

## Agenda April 10th

08:00-09:20	Open registration, coffee/tea/ breakfast
09:20-9:30	Welcome
<b>Session 1: Cheminformatics communications</b>	
9:30-10:00	State of the RDKit - Greg Landrum or Brian Kelley
10:00-10:30	Chemical Formats and the RDKit - Brian Kelley
10:30 - 10:45	<i>BREAK</i>
10:45-11:15	Erin Geno - Flare Therapeutics - how not to annoy chemists when showing them chemistry
11:15 - 11:45	Byron DeLaBarre - The Consulting Biochemist - TBA
<b>Lunch</b>	
12:00-13:15	<i>LUNCH</i>
<b>Session 2: Synthesis and planning</b>	
13:15-13:45	Mason Burlarge - Recursion- Synthesis automation/synthesis aware molecular design
13:45-14:15	Zhengkai Tu - MIT - ASKCOS: open-source, data-driven synthesis planning
14:15-14:45	Gabe Gomes - CMU - AI CoScientist
14:45 - 15:00	<i>BREAK</i>
<b>Session 3: Cheminformatics</b>	
15:00-15:30	David Deng - Novartis - The Role of Open-Source Toolkits in Advancing Chemical Registration Systems: A Case Study from Novartis
15:30-16:00	Nathan Morgan, Jackson Burns and Xiaorui Dong - MIT- RDKit for Deep Learning and Chemical Kinetics: Chemprop, RMG, and RDMC
16:00 - 16:15	<i>BREAK</i>
<b>Keynote</b>	
16:15-17:00	Pat Walters - Relay Therapeutics
<b>Networking</b>	
17:00 - 19:00	<i>Networking event</i>

## Agenda April 11th

08:00-8:50	breakfast, coffee/tea
08:50 - 9:00	Welcome and opening remarks
<b>Session 4: Beyond small molecule drug design</b>	
09:00 - 09:30	John Santa Maria - Parabilis Medicines - peptide design
09:30 - 10:00	Dan Nealschneider - Schrodinger - Building with Monomers in RDKit
10:00 - 10:30	Daniel Reker - Duke - Nanoparticle design
10:30 - 11:00	Jeremy Monat - Aionics, Inc. - Finding the Right Tautomer: A Case Study from Aionics
11:00-11:15	<i>BREAK</i>
<b>Session 5: Adding the third dimension</b>	
11:15-11:45	Olexandr Isayev - CMU - ML potentials + Auto3D
11:45-12:15	Guillaume Godin - OSMO - Mordred Descriptors
Lunch	
12:15 - 13:30	<i>Lunch</i>
<b>Session 6: Lightning talks</b>	
13:30 - 13:40	Fengbo Ren - Fovus - Supercharging Computational Drug Discovery with AI-Optimized Cloud HPC: Fovus in Action
13:40 - 13:50	Ryan Greenhalgh - Deep Mirror - TBA
13:50 - 14:00	Tugrul Kaynak - KNIME - TBA
14:00 - 14:10	Stephen Litster/Michael Tarselli - AWS
14:10 - 14:20	Questions for lightning talks
14:20 - 14:30	<i>BREAK</i>
14:30 - 14:40	Turki Alturaifi - UPitt- A Database of Steric and Electronic Properties of Heteroaryl Substituents
14:40-14:50	Babak Mahjour - MIT- RDCanon/SMARTS canonicalization
14:50-15:00	Jeff Wagner - Open Force Field - RDMol in the OMSF ecosystem
15:00:-15:10	Shitong Luo -MIT- TBA
15:10 - 15:20	Questions for lightning talks
<b>Closing</b>	
15:30-16:00	Closing remarks