# 7th RDKit UGM Agenda v1.1

19-21 September 2018
Cambridge, UK
Organizer: Andreas Bender (U. Cambridge)

## Extra notes on the agenda. Please read these! :-)

1. Locations. For both locations please use the East Entrance of the Chemistry building (near the Scott Polar Institute).
   a. On Wednesday and Thursday the UGM will be held in the BMS Lecture Theatre, Chemistry Department, University of Cambridge, Lensfield Road, Cambridge CB2 1EW.
   b. On Friday the Hackathon will be held in rooms U202/U203 in the Chemistry Department, University of Cambridge, Lensfield Road, Cambridge CB2 1EW.
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. If you have registered for the conference dinner on Wednesday: **please** remember to bring £55 with you when you check-in for the UGM on Wednesday morning. If your plans have changed and you no longer can attend the conference dinner, please let Andreas know by the end of the day on Monday the 10th of September.
5. If you would like to join us for dinner at Loch Fyne on Thursday, please complete the doodle poll here https://doodle.com/poll/cfesnen22u755ap9 to pick your meal by the end of the day on Monday the 10th of September.

6. We'll try to repeat the "RDKit Jogging" experiment from previous years 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.

## Wednesday 19 September: UGM

| Time | |
|---|---|
| **Time** | |
| **08:30 - 09:00** | Check in |
| **09:00 - 10:00** | Greg Landrum:<br>Welcome and Intro |
| **10:00 - 10:30** | Poster advertisements |
| **10:30 - 11:00** | Coffee Break + Posters |
| **11:00 - 11:30** | Pat Lorton: Similarity searching a billion compounds in real time |
| **11:30 - 12:00** | Sereina Riniker: News from 3D (new features of the conformer generator) |
| **12:00 - 12:30** | Alpha Lee: Uncertainty quantification with Bayesian molecular deep learning |
| **12:30 - 13:30** | Lunch + Posters |
| **13:30 - 14:00** | Lightning talks |
| **14:00 - 14:30** | Boran Adas: RDKit's new fingerprint generators |
| **14:30 - 15:00** | Susan Leung: GSoC RDKit MolVS Integration Project |
| **15:00 - 15:30** | Coffee break + Posters |
| **15:30 - 16:00** | Nicholas Firth: Multiparameter optimisation using RDKit and scipy: what's the chance of success? |
| **16:00 - 16:30** | Marina Fedorova: Computational tools for metabolic pathways prediction |
| **16:30 - 17:00** | Brian Cole: SMILES-driven de novo design engine |
| **17:00 - 17:30** | Pat Walters: A Few (Hopefully) Interesting Open Source Projects Built On The RDKit |
| **19:00 -** | Conference Dinner: Magdalene College |

## Thursday 20 September: UGM

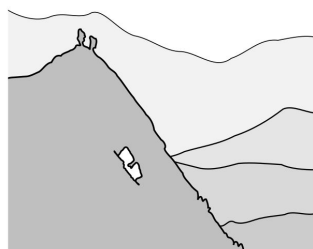| Time | |
|---|---|
| **Time** | |
| **08:30 - 09:00** | Check in |
| **09:00 - 09:30** | Joshua Meyers and Matthew Sellwood: Rediscovering R-Group Descriptors with RDKit |
| **09:30 - 10:00** | Noel O'Boyle: A de facto standard or a free-for-all? A benchmark for reading SMILES |
| **10:00 - 10:30** | Daria Goldmann: It's not just for Python! Interacting with chemical data using KNIME and the RDKit |
| **10:30 - 11:00** | Coffee Break + Posters |

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|---|---|
| **11:00 - 11:30** | Thomas Evangelidis: Ligand scaffold optimization guided by artificial intelligence. |
| **11:30 - 12:00** | Benjamin Tehan + Rob Smith: RDKit in the modern Biotech |
| **12:00 - 12:30** | Lewis Mervin + Natalia Aniceto: In silico protein target prediction with reliability-density neighbourhood applicability domain analysis |
| **12:30 - 13:30** | Lunch + Posters |
| **13:30 - 14:00** | Lightning talks |
| **14:00 - 14:30** | Marwin Segler: Computer aided synthesis planning |
| **14:30 - 15:00** | Jacob Spiegel: Genetic algorithm for de novo computer aided drug design |
| **15:00 - 15:30** | Coffee break + Posters |
| **15:30 - 16:00** | Andrea Morger: Machine learning and conformal prediction to support in silico toxicology |
| **16:00 - 16:30** | Lukas Pravda: The use of RDKit in the Protein Data Bank in Europe to handle small molecules chemistry and display protein-ligand interactions. |
| **16:30 - 17:00** | Roger Sayle: Deceptively Simple: How some cheminformatics problems can be more complicated than they appear. |
| **17:00 - 17:30** | Round table |
| **18:00 -** | Dinner: Loch Fyne |

## Friday 21 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 2018 RDKit UGM and allowing us to keep it free for participants.