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¹⁵N NMR of RNA Fragments Containing Specifically Labeled GU and GC Pairs

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Supplementary Material

5'-GAUGCGUCp-3' (1)

Temp (°C)	N1/GU	N2/GU	N1/GC	N2/GC	N6/AU	¹³ C/GU
20	141.7	69.4	145.0	71.7	80.0	147.6
30	141.9	69.3	145.2	71.8	79.9	147.7
40	142.2	69.2	145.3	71.7	79.4	148.1
50	143.1	69.5	145.2	71.4	78.0	148.8
60	144.3	69.9	145.0	70.7	76.1	149.6
70	145.0	69.8	145.0	70.2	75.1	149.9
80	145.2	69.9	145.2	70.0	74.8	150.0

5'-GGCGUGCCp-3' (2)

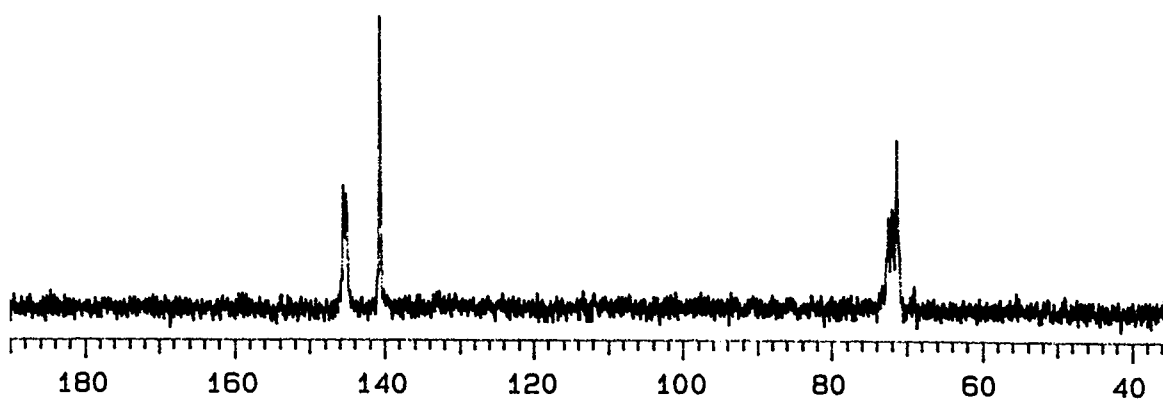
Temp (°C)	N1/GU	N2/GU	N1/GC	N2/GC	¹³ C/GU
20	141.9	69.8	145.5	72.2	147.4
30	142.1	69.6	145.5	72.2	147.5
40	142.4	69.5	145.7	72.2	147.7
50	142.8	69.4	145.7	72.2	147.9
60	143.6	69.5	145.8	71.7	148.5
70	144.5	69.8	145.3	70.5	149.4
80	145.5	70.0	145.5	70.0	149.8

5'-GGCUGGCCp-3' (3)

Temp (°C)	N1/GU	N2/GU	N1/GC	N2/GC	¹³ C/GU
25	139.7	70.1	145.8	72.6	146.9
35	139.9	70.0	146.0	72.6	147.0
45	140.1	70.0	146.0	72.5	147.1
55	140.3	69.8	146.3	72.3	147.2
65	N.A.	69.8	147.2	71.8	N.A.
75	146.3	69.8	148.2	70.7	149.7

5'-GGACUUCGGUCCp-3' (4)

Temp (°C)	N1/GU	N2/GU	N1/GC	N2/GC	¹³ C/GU
20	140.7	71.3	145.4	72.3	149.7
40	141.2	71.3	145.7	72.2	149.8
50	141.5	71.2	145.9	72.2	149.9
60	142.1	71.2	146.1	72.1	150.0
70	143.4	70.9	146.5	71.8	150.1
75	144.5	70.7	146.8	71.3	150.1
80	145.7	70.5	147.0	70.9	150.1
85	146.5	70.2	147.3	70.5	150.1
90					150.2



This is the spectrum of the tetraloop 12mer (4) at 20 °C. It was acquired at 40.5 MHz on a Varian XL400 spectrometer using a 1D experiment with a delay of 1 second. Chemical shifts are reported relative to NH₃ using external 1M [¹⁵N]urea in DMSO at 25°C at 77.0 ppm as a reference. The sample was in 100% D₂O, 0.1 M NaCl, 10 mM phosphate, and 0.1 mM EDTA at pH 6.7, with a total strand concentration of 11 mM.