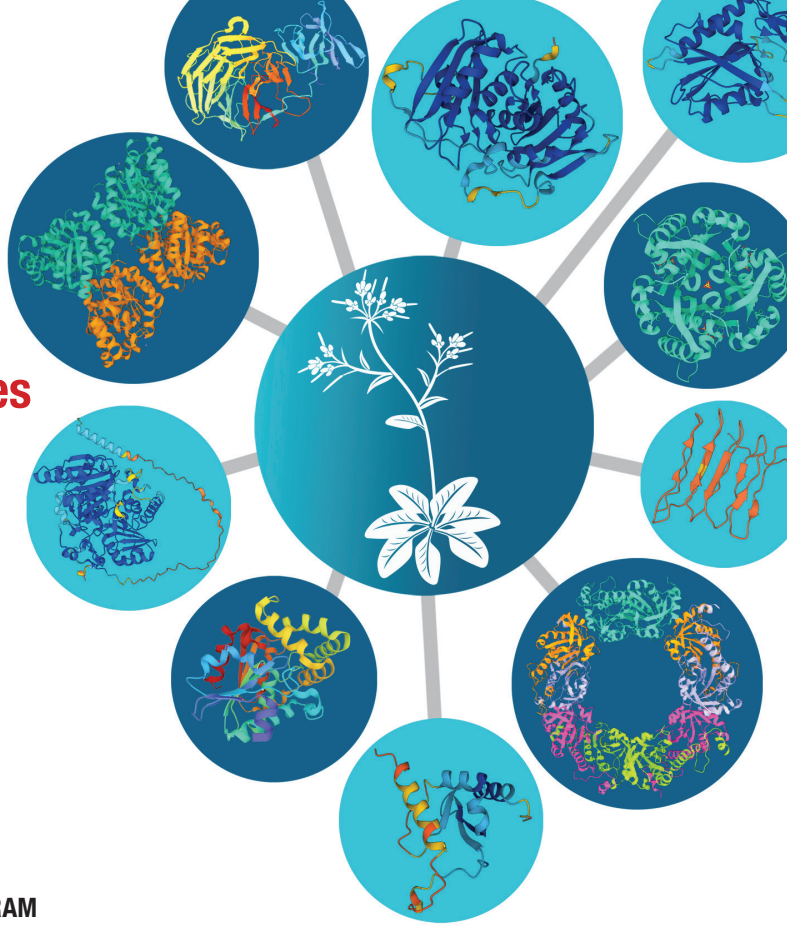
RUTGERS



DOE KNOWLEDGE-BASE/RCSB PROTEIN DATA BANK (DOE KBase/RCSB PDB) VIRTUAL CRASH COURSE

Using KBase to Access PDB Structures and Computed Structure Models from Artificial Intelligence/ Machine Learning

Thursday, November 10th 2022
1:00-5:00 PM EST

Registration: go.rutgers.edu/xfudv6m4*

LEARNING OBJECTIVES

The objective of this workshop is to introduce DOE, NSF, and NIH funded researchers to new protein structure-related tools, visualizations, and workflows that have been integrated into KBase as part of a collaboration with the RCSB PDB. We will demonstrate use of these tools to interested users, provide training for these tools, and gather feedback from users on how you would like us to further expand or enhance these tools. The training we will offer will cover these main topics:

- Importing experimental protein structure data into KBase from the RCSB PDB
- Uploading computed structure models of proteins from AlphaFold or RoseTTAFold into KBase
- Viewing experimental structures and computed structure models of proteins in KBase and linking to the broader KBase data resource
- Integrating protein structure analysis into the broader genomics workflows within KBase
- Using the PDB Mol* web-native graphics viewer for exploring protein structures within KBase

CONTACT

For comments or questions please contact **clermaortiz@anl.gov**

CO-ORGANIZERS

Stephen K. Burley (RCSB PDB Protein Data Bank, Rutgers University) and Christopher Henry (Systems Biology Knowledgebase, Argonne National Laboratory).

PROGRAM

1:00–1:05 PM *Welcome and Introduction*
Stephen K. Burley, M.D., D.Phil. - Founding Director, Institute for Quantitative Biomedicine

1:05–1:20 PM *Review of Joint DOE KBase/RCSB PDB Crash Course Objectives*
Christopher Henry, Ph.D. - KBase, Argonne National Laboratory

1:20–2:00 PM *Protein Candidates from Function Queries in KBase*
Janaka N. Edirisinghe, Ph.D. - KBase, Argonne National Laboratory

2:00–2:30 PM *Accessing Experimental Structures from the PDB*
Dennis Piehl, Ph.D. - RCSB Protein Data Bank, Rutgers University

2:30–3:00 PM *Accessing Computed Structure Models generated using AlphaFold2 or RoseTTAFold(2)*
Brinda Vallat, Ph.D. - RCSB Protein Data Bank, Rutgers University

3:00–3:15 PM *Break*

3:15–3:45 PM *Introduction to Mol* Molecular Graphics System*
Shuchismita Dutta, Ph.D. - RCSB Protein Data Bank, Rutgers University

3:45–4:15 PM *KBase Apps for Protein Structure Data Communication and Integration with RCSB PDB*
Qizhi Zhang, Ph.D. - KBase, Argonne National Laboratory

4:15–4:45 PM *Making the Best use of Protein Structure Data in KBase and PDB*
Christopher Henry, Ph.D. - KBase, Argonne National Laboratory

4:45–5:00 PM *Future Goals for KBase/RCSB PDB Collaboration*
Stephen K. Burley, M.D.,D. Phil. - RCSB Protein Data Bank, Rutgers

*LOGISTICS

The course will be broadcasted from a central virtual meeting site. We are asking the participants to fill out a registration form which will be available online from 12th September to 8th November. We will contact all the participants before the 10th of November with the central Zoom call address.

KBase PREDICTIVE BIOLOGY
kbase.us

RCSB PDB PROTEIN DATA BANK
rcsb.org

IQB
iqb.rutgers.edu