

*Supporting Materials*

# **The CAR mRNA-Interaction Surface is a Zipper Extension of the Ribosome A Site**

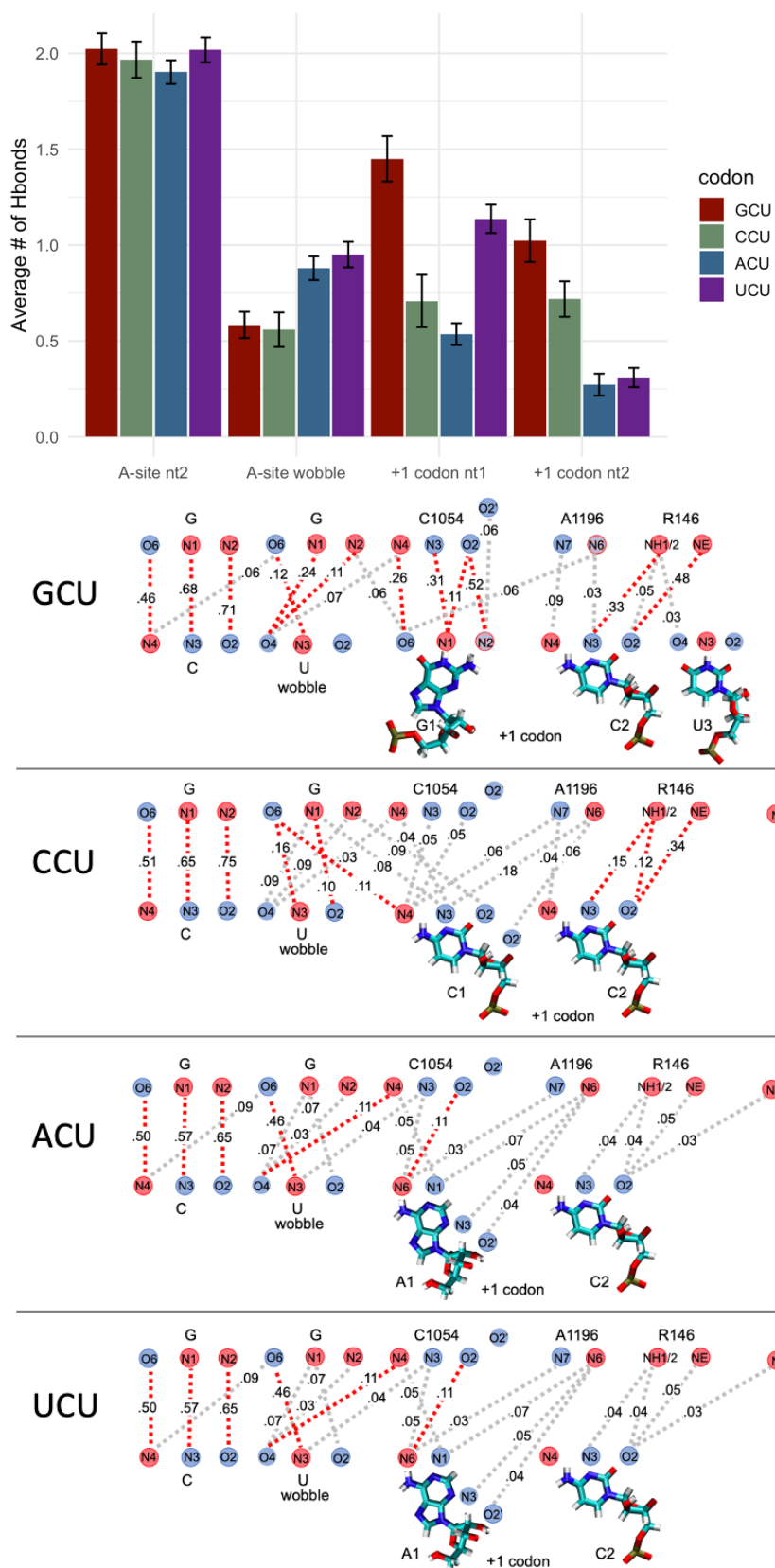
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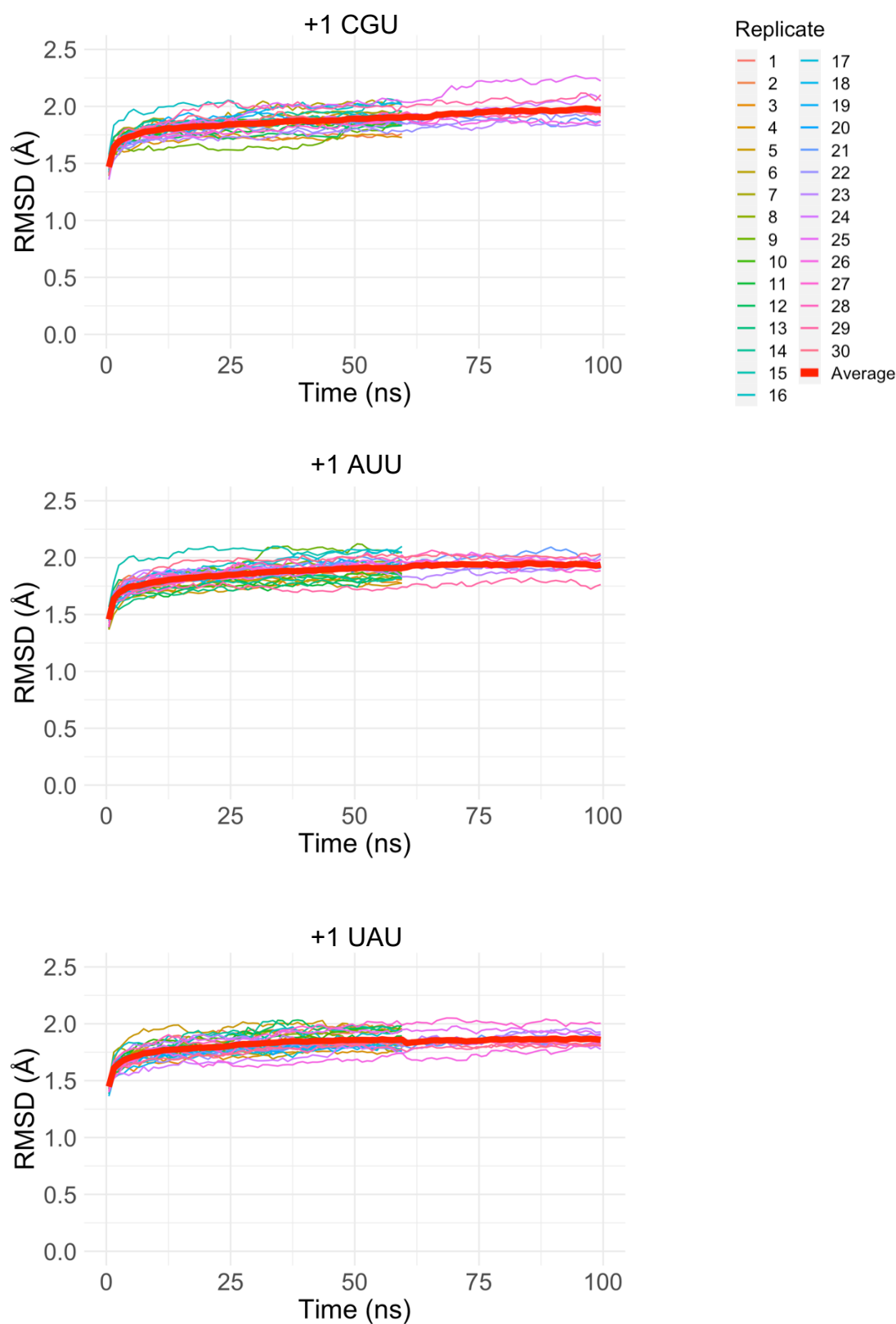
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## **1. Supplementary Materials**

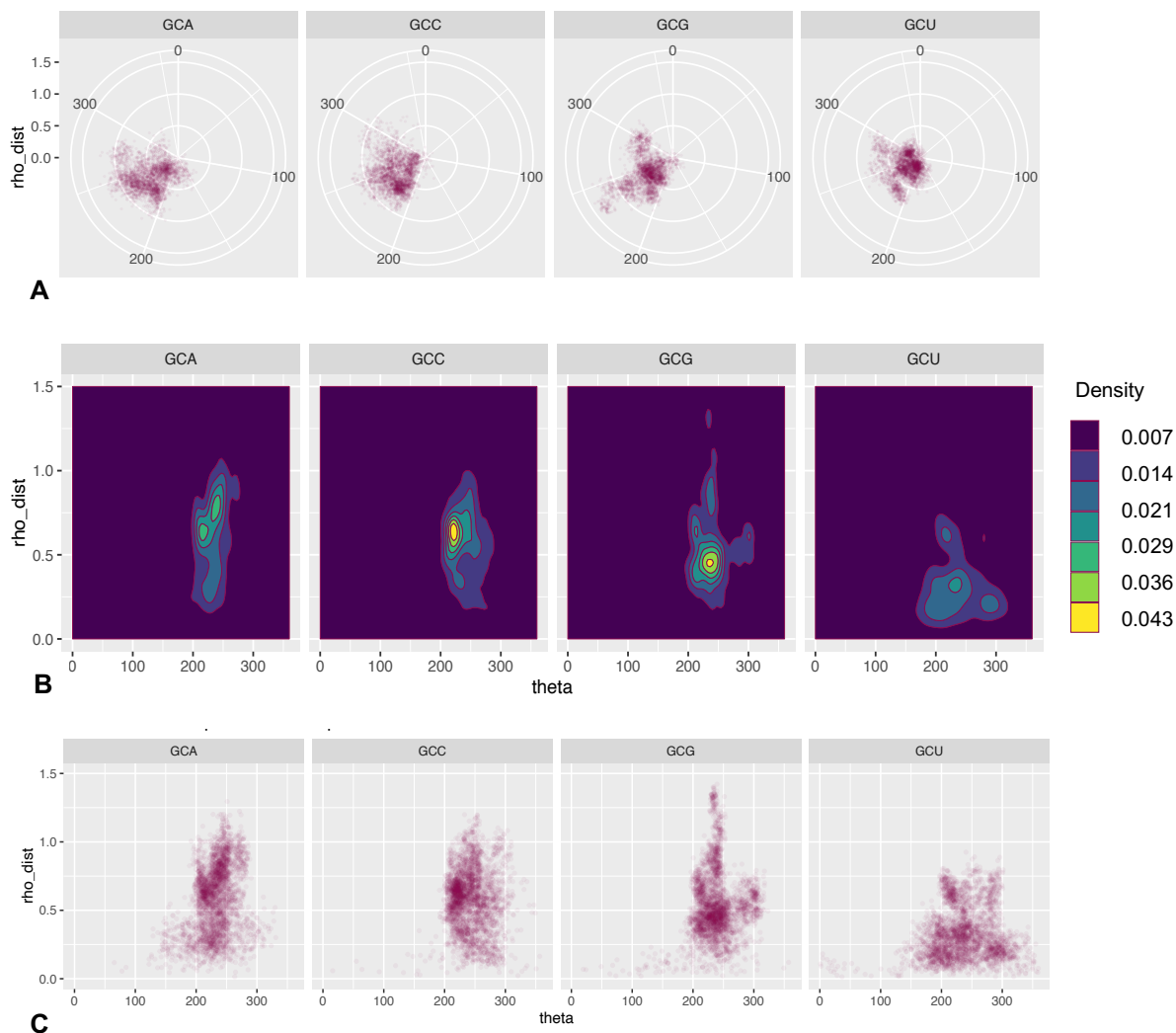
### *1.1 Supplementary Figures*



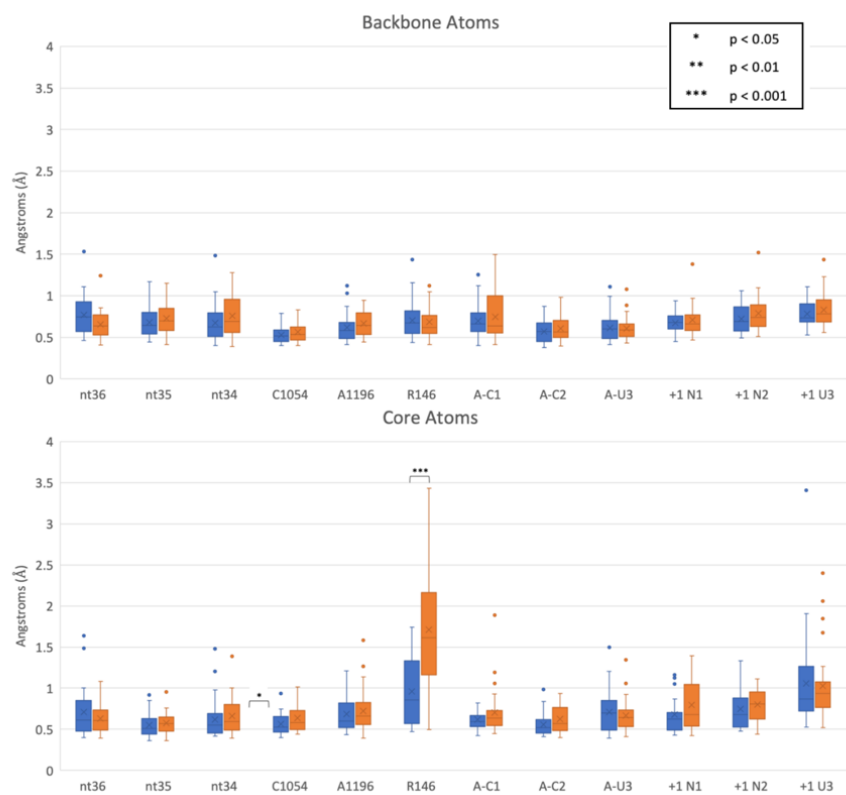
**Figure S1. H-bonding of CAR with +1 NCU codons.** +1 GCU codons have higher H-bonding with CAR compared with +1 CCU, +1 ACU and +1 UCU. Unlike the other +1 codons, H-bonding of the first nucleotide of +1 UCU is split between C1054 and A1196.



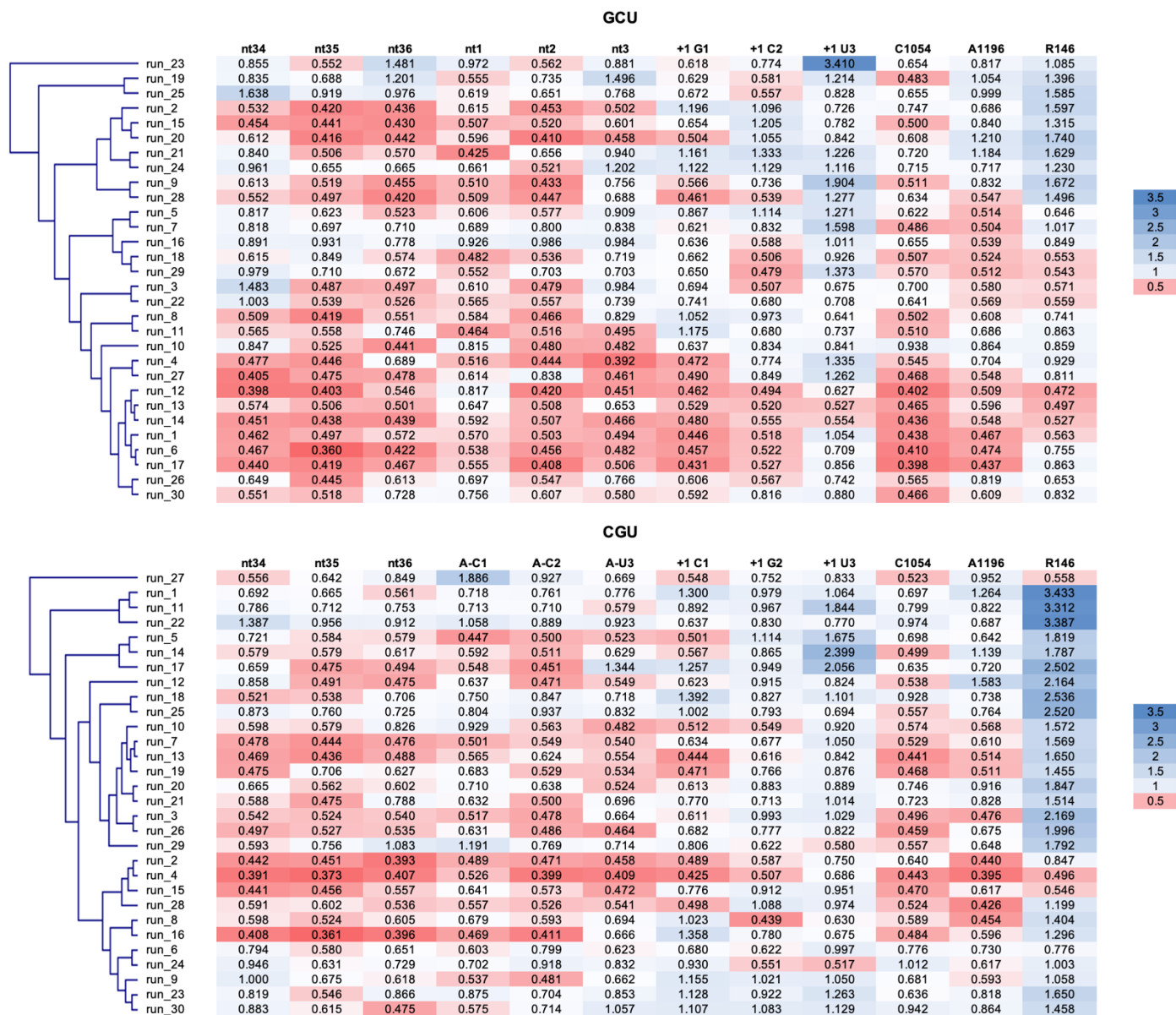
**Figure S2. RMSD profiles for trajectories.** Examples of RMSD profiles which were computed using as reference the structure at the end of equilibration. Subsystems with different +1 codons were analyzed using 60- and 100-ns trajectories. The trajectories stabilized by 20 ns and the first 20 ns of trajectories were not used for further analysis.



**Figure S3. Influences of nucleotide 3 of the +1 codon.** The stacking positions of G1 and C2 are compared in +1 GCA, GCC, GCG and GCU codons. The data in Figure 5D are illustrated here using scatterplot (A and C) and heat map (B) representations for the distributions of  $\rho$  (Å) and  $\theta$  (degrees; see Figures 5D) in 3200 frames (1600 ns) of +1 GCA, GCC, GCG and GCU trajectories. Converting the polar representation (A) to Cartesian coordinates (B and C) shows that the distribution of  $\rho$  values is lower for +1 GCU codons consistent with the better centered stacking of G1 and C2.



A



**B**

**Figure S4. RMSF comparison of +1 GCU and +1 CGU trajectories.** (A) R146 in +1 CGU trajectories has elevated RMSF (orange) compared to +1 GCU (blue;  $p < 0.001$  \*\*\*). RMSF was measured using “core” base heavy atoms of nucleotide bases (C2, C4, C5, C6, N1, N3 of C and U; C2, C4, C5, C6, C8, N1, N3, N7, and G) and the guanidinium group (CZ, NE, NH1, NH2). (B) RMSF measurements for each MD experiment (row).