# In silico Drug Discovery Workshop

hosted by the NCATS Assay Guidance Manual Program

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

## AGENDA: Day 1

**11:00 AM**  **Introductory Comments**
**TBD**
TBD, National Center for Advancing Translational Sciences (NCATS), National Institutes of Health (NIH)
**TBD**
TBD, BARDA

**11:20 AM**  **Overview of Workshop Objectives**
Sarine Markossian and Alexey Zakharov, NCATS, NIH

**11:30 AM**  **Keynote: Overview of in silico methods for preclinical drug discovery: Challenges and Opportunities**
Marti Head, Amgen

**12:10 PM**  **Lunch**

**12:40 PM**  **Session 1: Data sourcing for modeling and validation in in silico drug discovery**
Chair: Sarine Markossian, NCATS
12:40 PM        **15 years of ChEMBL: challenges & opportunities**
                Barbara Zdrazil, ChEMBL
1:10 PM         **Protein Data Bank: From Two Epidemics to the Global Pandemic to mRNA Vaccines and Paxlovid**
                Stephen K. Burley, Rutgers

**1:40 PM**  **Break**

**2:00 PM**  **Session 2: in silico methodologies used in drug discovery**
Chair: Alexander Tropsha, UNC
2:00 PM         **Data visualization (TBD)**
                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
3:30 PM         **Physics Based modeling (TBD)**
                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: Morgan Sherer, BARDA
4:15 PM         **Applying Artificial Intelligence in a Small Drug Discovery Company**
                Sean Ekins, Collaborations Pharmaceuticals, Inc.
4:45 PM         **TBD**
                Victoria Feher, Novartis Institutes for BioMedical Research (NIBR)

**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: Morgan Sherer, BARDA

            11:00 AM     **TBD**
                                Marissa Saunders, Recursion Pharmaceuticals

            11:30 AM     **TBD**
                                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     **Self-driving labs (TBD)**
                                TBD

            2:00 PM     **Protein therapeutics design (TBD)**
                                TBD

**2:30 PM**     **Break**

**3:00 PM**     **Panel Discussion: Bridging the gaps in translation**
Chair and moderator: Rommie Amaro, USCD
Panelists:

            3:00 PM     **Dangers of poor data (TBD)**
                                Pat Walters, Relay Therapeutics

            3:20 PM     **Team environment for better translation (TBD)**
                                Christopher Austin, GSK

            3:40 PM     **TBD**
                                TBD

            4:00 PM     **TBD**
                                TBD

            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; Rommie Amaro, USCD

**5:15 PM**     **Closing Statement and Adjourn**