ProteinsPlus: On-The-Fly Structure-Based Design on the Web

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The ProteinsPlus web server (https://proteins.plus)[1] offers modelling support for in-depth investigation of biomolecules. Its tools provide easy access to structure-based analyses for interdisciplinary researchers through an intuitive user interface. Users can perform computational studies for approx. 195,000 experimental protein structures from the Protein Data Bank (PDB)[2] and millions of predicted models from the AlphaFold Protein Structure Database.[3]

The services include structure quality analyses for X-ray models, structure preparation (hydrogen atom assignment, water placement, metal coordination), geometric analyses, pocket prediction and characterization, binding site comparison, automated molecular docking, 2D interaction visualization, protein-protein interface classification, and mutation analyses.

In this contribution, we will present services of the ProteinsPlus web server in a nutshell with implications on their potential application domains in structure-based design. We will also discuss several tools which are still in active development.

References

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