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Elucidating the function and mechanism of Glycoside Hydrolase 1 enzymes from Bacillus licheniformis

Sustainable, environmentally friendly energy is currently well sought after. Biomass is considered as one of the world's major energy sources, as the break-down of biomass leads to the production of biofuel and "green" chemicals. The degradation of biomass is however, recalcitrant and not yet sustainable. Researching the activity and mechanisms of the bacterial enzymes that utilize and bio-degrade biomass, contributes to a more sustainable bio-conversion process and also cuts the costs and time involved in finding novel industrial enzymes.

Glycoside Hydrolase 1 (GH1) enzymes hydrolyse the glycosidic bond between two or more carbohydrates or between a carbohydrate and a non-carbohydrate moiety. GH1's have a very conserved (α/β)8 barrel (TIM-barrel) structure and show a broad specificity for substrates, having 19 enzymatic activities including 6-P-β glucosidases, β-glucosidases, β-galactosidases and 6-P-β-galactosidases.

The Centre for High Performance Computing (CHPC) is a crucial part of structural bioinformatics research, as powerful computation is required to run the molecular dynamics (MD) simulations that are needed to reveal the inner-workings of enzymes. The GROningen MAchine for Chemical Simulations (GROMACS) tool, available on the CHPC, is used for MD simulations in this study. 10 nodes, 24 cores and 24 ranks (select=10:ncpus=24:mpiprocs=24) are utilized during my MD simulations. These MD simulations can inform us as to which substrates the enzymes utilize, which enzyme residues are involved in the binding and catalysis of these substrates, as well as the environmental properties in which the enzymes are most efficient. With the use of the CHPC, this research can be achieved in a significantly reduced time and therefore is extremely important.

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