

Abstract Submitted  
for the MAR06 Meeting of  
The American Physical Society

**An Inside Look at Traube's Rule: A Molecular Dynamics Study**

ALLISON DICKEY, ROLAND FALLER, UC Davis — According to Traube's Rule [1], the alcohol concentration required to maintain the interfacial tension ( $\gamma$ ) of a bilayer is reduced by a factor of three for each additional  $\text{CH}_2$  group that is added to the alkyl chain of the alcohol. Recent experimental work confirmed that Traube's Rule applies to 1-stearoyl, 2-oleoyl phosphatidylcholine (SOPC) lipid bilayers that are exposed to alcohol solutions of methanol, ethanol, propanol, and butanol [2]. To examine the molecular mechanisms leading to Traube's Rule, we use molecular dynamics simulations to study the interactions between a dipalmitoylphosphatidylcholine (DPPC) bilayer and ethanol, propanol, and butanol solutions. We first examine how the bilayer structure variation depends on alcohol chain length via the area per lipid headgroup, lipid chain disorder, and electron distribution functions. We also study the alcohol dynamics within the bilayer by monitoring the time length, number, and location of hydrogen bonds. Lipid mean squared displacements are also calculated to determine the extent to which lipid mobility is affected by alcohols.

- [1] I. Traube Liebigs Annalen (1891)
- [2] H. Ly, M. Longo Biophys J (2004)

Roland Faller  
UC Davis

Date submitted: 15 Nov 2005

Electronic form version 1.4