Thursday 19th September - Foyer			
10:30 – 10:50	Artem Cherkasov (invited speaker)	University of British Columbia	The Use of Active Learning for Effective Exploration of Chemical Universe
10:50 - 11:10	Rosa Friesacher	AstraZeneca, Katholieke Universiteit Leuven	Temporal Evaluation of Probability Calibration with Experimental Errors
11:10 - 11:30	Alessio Fallani	Janssen, University of Luxembourg	Atom-level Quantum Pretraining Enhances the Spectral Perception of Molecular Graphs in Graphormer
11:30 - 11:50	Mathias Hilfiker	AstraZeneca, University of Luxembourg	Leveraging quantum mechanical properties to predict solvent effects on large drug-like molecules
11:50 - 12:10	Muhammad Arslan Masood	Janssen, Aalto University	Balancing Imbalanced Toxicity predictor: Using MolBERT with Focal Loss
12:10 - 12:30	Mikhail Andronov	Pfizer, SUPSI	Curating reagents in chemical reaction data with an interactive reagent space map
12:30 - 14:00			**Lunch break**
14:00 - 14:20	Paula Torren Peraire	Janssen, Helmholtz Zentrum München	Improving Route Development Using Convergent Retrosynthesis Planning
14:20 - 14:40	Yasmine Nahal	Aalto University , AstraZeneca	Towards Interpretable Models of Chemist Preferences for Human-in-the-loop Assisted Drug Discovery
14:40 - 15:00	Marco Bertolini	Pfizer	Enhancing Interpretability in Molecular Property Prediction with Contextual Explanations of Molecular Graphical Depictions
15:00 - 15:20	Julian Cremer	Pfizer, Universitat Pompeu Fabra	Latent-Conditioned Equivariant Diffusion for Structure-Based De Novo Ligand Generation
15:20 - 15:40	Justin Diamond	Universität Basel	Neural SHAKE: Geometric Constraints in Graph Generative Models
15:40 - 16:00	Pedro Ballester	Imperial College	Scaffold Splits Overestimate Virtual Screening Performance
16:00 – 16:30			**Poster session with coffee**

Friday 20th September - Foyer			
10:10 - 10:30	Son Ha	Janssen, Johannes Gutenberg Universität Mainz	Cross Multimodal Learning of Cell Painting and Transcriptomics Data
10:30 - 11:00			**Poster session with coffee**
11:00 - 11:20	Fabrizio Ambrogi / Szymon Czaplak	Selvita	Target-Aware Drug Activity Model: A deep learning approach to virtual HTS
11:20 - 11:40	Emma Svensson	AstraZeneca, Johannes Kepler Universität Linz	Temporal Evaluation of Uncertainty Quantification under Distribution Shift
11:40 - 12:00	Eduardo Viganò	Mario Negri Institute for Pharmacological Research	Artificial Intelligence Methods for Evaluating Mitochondrial Dysfunction: Exploring Various Chemical Notations Suitable for Neural Language Processing Models
12:00 - 12:20	Regina Pikalyova	University of Strasbourg	Combinatorial Library Neural Network (CoLiNN) for Combinatorial Library Visualization without Compound Enumeration
12:20 - 12:40	Dragos Horvath	University of Strasbourg	De novo Drug Design – Do We Really Want To Be “Original”? A real-world case study on colchicine-site tubulin binders.
12:40			**Lunch break**