

Structure-Based Drug Discovery: The Next 25 Years

APS

Symposium

Tuesday May 09, 2017 Full Day

Bldg. 402, APS Lecture Hall

Organizers:

Lisa Keefe (IMCA-CAT / Hauptman-Woodward Medical Research Institute),

Barry Finzel (University of Minnesota)

Confirmed Speakers:

- Richard Alexander, *Janssen Pharmaceuticals*
- Matt Calabrese, *Pfizer*
- Srinivas Chakravarthy, *BioCAT / Illinois Institute of Technology*
- Vadim Cherezov, *University of Southern California*
- Artem Evdokimov, *HarkerBIO, LLC*
- Sarah L. Perry, *University of Massachusetts Amherst*
- Clint Potter, *New York Structural Biology Center and Nanolmaging Services, Inc.*
- Clemens Schulze-Briese, *DECTRIS Ltd.*
- Steven Sheriff, *Bristol-Myers Squibb Research & Development*
- Stephen M. Soisson, *Merck Research Laboratories*
- Vincent Stoll, *AbbVie*
- Stephen Streiffer, *Advanced Photon Source, Argonne National Laboratory*
- Suresh Sunderrajan, *Science & Technology Partnerships and Outreach, Argonne National Laboratory*

Full Description:

This symposium will bring together researchers in the pharmaceutical industry and experts in multiple aspects of structural biology to explore strategies that are effective for challenging projects and accelerating drug discovery.

Industry and academic researchers will showcase innovative drug discovery successes, highlight complementary and synchrotron-based techniques, and explore multi-faceted approaches to acquiring protein-ligand structural information.

Attendees will engage in open forum discussions to assess opportunities for incorporating emerging strategies into structural biology research programs.

Following the symposium, there will be a no-host dinner at the Argonne Guest House.

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Session Chair: Anne Mulichak (IMCA-CAT / Hauptman-Woodward Medical Research Institute)

- 8:30 – 8:40 IMCA-CAT: 25 Years of Shining a Light on Drug Discovery
Lisa Keefe (IMCA-CAT / Hauptman-Woodward Medical Research Institute)
- 8:40 – 8:50 Why has the Pharmaceutical Industry Invested in IMCA for 25 Years?
Vincent Stoll (AbbVie)
- 8:50 – 9:05 Argonne and Industry: A Partnership Built on Science and Technology
Suresh Sunderrajan (Science & Technology Partnerships and Outreach, Argonne Nat'l Laboratory)
- 9:05 – 9:15 Welcome from the Advanced Photon Source
Stephen Streiffer (Advanced Photon Source, Argonne National Laboratory)
- 9:15 – 10:00 Keynote – Toward Structure-Based Drug Design for GPCRs Using Synchrotrons and XFELs
Vadim Cherezov (University of Southern California)

10:00 – 10:15 Break

10:15- 11:00 Keynote - CryoEM from Academia to Industry
Clint Potter (New York Structural Biology Center and Nanomaging Services, Inc.)

11:00 – 11:30 Structurally Enabling Membrane Proteins to Accelerate Drug Discovery
Stephen M. Soisson (Merck Research Laboratories)

11:30 – 12:00 Driving Innovation and Turning Failure to Success for Patients, the Bcl-2 Story
Vincent Stoll (AbbVie)

12:00 – 1:15 Lunch

Session Chair: Kevin Battaile (IMCA-CAT / Hauptman-Woodward Medical Research Institute)

- 1:15 – 1:45 Structure of the Kinase Domain of TGF β R2
Steven Sheriff (Bristol-Myers Squibb Research & Development)
- 1:45 – 2:15 Opportunities in Industrial Crystallography: Fragment Based Crystallography as a Screening Tool
Richard Alexander (Janssen Pharmaceuticals)
- 2:15- 2:45 Flipping a New Switch on an Old Enzyme: AMPK Activators for Diabetic Nephropathy
Matt Calabrese (Pfizer)
- 2:45 – 3:00 Break
- 3:00 – 3:30 Graphene Microfluidics for Room Temperature Crystallography
Sarah L. Perry (University of Massachusetts Amherst)
- 3:30 – 4:00 Macromolecular Crystallization: The Old, The New, and The Inconvenient
Artem Evdokimov (HarkerBIO, LLC)
- 4:00 – 4:30 Pushing the Limits of Macromolecular Crystallography with EIGER
Clemens Schulze-Briese (DECTRIS Ltd.)
- 4:30 – 5:00 An Overview of the SAXS Program at the Biophysics Collaborative Access Team (BioCAT)
Srinivas Chakravarthy (BioCAT / Illinois Institute of Technology)
- 5:00 – 5:05 Concluding Remarks
Lisa Keefe (IMCA-CAT / Hauptman-Woodward Medical Research Institute)