

Challenges in Bridging the Gap Between Protein Structure Prediction and Functional Interpretation

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June 30, 2023

Abstract

The rapid evolution of protein structure prediction tools has significantly broadened access to protein structural data. Although predicted structure models have the potential to accelerate and impact fundamental and translational research significantly, it is essential to note that they are not validated and cannot be considered the ground truth. Thus, challenges persist, particularly in capturing protein dynamics, predicting multi-chain structures, interpreting protein function, and assessing model quality. Interdisciplinary collaborations are crucial to overcoming these obstacles. Databases like the AlphaFold Protein Structure Database, the ESM Metagenomic Atlas, and initiatives like the 3D-Beacons Network provide FAIR access to these data, enabling their interpretation and application across a broader scientific community. Whilst substantial advancements have been made in protein structure prediction, further progress is required to address the remaining challenges. Developing training materials, nurturing collaborations, and ensuring open data sharing will be paramount in this pursuit. The continued evolution of these tools and methodologies will deepen our understanding of protein function and accelerate disease pathogenesis and drug development discoveries.

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