Phosphorylation of Tyrosine 841 Plays a Significant Role in JAK3 Activation

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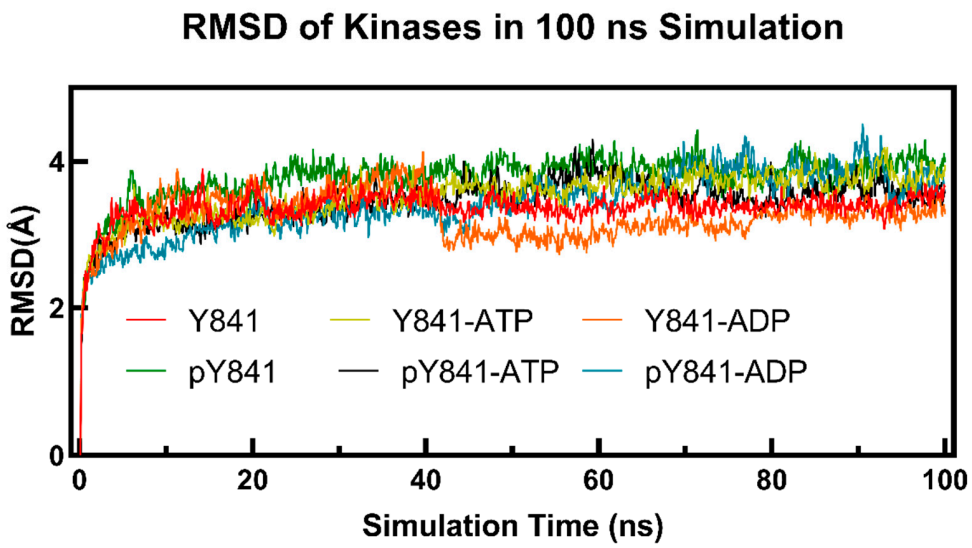


Figure S1: RMSD of the kinase Y841, pY841, and that with ADP or ATP.

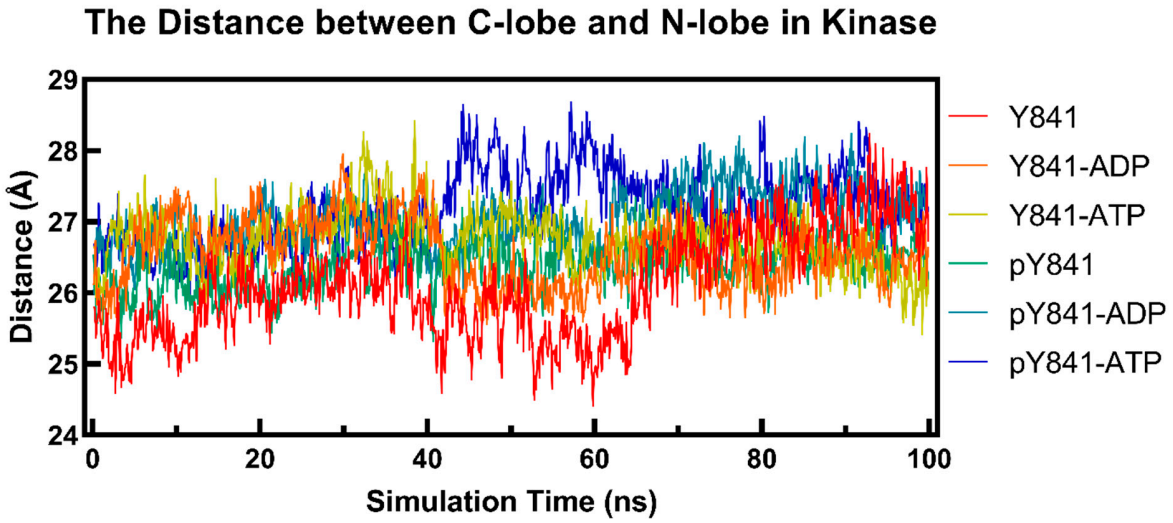


Figure S2: Cleft size of kinase Y841, pY841, and that with ADP or ATP.

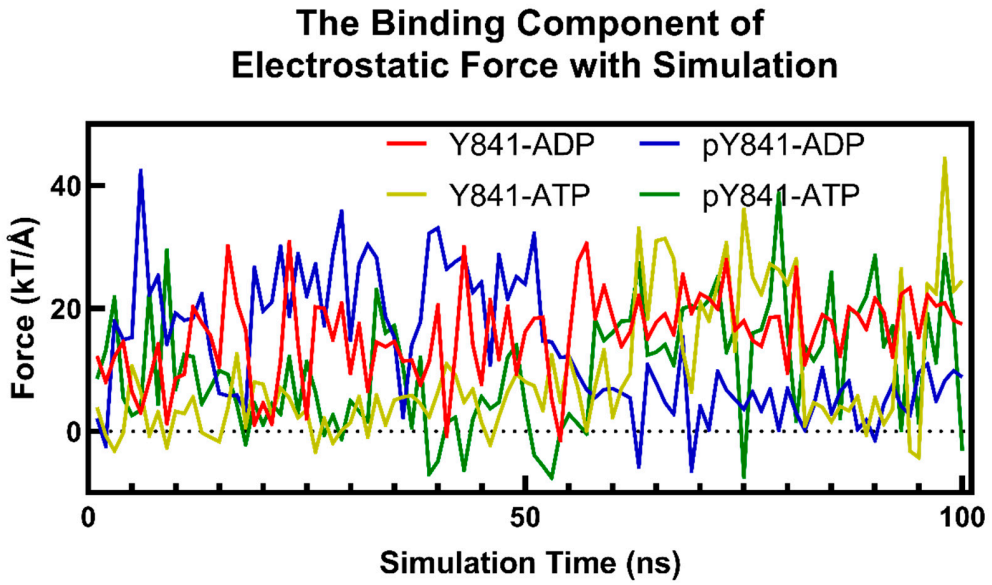


Figure S3: Binding components of electrostatic force between kinase and ADP/ATP in Y841, pY841.

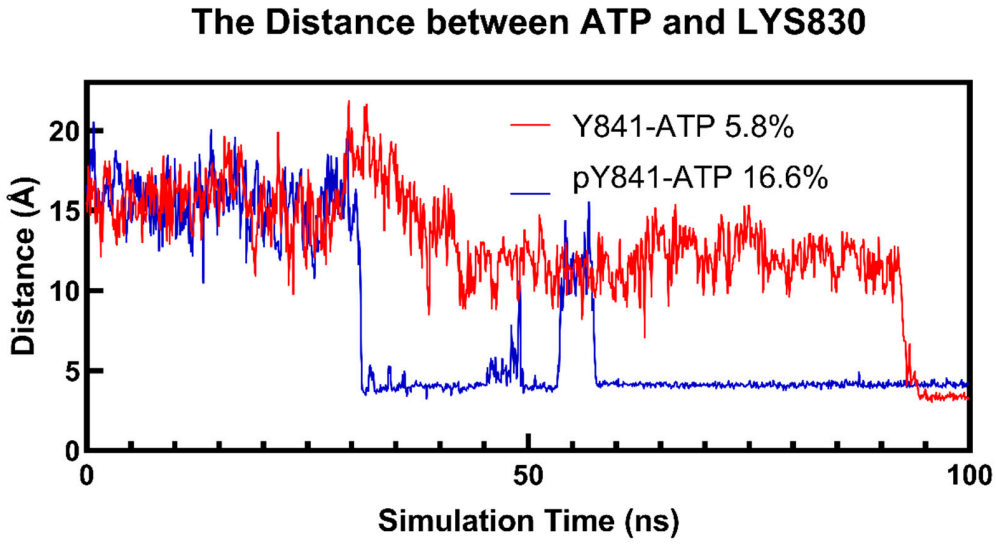


Figure S4: Distances between the salt bridge pairs LYS830/ATP in Y841 and pY841. The occupancy of LYS830/ATP in 5.8% while that in pY841 is 16.6%.

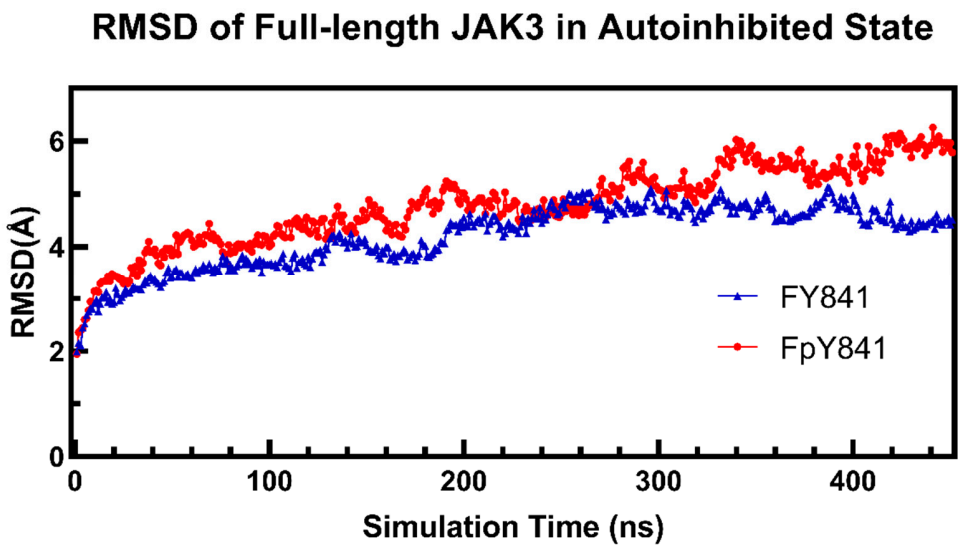


Figure S5: RMSD of full length JAK3 with non- phosphorated and phosphorated Y841 (FY841 and pY841) in auto-inhibited state

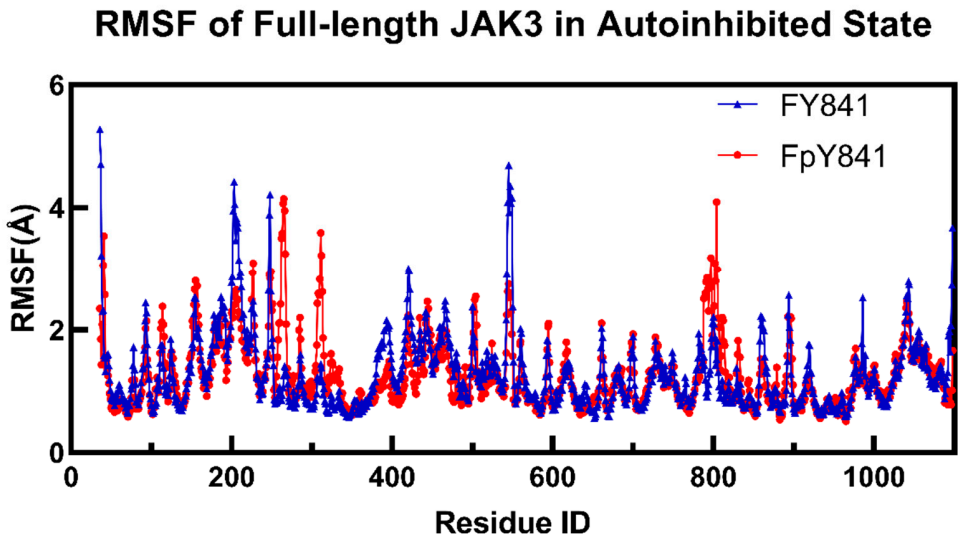


Figure S6: RMSF of full length JAK3 with non-phosphorated and phosphorated Y841 (FY841 and FpY841) in auto-inhibited state