

Using the classical molecular dynamics simulations, the interfacial partitioning of selected aromatic species, namely benzoic acid and neutral and zwitterionic form of L-phenylalanine, was studied in the three slab systems: a) aqueous organics solution, b) palmitic acid monolayer in tilted condensed phase at aqueous organics solution and c) palmitic acid monolayer in tilted condensed - 2D gas phase coexistence at aqueous organics solution. The surface activity and the tendency to aggregate in particular at the air-aqueous and palmitic acid-aqueous interface was confirmed for all of the investigated aromatic species. The results of the simulation performed for the system of palmitic acid monolayer at benzoic acid solution were compared with the literature results of a similar simulation that employed a different parametrization. The comparison showed that the behaviour of the aromatic species at the fatty acid monolayer-aqueous interface strongly depends on the force field. The structural properties of the palmitic acid Langmuir monolayers were evaluated by means of the chain tilt angle and the headgroup region dihedral angle distributions analysis depending on the surface film density and the adsorbed aromatic species. The simulations mimicking the isothermal compression of the mixed monolayer in the Langmuir trough resulted in the formation of a highly ordered L-phenylalanine cluster in a pore within the monolayer. The present simulations provided molecular level information relevant for the recently published experimental findings on mixed aromatic-aliphatic surfactant films.