4th RDKit User Group Meeting, 2.- 4. September 2015, ETH Zurich, Switzerland

RDKit
Open-Source Cheminformatics and Machine Learning

Time	2. September	3. September	4. September
08:30-09:00	**Registration and Coffee Break**	**Coffee Break**	**Coffee Break**
09:00-09:30	**Greg Landrum** Introduction and State of the Toolkit	**Guillaume Godin** tbd	**Hackathon**
09:30-10:00		**Riccardo Vianello** Development of python web applications using django and the RDKit	
10:00-10:30	**Lightning talks** David Hahn, Riccardo Vianello, Paul Czodrowski	**Tim Dudgeon** Using RDkit from the Java world	
10:30-10:45	**Break**	**Break**	
10:45-11:15	**Lightning talks** Greg Landrum, Brian Kelley	**Nadine Schneider** Get your atoms in order – reducing graph canonicalization to a sorting problem	
11:15-11:45	**Peter Ertl** Calculation of natural product likeness with RDKit	**Sereina Riniker** Teaching distance geometry about experimental torsion-angle preferences	
11:45-12:15	**Jasna Klicic** Designing a natural products library	**Samo Turk** Hinge binder extraction from PDBs with RDKit	
12:15-12:30	**Lunch + Poster**	**Lunch + Poster**	**Lunch**
12:30-13:00			
13:00-13:30			
13:30-14:00	**Paul Czodrowski** OCEAN: Optimized Cross rEActivity estimatioN	**Paolo Tosco** Resonance-aware substructure searching with RDKit	
14:00-14:30	**Jan Holst Jensen** RInChI: The IUPAC Reaction Identifier, coming to RDKit	**Jakub Gunera** Fragment-based similarity searching with infinite color space	
14:30-15:00	**Roger Sayle** Reaction perception and protein handling using RDKit	**Round-table discussion**	
15:00-15:30	**Coffee Break**	**Coffee Break**	
15:30-16:00	**Paul Barrett** ChemBio Hub: tools to help collaboration within the University of Oxford and beyond	**Round-table discussion**	
16:00-16:30	**Andrew Stretton** Tutorial: "Customising the ChemBio Hub ChemReg open source registration system"		Departure
18:00-22:00	Dinner at "Linde Oberstrass"	Dinner at "Commihalle"	

Coffee breaks and lunches sponsored by Open for Innovation KNIME Novartis Institutes for BioMedical Research

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich