

Methods for Quantitative Analysis of the Chirality of Protein Helical and Superhelical Structures

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Abstract: In this paper, we propose the methods for quantitative analysis of protein helical and superhelical structure chirality. A necessary and sufficient condition is the mutual arrangement of α -carbons, which allows a reduction of the amount of processed information and is a clear advantage when processing large data arrays. The analysis of the chirality sign of the protein helical structures is based on determining the mixed product of every three consecutive vectors between neighboring reference points - α -carbon atoms. The skeleton of α -carbons and the helix axis are directed from the C-terminus to the N-terminus. Structures of α -helices, 3-10-helices, π -helices, and polyprolines are considered. The method for evaluating the chirality sign of coiled coil structures is based on determining the direction and value of the angle between the coiled coil axis and the α -helices axes. The chirality sign of the coiled coil is calculated by averaging the value of the cosine of the corresponding angle for all helices forming the superhelix. The estimate of the chirality sign of the superhelix is calculated by averaging the cosine value of the corresponding angle for all helices forming the superhelix. The calculation for collagens is performed similarly. Chirality maps of helical and superhelical protein structures are presented. Based on the methods, computer programs in Python 3.7 are implemented. The programs allow to load a model from a file, display a list of helical structures, determine the sign of their chirality, and display a three-dimensional image using the matplotlib library. Input data are files with .pdb or .txt extension. The results obtained adequately reflect the data presented in the scientific literature. These approaches, tested on protein helical structures, are planned to be further developed for the β -structures and irregular secondary structures analysis.

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