# 6th RDKit UGM Agenda v1.1

20-22 September 2017
Berlin Germany
Organizers: Andrea Volkamer (Charité Berlin), Gerhard Wolber (FU Berlin)

## Extra notes on the agenda

1. Locations (please see the info sheet for maps):
    a. On Wednesday and Thursday the UGM will be held at the Freie Universität Berlin, Institute of Pharmacy, Königin-Luise-Str. 2+4.
    b. On Friday the Hackathon will be held at the Charité Berlin, CCM Innere Medizin, Seminar Room 1 + 4, Virchowweg 9.
2. Poster presenters: we will have a "poster advertisements" session on Wednesday morning. You have 2-3 minutes and up to one slide to describe your poster and get people interested. If you have a slide that you'd like to use, please make sure that you get a copy to Greg (via email or on a memory stick) before 9 a.m. on Wednesday.
3. As usual, we will have two Lightning Talk sessions. You can tell us in advance that you'd like to do a lightning talk (in which case we'll be sure you have a slot) or you can spontaneously decide to do one. The slots will be about 5 minutes long.
4. We'll try to repeat the "RDKit Jogging" experiment from last year on Thursday and/or Friday. Greg will come up with a route idea based on participants and where they are staying. We'll do a distance and speed that fits whoever's participating. This will likely take place in the early morning, but we could also think about doing it between the end of the program and dinner.
5. We will likely organize a walking tour of the "Regierungsviertel" area near the restaurant before dinner on Thursday. Details at the UGM.

## Wednesday 20 September: UGM

| Time | |
|---|---|
| 08:30 - 09:00 | Check in and coffee |
| 09:00 - 10:00 | Greg Landrum: <br> Welcome and Intro |
| 10:00 - 10:30 | Poster advertisements |
| 10:30 - 11:00 | Break + Posters |
| 11:00 - 11:30 | Enric Herrero: <br> Conformation generation with RDKit: Comparative study and application reproducing bioactive overlays with PharmScreen |
| 11:30 - 12:00 | Guillaume Godin: <br> 3D descriptors in RDKit |
| 12:00 - 12:30 | Paolo Tosco: <br> OpenMM Integration |
| 12:30 - 13:30 | Lunch + Posters |
| 13:30 - 13:50 | Lightning talks |
| 13:50 - 14:10 | Michael Beachy: <br> RDKit: Schrödinger use and contributions |
| 14:10 - 14:30 | Nicola Zonta: <br> 2D coordgen: chemistry in plane view |
| 14:30 - 15:00 | Alpha Lee: <br> Exploring chemical space using random matrix theory |
| 15:00 - 15:30 | Coffee break + Poster |
| 15:30 - 16:00 | Daniel Reker: <br> Active learning for drug discovery and chemogenomics |
| 16:00 - 16:30 | Nadine Schneider: <br> Chemical topics: TBD |
| 16:30 - 17:00 | Paul Czodrowski: <br> Automatic Generation of Neural Network Architectures Using a Genetic Algorithm |

| Time | |
|---|---|
| 18:00 - 22:00 | Dinner: Luise (http://www.luise-dahlem.de/) |

## Thursday 21 September: UGM

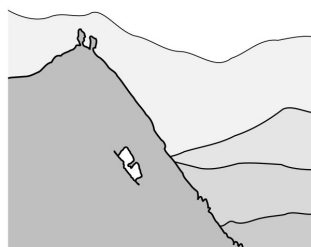| Time | |
|---|---|
| 08:30 - 09:00 | Check in and coffee |
| 09:00 - 09:30 | Anthony Bradley and Tim Dudgeon:<br>XChem and SQUONK - open-source tools for fragment-based drug design using the RDKit |
| 09:30 - 10:00 | Christian Kramer:<br>MMPDB: an RDKit-based MMP implementation for large datasets |
| 10:00 - 10:30 | Andrew Dalke:<br>MMPDB: Taming chiral structures for MMP prediction |
| 10:30 - 11:00 | Break + Posters |
| 11:00 - 11:30 | Samo Turk:<br>At the interface between SAR and machine learning - virtual compound optimization via MMP/ML |
| 11:30 - 12:00 | Marta Stepniewska-Dziubinska:<br>Pafnucy - A deep neural network for affinity prediction |
| 12:00 - 12:30 | Esben Jannick Bjerrum:<br>SMILES enumeration as Data Augmentation for Neural Network Modeling of Molecules |
| 12:30 - 13:30 | Lunch + Posters |
| 13:30 - 14:00 | Lightning talks |
| 14:00 - 14:30 | Thomas Evangelidis:<br>Ligand scaffold optimization guided by machine learning |
| 14:30 - 15:00 | Richard Sherhod:<br>Exploration of Patent Chemistry by Fuzzy MCS-led Fragment Decomposition |
| 15:00 - 15:30 | Coffee break + poster |
| 15:30 - 16:00 | Roger Sayle:<br>Recent improvements to the RDKit |
| 16:00 - 16:30 | Round table |

| 20:30 - 22:00 | Dinner: Zollpackhof (http://www.zollpackhof.de/index.php/de/) |
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## Friday 22 September: Hackathon

| Time | |
|---|---|
| 08:30 - 09:00 | Check in and organization |
| 09:00 - ??? | Hackathon |

# Sponsors

We're grateful to our sponsors for financially supporting the 2017 RDKit UGM and allowing us to keep it free for participants.