

IN SILICO DRUG DISCOVERY WORKSHOP

HOSTED BY THE NCATS ASSAY GUIDANCE MANUAL PROGRAM

OCTOBER 23-24, 2024

VIRTUAL AND FREE TO ATTEND

15+ TALKS BY EXPERTS FROM GOVERNMENT, PHARMA, BIOTECH & ACADEMIA

Keynote: Computer-Aided Drug Discovery Then and Now

Martha S. Head [Marti] (Amgen Inc.)

SESSION TOPICS

Session I: Data sourcing for *in silico* drug discovery

Chair: Sarine Markossian (NCATS, NIH); *Speakers:* Barbara Zdrazil (EMBL-EBI), Stephen K. Burley (Rutgers)

Session II: *In silico* methodologies used in drug discovery

Chair: Alexander Tropsha (UNC Chapel Hill); *Speakers:* Alexandre Varnek (The University of Strasbourg), Gisbert Schneider (ETH Zürich), Connor W. Coley (MIT), John D. Chodera (Memorial Sloan-Kettering Cancer Center)

Session III: Applications of *in silico* methodologies in drug discovery

Chair: Morgan Sherer (BARDA); *Speakers:* Sean Ekins (Collaborations Pharmaceuticals, Inc.), Victoria Feher (NIBR), Marissa Saunders (Recursion Pharmaceuticals), Alex Zhavoronkov (Insilico Medicine)

Session IV: Emerging trends in *in silico* drug discovery

Chair: Alexey Zakharov (NCATS); *Speakers:* Bryn Taylor (J&J Innovative Medicine), Cheryl H Arrowsmith (University of Toronto), Milad Abolhasani (North Carolina State University), David Baker (University of Washington)

Panel Discussion: Bridging the gaps in translation

Moderator: Rommie Amaro (USCD); *Panelists:* Pat Walters (Relay Therapeutics), Russ B Altman (Stanford University), Christopher Austin (GSK), Martha S. Head [Marti] (Amgen Inc.)

EVENT <https://ncats.corsizio.com/event/6628253bbb1a2115c082af51>



THE ASSAY GUIDANCE MANUAL



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