Poster

Mgy a novel metagenomic esterase as an excellent target for environment friendly degradation of polylactic acid

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Global plastic production is a major world concern due to the increasing plastic pollution and subsequent negative environmental impacts. Thus, in the last decade enzyme-catalyzed depolymerization of synthetic polyesters has become extremely developing field, providing a chance for plastic recycling. In this research we expressed, purified, and structurally characterized Mgy protein - a novel uncharacterized metagenomic esterase. We screened activity of Mgy against polylactic acid (PLA) in agarose gel and performed molecular dynamic simulations (MDS) for *Apo*Mgy as well as for the DL-PLA-Mgy and LD-PLA-Mgy complexes. Modelled structure showed that Mgy belongs to the class of α/β-hydrolases. Trajectories of DL-PLA-Mgy complex showed higher stability over the LD-PLA-Mgy complex suggesting chiral selective binding mode. MDSs revealed that PLA ligand binds in the Mgy active site in "U" bended conformation similarly as in its homologue MGS0156 which shows high hydrolytic activity against synthetic polyesters [1]. The major difference with respect to the MGS0156 is deeper PLA positioning in the binding hole. Using computational methods we found that Mgy enzyme contain a mobile lid and we identified its binding site and amino acids with the largest contribution to the substrate binding (Leu191, Val195, Val199, Leu200, Leu203, Phe206, Ile257, Ser261 i Lys264) as well as potential mutation targets (Fig. 1). To prove computational findings, we performed crystallization trials, but for the moment we obtained only low quality crystals. Since we mapped several regions with high flexibility (Fig. 1), particularly in the N-terminal region, truncated protein will be produced to obtain more rigid structure and consequently better diffracting crystals.

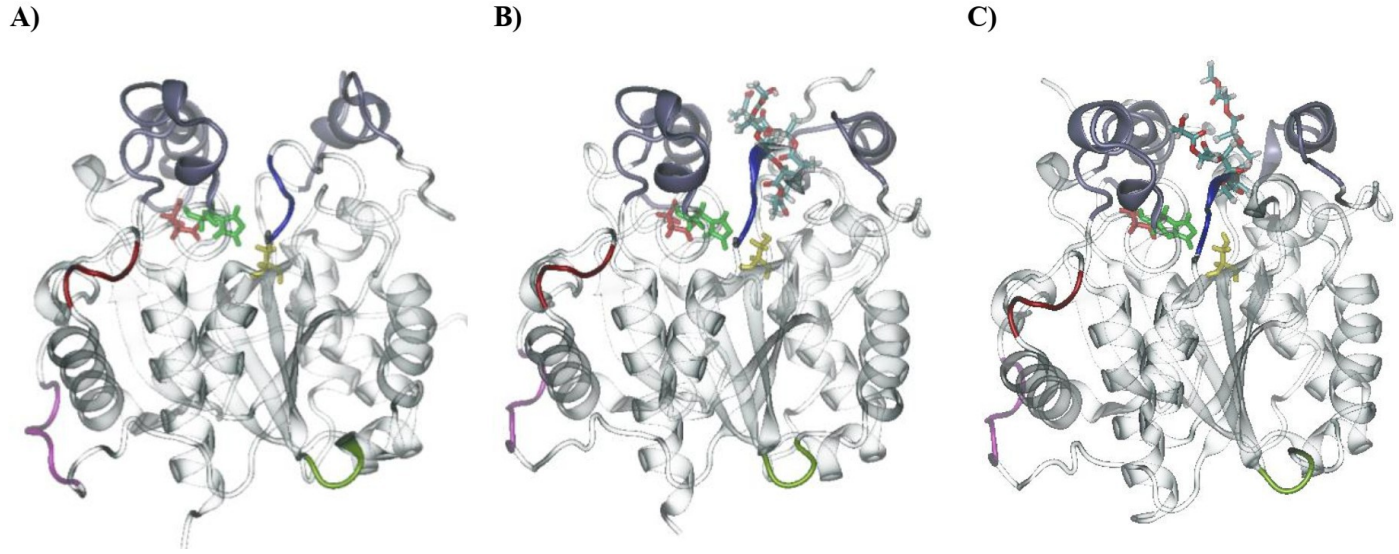

Figure 1. Ribbon representation of modelled Mgy in grey color: A) *Apo*, B) in complex with DL-PLA and C) in complex with LD-PLA. Substrate PLA (light-blue color) and catalytic triad (yellow serine, green histidine, and red aspartate) are shown as capped sticks. Flexible regions are highlighted - region around position 45 is marked in red, region around position 70 in lilac, around 100 in blue, around position 145 in yellow, and the regions around 200 and 310, which make lid in grey-blue color.

[1] Hajighasemi, M., Tchigvintsev, A., Nocek, B., Flick, R., Popovic, A., Hai, T., Khusnutdinova, A. N., Brown, G., Xu, X., Cui, H., Anstett, J., Chernikova, T. N., Brüls, T., Le Paslier, D., Yakimov, M. M., Joachimiak, A., Golyshina, O. V., Savchenko, A., Golyshin, P. N., Edwards, E. A. & Yakunin, A. F. (2018). Environ. Sci. Technol. 52(21) 12388–12401.