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Finding a strict relationship between distribution of residues in a sequence and protein fold

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The goal of this research is to find rules that describe the relationship between distribution of residues in a sequence and structural characteristics of a protein. The residue distribution rules identify 'key residues' that have to occupy certain positions in a sequence in order for polypeptide chain to form into a particular protein fold. The rules also specify which residues are 'unfavorable', i.e. incompatible with a given fold. These rules are based on statistical analysis of residue variability at different positions in polypeptide chains and investigation of residue-residue contact maps of proteins from different protein families but with similar structures. Our analysis focuses on beta proteins that are characterized by a specific arrangement of beta-strands in two beta sheets. These so-called 'sandwich structures' are typical of immunoglobulins, different types of cell receptors and many other proteins. We describe residue distribution rules for sandwich proteins and show that they allow one to correctly identify ~75% of sandwich proteins. The advantage of our approach is that it makes possible prediction of protein fold even in polypeptide chains that have very low global sequence similarities. Another potential benefit is that better understanding of which residues play essential roles for a given protein fold may facilitate rational protein engineering design.

Biography

Alexander Kister graduated from Moscow State University with a degree in Chemistry and received Ph.D in Biophysics from the Institute of Biophysics (Pushino, Russia). He worked in the National Institute of Genetics, in Moscow, Russia; Dana-Farber Cancer Institute in Boston; School of Health-Related Professions, University of Medicine and Dentistry of New Jersey; and now in the Department of Mathematics, Rutgers University, Piscataway, NJ. He has published about 90 papers in peer-reviewed journals, authored chapters in several books and an entry on "Immunoglobulin Fold" in Encyclopedia of Life Sciences, and is an editor of a volume on 'Supersecondary Structure of Proteins' in Methods in Molecular Biology (Springer).

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