



# 13th RDKit UGM Agenda v1.0

11-13 September 2024

Zürich, Switzerland

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/9HCRCkAKWu>

The Github repo for this year is here: [https://github.com/rdkit/UGM\\_2024](https://github.com/rdkit/UGM_2024)

The most recent version of this document, logistics information, and other practical details can be found in the [github repo](#).

## Wednesday 11 September

Time (CEST)	
08:30 - 09:00	Check-in / registration
09:00 - 10:00	<b>Greg Landrum</b> Welcome and State of the RDKit
10:00 - 10:30	<b>Javier Pineda</b> : The RDKit is getting Rust-y
10:30 - 11:30	Coffee and posters
11:30 - 12:00	<b>Jeffrey Wagner</b> : From RDKit to MD simulation in seconds: An introduction to Open Force Field
12:00 - 12:30	<b>Nauman Ulah Khan, Gerd Blanke</b> : InChI dynamics: canonical, unique and on-the-fly
12:30 - 13:30	Lunch and posters
13:30 - 14:00	Lightning talks 1
14:00 - 14:30	<b>Vladas Oleinikovas</b> : PLINDER: The protein-ligand interactions dataset and resource
14:30 - 15:00	<b>Benjamin Ries</b> : OpenFE: Kartograf & Konnektor tools for setting up free energy calculations
15:00 - 15:30	Coffee and posters
15:30 - 16:00	<b>Andrea Andrews-Morger</b> : Federated learning in computational toxicology: An industrial perspective on the effiris hackathon
16:00 - 16:30	<b>Martin Sicho</b> : Putting molecular generators to practice: Outlook and applications of open source software
16:30 - 17:00	<b>Gregori Gerebtzoff</b> : Deep learning models compared to experimental variability for the prediction of CYP3A4 time-dependent inhibition
18:00 - 22:00	Conference dinner

## Thursday 12 September

Time (CEST)	
08:30 - 09:00	Check-in / registration
09:00 - 09:30	What's new 2
09:30 - 10:00	<b>Jan Jensen:</b> RDKit and transition metal coordination compounds
10:00 - 10:30	t.b.d.
10:30 - 11:00	Coffee and posters
11:00 - 11:30	Lightning talks 2
11:30 - 12:00	<b>Paul Katzberger:</b> General graph neural network based implicit solvation model for organic molecules
12:00 - 12:30	<b>Christian W. Feldmann:</b> Model uncertainty: Evaluating the impact of neural fingerprints on probability calibration
12:30 - 13:30	Lunch and posters
13:30 - 14:00	What's new 3
14:00 - 14:30	<b>Rachael Pirie:</b> Double cubic lattice volume
14:30 - 15:00	<b>Joos Kiener:</b> RDKit-powered chemical registration
15:00 - 15:30	Coffee and posters
15:30 - 16:00	<b>Davit Rizhinashvili:</b> Light speed MMPA and UMAP using RDKit and WebGPU
16:00 - 16:30	<b>Roger Sayle:</b> Roger's talk
16:30 - 17:00	Wrap up

# Lightning Talks

## **Session 1**

Thomas Evangelidis

Nils van Staalduinen

Tom Daff

Markus Orsi

Guillaume Godin

## **Session 2**

Marco Stenta

Jessica Braun

Paolo Tosco

Wim Dehaen

## Friday 13 September

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.

In addition to the normal hackathon, we will have two workshops/tutorials on Friday morning:

1. Writing KNIME nodes in Python, presented by Alice Krebs and Tugrul Kaynak from KNIME
2. Exploring small molecule structure data in the PDB, presented by Ibrahim Roshan from EMBL-EBI

## Sponsors

The RDKit UGM can only take place in its current form thanks to the generous financial support of our sponsors.

### Gold



**Schrödinger**



### Silver



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