

5th RDKit UGM, 26-28 October 2016, Basel, Switzerland

Main Program

Time	26. October	27. October
08:30 - 09:00	Check-in	Check-in
09:00 - 09:30	Greg Landrum	Emanuel Ehmki & Christian Kramer Matched Molecular Series: Measuring SAR Transferability
09:30 - 10:00	Welcome, Intro, and State of the Toolkit	Manuel Schwarze How to develop new RDKit Nodes for KNIME Workflows
10:00 - 10:30	Greg Landrum & Nadine Schneider A quick RDKit-centric intro to Git and Github	Roger Sayle Five Not-so-easy Pieces: Tautomers, Nucleic Acids, Inorganics, Reactions and SMIRKS
10:30 - 11:00	Coffee Break	Coffee Break
11:00 - 11:30	Paul Czodrowski OCEAN, ctd: Optimized Cross rEActivity estimation	Nathan Brown The origin of three dimensionality in drug-like molecules
11:30 - 12:00	Simon Rüdisser Molecule selectivity prediction for serine proteases	Brian Kelley The Novartis Chemical Universe – Searching astronomically large spaces
12:00 - 12:30	Florian Flachsenberg Chemically meaningful ring perception: An open-source implementation of the Unique Ring Families approach	John May Higher Quality Chemical Depictions: Lessons Learned and Advice
12:30 - 13:30	Lunch (Sandwiches) + Posters	Lunch (SportsCloud) + Posters
13:30 - 14:00	Lightning Talk Round 1	
14:00 - 14:30	Nadine Schneider Let's talk about your chemical topics!	Lightning Talk Round 2
14:30 - 15:00	Paolo Tosco Boosting RDKit molecular simulations through OpenMM	Riccardo Vianello Faster similarity queries using RDKit, binary fingerprints and relational databases
15:00 - 15:30	Coffee break + Posters	Esben Jannik Bjerrum pI prediction of peptides and proteins using RDkit: Pseudoatoms, AA modifications and preliminary results for a machine learning pKa predictor
15:30 - 16:00	Sereina Riniker MDFP: Learning from Molecular Dynamics Data	Coffee break + Posters
16:00 - 16:30	Axel Pahl Data Pipelines and Mol_Lists: RDkit Tools for the Jupyter Notebook	Round table discussion
18:00 - 22:00	Dinner (Rhyschänzli)	Dinner (Da Gianni)

Coffee breaks and lunches sponsored by **Roche**, **KNIME.com** and the **Novartis Institutes for BioMedical Research**

5th RDKit UGM Hackathon Program, 28th October

Time	Track 1	Track 2
8:00 - 8:15	Meet at gate	Meet at gate
8:30 - 10:00	Nikolas Fechner QSAR/ML tutorial, Room 310.3.15	Hackathon Room 310.3.42
10:00 - 10:30	Coffee Break	Coffee Break
10:30 - 12:30	Manuel Schwarze Hands-on session implementing RDKit KNIME nodes, Room 310.3.15	Hackathon Room 310.3.42
12:30 - 13:30	Lunch	Lunch
13:30 - 16:00		Hackathon Room 310.3.15

Coffee break sponsored by **KNIME.com**