Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Molecular Dynamics study on the Micellization of Rhamnolipids.
ELANGO MUNUSAMY, STEVEN D. SCHWARTZ, Department of Chemistry and Biochemistry, University of Arizona, Tucson, AZ 85721 — Oil spills have become one of the most serious environmental and ecological problems owing to the growth of oil exploration, production and transportation. Millions of gallons of crude oil and refined products are spilled into marine waters worldwide each year. Large volumes of surfactants are applied to the ocean as a remediation strategy. Environmental and toxicity issues arise when such a voluminous amounts of chemical surfactants are applied. One prospective solution to this problem is to use greener surfactants that possess excellent biodegradation and toxicity characteristics relative to existing classes of commonly used surfactants. In this context, we are interested in designing and developing greener surfactants that are patterned after naturally occurring glycolipids. In the present work, we concentrate on one of the more commonly studied glycolipid, rhamnolipid ($Rha_1C_{10}C_{10}$). Despite the available experimental data, the molecular structure, shape and geometry of micelles formed by rhamnolipid is unknown. Molecular Dynamics (MD) simulations were performed to understand the aggregation behavior of rhamnolipids in aqueous solution and at air-water interface. All calculations were performed in NPT ensembles at 300 K using NAMD 2.8, a parallel code designed for high-performance simulation of large biological macromolecule using the CHARMM force field. The results obtained from MD simulations on the aggregation of rhamnolipids in water and at air-water interface will be presented.

Elango Munusamy
Department of Chemistry and Biochemistry,
University of Arizona, Tucson, AZ 85721

Date submitted: 14 Nov 2014 Electronic form version 1.4