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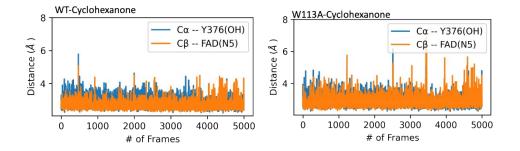


Figure S12. The interatomic distance of the axial proton located at the C $\alpha$  and C $\beta$  position of cyclohexanone in WT and W113A for the 500 ns trajectory.