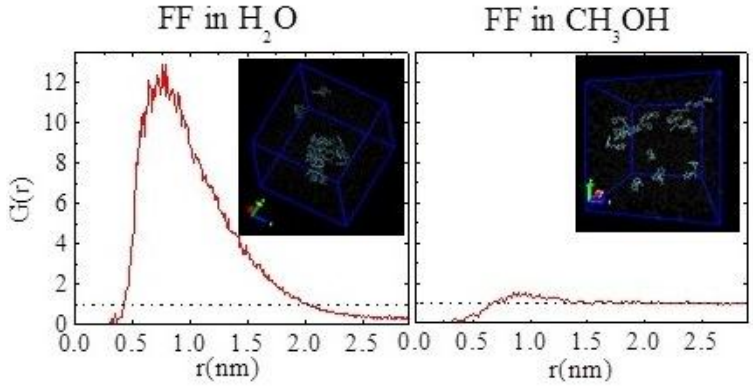
P.06 Effect of solvent on the self-assembly of Dialanine and Diphenylalanine Peptides

A N Rissanou[1,2], E Georgilis[3], E Kasotakis[3], A Mitraki[3,4] and V Harmandaris[1,2]

[1]Department of Applied Mathematics, University of Crete, Greece, [2]IACM FORTH, Greece, [3]Department of Materials Science and Technology, University of Crete, Greece, [4]Institute for Electronic Structure and Laser, FORTH, Greece

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. Finally, the simulation predictions were compared to new experimental data, which were produced in the framework of the present work. A very 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^3solvent) is presented. In the insets snapshots of FF in the corresponding solvents are shown.

[1] Rissanou, A. N.; Georgilis, E.; Kasotakis, E.; Mitraki, A.; Harmandaris, V., *Journal of Physical Chemistry B* 2013, *117*(15), 3962-75

[2] Tamamis, P.; Adler-Abramovich, L.; Reches, M.; Marshall, K.; Sikorski, P.; Serpell, L.; Gazit, E.; Archontis, G., *Biophys. J.* 2009, *96*, 5020-5029

[3] Villa, A.; van der Vegt, N. F. A.; Peter, C., *Phys. Chem. Chem Phys*. 2009, *11*, 2068-2076