

A MD Simulation Prediction for Regulation of N-terminal Modification on Binding of CD47 to CD172a in a force-dependent manner

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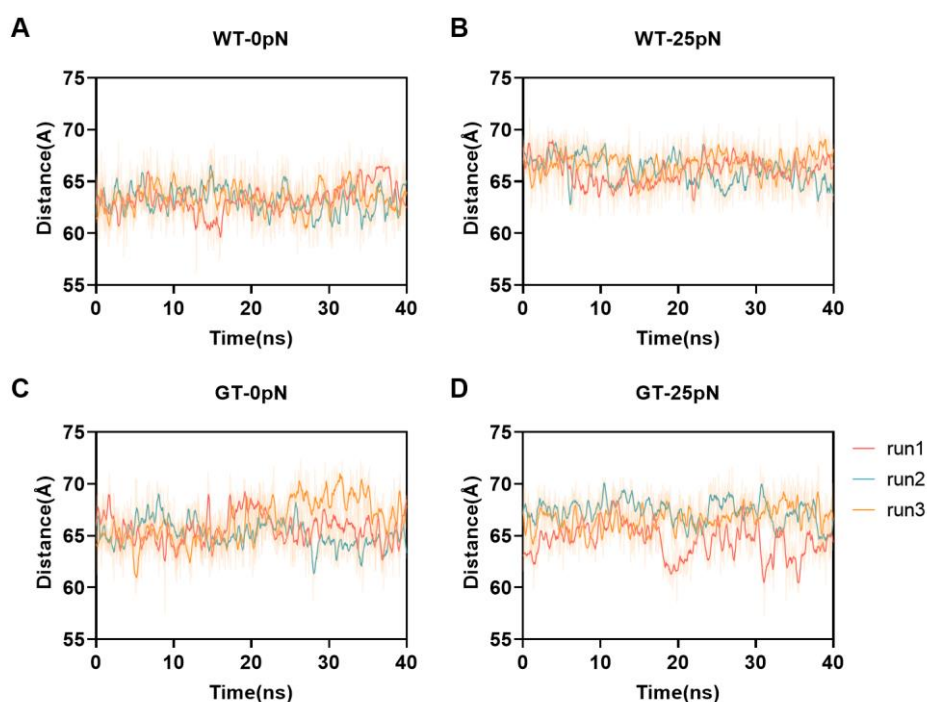


Figure S1. Time-courses of distance between Ca atom of VAL115 in CD47 and Ca atom of ALA115 in CD172. All data were sampled from “force-clamp” SMD runs of 40 ns thrice for WT-SS (A and B) and GT-SS (C and D) system at static state or under tensile force of 25 pN.

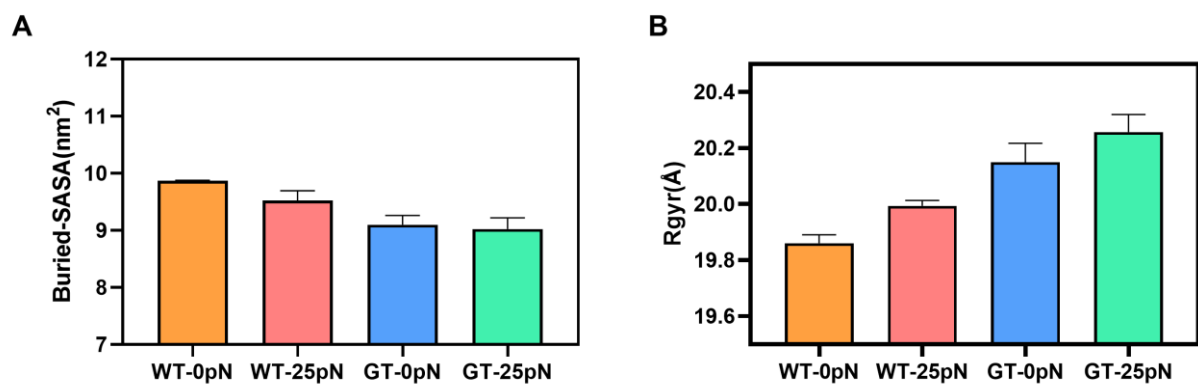


Figure S2. Tension-induced structural change of CD172a. The plots of the Buried-SASA (**A**) and the Rgyr (**B**) over thrice 40 ns “force-clamp” SMD runs for four systems, the WT-SS and GT-SS systems at static state or under tensile force of 25 pN.