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Online Protein Structure Analysis with Bio3D-web

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Summary: Here we describe Bio3D-web, an online application for interactive exploration and analysis of biomolecular structure data. Upon providing a single PDB identifier or protein sequence, Bio3D-web provides functionality for: (1) The identification of related protein structure sets to user specified thresholds of similarity; (2) Their multiple alignment and structure superposition; (3) Sequence and structure conservation analysis; (4) Inter-conformer relationship mapping with principal component analysis, and (5) comparison of predicted internal dynamics via ensemble normal mode analysis. This integrated functionality provides a complete workflow for the investigation of sequence-structure-dynamic relationships.

Results are available immediately through extensive in-browser visualization and plotting devices, as well as through downloading result files in commonly used formats. In addition to a convenient easy to use dynamic interface for exploring the effects of parameter and method choices, Bio3D-web also records the complete user input and subsequent graphical results of a user's session as a sharable reproducible report.

Bio3D-web is implemented entirely in the R language and is based on the Bio3D ^{1,2} and Shiny ³ R packages. It can be run from our online server or installed locally on any computer running R. Bio3D-web is open to all users and is provided free of charge under a GPL-3 open-source license from: <http://thegrantlab.org/bio3d/webapps>

Keywords: Protein structure analysis; Protein dynamics; Principal component analysis, Normal mode analysis.

Testing: Bio3D-web has been operational since the end of May 2016. Extensive testing in this 6-month period to date has involved application to more than 50 protein families by the authors and by an additional 12 researchers outside the authors immediate research groups. The server has also been tested simultaneously by 20 workshop participants at the University of Bergen.

References:

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