

The structural properties of a palmitic acid ( $\text{CH}_3(\text{CH}_2)_{14}\text{COOH}$ ) monolayer at the water-air interface are investigated in the present study via analysis of molecular dynamics simulation trajectories. The values are compared to known relevant experimental and computer simulation results, finding good agreement in terms of tilt angle of the chains, monolayer density profiles, and monolayer thickness. The alkyl chain length distribution for palmitic acid was found bimodal and the phenomenon was attributed to the  $\text{C}^1\text{-C}^2\text{-C}^3\text{-C}^4$  dihedral angle distribution. Simulations of 1-hexadecanol were carried out for comparison.