

P010 Towards a Virtual Outer Membrane: from Simulations to Systems
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The outer membrane of Gram negative bacteria provides a case study for developing a bridge between molecular simulations and systems descriptions of biological membranes. As a first step towards a systems description we are developing a high throughput MD simulation *pipeline* which will be used to populate a database of outer membrane protein (OMP) simulations. This database will eventually contain simulations of all outer membrane proteins of known three dimensional structure, plus simulations of a number of biomedically important homologues. Such a database will allow us to perform comparative analyses of multiple OMP simulations and will be used to develop a virtual outer membrane. The large volumes of simulation data generated by this approach will be stored and analysed using BioSimGrid (www.biosimgrid.org). As a case study for combining homology modelling and MD simulations, we are exploring the stability and pore dimensions of a model of the N-terminal domain of OprF, a homologue of *E. coli* OmpA from *Pseudomonas aeruginosa*. We are also exploring the use of an automated simulation procedure, using the National Grid Service (www.ngs.ac.uk), to compare models of a further five OmpA homologues. These latter studies employ a method that allows simulations of multiple models to be run quasi-simultaneously with inbuilt checking of simulation performance and stability. The results from these simulations will provide insights into the dynamics of the family of OmpA proteins.