Programme

Day 1: Monday 1st July

12:00 – 13:00	Registration and Lunch	
13:00 – 13:05	Daniel Cole	Welcome
Session 1: From Desktop to Benchtop and Back Chair: Natalie Tatum		
13:05 – 13:35 T1	**Frank von Delft** Diamond Light Source	Fast-Forward Fragments for rapidly progressing structure-based (XChem) fragment screens
13:35 – 13:55 T2	**Anna Duncan** Aarhus University	Why Losing a Lipid Tail Matters: Cardiolipin, and not Monolysocardiolipin, Preferentially Binds to the Interface of Complexes III and IV
13:55 – 14:15 T3	**Daniella Hares** Institute of Cancer Research	Decoding BCL6 Inhibitors: Computational Insights into the Impact of Water Networks on Potency
14:15 – 14:45 T4	**Giulio Tesei** University of Copenhagen	Data-driven Modelling of the Intrinsically Disordered Proteome
14:45 – 15:20	Coffee & Tea	
15:20 – 15:50 T5	**Matthieu Schapira (online)** University of Toronto	Lessons Learned from the First CACHE Challenge
15:50 – 16:10 T6	**Julian Streit** University College London	The Ribosome Lowers the Entropic Penalty of Protein Folding
16:10 – 16:30 T7	**Isabel Elliott** University of Southampton	Structure-guided Disulfide Engineering Restricts Antibody Conformation and Flexibility to Elicit TNFR Agonism in Anti-cancer Therapeutics
16:30 – 16:50 T8	**James Krieger** National Centre for Biotechnology, Madrid	Improving Continuous Heterogeneity Landscapes and Interpretations using Atomic Structures: A Case Study of SARS-CoV-2 Spike Variants
16:50 – 18:30	Poster session (odd numbers)	

Day 2: Tuesday 2nd July

Session 2: Molecular Modelling Methods Chair: Agnieszka Bronowska		
9:00 – 9:30 T9	**Antonia Mey** University of Edinburgh	From Active Learning to Zinc: Adventures with Alchemical Free Energy Calculations
9:30 – 9:50 T10	**Katarzyna Zator** University of Cambridge	Atom Surface Site Interaction Mapping of Protein-Ligand Complexes
9:50 – 10:10 T11	**Wojciech Kopec** Queen Mary University of London	Computational Electrophysiology of Potassium and Chloride Channels
10:10 – 10:30 T12	**Sofia Oliveira** University of Bristol	Using Dynamical-Nonequilibrium MD Simulations to Understand Drug Resistance and Allostery in Proteins
10:30 – 11:00	Coffee & Tea	
11:00 – 11:30 T13	**Marco de Vivo** Istituto Italiano di Tecnologia	Targeting the Conserved Active Site of Splicing Machines
11:30 – 11:50 T14	**Finlay Clark** University of Edinburgh	Automated Adaptive Absolute Binding Free Energy Calculations
11:50 – 12:20 T15	**Maria Kurnikova** Carnegie Mellon University	Active Learning Driven Hit Mining and Optimization based on Molecular Dynamics Simulated Free Energies
12:20 – 13:30	Lunch	

Day 2: Tuesday 2nd July
Afternoon

Session 3: Machine Learning Chair:		
13:30 – 14:00 T16	**Cecilia Clementi** (online) Freie Universität Berlin	Navigating protein landscapes with a machine-learned transferable coarse-grained model
14:00-14:20 T17	**Elliot Chan** University of Bristol	Electrostatic Embedding of Machine Learned Potentials for Accurate and Efficient Simulation of Enzyme Catalysis
14:20 – 14:40 T18	**Christopher Williams** University of Manchester	Stable and Accurate Simulations of Drug Molecules using Conformationally Generalisable Machine Learned Potentials
14:40 – 15:00 T19	**Francesc Sabanes** Acellera Therapeutics	Enhancing Protein-Ligand Binding Affinity Predictions using Neural Network Potentials
15:00 – 15:30	Coffee & Tea	
15:30 – 16:00 T20	**Mohammed AlQuraishi** Columbia University	The State of Protein Structure Prediction and Friends
16:00 – 16:20 T21	**Jonathan Heal** RxCelerate	Real World Comparison of Dynamic Ultra Large Library Screening with Commercial Library Screening against Different Target Classes
16:20 – 16:40 T22	**Will Gerrard** Kuano	Application of AI Augmented Design in Early Stage Drug Discovery
16:40 – 18:15	Poster Session (even numbers)	
18:15	Move to the Biscuit Factory	
19:00	**Conference Dinner**	

Day 3: Wednesday 3rd July

Session 4: Case Studies in Computer-Aided Design Chair:		
9:00 – 9:30 T23	**Giulia Rossetti** (online) Forschungszentrum Jülich	AI-based Identification of Therapeutic Agents Targeting GPCRs: Introducing Ligand Type Classifiers and Systems Biology
9:30 – 9:50 T24	**Richard Heath** Newcastle University	Using SeeSAR to Identify Novel Therapeutic Starting Points for Friedreich's Ataxia
9:50 – 10:10 T25	**Jordi Juarez-Jimenez** Universitat de Barcelona	Computational Tools for the Rational Design of Molecular Glues
10:10 – 10:30 T26	**Kin Chao** Imperial College London	Modulation of Class B1 GPCRs by the Plasma Membrane Environment
10:30 – 11:00	Coffee & Tea	
11:00 – 11:30 T27	**Joe Bluck** Bayer	Prioritizing Molecules for Synthesis using In-Silico Tools
11:30 – 11:50 T28	**Joshua Horton** Newcastle University	ASAP-Alchemy: A State-of-the-Art Open-Source Alchemical Free Energy Pipeline with Bespoke Force Fields
11:50 – 12:10 T29	**Stefano Serapian** University of Pavia	MD Simulations Map the Havoc Wreaked by One Mutation in $[Hsp60]_{14}$
12:10 – 12:30 T30	**Salome Llabres** Universitat de Barcelona	Unravelling the Energetics of a Small Molecule-Induced Disorder-to-Order Transition
12:30		Closing remarks
12:45	Conference closes & Lunch	