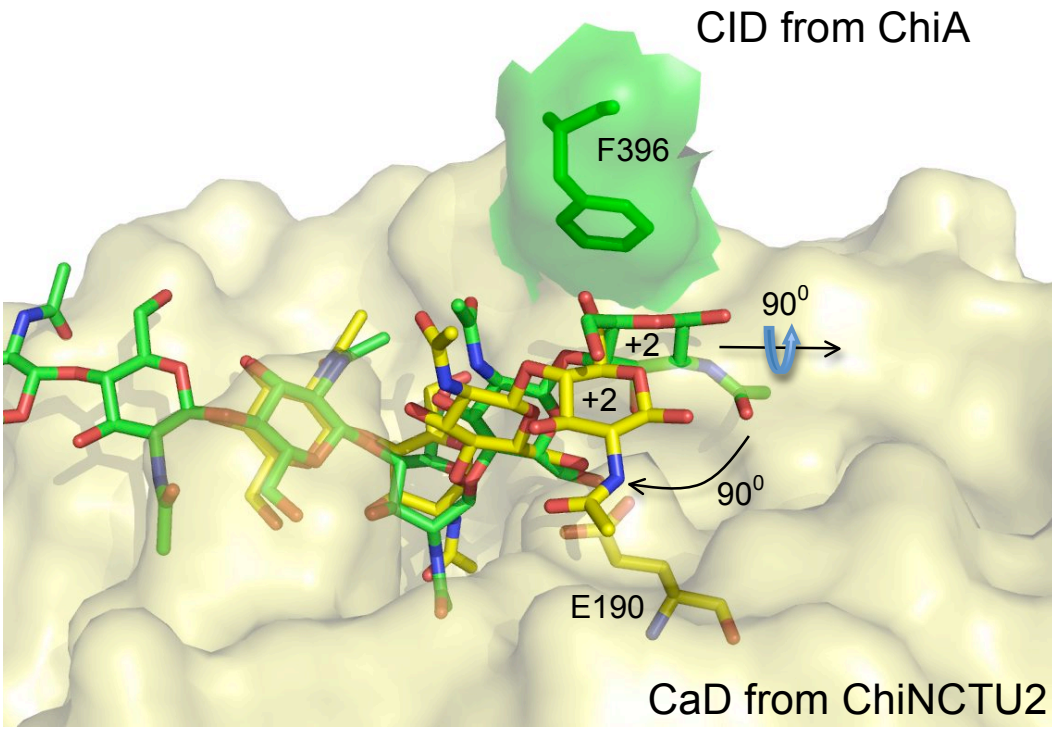
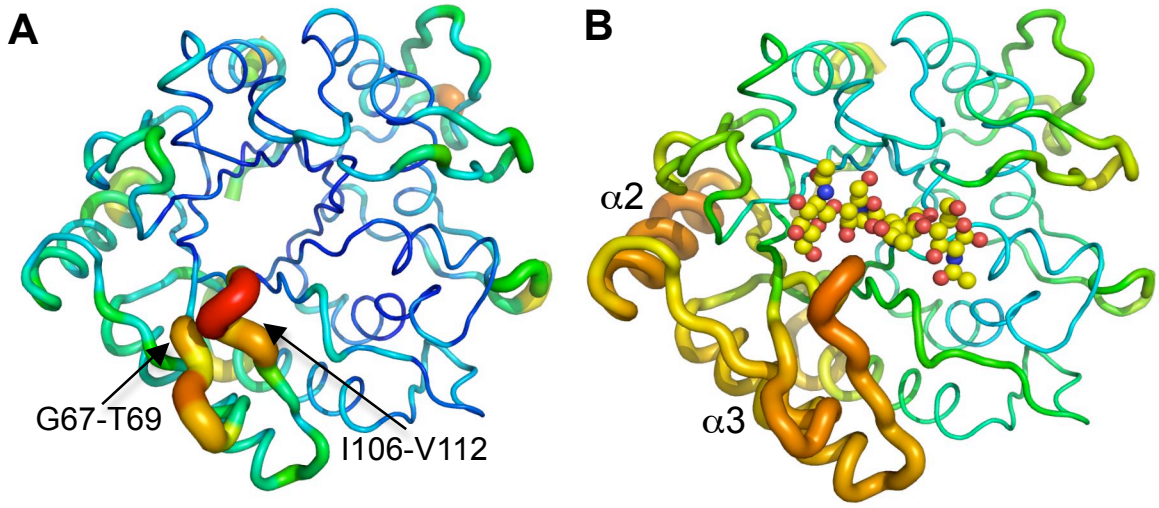
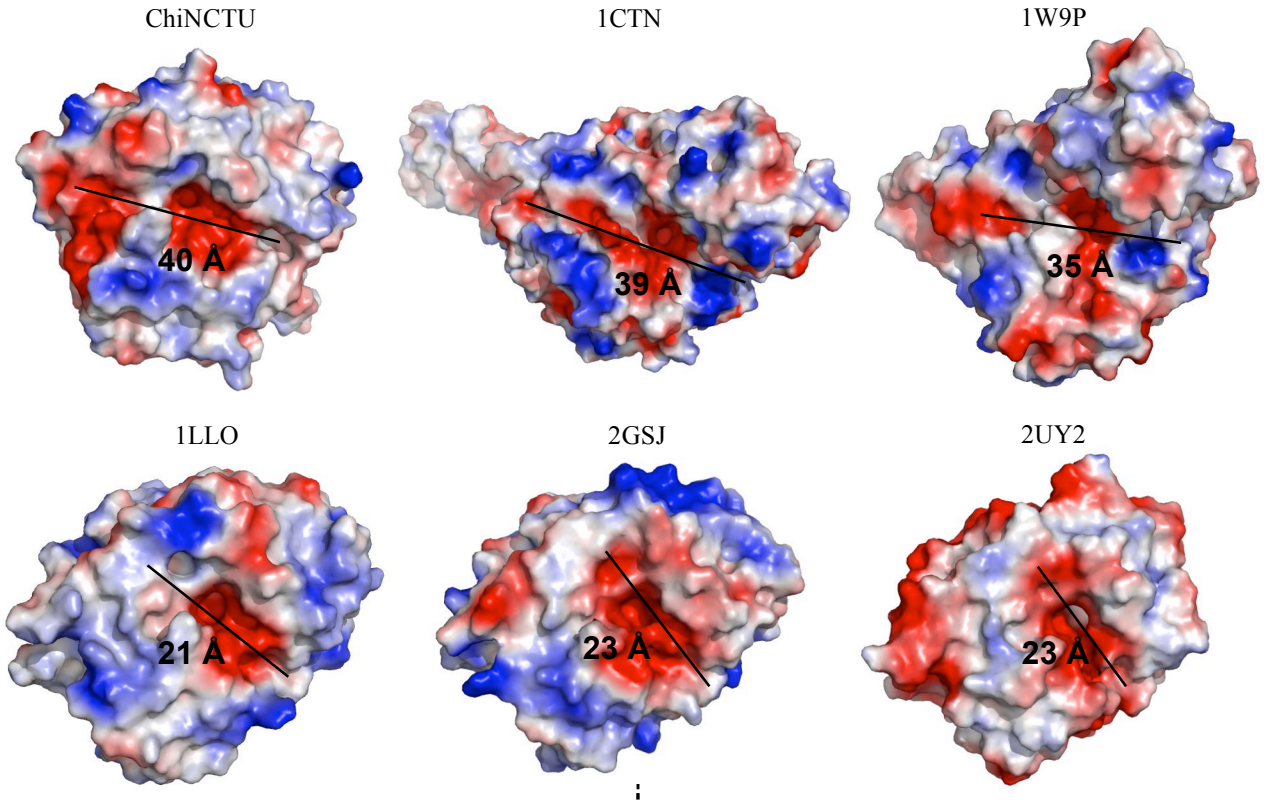
SUPPLEMENTARY FIGURES



SUPPLEMENTAL FIGURE 1. **The structural comparison of +2-(NAG) at the active sites of the complexes between ChiNCTU2 (an exochitinase without CID and CBD) and *Serratia marcescens* chitinase A (ChiA, an exochitinase with CID and CBD).** The orientation of +2-(NAG) (yellow sticks) in ChiNCTU2 (yellow surface) is different from that (green sticks) in *Serratia marcescens* chitinase A with an additional CID (shown partially in green surface) by rotating and bending ~ 90^0 toward the residue Glu190. The exochitinases, except ChiNCTU2, utilize the aromatic residues (Trp or Phe) of CID, such as Phe396 (green sticks) in the *Serratia marcescens* chitinase A, to stabilize +2-(NAG).



SUPPLEMENTAL FIGURE 2. **The *B*-factor labeled structure of ChiNCTU2 to show dynamic features.** The structure exhibits a high *B*-factor with red color and the larger caliber of the cartoon style. (A) The *B*-factor plot of wild-type native ChiNCTU2 structure shows two saccaride-binding loops with large *B*-factors, indicating that the two loops are dynamic in the (NAG)-free form. (B) The *B*-factor plot of mutant E145G/Y227F-$(NAG)_4$ complex structure shows that (NAG) (shown in spheres) binding induces the dynamic features of the neighboring α2 and α3 helices.



SUPPLEMENTAL FIGURE 3. **The electrostatic surfaces of chitinases.** The structural surface of ChiNCTU2 shows that the length of binding clef is ~ 40 Å, which is similar to the CaDs of *Serratia marcescens* chitinase A (1CTN) and *Aspergillus fumigatus* chitinase B1 (1W9P). The endochitinases of *Hevea brasiliensis* hevamine (1LLO), *Parkia platycephala* endochitinase (2GSJ) and *Saccharomyces cerevisiae* chitinase1 (2UY2) show that the binding clefs are smaller (~ 20 Å) than that of ChiNCTU2. The negative charge is shown in red and the positive charge is in blue.