Supporting Information

Studies of conformational changes of tubulin induced by interaction with kinesin using atomistic molecular dynamics simulations

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Supporting Figures

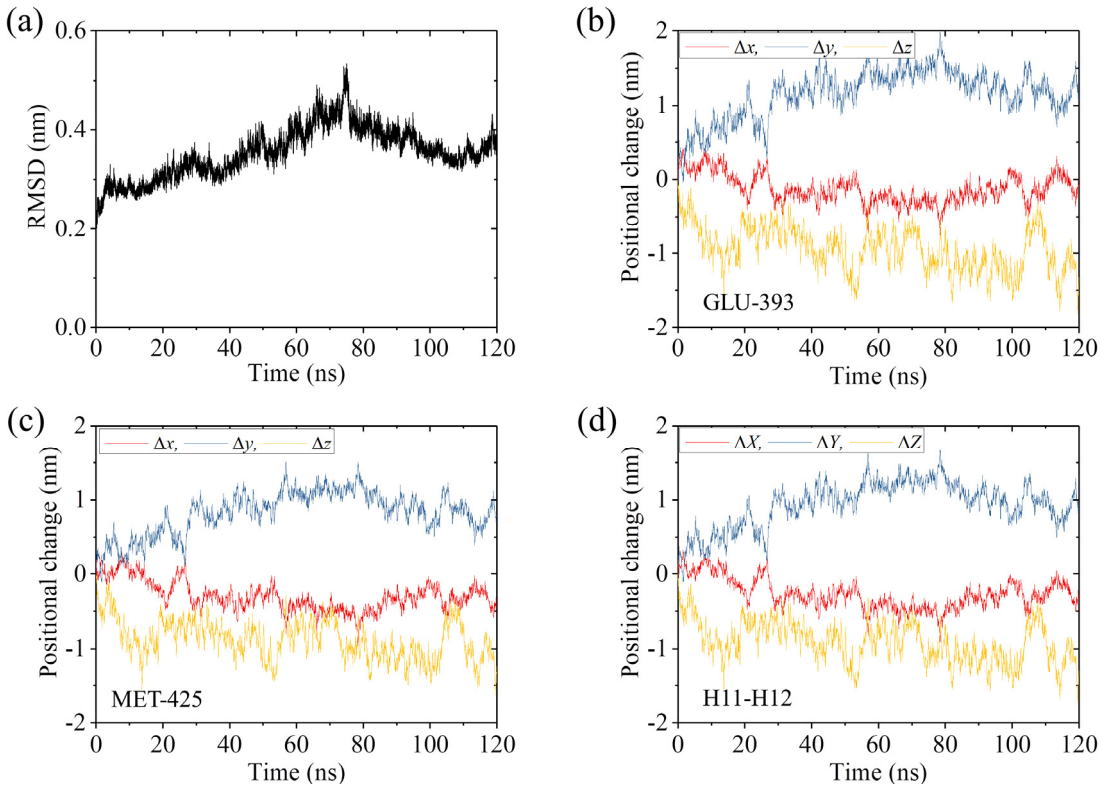

Figure S1. Equilibrium MD simulation results for APO-1 system. **(a)** Temporal evolution of RMSD value. **(b, c)** Temporal evolution of positional changes (Δx, Δy and Δz) of Cα atoms of GLU-393 in H11 and MET-425 in H12 of β-subunit relative to the corresponding ones at t = 0. **(d)** Temporal evolution of the average positional changes (ΔX, ΔY and ΔZ) of Cα atoms of all residues in H11 and H12 of β-subunit.

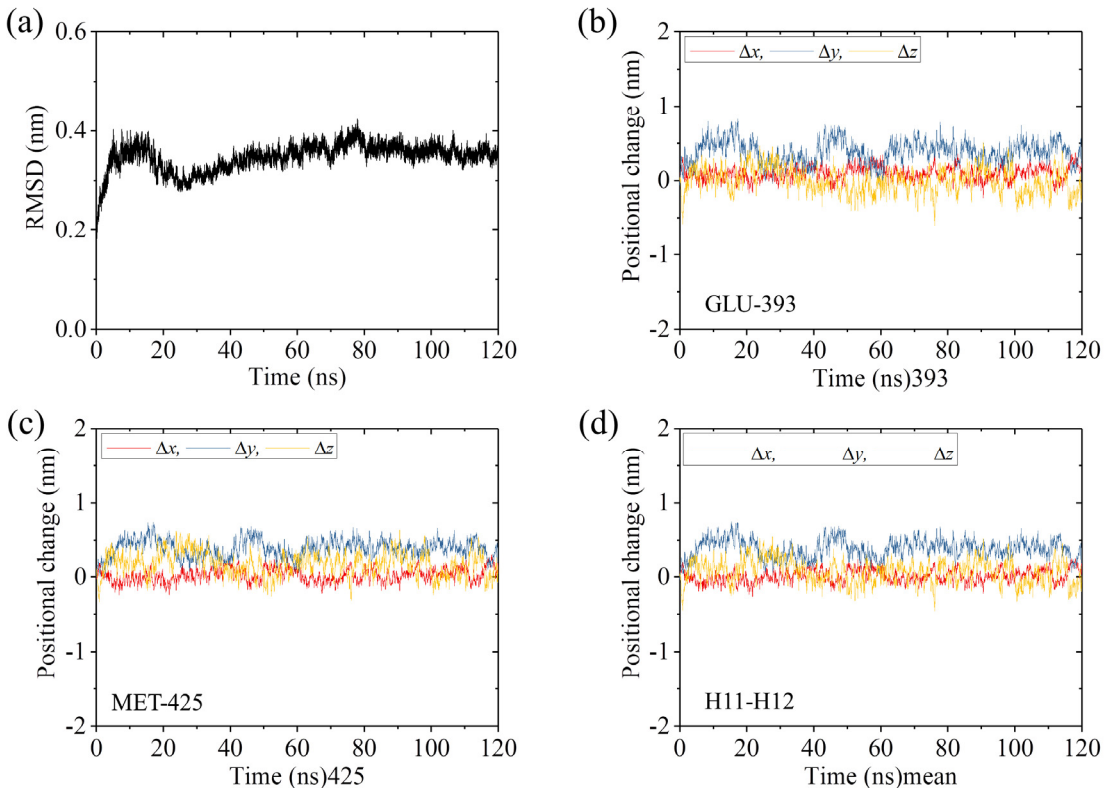

Figure S2. Equilibrium MD simulation results for ADP-2 system. **(a)** Temporal evolution of RMSD value. **(b, c)** Temporal evolution of positional changes (Δx, Δy and Δz) of Cα atoms of GLU-393 in H11 and MET-425 in H12 of β-subunit relative to the corresponding ones at t = 0. **(d)** Temporal evolution of the average positional changes (ΔX, ΔY and ΔZ) of Cα atoms of all residues in H11 and H12 of β-subunit.

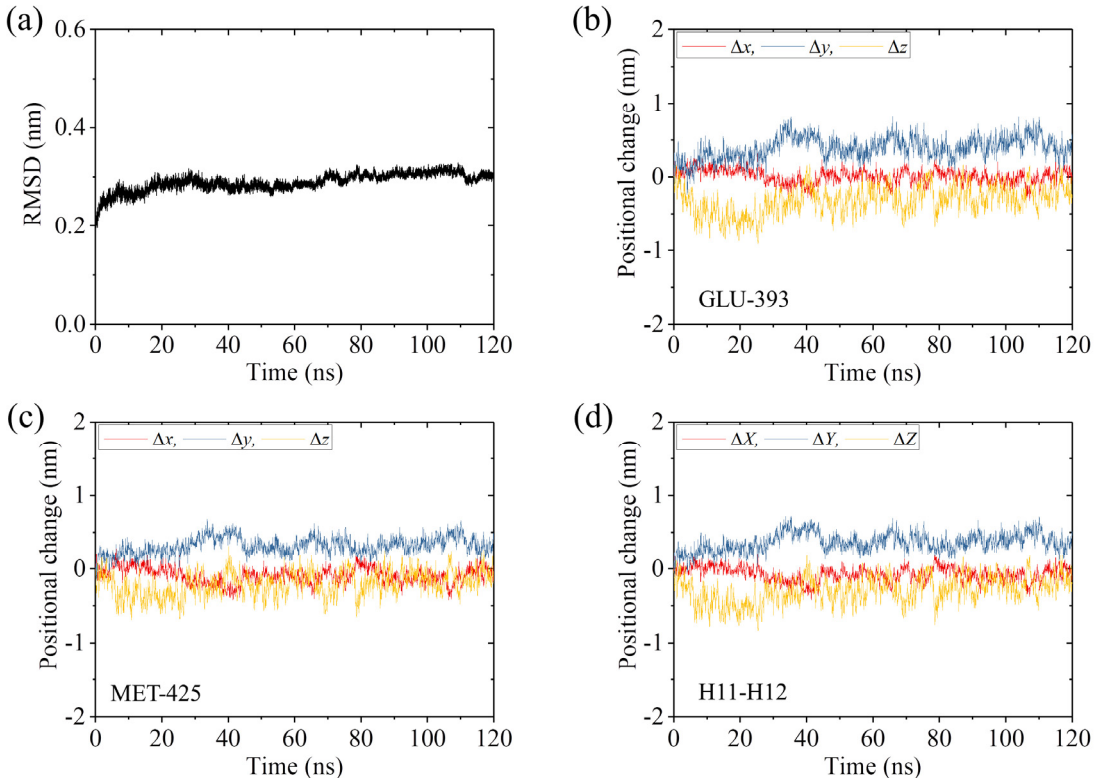

Figure S3. Equilibrium MD simulation results for isolated α/β-tubulin. **(a)** Temporal evolution of RMSD value. **(b, c)** Temporal evolution of positional changes (Δx, Δy and Δz) of Cα atoms of GLU-393 in H11 and MET-425 in H12 of β-subunit relative to the corresponding ones at t = 0. **(d)** Temporal evolution of the average positional changes (ΔX, ΔY and ΔZ) of Cα atoms of all residues in H11 and H12 of β-subunit.

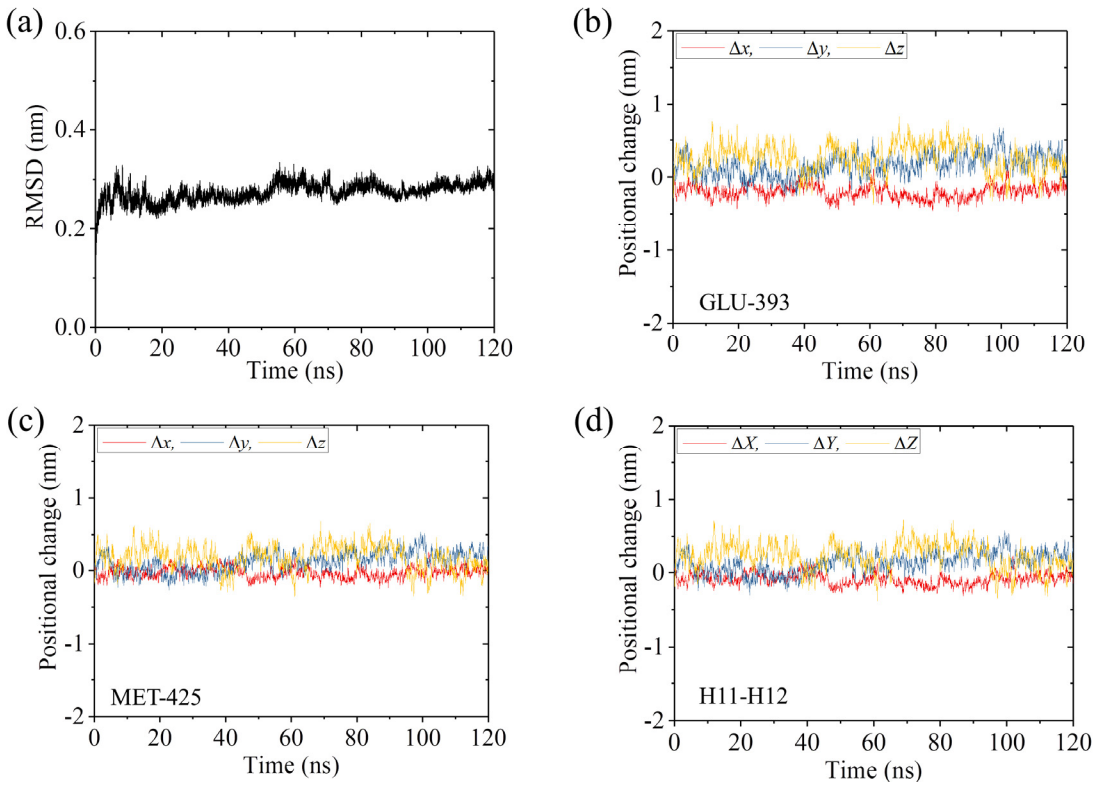

Figure S4. Equilibrium MD simulation results for ADP-1 system. **(a)** Temporal evolution of RMSD value. **(b, c)** Temporal evolution of positional changes (Δx, Δy and Δz) of Cα atoms of GLU-393 in H11 and MET-425 in H12 of β-subunit relative to the corresponding ones at t = 0. **(d)** Temporal evolution of the average positional changes (ΔX, ΔY and ΔZ) of Cα atoms of all residues in H11 and H12 of β-subunit.