Molecular Dynamics study on the Micellization of Rhamnolipids.
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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 gly-
colipids. In the present work, we concentrate on one of the more commonly studied
glycolipid, rhamnolipid (Rha\textsubscript{1}C\textsubscript{10}C\textsubscript{10}). Despite the available experimental data, the
molecular structure, shape and geometry of micelles formed by rhamnolipid is un-
known. 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 par-
allel 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.