

Abstract Submitted
for the SES05 Meeting of
The American Physical Society

Indole Localization in an Explicit Bilayer Revealed via Molecular Dynamics KRISTEN NORMAN, HUGH NYMEYER, Florida State University — It is well known that the amino-acid tryptophan is particularly stable in the interfacial region of biological membranes, and this preference is a property of the tryptophan side-chain. Analogues of this side-chain, such as indole, strongly localize in the interfacial region, especially near the glycerol moiety of the lipids in the bilayer. Using molecular dynamics calculations, we determine the potential of mean force (PMF) for indoles in the bilayer. We compare the calculated PMF for indole with that of benzene to show that exclusion from the center of the lipid bilayer does not occur in all aromatics, but is strong in indoles. We find three minima in the PMF. Indole is most stabilized near the glycerol moiety. A weaker binding location is found near the choline groups of the lipid molecules. An even weaker binding site is found near the center of the lipid hydrocarbon core. Comparisons between uncharged, weakly charged, and highly charged indoles demonstrate that the exclusion is caused by the charge distribution on the indole rather than the “lipo-phobic” effect. High temperature simulations are used to determine the relative contribution of enthalpy and entropy to indole localization. The orientation of indole is found to be largely charge independent and is a strong function of depth within the bilayer. We find good agreement between simulated S_{CD} order parameters for indole and experimentally determined order parameters.

Hugh Nymeyer
Florida State University

Date submitted: 09 Aug 2005

Electronic form version 1.4