3rd RDKit UGM Agenda v1.0

22-24 October 2014
Darmstadt Germany

Wednesday 22 October

9:00 - 9:30	Introduction by Greg: State of the Toolkit
9:30 - 11:00	lightning talks
	Daniel Kuhn,
	Christian Herhaus,
	Paul Czodrowski [...]
11:00 - 11:30	**coffee break**
11:30 - 12:00	George Papadatos (EBI)
	Patent chemoinformatics with SureChEMBL and RDKit
12:00 - 12:30	Sereina Rinker (ETH)
	Working with Conformers from Molecular Dynamics Simulations in the RDKit
12:30 - 13:00	round table discussion
13:00 - 14:00	**lunch break**
14:00 - 16:00	guided tour of campus
16:00 - 16:30	Christian Kramer (Innsbruck University)
	Nonadditivity analysis with the RDKit
16:30 - 17:00	Ilenia Giangreco (CCDC)
	Mining the CSD for matched molecular crystal structures
18:00 -	**Social activity/dinner**
	Darmstädter Ratskeller (http://www.ratskeller-darmstadt.de/) - Marktplatz 8, 64283 Darmstadt

Thursday 23 October

9:00 - 9:30	Michał Nowotka (EBI)
	Using RDKit *without RDKit - Beaker update*
9:30 - 10:00	Adrian Jasiński (Adamed)
	MolGears: *A cheminformatics tool for bioactive molecules*
10:00 - 10:30	Jan Holst Jensen (Biochemfusion)
	PYPL: An Oracle cartridge enabling RDKit functions in SQL and PL/SQL
10:30 - 11:00	Riccardo Vianello
	Python3 support in the RDKit
11:00 - 11:30	**coffee break**
11:30 - 12:00	Nadine Schneider (Novartis)
	Being more reactive - Expanded chemical reaction support in the RDKit
12:00 - 12:30	Roger Sayle (NextMove)
	Reaction Informatics with RDKit: An explosive combination
12:30 - 13:00	Grégori Gerebtzoff
	Matched Molecular Sequences: finding the missing pair
13:00 - 14:00	**lunch break**
14:00 - 14:30	Samo Turk (BioMedX)
	Scaffold analysis in Python with RDKit and pandas
14:30 - 15:00	Axel Pahl (Aviru)
	An interactive SDF viewer
15:00 - 15:30	Noel O'Boyle (Next Move)
	Using RDKit for Matched Molecular Series Analysis: When two are not enough
15:30 - 16:00	**coffee break**
16:00 - 16:30	Greg Landrum (Novartis)
	Open-source from/in the enterprise
16:30 - 17:00	round table discussion
18:00 -	**Social activity/dinner**
	Grohe Braurei (http://www.grohe-gastro.de) - Nieder-Ramstädter-Str. 3, 64283 Darmstadt

Friday 24 October

9:00-16:00 Hackathon.
Some possible topics here: https://github.com/rdkit/rdkit/labels/Sprint%20idea