Crystal structure of fungal tannase from Aspergillus niger

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Tannases are serine esterases that were first discovered in fungi more than one and a half centuries ago. They are commonly present in plants, animals, and microorganisms including bacteria, yeasts, and fungi. They catalyze the hydrolysis of the gallolyl ester bonds in gallotannins to release gallic acid, which is an important intermediate in the chemical and pharmaceutical industries. Since their discovery, fungal tannases have found wide industrial applications, although there is scarce knowledge about these enzymes at the molecular level, including their catalytic and substrate-binding sites. While this lack of knowledge hinders engineering efforts to modify the enzymes, many tannases have been isolated from various fungal strains in a search for the desired enzymatic properties. Here, the first crystal structure of a fungal tannase, that from Aspergillus niger, is reported. The enzyme possesses a typical /-hydrolase-fold domain with a large inserted cap domain, which together form a bowl-shaped hemispherical shape with a surface concavity surrounded by N-linked glycans. Gallic acid is bound at the junction of the two domains within the concavity by forming two hydrogen-bonding networks with neighbouring residues. One is formed around the carboxyl group of the gallic acid and involves residues from the hydrolase-fold domain, including those from the catalytic triad, which consists of Ser206, His485 and Asp439. The other is formed around the three hydroxyl groups of the compound, with the involvement of residues mainly from the cap domain, including Gln238, Gln239, His242 and Ser441. Gallic acid is bound in a sandwich-like mode by forming a hydrophobic contact with Ile442. All of these residues are found to be highly conserved among fungal and yeast tannases. Even though bacterial and fungal tannases are phylogenetically unrelated, structural comparison revealed that they share similarities in their binding interactions with gallic acid, which may facilitate engineering efforts for the modification of tannases in general [1,2].

Figure 1. The concave surface of the fungal tannase. Gallic acid is shown in ball-and-stick representation and N-linked glycans are shown in stick representation. The surface areas of the hydrolase-fold domain are coloured grey and those of the cap domain are coloured light orange.