Molecular mechanism for the substrate specificity of *Arthrobacter globiformis* M6 α-glucosidase CmmB, belonging to glycoside hydrolase family 13 subfamily 30

Supplementary materials

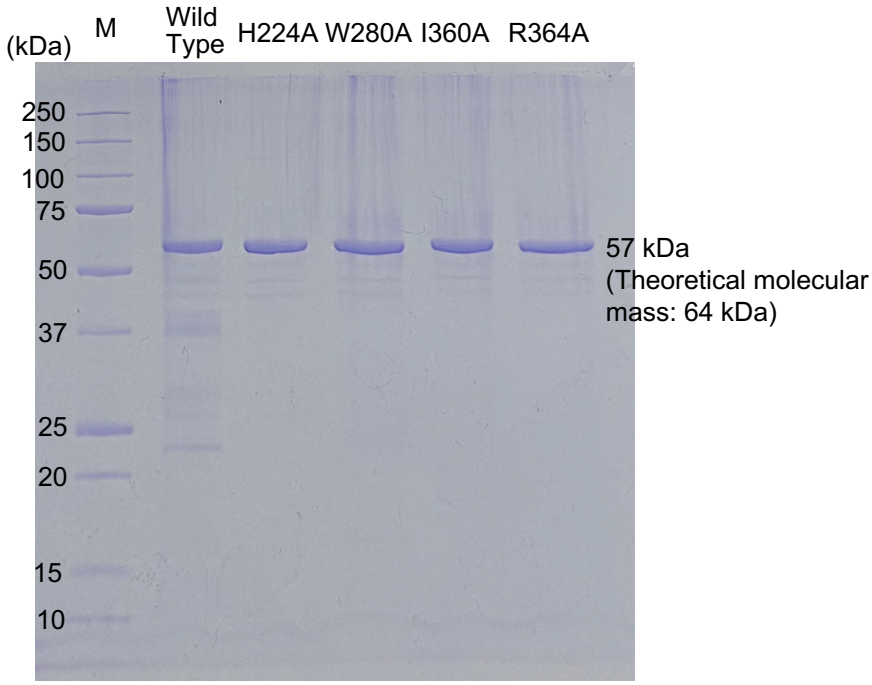

Fig. S1. SDS-PAGE analysis of purified CmmB variants.
One microgram of the purified sample was analyzed. Lane M, molecular size marker. Protein band was detected by the Coomassie Brilliant Blue staining.

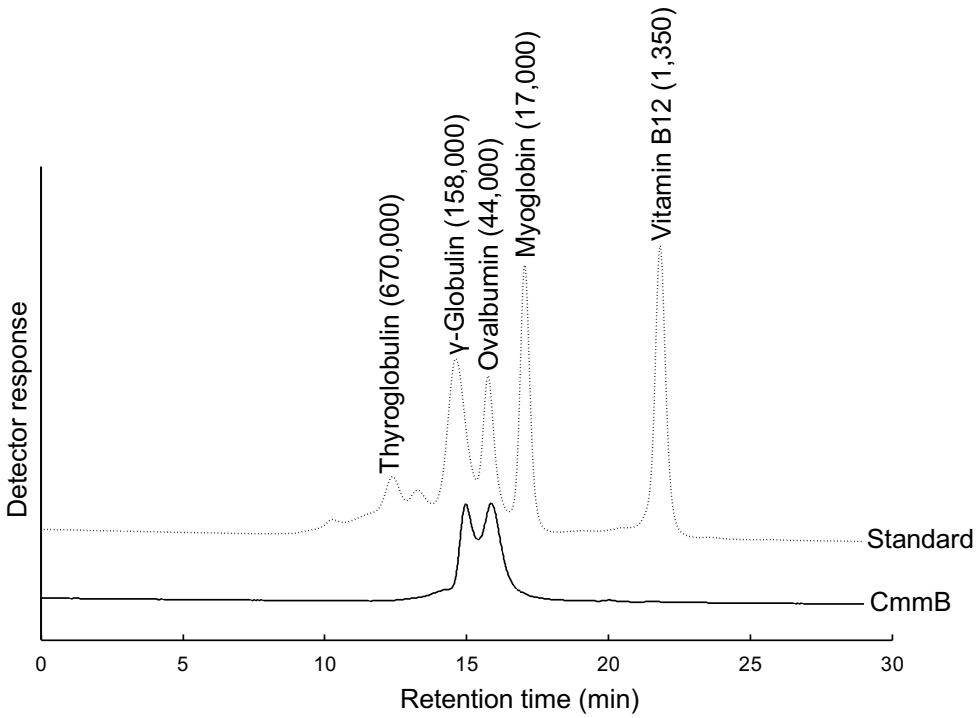

Fig. S2. Estimation of molecular mass of CmmB by gel filtration column chromatography.
Elution profiles of CmmB and standard proteins are shown in black solid and gray dotted lines, respectively. Molecular mass (Da) is indicated in the parentheses.

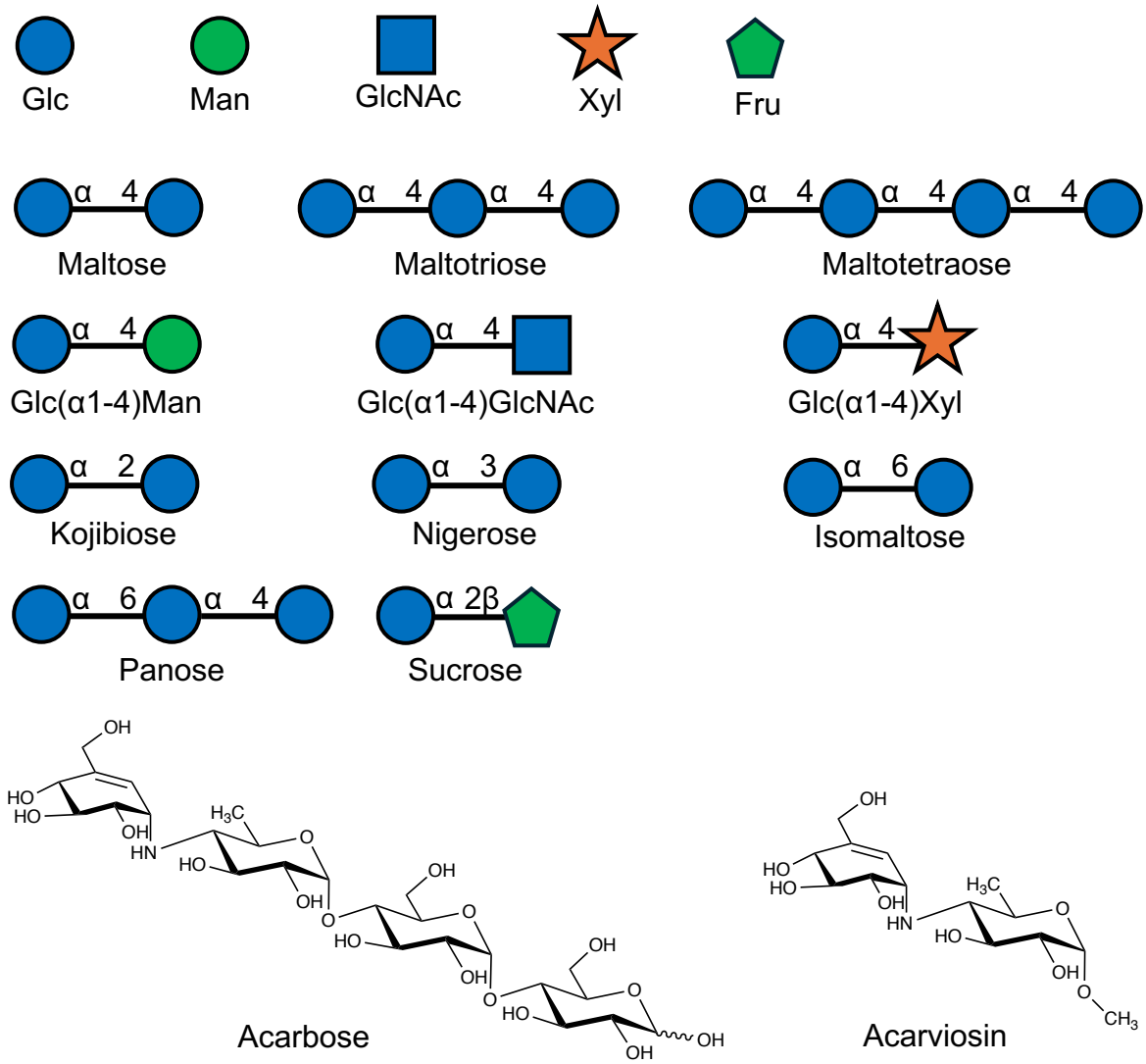

Fig. S3. Structures of the substrates and inhibitors tested in this study.

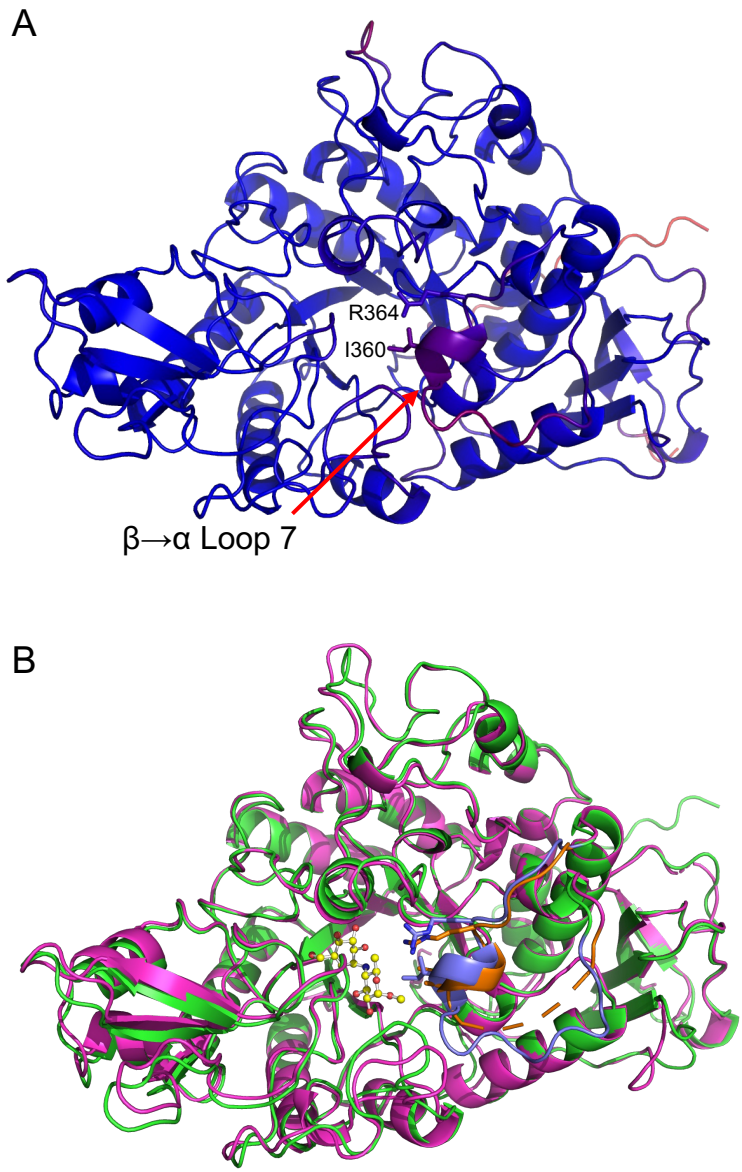

Fig. S4. Predicted structure of CmmB by Colabfold.
A, Mapping of predicted local distance difference test value. The overall structure is colored from high value (blue) to low value (red). B, Comparison between the predicted structure (green, but β→α loop 7 in purple) and the CmmB acarviosin complex (magenta, but β→α loop 7 in orange). Acarviosin is shown in stick and ball representation.

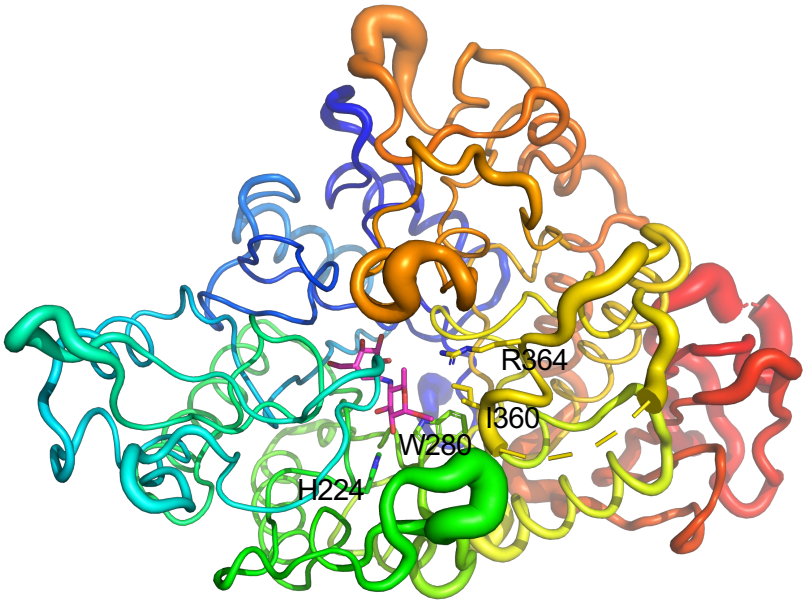

Fig. S5. Mapping of temperature factor of CmmB in complex with acarviosin. The bolder ribbon diagram shows a region with higher temperature factor. The overall structure is shown in rainbow coloring from N-terminal (blue) to C-terminal (red).

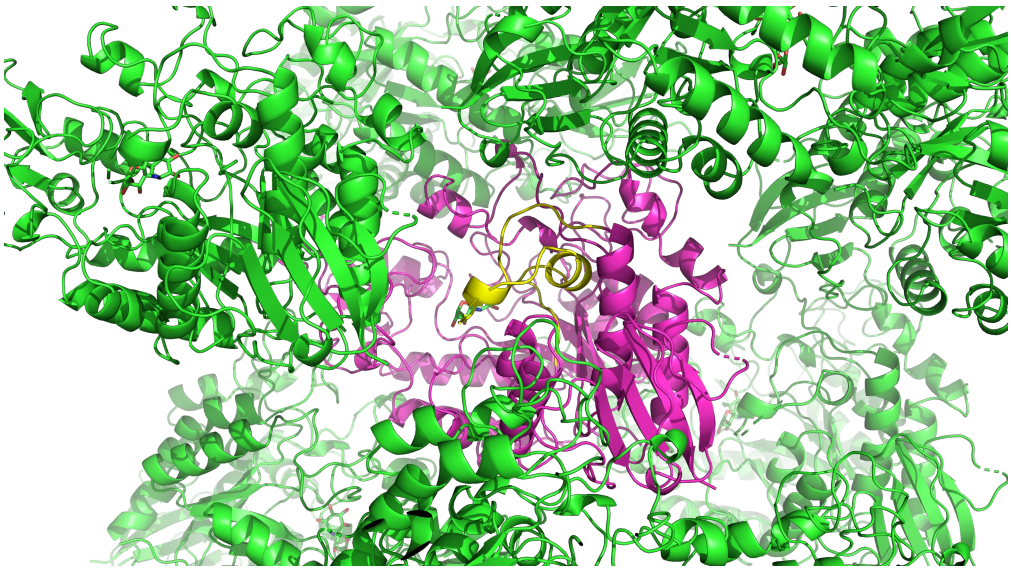

Fig. S6. Symmetry mates within 4Å from central CmmB acarviosin complex shown in magenta. β→α Loop 7 of the central molecule (magenta) is shown in yellow.

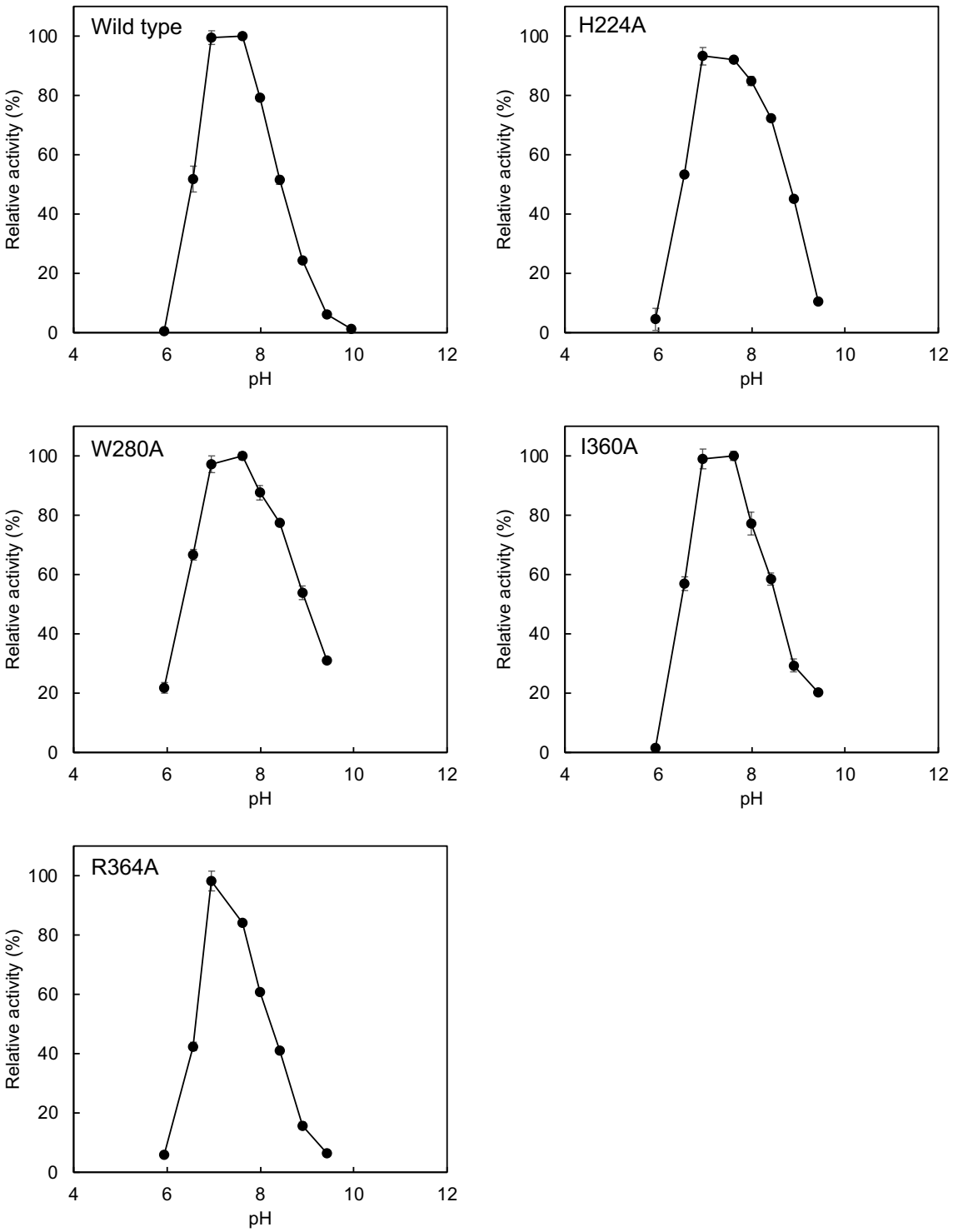

Fig. S7. pH activity curve of CmmB variants.
Hydrolytic velocity to 2 mM pNPG was measured at various pH values. Values are average of independent triplicated experiments, and error bars indicate standard deviation for the values.

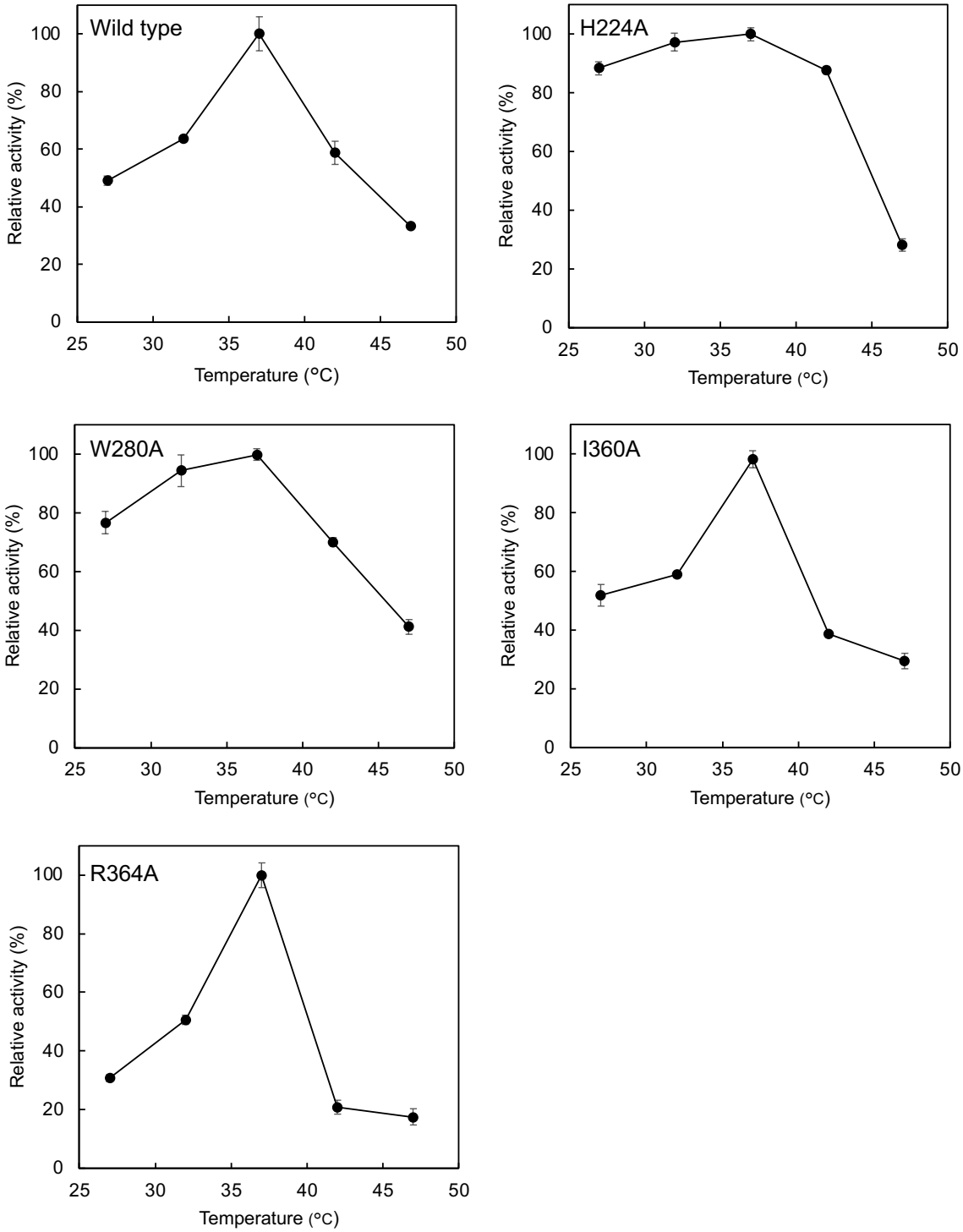

Fig. S8. Temperature activity curve of CmmB variants.
Hydrolytic velocity to 2 mM pNPG was measured at various temperatures. Values are average of independent triplicated experiments, and error bars indicate standard deviation for the values.