Supplementary Materials

Conformational Change of Pseudouridine 55 Synthase upon Its Association with RNA Substrate

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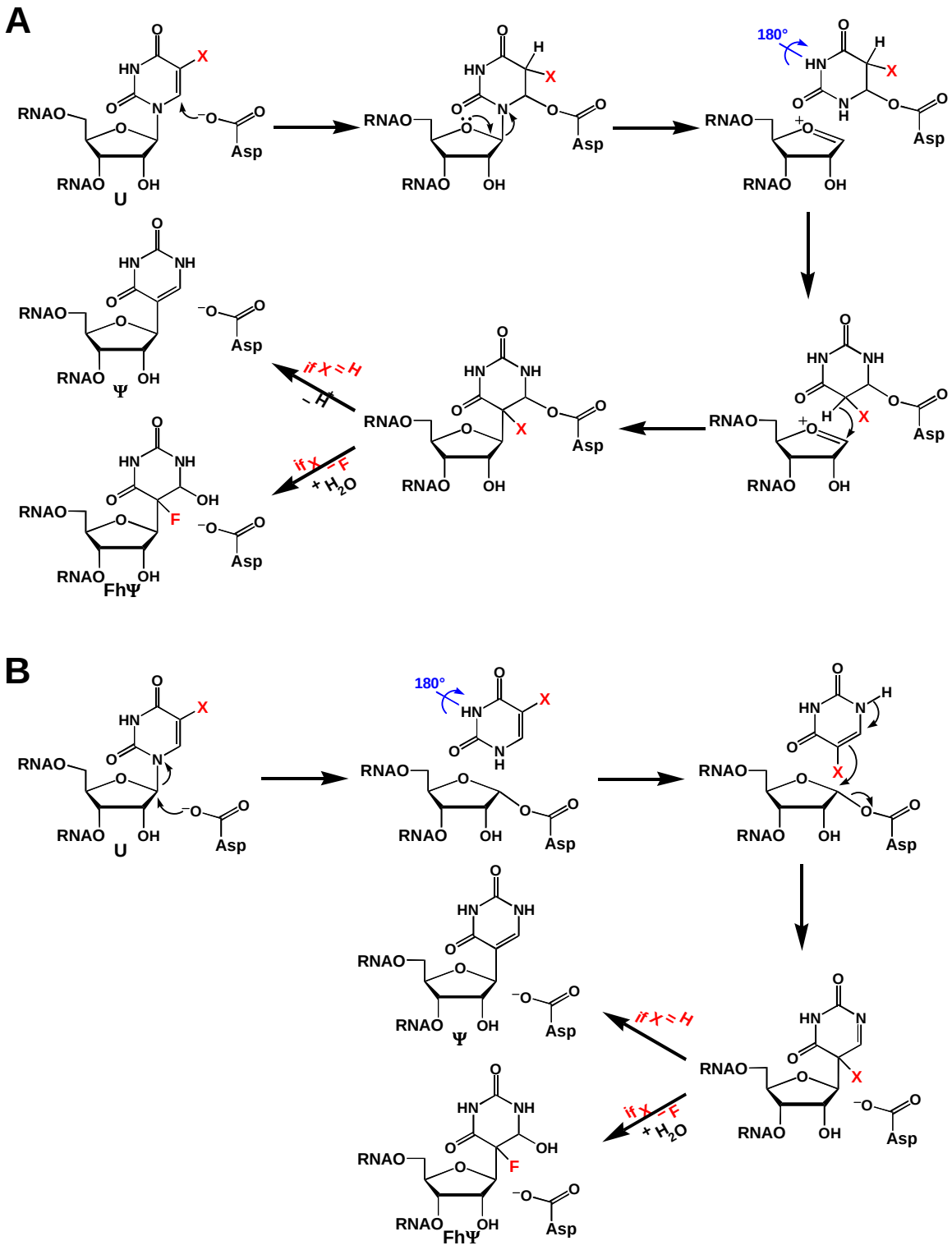

Figure S1. Two possible mechanisms of the ΨS-catalyzed reactions, modified from Mueller (16). When X=H, RNA is a substrate; when X=F, RNA is an inhibitor. **A.** The first possible mechanism involves nucleophilic attack of the conserved aspartic acid on the C6 of the base to assist the rotation of the base. **B.** The second possible mechanism involves nucleophilic attack of the conserved aspartic acid on the C1' of the ribose to assist the departure of the base.

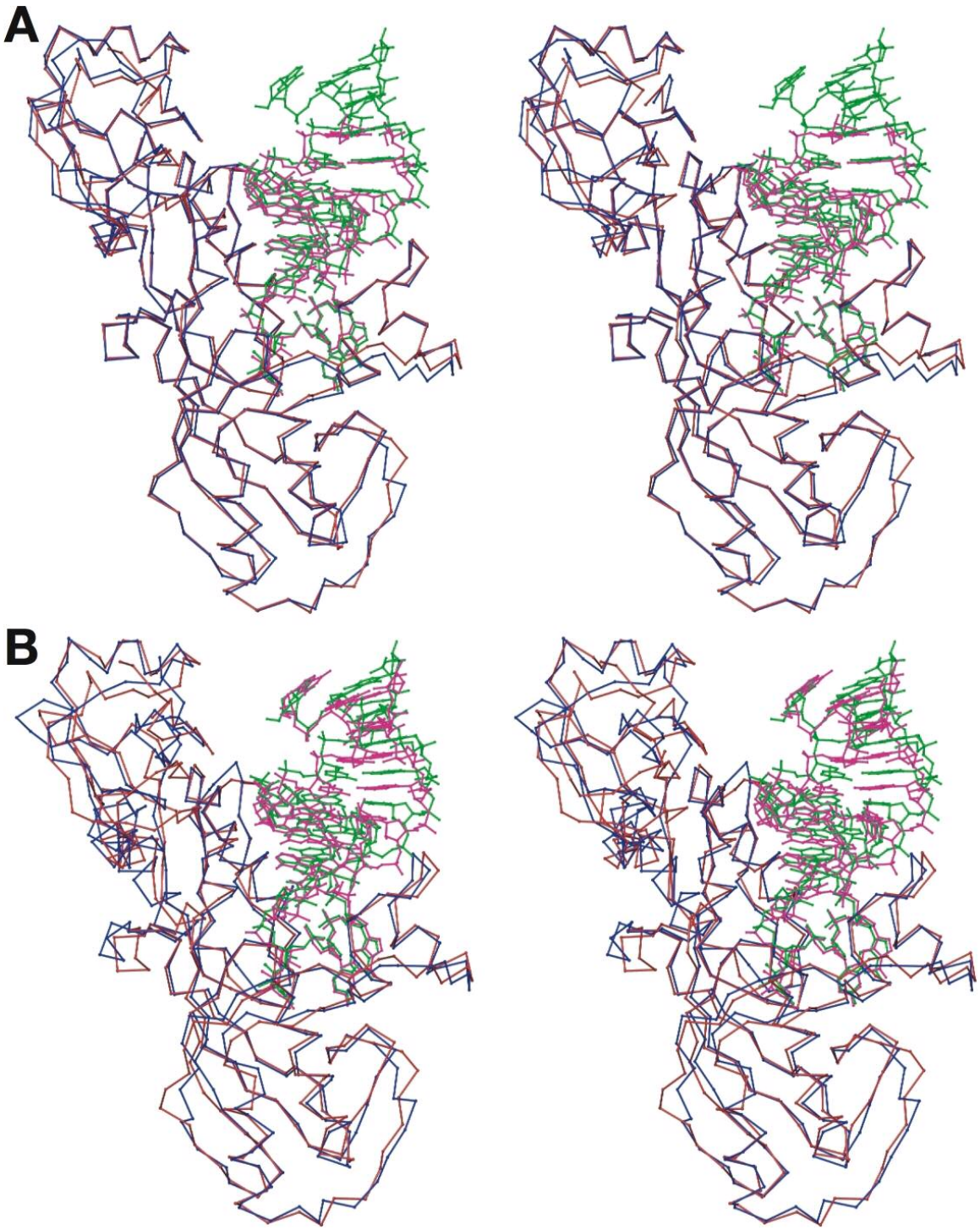

Figure S2. Superposition of the structure of Ψ55S-RNA complex presented in this paper with the one (PDB ID code: 1R3E) by Stroud and his coworkers (**A**), and the one (PDB ID code: 1R8W) by Hoang and Ferre-D'Amare (**B**). The protein and RNA in our structure are colored red and green, respectively. The protein and RNA from Stroud and his coworkers or from Hoang and Ferre-D'Amare are colored blue and magenta, respectively. The rmsd is 0.8 Å for 1R3E, and 1.8 Å for 1R8W. For comparison, the rmsd bwtween 1R3E and 1R8W is also 1.8 Å.