Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Membrane Disruption Effects of antimicrobial Peptide Protegrin-1 HAO WANG, JAMES KINDT, Department of Chemistry, Emory University, Atlanta, Georgia 30322, USA — Molecular dynamics simulations have been performed to better understand membrane disruption induced by antimicrobial peptide Protegrin-1 (PG-1). Two distinct setups were adopted for atomistic simulations for DMPC/PG-1 systems. One started from bilayered ribbons either with or without the PG-1 peptides embedded and another one started from random lipid mixtures in the presence of the PG-1 peptides. Line tensions deduced from the ribbon simulations were generally lower with the PG-1 peptides embedded in ribbon edge, which supports edge-active role of the peptides. The random mixtures self-assembled into various structures. Extended simulations are being carried out to investigate the relation between concentration of the PG-1 peptides and the resultant structures. Furthermore, coarse-grained models have been used to simulate larger DMPC bilayers with the PG-1 peptides embedded. The PG-1 peptides were found to self-assemble into clusters. However, pore formation was not observed within our simulation period up to 3 microseconds. (DMPC: 1,2-Dimyristoyl-sn-Glycero-3-Phosphocholine)

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Date submitted: 30 Nov 2008 Electronic form version 1.4