13th RDKit UGM Agenda v1.1

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	**Javier Pineda**: The RDKit is getting Rust-y
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	**Nauman Ulah Khan, Gerd Blanke**: 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	**Vladas Oleinikovas**: PLINDER: The protein-ligand interactions dataset and resource
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**: 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	**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	**Paul Katzberger**: General graph neural network based implicit solvation model for organic molecules
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**: Double cubic lattice volume
14:30 - 15:00	**Joos Kiener**: RDKit-powered chemical registration
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
Nils van Staalduinen
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.

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