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Role of ELA region in auto-activation of mutant KIT receptor: a molecular dynamics simulation insight — Source link 🖸

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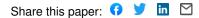
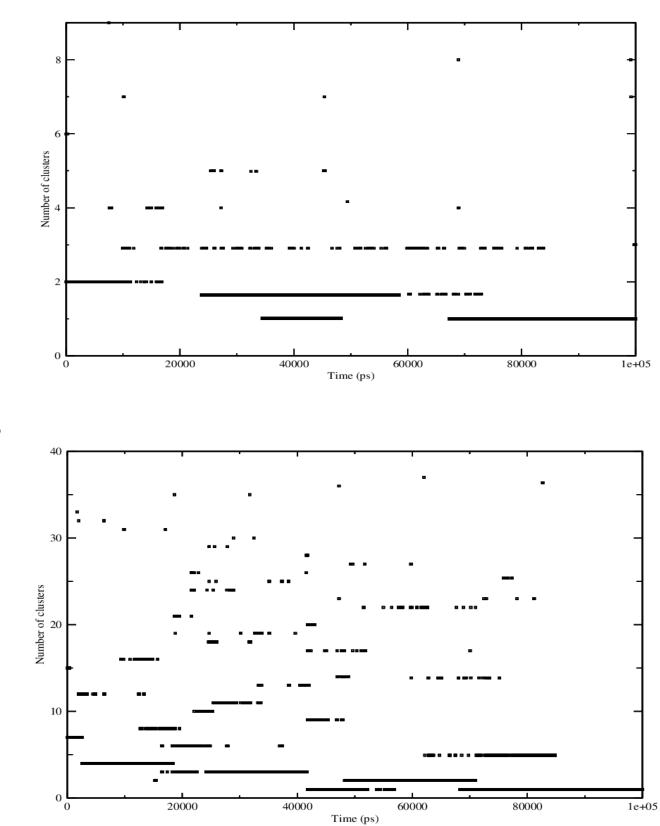


Figure S2. Number of populated clusters (C- α carbon atom) versus simulation time for (a) the wildtype and (b) mutant KIT protein trajectory. RMSD cut-off for two structures to be neighbor was 0.14 nm and gromos method was implemented for cluster determination. Results are shown for two independent clusterings. After 70 ns, the simulation appears equilibrated.



a

b