

RUTGERS

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
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VIRTUAL CRASH COURSE

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.



Development and management of the PDBx/mmCIF data dictionary is a collaborative effort involving RCSB PDB, Worldwide Protein Data Bank (wwPDB, wwpdb.org) partners, and members of the wwPDB PDBx/mmCIF Working Group (wwpdb.org/task/mmcif).

CO-SPONSORS



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RCSB PDB is a founding member of the wwPDB.