Supplemental Material to Accompany: **Chemically Accurate Relative Folding Stability of RNA Hairpins from Molecular Simulations**

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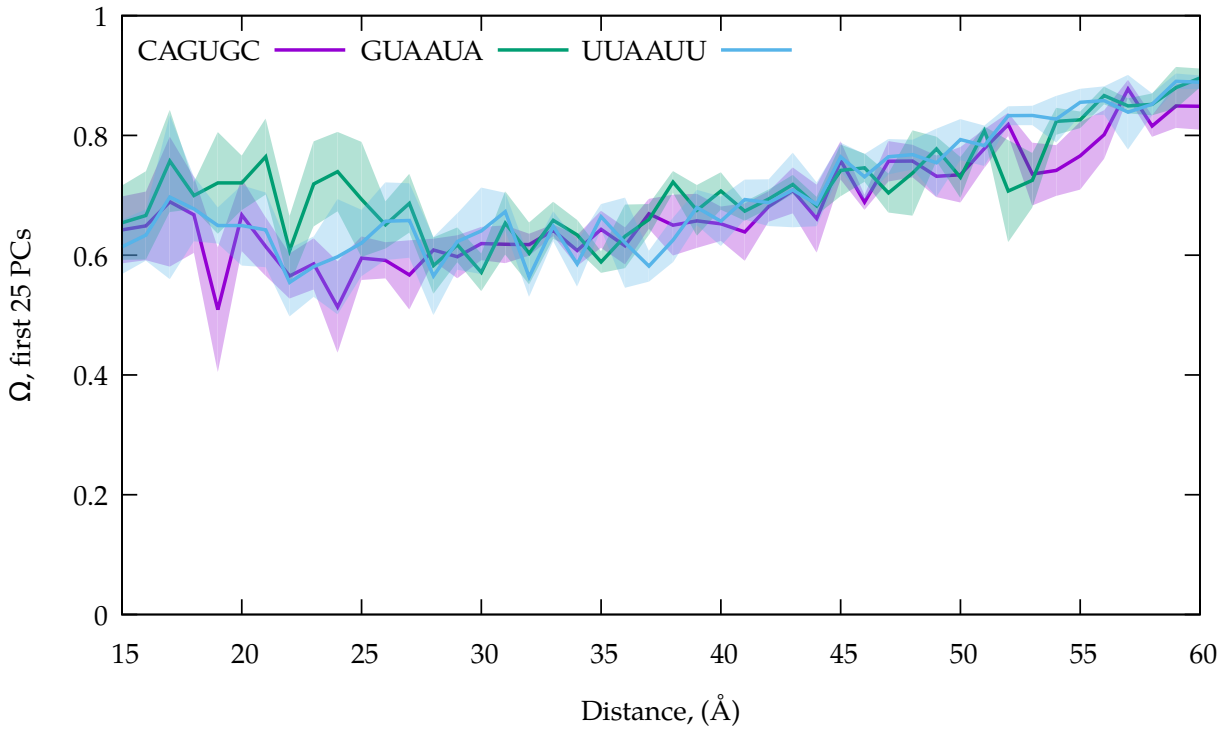
Supplementary Table 1: shows the average value of each coefficient for the polynomials fit to the basin (15-19 Å of the FEC). The standard error calculated from the variance in the coefficients is given after the ± symbol, with the error from the fit of the coefficient listed in parentheses. For each row, the name is the name of the loop sequence. The dataset used was the four full length replicas shown in Fig. 3.

Molecule	Third (kcal mol^{-1}Å^{-3})	Second (kcal mol^{-1}Å^{-2})	First (kcal mol^{-1}Å^{-1})	Constant (kcal mol^{-1})
CAGUGC	$(-7.88 \pm 1.01(2.13)) \times 10^{-2}$	$4.43 \pm 0.52(1.08)$	$(-8.18 \pm 0.88(1.83)) \times 10^{1}$	$(4.98 \pm 0.50(1.03) \times 10^{2})$
GUAAUA	$(-1.69 \pm 0.12(0.12)) \times 10^{-1}$	$9.18 \pm 0.60(0.59)$	$(-1.64 \pm 0.10(0.10)) \times 10^{2}$	$(9.74 \pm 0.56(0.57)) \times 10^{2}$
UUAAUU	$(-1.36 \pm 0.05(0.12)) \times 10^{-1}$	$7.36 \pm 0.24(0.63)$	$(-1.31 \pm 0.04(0.10)) \times 10^{2}$	$(7.73 \pm 0.24(0.60)) \times 10^{2}$
Average	$(-1.28 \pm 0.16(0.27)) \times 10^{-1}$	$6.99 \pm 0.83(1.38)$	$(-1.26 \pm 0.14(0.24)) \times 10^{2}$	$(7.49 \pm 0.79(1.32)) \times 10^{2}$

Supplementary Table 2: the average value of each coefficient for the polynomials fit to the stretched state (45-60 Å of the FEC). The standard error calculated from the variance in the coefficients is given after the ± symbol, with the variance from the fit of the coefficient propagated as a standard error listed in parentheses. For each row, the name is the name of the loop sequence. The dataset used was the four full length replicas shown in Fig. 3.

Molecule	Second (kcal mol^{-1}Å^{-2}	First (kcal mol^{-1}Å^{-1})	Constant (kcal mol^{-1})
CAGUGC	$(5.89 \pm 1.31(0.20)) \times 10^{-3}$	$(-3.00 \pm 1.39(0.20)) \times 10^{-1}$	$8.80 \pm 3.75(0.53)$
GUAAUA	$(6.92 \pm 0.51(0.24)) \times 10^{-3}$	$(-4.21 \pm 0.63(0.25)) \times 10^{-1}$	$(1.66 \pm 0.21(0.06)) \times 10^{1}$
UUAAUU	$(7.78 \pm 1.20(0.16)) \times 10^{-3}$	$(-5.29 \pm 1.22(0.12)) \times 10^{-1}$	$(1.70 \pm 0.29(0.04)) \times 10^{1}$
Average	$(6.86 \pm 1.85(0.35)) \times 10^{-3}$	$(-4.17 \pm 0.54(0.12)) \times 10^{-1}$	$(1.41 \pm 0.52(0.09)) \times 10^{1}$



Supplementary Figure 1: Shows the average subspace overlap for each window and the standard deviation of that quantity across the four replicas. The subspace was taken to be the first 25 modes of the all-heavy-atom principle component analysis of the motions of the trajectories representing each window. The envelopes around each line represent the standard deviation. Because the lower modes are less likely to constitute noise, and because the total volume of the state is smaller, the overlap is higher.