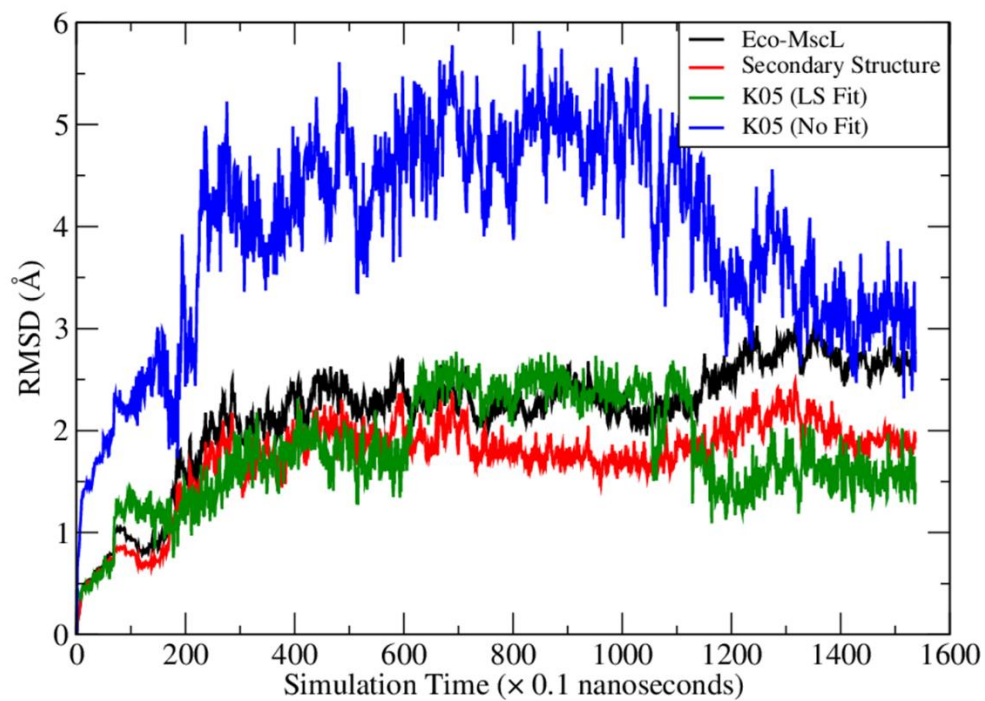


**Supplemental; Small compounds modulate and bind MscL similarly**

**S8 Fig. The RMSD (Root-mean-square deviation) ~ Simulation Time plot for Docking Pose 1.** According to the RMSDs of nonfit ligand (the blue curve), two conformation clusters can be observed. The first cluster is from 20 to 115 ns and second from 115 to 155 ns.