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Kinematic analyzing for a series of amino acids as an arm of nano-actuator

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Background and Aims: Bio nano-robotics is a prosperous technology which is expected to have a significant impact on medical sciences at the present time and in future. In this paper, molecular kinematic simulation is developed to analyze the geometric properties and conformational space of a string of amino acids for 2ZQM Pefoldin. 2ZQM Pefoldin is a heterohexameric molecular chaperone and forms a jellyfish-like structure.
Methods: Protein's functions are inherently correlated with their structures, therefore, the accuracy of secondary structure prediction is important for modeling the three dimensional structure of proteins. In this paper, the algorithm for analyzing the conformation space of molecular chains using Denavit-Hartenberg formulation is presented. Proteins are made up 20 different types of amino acids. The back-bone of amino acids is composed of three atoms (N-Cα-C) that connecting in a series such as a serial manipulator.The C-N bond joins two consecutive amino acids has a partial double-bond character, thus, is non-rotatable. Unlike C-N bond, N-Cα and Cα-C bonds are free to rotate.
Results: The dihedral angles are varied within the allowable ranges based on the Ramachandran plot and calculate the conformation of prefoldin. For instance, varying the first angle (N-CA bond) of amino acid 62 for this series of amino acids from -101.55 to -61.67 results in the coordinate change of the last atom of the corresponding arm from (9.49, 35.60, 29.64) to (-12.62, 33.41, 31.62) and changing this angle from 101.55 to -161.7 result in the coordinate change of the same atom from (9.49, 35.60, 29.64) to (50.79, 14.84, 35.91).
Conclusions: In this paper, a string of amino acids that made a branch of 2ZQM Prefoldin is considered as an arm of nano-actuator.The results show how molecular kinematic simulation can predict the coordinates of atoms and protein structure by changing the dihedral angles in allowable range.

Keywords: Bionanotechnology; Secondary structure; Molecular kinematic; Conformational space