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Coordenadores

Prof. Dr. Vanderlei Salvador Bagnato
Diretor do Instituto de Física de São Carlos – Universidade de São Paulo

Prof. Dr. Luiz Vitor de Souza Filho
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The crystal structure of Bl_Ylmd a putative multifunctional purine nucleoside enzyme YfiH-like from Bacillus licheniformis

ALMEIDA, L. R.[1]; ROSA, H. V. D.[1]; GREJO, M.[1]; SANTOS, J.[2]; BERNARDES, A.[1]; MUNIZ, J. R. C.[1]
al_leo@usp.br

[1]Instituto de Física de São Carlos - USP

[2]Instituto de Ciências Biomédicas - USP

The mesophilic bacteria *Bacillus licheniformis* has demonstrated great potential for industrial enzyme production, due to its high capacity to secrete proteases. (1) Based on proteomics and sequences analysis, a hypothetical protein CNF1/YfiH-like putative cysteine hydrolase from *B. licheniformis* (*Bl*_YlmD) drew attention because of their sequential similarities with well-known laccases domains and became the object of study in this research. We have heterologous expressed, purified *Bl*_YlmD and had its crystal structure determined at 2.6 Å resolution. *Bl*_YlmD is classified as an α/β protein that forms four layers of $\alpha/\beta/\beta/\alpha$ with mixed antiparallel beta-sheets and assembles into a dimer in the asymmetric unit. We applied bioinformatics tools to identify seven proteins in different organisms with reasonable sequence identity and structural homology to the CNF1/YfiH-like superfamily. Collectively, these sequences are assigned to the domain of multi-cooper polyphenol oxidoreductase laccase (PF02578 Cu-oxidase_4) and domain of the unknown function (DUF152). A comparative analysis of *Bl*_YlmD and its homologous structures showed that they share the hypothetical catalytic dyad, proposed for CNF1/YfiH-like putative cysteine hydrolases superfamily, which are Cys132 and His149 residues centrally positioned in the opened cavity revealed by *Caver 3.0*, a structural similarity that can be observed in these hypothetical proteins. Thus, the pathway accessibility and characteristic cysteine-histidine dyad representing the hypothetical catalytic domain from several bacterial cytotoxic necrotizing factor (CNF) proteins and the related dermonecrotic toxin (DNT) or to a peptidoglycan editing factor (PgeF).(2) Zinc ions are often present in structures of this superfamily, as with *Bl*_YlmD where two zinc ions are observed adopting tetrahedral coordination to cysteine residues. Recently, it was demonstrated that the Ylmd protein from *Geobacillus stearothermophilus* (PBD: 6T1B; 6T0Y, 55.38% identity) is able to phosphorolytically cleave adenosine into adenine and ribose-1 phosphate.(3)This protein, whose structure was obtained in complex with an inosine molecule as a ligand in the active region, refers to the C-terminal portion or DUF152 domain of the purine nucleoside phosphorylase (LACC1 gene) from *Homo sapiens*, also known as FAMIN (Fatty Acid Metabolism-Immunity Nexus), and which is strongly correlated with human disease. This truncated portion called FAMIN176 by the authors shares homology with other bacterial orthologs and contains several catalytic activities mentioned, functioning as: adenosine deaminase (EC 3.5.4.4), purine nucleoside phosphorylase (EC 2.4.2.1) and methylthioadenosine phosphorylase (EC 2.4.2.8). In the present work we carried out the discussion around some of the structural features related to these proteins, in purpose to compare catalytic pockets and ligand binding motifs.

Palavras-chave: Putative protein. Crystal structure. Bacillus licheniformis. PUFs .YlmD.

Referências:

1 DEGERING, C.; EGGERT, T.; PULS, M.; BONGAERTS, J.; EVERS, S.; MAURER, K.-H.; JAEGERr,

K.-E. Optimization of protease secretion in *Bacillus Subtilis* and *Bacillus licheniformis* by screening of homologous and heterologous signal peptides. **Applied Environmental Microbiololgy**. v.76 ,n.19, p.6370 LP – 6376,2010. DOI: https://doi.org/10.1128/AEM.01146-10.
2 PARVEEN, S.; REDDLY, M. Identification of YfiH (PgeF) as a factor contributing to the maintenance of bacterial peptidoglycan composition. **Molecular Microbiology,** v.105, n.5, p.705–720,2017. DOI: https://doi.org/10.1111/mmi.13730.
3 CADER, M. Z.*et. al.* FAMINis a multifunctional purine enzyme enabling the purine nucleotide cycle. **Cell**. v.180, n.2, p.278-295.e23,2020. DOI: https://doi.org/10.1016/j.cell.2019.12.017.