National Center for Advancing Translational Sciences

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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 **De novo Design**
  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 **From Concept to Clinic: Discovery of a non-CDN STING Agonist Using QM, MD, and ML**
  Woody Sherman, Psivant Therapeutics

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 **Benchmarking Machine Learning Models in Drug Discovery - You're Probably Doing It Wrong**
  Pat Walters, Relay Therapeutics
- 3:40 PM **Large Language Model Evaluation of Regulatory Submissions**
  Russ B Altman, Stanford University
- 4:00 PM **Team Environment for Better Translation**
  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**