Supporting Information for:

**Insight into the Underlying Synergy between Exo–Lytic Cellulases**

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**Table S1.** Simulation details of the molecular assemblies examined in this study.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| No. | Molecular  assemblies | Number of  atoms | Size of the simulation box (Å3) a | Simulation time (ns) | Runs b |
| 1 | *Te*Cel7Ac | 55,923 | 81×76×97 | 1500 | 1 |
| 2 | *Tr*Cel6Ad | 47,959 | 83×75×83 | 500 | 1 |
| 3 | EGe | 36,809 | 76×75×69 | 500 | 1 |
| 4 | BGf | 98,662 | 95×95×116 | 500 | 1 |
| 5 | *Te*Cel7A–*Tr*Cel6A | 86,388 | 133×85×82 | 1500 | 1 |
| 6 | *Te*Cel7A–EG | 104,000 | 125×94×96 | 500 | 1 |
| 7 | *Te*Cel7A–BG | 162,316 | 130×112×117 | 500 | 1 |
| 8 | *Te*Cel7A–*Te*Cel7A | 113,404 | 133×93×98 | 500 | 1 |

a The size of the water boxes guarantees a minimum distance of 15 Å from any atom of the enzyme to any edge of the simulation box.

b Independent MD runs.

c The initial structure of *Te*Cel7A (PDB code 3PFX).

d The initial structure of *Tr*Cel6A (PDB code 1HGW, in which A175 was mutated back to Asp).

e PDB code 1KS5

f Homologically modeled by SWISS-MODEL.

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**Fig. S1** Center-of-mass distance of two proteins in each complex structure.

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**Fig. S2.** Optimal docking poses of (a) *Te*Cel7A–EG, (b) *Te*Cel7A–BG and (c) *Te*Cel7A–*Te*Cel7A. The region of SELs is the area where enzymes are apt to bind.

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**Fig. S3** Final states of the complexes of (a) *Te*Cel7A–EG, (b) *Te*Cel7A–BG and (c) *Te*Cel7A–*Te*Cel7A.