

# ***In silico* Drug Discovery Workshop**

hosted by the NCATS Assay Guidance Manual Program

Wednesday, October 23, 2024 – Thursday, October 24, 2024 ~ Virtual (All times are in ET)

## **AGENDA: Day 1**

- 11:00 AM **Introductory Comments**  
Joni Rutter, National Center for Advancing Translational Sciences (NCATS), National Institutes of Health (NIH)  
Kimberly Sciarretta, Biomedical Advanced Research and Development Authority (BARDA)
- 11:20 AM **Overview of Workshop Objectives**  
Sarine Markossian and Alexey Zakharov, NCATS, NIH
- 11:30 AM **Keynote: Computer-Aided Drug Discovery Then and Now**  
Martha S. Head (Marti), Amgen Inc.
- 12:15 PM **Lunch**
- 12:45 PM **Session 1: Data sourcing for *in silico* drug discovery**  
Chair: Sarine Markossian, NCATS
- 12:45 PM **15 Years of ChEMBL: Challenges & Opportunities**  
Barbara Zdrazil, European Bioinformatics Institute (EMBL-EBI)
- 1:15 PM **Protein Data Bank: From Two Epidemics to the Global Pandemic to mRNA Vaccines and Paxlovid**  
Stephen K. Burley, Rutgers
- 1:45 PM **Break**
- 2:00 PM **Session 2: *In silico* methodologies used in drug discovery**  
Chair: Alexander Tropsha, University of North Carolina Chapel Hill
- 2:00 PM **Cartography-Guided Exploration of (Ultra)Large Chemical Spaces**  
Alexandre Varnek, The University of Strasbourg
- 2:30 PM **Virtual Screening (TBD)**  
Gisbert Schneider, ETH Zürich
- 3:00 PM **Synthesis-Aware Library Design and Optimal Experimental Design**  
Connor W. Coley, Massachusetts Institute of Technology (MIT)
- 3:30 PM **Physics-Based Modeling in Drug Discovery**  
John D. Chodera, Memorial Sloan-Kettering Cancer Center
- 4:00 PM **Break**
- 4:15 PM **Session 3: Applications of *in silico* methodologies in drug discovery**  
Chair: Shyam Rele, BARDA
- 4:15 PM **Applying Artificial Intelligence in a Small Drug Discovery Company**  
Sean Ekins, Collaborations Pharmaceuticals, Inc.
- 4:45 PM **The Computational Assay Driven Discovery of a Novel DHODH Inhibitor Series for Malarial Chemoprevention**  
Vicki Feher, Novartis BioMedical Research
- 5:15 PM **Summary of Day 1 and Adjourn**

## AGENDA: Day 2

- 11:00 AM **Session 3: Applications of *in silico* methodologies in drug discovery (continued)**  
Chair: Shyam Rele, BARDA
- 11:00 AM **Industrializing Early Drug Discovery at Scale**  
Marissa Saunders, Recursion Pharmaceuticals
- 11:30 AM **End-to-End Drug Discovery and Development Using Generative AI and Robotics**  
Alex Zhavoronkov, Insilico Medicine
- 12:00 PM **Lunch**
- 12:30 PM **Session 4: Emerging trends in *in silico* drug discovery**  
Chair: Alexey Zakharov, NCATS
- 12:30 PM **Understanding the Chameleonicity and Permeability of PROTACs Using Molecular Dynamics Simulations, Markov Models, and Deep Learning**  
Bryn Taylor, Johnson & Johnson Innovative Medicine
- 1:00 PM **Data Generation in Support of Computational Drug Discovery**  
Cheryl H Arrowsmith, University of Toronto
- 1:30 PM **Human-AI-Robot Collaboration to Accelerate Materials and Molecular Discovery**  
Milad Abolhasani, North Carolina State University
- 2:00 PM **Design of New Protein Functions Using Deep Learning**  
David Baker, University of Washington
- 2:30 PM **Break**
- 3:00 PM **Panel Discussion: Bridging the gaps in translation**  
Chair and moderator: Rommie Amaro, University of California San Diego (UCSD)  
Panelists: Pat Walters, Relay Therapeutics; Russ B Altman, Stanford University; Joel Karpiak, GSK; Martha S. Head (Marti), Amgen Inc.
- 3:00 PM **Introduction to the Session and Challenges Ahead**  
Rommie Amaro, UCSD
- 3:20 PM **Dangers of Poor Data (TBD)**  
Pat Walters, Relay Therapeutics
- 3:40 PM **Paying Attention to Attention in AI Generative Models**  
Russ B Altman, Stanford University
- 4:00 PM **Team Environment for Better Translation (TBD)**  
Joel Karpiak, GSK
- 4:20 PM **Discussion and Q&A**
- 5:00 PM **Closing Session: Summary of Discussions and Perspectives on the Challenges Ahead**  
Alexey Zakharov, NCATS; Alexander Tropsha, UNC Chapel Hill; Rommie Amaro, USCD
- 5:15 PM **Closing Statement and Adjourn**