

Invention unravels mystery of protein folding

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An Oak Ridge National Laboratory invention able to quickly predict three-dimensional structure of protein could have huge implications for drug discovery and human health.

While scientists have long studied [protein](#) structure and the mechanism of folding, this marks the first time they are able to computationally predict three-dimensional structure independent of size of the protein. Because the invention also determines possible intermediate states in the protein folding process, it provides a clearer picture and could open doors to designing new medicines for [neurodegenerative diseases](#) that are caused by incorrectly folded proteins.

Pratul Agarwal, inventor of the method and a member of the Department of Energy lab's Computer Science and Mathematics Division, believes this new method will provide benefits in many areas.

"This finding is relevant to energy, climate and health, which are all of tremendous significance today," Agarwal said. "We expect this approach to have many industrial applications through [protein engineering](#), for example, where we expect to be able to design more efficient enzymes."

Proteins often adopt a three-dimensional structure that allows them to carry out their designated function, but such a structure has provided a computationally challenging task. Using the fundamental insights of the protein structure, dynamics and function, the ORNL invention discloses a unique computational methodology to explore the conformational energy landscape of a protein.

"One of the main advantages of this approach is that it follows the natural intrinsic dynamics of the protein and by promoting the relevant dynamical modes allows rapid exploration of the folding pathway and prediction of the [protein structure](#)," Agarwal said.

In the area of drug development, Agarwal, a computational biophysicist, expects this discovery to help in the development of treatments with little or no side effects.

More information: This work is reflected in two recent papers published in *PLoS ONE* ("Discovering conformational sub-states relevant to protein function") and *The Journal of Physical Chemistry B* ("Redox-Promoting Protein Motions in Rubredoxin").

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Provided by Oak Ridge National Laboratory

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