

Tuesday, 6th of October

CEST time:	
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)

CEST time:	
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

CEST time:	
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 what 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

CEST time:	
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

CEST time:	
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

CEST time:	
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