



13th RDKit UGM Agenda v1.3

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

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	Greg Landrum Welcome and State of the RDKit
10:00 - 10:30	Joos Kiener : RDKit-powered chemical registration
10:30 - 11:30	Coffee and posters
11:30 - 12:00	Jeffrey Wagner : From RDKit to MD simulation in seconds: An introduction to Open Force Field
12:00 - 12:30	Paul Katzberger : General graph neural network based implicit solvation model for organic molecules
12:30 - 13:30	Lunch and posters
13:30 - 14:00	Lightning talks 1
14:00 - 14:30	Javier Pineda : The RDKit is getting Rust-y
14:30 - 15:00	Benjamin Ries : OpenFE: Kartograf & Konnektor tools for setting up free energy calculations
15:00 - 15:30	Coffee and posters
15:30 - 16:00	Andrea Andrews-Morger : Federated learning in computational toxicology: An industrial perspective on the effiris hackathon
16:00 - 16:30	Martin Sicho : Putting molecular generators to practice: Outlook and applications of open source software
16:30 - 17:00	Gregori Gerebtzoff : Towards human PK prediction: methods, models, and datasets
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	Jan Jensen: RDKit and transition metal coordination compounds
10:00 - 10:30	Afnan Sultan: Transformers for Molecular Property Prediction: A Review and a Recommendation for Efficient Training
10:30 - 11:00	Coffee and posters
11:00 - 11:30	Lightning talks 2
11:30 - 12:00	Nauman Ulah Khan, Gerd Blanke: InChI dynamics: canonical, unique and on-the-fly
12:00 - 12:30	Christian W. Feldmann: 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	Rachael Pirie: Resurrecting A Roger Relic: Implementing the Double Cubic Lattice Volume for RDKit
14:30 - 15:00	Vladas Oleinikovas: PLINDER: The protein-ligand interactions dataset and resource
15:00 - 15:30	Coffee and posters
15:30 - 16:00	Davit Rizhinashvili: Light speed MMPA and UMAP using RDKit and WebGPU
16:00 - 16:30	Roger Sayle: Roger's talk
16:30 - 17:00	Wrap up

Lightning Talks

Session 1

Thomas Evangelidis

Rachel Walker

Tom Daff

Markus Orsi

Guillaume Godin

Session 2

Marco Stenta

Jessica Braun

Paolo Tosco

Wim Dehaen

Antoine Lacour

Friday 13 September

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

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



GLYSADE