Programme

Monday, July 6th, 2026

12.00	Lunch and registration (put posters up)	
13:15	Opening & Session 1: Detailed Biological Insights from Biomolecular Simulation Chair: Robin Corey	
13:30	Phill Stansfeld University of Warwick	Keynote: CCD2MD: A Modular Toolkit for Preparing Co-Folded Biomolecular Complexes for Molecular Dynamics Simulations
14:20	Wojciech Kopec Queen Mary University	Accurate simulations of ion channels with charge-scaled force fields
14:45	Bryony Clifton University of Bristol	Open or closed? Revealing the proteolytic potential of an orphan rhomboid
15:10	Tea break	
15:40	Ariane Nunes Alves Brazilian Center for Research in Energy and Materials (CNPEM)	Combining τ-random accelerated molecular dynamics and machine learning to investigate protein-ligand dissociation
16:20	Eric Lang AstraZeneca	Molecular Modelling for Biocatalysis at AstraZeneca: Where We Are and What Lies Ahead
16:45	Jordan McIvor Syngenta	From Classical Methods to Generative AI: An Integrated Computational Framework for Agrochemical Discovery
17:10	Poster pitches I	Abbie Lear, Anushka Pahuja, Bjarne Feddersen, Callum Ellis, Carlos Ramos, Charlie Holdship, David Cheung, Harry Swift, Jonathan Colburn
17:40-19.15	Poster session I (odd numbers) and drinks	

Tuesday, July 7th, 2026

Session 2: Biomolecular Modelling for Efficient and Accurate Predictions I Chair: Sofia Oliveira		
9:00	Chris Wood University of Edinburgh	Data-Driven Methods for Reliable and Accessible Protein Design
9:40	Juno Underhill University of Bristol	Atomistic design and photophysical tuning of de novo flavoproteins: QM/MM in Protein Design
10:05	Konstantin Röder King's College London	Manipulating RNA structural dynamics through simulation-informed mutations
10:30	Coffee/Tea break	
11:00	Irfan Alibay Open Molecular Software Foundation	Large scale binding free energy benchmarking with OpenFE
11:40	Mina Moniri University of Oxford	Constitutive NMDA receptor activity: activation without canonical clamshell closure
12:05	Callum Ward University of Warwick	Predicting and Explaining Human Skin Permeability Using Molecular Simulation
12:30	Lunch buffet (& posters)	
13:40	Session 3: Biomolecular Modelling for Efficient and Accurate Predictions II Chair: Sarah Harris	
13:50	James Gebbie-Rayet STFC	Highlight: CCPBioSim training resources
14:00	Sereina Riniker ETH Zürich	Multiscale Neural Network Potential for the Simulation of Protein Dynamics and Enzymatic Reactions
14:30	Kirill Zinovjev Universitat de València	Surprising advantages of physics-based ML/MM potentials
15:05	James Davies Cardiff University	Integrating Molecular Dynamics and Machine Learning Reveals DNA Structural Determinants of OGG1-Mediated Repair
15:30	Tea break	

16:00	Paulo C. T. Souza École Normale Supérieure de Lyon	Martini 3 Across Scales: From Molecular Interactions to Biomolecular Design
16:40	George Hedger Imperial College London	Cardiolipin controls subcellular signalling by mitochondrial GPCRs: The predictive power of simulations integrated with structural native mass spectrometry
17:05	Gianluca Lattanzi University of Trento	Integrating Molecular Simulations with Experiments: Challenges in Complex Biomolecular Systems
17:20	Poster pitches II	Kakali Sen, Marco Hanzevacki, Michael Beer, Robert Welch, Sarah Fegan, Thilakan Kanesalingam, Victor Manuel Velasco Berrelleza
17:40-19:15	Poster session II (even numbers) and drinks	

Tuesday from 20.00 Conference Dinner at the Bristol Marriott Royal Hotel

College Green, Bristol, BS1 5TA

Wednesday, July 8th, 2026

Session 4: Computer-aided drug design and connecting simulations to experiment Chair: Rebecca Notman		
9:00	Daniel Cole Newcastle University	Data-driven interatomic potentials for computer-aided drug design
9:40	Kowit Hengphasatporn University of Tsukuba	Click, Dock, Discover: Rethinking Who Gets to Do Computational Drug Discovery
10:05	Yoav Shamir Weizmann Institute of Science	Discovery of Covalent Ligands with AlphaFold3
10:30	Coffee/Tea break	
10:55	Nicolas Foloppe Vernalis	Highlight: CCPBioSim Industry Talks
11:10	Vicky Higman & Hima Bindu Kolli CCP-N	Towards easy interfacing of MD with NMR
11:50	Parimala Shivaprasad University of Nottingham	Integrating Experimental Kinetics and Molecular Simulation to Tune Enzyme Selectivity to Valorise Horticulture Waste
12:15	Agnes Noy University of York	Towards modelling DNA in biological environments
12:55	Closing	
13:00	Lunch (take down posters)	