Computational biochemistry: enzyme catalysis, protein dynamics and drug design

Adrian Mulholland (Chemistry; lead, *BristolBridge*; Chair, UoB HPC Exec, Chair UK CCP Steering Panel)

- Biomolecular simulation (molecular dynamics simulations of proteins, e.g. 4-10 TB data per system; analyse effects of mutations, conditions)
- Antibiotic resistance (BristolBridge)
- Enzyme evolution and adaptation
- Catalyst design; synthetic biology
- Drug design: prediction of protein-ligand binding (e.g. smoking cessation; antivirals; antibiotics)
- Computational 'assays' of drug resistance
- Multiscale modelling; QM/MM