Tuesday, 6th of October

10:00 - 10:30	Welcome and organizational remarks
10:30 - 10:45	**Cédric Bouysset**: From RDKit to the Universe and back
10:45 - 11:00	**Manan Goel**: ANAKIN-ME and other Neural Network Potentials: Applications and Utilities in RDKit
11:00 - 11:30	**Anne Hersey**: ChEMBL's open source chemical structure curation pipeline
11:30 - 12:00	**Lukas Friedrich**: MELLODDY-TUNER: Data Standardization Framework for Federated Machine Learning
12:00 - 12:30	**Tuan Le**: Neuraldecipher – Reverse-engineering extended-connectivity fingerprints (ECFPs)

16:30 - 17:00	Virtual coffee & social time
17:00 - 17:30	Welcome and organizational remarks
17:30 - 18:00	**Greg Landrum**: State of the RDKit
18:00 - 18:30	**Jan Jensen**: Organometallica: Dealing with organometallic molecules in RDKit
18:30 - 19:00	**Eric Jonas**: Molecular Inverse Problems : Spectroscopy and RDKit
19:00 - 19:15	**Shrey Aryan**: t.b.d.
19:15 - 19:30	**Christopher Zou**: Mongo-rdkit: Chemistry in MongoDB

Wednesday, 7th of October

10:00 - 10:30	Virtual coffee & social time
10:30 - 11:00	Lightnings and Posters 1
11:00 - 11:30	**Roger Sayle**: Rolling SMARTS: You don't always find want you want, but if you try sometimes, you find what you need
11:30 - 12:00	**Marcel Baltruschat**: pKa predictions on top of the RDKit
12:00 - 12:30	**Carmen Esposito**: Automated procedure for class imbalance learning

16:30 - 17:00	Virtual coffee & social time
17:00 - 18:00	Panel: so you want a new feature added to the RDKit?
18:00 - 18:30	**Steven Kearnes & Connor Coley**: The Open Reaction Database

18:30 - 19:00	**Gareth Jones**: Using RDKit in Cheminformatics Visualizations
19:00 - 19:30	Lightnings and Posters 2

Thursday, 8th of October

10:00 - 10:30	Virtual coffee & social time
10:30 - 11:00	**Guillaume Godin**: Chemical Challenges in Deep learning
11:00 - 11:30	**Dominique Sydow**: KinFragLib: Subpocket-based kinase inhibitor fragmentation and recombination
11:30 - 12:00	**Ed Griffen & David Cosgrove**: Efficiently delivering better molecule depictions and highlighting: Why, What and How.
12:00 - 12:30	Lightnings and Posters 3
12:30	Closing remarks

16:30 - 17:00	Virtual coffee & social time
17:00 - 17:30	Lightnings and Posters 4
17:30 - 18:00	**Ricardo Rodriguez & Greg Landrum**: The New RDKit Chirality Code
18:00 - 18:30	**Esben Bjerrum**: RDKit derived reaction labels for improved retrosynthetic route finding
18:30 - 19:00	Closing remarks