeneous bilayers composed of a single phospholipid type, which may not work optimally or even fail when used in description of complex in homogeneous systems.

We will present preliminary results obtained from the comparison of MD simulations of different homogeneous and heterogeneous bacterial membrane models using different force fields (Slipids, CHARMM36, GROMOS 54A7 and Lipid17). Models consisting of five hundred lipids each one was studied, as gram-positive bacteria mimetic model, POPE/POPG (1:3) as gram-negative mimetic model, POPE/POPG (3:1) and POPG/POPC (3:7) as well as homogeneous bilayer models to simulate neutral membrane systems, anionic membrane systems or the outer layer of the membranes will be used respectively POPE, POPG and POPC. For comparation: area per lipid, thickness, number of hydrogen bonds, lateral diffusion, order parameters, lateral density, radial distribution function and number of clusters were used. These results would be useful to understand the behaviour of lipids at atomistic-level at lipid-bilayer/water interfaces and provide a point of reference for making the appropriate decision on the force field in bacterial membrane models MD simulations.

References

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Session Classification: Wine & cheese poster session