11th RDKit UGM Agenda v1.2

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/tcW6DQqAQf

The Github repo for this year is here: https://github.com/rdkit/UGM_2022

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

Wednesday 12 October, Artloft.berlin

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

Lightning talks 1 session

Richard Gowers Biopolymers in RDKit

Barak Akabayov Expanding the chemical space of a hit molecule obtained by NMR fragment screening using machine-learning

Matt Stahl RDKit Molecular Analytics

Dan Nealschneider Comparing molecules that have enhanced stereo labels

Miriana Di Stefano VenomPred: A Machine Learning Based Platform for Molecular Toxicity Predictions

Thursday 13 October, Artloft.berlin

Time (CEST)	
8:00 - 8:30	Check-in / registration
8:30 - 9:00	**Lightning talks 2**
9:00 - 9:30	**Hao Shen** Extending Rdkit Reactions and Some Use Cases
9:30 - 10:00	**Jess Stacey** Using Matched Molecular Pairs for CoreDesign®
10:00 - 10:30	**Rafał A. Bachorz** MOVAE: a generic framework for creating molecular variational autoencoders
10:30 - 11:30	Coffee and posters
11:30 - 12:00	**Lukas Friedrich** Three Years of Project MELLODDY: Insights from a Collaborative Machine Learning Endeavor in Drug Discovery
12:00 - 12:30	**Andrew Dalke** mmpdb 3.0
12:30 - 14:00	Lunch and posters
14:00 - 14:30	**Lightning talks 3**
14:30 - 15:00	**Roger Sayle** Understanding tautomerism (in 2½D)
15:00 - 15:30	Wrap up
15:30 - 17:00	Coffee and posters

Lightning talks 2 session

Markus Orsi Introducing an open-source version of MXFP (macromolecule extended atom-pair fingerprint)
Eduardo Mayo Expansion of The COMPAS Project: Heterocyclic Polyaromatics
Alice Krebs and Norbert Sas Developing KNIME Nodes in Python
Joos Kiener Slide Generator - Advanced MolsToGridImage
Stéphane Téletchéa DockNmine2: small scale virtual screening made easy
Bartosz Baranowski Laplacian Modified Naive Bayes implementation in python

Lightning talks 3 session

Jeffrey Wagner Open Force Field: Powered by RDKit
Rachel Walker Potential improvements to 2D coordinate generation
Rodrigo Ochoa pyPept: a python library to analyze peptides using BILN and RDKit representations
Ya Chen RDKit applications in cheminformatic analysis for natural products
Marco Stenta Moving beyond chemical cartridges by federating our chemical searches.

Friday 14 October, TUECHTIG

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.