

Insights into Resistance Mechanisms of Inhibitors to Mps1 C604Y Mutation via a Comprehensive Molecular Modeling Study

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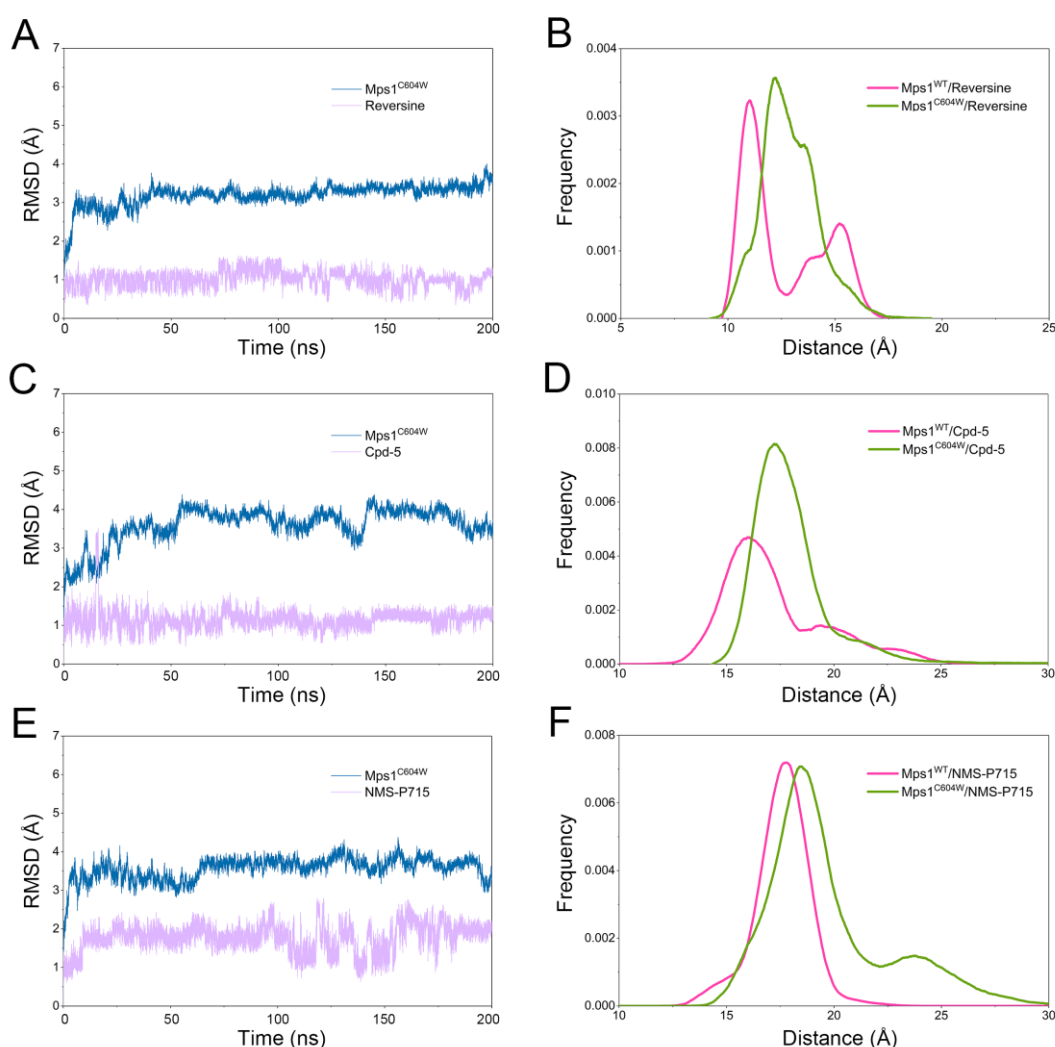


Figure S1. RMSD analysis of (A) Mps1^{C604W}/reversine, (C) Mps1^{C604W}/Cpd-5, (E) Mps1^{C604W}/NMS-P715 from classical MD simulations. The distribution of the opening degree of the A-loop between (B) Mps1^{WT}/reversine and Mps1^{C604W}/reversine, (D) Mps1^{WT}/Cpd-5 and Mps1^{C604W}/Cpd-5, (F) Mps1^{WT}/NMS-P715 and Mps1^{C604W}/NMS-P715.