RUTGERS

VIRTUAL CRASH COURSE

Enabling PROTEIN STRUCTURE PREDICTION with Artificial Intelligence at Rutgers and Beyond

Thursday, December 9th 2021 • 1:00 PM EST

Registration (required): go.rutgers.edu/dlqx9nfb

LEARNING OBJECTIVES

This Institute for Quantitative Biomedicine Crash Course will present a broad overview of how Artificial Intelligence/Machine Learning (AI/ML) methods are being used for *de novo* protein structure prediction and provide hands-on experience with both AlphaFold2 and RoseTTAFold.

CASP14 revealed that AlphaFold2, developed by Google DeepMind, Inc., can predict three-dimensional structures of small globular proteins with accuracies comparable to experimental methods. RoseTTAFold, developed at the University of Washington/Howard Hughes Medical Institute, approaches AlphaFold2 in terms of prediction accuracy while requiring fewer computational resources.

In this Crash Course, expert speakers will provide a solid foundation on the role of AI/ML in structural biology and showcase ongoing research efforts at Rutgers. During the hands-on tutorial, participants will learn how to utilize these new computational tools to compute structure models from amino acid sequences and download precomputed structure models from the AlphaFoldDB database. Local computing resources (Rutgers University Amarel Cluster) and access to Google Colab and the RoseTTAFold server will be made available during the hands-on session.

CO-ORGANIZERS:

Balamurugan Desinghu, Ph.D. and
Stephen K. Burley, M.D., D.Phil.

PROGRAM

1:00–1:05 PM *Introductions*
Stephen K. Burley, M.D., D.Phil.: Founding Director, Institute for Quantitative Biomedicine
J. Barr von Oehsen, Ph.D.: Associate Vice President, Office of Advanced Research Computing

1:05–1:10 PM *Welcome and Crash Course Learning Objectives*
Michael E. Zwick, Ph.D.: Senior Vice President, Office for Research

1:10–1:40 PM *De Novo Protein Structure Prediction: Disruptive Transformation of Biology in 3D*
Minkyung Baek, Ph.D.: University of Washington

1:40–2:10 PM *Primer on Artificial Intelligence: Statistical Underpinning and Vocabulary*
Sijian Wang, Ph.D.: IQB; SAS-Statistics

2:10–2:30 PM *Potential for Impact on Research in Cell/Molecular, Cancer, and Structural Biology*
Stephen K. Burley, M.D., D.Phil.: RCSB PDB; IQB; SAS-CCB; CINJ

Lightning Talks:

2:30–2:45 PM *Experience with Applications in Single-particle Cryo-Electron Microscopy*
Vasileios Petrou, Ph.D.: CII; RNJMS-MB&MG

2:45–3:00 PM *Experience with Applications in Computational Biology*
Guillaume Lamoureux, Ph.D.: CCIB; CCAS-Chemistry

3:00–3:15 PM *Experience with Applications in SARS-CoV-2 Protease Modeling and Drug Discovery*
Sagar Khare, Ph.D.: IQB; SAS-CCB; CINJ

3:15–3:30 PM *Break*

3:30–3:45 PM *Primer: Getting Access to Rutgers Infrastructure (Amarel, AlphaFold2, RoseTTAFold)*
Balamurugan Desinghu, Ph.D.: OARC

3:45–4:55 PM *Hands On De Novo Protein Structure Prediction Tutorial*
- Modeling/visualizing a small globular protein structure in real time
- Downloading pre-computed structure models from AlphaFoldDB
- Modeling your favorite protein using AlphaFold2 and RoseTTAFold (requires FASTA sequence or UniProt ID)

Balamurugan Desinghu, Ph.D., Paul Arias, Ph.D., Vlad Kholodovych Ph.D., Ehud Zelzion, Ph.D., Janet Chang, Ph.D.: OARC
Stephen K. Burley, M.D., D.Phil., Sagar Khare, Ph.D., Joseph Lubin, B.Sc.: IQB

5:00 PM *Closing Remarks and Acknowledgements*
Balamurugan Desinghu, Ph.D.: Senior Scientist, Office of Advanced Research Computing

CO-SPONSORS:

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