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Computational analysis of the intermolecular interaction driving the self-assembly of collagen

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Collagen self-assembly is an important phenomenon generating the biological alloy ECM and the structural/functional diversity of different tissue types. We explored the question of how the amino acid sequence determines structure resulted from the self-assembly. Studies investigating the collagen intermolecular interactions are mostly based on the experimental host-guest peptides representing small part of collagen alpha chain and their pairwise interaction. By the combination of given protein primary structures and the programming language python, we investigated the three main types of interaction including hydrophobic, polar, and electrostatic between molecules by taking the physicochemical properties of side chains in a certain range. D-periodic staggered arrangement of collagen molecules in fibrils is clarified by taking the amino acid sequence and calculating the corresponding interaction sliding one molecule another. Our amino acid based computational analysis provides a wide range of application to investigate the sequence effect on the structure and to understand the characterization of interactions and stabilization of other fibrillar macromolecules.

Biography

Esma Eryilmaz has completed her graduation in Physics and MS in Molecular Physics from Selcuk University, Turkey. She has completed her PhD from Texas A&M University Biophysics & Biomedical Engineering with a PhD fellowship by Turkish Ministry of Education in December 2015. She is an Assistant Professor at Selcuk University, Turkey and has published articles in both national and international refereed journals. Her research interest includes "self-assembly mechanism of biomolecules, intermolecular interactions, biomaterials and bioinformatics approaches".

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