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Τίτλος

**«Μελέτη Αυτο-οργάνωσης Boc-FF και Fmoc-FF
Ολιγοπεπτιδίων με Ατομιστικές Προσομοιώσεις Μοριακής
Δυναμικής»**

**«Study of Self-assembly of Boc-FF and Fmoc-FF
Oligopeptides through Atomistic Molecular Dynamics
Simulations»**

Τζέλη Δέσποινα

Μεταπτυχιακή Φοιτήτρια

Τμήματος Επιστήμης και Τεχνολογίας Υλικών, Πανεπιστημίου Κρήτης

Επιβλέπουσα Καθηγήτρια κ. Α. Μητράκη

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Αίθουσα A115, Κτίριο Τμήματος Επιστήμης Υπολογιστών,

Πανεπιστήμιο Κρήτης

Abstract

Diphenylalanine (FF) and chemically modified FF-peptides are very common peptides with many potential applications, both biological and technological, due to a large number of different nanostructures which they attain.

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. Simulations have been performed on two types of chemically modified diphenylalanine peptides named as Fmoc-FF and Boc-FF in water and their differences have been reported. Comparisons with FF-water solutions have been performed as well. Experimental findings on Boc-FF in a mixture of water and ethanol 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. On top of that Fmoc-FF peptide have been observed to form hydrogel under physiological conditions.

The current work concerns a detailed study of the self-assembled structures of Fmoc-FF in an aqueous (H₂O) through simulations. Detailed atomistic Molecular Dynamics (MD) simulations of Fmoc-FF in water have been performed, using an explicit solvent model. The self-assembling propensity of Fmoc-FF in water is obvious. We studied structural properties of Fmoc-FF in water and a comparison with a system of

diphenylalanine (FF) in the corresponding solvent was performed. In addition, temperature dependence studies were carried out. The simulation predictions were compared to new experimental data, which have shown that Fmoc-FF peptide forms hydrogel under physiological conditions. Good qualitative agreement between simulation and experimental observations was found. Simulations of Boc-FF peptides are in progress.