# Mechanistic insights into the interaction of DMSO with DMPC lipid bilayers: Implications for the development of effective cryopreservation protocols

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## Abstract

We present molecular dynamics simulations of dimyristoylphosphatidylcholine (DMPC) lipid bilayers in the presence of dimethylsulfoxide (DMSO). The MD simulations focus on understanding the effect of 3 mol % DMSO on structural and permeation properties of DMPC bilayers. The potential of mean force (PMF) and the diffusivity profiles along the normal direction to the bilayer were calculated for water and DMSO molecules in systems containing 0 and 3 mol % DMSO. Our simulation results indicate that while the presence of DMSO has only a small effect on diffusion coefficients of both water and DMSO molecules, it affects significantly the corresponding trans-membrane free energy profiles. Using the free energy profiles and diffusivities for water and DMSO and by employing an inhomogeneous solubility-diffusion model we calculated the permeability coefficients. Our simulations show that the increase of the concentration of DMSO in the solution to 3 mol % leads to a significant increase, by about 3 times, of the permeability of water through a DMPC bilayer; a permeability increase that might explain in part the unusual ability of DMSO, even at relatively low concentrations, to reduce the osmotic pressure imbalance present during cryopreservation protocols.

*Work supported in part by the NSF-EPSCoR, LA-SiGMA Grant # EPS-1003897. Computer resources were provided by LONI and by HPC@LSU.