Session 1: Wednesday 07.10, 10:30 – 11:00 (CEST)

Takayuki Serizawa	Automated Identification of Chemical Series with RDKit	Lightning
Tuomo Kalliokoski	Shuffling through a billion molecule database using RDKit-based tools while looking for CNS-relevant compounds	Lightning
Noel O'Boyle	An efficient algorithm to find matched pairs of a peptide	Lightning
Sascha Jung	Let it flow: VSFlow as versatile open source tool for virtual screening	Lightning
Nadine Schneider	Substructure filters re-visited – or fun with SMARTS	Lightning
Eric March Vila	Cleaning the dark corners of the chemical space. A structure curation tool for problematic substances	Poster

Session 2: Wednesday 07.10, 19:00 – 19:30 (CEST)

Joann Prescott-Roy	DeprotectLib	Lightning
Kevin Jernigan	RDKit and Amazon Aurora	Lightning
Jaime Rodriguez-Guerra & Dominique Sydow	TeachOpenCADD news	Lightning
Philippe Schwaller	Unsupervised Attention-Guided Atom-Mapping	Lightning
Vincent Scalfani	RDKit cookbook	Poster
Helge Vatheuer	Same same but different: investigations of two almost identical kinase inhibitors	Lightning

Session 3: Thursday 08.10, 12:00 – 12:30 (CEST)

Mahendra Awale	The Playbooks of Medicinal Chemistry Design Moves	Lightning
Aishvarya Tandon	Deep Painting, an amalgamation of Cell Painting and Machine Learning	Lightning
Jessica Lanini	Analysis and Benchmarking of Data-Driven Molecular Representations	Lightning
Stéphane Télétchéa	DockNmine, a Web Portal to Assemble and Analyse Virtual and Experimental Interaction Data	Lightning
Gerd Blanke	How are RDKit and MolVS used to prepare Elsevier's reaction data for synthetic route prediction	Poster
Talia Kimber	Cytotoxicity maps	Lightning

Session 4: Thursday 08.10, 17:00 – 17:30 (CEST)

Pratik Dhakal	Machine Learning-Enabled Accelerated Discovery of High Ionic Conductivity Ionic Liquids	Lightning

Pedro Reis	Fast and accurate protein pKa predictions with machine learning	Lightning
Eduardo Mayo	Genetic Algorithm for ligand design	Lightning
Joseph Ni	Curating a Minimal Set of Reaction Rules to Cover the Entire Space of Common Enzymatic Transformations	Poster
Fabio Le Piane	Predicting the properties of molecular materials: multiscale simulation workflows meet machine learning	Poster
José Teofilo Moreira-Filho	An Artificial Intelligence-Based Web App to Assess Acute Toxicity of Chemicals to Honey Bees	Lightning