	Wednesday		Thursday		Friday
08:30 - 09:00	Check-In/ Registration	08:30 - 09:00	Check-In/Organization	08:30 - 9:00	Check-In/Organization
09:00 - 10:00	Welcome & Introduction (Greg/Emanuel)	09:00 - 09:30	Dominique Sydow and Jaime Rodríguez-Guerra: TeachOpenCADD: An open source teaching platform for computer-aided drug design	09:00 - 16:00	Hackathon & Workshop
		09:30 - 10:00	Rob Smith: Traversing and Indexing Chemically Rich Documentation with RDKit to aid GPCR-based Drug Discovery		
10:00 - 10:30	Poster Advertising	10:00 - 10:30	Jan Halborg Jensen: Quantum chemistry meets cheminformatics		
10:30 - 11:15	Coffee & Posters	10:30 - 11:15	Coffee & Posters		
11:15 - 11:45	Floriane Montanari and Robin Winter: Utilizing in silico models in both directions: predicting and optimizing the properties of small molecules	11:15 - 11:45	Brian Kelley: "Learned" Molecule Representations - a technical comparison with data from real projects		
11:45 - 12:15	Mahendra Awale: SAR Transfer via Matched Molecular Series	11:45 - 12:15	Ya Chen: Applications of RDKit in Machine Learning		
12:15 -12:45	Martin Vogt: Systematic extraction of analogue series from large compound collections	12:15 -12:45	Christoph Bauer: Generation of Bimolecular 3D Complex Structures with RDKit		
12:45 - 14:00	Lunch & Posters	12:45 - 14:00	Lunch & Posters		
14:00 - 14:30	Lightning Talks	14:00 - 14:30	Lightning Talks		
14:30 - 15:00	Paul Czodrowski: Is bigger always better? Comparing two strategies for the generation of predictive models based on different computational resources	14:30 - 15:00	Suliman Sharif: Cocktail Shaker: An open source drug expansion and enumeration library using Python and RDKit		
15:00 - 15:30	Chaya Stern: Improving molecular models by generating high-quality quantum chemistry data	15:00 - 15:30	Florian Flachsenberg: LSL-BFGS: A gradient-based numerical optimization algorithm for molecular systems		
15:30 - 16:15	Coffee & Posters	15:30 - 16:15	Coffee & Posters		
16:15 - 16:45	Carmen Esposito: Ligand-Based Machine Learning Approach to Predict P-Glycoprotein Substrates and Multidrug Resistance	16:15 - 16:45	Susan Leung: Can Computers Find Hits Faster Than Humans? Using Bayesian Optimisation in Ligand-Based and Structure-Based Virtual Screening		
16:45 - 17:15	Esben Bjerrum: Molecular De Novo Design - using Deep Learning Encoders and Generators together with RDKit	16:45 - 17:15	Roger Sayle: 2D Similarity, Diversity and Clustering in RDKit		
17:15 - 17:45	Dan Neilschneider: Enhanced stereochemistry: vials vs files	17:15 - 17:45	Roundtable/Feedback		
17:45 - 18:15	Special Session on Stereochemistry				
19:00 - 23:00	Conference Dinner	18:00 -	Dinner		