10th RDKit UGM Agenda v1.1

14-15 October 2021

online

Thursday 14 October

Time (CEST)	
10:00 - 10:30	Welcome and organizational remarks
10:30 - 11:00	**Djork-Arné Clevert** Img2Mol – SMILES Recognition from Depictions of Chemical Structures
11:00 - 11:30	**Mahendra Awale** Modifying the Synthetic Accessibility Score to Identify Undesirable Virtual Compounds
11:30 - 12:00	**Christina Humer and Henry Heberle** ChemInformatics Model Explorer (CIME): Exploratory analysis of chemical model explanations
12:00 - 12:30	**Marek Noga** Using RDKit to build analytical assays for diagnosis of metabolic disorders
16:30 - 17:00	virtual coffee and social time
17:00 - 17:30	Welcome and organizational remarks
17:30 - 18:00	**Greg Landrum** State of the RDKit
18:00 - 18:30	**Yuliana Zabolotna** SYNTHI: a New Toolkit for Synthon-Based Library Design and Building Blocks Analysis
18:30 - 19:00	**Eduardo Mayo** MScreen: Molecular docking benchmarking made easy
19:00 - 19:30	Lightning talks 1

Friday 15 October

Time (CEST)	
10:00 - 10:30	virtual coffee and social time
10:30 - 11:00	**Sereina Riniker** Combining ETKDG and NOE-derived distance bounds”
11:00 - 11:30	**Amol Thakkar** Browser based exploration of the GDB chemical space using AI planned synthesis facilitates experimental engagement
11:30 - 12:00	**Jimmy Kromann** Building Quantum Chemistry Pipelines with RDKit
12:00 - 12:30	**Paolo Tosco** An RDKit-based JavaScript component for molecule visualization
16:30 - 17:00	virtual coffee and social time
17:00 - 17:30	Lightning talks 2
17:30 - 18:00	**Daniel Probst** RDKit-Powered Reaction Classification and Yield Prediction using the Differential Reaction Fingerprint DRFP
18:00 - 18:30	**Hadrien Mary** Datamol: Molecular Manipulation Made Easy
18:30 - 19:00	**Roger Sayle** Handling organometallic and inorganic stereochemistry in RDKit
19:00 - 19:15	Wrap-up and closing words

Lightning talks session 1: Thursday

Jonas Boström The value of shape and electrostatic similarities in deep generative methods
Christoph Bauer Multiobjective Reaction Similarity with the RDKit
Andrew Skalkin Datagrok: cheminformatics in the browser

Lightning talks session 2: Friday

Cédric Bouysset Interactive visualization and filtering of small molecule datasets with mols2grid
Dominique Sydow TeachOpenCADD update
Jacob Spiegel Automated Analog Generation and Retrosynthesis Predictions