OE 1 - Structure and Mechanism of Chitin Deacetylase

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To enable the use of chitin deacetylases in the enzymatic conversion of chitin to chitosan, a detailed understanding of their structure, reaction mechanism and substrate binding mode is required. The fungal pathogen *Colletotrichum lindemuthianum* secretes and endo-chitin de-N-acetylase (ClCDA) to modify exposed hyphal chitin during penetration and infection of plants. Although a significant amount of biochemical data is available on fungal chitin de-N-acetylases, no structural data exists. Here we describe the first crystal structures of a chitin deacetylase and chitin deacetylase homologues, together with detailed biochemical characterization and mutagenesis. A complex with a chitooligosaccharide is also discussed. The structural data in combination with biochemical data reveal that the chitin deacetylases possess a compact catalytic domain encompassing a mononuclear metallo-enzyme, which employs a conserved His-His-Asp zinc-binding triad closely associated with the conserved catalytic base (aspartic acid) and acid (histidine) to carry out acid-base catalysis. This is in contrast to previous reports claiming no metal dependency for this family of enzymes. Chitin deacetylases possess a highly conserved substrate-binding groove, with distinct subsites, explaining why the enzyme requires occupancy of at least the 0 and +1 subsites by (GlcNAc)2 for activity.
These data offer new opportunities for the biotechnological exploitation of chitin deacetylases for the enzymatic conversion of chitin to chitosan.