The aim of the thesis is to get insight into the interactions between amino acids with a hydrophobic side-chain and a phospholipid monolayer on the water-air interface via molecular dynamics. There were three simulations performed: a) simulation of leucine in aqueous solution, b) simulation of leucine at the solution - air interface c) simulation of leucine solution with DPPC phospholipid monolayer at its surface. These simulations demonstrate that leucine shows surface activity and tendency to aggregate, particularly at the water surface. This tendency also remains in the presence of DPPC monolayer. In addition, intercalation of leucine between DPPC molecules was observed, leading to creation of small pores in the DPPC monolayer. The results of the simulation with leucine were compared with the results of a previously done analogous simulation with phenylalanine. The comparison showed that phenylalanine penetrates into the DPPC monolayer more than leucine, however the depth of penetration between DPPC molecules is almost the same for both amino acids.