Agenda April 10th

Session 1: Cheminformatics communications 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 BREAK Erin Geno - Flare Therapeutics - how not to annoy chemists when showing them chemistry 11:15 - 11:45 Byron DeLaBarre - The Consulting Biochemist - TBA Lunch 12:00-13:15 LUNCH Session 2: Synthesis and planning 13:15-13:45 Mason Burlarge - Recursion- Synthesis automation/synthesis aware molecular design 13:45-14:15 Gabe Gomes - CMU - AI CoScientist 14:45 - 15:00 BREAK Session 3: Cheminformatics David Deng - Novartis - The Role of Open-Source Toolkits in Advancing Chemical Registration Systems: A Case Study from Novartis Nathan Morgan, Jackson Burns and Xiaorui Dong - MIT- RDKit for Deep Learning and Chemical Kinetics: Chemprop, RMG, and RDMC BREAK Keynote Pat Walters - Relay Therapeutics Networking	<u> </u>		
Session 1: Cheminformatics communications 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 BREAK Erin Geno - Flare Therapeutics - how not to annoy chemists when showing them chemistry 11:15 - 11:45 Byron DeLaBarre - The Consulting Biochemist - TBA Lunch 12:00-13:15 LUNCH Session 2: Synthesis and planning 13:15-13:45 Mason Burlarge - Recursion- Synthesis automation/synthesis aware molecular design 13:45-14:45 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: Cheminformatics David Deng - Novartis - The Role of Open-Source Toolkits in Advancing Chemical Registration Systems: A Case Study from Novartis Nathan Morgan, Jackson Burns and Xiaorui Dong - MIT- RDKit for Deep Learning and Chemical Kinetics: Chemprop, RMG, and RDMC Mathan Morgan, Jackson Burns and Registration Systems: A Case Study Form Novartis Nathan Morgan, Jackson Burns and Roma Roma Roma Roma Roma Roma Roma Roma	08:00-09:20	Open registration, coffee/tea/ breakfast	
9:30-10:00 State of the RDKit - Greg Landrum or Brian Kelley 10:30 - 10:45 BREAK Erin Geno - Flare Therapeutics - how not to annoy chemists when showing them chemistry 11:15 - 11:45 Byron DeLaBarre - The Consulting Biochemist - TBA Lunch 12:00-13:15 LUNCH Session 2: Synthesis and planning 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 - Al CoScientist 14:45 - 15:00 BREAK Session 3: Cheminformatics David Deng - Novartis - The Role of Open-Source Toolkits in Advancing Chemical Registration Systems: A Case Study from Novartis 15:30-16:00 Chemical Kinetics: Chemprop, RMG, and RDMC BREAK Keynote Pat Walters - Relay Therapeutics Networking	09:20-9:30	Welcome	
10:00-10:30 Chemical Formats and the RDKit - Brian Kelley 10:30 - 10:45 BREAK Erin Geno - Flare Therapeutics - how not to annoy chemists when showing them chemistry 11:15 - 11:45 Byron DeLaBarre - The Consulting Biochemist - TBA Lunch 12:00-13:15 LUNCH Session 2: Synthesis and planning 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 - Al CoScientist 14:45 - 15:00 BREAK Session 3: Cheminformatics David Deng - Novartis - The Role of Open-Source Toolkits in Advancing Chemical Registration Systems: A Case Study from Novartis 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	Session 1: Cheminformatics communications		
10:30 - 10:45 BREAK Erin Geno - Flare Therapeutics - how not to annoy chemists when showing them chemistry 11:15 - 11:45 Byron DeLaBarre - The Consulting Biochemist - TBA Lunch 12:00-13:15 LUNCH Session 2: Synthesis and planning 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 BREAK Session 3: Cheminformatics David Deng - Novartis - The Role of Open-Source Toolkits in Advancing Chemical Registration Systems: A Case Study from Novartis 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	9:30-10:00	State of the RDKit - Greg Landrum or Brian Kelley	
Erin Geno - Flare Therapeutics - how not to annoy chemists when showing them chemistry 11:15 - 11:45 Byron DeLaBarre - The Consulting Biochemist - TBA Lunch Lunch Session 2: Synthesis and planning 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 BREAK Session 3: Cheminformatics David Deng - Novartis - The Role of Open-Source Toolkits in Advancing Chemical Registration Systems: A Case Study from Novartis Nathan Morgan, Jackson Burns and Xiaorui Dong - MIT- RDKit for Deep Learning and Chemical Kinetics: Chemprop, RMG, and RDMC BREAK Keynote 16:15-17:00 Pat Walters - Relay Therapeutics Networking	10:00-10:30	Chemical Formats and the RDKit - Brian Kelley	
10:45-11:15 chemistry 11:15 - 11:45 Byron DeLaBarre - The Consulting Biochemist - TBA Lunch 12:00-13:15 LUNCH Session 2: Synthesis and planning 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 BREAK Session 3: Cheminformatics David Deng - Novartis - The Role of Open-Source Toolkits in Advancing Chemical Registration Systems: A Case Study from Novartis Nathan Morgan, Jackson Burns and Xiaorui Dong - MIT- RDKit for Deep Learning and Chemical Kinetics: Chemprop, RMG, and RDMC BREAK Keynote 16:15-17:00 Pat Walters - Relay Therapeutics Networking	10:30 - 10:45	BREAK	
Lunch 12:00-13:15 LUNCH Session 2: Synthesis and planning 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 BREAK Session 3: Cheminformatics David Deng - Novartis - The Role of Open-Source Toolkits in Advancing Chemical Registration Systems: A Case Study from Novartis 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	10:45-11:15	· · · · · · · · · · · · · · · · · · ·	
Session 2: Synthesis and planning 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 BREAK Session 3: Cheminformatics David Deng - Novartis - The Role of Open-Source Toolkits in Advancing Chemical Registration Systems: A Case Study from Novartis 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	11:15 - 11:45	Byron DeLaBarre - The Consulting Biochemist - TBA	
Session 2: Synthesis and planning 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 BREAK Session 3: Cheminformatics David Deng - Novartis - The Role of Open-Source Toolkits in Advancing Chemical Registration Systems: A Case Study from Novartis 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	Lunch		
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 BREAK Session 3: Cheminformatics David Deng - Novartis - The Role of Open-Source Toolkits in Advancing Chemical Registration Systems: A Case Study from Novartis Nathan Morgan, Jackson Burns and Xiaorui Dong - MIT- RDKit for Deep Learning and Chemical Kinetics: Chemprop, RMG, and RDMC 15:30-16:00 BREAK Keynote 16:15-17:00 Pat Walters - Relay Therapeutics Networking	12:00-13:15	LUNCH	
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: Cheminformatics David Deng - Novartis - The Role of Open-Source Toolkits in Advancing Chemical Registration Systems: A Case Study from Novartis 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	Session 2: Synthesis and planning		
14:15-14:45 Gabe Gomes - CMU - AI CoScientist 14:45 - 15:00 BREAK Session 3: Cheminformatics David Deng - Novartis - The Role of Open-Source Toolkits in Advancing Chemical Registration Systems: A Case Study from Novartis 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	13:15-13:45	Mason Burlarge - Recursion- Synthesis automation/synthesis aware molecular design	
Session 3: Cheminformatics David Deng - Novartis - The Role of Open-Source Toolkits in Advancing Chemical Registration Systems: A Case Study from Novartis 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	13:45-14:15	Zhengkai Tu - MIT - ASKCOS: open-source, data-driven synthesis planning	
Session 3: Cheminformatics David Deng - Novartis - The Role of Open-Source Toolkits in Advancing Chemical Registration Systems: A Case Study from Novartis 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	14:15-14:45	Gabe Gomes - CMU - AI CoScientist	
David Deng - Novartis - The Role of Open-Source Toolkits in Advancing Chemical Registration Systems: A Case Study from Novartis 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	14:45 - 15:00	BREAK	
15:00-15:30 Registration Systems: A Case Study from Novartis 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	Session 3: Cheminformatics		
15:30-16:00 Chemical Kinetics: Chemprop, RMG, and RDMC 16:00 - 16:15 BREAK Keynote 16:15-17:00 Pat Walters - Relay Therapeutics Networking	15:00-15:30		
Keynote 16:15-17:00 Pat Walters - Relay Therapeutics Networking	15:30-16:00		
16:15-17:00 Pat Walters - Relay Therapeutics Networking	16:00 - 16:15	BREAK	
Networking	Keynote		
	16:15-17:00	Pat Walters - Relay Therapeutics	
17:00 - 19:00 Networking event	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 - Nanoparticle design	
10:30 - 11:00	Jeremy Monat - Aionics, Inc Finding the Right Tautomer: A Case Study from Aionics	
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	
Lunch		
12:15 - 13:30	Lunch	
Session 6: Lightning talks		
13:30 - 13:40	Fengbo Ren - Fovus - Supercharging Computational Drug Discovery with Al-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	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- TBA	
15:10 - 15:20	Questions for lightning talks	
Closing		
15:30-16:00	Closing remarks	