

## 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

MolGears: A cheminformatics tool for bioactive molecules  Jan Holst Jensen (Biochemfusion)  PYPL: An Oracle cartridge enabling RDKit functions in SQL and PL/SQL  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 - 14:30 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	9:00 - 9:30	Michał Nowotka (EBI)
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Grone Braurei (http://www.grone-gastro.de) - Nieder-Ramstädter-Str. 3, 64283 Darmstadt		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: <a href="https://github.com/rdkit/rdkit/labels/Sprint%20idea">https://github.com/rdkit/rdkit/labels/Sprint%20idea</a>