Supporting Information for:

L-Proline and RNA Duplex *m*-Value Temperature Dependence

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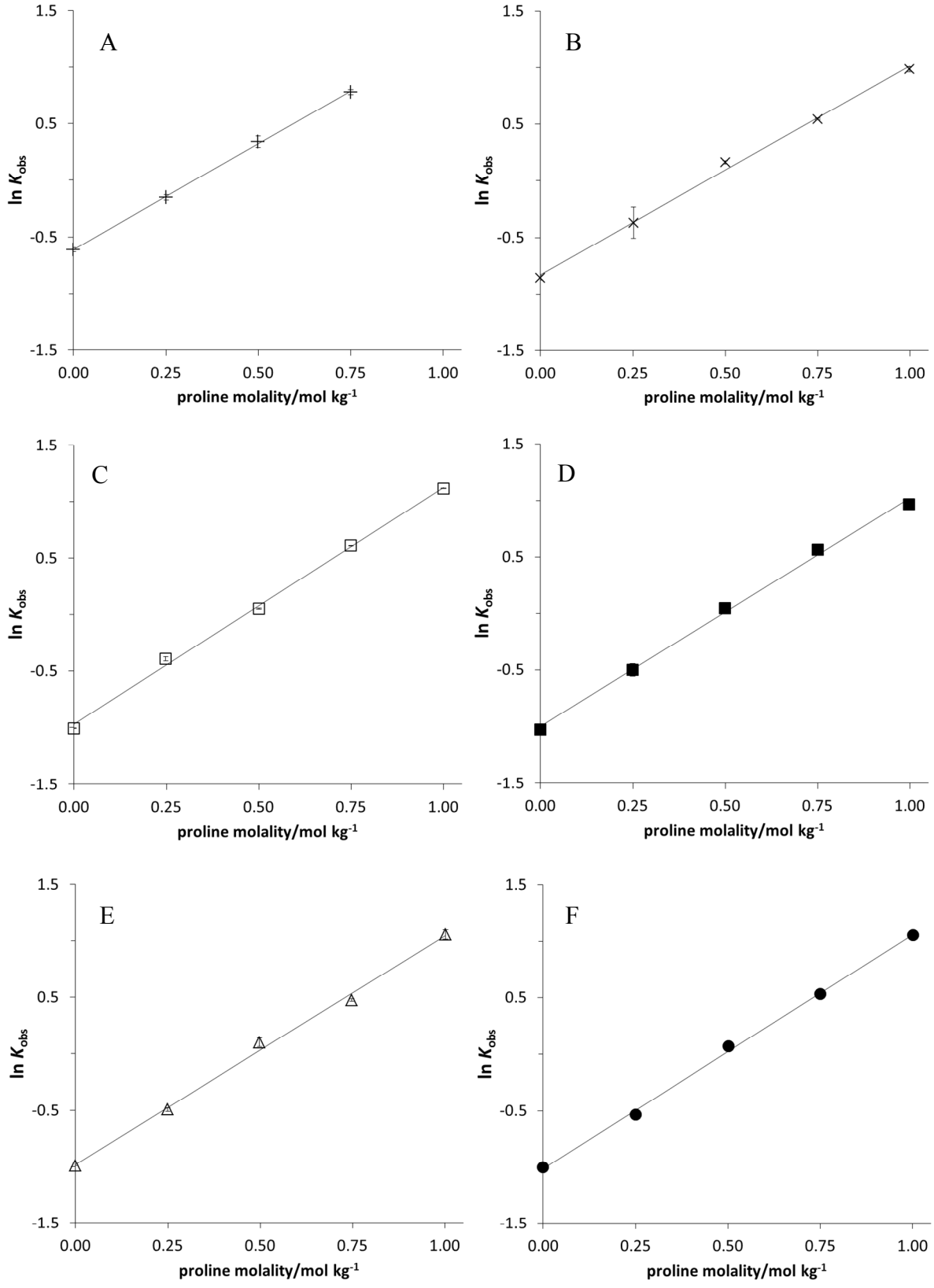

A
B
C
D
E
F
1.5
0.5
-0.5
-1.5
0.00
0.25
0.50
0.75
1.00
ln K_{obs}
proline molality/mol kg^{-1}

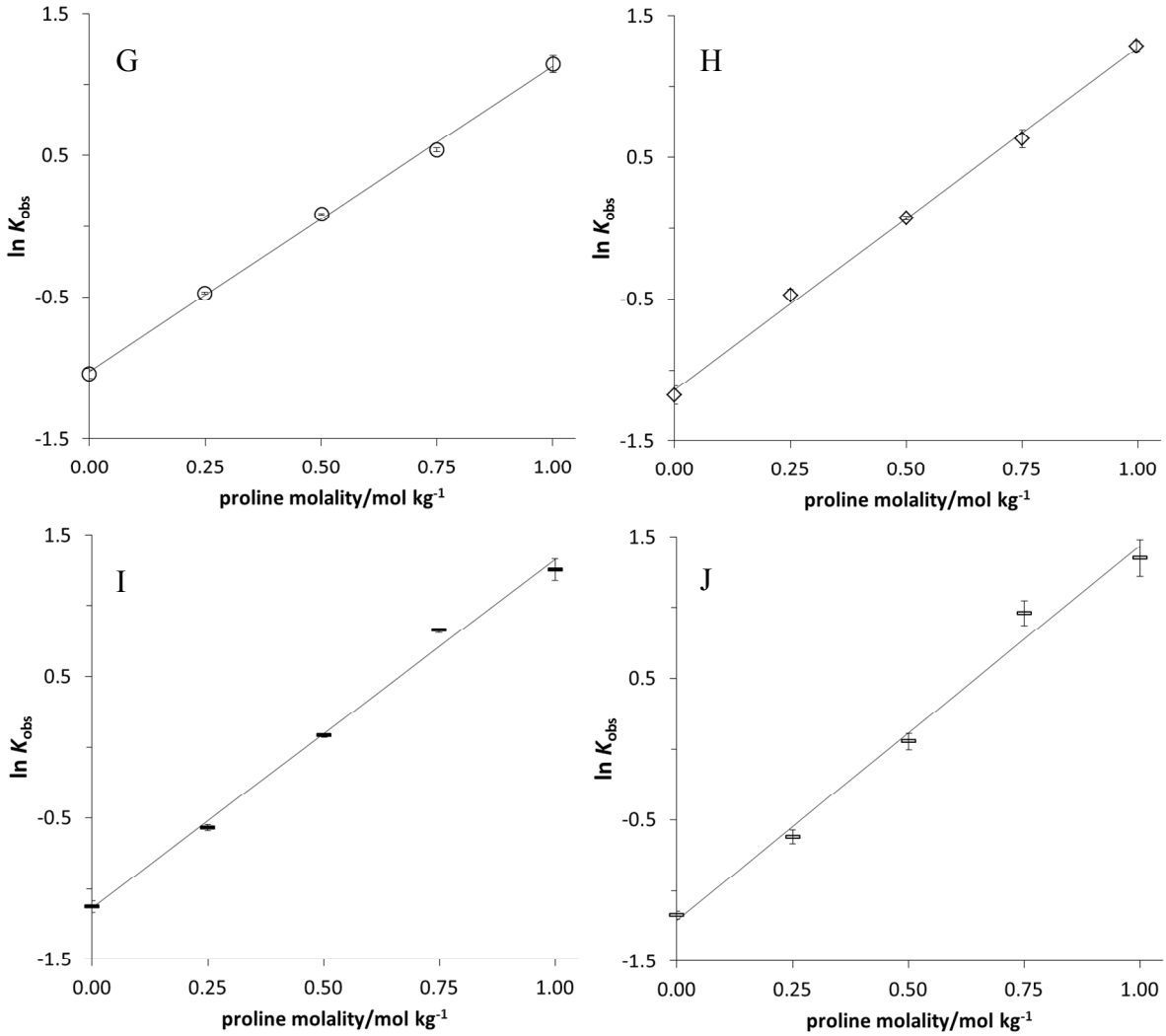
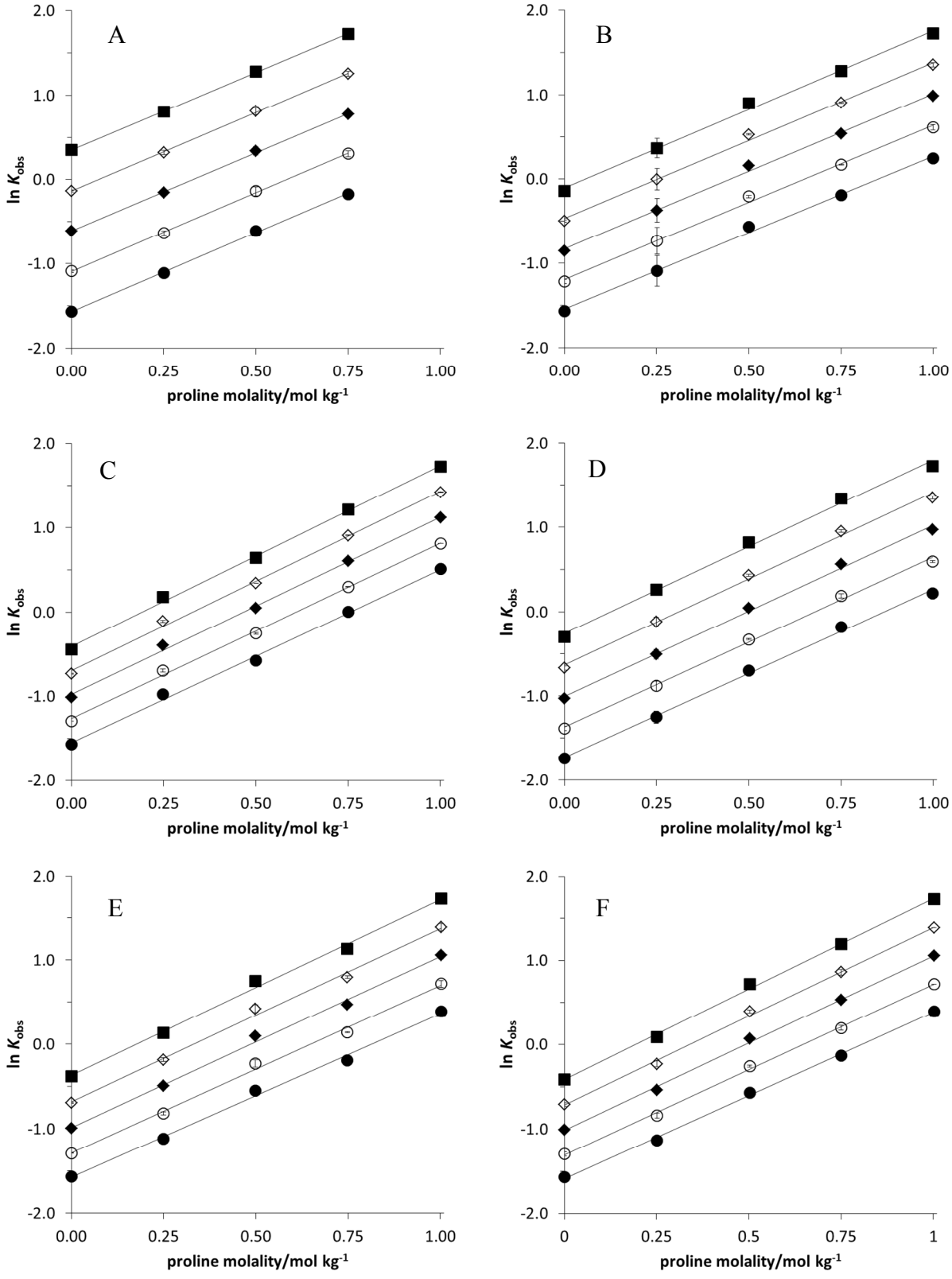


Figure S1. Natural logarithm of the observed unfolding equilibrium constant K_{obs} for thermal denaturation of RNA duplexes as a function of proline molality and temperature. The K_{obs} values were determined at the duplex transition temperature (fraction unfolded single strand equal to 0.5) in 0.5 molal proline. A) 5'-r(GAAAUUAUAAAG)-3' at 31.5 ^{o}C; B) 5'-r(GAAAGUAUAAAG)-3' at 38.1 ^{o}C; C) 5'-r(GAUAGUAGAUAG)-3' at 47.8 ^{o}C; D) 5'-r(GAAAGUAGAAAC)-3' at 44.3 ^{o}C; E) 5'-r(GCAAAGUAAACG)-3' at 47.9 ^{o}C; F) 5'-r(GCAUAGCAUACG)-3' at 55.7 ^{o}C; G) 5'-r(GCAAAGCAAACG)-3' at 53.0 ^{o}C; H) 5'-r(GCGAAGCCAACG)-3' at 64.8 ^{o}C; I) 5'-r(GCUCCGCCAACG)-3' at 71.8 ^{o}C, J) 5'-r(GCGCAGCCAGCG)-3' at 75.6 ^{o}C.

Values of ΔASA for the stacked and half-stacked RNA single strand conformations can be found in the Supporting Information of reference 27. The unstacked conformation ΔASA values are listed here in Table S1.

Table S1: Change in Solvent Accessible Surface Area (ΔASA) Values for RNA Duplex Dodecamers Assuming Unstacked Nucleobases in Single Strands

sequence	%GC	total ΔASA/Å^2	anionic oxygen ΔASA/Å^2	sugar ΔASA/Å^2	base aromatic ΔASA/Å^2	base amine ΔASA/Å^2	amide-like oxygen ΔASA/Å^2	aliphatic base ΔASA/Å^2
5'-r(GAAAUUAUAAAG)-3'	17	3533	-348	326	2010	843	705	0
5'-r(GAAAGUAUAAAG)-3'	25	3570	-348	334	1973	896	718	0
5'-r(GAUAGUAGAUAG)-3'	33	3608	-348	342	1939	949	729	0
5'-r(GAAAGUAGAAAC)-3'	33	3614	-352	335	1940	976	717	0
5'-r(GCAAAGUAAACG)-3'	42	3638	-348	348	1906	1000	735	0
5'-r(GCAAAGCAAACG)-3'	50	3672	-352	352	1873	1054	748	0
5'-r(GCAUAGCAUACG)-3'	50	3671	-352	350	1875	1056	745	0
5'-r(GCGAAGCCAACG)-3'	67	3640	-334	350	1749	1139	741	0
5'-r(GCGCCGCCGGCG)-3'	100	3892	-352	397	1666	1372	812	0


A
B
C
D
E
F
ln K_{obs}
proline molality/mol kg^{-1}
2.0
1.0
0.0
-1.0
-2.0
0.00
0.25
0.50
0.75
1.00
0
0.5
1

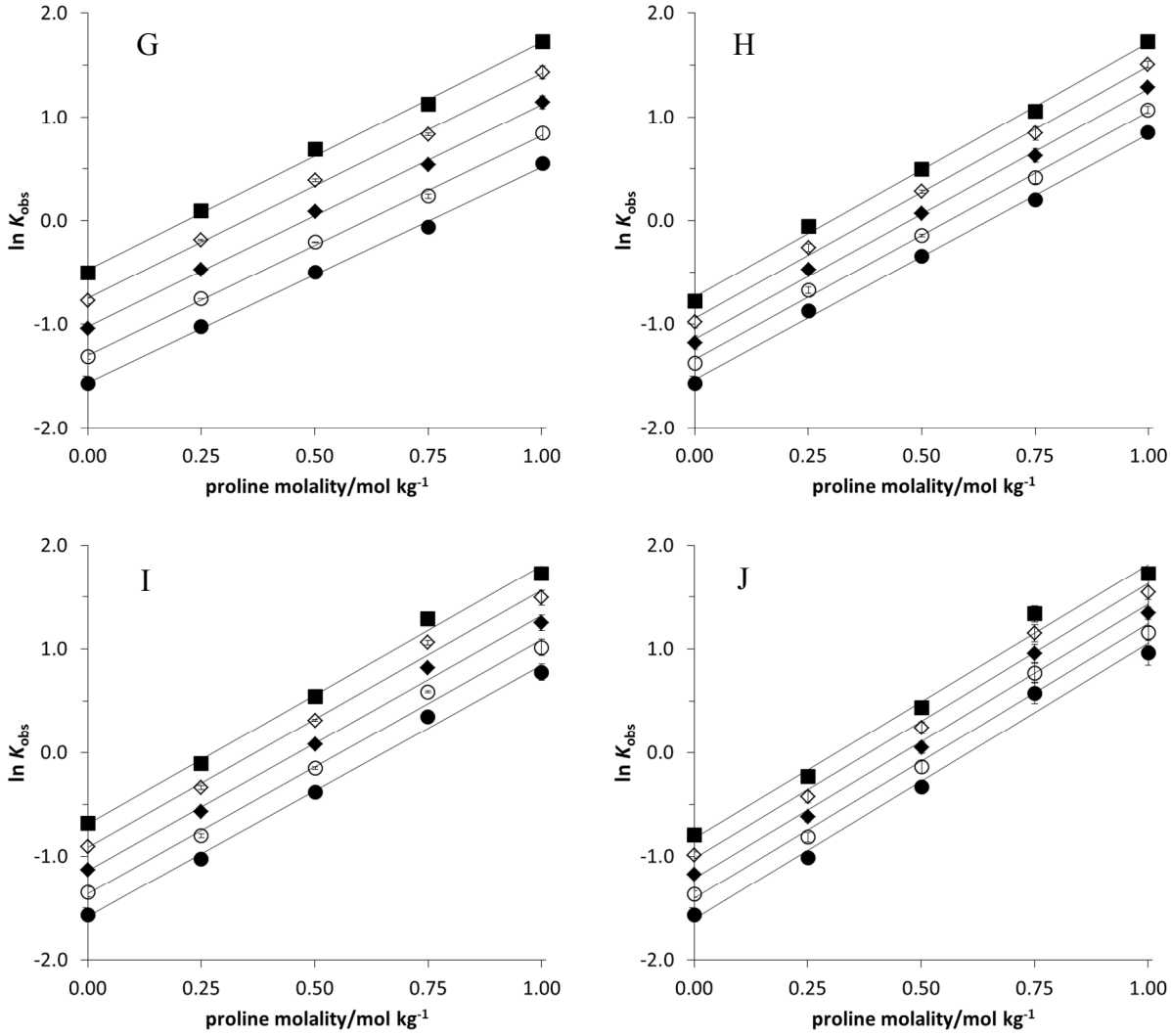


Figure S2. Natural logarithm of the observed unfolding equilibrium constant K_{obs} for thermal denaturation of RNA duplexes as a function of proline molality and temperature. The temperature at a fraction of unfolded duplex of 0.2 is given by filled circles and a fraction of unfolded duplex of 0.8 is given by filled squares. Temperatures in between these two temperatures follow the progression open diamonds > filled diamonds > open circles. A) 5'-r(GAAAUUAUAAAG)-3' at 29.5, 30.5, 31.5, 32.5, and 33.5 ^{o}C; B) 5'-r(GAAAGUAUAAAG)-3' at 36.5, 37.3, 38.1, 38.9, and 39.6 ^{o}C; C) 5'-r(GAUAGUAGAUAG)-3' at 46.6, 47.2, 47.8, 48.4, and 49.1 ^{o}C; D) 5'-r(GAAAGUAGAAAC)-3' at 42.6, 43.5, 44.3, 45.1, and 46.0 ^{o}C; E) 5'-r(GCAAAGUAAACG)-3' at 46.5, 47.2, 47.9, 48.6, and 49.3 ^{o}C; F) 5'-r(GCAUAGCAUACG)-3' at 54.3, 55.0, 55.7, 56.4, and 57.1 ^{o}C; G) 5'-r(GCAAAGCAAACG)-3' at 51.8, 52.4, 53.0, 53.6, and 54.3 ^{o}C; H) 5'-r(GCGAAGCCAACG)-3' at 63.9, 64.4, 64.8, 65.3, and 65.7 ^{o}C; I) 5'-r(GCUCCGCCAACG)-3' at 70.8, 71.3, 71.8, 72.2, and 72.7 ^{o}C; J) 5'-r(GCGCAGCCAGCG)-3' at 74.8, 75.2, 75.6, 76.0, and 76.4 ^{o}C. Linear regression slopes are equal to $-m$-value/RT.

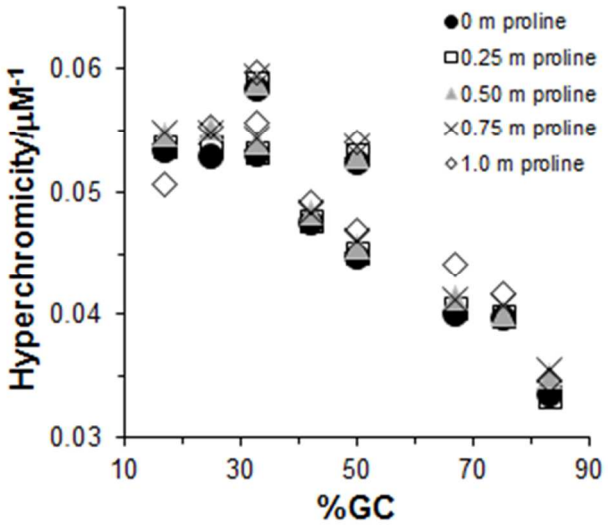


Figure S3. RNA duplex concentration-normalized transition region hyperchromicity (μM^{-1}) as a function of GC content and proline molality.