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The first crystal structure of a tannase-like feruloyl esterase in complex with a hydroxycinnamic acid

AUTHORS
Maria DIMAROGONA / UNIVERSITY OF PATRAS, KARATHEODORI1, PATRAS

PURPOSE OF THE ABSTRACT
Feruloyl esterases (FAEs) are enzymes implicated in plant biomass decomposition, by hydrolyzing the ester bond between hydroxycinnamic acids and arabinose residues [1]. They present biotechnological interest, not only for biomass saccharification but also for the generation of potent antioxidant compounds such as ferulic acid. Here, we report the crystal structure of an FAE from Fusarium oxysporum (FoFaeC) at 1.7 Å resolution in complex with p-coumaric acid (PCA), which is the first ligand-bound structure of a tannase-like FAE [2]. PCA is sandwiched between the lid and catalytic domain, with its carboxyl group being oriented towards the catalytic triad that is comprised of Ser201, His452 and Asp412 (Figure 1). A close inspection of the substrate binding site reveals two conformations of Ser201, possibly indicating a “resting” and an “active” state of the enzyme. Significant alterations are also observed in the hydrophobic core of the lid domain, the most pronounced ones being Met124 and Tyr351 side chains that shift towards the bound phenolic ring. The FoFaeC structure is discussed in relation to other known FAEs, but also to a bacterial mono-(2-hydroxyethyl) terephthalate esterase (MHETase) from Ideonella sakaiensis, which is its third closest structural homologue, and is implicated in polyethylene terephthalate (PET) degradation [3]. The enrichment of structural data of the tannase superfamily assists towards our fundamental understanding of the underlying mechanisms of these biotechnologically relevant enzymes.

FIGURES

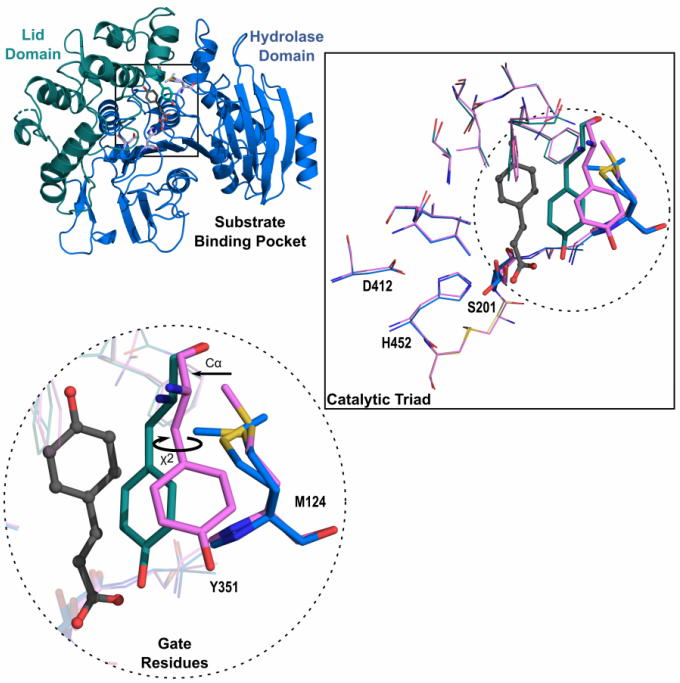

FIGURE 1

Figure 1.

Cartoon representation of FoFaeC monomer in complex with p-coumaric acid and close-up view of the substrate binding pocket.

FIGURE 2

KEYWORDS

feruloyl esterase | tannase superfamily | p-coumaric acid | X-ray crystallography

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