Self-Assembly of Diphenylalanine and Chemically Modified Diphenylalanine Peptides on Various Solvents

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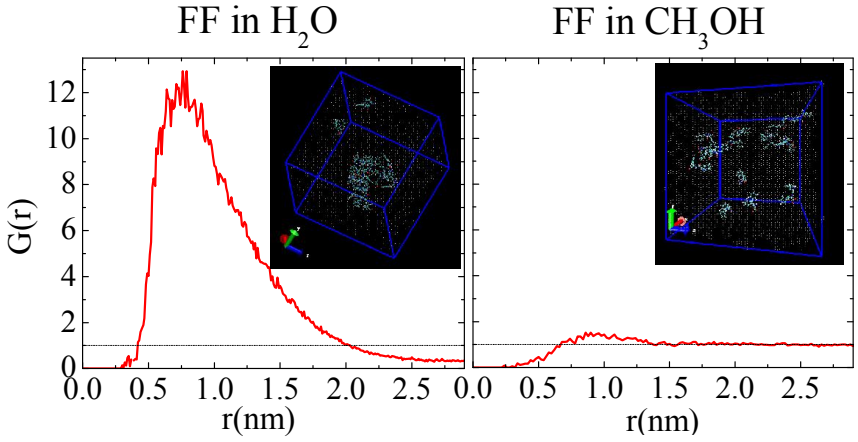
Diphenylalanine (FF) is a very common peptide with many potential applications, both biological and technological, due to a large number of different nanostructures which it attains. The current work concerns a detailed study of the self-assembled structures of FF in two different solvents, an aqueous (H_2O) and an organic (CH_3OH) through simulations and experiments. Detailed atomistic Molecular Dynamics (MD) simulations of FF in both solvents have been performed, using an explicit solvent model. The self -assembling propensity of FF in water is obvious while, in methanol a very weak self -assembling propensity is observed. We studied and compared structural properties of FF in the two different solvents and a comparison with a system of dialanine (AA) in the corresponding solvents was also performed. In addition, temperature dependence studies were carried out. The simulation predictions were compared to new experimental data, which were produced in the framework of the present work. Good qualitative agreement between simulation and experimental observations was found.



In the above figure the pair radial distribution function (rdf) calculated for the center of mass (cm) of peptides: (*left*) FF-FF in water and (*right*) FF-FF in methanol, at *T=300K* and *c=0.0385grFF/(cm*^{3}solvent) is presented. In the insets snapshots of FF in the corresponding solvents are shown. The difference between the two curves indicates the tendency for aggregation

of FF peptides in water in contrast to their behavior in methanol as is obvious in the snapshots as well.

On top of that experimental observations indicate that the properties of FF peptide can be modulated by N-termini blocking amino acid changes, or conjugation to other chemical moieties. Further simulations have been performed on two types of chemically modified diphenylalanine peptides named as Boc-FF and Fmoc-FF in water and their differences have been reported. Comparisons with FF-water solutions have been performed as well. Moreover mixed water-ethanol solutions are of particular interest. Experimental findings on Boc-FF show a nucleation process in multi-steps, starting from nanospheres, which then undergo ripening and structural conversions to form the final supramolecular assemblies, depending on the concentration ratio of the two solvents. Simulation studies of these systems are will be presented.

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