SEMINAR

On July 3, 2018, at 2:00 pm, in room 218 at the Institute of Information and Communication Technologies, BAS, Acad. G. Bonchev St., Block 25 A, **Ms. Yanzhen Hou, PhD Student at Beijing Institute of Technology (PR China)**, will give a presentation on:

A New 3D Visualization Method for Protein Structure Analysis

Abstract

In theoretical studies, the shape of a protein is usually modelled by the C_α atoms of its backbone referring to extrinsic geometry or intrinsic structures determined by the peptide planes. Different from all of them, here we develop a new 3D methodology for analysis and visualization of protein structure, based on the construction of series of right-handed orthonormal coordinate systems, along the intrinsic structures determined by protein side chains. Our method is validated by analyzing the *cis* peptide planes among all resolved structures in Protein Data Bank and the histidine residues in myoglobin, the results being in good agreement with actual biological structures. Therefore, our method can be employed as a valuable visual tool for protein side chain construction as well as for structure validation and refinement, complementary to widely used visualization tools like VMD, Jmol, PyMOL and backbone-based representations like Frenet, Bishop, and Ramachandran coordinates.