Enzyme kinetics by GH7 cellobiohydrolases on chromogenic substrates is dictated by non-productive binding: Insights from crystal structures and MD simulation

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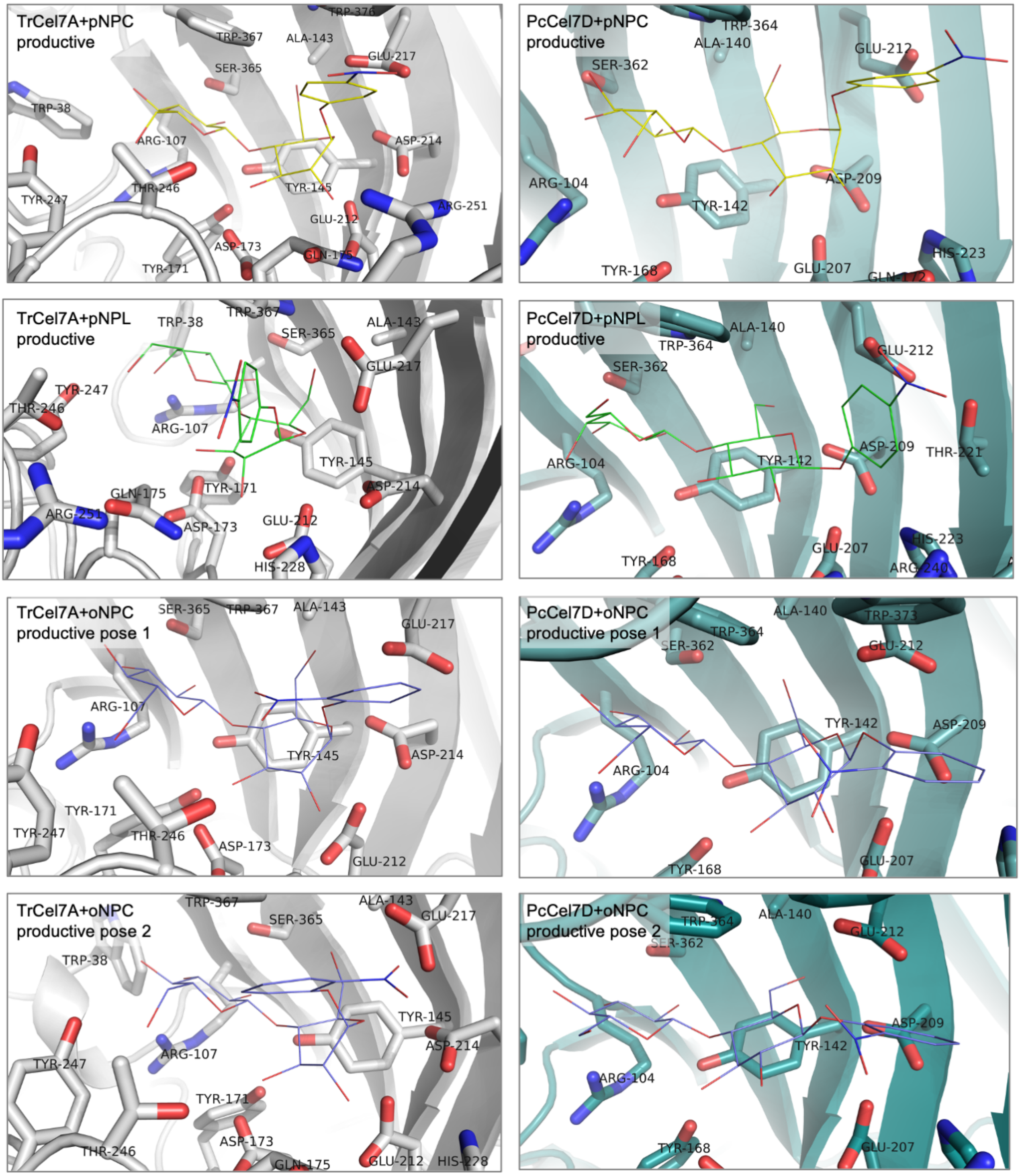
Supplementary Information

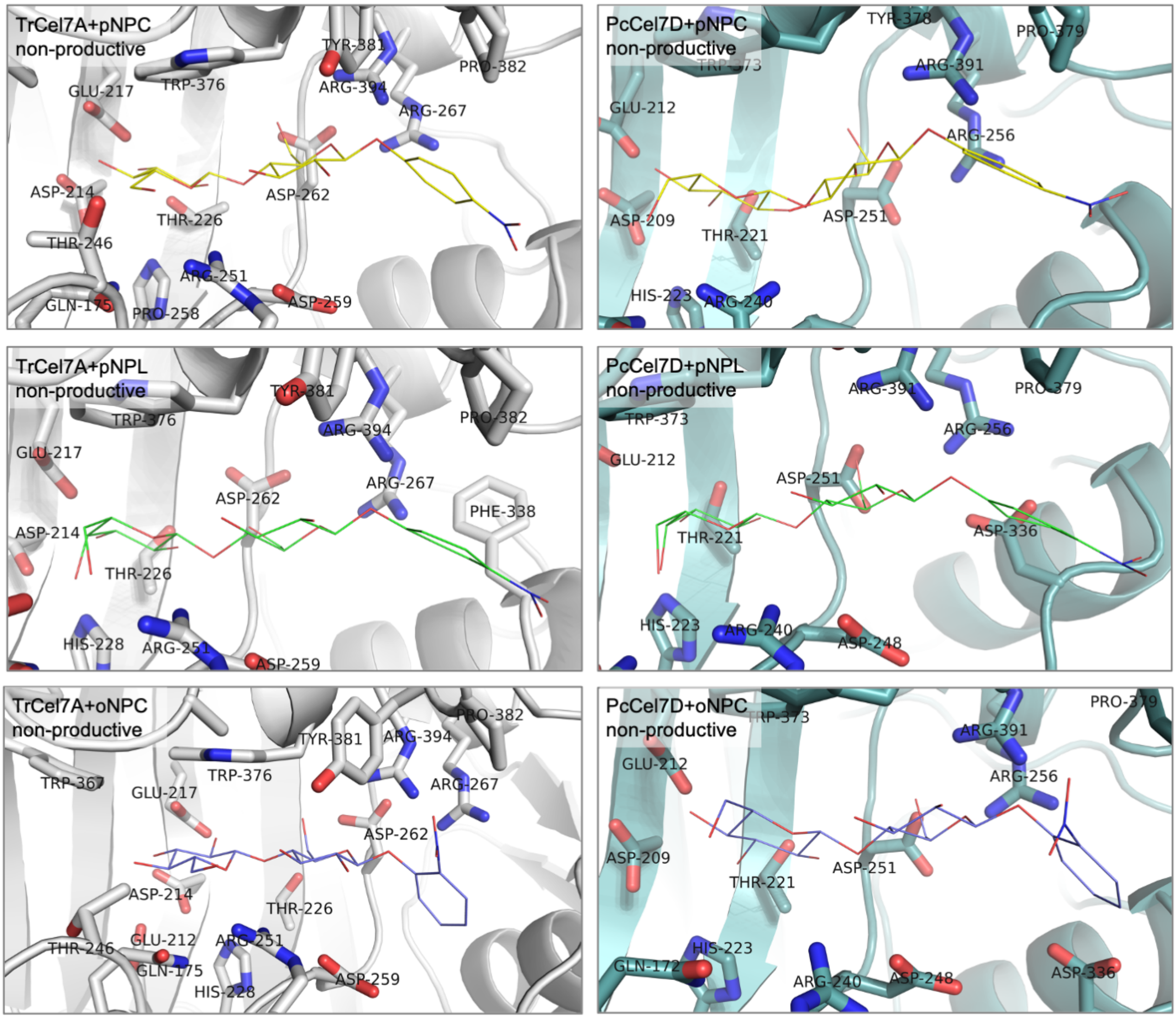
Supplementary Figure S1. Snapshots at 500 ps of MD simulation of substrate binding in productive mode at subsites -2/-1/+1 in TrCel7A and PcCel7D.

Supplementary Figure S2. Snapshots at 500 ps of MD simulation of substrate binding in non-productive mode at subsites +1/+2/+3 in TrCel7A and PcCel7D.

Supplementary Figure S3. Plots of distances between substrate and catalytic amino acids during 10 ns and 100 ns of MD simulations of productive binding mode at subsites -2/-1/+1 of pNPC, pNPL and oNPC, in TrCel7A and in PcCel7D.



Supplementary Figure S1. Snapshots at 500 ps of MD simulation of substrate binding in productive mode at subsites -2/-1/+1 in TrCel7A (white; left) and PcCel7D (teal; right)



TrCel7A+pNPC non-productive

PcCel7D+pNPC non-productive

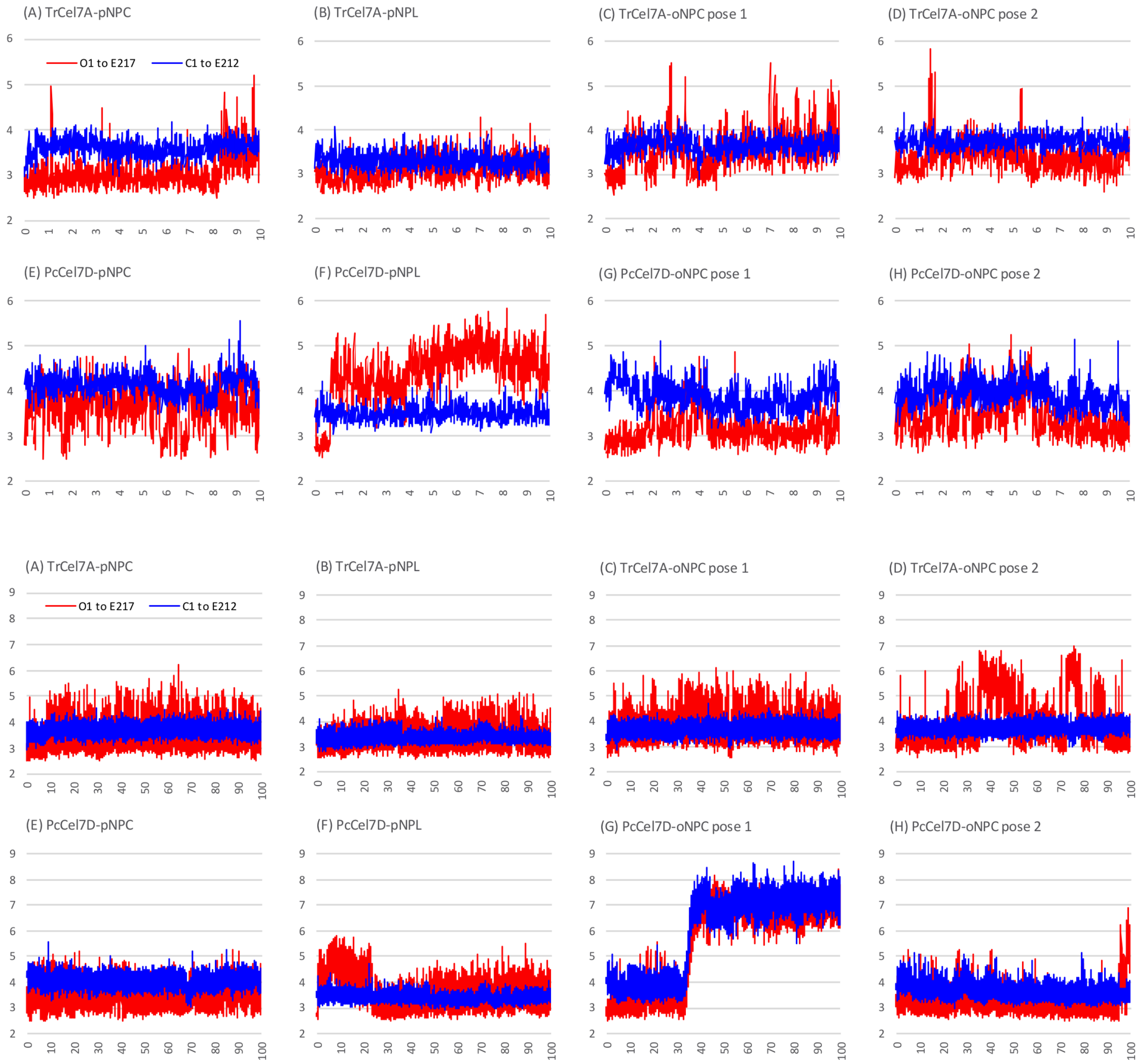
TrCel7A+pNPL non-productive

PcCel7D+pNPL non-productive

TrCel7A+oNPC non-productive

PcCel7D+oNPC non-productive

Supplementary Figure S2. Snapshots at 500 ps of MD simulation of substrate binding in non-productive mode at subsites +1/+2/+3 in TrCel7A (white; left) and PcCel7D (teal; right)



Supplementary Figure S3. Plots of distances (Å) between substrate and catalytic amino acids during 10 ns (top) and 100 ns (bottom) of MD simulations of productive binding mode at subsites -2/-1/+1 of pNPC, pNPL and oNPC, in TrCel7A (A-D) and in PcCel7D (E-H). The red line shows the shortest distance from the glycosidic oxygen O1 to the nearest O atom of the catalytic acid/base (Glu/E217 in TrCel7A; Glu/E212 in PcCel7D). The blue line shows the shortest distance from the anomeric carbon C1 to the nearest O atom of the catalytic nucleophile (Glu/E212 in TrCel7A; Glu/E207 in PcCel7D).