



11th RDKit UGM Agenda v1.0

12-14 October 2022

Berlin, Germany

The UGM will be an in-person event with the presentations lived-streamed via zoom. If you have registered for the virtual version of the UGM, you will get an email a day or two before it starts with the zoom link.

Since the discord server worked well over the past two years, we've set one up this year as well: <https://discord.gg/tcW6DQgAQf>

The Github repo for this year is here: https://github.com/rdkit/UGM_2022

Practical details and logistics information can be found in the [github repo](#).

Wednesday 12 October, [Artloft.berlin](https://artloft.berlin)

Time (CEST)	
8:00 - 8:30	Check-in / registration
8:30 - 9:30	Greg Landrum Welcome and State of the RDKit
9:30 - 10:00	Brian Kelley Two years of DMPK, Gaussian Processes and confidence
10:00 - 10:30	Hao Shen Extending Rdkit Reaction Utility
10:30 - 11:30	Coffee and posters
11:30 - 12:00	Lauren Reid SARKush: Automated Markush-like Structure Generation for SAR Communication
12:00 - 12:30	John Mayfield Bits and pieces for better fingerprints
12:30 - 13:30	Lunch and posters
13:30 - 14:00	Lightning talks 1
14:00 - 14:30	Christos Kannas Creating a Reaction Knowledge Graph with Open Source Software
14:30 - 15:00	Marco Bertolini Beyond Atoms and Bonds: Contextual Explainability via Molecular Graphical Depictions
15:00 - 15:30	Coffee and posters
15:30 - 16:00	Rachael Pirie Can You Hear the Shape of a Drug?
16:00 - 16:30	Jan Jensen Do machines dream of atoms? A quantitative molecular benchmark for explainable AI heatmaps.

Lightning talks 1 session

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Thursday 13 October, [Artloft.berlin](https://artloft.berlin)

Time (CEST)	
8:00 - 8:30	Check-in / registration
8:30 - 9:00	Lightning talks 2
9:00 - 9:30	Paolo Tosco Interactive rendering of 2D structures with RDKit
9:30 - 10:00	Jess Stacey Using Matched Molecular Pairs for CoreDesign®
10:00 - 10:30	Rafał A. Bachorz MOVAE: a generic framework for creating molecular variational autoencoders
10:30 - 11:30	Coffee and posters
11:30 - 12:00	Lukas Friedrich t.b.d.
12:00 - 12:30	Andrew Dalke mmpdb 3.0
12:30 - 14:00	Lunch and posters
14:00 - 14:30	Lightning talks 3
14:30 - 15:00	Roger Sayle Understanding tautomerism (in 2½D)
15:00 - 15:30	Wrap up
15:30 - 17:00	Coffee and posters

Lightning talks 2 session

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Lightning talks 3 session

t.b.d

Friday 14 October, [TUECHTIG](#)

Time (CEST)	
9:00 - 9:30	Check-in / registration
9:30 - 16:00	Hackathon!

The hackathon is, as always, spontaneously organized and informal. Additional information will be sent to those who said that they planned to attend via email.