12th RDKit UGM Agenda v1.7

20-22 September 2023
Mainz, 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/adCjKPzXfS

The Github repo for this year is here: https://github.com/rdkit/UGM_2023

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

About the "Ask the community" session

This is a new thing we're trying this year.
If you have a question about whether or not you can do something with the RDKit, or what the best way to do something is, this is the time to ask. People with questions will have a couple of minutes (and up to one slide) to ask their question to the community in attendance. The idea is that people with answers or ideas can then reach out to you during one of the breaks or via discord and provide an answer. We'll regularly check in on how things are going in terms of people having their questions answered. Maybe some of these questions will lead to new pieces of RDKit documentation, or blog posts, or something like that too, but the main thing is harness the expertise of all the people sitting in the room to get your questions answered.
We'll give priority to students, including PhD students, here (so, if you're a student and have questions about how to do stuff with the RDKit, please get ready to ask!), but if there aren't enough student questions, we'll open the floor.

Wednesday 20 September

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	**Susan Leung:** Why is it so difficult to replace the old with the new? Learnings from dealing with legacy systems in AstraZeneca and how RDKit can help
10:00 - 10:30	**Esben Bjerrum:** Faster and more diverse de novo molecular optimization with double-loop reinforcement learning using augmented SMILES
10:30 - 11:30	Coffee and posters
11:30 - 12:00	**Dmytro Radchenko:** Fragment-based substructure search in Enamine REAL Space
12:00 - 12:30	**Paolo Tosco:** RDKit Office Hours
12:30 - 13:30	Lunch and posters
13:30 - 14:00	**Lightning talks 1**
14:00 - 14:30	**Tim Vandermeersch:** CTSmarts: Compile time SMARTS expressions in C++20
14:30 - 15:00	**Jessica Braun:** Understanding and quantifying molecular flexibility: Torsion Angular Bin Strings
15:00 - 15:30	Coffee and posters
15:30 - 16:00	**Jessica Lanini:** PREFER: A New Predictive Modeling Framework for Molecular Discovery
16:00 - 16:30	**Aishvarya Tandon & Marcel Baltruschat:** eXplainable FingerPrints (X-FP)
16:30 - 17:00	Ask the community
19:00 - 23:00	Conference dinner

Thursday 21 September

Time (CEST)	
8:00 - 8:30	Check-in / registration
8:30 - 9:00	**Lightning talks 2**
9:00 - 9:30	What's new 2
9:30 - 10:00	**Francois Berenger:** 3D sensitive encoding of pharmacophore features
10:00 - 10:30	**Maximilian Beckers:** Leveraging historical small molecule data from the Novartis portfolio: From chemical series evolution to predictive modelling
10:30 - 11:30	Coffee and posters
11:30 - 12:00	**Noel O'Boyle:** SmiZip (2001) - Ancient Relic or Buried Treasure?
12:00 - 12:30	**Hannah Baumann:** Breaking free from ligand similarity restrictions in binding free energy calculations
12:30 - 13:30	Lunch and posters
13:30 - 14:00	**Lightning talks 3**
14:00 - 14:30	What's new 3
14:30 - 15:00	**Lauren Reid:** How to give the user what they want?: Challenges in Markush structure visualisation and exploitation"
15:00 - 15:30	**Roger Sayle:** t.b.d.
15:30 - 16:00	Wrap up
16:00 - 17:00	Coffee and posters

Lightning Talks

This is currently a partial list and subject to change.

Session 1

1. **Andrea Volkamer**: TeachOpenCADD goes DL
2. **Charles Tapley Hoyt**: Improving reproducibility of cheminformatics workflows with `chembl-downloader`
3. **Markus Orsi**: Encoding Stereochemistry in Molecular Fingerprints
4. **Patrick Penner**: Descriptive Grammar Analysis of Molecular File Formats
5. **Richard Gowers**: PDBinf: A rules based system for nonstandard amino acid and nucleotide recognition in RDKit
6. **Wouter Heyndrickx**: Ligand-based ML for virtual screening of anti-tuberculosis compounds:a viable option?

Session 2

1. **Paolo Tosco**: A stub a day keeps the docstrings at bay
2. **Torben Gutermuth**: SmartChemist - Communication about chemical structures made easy
3. **Rostislav Fedorov**: Decomposition of COFs
4. **David Kreutter**: Disconnection-Aware Triple Transformer Loop with a Route-Penalty Score for Multistep Retrosynthesis
5. **Rachael Piri**e: Filling in the gaps: Extracting implied reactions with RDKit
6. **Greg Landrum**: lwreg: chemical registration system for computational work

Session 3

1. **Tom Daff**: RDKit on AWS Lambda
2. **Jimmy Kromann**: Streamlining Quantum Chemistry for Tautomers, Protomers & Conformers using RDKit
3. **Grégori Gerebtzoff**: Putting RDKit in the hands of the users in a corporate environment: leveraging the power of Datagrok
4. **Michel Lim and Vinith Kowrithasan**: Tools developed in the Czodrowski Lab
5. **Michael Backenköhler, Joschka Groß**: Hybrid Docking as a Data Generation Approach for Kinase-Based Deep Learning Tasks
6. **Esben Bjerrum:** Scikit-Mol brings RDKit to Scikit-Learn

Friday 22 September

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 via email to those who said that they planned to attend.

Sponsors

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

Platinum

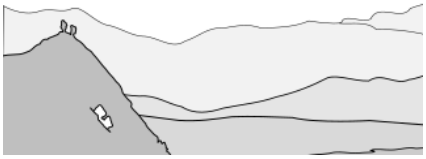
NextMove Software

Gold

CDD VAULT® Complexity Simplified

Open for Innovation KNIME

Schrödinger



MERCK

Silver

GLYSADE

Bronze

MedChemica

CREATING A STEP CHANGE IN MEDICINAL CHEMISTRY