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Analysis of protein-nucleic acid interactions in the PPI3D web server

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To perform their functions, proteins frequently interact with other proteins and nucleic acids. Detailed information on these interactions can be obtained from the three-dimensional structures of the corresponding protein-protein or protein-nucleic acid complexes. Since the experimental structure determination is often tedious and expensive, computational structure prediction methods are widely applied. Currently, the structures of protein-protein complexes can be modeled accurately by AlphaFold, but structures protein-nucleic acid complexes can be reliably inferred only based on homology. To facilitate the search and analysis of structural data on protein interactions based on sequence homology, we have developed the PPI3D web server. Here, we present its novel features related to the analysis of protein-nucleic acid interactions. Given the sequences of proteins, PPI3D can now identify not only protein-protein, but also protein-nucleic acid interactions available for homologous proteins in the Protein Data Bank. These structures in the PPI3D database are clustered according to similarity of both protein sequences and interaction interfaces. The identified protein-nucleic acid interfaces can be analyzed in detail at the sequence and structure levels. In addition, homology models of the interactions with nucleic acids can be generated for the query proteins. PPI3D web server is available at https://bioinformatics.lt/ppi3d.

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