

Crystal Structure Of A Fungal Polyglycine Hydrolase Using A Rosettafold Model

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Chitinase-modifying proteins (CMP) are a subclass of polyglycine hydrolases that are secreted by fungi in response to plant-fungal defense. These CMPs are responsible for inactivating plant chitinases through cleavage of their inter-domain linker region. Our work focused on the structural investigation of a chitinase-modifying protein originating from *Fusarium vanettenii*. We used a combinatorial approach of *in silico* and *in vitro* methods to determine the structure solution. Previous attempts at homology modelling failed to generate a reasonable model, suggesting unique structural features. Owing to recent developments in structure prediction, we were able to generate a full-length homology model using RoseTTAFold1 for our target protein. In combination with a native data set, we were able to solve the structure to 2.2 Angstroms. The structure solution revealed two distinct domains. The amino terminal domain revealed a putatively novel fold, thus explaining previous homology modelling difficulties, whereas the carboxyl terminal domain revealed a beta-lactamase-like region. Further work has focused on the crystallization of the catalytic mutant and co-crystallization of the substrate complex.

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