Supporting Information

Effect of Sodium Ions on RNA Duplex Stability

*Zexiang Chen and Brent M. Znosko**

Department of Chemistry, Saint Louis University; 3501 Laclede Ave., Saint Louis, MO 63103

Figure S1: ΔH° vs ln $[Na^{+}]$ for representative RNA oligomers of different G-C base pair contents: 100% GC, 5'-$(CGCGCG)_2$-3'; 66.7% GC, 5'-$(GCAUGC)_2$-3'; and 25% GC, 5'-$(AGAUAUCU)_2$-3'. 1.021 M data for these representative RNA oligomers are from Xia et al. (9).

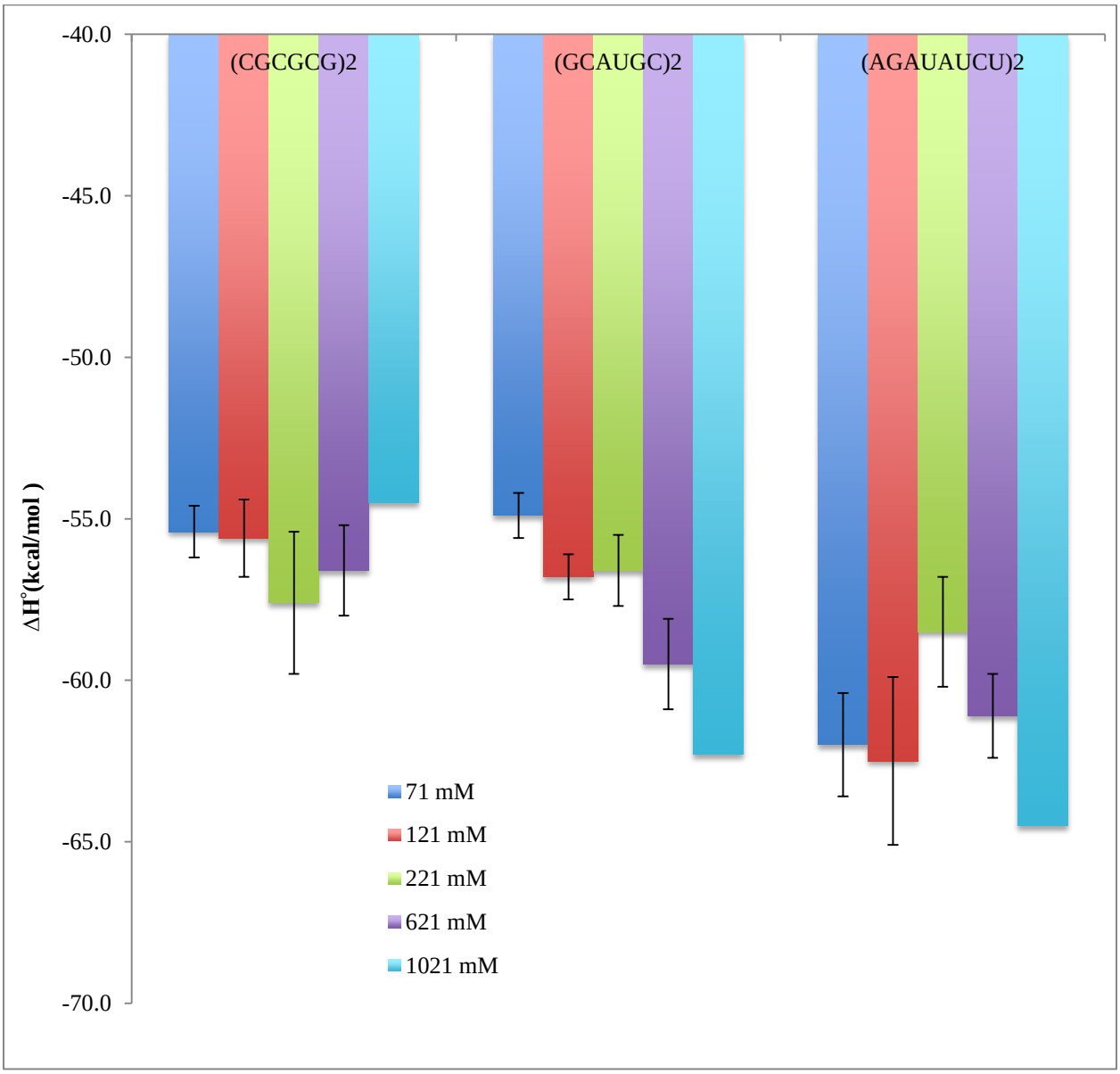

Figure S2: ΔS° vs ln [Na^{+}] for representative RNA oligomers of different G-C base pair contents: 100% GC, 5'-$(CGCGCG)_2$-3'; 66.7% GC, 5'-$(GCAUGC)_2$-3'; and 25% GC, 5'-$(AGAUAUCU)_2$-3'. 1.021 M data for these representative RNA oligomers are from Xia et al. (9).

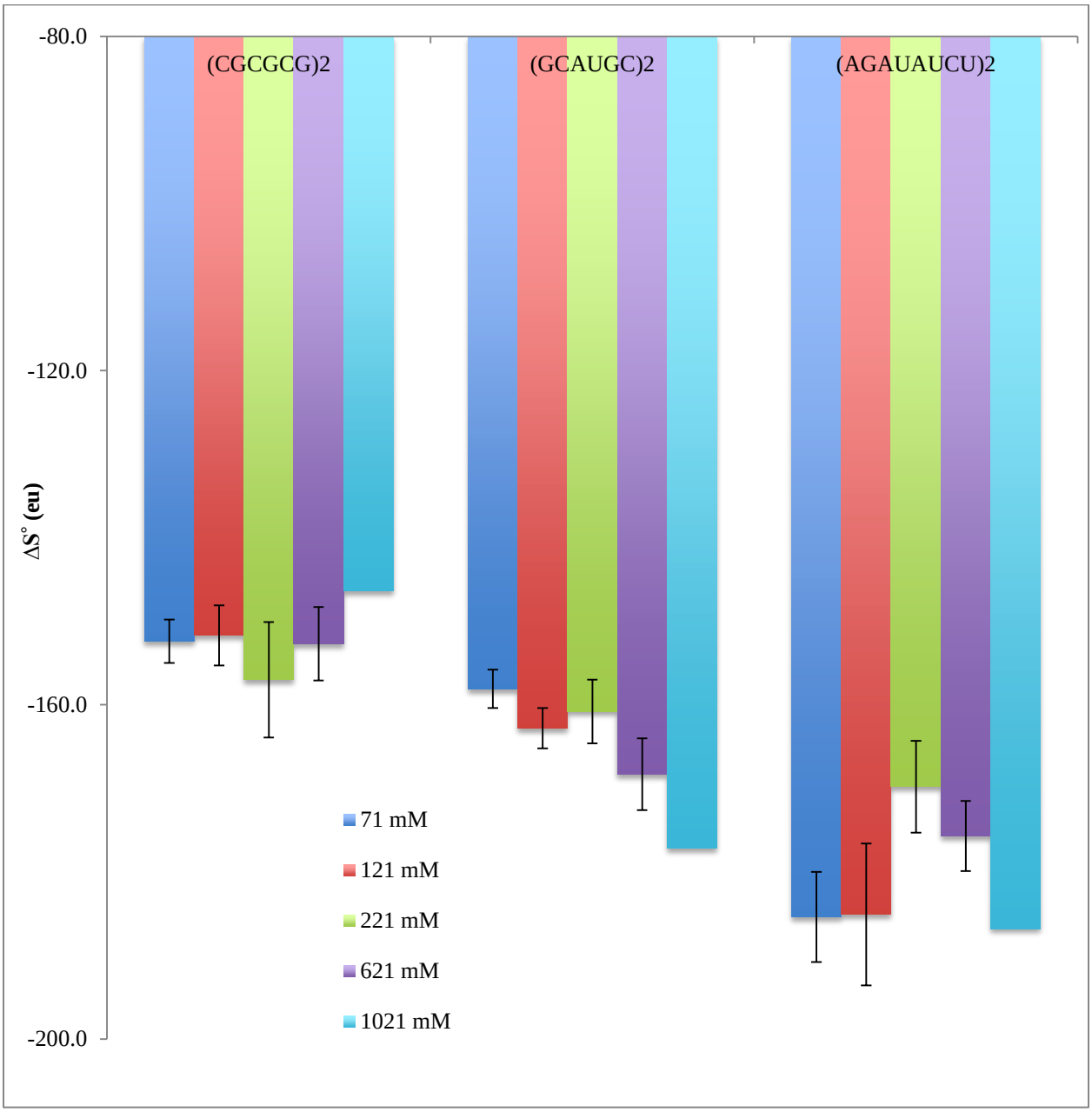

Table S1: Experimental RNA Thermodynamic Parameters for Duplex Formation

		Analysis of Curve Fits				Analysis of T_m^{-1} vs. ln C_t Plot			
Sequence[a]	**[Na^+]**	**ΔH° (kcal/mol)**	**ΔS° (eu)**	**ΔG°_{37} (kcal/mol)**	**T_m[c] ($^\circ$C)**	**ΔH° (kcal/mol)**	**ΔS° (eu)**	**ΔG°_{37} (kcal/mol)**	**T_m[c] ($^\circ$C)**
CGCGCG	71 mM	-53.3±2.1	-145.7±6.5	-8.07±0.07	51.6	-55.4±0.8	-152.4±2.6	-8.12±0.03	51.3
	121 mM	-54.0±2.2	-147.0±6.9	-8.47±0.10	53.9	-55.6±1.2	-151.7±3.6	-8.52±0.05	53.7
	221 mM	-56.2±1.5	-152.8±4.7	-8.81±0.09	55.3	-57.6±2.2	-157.0±6.9	-8.87±0.11	55.2
	621 mM	-56.0±3.2	-150.7±9.6	-9.22±0.21	58.0	-56.6±1.4	-152.7±4.4	-9.23±0.08	57.8
	1.021 M[b]	-53.8	-144.2	-9.08	57.9	-54.5	-146.4	-9.12	57.8
CGGCCG	71 mM	-54.0±2.2	-146.2±6.8	-8.71±0.11	55.4	-55.7±0.9	-151.2±2.9	-8.76±0.05	55.2
	121 mM	-53.7±2.1	-144.2±6.4	-9.02±0.10	57.6	-55.2±1.2	-148.8±3.8	-9.09±0.07	57.4
	221 mM	-53.5±1.7	-142.4±5.0	-9.38±0.10	60.1	-54.2±1.1	-144.4±3.3	-9.40±0.06	59.9
	621 mM	-54.2±2.3	-143.4±7.0	-9.73±0.17	62.1	-54.2±1.7	-143.3±5.0	-9.70±0.11	61.9
	1.021 M[b]	-56.6	-150.0	-10.11	63.3	-54.1	-142.6	-9.90	63.2
GCCGGC	71 mM	-63.6±3.1	-172.5±9.3	-10.13±0.19	60.3	-65.6±1.8	-178.5±5.4	-10.23±0.12	60.1
	121 mM	-64.5±2.8	-173.8±8.4	-10.63±0.20	62.8	-66.3±1.1	-179.1±3.4	-10.73±0.09	62.6
	221 mM	-62.7±1.5	-166.9±4.2	-10.88±0.16	65.1	-63.0±3.4	-168.1±10.2	-10.90±0.25	65.0
	621 mM	-64.4±1.4	-170.6±4.2	-11.46±0.15	67.6	-63.9±3.1	-169.2±9.2	-11.41±0.24	67.6
	1.021 M	-65.7±3.1	-174.6±9.3	-11.59±0.25	67.6	-67.3±2.5	-179.3±7.5	-11.69±0.21	67.4
GCGCGC	71 mM	-56.7±1.9	-154.2±5.9	-8.85±0.09	55.4	-57.2±1.3	-155.7±4.0	-8.85±0.06	55.3
	121 mM	-57.6±1.6	-155.8±5.0	-9.32±0.11	58.0	-58.0±1.5	-156.8±4.6	-9.32±0.09	57.8
	221 mM	-60.3±2.4	-162.6±7.4	-9.83±0.15	60.0	-60.5±1.6	-163.2±4.9	-9.83±0.11	59.9
	621 mM	-60.8±1.9	-162.9±5.7	-10.27±0.12	62.4	-61.3±2.6	-164.4±7.7	-10.29±0.18	62.3
	1.021 M	-61.2±3.6	-164.0±10.9	-10.38±0.22	62.8	-64.3±1.6	-173.4±4.7	-10.56±0.11	62.5

		Analysis of Curve Fits				Analysis of T_m^{-1} vs. ln C_t Plot			
Sequence[a]	**[Na^+]**	**ΔH° (kcal/mol)**	**ΔS° (eu)**	**ΔG°_{37} (kcal/mol)**	**T_m[c] ($^\circ$C)**	**ΔH° (kcal/mol)**	**ΔS° (eu)**	**ΔG°_{37} (kcal/mol)**	**T_m[c] ($^\circ$C)**
ACCGGU	71 mM	-48.0±5.1	-132.6±16.7	-6.82±0.15	44.6	-55.9±6.0	-158.0±19.3	-6.85±0.20	43.7
	121 mM	-48.5±4.1	-133.1±13.5	-7.23±0.09	47.3	-49.7±4.9	-136.7±15.4	-7.25±0.19	47.2
	221 mM	-48.8±3.0	-132.5±9.4	-7.66±0.22	50.1	-49.1±4.8	-133.6±15.0	-7.67±0.21	50.1
	621 mM	-51.9±4.4	-141.2±13.5	-8.12±0.35	52.3	-51.8±7.8	-141.0±24.2	-8.07±0.52	52.0
	1.021 M[b]	-53.2	-144.9	-8.26	52.8	-59.8	-164.5	-8.51	53.9
AGCGCU	71 mM	-47.3±5.4	-132.1±17.8	-6.33±0.19	41.3	-47.2±4.0	-131.7±12.9	-6.32±0.17	41.3
	121 mM	-45.6±2.3	-124.6±7.8	-6.92±0.12	45.7	-45.0±4.0	-122.8±12.6	-6.91±0.14	45.7
	221 mM	-46.9±4.7	-127.5±15.3	-7.33±0.14	48.4	-50.0±6.3	-137.5±19.9	-7.38±0.31	47.9
	621 mM	-47.7±5.1	-128.7±16.8	-7.81±0.21	51.5	-48.5±8.9	-131.1±27.5	-7.82±0.63	51.4
	1.021 M[b]	-50.9	-137.9	-8.13	52.7	-50.1	-135.7	-7.99	52.0
CACGUG	71 mM	-54.8±5.4	-160.2±17.4	-5.13±0.08	33.9	-53.2±1.1	-154.9±3.7	-5.10±0.02	33.6
	121 mM	-54.1±5.7	-156.5±18.7	-5.58±0.11	36.5	-54.1±1.6	-156.5±5.2	-5.54±0.03	36.2
	221 mM	-53.0±5.6	-151.7±18.2	-5.99±0.06	38.8	-53.5±2.1	-153.4±6.7	-5.94±0.03	38.5
	621 mM	-55.1±8.0	-156.5±26.0	-6.52±0.11	41.8	-60.4±3.4	-173.9±10.9	-6.45±0.06	41.0
	1.021 M[b]	-55.3	-156.8	-6.68	42.8	-50.3	-141.0	-6.59	42.8
CAGCUG	71 mM	-52.4±3.5	-151.5±11.3	-5.42±0.06	35.5	-53.3±1.0	-154.5±3.4	-5.37±0.01	35.3
	121 mM	-51.3±4.3	-146.9±14.0	-5.78±0.06	37.6	-52.4±1.8	-150.5±5.7	-5.72±0.02	37.2
	221 mM	-52.4±4.9	-148.8±15.9	-6.21±0.10	40.2	-57.5±2.6	-165.6±8.3	-6.18±0.03	39.7
	621 mM	-51.0±6.9	-143.1±22.2	-6.61±0.04	42.8	-57.0±2.2	-162.4±6.9	-6.60±0.03	42.1
	1.021 M[b]	-50.2	-140.0	-6.78	44.0	-51.6	-144.7	-6.68	43.1

		Analysis of Curve Fits				Analysis of T_m^{-1} vs. ln C_t Plot			
Sequence[a]	**[Na^+]**	**ΔH° (kcal/mol)**	**ΔS° (eu)**	**ΔG°_{37} (kcal/mol)**	**T_m[c] ($^\circ$C)**	**ΔH° (kcal/mol)**	**ΔS° (eu)**	**ΔG°_{37} (kcal/mol)**	**T_m[c] ($^\circ$C)**
CCAUGG	71 mM	-57.1±3.6	-166.5±11.6	-5.48±0.07	36.0	-57.9±2.5	-169.0±8.0	-5.44±0.04	35.7
	121 mM	-58.6±5.7	-170.4±18.6	-5.72±0.11	37.2	-56.7±2.3	-164.5±7.6	-5.68±0.03	37.0
	221 mM	-56.6±6.8	-161.7±22.0	-6.40±0.06	41.0	-61.3±1.5	-177.1±4.9	-6.34±0.01	40.4
	621 mM	-58.3±9.0	-165.3±29.0	-7.03±0.10	44.3	-65.9±4.4	-189.9±13.9	-7.02±0.09	43.5
	1.021 M[b]	-61.0	-172.5	-7.49	46.6	-56.9	-159.9	-7.30	46.4
CCUAGG	71 mM	-58.8±1.6	-169.6±5.2	-6.22±0.07	39.9	-62.6±1.4	-181.9±4.4	-6.22±0.01	39.7
	121 mM	-61.0±5.3	-174.9±17.0	-6.79±0.14	42.8	-63.7±2.6	-183.4±8.3	-6.76±0.03	42.4
	221 mM	-60.5±3.3	-171.8±10.5	-7.19±0.03	45.0	-62.3±1.1	-177.7±3.4	-7.18±0.02	44.7
	621 mM	-60.7±5.7	-170.9±18.2	-7.70±0.15	47.7	-62.0±4.8	-175.1±15.2	-7.68±0.15	47.4
	1.021 M[b]	-59.7	-166.5	-8.06	49.9	-54.1	-149.1	-7.80	50.0
CUGCAG	71 mM	-55.4±1.7	-160.3±5.6	-5.70±0.07	37.1	-57.2±1.7	-165.9±5.6	-5.69±0.02	37.1
	121 mM	-55.1±2.7	-157.5±8.8	-6.23±0.03	40.1	-56.4±0.6	-161.8±2.1	-6.20±0.00	39.9
	221 mM	-54.1±1.9	-153.2±6.3	-6.54±0.03	42.1	-55.6±0.8	-158.1±2.5	-6.53±0.01	41.9
	621 mM	-55.6±3.0	-156.5±9.4	-7.07±0.15	44.9	-55.5±1.7	-156.3±5.4	-7.03±0.03	44.8
	1.021 M[b]	-54.5	-153	-7.05	45.0	-55.4	-155.7	-7.11	45.3
GACGUC	71 mM	-57.1±4.9	-165.0±15.9	-5.95±0.08	38.5	-57.5±0.9	-166.1±3.0	-5.96±0.01	38.5
	121 mM	-56.8±3.4	-162.2±10.8	-6.47±0.04	41.4	-57.4±1.0	-164.3±3.4	-6.44±0.01	41.2
	221 mM	-55.7±2.2	-157.6±7.1	-6.78±0.06	43.3	-56.5±1.4	-160.2±4.5	-6.77±0.02	43.1
	621 mM	-54.9±2.6	-153.6±8.1	-7.26±0.08	46.2	-56.3±1.9	-158.2±6.1	-7.26±0.04	46.0
	1.021 M[b]	-57.3	-161.0	-7.37	46.4	-58.1	-163.5	-7.35	46.2

		Analysis of Curve Fits				Analysis of T_m^{-1} vs. ln C_t Plot			
Sequence[a]	**[Na^+]**	**ΔH° (kcal/mol)**	**ΔS° (eu)**	**ΔG°_{37} (kcal/mol)**	**T_m**[c] **(°C)**	**ΔH° (kcal/mol)**	**ΔS° (eu)**	**ΔG°_{37} (kcal/mol)**	**T_m**[c] **(°C)**
GAGCUC	71 mM	-54.7±1.8	-156.0±5.9	-6.26±0.04	40.3	-54.5±0.7	-155.6±2.4	-6.24±0.01	40.2
	121 mM	-55.7±2.7	-157.8±8.6	-6.72±0.09	42.9	-56.4±1.3	-160.2±4.0	-6.70±0.02	42.7
	221 mM	-55.6±2.4	-156.2±7.7	-7.11±0.06	45.2	-57.8±1.2	-163.2±3.8	-7.13±0.03	45.0
	621 mM	-56.5±2.6	-157.5±8.3	-7.60±0.07	47.9	-57.3±0.7	-160.3±2.3	-7.59±0.02	47.7
	1.021 M[b]	-58.3	-163.0	-7.75	48.4	-62.3	-175.3	-7.98	48.7
GCAUGC	71 mM	-55.2±2.5	-159.1±8.0	-5.84±0.03	37.9	-54.9±0.7	-158.1±2.3	-5.81±0.00	37.8
	121 mM	-56.7±2.6	-162.3±8.5	-6.30±0.03	40.4	-56.8±0.7	-162.8±2.4	-6.26±0.01	40.2
	221 mM	-55.4±3.6	-157.1±11.4	-6.71±0.05	42.9	-56.6±1.1	-160.8±3.8	-6.69±0.02	42.6
	621 mM	-58.5±3.8	-165.1±12.1	-7.34±0.09	46.1	-59.5±1.4	-168.3±4.3	-7.31±0.03	45.8
	1.021 M[b]	-59.6	-168.4	-7.41	46.3	-62.3	-177.2	-7.38	45.7
AACUAGUU	71 mM	-58.9±1.9	-173.5±6.1	-5.11±0.03	34.0	-59.0±1.2	-173.8±4.0	-5.09±0.03	34.0
	121 mM	-59.8±3.4	-174.5±11.1	-5.68±0.02	37.0	-58.4±1.5	-169.8±4.8	-5.68±0.02	37.0
	221 mM	-60.1±3.6	-173.5±11.6	-6.27±0.03	40.1	-59.6±0.7	-171.9±2.3	-6.24±0.00	40.0
	621 mM	-59.6±1.9	-169.8±6.0	-6.95±0.06	43.8	-58.2±1.6	-165.3±5.0	-6.92±0.02	43.8
	1.021 M[b]	-55.2	-155.0	-7.13	45.4	-54.6	-153.0	-7.16	45.7
ACUAUAGU	71 mM	-61.3±2.9	-182.0±9.4	-4.89±0.06	33.1	-61.3±1.6	-181.9±5.2	-4.86±0.04	32.9
	121 mM	-63.1±4.5	-185.6±14.5	-5.53±0.05	36.3	-59.4±0.6	-173.7±2.1	-5.53±0.01	36.2
	221 mM	-63.7±3.4	-185.8±11.1	-6.07±0.03	38.9	-63.8±1.0	-186.1±3.2	-6.04±0.01	38.8
	621 mM	-64.4±3.5	-185.4±11.3	-6.89±0.03	43.0	-65.5±1.3	-189.1±4.3	-6.87±0.01	42.7
	1.021 M[b]	-61.4	-175.0	-7.12	44.5	-59.2	-168.4	-6.98	44.0

		Analysis of Curve Fits				Analysis of T_m^{-1} vs. ln C_t Plot			
Sequence[a]	**[Na^+]**	**ΔH° (kcal/mol)**	**ΔS° (eu)**	**ΔG°_{37} (kcal/mol)**	**T_m[c] ($^\circ$C)**	**ΔH° (kcal/mol)**	**ΔS° (eu)**	**ΔG°_{37} (kcal/mol)**	**T_m[c] ($^\circ$C)**
ACUUAAGU	71 mM	-57.3±3.2	-171.0±10.5	-4.32±0.09	29.8	-55.1±1.3	-163.6±4.4	-4.37±0.05	29.8
	121 mM	-60.7±1.9	-180.3±6.1	-4.79±0.07	32.5	-61.2±1.8	-181.9±6.1	-4.76±0.05	32.4
	221 mM	-61.3±2.8	-180.0±9.2	-5.44±0.03	35.8	-58.8±1.1	-172.1±3.8	-5.46±0.02	35.8
	621 mM	-61.1±2.2	-177.1±7.2	-6.12±0.03	39.3	-60.5±0.6	-175.3±2.0	-6.11±0.01	39.3
	1.021 M[b]	-49.4	-139.0	-6.29	40.9	-47.2	-132.4	-6.16	40.3
AGAUAUCU	71 mM	-64.3±3.2	-193.0±10.6	-4.40±0.06	30.9	-62.0±1.6	-185.4±5.4	-4.45±0.05	31.0
	121 mM	-61.9±4.8	-183.2±15.8	-5.09±0.09	34.1	-62.5±2.6	-185.1±8.5	-5.05±0.06	33.9
	221 mM	-61.0±3.0	-177.9±9.7	-5.82±0.06	37.7	-58.5±1.7	-169.8±5.5	-5.82±0.02	37.7
	621 mM	-61.0±2.1	-175.5±6.7	-6.61±0.04	41.8	-61.1±1.3	-175.7±4.2	-6.59±0.01	41.7
	1.021 M[b]	-63.4	-183.0	-6.64	41.8	-64.5	-186.8	-6.58	41.4

[a] Sequences are written 5' to 3'. Due to the nature of the sequences, all samples formed self-complementary duplexes in solution.

[b] All 1.021 M data, except for GCCGGC and GCGCGC, are from Xia et al. [(9)].

[c] Calculated at 0.1 mM oligomer concentration.