Bilayers at the ILL

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Molecular dynamics simulations with cationic lipids

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Cationic lipids are widely used in modern drug delivery systems such as lipid nano-particles (LNPs). These drug carriers are multi-component systems (containing novel cationic lipids, cholesterol, phospholipids, siRNA/mRNA) with strongly pH-dependent structures, which are poorly characterized. Earlier experimental methods could provide the information about optimal sizes of LNPs, but their exact inner structures and mechanisms of actions were not determined.
In this work we use the combination of scattering techniques with multiscale computer simulations in order to refine structures of pharmaceutical LNPs and understand their pharmaco-kinetics. At the first step models for cationic lipids were developed for both neutral and ionized forms using the same methodology as the one which was employed for the derivation of atomistic SLipids force field. Parameters for lipids tails were adopted from the ones which were derived for polyunsaturated phospholipids and head-groups were mainly parametrized. Membranes containing cationic lipids and cholesterol were simulated using classical molecular dynamics (MD) approach employing newly delivered models at the ratio 50:38.5. From the preliminary analysis of MD trajectories it was observed that cholesterol molecules aggregate and water pores were formed in every simulated lipid bilayer. This information will be used for future simulations of more complex structures and the derivation of coarse-grained models.

Primary author(s) : ERMILOVA, Inna (Chalmers University of Technology); SWENSON, Jan (Chalmers University of Technology)

Presenter(s) : ERMILOVA, Inna (Chalmers University of Technology)

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