



# 11th RDKit UGM Agenda v1.1

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](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	<b>Greg Landrum</b> Welcome and State of the RDKit
9:30 - 10:00	<b>Brian Kelley</b> Two years of DMPK, Gaussian Processes and confidence
10:00 - 10:30	<b>Paolo Tosco</b> Interactive rendering of 2D structures with RDKit
10:30 - 11:30	Coffee and posters
11:30 - 12:00	<b>Lauren Reid</b> SARKush: Automated Markush-like Structure Generation for SAR Communication
12:00 - 12:30	<b>John Mayfield</b> Bits and pieces for better fingerprints
12:30 - 13:30	Lunch and posters
13:30 - 14:00	<b>Lightning talks 1</b>
14:00 - 14:30	<b>Christos Kannas</b> Creating a Reaction Knowledge Graph with Open Source Software
14:30 - 15:00	<b>Marco Bertolini</b> Beyond Atoms and Bonds: Contextual Explainability via Molecular Graphical Depictions
15:00 - 15:30	Coffee and posters
15:30 - 16:00	<b>Rachael Pirie</b> Can You Hear the Shape of a Drug?
16:00 - 16:30	<b>Jan Jensen</b> GABBY: Searching the REAL data base with genetic algorithms

### Lightning talks 1 session

t.b.d

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

Time (CEST)	
8:00 - 8:30	Check-in / registration
8:30 - 9:00	<b>Lightning talks 2</b>
9:00 - 9:30	<b>Hao Shen</b> Extending Rdkit Reactions and Some Use Cases
9:30 - 10:00	<b>Jess Stacey</b> Using Matched Molecular Pairs for CoreDesign®
10:00 - 10:30	<b>Rafał A. Bachorz</b> MOVAE: a generic framework for creating molecular variational autoencoders
10:30 - 11:30	Coffee and posters
11:30 - 12:00	<b>Lukas Friedrich</b> t.b.d.
12:00 - 12:30	<b>Andrew Dalke</b> mmpdb 3.0
12:30 - 14:00	Lunch and posters
14:00 - 14:30	<b>Lightning talks 3</b>
14:30 - 15:00	<b>Roger Sayle</b> Understanding tautomerism (in 2½D)
15:00 - 15:30	Wrap up
15:30 - 17:00	Coffee and posters

### Lightning talks 2 session

t.b.d

### Lightning talks 3 session

t.b.d

## Friday 14 October, [TUECHTIG](#)

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

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.