JCUP XII Agenda

Thursday, September 12

10:00 – 10:30	Registration
Morning Session:	
10:30 – 11:15	Welcome to JCUP XII – **Anthony Nicholls**, *OpenEye*
11:15 – 12:00	"Large Language models and AI at GSK" – **Kim Branson**, *GSK*
12:00 – 12:20	Break
Luncheon Seminar:	
12:20 – 12:50	"Innovative molecular design and collaboration with Orion®" – **Kalli Burley**, *OpenEye*
Poster Session:	
12:50 – 13:50	Poster Session I
13:50 – 14:00	Break
Afternoon Session:	
14:00 – 14:30	"Science Strategy at OpenEye" – **Geoff Skillman**, *OpenEye*
14:30 – 15:00	"Validation of New Methodology to Create Orally Available Cyclic Peptides for Intracellular Tough Targets" – **Yusuke Yamagishi**, *Chugai Pharma*
15:00 – 15:15	Break
15:15 – 15:45	"Expanding the druggable universe: Validation of a cryptic pocket detection workflow on several difficult-to-drug targets" – **David LeBard**, *OpenEye*
15:45 – 16:30	"Where art thou, easy button? Accelerating small-biotech discovery with computation" – **Katrina Lexa**, *Nico Therapeutics*
16:30 – 16:45	Break
16:45 – 17:15	"Advancing Molecular Fingerprints: Integrating Chemical Reactivity for Enhanced Precision" – **Kazufumi Ohkawa**, *Asahi-Kasei Pharma*
17:15 – 18:00	"Why Scientific Collaborations Matter: A Personal History" – **Eric Manas**, *Treeline Biosciences*
18:00 – 18:15	"Crystal Structure Prediction services at OpenEye" - **Geoff Skillman & Scott Parker**, *OpenEye*
Banquet:	
18:30 – 20:30	Banquet (on the 6th Floor)

Friday, September 13

9:30 – 10:00	Registration
Morning Session:	
10:00 – 10:30	"Faster, Larger, Smarter: Filling the funnel and advancing the scale of Virtual Screening" – **Matt Geballe**, *OpenEye*
10:30 – 11:15	"Molecular Dynamics Simulations for Protein Kinases" – **Mitsunori Ikeguchi**, *Yokohama City University*
11:15 – 11:45	"Optimizing Lead Compounds with Efficient Binding Free Energy Calculations" – **Chris Neale**, *OpenEye*
11:45 – 12:00	Break
Luncheon Seminar:	
12:00 – 12:30	"Rapid comparison of protein binding sites using shape and chemical features" – **Kalli Burley**, *OpenEye*
Poster Session:	
12:30 – 13:30	Poster Session II
13:30 – 13:45	Break
Afternoon Session:	
13:45 – 14:30	"Potency isn't Everything: Glucokinase as a Drug Target for Type 2 Diabetes" - **Kim Sharp**, *University of Pennsylvania*
14:30 – 15:15	"Mechanisms of Conformational Change, Association, and Dissociation of Proteins investigated by Parallel Cascade Selection Molecular Dynamics" – **Akio Kitao**, *Tokyo Institute of Technology*
15:15 – 15:30	Break
15:30 – 16:00	"Development-ability of Antibody Therapeutics" – **Jesper Sorensen**, *OpenEye*
16:00 – 16:45	"Is AI capable of real-world drug discovery? Lessons from my career" **- Georgia McGaughey**, *Trilligant, LLC*
16:45 – 17:00	Closing remarks – **Anthony Nicholls**, *OpenEye*