	Presenter	Affiliation	Title
1	David Marcus	GSK	QSARStudio: An enterprise platform for building and monitoring machine learning models
2	Peter Hunt	Optibrium Ltd.	Synergistic application of QuanSA & physics-based simulation in affinity prediction
3	Mark Gardner	AMG Consultants Ltd.	Models of unbound volume of distribution, Vdss and fraction unbound
4	Jiahao Yu	GSK / University of Bristol	Filling the gaps: Data Imputation Methods for Drug Discovery
5	Leonie Windeln	University of Southampton	How do autoencoders help explore the conformational space of MD simulations of cyclic peptides?
6	Andrew Henry	Chemical Computing Group	Database AutoPH4: Pharmacophore Analysis of Multiple Protein Structures
7	Noel O'Boyle	Sosei Heptares	Handling Ultra-large Chemical Spaces in Structure-Based Drug Design
8	Olga Obrezanova	AstraZeneca	Towards early prediction of human pharmacokinetics using AI approaches
9	Mirielle Krier	OpenEye	3D-QSAR meets ML for Binding Affinity Prediction
10	Nicolas Bosc	EMBL-EBI	The new SureChEMBL in a nutshell
11	Finlay Clark	University of Edinburgh	Robust Automated Equilibration Detection for Molecular Simulation
12	Ben Honoré	University of Bristol	The Application of Machine Learning to Predict and Solve NMR Spectra in Structure Elucidation
13	Johannes Reynisson	Keele University	Phosphatidylcholine-specific phospholipase C as a promising drug target
14	Syed Zayyan Masud	(Independent)	QITB: An interactive open-source web app for cheminformatics
15	Nikolai Nikolov	Technical University of Denmark	The Danish (Q)SAR Database and modelling software
16	Daniella Hares	Institute of Cancer Research	Computational study of water network influencing potency of BCL6 inhibitors
17	Oliver Hills	Cresset	Prioritization of new molecule design using QSAR models: 2D- and 3D-QSAR studies on SARS-CoV-2 Mpro inhibitors
18	Adriana Coricello	Università degli Studi di Urbino "Carlo Bo"	An MD-based workflow for predicting relative affinities of series of congeneric ligands
19	Joe Heeley	University of Nottingham	Solvent Surfer: interactive PCA for solvent selection
20	Jack Sawdon	University of Southampton	Machine Learning Driven Development of a Coarse-Grained Water Model Using ForceBalance
21	Terence Egbelo	University of Sheffield	Predicting Bioactivity by Traversing Knowledge Graphs
22	Joe Davies	University of Nottingham	Integrating sustainability into reaction planning for the AI4Green electronic laboratory notebook
23	Peter Curran	Pharmenable Tx	ChemXpander: Exploration of Ultra Large Small Molecule Libraries for Hit Discovery
24	James Middleton	University of Sheffield	Fusing spectral geometry and content-based image retrieval techniques to generate a 3D alignment-invariant shape and electrostatic molecular descriptor