

Characterising surfaces of Mycobacterial Lipids for the diagnosis of TB

HPC-Competence Center

High Performance Computing (HPC) Wales is Wales' national super-computing service provider. Host to the UK's largest national distributed supercomputing network, HPCWales provides businesses and researchers with local access to world-class technology and the support to fully exploit it.



Enterprise

Established in 2012 as a Point of Care diagnostics company, Diagnostig has technology that focuses on novel devices for the diagnosis of Mycobacterial infections (including Tuberculosis) using a proprietary lipid technology. Their core technology is based on the manufacture of specific mycolic acids which are components of the cell walls of mycobacteria.

How HPC makes the difference

The aim of the project was to characterise the three-dimensional surface for antibody binding created by mycolic acid antigen on a surface, for the diagnosis of TB. Different surfaces that correlate to in-house assays were modelled and the arrangement of numerous molecules were evaluated to find favourable antigenic traits in order to predict the best antigens.

A coarse grained model was used to minimise the number of interactions to be calculated, based on the open source molecular dynamics package Gromacs that is primarily designed for simulations of proteins, lipids and nucleic acids, together with the FFT library, FFTW, the GNU scientific Library (GSL) and OpenMPI. Combining the coarse grained approach with HPC facilities meant that large system sizes and long timescales could be simulated to more closely approximate real-life scenarios.

Access to HPC Wales enabled a new computational approach to protein stabilisation, allowing the simulation of more molecules together with reduced computation time as compared to an atomistic approach.

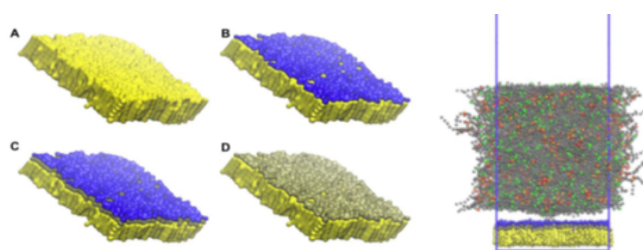


Fig: The composition of the solid surfaces used in the simulations is shown on the left. The simulation setup with lipids in relation to the surface is shown on the right..

