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**Supporting information for article:**

## Structural features underlying the selective cleavage of a novel exo-type maltose-forming amylase from *Pyrococcus* sp. ST04

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(a)

| Enzymes | Strains | Conserved regions I | II | III | IV | V |
|---|---|---|---|---|---|---|
| PSMA | *Pyrococcus* sp. ST04 | 10 H A Y Q P | 104 T H V E P T | 150 W L P E N V | 251 S S D L E S L V A N | 446 N H C S C P R F W |
| Amylopullulanase | *Pyrococcus furiosus* DSM 3638 | 39 H Q H Q P | 262 G N V E V T | 314 W A A E S A | 418 T L D G E N P W E H | 566 A E A S D W F W W |
| Branching enzyme | *Thermococcus kodakarensis* KOD1 | 10 H T H I P | 134 G Y V E V I | 180 W L P E C A | 352 P Y D T E L F G H W | 463 L E A S D W Q F L |
| 4-α-Glucanotransferase | *Thermococcus litoralis* | 11 H N H Q P | 76 G Q L E I V | 120 W L T E R V | 212 H D D G E K F G V W | 350 A Q C N D A Y W H |
| α-amylase AmyC | *Thermotoga maritima* | 10 H A H L P | 135 G K L E I V | 182 W L A E C G | 347 P F D A E L F G H W | 459 A Q S S D W A F I |

(b)


**Figure S1** Conserved sequence regions of PSMA. (a) Multiple sequence alignment of the conserved motifs for the Glycoside Hydrolases 57 family. The catalytic residues are indicated by gray box. (b) Sequence and secondary structure of PSMA. The numbering is shown on the right side. The conserved regions are shown in dotted yellow boxes.

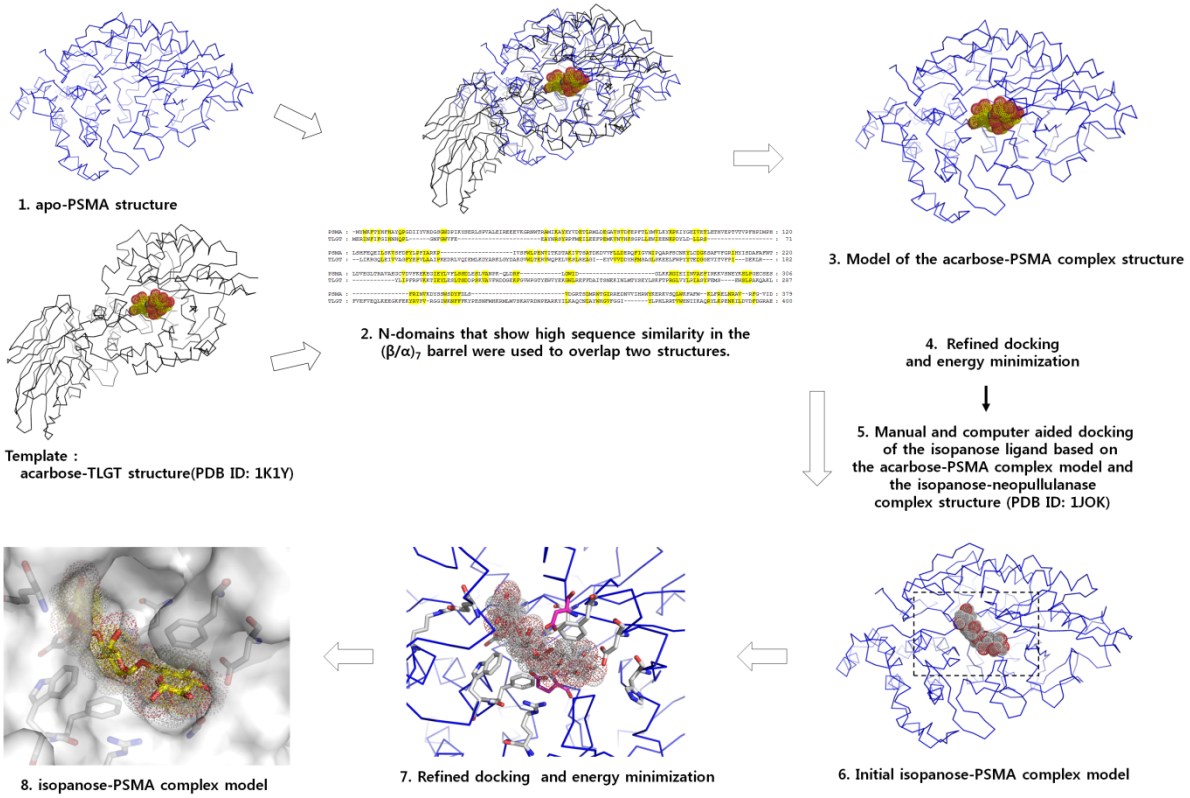


**Figure S2** Flow chart for the modeling of PSMA and isopanose complex.

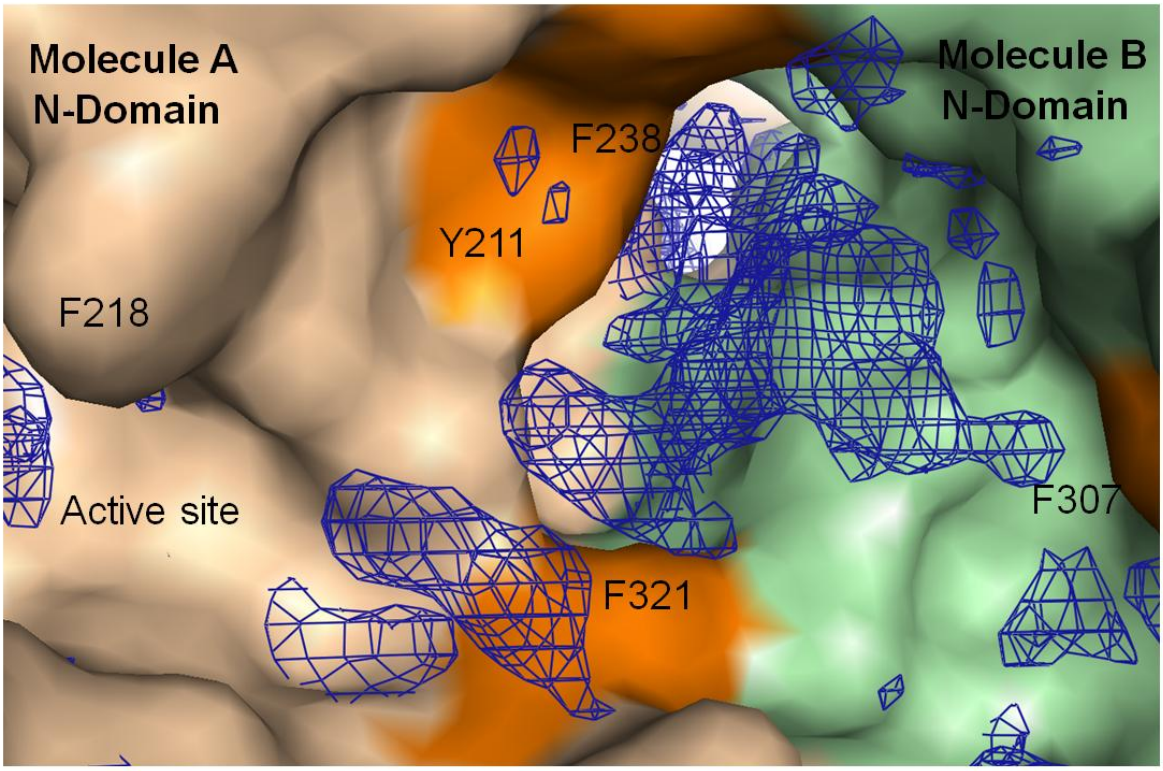


**Figure S3** Electron density for the ligand on the substrate binding channel. An obvious electron density on the substrate binding groove was observed in the omit map of Fo − Fc (3.1 σ) from the PSMA crystal that was soaked in a buffer containing 1mM maltose molecule. The data obtained from the crystal was refined to resolution 1.84Å ($R_{factor}$ =22.08, $R_{free}$=25.38)