USE PDB DATA TO THEIR FULL EXTENT: UNDERSTANDING PDBx/mmCIF

Wednesday, May 3rd 2023 | 1:00 PM EDT
Registration:* go.rutgers.edu/u3vpwjet

* This RCSB Protein Data Bank (PDB) virtual course will be broadcast on Zoom. Please fill out the registration form to receive the Zoom link. Registration will be available online from March 1, 2023 to May 3, 2023.

LEARNING OBJECTIVES
Understand the basics of PDBx/mmCIF data dictionary and file format that underpin archiving of more than 200,000 experimentally determined three-dimensional biostructures in the PDB. Learn about software tools for generating and working with PDBx/mmCIF files, and programmatic access for harvesting PDB data.

Main topics:
- PDBx/mmCIF format description and examples
- PDBx/mmCIF data model
- Software tools for generating, editing, and visualizing PDBx/mmCIF files
- PDBx/mmCIF dictionary extensions, including ModelCIF for computed structure models (CSM) from AI/ML
- Parsing data from PDBx/mmCIF files for your research

WHO SHOULD ATTEND
Professionals and graduate students interested in learning about strategies to take full advantage of PDB data in the fields of:
- Structural biology
- Cheminformatics and computational chemistry
- Bioinformatics and computational biology

CO-ORGANIZERS
RCSB PDB Biocurators: Gregg Crichlow, Justin Flatt, Sutapa Ghosh, Brian Hudson, Yuhe Liang, Ezra Peisach, Irina Persikova, Monica Sekharan, Chenghua Shao, Jasmine Young (Rutgers, The State University of New Jersey)

CONTACT
For comments or questions please contact michelle.sanghera@rcsb.org

PROGRAM
1:00–1:10 PM
Welcome
Stephen K. Burley, M.D., D.Phil.
Director, RCSB PDB and Founding Director,
Institute for Quantitative Biomedicine, Rutgers University

1:10–1:25 PM
Introduction and course objectives
Gregg Crichlow, Ph.D., RCSB PDB, Rutgers University

1:25–1:45 PM
PDBx/mmCIF format - Not your parents' legacy PDB format
Ezra Peisach, Ph.D., RCSB PDB, Rutgers University

1:45–2:05 PM
PDBx/mmCIF data files - Lifting the lid off the black box
Brian Hudson, Ph.D., RCSB PDB, Rutgers University

2:05–2:50 PM
Programmatic data access and analysis using PDBx/mmCIF files
Irina Persikova, Ph.D. and Chenghua Shao, Ph.D., RCSB PDB, Rutgers University

2:50–3:00 PM
Closing remarks and acknowledgements
Stephen K. Burley, M.D., D.Phil.

CO-SPONSORS
RCSB Protein Data Bank rcsb.org
Institute for Quantitative Biomedicine iqb.rutgers.edu

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RCSB PDB is a founding member of the wwPDB.