Posters list

	Presenter	Affiliation	Title
1	Adelaide Punt	University of Oxford	Investigating the impact and mitigation of noise in QSAR models
2	Alex Porter	Syngenta	Generative AI as a tool for metabolite identification
3	Charmaine Chu	Liverpool ChiroChem	Implementation of R-BIND Nearest Neighbour Search and ROBIN Machine Learning methods to generate a RNA focused Virtual Library
4	Federico Ricci	University of Urbino	KLig Enumerator: a Tool for Library Creation Based on Kinase X-Ray Structures.
5	Gwee Shu Hui Eunice	University of Dundee	Aminoacyl-tRNA synthetases (aaRSs) as drug targets
6	Kate Fieseler	University of Oxford	Synthesis directed elaborations by automated chemistry to maximally exploit the fragment-design space
7	Klaudia Caba	Imperial College London	Comprehensive machine learning boosts structure-based virtual screening for PARP1 inhibitors
8	Lukas Eberlein	OpenEye, Cadence	Automated Identification of Cryptic Pockets for Drug Discovery
9	Marek Szczygiel	ANYO Labs	iScore: Ultra-fast Virtual screening
10	Matteo Ferla	University of Oxford	Advancing Fragment-Based Drug Discovery in the ASAP Consortium with Fragmenstein
11	Matthew Habgood	Cresset	Active learning FEP using 3D-QSAR for prioritizing bioisosteres in medicinal chemistry
12	Mike Bodkin	Dundee University	FP-score for hotspot identification and efficient fragment-to-lead growth strategies
13	Nivya James	Imperial College London	Benchmarking Generic Classical SFs For Structure Based Virtual Screening Against TRPM8 Ion Channel
14	Peter E.G.F. Ibrahim	University of Dundee	FraGrow: Fully automated software for fragment growth and optimization
15	Qianrong Guo	Imperial College London	Artificial Intelligence for Phenotypic Virtual Screening
16	Ronald Cvek	University of Oxford	Prioritisation and Ranking of fragments from a high-throughput screen
17	Ruslan Kotlyarov	University of Cambridge	Towards Automated Reassignment of NMR Spectra
18	Simon Cross	Molecular Discovery	DEEPGRID: 3D image recognition using deep learning and grid molecular interaction fields

19	Sonja Peter	Nxera Pharma UK / University of Urbino	Comparative Study of Allosteric GPCR Binding Sites and Their Ligandability Potential
20	Swathi S	Unilever	Cheminformatics/QSAR approach for personal care formulation optimization
21	Syed Zayyan Masud	Molrus	Molrus – A cheminformatics library written in Rust
22	Vittorio Lembo	University of Urbino "Carlo Bo"	In Silico Identification of Readily Available Target Pairs for Dual-Target-directed Ligand Development
23	Wei Dai	Queen Mary University of London	Cheminformatics and Machine Learning Approaches for GPCR Computer-Aided Drug Design