10th RDKit UGM Agenda v1.0

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?**

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
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

Friday session

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