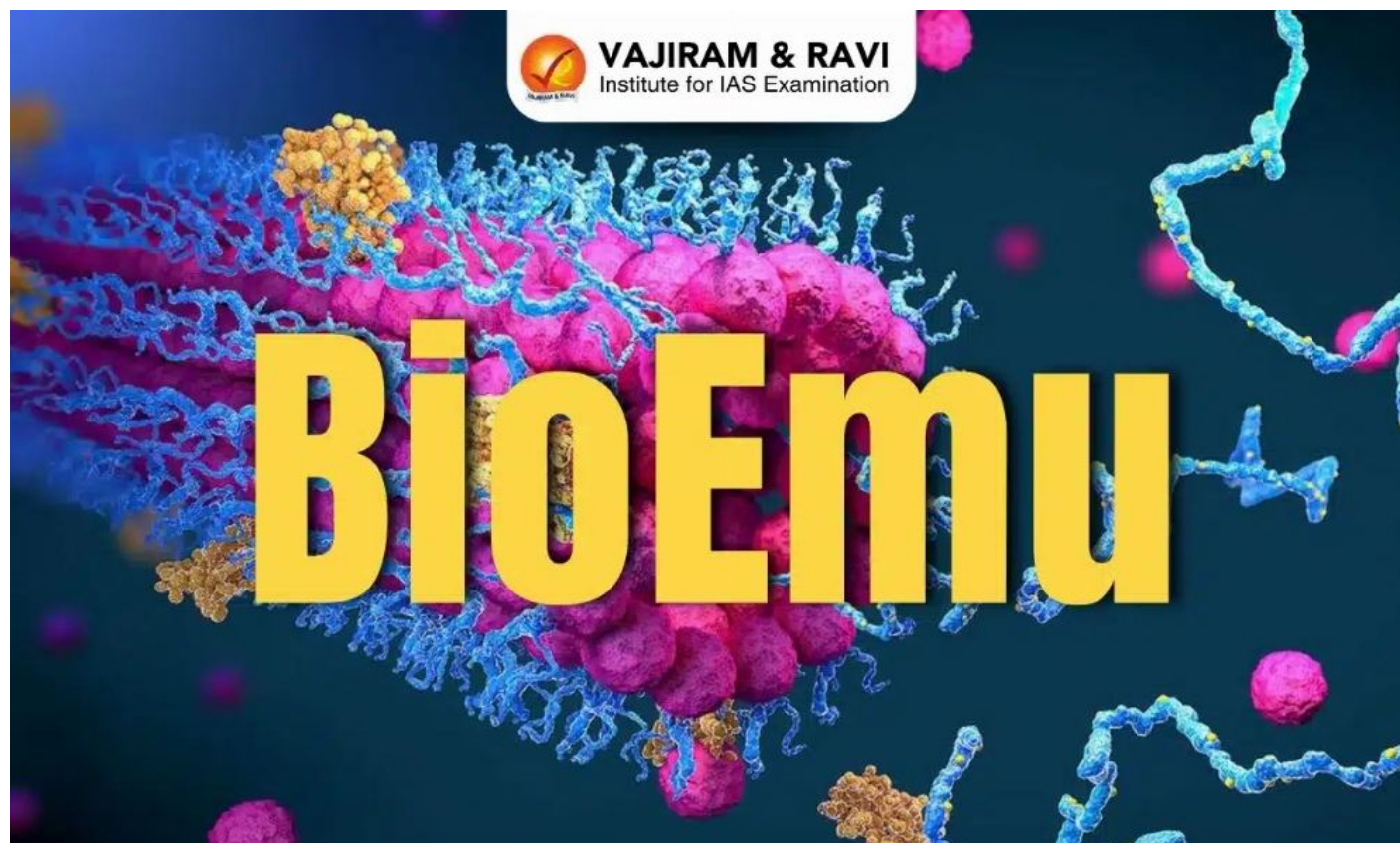


BioEmu

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BioEmu Latest News

A new deep learning system called BioEmu predicts the full range of shapes a protein naturally explores under biological conditions.

About BioEmu

- **Biomolecular Emulator** (BioEmu for short) is a generative **deep learning system**.
- It can **generate** thousands of statistically independent samples from the **protein structure ensemble** per hour on a single graphical processing unit
- It is a model that samples from the approximated **equilibrium distribution** of structures for a **protein monomer**, given its amino acid sequence.
- **Developed by:** It is **developed by Microsoft** and researchers at Rice University in the US and Freie Universität in Germany.

Working of BioEmu

- It **predicts the full range of shapes a protein** naturally explores under biological conditions.
- It promises to be faster and cheaper than classical approaches at predicting protein function
- It allows **high-resolution** protein flexibility modelling at scale, unlike slower, more classical approaches like **molecular dynamics (MD) which is slow and costly.**
- It captures large shape changes in enzymes, local unfolding that switches proteins on or off, and fleeting cryptic pockets, temporary crevices that can serve as drug docking sites, like in the cancer-linked protein Ras.
- It predicts 83% of large shifts and 70-81% of small changes accurately, including open and closed forms of a vital enzyme called adenylate kinase.
- It also handled **hard to predict proteins** that don't have a fixed 3D structure and how **mutations affect protein stability.**
- It quickly generates snapshots of all the stable shapes a protein is likely to adopt. It can **produce thousands of these structures** in minutes to hours on a single GPU.
- BioEmu **can't model cell walls**, drug molecules, **pH changes** or show prediction reliability like AlphaFold and also can't handle **temperature shifts, membranes**, and other conditions.

Source: TH

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