



**Figure S3.** Positive selection region in chloroplast  $\beta$ -amylase (CT-BMY). **(a)** Ka/Ks profile of *Agave americana* (Aa) versus *Arabidopsis thaliana* (At); **(b)** superimposed structures in Aa and At, with the positive selection region highlighted; **(c)** Ka/Ks profile of Aa versus *Oryza sativa* (Os); **(d)** superimposed structures in Aa and Os, with the positive selection region highlighted; **(e)** Ka/Ks profile of Aa versus *Zea mays* (Zm); **(f)** superimposed structures in Aa and Zm, with the positive selection region highlighted. **(g)** The structure model of CT-BMY (Aam049326). This model indicates that the beta-amylase (helices in red, strands in yellow and coils in white) may react with glucose or maltose. A D-glucose substrate (Glc, blue surface) is bound at the active site in the model. E24 (codon 73, purple spheres and sticks) is located in a mobile loop region that may act as a cover of the pocket that holds the substrate. A glucose (Glc) substrate that may bind to the Aa CT-BMY is marked by an arrow. The proteins are colored in grey for Aa, blue for At, green for Os and red for Zm.