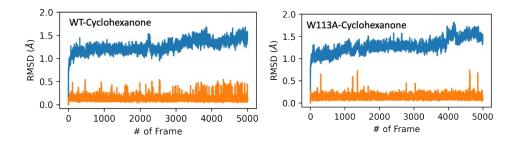
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**Figure S10.** The RMSD obtained from wild type CDH and W113A in complex with cyclohexanone ligand for 500 ns trajectory. The RMSD values of  $C\alpha$  atoms of the protein and the heavy atoms of cyclohexanone ligand are shown in blue and orange colours respectively.