



**Figure S3. (a) Total alignment** of three-dimensional structural alignment of 3D structures of LysB-D29 (red color) and its relative members of the  $\alpha/\beta$  hydrolase family including: *Fusarium solani* cutinase (blue color), *Humicola insolens* cutinase (purple color), *Trichoderma reesei* cutinase (orange color), *Penicillium purpureogenum* Acetylxyylan esterase (cyan color) showing the lid domain of *T. reesei* cutinase (Orange color), linker domain of LysB-D29 (red color). **(b) Focus view:** showing catalytic triad residues, oxyanion hole residues and GXP residues (each is shown in its color), co-crystallized inhibitor molecule (black), and the rest of protein (gray).