

RESORCINOLIC LIPIDS - DISTURB OR STABILIZE BIOLOGICAL MEMBRANES? MOLECULAR DYNAMICS SIMULATIONS

MAGDALENA E. SIWKO^{1*}, SIEWERT-JAN MARRINK², ARKADIUSZ KOZUBEK¹ and ALAN E. MARK²

¹University of Wrocław, Department of Lipids and Liposomes, Przybyszewskiego 63/77, 51-148 Wrocław, Poland, ²University of Groningen, Department of Biophysical Chemistry, Nijenborgh 4, 9747 AG Groningen, The Netherlands

Among many biological activities exerted by resorcinolic lipids very specific is their influence on the biological membranes. Experiments have shown that resorcinolic lipids have a dual effect on the cell membrane and also on the model membrane - liposome. Preincorporated, they occur stabilizing and ordering effect on the phospholipid membrane. The size of modified liposomes by resorcinols is kept unchanged much longer and marker is released much slower. If resorcinols are incorporated into liposomes suspension the instantaneous marker release and erythrocyte hemolysis is observed. Nowadays computer simulations methods are useful tool to understand the interaction of membranes and drugs and their influence on the disorder of the bilayer structure. We present the molecular dynamics simulations of phospholipid membrane with various homologs of resorcinolic lipids at the atomistic level and thereafter applying coarse grained model. A data from the simulations sustain experimental results. We observe increase of the order parameter and diminish area per lipid what suggests the growth of membrane stiffness when they are preincorporated. And also diffusion of water through the membrane is higher when resorcinol molecules are incorporated into the external leaflet from the water solution.

* E-mail: msiwko@ibmb.uni.wroc.pl