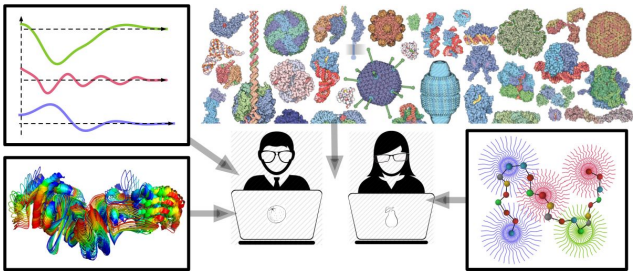

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From Interaction Prediction to Sequence Design: Unveiling PeSTo's Potential in Structural Biology

Wednesday, 14 February 2024 17:45 (30 minutes)

In the field of structural biology, predicting protein interactions and designing sequences based on backbone scaffolds remain pivotal yet challenging tasks. Built on the same deep learning architectural framework, Protein Structure Transformer (PeSTo) and its derivative, CARBonAra, address these challenges. PeSTo employs geometric transformers to proficiently predict diverse protein binding interfaces, setting a new benchmark in accuracy and computational efficiency. It enables high-throughput analyses and is compatible with the expansive AlphaFold foldome. CARBonAra, adapted from PeSTo, specializes in sequence recovery from backbone scaffolds and uniquely accounts for non-protein entities like nucleic acids and ligands. These methods combine speed, accuracy, and wide applicability, offering promising avenues for advancements in structural biology and biotechnology.

https://www.nature.com/articles/s41467-023-37701-8
https://www.biorxiv.org/content/10.1101/2023.06.19.545381v1

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