

Amino acid phenylalanine plays a key role in numerous biological processes and is also involved in amyloid fibril diseases. The aim of the thesis is to deepen our understanding of its behavior and partitioning at interfaces, and to investigate its clustering. Classical atomistic molecular dynamics simulations were performed for phenylalanine and three other aromatic molecules which chemical structure is derived from it - phenylglycine, phenylacetic acid and tyrosine. Molecules are simulated at both water-air and at water-DPPC-air interfaces. Phenylalanine, phenylglycine and phenylacetic acid demonstrate surface activity at the water-air interface, whereas tyrosine is not surface active. All molecules interact with the lipid monolayer at the water-DPPC-air interface but only phenylalanine penetrates deep into the monolayer. Formation of transient clusters is observed in the interfacial regions, mostly for phenylalanine.