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PharmaDesign and CBRC develop software to predict disorder regions in proteins

We are pleased to announce that PharmaDesign Inc. (Tokyo, Japan) and Protein Function team lead by Dr. Tamotsu Noguchi at Computational Biology Research Center (CBRC) of National Institute of Advanced Industrial Science and Technology (AIST), has developed POODLE (Prediction Of Orders and Disorder by machine LEarning), a new method to predict disorder regions (amino acid sequences that do not form certain three-dimensional structures) in proteins. POODLE has higher accuracy in prediction of disorder regions than existing methods, and will make protein structure analysis including X-ray crystallography and NMR analysis more effective.

It is well known that proteins need to form their unique three-dimensional structures in order to interact with other molecules and function properly. Enormous time and labors have been spent to solve those structures.

However, it has been experimentally proven that some sequences that do not form certain three-dimensional structures (hence called disorder regions or natively unfolded regions) play important roles especially in higher organisms. Many of them have been discovered in proteins involved in gene transcription and DNA binding proteins. Therefore, it is considered very important to unravel relationships between the disorder regions and their functions in terms of understanding proteins' functionality. In addition, since the disorder regions are known to prevent crystallization and spectral assignment, removing them beforehand will make analysis much easier. Thus, accurate prediction of the disorder regions has become very important in both structure and function analysis of proteins.

POODLE will be available online for free of charge at the CBRC website (<http://mbs.cbrc.jp/poodle>) from August 10, 2006, and its on-site version will become available from PharmaDesign this coming fall (pricing to be determined). PharmaDesign will start contract research services to identify disorder regions using POODLE as well as some other programs.

PharmaDesign also is scheduled to release a peptide library aimed for drug discovery based on the same disorder region prediction this coming December.

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