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Structural analysis of the nanostructures formed aromatic aminoacids

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In this work we have analyzed the nanostructures formed by tyrosine, tryptophan and phenylalanine, which have aromatic rings, in our molecular dynamics simulations. We have focused on the similarities and differences of these structures. The simulations are done by using Gromacs Molecular Dynamics simulation software. The force field chosen is OPLS-AA force field. The water molecules are included by TIP3P explicit water molecules. After NVT and NPT equilibration runs we have simulated the systems minimum up to 300 ns. The Berendsen thermostat kept temperature constant and the Parrinello-Rahman algorithm held the pressure at 1 bar. The integration step for all simulations was 2 fs. We have seen that concentration, temperature and acidity play an important role in obtaining the nanostructures. The structures seen are aggregated ones, crsytal-like one and 4-fold tubular ones. In each case of the pure systems the occurrences of these structures are often at different set of parameters. There are some differences of the structures with respect to the stability of the formed structure and the time to reach the equilibration. Furthermore, differently from our previous works, we have seen that one finds the structural similarities and differences between of the pure systems.

Biography

Sahin Uyaver has completed his PhD from Potsdam University, Germany. He has been working mainly computational researches on biophysical systems. Currently he is a Member of the Faculty of Science at Turkish-German University of Istanbul.

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