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Had a drink last night? How alcohol interacts with biological membranes MIKKO KARTTUNEN, Helsinki University of Technology, Finland, MICHAEL PATRA, Lund University, Sweden, EMPPU SALONEN, EMMA TERAMA, ILPO VATTULAINEN, Helsinki University of Technology, Finland, ROLAND FALLER, BRYAN LEE, University of California, Davis, JUHA HOLOPAINEN, University of Helsinki — We have performed extensive 100 ns molecular dynamics simulations to study the effect of methanol and ethanol on two different lipid bilayer systems (POPC and DPPC) in the fluid phase at 323 K [1,2]. We studied both structural changes induced by the alcohols and the dynamics of the system. It turned out that ethanol was able to penetrate the membranes whereas methanol was not able to do so. In particular, ethanol prefers to be accommodated in the vicinity of the lipid headgroup region. We also determined the dependence of lipid chain ordering on ethanol concentration and quite surprisingly found that to be non-monotonous. We explain that in terms of modified surface tension [2]. Finally, we determined lifetime of hydrogen bonds to be about 1 ns and found that be in excellent agreement with NMR results.

[1] B.W. Lee, et al, Fluid Phase Equilibria 225, 63-68 (2004)
[2] M. Patra et al, Biophys. J., in press 2005

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