Agenda April 10th

08:00-09:20	Open registration, coffee/tea/ breakfast
09:20-9:30	Welcome
Session 1: Cheminformatics communications	
9:30-10:10	State of the RDKit - Greg Landrum or Brian Kelley
10:10-10:30	Tad Hurst - Collaborative Drug Discovery - Rigorous Enhanced Stereo Chemistry and Read support for Self-Contained Sequence Representation (SCSR) in RDKit.
10:30 - 10:45	*BREAK*
10:45-11:15	Erin Geno - Flare Therapeutics - How not to annoy chemists when showing them chemistry
11:15 - 11:45	David Deng - Novartis - The Role of Open-Source Toolkits in Advancing Chemical Registration Systems: A Case Study from Novartis
Lunch	
12:00-13:15	*LUNCH*
Session 2: Synthesis and planning	
13:15-13:45	Mason Burlage - 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	*BREAK*
Session 3: Machine/Deep Learning	
15:00-15:30	Byron DeLaBarre - The Consulting BioChemist - Using RDKIT in a Machine Learning Workflow for Identifying Small Molecule Binding Sites Across the Human Proteome
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	*BREAK*
Keynote	
16:15-17:00	Pat Walters - Relay Therapeutics
Networking	
17:00 - 19:00	*Networking event*

Agenda April 11th

08:00-8:50	breakfast, coffee/tea
08:50 - 9:00	Welcome and opening remarks
Session 4: Beyond small molecule drug design	
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 - Cheminformatics for drug delivery and nanoparticle design
10:30 - 11:00	Jeremy Monat - Finding Tautomers
11:00-11:15	*BREAK*
Session 5: Adding the third dimension	
11:15-11:45	Olexandr Isayev - CMU - ML potentials + Auto3D
11:45-12:15	Guillaume Godin - OSMO - Mordred Descriptors and the RDKit
Lunch	
12:15 - 13:30	*Lunch*
Session 6: Lightning talks	
13:30 - 13:40	Fengbo Ren - Fovus - Supercharge computational drug discovery with AI-powered serverless high-performance computing (HPC)
13:40 - 13:50	Ryan Greenhalgh - Deep Mirror - TBA
13:50 - 14:00	Tugrul Kaynak - KNIME - From Python Code to KNIME Node: Share Custom Tools with Non-Coders
14:00 - 14:10	Stephen Litster/Michael Tarselli - AWS - TBA
14:10 - 14:20	Questions for lightning talks
14:20 - 14:30	*BREAK*
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- Generative AI-guided exploration of synthesizable chemical space with RDKit
15:10 - 15:20	Questions for lightning talks
Closing	
15:30-16:00	Closing remarks