

Supplementary Table: ¹H chemical shifts of RNA duplexes

A	H2/H5	H8/H6	H1'	H2'	H3'	Imino	Amino
C1	5.99	8.06	5.56	4.33	4.56	—	—
G2	—	7.78	5.76	4.55	4.71	12.33	5.77 / 7.86
C3	5.29	7.69	5.48	4.52	4.56	—	6.71 / 8.26
A4	6.71	7.94	5.85	4.63	4.71	—	6.30 / 7.74
A5	7.63	7.77	5.82	4.41	4.54	—	6.80 / 7.83
U6	4.99	7.53	5.41	4.28	4.40	13.94	—
U7	5.49	7.89	5.62	4.44	4.55	13.06	—
G8	—	7.69	5.74	4.42	4.57	13.00	—
C9	5.18	7.56	5.42	4.26	4.40	—	6.73 / 8.29
G10	—	7.53	5.79	4.18	4.24	12.78	—

B	H2/H5	H8/H6	H1'	H2'	H3'	Imino	Amino
C1	5.99	8.07	5.54	4.34	4.56	—	—
G2	—	7.80	5.78	4.56	4.72	12.39	5.90 / 8.00
C3	5.32	7.72	5.49	4.53	4.57	—	6.70 / 8.30
A4	6.67	7.96	5.88	4.67	4.72	—	6.35 / 7.84
A5	7.65	7.76	5.82	4.44	4.54	—	6.85 / —
U6	4.97	7.57	5.39	3.57	4.55	14.09	—
U7	5.50	7.83	5.59	4.55	4.48	13.00	—
G8	—	7.71	5.76	4.43	4.61	13.05	—
C9	5.20	7.57	5.43	4.28	4.43	—	6.77 / 8.32
G10	—	7.54	5.81	4.19	4.26	12.76	—

C	H2/H5	H8/H6	H1'	H2'	H3'	Imino	Amino
C1	6.00	8.09	5.56	4.34	4.57	—	—
G2	—	7.80	5.79	4.57	4.72	12.47	5.88 / 7.88
C3	5.32	7.72	5.48	4.49	4.57	—	6.76 / 8.35
A4	6.80	7.97	5.86	4.66	4.75	—	6.36 / 7.88
A5	7.70	7.83	5.82	4.34	4.56	—	7.03 / —
U6	5.03	7.70	5.32	3.82	4.68	14.65	—
U7	5.55	7.99	5.47	4.34	4.54	13.07	—
G8	—	7.71	5.74	4.41	4.55	13.10	—
C9	5.19	7.58	5.42	4.27	4.43	—	6.80 / 8.37
G10	—	7.54	5.81	4.19	4.27	12.77	—

Proton chemical shifts of (A) 2'-hydroxyl, (B) 2'-amino, and (C) 2'-ethylureido RNA duplexes used for molecular modeling. The chemical shift of the H₂O peak (at 15 °C) was used as a reference.