[MS5-P18] Crystal structures of two polysaccharide deacetylases from *Bacillus cereus.*

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Deacetylation of polysaccharides is a common modification process developed by many bacteria to overcome the defense mechanisms of their hosts [1]. When, for example a gram+ spore forming pathogenic bacterium attacks a mammalian cell, the latter uses a weapony of hydrolytic enzymes to destroy the peptidoglycan layer of the invader. The produced fragments are recognized by pattern recognition factors (Nod proteins), thus triggering the immune response of the host. Bacterial pathogens have evolved a mechanism to evade host defense which is based on chemical modifications of the saccharide residues of their peptidoglycans. Deacetylases of peptidoglycan are used to de-N-acetylate the N-acetyl glucosamine (GlcNAc) and/or the N-acetyl muramic acid (MurNAc) residues of this heteropolymer. As a result, the peptidoglycans cannot be recognized by the enzymes of the host and the pathogen is resistant to the defense mechanism of hosts [2]. Deacetylases of polysaccharides, belong to the family 4 of carbohydrate esterases (CE4), which also include chitin deacetylases and xylan esterases. The members of CE4 family are characterized by a conserved sequence core termed NodB homology domain. Conserved residues of the NodB homology domain line a substrate binding groove while a catalytic mechanism is not yet clarified for the family.

Here we present the crystal structures of two deacetylases from *Bacillus cereus*. *Bc*1960 has been characterized as a deacetylase of the peptidoglycan N-acetyl-glucosamine residue [3] while the specific substrate for the other one, named *Bc*0361, remains to be identified [4]. Our data confirms a conserved structural motif for the catalytic domain and reveals a modified active-site related proline residue. The C-terminal catalytic domain of these enzymes is folded as a deformed $(\beta/\alpha)_8$ TIM- like barrel with 7-strands and carries the His- His-Asp metal binding motif characteristic for the supefamily. The N-terminal is variable with, that of the *Bc*1960 being so flexible that we could not trace the electron density for the first 50 residues. The N-terminal of *Bc*0361 forms a two-layered (4+3) β-sandwich domain. Surprisingly, both enzymes display in structurally equivalent positions, a proline residue which is modified at its Cα-atom. The residue in question has been modeled as a hydroxyproline. A sequence alignment reveals that this proline is strictly conserved among the members of a wide subgroup of the CE4 family. This work was supported by EU funds from the InnovCrete project (FP7-REGPOT-2012/2013) and Marie Curie Reintegration Grant (FP_PEOPLE-2010-RG).

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