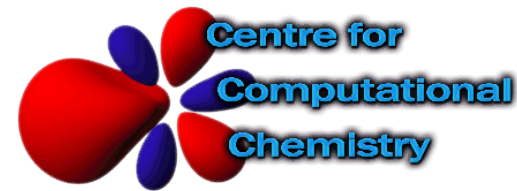


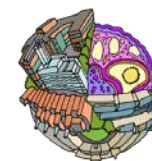
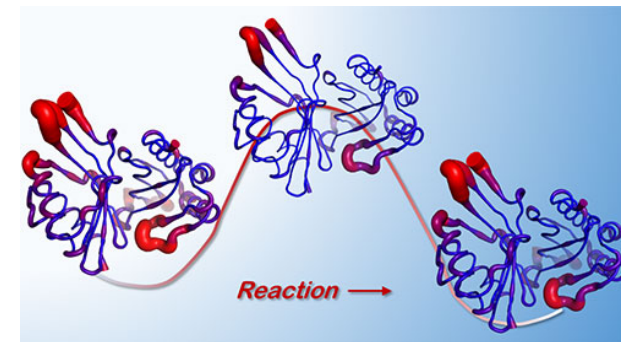
Computational biochemistry: enzyme catalysis, protein dynamics and drug design



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



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biomolecules to biosystems
from understanding to design