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Effect of Ion Binding in Palmitoyl-Oleoyl Phosphatidylserine Monolayers MATTHEW ECKLER, SILVINA MATYSIAK, University of Maryland - College Park — Molecular dynamics simulations of palmitoyl-oleoyl phosphatidylserine (POPS) monolayers at the air-water interface were performed with different ionic strengths with the aim of determining the specific organization and dynamics of counterion binding events. Na+ ions penetrated the monolayers into both the ester carbonyl and carboxylate regions of the phospholipids. The binding events increase with the addition of salt. Differences in lipid order parameter, headgroup orientation, and prevalence of inter- and intramolecular hydrogen bonding events between the amine group of the lipid and oxygen groups are observed depending on whether the Na+ is binding near the carboxylate or ester region of the lipid. The observed changes are explained in terms of the salting-out effect.

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