Developing Training and Educational Resources in Biomolecular Structural Biology for Diverse Audiences

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Understanding relationships between three-dimensional (3D) structure and function has paved the way for many discoveries and technical advances in fundamental biology, biomedicine, bioengineering, and energy sciences. The undergraduate biology education community identifies understanding "Structure and Function" as a core concept[1] and the ability to use "Modeling and Simulation" as a core competency. Several biological data resources provide open access to biomolecular sequences, 3D structures, and functional annotations. Biology educators, however, sometimes find it challenging to teach their students how to access relevant information from these data resources, understand their various representations and relationships, and meaningfully synthesize new knowledge. Herein, we describe resources for engaging diverse audiences to use 3D biostructure data.

Protein Data Bank[2] (PDB) is the single worldwide repository that archives and supports open access to 3D structures of biological macromolecules (proteins, nucleic acids, and carbohydrates), their complexes with one another, and with small-molecule ligands. The Global Core Biodata Coalition (globalbiodata.org) has designated PDB as a Global Core Biodata Resource of fundamental importance to the broad life science community and the long-term preservation of biological data. As a founding member of the Worldwide Protein Data Bank partnership (wwPDB.org), the US-funded Research Collaboratory for Structural Bioinformatics Protein Data Bank[3,4,5] (RCSB PDB) provides free access to more than 200,000 experimentally-determined structures alongside more than one million computed structure models, with no limitations on usage. In addition to providing tools and resources for visualizing and analyzing PDB data, the research-focused web portal (RCSB.org) integrates information from nearly 50 trusted external biological data resources that help in understanding biomolecular function and interactions. A second web portal, PDB-101[6] (PDB101.RCSB.org), provides access to introductory level and simplified views of PDB data for basic and applied researchers, their trainees, educators, students, and other users. It also presents a variety of training and education resources targeting diverse user communities. This talk will describe projects wherein researchers, educators, and students collaboratively developed resources for learning key concepts about the 3D structural and linked bioinformatics data. Examples of activities engaging diverse audiences and training them to use 3D structural data meaningfully will also be presented.

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