

Supplementary Information

For

Cyclization Reaction Catalyzed by Cyclodipeptide
Synthases Relies on a Conserved Tyrosine Residue

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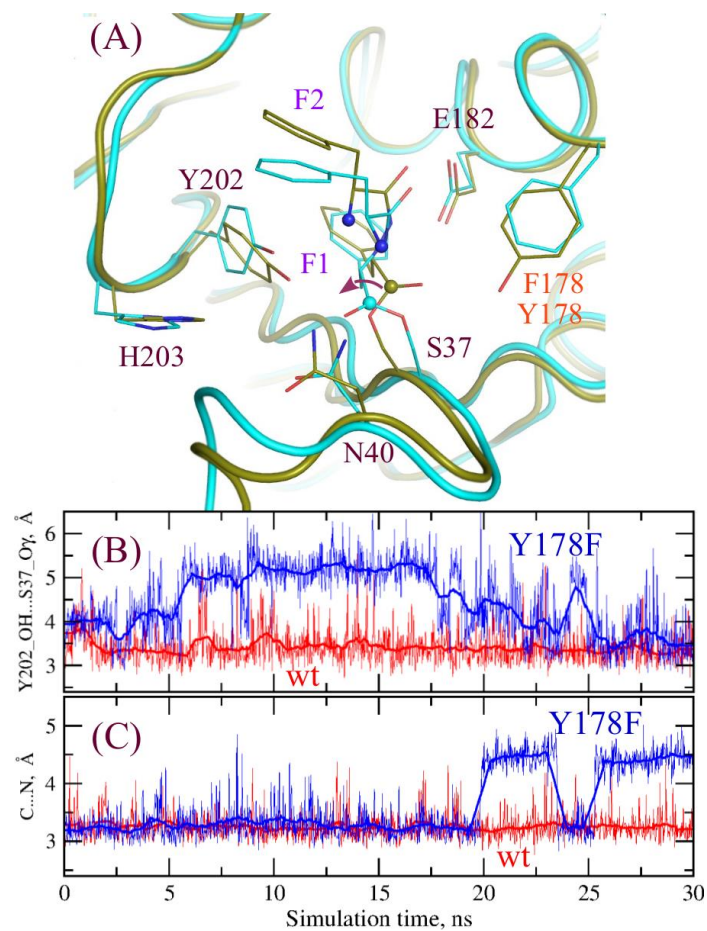


Figure SI-1. Effect of mutation Y178F on the geometry of the dipeptidyl-enzyme. (A) Snapshots from the MD simulations of the wild-type AlbC and Y178F mutant shown in dark green and cyan, respectively; (B) the distance between the hydroxyl oxygen of Y202 and the S37 hydroxyl oxygen in the simulations with the wild-type AlbC and Y178F mutant; (C) the distance between the N and C atoms of the dipeptide in the wild-type AlbC and Y178F simulations.