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BITS Pilani unveils AI tool for accurate prediction of DNA-binding residues

27 October 2026 | News

Accurately predicts DNA-interacting protein regions across both structured and intrinsically disordered segments

An international research study co-authored by Dr Sushmita Basu, Assistant Professor at Birla Institute of Technology and Science (BITS) Pilani, has developed DNAreader, an advanced AI-driven tool designed to identify the specific parts of proteins that interact with DNA in both structured and flexible regions.

The project was led by scientists at Virginia Commonwealth University (USA) and Xinyang Normal University (China) in collaboration with Hebei University of Technology (China).

Published in the prestigious journal Nucleic Acids Research, the study addresses an important challenge in understanding how proteins interact with DNA. These interactions are vital for processes such as controlling gene activity, copying and repairing DNA, and maintaining the organization of genetic material. However, identifying the exact parts of proteins involved in these interactions can be challenging, particularly in proteins that lack a fixed structure.

To solve this, the research team, developed a first-of-its-kind tool optimised to predict DNA-binding residues in both structured and disordered protein regions. Another challenge with existing DNA prediction tools is that they often incorrectly identify residues that interact with non-DNA molecules as DNA-binding residues.

DNAreader addresses this challenge through two combined innovations: A specially designed batch-training strategy that exposes the model to balanced examples of DNA-binding, other-ligand-binding and non-binding residues in both structured and disordered regions; A contrastive learning approach that sharpens the model's ability to distinguish between these residue types.