

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Interactions between non-steroidal anti-inflammatory drugs and lipid membranes¹ MOHAN BOGGARA, RAMANAN KRISHNAMOORTI, Dept of Chemical and Biomolecular Engg., Univ of Houston — Chronic usage of Non-steroidal anti-inflammatory drugs(NSAIDs) leads to gastrointestinal toxicity and clinical evidences point the cause to direct interactions between NSAIDs and phospholipid membranes. Also, NSAIDs pre-associated with phospholipid vesicles are shown to be safer and therapeutically more effective than unmodified ones. Our initial experiments and simulations on the partitioning of Aspirin and Ibuprofen clearly indicate role played by the drug structure in drug-membrane interactions. Those results motivated systematic molecular dynamics simulations of membranes with NSAIDs of different size, structure and pKa values. Our results suggest high partition coefficients for these NSAIDs in the membrane compared to water and thinning effect on the bilayer. Our small angle neutron scattering and reflectivity studies on DMPC-Ibuprofen systems indicate that the drug affects both ~ 5 nm thick bilayer and overall ~ 100 nm diameter vesicle, indicating that NSAIDs affect vesicles on various length scales. We will discuss the structural perturbations to membranes due to NSAIDs at clinically relevant molar ratios and their implications on the use of vesicles as delivery vehicles for NSAIDs.

¹NIST Center for Neutron Research is duly acknowledged.

Mohan Boggara
University of Houston

Date submitted: 29 Nov 2007

Electronic form version 1.4