



***Book of Abstracts***

**Faculty of Pharmacy Comenius University in Bratislava**



COMENIUS UNIVERSITY IN BRATISLAVA  
FACULTY OF PHARMACY



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Book of Abstracts



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## Cation-induced changes to the structure of lipid membranes

Norbert Kučerka,<sup>1,2</sup> *Ermuhammad Dushanov*,<sup>2</sup> *Kholmirzo T. Kholmurodov*,<sup>2</sup> and *Daniela Uhríková*<sup>1</sup>

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Cell membrane properties such as membrane fluidity, bending and rigidity moduli, electrostatics, and aggregation and fusion are tightly associated with ions that are prevalent in both the cytosol and the exterior of the membrane. Interestingly, the divalent metal cations were found to play a dominant role in affecting bilayer structure. For example, it is well known that  $Zn^{2+}$  plays a fundamental role in several critical cellular functions such as protein metabolism, gene expression, structural and functional integrity of biomembranes, and in metabolic processes, while  $Ca^{2+}$  was shown to alter a bacterial membrane in a manner limiting its water penetration. The cation binding depends strongly on the property of the cation and the membrane lipid head-group.

We have studied the interactions of calcium and zinc with the biomimetic membrane made of dipalmitoyl-phosphatidylcholine (DPPC). The small angle neutron diffraction (SAND) experiment on oriented multilamellar samples was employed to decouple effects due to electrostatic interactions from those of geometrical constraints found in curved vesicular bilayers. Attained results show clearly differences in the effects of the two cations. For both, a bilayer thickness increases due to divalent metal ion ( $Me^{2+}$ ) binding, reaching the maximum at stoichiometry  $Me^{2+}:DPPC \sim 1:7$  mol/mol. However, while the further increase in  $Ca^{2+}$  results in a bilayer thinning down to the level of pure DPPC, the  $Zn^{2+}$  binding indicates the behavior of a typical isotherm, reaching a level of saturation.

Our observations compared to those obtained for curved bilayers agree well with the notion that the effect can most likely be rationalized in terms of electrostatic interactions, rather than that of geometrical constraints due to bilayer curvature, and thus reinforcing the special importance of these cations. The electronic structure of zinc is different from that of divalent alkaline earth metal ions. Zinc cation possesses a higher affinity to electronegative groups and therefore, also other electronegative moieties such as ester oxygens and/or carbonyl groups of the lipid headgroup can be directly involved in complex formation. The molecular dynamics simulations have been performed to gain more detailed information, results of which will also be discussed.

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