NCI workshop on Rational Drug Discovery - *Final Program*

Day 1: October 18, 2021 (10:00am – 5:00pm EDT)

10:00am – 10:15am EDT	**NCI Welcome** Sharad Verma, PhD Rose Aurigemma, PhD James Doroshow, MD
10:15am – 12:45p EDT	*Artificial Intelligence (AI) in Drug Discovery* **Chair: Marti Head, PhD (Oak Ridge National Labs)** **Session topics:** Machine Learning/AI tools in drug discovery, Algorithm development to support drug discovery, Considerations in using AI for drug discovery **10:15am – 10:45am** Open data and open science as drivers of innovation and knowledge, Andrew Leach, PhD (EBI) **10:45am – 11:15am** AI in Drug Discovery - Some Aspects of Available Algorithms and Data, Andreas Bender, PhD (University of Cambridge) **11:15am – 11:45am** IMPROVE-ing the comparison of AI-based Predictive Models of Therapeutic Response, M.Ryan Weil, PhD (NCI) **11:45am – 12:15pm** Combining AI and physics-based computational methods to inform discovery decisions, Vicki Feher, PhD (Schrödinger) **Panel Discussion** Andreas Bender, PhD (University of Cambridge) Feixiong Cheng, PhD (Case Western Reserve University) Artem Cherkasov, PhD (University of British Columbia) Vicki Feher, PhD (Schrödinger) Marti Head, PhD (Oak Ridge National Labs) Andrew Leach, PhD (EBI) M. Ryan Weil, PhD (Frederick National Laboratory)
12:45pm – 1:15p EDT	**Break**
1:15pm – 2:00p EDT	**Day 1 Keynote Lecture** Use of Data Science and AI for Target Selection in Oncology Tudor Oprea, MD, PhD (University of New Mexico)
2:00pm – 4:30p EDT	*Novel Therapeutic Modalities* **Chair: Michelle Arkin, PhD (University of California, San Francisco)** **Session topics:** PROTACs and chemical degraders, Covalent inhibitors, Protein-Protein stabilizing drugs **2:00pm – 2:30pm** Functionalizing Covalent Binders, Nir London, PhD (Weizmann Institute) **2:30pm – 3:00pm** 14-3-3 molecular glues, Eline Sijbesma, PhD (Ambagon Therapeutics)

	3:00pm – 3:30pm Drugging the Undruggable with Molecular Glue, Mary Matyskiela, PhD (Neomorph) **3:30pm – 4:00pm** Tissue Targeted Drug Discovery: Prospects in the Design of New Epigenetic Modifiers, Yomi Oyelere, PhD (Georgia Institute Technology) **4:00pm – 4:30pm** The Chemical Logic of Signaling Metabolites, Alison Ondrus, PhD (California Institute Technology) **Panel Discussion** Michelle Arkin, PhD (University of California, San Francisco) Nir London, PhD (Weizmann Inst.) Mary Matyskiela, PhD (Neomorph) Alison Ondrus, PhD (California Institute Technology) Adeboyega Oyelere, PhD (Georgia Institute Technology) Eline Sijbesma, PhD (Ambagon Therapeutics)

Day 2: October 19, 2021 (10:00am – 5:00pm EDT)

10:00am – 12:30p EDT	*Structural Biology: From supramolecular complexes to breakthroughs in computational software* **Chair: Hao Wu, PhD (Harvard)** **Session topics:** Cryo-EM, Fragment based drug design with Cryo-EM, drug discovery *via* structural biology, structure prediction and protein design, new methods for solving Cryo-EM **10:00am – 10:30am** Cryo-EM of supramolecular complexes in HIV-1, a dissection of target-target interactions for drug discovery, Peijun Zhang, PhD (Oxford) **10:30am – 11:00am** Fragment Based Drug Discovery method: how drug candidates can be discovered once the target is chosen, Pamela Williams, D. Phil (Astex) **11:00am – 11:30am** Cryo-EM (meta)data processing in industry, with an artisanal touch, Alexis Rohou, PhD (Genentech) **11:30am – 12:00pm** High accuracy prediction and design of protein structures and interactions, David Baker, PhD (University of Washington) **Panel Discussion** David Baker, PhD (University of Washington) Susan Lea, D. Phil (National Cancer Institute) Marc Nicklaus, PhD (National Cancer Institute) Alexis Rohou, PhD (Genentech) Pamela Williams, D. Phil (Astex) Hao Wu, PhD (Harvard) Peijun Zhang, PhD (Oxford)
12:30pm – 1:00p EDT	**Break**
1:00pm – 1:45p EDT	**Day 2 Keynote Lecture** *In situ* Computational Microscopy Rommie Amaro PhD (University of California, San Diego)
1:45pm – 4:15p EDT	*Target Interrogation* **Chair: Yolanda Sanchez, PhD (Dartmouth)** **Session topics:** Single cell transcriptomics, CRISPR in target discovery, Emerging screening approaches **1:45pm – 2:15pm,** Target class approach to deubiquitinases, Sarah Buhrlage, PhD (Dana Farber) **2:15pm – 2:45pm**, Atlases as roadmaps to understanding tumors, Orit Rozenblatt-Rosen, PhD (Genentech) **2:45pm – 3:15pm,** High-throughput genomics for immunotherapy drug discovery, Ansuman Satpathy, MD, PhD (Stanford) **3:15pm – 3:45pm**, Drug Screening with Engineered 3D Tissue Models, Marc Ferrer, PhD (NCATS)

	Panel Discussion Marc Ferrer, PhD (NCATS) Orit Rozenblatt-Rosen, PhD (Genentech) Yolanda Sanchez, PhD (Dartmouth) Ansuman Satpathy, MD, PhD (Stanford) Min Shen, PhD (NCATS)
4:15pm – 4:30p EDT	**Closing Remarks** Rose Aurigemma, PhD (NCI) Sharad Verma, PhD (NCI)