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.

12:10 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 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 (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 **Industrializing early drug discovery at scale**
  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 **Human-AI-Robot Collaboration to Accelerate Materials and Molecular Discovery**
  Milad Abolhasani, North Carolina State University
- 2:00 PM **Protein therapeutics design (TBD)**
  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 (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 **Paying attention to attention in AI generative models**
  Russ B Altman, Stanford University
- 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**