Study predicts, verifies protein folding

October 4 2005

Houston scientists have combined theory and experiment for the first time to predict and verify protein-folding dynamics of a complex protein.

"Researchers have successfully combined computer modeling and experimental results in folding studies for small proteins, but this is the first effective combination for a large, multi-domain protein," said study co-author Kathleen Matthews, dean of Rice University's Wiess School of Natural Sciences.

Each cell in the human body contains thousands of proteins. A protein's function is tied to shape and every protein self-assembles into its characteristic shape within seconds of being created.

"The folded, functional form of the protein is what really matters, and our interest is in creating a folding roadmap of sorts, a plot of the thermodynamic route that the protein follows as it moves toward equilibrium," said co-author Cecilia Clementi, an assistant professor of chemistry.

The research appears in the Proceedings of the National Academy of Sciences.